Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:35 PM GMT

PDB ID	:	4ISM
Title	:	Crystal structure of ferritin from Pseudo-nitzschia multiseries soaked with zinc
Authors	:	Pfaffen, S.; Murphy, M.E.P.
Deposited on	:	2013-01-16
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
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:

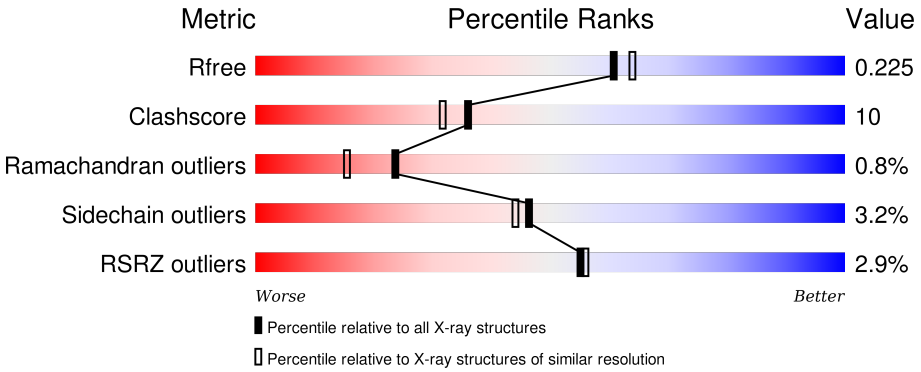
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 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 >=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	2% 79% 13% • 7%
1	B	168	5% 82% 11% • 5%
1	C	168	% 81% 10% • 8%
1	D	168	2% 77% 15% •• 5%
1	E	168	2% 78% 15% • 6%

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Mol	Chain	Length	Quality of chain
1	F	168	3% 80% 10% • 6%
1	G	168	4% 76% 18% • 5%
1	H	168	2% 81% 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
2	ZN	A	204	-	-	-	X
2	ZN	C	204	-	-	-	X
2	ZN	D	204	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11340 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	157	Total	C	N	O	S	0	8	0
			1296	813	217	261	5			
1	D	159	Total	C	N	O	S	0	8	0
			1318	827	218	268	5			
1	B	159	Total	C	N	O	S	0	6	0
			1302	818	217	261	6			
1	C	155	Total	C	N	O	S	0	7	0
			1285	804	214	261	6			
1	E	158	Total	C	N	O	S	0	5	0
			1284	805	212	262	5			
1	F	158	Total	C	N	O	S	0	7	0
			1301	817	215	263	6			
1	G	159	Total	C	N	O	S	0	8	0
			1320	829	221	265	5			
1	H	158	Total	C	N	O	S	0	6	0
			1290	809	216	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 ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is water.

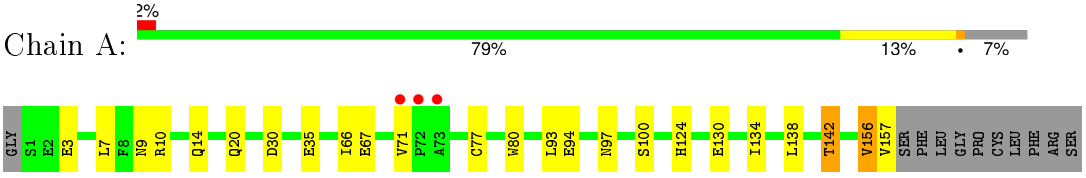
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	111	Total O 111 111	0	0
3	D	119	Total O 119 119	0	0
3	B	105	Total O 105 105	0	0
3	C	106	Total O 106 106	0	0
3	E	108	Total O 108 108	0	0
3	F	102	Total O 102 102	0	0
3	G	135	Total O 135 135	0	0
3	H	126	Total O 126 126	0	0

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.

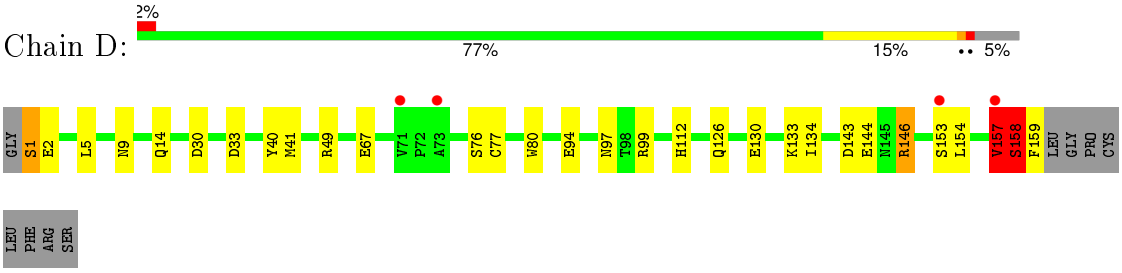
- Molecule 1: Ferritin

Chain A:



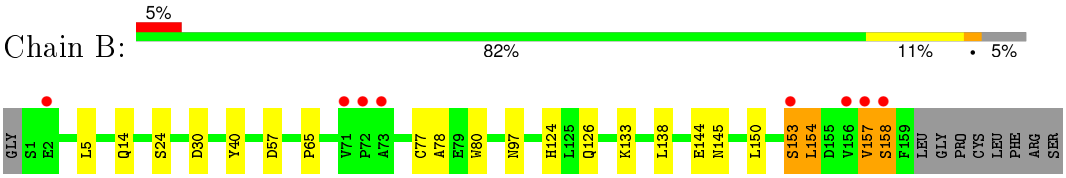
- Molecule 1: Ferritin

Chain D:



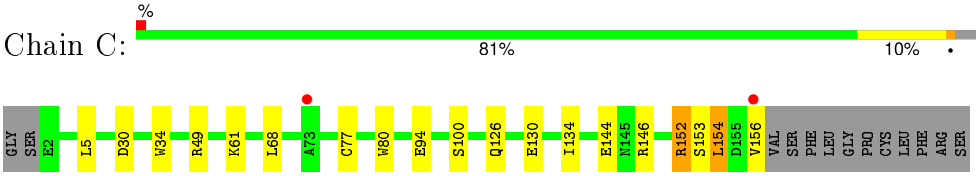
- Molecule 1: Ferritin

Chain B:



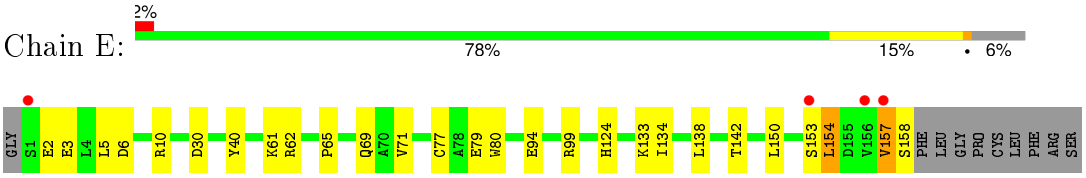
- Molecule 1: Ferritin

Chain C:



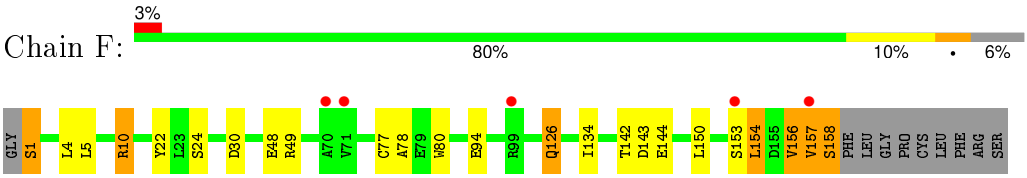
- Molecule 1: Ferritin

Chain E:



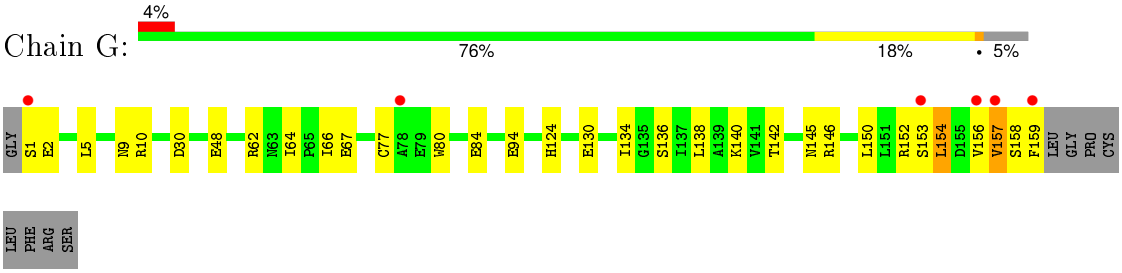
- Molecule 1: Ferritin

Chain F:



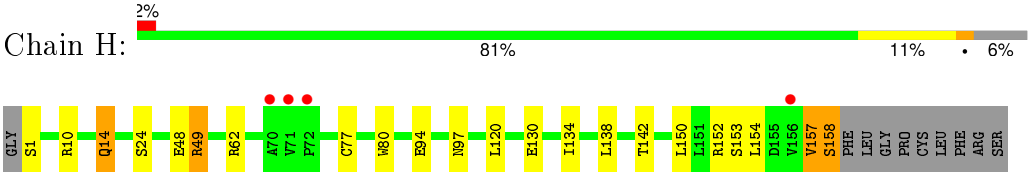
• Molecule 1: Ferritin

Chain G:



• Molecule 1: Ferritin

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 3	Depositor
Cell constants a, b, c, α, β, γ	175.11Å 175.11Å 175.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.51 – 2.00 42.47 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.5 (42.51-2.00) 97.5 (42.47-2.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	6.12 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.184 , 0.232 0.179 , 0.225	Depositor DCC
R_{free} test set	5895 reflections (5.29%)	DCC
Wilson B-factor (Å^2)	26.9	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 54.4	EDS
Estimated twinning fraction	0.037 for l,-k,h	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Outliers	3 of 117256 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	11340	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.14% 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: ZN, 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	1.05	0/1317	0.96	1/1792 (0.1%)
1	B	0.99	0/1314	0.92	2/1786 (0.1%)
1	C	1.03	1/1293 (0.1%)	0.98	2/1758 (0.1%)
1	D	1.06	1/1337 (0.1%)	1.02	5/1818 (0.3%)
1	E	1.03	0/1302	0.97	3/1771 (0.2%)
1	F	0.96	1/1309 (0.1%)	0.95	2/1781 (0.1%)
1	G	1.05	0/1339	0.96	1/1820 (0.1%)
1	H	1.09	1/1304 (0.1%)	0.98	3/1773 (0.2%)
All	All	1.03	4/10515 (0.0%)	0.97	19/14299 (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	A	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	76	SER	CB-OG	-5.73	1.34	1.42
1	F	22	TYR	CB-CG	-5.56	1.43	1.51
1	C	34	TRP	CE3-CZ3	5.14	1.47	1.38
1	H	48	GLU	CD-OE2	5.10	1.31	1.25

