



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:36 PM GMT

PDB ID : 4ITW  
Title : Anaerobic crystal structure of iron soaked (75 min) ferritin from Pseudonitzschia multiseriis  
Authors : Pfaffen, S.; Murphy, M.E.P.  
Deposited on : 2013-01-18  
Resolution : 2.00 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  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

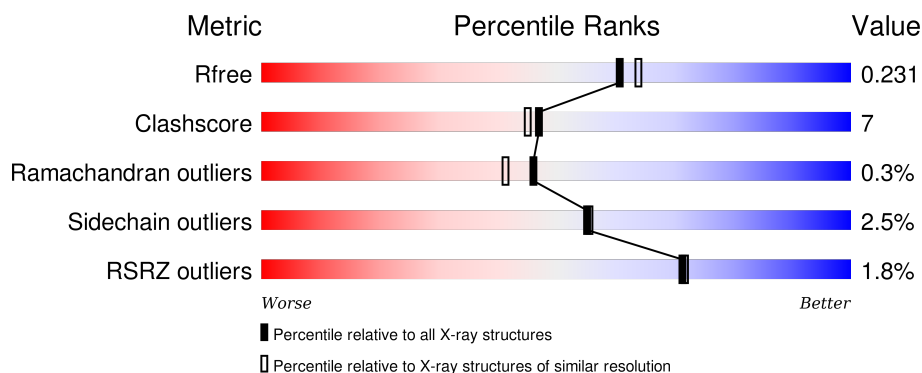
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
$R_{free}$	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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. 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	<div> <div>2%</div> <div>76% 15% • 7%</div> </div>
1	B	168	<div> <div>%</div> <div>85% 9% • 6%</div> </div>
1	C	168	<div> <div>2%</div> <div>81% 11% • 7%</div> </div>
1	D	168	<div> <div>2%</div> <div>80% 11% • 6%</div> </div>
1	E	168	<div> <div>2%</div> <div>83% 10% • 7%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	168	 83% 8% • 7%
1	G	168	 79% 13% • 8%
1	H	168	 82% 11% • 6%

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
1	YCM	E	77	-	-	X	-
1	YCM	H	77[A]	-	-	X	-

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11077 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
1	A	156	Total	C	N	O	S	0	6	0
			1277	803	211	258	5			
1	D	158	Total	C	N	O	S	0	7	0
			1298	813	216	264	5			
1	B	158	Total	C	N	O	S	0	5	0
			1284	806	213	259	6			
1	C	156	Total	C	N	O	S	0	3	0
			1260	790	210	254	6			
1	E	157	Total	C	N	O	S	0	3	0
			1265	794	210	256	5			
1	F	156	Total	C	N	O	S	0	5	0
			1274	801	211	256	6			
1	G	155	Total	C	N	O	S	0	7	0
			1277	805	211	255	6			
1	H	158	Total	C	N	O	S	0	4	0
			1281	802	214	259	6			

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).

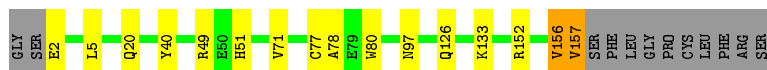
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total Fe 1 1	0	0
2	D	1	Total Fe 1 1	0	0
2	E	1	Total Fe 1 1	0	0
2	H	1	Total Fe 1 1	0	0
2	B	1	Total Fe 1 1	0	0
2	C	1	Total Fe 1 1	0	0
2	A	1	Total Fe 1 1	0	0
2	F	1	Total Fe 1 1	0	0

- Molecule 3 is water.


