



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 18, 2024 – 05:49 PM EDT

PDB ID : 4ITT
Title : Crystal structure of iron soaked (5 min) ferritin from Pseudo-nitzschia multi-series
Authors : Pfaffen, S.; Murphy, M.E.P.
Deposited on : 2013-01-18
Resolution : 2.10 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

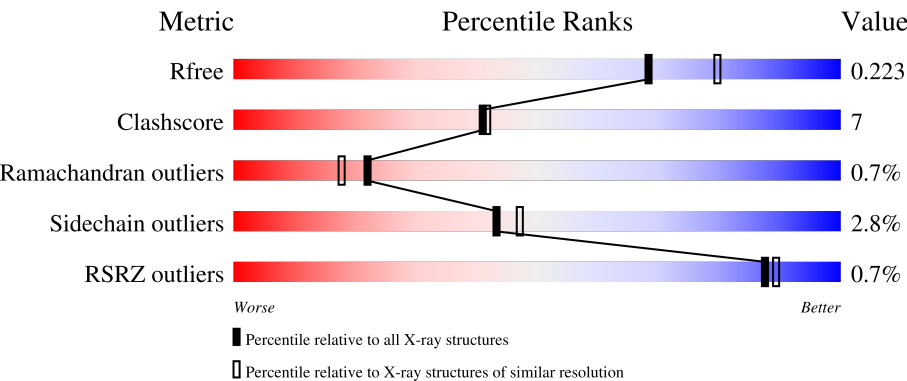
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	168	<div><div>%</div><div>85%8%• 5%</div></div>
1	B	168	<div><div>%</div><div>80%12%• 5%</div></div>
1	C	168	<div><div>%</div><div>83%10%•• 6%</div></div>
1	D	168	<div><div>%</div><div>88%5%• 6%</div></div>
1	E	168	<div><div>%</div><div>82%10%• 6%</div></div>

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Mol	Chain	Length	Quality of chain
1	F	168	<div><div>%</div><div><div></div><div>83%</div><div>8%</div><div>• •</div><div>7%</div></div></div>
1	G	168	<div><div>%</div><div><div></div><div>74%</div><div>13%</div><div>• •</div><div>7%</div></div></div>
1	H	168	<div><div></div><div><div>85%</div><div>8%</div><div>•</div><div>6%</div></div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11140 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	159	Total	C	N	O	S	0	5	0
			1298	815	215	262	6			
1	D	158	Total	C	N	O	S	0	6	0
			1296	810	217	263	6			
1	B	159	Total	C	N	O	S	0	4	0
			1292	811	215	260	6			
1	C	158	Total	C	N	O	S	0	4	0
			1281	803	214	258	6			
1	E	158	Total	C	N	O	S	0	7	0
			1297	813	215	263	6			
1	F	157	Total	C	N	O	S	0	3	0
			1265	794	210	256	5			
1	G	156	Total	C	N	O	S	0	7	0
			1285	806	215	258	6			
1	H	158	Total	C	N	O	S	0	7	0
			1299	814	216	263	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	D	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	E	1	Total Fe 1 1	0	0
2	G	1	Total Fe 1 1	0	0
2	H	1	Total Fe 1 1	0	0

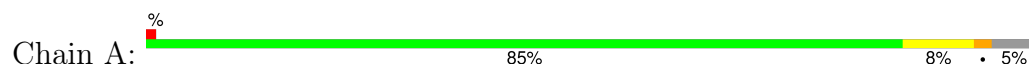
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	97	Total O 97 97	0	0
3	D	106	Total O 106 106	0	0
3	B	99	Total O 99 99	0	0
3	C	106	Total O 106 106	0	0
3	E	106	Total O 106 106	0	0
3	F	94	Total O 94 94	0	0
3	G	113	Total O 113 113	0	0
3	H	100	Total O 100 100	0	0

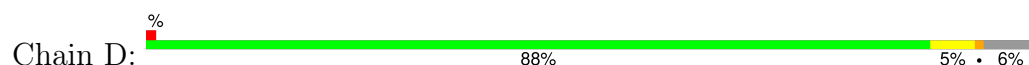
3 Residue-property plots [i](#)

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.

