Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:37 PM GMT

PDB ID	:	4IWK
Title	:	Crystal structure of iron soaked (overnight) ferritin from Pseudo-nitzschia multiseries
Authors	:	Pfaffen, S.; Murphy, M.E.P.
Deposited on	:	2013-01-23
Resolution	:	1.65 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

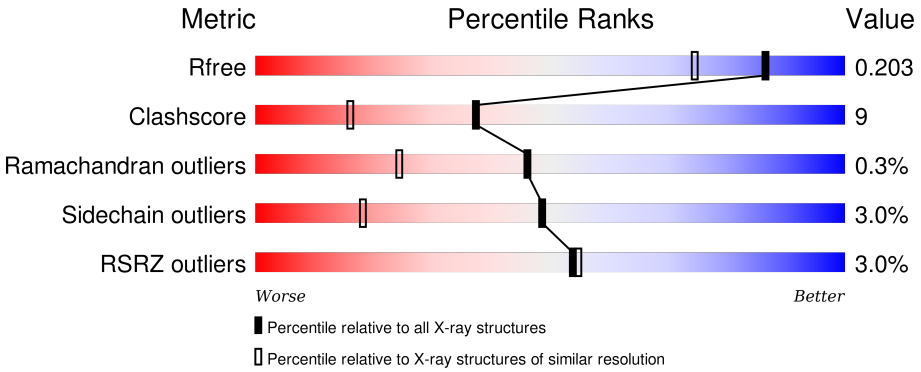
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.65 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	1226 (1.66-1.66)
Clashscore	102246	1323 (1.66-1.66)
Ramachandran outliers	100387	1295 (1.66-1.66)
Sidechain outliers	100360	1295 (1.66-1.66)
RSRZ outliers	91569	1227 (1.66-1.66)

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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	168	4% 76% 15% • 5%
1	B	168	2% 77% 14% • 7%
1	C	168	2% 80% 14% • 6%
1	D	168	3% 80% 12% • 5%
1	E	168	2% 74% 17% • 6%

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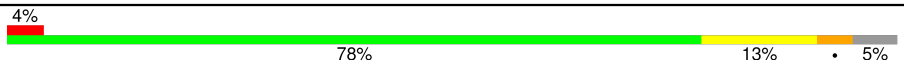
Mol	Chain	Length	Quality of chain
1	F	168	

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	A	77[A]	-	-	X	-
1	YCM	B	77[C]	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8599 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	8	0
			1303	826	213	258	6			
1	B	157	Total	C	N	O	S	0	6	0
			1272	803	209	254	6			
1	C	158	Total	C	N	O	S	0	4	0
			1271	800	212	254	5			
1	D	159	Total	C	N	O	S	0	7	0
			1299	818	215	260	6			
1	E	158	Total	C	N	O	S	0	5	0
			1276	804	209	258	5			
1	F	159	Total	C	N	O	S	0	5	0
			1282	809	210	257	6			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	EXPRESSION TAG	UNP B6DMH6
B	0	GLY	-	EXPRESSION TAG	UNP B6DMH6
C	0	GLY	-	EXPRESSION TAG	UNP B6DMH6
D	0	GLY	-	EXPRESSION TAG	UNP B6DMH6
E	0	GLY	-	EXPRESSION TAG	UNP B6DMH6
F	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	5	Total	Fe	0	0
			5	5		
2	E	4	Total	Fe	0	0
			4	4		
2	B	3	Total	Fe	0	0
			3	3		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	4	Total Fe 4 4	0	0
2	A	4	Total Fe 4 4	0	0
2	F	4	Total Fe 4 4	0	0

- Molecule 3 is water.

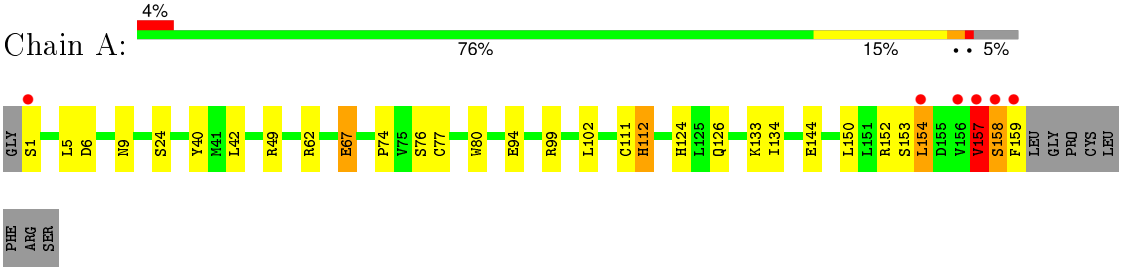
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	133	Total O 133 133	0	0
3	B	150	Total O 150 150	0	0
3	C	154	Total O 154 154	0	0
3	D	150	Total O 150 150	0	0
3	E	155	Total O 155 155	0	0
3	F	130	Total O 130 130	0	0

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 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.