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	97	Total O 97 97	0	0
3	D	114	Total O 114 114	0	0
3	B	115	Total O 115 115	0	0
3	C	103	Total O 103 103	0	0
3	E	116	Total O 116 116	0	0
3	F	103	Total O 103 103	0	0
3	G	108	Total O 108 108	0	0
3	H	97	Total O 97 97	0	0



Chain F:  83% 8% • 7%




• Molecule 1: Ferritin

Chain G:  79% 13% • 8%



• Molecule 1: Ferritin

Chain H:  82% 11% • 6%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	174.77Å 174.77Å 174.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.52 – 2.00 46.71 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.52-2.00) 99.8 (46.71-2.00)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.73 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.187 , 0.235 0.182 , 0.231	Depositor DCC
$R_{free}$ test set	5967 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	29.8	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 57.9	EDS
Estimated twinning fraction	0.037 for l,-k,h	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	1 of 119181 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	11077	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.04% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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	0.98	0/1295	0.95	3/1762 (0.2%)
1	B	0.98	0/1292	0.98	2/1757 (0.1%)
1	C	1.01	2/1265 (0.2%)	1.01	4/1720 (0.2%)
1	D	1.04	1/1316 (0.1%)	1.01	3/1790 (0.2%)
1	E	0.97	0/1280	1.02	3/1741 (0.2%)
1	F	0.96	0/1282	0.96	2/1744 (0.1%)
1	G	1.00	0/1288	0.99	2/1753 (0.1%)
1	H	1.04	0/1286	0.99	3/1749 (0.2%)
All	All	1.00	3/10304 (0.0%)	0.99	22/14016 (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	B	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	34	TRP	CE3-CZ3	6.49	1.49	1.38
1	D	76	SER	CB-OG	-5.55	1.35	1.42
1	C	6	ASP	CB-CG	-5.16	1.41	1.51

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	62	ARG	NE-CZ-NH1	-8.76	115.92	120.30
1	F	49	ARG	NE-CZ-NH1	-8.73	115.93	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	49	ARG	NE-CZ-NH1	-8.23	116.18	120.30
1	G	62	ARG	NE-CZ-NH1	-8.10	116.25	120.30
1	B	62	ARG	NE-CZ-NH1	-7.43	116.58	120.30
1	D	49	ARG	NE-CZ-NH1	-7.25	116.68	120.30
1	H	49	ARG	NE-CZ-NH1	-6.53	117.03	120.30
1	D	61	LYS	CD-CE-NZ	-6.43	96.90	111.70
1	E	62	ARG	NE-CZ-NH1	-6.30	117.15	120.30
1	F	49	ARG	NE-CZ-NH2	6.28	123.44	120.30
1	A	49	ARG	NE-CZ-NH1	-5.99	117.31	120.30
1	C	152	ARG	NE-CZ-NH1	5.97	123.28	120.30
1	C	5	LEU	CB-CG-CD2	5.71	120.71	111.00
1	H	150	LEU	CB-CG-CD2	-5.61	101.46	111.00
1	D	146	ARG	NE-CZ-NH2	-5.35	117.63	120.30
1	E	93	LEU	CB-CG-CD2	-5.33	101.93	111.00
1	A	33	ASP	CB-CG-OD1	5.28	123.05	118.30
1	G	113	ASP	CB-CG-OD1	5.25	123.02	118.30
1	C	152	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	B	152	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	H	62	ARG	CG-CD-NE	-5.09	101.10	111.80
1	C	6	ASP	CB-CG-OD2	-5.04	113.77	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	157	VAL	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	1277	0	1210	22	0
1	B	1284	0	1221	14	0
1	C	1260	0	1192	14	0
1	D	1298	0	1227	19	0
1	E	1265	0	1197	17	0
1	F	1274	0	1207	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	1277	0	1218	28	0
1	H	1281	0	1211	20	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	97	0	0	3	0
3	B	115	0	0	5	0
3	C	103	0	0	3	0
3	D	114	0	0	5	0
3	E	116	0	0	4	0
3	F	103	0	0	1	0
3	G	108	0	0	2	0
3	H	97	0	0	0	0
All	All	11077	0	9683	149	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 7.

