



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 22, 2021 – 12:23 PM EDT

PDB ID : 3DGG
Title : Crystal structure of FabOX108
Authors : Ren, J.; Nettleship, J.E.; Owens, R.J.; Oxford Protein Production Facility (OPPF)
Deposited on : 2008-06-13
Resolution : 2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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 ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.17.1
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) : 2.17.1

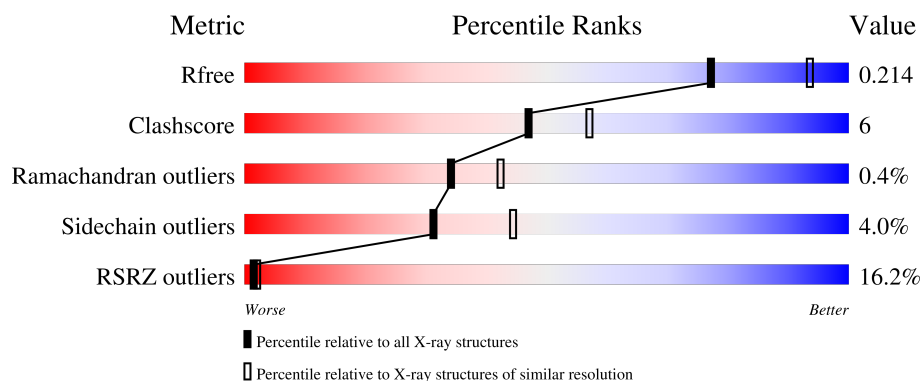
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 $\leq 5\%$. 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	217	<div> <div>11%</div> <div>84%</div> <div>15%</div> <div>.</div> </div>
1	C	217	<div> <div>19%</div> <div>83%</div> <div>14%</div> <div>..</div> </div>
2	B	229	<div> <div>17%</div> <div>83%</div> <div>8%</div> <div>.</div> <div>7%</div> </div>
2	D	229	<div> <div>16%</div> <div>83%</div> <div>10%</div> <div>6%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6976 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 called FabOX108 Light Chain Fragment.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	217	Total	C	N	O	S	0	0	0
			1675	1043	285	340	7			
1	C	215	Total	C	N	O	S	0	0	0
			1660	1035	283	336	6			

- Molecule 2 is a protein called FabOX108 Heavy Chain Fragment.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	212	Total	C	N	O	S	0	0	0
			1625	1034	260	323	8			
2	D	215	Total	C	N	O	S	0	0	0
			1643	1043	263	329	8			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	224	HIS	-	expression tag	PDB 3DGG
B	225	HIS	-	expression tag	PDB 3DGG
B	226	HIS	-	expression tag	PDB 3DGG
B	227	HIS	-	expression tag	PDB 3DGG
B	228	HIS	-	expression tag	PDB 3DGG
B	229	HIS	-	expression tag	PDB 3DGG
D	224	HIS	-	expression tag	PDB 3DGG
D	225	HIS	-	expression tag	PDB 3DGG
D	226	HIS	-	expression tag	PDB 3DGG
D	227	HIS	-	expression tag	PDB 3DGG
D	228	HIS	-	expression tag	PDB 3DGG
D	229	HIS	-	expression tag	PDB 3DGG

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total 3	Mg 3	0	0
3	C	2	Total 2	Mg 2	0	0
3	D	1	Total 1	Mg 1	0	0

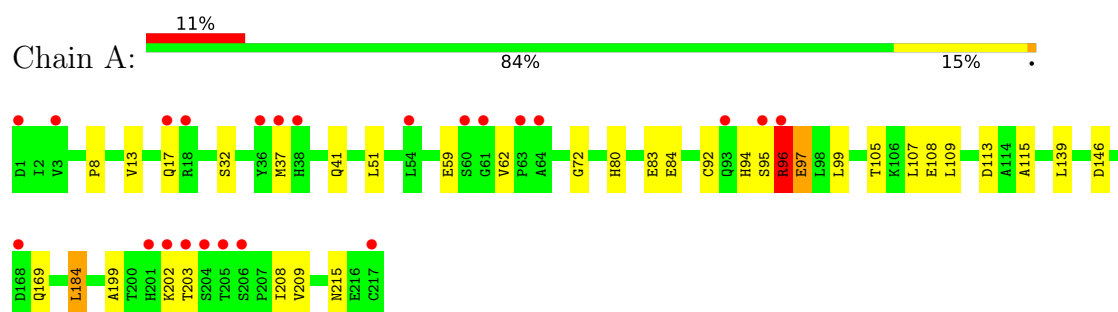
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	105	Total 105	O 105	0	0
4	B	83	Total 83	O 83	0	0
4	C	83	Total 83	O 83	0	0
4	D	96	Total 96	O 96	0	0

