

The binding of reducible N₂ in the reaction domain of nitrogenase.

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Supplementary Information

1. Protein model

The quantum computed protein model is an extract from crystal 3U7Q, shown in Chart S1. The six principal chains surrounding FeMo-co are highlighted with different colours, and the connecting hydrogen bonds are marked. Homocitrate, the His442 ligation of Mo, and relevant nearby water molecules are included (486 atoms total). Details, and the rationale for inclusion of amino acids and for truncation of uninvolved sidechains, are provided in the caption for Chart S1. Investigations of the protonation state of homocitrate using crystal structures at various pH (summarised in ref¹), vibrational circular dichroism spectroscopy,² QM/MM calculations,^{3,1} and quantum refinement,³ indicate that the coordinated alcoholate O atom is protonated. In the model used here this atom is not protonated. This difference is not expected to have significant consequences for the reaction steps of the mechanism described here because there are no potential hydrogen bonds or H transfer possibilities.

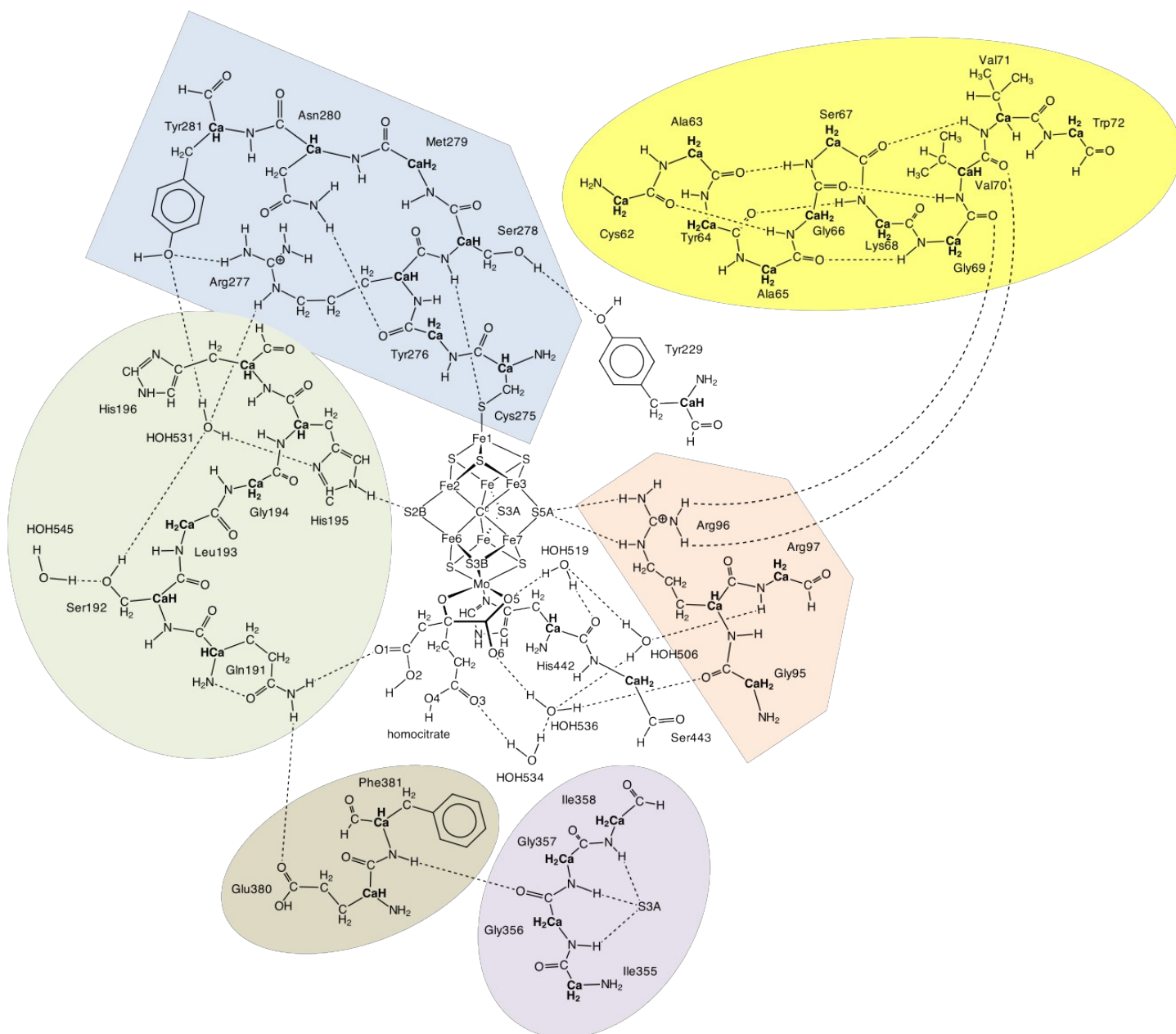


Chart S1. The quantum computed model, with residues and water molecules labelled according to *Azotobacter vinelandii* protein, crystal structure 3U7Q. Ca are labelled as Ca, and hydrogen bonds are broken lines. Non-influential sidechains are truncated to gly. In the ‘front’ chain (yellow highlight) that extends over the Fe2Fe3Fe6Fe7 face of FeMo-co the crucial residues Val70 and Val71 are complete, while 62, 63, 64, 65, 67, 68 and 72 are modelled as Gly. In the 191 to 196 chain (highlight green) the significant sidechains of Gln191, Ser193, His195 and His196 are complete. In the 275-281 chain (blue highlight) Cys275, Arg277, Ser278, Asn280, Tyr281 near the N_2 pathway are complete: Tyr229 is included in full because it borders the reaction domain and has an important hydrogen bond with Ser278. In chain 95-97 (salmon highlight) the sidechain of Arg96 is included because it forms crucial hydrogen bonds with S5A, Gly69 and Val70: the sidechain of Arg97 is not nearby and is truncated to gly. In the rear chain (mauve highlight) with hydrogen bonds to S5A, Ile355 and Ile358 are truncated to gly. Glu380 and Phe381 (fawn highlight) are included in full. Ligand His442 is complete and Ser443 is truncated to gly. Homocitrate is complete. HOH531 has hydrogen bonds with two chains, Ser192, His195 and Arg277, Tyr281, and is part of the putative proton transfer from surface water (HOH545) to His195.⁴

The four penultimate waters of the proton wire⁵ (HOH519, HOH506, HOH536 and HOH534) are included.

Experimental and computational studies are in general agreement that the redox level of the [CFe₇MoS₉] core of resting FeMo-co cluster is described by net charge -1,^{6,7,1,8} and so the net charge for the complete model in Chart S1 is -2 (-1 when the His195 side chain is protonated).

2. Constraints on the computed protein

Some constraints on the protein structure are required during optimization calculations because the modelled protein is incomplete and the bonding and dispersion influences of the complete protein outside the computational model are absent. The modelled protein must also maintain flexibility sufficient to accommodate the coordination of N₂ and of H₂, and the diffusion of these molecules to and from FeMo-co. The constraints used here involved the C α atoms at the ends of the modelled protein chains, allowing movement of the intermediate residues and all sidechains. The constraints maintained the crystallographic distances between C^c at the centre of FeMo-co and the C α atoms of residues 62, 95, 97, 191, 196, 229, 281, 355, 358, 380, 381, 443, and included C^c -- water distances. As previously explained⁹ trial calculations on the modes of diffusion and coordination of N₂ / H₂ led to the conclusion that the front chain near Val70 should move about 1Å away from FeMo-co. This is consistent with experimental data on mutation of amino acid 70 with smaller and larger side chains.¹⁰⁻¹² Therefore the C α (Trp72)-C^c distance was constrained to 14.1Å (13.08Å in the resting protein structure), and the C α (Val70)-C^c distance to 8.6Å (7.22Å in the resting protein). The lengths of the hydrogen bonds between the backside water HOH531 and Arg277, Tyr281 and Ser192 (Chart S1) were also constrained.

3. Density functional procedures

Density functional (DF) calculations use the DMol methodology of Delley,¹³⁻¹⁸ with accurate DNP (double numerical plus polarisation) basis sets.¹⁶ The real-space cutoff in the calculation of atomic basis sets was 9 au (4.76Å), which gives results within 0.1% of the limit for larger extensions of the basis sets. The gradient-corrected functional PBE¹⁹ was used because validation tests demonstrate that it is more accurate than other commonly used functionals when used with DMol.²⁰ See ref⁹ for results describing the accuracy with which the PBE/DMol method reproduces experimental enthalpy data on the binding of N₂. The calculations were all-electron, spin-unrestricted, with no imposed symmetry. The conductor-like screening model (COSMO)²¹⁻²³ was used with a dielectric constant of 5. Constraints on interatomic distances used the Lagrange Multiplier Algorithm. Control of electronic states was via the input spin populations for Fe1, Fe3, Fe4, Fe5 and Fe7. Output spin populations are calculated by the Mulliken method.²⁴

4. Preferred electronic states

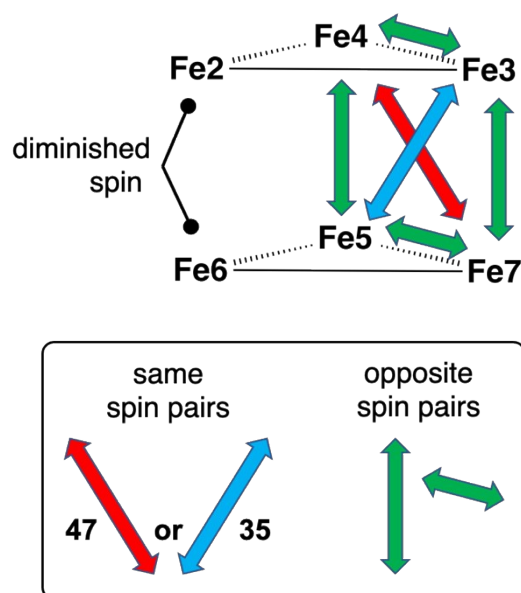


Chart S2. When the spin populations of Fe2 and Fe6 are diminished due to ligation, there are two pairs of negative spin, red *or* blue, that yield four oppositely signed (green) spin pairs along the shorter edges of the Fe3, Fe4, Fe5, Fe7 face where the spin populations have largest magnitude.

5. Distances for N₂ bound structures

Table S1. Non-bonding distances (Å)

	Structure	Fe2-Fe6	Fe2-S2B	Fe6-S3B	Structure	Fe2-Fe6	Fe2-S2B	Fe6-S3B
Fe-N ₂	His				His ⁺			
A hooked S2BH only								
Fe2-N ₂	1 , 47(2)	2.75			2 , 47(2)	2.76		
					2 , 35(2)	2.77		
Fe6-N ₂	3 , 47(2)	2.77						
B unhooked S2BH only								
Fe2-N ₂	9 , 35(1)	2.97			10 , 47(2)	2.89	3.22	
					10 , 35(1)	2.96	3.64	
Fe6-N ₂	11 , 35(1)	2.78			12 , 47(2)	2.78	4.03	
					12 , 35(1)	2.77	4.08	
C hooked S2HB + 6Hx								
Fe2-N ₂	5 , 47(1/2)	3.05			6 , 47(1/2)	3.07		
	5 , 47(3/2)	3.05			6 , 47(3/2)	3.06		
	5 , 47(5/2)	3.14			6 , 35(3/2)	3.04		
	5 , 35(3/2)	3.20			6 , 35(5/2)	3.04		
	5 , 35(5/2)	3.07						
Fe6-N ₂	7 , 47(5/2)	3.10			8 , 47(3/2)	3.30		
	7 , 35(3/2)	3.13			8 , 35(3/2)	3.27		

D unhooked S2HB + Fe2-H-Fe6								
Fe2-N ₂	13 , 47(3/2)	2.74	3.76		14 , 47(3/2)	2.75	3.81	
	13 , 47(5/2)	2.74	3.84		14 , 35(3/2)	2.73	3.85	
	13 , 35(3/2)	2.74	3.81					
Fe6-N ₂	15 , 47(3/2)	2.70	4.16		16 , 47(3/2)	2.69	4.13	
					16 , 35(1/2)	2.70	4.15	
E unhooked S2HB + 3b2								
Fe2-N ₂	17 , 47(5/2)	2.87	3.62	2.52	18 , 47(3/2)	2.89	3.67	2.59
					18 , 47(5/2)	2.88	3.63	2.61
Fe6-N ₂	19 , 47(3/2)	2.65			20 , 47(3/2)	2.67	3.98	2.65
					20 , 35(1/2)	2.64	4.03	2.73
					20 , 35(3/2)	2.64	4.01	2.73
F unhooked S2HB + 3b2 + Fe2-H-Fe6								
Fe2-N ₂	21 , 47(1)	2.68	3.91	2.93	22 , 47(2)	2.65	3.95	3.11
	21 , 47(2)	2.68	3.92	2.97	22 , 35(2)	2.66	3.91	2.99
Fe6-N ₂	23 , 47(1)	2.64	4.26	2.75	24 , 47(1)	2.63	4.24	2.63
	23 , 35(2)	2.66	4.29	2.83	24 , 47(2)	2.63	4.21	2.58
					24 , 35(2)	2.65	4.24	2.66

Table S2. Fe-N, N-N distances (Å)

Structure	<i>endo</i> N ₂ binding		<i>exo</i> -Fe2 N ₂ binding	
	Fe-N	N-N	Fe-N	N-N
1 , 47(2)	1.83	1.12	1.85	1.12
2 , 47(2)	1.85	1.12	1.84	1.13
2 , 35(2)	1.85	1.12	1.84	1.13
3 , 47(2)	1.80	1.13	1.79	1.13
9 , 35(1)	1.83	1.13	1.83	1.13
10 , 47(2)	1.83	1.12	1.83	1.13
10 , 35(1)	1.83	1.13	1.82	1.13
11 , 35(1)	1.80	1.13	1.80	1.13
12 , 47(2)	1.81	1.13	1.80	1.14
12 , 35(1)	1.80	1.13	1.79	1.14
5 , 47(1/2)	1.84	1.12	1.84	1.13
5 , 47(3/2)	1.85	1.12	1.85	1.13
5 , 47(5/2)	1.84	1.12	1.84	1.13
5 , 35(3/2)	1.84	1.12	1.85	1.12

5 , 35(5/2)	1.84	1.12	1.85	1.12
6 , 47(1/2)	1.83	1.12	1.83	1.13
6 , 47(3/2)	1.84	1.12	1.84	1.13
6 , 35(3/2)	1.83	1.12	1.84	1.13
6 , 35(5/2)	1.84	1.12	1.85	1.13
7 , 47(5/2)	1.82	1.13	1.80	1.13
7 , 35(3/2)	1.81	1.13	1.80	1.14
8 , 47(3/2)	1.82	1.13	1.80	1.14
8 , 35(3/2)	1.81	1.13	1.80	1.14
13 , 47(3/2)	1.84	1.12	1.84	1.13
14 , 47(3/2)	1.85	1.12	1.82	1.13
14 , 35(3/2)	1.85	1.12	1.84	1.13
15 , 47(3/2)	1.80	1.13	1.80	1.13
16 , 47(3/2)	1.81	1.13	1.79	1.13
16 , 35(1/2)	1.80	1.13	1.81	1.13
17 , 47(5/2)	1.80	1.13	1.83	1.13
18 , 47(3/2)	1.82	1.13	1.82	1.13
18 , 47(5/2)	1.81	1.13	1.81	1.13
19 , 47(3/2)	1.78	1.13	1.79	1.13
20 , 47(3/2)	1.79	1.13	1.78	1.14
20 , 35(1/2)	1.79	1.13	1.79	1.14
20 , 35(3/2)	1.79	1.13	1.79	1.14
21 , 47(1)	1.82	1.13	1.83	1.13
21 , 47(2)	1.82	1.13	1.83	1.13
22 , 47(2)	1.82	1.13	1.82	1.13
22 , 35(2)	1.82	1.13	1.82	1.13
23 , 47(1)	1.80	1.13	1.81	1.13
23 , 35(2)	1.80	1.13	1.81	1.13
24 , 47(1)	1.81	1.13	1.79	1.14
24 , 47(2)	1.82	1.13	1.80	1.14
24 , 35(2)	1.81	1.13	1.79	1.14

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7 Coordinates and spin populations for N₂ bound structures

structure, spin populations	filename, coordinates
1, 47(2)	bm12b2n2x2n2n47.car_3
Fe1 3.19	C1 -7.737101523 -5.428006885 1.000967941
Fe2 0.06	C2 -7.793593321 -6.751877513 0.232341760
Fe3 2.94	C3 -8.938811243 -3.372885836 1.611735901
Fe4 -2.67	C4 -8.693094133 -3.362372836 3.117840502
Fe5 2.26	C5 -8.850897006 -4.558795197 5.241291113
Fe6 -0.11	C6 -7.366019279 -4.664001527 5.608955447
Fe7 -2.22	C7 -5.132253945 -5.362675996 4.884011199
	C8 -4.447241041 -4.016175995 4.631145124
	C9 -4.354673672 -1.975332987 3.300007321
	C10 -4.644426338 -0.961120919 4.417116173
	C11 -6.184535943 -0.151921482 6.109474793

C12	-5.490305060	-0.485903455	7.438021031
C13	-5.028583309	-2.206282123	9.119792658
C14	-3.535602516	-2.520355965	9.268830221
C15	-1.511596306	-3.432733345	8.212248352
C16	-0.505725523	-2.522310621	7.500095188
C17	-0.255484169	-0.528731994	6.033458606
C18	-0.386718781	0.865936586	6.669074290
C19	-0.605291147	-0.564561626	4.524870985
C20	0.021083493	0.627387869	3.794501072
C21	-0.189294563	-1.909839545	3.918970192
C22	-1.779942367	2.849821276	7.034389625
C23	-1.861701298	2.879037650	8.570069338
C24	-2.992003794	3.526932822	6.351539906
C25	-3.256145406	4.916776935	6.940896117
C26	-2.775111050	3.630297536	4.834263206
C27	-2.784305816	1.918865530	10.597163297
C28	-1.445973167	1.878671618	11.304425242
C29	5.516735503	-9.959859741	7.251641425
C30	6.115797202	-8.865761207	6.365798092
C31	6.337741678	-6.382479265	6.168952743
C32	7.377321010	-5.734684747	7.102624709
C33	5.147004391	-5.448332636	5.892754652
C34	5.551289761	-4.110670028	5.268120370
C35	4.339446926	-3.388274801	4.672119727
C36	4.396278014	-0.895983800	4.439241715
C37	9.642757439	-4.815912836	7.268546571
C38	9.860458657	-3.346118579	6.980631711
C39	-4.962995397	-3.132971694	-1.730827418
C40	-5.441659076	-1.673449134	-1.664144342
C41	-3.443238314	-3.147163009	-1.448393217
C42	-2.815892072	-4.521840454	-1.124766359
C43	-2.326740100	-5.322602937	-2.330872737
C44	-5.897536657	0.323717617	-3.056191974
C45	-7.214412589	0.809968364	-2.456601096
C46	-5.723008851	0.642069431	-4.566820392
C47	-9.384961837	0.183312767	-1.510254895
C48	-9.158815326	0.593284526	-0.048244321
C49	-7.617293795	0.672968765	1.855323357
C50	-6.563375112	1.768280101	2.027442389
C51	-4.930691134	3.284760894	1.001880087
C52	-5.533890257	4.664739056	1.327052136
C53	-4.171593362	3.452903541	-0.324818811
C54	-3.386819309	2.282659876	-0.837266848
C55	-2.839961303	1.188839284	-0.201207276
C56	-2.293367677	1.152808255	-2.346737919
C57	-7.396914883	6.190340607	0.797031309
C58	-7.608241841	6.662044546	2.232271939
C59	-8.749796886	6.060447365	0.058219516
C60	-9.331961005	7.330420261	-0.488375795
C61	-9.439196845	8.591491023	0.064756502
C62	-10.347007747	8.556780028	-1.956316110
C63	8.462725775	2.767663150	4.452771987
C64	9.451272511	1.637728891	4.675538356
C65	7.089234769	2.112937288	4.174824663
C66	5.974853244	3.119250171	4.005233928
C67	5.220264528	3.575282181	5.101902562
C68	5.648395956	3.616057882	2.730178584
C69	4.176784222	4.493649442	4.934494298
C70	4.621177965	4.542008390	2.549294096
C71	3.879475254	4.973330995	3.651939461
C72	5.514857584	7.010542459	-1.883459317
C73	4.496467518	7.915900213	-2.587550347