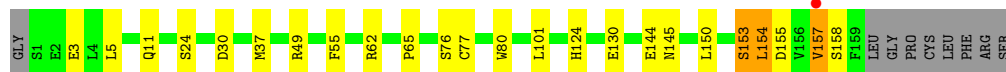
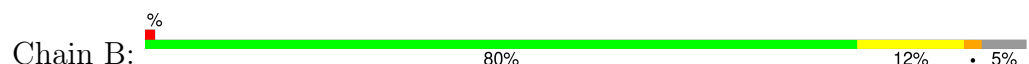
- Molecule 1: Ferritin



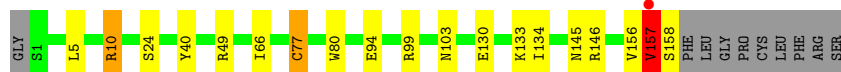
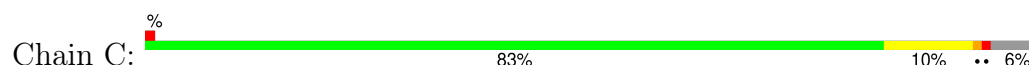
- Molecule 1: Ferritin



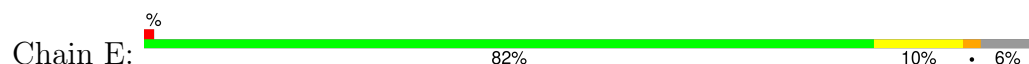
- Molecule 1: Ferritin



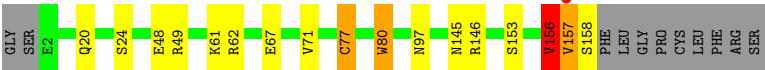
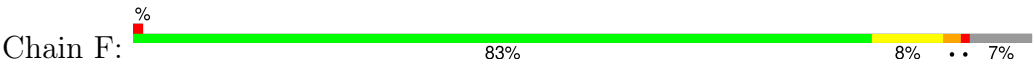
- Molecule 1: Ferritin



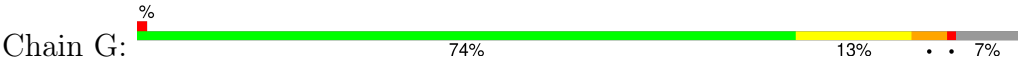
- Molecule 1: Ferritin



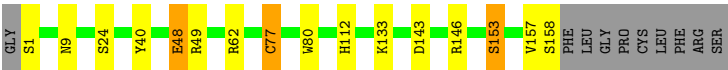
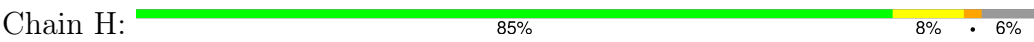
- Molecule 1: Ferritin



● Molecule 1: Ferritin



● Molecule 1: Ferritin



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 3	Depositor
Cell constants a, b, c, α , β , γ	175.28Å 175.28Å 175.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.55 – 2.10 42.51 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.6 (42.55-2.10) 99.6 (42.51-2.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.60 (at 2.10Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.176 , 0.225 0.174 , 0.223	Depositor DCC
R_{free} test set	5180 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	24.2	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 49.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.032 for l,-k,h	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11140	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.06% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: YCM, FE

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	0/1307	0.93	1/1778 (0.1%)
1	B	1.01	0/1298	0.95	2/1765 (0.1%)
1	C	1.05	0/1289	0.97	2/1753 (0.1%)
1	D	1.03	0/1301	0.97	2/1769 (0.1%)
1	E	0.98	0/1308	0.91	3/1779 (0.2%)
1	F	0.96	1/1280 (0.1%)	0.94	2/1741 (0.1%)
1	G	1.04	2/1293 (0.2%)	0.93	3/1759 (0.2%)
1	H	1.00	1/1310 (0.1%)	0.95	1/1782 (0.1%)
All	All	1.01	4/10386 (0.0%)	0.94	16/14126 (0.1%)

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	H	48	GLU	CD-OE1	-6.04	1.19	1.25
1	G	3	GLU	N-CA	5.56	1.57	1.46
1	G	79	GLU	CD-OE2	5.24	1.31	1.25
1	F	80	TRP	CG-CD1	5.07	1.43	1.36

