



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 07:30 pm BST

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

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

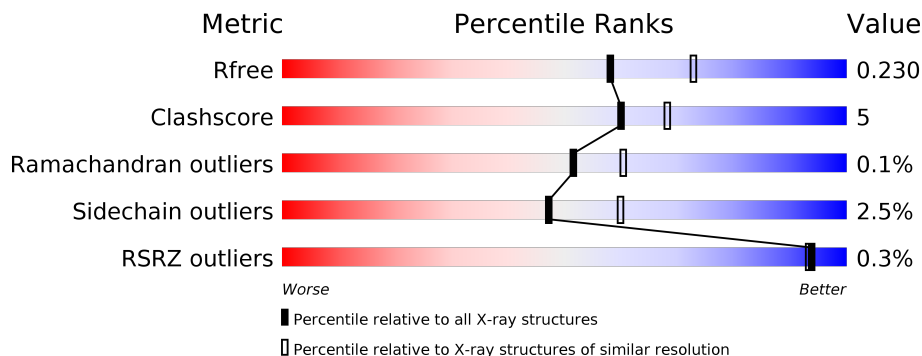
# 1 Overall quality at a glance

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	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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	168	
1	B	168	
1	C	168	
1	D	168	
1	E	168	
1	F	168	

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Mol	Chain	Length	Quality of chain
1	G	168	 77% 14% •• 7%
1	H	168	 80% 13% •• 5%

## 2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 10775 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	159	1276	803	211	257	5	0	2	0
1	D	159	1293	813	215	260	5	0	5	0
1	B	159	1270	800	210	255	5	0	1	0
1	C	159	1291	811	214	261	5	0	4	0
1	E	159	1281	808	211	257	5	0	3	0
1	F	158	1262	796	209	252	5	0	1	0
1	G	156	1250	788	208	249	5	0	2	0
1	H	159	1279	805	211	258	5	0	3	0

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

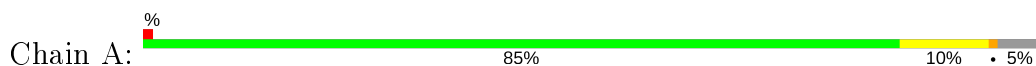
- Molecule 3 is water.

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 [i](#)

These plots are drawn for all protein, RNA and DNA 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.

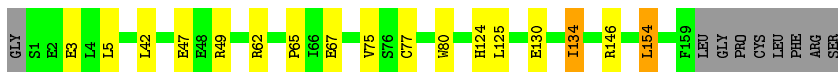
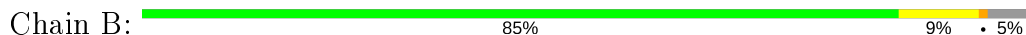
- Molecule 1: Ferritin



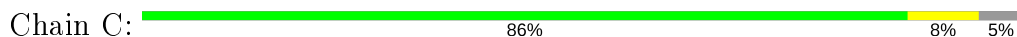
- Molecule 1: Ferritin



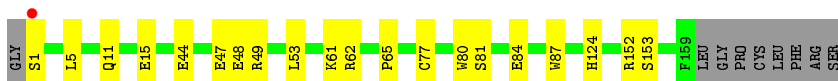
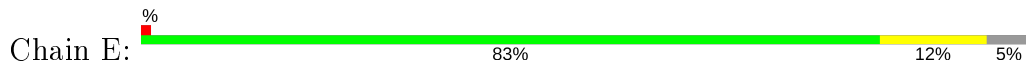
- Molecule 1: Ferritin



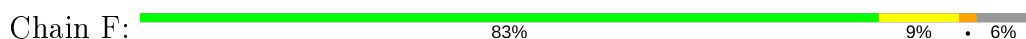
- Molecule 1: Ferritin



- Molecule 1: Ferritin



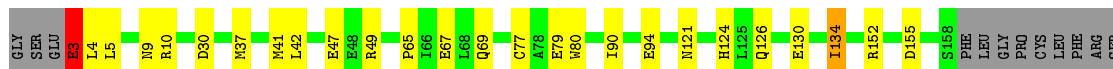
- Molecule 1: Ferritin





- Molecule 1: Ferritin

Chain G: 77% 14% 7%



- Molecule 1: Ferritin

Chain H: 80% 13% 5%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.64 (at 2.20Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.187 , 0.242 0.175 , 0.230	Depositor DCC
$R_{free}$ test set	4537 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.1	Xtrriage
Anisotropy	0.000	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 45.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.53$ , $\langle L^2 \rangle = 0.37$	Xtrriage
Estimated twinning fraction	0.049 for l,-k,h	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	10775	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtrriage'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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: 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

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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 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	1276	0	1207	10	0
1	B	1270	0	1203	9	0
1	C	1291	0	1218	11	0
1	D	1293	0	1229	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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

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 5.

