Full wwPDB X-ray Structure Validation Report (i)

Sep 24, 2024 – 02:11 PM JST

PDB ID	:	4ZTT
Title	:	Crystal structures of ferritin mutants reveal diferric-peroxo intermediates
Authors	:	Kim, S.; Park, Y.H.; Jung, S.W.; Seok, J.H.; Chung, Y.B.; Lee, D.B.; Gowda, G.; Lee, J.H.; Han, H.R.; Cho, A.E.; Lee, C.; Chung, M.S.; Kim, K.H.
Deposited on	:	2015-05-15
Resolution	:	1.83 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

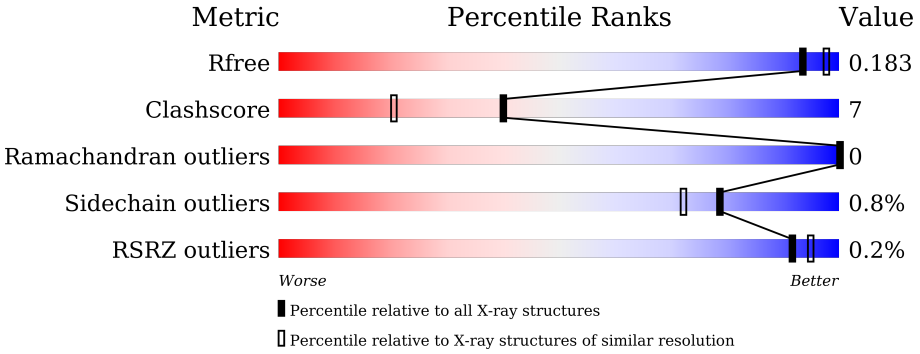
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.002 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.38.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.83 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}	164625	1150 (1.84-1.84)
Clashscore	180529	1248 (1.84-1.84)
Ramachandran outliers	177936	1240 (1.84-1.84)
Sidechain outliers	177891	1240 (1.84-1.84)
RSRZ outliers	164620	1149 (1.84-1.84)

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	166	82% 16% •
1	B	166	82% 16% ••
1	C	166	86% 11% •
1	D	166	83% 13% ••
1	E	166	% 83% 15% ••
2	F	166	% 90% 8% ••

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	FEO	E	201	-	-	X	-
5	GOL	A	204	-	-	X	-
5	GOL	C	205	-	-	X	-
5	GOL	C	208	-	-	X	-
5	GOL	E	204	-	X	-	-

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 9581 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 ferritin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	162	1426	906	228	281	11	0	11	0
1	B	164	1417	899	230	279	9	0	7	0
1	C	162	1414	898	229	278	9	0	9	0
1	D	162	1461	928	236	286	11	0	14	0
1	E	163	1454	925	234	285	10	0	13	0

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	HIS	-	expression tag	UNP C3T582
A	1	HIS	-	expression tag	UNP C3T582
A	20	ALA	SER	engineered mutation	UNP C3T582
B	0	HIS	-	expression tag	UNP C3T582
B	1	HIS	-	expression tag	UNP C3T582
B	20	ALA	SER	engineered mutation	UNP C3T582
C	0	HIS	-	expression tag	UNP C3T582
C	1	HIS	-	expression tag	UNP C3T582
C	20	ALA	SER	engineered mutation	UNP C3T582
D	0	HIS	-	expression tag	UNP C3T582
D	1	HIS	-	expression tag	UNP C3T582
D	20	ALA	SER	engineered mutation	UNP C3T582
E	0	HIS	-	expression tag	UNP C3T582
E	1	HIS	-	expression tag	UNP C3T582
E	20	ALA	SER	engineered mutation	UNP C3T582

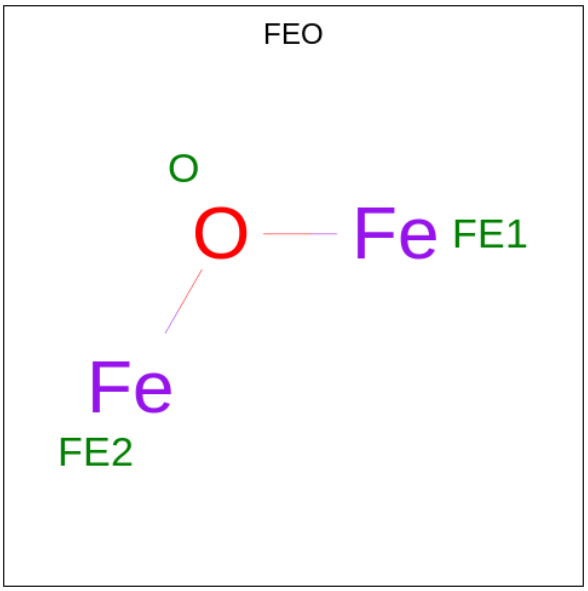
- Molecule 2 is a protein called ferritin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	F	164	1412	897	228	277	10	0	6	0

There are 3 discrepancies between the modelled and reference sequences:

