WORLDWIDE wwPDB PROTEIN DATA BANK

Preliminary Full wwPDB X-ray Structure Validation Report (i)

Jun 16, 2021 – 08:54 am BST

Deposition ID : D_1292116503

The following versions of software and data (see references (1)) were used in the production of this report:

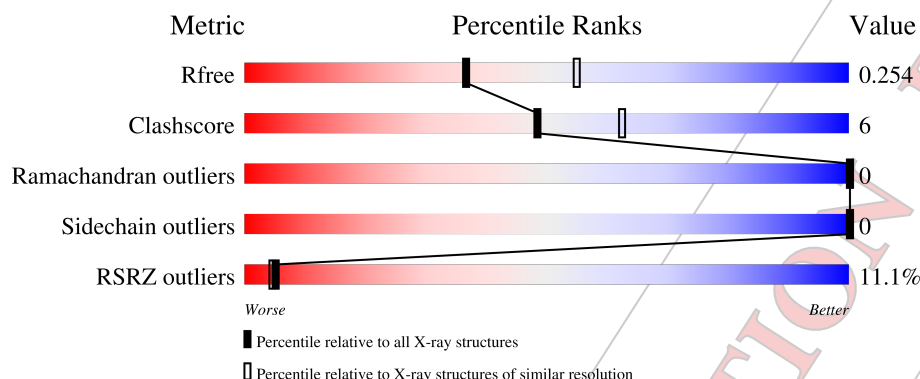|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.20
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.20

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.

Metric	Percentile Ranks	Value
Rfree		0.254
Clashscore		6
Ramachandran outliers		0
Sidechain outliers		0
RSRZ outliers		11.1%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

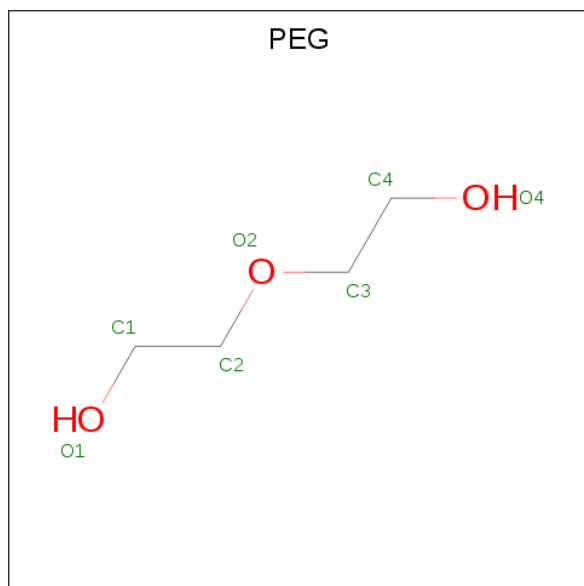| Mol	Chain	Length	Quality of chain
1	A	369	5% / 78% / 13% / 9%
1	B	369	6% / 81% / 9% / 9%
1	C	369	14% / 79% / 12% / 8%
1	D	369	15% / 80% / 11% / 9%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 10429 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	336	Total 2569	C 1608	N 441	O 495	P 1	S 24	0	0	0
1	B	334	Total 2551	C 1598	N 437	O 491	P 1	S 24	0	0	0
1	C	338	Total 2586	C 1617	N 443	O 499	P 1	S 26	0	0	0
1	D	335	Total 2560	C 1603	N 439	O 493	P 1	S 24	0	0	0