All (149) 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:10:ARG:HH11	1:D:10:ARG:HG3	1.08	1.16
1:H:24[A]:SER:OG	1:H:77[A]:YCM:OZ1	1.61	1.15
1:D:157:VAL:HG12	1:D:158:SER:H	1.02	1.11
1:G:94:GLU:HG3	1:G:134[A]:ILE:CD1	1.85	1.07
1:B:77[B]:YCM:HD2	1:B:78:ALA:H	1.15	1.07
1:B:77[B]:YCM:HD2	1:B:78:ALA:N	1.70	1.05
1:D:77:YCM:HB3	3:D:398:HOH:O	1.58	1.01
1:B:145:ASN:HB2	3:B:387:HOH:O	1.57	1.00
1:E:94:GLU:HG3	1:E:134:ILE:HD13	1.45	0.98
1:D:157:VAL:HG12	1:D:158:SER:N	1.79	0.96
1:B:157:VAL:HG12	1:B:158:SER:HB2	1.47	0.95
1:E:77:YCM:HB3	3:E:337:HOH:O	1.65	0.95
1:D:69:GLN:HG3	3:D:326:HOH:O	1.67	0.94
1:C:40:TYR:OH	1:C:133:LYS:HE2	1.70	0.92
1:D:10:ARG:CG	1:D:10:ARG:HH11	1.82	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:77[A]:YCM:SG	1:C:77[A]:YCM:O	2.31	0.86
1:E:94:GLU:HG3	1:E:134:ILE:CD1	2.05	0.86
1:G:3:GLU:OE1	1:G:5[B]:LEU:HD12	1.76	0.84
1:A:6[B]:ASP:OD2	1:A:10:ARG:NH2	2.13	0.81
1:E:77:YCM:HZ21	1:E:78:ALA:N	1.78	0.81
1:G:10:ARG:HH11	1:G:10:ARG:HG2	1.46	0.80
1:D:157:VAL:CG1	1:D:158:SER:H	1.87	0.80
1:D:10:ARG:CG	1:D:10:ARG:NH1	2.44	0.79
1:G:10:ARG:HH11	1:G:10:ARG:CG	1.95	0.79
1:D:146:ARG:NH2	3:D:314:HOH:O	2.16	0.79
1:A:94:GLU:HG3	1:A:134[A]:ILE:CD1	2.14	0.78
1:D:10:ARG:NH1	1:D:10:ARG:HG3	1.88	0.78
1:C:130:GLU:O	1:C:134:ILE:HD12	1.84	0.77
1:F:2:GLU:HA	1:F:2:GLU:OE1	1.84	0.76
1:H:76:SER:H	1:H:77[A]:YCM:HZ21	1.34	0.75
1:G:94:GLU:HG3	1:G:134[A]:ILE:HD13	1.67	0.75
1:E:157:VAL:O	1:E:157:VAL:HG12	1.85	0.73
1:E:1:SER:HA	1:E:4:LEU:HB3	1.69	0.72
1:A:5:LEU:HD13	1:A:65:PRO:HD2	1.70	0.72
1:D:157:VAL:CG1	1:D:158:SER:N	2.49	0.71
1:F:2:GLU:HG3	1:F:5[A]:LEU:HG	1.72	0.71
1:F:2:GLU:CG	1:F:5[A]:LEU:HG	2.21	0.70
1:C:155:ASP:O	1:C:156:VAL:HG13	1.92	0.70
1:G:153:SER:HB2	1:H:154:LEU:HD21	1.74	0.69
1:G:84:GLU:HG3	1:G:142[A]:THR:HG22	1.73	0.69
1:E:144:GLU:OE1	1:E:154:LEU:HG	1.92	0.69
1:H:77[B]:YCM:HB3	1:H:80:TRP:CZ3	2.28	0.68
1:H:24[B]:SER:OG	1:H:77[B]:YCM:HD2	1.94	0.68
1:H:94:GLU:HG3	1:H:134:ILE:HD13	1.76	0.67
1:B:24[A]:SER:HB2	1:B:77[A]:YCM:HZ21	1.61	0.66
1:C:40:TYR:OH	1:C:133:LYS:CE	2.43	0.65
1:B:48:GLU:OE2	3:B:357:HOH:O	2.14	0.64
1:A:94:GLU:HG3	1:A:134[A]:ILE:HD13	1.80	0.62
1:A:154:LEU:N	1:A:154:LEU:HD22	2.14	0.62
1:G:10:ARG:NH1	1:G:10:ARG:CG	2.59	0.62
1:H:51:HIS:CE1	1:H:126:GLN:HE22	2.18	0.62
1:F:97:ASN:HB3	3:F:387:HOH:O	1.99	0.61
