Full wwPDB X-ray Structure Validation Report (i)

Oct 4, 2023 – 12:11 PM EDT

PDB ID	:	6PBU
Title	:	ClpP1 from Mycobacterium smegmatis
Authors	:	Heras, B.; Nagpal, J.; Dougan, D.A.
Deposited on	:	2019-06-14
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
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 (1)) were used in the production of this report:

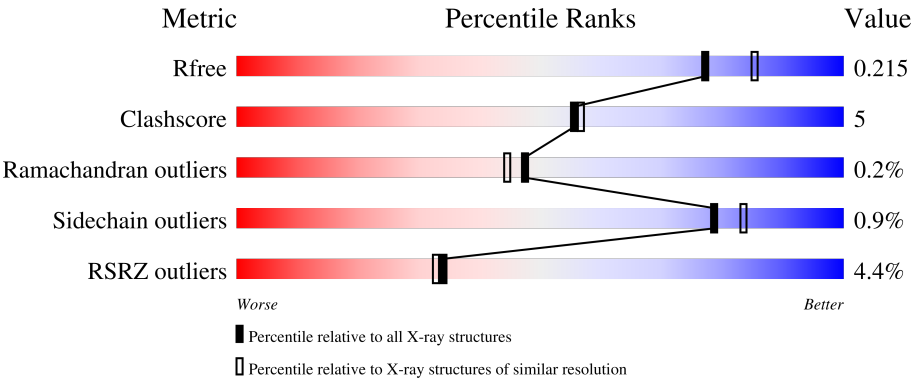
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.00 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}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (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 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	216	3% 78% 10% 12%
1	B	216	% 77% 12% 12%
1	C	216	6% 75% 12% 12%
1	D	216	3% 81% 8% 11%
1	E	216	3% 77% 10% 13%

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Mol	Chain	Length	Quality of chain
1	F	216	8% 73% 16% 11%
1	G	216	3% 79% 10% 11%

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	MLI	G	302	-	-	X	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 11314 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 ATP-dependent Clp protease proteolytic subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	190	Total	C	N	O	S	0	1	0
			1448	915	244	280	9			
1	B	191	Total	C	N	O	S	0	1	0
			1457	920	248	280	9			
1	C	190	Total	C	N	O	S	0	1	0
			1447	914	245	279	9			
1	D	192	Total	C	N	O	S	0	2	0
			1458	922	246	281	9			
1	E	188	Total	C	N	O	S	0	0	0
			1432	906	242	275	9			
1	F	192	Total	C	N	O	S	0	1	0
			1457	920	246	282	9			
1	G	193	Total	C	N	O	S	0	1	0
			1469	927	249	284	9			

There are 91 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	204	ALA	-	expression tag	UNP A0R198
A	205	ALA	-	expression tag	UNP A0R198
A	206	ALA	-	expression tag	UNP A0R198
A	207	HIS	-	expression tag	UNP A0R198
A	208	HIS	-	expression tag	UNP A0R198
A	209	HIS	-	expression tag	UNP A0R198
A	210	HIS	-	expression tag	UNP A0R198
A	211	HIS	-	expression tag	UNP A0R198
A	212	HIS	-	expression tag	UNP A0R198
A	213	HIS	-	expression tag	UNP A0R198
A	214	HIS	-	expression tag	UNP A0R198
A	215	HIS	-	expression tag	UNP A0R198
A	216	HIS	-	expression tag	UNP A0R198
B	204	ALA	-	expression tag	UNP A0R198
B	205	ALA	-	expression tag	UNP A0R198

