



Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 10:37 PM GMT

PDB ID : 4ISP
Title : Crystal structure of iron soaked (4h) ferritin from Pseudo-nitzschia multiseris
Authors : Pfaffen, S.; Murphy, M.E.P.
Deposited on : 2013-01-17
Resolution : 2.20 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

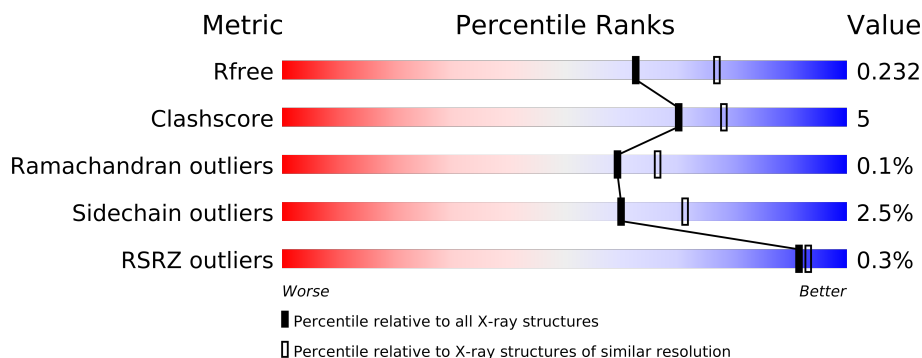
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	2938 (2.20-2.20)
Clashscore	79885	3751 (2.20-2.20)
Ramachandran outliers	78287	3681 (2.20-2.20)
Sidechain outliers	78261	3682 (2.20-2.20)
RSRZ outliers	66119	2939 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	168	
1	B	168	
1	C	168	
1	D	168	
1	E	168	
1	F	168	
1	G	168	
1	H	168	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	FE	A	202	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Geometry	Electron density
2	FE	E	204	-	X
2	FE	H	203	-	X
2	FE	H	204	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10775 atoms, of which 0 are hydrogen and 0 are deuterium.

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
1	A	159	Total	C	N	O	S	0	2	0
			1276	803	211	257	5			
1	D	159	Total	C	N	O	S	0	5	0
			1293	813	215	260	5			
1	B	159	Total	C	N	O	S	0	1	0
			1270	800	210	255	5			
1	C	159	Total	C	N	O	S	0	4	0
			1291	811	214	261	5			
1	E	159	Total	C	N	O	S	0	3	0
			1281	808	211	257	5			
1	F	158	Total	C	N	O	S	0	1	0
			1262	796	209	252	5			
1	G	156	Total	C	N	O	S	0	2	0
			1250	788	208	249	5			
1	H	159	Total	C	N	O	S	0	3	0
			1279	805	211	258	5			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	EXPRESSION TAG	UNP B6DMH6
D	0	GLY	-	EXPRESSION TAG	UNP B6DMH6
B	0	GLY	-	EXPRESSION TAG	UNP B6DMH6
C	0	GLY	-	EXPRESSION TAG	UNP B6DMH6
E	0	GLY	-	EXPRESSION TAG	UNP B6DMH6
F	0	GLY	-	EXPRESSION TAG	UNP B6DMH6
G	0	GLY	-	EXPRESSION TAG	UNP B6DMH6
H	0	GLY	-	EXPRESSION TAG	UNP B6DMH6

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	4	Total Fe 4 4	0	0
2	D	5	Total Fe 5 5	0	0
2	E	4	Total Fe 4 4	0	0
2	H	4	Total Fe 4 4	0	0
2	B	5	Total Fe 5 5	0	0
2	C	4	Total Fe 4 4	0	0
2	A	5	Total Fe 5 5	0	0
2	F	4	Total Fe 4 4	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	66	Total O 66 66	0	0
3	D	65	Total O 65 65	0	0
3	B	77	Total O 77 77	0	0
3	C	72	Total O 72 72	0	0
3	E	53	Total O 53 53	0	0
3	F	61	Total O 61 61	0	0
3	G	74	Total O 74 74	0	0
3	H	70	Total O 70 70	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 D: 