1:H:77[B]:YCM:SG	1:H:77[B]:YCM:O	2.58	0.61
1:H:51:HIS:HE1	1:H:126:GLN:HE22	1.49	0.61
1:A:154:LEU:N	1:A:154:LEU:CD2	2.64	0.60
1:C:6:ASP:OD2	1:C:10:ARG:NH2	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:94:GLU:HG3	1:G:134[A]:ILE:HD12	1.81	0.60
1:H:76:SER:N	1:H:77[A]:YCM:HZ21	2.01	0.59
1:A:153:SER:C	1:A:154:LEU:HD22	2.23	0.58
1:A:2:GLU:HG3	1:A:5:LEU:H	1.67	0.58
1:B:124:HIS:HE1	3:B:415:HOH:O	1.86	0.58
1:C:155:ASP:O	1:C:156:VAL:CG1	2.52	0.58
1:E:77:YCM:HZ21	1:E:77:YCM:C	2.17	0.58
1:D:138:LEU:O	1:D:142:THR:HG23	2.03	0.58
1:E:77:YCM:NZ2	1:E:78:ALA:N	2.52	0.57
1:H:157:VAL:HG12	1:H:158:SER:OG	2.03	0.57
1:F:77[B]:YCM:HA	1:F:80:TRP:CE3	2.39	0.57
1:G:5[A]:LEU:HD13	1:G:65:PRO:HD2	1.86	0.57
1:A:14:GLN:HE21	1:A:97:ASN:ND2	2.03	0.56
1:E:157:VAL:O	1:E:157:VAL:CG1	2.51	0.56
1:E:124:HIS:HE1	3:E:301:HOH:O	1.87	0.56
1:F:77[A]:YCM:HA	1:F:80:TRP:CE3	2.39	0.56
1:C:146:ARG:NH1	3:C:386:HOH:O	2.35	0.56
1:A:100[B]:SER:O	1:A:103:ASN:HB2	2.05	0.56
1:F:40:TYR:OH	1:F:133:LYS:HE3	2.06	0.56
1:B:157:VAL:CG1	1:B:158:SER:HB2	2.29	0.55
1:C:94:GLU:HG3	1:C:134:ILE:HD13	1.86	0.55
1:H:76:SER:N	1:H:77[A]:YCM:HD2	2.21	0.55
1:G:156:VAL:O	1:G:156:VAL:HG23	2.07	0.55
1:D:156:VAL:HG21	1:G:154:LEU:HD12	1.88	0.55
1:B:145:ASN:CB	3:B:387:HOH:O	2.32	0.54
1:G:94:GLU:HG3	1:G:134[A]:ILE:HD11	1.85	0.53
1:A:146:ARG:NH2	3:A:326:HOH:O	2.41	0.53
1:H:77[A]:YCM:HA	1:H:80:TRP:CE3	2.43	0.53
1:E:5:LEU:HD13	1:E:65:PRO:HD2	1.91	0.53
1:G:3:GLU:HG3	1:G:6[A]:ASP:H	1.73	0.53
1:F:77[A]:YCM:OZ1	1:F:78:ALA:N	2.41	0.53
1:G:77[B]:YCM:HA	1:G:80:TRP:CE3	2.44	0.52
1:A:51:HIS:HE1	1:A:126:GLN:HE22	1.58	0.52
1:G:153:SER:O	1:G:156:VAL:HG22	2.09	0.52
1:D:5:LEU:HD13	1:D:65:PRO:HD2	1.92	0.52
1:A:156:VAL:HG12	1:A:156:VAL:O	2.10	0.51
1:A:150:LEU:O	1:A:154:LEU:HD23	2.11	0.50
1:F:2:GLU:OE1	1:F:2:GLU:CA	2.52	0.50
1:C:77[B]:YCM:HD2	3:C:359:HOH:O	2.12	0.49
1:G:3:GLU:HG3	1:G:6[B]:ASP:H	1.77	0.49
1:A:14:GLN:HE21	1:A:97:ASN:HD22	1.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:24[A]:SER:HB2	1:G:77[A]:YCM:HD2	1.95	0.49
1:B:150:LEU:O	1:B:154:LEU:HD23	2.12	0.49
1:A:124:HIS:HE1	3:A:308:HOH:O	1.96	0.49
1:G:138:LEU:O	1:G:142[A]:THR:HG23	2.12	0.48
1:G:124:HIS:HE1	3:G:306:HOH:O	1.96	0.48
1:F:156:VAL:O	1:F:157:VAL:HG12	2.14	0.48
1:A:51:HIS:CE1	1:A:126:GLN:HE22	2.32	0.48