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	62	ARG	NE-CZ-NH1	-7.21	116.70	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	113	ASP	CB-CG-OD1	6.39	124.05	118.30
1	E	5	LEU	CB-CG-CD2	6.28	121.68	111.00
1	D	113	ASP	CB-CG-OD2	-6.24	112.69	118.30
1	H	62	ARG	NE-CZ-NH1	-6.07	117.26	120.30
1	G	93	LEU	CB-CG-CD2	5.93	121.08	111.00
1	G	62	ARG	NE-CZ-NH1	-5.88	117.36	120.30
1	E	41	MET	CG-SD-CE	5.80	109.49	100.20
1	E	62	ARG	NE-CZ-NH1	-5.80	117.40	120.30
1	A	62	ARG	NE-CZ-NH1	-5.76	117.42	120.30
1	B	101	LEU	CB-CG-CD1	-5.41	101.81	111.00
1	F	61	LYS	CD-CE-NZ	-5.38	99.31	111.70
1	B	62	ARG	NE-CZ-NH1	-5.35	117.62	120.30
1	C	99	ARG	NE-CZ-NH2	-5.27	117.67	120.30
1	G	6	ASP	CB-CG-OD2	5.15	122.94	118.30
1	C	103	ASN	CB-CA-C	-5.13	100.14	110.40

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 ⓘ

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	1298	0	1226	22	0
1	B	1292	0	1220	20	0
1	C	1281	0	1215	17	0
1	D	1296	0	1222	7	0
1	E	1297	0	1230	18	1
1	F	1265	0	1194	14	0
1	G	1285	0	1217	37	0
1	H	1299	0	1231	10	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	97	0	0	11	0
3	B	99	0	0	5	0
3	C	106	0	0	2	0
3	D	106	0	0	1	0
3	E	106	0	0	3	0
3	F	94	0	0	4	0
3	G	113	0	0	9	0
3	H	100	0	0	1	0
All	All	11140	0	9755	142	1