- Molecule 1: Ferritin

Chain B: 



- Molecule 1: Ferritin

Chain C: 



- Molecule 1: Ferritin

Chain E: 



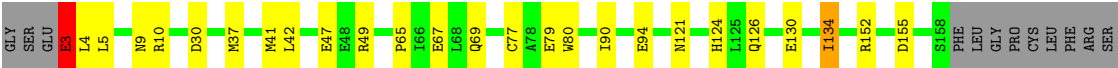
- Molecule 1: Ferritin

Chain F: 



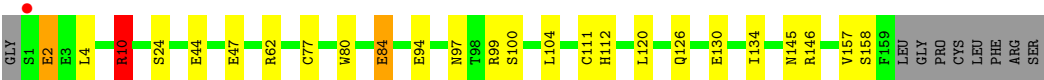
- Molecule 1: Ferritin

Chain G: 



● Molecule 1: Ferritin

Chain H: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 3	Depositor
Cell constants a, b, c, α , β , γ	175.45Å 175.45Å 175.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.59 – 2.20 41.35 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.7 (42.59-2.20) 99.7 (41.35-2.20)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.64 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.187 , 0.242 0.176 , 0.232	Depositor DCC
R_{free} test set	4537 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	26.1	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 27.5	EDS
Estimated twinning fraction	0.049 for l,-k,h	Xtriage
L-test for twinning	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtriage
Outliers	2 of 90432 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10775	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 14.45% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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, YCM

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	0.97	0/1292	0.94	1/1757 (0.1%)
1	B	0.98	0/1286	1.01	3/1749 (0.2%)
1	C	0.97	0/1307	0.92	3/1777 (0.2%)
1	D	1.01	0/1315	0.93	3/1787 (0.2%)
1	E	0.97	3/1300 (0.2%)	0.95	2/1768 (0.1%)
1	F	0.98	1/1278 (0.1%)	0.96	3/1738 (0.2%)
1	G	0.97	0/1265	0.94	3/1721 (0.2%)
1	H	0.98	0/1298	0.98	5/1765 (0.3%)
All	All	0.98	4/10341 (0.0%)	0.95	23/14062 (0.2%)

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	G	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	84	GLU	CD-OE2	5.65	1.31	1.25
1	E	44	GLU	CD-OE1	5.59	1.31	1.25
1	F	130	GLU	CD-OE2	5.37	1.31	1.25
1	E	87	TRP	CE3-CZ3	5.16	1.47	1.38

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	154	LEU	CA-CB-CG	8.69	135.28	115.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	152	ARG	NE-CZ-NH1	6.94	123.77	120.30
1	E	61	LYS	CD-CE-NZ	-6.61	96.50	111.70
1	F	49	ARG	NE-CZ-NH1	-6.38	117.11	120.30
1	H	146	ARG	NE-CZ-NH2	-6.30	117.15	120.30
1	G	134	ILE	CG1-CB-CG2	-6.23	97.69	111.40
1	F	42	LEU	CB-CG-CD2	-6.22	100.43	111.00
1	G	49	ARG	NE-CZ-NH1	-5.92	117.34	120.30
1	A	41	MET	CG-SD-CE	5.89	109.62	100.20
1	F	146	ARG	NE-CZ-NH1	5.87	123.23	120.30
1	B	146	ARG	NE-CZ-NH1	5.71	123.15	120.30
1	D	41	MET	CG-SD-CE	5.45	108.92	100.20
1	C	154	LEU	CB-CG-CD2	5.41	120.20	111.00
1	D	62	ARG	NE-CZ-NH1	-5.39	117.61	120.30
1	H	146	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	C	102	LEU	CB-CG-CD2	5.36	120.11	111.00
1	D	154	LEU	CB-CG-CD2	5.35	120.10	111.00
1	H	62	ARG	CG-CD-NE	-5.31	100.65	111.80
1	E	62	ARG	NE-CZ-NH1	-5.24	117.68	120.30
1	B	154	LEU	CB-CG-CD2	5.20	119.84	111.00
1	C	152	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	H	99	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	H	10	ARG	NE-CZ-NH1	5.02	122.81	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	3	GLU	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1276	0	1207	10	0
1	B	1270	0	1203	9	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1291	0	1218	11	0
1	D	1293	0	1229	9	0
1	E	1281	0	1219	10	0
1	F	1262	0	1196	10	0
1	G	1250	0	1191	21	0
1	H	1279	0	1212	15	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	4	0	0	1	0
2	D	5	0	0	0	0
2	E	4	0	0	0	0
2	F	4	0	0	0	0
2	G	4	0	0	0	0
2	H	4	0	0	0	0
3	A	66	0	0	4	0
3	B	77	0	0	4	0
3	C	72	0	0	6	0
3	D	65	0	0	3	0
3	E	53	0	0	4	0
3	F	61	0	0	2	0
3	G	74	0	0	5	0
3	H	70	0	0	5	0
All	All	10775	0	9675	92	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 5.