C74	4.825194281	5.731848276	-1.379738361
C75	3.669639400	8.760108821	-4.744773929
C76	2.274661408	8.155493179	-4.918093142
C77	0.848097904	6.157505364	-4.635634508
C78	0.083052831	6.312432431	-3.302166330
C79	1.068202747	4.684969975	-5.035609808
C80	-0.176590921	3.800970653	-5.186411175
C81	-1.091331041	4.090817191	-6.390030799
C82	-2.489978429	6.149780965	-6.590420155
C83	0.137550018	6.396788723	-0.865201477
C84	-0.104990901	7.866178308	-0.464250688
C85	0.875385942	5.702551082	0.284892014
C86	0.895817957	10.093362670	-0.332851143
C87	0.206642265	11.282205546	-0.995704744
C88	-1.202129117	12.097471704	-2.841151083
C89	-2.609091383	12.526157478	-2.374987003
C90	-1.204486537	11.760664123	-4.349500601
C91	-2.077901657	10.548444838	-4.653442380
C92	-4.592720296	11.933853779	-1.054078287
C93	-4.694872083	13.165078858	-0.161760846
C94	-5.127695344	10.687760772	-0.297405373
C95	-5.174008520	9.449882310	-1.164489754
C96	-6.276437706	9.204654897	-2.000530998
C97	-4.109428841	8.531811654	-1.182039024
C98	-6.311646260	8.087264501	-2.838734583
C99	-4.120275624	7.420078979	-2.028929669
C100	-5.222531454	7.213591839	-2.857932245
C101	5.556230159	-5.329224945	-7.378063361
C102	4.071380900	-5.100562229	-7.148330230
C103	2.371194643	-3.456681121	-6.393448919
C104	1.911403947	-2.273493399	-7.251544288
C105	2.178133660	0.127319797	-7.659413166
C106	3.286813512	1.167695461	-7.795430372
C107	5.485874015	1.997943149	-7.126263519
C108	6.532159367	1.780628619	-8.203469681
C109	-1.185678042	-5.354165651	-8.569531098
C110	-2.282777974	-4.282334073	-8.640242690
C111	-0.903651704	-5.715202568	-7.093147885
C112	-0.098073045	-7.023178921	-6.980664421
C113	0.408670034	-7.220671965	-5.569845404
C114	-2.842293121	-1.899398598	-8.492095050
C115	-2.308583458	-0.737172770	-9.307599256
C116	-3.381967792	-1.520203873	-7.091203196
C117	-2.279168748	-1.397192773	-6.073684696
C118	-1.502440086	-0.230353102	-5.981542293
C119	-1.932096036	-2.501502455	-5.278855259
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	O449	-1.142867427	6.513069760	-3.314555035
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	O453	-3.127708911	13.565718523	-2.807059187
	O454	-3.307384389	10.649633867	-4.785823989
	O455	-5.745265983	13.748942685	0.050323146
	O456	-5.194533844	6.116931407	-3.731707371
	O457	3.254029534	-6.042926918	-7.310700742
	O458	1.085903521	-2.415672940	-8.180677613
	O459	3.071405256	2.164996308	-8.504705035
	O460	7.531342437	2.474403905	-8.313050144
	O461	-3.476925254	-4.593450084	-8.789963841
	O462	-0.297535189	-7.621167605	-4.648469768
	O463	1.694126190	-6.893275061	-5.338483617
	O464	-2.602956336	0.435321127	-9.127017745
	O465	10.567905413	-5.365303325	-0.933844314
	O466	13.055576217	-6.397951551	1.237754959
	O467	0.032158800	-6.212857278	0.656279742
	O468	0.359559120	-8.056751432	1.858819002
	O469	5.606357277	-10.982781726	-0.110050576
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	O471	5.348841169	-5.629068238	0.632895390
	O472	5.050711262	-7.100191868	2.313081485
	O473	3.059132325	-6.187153879	-0.531362588
	O474	8.868520229	-5.713118747	3.681787507
	O475	7.148677718	-4.070855380	2.146787022
	O476	-4.037768547	3.796391605	-4.172036263
	O477	8.331388366	-10.184741788	1.175866300
	O478	7.523947333	-8.058347370	2.926052150
	S479	3.964298485	4.796872839	-2.724683371
	S480	2.358336762	1.168955648	-3.118622245
	S481	2.750886312	-3.780982887	-2.720967182
	S482	3.718736579	2.159667755	0.011503029
	S483	0.660102161	-1.440256561	-1.016729285
	S484	4.885158490	-1.453821230	-4.722225858
	S485	3.408630489	-3.189722858	0.835876494
	S486	5.982054413	1.475335409	-2.661784570
	S487	6.244100359	-3.346599349	-1.584818869
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	Fe1	3.20		
	Fe2	0.05		
	Fe3	2.92		
	Fe4	-2.67		
	Fe5	2.30		
	Fe6	-0.18		
	Fe7	-2.18		
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	C3	-8.792541878	2.731771322	3.024195470
	C4	-8.505755706	4.166247438	2.583039816
	C5	-8.576702679	6.544058672	3.129996990
	C6	-7.083088247	6.886792103	3.097990249
	C7	-4.846468769	6.329994771	3.925231268
	C8	-4.204105247	5.689580154	2.690139602
	C9	-4.195037814	3.829157676	1.111890092
	C10	-4.500998377	4.611042544	-0.174612824
	C11	-6.017844219	6.066691242	-1.387380390
	C12	-5.286926507	7.416330927	-1.452502379
	C13	-4.766736770	9.510831297	-0.294620707
	C14	-3.261451840	9.708794096	-0.076280624
	C15	-1.228487568	8.904102292	1.056790793
	C16	-0.254466731	7.931349794	0.382505058

C17	-0.091749258	5.968471114	-1.142200717
C18	-0.239241583	6.186591679	-2.659298635
C19	-0.493572550	4.548453873	-0.678838135
C20	0.073571298	3.486320737	-1.626502588
C21	-0.076356017	4.326360140	0.779317317
C22	-1.688120501	6.024161579	-4.635487872
C23	-1.743927288	7.491174272	-5.096164244
C24	-2.928573775	5.202767570	-5.058589194
C25	-3.231209877	5.388139364	-6.549029155
C26	-2.724660024	3.715135545	-4.739657226
C27	-2.605202977	9.728206459	-4.732501766
C28	-1.248114518	10.381700919	-4.910273947
C29	5.993345552	9.583780181	7.412089054
C30	6.537538138	8.415500343	6.589004273
C31	6.663055296	7.529670613	4.254395440
C32	7.701401082	8.220134957	3.348434876
C33	5.442112670	7.040442497	3.454997818
C34	5.801776231	6.060934086	2.335686984
C35	4.565182130	5.329545750	1.810192224
C36	4.532041413	4.387299443	-0.509776647
C37	9.939074763	8.062829003	2.363373690
C38	10.112074163	7.380876365	1.022274438
C39	-4.875102846	-0.622590442	3.631949902
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C42	-2.667610886	0.266191025	4.718883867
C43	-2.166967378	-0.693022616	5.796970971
C44	-6.067231419	-2.900736145	0.833937797
C45	-7.456734685	-2.564182239	0.281043714
C46	-5.837346096	-4.425834104	0.831573578
C47	-9.453326326	-1.166761377	0.499474548
C48	-9.182023143	0.079564929	-0.356602743
C49	-7.579900394	1.829083566	-0.998850440
C50	-6.553726855	1.664798686	-2.119099863
C51	-4.974765510	0.203559776	-3.302915363
C52	-5.615823658	0.130752242	-4.713606961
C53	-4.239209959	-1.132339751	-3.114452990
C54	-3.433442956	-1.316156678	-1.866909800
C55	-2.824838214	-0.460100006	-0.980541724
C56	-2.289592149	-2.533518125	-0.385069256
C57	-7.558340908	-0.735809666	-5.972363493
C58	-7.778325864	0.518539191	-6.816378235
C59	-8.912366949	-1.379967603	-5.593680905
C60	-9.552518492	-2.245630532	-6.639584174
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C67	5.185299516	3.781765411	-4.979557243
C68	5.548480903	1.486464602	-4.339651907
C69	4.101706230	3.396575819	-5.776836309
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C77	0.578211353	-6.171968928	-4.648540172
C78	-0.174006240	-4.907543129	-5.116642940

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C81	-1.324138711	-7.282321124	-2.137707522
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C86	0.564898633	-3.108215721	-9.615547358
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C89	-3.017004254	-5.653907385	-11.318073137
C90	-1.656694968	-7.389196024	-10.060779233
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H163	-4.646037954	2.828143657	1.051310139
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H165	-7.101171901	6.252851219	-1.383895246
H166	-0.534093338	5.079752939	1.438131587
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H169	-1.591676512	4.485554944	-0.724201178
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H173	-3.436279026	6.436263962	-6.809306856
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H177	-3.585296954	3.129569878	-5.094259434
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H184	-0.358777908	3.566416115	-2.633652676
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H189	4.175765165	0.038448310	-5.167517342
H190	6.067378867	0.736018994	-3.739037945
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H198	0.970688325	6.140837156	-0.921660237
H199	-3.189763710	9.865951201	-5.656931824
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H202	10.889127455	8.026991313	2.917613656

H203	-0.647773526	-0.958047794	7.144178855
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H205	-0.634961442	-4.730127911	9.578806008
H206	0.823392876	-5.448984596	8.847280565
H207	-1.775180093	-4.597586177	7.448103146
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H221	-1.826679554	0.877344476	4.361316790
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H224	-8.495755918	2.217861911	-1.463878782
H225	-7.244510924	0.243966153	0.394209994
H226	-7.348586830	-0.533615114	-3.847944355
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H238	-9.997586838	-1.880393291	-0.131819595
H239	-1.845784357	-3.367644345	0.151871406
H240	-10.112749863	-0.873678004	1.327850500
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C65	7.125160656	2.950191365	-3.455574750
C66	5.951142032	2.569284792	-4.327477066
C67	5.233495398	3.538052730	-5.053653696
C68	5.535296676	1.229634140	-4.426796034
C69	4.133188580	3.187300527	-5.843280676
C70	4.447202240	0.862994711	-5.218789239
C71	3.744614032	1.843711020	-5.923135627
C72	4.998922156	-4.174013546	-6.418167713
C73	3.878896726	-5.030930342	-7.021114447
C74	4.436889334	-3.281406864	-5.300268466
C75	2.895400374	-7.277781216	-7.180190834
C76	1.528903499	-7.160917936	-6.500821657
C77	0.240001469	-6.228741089	-4.611575421
C78	-0.458187192	-4.934523461	-5.080219364
C79	0.522249339	-6.239596038	-3.097617352
C80	-0.674491068	-6.056576674	-2.157624806
C81	-1.677596139	-7.220267955	-2.061369207
C82	-3.196344770	-7.914493751	-3.925063829
C83	-0.262179731	-2.631012163	-5.866654349

C84	-0.569683997	-2.632590784	-7.376546946
C85	0.583061290	-1.389234450	-5.552217937
C86	0.298473481	-3.193656696	-9.593540805
C87	-0.490948924	-4.111265355	-10.524380945
C88	-2.024344895	-6.024608488	-10.738547643
C89	-3.416679213	-5.589330664	-11.240459936
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C94	-5.688620956	-2.881705834	-9.993257035
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C96	-6.883028926	-4.015253838	-8.073140551
C97	-4.645377530	-3.203771541	-7.693986883
C98	-6.925573275	-4.528977643	-6.774383110
C99	-4.660048586	-3.733718837	-6.398699396
C100	-5.801049632	-4.400640551	-5.957318331
C101	5.425209710	-5.957206828	6.997125601
C102	3.947877952	-5.688694338	6.765472189
C103	2.202569168	-5.308143691	5.047036137
C104	1.610921379	-6.418956851	4.172655885
C105	1.714452445	-7.515215831	1.984149255
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C108	5.946494564	-8.774007517	0.400825861
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C113	0.508143421	-3.304756617	8.482846026
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C118	-1.883881416	-5.538930929	1.941266553
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C120	-0.712586580	-4.852377313	1.600988347
C121	-0.880944506	-3.533242348	3.618212616
C122	-0.191894923	-3.871082029	2.450324748
C123	8.991205824	-0.806586734	6.464991538
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C127	6.414546816	-1.818916632	8.281908127
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C133	3.724479250	2.315806952	6.269295807
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Fe141	5.073023761	-1.196874847	-0.459433902
Fe142	4.103544681	-3.337097414	0.646963430
Fe143	3.847364262	-3.013170615	-1.995155644
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H193	-0.714149759	8.811509596	2.099788956
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H226	-7.417766654	-0.236950113	-3.744107970
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H238	-10.064822074	-1.427413433	0.000221628
H239	-1.994114510	-3.294029979	0.184633175
H240	-10.127989170	-0.431577749	1.468870781
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H253	-1.204606299	-7.216098927	-7.496394845
H254	-2.726431161	-6.863211106	-6.714715143
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H266	1.020452345	-7.195399490	-2.865120571
H267	-3.773111623	-3.668393327	-5.765334683
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H278	-0.245936375	-5.914272836	-1.156152608
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H351	6.966550886	3.950205023	-3.025193370
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H364	-4.977384236	-2.047255079	-10.099611445
H365	-6.673030988	-2.513026046	-10.315480900
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H368	-1.473106212	-0.873259094	0.665374553
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N370	2.387028574	1.914540943	-0.193438929
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H197	3.609695635	3.496382540	6.663246312
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H206	0.683003575	-5.486825506	-8.849074538
H207	-1.880792271	-4.415531785	-7.539791478
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Fe6	-2.56	C6	-6.514946318	-5.615813393	5.764169727
Fe7	2.42	C7	-4.409242914	-6.159614756	4.637779006
		C8	-3.741790845	-4.786625243	4.507486793
		C9	-3.805461620	-2.558052449	3.514432058
		C10	-3.941839535	-1.734710355	4.804454056
		C11	-5.256281019	-1.205652701	6.773534279
		C12	-4.393212046	-1.729332807	7.930180892
		C13	-3.727327238	-3.680365199	9.251461617
		C14	-2.223931290	-3.972732052	9.162047605
		C15	-0.351718380	-4.674051610	7.727371847
		C16	0.561320391	-3.659859695	7.029850797
		C17	0.638515845	-1.463518932	5.859686283
		C18	0.590012138	-0.183678540	6.712108781
		C19	0.102946125	-1.266919104	4.423057204
		C20	0.633867756	0.035217180	3.815200842
		C21	0.430932156	-2.491216804	3.562259950
		C22	-0.760417320	1.686194807	7.554880499
		C23	-0.635856317	1.490075456	9.076062177
		C24	-2.064121334	2.415771441	7.146400044
		C25	-2.274790511	3.686019394	7.979143386
		C26	-2.052009911	2.758951644	5.650680340
		C27	-1.294839397	0.215544046	11.031640672
		C28	0.116770276	0.085225469	11.567626492
		C29	6.502562338	-10.784007805	4.791596335
		C30	6.974413536	-9.546384375	4.028428733
		C31	7.095567819	-7.052700140	4.179408057
		C32	8.253286212	-6.536324896	5.056327577

C33	5.873211447	-6.119618130	4.220684873
C34	6.173974078	-4.690522891	3.760669135
C35	4.884915167	-3.912558610	3.485751335
C36	4.817780591	-1.410284256	3.570437842
C37	10.525802622	-5.617983846	5.054990475
C38	10.739157689	-4.124277497	4.927705205
C39	-5.159220669	-2.953048734	-1.509149926
C40	-5.632044626	-1.532061686	-1.147695277
C41	-3.618624008	-2.976302966	-1.447408661
C42	-2.967489915	-4.374649556	-1.432410021
C43	-2.647947036	-4.961444762	-2.804256982
C44	-6.316168100	0.630247441	-2.161997749
C45	-7.563161294	0.995621268	-1.355362155
C46	-6.316121321	1.200684954	-3.614966547
C47	-9.518842735	0.149569218	-0.155050071
C48	-9.087542880	0.368103524	1.304506374
C49	-7.278547835	0.221272403	2.965078497
C50	-6.221747417	1.310745082	3.158038696
C51	-4.745002580	2.992427742	2.146281891
C52	-5.296421000	4.304919849	2.742650255
C53	-4.154940572	3.345997169	0.770214175
C54	-3.460018771	2.256406142	0.004378541
C55	-2.787003341	1.118101216	0.405124722
C56	-2.654713434	1.332398106	-1.790357712
C57	-7.236087267	5.841541729	2.745385336
C58	-7.250874708	6.079054475	4.251841482
C59	-8.675891796	5.796146546	2.181252771
C60	-9.334861237	7.123961024	1.943059705
C61	-9.339799046	8.280190915	2.699547526
C62	-10.546807216	8.553108586	0.861091929
C63	8.921800215	2.141080397	3.717644826
C64	9.925304486	1.005131322	3.654025633
C65	7.521281013	1.514377117	3.502062148
C66	6.404186046	2.523447709	3.624222468
C67	5.785630171	2.781522537	4.861770080
C68	5.951996642	3.238444909	2.500434406
C69	4.749537028	3.715253758	4.976996590
C70	4.930456644	4.182249826	2.602391854
C71	4.324757510	4.415514125	3.840456785
C72	5.251997946	7.422036897	-1.468633816
C73	4.120796129	8.361912940	-1.905486553
C74	4.676961135	6.038710659	-1.126270704
C75	2.997570210	9.469972498	-3.787241847
C76	1.592366552	8.866329190	-3.833928245
C77	0.220966783	6.820077872	-3.683921101
C78	-0.358136302	6.749394289	-2.255482632
C79	0.381647219	5.436879633	-4.338789191
C80	-0.867627869	4.553572207	-4.438267856
C81	-1.957340401	4.997728017	-5.431236255
C82	-3.372084057	7.029933163	-5.120527772
C83	0.016411275	6.436472039	0.134492556
C84	-0.157322279	7.816657613	0.797772003
C85	0.887861154	5.566865257	1.046329429
C86	0.841285515	10.022568747	1.138093557
C87	0.069619330	11.288778391	0.773067252
C88	-1.573791295	12.364451209	-0.710753744
C89	-2.894133302	12.699981297	0.015693076
C90	-1.798000055	12.265343858	-2.237617662
C91	-2.704913961	11.093184057	-2.595506537
C92	-4.687968105	11.878688541	1.478698940
C93	-4.657637660	12.943401983	2.569622915
C94	-5.125001194	10.518563728	2.088020520

