



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:06 PM UTC

PDB ID : 5C90 / pdb_00005c90
Title : Staphylococcus aureus ClpP mutant - Y63A
Authors : Ye, F.; Liu, H.; Zhang, J.; Gan, J.; Yang, C.-G.
Deposited on : 2015-06-26
Resolution : 1.75 Å(reported)

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

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<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

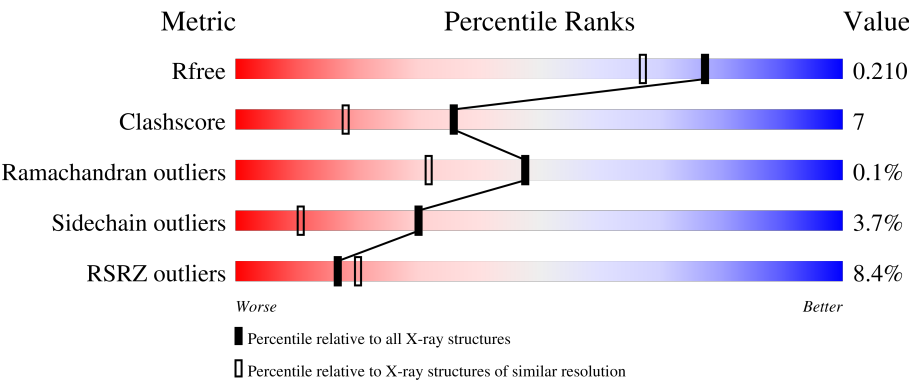
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 1.75 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}	180053	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (1.76-1.76)

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 $\leq 5\%$. 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	195	6% 81% 11% • 8%
1	B	195	9% 82% 11% • •
1	C	195	9% 82% 10% • 7%
1	D	195	7% 84% 7% •• 8%
1	E	195	7% 88% 7% 5%

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Mol	Chain	Length	Quality of chain
1	F	195	
1	G	195	
1	H	195	
1	I	195	
1	J	195	
1	K	195	
1	L	195	
1	M	195	
1	N	195	

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	201	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 21763 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	179	Total	C	N	O	S	0	4	0
			1391	879	235	270	7			
1	B	187	Total	C	N	O	S	0	4	0
			1457	918	246	285	8			
1	C	182	Total	C	N	O	S	0	6	0
			1429	901	243	277	8			
1	D	180	Total	C	N	O	S	0	3	0
			1392	880	235	270	7			
1	E	186	Total	C	N	O	S	0	6	0
			1460	924	246	283	7			
1	F	186	Total	C	N	O	S	0	3	0
			1445	910	245	283	7			
1	G	186	Total	C	N	O	S	0	3	0
			1442	909	244	282	7			
1	H	179	Total	C	N	O	S	0	3	0
			1386	873	236	271	6			
1	I	179	Total	C	N	O	S	0	2	0
			1381	871	234	269	7			
1	J	185	Total	C	N	O	S	0	3	0
			1435	903	244	281	7			
1	K	186	Total	C	N	O	S	0	4	0
			1453	914	249	284	6			
1	L	182	Total	C	N	O	S	0	3	0
			1408	890	237	274	7			
1	M	180	Total	C	N	O	S	0	4	0
			1400	884	236	273	7			
1	N	181	Total	C	N	O	S	0	3	0
			1406	886	238	275	7			

There are 14 discrepancies between the modelled and reference sequences:

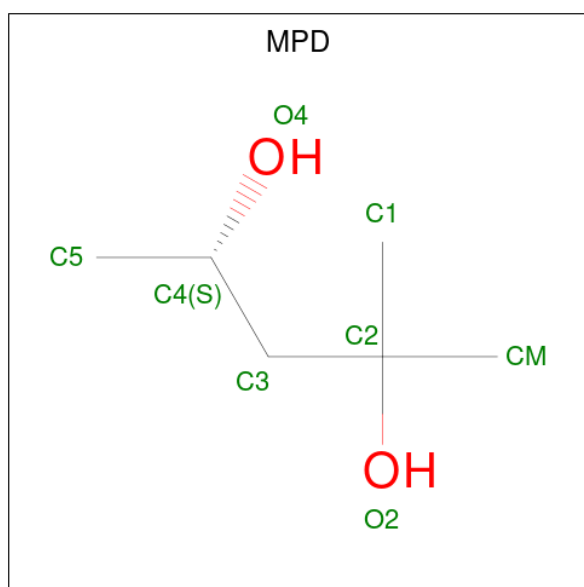
Chain	Residue	Modelled	Actual	Comment	Reference
A	63	ALA	TYR	engineered mutation	UNP Q2G036

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Chain	Residue	Modelled	Actual	Comment	Reference
B	63	ALA	TYR	engineered mutation	UNP Q2G036
C	63	ALA	TYR	engineered mutation	UNP Q2G036
D	63	ALA	TYR	engineered mutation	UNP Q2G036
E	63	ALA	TYR	engineered mutation	UNP Q2G036
F	63	ALA	TYR	engineered mutation	UNP Q2G036
G	63	ALA	TYR	engineered mutation	UNP Q2G036
H	63	ALA	TYR	engineered mutation	UNP Q2G036
I	63	ALA	TYR	engineered mutation	UNP Q2G036
J	63	ALA	TYR	engineered mutation	UNP Q2G036
K	63	ALA	TYR	engineered mutation	UNP Q2G036
L	63	ALA	TYR	engineered mutation	UNP Q2G036
M	63	ALA	TYR	engineered mutation	UNP Q2G036
N	63	ALA	TYR	engineered mutation	UNP Q2G036