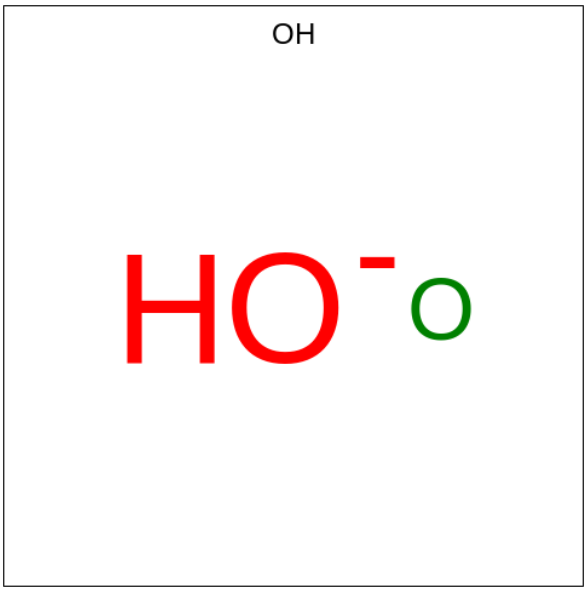
Chain	Residue	Modelled	Actual	Comment	Reference
F	0	HIS	-	expression tag	UNP C3T582
F	1	HIS	-	expression tag	UNP C3T582
F	20	ALA	SER	engineered mutation	UNP C3T582

- Molecule 3 is MU-OXO-DIIRON (three-letter code: FEO) (formula: Fe_2O).



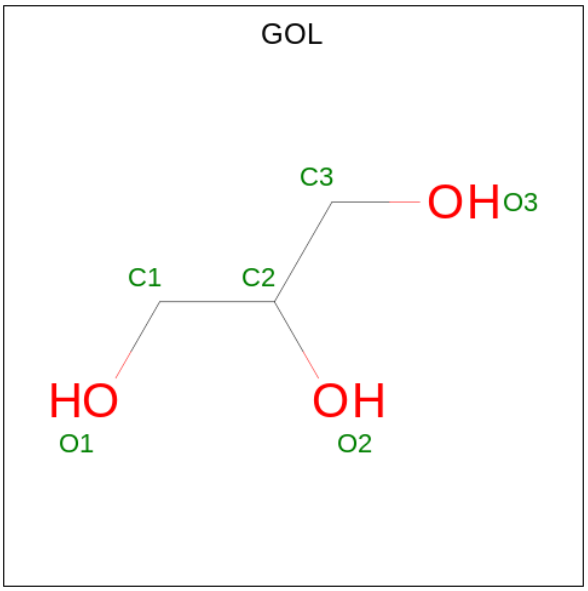
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	O		
3	A	1	3	2	1	0	0
3	B	1	3	2	1	0	0
3	E	1	3	2	1	0	0

- Molecule 4 is HYDROXIDE ION (three-letter code: OH) (formula: HO).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O 1 1	0	0
4	A	1	Total O 1 1	0	0
4	B	1	Total O 1 1	0	0
4	B	1	Total O 1 1	0	0
4	C	1	Total O 1 1	0	0
4	D	1	Total O 1 1	0	0
4	E	1	Total O 1 1	0	0
4	F	1	Total O 1 1	0	0
4	F	1	Total O 1 1	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	A	1	6	3	3	0	0
			Total	C	O		
5	A	1	6	3	3	0	0
			Total	C	O		
5	B	1	6	3	3	0	0
			Total	C	O		
5	B	1	6	3	3	0	0
			Total	C	O		
5	C	1	6	3	3	0	0
			Total	C	O		
5	C	1	6	3	3	0	0
			Total	C	O		
5	C	1	6	3	3	0	0
			Total	C	O		
5	C	1	6	3	3	0	0
			Total	C	O		
5	C	1	6	3	3	0	0
			Total	C	O		
5	D	1	6	3	3	0	0
			Total	C	O		
5	D	1	6	3	3	0	0
			Total	C	O		
5	E	1	6	3	3	0	0
			Total	C	O		
5	E	1	6	3	3	0	0
			Total	C	O		
5	F	1	6	3	3	0	0

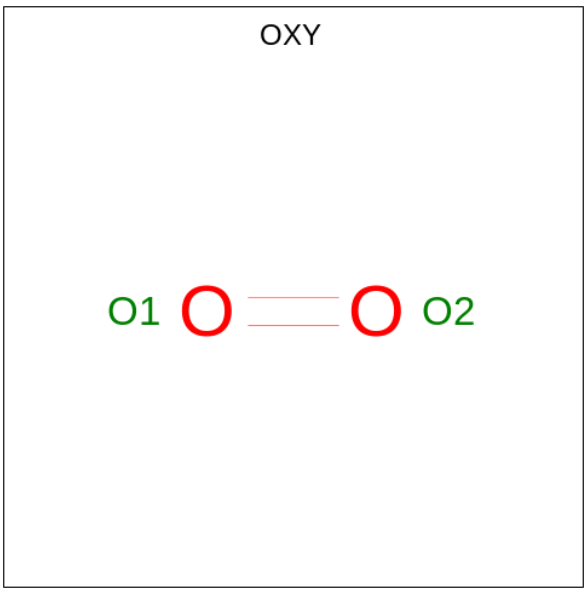
- Molecule 6 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Fe		
6	C	1	1	1	0	0
6	D	2	2	2	0	0
6	F	2	2	2	0	0

- Molecule 7 is FE (II) ION (three-letter code: FE2) (formula: Fe).

