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

Nov 8, 2021 – 11:20 AM JST

Deposition ID : D_1300025494

<div style="border: 1px solid red; padding: 1em;">

This is a Preliminary Full wwPDB X-ray Structure Validation Report.

This report is produced by the wwPDB Deposition System
during initial deposition but before annotation of the structure.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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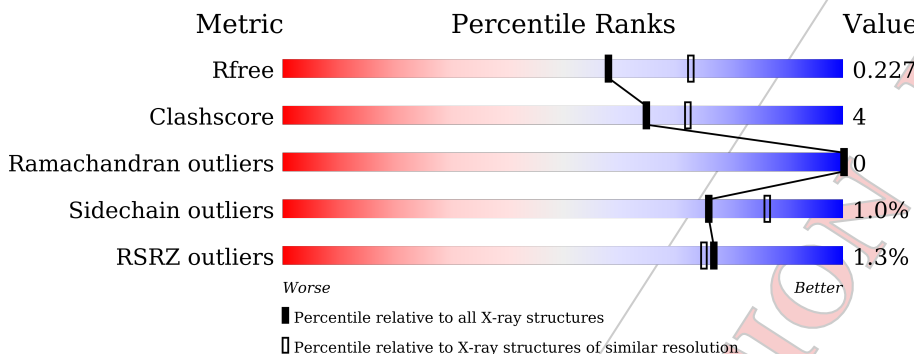The following versions of software and data (see references (i)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
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)	:	2.23.2

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 2.20 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.
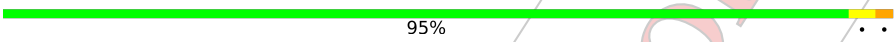
Metric	Percentile Ranks	Value
Rfree		0.227
Clashscore		4
Ramachandran outliers		0
Sidechain outliers		1.0%
RSRZ outliers		1.3%

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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	164	86% 13% ••
1	B	164	94% 6%
1	C	164	93% 7%
1	D	164	80% 19% •
1	E	164	92% 8%
1	F	164	88% 12%

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Mol	Chain	Length	Quality of chain
1	G	164	4% 86% 13%
1	H	164	95%

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 22289 atoms, of which 10540 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	H	164	Total 2686	C 874	H 1319	N 223	O 264	S 6	0	0	0
1	A	163	Total 2666	C 869	H 1307	N 222	O 263	S 5	0	0	0
1	B	164	Total 2686	C 874	H 1319	N 223	O 264	S 6	0	0	0
1	C	164	Total 2686	C 874	H 1319	N 223	O 264	S 6	0	0	0
1	D	164	Total 2686	C 874	H 1319	N 223	O 264	S 6	0	0	0
1	E	164	Total 2686	C 874	H 1319	N 223	O 264	S 6	0	0	0
1	F	164	Total 2686	C 874	H 1319	N 223	O 264	S 6	0	0	0
1	G	164	Total 2686	C 874	H 1319	N 223	O 264	S 6	0	0	0

- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	I	1	Total 1	Fe 1	0	0
2	I	1	Total 1	Fe 1	0	0
2	I	1	Total 1	Fe 1	0	0
2	I	1	Total 1	Fe 1	0	0
2	I	1	Total 1	Fe 1	0	0
2	I	1	Total 1	Fe 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	I	1	Total 1	Fe 1	0	0
2	I	1	Total 1	Fe 1	0	0
2	I	1	Total 1	Fe 1	0	0
2	I	1	Total 1	Fe 1	0	0
2	I	1	Total 1	Fe 1	0	0
2	I	1	Total 1	Fe 1	0	0
2	I	1	Total 1	Fe 1	0	0
2	I	1	Total 1	Fe 1	0	0
2	I	1	Total 1	Fe 1	0	0
2	I	1	Total 1	Fe 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	S	805	Total 805	O 805	0	0

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 H:

- Molecule 1:

Chain A:

- Molecule 1:

Chain B:

- Molecule 1:

Chain C:

- Molecule 1:

Chain D:

GLU164

• Molecule 1:

Chain E:

%

92% 8%

MET1 LYS10 LEU27 ALA30 PHE38 PHE41 ARG69 ILE75 ILE85 LYS86 ASN147 GLY148 LEU160 GLY161 GLN162 ARG163 GLU164

• Molecule 1:

Chain F:

%

88% 12%

MET1 LYS10 ASP14 GLN15 ARG18 TYR24 LEU25 TYR26 PHE38 PHE41 LYS47 GLU51 MET57 GLU96 ILE106 LEU107 GLU128 GLU132 LYS145 GLN149 TYR159 GLU164

• Molecule 1:

Chain G:

4%

86% 13%

MET1 LEU16 TYR24 MET29 ALA35 GLU36 GLY37 PHE38 LYS39 GLY40 MET45 ARG66 ASN83 GLY84 ILE85 ILE103 SER111 PHE125 GLU128 GLU132 VAL152 ILE153 PHE154 GLN155 LEU156 ASP157 ARG158 TYR159 GLN162 ARG163 GLU164

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	176.19Å 176.19Å 357.51Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	38.69 – 2.20 38.69 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (38.69-2.20) 99.9 (38.69-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.32 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.180 , 0.227 0.180 , 0.227	Depositor DCC
R_{free} test set	2000 reflections (1.85%)	wwPDB-VP
Wilson B-factor (Å^2)	32.8	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.42 , 47.5	EDS
L-test for twinning [2]	$< |L| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	22289	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.49% 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 (i)

5.1   Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: FE

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	0.68	0/1388	0.77	3/1866 (0.2%)
1	B	0.68	0/1396	0.73	3/1876 (0.2%)
1	C	0.62	1/1396 (0.1%)	0.67	1/1876 (0.1%)
1	D	0.64	0/1396	0.69	3/1876 (0.2%)
1	E	0.53	0/1396	0.61	0/1876
1	F	0.65	1/1396 (0.1%)	0.66	1/1876 (0.1%)
1	G	0.55	0/1396	0.56	0/1876
1	H	0.70	2/1396 (0.1%)	0.81	5/1876 (0.3%)
All	All	0.63	4/11160 (0.0%)	0.69	16/14998 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	51	GLU	CB-CG	5.56	1.62	1.52
1	H	61	GLU	CG-CD	5.29	1.59	1.51
1	H	69	ARG	CZ-NH1	5.11	1.39	1.33
1	F	149	GLN	CG-CD	5.06	1.62	1.51

All (16) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	69	ARG	NE-CZ-NH2	-10.58	115.01	120.30
1	H	69	ARG	NE-CZ-NH1	9.37	124.99	120.30
1	A	147	ASN	C-N-CA	-9.14	103.09	122.30
1	C	45	MET	CG-SD-CE	8.55	113.88	100.20
1	H	9	ARG	NE-CZ-NH2	-8.07	116.27	120.30
1	B	147	ASN	C-N-CA	-7.88	105.75	122.30
1	A	45	MET	CG-SD-CE	7.72	112.55	100.20
1	H	9	ARG	NE-CZ-NH1	7.44	124.02	120.30
1	D	69	ARG	NE-CZ-NH2	-7.17	116.71	120.30
1	D	45	MET	CG-SD-CE	6.68	110.89	100.20
1	H	18	ARG	NE-CZ-NH2	-6.65	116.98	120.30
1	F	57	MET	CG-SD-CE	6.49	110.58	100.20
1	B	2	MET	CG-SD-CE	5.95	109.72	100.20
1	B	150	MET	CG-SD-CE	5.43	108.89	100.20
1	A	57	MET	CG-SD-CE	5.30	108.68	100.20
1	D	69	ARG	CG-CD-NE	-5.00	101.30	111.80

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	148	GLY	Peptide
1	B	148	GLY	Peptide

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	1359	1307	1307	24	0
1	B	1367	1319	1319	3	0
1	C	1367	1319	1319	6	0
1	D	1367	1319	1319	19	0
1	E	1367	1319	1319	9	0
1	F	1367	1319	1319	10	1
1	G	1367	1319	1319	17	1
1	H	1367	1319	1319	4	0
2	I	16	0	0	0	0
3	S	805	0	0	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	11749	10540	10540	87	1

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 4.