C95	-5.291892743	9.432249789	1.048256510
C96	-6.481525551	9.330661643	0.309007765
C97	-4.259393697	8.519743903	0.770264737
C98	-6.641421459	8.357459545	-0.679850506
C99	-4.394037816	7.551106345	-0.228763985
C100	-5.586877834	7.480653954	-0.947643062
C101	4.510615968	-4.005026367	-8.810677266
C102	3.073012877	-3.853040296	-8.342469514
C103	1.483555588	-2.385459150	-7.124716731
C104	0.905038835	-1.086087669	-7.691087562
C105	1.098187170	1.355313187	-7.705127884
C106	2.173607899	2.424847196	-7.864000539
C107	4.449711202	3.204041168	-7.435711543
C108	5.321263821	3.171013669	-8.673533622
C109	-2.345707548	-3.997911146	-9.088384242
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C112	-1.048943478	-5.856677630	-7.928841339
C113	-0.364429184	-6.266116864	-6.643959618
C114	-3.983215193	-0.636057293	-8.264841498
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C117	-3.069595418	-0.488257269	-5.892297174
C118	-2.326524216	0.685823739	-5.677717169
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C123	8.381296733	-5.872467979	-4.246010858
C124	9.537828191	-5.850680687	-3.233169279
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C126	5.860713723	-6.317756383	-4.506469104
C127	5.632472730	-6.960586825	-5.706881513
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C134	3.283519025	-8.329571813	-1.309446171
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Fe139	4.025532250	-1.911453747	-3.672922170
Fe140	2.356181103	0.806348787	-1.278052934
Fe141	5.062111462	0.686430353	-1.320112669
Fe142	4.005242335	0.640915023	-3.675491418
Fe143	4.029673217	2.969505713	-2.290209079
Fe144	4.898357987	-1.867736715	-1.244046004
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H148	-9.498250339	-5.189637200	0.930001948
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H153	-9.635896949	-3.337448203	2.280084123
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H162	-4.029603315	-6.615198467	5.560341546
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H164	-4.923798596	-3.680412760	7.483316312
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H166	0.036403230	-3.413104547	4.015859841
H167	-0.015645926	-2.385540174	2.561935409
H168	1.516586967	-2.602190583	3.425039408
H169	-0.993377718	-1.185890921	4.490941598
H170	-4.233089038	-4.634890871	9.457069199
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H172	-1.982773572	-0.092164165	9.038169800
H173	-2.346212535	3.476465524	9.055774655
H174	0.245925594	0.159949004	2.795243643
H175	1.730935284	0.029618583	3.750538612
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H177	-2.967950718	3.303060298	5.379447458
H178	-3.204861868	4.182315443	7.664951281
H179	-1.190486862	3.403363903	5.410892264
H180	-1.443603484	4.393227681	7.827203060
H181	-2.906971342	1.728870989	7.343901803
H182	0.100682594	2.317100369	7.282283903
H183	-1.434495631	0.051825765	6.327560009
H184	0.326234157	0.913578320	4.400159111
H185	1.074008972	4.602965850	0.543664588
H186	0.305507984	5.377496180	1.962284655
H187	2.446935503	5.888266946	2.196860642
H188	2.912527047	5.369803748	4.770367056
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H195	-2.368311589	-4.359208560	7.125381489
H196	-3.863701393	-3.023667225	10.120261054
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H202	11.424584332	-6.145242070	4.701699848
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H206	-0.305777141	-5.718266832	-8.727445264
H207	-2.718570709	-4.771639653	-7.076931051
H208	-2.997173704	0.495818438	-9.900125335
H209	-2.867276781	-4.810324788	-9.617057843
H210	-3.223468344	-2.385202457	-2.288255349
H211	-3.626561142	-5.097466257	-0.918355487
H212	-2.028018667	-1.491145747	-8.462347727
H213	-4.920497332	-0.932427400	-8.777222471
H214	-0.683548321	-2.829674754	-9.515777345
H215	-0.827140541	-5.688222860	-2.119336019
H216	-1.255257901	-3.795876885	-7.224533225
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H224	-8.119069786	0.470762998	3.626843217
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H226	-7.148670080	3.829686218	2.004672025
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H232	-3.450357736	4.178249001	0.935443121
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H239	-2.376168259	1.113990205	-2.816133576
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H268	2.918370604	10.390100599	-3.192790461
H269	-2.436402843	7.164580194	-6.949972420
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H274	-5.491787154	1.113455387	-1.618686983
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H279	0.584721947	9.796526725	2.184347984
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H281	-0.917346360	13.225454282	-0.518692576
H282	1.907543557	10.284799517	1.102346568
H283	-2.875753642	10.870379908	0.921921910
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H285	5.056879199	-4.466542511	-7.961754810
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H288	4.010698694	-5.641868547	-9.909106445
H289	5.513178030	5.390348330	-0.833844273
H290	5.296428064	8.188703545	0.417211633
H291	4.669048224	8.136240151	-3.872757824
H292	3.984910724	6.132421131	-0.275845655
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H304	2.206097678	-0.067602977	-6.491855527
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H311	5.626318397	-11.162728527	4.243393310
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H313	6.928743911	-10.612269830	6.798368396
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C132	2.359283690	-6.572903583	0.814773925
C133	3.420496237	-6.816568793	-0.333470594
C134	3.432417098	-8.323227777	-0.720116927
C135	4.566707138	-8.677407363	-1.697630621
C136	4.786948002	-10.156239464	-1.849882870
C137	4.815251328	-6.500914993	0.290796460
C138	3.895177562	-0.672073160	-1.697776100
Fe139	4.495073652	-1.977518034	-3.163693967
Fe140	2.385666867	0.717137050	-1.030016790
Fe141	5.129339051	0.656570343	-0.752933659
Fe142	4.346783074	0.562170646	-3.240950541
Fe143	4.099906679	2.901728041	-2.046373262
Fe144	5.021503250	-1.911041908	-0.630395723
Fe145	2.615635429	-2.126218810	-1.467489272
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O453	0.142883159	12.367907121	1.061697606
O454	-3.424725150	13.738739962	-0.930297326
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O457	-5.461938206	6.487539287	-2.783337288
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O461	7.207373986	3.694368966	-8.165239329
O462	-3.643866442	-3.529271278	-9.210343281
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	O473	5.259821056	-7.202964523	1.228273749
	O474	3.155456328	-6.007524184	-1.422093302
	O475	9.091757798	-5.913656032	2.696477455
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	O477	-4.192410172	4.287126883	-3.464060412
	O478	8.587370263	-10.056883718	-0.339446228
	O479	7.781626297	-8.183323890	1.688775275
	S480	3.978159414	5.217222731	-2.238518050
	S481	2.476743044	1.786372261	-3.161240632
	S482	2.726344409	-3.342519971	-3.289447860
	S483	3.754562276	2.229250921	0.140487653
	S484	0.379623003	-1.792605543	-1.192107760
	S485	4.824373648	-0.744000500	-4.990976358
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Fe1	3.17	C1	-7.791551104	-5.321974483
Fe2	0.43	C2	-7.964573617	-6.562854872
Fe3	-2.56	C3	-8.869458016	-3.350147738
Fe4	2.89	C4	-8.460408988	-3.545311903
Fe5	-2.41	C5	-8.452402700	-5.006057597
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		C8	-4.099049481	-4.519641284
		C9	-4.027021820	-2.319278868
		C10	-4.181505532	-1.447818770
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		C12	-4.730621590	-1.359577614
		C13	-4.195216551	-3.299676479
		C14	-2.705936229	-3.664154862
		C15	-0.817033409	-4.479562791
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		C25	-2.377942406	3.961331096
		C26	-2.119682013	2.967078867
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		C28	-0.289791440	0.346280983
		C29	5.859813635	-10.943393338
		C30	6.410435522	-9.742887678
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		C32	7.784284135	-6.771232491
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		C37	10.092491371	-5.949460201
		C38	10.379332186	-4.471412617
		C39	-5.202693181	-2.799616539
		C40	-5.624162548	-1.345249159
		C41	-3.669544039	-2.891185141
		C42	-3.080467810	-4.315325778
		C43	-2.725453718	-4.934272186

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C45	-7.573449767	1.193610194	-1.817006791
C46	-6.133706715	1.358583148	-3.886598024
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C48	-9.102107200	0.794533838	0.992153532
C49	-7.355445147	0.607866367	2.713277626
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C51	-4.663499942	3.224664624	1.906437614
C52	-5.162450193	4.601154337	2.421919010
C53	-3.988593390	3.492154918	0.551788699
C54	-3.303439058	2.351101846	-0.138445975
C55	-2.715992344	1.177071088	0.271981693
C56	-2.398400461	1.344554852	-1.916771771
C57	-7.050705254	6.206654633	2.357494520
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C61	-9.053284653	8.721721408	2.165940310
C62	-10.179551822	8.998759825	0.277060240
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C64	9.826261107	0.659198990	4.032921885
C65	7.459172605	1.268712245	3.757661618
C66	6.378368738	2.323464999	3.812980549
C67	5.728548618	2.641194538	5.020634173
C68	5.995464615	3.026060379	2.656930479
C69	4.726502795	3.617198362	5.075327264
C70	5.008502821	4.012149799	2.697715878
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C73	4.546205742	8.122169497	-1.925099767
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C76	2.127844973	8.697012324	-3.963822694
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H188	2.982666615	5.356035383	4.767335596
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H261	2.787754495	6.782722221	-3.558031203
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C84	-0.335802597	7.770620394	1.171336438
C85	0.728914294	5.512935158	1.272067179
C86	0.597366373	9.985843993	1.626868271
C87	-0.208448161	11.246568452	1.321877552
C88	-1.860002466	12.356741759	-0.127022485
C89	-3.189356312	12.630439700	0.609215415
C90	-2.083168305	12.323150162	-1.656692351
C91	-2.967978113	11.153322562	-2.073192674
C92	-4.968387305	11.702865827	2.027949793
C93	-4.965338479	12.733471179	3.150188947
C94	-5.362611199	10.311451250	2.596750418
C95	-5.501470191	9.257715346	1.519429320
C96	-6.698991157	9.127487349	0.798938872
C97	-4.433683982	8.410883769	1.177287284
C98	-6.831149868	8.191194077	-0.229934657
C99	-4.541010222	7.484960417	0.134150146
C100	-5.741961907	7.384672530	-0.566343888
C101	4.545018798	-3.495813485	-8.980913164
C102	3.107355998	-3.399182623	-8.496360960
C103	1.524592082	-2.036370551	-7.144045847
C104	0.919012212	-0.731899586	-7.671838607
C105	1.067806292	1.710147418	-7.637249608
C106	2.115115643	2.810003799	-7.778225773
C107	4.374532838	3.632295253	-7.343144746
C108	5.227508817	3.675484972	-8.594218697
C109	-2.289391248	-3.612998933	-9.208591062
C110	-3.406315753	-2.598567512	-8.929504386

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C113	-0.258299796	-5.975466886	-6.906999856
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C115	-3.626273785	0.999079092	-8.888805930
C116	-4.283663399	-0.233345749	-6.720779875
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C118	-2.279463510	0.888405941	-5.622697609
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C127	5.595665919	-6.461043671	-6.020250575
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C138	3.709505099	-0.355559422	-2.177066924
Fe139	4.059012670	-1.654421213	-3.698177067
Fe140	2.503945944	1.204030788	-1.782448975
Fe141	5.042262480	0.919455708	-1.362806381
Fe142	4.076942157	0.884710287	-3.765394081
Fe143	4.090470529	3.232114395	-2.371501862
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Fe145	2.294766077	-1.519220903	-1.289280761
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H178	-3.289739284	3.736458452	7.850690128
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H180	-1.531416566	3.967804025	8.019121866
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H190	6.314702294	2.994370251	1.594316126
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H246	-4.172424354	3.662828933	-2.144920959
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		C20	-0.267143055	-0.292855635	3.816491534
		C21	-0.417994560	-2.786819630	3.347894134
		C22	-2.272188734	1.166825713	7.335271364
		C23	-2.472903105	0.849152197	8.827354120
		C24	-3.438116320	1.990211479	6.735139629
		C25	-3.755387619	3.214635770	7.601981426
		C26	-3.117676436	2.427284537	5.299035397
		C27	-3.583359399	-0.514457278	10.496693017
		C28	-2.317950759	-0.780958401	11.286873467
		C29	4.825499440	-11.498439460	5.058511442
		C30	5.525667508	-10.245072426	4.537067646
		C31	5.758858590	-7.794598088	4.964168765
		C32	6.730816570	-7.417508490	6.098391184
		C33	4.594462641	-6.796800968	4.845390845
		C34	5.038221936	-5.358301005	4.571372640
		C35	3.857094738	-4.499244052	4.115115418
		C36	3.884225031	-2.009386256	4.399101228
		C37	8.981616594	-6.620073527	6.640235848
		C38	9.261411798	-5.133528149	6.703152396
		C39	-4.782951634	-2.535481278	-2.781202112
		C40	-5.257634423	-1.107959318	-2.457739710
		C41	-3.297155483	-2.656293312	-2.395642609
		C42	-2.724154222	-4.087075683	-2.349769498
		C43	-2.153551277	-4.602810011	-3.667369320
		C44	-5.708824499	1.090891102	-3.456605697
		C45	-7.124793278	1.477210456	-3.011786314
		C46	-5.329444166	1.836590939	-4.752410279
		C47	-9.254136834	0.708011280	-2.092847591
		C48	-9.117201935	0.818076309	-0.566882770
		C49	-7.699986925	0.459371892	1.408285748
		C50	-6.651677355	1.451573529	1.911828512
		C51	-4.918001966	3.106589861	1.357495312
		C52	-5.504942068	4.432062865	1.906591419
		C53	-4.019584806	3.495044415	0.171778957
		C54	-3.239958931	2.403727459	-0.495144312
		C55	-2.745356366	1.185938010	-0.092420811
		C56	-2.057897017	1.523096220	-2.172051251
		C57	-7.362389556	6.051225872	1.678145170
		C58	-7.680443516	6.174274586	3.166673370
		C59	-8.654346212	6.125212283	0.832651902

C60	-9.186314280	7.502608361	0.563731727
C61	-9.251768927	8.619508947	1.374007624
C62	-10.090423053	9.066379565	-0.627691820
C63	8.059301064	1.330648545	5.690217862
C64	9.016710418	0.153082336	5.725561061
C65	6.712579654	0.793678319	5.145438623
C66	5.633260081	1.850254823	5.087732048
C67	4.805888079	2.118740187	6.193769354
C68	5.424915853	2.597214002	3.913932207
C69	3.799753260	3.090148010	6.129222755
C70	4.434037924	3.575851890	3.837093827
C71	3.617708951	3.818357865	4.945883619
C72	5.827776048	7.198974080	0.272700474
C73	4.825114470	8.211370490	-0.294019471
C74	5.198784830	5.796012260	0.305483176
C75	4.153400977	9.543656615	-2.244544558
C76	2.774939081	9.008557148	-2.630275987
C77	1.333341695	7.043631473	-2.970869434
C78	0.441339354	6.889022060	-1.722269524
C79	1.571407174	5.705130525	-3.691614240
C80	0.335545298	4.908562075	-4.122456006
C81	-0.490252471	5.481557650	-5.290233251
C82	-1.840512443	7.580480048	-5.142548897
C83	0.267538590	6.404391260	0.665703564
C84	0.028025029	7.733210753	1.411524640
C85	0.869336155	5.389406292	1.641087475
C86	1.018186899	9.846230457	2.146461261
C87	0.404253404	11.180283768	1.726961678
C88	-0.823785836	12.458562941	0.020517157
C89	-2.255684867	12.826525198	0.470146014
C90	-0.713784692	12.487211455	-1.520958801
C91	-1.579977539	11.413043075	-2.168098139
C92	-4.358788287	12.014640487	1.458238260
C93	-4.514136435	13.036077667	2.578631340
C94	-4.946513282	10.644798229	1.897274349
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C96	-5.985492969	9.667523340	-0.190475284
C97	-3.929402841	8.696924009	0.606545783
C98	-5.978539194	8.805887415	-1.289560107
C99	-3.895305731	7.838820132	-0.497894698
C100	-4.920428971	7.907357089	-1.438685016
C101	6.090799684	-3.636155546	-7.956745448
C102	4.593066655	-3.442777346	-7.779011868
C103	2.859801009	-1.986830421	-6.749951634
C104	2.479155909	-0.619137194	-7.327691864
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C106	3.924197941	2.825691910	-6.990992009
C107	6.106842758	3.441065028	-6.079483041
C108	7.223266005	3.446706481	-7.105040484
C109	-0.536843596	-3.183637887	-9.618355309
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C118	-0.946014074	1.225368547	-5.934407201
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C132	1.933862120	-6.813079114	0.374789511
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Fe140	2.933018914	1.043467629	-1.159633210
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H211	-3.502395546	-4.799811264	-2.024603212
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H226	-7.229992119	4.070789602	0.863998545
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H289	5.786391875	-5.181144322	-9.248033913
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Fe141	5.048809371	-1.382125993	-0.218784647
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Fe145	2.497013756	-0.490620023	2.709550183
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	O449	0.484295305	-7.656977472	-7.100117793		
	O450	-1.686680760	-4.819868436	-5.386000488		
	O451	-1.256945911	-1.815704658	-7.924136088		
	O452	1.878900676	-1.347481937	-6.436172680		
	O453	-0.109113890	-3.923716081	-11.806177615		
	O454	-3.850560895	-6.026318702	-12.296402764		
	O455	-4.165095050	-7.090742648	-8.956781678		
	O456	-6.215781451	-3.082785815	-13.228773607		
	O457	-5.790523899	-4.662855581	-4.885446193		
	O458	2.634653278	-5.705532002	7.795192376		
	O459	0.251597833	-7.278196708	4.578372812		
	O460	2.061502006	-9.106665678	0.274420851		
	O461	6.501701304	-9.420603958	-0.107143384		
	O462	-4.266330189	-6.707157654	6.817807461		
	O463	-0.548139079	-2.322713190	8.618820135		
	O464	1.323735773	-3.406337392	8.074809961		
	O465	-3.606364964	-8.570007962	2.100408667		
	O466	10.562149183	-0.620364582	5.379540488		
	O467	13.292822397	1.491124534	5.752259384		
	O468	0.339515821	2.368370091	5.902187041		
	O469	0.920622010	4.020563296	7.272418767		
	O470	5.962809427	2.321239044	10.613687198		
	O471	3.772088113	1.859834342	10.912486798		
	O472	5.638724849	1.515506600	5.308560788		
	O473	5.552337559	3.591691123	6.184743466		
	O474	3.248552271	0.843893753	6.171684971		
	O475	9.401070344	4.074307462	4.414457961		
	O476	7.457549510	2.347906557	3.300572592		
	O477	-4.605900979	-4.550654428	-2.540029444		
	O478	8.744684365	2.953224811	9.424532952		
	O479	8.094063065	4.130837198	6.887352347		
	S480	3.491795637	-4.241125118	-3.928592903		
	S481	2.120864193	-3.638945478	-0.472185988		
	S482	2.519781166	-1.792010361	4.482118275		
	S483	3.765100615	-1.198389814	-2.044418645		
	S484	0.645454971	-1.023692962	1.513680252		
	S485	4.279982018	-4.647221960	2.652804211		
	S486	3.720460529	1.327316562	2.923752172		
	S487	5.736279208	-3.550305627	-0.629967314		
	S488	6.065026938	-1.436465243	3.660812031		
	S489	6.370970429	0.312331020	0.398161535		
	5, 47(3/2)		bm12b2n2x6x2n2ndtc.car_5			
	Fe1	3.20	C1	-7.414842655	3.319935046	4.975277818
	Fe2	0.05	C2	-7.501236745	2.967292400	6.463325615
	Fe3	2.83	C3	-8.605965162	3.454433938	2.830585804
	Fe4	-2.65	C4	-8.187686038	4.858989595	2.403462817
	Fe5	2.35	C5	-8.081978811	7.236084799	2.953782248
	Fe6	-1.11	C6	-6.564303783	7.448048425	2.950255310
			C7	-4.397115591	6.709914739	3.818254995

Fe7 -2.29

C8	-3.768086116	6.018055763	2.604316134
C9	-3.868696284	4.172827417	1.011633240
C10	-4.085644764	4.989122801	-0.272447077
C11	-5.470356660	6.543275201	-1.516128260
C12	-4.624062185	7.823305475	-1.561620271
C13	-3.962406840	9.868008042	-0.386103384
C14	-2.455610370	9.949016215	-0.111516373
C15	-0.528152973	8.977907442	1.068101479
C16	0.389556101	7.963173323	0.376498933
C17	0.439586674	5.984351653	-1.133628748
C18	0.342825337	6.204533154	-2.653719001
C19	-0.075078251	4.596406384	-0.680479314
C20	0.423766050	3.490160983	-1.615037726
C21	0.297682464	4.334971640	0.784067910
C22	-1.070004935	6.162818018	-4.660483313
C23	-1.006563002	7.626115833	-5.130014596
C24	-2.360874524	5.437978763	-5.112462502
C25	-2.606766141	5.630049211	-6.612837486
C26	-2.294727239	3.942994195	-4.768460061
C27	-1.702279217	9.921559435	-4.793677083
C28	-0.307438036	10.493301319	-4.953322098
C29	6.597317264	9.016272304	7.570307225
C30	7.045907109	7.803956817	6.751911790
C31	7.159858377	6.923570464	4.415349717
C32	8.278576298	7.531507567	3.546695395
C33	5.927209044	6.538595837	3.579785221
C34	6.229535450	5.529523695	2.469855428
C35	4.944949957	4.925946585	1.898636512
C36	4.855633302	3.920483217	-0.396142706
C37	10.508676417	7.175072283	2.597507992
C38	10.661142573	6.476597147	1.263205173
C39	-5.038696497	-0.237646026	3.488126783
C40	-5.556252914	-0.517028424	2.066084551
C41	-3.496342106	-0.154464740	3.405032819
C42	-2.774236631	0.464864102	4.620481586
C43	-2.393817204	-0.519565986	5.724241411
C44	-6.202889608	-2.347135949	0.525518160
C45	-7.464677004	-1.762589884	-0.115242808
C46	-6.207365809	-3.899605196	0.618802980
C47	-9.499098193	-0.439960340	0.235725059
C48	-9.128073854	0.822697105	-0.555537474
C49	-7.390888396	2.451695004	-1.145815103
C50	-6.366224570	2.198255374	-2.253998299
C51	-4.916135051	0.623259739	-3.451319706
C52	-5.555867475	0.649467196	-4.855962701
C53	-4.308744283	-0.777761630	-3.278979945
C54	-3.543144006	-1.046516560	-2.019626219
C55	-2.923943129	-0.196598008	-1.126877556
C56	-2.581504458	-2.300907785	-0.524068281
C57	-7.514306517	-0.102333947	-6.149530056
C58	-7.607500759	1.168489547	-6.989487097
C59	-8.922281083	-0.639482513	-5.803340735
C60	-9.609330604	-1.439909785	-6.870831431
C61	-9.657989611	-1.273069740	-8.241364136
C62	-10.830612786	-3.054075167	-7.637835019
C63	8.733204005	2.644924997	-3.891359992
C64	9.768901333	3.071788389	-2.866185380
C65	7.358231773	2.688896739	-3.186200286
C66	6.204608983	2.363160946	-4.105346688
C67	5.538005682	3.367054431	-4.832256944
C68	5.750431896	1.039372481	-4.243056059
C69	4.450962556	3.063112329	-5.660047047