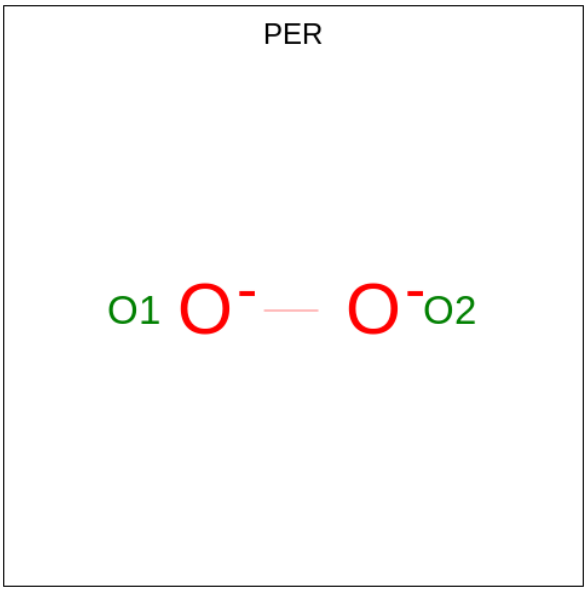
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Fe		
7	C	1	1	1	0	0
7	E	1	1	1	0	0

- Molecule 8 is OXYGEN MOLECULE (three-letter code: OXY) (formula: O_2).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	C	1	2	2	0	0

- Molecule 9 is PEROXIDE ION (three-letter code: PER) (formula: O_2).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	D	1	Total O 2 2	0	0

- Molecule 10 is OXYGEN ATOM (three-letter code: O) (formula: O).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	F	1	Total O 1 1	0	0

- Molecule 11 is water.

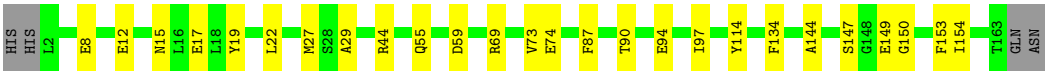
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	151	Total O 151 151	0	0
11	B	153	Total O 153 153	0	0
11	C	140	Total O 140 140	0	0
11	D	141	Total O 141 141	0	0
11	E	153	Total O 153 153	0	0
11	F	145	Total O 145 145	0	0

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.

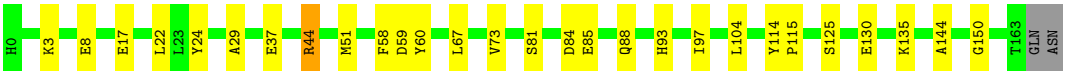
• Molecule 1: ferritin

Chain A:



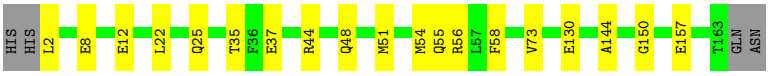
• Molecule 1: ferritin

Chain B:



• Molecule 1: ferritin

Chain C:



• Molecule 1: ferritin

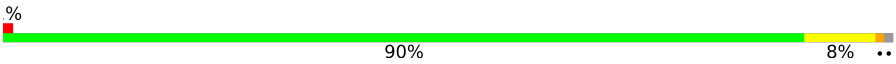
Chain D:

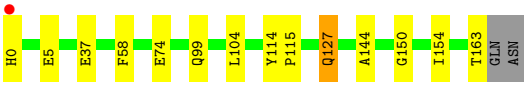
• Molecule 1: ferritin

Chain E:

• Molecule 2: ferritin

Chain F:




HO
E5
E37
F58
E74
Q99
L104
Y114
P115
Q127
A144
G150
I154
T163
GLN
ASN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α, β, γ	128.82Å 128.82Å 172.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.66 – 1.83 19.66 – 1.83	Depositor EDS
% Data completeness (in resolution range)	98.9 (19.66-1.83) 98.8 (19.66-1.83)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.22 (at 1.84Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.156 , 0.192 0.154 , 0.183	Depositor DCC
R_{free} test set	5691 reflections (4.71%)	wwPDB-VP
Wilson B-factor (Å^2)	27.3	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.43 , 57.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.020 for -h,k,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	9581	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% of the height of the origin peak. No significant pseudotranslation is detected.*

[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, A1L4B, FE2, OXY, OH, PER, GOL, FEO, O

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	1.22	1/1457 (0.1%)	1.10	4/1965 (0.2%)
1	B	1.23	5/1450 (0.3%)	1.05	4/1957 (0.2%)
1	C	1.21	3/1445 (0.2%)	1.00	1/1949 (0.1%)
1	D	1.21	5/1492 (0.3%)	1.12	12/2010 (0.6%)
1	E	1.22	3/1486 (0.2%)	1.14	7/2004 (0.3%)
2	F	1.18	1/1434 (0.1%)	1.04	0/1933
All	All	1.21	18/8764 (0.2%)	1.08	28/11818 (0.2%)