- Molecule 2 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 7	C 4	O 3	0	0
2	B	1	Total 7	C 4	O 3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	O	0	0
			7	4	3		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).
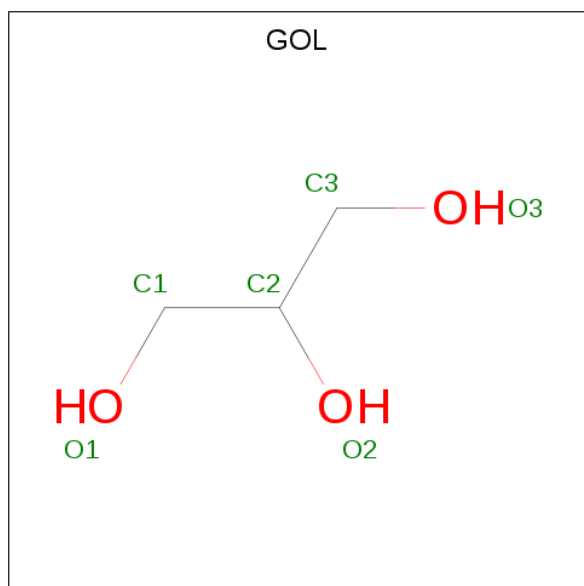
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	F	124	Total	O	0	0
			124	124		

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1:

Chain A:

5% — 78% — 13% — 9%

MET HIS HIS HIS HIS HIS HIS HIS HIS HIS LEU GLU VAL LEU PHE GLN GLY PRO SER PRO ASP THR THR SER LEU ASN ILE9 ALA10 ASP11 LEU23 PHE26 PRO27 MET MET GLU GLN31 PHE34 GLN35 THR36 ARG37 GLU38 GLU39 GLN40 VAL41 ALA42 PRO47 ALA51 GLN55 MET58 ASP61

ASP64 ALA89 ILE90 GLY112 MET115 GLY122 ALA126 ASP142 CYS146 LEU147 SER148 PRO149 SER150 SER151 ALA152 PRO153 GLU154 VAL155 ALA156 PRO157 ALA160 TRP171 ALA189 GLY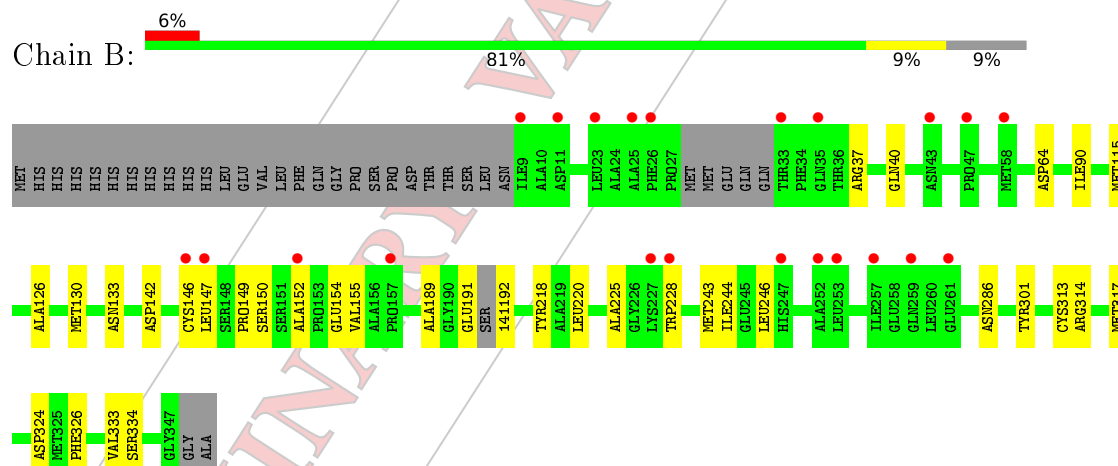190 GLU191 SER 141192 ILE211 TYR218 ALA219 LEU220 ALA225 TRP228 MET243 ILE244 GLU245 LEU246 GLU275 ILE285 ASN286 ARG312 CYS313

ARG314 ALA322 GLY323 ASP324 MET325 PHE326 SER334 GLY347 GLY ALA

- Molecule 1:

Chain B:

6% — 81% — 9% — 9%

MET HIS HIS HIS HIS HIS HIS HIS HIS HIS LEU GLU VAL LEU PHE GLN GLY PRO SER PRO ASP THR THR SER LEU ASN ILE9 ALA10 ASP11 LEU23 ALA24 ALA25 PHE26 PRO27 MET MET GLU GLN GLN THR33 PHE34 GLN35 THR36 ARG37 GLN40 ASN43 PRO47 MET58 ASP64 ILE90 MET115