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 (142) 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:F:77:YCM:HB2	3:F:278:HOH:O	1.17	1.34
1:G:5[A]:LEU:HD22	1:G:5[A]:LEU:H	1.38	0.89
1:C:40:TYR:OH	1:C:133:LYS:HE3	1.72	0.89
1:G:94:GLU:HG3	1:G:134:ILE:HD13	1.55	0.88
1:G:5[A]:LEU:HD22	1:G:5[A]:LEU:N	1.92	0.83
1:A:77[A]:YCM:SG	3:A:245:HOH:O	2.35	0.83
1:F:48:GLU:OE2	3:F:291:HOH:O	1.96	0.83
1:E:4[B]:LEU:C	1:E:4[B]:LEU:HD23	2.00	0.80
1:G:9:ASN:HD21	1:G:67:GLU:H	1.26	0.80
1:H:40:TYR:OH	1:H:133:LYS:HE3	1.81	0.80
1:C:146:ARG:NH1	3:C:394:HOH:O	2.16	0.79
1:G:94:GLU:HG3	1:G:134:ILE:CD1	2.12	0.79
1:G:5[A]:LEU:H	1:G:5[A]:LEU:CD2	1.95	0.79
1:G:69:GLN:HG3	3:G:385:HOH:O	1.83	0.78
1:A:1:SER:O	1:A:5:LEU:HG	1.83	0.77
1:F:157:VAL:CG1	1:F:157:VAL:O	2.33	0.76
1:F:157:VAL:O	1:F:157:VAL:HG12	1.83	0.76
1:E:94:GLU:HG3	1:E:134:ILE:CD1	2.17	0.74
1:B:130:GLU:HG3	3:B:386:HOH:O	1.86	0.74
1:G:10:ARG:HG2	1:G:10:ARG:HH11	1.52	0.73
1:D:24[B]:SER:OG	1:D:77[B]:YCM:NZ2	2.21	0.73
1:E:157:VAL:HG12	1:E:158:SER:H	1.52	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:10:ARG:HH11	1:G:10:ARG:CG	2.02	0.72
1:A:154:LEU:HD11	1:H:153:SER:HB3	1.72	0.70
1:B:157:VAL:HG12	1:B:158:SER:N	2.07	0.70
1:A:48:GLU:OE2	3:A:296:HOH:O	2.10	0.70
1:D:1:SER:O	1:D:5:LEU:HG	1.92	0.68
1:B:30:ASP:CB	3:B:391:HOH:O	2.42	0.68
1:B:30:ASP:HB3	3:B:391:HOH:O	1.92	0.68
1:C:10:ARG:CG	1:C:10:ARG:HH21	2.06	0.67
1:E:4[B]:LEU:HD23	1:E:4[B]:LEU:O	1.94	0.67
1:C:130:GLU:O	1:C:134:ILE:HD12	1.95	0.67
1:E:144:GLU:OE1	1:E:154:LEU:HG	1.94	0.66
1:G:77[A]:YCM:HZ22	1:G:78:ALA:HB2	1.61	0.66
1:G:84:GLU:OE1	1:G:145[B]:ASN:ND2	2.28	0.66
1:F:24[B]:SER:HB2	1:F:77:YCM:HZ21	1.60	0.65
1:D:2:GLU:HA	1:D:2:GLU:OE1	1.97	0.65
1:B:157:VAL:HG12	1:B:158:SER:H	1.63	0.64
1:G:97[B]:ASN:ND2	3:G:412:HOH:O	2.18	0.63
1:B:77[B]:YCM:SG	1:B:77[B]:YCM:O	2.56	0.63
1:G:130:GLU:HG3	3:G:411:HOH:O	2.00	0.62
1:F:145:ASN:HB3	3:F:288:HOH:O	1.98	0.62
1:G:24[B]:SER:HB2	1:G:77[B]:YCM:HZ21	1.63	0.61
1:A:77[A]:YCM:CD	3:A:245:HOH:O	2.48	0.61
1:E:157:VAL:HG12	1:E:158:SER:N	2.13	0.61
1:B:124:HIS:HE1	3:B:378:HOH:O	1.83	0.61
1:G:9:ASN:HD21	1:G:67:GLU:N	1.98	0.60
1:A:153:SER:HB2	1:A:154:LEU:HD22	1.83	0.59
1:F:156:VAL:HG23	1:F:156:VAL:O	2.02	0.59
1:B:30:ASP:CG	3:B:391:HOH:O	2.42	0.59
1:F:156:VAL:O	1:F:157:VAL:HG23	2.03	0.58
1:G:77[B]:YCM:HA	1:G:80:TRP:CE3	2.38	0.58
1:H:48:GLU:HA	1:H:48:GLU:OE2	2.04	0.58
1:G:157:VAL:HG12	1:G:157:VAL:O	2.04	0.57
1:G:5[B]:LEU:HD13	1:G:65:PRO:HD2	1.87	0.57
1:E:4[B]:LEU:C	1:E:4[B]:LEU:CD2	2.74	0.56
1:A:153:SER:HB2	1:A:154:LEU:CD2	2.36	0.56
1:E:124:HIS:HE1	3:E:307:HOH:O	1.89	0.56
1:G:77[A]:YCM:HA	1:G:80:TRP:CE3	2.40	0.56
1:B:150:LEU:O	1:B:154:LEU:HD23	2.07	0.55
1:D:145[A]:ASN:ND2	3:D:385:HOH:O	2.39	0.55
1:B:153:SER:HB3	1:B:154:LEU:HD22	1.89	0.55
1:C:10:ARG:CG	1:C:10:ARG:NH2	2.68	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:10:ARG:CG	1:G:10:ARG:NH1	2.65	0.54
1:E:94:GLU:HG3	1:E:134:ILE:HD12	1.90	0.54
1:G:124:HIS:HE1	3:G:309:HOH:O	1.89	0.54
1:G:3:GLU:OE1	1:G:5[A]:LEU:HD23	2.08	0.54
1:A:77[A]:YCM:HA	1:A:80:TRP:CE3	2.43	0.53
1:A:142[A]:THR:CG2	3:A:216:HOH:O	2.54	0.53