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	125	SER	CB-OG	-8.70	1.30	1.42
1	B	125	SER	CB-OG	-8.35	1.31	1.42
1	E	49	GLU	CD-OE2	6.77	1.33	1.25
1	E	94	GLU	CD-OE1	6.38	1.32	1.25
1	D	130	GLU	CD-OE1	6.29	1.32	1.25
1	B	130	GLU	CD-OE1	6.28	1.32	1.25
1	E	125	SER	CB-OG	-5.88	1.34	1.42
1	C	130	GLU	CD-OE1	5.85	1.32	1.25
1	D	96	LEU	C-O	5.49	1.33	1.23
1	B	81	SER	CB-OG	5.45	1.49	1.42
1	A	114	TYR	CB-CG	-5.43	1.43	1.51
2	F	5	GLU	CD-OE2	-5.23	1.20	1.25
1	D	12[A]	GLU	CD-OE1	5.21	1.31	1.25
1	D	12[B]	GLU	CD-OE1	5.21	1.31	1.25
1	C	157	GLU	CD-OE2	-5.18	1.20	1.25
1	B	17	GLU	CD-OE2	5.02	1.31	1.25
1	B	24	TYR	CZ-OH	5.01	1.46	1.37
1	C	8	GLU	CG-CD	5.00	1.59	1.51

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	44	ARG	NE-CZ-NH2	12.58	126.59	120.30
1	A	44	ARG	NE-CZ-NH2	10.35	125.47	120.30
1	D	44	ARG	NE-CZ-NH2	10.21	125.40	120.30
1	A	69	ARG	NE-CZ-NH2	8.44	124.52	120.30
1	D	59	ASP	CB-CG-OD2	-7.86	111.23	118.30
1	D	12[A]	GLU	CG-CD-OE2	-7.74	102.82	118.30
1	D	12[B]	GLU	CG-CD-OE2	-7.74	102.82	118.30
1	A	17	GLU	OE1-CD-OE2	-7.11	114.77	123.30
1	E	69[A]	ARG	NE-CZ-NH2	7.03	123.81	120.30
1	E	69[B]	ARG	NE-CZ-NH2	7.03	123.81	120.30
1	D	12[A]	GLU	CG-CD-OE1	6.54	131.37	118.30
1	D	12[B]	GLU	CG-CD-OE1	6.54	131.37	118.30
1	D	44	ARG	NE-CZ-NH1	-6.53	117.03	120.30
1	D	56	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	D	45	ARG	NE-CZ-NH2	6.50	123.55	120.30
1	B	44	ARG	NE-CZ-NH2	6.42	123.51	120.30
1	D	59	ASP	CB-CG-OD1	6.01	123.71	118.30
1	E	44	ARG	NE-CZ-NH1	-5.87	117.37	120.30
1	A	44	ARG	NE-CZ-NH1	-5.87	117.37	120.30
1	D	44	ARG	CA-CB-CG	5.74	126.02	113.40
1	E	59	ASP	CB-CG-OD1	5.50	123.25	118.30
1	C	56	ARG	NE-CZ-NH2	5.31	122.95	120.30
1	E	23	LEU	CB-CG-CD1	5.23	119.90	111.00
1	D	63	ASP	CB-CG-OD1	5.23	123.01	118.30
1	E	125	SER	N-CA-CB	5.17	118.26	110.50
1	B	17	GLU	OE1-CD-OE2	-5.11	117.17	123.30
1	B	60	TYR	CD1-CE1-CZ	-5.05	115.26	119.80
1	B	59	ASP	CB-CG-OD2	-5.02	113.78	118.30

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	1426	0	1355	29	0
1	B	1417	0	1339	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1414	0	1346	15	0
1	D	1461	0	1390	21	0
1	E	1454	0	1379	20	0
2	F	1412	0	1329	11	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
3	E	3	0	0	2	0
4	A	2	0	0	1	0
4	B	2	0	0	1	0
4	C	1	0	0	0	0
4	D	1	0	0	1	0
4	E	1	0	0	0	0
4	F	2	0	0	0	0
5	A	12	0	16	11	0
5	B	12	0	15	0	0
5	C	30	0	39	9	0
5	D	12	0	16	2	0
5	E	12	0	15	2	0
5	F	6	0	8	0	0
6	C	1	0	0	0	0
6	D	2	0	0	0	0
6	F	2	0	0	0	0
7	C	1	0	0	0	0
7	E	1	0	0	0	0
8	C	2	0	0	0	0
9	D	2	0	0	0	0
10	F	1	0	0	1	0
11	A	151	0	0	8	0
11	B	153	0	0	9	1
11	C	140	0	0	3	1
11	D	141	0	0	4	0
11	E	153	0	0	15	0
11	F	145	0	0	5	2
All	All	9581	0	8247	111	2

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 7.