All (92) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:77:YCM:HB2	3:D:365:HOH:O	1.65	0.95
1:H:44:GLU:OE1	3:H:351:HOH:O	1.91	0.88
1:H:84:GLU:HG2	3:H:317:HOH:O	1.75	0.86
1:G:9:ASN:HD21	1:G:67:GLU:H	1.27	0.81
1:H:10:ARG:HG2	1:H:10:ARG:HH11	1.47	0.80
1:E:47:GLU:OE1	3:E:349:HOH:O	2.00	0.78
1:D:24[A]:SER:HB2	1:D:77:YCM:HZ21	1.47	0.78
1:A:44:GLU:OE1	3:A:365:HOH:O	2.05	0.74
1:H:84:GLU:CG	3:H:317:HOH:O	2.36	0.73
1:H:47:GLU:OE2	1:H:130:GLU:OE2	2.08	0.71
1:A:126:GLN:NE2	3:A:351:HOH:O	2.24	0.71
1:C:24[A]:SER:HB2	1:C:77:YCM:HZ21	1.56	0.70
1:B:47:GLU:OE1	3:B:374:HOH:O	2.11	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:24[A]:SER:HB2	1:H:77:YCM:HZ21	1.61	0.66
2:C:204:FE:FE	3:C:354:HOH:O	1.47	0.65
1:G:47:GLU:OE1	3:G:370:HOH:O	2.15	0.65
1:D:47:GLU:OE2	3:D:362:HOH:O	2.14	0.64
1:G:126:GLN:NE2	3:G:371:HOH:O	2.09	0.64
1:F:146:ARG:HG2	1:F:146:ARG:HH11	1.63	0.63
1:G:9:ASN:ND2	1:G:67:GLU:H	1.97	0.62
1:H:47:GLU:OE1	3:H:369:HOH:O	2.16	0.62
1:F:152:ARG:O	1:F:156:VAL:HG13	2.00	0.62
1:G:9:ASN:HD21	1:G:67:GLU:N	1.98	0.59
1:G:3:GLU:HG2	1:G:4:LEU:H	1.67	0.59
1:C:10:ARG:HG2	1:C:10:ARG:HH11	1.67	0.58
1:E:48:GLU:OE2	3:E:309:HOH:O	2.17	0.57
1:D:77:YCM:CB	3:D:365:HOH:O	2.38	0.57
1:C:126:GLN:NE2	3:C:367:HOH:O	2.37	0.56
1:G:124:HIS:HE1	3:G:310:HOH:O	1.88	0.56
1:G:10:ARG:HH11	1:G:10:ARG:HG2	1.71	0.55
1:A:94:GLU:HG3	1:A:134:ILE:CD1	2.38	0.54
1:C:47:GLU:OE1	3:C:371:HOH:O	2.19	0.53
1:E:1:SER:O	1:E:5[A]:LEU:HG	2.09	0.52
1:B:5:LEU:HD13	1:B:65:PRO:HD2	1.89	0.52
1:E:124:HIS:HE1	3:E:303:HOH:O	1.92	0.52
1:A:124:HIS:HD2	3:A:358:HOH:O	1.92	0.52
1:D:152:ARG:O	1:D:156:VAL:HG13	2.11	0.51
1:B:124:HIS:HE1	3:B:303:HOH:O	1.94	0.50
1:D:94:GLU:HG3	1:D:134:ILE:HD13	1.92	0.50
1:H:10:ARG:HG2	1:H:10:ARG:NH1	2.17	0.49
1:G:47:GLU:OE2	3:G:371:HOH:O	2.19	0.49
1:B:124:HIS:HD2	3:B:363:HOH:O	1.95	0.49
1:F:94:GLU:HG3	1:F:134:ILE:HD13	1.95	0.48
1:G:94:GLU:HG3	1:G:134:ILE:HD13	1.95	0.48
1:F:69:GLN:HG3	3:F:306:HOH:O	2.13	0.48
1:C:77:YCM:HB2	3:C:302:HOH:O	2.14	0.48
1:C:77:YCM:CB	3:C:302:HOH:O	2.62	0.48
1:G:79:GLU:HG3	3:G:309:HOH:O	2.13	0.48
1:B:77:YCM:HA	1:B:80:TRP:CE3	2.48	0.47
1:B:62:ARG:NH1	3:B:369:HOH:O	2.45	0.46
1:G:3:GLU:CD	1:G:3:GLU:N	2.69	0.46