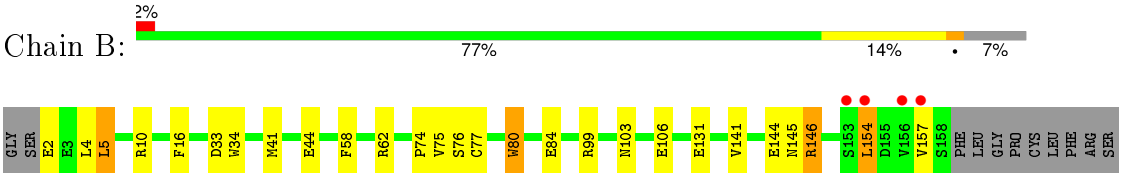
- Molecule 1: Ferritin

Chain A:



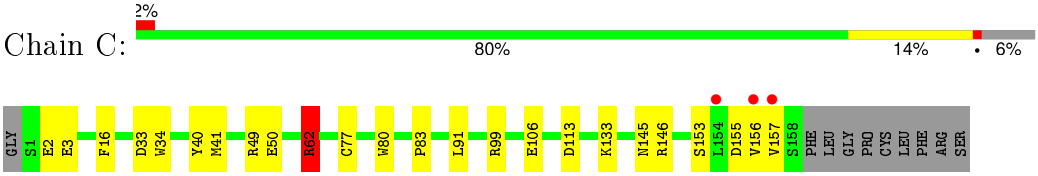
- Molecule 1: Ferritin

Chain B:



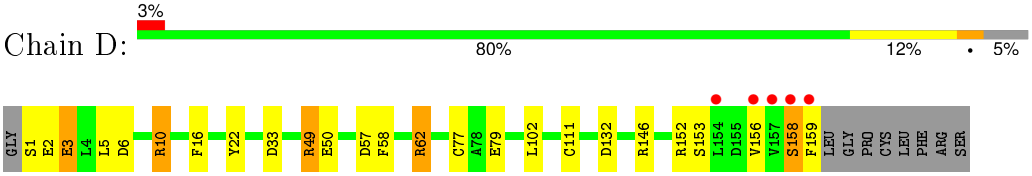
- Molecule 1: Ferritin

Chain C:



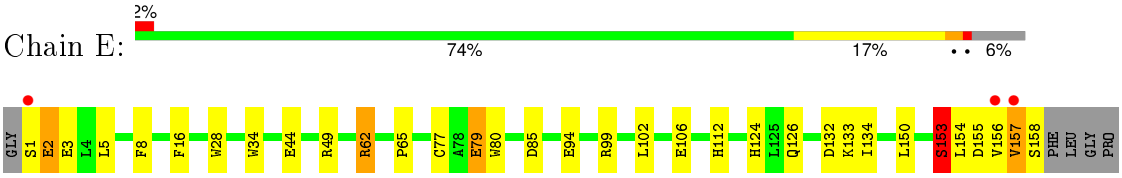
- Molecule 1: Ferritin

Chain D:



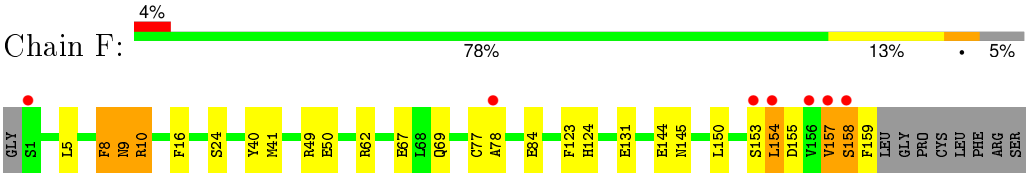
- Molecule 1: Ferritin

Chain E:



- Molecule 1: Ferritin

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α, β, γ	126.25Å 126.25Å 170.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.95 – 1.65 47.06 – 1.65	Depositor EDS
% Data completeness (in resolution range)	99.2 (47.95-1.65) 99.2 (47.06-1.65)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.08 (at 1.65Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.176 , 0.205 0.174 , 0.203	Depositor DCC
R_{free} test set	8205 reflections (5.29%)	DCC
Wilson B-factor (Å^2)	22.4	Xtriage
Anisotropy	0.029	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 53.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Outliers	3 of 163305 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	8599	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 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	1.18	0/1330	1.17	6/1809 (0.3%)
1	B	1.32	3/1295 (0.2%)	1.32	11/1761 (0.6%)
1	C	1.32	4/1298 (0.3%)	1.50	11/1764 (0.6%)
1	D	1.35	3/1323 (0.2%)	1.43	14/1798 (0.8%)
1	E	1.42	3/1303 (0.2%)	1.42	15/1772 (0.8%)
1	F	1.32	4/1307 (0.3%)	1.26	9/1777 (0.5%)
All	All	1.32	17/7856 (0.2%)	1.35	66/10681 (0.6%)