All (111) 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:F:127:A1L4B:O2	10:F:203:O:O	1.63	1.16
1:E:37:GLU:OE1	11:E:302:HOH:O	1.69	1.11
5:C:205:GOL:H32	1:D:51:MET:HE1	1.20	1.11
3:E:201:FEO:FE2	11:E:303:HOH:O	1.06	1.07
1:C:37:GLU:OE1	11:C:302:HOH:O	1.73	1.05
1:E:130:GLU:OE2	11:E:303:HOH:O	1.75	1.04
3:E:201:FEO:O	11:E:303:HOH:O	1.76	1.02
5:C:205:GOL:H32	1:D:51:MET:CE	1.91	0.99
1:B:44:ARG:HD3	11:B:346:HOH:O	1.63	0.98
4:D:204:OH:O	11:D:301:HOH:O	1.84	0.96
1:E:53:HIS:CB	11:E:301:HOH:O	2.25	0.82
2:F:37:GLU:OE1	11:F:302:HOH:O	1.99	0.80
1:B:8:GLU:OE1	11:B:302:HOH:O	2.00	0.80
1:A:15:ASN:O	5:A:204:GOL:H11	1.82	0.79
1:A:97:ILE:HD13	4:A:203:OH:O	1.81	0.79
1:E:50:GLU:OE2	11:E:303:HOH:O	1.98	0.79
1:A:73:VAL:HA	5:A:204:GOL:H31	1.66	0.77
1:A:94:GLU:OE1	11:A:301:HOH:O	2.01	0.77
1:A:147:SER:OG	1:A:149[B]:GLU:OE1	2.03	0.76
1:E:84[B]:ASP:OD1	11:E:304:HOH:O	2.04	0.75
1:C:12:GLU:OE2	11:C:303:HOH:O	2.05	0.74
1:E:53:HIS:CG	11:E:301:HOH:O	2.36	0.73
5:C:208:GOL:O2	11:C:304:HOH:O	2.07	0.73
5:C:205:GOL:C3	1:D:51:MET:CE	2.66	0.73
1:A:8:GLU:OE1	11:A:302:HOH:O	2.08	0.72
1:B:37:GLU:OE1	11:B:303:HOH:O	2.08	0.71
1:D:156:LYS:HE3	11:D:315:HOH:O	1.90	0.69
1:A:147:SER:OG	1:A:149[B]:GLU:CD	2.32	0.68
1:C:25:GLN:HE22	1:D:55[B]:GLN:HE22	1.42	0.68
5:A:204:GOL:H2	11:A:305:HOH:O	1.95	0.66
1:E:139:ASP:OD2	11:E:305:HOH:O	2.14	0.66
5:A:204:GOL:C2	11:A:305:HOH:O	2.42	0.66
1:B:93:HIS:NE2	11:B:305:HOH:O	2.18	0.65
1:E:69[A]:ARG:NH1	5:E:204:GOL:O3	2.28	0.65
1:A:147:SER:HG	1:A:149[B]:GLU:CD	2.00	0.64
1:C:44:ARG:NE	5:C:208:GOL:O3	2.26	0.64
1:E:8:GLU:OE1	11:E:306:HOH:O	2.14	0.63
1:C:44:ARG:HE	5:C:208:GOL:HO3	1.46	0.63
2:F:163:THR:C	11:F:337:HOH:O	2.36	0.63
5:A:204:GOL:H12	11:A:309:HOH:O	1.99	0.62
1:C:55[A]:GLN:OE1	1:D:44:ARG:HD2	2.01	0.60
1:E:144:ALA:O	1:E:150:GLY:HA3	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149[B]:GLU:HG3	1:D:149:GLU:OE1	2.01	0.60
1:B:51:MET:HE2	11:E:399:HOH:O	2.01	0.60
1:B:84[A]:ASP:OD2	11:B:304:HOH:O	2.16	0.59
1:C:51:MET:O	1:C:55[B]:GLN:HG3	2.04	0.58
1:A:149[B]:GLU:CG	1:D:149:GLU:OE1	2.52	0.58
1:A:147:SER:CB	1:A:149[B]:GLU:OE1	2.51	0.57
1:A:144:ALA:HB3	1:A:154:ILE:HD11	1.85	0.57
1:C:144:ALA:O	1:C:150:GLY:HA3	2.03	0.57
2:F:144:ALA:HB3	2:F:154:ILE:HD11	1.86	0.57
1:C:44:ARG:HH21	5:C:208:GOL:H32	1.69	0.56
1:B:44:ARG:CG	11:B:346:HOH:O	2.53	0.55
1:D:144:ALA:O	1:D:150:GLY:HA3	2.07	0.55
5:A:205:GOL:O1	11:A:303:HOH:O	2.18	0.55