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	49	ARG	NE-CZ-NH1	-7.50	116.55	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	62	ARG	NE-CZ-NH1	-7.41	116.60	120.30
1	E	61	LYS	CD-CE-NZ	-7.10	95.37	111.70
1	D	49	ARG	NE-CZ-NH1	-6.48	117.06	120.30
1	H	62	ARG	NE-CZ-NH1	-6.24	117.18	120.30
1	F	143	ASP	CB-CG-OD1	5.94	123.65	118.30
1	B	138	LEU	CB-CG-CD2	-5.84	101.08	111.00
1	D	49	ARG	NE-CZ-NH2	5.83	123.21	120.30
1	D	99	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	E	62	ARG	NE-CZ-NH1	-5.61	117.50	120.30
1	D	146	ARG	NE-CZ-NH1	-5.49	117.55	120.30
1	C	154	LEU	CA-CB-CG	-5.43	102.81	115.30
1	H	49[A]	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	H	49[B]	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	A	93	LEU	CB-CG-CD2	-5.20	102.17	111.00
1	B	57	ASP	CB-CG-OD2	5.11	122.89	118.30
1	D	41	MET	CG-SD-CE	5.06	108.30	100.20
1	E	99	ARG	NE-CZ-NH1	5.03	122.82	120.30
1	C	61	LYS	CD-CE-NZ	-5.02	100.15	111.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	156	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	1296	0	1236	27	0
1	B	1302	0	1239	23	0
1	C	1285	0	1205	23	0
1	D	1318	0	1241	24	0
1	E	1284	0	1214	28	0
1	F	1301	0	1236	26	0
1	G	1320	0	1253	39	0
1	H	1290	0	1232	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	4	0	0	0	0
2	B	4	0	0	0	0
2	C	4	0	0	0	0
2	D	4	0	0	0	0
2	E	4	0	0	0	0
2	F	4	0	0	0	0
2	G	4	0	0	0	0
2	H	4	0	0	0	0
3	A	111	0	0	3	0
3	B	105	0	0	4	0
3	C	106	0	0	3	0
3	D	119	0	0	4	0
3	E	108	0	0	4	0
3	F	102	0	0	6	0
3	G	135	0	0	6	0
3	H	126	0	0	2	0
All	All	11340	0	9856	195	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 10.

