Full wwPDB X-ray Structure Validation Report (i)

Oct 9, 2023 – 11:09 PM EDT

PDB ID	:	7M1M
Title	:	Crystal structure of Pseudomonas aeruginosa ClpP1
Authors	:	Mawla, G.D.; Grant, R.A.; Baker, T.A.; Sauer, R.T.
Deposited on	:	2021-03-13
Resolution	:	2.60 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:

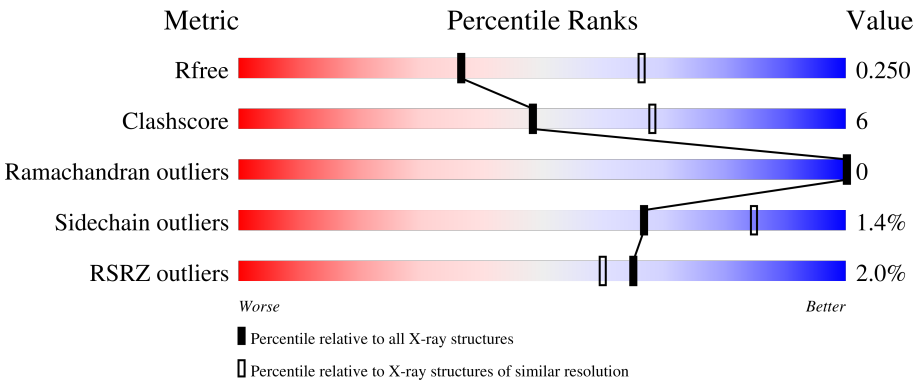
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	210	.% 80% 6% 13%
1	B	210	2% 77% 9% • 13%
1	C	210	2% 77% 10% 13%
1	D	210	3% 73% 13% 13%
1	E	210	2% 79% 8% • 12%

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Mol	Chain	Length	Quality of chain
1	F	210	%, 78%, 9%, 13%
1	G	210	2%, 76%, 10%, 13%
1	H	210	2%, 75%, 11%, 13%
1	I	210	2%, 80%, 7%, 13%
1	J	210	76%, 11%, 13%
1	K	210	%, 75%, 11%, 13%
1	L	210	%, 80%, 6%, 13%
1	M	210	%, 72%, 15%, 13%
1	N	210	2%, 78%, 9%, 13%

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	MPD	B	302	-	-	X	-
2	MPD	H	301	-	-	X	-
2	MPD	L	301	-	-	X	-
2	MPD	N	301	-	-	X	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 40456 atoms, of which 20313 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
			Total	C	H	N	O	S			
1	A	182	2844	898	1430	244	260	12	0	0	0
1	B	182	2844	898	1430	244	260	12	0	0	0
1	C	183	2860	903	1439	245	261	12	0	0	0
1	D	183	2856	902	1434	245	263	12	0	0	0
1	E	184	2875	908	1445	246	264	12	0	0	0
1	F	182	2844	898	1430	244	260	12	0	0	0
1	G	182	2844	898	1430	244	260	12	0	0	0
1	H	182	2844	898	1430	244	260	12	0	0	0
1	I	182	2844	898	1430	244	260	12	0	0	0
1	J	183	2860	903	1439	245	261	12	0	0	0
1	K	183	2856	902	1434	245	263	12	0	0	0
1	L	182	2844	898	1430	244	260	12	0	0	0
1	M	182	2844	898	1430	244	260	12	0	0	0
1	N	182	2844	898	1430	244	260	12	0	0	0

There are 168 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	199	SER	-	expression tag	UNP A0A072ZHR6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	200	GLY	-	expression tag	UNP A0A072ZHR6
A	201	SER	-	expression tag	UNP A0A072ZHR6
A	202	GLY	-	expression tag	UNP A0A072ZHR6
A	203	SER	-	expression tag	UNP A0A072ZHR6
A	204	GLY	-	expression tag	UNP A0A072ZHR6
A	205	HIS	-	expression tag	UNP A0A072ZHR6
A	206	HIS	-	expression tag	UNP A0A072ZHR6
A	207	HIS	-	expression tag	UNP A0A072ZHR6
A	208	HIS	-	expression tag	UNP A0A072ZHR6
A	209	HIS	-	expression tag	UNP A0A072ZHR6
A	210	HIS	-	expression tag	UNP A0A072ZHR6
B	199	SER	-	expression tag	UNP A0A072ZHR6
B	200	GLY	-	expression tag	UNP A0A072ZHR6
B	201	SER	-	expression tag	UNP A0A072ZHR6
B	202	GLY	-	expression tag	UNP A0A072ZHR6
B	203	SER	-	expression tag	UNP A0A072ZHR6
B	204	GLY	-	expression tag	UNP A0A072ZHR6
B	205	HIS	-	expression tag	UNP A0A072ZHR6
B	206	HIS	-	expression tag	UNP A0A072ZHR6
B	207	HIS	-	expression tag	UNP A0A072ZHR6
B	208	HIS	-	expression tag	UNP A0A072ZHR6
B	209	HIS	-	expression tag	UNP A0A072ZHR6
B	210	HIS	-	expression tag	UNP A0A072ZHR6
C	199	SER	-	expression tag	UNP A0A072ZHR6
C	200	GLY	-	expression tag	UNP A0A072ZHR6
C	201	SER	-	expression tag	UNP A0A072ZHR6
C	202	GLY	-	expression tag	UNP A0A072ZHR6
C	203	SER	-	expression tag	UNP A0A072ZHR6
C	204	GLY	-	expression tag	UNP A0A072ZHR6
C	205	HIS	-	expression tag	UNP A0A072ZHR6
C	206	HIS	-	expression tag	UNP A0A072ZHR6
C	207	HIS	-	expression tag	UNP A0A072ZHR6
C	208	HIS	-	expression tag	UNP A0A072ZHR6
C	209	HIS	-	expression tag	UNP A0A072ZHR6
C	210	HIS	-	expression tag	UNP A0A072ZHR6
D	199	SER	-	expression tag	UNP A0A072ZHR6
D	200	GLY	-	expression tag	UNP A0A072ZHR6
D	201	SER	-	expression tag	UNP A0A072ZHR6
D	202	GLY	-	expression tag	UNP A0A072ZHR6
D	203	SER	-	expression tag	UNP A0A072ZHR6
D	204	GLY	-	expression tag	UNP A0A072ZHR6
D	205	HIS	-	expression tag	UNP A0A072ZHR6

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Chain	Residue	Modelled	Actual	Comment	Reference
D	206	HIS	-	expression tag	UNP A0A072ZHR6
D	207	HIS	-	expression tag	UNP A0A072ZHR6
D	208	HIS	-	expression tag	UNP A0A072ZHR6
D	209	HIS	-	expression tag	UNP A0A072ZHR6
D	210	HIS	-	expression tag	UNP A0A072ZHR6
E	199	SER	-	expression tag	UNP A0A072ZHR6
E	200	GLY	-	expression tag	UNP A0A072ZHR6
E	201	SER	-	expression tag	UNP A0A072ZHR6
E	202	GLY	-	expression tag	UNP A0A072ZHR6
E	203	SER	-	expression tag	UNP A0A072ZHR6
E	204	GLY	-	expression tag	UNP A0A072ZHR6
E	205	HIS	-	expression tag	UNP A0A072ZHR6
E	206	HIS	-	expression tag	UNP A0A072ZHR6
E	207	HIS	-	expression tag	UNP A0A072ZHR6
E	208	HIS	-	expression tag	UNP A0A072ZHR6
E	209	HIS	-	expression tag	UNP A0A072ZHR6
E	210	HIS	-	expression tag	UNP A0A072ZHR6
F	199	SER	-	expression tag	UNP A0A072ZHR6
F	200	GLY	-	expression tag	UNP A0A072ZHR6
F	201	SER	-	expression tag	UNP A0A072ZHR6
F	202	GLY	-	expression tag	UNP A0A072ZHR6
F	203	SER	-	expression tag	UNP A0A072ZHR6
F	204	GLY	-	expression tag	UNP A0A072ZHR6
F	205	HIS	-	expression tag	UNP A0A072ZHR6
F	206	HIS	-	expression tag	UNP A0A072ZHR6
F	207	HIS	-	expression tag	UNP A0A072ZHR6
F	208	HIS	-	expression tag	UNP A0A072ZHR6
F	209	HIS	-	expression tag	UNP A0A072ZHR6
F	210	HIS	-	expression tag	UNP A0A072ZHR6
G	199	SER	-	expression tag	UNP A0A072ZHR6
G	200	GLY	-	expression tag	UNP A0A072ZHR6
G	201	SER	-	expression tag	UNP A0A072ZHR6
G	202	GLY	-	expression tag	UNP A0A072ZHR6
G	203	SER	-	expression tag	UNP A0A072ZHR6
G	204	GLY	-	expression tag	UNP A0A072ZHR6
G	205	HIS	-	expression tag	UNP A0A072ZHR6
G	206	HIS	-	expression tag	UNP A0A072ZHR6
G	207	HIS	-	expression tag	UNP A0A072ZHR6
G	208	HIS	-	expression tag	UNP A0A072ZHR6
G	209	HIS	-	expression tag	UNP A0A072ZHR6
G	210	HIS	-	expression tag	UNP A0A072ZHR6
H	199	SER	-	expression tag	UNP A0A072ZHR6

