Full wwPDB X-ray Structure Validation Report (i)

Nov 16, 2023 – 10:13 AM JST

PDB ID	:	6LKW
Title	:	Structural and functional insights into macrophage migration inhibitory factor from Oncomelania hupensis, the intermediate host of Schistosoma japonicum
Authors	:	Su, Z.M.; Tian, X.Y.; Li, H.J.; Wei, Z.M.; Chen, L.F.; Ren, H.X.; Peng, W.F.; Tang, C.T.
Deposited on	:	2019-12-20
Resolution	:	3.20 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

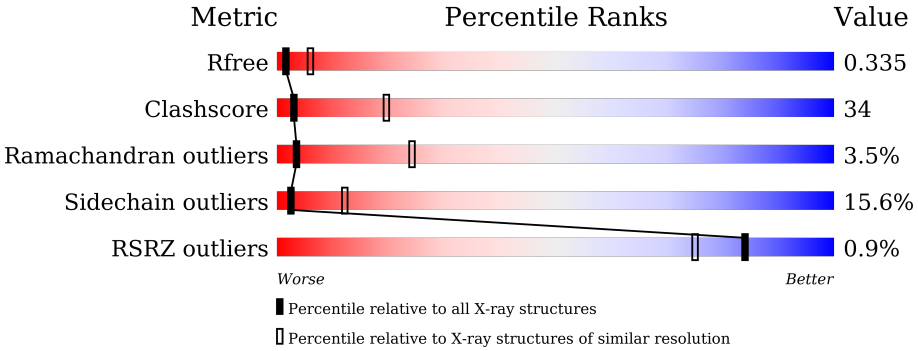
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 <=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	138	63% 28% 8% •
2	B	139	% 62% 35% •
3	D	137	% 45% 43% 12%
4	C	134	2% 43% 40% 16% •

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 4383 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 Macrophage migration inhibitory factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	138	1081	682	192	195	12	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	89	ASN	LYS	See sequence details	UNP A0A1U9W5E8
A	90	VAL	ILE	See sequence details	UNP A0A1U9W5E8
A	125	ILE	ASN	See sequence details	UNP A0A1U9W5E8
A	132	TYR	-	expression tag	UNP A0A1U9W5E8
A	133	LEU	-	expression tag	UNP A0A1U9W5E8
A	134	HIS	-	expression tag	UNP A0A1U9W5E8
A	135	HIS	-	expression tag	UNP A0A1U9W5E8
A	136	HIS	-	expression tag	UNP A0A1U9W5E8
A	137	HIS	-	expression tag	UNP A0A1U9W5E8
A	138	HIS	-	expression tag	UNP A0A1U9W5E8

- Molecule 2 is a protein called Macrophage migration inhibitory factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	139	1090	688	194	196	12	0	0	0

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	89	ASN	LYS	See sequence details	UNP A0A1U9W5E8
B	90	VAL	ILE	See sequence details	UNP A0A1U9W5E8
B	125	ILE	ASN	See sequence details	UNP A0A1U9W5E8
B	132	TYR	-	expression tag	UNP A0A1U9W5E8
B	133	LEU	-	expression tag	UNP A0A1U9W5E8
B	134	HIS	-	expression tag	UNP A0A1U9W5E8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	135	HIS	-	expression tag	UNP A0A1U9W5E8
B	136	HIS	-	expression tag	UNP A0A1U9W5E8
B	137	ALA	-	expression tag	UNP A0A1U9W5E8
B	138	HIS	-	expression tag	UNP A0A1U9W5E8
B	139	HIS	-	expression tag	UNP A0A1U9W5E8

- Molecule 3 is a protein called Macrophage migration inhibitory factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	D	137	1057	665	189	191	12	0	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	89	ASN	LYS	See sequence details	UNP A0A1U9W5E8
D	90	VAL	ILE	See sequence details	UNP A0A1U9W5E8
D	125	ILE	ASN	See sequence details	UNP A0A1U9W5E8
D	132	ALA	-	expression tag	UNP A0A1U9W5E8
D	133	ALA	-	expression tag	UNP A0A1U9W5E8
D	134	HIS	-	expression tag	UNP A0A1U9W5E8
D	135	HIS	-	expression tag	UNP A0A1U9W5E8
D	136	HIS	-	expression tag	UNP A0A1U9W5E8
D	137	ALA	-	expression tag	UNP A0A1U9W5E8

- Molecule 4 is a protein called Macrophage migration inhibitory factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	C	134	1039	657	182	189	11	0	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	89	ASN	LYS	See sequence details	UNP A0A1U9W5E8
C	90	VAL	ILE	See sequence details	UNP A0A1U9W5E8
C	125	ILE	ASN	See sequence details	UNP A0A1U9W5E8
C	132	TYR	-	expression tag	UNP A0A1U9W5E8
C	133	LEU	-	expression tag	UNP A0A1U9W5E8
C	134	HIS	-	expression tag	UNP A0A1U9W5E8
C	135	ALA	-	expression tag	UNP A0A1U9W5E8

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
5	A	1	1	1	0	0
5	B	1	1	1	0	0

- Molecule 6 is water.

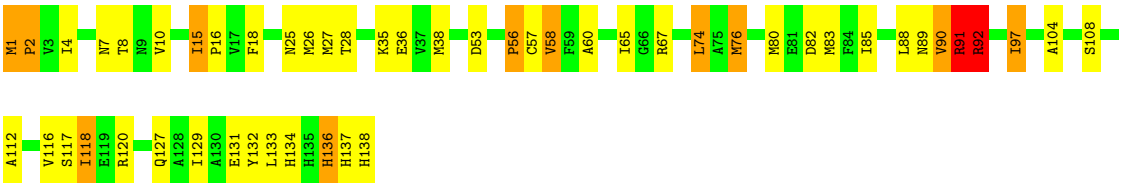
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	40	40	40	0	0
6	B	27	27	27	0	0
6	D	22	22	22	0	0
6	C	25	25	25	0	0

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.