All (92) 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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (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:A:124:HIS:HD2	3:A:358:HOH:O	1.92	0.52
1:E:124:HIS:HE1	3:E:303: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:B:124:HIS:HD2	3:B:363:HOH:O	1.95	0.49
1:G:47:GLU:OE2	3:G:371:HOH:O	2.19	0.49
1:F:94:GLU:HG3	1:F:134:ILE:HD13	1.95	0.48
1:F:69:GLN:HG3	3:F:306:HOH:O	2.13	0.48
1:G:94:GLU:HG3	1:G:134:ILE:HD13	1.95	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:A:49:ARG:HD3	1:E:49:ARG:HD3	1.98	0.46
1:G:3:GLU:CD	1:G:3:GLU:N	2.69	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:130:GLU:OE2	3:C:366:HOH:O	2.21	0.45
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:C:106:GLU:OE2	1:F:112:HIS:ND1	2.51	0.44
1:H:104:LEU:HG	1:H:120:LEU:HD11	1.99	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:B:130:GLU:O	1:B:134:ILE:HD13	2.18	0.43
1:G:130:GLU:O	1:G:134:ILE:HD12	2.19	0.43
1:H:145:ASN:ND2	3:H:317:HOH:O	2.51	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:A:5:LEU:HD22	1:A:64:ILE:HG23	2.01	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: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:A:77:YCM:HA	1:A:80:TRP:CE3	2.56	0.40
1:G:10:ARG:HH12	1:G:69:GLN:HE22	1.69	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 [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	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%)	25	26
All	All	1265/1344 (94%)	1249 (99%)	15 (1%)	1 (0%)	51	60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	2	GLU

### 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	138/143 (96%)	134 (97%)	4 (3%)	42	54
1	B	137/143 (96%)	131 (96%)	6 (4%)	28	35
1	C	140/143 (98%)	139 (99%)	1 (1%)	84	91
1	D	141/143 (99%)	141 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	E	139/143 (97%)	135 (97%)	4 (3%)	42 54
1	F	136/143 (95%)	131 (96%)	5 (4%)	34 43
1	G	135/143 (94%)	133 (98%)	2 (2%)	65 78
1	H	139/143 (97%)	133 (96%)	6 (4%)	29 36
All	All	1105/1144 (97%)	1077 (98%)	28 (2%)	47 60

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
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 [i](#)

There are no RNA molecules in this entry.

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

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	G	77	1	7,9,10	1.75	1 (14%)	4,10,12	0.83	0
1	YCM	H	77	1	7,9,10	0.92	0	4,10,12	0.70	0
1	YCM	F	77	1	7,9,10	1.28	0	4,10,12	0.64	0
1	YCM	D	77	1	7,9,10	1.39	1 (14%)	4,10,12	0.56	0
1	YCM	B	77	1	7,9,10	1.17	1 (14%)	4,10,12	0.88	0
1	YCM	E	77	1	7,9,10	1.81	2 (28%)	4,10,12	0.89	0
1	YCM	C	77	1	7,9,10	1.50	1 (14%)	4,10,12	1.46	1 (25%)
1	YCM	A	77	1	7,9,10	2.24	2 (28%)	4,10,12	0.34	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	G	77	1	-	0/6/8/10	-
1	YCM	H	77	1	-	1/6/8/10	-
1	YCM	F	77	1	-	1/6/8/10	-
1	YCM	D	77	1	-	1/6/8/10	-
1	YCM	B	77	1	-	1/6/8/10	-
1	YCM	E	77	1	-	2/6/8/10	-
1	YCM	C	77	1	-	1/6/8/10	-
1	YCM	A	77	1	-	3/6/8/10	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	77	YCM	CB-SG	3.95	1.96	1.80
1	A	77	YCM	CD-SG	3.76	1.91	1.81
1	G	77	YCM	CD-SG	3.66	1.91	1.81
1	C	77	YCM	CB-SG	3.63	1.95	1.80
1	E	77	YCM	CB-SG	3.07	1.93	1.80
1	E	77	YCM	CD-SG	3.06	1.89	1.81
1	D	77	YCM	CB-SG	2.90	1.92	1.80
1	B	77	YCM	CD-SG	2.19	1.87	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	77	YCM	CE-CD-SG	-2.69	105.68	113.59

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	E	77	YCM	SG-CD-CE-NZ2
1	A	77	YCM	SG-CD-CE-OZ1
1	A	77	YCM	SG-CD-CE-NZ2
1	H	77	YCM	CA-CB-SG-CD
1	F	77	YCM	CA-CB-SG-CD
1	D	77	YCM	CA-CB-SG-CD
1	B	77	YCM	CA-CB-SG-CD

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Mol	Chain	Res	Type	Atoms
1	C	77	YCM	CA-CB-SG-CD
1	A	77	YCM	CE-CD-SG-CB
1	E	77	YCM	CA-CB-SG-CD

There are no ring outliers.