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Chain	Residue	Modelled	Actual	Comment	Reference
B	206	ALA	-	expression tag	UNP A0R198
B	207	HIS	-	expression tag	UNP A0R198
B	208	HIS	-	expression tag	UNP A0R198
B	209	HIS	-	expression tag	UNP A0R198
B	210	HIS	-	expression tag	UNP A0R198
B	211	HIS	-	expression tag	UNP A0R198
B	212	HIS	-	expression tag	UNP A0R198
B	213	HIS	-	expression tag	UNP A0R198
B	214	HIS	-	expression tag	UNP A0R198
B	215	HIS	-	expression tag	UNP A0R198
B	216	HIS	-	expression tag	UNP A0R198
C	204	ALA	-	expression tag	UNP A0R198
C	205	ALA	-	expression tag	UNP A0R198
C	206	ALA	-	expression tag	UNP A0R198
C	207	HIS	-	expression tag	UNP A0R198
C	208	HIS	-	expression tag	UNP A0R198
C	209	HIS	-	expression tag	UNP A0R198
C	210	HIS	-	expression tag	UNP A0R198
C	211	HIS	-	expression tag	UNP A0R198
C	212	HIS	-	expression tag	UNP A0R198
C	213	HIS	-	expression tag	UNP A0R198
C	214	HIS	-	expression tag	UNP A0R198
C	215	HIS	-	expression tag	UNP A0R198
C	216	HIS	-	expression tag	UNP A0R198
D	204	ALA	-	expression tag	UNP A0R198
D	205	ALA	-	expression tag	UNP A0R198
D	206	ALA	-	expression tag	UNP A0R198
D	207	HIS	-	expression tag	UNP A0R198
D	208	HIS	-	expression tag	UNP A0R198
D	209	HIS	-	expression tag	UNP A0R198
D	210	HIS	-	expression tag	UNP A0R198
D	211	HIS	-	expression tag	UNP A0R198
D	212	HIS	-	expression tag	UNP A0R198
D	213	HIS	-	expression tag	UNP A0R198
D	214	HIS	-	expression tag	UNP A0R198
D	215	HIS	-	expression tag	UNP A0R198
D	216	HIS	-	expression tag	UNP A0R198
E	204	ALA	-	expression tag	UNP A0R198
E	205	ALA	-	expression tag	UNP A0R198
E	206	ALA	-	expression tag	UNP A0R198
E	207	HIS	-	expression tag	UNP A0R198
E	208	HIS	-	expression tag	UNP A0R198

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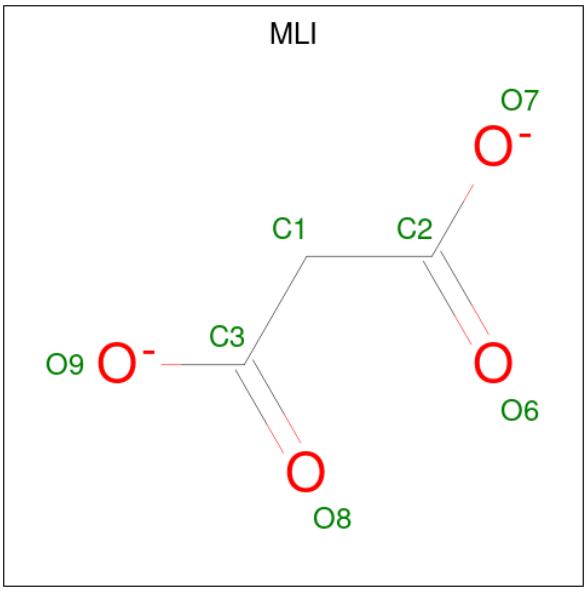
Chain	Residue	Modelled	Actual	Comment	Reference
E	209	HIS	-	expression tag	UNP A0R198
E	210	HIS	-	expression tag	UNP A0R198
E	211	HIS	-	expression tag	UNP A0R198
E	212	HIS	-	expression tag	UNP A0R198
E	213	HIS	-	expression tag	UNP A0R198
E	214	HIS	-	expression tag	UNP A0R198
E	215	HIS	-	expression tag	UNP A0R198
E	216	HIS	-	expression tag	UNP A0R198
F	204	ALA	-	expression tag	UNP A0R198
F	205	ALA	-	expression tag	UNP A0R198
F	206	ALA	-	expression tag	UNP A0R198
F	207	HIS	-	expression tag	UNP A0R198
F	208	HIS	-	expression tag	UNP A0R198
F	209	HIS	-	expression tag	UNP A0R198
F	210	HIS	-	expression tag	UNP A0R198
F	211	HIS	-	expression tag	UNP A0R198
F	212	HIS	-	expression tag	UNP A0R198
F	213	HIS	-	expression tag	UNP A0R198
F	214	HIS	-	expression tag	UNP A0R198
F	215	HIS	-	expression tag	UNP A0R198
F	216	HIS	-	expression tag	UNP A0R198
G	204	ALA	-	expression tag	UNP A0R198
G	205	ALA	-	expression tag	UNP A0R198
G	206	ALA	-	expression tag	UNP A0R198
G	207	HIS	-	expression tag	UNP A0R198
G	208	HIS	-	expression tag	UNP A0R198
G	209	HIS	-	expression tag	UNP A0R198
G	210	HIS	-	expression tag	UNP A0R198
G	211	HIS	-	expression tag	UNP A0R198
G	212	HIS	-	expression tag	UNP A0R198
G	213	HIS	-	expression tag	UNP A0R198
G	214	HIS	-	expression tag	UNP A0R198
G	215	HIS	-	expression tag	UNP A0R198
G	216	HIS	-	expression tag	UNP A0R198