1:A:12:GLU:OE1	11:A:304:HOH:O	2.18	0.54
1:E:53:HIS:HB3	11:E:301:HOH:O	1.98	0.54
2:F:144:ALA:O	2:F:150:GLY:HA3	2.08	0.54
5:C:205:GOL:C3	1:D:51:MET:HE2	2.37	0.53
1:E:9:LYS:HE2	11:E:420:HOH:O	2.08	0.53
1:B:44:ARG:CD	11:B:346:HOH:O	2.37	0.53
1:C:48[A]:GLN:HG2	5:C:205:GOL:O1	2.10	0.52
1:D:156:LYS:CE	11:D:315:HOH:O	2.55	0.52
1:B:3:LYS:NZ	11:B:307:HOH:O	2.34	0.52
1:A:19:TYR:HB2	5:A:204:GOL:C1	2.41	0.51
1:B:144:ALA:O	1:B:150:GLY:HA3	2.11	0.51
1:D:2:LEU:N	11:D:314:HOH:O	2.44	0.50
1:A:144:ALA:O	1:A:150:GLY:HA3	2.12	0.50
1:A:147:SER:HB2	1:A:149[B]:GLU:OE1	2.11	0.49
1:B:29:ALA:HB2	1:E:58:PHE:CZ	2.47	0.49
1:B:135:LYS:NZ	11:B:308:HOH:O	2.35	0.49
1:A:73:VAL:HG22	11:A:339:HOH:O	2.12	0.49
1:E:88:GLN:N	1:E:138[B]:ILE:HD11	2.28	0.49
1:D:54[B]:MET:C	1:D:54[B]:MET:SD	2.91	0.48
1:C:25:GLN:NE2	1:D:55[B]:GLN:HE22	2.11	0.48
1:A:15:ASN:O	5:A:204:GOL:C1	2.58	0.47
1:C:54[B]:MET:C	1:C:54[B]:MET:SD	2.93	0.47
1:E:22:LEU:HD12	1:E:73:VAL:HG11	1.95	0.47
2:F:99[A]:GLN:NE2	11:F:312:HOH:O	2.48	0.47
1:C:25:GLN:HE22	1:D:55[B]:GLN:NE2	2.09	0.47
1:C:58:PHE:CZ	1:D:29:ALA:HB2	2.51	0.46
1:D:144:ALA:HB3	1:D:154[A]:ILE:HD11	1.97	0.46
1:A:149[B]:GLU:HG2	1:A:150:GLY:N	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:LEU:HD12	1:B:73:VAL:HG11	1.99	0.45
1:D:114:TYR:N	1:D:115:PRO:CD	2.80	0.45
5:E:203:GOL:H32	11:E:306:HOH:O	2.17	0.44
2:F:74:GLU:OE2	11:F:303:HOH:O	2.21	0.44
1:A:73:VAL:HG13	5:A:204:GOL:O1	2.17	0.44
1:C:22:LEU:HD12	1:C:73:VAL:HG11	1.99	0.44
2:F:0:HIS:NE2	11:F:305:HOH:O	2.34	0.44
1:B:114:TYR:N	1:B:115:PRO:CD	2.81	0.43
1:A:74:GLU:HG3	5:A:204:GOL:O3	2.18	0.43
1:E:138[B]:ILE:HG23	11:E:307:HOH:O	2.18	0.43
1:D:99[A]:GLN:NE2	5:D:205:GOL:O1	2.43	0.43
2:F:114:TYR:N	2:F:115:PRO:CD	2.82	0.43
1:B:84[A]:ASP:O	1:B:88:GLN:HG2	2.18	0.43
1:D:99[A]:GLN:HE22	5:D:205:GOL:HO1	1.65	0.43
1:A:153:PHE:CD2	1:D:153:PHE:HZ	2.37	0.42
1:A:29:ALA:HB2	2:F:58:PHE:CZ	2.54	0.42
1:A:90[B]:THR:HG23	1:A:134:PHE:CD1	2.55	0.42
1:A:55[B]:GLN:NE2	1:A:59:ASP:OD1	2.35	0.42
1:B:58:PHE:CZ	1:E:29:ALA:HB2	2.55	0.42
2:F:99[B]:GLN:O	2:F:99[B]:GLN:HG3	2.19	0.42
1:B:67:LEU:HD21	1:E:77[A]:PHE:CZ	2.56	0.41
1:E:154[B]:ILE:HD13	1:E:154[B]:ILE:HA	1.80	0.41
1:E:14[B]:MET:C	1:E:14[B]:MET:SD	2.99	0.41
1:B:97:ILE:HD13	4:B:203:OH:O	2.21	0.41
1:A:22:LEU:HD12	1:A:73:VAL:HG11	2.03	0.40
1:A:27:MET:SD	1:A:90[A]:THR:HG22	2.61	0.40
1:A:15:ASN:HB3	5:A:204:GOL:H12	2.03	0.40
1:A:87:PHE:O	1:A:90[B]:THR:HG22	2.22	0.40