1:A:49:ARG:HD3	1:E:49:ARG:HD3	1.98	0.46
1:D:143:ASP:O	1:D:146[B]:ARG:HG3	2.15	0.45
1:F:77:YCM:HA	1:F:80:TRP:CE3	2.52	0.45
1:C:130:GLU:OE2	3:C:366:HOH:O	2.21	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:41:MET:CE	1:G:90:ILE:HG13	2.47	0.45
1:H:94:GLU:HG3	1:H:134:ILE:CD1	2.47	0.44
1:G:37:MET:HG3	1:G:155:ASP:OD1	2.17	0.44
1:H:104:LEU:HG	1:H:120:LEU:HD11	1.99	0.44
1:C:106:GLU:OE2	1:F:112:HIS:ND1	2.51	0.44
1:A:144:GLU:OE1	1:A:154:LEU:HB2	2.18	0.44
1:F:62:ARG:HD3	3:F:348:HOH:O	2.18	0.44
1:G:77:YCM:HA	1:G:80:TRP:CE3	2.52	0.44
1:E:11:GLN:O	1:E:15:GLU:HG2	2.18	0.44
1:H:77:YCM:HA	1:H:80:TRP:CE3	2.52	0.43
1:H:97:ASN:O	1:H:100:SER:HB3	2.19	0.43
1:B:49:ARG:HD3	1:F:49:ARG:HD3	1.99	0.43
1:D:11:GLN:HG2	1:D:55:PHE:CE2	2.54	0.43
1:H:145:ASN:ND2	3:H:317:HOH:O	2.51	0.43
1:G:130:GLU:O	1:G:134:ILE:HD12	2.19	0.43
1:B:130:GLU:O	1:B:134:ILE:HD13	2.18	0.43
1:B:125:LEU:HA	1:B:125:LEU:HD23	1.76	0.42
1:A:157:VAL:HG11	1:H:157:VAL:HG22	2.01	0.42
1:G:3:GLU:OE1	1:G:3:GLU:N	2.52	0.42
1:D:48:GLU:OE1	1:D:48:GLU:HA	2.20	0.42
1:H:111:CYS:O	1:H:112:HIS:HB2	2.20	0.42
1:G:5[B]:LEU:HD13	1:G:65:PRO:HD2	2.02	0.42
1:F:11:GLN:HG2	1:F:55:PHE:CE2	2.55	0.42
1:E:124:HIS:HD2	3:E:336:HOH:O	2.03	0.42
1:F:130:GLU:O	1:F:134:ILE:HD12	2.19	0.42
1:A:5:LEU:HD22	1:A:64:ILE:HG23	2.01	0.42
1:E:53:LEU:HD23	1:E:53:LEU:HA	1.80	0.41
1:C:10:ARG:HG2	1:C:10:ARG:NH1	2.35	0.41
1:A:124:HIS:HE1	3:A:309:HOH:O	2.02	0.41
1:C:41:MET:HE1	1:C:87:TRP:CZ3	2.56	0.41
1:C:130:GLU:O	1:C:134:ILE:HD12	2.21	0.41
1:E:77:YCM:HA	1:E:80:TRP:CE3	2.56	0.40
1:E:5[B]:LEU:HD13	1:E:65:PRO:HD2	2.03	0.40
1:G:10:ARG:HH12	1:G:69:GLN:HE22	1.69	0.40
1:A:77:YCM:HA	1:A:80:TRP:CE3	2.56	0.40
1:G:121:ASN:HD22	1:G:121:ASN:HA	1.72	0.40
1:G:42:LEU:HD12	1:G:42:LEU:HA	1.82	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	158/168 (94%)	155 (98%)	3 (2%)	0	100	100
1	B	157/168 (94%)	155 (99%)	2 (1%)	0	100	100
1	C	160/168 (95%)	159 (99%)	1 (1%)	0	100	100
1	D	161/168 (96%)	158 (98%)	3 (2%)	0	100	100
1	E	159/168 (95%)	158 (99%)	1 (1%)	0	100	100
1	F	156/168 (93%)	155 (99%)	1 (1%)	0	100	100
1	G	155/168 (92%)	154 (99%)	1 (1%)	0	100	100
1	H	159/168 (95%)	155 (98%)	3 (2%)	1 (1%)	33	32
All	All	1265/1344 (94%)	1249 (99%)	15 (1%)	1 (0%)	59	66