1:A:77:YCM:HA	1:A:80:TRP:CE3	2.49	0.47
1:H:24[A]:SER:CB	1:H:77[A]:YCM:OZ1	2.58	0.47
1:G:6[A]:ASP:OD2	1:G:10:ARG:NE	2.42	0.47
1:D:40:TYR:OH	1:D:133:LYS:HE3	2.15	0.47
1:F:20:GLN:HG3	1:F:71:VAL:HG11	1.97	0.46
1:B:146:ARG:NH1	3:B:343:HOH:O	2.48	0.46
1:H:154:LEU:CD2	1:H:154:LEU:N	2.79	0.46
1:F:51:HIS:CE1	1:F:126:GLN:HE22	2.33	0.46
1:D:145[B]:ASN:ND2	3:D:383:HOH:O	2.48	0.45
1:E:77:YCM:HD2	3:E:404:HOH:O	2.16	0.45
1:G:3:GLU:CD	1:G:5[B]:LEU:HD12	2.35	0.45
1:H:154:LEU:HD22	1:H:154:LEU:N	2.32	0.45
1:C:5:LEU:O	1:C:5:LEU:HG	1.98	0.45
1:F:156:VAL:HG23	1:F:156:VAL:O	2.18	0.44
3:D:388:HOH:O	1:G:140:LYS:HE3	2.18	0.44
1:B:77[A]:YCM:HA	1:B:80:TRP:CE3	2.53	0.44
1:G:77[A]:YCM:HA	1:G:80:TRP:CE3	2.53	0.44
1:F:51:HIS:HE1	1:F:126:GLN:HE22	1.65	0.43
1:A:124:HIS:HD2	3:A:370:HOH:O	2.02	0.43
1:C:77[B]:YCM:HA	1:C:80:TRP:CE3	2.54	0.43
1:C:5:LEU:HD11	1:C:65:PRO:O	2.19	0.43
1:A:77:YCM:HB2	1:A:80:TRP:CZ3	2.54	0.43
1:A:77:YCM:HA	1:A:80:TRP:CD2	2.54	0.43
1:B:77[B]:YCM:HA	1:B:80:TRP:CE3	2.54	0.43
1:C:134:ILE:HD11	3:C:305:HOH:O	2.18	0.43
1:E:1:SER:HA	1:E:4:LEU:CB	2.46	0.43
1:G:94:GLU:CG	1:G:134[A]:ILE:HD13	2.43	0.43
1:E:77:YCM:HA	1:E:80:TRP:CE3	2.53	0.43
1:F:20:GLN:CG	1:F:71:VAL:HG11	2.49	0.42
1:H:76:SER:CA	1:H:77[A]:YCM:HD2	2.45	0.42
1:D:140:LYS:O	1:D:144:GLU:HG3	2.20	0.42
1:E:146:ARG:NH1	3:E:320:HOH:O	2.52	0.42
1:H:7:LEU:HD23	1:H:7:LEU:HA	1.73	0.42
1:G:146:ARG:NH1	3:G:394:HOH:O	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:77[A]:YCM:OZ1	1:F:78:ALA:HB2	2.19	0.42
1:H:116:VAL:O	1:H:120:LEU:HG	2.20	0.41
1:E:77:YCM:NZ2	1:E:78:ALA:CA	2.84	0.41
1:H:6:ASP:O	1:H:10:ARG:HB3	2.21	0.41
1:F:20:GLN:HG3	1:F:71:VAL:CG1	2.51	0.41
1:A:84:GLU:CD	1:A:142[A]:THR:HG22	2.41	0.41
1:D:51:HIS:CE1	1:D:126:GLN:OE1	2.75	0.40
1:G:116:VAL:O	1:G:120:LEU:HG	2.21	0.40
1:D:125:LEU:HD23	1:D:125:LEU:HA	1.94	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	159/168 (95%)	157 (99%)	1 (1%)	1 (1%)	30	22
1	B	159/168 (95%)	155 (98%)	3 (2%)	1 (1%)	30	22
1	C	155/168 (92%)	153 (99%)	2 (1%)	0	100	100
1	D	162/168 (96%)	160 (99%)	1 (1%)	1 (1%)	30	22
1	E	157/168 (94%)	153 (98%)	4 (2%)	0	100	100
1	F	157/168 (94%)	154 (98%)	2 (1%)	1 (1%)	30	22
1	G	158/168 (94%)	156 (99%)	2 (1%)	0	100	100
1	H	158/168 (94%)	155 (98%)	3 (2%)	0	100	100
All	All	1265/1344 (94%)	1243 (98%)	18 (1%)	4 (0%)	46	41