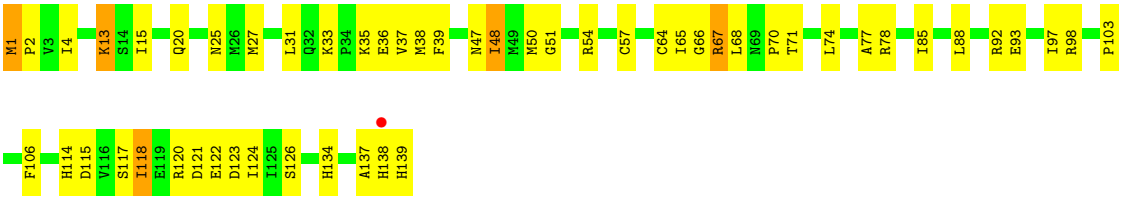
• Molecule 1: Macrophage migration inhibitory factor

Chain A:



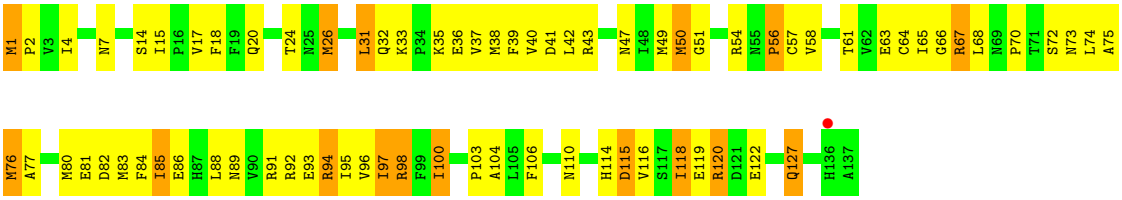
• Molecule 2: Macrophage migration inhibitory factor

Chain B:



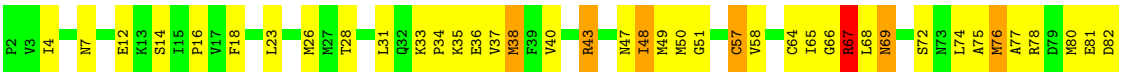
• Molecule 3: Macrophage migration inhibitory factor

Chain D:



• Molecule 4: Macrophage migration inhibitory factor

Chain C:



M83
F84
I85
E86
V90
R91
R92
I95
R98
F99
I100
P101
V102
P103
A104
L105
F106
C107
S108
F109
N110
G111
A112
L113
H114
D115
V116
S117
I118
E119
R120
D121
E122
D123
I124
I125
S126
Q127
A128
I129
A130
E131
Y132
L133
H134
A135

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 3 2	Depositor
Cell constants a, b, c, α, β, γ	172.84Å 172.84Å 172.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.95 – 3.20 25.48 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.4 (49.95-3.20) 99.7 (25.48-3.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	6.99 (at 3.17Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.230 , 0.333 0.234 , 0.335	Depositor DCC
R_{free} test set	735 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å^2)	60.4	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 50.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	4383	wwPDB-VP
Average B, all atoms (Å^2)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.25% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.69	0/1102	0.90	0/1492
2	B	0.65	0/1111	0.86	0/1503
3	D	0.65	0/1076	0.89	0/1457
4	C	0.65	0/1057	0.95	1/1431 (0.1%)
All	All	0.66	0/4346	0.90	1/5883 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	114	HIS	CB-CA-C	5.08	120.56	110.40

There are no chirality outliers.

There are no planarity outliers.

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	1081	0	1076	50	0
2	B	1090	0	1092	48	0
3	D	1057	0	1058	100	0
4	C	1039	0	1043	118	0
5	A	1	0	0	0	0
5	B	1	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	40	0	0	2	0
6	B	27	0	0	0	0
6	C	25	0	0	1	0
6	D	22	0	0	3	0
All	All	4383	0	4269	293	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 34.