ALA126 MET130 ASN133 ASP142 CYS146 LEU147 SER148 PRO149 SER150 SER151 ALA152 PRO153 GLU154 VAL155 ALA156 PRO157 ALA189 GLY190 GLU191 SER 141192 TYR218 ALA219 LEU220 ALA225 GLY226 LYS227 TRP228 MET243 ILE244 GLU245 LEU246 HIS247 ALA252 LEU253 ILE257 GLU258 GLN259 LEU260 GLU261 ASN286 TYR301 CYS313 ARG314 MET317

ASP324 MET325 PHE326 VAL333 SER334 GLY347 GLY ALA

- Molecule 1:

Chain C:

14% — 79% — 12% — 8%

MET HIS HIS HIS HIS HIS HIS HIS HIS HIS LEU GLU VAL LEU PHE GLN GLY PRO SER PRO ASP THR THR SER LEU ASN ILE ALA10 MET22 LEU23 ALA24 ALA25 PHE26 PRO27 MET28 MET29 GLU30 GLN31 GLN32 GLN35 THR36 ARG37 GLN40 VAL41 ALA42 ASN43 PRO47 THR50 ALA51 ALA52 ARG53 GLU54 MET58

MET59 MET60 ASP61 MET62 MET63 ASP64 SER84 ALA89 ILE90 LYS91 ILE92 MET115 ILE116 MET117 TYR121 GLY122 ALA126 GLY135 ASP142 CYS146 LEU147 PRO149 SER150 SER151 ALA152 PRO153 GLU154 VAL155 ALA156 PRO157 ALA160 SER167 GLU174 ASN175 GLU178 LEU179 ALA189 GLY190 GLY191 SER 141192 LYS204 ASP212

TYR218 ALA219 LEU220 ALA225 GLY226 LYS227 TRP228 MET243 ILE244 GLU245 LEU246 HIS247 ASN248 ASN249 GLN250 GLY251 ALA252 LEU253 ALA254 ILE257 GLU261 ALA274 GLU314 ILE285 ASN286 ARG312 CYS313 ARG314 HIS321 ASP324 ILE330 SER334 GLY347 GLY ALA

• Molecule 1:

15%

Chain D: 80%   11%   9%

MET HIS HIS HIS HIS HIS HIS HIS HIS HIS LEU GLU VAL LEU PHE GLN GLY PRO SER PRO ASP THR THR SER LEU ASN ILE9 ASP12 VAL13 MET22 LEU23 ALA24 ALA25 PHE26 PRO27 MET MET GLU GLN GLN32 THR33 PHE34 GLN35 THR36 ARG37 GLU38 ALA42 ASN43 ALA44 PRO47 GLU48 ALA49 THR50 ALA51 ALA52

ARG53 GLU54 GLN55 LEU56 LYS57 MET58 MET59 MET60 ASP61 MET62 MET63 ASP64 GLU80 PHE81 PRO85 ILE90 LYS91 ILE92 GLN93 PHE94 MET115 ILE116 PHE120 TYR121 GLY122 ALA126 ASP142 ASN145 CYS146 LEU147 SER148 PRO149 SER150 SER151 ALA152 PRO153 GLU154 VAL155 ALA156 PRO157 PHE158 PRO159 ALA160 ASN163 SER167 VAL172 ALA189 GLY190

GLU191 SER 141192 THR201 LYS204 TYR218 ALA219 LEU220 TYR223 ILE224 ALA225 TRP228 ILE244 GLU245 LEU246 HIS247 LEU253 ALA254 TYR255 GLY256 ILE257 LEU266 ALA267 ALA274 GLU275 GLN278 ILE285 ASN286 CYS313 ARG314 MET317 ASP324 ILE330 VAL333 SER334 GLY347 GLY ALA