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Chain	Residue	Modelled	Actual	Comment	Reference
H	200	GLY	-	expression tag	UNP A0A072ZHR6
H	201	SER	-	expression tag	UNP A0A072ZHR6
H	202	GLY	-	expression tag	UNP A0A072ZHR6
H	203	SER	-	expression tag	UNP A0A072ZHR6
H	204	GLY	-	expression tag	UNP A0A072ZHR6
H	205	HIS	-	expression tag	UNP A0A072ZHR6
H	206	HIS	-	expression tag	UNP A0A072ZHR6
H	207	HIS	-	expression tag	UNP A0A072ZHR6
H	208	HIS	-	expression tag	UNP A0A072ZHR6
H	209	HIS	-	expression tag	UNP A0A072ZHR6
H	210	HIS	-	expression tag	UNP A0A072ZHR6
I	199	SER	-	expression tag	UNP A0A072ZHR6
I	200	GLY	-	expression tag	UNP A0A072ZHR6
I	201	SER	-	expression tag	UNP A0A072ZHR6
I	202	GLY	-	expression tag	UNP A0A072ZHR6
I	203	SER	-	expression tag	UNP A0A072ZHR6
I	204	GLY	-	expression tag	UNP A0A072ZHR6
I	205	HIS	-	expression tag	UNP A0A072ZHR6
I	206	HIS	-	expression tag	UNP A0A072ZHR6
I	207	HIS	-	expression tag	UNP A0A072ZHR6
I	208	HIS	-	expression tag	UNP A0A072ZHR6
I	209	HIS	-	expression tag	UNP A0A072ZHR6
I	210	HIS	-	expression tag	UNP A0A072ZHR6
J	199	SER	-	expression tag	UNP A0A072ZHR6
J	200	GLY	-	expression tag	UNP A0A072ZHR6
J	201	SER	-	expression tag	UNP A0A072ZHR6
J	202	GLY	-	expression tag	UNP A0A072ZHR6
J	203	SER	-	expression tag	UNP A0A072ZHR6
J	204	GLY	-	expression tag	UNP A0A072ZHR6
J	205	HIS	-	expression tag	UNP A0A072ZHR6
J	206	HIS	-	expression tag	UNP A0A072ZHR6
J	207	HIS	-	expression tag	UNP A0A072ZHR6
J	208	HIS	-	expression tag	UNP A0A072ZHR6
J	209	HIS	-	expression tag	UNP A0A072ZHR6
J	210	HIS	-	expression tag	UNP A0A072ZHR6
K	199	SER	-	expression tag	UNP A0A072ZHR6
K	200	GLY	-	expression tag	UNP A0A072ZHR6
K	201	SER	-	expression tag	UNP A0A072ZHR6
K	202	GLY	-	expression tag	UNP A0A072ZHR6
K	203	SER	-	expression tag	UNP A0A072ZHR6
K	204	GLY	-	expression tag	UNP A0A072ZHR6
K	205	HIS	-	expression tag	UNP A0A072ZHR6

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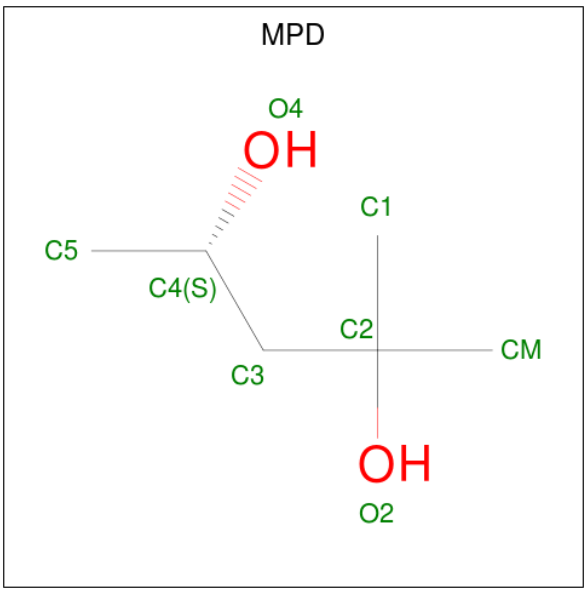
Chain	Residue	Modelled	Actual	Comment	Reference
K	206	HIS	-	expression tag	UNP A0A072ZHR6
K	207	HIS	-	expression tag	UNP A0A072ZHR6
K	208	HIS	-	expression tag	UNP A0A072ZHR6
K	209	HIS	-	expression tag	UNP A0A072ZHR6
K	210	HIS	-	expression tag	UNP A0A072ZHR6
L	199	SER	-	expression tag	UNP A0A072ZHR6
L	200	GLY	-	expression tag	UNP A0A072ZHR6
L	201	SER	-	expression tag	UNP A0A072ZHR6
L	202	GLY	-	expression tag	UNP A0A072ZHR6
L	203	SER	-	expression tag	UNP A0A072ZHR6
L	204	GLY	-	expression tag	UNP A0A072ZHR6
L	205	HIS	-	expression tag	UNP A0A072ZHR6
L	206	HIS	-	expression tag	UNP A0A072ZHR6
L	207	HIS	-	expression tag	UNP A0A072ZHR6
L	208	HIS	-	expression tag	UNP A0A072ZHR6
L	209	HIS	-	expression tag	UNP A0A072ZHR6
L	210	HIS	-	expression tag	UNP A0A072ZHR6
M	199	SER	-	expression tag	UNP A0A072ZHR6
M	200	GLY	-	expression tag	UNP A0A072ZHR6
M	201	SER	-	expression tag	UNP A0A072ZHR6
M	202	GLY	-	expression tag	UNP A0A072ZHR6
M	203	SER	-	expression tag	UNP A0A072ZHR6
M	204	GLY	-	expression tag	UNP A0A072ZHR6
M	205	HIS	-	expression tag	UNP A0A072ZHR6
M	206	HIS	-	expression tag	UNP A0A072ZHR6
M	207	HIS	-	expression tag	UNP A0A072ZHR6
M	208	HIS	-	expression tag	UNP A0A072ZHR6
M	209	HIS	-	expression tag	UNP A0A072ZHR6
M	210	HIS	-	expression tag	UNP A0A072ZHR6
N	199	SER	-	expression tag	UNP A0A072ZHR6
N	200	GLY	-	expression tag	UNP A0A072ZHR6
N	201	SER	-	expression tag	UNP A0A072ZHR6
N	202	GLY	-	expression tag	UNP A0A072ZHR6
N	203	SER	-	expression tag	UNP A0A072ZHR6
N	204	GLY	-	expression tag	UNP A0A072ZHR6
N	205	HIS	-	expression tag	UNP A0A072ZHR6
N	206	HIS	-	expression tag	UNP A0A072ZHR6
N	207	HIS	-	expression tag	UNP A0A072ZHR6
N	208	HIS	-	expression tag	UNP A0A072ZHR6
N	209	HIS	-	expression tag	UNP A0A072ZHR6
N	210	HIS	-	expression tag	UNP A0A072ZHR6

- Molecule 2 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula:

$C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
2	A	1	22	6	14	2	0	0
2	B	1	22	6	14	2	0	0
2	B	1	22	6	14	2	0	0
2	C	1	22	6	14	2	0	0
2	C	1	22	6	14	2	0	0
2	D	1	22	6	14	2	0	0
2	E	1	22	6	14	2	0	0
2	F	1	22	6	14	2	0	0
2	G	1	22	6	14	2	0	0
2	H	1	22	6	14	2	0	0
2	I	1	22	6	14	2	0	0
2	J	1	22	6	14	2	0	0
2	J	1	22	6	14	2	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
2	K	1	22	6	14	2	0	0
2	L	1	22	6	14	2	0	0
2	M	1	22	6	14	2	0	0
2	M	1	22	6	14	2	0	0
2	N	1	22	6	14	2	0	0

- Molecule 3 is water.