All (293) 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)
3:D:98:ARG:NH1	3:D:100:ILE:HD13	1.43	1.30
4:C:16:PRO:HB3	4:C:18:PHE:CE1	1.73	1.22
4:C:28:THR:HA	4:C:38:MET:HE1	1.27	1.13
4:C:81:GLU:O	4:C:85:ILE:HD12	1.48	1.11
3:D:51:GLY:HA2	4:C:35:LYS:O	1.48	1.10
3:D:50:MET:CE	3:D:57:CYS:HB2	1.82	1.09
3:D:73:ASN:ND2	4:C:106:PHE:CD2	2.20	1.09
3:D:98:ARG:HH11	3:D:100:ILE:HD13	0.95	1.09
1:A:16:PRO:HB3	1:A:18:PHE:CE1	1.90	1.07
3:D:73:ASN:ND2	4:C:106:PHE:HD2	1.51	1.05
3:D:98:ARG:NH1	3:D:100:ILE:HG23	1.73	1.03
2:B:1:MET:HB2	2:B:64:CYS:HA	1.43	0.99
3:D:1:MET:HB2	3:D:64:CYS:HA	1.45	0.99
3:D:15:ILE:HD13	3:D:88:LEU:HD23	1.43	0.98
4:C:26:MET:HE1	4:C:83:MET:SD	2.04	0.97
2:B:118:ILE:HG23	2:B:123:ASP:OD1	1.63	0.97
4:C:31:LEU:O	4:C:67:ARG:HD2	1.62	0.97
4:C:26:MET:CE	4:C:83:MET:SD	2.54	0.96
4:C:28:THR:CA	4:C:38:MET:HE1	1.96	0.96
3:D:98:ARG:HH11	3:D:100:ILE:CD1	1.80	0.94
2:B:25:ASN:HD21	2:B:35:LYS:HE3	1.32	0.94
4:C:113:LEU:HD12	4:C:113:LEU:H	1.33	0.93
4:C:107:CYS:SG	4:C:107:CYS:O	2.27	0.93
3:D:96:VAL:HG22	4:C:109:PHE:HB2	1.52	0.92
4:C:16:PRO:HB3	4:C:18:PHE:HE1	1.32	0.92
2:B:25:ASN:ND2	2:B:35:LYS:HE3	1.85	0.91
3:D:31:LEU:HD21	3:D:76:MET:SD	2.11	0.90
4:C:118:ILE:N	4:C:122:GLU:CB	2.35	0.90
3:D:74:LEU:HB2	4:C:113:LEU:HD11	1.55	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:98:ARG:NH1	3:D:100:ILE:CD1	2.35	0.89
3:D:98:ARG:NH1	3:D:100:ILE:CG2	2.35	0.88
3:D:92:ARG:HD2	4:C:110:ASN:OD1	1.74	0.88
3:D:50:MET:HE3	3:D:57:CYS:HB2	1.55	0.86
2:B:51:GLY:HA2	3:D:35:LYS:O	1.74	0.86
4:C:28:THR:HA	4:C:38:MET:CE	2.05	0.86
4:C:33:LYS:CE	4:C:67:ARG:NH1	2.39	0.85
1:A:74:LEU:O	1:A:74:LEU:HD12	1.76	0.85
4:C:31:LEU:HD21	4:C:76:MET:HE1	1.57	0.85
2:B:35:LYS:O	4:C:51:GLY:HA2	1.79	0.83
3:D:31:LEU:O	3:D:67:ARG:HD2	1.77	0.83
2:B:1:MET:HG2	2:B:65:ILE:HG13	1.57	0.83
3:D:84:PHE:HD2	3:D:95:ILE:HD13	1.44	0.83
3:D:15:ILE:HD13	3:D:88:LEU:CD2	2.09	0.82
4:C:31:LEU:CD2	4:C:76:MET:CE	2.57	0.82
1:A:16:PRO:HB3	1:A:18:PHE:HE1	1.43	0.81
3:D:31:LEU:CD2	3:D:76:MET:SD	2.69	0.81
4:C:33:LYS:HE3	4:C:67:ARG:NH1	1.96	0.80
4:C:31:LEU:CD2	4:C:76:MET:HE3	2.12	0.80
1:A:85:ILE:HD11	1:A:92:ARG:HB2	1.62	0.80
4:C:118:ILE:H	4:C:122:GLU:CB	1.94	0.80
1:A:1:MET:HB2	1:A:65:ILE:HG13	1.65	0.79
2:B:118:ILE:HG23	2:B:123:ASP:CG	2.02	0.79
2:B:85:ILE:HD11	2:B:92:ARG:HB2	1.65	0.78
4:C:16:PRO:CB	4:C:18:PHE:CE1	2.64	0.77
4:C:108:SER:CB	4:C:114:HIS:H	1.97	0.77
4:C:26:MET:HE2	4:C:83:MET:SD	2.24	0.77
4:C:33:LYS:HE2	4:C:67:ARG:NH1	1.99	0.77
4:C:105:LEU:HD22	4:C:116:VAL:HB	1.66	0.76
4:C:105:LEU:CD2	4:C:116:VAL:HB	2.15	0.76
2:B:118:ILE:CG2	2:B:123:ASP:OD1	2.33	0.76
2:B:1:MET:HG2	2:B:65:ILE:CG1	2.17	0.75
4:C:108:SER:HB3	4:C:113:LEU:HA	1.67	0.75
1:A:133:LEU:N	1:A:133:LEU:HD23	2.00	0.75
3:D:81:GLU:HB2	3:D:92:ARG:NH1	2.02	0.75
1:A:1:MET:CG	1:A:65:ILE:HG13	2.17	0.75
3:D:77:ALA:O	3:D:81:GLU:HG3	1.87	0.74
3:D:98:ARG:HH12	3:D:100:ILE:CG2	2.00	0.74
3:D:1:MET:HG2	3:D:65:ILE:HG13	1.68	0.74
4:C:31:LEU:HD21	4:C:76:MET:CE	2.18	0.74
3:D:80:MET:HE1	3:D:97:ILE:HG21	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:31:LEU:HG	4:C:76:MET:CE	2.18	0.74
3:D:1:MET:HG2	3:D:65:ILE:CG1	2.18	0.73
1:A:16:PRO:CB	1:A:18:PHE:CE1	2.72	0.72