- Molecule 2 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			8	6	2		
2	B	1	Total	C	O	0	0
			8	6	2		
2	C	1	Total	C	O	0	0
			8	6	2		
2	D	1	Total	C	O	0	0
			8	6	2		
2	E	1	Total	C	O	0	0
			8	6	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	F	1	Total C O 8 6 2	0	0
2	G	1	Total C O 8 6 2	0	0
2	H	1	Total C O 8 6 2	0	0
2	I	1	Total C O 8 6 2	0	0
2	J	1	Total C O 8 6 2	0	0
2	K	1	Total C O 8 6 2	0	0
2	L	1	Total C O 8 6 2	0	0
2	M	1	Total C O 8 6 2	0	0
2	N	1	Total C O 8 6 2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	139	Total O 139 139	0	0
3	B	84	Total O 84 84	0	0
3	C	103	Total O 103 103	0	0
3	D	96	Total O 96 96	0	0
3	E	146	Total O 146 146	0	0
3	F	168	Total O 168 168	0	0
3	G	163	Total O 163 163	0	0
3	H	87	Total O 87 87	0	0
3	I	143	Total O 143 143	0	0
3	J	163	Total O 163 163	0	0

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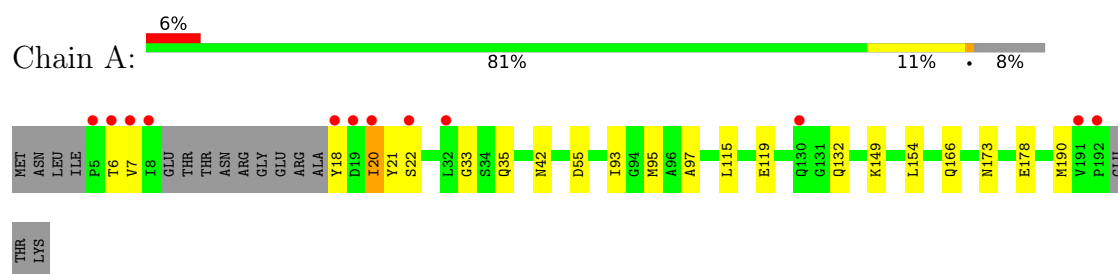
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	K	162	Total 162	O 162	0	0
3	L	137	Total 137	O 137	0	0
3	M	94	Total 94	O 94	0	0
3	N	81	Total 81	O 81	0	0

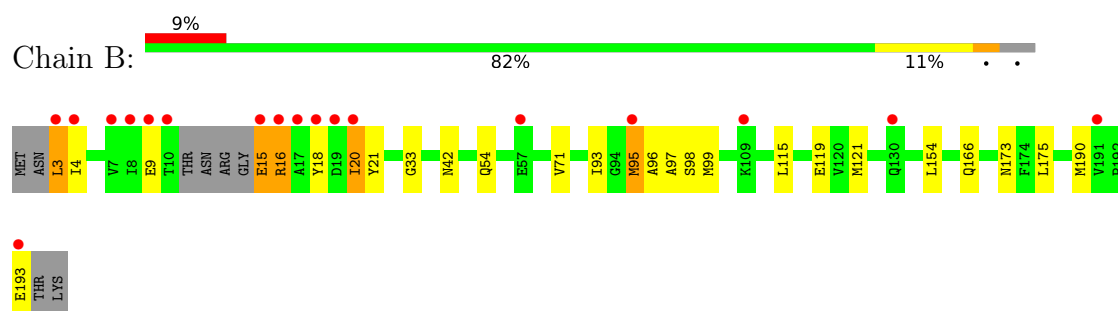
3 Residue-property plots [i](#)

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.

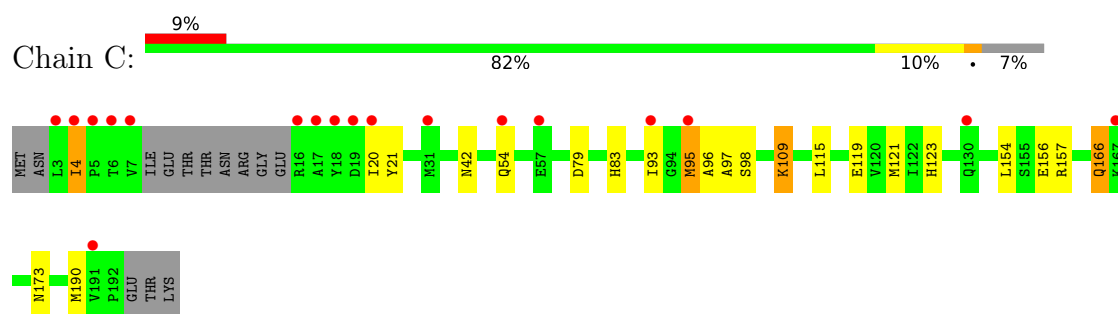
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



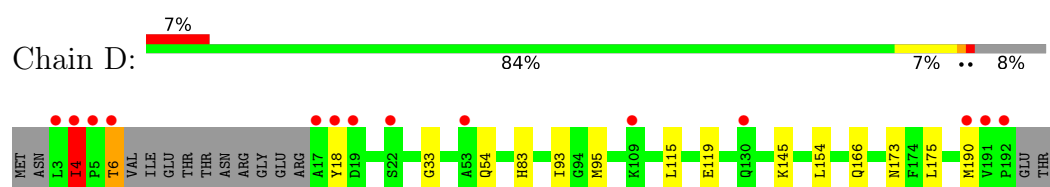
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