All (195) 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:B:145:ASN:HB2	3:B:388:HOH:O	1.30	1.29
1:G:77:YCM:HB3	3:G:395:HOH:O	1.41	1.17
1:A:71[B]:VAL:HG12	1:E:71:VAL:HB	1.34	1.10
1:A:130:GLU:HG3	3:A:377:HOH:O	1.51	1.08
1:H:130:GLU:HG3	3:H:397:HOH:O	1.52	1.05
1:G:130:GLU:HG3	3:G:386:HOH:O	1.58	1.01
1:E:77:YCM:HB3	3:E:302:HOH:O	1.62	0.97
1:A:71[B]:VAL:CG1	1:E:71:VAL:HB	1.99	0.91
1:E:157:VAL:HG12	1:E:158:SER:H	1.37	0.90
1:F:1:SER:HA	3:F:381:HOH:O	1.71	0.89
1:B:77[A]:YCM:HD2	1:B:78:ALA:N	1.90	0.86
1:D:77:YCM:HB3	3:D:388:HOH:O	1.76	0.85
1:G:9:ASN:HD21	1:G:67:GLU:H	1.24	0.83
1:A:9:ASN:HD21	1:A:67:GLU:H	1.28	0.82
1:H:153:SER:O	1:H:154:LEU:HD22	1.81	0.80
1:D:153:SER:O	1:D:154:LEU:HD22	1.82	0.79
1:B:77[A]:YCM:HD2	1:B:78:ALA:H	1.49	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:153:SER:HB2	1:G:154:LEU:HD11	1.68	0.74
1:H:24[A]:SER:OG	1:H:77[A]:YCM:HD2	1.86	0.74
1:B:14:GLN:HE21	1:B:97:ASN:ND2	1.85	0.73
1:B:14:GLN:HE21	1:B:97:ASN:HD22	1.37	0.73
1:A:71[B]:VAL:HG13	1:A:71[B]:VAL:O	1.88	0.73
1:D:112:HIS:CE1	3:D:415:HOH:O	2.42	0.72
1:G:48:GLU:OE2	3:G:405:HOH:O	2.05	0.72
1:F:48:GLU:OE2	3:F:367:HOH:O	2.06	0.72
1:E:157:VAL:HG12	1:E:158:SER:N	2.04	0.70
1:H:153:SER:C	1:H:154:LEU:HD22	2.13	0.69
1:H:157:VAL:O	1:H:158:SER:HB2	1.91	0.69
1:C:126:GLN:NE2	3:C:373:HOH:O	2.27	0.68
1:F:156:VAL:C	1:F:158:SER:H	1.97	0.67
1:E:153:SER:HB2	1:F:154:LEU:HD21	1.75	0.67
1:B:153:SER:OG	1:C:154:LEU:HD11	1.95	0.66
1:G:2:GLU:OE2	1:G:5[A]:LEU:HD12	1.95	0.66
1:G:10:ARG:HH11	1:G:10:ARG:HG2	1.59	0.66
1:B:150:LEU:O	1:B:154:LEU:HD23	1.97	0.65
1:D:9:ASN:HD21	1:D:67:GLU:H	1.45	0.65
1:D:112:HIS:ND1	3:D:415:HOH:O	2.29	0.64
1:E:94:GLU:HG3	1:E:134:ILE:CD1	2.27	0.64
1:D:153:SER:HB2	1:G:154:LEU:CD1	2.28	0.64
1:E:40:TYR:OH	1:E:133:LYS:CE	2.46	0.63
1:A:94:GLU:HG3	1:A:134:ILE:CD1	2.29	0.62
1:F:94:GLU:HG3	1:F:134[A]:ILE:CD1	2.28	0.62
1:G:94:GLU:HG3	1:G:134:ILE:CD1	2.29	0.62
1:H:157:VAL:HG12	1:H:158:SER:H	1.65	0.61
1:A:71[B]:VAL:CG1	1:E:71:VAL:CB	2.74	0.61
1:F:4[B]:LEU:HD23	1:F:4[B]:LEU:C	2.20	0.61
1:H:14:GLN:HG2	1:H:97[A]:ASN:OD1	2.00	0.61
1:E:6[B]:ASP:OD2	1:E:10:ARG:NH1	2.34	0.61
1:D:33:ASP:OD2	3:D:416:HOH:O	2.15	0.60
1:H:49[B]:ARG:HD3	3:H:340:HOH:O	2.00	0.60
1:B:153:SER:C	1:B:154:LEU:HD22	2.21	0.60
1:B:124:HIS:HD2	3:B:363:HOH:O	1.84	0.59
1:B:153:SER:OG	1:C:154:LEU:CD1	2.50	0.59
1:G:157:VAL:HG12	1:G:158:SER:N	2.18	0.59
1:D:158:SER:O	1:D:159:PHE:HB2	2.02	0.59
1:F:10:ARG:HG3	3:F:355:HOH:O	2.03	0.59
1:G:9:ASN:ND2	1:G:67:GLU:H	2.00	0.58
1:C:154:LEU:HD12	1:C:154:LEU:N	2.17	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:152:ARG:O	1:G:156:VAL:HG23	2.03	0.58
1:D:153:SER:HB2	1:G:154:LEU:CG	2.35	0.57
1:E:5:LEU:HD13	1:E:65:PRO:HD2	1.87	0.57
1:D:144:GLU:OE1	1:D:154:LEU:HG	2.05	0.57
1:F:77[A]:YCM:HD2	3:F:384:HOH:O	2.04	0.56
1:B:145:ASN:CB	3:B:388:HOH:O	2.11	0.56
1:C:49:ARG:HD3	1:H:49[A]:ARG:CD	2.36	0.56
1:G:146:ARG:NH1	3:G:314:HOH:O	2.38	0.56
1:G:5[B]:LEU:HD13	1:G:64:ILE:HG23	1.87	0.56
1:D:14:GLN:HG2	1:D:97[A]:ASN:OD1	2.05	0.56