3:D:84:PHE:CD2	3:D:95:ILE:HD13	2.24	0.71
1:A:65:ILE:HD13	1:A:104:ALA:HA	1.73	0.70
2:B:31:LEU:O	2:B:67:ARG:HD2	1.92	0.69
4:C:28:THR:OG1	4:C:38:MET:HE3	1.92	0.69
4:C:74:LEU:O	4:C:78:ARG:HG2	1.91	0.69
3:D:81:GLU:O	3:D:85:ILE:HG12	1.92	0.69
2:B:74:LEU:O	2:B:78:ARG:HG2	1.92	0.69
1:A:82:ASP:OD1	1:A:92:ARG:NH2	2.26	0.69
3:D:127:GLN:O	3:D:127:GLN:NE2	2.26	0.68
1:A:127:GLN:O	1:A:131:GLU:HG3	1.93	0.68
3:D:92:ARG:HG3	3:D:92:ARG:HH11	1.58	0.68
4:C:67:ARG:CG	4:C:67:ARG:HH11	2.06	0.68
4:C:81:GLU:C	4:C:85:ILE:HD12	2.13	0.68
1:A:1:MET:CB	1:A:65:ILE:HG13	2.22	0.68
3:D:81:GLU:CB	3:D:92:ARG:NH1	2.56	0.68
4:C:108:SER:CB	4:C:113:LEU:HA	2.23	0.68
4:C:67:ARG:HH21	4:C:124:ILE:HG22	1.58	0.68
4:C:16:PRO:HB3	4:C:18:PHE:CD1	2.29	0.67
4:C:33:LYS:CE	4:C:67:ARG:HH12	2.07	0.67
3:D:15:ILE:CD1	3:D:88:LEU:CD2	2.73	0.67
3:D:92:ARG:NH1	3:D:92:ARG:HG3	2.09	0.67
1:A:1:MET:N	1:A:2:PRO:HD2	2.10	0.66
3:D:50:MET:HE2	3:D:57:CYS:HB2	1.75	0.66
4:C:118:ILE:O	4:C:121:ASP:N	2.28	0.65
4:C:31:LEU:HG	4:C:76:MET:HE3	1.76	0.65
1:A:1:MET:HG2	1:A:65:ILE:HG13	1.78	0.64
3:D:50:MET:O	3:D:94:ARG:NH2	2.30	0.64
4:C:82:ASP:OD1	4:C:92:ARG:NH2	2.30	0.64
4:C:108:SER:HB2	4:C:114:HIS:H	1.62	0.64
2:B:50:MET:HB2	3:D:39:PHE:CD1	2.33	0.64
3:D:80:MET:CE	3:D:97:ILE:HG21	2.27	0.63
4:C:31:LEU:CG	4:C:76:MET:CE	2.76	0.63
5:B:201:CL:CL	4:C:98:ARG:NH2	2.65	0.63
4:C:77:ALA:O	4:C:81:GLU:HG3	1.98	0.62
1:A:76:MET:O	1:A:80:MET:HG3	1.99	0.62
4:C:125:ILE:HD12	4:C:125:ILE:H	1.65	0.62
3:D:82:ASP:O	3:D:86:GLU:HG2	2.00	0.62
4:C:31:LEU:CG	4:C:76:MET:HE3	2.28	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:127:GLN:OE1	4:C:127:GLN:HA	1.99	0.62
2:B:13:LYS:HD3	2:B:13:LYS:N	2.15	0.61
3:D:82:ASP:O	3:D:86:GLU:CG	2.49	0.61
1:A:4:ILE:HD13	1:A:38:MET:SD	2.41	0.61
4:C:28:THR:CA	4:C:38:MET:CE	2.73	0.60
4:C:122:GLU:C	4:C:125:ILE:CD1	2.69	0.60
3:D:98:ARG:HH12	3:D:100:ILE:HG21	1.66	0.60
4:C:65:ILE:HD12	4:C:65:ILE:N	2.17	0.60
1:A:56:PRO:C	1:A:90:VAL:HG13	2.21	0.60
4:C:31:LEU:HD23	4:C:76:MET:HE3	1.83	0.60
4:C:116:VAL:HG22	4:C:116:VAL:O	2.01	0.60
3:D:81:GLU:CB	3:D:92:ARG:HH11	2.14	0.59
2:B:2:PRO:HG3	2:B:33:LYS:HD3	1.85	0.59
1:A:74:LEU:HD12	1:A:74:LEU:C	2.20	0.59
4:C:33:LYS:HE2	4:C:67:ARG:HH12	1.64	0.59
2:B:2:PRO:HD2	2:B:37:VAL:O	2.02	0.59
2:B:47:ASN:OD1	2:B:54:ARG:NH1	2.34	0.59
2:B:39:PHE:CZ	4:C:50:MET:SD	2.96	0.59
3:D:24:THR:OG1	3:D:40:VAL:HG21	2.02	0.59
1:A:118:ILE:HD13	1:A:118:ILE:N	2.18	0.58
4:C:76:MET:O	4:C:80:MET:HG3	2.03	0.58
3:D:47:ASN:OD1	3:D:54:ARG:NH2	2.36	0.58
3:D:81:GLU:HB3	3:D:92:ARG:HG3	1.84	0.58
3:D:103:PRO:HB2	3:D:106:PHE:HB2	1.86	0.58
3:D:81:GLU:HB2	3:D:92:ARG:HH12	1.68	0.58
2:B:36:GLU:OE1	2:B:36:GLU:N	2.35	0.58
2:B:4:ILE:HD12	2:B:4:ILE:N	2.19	0.57
1:A:4:ILE:N	1:A:4:ILE:HD12	2.18	0.57
1:A:36:GLU:OE1	1:A:36:GLU:N	2.34	0.57
4:C:121:ASP:O	4:C:125:ILE:HD11	2.03	0.57
3:D:98:ARG:HH21	4:C:100:ILE:HG21	1.69	0.57
2:B:4:ILE:HD13	2:B:38:MET:SD	2.44	0.57
3:D:24:THR:OG1	3:D:40:VAL:CG2	2.53	0.57
4:C:31:LEU:CD2	4:C:76:MET:HE1	2.21	0.57
4:C:4:ILE:N	4:C:4:ILE:HD12	2.20	0.57
4:C:75:ALA:HA	6:C:212:HOH:O	2.05	0.57
3:D:85:ILE:O	3:D:89:ASN:HA	2.05	0.56
1:A:132:TYR:O	1:A:136:HIS:HB2	2.05	0.56
4:C:129:ILE:HG13	4:C:129:ILE:O	2.05	0.56