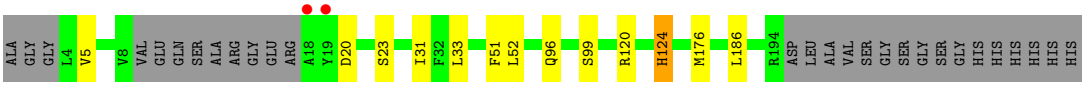
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	11	11	11	0	0
3	B	13	13	13	0	0
3	C	10	10	10	0	0
3	D	9	9	9	0	0
3	E	9	9	9	0	0
3	F	15	15	15	0	0
3	G	6	6	6	0	0
3	H	11	11	11	0	0
3	I	9	9	9	0	0
3	J	14	14	14	0	0
3	K	17	17	17	0	0
3	L	6	6	6	0	0
3	M	16	16	16	0	0
3	N	11	11	11	0	0

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.

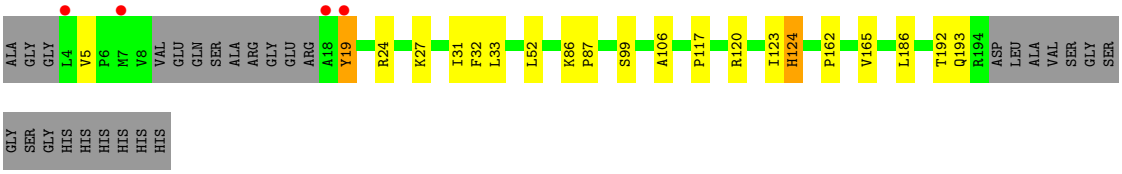
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain A:



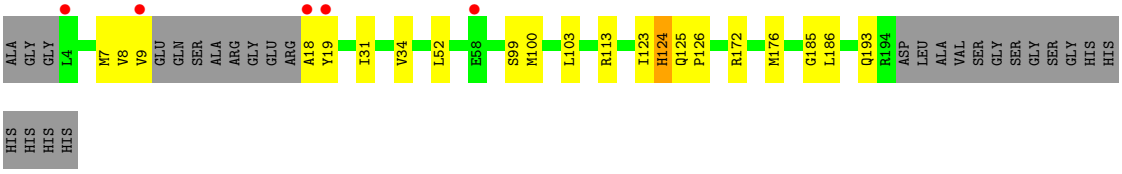
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain B:



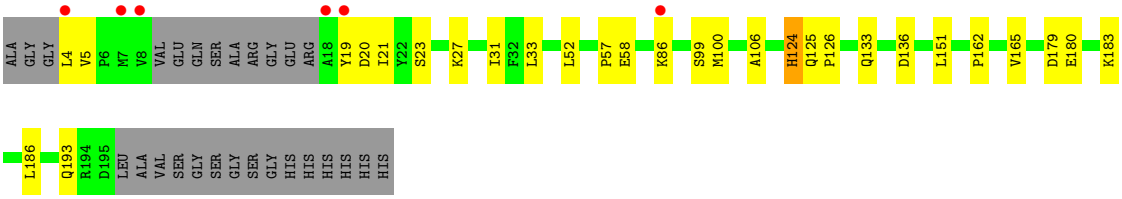
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain C:



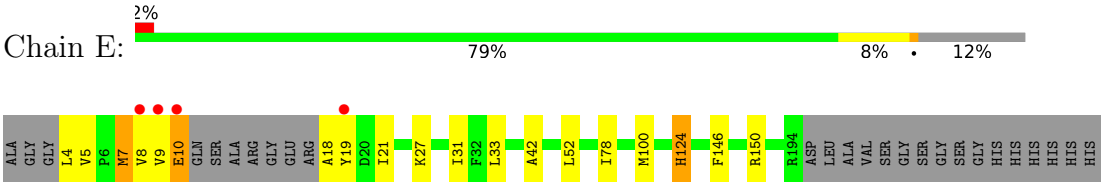
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain D:



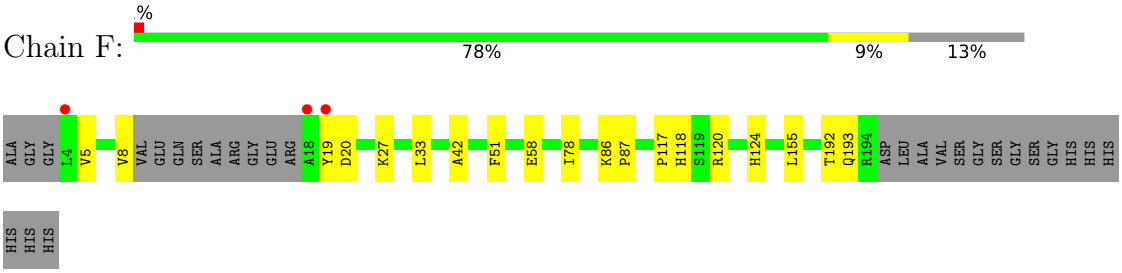
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain E:



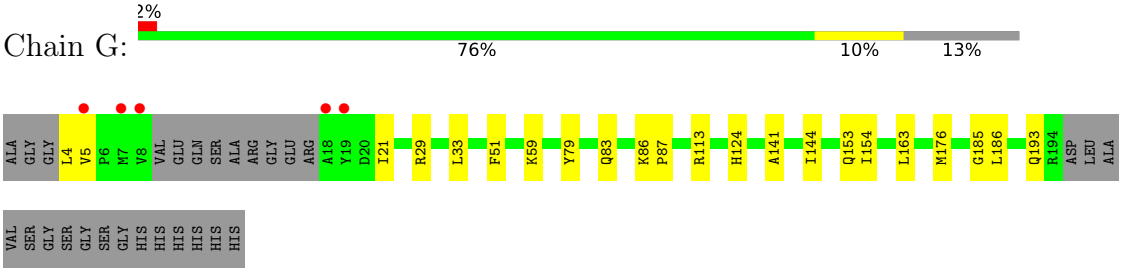
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain F:



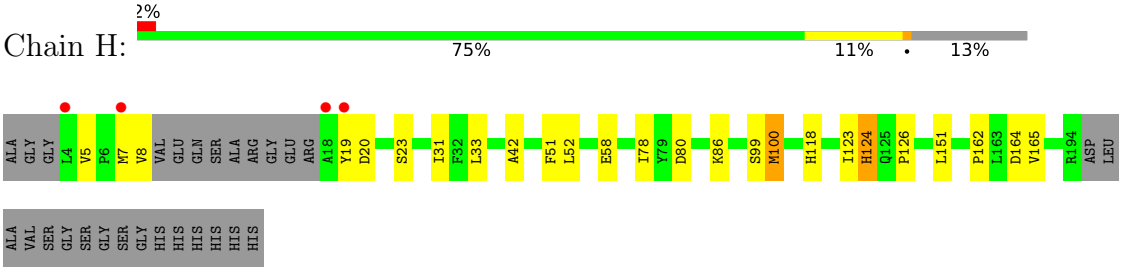
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain G:



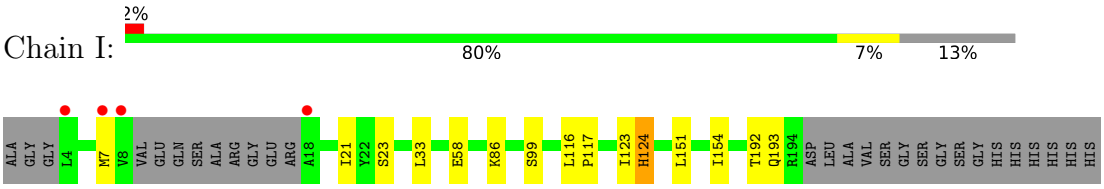
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain H:



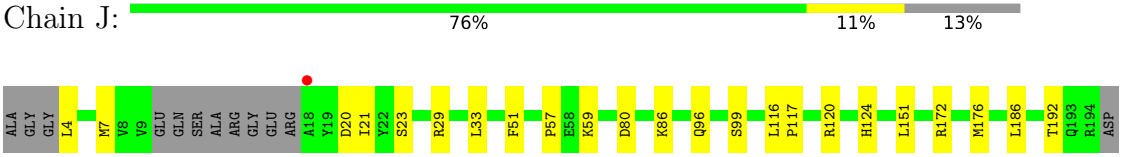
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

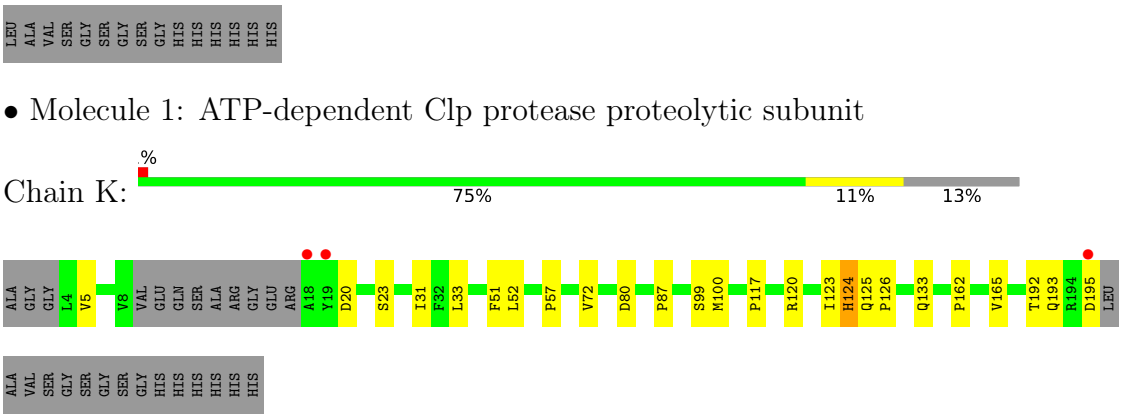
Chain I:



• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain J:




LEU ALA VAL SER GLY SER GLY SER GLY HIS HIS HIS HIS HIS HIS
• Molecule 1: ATP-dependent Clp protease proteolytic subunit
Chain K:
%
75%
11%
13%
ALA GLY GLY L4 V5 V8 VAL GLU GLN SER ALA ARG GLY GLU ARG A18 Y19 D20 S23 I31 F32 L33 F51 L52 P57 V72 D80 P87 S99 M100 P117 R120 I123 H124 Q125 P126 Q133 P162 V165 T192 Q193 R194 D195 LEU
ALA VAL SER GLY SER GLY SER GLY HIS HIS HIS HIS HIS HIS HIS
• Molecule 1: ATP-dependent Clp protease proteolytic subunit
Chain L:
%
80%
6%
13%
ALA GLY GLY L4 M7 V8 VAL GLU GLN SER ALA ARG GLY GLU ARG A18 Y19 D20 I21 L33 A42 I78 K86 P87 S99 H124 E143 L151 L155 M176 L186 R194 ASP LEU ALA VAL SER GLY SER GLY SER GLY HIS HIS HIS HIS HIS
HIS
• Molecule 1: ATP-dependent Clp protease proteolytic subunit
Chain M:
%
72%
15%
13%
ALA GLY GLY L4 M7 V8 VAL GLU GLN SER ALA ARG GLY GLU ARG A18 Y19 D20 I21 Y22 S23 I31 F32 L33 A42 F51 L52 I78 K86 P87 S99 M100 A106 R113 P117 H124 Q125 P126 D136 F146 R150 L151 D169 Y184
G185 L186 M191 T192 Q193 R194 ASP LEU ALA VAL SER GLY SER GLY SER GLY HIS HIS HIS HIS HIS HIS
• Molecule 1: ATP-dependent Clp protease proteolytic subunit
Chain N:
2%
78%
9%
13%
ALA GLY GLY L4 V5 P6 M7 V8 VAL GLU GLN SER ALA ARG GLY GLU ARG A18 Y19 D20 I21 Y22 S23 I31 F32 L33 F51 L52 K86 P87 S99 M100 L116 I123 H124 L151 L155 M176 L186 R194 ASP LEU ALA VAL SER GLY SER GLY SER
GLY HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	96.97Å 97.12Å 108.35Å 66.99° 85.93° 77.17°	Depositor
Resolution (Å)	48.54 – 2.60 48.54 – 2.60	Depositor EDS
% Data completeness (in resolution range)	94.3 (48.54-2.60) 88.2 (48.54-2.60)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.74 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.17.1	Depositor
R, R_{free}	0.207 , 0.250 0.207 , 0.250	Depositor DCC
R_{free} test set	2000 reflections (1.94%)	wwPDB-VP
Wilson B-factor (Å^2)	35.8	Xtriage
Anisotropy	0.885	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 41.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	40456	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.38% 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: MPD

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	0.33	0/1438	0.54	0/1939
1	B	0.39	1/1438 (0.1%)	0.57	1/1939 (0.1%)
1	C	0.37	0/1445	0.55	0/1949
1	D	0.35	0/1446	0.54	0/1950
1	E	0.32	0/1454	0.54	0/1961
1	F	0.32	0/1438	0.52	0/1939
1	G	0.34	0/1438	0.55	0/1939
1	H	0.32	0/1438	0.52	0/1939
1	I	0.33	0/1438	0.55	0/1939
1	J	0.32	0/1445	0.54	0/1949
1	K	0.34	0/1446	0.54	0/1950
1	L	0.33	0/1438	0.55	0/1939
1	M	0.30	0/1438	0.53	0/1939
1	N	0.32	0/1438	0.53	0/1939
All	All	0.34	1/20178 (0.0%)	0.54	1/27210 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	19	TYR	CD2-CE2	-5.99	1.30	1.39

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	19	TYR	CZ-CE2-CD2	6.91	126.02	119.80

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	1414	1430	1429	13	0
1	B	1414	1430	1429	20	0
1	C	1421	1439	1438	18	0
1	D	1422	1434	1433	23	0
1	E	1430	1445	1444	18	0
1	F	1414	1430	1429	19	0
1	G	1414	1430	1429	18	0
1	H	1414	1430	1429	23	0
1	I	1414	1430	1429	11	0
1	J	1421	1439	1438	18	0
1	K	1422	1434	1433	22	0
1	L	1414	1430	1429	17	0
1	M	1414	1430	1429	24	0
1	N	1414	1430	1429	23	0
2	A	8	14	14	4	0
2	B	16	28	28	7	0
2	C	16	28	28	7	0
2	D	8	14	14	3	0
2	E	8	14	14	3	0
2	F	8	14	14	2	0
2	G	8	14	14	0	0
2	H	8	14	14	9	0
2	I	8	14	14	2	0
2	J	16	28	28	5	0
2	K	8	14	14	5	0
2	L	8	14	14	6	0
2	M	16	28	28	5	0
2	N	8	14	14	9	0
3	A	11	0	0	0	0
3	B	13	0	0	0	0
3	C	10	0	0	0	0
3	D	9	0	0	1	0
3	E	9	0	0	0	0
3	F	15	0	0	0	0
3	G	6	0	0	0	0
3	H	11	0	0	0	0
3	I	9	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	J	14	0	0	0	0
3	K	17	0	0	1	0
3	L	6	0	0	0	0
3	M	16	0	0	1	0
3	N	11	0	0	0	0
All	All	20143	20313	20299	243	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 6.