C70	4.675636157	0.719687643	-5.072568057
C71	4.023467548	1.733927972	-5.777337777
C72	5.075826340	-4.337404414	-6.302472121
C73	3.939467490	-5.144864047	-6.944042603
C74	4.512674407	-3.423136782	-5.204028865
C75	2.860051358	-7.341848097	-7.146590988
C76	1.476792142	-7.167186639	-6.516464749
C77	0.159036195	-6.207757394	-4.665780887
C78	-0.459793860	-4.888454708	-5.174216986
C79	0.373018136	-6.228564162	-3.140624379
C80	-0.848731248	-5.972042064	-2.250230981
C81	-1.915861945	-7.080670783	-2.183639251
C82	-3.392565208	-7.698400224	-4.104035586
C83	-0.152694055	-2.585550612	-5.909717829
C84	-0.413838480	-2.580898437	-7.428207250
C85	0.727671595	-1.375209211	-5.576105374
C86	0.516705167	-3.160578910	-9.614380506
C87	-0.286373253	-4.028001740	-10.580212422
C88	-1.895507271	-5.866082158	-10.871173006
C89	-3.253210384	-5.380140583	-11.419550707
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C92	-5.078079516	-3.750946371	-11.206210027
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C95	-5.586343166	-3.100135122	-8.791688816
C96	-6.770737345	-3.688681065	-8.321830495
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C100	-5.753026139	-4.118720075	-6.182058045
C101	4.893932420	-6.205977416	7.117435017
C102	3.433046155	-5.889186551	6.844123729
C103	1.761051099	-5.431602626	5.067932872
C104	1.169323973	-6.527295250	4.173988996
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C108	5.550639142	-9.001585692	0.538837004
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C112	-0.623567704	-4.735449242	8.664207073
C113	0.036661835	-3.389189958	8.466781272
C114	-3.692162184	-7.268735315	4.158862394
C115	-3.279163047	-8.424772821	3.267909575
C116	-4.107429016	-5.981787303	3.401481160
C117	-2.902391254	-5.183694176	2.984447461
C118	-2.183150112	-5.511082102	1.823475769
C119	-2.388085306	-4.197136193	3.843108822
C120	-0.945415003	-4.912742634	1.570184616
C121	-1.148305328	-3.603612484	3.590139226
C122	-0.411524562	-3.986252895	2.467436404
C123	8.687654459	-1.243116508	6.794766227
C124	9.796749381	-0.297596443	6.307105537
C125	7.387621711	-0.493882425	7.125018127
C126	6.198532276	-1.350858302	7.433456312
C127	6.006244113	-2.170373318	8.528532541
C128	4.157152255	-2.117040595	7.309465421
C129	11.031428707	1.780715328	6.549431154
C130	12.373740817	1.089839317	6.458521534
C131	1.224106599	3.131423004	6.275472442

C132	2.629715566	3.171358475	5.746655552
C133	3.603563810	2.144072905	6.457117410
C134	3.608335380	2.404262193	7.990843720
C135	4.647782671	1.535374901	8.718946266
C136	4.883846645	1.945641192	10.144177239
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Fe141	5.041322473	-1.384084499	-0.230521734
Fe142	3.971619889	-3.493420274	0.781913136
Fe143	3.763412986	-3.277870218	-1.838293626
Fe144	5.035075469	-0.278885385	2.062448748
Fe145	2.502259743	-0.488783747	2.708707470
H146	-5.562499141	3.412003365	6.912794588
H147	-5.836240937	1.811504726	6.739611629
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H149	-8.195618471	2.124653834	6.602969007
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H151	-7.937331800	2.756274312	2.306906996
H152	-8.969942494	5.663023397	4.124005358
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H154	-8.529747665	7.901501794	3.703831047
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H156	-8.447389529	7.540210395	1.964479423
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H158	-5.089446353	4.436659887	2.766643531
H159	-4.041910357	6.228880743	4.740066047
H160	-5.248425713	5.970861089	-2.425448514
H161	-5.954125203	5.615994475	0.366091607
H162	-4.047909828	7.748826987	3.812464040
H163	-4.391363921	3.207826017	0.933997655
H164	-5.100524759	8.245066831	0.409443878
H165	-6.533103529	6.824288978	-1.525972717
H166	-0.115297341	5.113261156	1.443130537
H167	-0.109076286	3.365814303	1.112306298
H168	1.388309142	4.297430890	0.924299269
H169	-1.174204879	4.618780811	-0.744538194
H170	-4.467337869	10.462805838	0.389597112
H171	-2.227654008	3.764237686	-3.686692702
H172	-2.304935086	8.240107289	-3.624268016
H173	-2.754626196	6.686485679	-6.880925741
H174	0.086771987	2.510543884	-1.247386415
H175	1.520909043	3.466128577	-1.660208416
H176	8.727639511	3.410730109	-4.691747058
H177	-3.199644210	3.433655558	-5.129534819
H178	-3.505532781	5.073033146	-6.914979210
H179	-1.421953516	3.473883655	-5.251241108
H180	-1.757202487	5.248800573	-7.201875996
H181	-3.207541518	5.888469233	-4.562787312
H182	-0.204067420	5.680437607	-5.140321410
H183	-1.681345698	5.746680290	-2.641149187
H184	0.039396232	3.613995795	-2.636987272
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H186	0.106197595	-0.477974848	-5.726243231
H187	2.205344974	-0.423377295	-6.441755922
H188	2.536266047	2.162111479	-6.951541751
H189	4.313416607	-0.306190483	-5.135550414
H190	6.212310114	0.246493552	-3.650810968
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H199	-2.258134742	10.078431715	-5.732486494
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H201	0.478375565	9.996201004	-4.337630089
H202	11.436132426	7.059714528	3.178920063
H203	-0.923538519	-0.921604001	7.093675406
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H206	0.138650647	-5.508480499	8.837990520
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H208	-2.656281163	-9.195350047	3.780520015
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H221	-1.869339886	0.983766587	4.272714620
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H223	-2.851483060	0.885043514	-1.075975821
H224	-8.262033048	2.922953278	-1.619795286
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H238	-10.132959633	-1.043099839	-0.427584585
H239	-2.216293779	-3.144299240	0.056452022
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H244	-1.132254103	-2.424862866	-5.436653544
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H259	-4.712454955	-6.355283748	-4.937578711
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C81	-1.911440742	-7.060647610	-2.178296187
C82	-3.386637593	-7.685623451	-4.097574169
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C84	-0.409548702	-2.584264469	-7.437230139
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H210	-2.827567841	-2.465662029	-2.679666773
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	C20	-0.045101599	0.114162488	3.869513046
	C21	-0.180580253	-2.422422423	3.684101834
	C22	-1.957706028	1.881456897	7.312949914
	C23	-2.077120032	1.738020112	8.839629536

C24	-3.170600155	2.597778138	6.671544564
C25	-3.489335864	3.904961630	7.405273464
C26	-2.915165787	2.870763844	5.182610458
C27	-3.027803598	0.537043758	10.719565968
C28	-1.712141717	0.447841922	11.467178142
C29	5.763186366	-10.582773157	6.068130507
C30	6.330373556	-9.362009454	5.341817516
C31	6.455423830	-6.869588004	5.462465993
C32	7.465492265	-6.324841280	6.490634940
C33	5.246008034	-5.934189268	5.289972245
C34	5.623896842	-4.521536730	4.838908711
C35	4.397027954	-3.742800581	4.359071535
C36	4.344181717	-1.238378795	4.317017851
C37	9.681505408	-5.333907706	6.809944118
C38	9.868235801	-3.835225633	6.705891285
C39	-4.849329374	-3.055331689	-2.198452635
C40	-5.383874943	-1.633124976	-1.956564543
C41	-3.333107690	-3.031518532	-1.896727124
C42	-2.643975363	-4.401570162	-1.724702767
C43	-2.109281765	-5.035762172	-3.007946324
C44	-5.852131293	0.519910629	-3.096131639
C45	-7.191668174	0.899407789	-2.459696236
C46	-5.685645382	1.040569917	-4.551292186
C47	-9.361776347	0.087877674	-1.653373068
C48	-9.178683804	0.301758956	-0.143929634
C49	-7.669284419	0.182940749	1.787344137
C50	-6.658903307	1.287577676	2.107967626
C51	-5.084936407	2.990152241	1.313673484
C52	-5.766469292	4.282586982	1.811517631
C53	-4.307317716	3.374342190	0.044557003
C54	-3.465954007	2.313588999	-0.596097582
C55	-2.923572084	1.147957682	-0.098772555
C56	-2.302242521	1.425110490	-2.207376016
C57	-7.671874177	5.795671779	1.399118230
C58	-7.947899140	6.070160650	2.873801778
C59	-8.993456282	5.704578407	0.599987278
C60	-9.620644666	7.007050761	0.201340632
C61	-9.736229663	8.201819976	0.885006153
C62	-10.666998369	8.365400067	-1.119696038
C63	8.215399524	2.431317947	4.996940283
C64	9.230366269	1.309425901	5.112713216
C65	6.872858601	1.779168994	4.589456351
C66	5.731372446	2.765339030	4.511792412
C67	4.932066812	3.056372572	5.632087584
C68	5.430172723	3.417054552	3.302336890
C69	3.863944537	3.957007709	5.550081903
C70	4.377464536	4.326265793	3.207581687
C71	3.590338515	4.591972778	4.331411378
C72	5.315085760	7.429019564	-0.880128399
C73	4.259746782	8.351595999	-1.503133544
C74	4.693467796	6.061827626	-0.555480933
C75	3.438586794	9.413567791	-3.561923033
C76	2.064349544	8.788417155	-3.807209360
C77	0.711379664	6.723874585	-3.819359713
C78	-0.078713411	6.681119497	-2.494626461
C79	0.985119613	5.325478561	-4.402673601
C80	-0.224295305	4.421625087	-4.668383656
C81	-1.147108640	4.810299003	-5.838567706
C82	-2.612108838	6.835691068	-5.833105943
C83	-0.067901774	6.454305225	-0.066449781
C84	-0.376017410	7.852818110	0.503244606
C85	0.682533871	5.660054220	1.010563189

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C87	-0.187080340	11.322255383	0.418572999
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C89	-3.020171527	12.658954670	-0.846781081
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C91	-2.391421630	10.999490403	-3.346341949
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C93	-5.185919331	12.961531364	1.362231184
C94	-5.513405136	10.501080473	0.934199233
C95	-5.508538822	9.375953791	-0.074737278
C96	-6.592335149	9.195348318	-0.949360155
C97	-4.409056975	8.509460845	-0.195471181
C98	-6.575472911	8.196257931	-1.927039845
C99	-4.364055768	7.518277714	-1.181629355
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C102	4.342049135	-4.028334238	-7.633133606
C103	2.563465373	-2.555411117	-6.725258146
C104	2.077259221	-1.296105961	-7.449958623
C105	2.276591177	1.139066865	-7.582555156
C106	3.344673732	2.226714096	-7.554083537
C107	5.484704916	3.049588830	-6.713645121
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		C22	-1.135696555	6.154956002	-4.635873833
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H163	-4.325242224	3.219622416	1.076438555
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O452	-1.489911792	-1.813803539	-7.856932043
O453	1.686970448	-1.356708475	-6.472007224
O454	-0.441394550	-3.933572214	-11.773809792
O455	-4.179360119	-6.024307665	-12.178823090
O456	-4.425586634	-7.067430864	-8.801703710
O457	-6.532903106	-3.100213238	-13.081288667
O458	-5.965570696	-4.684276261	-4.766278058
O459	2.840308901	-5.663993874	7.740315419
O460	0.344789126	-7.240604171	4.586232770
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O462	6.474937175	-9.430347429	-0.233491970

	O463	-4.079877083	-6.672578281	6.968043673
	O464	-0.313362359	-2.274054802	8.614992304
	O465	1.545840538	-3.359266696	8.032667599
	O466	-3.615109744	-8.483543764	2.222549900
	O467	10.733103916	-0.637965188	5.087562349
	O468	13.477397645	1.483888260	5.386897767
	O469	0.522559115	2.405700460	5.904715322
	O470	1.152905026	4.078957456	7.224995272
	O471	6.257817399	2.327793153	10.454088572
	O472	4.068490105	1.886137444	10.792161559
	O473	5.789192909	1.516409112	5.135324114
	O474	5.745876298	3.585751838	6.028618991
	O475	3.415261482	0.862151319	6.054981593
	O476	9.549149816	4.064421038	4.129919264
	O477	7.571251847	2.331668379	3.091011247
	O478	-4.618986954	-4.540650875	-2.511730584
	O479	9.032419767	2.956968467	9.164319867
	O480	8.313646997	4.129752916	6.640118159
	S481	3.393035250	-4.280337058	-3.997589877
	S482	2.095728830	-3.692698306	-0.498333757
	S483	2.624830748	-1.746073995	4.402762361
	S484	3.727465060	-1.250088548	-2.141736415
	S485	0.660025893	-0.972816672	1.467637518
	S486	4.348640743	-4.638097373	2.580772905
	S487	3.826826578	1.340313711	2.782098282
	S488	5.703262528	-3.625722550	-0.753568258
	S489	6.167507422	-1.436109028	3.500310466
	S490	6.402217839	0.255951148	0.205812756
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	Fe1	3.20		
	Fe2	0.05		
	Fe3	2.82		
	Fe4	-2.66		
	Fe5	2.36		
	Fe6	-1.13		
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	C2	-7.513939390	2.835028821	6.510168043
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	C4	-8.295515800	4.650706617	2.434163041
	C5	-8.250734926	7.038710617	2.947201217
	C6	-6.740073433	7.298267987	2.929605464
	C7	-4.543896115	6.633953738	3.788840848
	C8	-3.907024646	5.945791904	2.577406615
	C9	-3.975703265	4.076902972	1.010084338
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	C11	-5.664628676	6.375203527	-1.528126907
	C12	-4.849118948	7.675220551	-1.594590279
	C13	-4.238528407	9.758879663	-0.464049410
	C14	-2.728088359	9.874157875	-0.223122391
	C15	-0.763057091	8.975463617	0.956614323
	C16	0.173619054	7.970656973	0.276833097
	C17	0.258723881	5.985617172	-1.223804601
	C18	0.133612876	6.184305751	-2.744926885
	C19	-0.206187669	4.588067794	-0.748632888
	C20	0.319183622	3.484671334	-1.672769415
	C21	0.188897207	4.354474598	0.714720781
	C22	-1.303214270	6.081083073	-4.731608578
	C23	-1.283279465	7.540138541	-5.221967474
	C24	-2.575767069	5.312079204	-5.160000867
	C25	-2.841711633	5.476541918	-6.660198866
	C26	-2.460769581	3.824504950	-4.796608898
	C27	-2.021908457	9.826277363	-4.889189155
	C28	-0.640931440	10.427372615	-5.062211148
	C29	6.421589030	9.310293682	7.395621830
	C30	6.891496030	8.101763947	6.585110276
	C31	7.013991237	7.205025603	4.256712237
	C32	8.108255547	7.832762867	3.370304895

C33	5.784954624	6.778875429	3.434305128
C34	6.104452639	5.754102741	2.342607507
C35	4.831261617	5.121324565	1.778936608
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C37	10.335931279	7.521112632	2.396969996
C38	10.503670237	6.797225590	1.078790382
C39	-4.970931818	-0.315389073	3.586068624
C40	-5.500181873	-0.676055445	2.188081071
C41	-3.432464816	-0.192746798	3.476401710
C42	-2.711674725	0.459484902	4.674514545
C43	-2.282393307	-0.507465725	5.777247049
C44	-6.231906611	-2.552167185	0.783661303
C45	-7.588051117	-2.137516872	0.198440819
C46	-6.094799726	-4.088048862	0.797415505
C47	-9.510230293	-0.633241610	0.373524748
C48	-9.158302492	0.592128936	-0.481455001
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C50	-6.425329668	2.002715114	-2.228693198
C51	-4.937947988	0.435189475	-3.397343361
C52	-5.563831454	0.385563921	-4.814872818
C53	-4.288605021	-0.940552602	-3.190903269
C54	-3.495359844	-1.162585693	-1.942222694
C55	-2.834457924	-0.342215675	-1.060204657
C56	-2.426156795	-2.443913288	-0.457935544
C57	-7.543424663	-0.376045663	-6.087556954
C58	-7.691523472	0.874052275	-6.953350401
C59	-8.925429303	-0.956622051	-5.709081422
C60	-9.604150213	-1.795830775	-6.750890638
C61	-9.686892928	-1.650208654	-8.122680640
C62	-10.785736751	-3.461163568	-7.469180100
C63	8.633301859	2.838368251	-4.022299876
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C68	5.680632628	1.149888770	-4.298771946
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C70	4.603563576	0.791527960	-5.109051025
C71	3.928382104	1.776863694	-5.833385579
C72	5.139682237	-4.255150261	-6.294200878
C73	4.020984128	-5.108299354	-6.907214908
C74	4.560719215	-3.340010470	-5.205714340
C75	3.016198810	-7.344125932	-7.070733150
C76	1.634296271	-7.197783353	-6.432645883
C77	0.305209853	-6.249876590	-4.583753613
C78	-0.362375706	-4.949378278	-5.082953984
C79	0.535176598	-6.255596909	-3.060764377
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C83	-0.122313619	-2.657955500	-5.883547465
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C85	0.729883304	-1.420726382	-5.572072783
C86	0.524528436	-3.261798647	-9.588424748
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C89	-3.200658832	-5.608840146	-11.315762131
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C94	-5.479898030	-2.880159790	-10.143656892

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C103	1.986878833	-5.299467310	5.119115517
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H148	-9.428330933	2.621787257	4.792613852
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H151	-7.991801648	2.557095187	2.368924337
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H163	-4.470724932	3.096235664	0.956840905
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H165	-6.734471222	6.627738377	-1.529982220
H166	-0.249062942	5.121575176	1.371217441
H167	-0.177854241	3.373120512	1.054903497
H168	1.281501246	4.360613532	0.847072011
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H173	-3.012045796	6.526097885	-6.940184050
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H177	-3.346320337	3.279942912	-5.155419426
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H208	-2.368130557	-9.220975582	3.926570261
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H238	-10.081434687	-1.319080778	-0.264046578
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H251	-0.929658662	-7.757578421	-9.798570552
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O460	0.510486262	-7.178227916	4.653988462
O461	2.317079791	-8.984978037	0.333982797
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C81	-2.164812214	-6.720963666	-3.091306670
C82	-3.796811997	-7.032935767	-4.963754646
C83	-0.629336260	-1.647419867	-6.186395663
C84	-0.999576970	-1.397999113	-7.662471555
C85	0.299299857	-0.511751146	-5.737462890
C86	-0.253305630	-1.642437324	-9.977156431
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C93	-6.079199654	-1.256698505	-12.580489417
C94	-6.235515180	-0.979089223	-10.078076348
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C96	-7.408120259	-2.352055108	-8.307685420
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C103	2.060766080	-6.134131629	4.048452762
C104	1.385156237	-7.073835672	3.043547210
C105	1.359064291	-7.840642525	0.719287004
C106	2.319821593	-8.215695857	-0.405724892
C107	4.454043586	-7.883979324	-1.551073533
C108	5.443590890	-8.995719832	-1.255817530
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C133	4.116021170	1.130888605	6.409139545
C134	4.233512800	1.141420797	7.959637292
C135	5.324613562	0.187423451	8.474330191
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C137	5.512873615	1.534287405	5.840758816
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	C32	6.911485528	-7.300116886	6.063350510
	C33	4.736389159	-6.667150490	4.890413018
	C34	5.223342363	-5.258827136	4.540754097
	C35	4.063024924	-4.362108821	4.104743767
	C36	4.179027900	-1.858061321	4.213049561
	C37	9.203382354	-6.519546531	6.442400057
	C38	9.502194642	-5.036014320	6.442626297
	C39	-5.052015093	-2.521132284	-2.407995838
	C40	-5.475444047	-1.081581284	-2.067154337
	C41	-3.541800412	-2.638351559	-2.098138094
	C42	-2.964269677	-4.066391789	-2.015349376
	C43	-2.474121880	-4.656100193	-3.335474389
	C44	-5.742945355	1.179268903	-3.043783802