- Molecule 2 is MALONATE ION (three-letter code: MLI) (formula: $C_3H_2O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C O 7 3 4	0	0
2	C	1	Total C O 7 3 4	0	0
2	C	1	Total C O 7 3 4	0	0
2	D	1	Total C O 7 3 4	0	0
2	E	1	Total C O 7 3 4	0	0
2	F	1	Total C O 7 3 4	0	0
2	G	1	Total C O 7 3 4	0	0
2	G	1	Total C O 7 3 4	0	0
2	G	1	Total C O 7 3 4	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	154	Total O 154 154	0	0
3	B	162	Total O 162 162	0	0
3	C	127	Total O 127 127	0	0

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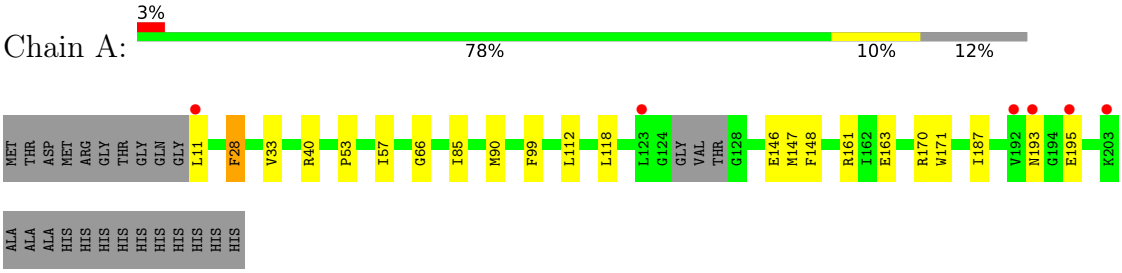
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	162	Total O 162 162	0	0
3	E	164	Total O 164 164	0	0
3	F	134	Total O 134 134	0	0
3	G	180	Total O 180 180	0	0

3 Residue-property plots

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.

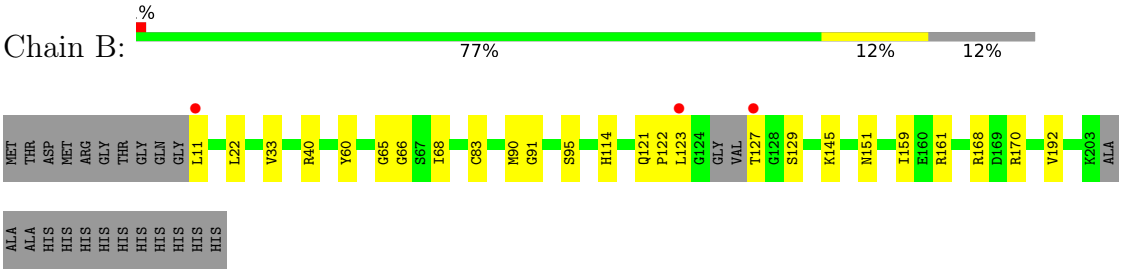
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain A:



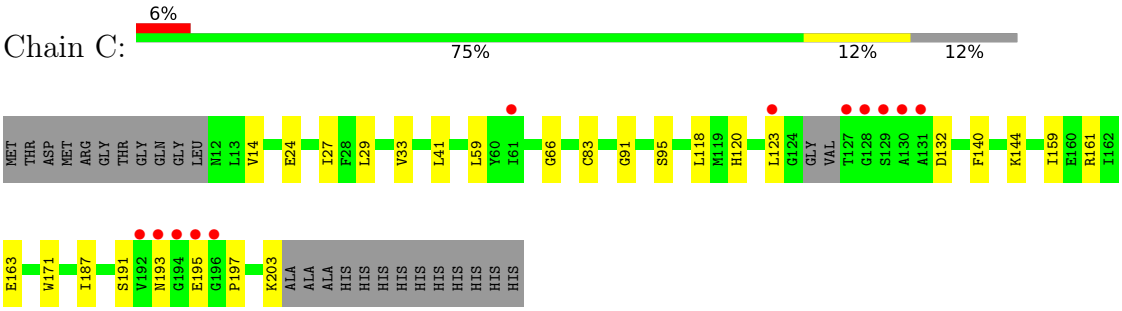
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain B:



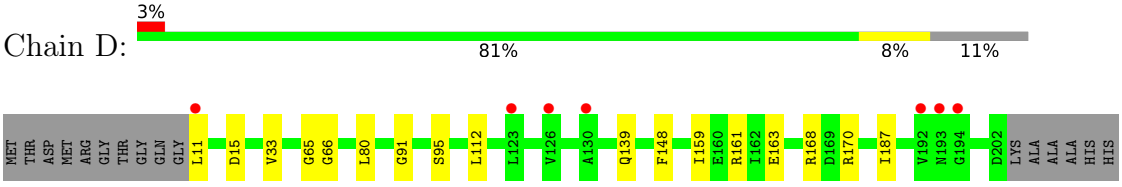
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain C:



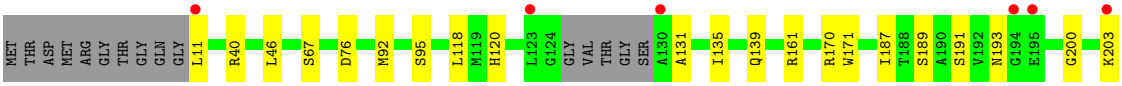
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain D:



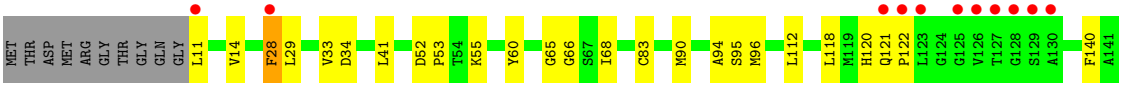
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

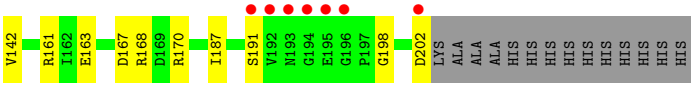
Chain E:



• Molecule 1: ATP-dependent Clp protease proteolytic subunit

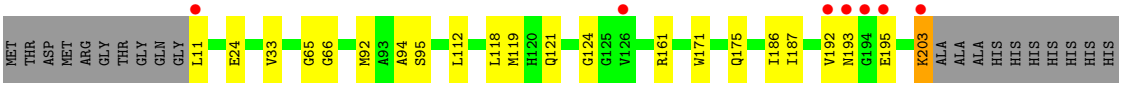
Chain F:





• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain G:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α, β, γ	169.62Å 169.62Å 114.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.15 – 2.00 37.15 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.3 (37.15-2.00) 99.3 (37.15-2.00)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.87 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.178 , 0.215 0.178 , 0.215	Depositor DCC
R_{free} test set	5585 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	26.7	Xtriage
Anisotropy	0.389	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 52.8	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	0.96	EDS
Total number of atoms	11314	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.44% 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

5.1 Standard geometry

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

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	0.37	0/1475	0.54	0/1994
1	B	0.40	0/1484	0.56	0/2006
1	C	0.41	1/1474 (0.1%)	0.57	0/1992
1	D	0.38	0/1489	0.56	0/2015
1	E	0.37	0/1456	0.57	0/1969
1	F	0.40	1/1485 (0.1%)	0.58	1/2012 (0.0%)
1	G	0.41	0/1494	0.56	0/2023
All	All	0.39	2/10357 (0.0%)	0.56	1/14011 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	83	CYS	CB-SG	-6.28	1.71	1.82
1	F	83	CYS	CB-SG	-5.50	1.72	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	34	ASP	CB-CG-OD1	5.23	123.01	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1448	0	1431	15	0
1	B	1457	0	1445	19	0
1	C	1447	0	1434	13	0
1	D	1458	0	1446	11	0
1	E	1432	0	1417	17	0
1	F	1457	0	1440	24	0
1	G	1469	0	1453	17	0
2	B	7	0	2	1	0
2	C	14	0	4	1	0
2	D	7	0	2	0	0
2	E	7	0	2	0	0
2	F	7	0	2	0	0
2	G	21	0	6	4	0
3	A	154	0	0	1	0
3	B	162	0	0	5	0
3	C	127	0	0	1	0
3	D	162	0	0	0	0
3	E	164	0	0	3	0
3	F	134	0	0	1	0
3	G	180	0	0	2	0
All	All	11314	0	10084	103	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 5.