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	2	GLU

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	138/143 (96%)	134 (97%)	4 (3%)	55	66
1	B	137/143 (96%)	131 (96%)	6 (4%)	39	45
1	C	140/143 (98%)	139 (99%)	1 (1%)	91	96
1	D	141/143 (99%)	141 (100%)	0	100	100
1	E	139/143 (97%)	135 (97%)	4 (3%)	55	66
1	F	136/143 (95%)	131 (96%)	5 (4%)	45	54

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	135/143 (94%)	133 (98%)	2 (2%)	76	86
1	H	139/143 (97%)	133 (96%)	6 (4%)	40	47
All	All	1105/1144 (97%)	1077 (98%)	28 (2%)	60	71

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	ASP
1	A	67	GLU
1	A	75	VAL
1	A	126	GLN
1	B	3	GLU
1	B	42	LEU
1	B	67	GLU
1	B	75	VAL
1	B	134	ILE
1	B	154	LEU
1	C	3	GLU
1	E	81[A]	SER
1	E	81[B]	SER
1	E	152	ARG
1	E	153	SER
1	F	10	ARG
1	F	75	VAL
1	F	81	SER
1	F	153	SER
1	F	156	VAL
1	G	3	GLU
1	G	30	ASP
1	H	2	GLU
1	H	4	LEU
1	H	10	ARG
1	H	84	GLU
1	H	126	GLN
1	H	158	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	121	ASN
1	A	124	HIS
1	B	121	ASN
1	B	124	HIS
1	E	121	ASN
1	E	124	HIS
1	G	9	ASN
1	G	31	GLN
1	G	69	GLN
1	G	121	ASN
1	G	124	HIS
1	H	63	ASN
1	H	69	GLN
1	H	126	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