1:E:40:TYR:OH	1:E:133:LYS:HE3	2.05	0.56
1:B:154:LEU:CD2	1:B:154:LEU:N	2.69	0.55
1:G:153:SER:C	1:G:154:LEU:HD22	2.27	0.55
1:A:9:ASN:ND2	1:A:67:GLU:H	2.00	0.55
1:C:126:GLN:O	1:C:130[B]:GLU:HG3	2.06	0.55
1:G:153:SER:HB2	1:H:154:LEU:HD11	1.87	0.55
1:H:94:GLU:HG3	1:H:134:ILE:CD1	2.37	0.55
1:E:40:TYR:OH	1:E:133:LYS:HE2	2.07	0.54
1:A:97[A]:ASN:ND2	1:A:100[A]:SER:OG	2.40	0.54
1:A:124:HIS:HE1	3:A:314:HOH:O	1.91	0.54
1:E:153:SER:CB	1:F:154:LEU:HD21	2.37	0.53
1:C:94:GLU:HG3	1:C:134:ILE:CD1	2.39	0.53
1:G:154:LEU:HD22	1:G:154:LEU:N	2.24	0.53
1:H:150:LEU:O	1:H:154:LEU:HD23	2.10	0.52
1:A:7:LEU:CD2	1:A:10[B]:ARG:HH11	2.23	0.52
1:A:138:LEU:O	1:A:142[A]:THR:CG2	2.58	0.52
1:G:153:SER:HB2	1:H:154:LEU:HD21	1.91	0.52
1:G:5[B]:LEU:HD12	1:G:5[B]:LEU:O	2.10	0.52
1:E:157:VAL:CG1	1:E:158:SER:N	2.72	0.52
1:B:77[B]:YCM:HA	1:B:80:TRP:CE3	2.45	0.51
1:C:49:ARG:CD	1:H:49[A]:ARG:HD2	2.40	0.51
1:E:77:YCM:HZ21	1:E:77:YCM:C	2.23	0.51
1:F:77[A]:YCM:HA	1:F:80:TRP:CE3	2.44	0.51
1:B:5:LEU:HD13	1:B:65:PRO:HD2	1.92	0.51
1:H:138:LEU:O	1:H:142[B]:THR:HG23	2.10	0.51
1:A:71[B]:VAL:HG12	1:E:71:VAL:CB	2.23	0.51
1:D:158:SER:O	1:D:159:PHE:CB	2.58	0.51
1:A:138:LEU:O	1:A:142[B]:THR:HG23	2.11	0.51
1:B:24[B]:SER:OG	1:B:77[B]:YCM:OZ1	2.20	0.50
1:H:77[A]:YCM:HA	1:H:80:TRP:CE3	2.46	0.50
1:F:150:LEU:O	1:F:153:SER:HB2	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:5:LEU:O	1:E:5:LEU:HD12	2.12	0.50
1:F:157:VAL:O	1:F:157:VAL:HG12	2.12	0.50
1:G:77:YCM:HA	1:G:80:TRP:CE3	2.47	0.50
1:G:10:ARG:HH11	1:G:10:ARG:CG	2.25	0.50
1:G:84:GLU:HG3	1:G:142[A]:THR:HG22	1.93	0.49
1:A:9:ASN:HD21	1:A:67:GLU:N	2.06	0.49
1:A:7:LEU:HD23	1:A:10[B]:ARG:HH11	1.76	0.49
1:D:1:SER:OG	1:D:5:LEU:HD11	2.13	0.49
1:D:153:SER:C	1:D:154:LEU:HD22	2.31	0.49
1:C:153:SER:C	1:C:154:LEU:HD12	2.32	0.49
1:A:14:GLN:HE21	1:A:97[A]:ASN:HD22	1.61	0.49
1:B:77[A]:YCM:HA	1:B:80:TRP:CE3	2.47	0.49
1:A:71[B]:VAL:O	1:A:71[B]:VAL:CG1	2.58	0.49
1:G:9:ASN:HD21	1:G:67:GLU:N	2.02	0.49
1:G:124:HIS:HE1	3:G:304:HOH:O	1.96	0.49
1:D:143:ASP:OD1	1:D:146:ARG:NH1	2.46	0.48
1:G:136[B]:SER:O	1:G:140:LYS:HG3	2.14	0.48
1:E:77:YCM:C	1:E:77:YCM:NZ2	2.77	0.48
1:G:157:VAL:HG22	1:H:157:VAL:HG11	1.96	0.48
1:F:156:VAL:C	1:F:158:SER:N	2.67	0.48
1:G:145[A]:ASN:ND2	3:G:302:HOH:O	2.46	0.48
1:F:77[B]:YCM:HZ22	1:F:78:ALA:HB2	1.79	0.47
1:B:24[B]:SER:O	1:B:77[B]:YCM:OZ1	2.31	0.47
1:G:150:LEU:O	1:G:154:LEU:HD23	2.14	0.47
1:C:77[B]:YCM:HD2	3:C:387:HOH:O	2.14	0.47
1:F:77[B]:YCM:HA	1:F:80:TRP:CE3	2.48	0.47
1:G:2:GLU:OE2	1:G:2:GLU:HA	2.14	0.47
1:G:138:LEU:O	1:G:142[A]:THR:HG23	2.14	0.47
1:G:157:VAL:CG2	1:H:157:VAL:HG11	2.45	0.47
1:A:9:ASN:HD22	1:A:66:ILE:HA	1.78	0.47
1:B:144:GLU:OE1	1:B:154:LEU:HG	2.14	0.47
1:E:69:GLN:HG3	3:E:326:HOH:O	2.15	0.47
1:D:40:TYR:OH	1:D:133:LYS:HE3	2.16	0.46
1:E:124:HIS:HE1	3:E:306:HOH:O	1.97	0.46
1:C:49:ARG:HD3	1:H:49[A]:ARG:HD2	1.97	0.46
1:H:77[B]:YCM:HA	1:H:80:TRP:CE3	2.50	0.46
1:B:154:LEU:HD22	1:B:154:LEU:N	2.30	0.46
1:F:153:SER:C	1:F:154:LEU:HD22	2.37	0.46