All (87) 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:96:GLU:OE2	3:S:864:HOH:O	1.77	1.00
1:F:10:LYS:NZ	3:S:550:HOH:O	2.01	0.91
1:A:26:TYR:CD1	1:A:45:MET:HE3	2.06	0.90
1:A:26:TYR:CD1	1:A:45:MET:CE	2.57	0.87
1:A:26:TYR:HD1	1:A:45:MET:CE	1.89	0.85
1:A:26:TYR:HD1	1:A:45:MET:HE1	1.52	0.74
1:A:81:ASN:HB3	3:S:58:HOH:O	1.90	0.70
1:A:26:TYR:CG	1:A:45:MET:HE3	2.30	0.66
1:E:38:PHE:CE2	1:E:85:ILE:HD11	2.34	0.63
1:A:29:MET:HB2	1:A:45:MET:HE2	1.80	0.62
1:A:26:TYR:CB	1:A:45:MET:HE3	2.29	0.61
1:E:69:ARG:HG3	1:G:35:ALA:HB2	1.82	0.61
1:A:26:TYR:CD1	1:A:45:MET:HE1	2.29	0.60
1:A:26:TYR:OH	1:A:96:GLU:OE2	2.15	0.60
1:G:29:MET:SD	1:G:45:MET:CE	2.90	0.60
1:G:83:ASN:ND2	3:S:858:HOH:O	2.25	0.58
1:F:51:GLU:OE1	3:S:88:HOH:O	2.17	0.56
1:D:155:GLN:HA	1:D:158:ARG:HD2	1.88	0.56
1:A:123:LYS:HD2	1:C:123:LYS:HE3	1.88	0.55
1:A:29:MET:SD	1:A:45:MET:HE1	2.47	0.55
1:G:29:MET:SD	1:G:45:MET:HE1	2.48	0.54
1:H:69:ARG:HG3	1:A:35:ALA:HB2	1.90	0.54
1:A:18:ARG:NH2	3:S:116:HOH:O	2.38	0.53
1:E:86:LYS:HE2	3:S:514:HOH:O	2.09	0.52
1:A:26:TYR:HA	1:A:45:MET:CE	2.41	0.51
1:D:159:TYR:O	1:D:162:GLN:HB2	2.11	0.51
1:H:18:ARG:NH2	3:S:8:HOH:O	2.36	0.51
1:F:10:LYS:HE2	1:F:14:ASP:OD1	2.11	0.51
1:E:75:ILE:HD11	1:G:24:TYR:CZ	2.46	0.50
1:D:38:PHE:CE2	1:D:85:ILE:HD11	2.46	0.50
1:D:135:GLN:O	3:S:730:HOH:O	2.19	0.50
1:A:15:GLN:HB2	1:A:106:ILE:HD11	1.94	0.50
1:B:15:GLN:HB2	1:B:106:ILE:HD11	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:51:GLU:OE2	1:D:132:GLU:OE2	2.30	0.50
1:D:151:SER:OG	3:S:629:HOH:O	2.20	0.50
1:A:26:TYR:HB3	1:A:45:MET:HE3	1.92	0.49
1:F:15:GLN:HB2	1:F:106:ILE:HD11	1.95	0.49
1:G:103:ILE:HD13	1:G:125:PHE:HB3	1.93	0.49
1:E:41:PHE:CD1	1:E:160:LEU:HD12	2.48	0.48
1:D:41:PHE:HE2	1:D:85:ILE:HD13	1.78	0.48
1:B:80:SER:OG	3:S:493:HOH:O	2.19	0.48
1:F:107:LEU:O	1:F:107:LEU:HD23	2.14	0.47
1:D:48:GLN:NE2	1:D:132:GLU:OE1	2.47	0.47
1:G:38:PHE:CE2	1:G:85:ILE:HD11	2.50	0.47
1:D:143:LEU:HD23	1:D:156:LEU:HD12	1.96	0.47
1:A:38:PHE:HB3	1:A:41:PHE:HD2	1.80	0.46
1:D:15:GLN:HB2	1:D:106:ILE:HD11	1.97	0.46
1:D:32:TYR:HH	1:D:84:GLY:H	1.61	0.46
1:E:41:PHE:CE1	1:E:160:LEU:HD12	2.51	0.46
1:C:103:ILE:HD13	1:C:125:PHE:HB3	1.98	0.46
1:C:10:LYS:HD2	3:S:254:HOH:O	2.16	0.46
1:G:29:MET:SD	1:G:45:MET:HE3	2.56	0.46
1:A:103:ILE:HD13	1:A:125:PHE:HB3	1.98	0.45
1:G:16:LEU:C	1:G:16:LEU:HD23	2.36	0.45
1:G:128:GLU:O	1:G:132:GLU:HG2	2.16	0.45
1:A:26:TYR:HA	1:A:45:MET:HE2	1.98	0.45
1:B:103:ILE:HD13	1:B:125:PHE:HB3	1.99	0.44
1:C:3:VAL:HG11	1:D:137:ARG:NH2	2.33	0.44
1:C:15:GLN:HB2	1:C:106:ILE:HD11	1.98	0.44
1:F:128:GLU:O	1:F:132:GLU:HG2	2.17	0.44
1:E:164:GLU:HA	1:E:164:GLU:OE1	2.18	0.44
1:F:38:PHE:HB3	1:F:41:PHE:HD2	1.83	0.44
1:D:79:PRO:HB2	1:D:82:TRP:CZ2	2.53	0.44
1:F:26:TYR:OH	1:F:96:GLU:HG2	2.18	0.43
1:F:18:ARG:NH2	3:S:167:HOH:O	2.44	0.43
1:H:1:MET:HG2	1:H:2:MET:N	2.33	0.43
1:G:155:GLN:HE21	1:G:155:GLN:HB2	1.63	0.42
1:A:97:GLU:OE1	3:S:379:HOH:O	2.21	0.42
1:E:147:ASN:HB3	1:E:148:GLY:H	1.75	0.42
1:A:106:ILE:HG22	1:A:122:LEU:HD11	2.01	0.42
1:G:38:PHE:HB3	1:G:157:ASP:OD1	2.19	0.42
1:G:66:ARG:HA	1:G:66:ARG:HD2	1.83	0.41
1:F:47:LYS:HE3	1:F:164:GLU:OXT	2.20	0.41
1:D:30:ALA:O	1:D:34:ASP:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:38:PHE:HE1	1:D:154:PHE:CE1	2.38	0.41
1:H:15:GLN:HB2	1:H:106:ILE:HD11	2.03	0.41
1:D:16:LEU:C	1:D:16:LEU:HD23	2.41	0.41
1:D:149:GLN:HG2	3:S:629:HOH:O	2.20	0.41
1:C:41:PHE:CD1	1:C:160:LEU:HD12	2.56	0.41
1:D:66:ARG:HA	1:D:66:ARG:HD2	1.90	0.41
1:G:40:GLY:HA3	1:G:157:ASP:O	2.21	0.40
1:G:159:TYR:O	1:G:162:GLN:HB2	2.21	0.40
1:A:55:HIS:HE1	1:A:132:GLU:OE1	2.05	0.40
1:E:27:LEU:O	1:E:30:ALA:HB3	2.22	0.40
1:G:38:PHE:CE1	1:G:154:PHE:CE2	3.09	0.40
1:G:152:VAL:HA	1:G:155:GLN:HE21	1.85	0.40
1:D:152:VAL:HG23	3:S:629:HOH:O	2.20	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:145:LYS:NZ	1:G:37:GLY:O[12_555]	2.11	0.09