1:F:97:ASN:HB3	3:F:202:HOH:O	2.08	0.53
1:F:77:YCM:HA	1:F:80:TRP:CE3	2.44	0.53
1:B:5:LEU:HD13	1:B:65:PRO:HD2	1.89	0.53
1:G:146:ARG:NH1	3:G:392:HOH:O	2.41	0.53
1:C:77[B]:YCM:HA	1:C:80:TRP:CE3	2.45	0.51
1:H:40:TYR:HH	1:H:133:LYS:HE3	1.73	0.51
1:C:156:VAL:C	1:C:158:SER:H	2.13	0.51
1:C:10:ARG:NH2	1:C:10:ARG:HG3	2.24	0.51
1:C:94:GLU:HG3	1:C:134:ILE:HD13	1.92	0.51
1:G:9:ASN:ND2	1:G:67:GLU:H	2.03	0.51
1:E:77[B]:YCM:HA	1:E:80:TRP:CE3	2.45	0.51
1:D:77[B]:YCM:HA	1:D:80:TRP:CE3	2.46	0.50
1:B:37:MET:HG3	1:B:155:ASP:OD1	2.11	0.50
1:G:153:SER:C	1:G:154:LEU:HD22	2.33	0.49
1:D:28:TRP:HB2	1:D:77[B]:YCM:HD2	1.95	0.49
1:B:157:VAL:CG1	1:B:158:SER:N	2.75	0.49
1:C:10:ARG:HH21	1:C:10:ARG:HG3	1.78	0.49
1:E:77[A]:YCM:HA	1:E:80:TRP:CE3	2.47	0.49
1:G:144:GLU:OE1	1:G:154:LEU:HG	2.12	0.49
1:B:144:GLU:OE1	1:B:154:LEU:HG	2.13	0.48
1:G:130:GLU:O	1:G:134:ILE:HD12	2.13	0.48
1:A:77[A]:YCM:HD3	3:A:245:HOH:O	2.13	0.48
1:G:3:GLU:OE1	1:G:5[A]:LEU:CD2	2.62	0.48
1:G:156:VAL:C	1:G:158:SER:H	2.16	0.48
1:A:124:HIS:HD2	3:A:273:HOH:O	1.97	0.48
1:A:153:SER:C	1:A:154:LEU:HD22	2.35	0.47
1:A:97:ASN:HB3	3:A:242:HOH:O	2.15	0.47
1:G:24[B]:SER:CB	1:G:77[B]:YCM:HZ21	2.27	0.47
1:E:11:GLN:HG2	1:E:55:PHE:CE2	2.49	0.47
1:A:77[B]:YCM:HA	1:A:80:TRP:CE3	2.49	0.47
1:F:20:GLN:HG3	1:F:71:VAL:HG11	1.96	0.47
1:H:9[A]:ASN:ND2	3:H:303:HOH:O	2.47	0.47
1:H:77[B]:YCM:HA	1:H:80:TRP:CE3	2.50	0.46
1:H:77[A]:YCM:HA	1:H:80:TRP:CE3	2.50	0.46
1:A:154:LEU:HD22	1:A:154:LEU:N	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77[B]:YCM:HD2	3:A:264:HOH:O	2.15	0.46
1:B:49:ARG:HD3	1:F:49:ARG:HD3	1.97	0.46
1:E:157:VAL:O	1:E:158:SER:C	2.55	0.46
1:E:148:PRO:HB3	1:F:146:ARG:CZ	2.46	0.45
1:G:3:GLU:HB2	1:G:4:LEU:H	1.59	0.45
1:E:69:GLN:NE2	3:E:402:HOH:O	2.48	0.45
1:A:157:VAL:HG12	1:A:158:SER:N	2.31	0.45
1:A:146:ARG:NH1	3:A:250:HOH:O	2.45	0.45
1:G:152:ARG:O	1:G:156:VAL:HG23	2.17	0.45
1:G:79:GLU:O	1:G:79:GLU:HG2	2.17	0.44
1:C:157:VAL:HG23	1:C:157:VAL:O	2.18	0.44
1:B:11:GLN:HG2	1:B:55:PHE:CE2	2.53	0.44
1:G:145[A]:ASN:ND2	3:G:302:HOH:O	2.50	0.44
1:B:76:SER:O	1:B:77[A]:YCM:C	2.64	0.43
1:C:77[B]:YCM:HA	1:C:80:TRP:CD2	2.52	0.43
1:G:124:HIS:HD2	3:G:384:HOH:O	2.01	0.43
1:A:24:SER:HB2	1:A:77[A]:YCM:HZ21	1.83	0.43
1:G:77[A]:YCM:NZ2	1:G:78:ALA:HB2	2.30	0.42
1:A:142[A]:THR:HG23	3:A:216:HOH:O	2.19	0.42
1:C:145[B]:ASN:ND2	3:C:301:HOH:O	2.52	0.42
1:F:156:VAL:O	1:F:156:VAL:CG2	2.67	0.42
1:G:77[A]:YCM:HD2	3:G:327:HOH:O	2.19	0.42
1:B:77[A]:YCM:HA	1:B:80:TRP:CE3	2.55	0.42
1:A:124:HIS:HE1	3:A:206:HOH:O	2.02	0.42
1:B:77[B]:YCM:HB3	1:B:80:TRP:CZ3	2.54	0.42
1:B:24[B]:SER:CB	1:B:77[B]:YCM:HZ21	2.32	0.42
1:C:24[B]:SER:OG	1:C:77[B]:YCM:NZ2	2.53	0.41
1:H:24[B]:SER:OG	1:H:77[B]:YCM:HD2	2.20	0.41
1:D:2:GLU:OE1	1:D:2:GLU:CA	2.66	0.41
1:C:66:ILE:HD13	1:C:66:ILE:HA	1.79	0.41
1:A:154:LEU:CD2	1:A:154:LEU:N	2.83	0.41
1:C:10:ARG:HH21	1:C:10:ARG:HG2	1.83	0.41
1:E:4[A]:LEU:HD12	1:E:4[A]:LEU:HA	1.87	0.41
1:H:143:ASP:HA	1:H:146:ARG:HD3	2.02	0.41
1:E:24[B]:SER:HB2	1:E:77[B]:YCM:HZ21	1.86	0.41
1:E:124:HIS:HD2	3:E:327:HOH:O	2.04	0.41
1:C:49:ARG:HD3	1:H:49:ARG:HD3	2.03	0.40