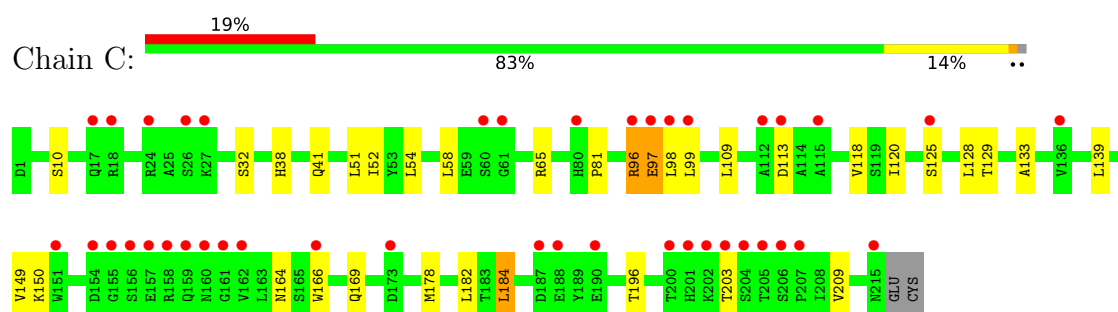
3 Residue-property plots [i](#)

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.

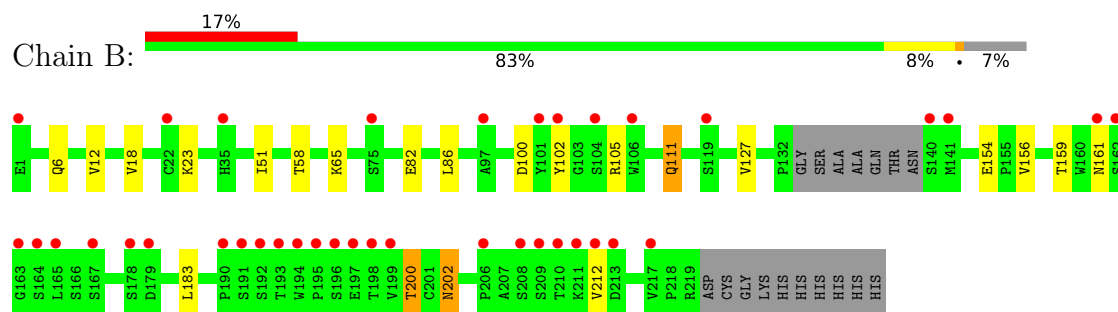
• Molecule 1: FabOX108 Light Chain Fragment



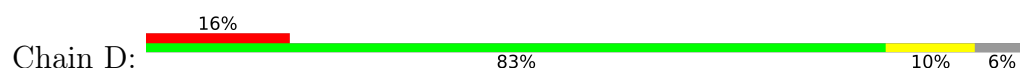
• Molecule 1: FabOX108 Light Chain Fragment