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	161/164 (98%)	159 (99%)	2 (1%)	0	100	100
1	B	162/164 (99%)	161 (99%)	1 (1%)	0	100	100
1	C	162/164 (99%)	160 (99%)	2 (1%)	0	100	100
1	D	162/164 (99%)	157 (97%)	5 (3%)	0	100	100
1	E	162/164 (99%)	159 (98%)	3 (2%)	0	100	100
1	F	162/164 (99%)	159 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	162/164 (99%)	160 (99%)	2 (1%)	0	100	100
1	H	162/164 (99%)	159 (98%)	3 (2%)	0	100	100
All	All	1295/1312 (99%)	1274 (98%)	21 (2%)	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	143/144 (99%)	142 (99%)	1 (1%)	84	91
1	B	144/144 (100%)	143 (99%)	1 (1%)	84	91
1	C	144/144 (100%)	143 (99%)	1 (1%)	84	91
1	D	144/144 (100%)	141 (98%)	3 (2%)	53	67
1	E	144/144 (100%)	143 (99%)	1 (1%)	84	91
1	F	144/144 (100%)	143 (99%)	1 (1%)	84	91
1	G	144/144 (100%)	141 (98%)	3 (2%)	53	67
1	H	144/144 (100%)	143 (99%)	1 (1%)	84	91
All	All	1151/1152 (100%)	1139 (99%)	12 (1%)	76	86