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	56.76Å 189.39Å 75.95Å 90.00° 111.93° 90.00°	Depositor
Resolution (Å)	47.35 – 2.40 47.35 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.35-2.40) 99.9 (47.35-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.21 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.244 , 0.253 0.245 , 0.254	Depositor DCC
R_{free} test set	2927 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	34.1	Xtriage
Anisotropy	0.602	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 19.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.43, < L^2 > = 0.25$	Xtriage
Estimated twinning fraction	0.398 for h,-k,-h-l	Xtriage
Reported twinning fraction	0.597 for H, K, L 0.403 for -H, -K, H+L	Depositor
Outliers	1 of 57868 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	10429	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.53% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< \|L\| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 141, GOL, PEG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z|>5	RMSZ	#|Z|>5
1	A	0.69	0/2590	0.80	0/3506
1	B	0.67	0/2572	0.80	0/3482
1	C	0.68	0/2608	0.81	0/3530
1	D	0.68	0/2581	0.80	0/3494
All	All	0.68	0/10351	0.80	0/14012

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2569	0	2484	34	0
1	B	2551	0	2468	25	0
1	C	2586	0	2498	38	0
1	D	2560	0	2476	28	0
2	A	7	0	10	0	0
2	B	7	0	10	3	0
2	C	7	0	10	3	0
3	C	12	0	16	0	0
3	D	6	0	8	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	F	124	0	0	1	0
All	All	10429	0	9980	121	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (121) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:ARG:HA	1:A:40:GLN:OE1	1.79	0.82
1:D:90:ILE:HG23	1:D:142:ASP:O	1.80	0.81
1:A:90:ILE:HG23	1:A:142:ASP:O	1.80	0.81
1:B:90:ILE:HG23	1:B:142:ASP:O	1.80	0.80
1:C:90:ILE:HG23	1:C:142:ASP:O	1.81	0.79
1:C:50:THR:HG23	1:C:53:ARG:NH2	2.02	0.73
1:C:50:THR:HG23	1:C:53:ARG:HH21	1.56	0.70
1:C:135:GLY:HA3	2:C:401:PEG:H32	1.73	0.70
1:A:34:PHE:CD1	1:A:40:GLN:HG2	2.29	0.67
1:A:9:ILE:HG21	1:A:11:ASP:OD2	1.94	0.67
1:D:53:ARG:O	1:D:56:LEU:HG	1.95	0.66
1:A:149:PRO:HG3	1:A:155:VAL:CG2	2.27	0.65
1:D:115:MET:HG2	1:D:146:CYS:SG	2.39	0.62
1:D:156:ALA:HB1	1:D:157:PRO:HD2	1.80	0.62
1:C:50:THR:CB	1:C:53:ARG:HH21	2.13	0.61
1:B:130:MET:HG2	2:B:401:PEG:H22	1.83	0.61
1:B:115:MET:HG2	1:B:146:CYS:SG	2.43	0.58
1:C:50:THR:CG2	1:C:53:ARG:HH21	2.15	0.58
1:C:115:MET:HG3	1:C:147:LEU:HB3	1.86	0.58
1:C:135:GLY:HA2	2:C:401:PEG:H22	1.85	0.58
1:A:37:ARG:HA	1:A:40:GLN:CD	2.24	0.57
1:A:61:ASP:HA	1:A:122:GLY:HA3	1.86	0.57
1:A:149:PRO:HG3	1:A:155:VAL:HG23	1.87	0.56
1:C:204:LYS:HG2	1:C:204:LYS:O	2.05	0.56