All (2) 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)
11:C:395:HOH:O	11:F:324:HOH:O[3_755]	2.13	0.07
11:B:343:HOH:O	11:F:392:HOH:O[6_775]	2.17	0.03

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	171/166 (103%)	168 (98%)	3 (2%)	0	100	100
1	B	169/166 (102%)	164 (97%)	5 (3%)	0	100	100
1	C	169/166 (102%)	167 (99%)	2 (1%)	0	100	100
1	D	174/166 (105%)	170 (98%)	4 (2%)	0	100	100
1	E	174/166 (105%)	171 (98%)	3 (2%)	0	100	100
2	F	167/166 (101%)	167 (100%)	0	0	100	100
All	All	1024/996 (103%)	1007 (98%)	17 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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	157/150 (105%)	157 (100%)	0	100	100
1	B	155/150 (103%)	153 (99%)	2 (1%)	65	53
1	C	155/150 (103%)	153 (99%)	2 (1%)	65	53
1	D	160/150 (107%)	157 (98%)	3 (2%)	52	36
1	E	159/150 (106%)	159 (100%)	0	100	100
2	F	153/149 (103%)	152 (99%)	1 (1%)	81	76
All	All	939/899 (104%)	931 (99%)	8 (1%)	79	67

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	85	GLU
1	B	104	LEU
1	C	2	LEU
1	C	35	THR
1	D	12[A]	GLU
1	D	12[B]	GLU
1	D	163	THR
2	F	104	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	112	GLN
1	C	127	GLN
2	F	34	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	A1L4B	F	127	6,2	6,9,10	3.20	2 (33%)	1,10,12	1.69	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	A1L4B	F	127	6,2	-	1/6/9/11	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	127	A1L4B	OE1-CD	6.58	1.31	1.22
2	F	127	A1L4B	O2-NE2	3.93	1.40	1.27

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	127	A1L4B	O-C-CA-CB

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	127	A1L4B	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 36 ligands modelled in this entry, 9 are modelled with single atom and 8 are monoatomic - leaving 19 for Mogul analysis.

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	$\#\|Z\| > 2$
3	FEO	B	201	11,1,4	0,2,2	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	GOL	B	204	-	5,5,5	1.18	0	5,5,5	1.63	2 (40%)
5	GOL	B	205	-	5,5,5	0.55	0	5,5,5	0.82	0
5	GOL	C	206	-	5,5,5	0.47	0	5,5,5	1.30	1 (20%)
5	GOL	D	205	-	5,5,5	0.64	0	5,5,5	1.22	1 (20%)
3	FEO	A	201	11,1,4	0,2,2	-	-	-		
5	GOL	A	205	-	5,5,5	0.49	0	5,5,5	1.04	0
5	GOL	A	204	-	5,5,5	0.71	0	5,5,5	0.98	0
5	GOL	C	205	-	5,5,5	0.88	0	5,5,5	1.53	1 (20%)
5	GOL	D	206	-	5,5,5	0.24	0	5,5,5	0.86	0
5	GOL	F	206	-	5,5,5	1.19	1 (20%)	5,5,5	1.03	0
5	GOL	C	209	-	5,5,5	0.32	0	5,5,5	0.66	0
3	FEO	E	201	1,4	0,2,2	-	-	-		
5	GOL	E	204	-	5,5,5	2.67	1 (20%)	5,5,5	2.19	2 (40%)
5	GOL	C	207	-	5,5,5	0.34	0	5,5,5	0.62	0
9	PER	D	203	6	0,1,1	-	-	-		
5	GOL	C	208	-	5,5,5	0.28	0	5,5,5	0.70	0
5	GOL	E	203	-	5,5,5	0.32	0	5,5,5	0.92	0
8	OXY	C	203	7,6	1,1,1	0.11	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
5	GOL	D	205	-	-	2/4/4/4	-
5	GOL	C	207	-	-	2/4/4/4	-
5	GOL	A	205	-	-	2/4/4/4	-
5	GOL	A	204	-	-	2/4/4/4	-
5	GOL	C	205	-	-	2/4/4/4	-
5	GOL	E	204	-	-	3/4/4/4	-
5	GOL	B	204	-	-	1/4/4/4	-
5	GOL	D	206	-	-	2/4/4/4	-
5	GOL	B	205	-	-	2/4/4/4	-
5	GOL	C	208	-	-	1/4/4/4	-
5	GOL	F	206	-	-	1/4/4/4	-
5	GOL	E	203	-	-	4/4/4/4	-
5	GOL	C	206	-	-	2/4/4/4	-
5	GOL	C	209	-	-	4/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	204	GOL	O2-C2	-5.57	1.26	1.43
5	F	206	GOL	O2-C2	2.50	1.50	1.43

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	204	GOL	O2-C2-C1	-3.52	93.62	109.12
5	B	204	GOL	O3-C3-C2	-2.74	97.06	110.20
5	B	204	GOL	C3-C2-C1	-2.24	102.98	111.70
5	D	205	GOL	O1-C1-C2	-2.21	99.62	110.20
5	E	204	GOL	O1-C1-C2	-2.18	99.76	110.20
5	C	205	GOL	O3-C3-C2	-2.16	99.85	110.20
5	C	206	GOL	O1-C1-C2	-2.07	100.30	110.20