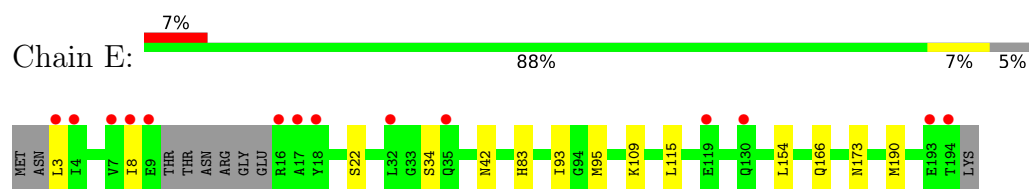
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



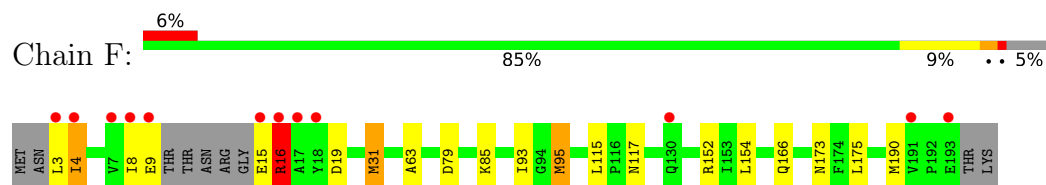
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



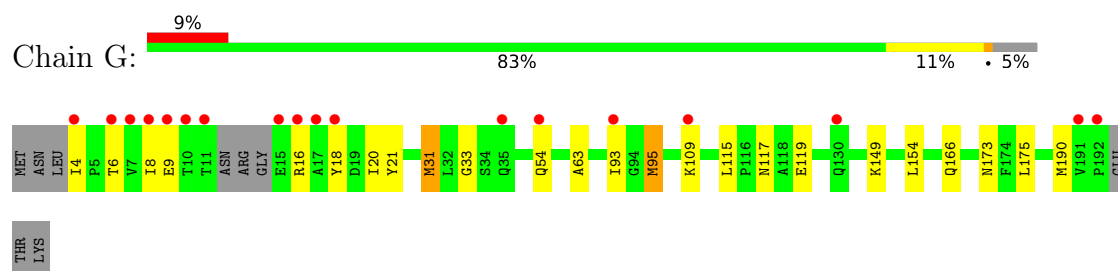
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



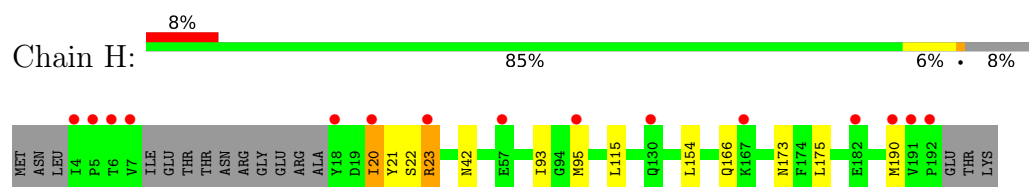
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



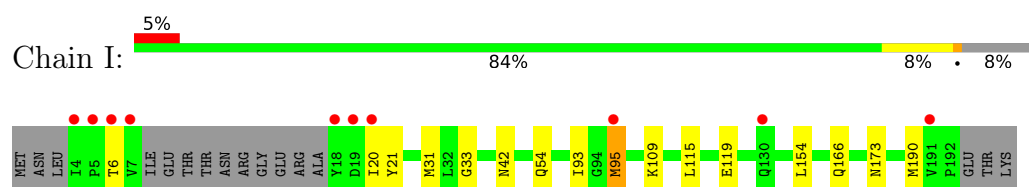
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



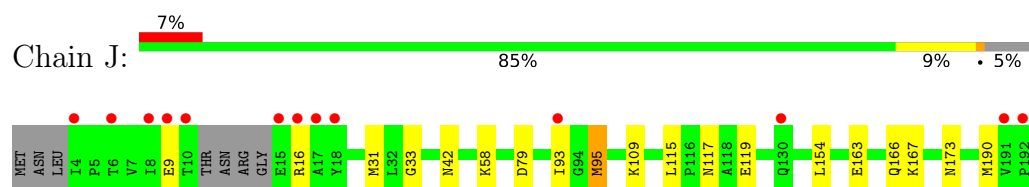
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



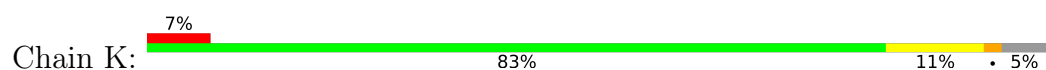
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