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	156	VAL

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Mol	Chain	Res	Type
1	D	157	VAL
1	F	156	VAL
1	B	157	VAL

### 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	139/143 (97%)	134 (96%)	5 (4%)	42	39
1	B	139/143 (97%)	137 (99%)	2 (1%)	74	77
1	C	135/143 (94%)	129 (96%)	6 (4%)	35	30
1	D	142/143 (99%)	139 (98%)	3 (2%)	61	63
1	E	137/143 (96%)	134 (98%)	3 (2%)	60	62
1	F	137/143 (96%)	135 (98%)	2 (2%)	72	75
1	G	138/143 (96%)	136 (99%)	2 (1%)	74	77
1	H	138/143 (96%)	133 (96%)	5 (4%)	42	39
All	All	1105/1144 (97%)	1077 (98%)	28 (2%)	55	55

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

Mol	Chain	Res	Type
1	A	5	LEU
1	A	26[A]	SER
1	A	26[B]	SER
1	A	75	VAL
1	A	154	LEU
1	D	10	ARG
1	D	153	SER
1	D	158	SER
1	B	1	SER
1	B	106	GLU
1	C	2	GLU
1	C	3	GLU

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Mol	Chain	Res	Type
1	C	5	LEU
1	C	6	ASP
1	C	79	GLU
1	C	153	SER
1	E	3	GLU
1	E	5	LEU
1	E	154	LEU
1	F	152	ARG
1	F	157	VAL
1	G	10	ARG
1	G	154	LEU
1	H	2	GLU
1	H	10	ARG
1	H	152	ARG
1	H	154	LEU
1	H	158	SER

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

Mol	Chain	Res	Type
1	A	20	GLN
1	A	51	HIS
1	A	97	ASN
1	A	121	ASN
1	A	124	HIS
1	D	51	HIS
1	D	69	GLN
1	D	95	GLN
1	B	63	ASN
1	B	69	GLN
1	B	121	ASN
1	B	124	HIS
1	C	63	ASN
1	E	63	ASN
1	E	121	ASN
1	E	124	HIS
1	F	126	GLN
1	G	121	ASN
1	G	124	HIS
1	H	51	HIS
1	H	69	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