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	E	0	1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	62	ARG	CZ-NH1	7.66	1.43	1.33
1	F	9	ASN	N-CA	-6.08	1.34	1.46
1	C	16	PHE	CG-CD2	5.90	1.47	1.38
1	F	69	GLN	CG-CD	5.58	1.63	1.51
1	B	80	TRP	CZ3-CH2	5.57	1.49	1.40
1	D	58	PHE	CD2-CE2	5.55	1.50	1.39
1	E	28	TRP	CZ3-CH2	5.46	1.48	1.40
1	C	50	GLU	CD-OE1	5.32	1.31	1.25
1	B	34	TRP	CE3-CZ3	5.27	1.47	1.38
1	B	80	TRP	CE3-CZ3	5.16	1.47	1.38
1	D	50	GLU	CD-OE1	5.15	1.31	1.25
1	F	50	GLU	CD-OE1	5.13	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	34	TRP	CE3-CZ3	5.11	1.47	1.38
1	D	3	GLU	CD-OE2	5.07	1.31	1.25
1	E	34	TRP	CE3-CZ3	5.06	1.47	1.38
1	F	123	PHE	CG-CD1	5.04	1.46	1.38
1	E	106	GLU	CD-OE1	5.03	1.31	1.25

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	62	ARG	NE-CZ-NH2	-27.64	106.48	120.30
1	C	62	ARG	NE-CZ-NH1	21.06	130.83	120.30
1	E	62	ARG	NE-CZ-NH2	-16.51	112.05	120.30
1	D	49	ARG	NE-CZ-NH1	-11.40	114.60	120.30
1	A	62	ARG	NE-CZ-NH1	-10.20	115.20	120.30
1	E	102	LEU	CB-CG-CD2	9.03	126.36	111.00
1	F	49	ARG	NE-CZ-NH1	-8.79	115.91	120.30
1	D	33	ASP	CB-CG-OD1	8.60	126.04	118.30
1	E	62	ARG	NE-CZ-NH1	8.46	124.53	120.30
1	B	76	SER	CB-CA-C	8.42	126.10	110.10
1	F	49	ARG	NE-CZ-NH2	8.35	124.48	120.30
1	D	62	ARG	NE-CZ-NH1	-8.17	116.22	120.30
1	D	16	PHE	CB-CG-CD2	-7.96	115.23	120.80
1	A	6	ASP	CB-CG-OD2	7.91	125.42	118.30
1	F	155	ASP	CB-CG-OD2	7.65	125.19	118.30
1	C	33	ASP	CB-CG-OD2	-7.56	111.50	118.30
1	D	49	ARG	CD-NE-CZ	-7.29	113.39	123.60
1	F	49	ARG	CD-NE-CZ	-7.08	113.69	123.60
1	B	62	ARG	NE-CZ-NH1	-6.87	116.86	120.30
1	A	152	ARG	NE-CZ-NH1	-6.76	116.92	120.30
1	F	62	ARG	NE-CZ-NH1	-6.69	116.95	120.30
1	E	16	PHE	CB-CG-CD2	-6.65	116.15	120.80
1	F	8	PHE	CB-CG-CD2	-6.54	116.22	120.80
1	D	16	PHE	CB-CG-CD1	6.47	125.33	120.80
1	F	10	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	C	49	ARG	NE-CZ-NH1	-6.42	117.09	120.30
1	A	42	LEU	CB-CG-CD2	-6.27	100.34	111.00
1	C	155	ASP	CB-CG-OD2	6.19	123.87	118.30
1	B	5	LEU	CB-CG-CD2	6.18	121.50	111.00
1	B	75	VAL	CG1-CB-CG2	-6.05	101.21	110.90
1	B	16	PHE	CB-CG-CD2	-6.01	116.59	120.80
1	B	41	MET	CG-SD-CE	6.01	109.82	100.20
1	D	5	LEU	CB-CG-CD2	5.94	121.10	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	62	ARG	CG-CD-NE	-5.92	99.37	111.80
1	F	16	PHE	CB-CG-CD2	-5.90	116.67	120.80
1	E	49	ARG	CD-NE-CZ	-5.83	115.44	123.60
1	D	33	ASP	CB-CG-OD2	-5.82	113.06	118.30
1	C	49	ARG	NE-CZ-NH2	5.76	123.18	120.30
1	E	85	ASP	CB-CG-OD2	-5.75	113.12	118.30
1	E	8	PHE	CB-CG-CD2	-5.75	116.78	120.80
1	B	131	GLU	OE1-CD-OE2	-5.74	116.41	123.30
1	E	99	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	D	57	ASP	CB-CG-OD2	-5.73	113.14	118.30
1	D	132	ASP	CB-CG-OD1	-5.58	113.28	118.30
1	D	22	TYR	CB-CG-CD2	-5.53	117.68	121.00
1	A	49	ARG	NE-CZ-NH2	5.53	123.06	120.30
1	C	91	LEU	CB-CG-CD2	-5.49	101.66	111.00
1	E	153	SER	N-CA-C	5.43	125.67	111.00
1	D	153	SER	N-CA-C	5.43	125.66	111.00
1	D	102	LEU	CB-CG-CD2	5.41	120.20	111.00
1	C	16	PHE	CB-CG-CD2	-5.33	117.07	120.80
1	E	106	GLU	OE1-CD-OE2	5.33	129.69	123.30
1	F	131	GLU	OE1-CD-OE2	-5.31	116.93	123.30
1	A	102	LEU	CB-CG-CD2	5.30	120.01	111.00
1	C	49	ARG	CD-NE-CZ	-5.27	116.22	123.60
1	B	10	ARG	CA-CB-CG	-5.24	101.88	113.40
1	E	155	ASP	CB-CG-OD2	5.13	122.92	118.30
1	B	146	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	E	132	ASP	CB-CG-OD2	5.06	122.86	118.30
1	B	58	PHE	CG-CD1-CE1	-5.05	115.25	120.80
1	B	33	ASP	CB-CG-OD2	-5.03	113.77	118.30
1	E	150	LEU	CB-CG-CD2	-5.03	102.44	111.00
1	C	155	ASP	CB-CG-OD1	-5.02	113.78	118.30
1	D	10	ARG	NE-CZ-NH1	5.01	122.80	120.30
1	E	16	PHE	CB-CG-CD1	5.00	124.30	120.80
1	E	156	VAL	CB-CA-C	5.00	120.90	111.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	1	SER	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	1303	0	1260	38	0
1	B	1272	0	1225	31	0
1	C	1271	0	1222	17	0
1	D	1299	0	1243	10	0
1	E	1276	0	1221	22	0
1	F	1282	0	1226	22	1
2	A	4	0	0	0	0
2	B	3	0	0	1	0
2	C	4	0	0	1	0
2	D	5	0	0	0	0
2	E	4	0	0	1	0
2	F	4	0	0	0	0
3	A	133	0	0	7	0
3	B	150	0	0	11	0
3	C	154	0	0	7	0
3	D	150	0	0	3	0
3	E	155	0	0	10	0
3	F	130	0	0	8	0
All	All	8599	0	7397	141	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 9.