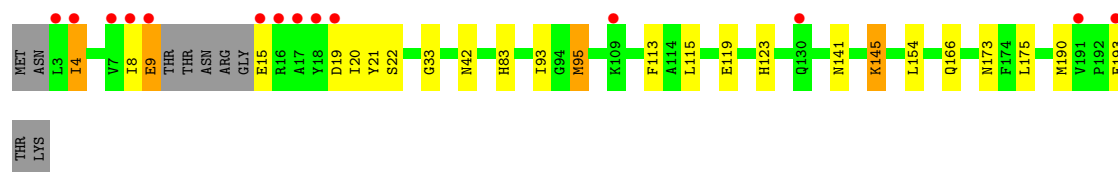


- Molecule 1: ATP-dependent Clp protease proteolytic subunit

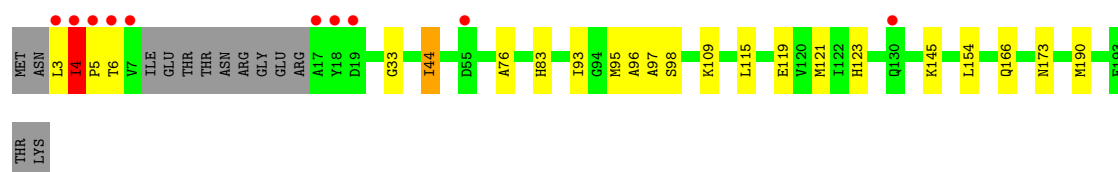
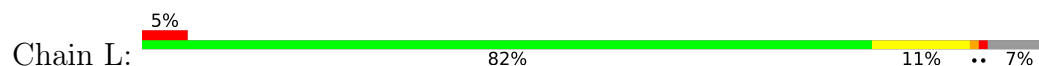


- Molecule 1: ATP-dependent Clp protease proteolytic subunit

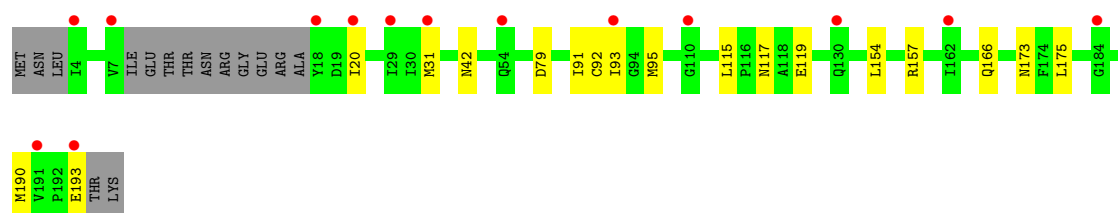
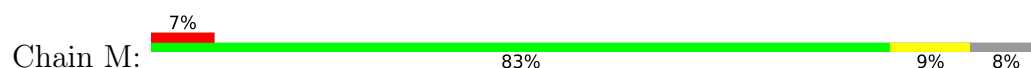




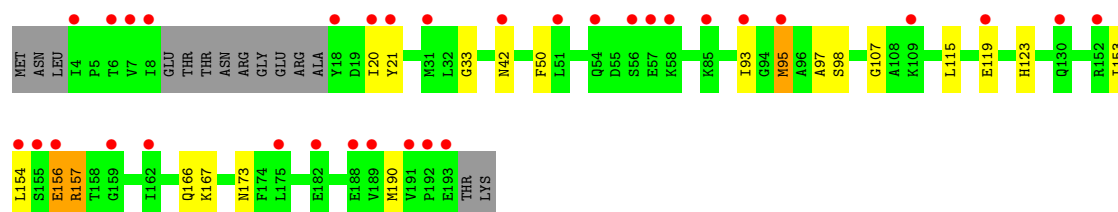
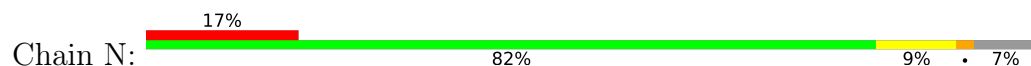
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



- Molecule 1: ATP-dependent Clp protease proteolytic subunit



- Molecule 1: ATP-dependent Clp protease proteolytic subunit



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	94.36Å 126.24Å 145.65Å 90.00° 93.74° 90.00°	Depositor
Resolution (Å)	30.00 – 1.75 30.00 – 1.75	Depositor EDS
% Data completeness (in resolution range)	99.4 (30.00-1.75) 99.4 (30.00-1.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.33 (at 1.75Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.182 , 0.202 0.195 , 0.210	Depositor DCC
R_{free} test set	17181 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	21.8	Xtriage
Anisotropy	0.431	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 38.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	21763	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.02% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: 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	0.80	2/1420 (0.1%)	0.83	2/1915 (0.1%)
1	B	0.64	0/1486	0.80	0/2004
1	C	0.66	0/1461	0.80	1/1970 (0.1%)
1	D	0.67	0/1418	0.85	4/1913 (0.2%)
1	E	0.76	1/1492 (0.1%)	0.85	0/2016
1	F	0.78	0/1471	0.86	1/1984 (0.1%)
1	G	0.77	0/1468	0.86	0/1981
1	H	0.62	0/1412	0.79	0/1906
1	I	0.75	0/1404	0.82	0/1894
1	J	0.81	2/1461 (0.1%)	0.92	2/1971 (0.1%)
1	K	0.78	1/1482 (0.1%)	0.85	0/1999
1	L	0.77	2/1434 (0.1%)	0.87	4/1935 (0.2%)
1	M	0.71	2/1429 (0.1%)	0.87	6/1928 (0.3%)
1	N	0.65	1/1429 (0.1%)	0.83	1/1928 (0.1%)
All	All	0.73	11/20267 (0.1%)	0.84	21/27344 (0.1%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	31[A]	MET	CA-C	9.58	1.64	1.52
1	M	31[B]	MET	CA-C	9.58	1.64	1.52
1	E	154	LEU	C-O	-6.51	1.16	1.24
1	A	55	ASP	C-O	-5.79	1.16	1.24
1	J	31[A]	MET	CA-C	5.62	1.59	1.52
1	J	31[B]	MET	CA-C	5.62	1.59	1.52
1	K	145	LYS	CA-CB	5.54	1.61	1.53
1	N	157	ARG	C-O	-5.41	1.17	1.24
1	A	154	LEU	C-O	-5.17	1.18	1.24
1	L	154	LEU	C-O	-5.13	1.18	1.24
1	L	4	ILE	CA-CB	5.12	1.60	1.54