8 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	YCM	A	77	1	9,9,10	7.20	3 (33%)	8,10,12	1.61	2 (25%)
1	YCM	B	77	1	9,9,10	7.29	3 (33%)	8,10,12	1.46	1 (12%)
1	YCM	C	77	1	9,9,10	6.70	2 (22%)	8,10,12	1.55	2 (25%)
1	YCM	D	77	1	9,9,10	7.59	2 (22%)	8,10,12	1.04	1 (12%)
1	YCM	E	77	1	9,9,10	7.29	3 (33%)	8,10,12	1.15	1 (12%)
1	YCM	F	77	1	9,9,10	7.88	3 (33%)	8,10,12	0.96	0
1	YCM	G	77	1	9,9,10	7.82	4 (44%)	8,10,12	1.78	1 (12%)
1	YCM	H	77	1	9,9,10	7.63	2 (22%)	8,10,12	0.92	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
1	YCM	A	77	1	-	0/6/8/10	0/0/0/0
1	YCM	B	77	1	-	0/6/8/10	0/0/0/0
1	YCM	C	77	1	-	0/6/8/10	0/0/0/0
1	YCM	D	77	1	-	0/6/8/10	0/0/0/0
1	YCM	E	77	1	-	0/6/8/10	0/0/0/0
1	YCM	F	77	1	-	0/6/8/10	0/0/0/0
1	YCM	G	77	1	-	0/6/8/10	0/0/0/0
1	YCM	H	77	1	-	0/6/8/10	0/0/0/0

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	77	YCM	O-C	22.98	1.27	1.11
1	H	77	YCM	O-C	22.53	1.27	1.11
1	G	77	YCM	O-C	22.38	1.26	1.11
1	D	77	YCM	O-C	21.96	1.26	1.11
1	B	77	YCM	O-C	21.43	1.26	1.11
1	E	77	YCM	O-C	20.48	1.25	1.11
1	A	77	YCM	O-C	19.28	1.24	1.11
1	C	77	YCM	O-C	18.66	1.24	1.11
1	A	77	YCM	CB-SG	7.65	1.96	1.81
1	C	77	YCM	CB-SG	7.02	1.95	1.81
1	E	77	YCM	CB-SG	5.91	1.93	1.81
1	D	77	YCM	CB-SG	5.57	1.92	1.81
1	A	77	YCM	CD-SG	5.31	1.91	1.81
1	G	77	YCM	CD-SG	5.17	1.91	1.81
1	E	77	YCM	CD-SG	4.31	1.89	1.81
1	H	77	YCM	CA-C	3.55	1.55	1.48
1	G	77	YCM	CB-SG	3.50	1.88	1.81
1	F	77	YCM	CB-SG	3.48	1.88	1.81
1	F	77	YCM	CA-C	3.40	1.54	1.48
1	G	77	YCM	CA-C	3.13	1.54	1.48
1	B	77	YCM	CD-SG	3.09	1.87	1.81
1	B	77	YCM	CA-C	2.02	1.52	1.48

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	77	YCM	CB-SG-CD	-4.11	95.21	101.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	77	YCM	C-CA-N	-3.43	110.41	113.83
1	A	77	YCM	C-CA-N	3.19	117.01	113.83
1	C	77	YCM	CE-CD-SG	-2.85	105.68	112.87
1	D	77	YCM	CB-CA-N	2.48	114.48	110.27
1	A	77	YCM	CD-CE-NZ2	2.38	119.09	115.59
1	C	77	YCM	CB-CA-N	2.31	114.18	110.27
1	E	77	YCM	CB-CA-N	2.16	113.93	110.27

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 35 ligands modelled in this entry, 35 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.