All (141) 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:A:74:PRO:HB2	1:A:77[A]:YCM:HD2	1.29	1.15
1:E:2:GLU:OE1	1:E:2:GLU:HA	1.47	1.15
1:E:77:YCM:HB3	3:E:447:HOH:O	1.51	1.10
1:E:157:VAL:HG23	1:E:158:SER:N	1.79	0.92
1:A:74:PRO:CB	1:A:77[A]:YCM:HD2	1.99	0.92
1:E:157:VAL:HG23	1:E:158:SER:H	1.31	0.91
1:A:40:TYR:OH	1:A:133:LYS:HE2	1.71	0.90
1:A:77[A]:YCM:NZ2	1:A:80:TRP:CH2	2.41	0.89
1:A:144:GLU:OE1	1:A:154:LEU:HG	1.71	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:157:VAL:CG2	1:E:158:SER:H	1.91	0.84
1:A:24[A]:SER:OG	1:A:77[A]:YCM:NZ2	2.11	0.84
1:F:77[B]:YCM:SG	3:F:408:HOH:O	2.38	0.81
1:B:77[C]:YCM:OZ1	1:B:80:TRP:CH2	2.34	0.81
1:B:77[C]:YCM:CE	1:B:77[C]:YCM:H	1.94	0.81
1:F:144:GLU:OE1	1:F:154:LEU:HG	1.81	0.80
1:A:77[A]:YCM:H	1:A:77[A]:YCM:CD	1.96	0.79
1:B:74:PRO:HB2	1:B:77[C]:YCM:CD	2.12	0.78
1:E:157:VAL:CG2	1:E:158:SER:N	2.47	0.78
1:B:74:PRO:HB2	1:B:77[C]:YCM:HD2	1.63	0.78
1:E:2:GLU:CA	1:E:2:GLU:OE1	2.29	0.77
1:F:153:SER:C	1:F:154:LEU:HD22	2.06	0.76
1:E:126:GLN:NE2	3:E:367:HOH:O	2.19	0.76
1:A:112:HIS:HD2	1:B:106:GLU:OE1	1.70	0.75
1:A:94:GLU:HG3	1:A:134[A]:ILE:CD1	2.17	0.75
1:D:146[A]:ARG:NH1	3:D:431:HOH:O	2.20	0.74
1:B:84:GLU:HG3	3:B:418:HOH:O	1.88	0.73
1:A:99:ARG:HD3	3:A:337:HOH:O	1.86	0.73
1:E:94:GLU:HG3	1:E:134[B]:ILE:CD1	2.20	0.72
1:F:24:SER:OG	1:F:77[B]:YCM:HD2	1.89	0.71
1:B:77[B]:YCM:SG	3:B:445:HOH:O	2.48	0.71
1:B:157:VAL:HG12	1:B:157:VAL:O	1.91	0.71
1:B:146:ARG:NH2	3:B:373:HOH:O	2.23	0.71
1:F:150:LEU:O	1:F:154:LEU:HD23	1.91	0.70
1:F:158:SER:O	1:F:159:PHE:C	2.29	0.70
1:B:44:GLU:OE2	3:B:450:HOH:O	2.10	0.70
2:B:203:FE:FE	3:B:434:HOH:O	1.44	0.69
1:B:77[B]:YCM:CD	3:B:445:HOH:O	2.41	0.68
2:C:202:FE:FE	3:C:454:HOH:O	1.43	0.68
1:A:153:SER:C	1:A:154:LEU:HD22	2.14	0.68
1:A:126:GLN:NE2	3:A:381:HOH:O	2.27	0.68
1:E:79:GLU:HB2	3:E:441:HOH:O	1.93	0.67
1:D:152:ARG:O	1:D:156:VAL:HG13	1.96	0.66
1:A:77[B]:YCM:HD3	3:A:405:HOH:O	1.95	0.65
1:E:94:GLU:HG3	1:E:134[B]:ILE:HD12	1.77	0.65
1:D:77[A]:YCM:SG	3:D:446:HOH:O	2.55	0.65
1:B:2:GLU:HB3	1:B:5:LEU:H	1.61	0.65
1:F:154:LEU:CD2	1:F:154:LEU:N	2.60	0.65
1:A:1:SER:HB2	1:A:111:CYS:SG	2.37	0.65
1:A:77[B]:YCM:CD	3:A:405:HOH:O	2.45	0.64
1:D:6[A]:ASP:OD2	1:D:10:ARG:CZ	2.45	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:77[A]:YCM:SG	3:F:413:HOH:O	2.55	0.64
1:B:145:ASN:ND2	3:B:418:HOH:O	2.29	0.64
1:A:157:VAL:HG12	1:A:158:SER:H	1.63	0.64
1:C:146[A]:ARG:NH2	3:C:439:HOH:O	2.26	0.62
2:E:202:FE:FE	3:E:451:HOH:O	1.52	0.61
1:A:158:SER:O	1:A:159:PHE:HB2	2.01	0.60
1:A:99:ARG:HG3	3:A:358:HOH:O	2.02	0.58
1:E:79:GLU:CB	3:E:441:HOH:O	2.50	0.58
1:E:124:HIS:HD2	3:E:416:HOH:O	1.85	0.58
1:A:153:SER:OG	1:A:154:LEU:CD2	2.52	0.58
1:F:84:GLU:HG3	3:F:419:HOH:O	2.04	0.58
1:B:103:ASN:HB2	3:B:367:HOH:O	2.05	0.57
1:F:154:LEU:HD22	1:F:154:LEU:N	2.18	0.57
1:C:106:GLU:OE1	1:E:112:HIS:HD2	1.88	0.56
1:A:150:LEU:O	1:A:154:LEU:HD23	2.05	0.56
1:A:76:SER:N	1:A:77[A]:YCM:HD3	2.20	0.56