8 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	G	77	YCM	1	0
1	H	77	YCM	2	0
1	F	77	YCM	1	0
1	D	77	YCM	3	0
1	B	77	YCM	1	0
1	E	77	YCM	1	0
1	C	77	YCM	3	0
1	A	77	YCM	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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.

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

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	158/168 (94%)	-0.53	1 (0%) 89   88	16, 26, 46, 68	0
1	B	158/168 (94%)	-0.57	0 100   100	15, 25, 47, 72	0
1	C	158/168 (94%)	-0.52	0 100   100	16, 26, 49, 76	0
1	D	158/168 (94%)	-0.49	0 100   100	14, 25, 46, 73	0
1	E	158/168 (94%)	-0.51	1 (0%) 89   88	17, 25, 51, 71	0
1	F	157/168 (93%)	-0.55	0 100   100	16, 25, 50, 68	0
1	G	155/168 (92%)	-0.56	0 100   100	15, 24, 44, 60	0
1	H	158/168 (94%)	-0.49	2 (1%) 77   75	16, 26, 49, 72	0
All	All	1260/1344 (93%)	-0.53	4 (0%) 94   93	14, 25, 49, 76	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	1	SER	2.5
1	A	72	PRO	2.3
1	E	1	SER	2.2
1	H	71	VAL	2.0

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	YCM	A	77	10/11	0.88	0.15	26,31,46,62	0
1	YCM	G	77	10/11	0.91	0.12	26,39,40,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	YCM	C	77	10/11	0.92	0.12	29,35,38,43	0
1	YCM	F	77	10/11	0.93	0.13	29,41,44,45	0
1	YCM	D	77	10/11	0.93	0.12	31,35,43,45	0
1	YCM	H	77	10/11	0.94	0.13	27,37,44,45	0
1	YCM	B	77	10/11	0.95	0.10	27,30,33,37	0
1	YCM	E	77	10/11	0.95	0.08	31,33,42,42	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates 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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
2	FE	D	205	1/1	0.85	0.09	42,42,42,42	1
2	FE	E	204	1/1	0.85	0.15	44,44,44,44	1
2	FE	H	203	1/1	0.86	0.18	36,36,36,36	1
2	FE	B	205	1/1	0.86	0.14	39,39,39,39	1
2	FE	C	203	1/1	0.89	0.07	43,43,43,43	1
2	FE	F	203	1/1	0.90	0.12	43,43,43,43	1
2	FE	D	204	1/1	0.91	0.07	46,46,46,46	1
2	FE	B	203	1/1	0.93	0.06	46,46,46,46	1
2	FE	G	203	1/1	0.94	0.08	42,42,42,42	1
2	FE	D	203	1/1	0.94	0.12	47,47,47,47	1
2	FE	F	204	1/1	0.94	0.09	41,41,41,41	1
2	FE	E	203	1/1	0.94	0.12	47,47,47,47	1
2	FE	H	202	1/1	0.95	0.10	40,40,40,40	1
2	FE	H	204	1/1	0.96	0.28	33,33,33,33	1
2	FE	A	205	1/1	0.97	0.05	39,39,39,39	1
2	FE	B	204	1/1	0.97	0.13	43,43,43,43	1
2	FE	C	204	1/1	0.97	0.11	37,37,37,37	1
2	FE	F	202	1/1	0.97	0.09	46,46,46,46	1
2	FE	G	204	1/1	0.97	0.08	47,47,47,47	1
2	FE	C	201	1/1	0.98	0.04	38,38,38,38	0
2	FE	G	202	1/1	0.98	0.04	39,39,39,39	0
2	FE	E	202	1/1	0.98	0.10	44,44,44,44	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	FE	D	202	1/1	0.98	0.06	42,42,42,42	1
2	FE	A	203	1/1	0.98	0.06	52,52,52,52	1
2	FE	A	204	1/1	0.98	0.12	39,39,39,39	1
2	FE	D	201	1/1	0.99	0.06	38,38,38,38	1
2	FE	E	201	1/1	0.99	0.08	39,39,39,39	1
2	FE	B	201	1/1	0.99	0.06	38,38,38,38	1
2	FE	A	201	1/1	0.99	0.09	39,39,39,39	1
2	FE	A	202	1/1	0.99	0.11	42,42,42,42	1
2	FE	C	202	1/1	0.99	0.05	43,43,43,43	1
2	FE	G	201	1/1	0.99	0.07	40,40,40,40	0
2	FE	B	202	1/1	0.99	0.07	41,41,41,41	1
2	FE	F	201	1/1	0.99	0.05	42,42,42,42	0
2	FE	H	201	1/1	0.99	0.10	38,38,38,38	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.