13 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	8,9,10	1.64	1 (12%)	5,10,12	1.00	1 (20%)
1	YCM	B	77[A]	-	8,9,10	1.93	2 (25%)	5,10,12	1.59	2 (40%)
1	YCM	B	77[B]	-	8,9,10	1.23	2 (25%)	5,10,12	1.33	0
1	YCM	C	77[A]	1	8,9,10	1.64	1 (12%)	5,10,12	1.59	2 (40%)
1	YCM	C	77[B]	1	8,9,10	0.66	0	5,10,12	1.08	1 (20%)
1	YCM	D	77	1	8,9,10	2.03	1 (12%)	5,10,12	1.17	1 (20%)
1	YCM	E	77	1	8,9,10	0.94	0	5,10,12	1.64	1 (20%)
1	YCM	F	77[A]	-	8,9,10	1.35	1 (12%)	5,10,12	1.13	1 (20%)
1	YCM	F	77[B]	-	8,9,10	1.82	1 (12%)	5,10,12	1.22	1 (20%)
1	YCM	G	77[A]	1	8,9,10	2.03	2 (25%)	5,10,12	1.65	1 (20%)
1	YCM	G	77[B]	1	8,9,10	0.67	0	5,10,12	0.93	0
1	YCM	H	77[A]	1	8,9,10	2.21	1 (12%)	5,10,12	1.77	1 (20%)
1	YCM	H	77[B]	1	8,9,10	1.71	1 (12%)	5,10,12	1.80	2 (40%)

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[A]	-	-	0/6/8/10	0/0/0/0
1	YCM	B	77[B]	-	-	0/6/8/10	0/0/0/0
1	YCM	C	77[A]	1	-	0/6/8/10	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	YCM	C	77[B]	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[A]	-	-	0/6/8/10	0/0/0/0
1	YCM	F	77[B]	-	-	0/6/8/10	0/0/0/0
1	YCM	G	77[A]	1	-	0/6/8/10	0/0/0/0
1	YCM	G	77[B]	1	-	0/6/8/10	0/0/0/0
1	YCM	H	77[A]	1	-	0/6/8/10	0/0/0/0
1	YCM	H	77[B]	1	-	0/6/8/10	0/0/0/0

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	77[B]	YCM	CD-SG	-2.15	1.77	1.81
1	B	77[B]	YCM	CB-SG	2.29	1.85	1.81
1	F	77[A]	YCM	CB-SG	2.47	1.86	1.81
1	G	77[A]	YCM	CB-SG	3.23	1.87	1.81
1	B	77[A]	YCM	CB-SG	3.45	1.88	1.81
1	B	77[A]	YCM	CD-SG	4.06	1.90	1.81
1	G	77[A]	YCM	CD-SG	4.10	1.90	1.81
1	H	77[B]	YCM	CD-SG	4.12	1.90	1.81
1	C	77[A]	YCM	CB-SG	4.24	1.89	1.81
1	F	77[B]	YCM	CD-SG	4.34	1.90	1.81
1	A	77	YCM	CB-SG	4.45	1.90	1.81
1	D	77	YCM	CB-SG	5.48	1.92	1.81
1	H	77[A]	YCM	CD-SG	5.55	1.93	1.81

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	77	YCM	O-C-CA	-2.67	118.54	125.49
1	B	77[A]	YCM	O-C-CA	-2.65	118.60	125.49
1	C	77[A]	YCM	O-C-CA	-2.44	119.14	125.49
1	F	77[B]	YCM	O-C-CA	-2.43	119.17	125.49
1	D	77	YCM	O-C-CA	-2.40	119.23	125.49
1	C	77[A]	YCM	CA-CB-SG	-2.34	107.31	112.84
1	C	77[B]	YCM	O-C-CA	-2.33	119.41	125.49
1	H	77[B]	YCM	O-C-CA	-2.23	119.67	125.49
1	A	77	YCM	O-C-CA	-2.14	119.91	125.49
1	F	77[A]	YCM	O-C-CA	-2.13	119.94	125.49
1	B	77[A]	YCM	CD-CE-NZ2	2.25	117.96	115.48
1	G	77[A]	YCM	CD-CE-NZ2	2.71	118.47	115.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	77[B]	YCM	CD-CE-NZ2	2.96	118.75	115.48
1	H	77[A]	YCM	CD-CE-NZ2	3.38	119.21	115.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