All (243) 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:D:58:GLU:OE2	1:D:86:LYS:NZ	1.73	1.19
1:H:151:LEU:HD13	2:H:301:MPD:H13	1.41	1.01
1:B:124:HIS:O	2:B:302:MPD:O4	1.78	0.99
1:N:151:LEU:HD13	2:N:301:MPD:C1	1.94	0.97
1:D:151:LEU:HD13	2:D:301:MPD:H52	1.48	0.94
1:K:124:HIS:O	2:K:301:MPD:O4	1.84	0.94
1:B:19:TYR:CE2	1:B:27:LYS:HD2	2.08	0.88
1:B:19:TYR:HE2	1:B:27:LYS:HD2	1.41	0.86
1:C:9:VAL:HG22	1:C:18:ALA:HA	1.61	0.81
1:D:180:GLU:HA	1:D:183:LYS:HE3	1.62	0.80
1:M:20:ASP:OD1	1:M:23:SER:OG	2.03	0.77
1:N:123:ILE:HG22	2:N:301:MPD:H51	1.67	0.75
1:L:124:HIS:O	2:L:301:MPD:O4	2.05	0.74
1:J:20:ASP:OD1	1:J:23:SER:OG	2.06	0.73
1:K:117:PRO:HG3	1:K:192:THR:HG22	1.70	0.72
1:N:176:MET:CE	1:N:186:LEU:HD22	2.19	0.72
1:F:19:TYR:CE2	1:F:27:LYS:HD2	2.30	0.67
1:D:57:PRO:HB2	1:D:86:LYS:HD3	1.75	0.67
1:N:176:MET:HE1	1:N:186:LEU:HD22	1.78	0.66
1:J:151:LEU:HD13	2:J:302:MPD:H13	1.78	0.66
1:D:99:SER:HG	1:D:124:HIS:CE1	2.12	0.66
2:J:301:MPD:H52	3:K:413:HOH:O	1.96	0.65
1:E:9:VAL:HG22	1:E:10:GLU:HG2	1.78	0.64
1:D:4:LEU:CD2	1:E:4:LEU:HD11	2.28	0.63
1:D:20:ASP:OD1	1:D:23:SER:OG	2.14	0.63
1:D:58:GLU:OE2	1:D:86:LYS:CE	2.46	0.63
1:L:151:LEU:HD13	2:L:301:MPD:H13	1.80	0.63
1:C:124:HIS:HD2	2:C:302:MPD:HM1	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:117:PRO:HG3	1:F:192:THR:HG22	1.81	0.61
1:K:99:SER:HG	1:K:124:HIS:CE1	2.17	0.61
1:H:100:MET:N	2:H:301:MPD:HM3	2.16	0.61
1:N:155:LEU:HD11	2:N:301:MPD:H53	1.83	0.61
1:C:123:ILE:HG22	2:C:302:MPD:H51	1.83	0.61
1:E:100:MET:HE1	2:E:301:MPD:H52	1.82	0.60
1:J:29:ARG:NH2	1:J:59:LYS:O	2.34	0.60
1:H:124:HIS:O	2:H:301:MPD:O4	2.19	0.60
1:M:4:LEU:CD2	1:N:5:VAL:HG21	2.31	0.60
1:A:176:MET:CE	1:A:186:LEU:HD22	2.32	0.59
1:H:151:LEU:CD1	2:H:301:MPD:H13	2.27	0.59
1:A:124:HIS:O	2:A:301:MPD:H13	2.03	0.59
1:D:4:LEU:HD22	1:E:4:LEU:HD11	1.85	0.59
1:K:31:ILE:HD11	1:K:52:LEU:HD12	1.82	0.58
1:M:151:LEU:HD13	2:M:302:MPD:H13	1.84	0.58
1:N:151:LEU:HD13	2:N:301:MPD:H11	1.81	0.58
1:A:124:HIS:O	2:A:301:MPD:O4	2.19	0.58
1:H:20:ASP:OD1	1:H:23:SER:OG	2.18	0.58
1:M:4:LEU:HD23	1:N:5:VAL:HG21	1.86	0.58
1:C:176:MET:CE	1:C:186:LEU:HD22	2.34	0.57
1:C:8:VAL:N	1:C:19:TYR:O	2.30	0.57
1:C:9:VAL:HG22	1:C:18:ALA:CA	2.34	0.56
1:E:146:PHE:CZ	1:E:150:ARG:HD2	2.41	0.56
1:B:19:TYR:HE2	1:B:27:LYS:CD	2.15	0.56
1:I:21:ILE:HD11	1:J:51:PHE:CB	2.35	0.56
1:M:146:PHE:O	1:M:150:ARG:HG2	2.05	0.56
1:K:99:SER:HB3	2:K:301:MPD:H13	1.88	0.56
1:H:100:MET:HE2	2:H:301:MPD:H11	1.88	0.55
1:N:100:MET:HE2	2:N:301:MPD:HM3	1.87	0.55
1:C:124:HIS:CD2	2:C:302:MPD:HM1	2.42	0.55
1:B:99:SER:HB3	2:B:302:MPD:HM3	1.89	0.54
1:H:8:VAL:N	1:H:19:TYR:O	2.29	0.54
1:F:155:LEU:HD11	2:F:301:MPD:H12	1.90	0.53
1:N:99:SER:HG	1:N:124:HIS:CE1	2.25	0.53
1:B:124:HIS:HD2	2:B:302:MPD:HM1	1.74	0.53
1:J:57:PRO:HB2	1:J:86:LYS:HD3	1.91	0.53
1:M:100:MET:HE2	2:M:302:MPD:H11	1.91	0.53
1:F:19:TYR:HE2	1:F:27:LYS:HD2	1.73	0.53
1:N:151:LEU:HD13	2:N:301:MPD:H13	1.89	0.53
1:F:155:LEU:HD11	2:F:301:MPD:C1	2.39	0.53
1:A:20:ASP:OD1	1:A:23:SER:OG	2.18	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:176:MET:CE	1:L:186:LEU:HD22	2.38	0.52
1:G:29:ARG:NH2	1:G:59:LYS:O	2.40	0.52
1:M:117:PRO:HG3	1:M:192:THR:HG22	1.91	0.52
1:I:21:ILE:HD11	1:J:51:PHE:HB2	1.92	0.52
1:C:176:MET:HE3	1:C:186:LEU:HD22	1.91	0.52
1:H:80:ASP:HB3	1:N:116:LEU:HD13	1.92	0.52
1:D:100:MET:HE2	2:D:301:MPD:H53	1.91	0.51
1:N:176:MET:HE3	1:N:186:LEU:HD22	1.90	0.51
1:E:4:LEU:HG	1:E:5:VAL:H	1.74	0.51
1:F:42:ALA:HA	1:F:78:ILE:HD11	1.93	0.51
1:J:176:MET:HE3	1:J:186:LEU:HD22	1.92	0.51
1:K:120:ARG:NE	1:L:143:GLU:OE2	2.41	0.51
1:D:19:TYR:CZ	1:D:27:LYS:HD2	2.46	0.51
1:H:58:GLU:OE2	1:H:86:LYS:NZ	2.30	0.51
1:F:58:GLU:OE2	1:F:86:LYS:NZ	2.33	0.51
2:J:301:MPD:O4	2:J:301:MPD:O2	2.26	0.50
1:K:20:ASP:OD1	1:K:23:SER:OG	2.14	0.50
1:B:124:HIS:CD2	2:B:302:MPD:HM1	2.47	0.50
1:M:100:MET:CE	2:M:302:MPD:H11	2.42	0.49
1:F:8:VAL:HG11	1:G:51:PHE:CZ	2.47	0.49
1:H:100:MET:CE	2:H:301:MPD:H11	2.42	0.49
1:M:33:LEU:C	1:M:33:LEU:HD23	2.32	0.49