1:B:77[C]:YCM:H	1:B:77[C]:YCM:CD	2.17	0.55
1:E:5:LEU:HD12	1:E:65:PRO:HD2	1.88	0.55
1:A:157:VAL:CG1	1:A:158:SER:N	2.70	0.55
1:A:154:LEU:N	1:A:154:LEU:CD2	2.70	0.55
1:F:9:ASN:HD21	1:F:67:GLU:H	1.53	0.55
1:B:74:PRO:HB2	1:B:77[C]:YCM:HD3	1.89	0.55
1:B:74:PRO:C	1:B:77[C]:YCM:HD3	2.28	0.54
1:A:77[A]:YCM:H	1:A:77[A]:YCM:HD3	1.72	0.53
1:E:124:HIS:HE1	3:E:302:HOH:O	1.92	0.53
1:A:94:GLU:HG3	1:A:134[A]:ILE:HD13	1.89	0.52
1:F:77[B]:YCM:CD	3:F:408:HOH:O	2.57	0.52
1:F:124:HIS:HD2	3:F:304:HOH:O	1.93	0.52
1:B:154:LEU:CB	3:B:315:HOH:O	2.58	0.52
1:F:5:LEU:O	1:F:5:LEU:HD12	2.11	0.51
1:F:40:TYR:HD2	1:F:41:MET:CE	2.24	0.51
1:D:6[A]:ASP:OD2	1:D:10:ARG:NH1	2.44	0.51
1:C:153:SER:O	1:C:157:VAL:HB	2.10	0.50
1:E:77:YCM:HA	1:E:80:TRP:CE3	2.46	0.50
1:D:158:SER:O	1:D:159:PHE:HB2	2.12	0.50
1:E:153:SER:HB2	3:E:326:HOH:O	2.11	0.50
1:C:145:ASN:HB3	3:C:437:HOH:O	2.12	0.49
1:C:40:TYR:OH	1:C:133:LYS:HE2	2.12	0.49
1:C:40:TYR:HD2	1:C:41:MET:HE2	1.77	0.49
1:A:157:VAL:CG1	1:A:158:SER:H	2.24	0.49
1:B:157:VAL:CG1	1:B:157:VAL:O	2.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2:GLU:CB	1:B:5:LEU:H	2.26	0.48
1:A:124:HIS:HD2	3:A:406:HOH:O	1.95	0.48
1:E:44:GLU:OE2	3:E:453:HOH:O	2.20	0.48
1:B:154:LEU:HB2	3:B:315:HOH:O	2.14	0.48
1:A:9[A]:ASN:HD21	1:A:67:GLU:H	1.61	0.48
1:A:5[B]:LEU:HD12	1:A:9[B]:ASN:HD22	1.78	0.48
1:C:106:GLU:OE1	1:E:112:HIS:CD2	2.66	0.47
1:F:157:VAL:HG12	1:F:158:SER:N	2.29	0.47
1:A:40:TYR:HH	1:A:133:LYS:HE2	1.74	0.47
1:B:154:LEU:HD12	1:C:156:VAL:HG11	1.96	0.47
1:C:77:YCM:CD	3:C:446:HOH:O	2.64	0.46
1:E:157:VAL:HG23	1:E:158:SER:OG	2.15	0.46
1:C:62:ARG:NH2	1:C:113:ASP:OD1	2.45	0.46
1:F:145:ASN:ND2	3:F:419:HOH:O	2.49	0.46
1:C:40:TYR:HD2	1:C:41:MET:CE	2.29	0.46
1:F:40:TYR:HD2	1:F:41:MET:HE3	1.80	0.46
1:B:84:GLU:HG2	1:B:141:VAL:HG12	1.98	0.45
1:F:153:SER:OG	1:F:154:LEU:CD2	2.64	0.45
1:A:154:LEU:N	1:A:154:LEU:HD22	2.31	0.45
1:C:99:ARG:HG3	3:C:436:HOH:O	2.15	0.45
1:B:77[B]:YCM:HA	1:B:80:TRP:CE3	2.51	0.45
1:A:158:SER:O	1:A:159:PHE:CB	2.64	0.45
1:B:144:GLU:OE2	1:B:154:LEU:HG	2.17	0.45
1:C:77:YCM:HA	1:C:80:TRP:CE3	2.51	0.45
1:D:2:GLU:HA	1:D:2:GLU:OE2	2.18	0.44
1:B:2:GLU:HB2	1:B:5:LEU:HB3	1.99	0.44
1:B:77[B]:YCM:HD3	3:B:445:HOH:O	2.10	0.43
1:C:145:ASN:ND2	3:C:313:HOH:O	2.50	0.43
1:A:124:HIS:HE1	3:A:303:HOH:O	2.01	0.43
1:E:133:LYS:HG3	3:E:368:HOH:O	2.19	0.43
1:A:74:PRO:C	1:A:77[A]:YCM:HD2	2.39	0.43
1:A:1:SER:CB	1:A:111:CYS:SG	3.06	0.42
1:C:62:ARG:HH22	1:C:113:ASP:CG	2.23	0.42
1:A:77[B]:YCM:HA	1:A:80:TRP:CE3	2.54	0.42
1:C:77:YCM:HD3	3:C:446:HOH:O	2.19	0.42
1:B:77[C]:YCM:HA	1:B:80:TRP:CE3	2.54	0.42
1:D:79:GLU:HB2	3:D:433:HOH:O	2.19	0.41
1:D:49:ARG:HH11	1:D:49:ARG:HD3	1.40	0.41
1:F:24:SER:HG	1:F:77[B]:YCM:HD2	1.84	0.41
1:C:62:ARG:O	1:C:62:ARG:HD2	2.20	0.41
1:A:24[B]:SER:OG	1:A:77[B]:YCM:NZ2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:157:VAL:CG1	1:F:158:SER:N	2.83	0.41
1:D:1:SER:HB2	1:D:111:CYS:SG	2.61	0.41
1:F:9:ASN:ND2	1:F:67:GLU:H	2.16	0.41