All (1) 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)
1:E:10:ARG:NH1	1:E:10:ARG:NH1[4_565]	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	160/168 (95%)	156 (98%)	3 (2%)	1 (1%)	25	21
1	B	159/168 (95%)	154 (97%)	4 (2%)	1 (1%)	25	21
1	C	158/168 (94%)	154 (98%)	3 (2%)	1 (1%)	25	21
1	D	160/168 (95%)	156 (98%)	3 (2%)	1 (1%)	25	21
1	E	161/168 (96%)	158 (98%)	2 (1%)	1 (1%)	25	21
1	F	157/168 (94%)	153 (98%)	2 (1%)	2 (1%)	12	7
1	G	159/168 (95%)	157 (99%)	1 (1%)	1 (1%)	25	21
1	H	161/168 (96%)	157 (98%)	3 (2%)	1 (1%)	25	21
All	All	1275/1344 (95%)	1245 (98%)	21 (2%)	9 (1%)	22	18

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	157	VAL
1	B	157	VAL
1	C	157	VAL
1	E	157	VAL
1	F	157	VAL
1	D	157	VAL
1	G	157	VAL
1	F	156	VAL
1	H	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	140/143 (98%)	137 (98%)	3 (2%)	53	59
1	B	139/143 (97%)	134 (96%)	5 (4%)	35	36
1	C	138/143 (96%)	135 (98%)	3 (2%)	52	57
1	D	140/143 (98%)	139 (99%)	1 (1%)	84	88
1	E	141/143 (99%)	137 (97%)	4 (3%)	43	47
1	F	137/143 (96%)	133 (97%)	4 (3%)	42	46
1	G	139/143 (97%)	131 (94%)	8 (6%)	20	17
1	H	141/143 (99%)	137 (97%)	4 (3%)	43	47
All	All	1115/1144 (98%)	1083 (97%)	32 (3%)	43	46

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	GLU
1	A	126	GLN
1	A	154	LEU
1	D	2	GLU
1	B	3	GLU
1	B	145[A]	ASN
1	B	145[B]	ASN
1	B	153	SER
1	B	154	LEU
1	C	5	LEU
1	C	10	ARG
1	C	157	VAL
1	E	79	GLU
1	E	152	ARG
1	E	154	LEU
1	E	158	SER
1	F	67	GLU
1	F	153	SER
1	F	156	VAL

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Mol	Chain	Res	Type
1	F	158	SER
1	G	3	GLU
1	G	5[A]	LEU
1	G	5[B]	LEU
1	G	10	ARG
1	G	79	GLU
1	G	93	LEU
1	G	154	LEU
1	G	158	SER
1	H	1	SER
1	H	112	HIS
1	H	153	SER
1	H	158	SER