1:B:117:PRO:HG3	1:B:192:THR:HG22	1.94	0.49
1:L:99:SER:HB3	2:L:301:MPD:HM3	1.94	0.49
1:N:151:LEU:HD13	2:N:301:MPD:H12	1.87	0.49
1:J:176:MET:CE	1:J:186:LEU:HD22	2.42	0.49
2:A:301:MPD:H13	2:A:301:MPD:O4	2.13	0.49
1:L:99:SER:HG	1:L:124:HIS:CE1	2.28	0.49
1:B:19:TYR:HD2	1:B:24:ARG:HA	1.78	0.48
1:H:118:HIS:CD2	1:I:154:ILE:HD11	2.49	0.48
1:D:100:MET:CE	2:D:301:MPD:H53	2.43	0.48
1:G:113:ARG:NH2	1:G:185:GLY:O	2.43	0.48
1:D:136:ASP:OD2	3:D:401:HOH:O	2.19	0.48
1:F:118:HIS:NE2	1:G:154:ILE:HD11	2.29	0.48
1:G:153:GLN:HG2	1:G:163:LEU:HD12	1.96	0.48
1:H:123:ILE:HG22	2:H:301:MPD:H51	1.96	0.48
1:C:99:SER:HB3	2:C:302:MPD:HM3	1.96	0.48
1:L:155:LEU:HD11	2:L:301:MPD:H53	1.95	0.48
1:I:151:LEU:HD13	2:I:301:MPD:H11	1.96	0.48
1:L:176:MET:HE1	1:L:186:LEU:HD22	1.96	0.48
1:I:117:PRO:HG3	1:I:192:THR:HG22	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:99:SER:HA	2:B:302:MPD:H4	1.96	0.47
1:K:99:SER:HA	2:K:301:MPD:H4	1.96	0.47
1:B:32:PHE:HB2	2:B:301:MPD:H13	1.96	0.47
1:M:4:LEU:HD22	1:N:5:VAL:HG11	1.96	0.47
1:F:5:VAL:CG2	1:F:20:ASP:HB2	2.45	0.47
1:G:4:LEU:HG	1:G:5:VAL:H	1.77	0.47
1:G:176:MET:CE	1:G:186:LEU:HD22	2.45	0.47
1:K:33:LEU:C	1:K:33:LEU:HD23	2.35	0.47
1:G:4:LEU:CG	1:G:5:VAL:H	2.28	0.47
1:D:5:VAL:CG2	1:D:21:ILE:HG22	2.44	0.47
1:M:99:SER:HB3	2:M:302:MPD:HM3	1.96	0.47
1:G:163:LEU:HD23	1:G:163:LEU:O	2.15	0.47
1:B:33:LEU:HD23	1:B:33:LEU:C	2.36	0.47
1:G:4:LEU:HG	1:G:5:VAL:HG12	1.97	0.46
1:H:7:MET:O	1:I:23:SER:OG	2.20	0.46
1:E:100:MET:CE	2:E:301:MPD:H52	2.45	0.46
1:B:106:ALA:HB2	1:B:186:LEU:HD12	1.97	0.46
1:E:8:VAL:O	1:E:18:ALA:HA	2.15	0.46
1:I:99:SER:HG	1:I:124:HIS:CD2	2.26	0.46
1:J:21:ILE:HD11	1:K:51:PHE:CB	2.45	0.46
1:C:124:HIS:O	2:C:302:MPD:O4	2.24	0.46
1:F:118:HIS:CD2	1:G:154:ILE:HD11	2.50	0.46
1:I:116:LEU:HD13	1:J:80:ASP:HB3	1.98	0.46
1:K:123:ILE:HA	2:K:301:MPD:H51	1.98	0.46
1:M:136:ASP:OD2	3:M:401:HOH:O	2.20	0.46
1:D:5:VAL:HG23	1:D:21:ILE:HG22	1.97	0.45
1:N:5:VAL:O	1:N:5:VAL:HG13	2.17	0.45
1:L:33:LEU:C	1:L:33:LEU:HD23	2.36	0.45
1:A:51:PHE:CB	1:G:21:ILE:HD11	2.47	0.45
1:M:42:ALA:HA	1:M:78:ILE:HD11	1.99	0.45
1:C:34:VAL:HG21	2:C:301:MPD:HM2	1.98	0.45
1:E:4:LEU:CG	1:E:5:VAL:H	2.29	0.45
1:G:141:ALA:O	1:G:144:ILE:HG22	2.17	0.45
1:E:42:ALA:HA	1:E:78:ILE:HD11	1.99	0.45
1:E:19:TYR:CZ	1:E:27:LYS:HD2	2.51	0.45
1:H:33:LEU:C	1:H:33:LEU:HD23	2.36	0.45
1:C:125:GLN:HB2	1:C:126:PRO:HD2	1.99	0.45
1:K:72:VAL:HA	1:K:100:MET:CE	2.47	0.45
1:B:162:PRO:HG2	1:B:165:VAL:CG2	2.48	0.44
1:C:31:ILE:HD11	1:C:52:LEU:HD12	1.99	0.44
1:E:21:ILE:HD11	1:F:51:PHE:CB	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:5:VAL:O	1:E:7:MET:CE	2.66	0.44
1:E:33:LEU:C	1:E:33:LEU:HD23	2.38	0.44
1:N:31:ILE:HD11	1:N:52:LEU:HD12	2.00	0.44
2:A:301:MPD:H13	2:A:301:MPD:HO4	1.81	0.44
1:J:4:LEU:HD21	1:K:5:VAL:HG21	1.98	0.44
1:L:124:HIS:CD2	2:L:301:MPD:HM1	2.52	0.44
2:N:301:MPD:HO4	2:N:301:MPD:HO2	1.65	0.44
1:E:31:ILE:HD11	1:E:52:LEU:HD12	1.98	0.44
1:M:106:ALA:HB2	1:M:186:LEU:HD12	1.99	0.44
1:M:86:LYS:N	1:M:87:PRO:HD2	2.33	0.44
1:A:120:ARG:HD2	1:A:120:ARG:HA	1.86	0.44
1:A:176:MET:HE3	1:A:186:LEU:HD22	2.00	0.44
1:D:33:LEU:HD23	1:D:33:LEU:C	2.38	0.44
1:H:42:ALA:HA	1:H:78:ILE:HD11	2.00	0.44
1:E:124:HIS:H	2:E:301:MPD:HO2	1.66	0.44
1:G:86:LYS:N	1:G:87:PRO:HD2	2.33	0.44
1:M:169:ASP:OD2	1:M:184:TYR:OH	2.26	0.44
1:A:5:VAL:HG13	1:A:5:VAL:O	2.17	0.43
1:D:162:PRO:HG2	1:D:165:VAL:CG2	2.48	0.43
1:N:33:LEU:HD23	1:N:33:LEU:C	2.38	0.43
1:F:5:VAL:HG22	1:F:20:ASP:HB2	2.01	0.43
1:H:51:PHE:CB	1:N:21:ILE:HD11	2.48	0.43
1:D:125:GLN:HB2	1:D:126:PRO:HD2	2.00	0.43
1:L:21:ILE:HD11	1:M:51:PHE:CB	2.48	0.43
1:M:113:ARG:NH2	1:M:185:GLY:O	2.49	0.43
1:H:31:ILE:HD11	1:H:52:LEU:HD12	2.01	0.43
1:J:33:LEU:C	1:J:33:LEU:HD23	2.38	0.43
1:G:163:LEU:HD23	1:G:163:LEU:C	2.39	0.43
1:H:162:PRO:HB2	1:H:164:ASP:OD1	2.19	0.43
1:I:33:LEU:HD23	1:I:33:LEU:C	2.39	0.43
1:M:31:ILE:HD11	1:M:52:LEU:HD12	2.00	0.43
1:A:99:SER:HG	1:A:124:HIS:CE1	2.33	0.43
1:F:5:VAL:HG13	1:F:5:VAL:O	2.19	0.43
1:G:176:MET:HE1	1:G:186:LEU:HD22	1.99	0.43