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	204	GOL	O1-C1-C2-C3
5	A	205	GOL	C1-C2-C3-O3
5	C	205	GOL	C1-C2-C3-O3
5	C	209	GOL	O1-C1-C2-O2
5	C	209	GOL	O1-C1-C2-C3
5	C	209	GOL	C1-C2-C3-O3
5	D	205	GOL	O1-C1-C2-C3
5	E	204	GOL	O1-C1-C2-O2
5	B	204	GOL	O1-C1-C2-C3
5	B	205	GOL	C1-C2-C3-O3
5	C	206	GOL	C1-C2-C3-O3
5	C	207	GOL	O1-C1-C2-C3
5	D	206	GOL	C1-C2-C3-O3
5	E	203	GOL	O1-C1-C2-C3
5	E	203	GOL	C1-C2-C3-O3
5	E	204	GOL	O1-C1-C2-C3
5	F	206	GOL	O1-C1-C2-C3
5	A	204	GOL	O1-C1-C2-O2
5	C	205	GOL	O2-C2-C3-O3
5	C	209	GOL	O2-C2-C3-O3
5	D	206	GOL	O2-C2-C3-O3
5	A	205	GOL	O2-C2-C3-O3
5	D	205	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
5	B	205	GOL	O2-C2-C3-O3
5	E	203	GOL	O2-C2-C3-O3
5	C	206	GOL	O2-C2-C3-O3
5	E	203	GOL	O1-C1-C2-O2
5	C	208	GOL	O1-C1-C2-O2
5	E	204	GOL	O2-C2-C3-O3
5	C	207	GOL	O1-C1-C2-O2

There are no ring outliers.

8 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	205	GOL	2	0
5	A	205	GOL	1	0
5	A	204	GOL	10	0
5	C	205	GOL	5	0
3	E	201	FEO	2	0
5	E	204	GOL	1	0
5	C	208	GOL	4	0
5	E	203	GOL	1	0

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 (i)

6.1 Protein, DNA and RNA chains (i)

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	162/166 (97%)	-0.54	0	100	100	10, 24, 40, 58	11 (6%)
1	B	164/166 (98%)	-0.60	0	100	100	10, 23, 38, 55	8 (4%)
1	C	162/166 (97%)	-0.55	0	100	100	10, 25, 39, 53	10 (6%)
1	D	162/166 (97%)	-0.49	0	100	100	10, 25, 40, 55	15 (9%)
1	E	163/166 (98%)	-0.49	1 (0%)	85	91	9, 24, 40, 55	15 (9%)
2	F	163/166 (98%)	-0.55	1 (0%)	85	91	9, 24, 42, 59	6 (3%)
All	All	976/996 (97%)	-0.54	2 (0%)	92	95	9, 24, 41, 59	65 (6%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	1	HIS	2.5
2	F	0	HIS	2.3

6.2 Non-standard residues in protein, DNA, RNA chains (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(Å^2)	Q<0.9
2	A1L4B	F	127	10/11	0.97	0.08	15,17,22,39	10

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(Å^2)	Q<0.9
5	GOL	B	205	6/6	0.81	0.16	36,42,49,59	6
5	GOL	D	206	6/6	0.82	0.16	39,49,52,63	6
5	GOL	D	205	6/6	0.87	0.16	32,47,54,67	6
5	GOL	C	208	6/6	0.89	0.14	28,51,56,57	6
5	GOL	C	206	6/6	0.89	0.12	44,45,50,51	6
5	GOL	C	207	6/6	0.89	0.10	41,48,53,54	6
5	GOL	E	204	6/6	0.89	0.18	26,27,46,47	6
5	GOL	E	203	6/6	0.90	0.10	42,43,47,53	6
5	GOL	C	205	6/6	0.90	0.13	28,31,36,38	6
5	GOL	A	205	6/6	0.91	0.12	33,42,45,54	6
5	GOL	C	209	6/6	0.91	0.12	27,44,49,55	6
5	GOL	A	204	6/6	0.93	0.09	35,39,40,57	6
7	FE2	E	205	1/1	0.93	0.17	500,500,500,500	1
5	GOL	F	206	6/6	0.94	0.09	23,26,28,30	6
5	GOL	B	204	6/6	0.95	0.07	23,26,30,31	6
4	OH	A	203	1/1	0.97	0.35	19,19,19,19	1
4	OH	D	204	1/1	0.98	0.05	22,22,22,22	0
4	OH	B	203	1/1	0.98	0.22	26,26,26,26	1
9	PER	D	203	2/2	0.98	0.12	10,10,10,17	2
4	OH	C	204	1/1	0.99	0.05	22,22,22,22	0
4	OH	B	202	1/1	0.99	0.04	17,17,17,17	0
4	OH	F	204	1/1	0.99	0.03	19,19,19,19	0
4	OH	F	205	1/1	0.99	0.15	27,27,27,27	1
8	OXY	C	203	2/2	0.99	0.09	10,10,10,18	2
4	OH	A	202	1/1	0.99	0.03	16,16,16,16	0
10	O	F	203	1/1	0.99	0.09	21,21,21,21	0
6	FE	C	201	1/1	1.00	0.02	17,17,17,17	0
6	FE	D	201	1/1	1.00	0.02	17,17,17,17	0
6	FE	D	202	1/1	1.00	0.01	20,20,20,20	0
6	FE	F	201	1/1	1.00	0.01	18,18,18,18	0
6	FE	F	202	1/1	1.00	0.01	16,16,16,16	0
7	FE2	C	202	1/1	1.00	0.01	18,18,18,18	0
3	FEO	A	201	3/3	1.00	0.01	17,17,17,18	0
3	FEO	B	201	3/3	1.00	0.02	15,15,17,17	0
3	FEO	E	201	3/3	1.00	0.01	16,16,18,18	0
4	OH	E	202	1/1	1.00	0.02	16,16,16,16	0

6.5 Other polymers (i)

There are no such residues in this entry.