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

Mol	Chain	Res	Type
1	A	69	GLN
1	A	121	ASN
1	A	124	HIS
1	D	63	ASN
1	D	112	HIS
1	B	63	ASN
1	B	69	GLN
1	B	121	ASN
1	B	124	HIS
1	E	63	ASN
1	E	121	ASN
1	E	124	HIS
1	G	9	ASN
1	G	121	ASN
1	G	124	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

15 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	C	77[A]	1	7,9,10	0.68	0	5,10,12	0.71	0
1	YCM	C	77[B]	1	7,9,10	1.30	1 (14%)	5,10,12	0.43	0
1	YCM	H	77[A]	-	7,9,10	1.00	1 (14%)	5,10,12	0.69	0
1	YCM	H	77[B]	-	7,9,10	1.45	2 (28%)	5,10,12	0.47	0
1	YCM	D	77[A]	1	7,9,10	1.16	1 (14%)	5,10,12	1.00	1 (20%)
1	YCM	D	77[B]	1	7,9,10	1.46	1 (14%)	5,10,12	0.71	0
1	YCM	A	77[A]	1	7,9,10	2.27	2 (28%)	5,10,12	0.68	0
1	YCM	A	77[B]	1	7,9,10	1.08	1 (14%)	5,10,12	1.25	1 (20%)
1	YCM	E	77[A]	-	7,9,10	0.92	0	5,10,12	0.66	0
1	YCM	E	77[B]	-	7,9,10	1.69	2 (28%)	5,10,12	0.88	0
1	YCM	B	77[A]	1	7,9,10	0.96	0	5,10,12	0.70	0
1	YCM	B	77[B]	1	7,9,10	1.01	0	5,10,12	0.57	0
1	YCM	G	77[B]	-	7,9,10	1.90	1 (14%)	5,10,12	0.54	0
1	YCM	G	77[A]	-	7,9,10	0.82	0	5,10,12	0.62	0
1	YCM	F	77	1	7,9,10	2.52	2 (28%)	5,10,12	0.38	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	C	77[A]	1	-	2/6/8/10	-
1	YCM	C	77[B]	1	-	1/6/8/10	-
1	YCM	H	77[A]	-	-	1/6/8/10	-
1	YCM	H	77[B]	-	-	1/6/8/10	-
1	YCM	D	77[A]	1	-	1/6/8/10	-
1	YCM	D	77[B]	1	-	1/6/8/10	-
1	YCM	A	77[A]	1	-	0/6/8/10	-
1	YCM	A	77[B]	1	-	2/6/8/10	-
1	YCM	E	77[A]	-	-	3/6/8/10	-
1	YCM	E	77[B]	-	-	1/6/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	YCM	B	77[A]	1	-	3/6/8/10	-
1	YCM	B	77[B]	1	-	1/6/8/10	-
1	YCM	G	77[B]	-	-	1/6/8/10	-
1	YCM	G	77[A]	-	-	3/6/8/10	-
1	YCM	F	77	1	-	0/6/8/10	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	77	YCM	CD-SG	5.61	1.95	1.81
1	A	77[A]	YCM	CD-SG	5.38	1.95	1.81
1	G	77[B]	YCM	CD-SG	3.98	1.91	1.81
1	D	77[A]	YCM	CD-SG	-2.86	1.74	1.81
1	E	77[B]	YCM	CD-SG	2.85	1.88	1.81
1	E	77[B]	YCM	CB-SG	2.67	1.91	1.81
1	F	77	YCM	CB-SG	2.44	1.90	1.81
1	H	77[B]	YCM	CD-SG	2.34	1.87	1.81
1	A	77[B]	YCM	CD-SG	-2.23	1.76	1.81
1	C	77[B]	YCM	CD-SG	2.23	1.87	1.81
1	H	77[A]	YCM	O-C	2.19	1.28	1.20
1	H	77[B]	YCM	O-C	2.19	1.28	1.20
1	A	77[A]	YCM	CB-SG	2.14	1.89	1.81
1	D	77[B]	YCM	CB-SG	2.12	1.89	1.81

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	77[B]	YCM	CE-CD-SG	-2.17	106.95	113.81
1	D	77[A]	YCM	CE-CD-SG	-2.03	107.41	113.81

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	77[B]	YCM	C-CA-CB-SG
1	D	77[B]	YCM	SG-CD-CE-NZ2
1	B	77[A]	YCM	N-CA-CB-SG
1	B	77[A]	YCM	C-CA-CB-SG
1	C	77[A]	YCM	N-CA-CB-SG
1	C	77[A]	YCM	C-CA-CB-SG
1	E	77[A]	YCM	C-CA-CB-SG

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

There are no ring outliers.