1:N:20:ASP:OD1	1:N:23:SER:OG	2.16	0.43
1:C:100:MET:HE3	1:C:103:LEU:HD22	2.00	0.43
1:C:176:MET:HE1	1:C:186:LEU:HD22	2.00	0.43
1:M:126:PRO:HG3	1:M:151:LEU:HD12	2.01	0.43
1:C:172:ARG:NH1	1:D:133:GLN:OE1	2.35	0.43
1:H:126:PRO:HG3	1:H:151:LEU:HD12	2.01	0.42
1:A:33:LEU:C	1:A:33:LEU:HD23	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:106:ALA:HB2	1:D:186:LEU:HD12	2.01	0.42
1:I:123:ILE:HG22	2:I:301:MPD:H51	2.00	0.42
1:J:117:PRO:HG3	1:J:192:THR:HG22	2.00	0.42
1:G:33:LEU:C	1:G:33:LEU:HD23	2.39	0.42
1:M:99:SER:CA	2:M:302:MPD:HM3	2.49	0.42
1:H:99:SER:HA	2:H:301:MPD:HM1	2.01	0.42
1:J:99:SER:HA	2:J:302:MPD:CM	2.49	0.42
1:B:86:LYS:N	1:B:87:PRO:HD2	2.34	0.42
1:H:162:PRO:HG2	1:H:165:VAL:HG23	2.01	0.42
1:K:124:HIS:CD2	2:K:301:MPD:H11	2.54	0.42
1:L:7:MET:N	1:M:23:SER:OG	2.40	0.42
1:H:99:SER:HA	2:H:301:MPD:H4	2.02	0.42
1:K:99:SER:HG	1:K:124:HIS:CD2	2.31	0.42
1:C:34:VAL:CG2	2:C:301:MPD:HM2	2.49	0.42
1:G:79:TYR:O	1:G:83:GLN:HG2	2.20	0.42
1:K:162:PRO:HG2	1:K:165:VAL:HG23	2.02	0.42
1:M:117:PRO:HD3	1:M:191:MET:O	2.19	0.42
1:N:86:LYS:N	1:N:87:PRO:HD2	2.35	0.42
1:B:31:ILE:HD11	1:B:52:LEU:HD12	2.02	0.42
1:K:125:GLN:HB2	1:K:126:PRO:HD2	2.02	0.42
1:I:58:GLU:OE2	1:I:86:LYS:CE	2.67	0.41
1:K:120:ARG:NH2	1:L:143:GLU:OE1	2.53	0.41
1:D:58:GLU:CD	1:D:86:LYS:HE2	2.40	0.41
1:D:179:ASP:O	1:D:183:LYS:HG3	2.20	0.41
1:E:21:ILE:HD11	1:F:51:PHE:HB2	2.02	0.41
1:A:176:MET:HE1	1:A:186:LEU:HD22	2.02	0.41
1:F:86:LYS:N	1:F:87:PRO:HD2	2.36	0.41
1:N:99:SER:HA	2:N:301:MPD:H4	2.01	0.41
1:D:31:ILE:HD11	1:D:52:LEU:HD12	2.02	0.41
1:H:5:VAL:HG13	1:H:5:VAL:O	2.20	0.41
1:L:124:HIS:HD2	2:L:301:MPD:HM1	1.85	0.41
1:J:96:GLN:HA	1:J:120:ARG:O	2.21	0.41
1:L:86:LYS:N	1:L:87:PRO:CD	2.84	0.41
1:F:33:LEU:C	1:F:33:LEU:HD23	2.41	0.41
1:B:5:VAL:HG13	1:B:5:VAL:O	2.21	0.41
1:L:42:ALA:HA	1:L:78:ILE:HD11	2.03	0.41
1:B:162:PRO:HG2	1:B:165:VAL:HG23	2.02	0.41
1:A:96:GLN:HA	1:A:120:ARG:O	2.21	0.40
1:J:172:ARG:NH1	1:K:133:GLN:OE1	2.39	0.40
1:J:99:SER:CA	2:J:302:MPD:HM3	2.51	0.40
1:B:120:ARG:HA	1:B:120:ARG:HD2	1.90	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:ILE:HB	2:B:302:MPD:H51	2.03	0.40
1:C:113:ARG:NH2	1:C:185:GLY:O	2.53	0.40
1:J:116:LEU:HD13	1:K:80:ASP:HB3	2.03	0.40
1:A:31:ILE:HD11	1:A:52:LEU:HD12	2.04	0.40
1:K:5:VAL:HG13	1:K:5:VAL:O	2.21	0.40
1:K:57:PRO:HA	1:K:87:PRO:HG3	2.04	0.40
1:L:176:MET:HE3	1:L:186:LEU:HD22	2.03	0.40
1:M:21:ILE:HD11	1:N:51:PHE:CB	2.52	0.40
1:E:9:VAL:HB	1:F:19:TYR:OH	2.21	0.40
1:F:120:ARG:HD2	1:F:120:ARG:HA	1.92	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	178/210 (85%)	174 (98%)	4 (2%)	0	100	100
1	B	178/210 (85%)	175 (98%)	3 (2%)	0	100	100
1	C	179/210 (85%)	176 (98%)	3 (2%)	0	100	100
1	D	179/210 (85%)	175 (98%)	4 (2%)	0	100	100
1	E	180/210 (86%)	177 (98%)	3 (2%)	0	100	100
1	F	178/210 (85%)	175 (98%)	3 (2%)	0	100	100
1	G	178/210 (85%)	175 (98%)	3 (2%)	0	100	100
1	H	178/210 (85%)	174 (98%)	4 (2%)	0	100	100
1	I	178/210 (85%)	174 (98%)	4 (2%)	0	100	100
1	J	179/210 (85%)	175 (98%)	4 (2%)	0	100	100
1	K	179/210 (85%)	175 (98%)	4 (2%)	0	100	100
1	L	178/210 (85%)	174 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	M	178/210 (85%)	175 (98%)	3 (2%)	0	100	100
1	N	178/210 (85%)	175 (98%)	3 (2%)	0	100	100
All	All	2498/2940 (85%)	2449 (98%)	49 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	152/171 (89%)	151 (99%)	1 (1%)	84	94
1	B	152/171 (89%)	150 (99%)	2 (1%)	69	86
1	C	153/171 (90%)	150 (98%)	3 (2%)	55	78
1	D	153/171 (90%)	151 (99%)	2 (1%)	69	86
1	E	154/171 (90%)	151 (98%)	3 (2%)	57	79
1	F	152/171 (89%)	150 (99%)	2 (1%)	69	86
1	G	152/171 (89%)	150 (99%)	2 (1%)	69	86
1	H	152/171 (89%)	150 (99%)	2 (1%)	69	86
1	I	152/171 (89%)	149 (98%)	3 (2%)	55	78
1	J	153/171 (90%)	151 (99%)	2 (1%)	69	86
1	K	153/171 (90%)	150 (98%)	3 (2%)	55	78
1	L	152/171 (89%)	151 (99%)	1 (1%)	84	94
1	M	152/171 (89%)	149 (98%)	3 (2%)	55	78
1	N	152/171 (89%)	151 (99%)	1 (1%)	84	94
All	All	2134/2394 (89%)	2104 (99%)	30 (1%)	67	85