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	9	ARG
1	A	69	ARG
1	B	1	MET
1	C	154	PHE
1	D	9	ARG
1	D	34	ASP
1	D	147	ASN
1	E	10	LYS
1	F	24	TYR

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Mol	Chain	Res	Type
1	G	1	MET
1	G	24	TYR
1	G	111	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	83	ASN
1	C	50	GLN
1	E	135	GLN
1	E	155	GLN
1	G	155	GLN

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 ⓘ

Of 16 ligands modelled in this entry, 16 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7　Other polymers　ⓘ

There are no such residues in this entry.

5.8　Polymer linkage issues　ⓘ

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	163/164 (99%)	-0.43	2 (1%)	79	77	21, 30, 43, 60	0
1	B	164/164 (100%)	-0.26	2 (1%)	79	77	23, 34, 47, 68	0
1	C	164/164 (100%)	-0.52	1 (0%)	89	88	27, 36, 53, 68	0
1	D	164/164 (100%)	-0.20	2 (1%)	79	77	26, 41, 67, 82	0
1	E	164/164 (100%)	-0.41	2 (1%)	79	77	29, 41, 64, 70	0
1	F	164/164 (100%)	-0.41	2 (1%)	79	77	25, 36, 53, 64	0
1	G	164/164 (100%)	-0.24	6 (3%)	41	39	35, 47, 67, 75	0
1	H	164/164 (100%)	-0.51	0	100	100	21, 30, 49, 65	0
All	All	1311/1312 (99%)	-0.37	17 (1%)	77	75	21, 37, 60, 82	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	159	TYR	4.2
1	G	156	LEU	4.1
1	B	1	MET	3.9
1	G	1	MET	3.3
1	D	159	TYR	3.1
1	G	164	GLU	3.0
1	G	162	GLN	2.8
1	F	164	GLU	2.7
1	E	162	GLN	2.6
1	A	164	GLU	2.6
1	D	164	GLU	2.5
1	F	159	TYR	2.5
1	E	164	GLU	2.3
1	G	154	PHE	2.2
1	A	159	TYR	2.1
1	C	164	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	162	GLN	2.1

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	FE	I	14	1/?	0.77	0.14	51,51,51,51	1
2	FE	I	15	1/?	0.78	0.09	57,57,57,57	1
2	FE	I	11	1/?	0.86	0.12	58,58,58,58	1
2	FE	I	12	1/?	0.86	0.14	53,53,53,53	1
2	FE	I	9	1/?	0.92	0.09	49,49,49,49	1
2	FE	I	16	1/?	0.94	0.12	52,52,52,52	1
2	FE	I	17	1/?	0.95	0.06	60,60,60,60	1
2	FE	I	10	1/?	0.96	0.06	52,52,52,52	1
2	FE	I	4	1/?	0.98	0.15	34,34,34,34	0
2	FE	I	1	1/?	0.99	0.13	28,28,28,28	0
2	FE	I	5	1/?	0.99	0.12	35,35,35,35	0
2	FE	I	6	1/?	0.99	0.11	40,40,40,40	0
2	FE	I	8	1/?	0.99	0.17	48,48,48,48	0
2	FE	I	2	1/?	0.99	0.14	35,35,35,35	0
2	FE	I	3	1/?	0.99	0.09	36,36,36,36	0
2	FE	I	7	1/?	1.00	0.07	38,38,38,38	0

6.5   Other polymers ⓘ

There are no such residues in this entry.