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	159/168 (94%)	-0.47	1 (0%) 86 88	16, 26, 46, 68	0
1	B	159/168 (94%)	-0.52	0 100 100	15, 25, 47, 72	0
1	C	159/168 (94%)	-0.48	0 100 100	16, 26, 49, 76	0
1	D	159/168 (94%)	-0.43	0 100 100	14, 25, 46, 73	0
1	E	159/168 (94%)	-0.48	1 (0%) 86 88	17, 25, 51, 71	0
1	F	158/168 (94%)	-0.50	0 100 100	16, 25, 50, 68	0
1	G	156/168 (92%)	-0.52	0 100 100	15, 24, 44, 60	0
1	H	159/168 (94%)	-0.45	1 (0%) 86 88	16, 26, 49, 72	0
All	All	1268/1344 (94%)	-0.48	3 (0%) 91 94	14, 25, 48, 76	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	1	SER	2.4
1	E	1	SER	2.1
1	A	72	PRO	2.0

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

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	YCM	A	77	10/11	0.15	1.29	26,31,46,62	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
1	YCM	F	77	10/11	0.14	1.28	29,41,44,45	0
1	YCM	C	77	10/11	0.11	-0.17	29,35,38,43	0
1	YCM	D	77	10/11	0.11	-0.32	31,35,43,45	0
1	YCM	B	77	10/11	0.10	-0.35	27,30,33,37	0
1	YCM	G	77	10/11	0.10	-0.45	26,39,40,46	0
1	YCM	H	77	10/11	0.10	-0.57	27,37,44,45	0
1	YCM	E	77	10/11	0.07	-0.92	31,33,42,42	0

6.3 Carbohydrates

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	FE	H	204	1/1	0.27	17.95	33,33,33,33	1
2	FE	E	204	1/1	0.17	4.92	44,44,44,44	1
2	FE	A	202	1/1	0.12	2.72	42,42,42,42	1
2	FE	H	203	1/1	0.18	2.60	36,36,36,36	1
2	FE	E	203	1/1	0.14	1.45	47,47,47,47	1
2	FE	A	204	1/1	0.13	1.11	39,39,39,39	1
2	FE	E	202	1/1	0.11	1.10	44,44,44,44	1
2	FE	H	202	1/1	0.10	0.64	40,40,40,40	1
2	FE	F	202	1/1	0.10	0.62	46,46,46,46	1
2	FE	B	204	1/1	0.12	0.43	43,43,43,43	1
2	FE	B	205	1/1	0.14	0.31	39,39,39,39	1
2	FE	C	204	1/1	0.10	0.22	37,37,37,37	1
2	FE	F	203	1/1	0.13	0.11	43,43,43,43	1
2	FE	D	203	1/1	0.12	-0.09	47,47,47,47	1
2	FE	A	201	1/1	0.11	-0.10	39,39,39,39	1
2	FE	H	201	1/1	0.10	-0.12	38,38,38,38	1
2	FE	F	204	1/1	0.10	-0.19	41,41,41,41	1
2	FE	G	203	1/1	0.09	-0.76	42,42,42,42	1
2	FE	B	203	1/1	0.08	-0.80	46,46,46,46	1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	FE	D	204	1/1	0.08	-0.90	46,46,46,46	1
2	FE	C	203	1/1	0.08	-1.01	43,43,43,43	1
2	FE	D	205	1/1	0.08	-1.09	42,42,42,42	1
2	FE	E	201	1/1	0.09	-1.15	39,39,39,39	1
2	FE	A	203	1/1	0.07	-1.22	52,52,52,52	1
2	FE	B	202	1/1	0.08	-1.26	41,41,41,41	1
2	FE	A	205	1/1	0.06	-1.33	39,39,39,39	1
2	FE	G	201	1/1	0.07	-1.47	40,40,40,40	0
2	FE	G	204	1/1	0.08	-1.52	47,47,47,47	1
2	FE	B	201	1/1	0.07	-1.67	38,38,38,38	1
2	FE	F	201	1/1	0.05	-2.02	42,42,42,42	0
2	FE	C	202	1/1	0.05	-2.40	43,43,43,43	1
2	FE	D	202	1/1	0.07	-2.64	42,42,42,42	1
2	FE	C	201	1/1	0.05	-2.81	38,38,38,38	0
2	FE	G	202	1/1	0.06	-2.91	39,39,39,39	0
2	FE	D	201	1/1	0.05	-4.21	38,38,38,38	1

6.5 Other polymers ⓘ

There are no such residues in this entry.