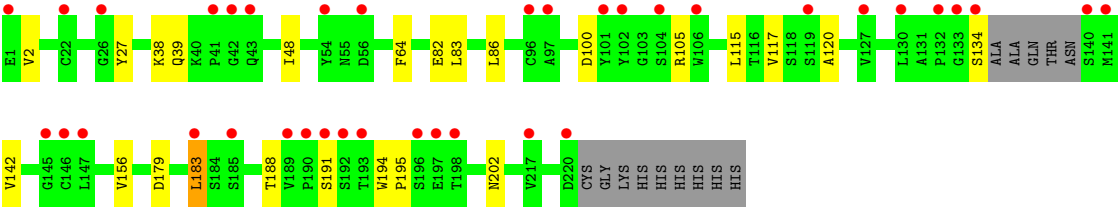


• Molecule 2: FabOX108 Heavy Chain Fragment



• Molecule 2: FabOX108 Heavy Chain Fragment





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	78.22Å 52.14Å 112.12Å 90.00° 103.14° 90.00°	Depositor
Resolution (Å)	30.00 – 2.30 29.73 – 2.27	Depositor EDS
% Data completeness (in resolution range)	98.6 (30.00-2.30) 96.9 (29.73-2.27)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 2.26Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.187 , 0.246 0.228 , 0.214	Depositor DCC
R_{free} test set	2004 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	34.3	Xtriage
Anisotropy	0.315	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 50.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6976	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.56% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: MG

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	0.38	0/1713	0.55	0/2327
1	C	0.37	0/1698	0.54	0/2307
2	B	0.35	0/1671	0.52	0/2282
2	D	0.39	0/1689	0.51	0/2306
All	All	0.37	0/6771	0.53	0/9222

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 [i](#)