All (103) 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:G:124:GLY:H	2:G:302:MLI:H11	1.27	0.98
1:G:161:ARG:NH1	3:G:401:HOH:O	2.14	0.81
1:F:33:VAL:HB	1:F:66:GLY:HA3	1.62	0.79
1:G:193:ASN:OD1	1:G:195:GLU:HB3	1.85	0.75
1:A:118:LEU:HD23	1:A:171:TRP:HB3	1.70	0.74
1:E:11:LEU:HD22	1:F:11:LEU:HD22	1.72	0.71
1:G:124:GLY:N	2:G:302:MLI:H11	2.05	0.69
1:G:112:LEU:HD23	1:G:187:ILE:HG23	1.76	0.68
1:C:118:LEU:HD23	1:C:171:TRP:HB3	1.77	0.67
1:E:193:ASN:OD1	3:E:401:HOH:O	2.13	0.67
1:E:40:ARG:HG3	1:F:14:VAL:HG22	1.79	0.65
1:D:11:LEU:HD22	1:D:15:ASP:HB3	1.78	0.64
2:C:301:MLI:O7	3:C:401:HOH:O	2.15	0.64
1:D:33:VAL:HB	1:D:66:GLY:HA3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:LEU:HD23	1:A:187:ILE:HG23	1.78	0.64
1:D:161:ARG:HH21	1:D:170:ARG:HH12	1.45	0.64
1:E:139:GLN:HE22	1:F:118:LEU:HD21	1.63	0.63
1:D:112:LEU:HD23	1:D:187:ILE:HG23	1.82	0.61
1:A:11:LEU:HG	1:B:11:LEU:O	2.02	0.60
1:E:11:LEU:N	3:E:404:HOH:O	2.35	0.59
1:F:52:ASP:OD2	1:F:55:LYS:HD3	2.03	0.59
1:A:193:ASN:OD1	1:A:195:GLU:HB2	2.03	0.59
1:G:92:MET:HE2	1:G:94:ALA:HB2	1.86	0.58
1:F:121[A]:GLN:HE21	1:F:140:PHE:HZ	1.51	0.58
1:A:57:ILE:HB	1:A:85:ILE:HD13	1.86	0.57
1:F:68:ILE:HG12	1:F:122:PRO:HG2	1.85	0.57
1:D:148:PHE:CD2	1:D:163[B]:GLU:HG2	2.40	0.57
1:F:112:LEU:HD23	1:F:187:ILE:HG23	1.87	0.57
1:B:159:ILE:HG13	3:B:496:HOH:O	2.05	0.57
1:D:161:ARG:NH2	1:D:170:ARG:HH12	2.02	0.56
1:B:40:ARG:HG2	3:B:512:HOH:O	2.05	0.55
1:E:95:SER:HB2	1:E:120:HIS:HB3	1.88	0.55
1:E:200:GLY:HA2	1:E:203:LYS:NZ	2.22	0.55
1:E:118:LEU:HD12	1:E:171:TRP:HB3	1.87	0.55
1:B:33:VAL:HB	1:B:66:GLY:HA3	1.88	0.55
1:G:124:GLY:H	2:G:302:MLI:C1	2.11	0.54
1:B:65:GLY:HA2	1:B:95:SER:HB3	1.90	0.54
1:G:118:LEU:HG	1:G:171:TRP:HB3	1.89	0.53
1:F:121[B]:GLN:NE2	1:F:167:ASP:OD1	2.41	0.53
1:A:193:ASN:H	1:A:193:ASN:HD22	1.58	0.52
1:F:53:PRO:HB2	1:G:192:VAL:HG11	1.92	0.52
1:A:161:ARG:NH2	1:A:170:ARG:HH12	2.08	0.52
1:G:203:LYS:HG3	3:G:455:HOH:O	2.10	0.52
1:F:168:ARG:NH2	1:F:170:ARG:HD2	2.25	0.51
1:D:159:ILE:O	1:D:163[B]:GLU:HG3	2.10	0.51
1:B:161[B]:ARG:HH21	1:B:170:ARG:HH12	1.59	0.51
1:E:76:ASP:HB3	1:F:112:LEU:HD13	1.93	0.51
1:D:65:GLY:HA2	1:D:95:SER:HB3	1.93	0.51
1:A:193:ASN:H	1:A:193:ASN:ND2	2.09	0.51
1:C:95:SER:HB2	1:C:120:HIS:HB3	1.94	0.49
1:F:60:TYR:CD2	1:F:90:MET:HE3	2.47	0.49
1:G:33:VAL:HB	1:G:66:GLY:HA3	1.95	0.49
1:A:148:PHE:CD2	1:A:163[B]:GLU:HG2	2.47	0.49
1:E:46:LEU:HD12	1:F:28:PHE:HE1	1.79	0.48
1:A:33:VAL:HB	1:A:66:GLY:HA3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:LYS:NZ	3:B:401:HOH:O	2.16	0.48