1:C:115:MET:HG3	1:C:147:LEU:CB	2.36	0.55
1:B:133:ASN:HB2	2:B:401:PEG:H21	1.91	0.53
1:C:50:THR:HA	1:C:53:ARG:HH21	1.75	0.52
1:A:64:ASP:HA	1:A:126:ALA:HB2	1.92	0.52
1:C:135:GLY:CA	2:C:401:PEG:H32	2.38	0.52
1:B:64:ASP:HA	1:B:126:ALA:HB2	1.92	0.52
1:A:243:MET:HE1	1:A:326:PHE:HE2	1.74	0.51
1:B:189:ALA:HA	1:B:218:TYR:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:189:ALA:HA	1:C:218:TYR:O	2.11	0.51
1:A:23:LEU:HA	1:A:26:PHE:HB2	1.93	0.51
1:A:23:LEU:HA	1:A:26:PHE:CB	2.41	0.50
1:C:37:ARG:O	1:C:40:GLN:HB2	2.12	0.50
1:A:23:LEU:O	1:A:26:PHE:HB3	2.11	0.49
1:C:64:ASP:HA	1:C:126:ALA:HB2	1.94	0.49
1:D:64:ASP:HA	1:D:126:ALA:HB2	1.94	0.49
1:D:189:ALA:HA	1:D:218:TYR:O	2.12	0.49
1:A:189:ALA:HA	1:A:218:TYR:O	2.12	0.49
1:B:37:ARG:O	1:B:40:GLN:HB2	2.13	0.49
1:B:225:ALA:HB3	1:B:228:TRP:CE2	2.48	0.49
1:D:44:ALA:HB1	1:D:53:ARG:NH2	2.28	0.49
1:C:225:ALA:HB3	1:C:228:TRP:CE2	2.48	0.48
1:D:225:ALA:HB3	1:D:228:TRP:CE2	2.47	0.48
1:D:56:LEU:HD12	1:D:57:LYS:N	2.28	0.48
1:A:36:THR:HB	1:A:38:GLU:OE1	2.14	0.48
1:A:225:ALA:HB3	1:A:228:TRP:CE2	2.48	0.48
1:A:244:ILE:HD12	1:A:246:LEU:HD21	1.96	0.48
1:C:175:ASN:HA	1:C:178:GLU:OE1	2.13	0.48
1:B:40:GLN:HB3	1:B:147:LEU:HD11	1.96	0.48
1:D:36:THR:HB	1:D:38:GLU:OE1	2.13	0.48
1:D:330:ILE:O	1:D:330:ILE:HG13	2.13	0.48
1:A:55:GLN:HA	1:A:58:MET:HB2	1.96	0.48
1:B:243:MET:HE1	1:B:326:PHE:HE2	1.78	0.48
1:D:34:PHE:HZ	1:D:43:ASN:HD22	1.62	0.47
1:C:286:ASN:ND2	1:C:314:ARG:HE	2.12	0.47
1:D:286:ASN:ND2	1:D:314:ARG:HE	2.13	0.47
1:D:61:ASP:HA	1:D:122:GLY:HA3	1.95	0.47
1:B:286:ASN:ND2	1:B:314:ARG:HE	2.13	0.47
1:C:244:ILE:HD12	1:C:246:LEU:HD21	1.97	0.47
1:D:244:ILE:HD12	1:D:246:LEU:HD21	1.97	0.47
1:A:286:ASN:HD22	1:A:314:ARG:HE	1.63	0.47
1:B:244:ILE:HD12	1:B:246:LEU:HD21	1.97	0.46
1:C:286:ASN:HD22	1:C:314:ARG:HE	1.62	0.46
1:D:286:ASN:HD22	1:D:314:ARG:HE	1.63	0.46
1:B:154:GLU:HG3	4:F:103:HOH:O	2.16	0.46
1:B:286:ASN:HD22	1:B:314:ARG:HE	1.62	0.46
1:C:29:MET:O	1:C:29:MET:HG3	2.15	0.46
1:D:150:SER:OG	1:D:152:ALA:HB3	2.16	0.45
1:D:13:VAL:HG12	3:D:401:GOL:H32	1.98	0.45
1:C:35:GLN:O	1:C:253:LEU:HD21	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:SER:OG	1:B:152:ALA:HB3	2.17	0.45
1:C:150:SER:OG	1:C:152:ALA:HB3	2.16	0.45
1:C:50:THR:HA	1:C:53:ARG:HE	1.81	0.45
1:A:312:ARG:HG3	1:B:333:VAL:HG22	1.99	0.45
1:A:150:SER:OG	1:A:152:ALA:HB3	2.17	0.44
1:B:149:PRO:HA	1:B:155:VAL:HG22	2.00	0.44
1:C:26:PHE:CG	1:C:27:PRO:HD2	2.52	0.44
1:C:50:THR:CA	1:C:53:ARG:HH21	2.31	0.44
1:C:115:MET:HA	1:C:146:CYS:SG	2.57	0.44
1:D:12:ASP:HA	3:D:401:GOL:O2	2.17	0.44
1:D:324:ASP:O	1:D:334:SER:HA	2.18	0.44
1:C:312:ARG:HG3	1:D:333:VAL:HG22	2.00	0.43
1:A:115:MET:HA	1:A:146:CYS:SG	2.58	0.43
1:A:153:PRO:HD2	1:A:154:GLU:H	1.82	0.43