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	31[A]	MET	CA-C-O	8.96	130.46	120.43
1	J	31[B]	MET	CA-C-O	8.96	130.46	120.43
1	M	31[A]	MET	CA-C-O	8.44	129.39	120.36
1	M	31[B]	MET	CA-C-O	8.44	129.39	120.36
1	N	167	LYS	CG-CD-CE	7.79	129.23	111.30
1	D	18	TYR	N-CA-C	-7.03	97.79	109.46
1	D	4	ILE	CA-C-N	-6.71	113.39	120.03
1	D	4	ILE	C-N-CA	-6.71	113.39	120.03
1	L	44	ILE	CA-CB-CG1	-6.29	99.71	110.40
1	D	4	ILE	CB-CA-C	5.94	122.18	111.36
1	C	4	ILE	N-CA-CB	5.74	119.24	111.21
1	L	4	ILE	CA-C-N	-5.66	114.43	120.03
1	L	4	ILE	C-N-CA	-5.66	114.43	120.03
1	L	4	ILE	N-CA-C	-5.42	97.18	108.88
1	M	31[A]	MET	CA-C-N	-5.19	115.09	122.77
1	M	31[A]	MET	C-N-CA	-5.19	115.09	122.77
1	M	31[B]	MET	CA-C-N	-5.19	115.09	122.77
1	M	31[B]	MET	C-N-CA	-5.19	115.09	122.77
1	A	20	ILE	CB-CA-C	-5.16	103.90	112.26
1	F	16	ARG	N-CA-C	5.15	116.90	108.55
1	A	20	ILE	N-CA-CB	5.11	120.02	110.77

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	1391	0	1424	25	0
1	B	1457	0	1486	53	0
1	C	1429	0	1461	32	0
1	D	1392	0	1424	12	0
1	E	1460	0	1501	17	0
1	F	1445	0	1470	24	0
1	G	1442	0	1472	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	1386	0	1409	17	0
1	I	1381	0	1406	16	0
1	J	1435	0	1460	16	0
1	K	1453	0	1480	30	0
1	L	1408	0	1439	35	0
1	M	1400	0	1429	26	0
1	N	1406	0	1428	22	0
2	A	8	0	14	0	0
2	B	8	0	14	19	0
2	C	8	0	14	5	0
2	D	8	0	14	0	0
2	E	8	0	14	0	0
2	F	8	0	14	0	0
2	G	8	0	14	0	0
2	H	8	0	14	0	0
2	I	8	0	14	0	0
2	J	8	0	14	0	0
2	K	8	0	14	0	0
2	L	8	0	14	5	0
2	M	8	0	14	0	0
2	N	8	0	14	0	0
3	A	139	0	0	4	0
3	B	84	0	0	3	0
3	C	103	0	0	6	0
3	D	96	0	0	5	0
3	E	146	0	0	5	0
3	F	168	0	0	4	0
3	G	163	0	0	6	0
3	H	87	0	0	2	0
3	I	143	0	0	4	0
3	J	163	0	0	5	0
3	K	162	0	0	6	0
3	L	137	0	0	4	0
3	M	94	0	0	5	0
3	N	81	0	0	1	0
All	All	21763	0	20485	294	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 7.