C45	-7.031498009	1.624110636	-2.351107020
C46	-5.571463516	1.792914883	-4.460565410
C47	-9.293760765	0.986190258	-1.647959989
C48	-9.114430918	1.064292702	-0.125559155
C49	-7.641165881	0.665155093	1.796697083
C50	-6.545138949	1.661471334	2.184851914
C51	-4.851025257	3.293161566	1.502094594
C52	-5.428922945	4.597003551	2.085547610
C53	-4.041034347	3.701702900	0.261753089
C54	-3.286290734	2.617282674	-0.442075471
C55	-2.880677700	1.370644367	-0.021789251
C56	-2.181970431	1.728482958	-2.094681347
C57	-7.188495489	6.288169055	1.761591088
C58	-7.438789594	6.480658911	3.255199411
C59	-8.516174686	6.357784933	0.971775924
C60	-9.042295881	7.730467605	0.674312961
C61	-9.060330295	8.877676278	1.442750387
C62	-9.986288730	9.256451587	-0.534474364
C63	8.366533290	1.450162083	5.140836204
C64	9.290062756	0.247588759	5.183989184
C65	6.979964374	0.926092687	4.691831924
C66	5.916302944	1.999442677	4.674091380
C67	5.145176648	2.286403164	5.815042671
C68	5.660296582	2.739124034	3.505738376
C69	4.151228241	3.272643855	5.791995459
C70	4.679779309	3.731745345	3.469290256
C71	3.923274573	3.996735368	4.614083866
C72	5.885173450	7.032438379	-0.367569739
C73	4.910822009	8.074577319	-0.931101871
C74	5.154472332	5.705285310	-0.111430946
C75	4.189931210	9.330914349	-2.914685295
C76	2.773185588	8.836219919	-3.214085649
C77	1.260963318	6.892249022	-3.358566047
C78	0.463693526	6.824790211	-2.038611831
C79	1.428202146	5.517688630	-4.030428061
C80	0.156435209	4.723804566	-4.346607089
C81	-0.729823358	5.250013220	-5.490541126
C82	-2.030802477	7.380975436	-5.350154877
C83	0.445399281	6.437430928	0.367127593
C84	0.244327076	7.810612654	1.034977476
C85	1.118589263	5.503312460	1.380871794
C86	1.314247097	9.933857650	1.607771140
C87	0.689204670	11.257817493	1.175551766
C88	-0.609423335	12.482948045	-0.519405104
C89	-2.008872435	12.892035217	-0.009862294
C90	-0.579416665	12.434925736	-2.063982068
C91	-1.506132280	11.352557079	-2.607013493
C92	-4.067823830	12.150269012	1.112322106
C93	-4.163960653	13.209435131	2.204280280
C94	-4.658617812	10.810057866	1.626386529
C95	-4.742128361	9.755981183	0.543625135
C96	-5.842328472	9.720156031	-0.327378279
C97	-3.716782533	8.815464227	0.354319036
C98	-5.914238740	8.788856034	-1.366531838
C99	-3.759122438	7.891139724	-0.695215635
C100	-4.862080900	7.888092632	-1.547921412
C101	5.546886918	-4.095264589	-8.103268946
C102	4.063958410	-3.851206552	-7.879399833
C103	2.402684774	-2.299043400	-6.876588764
C104	2.019373516	-0.962224971	-7.523495467
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C106	3.566911509	2.452198648	-7.403820546

C107	5.749308403	3.064243667	-6.481381391
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C112	-0.186482933	-5.573862317	-8.165769699
C113	0.274755292	-6.056114727	-6.808821138
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C115	-2.056030934	1.136123411	-9.323551513
C116	-3.266862511	0.011956829	-7.338646451
C117	-2.185068879	-0.086419696	-6.299637771
C118	-1.396548226	1.029471639	-5.980931136
C119	-1.842189983	-1.337728813	-5.758498136
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C121	-0.683766193	-1.488841237	-4.991150706
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Fe140	2.423320118	0.693058587	-1.063034193
Fe141	5.181474224	0.326513391	-0.517104427
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Fe145	2.368048397	-2.393654717	-0.836016254
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H147	-6.276309328	-6.235033084	-2.145567184
H148	-9.857351908	-4.509741731	-0.778716273
H149	-8.649004110	-6.008253081	-2.088079543
H150	-8.702270900	-7.104704267	-0.710588284
H151	-8.328698180	-2.489743999	0.436642937
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H153	-10.088199468	-2.691608931	0.600314273
H154	-9.778476958	-5.920166217	4.298428127
H155	-7.301940493	-5.790538933	2.520288122
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H158	-5.807137221	-3.912717383	2.065999484
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H160	-6.023768153	0.046277325	5.753380905
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H162	-5.319723888	-6.436287176	4.623576810
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H164	-6.304561161	-3.504403839	6.489522497
H165	-7.453845444	-1.004307739	5.939284841
H166	-0.924205816	-3.521674458	3.884880846
H167	-0.644151342	-2.477526431	2.471300143
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H174	-0.217348983	0.030598040	2.806063081
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H182	-0.915796372	2.110703490	7.313934436
H183	-2.451661006	-0.006345214	6.056811887
H184	-0.381683390	0.761196532	4.413705055
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H187	2.461359167	5.709287379	2.796247003
H188	2.435994296	5.004396477	5.350304526
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H208	-1.325655038	0.963112868	-10.149142470
H209	-1.665920287	-4.342954265	-10.062790805
H210	-2.986992072	-2.048098098	-2.846030369
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H222	-4.197454670	2.867979290	2.276639241
H223	-3.013014639	0.836520571	0.911967628
H224	-8.553371188	0.970795798	2.325984778
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H226	-7.070032661	4.342271055	0.881354481
H227	-8.692071703	9.094191142	2.439454960
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H234	-9.822377694	10.807204876	0.914366858
H235	-8.344720209	5.875547241	-0.003173735
H236	-6.168827481	2.183095353	0.208055352
H237	-7.347703427	-0.313624785	2.202772629
H238	-9.777521737	1.926105293	-1.949174815
H239	-1.692539465	1.547853219	-3.047915472
H240	-9.994376763	0.168422344	-1.867561631
H241	9.679916442	2.927867536	4.603981574
H242	8.178164597	3.133425934	3.991745351
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H244	-0.564369212	6.046507690	0.174604511
H245	1.991100392	8.501318716	0.212040681
H246	-3.349363755	4.070463818	-2.770013760
H247	-4.991218683	3.665510859	-4.088858437
H248	-4.192022190	5.426548581	-2.884900464
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H264	4.651430505	9.633175571	-3.865056496
H265	-5.453180884	-0.755407656	-4.037392152
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H267	-2.926294694	7.205383967	-0.861087439
H268	4.077604180	10.230566754	-2.294287742
H269	-0.809012793	7.481045137	-7.003389625
H270	-3.367036170	8.909309690	-5.136662885
H271	-4.631040439	-3.488871579	-4.171340702
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H286	8.506331623	-5.306604435	-3.374040423
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H288	5.127566703	-5.678510736	-9.310281367
H289	5.891470495	4.967027486	0.229160288
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H298	4.700493018	1.251874123	-6.126205672
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H311	4.061515015	-11.678630925	4.684418026
H312	1.066403486	-0.490848617	-4.193313562
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H314	3.530674114	-11.714382202	6.875477285
H315	4.991571035	-2.997265638	2.768370205
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H317	-2.476627267	-2.204831203	-5.955079268
H318	7.600251587	-9.991684189	0.170101950
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H322	6.633215235	2.216697511	-8.350878363
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H324	2.192661285	-7.345218959	1.434318505
H325	4.504456038	-2.131373335	-6.852601829
H326	2.957206084	-9.190550728	-0.177277601
H327	4.325068771	-7.033621638	-6.414232837
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H329	5.624029565	-12.195627553	5.325742550
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H178	-4.051873515	4.262192131	7.189559228
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H186	0.376220759	5.298530130	2.169759261
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H188	2.445278345	5.008842370	5.348388479
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O478	7.875552548	-10.569542166	-0.589905443
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S480	4.300578960	5.015897079	-1.630936042
S481	2.704132722	1.996960427	-2.965591464
S482	2.513347630	-3.341851103	-2.941086553
S483	3.806572464	1.713392419	0.493315834

	S484	0.869165274	-0.913097715	-1.640270449
	S485	4.820257594	-0.784092982	-4.772640652
	S486	3.728501173	-3.709003897	0.431515098
	S487	6.210294321	1.556892790	-2.121930270
	S488	6.114843761	-3.223228409	-2.204300716
	S489	6.327693460	-1.032955518	0.836472324
8, 47(3/2)	bm22b2n2x6x6n2ncnxdtr.car_3			
Fe1	2.86	C1	2.011406082	0.661737048
Fe2	-1.17	C2	3.375613270	0.178647804
Fe3	2.75	C3	0.289225886	2.403860015
Fe4	-2.34	C4	-0.941426594	1.536051043
Fe5	2.52	C5	-2.013873167	-0.151848772
Fe6	-0.01	C6	-2.196768292	-1.278397570
Fe7	-2.04	C7	-1.123283955	-2.730747979
		C8	-1.646950946	-2.162218011
		C9	-1.700971417	-0.275939558
		C10	-3.203263372	0.043746755
		C11	-5.117474228	0.681319986
		C12	-5.989232237	-0.582073972
		C13	-6.393569096	-2.742795166
		C14	-6.280900686	-3.937738110
		C15	-4.820535210	-5.260698862
		C16	-4.710796254	-4.968688723
		C17	-4.656111004	-3.156202647
		C18	-5.969514810	-2.485499685
		C19	-3.413206402	-2.248050716
		C20	-3.454181950	-1.500873977
		C21	-2.129987456	-3.066029570
		C22	-7.453610158	-0.538964877
		C23	-8.750250792	-1.170131965
		C24	-7.297893817	0.949353309
		C25	-8.572449717	1.743567584
		C26	-6.095162904	1.579980350
		C27	-9.933052375	-2.144138347
		C28	-10.426955018	-3.345375647
		C29	-0.050497448	-13.175602408
		C30	0.061265276	-12.404801214
		C31	-1.183634558	-10.820831026
		C32	-2.282760882	-11.478661676
		C33	-1.538694102	-9.372178103
		C34	-1.770739203	-8.472511397
		C35	-1.819646162	-6.998473827
		C36	-2.923504929	-5.221016389
		C37	-2.864215099	-12.331859339
		C38	-3.441978498	-11.397318174
		C39	2.995113651	1.758421630
		C40	2.134820567	2.981385473
		C41	2.832825127	0.734906875
		C42	3.357526453	-0.689173822
		C43	4.824274096	-0.922184963
		C44	2.216952394	5.233609983
		C45	1.518866950	6.158230774
		C46	3.181407342	6.037657706
		C47	0.730190639	6.432233348
		C48	-0.697979816	5.866767292
		C49	-2.225676479	4.077596660
		C50	-2.971498142	4.101492705
		C51	-2.921035558	4.567722853
		C52	-3.995859809	5.677022781
		C53	-1.913858731	4.857319038
		C54	-0.787926801	3.890751305

C55	-0.596148510	2.569565295	-1.592194528
C56	1.189195441	3.250913794	-0.451298746
C57	-4.473793313	8.035536723	-3.043650328
C58	-5.923012219	7.803664959	-3.467147864
C59	-3.804288645	9.100465402	-3.942670711
C60	-4.091429801	10.533101320	-3.598104237
C61	-5.260181078	11.148583741	-3.193709661
C62	-3.614623872	12.626635428	-3.327342974
C63	-5.007686909	-5.462722231	6.576714124
C64	-4.520782877	-6.895807752	6.692906904
C65	-4.421888271	-4.902607799	5.260576375
C66	-4.872182588	-3.492274310	4.957261992
C67	-6.057485181	-3.244564816	4.239612560
C68	-4.106868999	-2.385983376	5.365143091
C69	-6.465290913	-1.940615844	3.937279530
C70	-4.504016052	-1.079503521	5.077654943
C71	-5.685177225	-0.858053404	4.362606248
C72	-2.331853787	2.107817504	8.605644055
C73	-2.269175917	3.631904340	8.443838952
C74	-2.068928871	1.419471900	7.258180799
C75	-1.010014379	5.687195990	8.910660022
C76	-0.575135170	6.217750584	7.543841293
C77	0.281466325	5.660339882	5.297583690
C78	-0.901692772	5.555833105	4.311091982
C79	1.490995598	4.806477077	4.878037362
C80	2.086632835	5.055110141	3.488577071
C81	2.863421882	6.368155095	3.279650578
C82	1.805980778	8.637840192	3.271487562
C83	-2.948650847	4.419955068	3.628341339
C84	-4.132131205	5.317325346	4.041481832
C85	-3.466546868	2.980217713	3.508900002
C86	-5.490909728	6.086200658	5.922946646
C87	-5.670652790	7.577683693	6.189701556
C88	-4.681745522	9.830311880	6.107937619
C89	-5.375669885	10.729253365	5.061507202
C90	-3.256779916	10.346887356	6.410600014
C91	-2.347952501	10.242019311	5.192022573
C92	-6.198832944	10.913810266	2.755424132
C93	-7.628082570	11.371032013	3.028283290
C94	-6.153470077	10.065424367	1.456586549
C95	-4.738119110	9.726468814	1.046548012
C96	-3.967356056	10.652618399	0.325778205
C97	-4.139262069	8.510895293	1.419645492
C98	-2.635073407	10.388365396	0.002962514
C99	-2.799873145	8.237725800	1.124661305
C100	-2.061278378	9.188388600	0.423926608
C101	9.280499674	-3.217484564	4.098013628
C102	8.906496143	-2.308093887	2.940244446
C103	7.293802481	-0.587351693	2.162599632
C104	7.300592094	0.864085003	2.659227038
C105	6.304817141	2.442854005	4.242372570
C106	5.853542808	2.518100665	5.698252494
C107	4.869675501	1.437066099	7.658585872
C108	5.903015170	1.129590934	8.726006925
C109	10.020390430	1.345072720	-0.938073771
C110	9.428413348	2.726610571	-1.248322192
C111	9.020003376	0.243504693	-1.354706444
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C113	8.662141147	-2.230446677	-1.563050946
C114	7.915731122	4.518582664	-0.555305744
C115	7.908377929	5.348874225	0.713160900
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C124	4.769064180	-9.460360676	4.932789989
C125	5.612534947	-8.152476364	2.909755318
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C127	7.753416465	-6.885160810	2.219100759
C128	6.786043455	-5.132978928	1.269652108
C129	3.597896882	-11.570710444	4.634229297
C130	3.923145530	-12.054750866	6.029753523
C131	2.868370622	-5.665287619	-3.291476589
C132	2.387979692	-6.356537247	-2.044960666
C133	3.564578617	-6.751930981	-1.065858967
C134	4.607212833	-7.629116624	-1.822186929
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C136	6.506061195	-9.294173288	-1.511316430
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C138	1.864918149	-2.247592757	3.138815659
Fe139	3.771323357	-2.869549091	3.108875271
Fe140	0.817366630	-0.305071763	2.678231879
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H148	2.162030264	2.364844707	-10.411475235
H149	4.043879349	1.042981511	-9.899261840
H150	3.208178245	-0.239020751	-10.770414207
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H154	-1.839118859	-0.597796310	-12.032623934
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H157	-1.551787151	-0.916685390	-4.622055779
H158	-0.479618967	-0.468587867	-7.265347490
H159	-0.115778916	-3.141188096	-8.213824436
H160	-5.468586396	1.295098982	-6.072899915
H161	-3.063990082	0.581899656	-7.554919773
H162	-1.790868290	-3.552644370	-8.653211915
H163	-1.131560283	0.652760883	-5.350351550
H164	-4.712858911	-1.460480206	-8.322009173
H165	-5.271901034	1.238905389	-7.846072756
H166	-2.106159913	-3.546862293	-3.399082573
H167	-1.244950448	-2.415787056	-2.327692169
H168	-2.037988130	-3.846702751	-1.641137918
H169	-3.444310145	-1.496018060	-3.031185279
H170	-6.155724493	-3.106032940	-9.040914128
H171	-5.146265781	1.093910018	-2.112875218
H172	-7.950636738	-1.349212555	-4.616410009
H173	-9.441460438	1.368654043	-2.816030947
H174	-2.520760663	-0.939893252	-0.738611418
H175	-3.552855792	-2.193029965	-0.042389206
H176	-6.109498187	-5.501077134	6.467570566
H177	-6.010176656	2.642274437	-2.117962713
H178	-8.422408740	2.799429651	-2.527906613

H179	-6.221957295	1.517566716	-0.752721408
H180	-8.813490851	1.699358984	-1.183055011
H181	-7.119091554	0.987475494	-3.652671834
H182	-7.543894502	-0.608810913	-1.070947597
H183	-5.608687368	-0.878952881	-3.213600055
H184	-4.287693214	-0.785716891	-0.849010847
H185	-2.611315875	2.304667363	3.346744799
H186	-4.116101705	2.945371336	2.618925687
H187	-4.796272099	1.884614023	4.443497462
H188	-6.835080300	0.478548182	3.547053608
H189	-3.882818162	-0.235081603	5.378332078
H190	-3.158553524	-2.545417350	5.883061466
H191	-6.669808236	-4.083886898	3.896974205
H192	-4.868964008	-2.985681331	-4.517687648
H193	-3.881765627	-5.747639456	-5.906483532
H194	-5.637738276	-5.981706002	-5.737899454
H195	-4.280765919	-3.517001428	-6.695452157
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H199	-10.756895474	-1.416625797	-4.671888894
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H208	8.762178347	5.145018954	1.400909528
H209	10.886365401	1.279541513	-1.614867741
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H218	4.599691789	2.281671468	-6.211543847
H219	1.755398041	0.659487973	-3.664585512
H220	8.845317626	-2.577235422	0.366458588
H221	2.733967992	-1.408615345	-3.593181178
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H223	-1.223358132	1.864764803	-2.125444002
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H257	-2.049018474	11.113067636	-0.568029063
H258	-4.717603829	7.745752594	1.945788686
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H261	-0.130067583	4.307793579	6.901966225
H262	1.315153256	4.953314456	2.709490684
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H266	2.275593332	4.957220515	5.637523571
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H278	2.795311750	4.232700258	3.321722649
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H301	7.286780996	2.931193334	4.182250839
H302	5.062279370	0.017940908	-0.693717036