3:D:4:ILE:HD12	3:D:4:ILE:N	2.20	0.56
3:D:80:MET:SD	3:D:97:ILE:HD12	2.46	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:ARG:O	1:A:92:ARG:HB3	2.05	0.56
4:C:108:SER:CB	4:C:114:HIS:N	2.68	0.56
3:D:2:PRO:HD2	3:D:37:VAL:O	2.06	0.56
3:D:92:ARG:CD	4:C:110:ASN:OD1	2.49	0.55
1:A:133:LEU:HD23	1:A:133:LEU:H	1.70	0.55
1:A:2:PRO:HB2	1:A:38:MET:CE	2.37	0.55
2:B:4:ILE:HG12	2:B:27:MET:HG3	1.89	0.55
2:B:48:ILE:CG2	2:B:57:CYS:SG	2.95	0.55
4:C:121:ASP:N	4:C:121:ASP:OD2	2.40	0.55
4:C:72:SER:O	4:C:75:ALA:HB3	2.07	0.55
3:D:91:ARG:NH1	3:D:93:GLU:OE1	2.37	0.55
1:A:28:THR:HG21	1:A:35:LYS:HB2	1.87	0.55
3:D:98:ARG:NH2	4:C:100:ILE:HG21	2.21	0.54
1:A:4:ILE:HG12	1:A:27:MET:HG3	1.90	0.54
4:C:28:THR:N	4:C:38:MET:HE1	2.22	0.54
4:C:67:ARG:HH11	4:C:67:ARG:HG2	1.73	0.54
4:C:122:GLU:C	4:C:125:ILE:HD11	2.27	0.54
3:D:58:VAL:HG11	3:D:84:PHE:CE2	2.42	0.53
2:B:67:ARG:HH11	2:B:67:ARG:HG2	1.73	0.53
1:A:60:ALA:HB3	1:A:97:ILE:HG23	1.91	0.53
4:C:66:GLY:C	4:C:68:LEU:H	2.11	0.53
1:A:10:VAL:HG12	1:A:15:ILE:HD12	1.91	0.53
3:D:80:MET:SD	3:D:97:ILE:CD1	2.97	0.52
1:A:134:HIS:O	1:A:138:HIS:CA	2.57	0.52
4:C:33:LYS:HE3	4:C:67:ARG:HH11	1.70	0.52
4:C:65:ILE:HD11	4:C:107:CYS:SG	2.50	0.52
1:A:56:PRO:CB	1:A:90:VAL:HA	2.38	0.52
1:A:27:MET:CE	1:A:76:MET:HG2	2.40	0.52
2:B:50:MET:SD	3:D:39:PHE:CZ	3.03	0.52
3:D:104:ALA:O	3:D:114:HIS:HB2	2.09	0.52
4:C:90:VAL:HG13	4:C:95:ILE:HD11	1.91	0.52
2:B:50:MET:HB2	3:D:39:PHE:CE1	2.44	0.51
2:B:31:LEU:O	2:B:67:ARG:CD	2.56	0.51
3:D:81:GLU:HB3	3:D:92:ARG:HH11	1.75	0.51
1:A:1:MET:CG	1:A:65:ILE:CG1	2.88	0.51
4:C:109:PHE:CD1	4:C:109:PHE:C	2.85	0.50
3:D:32:GLN:HG3	6:D:206:HOH:O	2.10	0.50
4:C:132:TYR:CG	4:C:132:TYR:O	2.61	0.50
3:D:91:ARG:HH11	3:D:93:GLU:CD	2.15	0.50
1:A:56:PRO:O	1:A:90:VAL:HG13	2.12	0.50
2:B:93:GLU:HB3	3:D:110:ASN:ND2	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:67:ARG:HG2	3:D:67:ARG:HH11	1.76	0.50
3:D:120:ARG:HD3	3:D:122:GLU:OE1	2.12	0.50
3:D:1:MET:HG2	3:D:65:ILE:CB	2.42	0.49
3:D:20:GLN:NE2	3:D:42:LEU:HB2	2.27	0.49
3:D:81:GLU:HB3	3:D:92:ARG:NH1	2.26	0.49
3:D:31:LEU:O	3:D:67:ARG:CD	2.57	0.49
1:A:56:PRO:HB2	1:A:90:VAL:HA	1.95	0.48
2:B:48:ILE:HG23	2:B:57:CYS:SG	2.53	0.48
4:C:132:TYR:CD1	4:C:132:TYR:C	2.86	0.48
4:C:68:LEU:HD22	4:C:99:PHE:HB3	1.95	0.48
4:C:132:TYR:C	4:C:134:HIS:H	2.17	0.48
3:D:82:ASP:O	3:D:86:GLU:HG3	2.13	0.47
1:A:129:ILE:O	1:A:132:TYR:HB3	2.15	0.47
3:D:116:VAL:O	3:D:120:ARG:HD2	2.15	0.47
3:D:74:LEU:HD13	4:C:112:ALA:HA	1.96	0.47
1:A:27:MET:HE1	1:A:76:MET:HG2	1.95	0.47
1:A:108:SER:O	1:A:108:SER:OG	2.28	0.47
2:B:48:ILE:HG13	3:D:41:ASP:CB	2.44	0.47
3:D:120:ARG:HB2	3:D:122:GLU:HG3	1.96	0.47
4:C:113:LEU:H	4:C:113:LEU:CD1	2.09	0.47
2:B:92:ARG:HG2	3:D:110:ASN:HA	1.96	0.46
3:D:26:MET:CE	3:D:83:MET:SD	3.03	0.46
4:C:12:GLU:O	4:C:12:GLU:HG2	2.14	0.46
4:C:23:LEU:HB2	4:C:83:MET:HE2	1.98	0.46
4:C:48:ILE:HG23	4:C:57:CYS:SG	2.56	0.46
3:D:66:GLY:C	3:D:68:LEU:H	2.19	0.46
3:D:50:MET:HE3	3:D:57:CYS:CB	2.36	0.45
1:A:8:THR:HB	1:A:58:VAL:HG22	1.98	0.45
3:D:20:GLN:HE21	3:D:42:LEU:HB2	1.80	0.45
4:C:69:ASN:C	4:C:69:ASN:HD22	2.20	0.45
1:A:1:MET:H3	1:A:2:PRO:HD2	1.81	0.45
2:B:115:ASP:O	2:B:118:ILE:HG13	2.17	0.45