All (294) 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:F:4:ILE:CD1	1:F:19:ASP:HB2	1.64	1.27
1:B:95[B]:MET:HE2	1:B:97:ALA:HB2	1.28	1.14
1:M:93:ILE:HD12	1:M:115:LEU:CD1	1.77	1.14
1:L:95[A]:MET:HE2	1:L:97:ALA:HB2	1.25	1.10
1:C:95[B]:MET:HE2	1:C:97:ALA:HB2	1.25	1.09
1:B:15:GLU:HG2	1:B:16:ARG:HD3	1.28	1.06
1:M:93:ILE:HG23	1:M:115:LEU:HD12	1.36	1.05
1:L:95[A]:MET:SD	1:L:119:GLU:HG2	2.08	0.94
1:F:4:ILE:HD13	1:F:19:ASP:HB2	1.45	0.93
1:C:95[B]:MET:SD	1:C:119:GLU:HG2	2.10	0.91
1:K:4:ILE:HD12	1:K:21:TYR:CE2	2.06	0.91
1:A:95[A]:MET:SD	1:A:119:GLU:HG2	2.10	0.91
1:B:95[B]:MET:SD	1:B:119:GLU:HG2	2.10	0.90
1:C:121:MET:HE2	3:C:309:HOH:O	1.72	0.88
1:F:4:ILE:CD1	1:F:19:ASP:CB	2.51	0.87
1:M:93:ILE:HD12	1:M:115:LEU:HD12	1.55	0.87
1:A:18:TYR:CE1	1:G:8:ILE:HD12	2.10	0.86
1:B:98[A]:SER:HB2	2:B:201:MPD:H11	1.56	0.86
1:B:99[A]:MET:CE	2:B:201:MPD:HM2	2.05	0.86
1:H:23:ARG:HD2	1:N:50:PHE:CE1	2.12	0.84
1:C:109:LYS:HE2	3:C:310:HOH:O	1.77	0.84
1:K:113:PHE:CG	1:K:190:MET:HE3	2.13	0.83
1:M:91:ILE:HG22	1:M:93:ILE:HD11	1.62	0.82
1:K:4:ILE:CD1	1:K:21:TYR:CD2	2.63	0.81
1:B:193:GLU:C	3:B:4171:HOH:O	2.24	0.81
1:F:4:ILE:HD11	1:F:19:ASP:HB2	1.60	0.80
1:J:58:LYS:HE2	3:J:443:HOH:O	1.81	0.80
1:K:141:ASN:HB3	3:K:423:HOH:O	1.81	0.79
1:L:95[A]:MET:CE	1:L:97:ALA:HB2	2.12	0.78
1:B:98[A]:SER:HB2	2:B:201:MPD:C1	2.15	0.77
1:C:95[B]:MET:CE	1:C:97:ALA:HB2	2.12	0.77
1:M:93:ILE:HD12	1:M:115:LEU:HD11	1.65	0.76
1:B:95[B]:MET:CE	1:B:97:ALA:HB2	2.13	0.74
1:F:4:ILE:HD11	1:F:19:ASP:CB	2.16	0.73
1:M:173:ASN:ND2	3:M:301:HOH:O	2.20	0.73
1:A:95[B]:MET:HE2	1:A:97:ALA:HB2	1.70	0.72
1:A:95[A]:MET:HE3	1:A:97:ALA:HB2	1.72	0.71
1:L:4:ILE:HB	1:L:5:PRO:CD	2.20	0.71
1:L:95[A]:MET:HE2	1:L:97:ALA:CB	2.14	0.71
1:J:16:ARG:HD2	1:K:8:ILE:HG21	1.72	0.70
1:K:173:ASN:ND2	3:K:302:HOH:O	2.25	0.70
1:B:173:ASN:ND2	3:B:4101:HOH:O	2.25	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95[A]:MET:CE	1:A:119:GLU:OE2	2.40	0.69
1:M:93:ILE:HD12	1:M:115:LEU:CG	2.21	0.69
1:I:54:GLN:HG3	3:I:373:HOH:O	1.91	0.69
1:M:92:CYS:O	1:M:93:ILE:HD13	1.93	0.69
1:N:173:ASN:ND2	3:N:301:HOH:O	2.26	0.69
1:F:3:LEU:CD1	1:G:4:ILE:CD1	2.72	0.68
3:A:2105:HOH:O	1:K:123:HIS:HB2	1.93	0.68
1:B:95[B]:MET:HE2	1:B:97:ALA:CB	2.16	0.68
2:B:201:MPD:H12	2:B:201:MPD:O4	1.94	0.67
1:J:173:ASN:ND2	3:J:301:HOH:O	2.27	0.67
1:M:93:ILE:CD1	1:M:115:LEU:HG	2.25	0.67
1:B:98[B]:SER:HB3	2:B:201:MPD:H11	1.76	0.67
1:C:95[B]:MET:HE2	1:C:97:ALA:CB	2.14	0.67
1:A:33:GLY:HA3	1:B:42[B]:ASN:ND2	2.09	0.67
1:B:95[B]:MET:SD	1:B:119:GLU:CG	2.83	0.67
1:H:23:ARG:HD2	1:N:50:PHE:CD1	2.30	0.67
1:B:33:GLY:HA3	1:C:42[B]:ASN:ND2	2.10	0.66
1:L:95[A]:MET:HE3	1:L:96:ALA:C	2.20	0.66
1:F:3:LEU:HD11	1:G:4:ILE:HD12	1.76	0.66
1:C:54:GLN:HG3	3:C:333:HOH:O	1.96	0.66
1:K:42[B]:ASN:ND2	1:L:33:GLY:HA3	2.10	0.66
1:L:95[A]:MET:SD	1:L:119:GLU:CG	2.82	0.66
1:B:99[A]:MET:CE	2:B:201:MPD:CM	2.73	0.66
1:C:95[B]:MET:SD	1:C:119:GLU:CG	2.83	0.65
1:G:173:ASN:ND2	3:G:301:HOH:O	2.28	0.65
1:L:173:ASN:ND2	3:L:301:HOH:O	2.28	0.65