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	1675	0	1611	25	0
1	C	1660	0	1600	18	0
2	B	1625	0	1577	22	0
2	D	1643	0	1589	19	0
3	A	3	0	0	0	0
3	C	2	0	0	0	0
3	D	1	0	0	0	0
4	A	105	0	0	0	0
4	B	83	0	0	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	83	0	0	0	0
4	D	96	0	0	3	0
All	All	6976	0	6377	81	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 (81) 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)
2:B:12:VAL:HG11	2:B:18:VAL:CG1	1.86	1.06
1:C:65:ARG:HD2	1:C:81:PRO:O	1.79	0.81
1:A:84:GLU:HA	1:A:109:LEU:CD2	2.12	0.79
2:B:12:VAL:HG11	2:B:18:VAL:HG12	1.67	0.77
1:A:84:GLU:HA	1:A:109:LEU:HD21	1.71	0.73
2:B:12:VAL:HG11	2:B:18:VAL:HG11	1.71	0.72
1:C:120:ILE:HG22	2:D:134:SER:HB3	1.73	0.71
1:C:118:VAL:HG22	1:C:139:LEU:HD22	1.73	0.69
1:C:41:GLN:HB2	1:C:51:LEU:HD11	1.73	0.68
1:A:109:LEU:H	1:A:169:GLN:HE22	1.43	0.67
2:B:12:VAL:HG21	2:B:86:LEU:HD13	1.78	0.66
2:B:100:ASP:OD2	4:B:249:HOH:O	2.12	0.66
2:D:100:ASP:OD2	4:D:508:HOH:O	2.14	0.66
2:D:48:ILE:HD12	2:D:64:PHE:CE2	2.31	0.65
1:C:109:LEU:H	1:C:169:GLN:HE22	1.43	0.64
1:C:133:ALA:O	1:C:184:LEU:HD23	1.96	0.64
1:A:184:LEU:HD23	1:A:184:LEU:N	2.16	0.60
2:B:159:THR:HG23	2:B:202:ASN:ND2	2.16	0.60
1:A:107:LEU:C	1:A:107:LEU:HD23	2.22	0.60
2:B:6:GLN:H	2:B:111:GLN:HE22	1.51	0.59
1:C:113:ASP:HB3	1:C:203:THR:HG22	1.87	0.56
1:A:139:LEU:HD23	1:A:199:ALA:HB2	1.86	0.56
1:A:37:MET:HE1	1:A:92:CYS:HB2	1.89	0.54
1:A:84:GLU:HA	1:A:109:LEU:HD22	1.89	0.54
1:C:118:VAL:HG22	1:C:139:LEU:CD2	2.36	0.54
1:C:164:ASN:HB3	1:C:178:MET:HE2	1.90	0.54
2:D:39:GLN:NE2	4:D:503:HOH:O	2.41	0.54
2:D:115:LEU:HD22	2:D:117:VAL:HG23	1.88	0.54
1:A:32:SER:HB2	1:C:99:LEU:HD11	1.89	0.54
1:A:37:MET:CE	1:A:92:CYS:HB2	2.38	0.53
1:A:115:ALA:HB1	1:A:208:ILE:HD11	1.88	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:159:THR:HG23	2:B:202:ASN:HD22	1.73	0.53
2:B:154:GLU:OE2	4:B:237:HOH:O	2.18	0.53
1:A:8:PRO:O	1:A:105:THR:HG23	2.09	0.53
1:A:96:ARG:HG2	1:A:97:GLU:HG2	1.90	0.53
1:C:52:ILE:HD13	1:C:58:LEU:HD23	1.91	0.52
1:A:41:GLN:HB2	1:A:51:LEU:HD11	1.90	0.52
1:A:95:SER:HB3	1:A:99:LEU:HD12	1.91	0.52
2:B:111:GLN:NE2	2:B:111:GLN:H	2.08	0.52
2:D:183:LEU:C	2:D:183:LEU:HD12	2.30	0.51
1:A:139:LEU:CD2	1:A:199:ALA:HB2	2.40	0.51
2:B:159:THR:HG22	2:B:202:ASN:HB2	1.93	0.51
1:C:125:SER:O	1:C:129:THR:HG23	2.11	0.51
1:A:95:SER:O	1:A:97:GLU:N	2.44	0.50
2:B:127:VAL:HG21	2:B:212:VAL:HG21	1.94	0.49
2:D:115:LEU:CD2	2:D:117:VAL:HG23	2.42	0.49
2:B:111:GLN:H	2:B:111:GLN:HE21	1.60	0.49
2:D:120:ALA:HB2	2:D:179:ASP:HB3	1.96	0.48
2:B:51:ILE:HD12	2:B:58:THR:CG2	2.43	0.48
2:D:38:LYS:HB2	2:D:48:ILE:HD11	1.95	0.48
2:B:12:VAL:CG1	2:B:18:VAL:HG11	2.41	0.48
2:D:100:ASP:HB3	4:D:525:HOH:O	2.14	0.47
2:B:127:VAL:HG21	2:B:212:VAL:CG2	2.45	0.46
1:A:59:GLU:O	1:A:62:VAL:HG22	2.15	0.46
2:B:51:ILE:HD12	2:B:58:THR:HG23	1.98	0.46
2:D:188:THR:HG23	2:D:188:THR:O	2.16	0.46
1:A:94:HIS:CE1	1:A:96:ARG:HB3	2.51	0.45
1:C:96:ARG:O	1:C:98:LEU:N	2.49	0.45
1:C:38:HIS:HD2	1:C:54:LEU:H	1.63	0.45
1:C:139:LEU:HD11	1:C:149:VAL:HG22	1.99	0.45
1:C:166:TRP:CH2	1:C:178:MET:HE3	2.51	0.45
2:B:18:VAL:HG22	2:B:86:LEU:HD11	1.99	0.45
2:D:100:ASP:HB2	2:D:105:ARG:HG2	2.00	0.43
2:D:142:VAL:HG23	2:D:191:SER:HA	2.00	0.43
2:D:194:TRP:CG	2:D:195:PRO:HA	2.54	0.43
1:C:120:ILE:HG22	2:D:134:SER:CB	2.46	0.42
2:D:2:VAL:HG13	2:D:27:TYR:CD1	2.54	0.42
2:B:12:VAL:HG21	2:B:86:LEU:CD1	2.48	0.42
2:D:48:ILE:HD12	2:D:64:PHE:CD2	2.54	0.42
1:A:113:ASP:HB3	1:A:203:THR:HG22	2.02	0.42
1:C:196:THR:CG2	1:C:209:VAL:HG23	2.50	0.42
2:B:100:ASP:HB2	2:B:105:ARG:HG2	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:VAL:HG12	1:A:17:GLN:NE2	2.35	0.41
2:B:159:THR:CG2	2:B:202:ASN:HB2	2.50	0.41
2:D:38:LYS:CB	2:D:48:ILE:HD11	2.50	0.41
1:A:96:ARG:CG	1:A:97:GLU:HG2	2.51	0.41
1:A:96:ARG:HG3	1:A:97:GLU:N	2.35	0.41
1:A:107:LEU:HD23	1:A:108:GLU:N	2.35	0.41
2:D:83:LEU:HB3	2:D:86:LEU:HD21	2.02	0.41
2:B:161:ASN:HD22	2:B:200:THR:HG23	1.86	0.40
1:A:94:HIS:NE2	1:A:96:ARG:HB3	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	215/217 (99%)	203 (94%)	10 (5%)	2 (1%)	17	20
1	C	213/217 (98%)	205 (96%)	7 (3%)	1 (0%)	29	35
2	B	208/229 (91%)	203 (98%)	5 (2%)	0	100	100
2	D	211/229 (92%)	207 (98%)	4 (2%)	0	100	100
All	All	847/892 (95%)	818 (97%)	26 (3%)	3 (0%)	34	42