4:C:109:PHE:CD1	4:C:109:PHE:O	2.70	0.45
4:C:124:ILE:C	4:C:124:ILE:HD12	2.38	0.45
4:C:64:CYS:HB3	4:C:68:LEU:HD11	1.98	0.45
2:B:1:MET:HG2	2:B:65:ILE:CB	2.47	0.44
4:C:69:ASN:ND2	4:C:69:ASN:O	2.49	0.44
4:C:102:VAL:HG11	4:C:107:CYS:SG	2.58	0.44
4:C:66:GLY:O	4:C:68:LEU:N	2.48	0.44
4:C:102:VAL:CG1	4:C:107:CYS:HB3	2.47	0.44
3:D:116:VAL:HG21	6:D:221:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:34:PRO:HB2	4:C:37:VAL:HG22	1.99	0.44
2:B:98:ARG:NH1	3:D:63:GLU:OE2	2.48	0.44
2:B:120:ARG:NE	2:B:122:GLU:OE2	2.43	0.44
1:A:137:HIS:CE1	6:A:306:HOH:O	2.70	0.44
2:B:2:PRO:HG2	2:B:38:MET:HE2	1.98	0.44
4:C:58:VAL:HG23	4:C:90:VAL:HG21	2.00	0.44
3:D:116:VAL:O	3:D:119:GLU:HB3	2.17	0.44
4:C:67:ARG:NH1	4:C:67:ARG:HG2	2.31	0.44
2:B:1:MET:HB2	2:B:64:CYS:CA	2.32	0.43
2:B:121:ASP:O	2:B:124:ILE:HG13	2.18	0.43
2:B:20:GLN:NE2	4:C:47:ASN:OD1	2.38	0.43
2:B:67:ARG:HG2	2:B:67:ARG:NH1	2.33	0.43
3:D:72:SER:O	3:D:75:ALA:HB3	2.17	0.43
1:A:85:ILE:O	1:A:89:ASN:HA	2.17	0.43
4:C:123:ASP:N	4:C:125:ILE:CD1	2.81	0.43
1:A:15:ILE:HD11	1:A:88:LEU:CD2	2.47	0.43
4:C:67:ARG:HH11	4:C:67:ARG:HG3	1.82	0.43
3:D:1:MET:CB	3:D:64:CYS:HA	2.32	0.43
2:B:15:ILE:HD13	2:B:88:LEU:CD2	2.48	0.43
3:D:36:GLU:CB	6:D:218:HOH:O	2.67	0.43
3:D:61:THR:HB	3:D:100:ILE:HD11	2.00	0.43
4:C:90:VAL:CG1	4:C:95:ILE:HD11	2.49	0.43
1:A:2:PRO:HB2	1:A:38:MET:HE2	2.00	0.43
1:A:2:PRO:CB	1:A:38:MET:CE	2.97	0.43
4:C:69:ASN:C	4:C:69:ASN:ND2	2.72	0.42
2:B:48:ILE:HG13	3:D:41:ASP:HB2	2.00	0.42
4:C:118:ILE:CA	4:C:122:GLU:CB	2.97	0.42
1:A:112:ALA:HB3	6:A:315:HOH:O	2.20	0.42
3:D:67:ARG:HG2	3:D:67:ARG:NH1	2.34	0.42
1:A:132:TYR:HB3	1:A:133:LEU:HD23	2.01	0.42
3:D:31:LEU:HD23	3:D:76:MET:SD	2.57	0.42
4:C:28:THR:OG1	4:C:38:MET:CE	2.64	0.42
4:C:123:ASP:N	4:C:125:ILE:HD12	2.34	0.42
2:B:77:ALA:HA	2:B:97:ILE:HD12	2.01	0.42
3:D:118:ILE:H	3:D:118:ILE:HG12	1.75	0.42
4:C:26:MET:HE1	4:C:83:MET:CG	2.49	0.42
1:A:56:PRO:HB3	1:A:90:VAL:HA	2.00	0.42
2:B:66:GLY:C	2:B:68:LEU:H	2.23	0.42
3:D:73:ASN:ND2	4:C:106:PHE:CE2	2.58	0.42
4:C:113:LEU:HD12	4:C:113:LEU:N	2.16	0.42
3:D:98:ARG:HH11	3:D:100:ILE:CG1	2.31	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:65:ILE:CD1	2:B:114:HIS:ND1	2.83	0.41
3:D:33:LYS:HE2	3:D:67:ARG:HG3	2.01	0.41
4:C:123:ASP:CA	4:C:125:ILE:HD12	2.50	0.41
4:C:126:SER:O	4:C:130:ALA:N	2.52	0.41
3:D:18:PHE:CD1	3:D:18:PHE:C	2.94	0.41
2:B:2:PRO:CD	2:B:37:VAL:HG23	2.49	0.41
4:C:122:GLU:CA	4:C:125:ILE:HD11	2.50	0.41
3:D:26:MET:HE3	3:D:83:MET:SD	2.61	0.41
3:D:120:ARG:NH2	3:D:122:GLU:OE1	2.54	0.41
4:C:4:ILE:O	4:C:40:VAL:HA	2.21	0.41
4:C:7:ASN:OD1	4:C:43:ARG:NH1	2.53	0.41
1:A:116:VAL:HG22	1:A:120:ARG:NH1	2.35	0.41
4:C:65:ILE:N	4:C:65:ILE:CD1	2.81	0.41
1:A:25:ASN:OD1	1:A:35:LYS:HE2	2.22	0.40
4:C:104:ALA:HB3	4:C:116:VAL:HA	2.02	0.40
4:C:121:ASP:O	4:C:125:ILE:CD1	2.68	0.40
3:D:2:PRO:HB2	3:D:38:MET:SD	2.62	0.40
2:B:103:PRO:HB2	2:B:106:PHE:HB2	2.03	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	136/138 (99%)	116 (85%)	14 (10%)	6 (4%)	2 19
2	B	137/139 (99%)	121 (88%)	12 (9%)	4 (3%)	4 28
3	D	135/137 (98%)	112 (83%)	19 (14%)	4 (3%)	4 28
4	C	132/134 (98%)	111 (84%)	16 (12%)	5 (4%)	3 22
All	All	540/548 (98%)	460 (85%)	61 (11%)	19 (4%)	3 24