13 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	77[B]	YCM	3	0
1	H	77[A]	YCM	1	0
1	H	77[B]	YCM	2	0
1	D	77[B]	YCM	3	0
1	A	77[A]	YCM	5	0
1	A	77[B]	YCM	2	0
1	E	77[A]	YCM	1	0
1	E	77[B]	YCM	2	0
1	B	77[A]	YCM	2	0
1	B	77[B]	YCM	3	0
1	G	77[B]	YCM	3	0
1	G	77[A]	YCM	4	0
1	F	77	YCM	3	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9
1	A	158/168 (94%)	-0.42	1 (0%) 89 91	16, 25, 54, 77	1 (0%)
1	B	158/168 (94%)	-0.49	1 (0%) 89 91	17, 25, 49, 78	1 (0%)
1	C	157/168 (93%)	-0.46	1 (0%) 89 91	17, 25, 46, 77	1 (0%)
1	D	157/168 (93%)	-0.48	1 (0%) 89 91	15, 23, 45, 75	0
1	E	157/168 (93%)	-0.44	2 (1%) 77 80	18, 25, 53, 76	0
1	F	156/168 (92%)	-0.48	1 (0%) 89 91	18, 26, 47, 75	0
1	G	155/168 (92%)	-0.46	2 (1%) 77 80	15, 23, 40, 71	1 (0%)
1	H	157/168 (93%)	-0.42	0 100 100	16, 24, 52, 70	0
All	All	1255/1344 (93%)	-0.46	9 (0%) 87 89	15, 24, 49, 78	4 (0%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	157	VAL	3.3
1	C	157	VAL	2.8
1	B	157	VAL	2.6
1	E	157	VAL	2.5
1	F	157	VAL	2.4
1	G	156	VAL	2.4
1	A	157	VAL	2.3
1	E	156	VAL	2.2
1	G	157	VAL	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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column

labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	YCM	E	77[A]	10/11	0.82	0.21	32,36,39,40	7
1	YCM	E	77[B]	10/11	0.82	0.21	30,33,36,38	7
1	YCM	F	77	10/11	0.82	0.16	29,39,55,56	0
1	YCM	G	77[A]	10/11	0.85	0.18	30,33,37,38	7
1	YCM	G	77[B]	10/11	0.85	0.18	24,31,35,38	7
1	YCM	A	77[B]	10/11	0.86	0.20	22,25,29,29	10
1	YCM	A	77[A]	10/11	0.86	0.20	23,27,30,30	10
1	YCM	H	77[A]	10/11	0.87	0.18	28,33,37,38	7
1	YCM	H	77[B]	10/11	0.87	0.18	23,31,36,37	7
1	YCM	C	77[B]	10/11	0.90	0.21	19,24,29,30	10
1	YCM	C	77[A]	10/11	0.90	0.21	28,31,33,35	10
1	YCM	D	77[B]	10/11	0.92	0.19	20,24,28,28	10
1	YCM	B	77[A]	10/11	0.92	0.19	25,31,35,40	10
1	YCM	B	77[B]	10/11	0.92	0.19	17,21,25,26	10
1	YCM	D	77[A]	10/11	0.92	0.19	19,23,29,29	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(\AA^2)	Q<0.9
2	FE	H	201	1/1	0.94	0.11	46,46,46,46	1
2	FE	C	201	1/1	0.96	0.05	39,39,39,39	1
2	FE	D	201	1/1	0.97	0.06	34,34,34,34	1
2	FE	E	201	1/1	0.98	0.05	41,41,41,41	1
2	FE	G	201	1/1	0.98	0.09	36,36,36,36	1
2	FE	B	201	1/1	0.98	0.04	37,37,37,37	1

6.5 Other polymers [i](#)

There are no such residues in this entry.