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	96	ARG
1	C	97	GLU
1	A	72	GLY

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	190/190 (100%)	181 (95%)	9 (5%)	26	37
1	C	188/190 (99%)	180 (96%)	8 (4%)	29	40
2	B	186/199 (94%)	177 (95%)	9 (5%)	25	36
2	D	188/199 (94%)	184 (98%)	4 (2%)	53	70
All	All	752/778 (97%)	722 (96%)	30 (4%)	31	44

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	80	HIS
1	A	83	GLU
1	A	96	ARG
1	A	97	GLU
1	A	146	ASP
1	A	184	LEU
1	A	202	LYS
1	A	209	VAL
1	A	215	ASN
2	B	23	LYS
2	B	65	LYS
2	B	82	GLU
2	B	102	TYR
2	B	111	GLN
2	B	156	VAL
2	B	183	LEU
2	B	200	THR
2	B	202	ASN
1	C	10	SER
1	C	32	SER
1	C	96	ARG
1	C	97	GLU
1	C	128	LEU
1	C	150	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	182	LEU
1	C	184	LEU
2	D	82	GLU
2	D	156	VAL
2	D	183	LEU
2	D	202	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	GLN
1	A	38	HIS
1	A	41	GLN
1	A	42	GLN
1	A	160	ASN
1	A	169	GLN
1	A	193	ASN
1	A	215	ASN
2	B	39	GLN
2	B	111	GLN
2	B	161	ASN
2	B	202	ASN
1	C	38	HIS
1	C	41	GLN
1	C	42	GLN
1	C	46	GLN
1	C	93	GLN
1	C	164	ASN
1	C	169	GLN
2	D	39	GLN
2	D	59	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 [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 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 [i](#)

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	217/217 (100%)	0.86	23 (10%) 6 8	37, 51, 73, 90	0
1	C	215/217 (99%)	1.15	41 (19%) 1 1	40, 52, 70, 79	0
2	B	212/229 (92%)	1.10	38 (17%) 1 1	36, 52, 66, 74	2 (0%)
2	D	215/229 (93%)	0.98	37 (17%) 1 1	37, 52, 67, 85	2 (0%)
All	All	859/892 (96%)	1.02	139 (16%) 1 2	36, 52, 69, 90	4 (0%)