1:E:150:LEU:O	1:E:154:LEU:HD23	2.16	0.45
1:C:77[A]:YCM:HA	1:C:80:TRP:CE3	2.51	0.45
1:H:157:VAL:O	1:H:158:SER:CB	2.58	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:77[B]:YCM:HA	1:C:80:TRP:CE3	2.51	0.45
1:A:138:LEU:O	1:A:142[A]:THR:HG22	2.15	0.45
1:A:20:GLN:HG3	1:A:71[B]:VAL:HG21	1.98	0.45
1:B:124:HIS:HE1	3:B:305:HOH:O	1.99	0.45
1:F:157:VAL:O	1:F:157:VAL:CG1	2.65	0.45
1:C:5:LEU:HD12	1:C:5:LEU:O	2.17	0.44
1:G:154:LEU:N	1:G:154:LEU:CD2	2.81	0.44
1:G:1:SER:O	1:G:2:GLU:C	2.56	0.44
1:B:157:VAL:HB	1:B:158:SER:H	1.60	0.44
1:G:10:ARG:NH1	1:G:10:ARG:CG	2.80	0.44
1:E:124:HIS:HD2	3:E:313:HOH:O	2.01	0.44
1:H:138:LEU:O	1:H:142[B]:THR:CG2	2.65	0.44
1:F:144:GLU:OE1	1:F:154:LEU:HG	2.18	0.43
1:A:71[B]:VAL:CG1	1:E:71:VAL:CG2	2.97	0.43
1:A:77:YCM:HA	1:A:80:TRP:CE3	2.52	0.43
1:F:154:LEU:CD2	1:F:154:LEU:N	2.82	0.43
1:D:157:VAL:O	1:D:158:SER:C	2.56	0.43
1:A:124:HIS:HD2	3:A:321:HOH:O	2.01	0.43
1:C:153:SER:CB	1:C:154:LEU:HD12	2.48	0.43
1:F:4[B]:LEU:O	1:F:4[B]:LEU:HD23	2.17	0.43
1:C:144:GLU:OE2	1:C:154:LEU:HD22	2.19	0.43
1:F:1:SER:O	1:F:5:LEU:HG	2.18	0.42
1:C:94:GLU:HG3	1:C:134:ILE:HD12	2.01	0.42
1:H:157:VAL:HG12	1:H:158:SER:N	2.34	0.42
1:C:49:ARG:HD3	1:H:49[B]:ARG:HD2	1.99	0.42
1:F:10:ARG:HD2	1:F:10:ARG:O	2.19	0.42
1:A:20:GLN:HG3	1:A:71[B]:VAL:CG2	2.50	0.42
1:D:77:YCM:HA	1:D:80:TRP:CE3	2.54	0.42
1:A:10[A]:ARG:HG2	1:A:10[A]:ARG:HH11	1.84	0.42
1:D:146:ARG:HD3	1:D:146:ARG:HH11	1.71	0.42
1:B:40:TYR:OH	1:B:133:LYS:HE3	2.20	0.41
1:E:153:SER:C	1:E:154:LEU:HD22	2.41	0.41
1:G:66:ILE:HD13	1:G:66:ILE:HA	1.82	0.41
1:D:1:SER:HA	1:D:2:GLU:HA	1.76	0.41
1:D:153:SER:HB2	1:G:154:LEU:HG	2.03	0.41
1:H:152:ARG:C	1:H:154:LEU:H	2.24	0.41
1:F:24[A]:SER:OG	1:F:77[A]:YCM:HB3	2.20	0.41
1:C:146:ARG:NH1	3:C:347:HOH:O	2.53	0.41
1:E:138:LEU:O	1:E:142[A]:THR:HG23	2.21	0.41
1:G:153:SER:CB	1:H:154:LEU:HD21	2.51	0.41
1:E:154:LEU:CD2	1:E:154:LEU:N	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:152:ARG:O	1:C:153:SER:C	2.58	0.41
1:A:138:LEU:O	1:A:142[A]:THR:HG23	2.20	0.41
1:D:126[B]:GLN:O	1:D:130[B]:GLU:HG3	2.21	0.41
1:F:154:LEU:HD22	1:F:154:LEU:N	2.36	0.41
1:F:126:GLN:NE2	3:F:331:HOH:O	2.53	0.41
1:E:77:YCM:HA	1:E:80:TRP:CE3	2.55	0.41
1:B:153:SER:HA	1:C:154:LEU:HD21	2.02	0.41
1:C:68:LEU:H	1:H:77[A]:YCM:HZ22	1.69	0.40
1:D:94:GLU:HG3	1:D:134:ILE:CD1	2.51	0.40
1:G:158:SER:OG	1:G:159:PHE:N	2.49	0.40
1:C:152:ARG:HA	1:C:152:ARG:HD3	1.84	0.40
1:F:142[B]:THR:HG23	3:F:352:HOH:O	2.19	0.40
1:H:138:LEU:O	1:H:142[A]:THR:HG23	2.21	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	162/168 (96%)	158 (98%)	3 (2%)	1 (1%)	30	22
1	B	161/168 (96%)	156 (97%)	3 (2%)	2 (1%)	16	8
1	C	158/168 (94%)	155 (98%)	3 (2%)	0	100	100
1	D	164/168 (98%)	160 (98%)	2 (1%)	2 (1%)	16	8
1	E	160/168 (95%)	157 (98%)	1 (1%)	2 (1%)	15	7
1	F	161/168 (96%)	158 (98%)	2 (1%)	1 (1%)	30	22
1	G	164/168 (98%)	161 (98%)	2 (1%)	1 (1%)	30	22
1	H	160/168 (95%)	155 (97%)	4 (2%)	1 (1%)	30	22
All	All	1290/1344 (96%)	1260 (98%)	20 (2%)	10 (1%)	24	15