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H307	-0.698541796	-8.984011245	-1.119843604
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Fe140	2.571668218	0.975038250	-0.586150139
Fe141	5.091971666	0.781869070	0.794752137
Fe142	5.037999541	0.705305632	-1.780833654
Fe143	4.335758623	2.995735999	-0.450565987
Fe144	5.190818609	-1.727291236	0.888500853
Fe145	2.671748254	-2.234617832	0.015958621
H146	-5.281293416	-7.702918609	-1.826603960
H147	-5.014105780	-6.887227012	-3.216512016
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H153	-9.673294333	-3.576997177	-1.735121415
H154	-10.012009937	-6.613242921	2.119003473
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H157	-3.757079202	-2.626114755	1.899781870
H158	-5.794635093	-4.351285119	0.802683178
H159	-5.125679796	-6.873980098	1.939618218
H160	-7.212347164	-0.235225269	4.047873239
H161	-7.343318017	-2.658927558	2.435100441
H162	-5.767312442	-6.676096364	3.587966487
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H166	-1.608746470	-3.450862631	3.760420936
H167	-1.045736302	-2.453961025	2.397684674
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H173	-5.798703132	3.501708944	7.291334746
H174	-0.888495306	0.066158031	2.644433093
H175	0.009893637	0.072269659	4.165606129
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H178	-5.991872536	4.177364083	5.656248451
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H188	0.598222638	5.449589658	5.442213277
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H190	5.112311251	3.124630018	3.908751284
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O456	-2.801809038	11.078582873	-4.039438747
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O459	5.552467073	-4.774866903	-6.818223530
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O476	8.022598745	-5.741011213	5.235542620
O477	6.679992497	-4.043421621	3.422638347
O478	-3.060250463	4.316881930	-4.500885651
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O480	7.158790020	-8.010284663	3.844564153
S481	4.159203831	5.283066558	-0.797550747
S482	3.361336338	2.131661895	-2.369333782
S483	3.365998291	-3.233972384	-1.970368986
S484	3.324069706	2.056864183	1.305888116
S485	1.207422364	-0.859471143	-1.135282248
S486	5.938464856	-0.610639975	-3.339544394
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Fe3 2.86
Fe4 -2.57
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C78	-1.116186252	-4.518772716	-5.376903717
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C81	-1.999116458	-6.925004927	-2.364031702
C82	-3.705973196	-7.475227665	-4.107024603
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C84	-1.469823088	-2.028048579	-7.488992505
C85	-0.126821131	-0.953894392	-5.677201397
C86	-0.884261414	-2.423912275	-9.830509100
C87	-1.810905666	-3.253531424	-10.716949346
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C91	-4.055067037	-6.489175311	-8.828370539
C92	-6.641307148	-3.116061243	-10.531783550
C93	-6.941227067	-2.509423891	-11.899484451
C94	-6.917055842	-2.071842646	-9.417560030
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C98	-7.746852156	-3.947361343	-6.192224919
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C104	2.057959635	-6.726375904	3.410289317
C105	1.873384937	-7.602490336	1.133613057
C106	2.773985374	-8.047544854	-0.013481533
C107	4.852348746	-7.794993042	-1.278883945
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C127	7.235890671	-2.440967228	7.201242186
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C133	4.338745592	1.833972429	5.921007067
C134	4.612091755	1.935727693	7.448924361
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C18	-0.424099504	-0.095069142	6.642265964
C19	-0.341750417	-1.322913594	4.369684762
C20	-0.069621855	0.058401457	3.773818851
C21	0.413475431	-2.433017221	3.633912477
C22	-2.259384161	1.402844915	7.292424789
C23	-2.302610520	1.208604480	8.818435066
C24	-3.621270597	1.843840180	6.703190096
C25	-4.195978369	3.035145355	7.480150529
C26	-3.484655324	2.192256407	5.215882962
C27	-2.949644869	-0.196777699	10.686906323
C28	-1.628061326	-0.019085178	11.406050135
C29	7.639949780	-9.358878332	5.814421945
C30	7.999714512	-8.038119063	5.140159576
C31	7.667173420	-5.566123716	5.341948260
C32	8.568636361	-4.842217607	6.359135961
C33	6.281629969	-4.907546523	5.221115821
C34	6.330408101	-3.433069697	4.814728722
C35	4.960778662	-2.945939746	4.336905660
C36	4.356956838	-0.515509109	4.422935052
C37	10.575078159	-3.468832468	6.649126641
C38	10.496106966	-1.961240137	6.542598063
C39	-4.113570077	-3.869855948	-2.219474550
C40	-4.920307885	-2.582202475	-1.965247425
C41	-2.629551137	-3.603636810	-1.914943029
C42	-1.738917458	-4.855417684	-1.769454141
C43	-1.118478855	-5.385677499	-3.059509265
C44	-5.882860062	-0.603404729	-3.108865158
C45	-7.280222941	-0.513474199	-2.493470460
C46	-5.796682472	-0.044250894	-4.555980815
C47	-9.187900071	-1.761649709	-1.596954524
C48	-9.031913880	-1.484523510	-0.095025954
C49	-7.514187342	-1.245599453	1.816355658
C50	-6.719191049	0.018318252	2.145906864
C51	-5.505060200	1.997248935	1.354444533
C52	-6.384375382	3.168259331	1.837696786
C53	-4.783627540	2.484643290	0.086346147
C54	-3.772296693	1.560079736	-0.526894596
C55	-2.910632283	0.638137493	0.035275326
C56	-2.566767624	0.738488651	-2.138703294
C57	-8.554319112	4.296430966	1.532121824
C58	-8.805071890	4.537477536	3.018010780
C59	-9.874456665	3.970271371	0.793784212
C60	-10.735951581	5.145558259	0.433327434
C61	-11.059456899	6.280631730	1.151242568
C62	-12.057784035	6.306601339	-0.826597053
C63	7.729980181	3.894224070	4.969133286
C64	8.960358477	3.010377009	5.045977865
C65	6.548922765	2.979581023	4.548618341
C66	5.237358074	3.721200929	4.447572231
C67	4.407062252	3.896170546	5.571056118
C68	4.804935632	4.254032150	3.220611794
C69	3.188331864	4.576922415	5.475079395
C70	3.598609184	4.945700165	3.111165622
C71	2.788355795	5.104573220	4.240703775
C72	3.913677477	8.348080778	-0.855994705
C73	2.656181144	8.990008632	-1.456283701
C74	3.713258918	6.830036269	-0.722712225
C75	1.599836040	9.921892974	-3.464793652

C76	0.374542492	9.031736901	-3.679842268
C77	-0.560662212	6.755577370	-3.750760751
C78	-1.346396180	6.541290836	-2.441047903
C79	-0.027335979	5.435908333	-4.338693455
C80	-1.030873989	4.300707814	-4.575511741
C81	-2.045042768	4.478595017	-5.721306154
C82	-3.831655303	6.219209702	-5.680558636
C83	-1.314117279	6.369075400	0.002264142
C84	-1.823652219	7.674453622	0.643464035
C85	-0.441596180	5.621754365	1.013505046
C86	-1.365707574	10.040333651	1.064615395
C87	-2.300220254	11.127097238	0.537597634
C88	-3.891749578	11.828473959	-1.206172143
C89	-5.356386766	11.886182600	-0.720348101
C90	-3.834312262	11.686522533	-2.744673644
C91	-4.430421200	10.363557959	-3.214574700
C92	-7.155516316	10.713725379	0.483670193
C93	-7.514288505	11.767673658	1.525096114
C94	-7.382243837	9.288973887	1.061424307
C95	-7.160623368	8.196653152	0.036943566
C96	-8.195031394	7.817390319	-0.834423019
C97	-5.918313369	7.552331666	-0.093918592
C98	-8.000295596	6.836748246	-1.809504561
C99	-5.697897397	6.585540795	-1.079076684
C100	-6.745869247	6.235649618	-1.931221339
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C103	3.004660816	-1.993882243	-6.637176000
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C106	2.891539868	2.844566892	-7.507873750
C107	4.925183529	4.029089333	-6.855318052
C108	5.936697794	4.174419412	-7.973330602
C109	-0.103643551	-4.272995625	-9.191428595
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C113	1.862058391	-6.199200644	-6.467465954
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C119	-1.429734177	-2.149599836	-5.583506690
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C131	2.250203713	-6.838500702	0.517865183
C132	3.466375192	-6.069276788	0.961002503
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C134	4.962805670	-7.497052398	-0.550172633
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C137	5.870415037	-5.452485118	0.590666243

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Fe140	2.417152986	1.594440849	-1.670031262
Fe141	4.926838720	1.781260018	-0.548607710
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Fe144	5.126674506	-0.780561154	-0.376211922
Fe145	2.608807407	-0.971714440	-0.845860218
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H148	-8.239298042	-6.926497806	-0.447799770
H149	-6.623393080	-8.085858310	-1.700875302
H150	-6.474899054	-9.098601000	-0.268306260
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H153	-8.962206440	-5.155113884	0.821048106
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H166	0.235167868	-3.416165793	4.094750315
H167	0.087962073	-2.493486952	2.585301462
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H173	-4.380672805	2.793254321	8.536795541
H174	-0.277894431	0.058957013	2.695447339
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H183	-2.395529487	-0.350966067	6.050975644
H184	-0.697395652	0.833035976	4.237320875
H185	-0.106625573	4.673762152	0.557936884
H186	-1.073067350	5.391057251	1.886187086
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H188	1.095274588	5.779704994	4.909844890
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H191	4.711174226	3.481782656	6.536507974
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H211	-2.319323702	-5.683281510	-1.323427394
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H213	-3.232776720	-1.753437315	-9.373505380
H214	1.379480226	-2.827168872	-9.329976553
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H225	-6.966624718	-1.764239118	-0.183770015
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H265	-5.031931125	-2.445574303	-3.950908074
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H289	4.637380625	6.395986776	-0.321855992
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H318	9.921244840	-7.586237994	0.584074309
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H320	8.160521310	-6.233705196	1.665368950
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Fe140	2.484409597	1.571610089	-1.579123527
Fe141	5.021629336	1.495762528	-0.529793603
Fe142	4.575382749	1.414747120	-3.056349706

Fe143	3.980654660	3.717558388	-1.892565215
Fe144	5.064959789	-1.081648292	-0.564905307
Fe145	2.508013657	-1.047629330	-0.969298293
H146	-4.606254963	-8.222585580	-0.811189011
H147	-4.782177218	-7.343065810	-2.176214074
H148	-8.671854981	-6.425788765	-0.737794436
H149	-7.150350875	-7.551905813	-2.136901476
H150	-7.016136455	-8.664556230	-0.778018668
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H153	-9.262546747	-4.708618799	0.664911584
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H169	-1.410488970	-1.767598377	4.208877874
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O449	2.188131328	9.170423983	-0.096071462
O450	-0.201483242	9.870753402	-3.192307237
O451	-2.215227070	6.689560330	-1.908414913
O452	-2.226596139	7.622361208	2.123689780

	O453	1.078715243	6.300806689	1.905587885
	O454	-1.556535258	12.194721985	2.118987819
	O455	-5.286977104	13.209558351	0.138129039
	O456	-5.073847756	10.753526268	-2.418004025
	O457	-7.835041897	12.405430307	2.957611127
	O458	-6.232326274	5.934160390	-2.353078551
	O459	3.946341612	-3.800165175	-8.373395539
	O460	1.256466826	-0.467985731	-8.369492271
	O461	2.506629355	4.291601850	-7.850427031
	O462	6.847822144	5.308969111	-7.760566211
	O463	-2.938269101	-3.116198543	-9.534440887
	O464	0.775938597	-6.502371872	-6.168391308
	O465	2.574191688	-5.271347349	-6.648710807
	O466	-2.831728307	1.958729645	-8.831095832
	O467	11.080304780	-3.302432479	-1.979324162
	O468	13.846774059	-4.352202879	-0.119984689
	O469	0.975767244	-6.430151857	-0.692842132
	O470	1.703269421	-8.318620538	0.225937191
	O471	7.276776258	-9.650218460	-2.407987868
	O472	5.150384953	-9.952772039	-3.112677501
	O473	6.017989652	-4.685135980	-0.381193643
	O474	6.113660369	-6.561222569	0.861580140
	O475	3.897048008	-5.430047013	-1.723321716
	O476	9.745018066	-4.831730311	2.412222668
	O477	7.672859080	-3.202216620	1.339665815
	O478	-4.705019163	3.964085117	-3.191552410
	O479	9.845977505	-8.668829121	-1.023841112
	O480	8.763732686	-7.125482519	1.151483144
	S481	3.612537315	5.968026578	-1.918435653
	S482	2.799888235	2.697387956	-3.472858647
	S483	2.879450665	-2.508157505	-2.952486931
	S484	3.333465501	2.891435095	0.089765669
	S485	0.266157636	-1.840753810	-0.875767754
	S486	5.093066620	0.186790107	-4.832026776
	S487	3.675423393	-2.645579875	0.225320383
	S488	6.053022246	2.788915240	-2.147101482
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	C5	-7.869065760	-6.859482391	4.086807531
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	C9	-3.821853978	-3.314817336	2.844098901
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	C12	-5.117796092	-2.935801586	7.155932067
	C13	-4.313533817	-4.869168504	8.422613573
	C14	-2.784101484	-4.937370011	8.522846935
	C15	-0.656916814	-5.246675725	7.323313446
	C16	0.177401931	-4.069097912	6.804425714
	C17	0.067520184	-1.811159068	5.755866580
	C18	-0.275639107	-0.597644710	6.638215250
	C19	-0.315223044	-1.639379422	4.269718678
	C20	0.023117480	-0.232731383	3.777483559
	C21	0.363804255	-2.728698667	3.433394890
	C22	-1.998371305	0.956519486	7.446002255

C23	-2.025539594	0.635532282	8.952023185
C24	-3.340561600	1.524727198	6.929181869
C25	-3.815687886	2.693659919	7.800894212
C26	-3.219351465	1.971645311	5.465433524
C27	-2.723693589	-0.879721985	10.714077891
C28	-1.385633723	-0.817876385	11.422626883
C29	7.192292683	-10.219806858	4.882831369
C30	7.626632021	-8.872292560	4.307230635
C31	7.433718478	-6.408384009	4.693353378
C32	8.397710678	-5.824326368	5.742746712
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C36	4.429797118	-1.109059174	4.223693467
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C43	-1.466354237	-5.066659497	-3.421036694
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C50	-6.644188183	0.247565441	2.343073412
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C52	-6.104955907	3.405768856	2.218337942
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C54	-3.616818116	1.773628547	-0.257851411
C55	-2.827661857	0.734095571	0.175941356
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C57	-8.230092964	4.657660006	2.094500759
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C65	6.820749593	2.214682837	4.605756798
C66	5.557361112	3.042642132	4.593935367
C67	4.758971336	3.172831052	5.745690958
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C69	3.584393282	3.932842813	5.735099056
C70	3.978941353	4.478142137	3.403603738
C71	3.197603518	4.585864373	4.557877264
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C73	3.172994497	8.929717337	-0.818985099
C74	4.092625780	6.646603335	-0.291721877
C75	2.131740891	10.055942419	-2.732747815
C76	0.854879605	9.253296021	-2.974416926
C77	-0.211291216	7.050235845	-3.196578648
C78	-0.981904087	6.774000633	-1.890152747
C79	0.226760340	5.757032251	-3.908613821
C80	-0.851330831	4.709205221	-4.209811005
C81	-1.867796257	5.033731009	-5.320873422
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C90	-3.165511557	12.062892330	-1.733252177
C91	-3.842412139	10.812691255	-2.283303980
C92	-6.458897402	11.051781670	1.507581091
C93	-6.726295626	12.049985136	2.628835751
C94	-6.769460537	9.610299485	1.992431262
C95	-6.653211601	8.584232532	0.887774028
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C112	0.779214476	-5.347814387	-8.300927562
C113	1.362059414	-5.775820926	-6.972678758
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C115	-2.386628525	0.918070075	-9.272486915
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C117	-2.171336276	-0.411991626	-6.227497629
C118	-1.565924455	0.796904156	-5.837652866
C119	-1.680390326	-1.611245061	-5.684550160
C120	-0.480009519	0.794196480	-4.952766249
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H148	-8.663144099	-6.423022955	-0.744886921
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H150	-7.003812987	-8.657039813	-0.788650553
H151	-7.583043043	-4.127553755	0.490398574
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H155	-5.887233095	-7.259657839	2.494393585
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H158	-4.796828218	-5.070267936	2.068023246
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H160	-5.804649226	-1.355534311	5.892637978
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H163	-4.294957972	-2.818141010	1.984319118
H164	-5.259455718	-4.895630593	6.507802101
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H167	0.003011230	-2.707565225	2.394672157
H168	1.454685293	-2.583185575	3.404683988
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H188	1.561167862	5.302485730	5.319595755
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H203	0.176676765	-5.964765288	-4.251440970
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H234	-11.793185297	8.541756169	1.441568039
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H237	-7.054766919	-1.852147354	2.317922631
H238	-9.972552440	-0.311984149	-1.783407302
H239	-1.972171123	0.907949326	-2.965892792
H240	-9.849473912	-2.073573046	-1.610581526
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H242	7.482295506	4.663483515	3.987962573
H243	0.769424686	6.650403853	-0.796522288
H244	-1.836197015	5.856950817	0.321534444
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H249	-4.853390260	0.606437766	-4.758051757
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H251	-2.123061501	12.143452512	-2.074181928
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H253	-2.001680892	9.854636387	-2.637964772
H254	-3.437427359	8.884235888	-2.821020565
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H257	-8.468656035	7.271743387	-1.708937062
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C75	2.968888665	9.927743165	2.419548548
C76	1.702940414	9.489504691	1.680872826
C77	0.562483204	7.727815730	0.389941022
C78	-0.378575065	6.985124236	1.361036807
C79	1.022803461	6.848762531	-0.787316932
C80	-0.066120118	6.201830683	-1.652083698
C81	-0.884722052	7.133353243	-2.565735757
C82	-2.521274392	8.812648884	-1.708258001
C83	-0.650362824	5.510928487	3.286331690
C84	-1.133049225	6.379609439	4.465073047
C85	0.013942224	4.251238436	3.853063073
C86	-0.489073111	8.066295941	6.115870868
C87	-1.247003796	9.387279349	6.217730252

C88	-2.527071494	11.139250601	5.054335536
C89	-4.021793799	11.139181550	5.441482275
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C91	-2.978017239	11.028335157	2.558308186
C92	-6.058684039	9.793613079	5.729094359
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C95	-6.279967937	7.919974627	4.002085125
C96	-7.219224886	8.234406232	3.007142707
C97	-5.112832795	7.238869506	3.617766877
C98	-6.998492285	7.898962213	1.668679429
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C100	-5.814748871	7.246181331	1.315740651
C101	7.098061751	0.694232318	-7.935379132
C102	5.579172882	0.663758397	-7.883970325
C103	3.587370588	1.397696885	-6.593027630
C104	3.070168591	2.839503989	-6.603272851
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C111	0.764229435	0.014615173	-9.144998931
C112	1.720509451	-1.047349209	-9.717671090
C113	2.067800773	-2.083526272	-8.669874319
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C116	-2.226911789	3.193316859	-7.026245393
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C118	-0.724416465	3.558907990	-5.010408577
C119	-0.889005153	1.341702174	-5.954304952
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C127	7.572157362	-3.459889222	-6.492955528
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H206	-0.714857791	-5.743986798	-8.696404135
H207	-3.044192086	-4.754073942	-6.954146109
H208	-3.375153313	0.533267463	-9.815102736
H209	-3.293174864	-4.776385589	-9.482306446
H210	-3.313712760	-2.357301800	-2.143951799
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H268	-7.227529953	2.859156779	-2.569329493
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	O471	5.325930489	-10.832347515	-2.761221264	
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		C13	-3.450214830	-3.584408119	9.407545282
		C14	-1.956943225	-3.896452677	9.254503223
		C15	-0.159534000	-4.646820212	7.754032935
		C16	0.745465075	-3.660498765	7.009060977
		C17	0.825217845	-1.460991012	5.845901213
		C18	0.826848660	-0.178328440	6.694804708
		C19	0.246187837	-1.259069699	4.427615539
		C20	0.781411068	0.029975868	3.796527023
		C21	0.522652943	-2.492323996	3.560186928
		C22	-0.460257768	1.717764217	7.574469940
		C23	-0.282513018	1.524643185	9.090894248
		C24	-1.762280143	2.470976448	7.207869055
		C25	-1.917102888	3.748895314	8.040638175
		C26	-1.791785891	2.808024009	5.710717089
		C27	-0.889368819	0.274225104	11.079942450
		C28	0.542060416	0.149580770	11.561947995
		C29	6.471580933	-10.881903215	4.608314384
		C30	6.916899661	-9.655349292	3.811452240
		C31	7.138777350	-7.167455162	3.968741252
		C32	8.342384330	-6.673354275	4.795086500
		C33	5.941440436	-6.205393543	4.067588337
		C34	6.255553560	-4.781815311	3.598856755