All (139) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	203	THR	8.2
1	A	203	THR	7.8
2	B	196	SER	6.1
2	B	193	THR	6.1
1	A	206	SER	6.1
1	A	205	THR	6.0
2	D	22	CYS	6.0
2	B	198	THR	5.7
1	C	204	SER	5.7
1	C	160	ASN	5.5
2	B	195	PRO	5.5
2	B	22	CYS	5.5
1	A	217	CYS	5.3
2	D	140	SER	5.3
2	B	192	SER	5.2
1	C	206	SER	5.2
2	B	162	SER	5.0
1	C	215	ASN	5.0
2	B	165	LEU	5.0
1	C	161	GLY	5.0
2	B	197	GLU	4.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	192	SER	4.9
1	C	187	ASP	4.7
2	D	197	GLU	4.7
2	B	194	TRP	4.6
2	B	217	VAL	4.6
2	B	164	SER	4.5
2	B	212	VAL	4.5
2	B	211	LYS	4.4
1	C	98	LEU	4.4
1	A	3	VAL	4.2
2	D	220	ASP	4.1
2	D	193	THR	4.1
1	C	158	ARG	4.0
1	C	155	GLY	4.0
2	B	167	SER	3.9
2	D	141	MET	3.9
2	B	141	MET	3.8
2	B	209	SER	3.8
1	C	205	THR	3.8
1	C	159	GLN	3.7
2	D	196	SER	3.6
1	C	80	HIS	3.6
2	D	42	GLY	3.6
2	B	140	SER	3.6
2	D	54	TYR	3.5
2	B	208	SER	3.5
2	D	190	PRO	3.4
1	A	201	HIS	3.4
2	D	56	ASP	3.4
2	B	1	GLU	3.3
2	D	1	GLU	3.3
2	B	119	SER	3.3
2	D	102	TYR	3.3
2	B	213	ASP	3.3
1	C	99	LEU	3.3
1	C	60	SER	3.3
1	A	64	ALA	3.2
1	A	36	TYR	3.2
1	C	190	GLU	3.2
1	C	115	ALA	3.1
2	B	190	PRO	3.1
1	A	60	SER	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	95	SER	3.1
2	B	161	ASN	3.1
2	B	104	SER	3.0
2	D	96	CYS	3.0
1	A	63	PRO	3.0
1	C	157	GLU	2.9
1	C	207	PRO	2.9
2	B	206	PRO	2.9
2	B	102	TYR	2.9
1	A	1	ASP	2.9
1	C	200	THR	2.8
2	D	147	LEU	2.8
1	A	54	LEU	2.8
2	B	210	THR	2.8
1	C	61	GLY	2.7
1	C	24	ARG	2.7
2	D	133	GLY	2.7
2	D	217	VAL	2.7
1	C	202	LYS	2.7
1	A	61	GLY	2.7
2	D	198	THR	2.7
2	B	191	SER	2.7
2	D	104	SER	2.6
2	D	43	GLN	2.6
1	C	151	TRP	2.6
2	D	130	LEU	2.5
2	D	146	CYS	2.5
2	D	26	GLY	2.5
1	C	136	VAL	2.5
1	C	112	ALA	2.5
1	C	18	ARG	2.5
1	C	96	ARG	2.5
1	C	188	GLU	2.5
1	A	204	SER	2.5
1	C	154	ASP	2.5
2	D	119	SER	2.4
2	D	191	SER	2.4
2	D	41	PRO	2.4
2	B	97	ALA	2.4
2	B	75	SER	2.4
2	D	189	VAL	2.4
1	C	27	LYS	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	113	ASP	2.4
2	D	183	LEU	2.4
2	B	179	ASP	2.3
2	B	106	TRP	2.3
2	D	101	TYR	2.3
1	A	37	MET	2.3
2	D	134	SER	2.3
1	A	93	GLN	2.3
2	D	185	SER	2.3
2	D	106	TRP	2.3
2	D	127	VAL	2.3
2	D	132	PRO	2.3
1	A	202	LYS	2.3
2	B	163	GLY	2.3
2	B	199	VAL	2.2
1	A	168	ASP	2.2
1	C	156	SER	2.2
1	A	17	GLN	2.2
2	B	35	HIS	2.2
2	D	97	ALA	2.2
1	A	96	ARG	2.2
1	C	125	SER	2.2
1	C	17	GLN	2.1
1	A	38	HIS	2.1
2	B	101	TYR	2.1
1	C	173	ASP	2.1
1	C	26	SER	2.1
1	C	166	TRP	2.1
2	D	145	GLY	2.1
1	C	201	HIS	2.0
2	B	178	SER	2.0
1	C	162	VAL	2.0
1	C	97	GLU	2.0
1	A	18	ARG	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 [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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(\AA^2)	Q<0.9
3	MG	D	456	1/1	0.80	0.33	72,72,72,72	0
3	MG	C	451	1/1	0.84	0.32	64,64,64,64	0
3	MG	A	455	1/1	0.89	0.41	80,80,80,80	0
3	MG	C	453	1/1	0.91	0.25	69,69,69,69	0
3	MG	A	452	1/1	0.94	0.28	63,63,63,63	0
3	MG	A	454	1/1	0.95	0.43	43,43,43,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.