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:F:10:ARG:NH1	1:F:10:ARG:NH1[7_554]	1.89	0.31

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	163/168 (97%)	161 (99%)	1 (1%)	1 (1%)	30 9
1	B	159/168 (95%)	157 (99%)	2 (1%)	0	100 100
1	C	159/168 (95%)	158 (99%)	1 (1%)	0	100 100
1	D	162/168 (96%)	161 (99%)	1 (1%)	0	100 100
1	E	160/168 (95%)	155 (97%)	4 (2%)	1 (1%)	30 9
1	F	160/168 (95%)	155 (97%)	4 (2%)	1 (1%)	30 9
All	All	963/1008 (96%)	947 (98%)	13 (1%)	3 (0%)	46 24

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	157	VAL
1	F	78	ALA
1	E	157	VAL

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	143/143 (100%)	138 (96%)	5 (4%)	43 14
1	B	139/143 (97%)	137 (99%)	2 (1%)	74 53
1	C	139/143 (97%)	135 (97%)	4 (3%)	50 19
1	D	142/143 (99%)	139 (98%)	3 (2%)	61 34
1	E	140/143 (98%)	134 (96%)	6 (4%)	35 9
1	F	140/143 (98%)	136 (97%)	4 (3%)	50 19
All	All	843/858 (98%)	819 (97%)	24 (3%)	48 21

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	GLU
1	A	112	HIS
1	A	154	LEU
1	A	157	VAL
1	A	158	SER
1	B	99	ARG
1	B	154	LEU
1	C	2	GLU
1	C	3	GLU
1	C	62	ARG
1	C	83	PRO
1	D	3	GLU
1	D	62	ARG
1	D	158	SER
1	E	2	GLU
1	E	3	GLU
1	E	62	ARG
1	E	79	GLU
1	E	153	SER
1	E	154	LEU
1	F	8	PHE
1	F	154	LEU

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Mol	Chain	Res	Type
1	F	157	VAL
1	F	158	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	112	HIS
1	A	121	ASN
1	A	124	HIS
1	A	126	GLN
1	B	31	GLN
1	B	121	ASN
1	B	145	ASN
1	C	121	ASN
1	C	145	ASN
1	E	31	GLN
1	E	112	HIS
1	E	121	ASN
1	E	124	HIS
1	E	126	GLN
1	E	145	ASN
1	F	9	ASN
1	F	121	ASN
1	F	124	HIS
1	F	145	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