C35	4.974578479	-3.972407328	3.383947342
C36	4.939248455	-1.465474412	3.442884878
C37	10.621890420	-5.780503328	4.702385590
C38	10.856729810	-4.292042463	4.558112904
C39	-5.236746432	-2.898322333	-1.315056873
C40	-5.677748382	-1.461836637	-0.983214611
C41	-3.695439254	-2.947268907	-1.292705916
C42	-3.057442554	-4.351169934	-1.307745853
C43	-2.798092403	-4.937941889	-2.693244074
C44	-6.446831139	0.639398149	-1.998812969
C45	-7.715309298	1.030761765	-1.230928849
C46	-6.449569400	1.280150629	-3.402284536
C47	-9.531834491	0.289324924	0.228015677
C48	-9.028081539	0.528275312	1.658849427
C49	-7.148934137	0.358628978	3.234429771
C50	-6.065496802	1.425229131	3.386309452
C51	-4.600993424	3.073745445	2.301094518
C52	-5.096580455	4.423321341	2.883170510
C53	-4.033965574	3.390687085	0.907819410
C54	-3.371472696	2.283441686	0.144450940
C55	-2.712103503	1.124468711	0.481564353
C56	-2.592295952	1.334678917	-1.722552387
C57	-7.020462456	5.980044817	2.985753158
C58	-6.987582826	6.207424598	4.494978707
C59	-8.477316989	5.954363180	2.467028119
C60	-9.123149949	7.290743066	2.242483355
C61	-9.102838558	8.445660451	3.000280167
C62	-10.345084103	8.732338642	1.187907771
C63	9.090881808	1.997361745	3.413616088
C64	10.077096510	0.850024537	3.302098971
C65	7.674019671	1.393337051	3.246024970
C66	6.578007477	2.422102594	3.399042435
C67	5.999855564	2.692957725	4.653341420
C68	6.104365630	3.141513016	2.286760784
C69	4.983325812	3.643999181	4.797205654
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C71	4.537573972	4.348536026	3.671148351
C72	5.336789047	7.333551210	-1.676792371
C73	4.199129823	8.285463904	-2.068846466
C74	4.759840643	5.956472427	-1.312460643
C75	3.028492917	9.417092262	-3.907810111
C76	1.617989923	8.826702388	-3.908747411
C77	0.224767533	6.802944324	-3.709298506
C78	-0.314563558	6.727618163	-2.266021198
C79	0.335180317	5.419968541	-4.376306824
C80	-0.938881580	4.569232759	-4.442867129
C81	-2.042243587	5.039890393	-5.409912186
C82	-3.416900313	7.097411444	-5.063621058
C83	0.135707500	6.435611145	0.115029079
C84	0.004829652	7.823597933	0.774108465
C85	1.023689734	5.556748507	1.001723699
C86	1.060231578	10.011742313	1.067532988
C87	0.287292500	11.285777283	0.736882976
C88	-1.383365494	12.387828991	-0.695899863
C89	-2.671855113	12.747316025	0.073872568
C90	-1.663238397	12.289536439	-2.213302710
C91	-2.596040525	11.128192425	-2.533725174
C92	-4.413433955	11.966295558	1.619270116
C93	-4.316220514	13.044164899	2.694755172
C94	-4.852370348	10.620983504	2.257211397
C95	-5.089346967	9.539017323	1.228270839
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C98	-6.530576699	8.488504466	-0.435344250
C99	-4.265409799	7.668575951	-0.113470265
C100	-5.493941001	7.615321643	-0.768817654
C101	4.132048877	-4.107363788	-8.936832724
C102	2.713767916	-3.931301295	-8.421994923
C103	1.199949780	-2.436688379	-7.137614520
C104	0.623388032	-1.132589891	-7.695653305
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C106	1.942599731	2.361489705	-7.936352644
C107	4.244765959	3.102662276	-7.594785186
C108	5.085122105	3.044074405	-8.854853841
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H167	0.053252243	-2.375022164	2.571167624
H168	1.600986895	-2.633597433	3.396090463
H169	-0.846039110	-1.160055241	4.529352530
H170	-3.960327208	-4.530059767	9.640919830
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H173	-1.952718868	3.545587731	9.120351090
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H183	-1.206027048	0.093358365	6.377307349
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H186	0.473418856	5.384400273	1.940832486
H187	2.637142550	5.849867190	2.082007198
H188	3.180282224	5.341297867	4.642854083
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H190	6.496406982	2.922651254	1.291251733
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H206	-0.711337044	-5.746767235	-8.685866100
H207	-3.039063167	-4.750944671	-6.945444701
H208	-3.363339366	0.532006070	-9.801649428
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H210	-3.310539665	-2.353249355	-2.136183826
H211	-3.696559504	-5.069522125	-0.764420731
H212	-2.331366716	-1.465276225	-8.402052024
H213	-5.222660594	-0.863927658	-8.593876235
H214	-1.045199071	-2.860862360	-9.454483094
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H239	-2.336123365	1.149244459	-2.763045988
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H268	-7.225363256	2.865259991	-2.571432617
H269	2.977427806	10.337203294	-3.309908795
H270	-2.539989467	7.204239640	-6.925307118
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H278	-0.614607556	3.577275150	-4.784778752
H279	-3.616496542	5.377401209	-4.003558728
H280	0.864817469	9.792763654	2.127918590
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H282	-0.705594936	13.237625899	-0.528302277

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H294	6.584466831	8.713395690	-0.819111986
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H299	3.437650395	1.210065670	-7.048191547
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H315	5.489347351	-11.238879892	6.381607868
H316	5.532169058	-2.574761241	1.875179784
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H319	8.046648356	-9.574996684	-1.038748403
H320	6.959140821	-7.583606641	-3.581860483
H321	6.864057748	-7.890903025	0.252276324
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		C16	1.014145293	-3.779812190	6.887941439
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C95	-6.121580315	8.892286949	1.434631153
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O447	2.863413600	5.427187227	3.855132504
O448	2.486364619	9.101742735	-0.834977690
O449	-0.328892755	9.738521787	-3.595502889
O450	-2.241127701	6.788124012	-1.875235825
O451	-1.634520809	7.798028252	2.056804965
O452	1.557359910	6.287585226	1.399315332
O453	-0.791212578	12.331813164	1.763789860
O454	-4.723596389	13.456503777	0.310194071
O455	-5.001366962	10.869635515	-2.094405350
O456	-6.921375847	12.826528703	3.476356934
O457	-6.288103667	6.033208990	-1.654858769
O458	2.472454217	-4.291430798	-8.707221045
O459	-0.073230714	-0.844957072	-8.454928599
O460	1.459603937	3.845236156	-8.397393990
O461	5.766187034	4.667906113	-8.967218314
O462	-4.486567929	-3.370119049	-8.848713984
O463	-0.423080266	-6.750409837	-5.919927326
O464	1.324264282	-5.635267052	-6.741910366
O465	-4.131744841	1.724600688	-8.425937940
O466	10.551951237	-3.854430511	-3.538589837
O467	13.493723753	-4.953411213	-2.026482471
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O470	6.483109234	-10.089295229	-3.042040106
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	O473	5.954464184	-6.807700062	0.244917405	
	O474	3.450916939	-5.683653615	-2.061091205	
	O475	9.802511441	-5.110031727	1.134584786	
	O476	7.645752651	-3.463535154	0.287529941	
	O477	-5.060123164	3.957884675	-2.704617536	
	O478	9.242246886	-9.102004747	-2.097937792	
	O479	8.575059554	-7.414538712	0.143130737	
	S480	3.544949972	5.752007851	-2.734091385	
	S481	2.276051205	2.449806182	-3.885027086	
	S482	2.355234970	-2.831826345	-3.183534180	
	S483	3.505654586	2.764413028	-0.526337604	
	S484	0.108438534	-1.800030828	-0.993024100	
	S485	4.215817780	-0.247099501	-5.548208833	
	S486	3.942390736	-3.047865326	-0.020221642	
	S487	5.764842536	2.391208728	-3.214576138	
	S488	6.034643135	-2.245595308	-2.960306806	
	S489	6.209499629	-0.051229079	-0.039181967	
20, 47(3/2)	bm2unh2b2n2x6n2n3b2.car_4				
Fe1	2.73	C1	-7.177769453	-6.051855740	1.092957729
Fe2	-1.01	C2	-7.269739477	-7.254381533	0.148916576
Fe3	2.85	C3	-8.390929800	-4.218184611	2.186302585
Fe4	-2.06	C4	-7.935729812	-4.419902262	3.630089246
Fe5	2.58	C5	-7.738933092	-5.928526873	5.539533028
Fe6	0.19	C6	-6.215100490	-6.021395091	5.678056866
Fe7	-1.86	C7	-4.087102551	-6.469073906	4.553700941
		C8	-3.483134320	-5.065309477	4.445278835
		C9	-3.663468998	-2.818438734	3.515384569
		C10	-3.839439180	-2.030493558	4.823458428
		C11	-5.177269272	-1.610220116	6.804908619
		C12	-4.280344402	-2.117371045	7.943512360
		C13	-3.491290354	-4.057336959	9.209038003
		C14	-1.969354153	-4.222538365	9.099035988
		C15	-0.070381194	-4.800359310	7.644480284
		C16	0.772116749	-3.718657227	6.960809199
		C17	0.710471916	-1.512328977	5.815752163
		C18	0.594947707	-0.236764282	6.670604287
		C19	0.164229130	-1.343616166	4.379973268
		C20	0.593874358	-0.001492492	3.784794234
		C21	0.599341866	-2.526096194	3.507546305
		C22	-0.867890998	1.512155712	7.586511564
		C23	-0.719477186	1.291860119	9.103247085
		C24	-2.213067455	2.171376725	7.195160723
		C25	-2.491590973	3.411923472	8.052886178
		C26	-2.218899274	2.543707192	5.706617885
		C27	-1.260573849	-0.065131352	11.038872299
		C28	0.171480706	-0.131188833	11.531531041
		C29	7.006879110	-10.548800100	4.510965846
		C30	7.451355651	-9.272284597	3.798955835
		C31	7.496884272	-6.786728680	4.049298720
		C32	8.641649504	-6.230324163	4.917458287
		C33	6.232791281	-5.916169110	4.145192613
		C34	6.462914577	-4.461341635	3.731810034
		C35	5.135975646	-3.724064343	3.552722138
		C36	4.904434973	-1.230533815	3.700901931
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		C38	10.965619983	-3.660756606	4.813285239
		C39	-4.945137857	-3.210334592	-1.546328382
		C40	-5.509110764	-1.819028336	-1.207704963
		C41	-3.406594639	-3.139674297	-1.484543912
		C42	-2.666696455	-4.492585521	-1.482783206
		C43	-2.330772761	-5.058197625	-2.860984935

C44	-6.397352136	0.238375783	-2.216254414
C45	-7.721596014	0.518708129	-1.498273786
C46	-6.389895451	0.903803889	-3.608418480
C47	-9.516800331	-0.376749381	-0.102898832
C48	-9.082302428	-0.129383777	1.349080647
C49	-7.249167815	-0.180219745	2.987526427
C50	-6.234188398	0.940199340	3.204024661
C51	-4.865199033	2.729701415	2.219138499
C52	-5.462045022	4.025289169	2.821336019
C53	-4.289794248	3.133470265	0.852999137
C54	-3.548258730	2.090043289	0.075640031
C55	-2.824250956	0.969109214	0.406009601
C56	-2.684294670	1.219320330	-1.789006231
C57	-7.482970504	5.448091184	2.896764684
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C64	9.960675777	1.507993135	3.581462549
C65	7.526932383	1.860955050	3.500191819
C66	6.344979642	2.794503451	3.615101025
C67	5.736964639	3.057707317	4.856632651
C68	5.809881865	3.419458729	2.473698373
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C71	4.119688716	4.514625149	3.802758062
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C73	3.719586159	8.587655212	-1.775472655
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C76	1.161789461	8.989304522	-3.653891260
C77	-0.089071494	6.875117811	-3.583434238
C78	-0.694797611	6.743772990	-2.172623822
C79	0.142784883	5.505264170	-4.245289204
C80	-1.063420912	4.563863302	-4.345797209
C81	-2.173746786	4.950217156	-5.342568698
C82	-3.679899487	6.924707364	-5.033020846
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C84	-0.550891768	7.811310694	0.938326283
C85	0.567844777	5.580056439	1.105294088
C86	0.322528449	10.063638556	1.329140285
C87	-0.510652279	11.292260206	0.972628819
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C90	-2.429486274	12.197284483	-2.031257652
C91	-3.267225933	10.979363895	-2.398734920
C92	-5.293819138	11.630130085	1.670522849
C93	-5.351985925	12.706192478	2.749730518
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C115	-3.623052064	0.635848484	-8.920174009
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H162	-3.688824007	-6.920712960	5.470415098
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H172	-1.979016810	-0.363628775	9.053976519
H173	-2.574254490	3.172060977	9.122369682
H174	0.208335669	0.103277678	2.761201894
H175	1.687443564	0.079068246	3.723513926
H176	8.913282935	2.940870943	4.761253492
H177	-3.172378653	3.021826906	5.438508249
H178	-3.434902520	3.879212023	7.733286467
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H181	-3.017212905	1.435961277	7.378411082
H182	-0.048507301	2.200805006	7.327769263
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H188	2.675462917	5.418220139	4.736486388
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H238	-10.138619221	0.477347927	-0.399840406
H239	-2.402369421	1.068845228	-2.828544329
H240	-10.147814331	-1.274818335	-0.126336049
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H244	-1.317624802	5.984830851	0.178367105
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C75	2.517547802	9.693260888	-3.608966584
C76	1.162495686	8.989333375	-3.647450161
C77	-0.087840827	6.875995008	-3.581276522
C78	-0.697631178	6.743123201	-2.172267847
C79	0.146389138	5.507035369	-4.243917865
C80	-1.055924625	4.561775031	-4.343945512
C81	-2.166381699	4.941431442	-5.342516712
C82	-3.668855511	6.918843364	-5.032481506
C83	-0.332552345	6.471929262	0.234091499
C84	-0.551523643	7.822884462	0.944886158
C85	0.558310270	5.586164516	1.107461378
C86	0.321674984	10.075267067	1.335286441
C87	-0.513886153	11.301522589	0.977209403
C88	-2.207524697	12.300819862	-0.504062769
C89	-3.543507053	12.568580578	0.221522060
C90	-2.430976360	12.193211983	-2.030502537
C91	-3.267671377	10.973227701	-2.394344147
C92	-5.301150600	11.630331679	1.666302165
C93	-5.364073815	12.706115975	2.744919976
C94	-5.636783111	10.243078468	2.280828822
C95	-5.761816732	9.157898457	1.234195005
C96	-6.971958825	8.972465021	0.546272310
C97	-4.672960014	8.339664228	0.891038827
C98	-7.092846669	8.014163704	-0.462408808
C99	-4.767968567	7.391354890	-0.132981876
C100	-5.980949453	7.244409509	-0.803613623
C101	4.658453849	-3.657621530	-8.842424923
C102	3.215803930	-3.593564762	-8.369574845
C103	1.594298542	-2.230942113	-7.060253474
C104	0.962667074	-0.948783679	-7.614388676
C105	1.069520979	1.495216403	-7.649004573
C106	2.103133426	2.596802255	-7.863782835
C107	4.343319239	3.488548954	-7.474947893
C108	5.198470762	3.488623629	-8.726107031
C109	-2.155052734	-3.948647780	-9.097371046

C110	-3.299902899	-2.961545762	-8.834376338
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C112	-0.807772148	-5.804621155	-7.989196909
C113	-0.083643524	-6.206413454	-6.724208455
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C119	-2.519681227	-1.727919046	-5.304164051
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C122	-0.618754200	-0.562983193	-4.350490355
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C124	9.710269213	-5.336531774	-3.390895310
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C126	6.015607626	-5.832016222	-4.578280937
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C133	3.668973312	-6.706129939	-0.915334057
C134	3.720044509	-8.184928624	-1.389361405
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C136	5.022453868	-9.846268666	-2.825115529
C137	5.098226598	-6.327728197	-0.414868728
C138	3.722929299	-0.300680660	-2.156069779
Fe139	4.086613861	-1.668948490	-3.584258516
Fe140	2.465923969	1.279647474	-1.855777785
Fe141	5.013064682	0.997956162	-1.366888055
Fe142	4.137569919	0.857580634	-3.806636661
Fe143	4.072499727	3.262086977	-2.512622565
Fe144	4.844060074	-1.581125250	-1.152618796
Fe145	2.262535807	-1.288485513	-1.295211822
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H168	1.689565580	-2.530668517	3.348896471
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H185	0.695992701	4.613681879	0.602617325
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H187	2.185760977	5.894292607	2.162892594
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H212	-1.955880986	-1.421218290	-8.493355323
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		C11	-5.998721586	-1.864412292
		C12	-5.259142466	-2.481513177
		C13	-4.655918750	-4.536218874
		C14	-3.134250533	-4.720950095
		C15	-1.078042420	-5.221520736
		C16	-0.146366653	-4.111831026
		C17	-0.044819334	-1.837173196
		C18	-0.253687297	-0.636318675
		C19	-0.405009846	-1.547725437
		C20	0.113370875	-0.173161188
		C21	0.113327159	-2.675900892
		C22	-1.779865088	1.077807581
		C23	-1.786804841	0.724006574
		C24	-3.078559868	1.781193878
		C25	-3.405058467	2.978758004
		C26	-2.970716850	2.232392976
		C27	-2.558776759	-0.778143192
		C28	-1.198192745	-0.893390908
		C29	6.082421001	-11.056077985
		C30	6.645886281	-9.755983302
		C31	6.756716409	-7.296153020
		C32	7.809177145	-6.828055784
		C33	5.506375472	-6.401241499
		C34	5.801319342	-4.931357133
		C35	4.517959767	-4.170304646
		C36	4.400605116	-1.679195433
		C37	10.042645889	-5.860708574
		C38	10.158556746	-4.352985502
		C39	-4.821384848	-2.896135879
		C40	-5.374777468	-1.526493376
		C41	-3.303908514	-2.924564544
		C42	-2.645688169	-4.319834964
		C43	-2.149471145	-4.796543751
		C44	-5.949298095	0.728078705
		C45	-7.241110176	0.996319262
		C46	-5.931035996	1.404826813
		C47	-9.387171475	0.087078827
		C48	-9.154615884	0.119158601
		C49	-7.561875367	-0.170843442
		C50	-6.536835024	0.899120237
		C51	-5.053603371	2.722414917
		C52	-5.692732054	3.976831782
		C53	-4.290369377	3.195665012
		C54	-3.468678027	2.183502725
		C55	-2.839338149	1.025467673