1:H:42[B]:ASN:OD1	1:I:31[B]:MET:HE1	1.96	0.64
1:F:4:ILE:HD12	1:F:19:ASP:HB2	1.76	0.64
1:A:95[A]:MET:SD	1:A:119:GLU:CG	2.86	0.64
1:A:95[A]:MET:HE2	1:A:119:GLU:OE2	1.98	0.64
1:K:42[B]:ASN:ND2	1:L:33:GLY:O	2.29	0.64
1:B:71:VAL:HG22	1:B:99[A]:MET:HE3	1.80	0.63
1:D:173:ASN:ND2	3:D:301:HOH:O	2.31	0.63
1:L:93[B]:ILE:HG23	1:L:115:LEU:HD12	1.81	0.63
1:F:173:ASN:ND2	3:F:302:HOH:O	2.31	0.63
1:K:22:SER:HB3	1:L:6:THR:O	1.99	0.63
1:J:42[A]:ASN:ND2	1:K:33:GLY:HA3	2.14	0.62
1:H:42[B]:ASN:ND2	1:I:33:GLY:HA3	2.13	0.62
1:H:173:ASN:ND2	3:H:301:HOH:O	2.33	0.62
1:C:95[B]:MET:HE3	1:C:96:ALA:C	2.25	0.62
1:D:93:ILE:HG23	1:D:115:LEU:HD12	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:113:PHE:CD1	1:K:190:MET:HE3	2.34	0.62
1:B:95[B]:MET:HE3	1:B:96:ALA:C	2.25	0.61
1:J:93:ILE:HG23	1:J:115:LEU:HD12	1.81	0.61
1:K:4:ILE:CD1	1:K:20:ILE:HG22	2.31	0.61
1:M:91:ILE:CG2	1:M:93:ILE:HD11	2.30	0.61
2:B:201:MPD:O2	2:B:201:MPD:H53	2.01	0.61
1:B:190:MET:HE3	1:C:83:HIS:NE2	2.16	0.61
1:F:93:ILE:HG23	1:F:115:LEU:HD12	1.82	0.60
1:D:4:ILE:HG22	3:E:318:HOH:O	2.00	0.60
1:G:119:GLU:HG2	3:G:384:HOH:O	2.01	0.60
1:A:18:TYR:CD1	1:G:8:ILE:HD12	2.36	0.59
1:C:123:HIS:H	2:C:201:MPD:H11	1.68	0.59
1:K:4:ILE:CD1	1:K:21:TYR:CE2	2.80	0.59
1:B:98[B]:SER:HB3	2:B:201:MPD:C1	2.33	0.58
1:D:33:GLY:HA3	1:E:42:ASN:ND2	2.18	0.58
1:L:4:ILE:HB	1:L:5:PRO:HD3	1.85	0.58
1:L:95[A]:MET:HE3	1:L:96:ALA:O	2.03	0.58
1:J:163:GLU:HG3	1:J:167:LYS:HE2	1.85	0.58
1:K:4:ILE:HD12	1:K:21:TYR:CD2	2.30	0.58
1:M:42[A]:ASN:HD21	1:N:33:GLY:HA3	1.68	0.58
1:J:16:ARG:CD	1:K:8:ILE:HG21	2.33	0.58
1:N:156:GLU:HG3	1:N:157:ARG:N	2.19	0.57
1:A:42[A]:ASN:ND2	1:G:33:GLY:HA3	2.19	0.57
1:B:98[A]:SER:CB	2:B:201:MPD:H11	2.29	0.57
1:L:95[A]:MET:HE1	1:L:121:MET:CB	2.35	0.57
1:C:123:HIS:H	2:C:201:MPD:C1	2.17	0.56
1:C:95[B]:MET:HE3	1:C:96:ALA:O	2.05	0.56
1:B:15:GLU:C	1:B:16:ARG:HD3	2.30	0.56
1:K:145:LYS:HE3	3:K:423:HOH:O	2.06	0.56
1:L:123:HIS:H	2:L:201:MPD:C1	2.18	0.56
1:M:93:ILE:HD12	1:M:115:LEU:HG	1.86	0.55
1:A:42[B]:ASN:HB3	1:G:21:TYR:OH	2.06	0.55
1:B:95[B]:MET:HE3	1:B:96:ALA:O	2.05	0.55
1:D:119:GLU:HG2	3:D:350:HOH:O	2.05	0.55
1:F:85:LYS:NZ	3:F:301:HOH:O	2.22	0.55
1:L:98[A]:SER:HA	2:L:201:MPD:H12	1.89	0.55
1:A:7:VAL:O	1:A:18:TYR:N	2.40	0.55
1:M:93:ILE:HG23	1:M:115:LEU:CD1	2.25	0.55
1:C:95[B]:MET:SD	1:C:119:GLU:OE2	2.65	0.55
1:F:117:ASN:HD22	1:G:149:LYS:HD2	1.71	0.55
1:B:3:LEU:CD1	1:C:4:ILE:HD13	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:123:HIS:H	2:L:201:MPD:H11	1.72	0.54
1:B:33:GLY:O	1:C:42[B]:ASN:ND2	2.40	0.54
1:J:16:ARG:HD2	1:K:8:ILE:CG2	2.38	0.54
1:C:95[B]:MET:HE1	1:C:121:MET:CB	2.38	0.54
1:E:93:ILE:HG22	1:E:115[B]:LEU:HD23	1.91	0.53
1:N:95[B]:MET:HE1	1:N:119:GLU:HG2	1.89	0.53
1:B:95[B]:MET:SD	1:B:119:GLU:OE2	2.66	0.53
1:L:95[A]:MET:HE1	1:L:121:MET:HB2	1.90	0.53
1:N:95[B]:MET:CE	1:N:119:GLU:HG2	2.38	0.53
1:B:115:LEU:HD13	1:C:79:ASP:HB3	1.90	0.53
1:C:173:ASN:ND2	3:C:301:HOH:O	2.40	0.53
1:A:22:SER:HB3	1:G:6:THR:O	2.07	0.53
1:C:98[B]:SER:HA	2:C:201:MPD:H12	1.90	0.53
1:M:42[A]:ASN:ND2	1:N:33:GLY:HA3	2.23	0.53