1:B:225:ALA:HB3	1:B:228:TRP:CZ2	2.54	0.43
1:A:225:ALA:HB3	1:A:228:TRP:CZ2	2.53	0.43
1:C:324:ASP:O	1:C:334:SER:HA	2.19	0.43
1:B:115:MET:CG	1:B:146:CYS:SG	3.07	0.43
1:C:313:CYS:HB3	1:D:317:MET:HB2	2.01	0.43
1:D:53:ARG:HA	1:D:56:LEU:CD2	2.49	0.43
1:A:286:ASN:ND2	1:A:314:ARG:HE	2.16	0.42
1:A:324:ASP:O	1:A:334:SER:HA	2.19	0.42
1:B:191:GLU:HA	1:B:220:LEU:HB2	1.99	0.42
1:B:324:ASP:O	1:B:334:SER:HA	2.19	0.42
1:D:149:PRO:HA	1:D:155:VAL:HG22	2.01	0.42
1:C:225:ALA:HB3	1:C:228:TRP:CZ2	2.55	0.42
1:A:313:CYS:HB3	1:B:317:MET:HB2	2.00	0.42
1:B:130:MET:CG	2:B:401:PEG:H22	2.50	0.42
1:D:225:ALA:HB3	1:D:228:TRP:CZ2	2.54	0.42
1:C:191:GLU:HA	1:C:220:LEU:HB2	2.00	0.42
1:C:22:MET:O	1:C:26:PHE:HB2	2.19	0.42
1:A:112:GLY:HA2	1:A:192:141:O03	2.20	0.42
1:C:243:MET:HE1	1:C:321:HIS:O	2.19	0.42
1:D:191:GLU:HA	1:D:220:LEU:HB2	2.01	0.42
1:B:301:TYR:CG	1:B:313:CYS:HB2	2.55	0.41
1:C:285:ILE:O	1:C:313:CYS:HA	2.20	0.41
1:C:330:ILE:HG13	1:C:330:ILE:O	2.19	0.41
1:A:285:ILE:O	1:A:313:CYS:HA	2.21	0.41
1:C:149:PRO:HA	1:C:155:VAL:HG22	2.03	0.41
1:A:115:MET:HG2	1:A:146:CYS:SG	2.60	0.41
1:A:149:PRO:HA	1:A:155:VAL:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:GLU:HA	1:A:220:LEU:HB2	2.01	0.41
1:A:322:ALA:O	1:A:325:MET:HG2	2.21	0.41
1:A:211:ILE:HD12	1:A:211:ILE:HA	1.98	0.41
1:D:115:MET:HA	1:D:146:CYS:SG	2.61	0.41
1:D:285:ILE:O	1:D:313:CYS:HA	2.21	0.41
1:B:115:MET:HE2	1:B:192:141:C06	2.51	0.40
1:C:61:ASP:HA	1:C:122:GLY:HA3	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	331/369 (90%)	303 (92%)	28 (8%)	0	100	100
1	B	329/369 (89%)	302 (92%)	27 (8%)	0	100	100
1	C	335/369 (91%)	306 (91%)	29 (9%)	0	100	100
1	D	330/369 (89%)	302 (92%)	28 (8%)	0	100	100
All	All	1325/1476 (90%)	1213 (92%)	112 (8%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	268/298 (90%)	268 (100%)	0	100	100
1	B	266/298 (89%)	266 (100%)	0	100	100
1	C	270/298 (91%)	270 (100%)	0	100	100
1	D	267/298 (90%)	267 (100%)	0	100	100
All	All	1071/1192 (90%)	1071 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	286	ASN
1	B	286	ASN
1	C	286	ASN
1	D	286	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	PEG	C	401	-	6,6,6	0.13	0	5,5,5	0.11	0
2	PEG	B	401	-	6,6,6	0.26	0	5,5,5	0.12	0
2	PEG	A	401	-	6,6,6	0.16	0	5,5,5	0.06	0
3	GOL	C	501	-	5,5,5	0.13	0	5,5,5	0.31	0
3	GOL	C	601	-	5,5,5	0.16	0	5,5,5	0.28	0
3	GOL	D	401	-	5,5,5	0.08	0	5,5,5	0.30	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PEG	C	401	-	-	0/4/4/4	-
2	PEG	B	401	-	-	1/4/4/4	-
2	PEG	A	401	-	-	1/4/4/4	-
3	GOL	C	501	-	-	0/4/4/4	-
3	GOL	C	601	-	-	0/4/4/4	-
3	GOL	D	401	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	401	PEG	C1-C2-O2-C3
2	A	401	PEG	C4-C3-O2-C2