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	157	VAL
1	B	157	VAL
1	E	157	VAL
1	F	157	VAL
1	H	157	VAL
1	A	156	VAL
1	E	2	GLU
1	G	157	VAL
1	D	158	SER
1	B	158	SER

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	142/143 (99%)	136 (96%)	6 (4%)	36	31
1	B	141/143 (99%)	137 (97%)	4 (3%)	51	50
1	C	138/143 (96%)	134 (97%)	4 (3%)	50	49
1	D	144/143 (101%)	140 (97%)	4 (3%)	51	50
1	E	140/143 (98%)	136 (97%)	4 (3%)	50	49
1	F	141/143 (99%)	134 (95%)	7 (5%)	30	24
1	G	144/143 (101%)	142 (99%)	2 (1%)	74	77
1	H	140/143 (98%)	135 (96%)	5 (4%)	42	39
All	All	1130/1144 (99%)	1094 (97%)	36 (3%)	46	44

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLU
1	A	30	ASP
1	A	35	GLU
1	A	142[A]	THR

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Mol	Chain	Res	Type
1	A	142[B]	THR
1	A	157	VAL
1	D	1	SER
1	D	30	ASP
1	D	157	VAL
1	D	158	SER
1	B	30	ASP
1	B	126	GLN
1	B	153	SER
1	B	154	LEU
1	C	30	ASP
1	C	100	SER
1	C	152	ARG
1	C	156	VAL
1	E	3	GLU
1	E	30	ASP
1	E	79	GLU
1	E	154	LEU
1	F	1	SER
1	F	10	ARG
1	F	30	ASP
1	F	126	GLN
1	F	154	LEU
1	F	156	VAL
1	F	158	SER
1	G	30	ASP
1	G	154	LEU
1	H	1	SER
1	H	10	ARG
1	H	14	GLN
1	H	120	LEU
1	H	158	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	11	GLN
1	A	63	ASN
1	A	103	ASN
1	A	121	ASN
1	A	124	HIS

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Mol	Chain	Res	Type
1	D	9	ASN
1	D	14	GLN
1	D	63	ASN
1	B	95	GLN
1	B	97	ASN
1	B	121	ASN
1	B	124	HIS
1	B	126	GLN
1	C	63	ASN
1	C	126	GLN
1	E	121	ASN
1	E	124	HIS
1	F	69	GLN
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

12 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	1.09	1 (12%)	5,10,12	1.25	1 (20%)
1	YCM	B	77[A]	-	8,9,10	1.10	1 (12%)	5,10,12	1.51	1 (20%)
1	YCM	B	77[B]	-	8,9,10	2.78	2 (25%)	5,10,12	2.50	2 (40%)
1	YCM	C	77[A]	-	8,9,10	2.28	1 (12%)	5,10,12	1.40	1 (20%)
1	YCM	C	77[B]	-	8,9,10	1.22	1 (12%)	5,10,12	1.04	1 (20%)
1	YCM	D	77	1	8,9,10	1.94	1 (12%)	5,10,12	1.21	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	YCM	E	77	1	8,9,10	0.93	0	5,10,12	1.15	0
1	YCM	F	77[A]	1	8,9,10	1.32	1 (12%)	5,10,12	1.07	1 (20%)
1	YCM	F	77[B]	1	8,9,10	0.98	1 (12%)	5,10,12	1.13	1 (20%)
1	YCM	G	77	1	8,9,10	1.46	1 (12%)	5,10,12	0.92	0
1	YCM	H	77[A]	-	8,9,10	2.53	3 (37%)	5,10,12	2.15	2 (40%)
1	YCM	H	77[B]	-	8,9,10	0.73	0	5,10,12	0.91	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	YCM	A	77	1	-	0/6/8/10	0/0/0/0
1	YCM	B	77[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]	-	-	0/6/8/10	0/0/0/0
1	YCM	C	77[B]	-	-	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]	1	-	0/6/8/10	0/0/0/0
1	YCM	F	77[B]	1	-	0/6/8/10	0/0/0/0
1	YCM	G	77	1	-	0/6/8/10	0/0/0/0
1	YCM	H	77[A]	-	-	0/6/8/10	0/0/0/0
1	YCM	H	77[B]	-	-	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[A]	YCM	CB-SG	2.04	1.85	1.81
1	F	77[B]	YCM	CB-SG	2.10	1.85	1.81
1	H	77[A]	YCM	CE-NZ2	2.47	1.40	1.32
1	A	77	YCM	CB-SG	2.75	1.86	1.81
1	C	77[B]	YCM	CB-SG	3.01	1.87	1.81
1	F	77[A]	YCM	CD-SG	3.18	1.88	1.81
1	G	77	YCM	CD-SG	3.68	1.89	1.81
1	H	77[A]	YCM	CD-SG	3.69	1.89	1.81
1	H	77[A]	YCM	CB-SG	4.84	1.90	1.81
1	B	77[B]	YCM	CD-SG	4.99	1.92	1.81
1	D	77	YCM	CB-SG	5.20	1.91	1.81
1	B	77[B]	YCM	CB-SG	5.40	1.92	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	77[A]	YCM	CB-SG	6.16	1.93	1.81

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	77[A]	YCM	O-C-CA	-3.00	117.67	125.49
1	B	77[B]	YCM	O-C-CA	-2.79	118.23	125.49
1	D	77	YCM	O-C-CA	-2.38	119.28	125.49
1	A	77	YCM	O-C-CA	-2.38	119.29	125.49
1	F	77[A]	YCM	O-C-CA	-2.33	119.43	125.49
1	C	77[B]	YCM	O-C-CA	-2.07	120.10	125.49
1	F	77[B]	YCM	O-C-CA	-2.07	120.10	125.49
1	B	77[A]	YCM	O-C-CA	-2.03	120.21	125.49
1	H	77[A]	YCM	CA-CB-SG	2.69	119.21	112.84
1	H	77[A]	YCM	CD-CE-NZ2	3.12	118.92	115.48
1	B	77[B]	YCM	CD-CE-NZ2	4.48	120.42	115.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 28 short contacts:

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 32 ligands modelled in this entry, 32 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^{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	156/168 (92%)	-0.15	3 (1%)	70	70	18, 27, 45, 67	0
1	B	158/168 (94%)	-0.08	8 (5%)	32	33	19, 30, 52, 75	0
1	C	154/168 (91%)	-0.22	2 (1%)	79	80	18, 26, 42, 67	0
1	D	158/168 (94%)	-0.15	4 (2%)	61	61	16, 25, 47, 86	0
1	E	157/168 (93%)	-0.11	4 (2%)	61	61	19, 27, 54, 78	0
1	F	157/168 (93%)	-0.09	5 (3%)	51	52	20, 28, 53, 76	0
1	G	158/168 (94%)	-0.10	6 (3%)	44	45	16, 25, 49, 85	0
1	H	157/168 (93%)	-0.13	4 (2%)	61	61	17, 25, 52, 67	0
All	All	1255/1344 (93%)	-0.13	36 (2%)	55	56	16, 27, 50, 86	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	156	VAL	5.8
1	G	157	VAL	5.3
1	H	156	VAL	4.2
1	E	1	SER	3.8
1	C	156	VAL	3.7
1	G	153	SER	3.3
1	F	157	VAL	3.2
1	E	153	SER	3.1
1	H	71	VAL	3.1
1	D	157	VAL	3.0
1	G	156	VAL	2.9
1	A	71[A]	VAL	2.9
1	E	156	VAL	2.9
1	E	157	VAL	2.9
1	F	70	ALA	2.6
1	B	157	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	H	70	ALA	2.6
1	A	72	PRO	2.5
1	B	71	VAL	2.5
1	F	71	VAL	2.5
1	G	159	PHE	2.5
1	D	73	ALA	2.4
1	F	153	SER	2.4
1	C	73	ALA	2.4
1	A	73	ALA	2.3
1	B	73	ALA	2.3
1	B	2	GLU	2.3
1	H	72	PRO	2.2
1	D	71	VAL	2.2
1	B	153	SER	2.2
1	B	158	SER	2.1
1	F	99	ARG	2.0
1	B	72	PRO	2.0
1	D	153	SER	2.0
1	G	1	SER	2.0
1	G	78	ALA	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	B	77[A]	10/11	0.81	0.28	-	32,36,40,47	7
1	YCM	B	77[B]	10/11	0.81	0.28	-	25,33,36,39	7
1	YCM	D	77	10/11	0.95	0.10	-	29,37,49,54	0
1	YCM	H	77[A]	10/11	0.81	0.21	-	18,35,41,43	7
1	YCM	C	77[B]	10/11	0.87	0.26	-	29,32,35,36	7
1	YCM	C	77[A]	10/11	0.87	0.26	-	23,30,32,33	7
1	YCM	F	77[A]	10/11	0.87	0.18	-	30,37,40,44	10
1	YCM	G	77	10/11	0.94	0.10	-	31,39,54,55	0
1	YCM	F	77[B]	10/11	0.87	0.18	-	33,38,42,44	10
1	YCM	E	77	10/11	0.94	0.10	-	36,46,61,68	0
1	YCM	A	77	10/11	0.96	0.09	-	31,39,50,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
1	YCM	H	77[B]	10/11	0.81	0.21	-	31,37,41,43	7

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	ZN	C	204	1/1	0.85	0.26	5.80	49,49,49,49	1
2	ZN	D	204	1/1	0.92	0.17	3.72	44,44,44,44	1
2	ZN	A	204	1/1	0.76	0.17	2.80	48,48,48,48	1
2	ZN	H	204	1/1	0.83	0.14	0.77	50,50,50,50	1
2	ZN	B	204	1/1	0.73	0.11	0.02	50,50,50,50	1
2	ZN	G	204	1/1	0.84	0.11	-0.13	48,48,48,48	1
2	ZN	H	201	1/1	1.00	0.07	-1.27	26,26,26,26	0
2	ZN	C	201	1/1	1.00	0.05	-1.30	27,27,27,27	0
2	ZN	E	204	1/1	0.88	0.06	-1.69	53,53,53,53	1
2	ZN	E	201	1/1	1.00	0.05	-1.71	29,29,29,29	0
2	ZN	A	203	1/1	1.00	0.04	-1.88	37,37,37,37	1
2	ZN	C	203	1/1	0.99	0.04	-1.88	36,36,36,36	0
2	ZN	B	203	1/1	0.99	0.04	-1.94	40,40,40,40	0
2	ZN	H	203	1/1	1.00	0.04	-1.97	33,33,33,33	1
2	ZN	D	201	1/1	1.00	0.04	-1.99	26,26,26,26	0
2	ZN	F	204	1/1	0.94	0.07	-2.04	48,48,48,48	1
2	ZN	A	201	1/1	1.00	0.06	-2.11	29,29,29,29	0
2	ZN	D	203	1/1	1.00	0.04	-2.21	34,34,34,34	1
2	ZN	G	203	1/1	0.99	0.04	-2.57	35,35,35,35	0
2	ZN	E	202	1/1	0.99	0.03	-2.62	35,35,35,35	1
2	ZN	F	203	1/1	0.99	0.03	-3.20	35,35,35,35	1
2	ZN	C	202	1/1	0.97	0.04	-3.41	36,36,36,36	1
2	ZN	D	202	1/1	0.99	0.04	-3.72	37,37,37,37	1
2	ZN	E	203	1/1	0.99	0.04	-4.06	39,39,39,39	1
2	ZN	G	202	1/1	0.97	0.04	-	33,33,33,33	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	ZN	A	202	1/1	0.98	0.04	-	38,38,38,38	1
2	ZN	B	201	1/1	1.00	0.06	-	31,31,31,31	0
2	ZN	F	202	1/1	0.94	0.08	-	41,41,41,41	1
2	ZN	F	201	1/1	1.00	0.06	-	30,30,30,30	0
2	ZN	G	201	1/1	1.00	0.06	-	26,26,26,26	0
2	ZN	B	202	1/1	0.98	0.03	-	42,42,42,42	1
2	ZN	H	202	1/1	0.97	0.05	-	37,37,37,37	1

6.5 Other polymers

There are no such residues in this entry.