10 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[A]	1	8,9,10	2.60	3 (37%)	5,10,12	1.23	1 (20%)
1	YCM	A	77[B]	1	8,9,10	2.31	3 (37%)	5,10,12	1.41	1 (20%)
1	YCM	B	77[B]	-	8,9,10	3.37	4 (50%)	5,10,12	1.78	1 (20%)
1	YCM	B	77[C]	-	8,9,10	1.70	2 (25%)	5,10,12	0.96	0
1	YCM	C	77	1	8,9,10	2.92	3 (37%)	5,10,12	1.67	1 (20%)
1	YCM	D	77[A]	1	8,9,10	2.45	2 (25%)	5,10,12	1.96	2 (40%)
1	YCM	D	77[B]	1	8,9,10	2.23	3 (37%)	5,10,12	1.38	1 (20%)
1	YCM	E	77	1	8,9,10	1.70	3 (37%)	5,10,12	1.29	0
1	YCM	F	77[A]	-	4,5,10	1.56	1 (25%)	3,5,12	2.21	1 (33%)
1	YCM	F	77[B]	-	8,9,10	4.98	4 (50%)	5,10,12	4.49	4 (80%)

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[A]	1	-	0/6/8/10	0/0/0/0
1	YCM	A	77[B]	1	-	0/6/8/10	0/0/0/0
1	YCM	B	77[B]	-	-	0/6/8/10	0/0/0/0
1	YCM	B	77[C]	-	-	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[A]	1	-	0/6/8/10	0/0/0/0
1	YCM	D	77[B]	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]	-	-	0/1/4/10	0/0/0/0
1	YCM	F	77[B]	-	-	0/6/8/10	0/0/0/0

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	77[A]	YCM	CD-SG	-3.58	1.74	1.81
1	D	77[B]	YCM	CE-NZ2	-3.52	1.21	1.32
1	A	77[B]	YCM	CE-NZ2	-3.07	1.22	1.32
1	B	77[C]	YCM	CD-SG	-2.99	1.75	1.81
1	A	77[A]	YCM	CB-SG	2.08	1.85	1.81
1	E	77	YCM	CD-SG	2.08	1.86	1.81
1	D	77[B]	YCM	OZ1-CE	2.09	1.30	1.24
1	E	77	YCM	O-C	2.16	1.29	1.19
1	B	77[B]	YCM	CB-CA	2.29	1.59	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	77[B]	YCM	CA-N	2.29	1.55	1.47
1	F	77[B]	YCM	CB-CA	2.50	1.60	1.53
1	F	77[A]	YCM	CB-SG	2.52	1.87	1.81
1	A	77[A]	YCM	OZ1-CE	2.77	1.32	1.24
1	C	77	YCM	OZ1-CE	2.89	1.33	1.24
1	B	77[C]	YCM	CB-SG	2.99	1.87	1.81
1	E	77	YCM	CB-SG	3.33	1.87	1.81
1	A	77[B]	YCM	CB-SG	3.50	1.88	1.81
1	A	77[B]	YCM	CD-SG	3.79	1.89	1.81
1	B	77[B]	YCM	CD-SG	3.86	1.89	1.81
1	D	77[B]	YCM	CD-SG	4.36	1.90	1.81
1	C	77	YCM	CB-SG	4.73	1.90	1.81
1	F	77[B]	YCM	CE-NZ2	4.76	1.48	1.32
1	D	77[A]	YCM	CB-SG	5.44	1.92	1.81
1	C	77	YCM	CD-SG	5.95	1.94	1.81
1	A	77[A]	YCM	CD-SG	6.21	1.94	1.81
1	B	77[B]	YCM	CB-SG	7.75	1.96	1.81
1	F	77[B]	YCM	CD-SG	8.27	1.99	1.81
1	F	77[B]	YCM	CB-SG	9.78	2.00	1.81

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	77[B]	YCM	OZ1-CE-CD	-3.07	114.25	121.03
1	F	77[A]	YCM	CA-CB-SG	-2.73	108.23	114.48
1	D	77[A]	YCM	CA-CB-SG	-2.71	106.42	112.84
1	A	77[B]	YCM	O-C-CA	-2.68	118.50	125.49
1	F	77[B]	YCM	O-C-CA	-2.68	118.52	125.49
1	A	77[A]	YCM	O-C-CA	-2.59	118.74	125.49
1	D	77[B]	YCM	CA-CB-SG	2.48	118.70	112.84
1	D	77[A]	YCM	CD-CE-NZ2	2.57	118.32	115.48
1	C	77	YCM	CD-CE-NZ2	3.15	118.96	115.48
1	B	77[B]	YCM	CA-CB-SG	3.39	120.86	112.84
1	F	77[B]	YCM	CD-CE-NZ2	6.09	122.19	115.48
1	F	77[B]	YCM	CA-CB-SG	6.87	129.09	112.84