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	401	PEG	3	0
2	B	401	PEG	3	0
3	D	401	GOL	2	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	335/369 (90%)	0.41	18 (5%)	25	24	17, 39, 71, 85	0
1	B	333/369 (90%)	0.49	22 (6%)	18	17	14, 39, 71, 79	0
1	C	337/369 (91%)	0.90	53 (15%)	2	1	17, 49, 80, 99	0
1	D	334/369 (90%)	0.97	55 (16%)	1	1	16, 50, 73, 85	0
All	All	1339/1476 (90%)	0.69	148 (11%)	5	4	14, 43, 74, 99	0

All (148) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	253	LEU	6.2
1	C	147	LEU	5.1
1	D	51	ALA	5.0
1	D	62	MET	5.0
1	D	155	VAL	4.7
1	D	121	TYR	4.6
1	D	266	LEU	4.6
1	D	167	SER	4.6
1	C	59	MET	4.5
1	D	153	PRO	4.4
1	C	35	GLN	4.3
1	D	35	GLN	4.3
1	D	159	PRO	4.3
1	C	62	MET	4.2
1	A	51	ALA	4.0
1	C	249	ASN	4.0
1	C	117	MET	4.0
1	A	155	VAL	3.9
1	C	151	SER	3.9
1	C	157	PRO	3.9
1	D	255	TYR	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	9	ILE	3.8
1	D	27	PRO	3.8
1	D	115	MET	3.7
1	D	55	GLN	3.7
1	D	147	LEU	3.7
1	D	90	ILE	3.7
1	C	156	ALA	3.5
1	B	253	LEU	3.5
1	C	29	MET	3.5
1	C	153	PRO	3.5
1	B	33	THR	3.4
1	C	31	GLN	3.4
1	C	257	ILE	3.4
1	A	147	LEU	3.4
1	C	247	HIS	3.4
1	C	90	ILE	3.3
1	A	27	PRO	3.3
1	C	23	LEU	3.3
1	C	252	ALA	3.3
1	C	92	ILE	3.2
1	D	152	ALA	3.2
1	C	253	LEU	3.2
1	A	275	GLU	3.1
1	D	145	ASN	3.1
1	B	247	HIS	3.1
1	D	172	VAL	3.1
1	D	275	GLU	3.1
1	C	154	GLU	3.0
1	A	153	PRO	3.0
1	D	26	PHE	2.9
1	A	26	PHE	2.9
1	C	228	TRP	2.9
1	D	257	ILE	2.9
1	C	51	ALA	2.9
1	B	11	ASP	2.9
1	D	22	MET	2.9
1	A	39	GLU	2.8
1	D	160	ALA	2.8
1	B	23	LEU	2.8
1	D	148	SER	2.8
1	D	42	ALA	2.8
1	D	59	MET	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	254	ALA	2.8
1	D	47	PRO	2.8
1	B	35	GLN	2.7
1	C	32	GLN	2.7
1	C	41	VAL	2.7
1	D	149	PRO	2.7
1	A	58	MET	2.7
1	C	43	ASN	2.7
1	C	47	PRO	2.7
1	A	35	GLN	2.7
1	C	274	ALA	2.6