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	134	HIS
3	D	115	ASP
1	A	92	ARG
2	B	67	ARG
3	D	67	ARG
4	C	116	VAL
4	C	119	GLU
1	A	2	PRO
1	A	67	ARG
2	B	137	ALA
1	A	91	ARG
3	D	56	PRO
1	A	90	VAL
4	C	67	ARG
4	C	107	CYS
4	C	115	ASP
2	B	70	PRO
3	D	70	PRO
1	A	56	PRO

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	119/121 (98%)	103 (87%)	16 (13%)	4 18
2	B	120/121 (99%)	111 (92%)	9 (8%)	13 45
3	D	115/117 (98%)	95 (83%)	20 (17%)	2 10
4	C	114/116 (98%)	86 (75%)	28 (25%)	0 2
All	All	468/475 (98%)	395 (84%)	73 (16%)	2 12

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	7	ASN
1	A	15	ILE

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Mol	Chain	Res	Type
1	A	26	MET
1	A	53	ASP
1	A	57	CYS
1	A	58	VAL
1	A	74	LEU
1	A	76	MET
1	A	83	MET
1	A	91	ARG
1	A	92	ARG
1	A	97	ILE
1	A	117	SER
1	A	118	ILE
1	A	136	HIS
2	B	1	MET
2	B	13	LYS
2	B	48	ILE
2	B	71	THR
2	B	117	SER
2	B	118	ILE
2	B	126	SER
2	B	138	HIS
2	B	139	HIS
3	D	1	MET
3	D	7	ASN
3	D	14	SER
3	D	17	VAL
3	D	26	MET
3	D	31	LEU
3	D	43	ARG
3	D	49	MET
3	D	50	MET
3	D	56	PRO
3	D	76	MET
3	D	85	ILE
3	D	94	ARG
3	D	97	ILE
3	D	98	ARG
3	D	100	ILE
3	D	115	ASP
3	D	118	ILE
3	D	120	ARG
3	D	127	GLN

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Mol	Chain	Res	Type
4	C	14	SER
4	C	36	GLU
4	C	38	MET
4	C	43	ARG
4	C	48	ILE
4	C	49	MET
4	C	57	CYS
4	C	67	ARG
4	C	69	ASN
4	C	76	MET
4	C	86	GLU
4	C	98	ARG
4	C	105	LEU
4	C	107	CYS
4	C	108	SER
4	C	109	PHE
4	C	113	LEU
4	C	115	ASP
4	C	117	SER
4	C	118	ILE
4	C	121	ASP
4	C	124	ILE
4	C	125	ILE
4	C	126	SER
4	C	127	GLN
4	C	129	ILE
4	C	132	TYR
4	C	133	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	25	ASN
2	B	135	HIS
2	B	136	HIS
3	D	127	GLN
3	D	136	HIS
4	C	20	GLN
4	C	69	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 2 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 (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	138/138 (100%)	-0.47	0	100	100	29, 51, 88, 115	0
2	B	139/139 (100%)	-0.46	1 (0%)	87	81	32, 53, 77, 112	0
3	D	137/137 (100%)	-0.10	1 (0%)	87	81	42, 77, 109, 135	0
4	C	134/134 (100%)	-0.14	3 (2%)	62	48	36, 71, 119, 131	0
All	All	548/548 (100%)	-0.29	5 (0%)	84	75	29, 63, 107, 135	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	C	134	HIS	3.4
4	C	132	TYR	3.1
4	C	116	VAL	2.5
3	D	136	HIS	2.2
2	B	138	HIS	2.2

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

There are no non-standard protein/DNA/RNA residues in this entry.