C56	-2.426613882	1.383733483	-1.948837194
C57	-7.626085985	5.502594150	2.329602931
C58	-7.746123859	5.614181062	3.846766123
C59	-9.026204738	5.488742250	1.668266312
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C61	-9.788935086	7.904409743	2.341771617
C62	-10.776928818	8.354495585	0.410192913
C63	8.484457887	2.036533779	4.832790638
C64	9.521705087	0.934935487	4.727889433
C65	7.129385634	1.416106759	4.406681843
C66	5.980999337	2.392579846	4.487690249
C67	5.235941694	2.555565038	5.671192035
C68	5.617866119	3.161804089	3.370065853
C69	4.161712691	3.451045067	5.735675362
C70	4.559980891	4.069353722	3.423049562
C71	3.828955466	4.209032972	4.606356968
C72	5.234936113	7.655870449	-0.257673136
C73	4.106681878	8.572974555	-0.746159515
C74	4.765340769	6.191749448	-0.236090054
C75	3.167413025	9.813011501	-2.644221595
C76	1.799845953	9.165444454	-2.862109262
C77	0.489866021	7.091483121	-3.057021531
C78	-0.260257953	6.904580709	-1.722835130
C79	0.760298985	5.755659865	-3.774584732
C80	-0.438185420	4.838874372	-4.048694213
C81	-1.442310770	5.283980091	-5.129071274
C82	-2.904911732	7.288216174	-4.827783992
C83	-0.150559434	6.472499917	0.684360016
C84	-0.429781075	7.785018977	1.442093287
C85	0.647912052	5.538432762	1.599886890
C86	0.445882914	9.987266345	2.047729626
C87	-0.339113255	11.248011179	1.694086431
C88	-1.843662199	12.372062897	0.101064829
C89	-3.250112952	12.613477735	0.688681883
C90	-1.895802192	12.361890884	-1.444642934
C91	-2.710065305	11.183040150	-1.966824188
C92	-5.174852255	11.625027914	1.851370717
C93	-5.336807377	12.628677566	2.987176116
C94	-5.619870098	10.211812744	2.316803358
C95	-5.632915844	9.198598932	1.193717277
C96	-6.748864228	9.090203298	0.348800855
C97	-4.528217500	8.368242787	0.938736033
C98	-6.764144045	8.193484668	-0.723219750
C99	-4.515438169	7.482796536	-0.144366255
C100	-5.637867697	7.404384136	-0.967574510
C101	5.576099449	-3.229886131	-8.499481350
C102	4.091633409	-3.118903399	-8.193005790
C103	2.373251893	-1.761048128	-7.019457926
C104	1.843431476	-0.433222021	-7.564468652
C105	1.964809344	2.005102395	-7.366134874
C106	3.028405661	3.098129679	-7.324142620
C107	5.255086155	3.845368940	-6.650292668
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C109	-1.154039792	-3.245127072	-9.582843132
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C113	0.542227098	-5.734472923	-7.142534427
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C138	3.941211373	-0.306539526	-1.744277010
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Fe144	4.951425272	-1.667788347	-0.743151004
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H151	-7.988715008	-3.236662618	0.644488768
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H153	-9.715121947	-3.620219630	0.827204887
H154	-9.007256593	-7.000309892	4.329906655
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H156	-8.937966871	-5.309868560	4.881801509
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H159	-4.371945254	-7.154208243	2.747407485
H160	-5.756467869	-0.793861930	6.015759705
H161	-6.367137001	-2.997293657	4.237735960
H162	-4.508537635	-7.110735035	4.522845611
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H166	-0.281385165	-3.651022377	3.669430525
H167	-0.188063438	-2.515383926	2.300925332
H168	1.212633291	-2.720059195	3.364753458
H169	-1.503856016	-1.530574837	4.176575731
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H173	-3.557593644	2.686023409	9.010928189
H174	-0.126587385	0.000688659	2.752530470
H175	1.204815665	-0.101501827	3.915851488
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H177	-3.898276548	2.735061076	5.288210192
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H182	-0.937068075	1.776280022	7.400514082
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H184	-0.346085309	0.638437321	4.393567067
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H186	-0.003718616	5.270419371	2.447373653
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H207	-1.774220874	-4.217481370	-7.724642850
H208	-1.806116686	1.308325325	-10.125296090
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H210	-2.806216361	-2.264759107	-2.854187559
H211	-3.358515634	-5.080012966	-1.778722782
H212	-0.955111314	-0.773202927	-8.769871518
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H216	-0.318381585	-3.227331087	-7.581203015
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H219	-3.131329194	-2.489530454	-1.131995970
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H222	-4.361586367	2.325577417	2.532057511
H223	-2.801637737	0.517089629	1.153156329
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H227	-9.424461410	8.076774616	3.348631038
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H246	-3.885894267	3.711077993	-2.480379057
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H251	-0.863564841	12.344006931	-1.823658576
H252	-2.377219691	13.293501848	-1.769401724
H253	-0.976614306	10.079717905	-2.444997685
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H265	-5.468244061	-1.117030997	-3.905156579
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H268	2.990788858	10.695410810	-2.014117933
H269	-1.712461737	7.599090268	-6.474504074
H270	-4.332153247	8.711037319	-4.486592226
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H294	5.797697385	3.689142074	-5.704605886
H295	6.086178753	7.737118083	-0.952182903
H296	5.004887681	-6.497233323	5.413723509
H297	7.194657239	-7.300563714	3.424200772
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H318	8.440778177	-9.218181093	-0.592092981
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H322	6.057762534	3.214949873	-8.637387269
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H326	3.716673615	-8.823806011	-0.714886621
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H162	-4.509469418	-7.109249592	4.524567392
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H169	-1.505295550	-1.537592669	4.178815792
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H172	-3.056432133	-0.888827723	8.694147521
H173	-3.548796894	2.686106830	9.008514993
H174	-0.133125464	-0.001646294	2.755194929
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	O455	-3.823007012	13.699883225	0.523266401
	O456	-3.947051079	11.224757437	-2.012717373
	O457	-6.414724258	13.070877902	3.344342125
	O458	-5.585091289	6.530301847	-2.063387039
	O459	3.298580943	-4.025745251	-8.548481597
	O460	1.022985437	-0.392826288	-8.512520749
	O461	2.718931414	4.227798720	-7.752119408
	O462	7.201504556	4.683521594	-7.785081949
	O463	-3.482703122	-2.561514628	-9.562053731
	O464	-0.115933325	-6.401562593	-6.353334107
	O465	1.808659967	-5.382948439	-6.834096845
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	O467	10.661139651	-4.463171843	-2.308449297
	O468	13.327341831	-5.995861471	-0.567335371
	O469	0.216491927	-6.539480096	-0.884840979
	O470	0.774714123	-8.458852040	0.088873520
	O471	6.040104520	-10.322179832	-2.756384607
	O472	3.886328590	-10.392063419	-3.432198908
	O473	5.513872667	-5.387700617	-0.766628879
	O474	5.323239068	-7.196986466	0.562703885
	O475	3.206826109	-5.762530613	-1.961635585
	O476	9.154646480	-5.957311894	2.080403805
	O477	7.281247063	-4.099741541	1.033721753
	O478	-4.383478881	4.405841217	-3.043027436
	O479	8.748912801	-9.721120761	-1.384244593
	O480	7.881665541	-8.106502501	0.820759159
	S481	4.170498840	5.597354646	-1.887714782
	S482	2.632207520	2.245293426	-3.068903126
	S483	2.667499007	-2.911396021	-3.442164165
	S484	3.835322379	2.475076927	0.299994477
	S485	0.312683075	-2.254565709	-1.077638669
	S486	4.919440524	-0.214404806	-5.018754542
	S487	3.671876609	-3.344585222	0.259190194
	S488	6.173225415	2.164893692	-2.300061232
	S489	6.213996939	-2.598994293	-2.336411246
	S490	6.210065324	-0.509483946	0.673713574
22, 47(2) Fe1 3.22	bm2unh2b2n2x263b22n2nas.car_4			
	C1	-6.779387555	-6.547437036	-0.530906275

Fe2	-0.01	C2	-6.814651845	-7.452806607	-1.765702395
Fe3	2.51	C3	-8.084232191	-5.157959816	1.016489186
Fe4	-2.76	C4	-7.582964072	-5.704462631	2.351148322
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Fe7	-2.50	C7	-3.603730751	-7.677720642	2.707619033
		C8	-3.082157501	-6.262920039	2.978948938
		C9	-3.405803781	-3.864471686	2.675442600
		C10	-3.613920981	-3.469691394	4.146336644
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		C14	-1.539278328	-6.587288062	7.682854305
		C15	0.369279694	-6.620486421	6.129886677
		C16	1.136382913	-5.353861304	5.736905521
		C17	0.918374697	-2.933467758	5.200034793
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		C29	7.689155231	-10.897167214	1.545979405
		C30	8.038546780	-9.451879140	1.198315441
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		C35	5.393747534	-4.192683517	2.417191259
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		C47	-9.455641512	-0.933866311	-0.184621308
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		C50	-6.195575698	-0.323044621	3.345119722
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		C54	-3.583220128	1.738675432	0.653558088
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C73	3.167237463	8.973651583	0.538690619
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C76	0.556863247	9.670670714	-1.141079587
C77	-0.559433093	7.539433237	-1.627400215
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C79	-0.266182966	6.423056066	-2.646579262
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C94	-6.203013030	8.914584838	4.922796914
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C113	0.150500951	-4.216936290	-8.126519241
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C121	-1.381549611	-0.600022813	-4.904308577
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C78	-0.305710773	6.812468050	-1.949393338
C79	0.381806918	5.592955512	-4.090996803
C80	-0.875335036	4.719828306	-4.173016484
C81	-1.993938081	5.172978889	-5.130724185
C82	-3.331557684	7.247386539	-4.720603130
C83	0.133628412	6.494073872	0.439732358
C84	0.004744143	7.849820863	1.162962816
C85	1.016416489	5.568270634	1.282122826
C86	1.043221268	10.030495334	1.555683914
C87	0.257767261	11.305620592	1.260300125
C88	-1.433044726	12.417171508	-0.144549459
C89	-2.737182547	12.732040798	0.616833758
C90	-1.698548654	12.349404716	-1.667037997
C91	-2.614667671	11.184973338	-2.026636825
C92	-4.496953410	11.864595303	2.093938541
C93	-4.444087000	12.897858120	3.214991315
C94	-4.925780497	10.488525778	2.670198376
C95	-5.138755357	9.442661000	1.599366160
C96	-6.373460173	9.342078612	0.938746131
C97	-4.106811699	8.571539355	1.210986183
C98	-6.572803091	8.414941940	-0.086884843
C99	-4.279742743	7.652692639	0.171033485
C100	-5.514596216	7.591073780	-0.471549354
C101	4.238419526	-3.723933571	-9.049459842
C102	2.812075029	-3.542378028	-8.557981028
C103	1.314416482	-2.102071094	-7.197094688
C104	0.749307750	-0.775023446	-7.712608716
C105	0.982060960	1.664556123	-7.640251367
C106	2.076805918	2.713333152	-7.816709656
C107	4.385501118	3.427335164	-7.456020966
C108	5.193416723	3.451150266	-8.737710773
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C110	-3.647581316	-2.504286866	-8.875129174
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C112	-1.330489372	-5.520411269	-8.134845737
C113	-0.595391030	-5.993732722	-6.901410796
C114	-4.131793007	-0.199206001	-8.197466055
C115	-3.696275919	1.105492834	-8.836908181
C116	-4.440946034	-0.107030516	-6.681372048
C117	-3.203829086	-0.182818297	-5.820398360
C118	-2.413462139	0.952391158	-5.568507155
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C122	-0.768049067	-0.410460174	-4.408463181
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Fe140	2.351095221	0.943108593	-1.340529195
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Fe142	3.995260613	0.741231657	-3.823314256
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Fe145	2.077101454	-1.622053275	-1.990747261
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	O457	-3.848562971	11.273500251	-1.935621624
	O458	-5.441403300	13.409782189	3.695746021
	O459	-5.659387094	6.692965262	-1.544285471
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	O462	1.755963679	3.821669805	-8.277617656
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	O471	0.525762564	-8.464350857	0.334178369
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	O474	5.180195251	-5.578057975	-1.271199567
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	O477	9.199392512	-6.187118292	1.025451891
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	O480	8.222537311	-10.048295722	-2.192760948
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C15	-0.602132131	-6.884688307	5.806636678
C16	0.205876723	-5.598815323	5.600967981
C17	0.057548214	-3.155783654	5.138736545
C18	-0.315273391	-2.200291805	6.287732104
C19	-0.314505558	-2.623334464	3.737974846
C20	0.008442381	-1.133788513	3.614968601
C21	0.385900652	-3.459175504	2.661658102
C22	-2.082395874	-0.927222745	7.428414785
C23	-2.115247841	-1.599190604	8.812700016
C24	-3.438331906	-0.285869099	7.041645832
C25	-3.962165185	0.619085307	8.163572940
C26	-3.311408579	0.511952559	5.737256729
C27	-2.786112350	-3.504331493	10.150165427
C28	-1.451836379	-3.604628045	10.860089267
C29	7.409474526	-10.918642862	2.320479098
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C31	7.550825857	-7.175353193	3.074110149
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C33	6.195874565	-6.462311525	3.218013232
C34	6.309790317	-4.938413936	3.286311184
C35	4.947864851	-4.276985658	3.074725558
C36	4.417652616	-1.977100794	3.920905012
C37	10.548858834	-5.686780471	4.903768943
C38	10.515920351	-4.222932697	5.287536602
C39	-4.300349653	-2.844138982	-3.224858438
C40	-5.046178891	-1.680987442	-2.547272649
C41	-2.801560126	-2.733279004	-2.893299730
C42	-1.954197648	-3.991625474	-3.171367745
C43	-1.366712265	-4.102674493	-4.574721439
C44	-5.939434809	0.597333660	-2.955997640
C45	-7.307319865	0.508969129	-2.278566361
C46	-5.891686389	1.580866145	-4.157895726
C47	-9.264450443	-0.883705309	-1.812950488
C48	-9.074373551	-1.102564929	-0.304969627
C49	-7.521159501	-1.559663095	1.537987892
C50	-6.693345382	-0.471880771	2.225460614
C51	-5.424524721	1.620417578	2.057236020
C52	-6.255956324	2.587847340	2.926086763
C53	-4.721264640	2.470953739	0.986058133
C54	-3.741980492	1.774790332	0.088705278
C55	-2.921943359	0.682629406	0.293837489
C56	-2.570761670	1.508278689	-1.723946633
C57	-8.393092392	3.816374035	3.058128093
C58	-8.605345913	3.570560978	4.549378198
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C61	-10.824141048	5.901035107	3.377549452
C62	-11.858034915	6.566558279	1.533814218
C63	7.936481765	1.898159710	5.731308348
C64	9.135997198	0.997097765	5.507851292
C65	6.719931635	1.198191854	5.072706670
C66	5.434499371	1.969419864	5.254036971
C67	4.638615039	1.804197108	6.403572834
C68	4.992446005	2.874419639	4.273031313
C69	3.438823359	2.507235724	6.565486084
C70	3.806112377	3.593464420	4.425755514
C71	3.026736017	3.405278825	5.571919037
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C75	1.881241911	10.475636434	-0.186053441
C76	0.624373538	9.724017519	-0.624226496
C77	-0.384796408	7.616574512	-1.388882944
C78	-1.155334073	7.036387775	-0.186448265
C79	0.089987558	6.531396482	-2.372341056
C80	-0.959604056	5.556964332	-2.920357454
C81	-1.979783820	6.111448314	-3.931383881
C82	-3.711373559	7.801661879	-3.308715963
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C84	-1.554458732	7.116820234	3.074281367
C85	-0.221747313	5.023543550	2.778039466
C86	-0.991296955	9.203251013	4.221936493
C87	-1.915077385	10.414587511	4.115934328
C88	-3.494798912	11.700077028	2.733902350
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C91	-4.128045605	10.974452885	0.380014320
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C93	-7.089317513	10.884129109	5.394846360
C94	-7.052035142	8.686646008	4.162490420
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C97	-5.670352909	7.352217253	2.489909867
C98	-7.791036474	7.294278656	0.675947106
C99	-5.495282740	6.741899359	1.244628147
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C103	2.798753928	0.134272111	-7.007813605
C104	2.119713080	1.481992891	-7.275907871
C105	1.945618637	3.821666167	-6.578315095
C106	2.874810457	5.001588974	-6.311459602
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C108	5.888073964	6.373000980	-6.410655082
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Fe141	4.409109064	-0.476944229	-2.939550030
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Fe144	4.798385714	-1.941045076	-0.840723744
Fe145	2.115633855	-1.812083723	-0.435180022
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H147	-4.191572062	-5.175849289	6.121345810
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H150	-5.673875824	-4.421015009	8.558335842
H151	-6.445883738	-0.687755671	5.729940920
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H153	-7.902916331	-0.602788220	6.751454072
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H158	-3.229068164	-0.464560157	6.523285490
H159	-1.526462820	-1.548271412	8.537455234
H160	-3.500189604	4.906218854	5.796443288
H161	-3.963717626	2.232696637	6.833837061
H162	-1.167157209	-0.082405409	9.483370241
H163	-3.105680888	0.675187682	4.516309377
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H167	1.082042733	0.363633693	3.410484698
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H170	-1.085822812	4.182029129	10.522520560
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H176	8.827954651	5.468031236	-1.716808836
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O455	-2.512717221	9.026799915	-8.209946960
O456	-6.736497481	8.680830706	-9.052316738
O457	-6.980051035	5.202846919	-8.464165261
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O461	-1.307194016	-7.132204112	-4.336582001
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O463	3.387058565	-4.242617151	-10.261749802
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O469	13.636629322	-4.964046583	-0.462219027
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O472	7.459328610	-8.768269043	4.467556632
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O475	6.925251481	-4.158853997	4.003091290
O476	3.929556072	-5.222658054	2.347951766
O477	10.579563349	-2.538390050	2.388482309
O478	8.076395186	-2.103203055	1.107596747
O479	-5.944903626	0.556322208	-3.536896756
O480	10.167085120	-7.520099112	3.639051461
O481	9.587259925	-4.705108181	3.850593254
S482	1.999291118	1.340908257	-6.820035900
S483	1.152658725	-1.627535740	-4.746282642
S484	2.201704752	-4.300005359	-0.312220701
S485	2.879224257	1.182582074	-3.249436250
S486	0.218930399	-1.800566455	1.058084925
S487	3.269831445	-4.623988309	-4.096125285
S488	4.046044406	-1.996988144	1.347944893
S489	4.650429245	-1.213361722	-5.113595988
S490	5.754205055	-3.885051792	-1.389791430
S491	6.087713615	-0.253977686	-1.484683238
24, 47(2)			
Fe1	2.76	bm2unh2b2n2x263b26n2n472.car_1	
Fe2	-1.01	C1	-5.488949175 -2.882958036 7.107221556
Fe3	2.88	C2	-5.504277528 -4.371217917 7.468458218
Fe4	-2.14	C3	-6.834861184 -0.861788446 6.739623739
Fe5	2.48	C4	-6.092883360 0.117667617 7.647685194
Fe6	-0.22	C5	-5.260962691 0.629926802 9.886947742
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		C7	-1.808309074 -0.498490048 8.700199093
		C8	-1.530194522 0.303397374 7.424109441
		C9	-2.320780863 0.995613310 5.223348036
		C10	-2.426493225 2.508829421 5.473049207
		C11	-3.443883151 4.319941612 6.726421256
		C12	-2.272450023 4.880409216 7.545832971
		C13	-0.879558289 4.639840850 9.542608892
		C14	0.601981847 4.408387634 9.218901306
		C15	2.284396334 2.900402422 8.246040038
		C16	2.760520205 3.043921827 6.796356279
		C17	2.038030779 3.537134960 4.464709388
		C18	1.816655357 5.005565194 4.054763793
		C19	1.209582053 2.525310681 3.647229825

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C21	1.734724791	1.107960173	3.893281266
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C24	-1.275394623	6.979931443	3.332746500
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C26	-1.642035977	6.053015144	2.164491407
C27	0.774135662	8.528694472	7.073521800
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C31	9.307319701	-1.240425818	5.510524743
C32	10.446021215	-0.220552807	5.315971096
C33	7.927569351	-0.609436978	5.259490750
C34	7.780052506	-0.004455485	3.862889305
C35	6.315799530	0.286074215	3.534828525
C36	5.624893785	1.980501905	1.821721786
C37	12.363679242	0.408978552	3.925547407
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C39	-4.382831413	-3.164336877	2.777675534
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C46	-6.993085057	-2.133735179	-1.149637801
C47	-9.094583669	-0.204748134	2.781753006
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C51	-4.827703220	3.497335993	0.602790473
C52	-5.564408453	4.782382545	0.150482756
C53	-4.576690065	2.677088410	-0.672678380
C54	-3.753511664	1.433571136	-0.542530791
C55	-2.758542689	1.020883730	0.311530341
C56	-3.016427843	-0.566341890	-1.208800627
C57	-7.782441904	5.770679951	-0.308098053
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C59	-9.246807671	5.294904890	-0.166110304
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C79	-1.750282117	0.182173267	-6.735186396
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H164	-2.352038620	3.262702229	8.834784821
H165	-4.374433303	4.468151940	7.291533480
H166	1.760923178	0.874588711	4.967595608
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H168	2.748543108	0.981594905	3.484034929
H169	0.172132148	2.579566986	4.011329946
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H178	-2.682446120	8.504448677	2.701278489
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H181	-1.868887807	6.682264775	4.215913934
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H192	0.852408586	3.488765378	6.248460903
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H240	-9.509454685	-0.789106861	3.613578159
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C84	-1.928925753	5.679093701	-5.128144441

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C98	-8.518844820	4.792729103	-4.391159434
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C101	3.646479365	-9.211804767	-3.870291519
C102	2.332717894	-8.778036275	-3.242700475
C103	0.730729481	-6.886508777	-3.028799415
C104	-0.241630348	-6.499734538	-4.148782571
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C112	-1.032185997	-9.834883241	-0.269290537
C113	-0.028069487	-9.118658326	0.604833012
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C115	-5.180437308	-6.458885183	-4.906021573
C116	-5.206860315	-5.489905518	-2.514840603
C117	-3.866433151	-4.823404792	-2.318802229
C118	-3.347848360	-3.919697019	-3.262554537
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