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	124	HIS

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Mol	Chain	Res	Type
1	B	124	HIS
1	B	193	GLN
1	C	7	MET
1	C	124	HIS
1	C	193	GLN
1	D	124	HIS
1	D	193	GLN
1	E	7	MET
1	E	10	GLU
1	E	124	HIS
1	F	124	HIS
1	F	193	GLN
1	G	124	HIS
1	G	193	GLN
1	H	100	MET
1	H	124	HIS
1	I	7	MET
1	I	124	HIS
1	I	193	GLN
1	J	7	MET
1	J	124	HIS
1	K	124	HIS
1	K	193	GLN
1	K	195	ASP
1	L	124	HIS
1	M	7	MET
1	M	124	HIS
1	M	193	GLN
1	N	124	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	193	GLN
1	I	36	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)

18 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	MPD	D	301	-	7,7,7	0.11	0	9,10,10	0.35	0
2	MPD	L	301	-	7,7,7	0.13	0	9,10,10	0.36	0
2	MPD	F	301	-	7,7,7	0.17	0	9,10,10	0.27	0
2	MPD	J	302	-	7,7,7	0.17	0	9,10,10	0.33	0
2	MPD	A	301	-	7,7,7	0.14	0	9,10,10	0.21	0
2	MPD	G	301	-	7,7,7	0.09	0	9,10,10	0.37	0
2	MPD	N	301	-	7,7,7	0.17	0	9,10,10	0.36	0
2	MPD	J	301	-	7,7,7	0.20	0	9,10,10	0.45	0
2	MPD	K	301	-	7,7,7	0.16	0	9,10,10	0.34	0
2	MPD	M	302	-	7,7,7	0.16	0	9,10,10	0.37	0
2	MPD	B	302	-	7,7,7	0.10	0	9,10,10	0.44	0
2	MPD	C	302	-	7,7,7	0.21	0	9,10,10	0.29	0
2	MPD	C	301	-	7,7,7	0.14	0	9,10,10	0.29	0
2	MPD	E	301	-	7,7,7	0.10	0	9,10,10	0.28	0
2	MPD	H	301	-	7,7,7	0.12	0	9,10,10	0.43	0
2	MPD	I	301	-	7,7,7	0.11	0	9,10,10	0.46	0
2	MPD	M	301	-	7,7,7	0.11	0	9,10,10	0.28	0
2	MPD	B	301	-	7,7,7	0.09	0	9,10,10	0.35	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	MPD	D	301	-	-	0/5/5/5	-
2	MPD	L	301	-	-	0/5/5/5	-
2	MPD	F	301	-	-	0/5/5/5	-
2	MPD	J	302	-	-	0/5/5/5	-
2	MPD	A	301	-	-	0/5/5/5	-
2	MPD	G	301	-	-	0/5/5/5	-
2	MPD	N	301	-	-	0/5/5/5	-
2	MPD	J	301	-	-	1/5/5/5	-
2	MPD	K	301	-	-	0/5/5/5	-
2	MPD	M	302	-	-	1/5/5/5	-
2	MPD	B	302	-	-	0/5/5/5	-
2	MPD	C	302	-	-	0/5/5/5	-
2	MPD	C	301	-	-	0/5/5/5	-
2	MPD	E	301	-	-	0/5/5/5	-
2	MPD	H	301	-	-	0/5/5/5	-
2	MPD	I	301	-	-	0/5/5/5	-
2	MPD	M	301	-	-	0/5/5/5	-
2	MPD	B	301	-	-	0/5/5/5	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	J	301	MPD	O2-C2-C3-C4
2	M	302	MPD	CM-C2-C3-C4

There are no ring outliers.

16 monomers are involved in 67 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	301	MPD	3	0
2	L	301	MPD	6	0
2	F	301	MPD	2	0
2	J	302	MPD	3	0
2	A	301	MPD	4	0
2	N	301	MPD	9	0
2	J	301	MPD	2	0
2	K	301	MPD	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	M	302	MPD	5	0
2	B	302	MPD	6	0
2	C	302	MPD	5	0
2	C	301	MPD	2	0
2	E	301	MPD	3	0
2	H	301	MPD	9	0
2	I	301	MPD	2	0
2	B	301	MPD	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 (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	182/210 (86%)	-0.01	2 (1%)	80	78	28, 38, 59, 82	0
1	B	182/210 (86%)	0.01	4 (2%)	62	56	28, 37, 61, 90	0
1	C	183/210 (87%)	0.04	5 (2%)	54	48	28, 37, 63, 84	0
1	D	183/210 (87%)	-0.02	6 (3%)	46	39	29, 39, 63, 83	0
1	E	184/210 (87%)	0.05	4 (2%)	62	56	28, 37, 60, 94	0
1	F	182/210 (86%)	-0.05	3 (1%)	72	68	27, 39, 61, 90	0
1	G	182/210 (86%)	-0.11	5 (2%)	54	48	26, 38, 63, 92	0
1	H	182/210 (86%)	0.03	4 (2%)	62	56	28, 39, 62, 85	0
1	I	182/210 (86%)	0.19	4 (2%)	62	56	28, 38, 61, 99	0
1	J	183/210 (87%)	-0.10	1 (0%)	91	89	29, 39, 60, 78	0
1	K	183/210 (87%)	-0.10	3 (1%)	72	68	27, 37, 63, 85	0
1	L	182/210 (86%)	0.00	3 (1%)	72	68	28, 36, 60, 78	0
1	M	182/210 (86%)	-0.00	3 (1%)	72	68	29, 39, 61, 89	0
1	N	182/210 (86%)	0.05	5 (2%)	54	48	29, 38, 62, 80	0
All	All	2554/2940 (86%)	-0.00	52 (2%)	65	60	26, 38, 63, 99	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	18	ALA	9.1
1	I	7	MET	7.9
1	E	9	VAL	5.7
1	N	18	ALA	5.7
1	H	4	LEU	5.4
1	F	18	ALA	5.4
1	H	18	ALA	5.1
1	B	18	ALA	5.1

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Mol	Chain	Res	Type	RSRZ
1	G	7	MET	4.6
1	K	18	ALA	4.5
1	B	19	TYR	4.5
1	H	19	TYR	4.5
1	D	18	ALA	4.5
1	C	9	VAL	4.2
1	M	18	ALA	4.2
1	M	4	LEU	3.8
1	E	8	VAL	3.7
1	K	195	ASP	3.7
1	C	18	ALA	3.7
1	C	4	LEU	3.6
1	M	19	TYR	3.5
1	L	19	TYR	3.2
1	I	4	LEU	2.9
1	L	18	ALA	2.9
1	B	4	LEU	2.8
1	C	19	TYR	2.8
1	N	8	VAL	2.8
1	F	4	LEU	2.7
1	E	10	GLU	2.7
1	N	19	TYR	2.6
1	A	18	ALA	2.6
1	K	19	TYR	2.6
1	N	4	LEU	2.6
1	C	58	GLU	2.5
1	D	86	LYS	2.4
1	D	7	MET	2.4
1	G	18	ALA	2.4
1	D	19	TYR	2.3
1	N	7	MET	2.3
1	I	8	VAL	2.3
1	B	7	MET	2.3
1	G	8	VAL	2.2
1	G	5	VAL	2.2
1	D	8	VAL	2.1
1	J	18	ALA	2.1
1	A	19	TYR	2.1
1	D	4	LEU	2.1
1	G	19	TYR	2.1
1	L	4	LEU	2.1
1	E	19	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	7	MET	2.0
1	F	19	TYR	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, 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
2	MPD	B	302	8/8	0.89	0.22	49,62,77,78	0
2	MPD	C	301	8/8	0.90	0.21	25,50,55,61	0
2	MPD	E	301	8/8	0.90	0.28	48,61,78,78	0
2	MPD	G	301	8/8	0.90	0.22	44,58,67,67	0
2	MPD	J	302	8/8	0.91	0.26	35,52,69,70	0
2	MPD	K	301	8/8	0.91	0.22	49,62,68,78	0
2	MPD	J	301	8/8	0.92	0.20	37,54,68,70	0
2	MPD	A	301	8/8	0.92	0.26	36,54,68,68	0
2	MPD	C	302	8/8	0.92	0.47	45,61,68,70	0
2	MPD	L	301	8/8	0.92	0.41	40,58,72,76	0
2	MPD	B	301	8/8	0.93	0.17	31,43,53,62	0
2	MPD	D	301	8/8	0.93	0.26	33,55,68,68	0
2	MPD	N	301	8/8	0.93	0.28	45,62,83,83	0
2	MPD	I	301	8/8	0.94	0.20	48,62,76,81	0
2	MPD	M	302	8/8	0.94	0.23	45,57,60,61	0
2	MPD	H	301	8/8	0.94	0.31	41,57,69,76	0
2	MPD	M	301	8/8	0.95	0.24	36,46,72,72	0
2	MPD	F	301	8/8	0.96	0.29	36,54,75,75	0

6.5 Other polymers (i)

There are no such residues in this entry.