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,

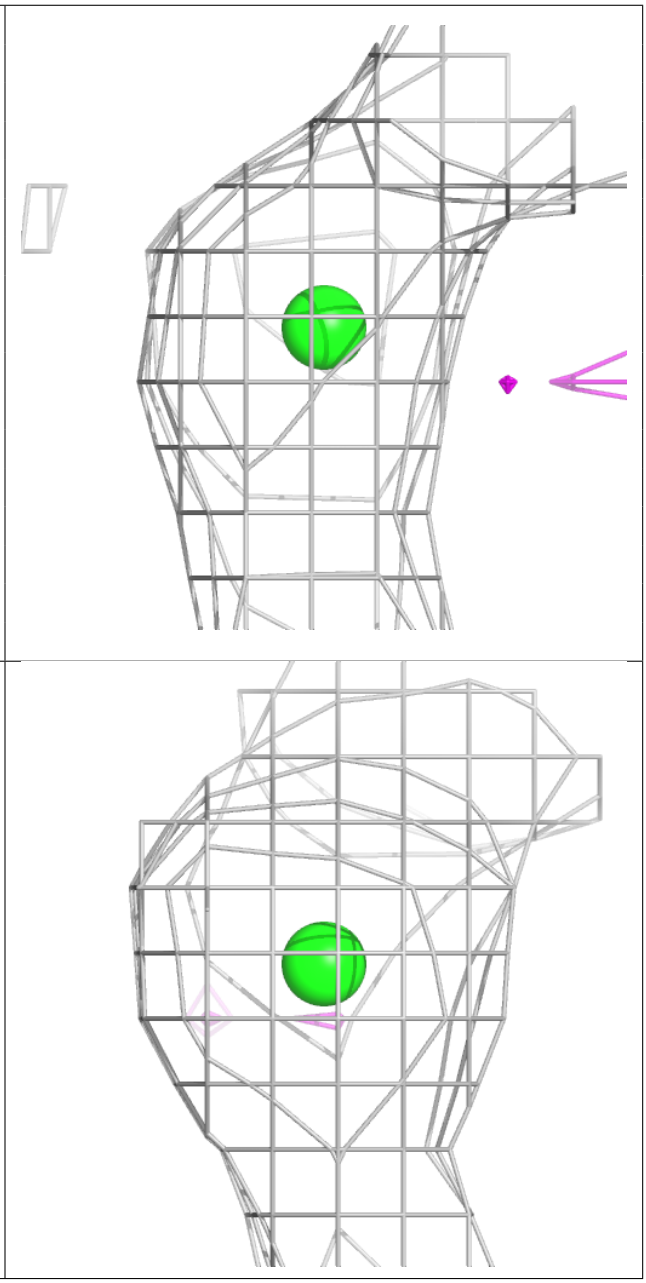
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	CL	B	201	1/1	0.95	0.21	38,38,38,38	0
5	CL	A	201	1/1	0.99	0.08	36,36,36,36	1

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

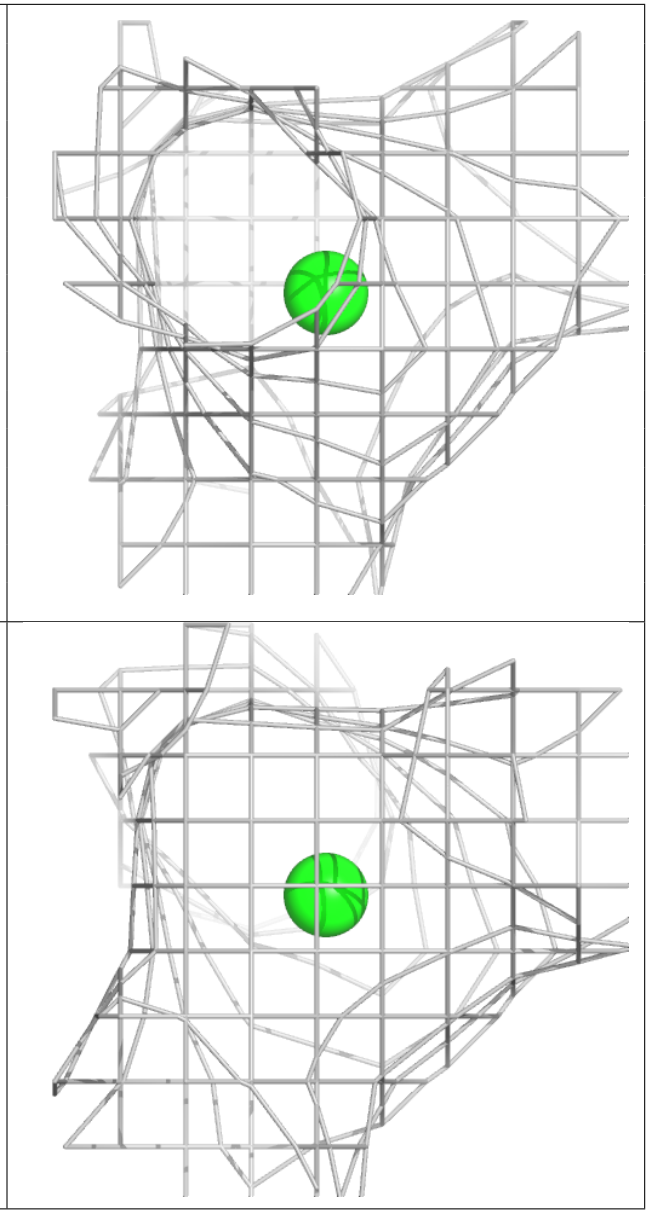
Electron density around CL B 201:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)



Electron density around CL A 201:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.