1:C:29:LEU:HB2	1:C:41:LEU:HD21	1.95	0.47
1:C:132:ASP:OD2	1:C:132:ASP:N	2.42	0.47
1:F:163:GLU:OE2	3:F:1001:HOH:O	2.20	0.47
1:C:140:PHE:CE2	1:C:144[B]:LYS:HD2	2.50	0.47
1:E:131:ALA:HB1	1:E:135:ILE:HG13	1.97	0.46
1:C:191:SER:OG	1:C:193:ASN:HB2	2.16	0.46
1:B:121:GLN:O	1:B:123:LEU:HD22	2.16	0.46
1:F:142:VAL:HG21	2:G:301:MLI:O9	2.15	0.46
1:C:159:ILE:O	1:C:163:GLU:HG3	2.16	0.45
1:A:146:GLU:HG2	1:B:114:HIS:CD2	2.51	0.45
1:F:191:SER:O	1:F:198:GLY:HA2	2.17	0.45
1:D:168:ARG:NH2	1:D:170:ARG:HD2	2.32	0.45
3:E:431:HOH:O	1:F:202:ASP:HB2	2.16	0.45
1:F:65:GLY:HA2	1:F:94:ALA:O	2.17	0.44
1:C:27:ILE:HG13	1:C:59:LEU:HD13	1.98	0.44
1:G:121[B]:GLN:HG3	1:G:121[B]:GLN:O	2.17	0.44
1:A:40:ARG:NH2	3:A:306:HOH:O	2.51	0.44
1:B:145:LYS:NZ	3:B:409:HOH:O	2.50	0.44
1:E:161:ARG:HH21	1:E:170:ARG:HH12	1.65	0.44
1:B:22:LEU:HD12	1:B:22:LEU:HA	1.87	0.43
1:D:80:LEU:HA	1:E:189:SER:HA	1.99	0.43
1:G:175:GLN:HA	1:G:186:ILE:HD11	2.00	0.43
1:B:60:TYR:CD2	1:B:90:MET:HE3	2.53	0.43
1:B:40:ARG:HG3	1:C:14:VAL:HG22	1.99	0.43
1:B:68:ILE:CG1	1:B:122:PRO:HG2	2.49	0.43
1:A:99:PHE:CE1	1:A:147:MET:HG2	2.54	0.43
1:E:200:GLY:HA2	1:E:203:LYS:HZ2	1.84	0.43
1:B:83:CYS:O	2:B:301:MLI:O8	2.37	0.42
1:D:139:GLN:OE1	1:E:92:MET:HE1	2.20	0.42
1:F:120:HIS:O	1:F:122:PRO:HD3	2.19	0.42
1:C:24:GLU:O	1:C:203:LYS:HE2	2.20	0.42
1:G:24:GLU:OE1	1:G:203:LYS:HE2	2.20	0.42
1:C:187:ILE:HD12	1:C:197:PRO:HG2	2.01	0.42
1:E:46:LEU:HD12	1:F:28:PHE:CE1	2.55	0.42
1:B:127:THR:C	1:B:129:SER:H	2.22	0.41
1:C:33:VAL:HB	1:C:66:GLY:HA3	2.01	0.41
1:G:118:LEU:HD23	1:G:119:MET:O	2.20	0.41
1:F:11:LEU:HD11	1:G:11:LEU:HD13	2.01	0.41
1:F:95:SER:OG	1:F:96:MET:N	2.53	0.41
1:E:187:ILE:HD13	1:E:187:ILE:HG21	1.80	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:193:ASN:HB3	1:C:195:GLU:H	1.85	0.41
1:B:168:ARG:NH2	1:B:170:ARG:HD2	2.36	0.41
1:A:53:PRO:HB2	1:B:192:VAL:HG11	2.03	0.41
1:A:28:PHE:CE1	1:A:90:MET:HE1	2.56	0.40
1:B:40:ARG:NH1	3:B:411:HOH:O	2.54	0.40
1:F:29:LEU:HB2	1:F:41:LEU:HD11	2.04	0.40
1:G:65:GLY:HA2	1:G:95:SER:HB3	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	187/216 (87%)	179 (96%)	8 (4%)	0	100	100
1	B	188/216 (87%)	182 (97%)	5 (3%)	1 (0%)	29	23
1	C	187/216 (87%)	183 (98%)	3 (2%)	1 (0%)	29	23
1	D	192/216 (89%)	186 (97%)	5 (3%)	1 (0%)	29	23
1	E	184/216 (85%)	178 (97%)	6 (3%)	0	100	100
1	F	191/216 (88%)	183 (96%)	8 (4%)	0	100	100
1	G	192/216 (89%)	186 (97%)	6 (3%)	0	100	100
All	All	1321/1512 (87%)	1277 (97%)	41 (3%)	3 (0%)	47	44