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 37 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	77[A]	YCM	8	0
1	A	77[B]	YCM	4	0
1	B	77[B]	YCM	4	0
1	B	77[C]	YCM	10	0
1	C	77	YCM	3	0
1	D	77[A]	YCM	1	0
1	E	77	YCM	2	0
1	F	77[A]	YCM	1	0
1	F	77[B]	YCM	4	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 24 ligands modelled in this entry, 24 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, 95^{th} 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%)	-0.19	6 (3%)	44	44	17, 23, 46, 66	0
1	B	156/168 (92%)	-0.23	4 (2%)	59	60	15, 22, 42, 69	0
1	C	157/168 (93%)	-0.29	3 (1%)	70	73	16, 22, 39, 64	0
1	D	158/168 (94%)	-0.09	5 (3%)	51	52	13, 21, 45, 70	0
1	E	157/168 (93%)	-0.23	3 (1%)	70	73	14, 20, 43, 66	0
1	F	158/168 (94%)	-0.16	7 (4%)	38	37	16, 22, 47, 70	0
All	All	944/1008 (93%)	-0.20	28 (2%)	54	55	13, 22, 45, 70	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	157	VAL	7.5
1	D	157	VAL	7.3
1	C	156	VAL	6.9
1	A	156	VAL	6.5
1	A	157	VAL	5.0
1	D	156	VAL	4.9
1	D	159	PHE	4.4
1	B	157	VAL	4.2
1	F	157	VAL	4.1
1	B	156	VAL	3.9
1	E	156	VAL	3.7
1	F	156	VAL	3.7
1	E	157	VAL	3.6
1	B	153	SER	3.0
1	B	154	LEU	2.8
1	A	159	PHE	2.8
1	D	158	SER	2.7
1	A	154	LEU	2.7
1	A	158	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	1	SER	2.6
1	A	1	SER	2.4
1	F	153	SER	2.4
1	F	1	SER	2.3
1	C	154	LEU	2.2
1	F	154	LEU	2.2
1	F	78	ALA	2.2
1	F	158	SER	2.1
1	D	154	LEU	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^{th} 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^2)	Q<0.9
1	YCM	F	77[A]	6/11	0.73	0.17	-	33,35,43,49	3
1	YCM	E	77	10/11	0.95	0.10	-	22,27,52,56	0
1	YCM	A	77[A]	10/11	0.86	0.17	-	22,30,33,35	10
1	YCM	D	77[A]	10/11	0.92	0.13	-	19,25,31,34	10
1	YCM	B	77[B]	10/11	0.88	0.16	-	21,22,31,32	7
1	YCM	A	77[B]	10/11	0.86	0.17	-	18,22,29,30	10
1	YCM	D	77[B]	10/11	0.92	0.13	-	15,17,24,24	10
1	YCM	B	77[C]	10/11	0.88	0.16	-	20,26,32,39	7
1	YCM	F	77[B]	10/11	0.73	0.17	-	20,33,43,49	7
1	YCM	C	77	10/11	0.91	0.10	-	24,27,31,32	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. 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^{th} 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^2)	Q<0.9
2	FE	C	201	1/1	0.99	0.07	0.30	22,22,22,22	1
2	FE	C	203	1/1	0.94	0.08	0.26	38,38,38,38	1
2	FE	D	202	1/1	0.94	0.08	-0.13	35,35,35,35	1
2	FE	A	204	1/1	0.98	0.09	-0.22	39,39,39,39	1
2	FE	B	202	1/1	0.99	0.06	-0.23	22,22,22,22	1
2	FE	F	203	1/1	0.95	0.08	-0.37	32,32,32,32	1
2	FE	A	201	1/1	0.99	0.06	-0.82	24,24,24,24	0
2	FE	E	203	1/1	0.98	0.07	-1.12	35,35,35,35	1
2	FE	B	201	1/1	0.95	0.05	-1.20	38,38,38,38	1
2	FE	E	201	1/1	0.99	0.07	-1.28	22,22,22,22	1
2	FE	A	203	1/1	0.99	0.04	-1.76	23,23,23,23	1
2	FE	C	202	1/1	0.99	0.04	-1.84	21,21,21,21	1
2	FE	F	202	1/1	0.99	0.03	-2.27	22,22,22,22	1
2	FE	F	201	1/1	0.99	0.05	-2.53	23,23,23,23	0
2	FE	D	201	1/1	0.99	0.06	-2.59	21,21,21,21	0
2	FE	B	203	1/1	0.99	0.04	-2.63	21,21,21,21	1
2	FE	E	202	1/1	0.99	0.04	-2.68	20,20,20,20	1
2	FE	D	204	1/1	0.98	0.04	-2.98	21,21,21,21	1
2	FE	D	205	1/1	0.93	0.09	-	34,34,34,34	1
2	FE	D	203	1/1	0.78	0.09	-	40,40,40,40	1
2	FE	F	204	1/1	0.81	0.10	-	35,35,35,35	1
2	FE	C	204	1/1	0.92	0.10	-	36,36,36,36	1
2	FE	A	202	1/1	0.77	0.12	-	40,40,40,40	1
2	FE	E	204	1/1	0.91	0.07	-	38,38,38,38	1

6.5 Other polymers (i)

There are no such residues in this entry.