1:L:95[A]:MET:SD	1:L:119:GLU:OE2	2.66	0.52
1:B:99[A]:MET:HE3	2:B:201:MPD:HM2	1.87	0.52
1:B:98[B]:SER:HA	2:B:201:MPD:H12	1.91	0.52
1:J:79:ASP:HB3	1:K:115:LEU:HD13	1.92	0.52
1:M:91:ILE:HG22	1:M:93:ILE:CD1	2.36	0.52
1:B:21:TYR:OH	1:C:42[A]:ASN:HB3	2.10	0.52
1:B:54:GLN:HG3	3:B:4112:HOH:O	2.11	0.51
1:C:95[B]:MET:HE1	1:C:121:MET:HB2	1.92	0.51
1:F:95:MET:HE3	3:G:318:HOH:O	2.10	0.51
1:B:98[A]:SER:CB	2:B:201:MPD:C1	2.87	0.51
1:J:42[A]:ASN:ND2	1:K:33:GLY:O	2.44	0.51
1:E:115[A]:LEU:HD13	1:F:79:ASP:HB3	1.93	0.51
1:K:4:ILE:HD11	1:K:20:ILE:HG22	1.93	0.51
1:M:42[A]:ASN:HB3	1:N:21:TYR:OH	2.11	0.51
1:F:3:LEU:CD1	1:G:4:ILE:HD13	2.41	0.50
1:L:98[B]:SER:HA	2:L:201:MPD:H12	1.92	0.50
1:B:98[A]:SER:HA	2:B:201:MPD:H12	1.93	0.50
1:F:152:ARG:NE	3:F:303:HOH:O	2.32	0.50
1:B:95[B]:MET:HE1	1:B:121:MET:CB	2.41	0.50
1:D:145:LYS:HD3	3:D:383:HOH:O	2.11	0.50
1:L:145:LYS:CE	3:L:311:HOH:O	2.59	0.49
1:M:92:CYS:C	1:M:93:ILE:HD13	2.38	0.49
1:H:21:TYR:OH	1:N:42[A]:ASN:HB3	2.13	0.49
1:M:117:ASN:ND2	3:M:303:HOH:O	2.45	0.49
1:C:98[A]:SER:HA	2:C:201:MPD:H12	1.94	0.49
1:C:156[B]:GLU:HG3	1:C:157:ARG:N	2.27	0.49
1:A:21:TYR:OH	1:B:42[A]:ASN:HB3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:119:GLU:HG2	3:J:406:HOH:O	2.12	0.49
1:N:97:ALA:C	1:N:98[A]:SER:OG	2.55	0.49
1:A:95[A]:MET:SD	1:A:119:GLU:OE2	2.70	0.48
1:B:99[A]:MET:HE2	2:B:201:MPD:HM2	1.90	0.48
1:F:3:LEU:HD11	1:G:4:ILE:CD1	2.37	0.48
1:A:93:ILE:HG13	1:A:93:ILE:O	2.13	0.48
1:B:15:GLU:CG	1:B:16:ARG:HD3	2.20	0.48
1:B:98[B]:SER:HA	2:B:201:MPD:C1	2.43	0.48
1:A:178:GLU:OE1	3:A:2101:HOH:O	2.20	0.48
1:E:173:ASN:ND2	3:E:305:HOH:O	2.47	0.48
1:G:93:ILE:HG13	1:G:93:ILE:O	2.14	0.48
1:K:4:ILE:HG12	1:K:19:ASP:HB2	1.96	0.48
1:C:93:ILE:HG13	1:C:93:ILE:O	2.14	0.48
1:M:119:GLU:HG2	3:M:369:HOH:O	2.12	0.48
1:B:95[B]:MET:HE1	1:B:121:MET:HB2	1.94	0.48
1:I:93:ILE:HG13	1:I:93:ILE:O	2.14	0.48
1:K:93:ILE:HG13	1:K:93:ILE:O	2.14	0.48
1:H:42[A]:ASN:HB3	1:I:21:TYR:OH	2.13	0.48
1:M:42[A]:ASN:HB3	1:N:21:TYR:HH	1.79	0.48
1:M:157:ARG:HD3	3:M:321:HOH:O	2.14	0.47
1:D:54:GLN:HG3	3:D:380:HOH:O	2.14	0.47
1:E:8:ILE:HD13	1:F:16:ARG:HB2	1.97	0.47
1:B:99[A]:MET:HE1	2:B:201:MPD:CM	2.44	0.47
1:K:22:SER:OG	1:L:6:THR:N	2.37	0.47
1:B:98[A]:SER:CA	2:B:201:MPD:H11	2.45	0.47
1:E:93:ILE:O	1:E:93:ILE:HG13	2.14	0.47
3:D:349:HOH:O	1:E:83:HIS:HD2	1.97	0.47
1:N:93:ILE:O	1:N:93:ILE:HG13	2.14	0.47
1:F:173:ASN:C	1:F:173:ASN:HD22	2.21	0.47
1:B:93:ILE:HG13	1:B:93:ILE:O	2.14	0.46
1:H:42[B]:ASN:CB	1:I:31[B]:MET:HE3	2.45	0.46
1:H:93:ILE:HG13	1:H:93:ILE:O	2.14	0.46
1:L:95[B]:MET:HE3	3:L:411:HOH:O	2.14	0.46
1:N:173:ASN:C	1:N:173:ASN:HD22	2.23	0.46
1:B:95[B]:MET:HE1	1:B:121:MET:N	2.30	0.46
1:L:115:LEU:HD21	1:L:190:MET:CE	2.45	0.46
1:K:119:GLU:HG2	3:K:398:HOH:O	2.14	0.46
1:C:109:LYS:CE	3:C:310:HOH:O	2.50	0.46
1:D:6:THR:O	1:E:22:SER:HB3	2.16	0.46
3:H:363:HOH:O	1:I:95:MET:HE3	2.16	0.46
1:L:95[A]:MET:HE1	1:L:121:MET:N	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:9:GLU:O	1:K:15:GLU:HA	2.15	0.46
1:K:173:