1	D	92	ILE	2.6
1	A	157	PRO	2.6
1	B	252	ALA	2.6
1	B	147	LEU	2.6
1	D	24	ALA	2.6
1	D	274	ALA	2.6
1	C	179	LEU	2.6
1	B	257	ILE	2.6
1	C	26	PHE	2.6
1	D	247	HIS	2.6
1	D	223	TYR	2.6
1	C	25	ALA	2.5
1	B	47	PRO	2.5
1	C	152	ALA	2.5
1	D	267	ALA	2.5
1	B	261	GLU	2.4
1	D	57	LYS	2.4
1	D	278	GLN	2.4
1	D	201	THR	2.4
1	D	54	GLU	2.4
1	C	155	VAL	2.4
1	B	228	TRP	2.4
1	A	47	PRO	2.4
1	D	81	PHE	2.4
1	B	227	LYS	2.4
1	A	160	ALA	2.4
1	A	55	GLN	2.4
1	B	43	ASN	2.4
1	B	9	ILE	2.4
1	A	42	ALA	2.3
1	C	89	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	275	GLU	2.3
1	A	171	TRP	2.3
1	C	212	ASP	2.3
1	D	163	ASN	2.3
1	C	246	LEU	2.3
1	D	48	GLU	2.3
1	D	116	ILE	2.3
1	D	94	PHE	2.3
1	D	56	LEU	2.3
1	A	89	ALA	2.3
1	B	146	CYS	2.3
1	C	174	GLU	2.3
1	D	91	LYS	2.2
1	C	243	MET	2.2
1	C	63	MET	2.2
1	C	244	ILE	2.2
1	C	251	GLY	2.2
1	D	85	PRO	2.2
1	C	22	MET	2.2
1	B	26	PHE	2.2
1	A	150	SER	2.2
1	C	167	SER	2.2
1	C	58	MET	2.2
1	C	121	TYR	2.1
1	B	25	ALA	2.1
1	D	80	GLU	2.1
1	D	120	PHE	2.1
1	C	52	ALA	2.1
1	C	54	GLU	2.1
1	C	261	GLU	2.1
1	D	254	ALA	2.1
1	C	84	SER	2.1
1	C	61	ASP	2.1
1	B	58	MET	2.1
1	B	157	PRO	2.1
1	D	256	GLY	2.1
1	C	160	ALA	2.1
1	D	52	ALA	2.1
1	B	152	ALA	2.0
1	B	259	GLN	2.0
1	D	204	LYS	2.0
1	D	49	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	226	GLY	2.0

6.2   Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3   Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4   Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	PEG	C	401	7/?	0.64	0.35	56,58,58,60	0
2	PEG	B	401	7/?	0.83	0.21	31,34,36,38	0
3	GOL	D	401	6/?	0.84	0.20	52,55,56,57	0
3	GOL	C	501	6/?	0.85	0.19	42,47,49,50	0
2	PEG	A	401	7/?	0.86	0.19	47,47,49,49	0
3	GOL	C	601	6/?	0.87	0.16	26,26,27,28	0

6.5   Other polymers ⓘ

There are no such residues in this entry.