13 monomers are involved in 37 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	77	YCM	3	0
1	B	77[A]	YCM	2	0
1	B	77[B]	YCM	4	0
1	C	77[A]	YCM	1	0
1	C	77[B]	YCM	2	0
1	D	77	YCM	1	0
1	E	77	YCM	7	0
1	F	77[A]	YCM	3	0
1	F	77[B]	YCM	1	0
1	G	77[A]	YCM	2	0
1	G	77[B]	YCM	1	0
1	H	77[A]	YCM	7	0
1	H	77[B]	YCM	3	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	155/168 (92%)	-0.23	3 (1%) 70 70	22, 30, 46, 70	0
1	B	157/168 (93%)	-0.22	2 (1%) 79 80	20, 28, 46, 71	0
1	C	155/168 (92%)	-0.22	4 (2%) 59 60	21, 30, 47, 86	0
1	D	157/168 (93%)	-0.20	3 (1%) 70 70	18, 26, 49, 82	0
1	E	156/168 (92%)	-0.12	4 (2%) 59 60	21, 30, 49, 71	0
1	F	155/168 (92%)	-0.22	0 100 100	20, 29, 46, 69	0
1	G	154/168 (91%)	-0.23	2 (1%) 79 80	18, 26, 42, 69	0
1	H	157/168 (93%)	-0.09	4 (2%) 61 61	20, 28, 52, 68	0
All	All	1246/1344 (92%)	-0.19	22 (1%) 71 72	18, 28, 48, 86	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	156	VAL	6.5
1	B	157	VAL	6.3
1	H	157	VAL	6.0
1	E	156	VAL	5.2
1	G	153	SER	5.1
1	E	1	SER	4.8
1	B	156	VAL	4.8
1	D	157	VAL	3.5
1	H	154	LEU	3.4
1	H	153	SER	3.3
1	E	153	SER	3.2
1	C	1	SER	3.2
1	E	157	VAL	3.1
1	G	156	VAL	3.0
1	A	156	VAL	2.7
1	D	156	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	157	VAL	2.5
1	D	1	SER	2.4
1	A	153	SER	2.4
1	C	2	GLU	2.3
1	C	5	LEU	2.1
1	C	156	VAL	2.1

## 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. 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, 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	YCM	A	77	10/11	0.94	0.10	-	33,44,55,63	0
1	YCM	G	77[B]	10/11	0.80	0.22	-	27,34,37,37	10
1	YCM	C	77[A]	10/11	0.89	0.21	-	20,31,34,36	10
1	YCM	G	77[A]	10/11	0.80	0.22	-	21,38,42,42	10
1	YCM	E	77	10/11	0.93	0.13	-	38,49,58,61	0
1	YCM	H	77[A]	10/11	0.76	0.25	-	21,32,37,45	10
1	YCM	D	77	10/11	0.95	0.10	-	32,38,45,46	0
1	YCM	B	77[B]	10/11	0.92	0.19	-	29,32,36,43	7
1	YCM	B	77[A]	10/11	0.92	0.19	-	28,29,32,34	7
1	YCM	F	77[B]	10/11	0.79	0.22	-	24,34,37,42	7
1	YCM	H	77[B]	10/11	0.76	0.25	-	21,34,38,39	10
1	YCM	F	77[A]	10/11	0.79	0.22	-	30,35,42,43	7
1	YCM	C	77[B]	10/11	0.89	0.21	-	28,34,38,38	10

## 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. 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, 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	FE	H	201	1/1	0.99	0.11	0.29	35,35,35,35	1
2	FE	A	201	1/1	0.98	0.08	-	41,41,41,41	1
2	FE	D	201	1/1	0.97	0.12	-	42,42,42,42	1
2	FE	G	201	1/1	0.97	0.12	-	38,38,38,38	1
2	FE	B	201	1/1	0.95	0.09	-	42,42,42,42	1
2	FE	C	201	1/1	0.98	0.05	-	44,44,44,44	1
2	FE	E	201	1/1	0.97	0.11	-	40,40,40,40	1
2	FE	F	201	1/1	0.97	0.12	-	45,45,45,45	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.