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	91	GLY
1	D	91	GLY
1	B	91	GLY

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	149/167 (89%)	148 (99%)	1 (1%)	84 88
1	B	150/167 (90%)	149 (99%)	1 (1%)	84 88
1	C	149/167 (89%)	147 (99%)	2 (1%)	69 74
1	D	150/167 (90%)	150 (100%)	0	100 100
1	E	147/167 (88%)	145 (99%)	2 (1%)	67 72
1	F	150/167 (90%)	148 (99%)	2 (1%)	69 74
1	G	151/167 (90%)	150 (99%)	1 (1%)	84 88
All	All	1046/1169 (90%)	1037 (99%)	9 (1%)	78 83

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	PHE
1	B	151	ASN
1	C	123	LEU
1	C	161	ARG
1	E	67	SER
1	E	191	SER
1	F	28	PHE
1	F	161	ARG
1	G	203	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	151	ASN
1	D	121	GLN
1	E	139	GLN

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)

9 ligands 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	$\#\|Z\| > 2$
2	MLI	C	301	-	6,6,6	1.42	0	7,7,7	0.87	0
2	MLI	G	303	-	6,6,6	1.28	0	7,7,7	1.18	0
2	MLI	E	301	-	6,6,6	1.41	0	7,7,7	0.92	0
2	MLI	B	301	-	6,6,6	1.19	0	7,7,7	1.17	1 (14%)
2	MLI	C	302	-	6,6,6	1.33	0	7,7,7	0.89	0
2	MLI	F	301	-	6,6,6	1.14	0	7,7,7	1.27	0
2	MLI	D	301	-	6,6,6	1.12	0	7,7,7	1.21	0
2	MLI	G	302	-	6,6,6	1.39	0	7,7,7	0.71	0
2	MLI	G	301	-	6,6,6	1.32	1 (16%)	7,7,7	0.73	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
2	MLI	C	301	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MLI	G	303	-	-	4/4/4/4	-
2	MLI	E	301	-	-	0/4/4/4	-
2	MLI	B	301	-	-	0/4/4/4	-
2	MLI	C	302	-	-	2/4/4/4	-
2	MLI	F	301	-	-	4/4/4/4	-
2	MLI	D	301	-	-	2/4/4/4	-
2	MLI	G	302	-	-	0/4/4/4	-
2	MLI	G	301	-	-	0/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	301	MLI	O9-C3	-2.10	1.23	1.30

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	301	MLI	C3-C1-C2	-2.22	105.07	112.87

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	303	MLI	C3-C1-C2-O6
2	G	303	MLI	C2-C1-C3-O8
2	C	302	MLI	C2-C1-C3-O8
2	C	302	MLI	C2-C1-C3-O9
2	G	303	MLI	C2-C1-C3-O9
2	D	301	MLI	C3-C1-C2-O6
2	G	303	MLI	C3-C1-C2-O7
2	C	301	MLI	C2-C1-C3-O9
2	D	301	MLI	C3-C1-C2-O7
2	F	301	MLI	C3-C1-C2-O6
2	F	301	MLI	C3-C1-C2-O7
2	C	301	MLI	C2-C1-C3-O8
2	F	301	MLI	C2-C1-C3-O8
2	F	301	MLI	C2-C1-C3-O9

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	301	MLI	1	0
2	B	301	MLI	1	0
2	G	302	MLI	3	0
2	G	301	MLI	1	0

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	190/216 (87%)	-0.16	6 (3%) 47 46	18, 28, 55, 89	0
1	B	191/216 (88%)	-0.19	3 (1%) 72 70	18, 27, 46, 73	0
1	C	190/216 (87%)	0.11	12 (6%) 20 19	18, 28, 59, 87	0
1	D	192/216 (88%)	-0.13	7 (3%) 42 42	17, 27, 54, 70	0
1	E	188/216 (87%)	-0.24	6 (3%) 47 46	18, 27, 53, 78	0
1	F	192/216 (88%)	0.17	18 (9%) 8 8	18, 27, 65, 104	0
1	G	193/216 (89%)	-0.17	7 (3%) 42 42	16, 25, 55, 92	0
All	All	1336/1512 (88%)	-0.09	59 (4%) 34 33	16, 27, 55, 104	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	195	GLU	9.0
1	F	194	GLY	8.8
1	F	193	ASN	7.7
1	B	123	LEU	7.3
1	F	130	ALA	6.7
1	C	193	ASN	6.2
1	A	195	GLU	6.2
1	A	193	ASN	5.8
1	G	193	ASN	5.7
1	D	11	LEU	5.2
1	C	130	ALA	5.2
1	C	195	GLU	5.1
1	B	11	LEU	5.1
1	A	11	LEU	5.1
1	E	11	LEU	4.9
1	G	195	GLU	4.8
1	F	192	VAL	4.4

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Mol	Chain	Res	Type	RSRZ
1	F	123	LEU	4.2
1	D	193	ASN	4.2
1	G	11	LEU	4.1
1	F	122	PRO	3.9
1	C	127	THR	3.8
1	F	128	GLY	3.8
1	E	203	LYS	3.8
1	C	194	GLY	3.8
1	E	130	ALA	3.6
1	F	126	VAL	3.5
1	F	127	THR	3.5
1	D	192	VAL	3.4
1	G	203	LYS	3.4
1	D	123	LEU	3.3
1	G	194	GLY	3.3
1	F	191	SER	3.3
1	F	11	LEU	3.3
1	C	128	GLY	3.2
1	F	129	SER	3.2
1	D	126	VAL	3.2
1	A	123	LEU	3.1
1	F	196	GLY	3.0
1	C	129	SER	2.9
1	F	121[A]	GLN	2.9
1	E	195	GLU	2.8
1	B	127	THR	2.8
1	G	126	VAL	2.7
1	F	125	GLY	2.6
1	C	123	LEU	2.5
1	A	192	VAL	2.5
1	F	202	ASP	2.4
1	D	194	GLY	2.3
1	E	194	GLY	2.3
1	D	130	ALA	2.2
1	C	131	ALA	2.2
1	E	123	LEU	2.2
1	C	61	ILE	2.1
1	C	196	GLY	2.1
1	C	192	VAL	2.0
1	F	28	PHE	2.0
1	A	203	LYS	2.0
1	G	192	VAL	2.0

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, 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	B-factors(Å^2)	Q<0.9
2	MLI	B	301	7/7	0.70	0.28	45,47,52,55	0
2	MLI	G	303	7/7	0.75	0.30	48,52,54,56	0
2	MLI	D	301	7/7	0.78	0.28	47,51,54,58	0
2	MLI	C	301	7/7	0.80	0.28	49,50,52,52	0
2	MLI	F	301	7/7	0.81	0.26	53,57,67,68	0
2	MLI	G	302	7/7	0.82	0.26	49,50,54,57	0
2	MLI	G	301	7/7	0.82	0.27	36,44,59,61	0
2	MLI	C	302	7/7	0.90	0.16	37,45,54,56	0
2	MLI	E	301	7/7	0.91	0.32	41,43,45,46	0

6.5 Other polymers (i)

There are no such residues in this entry.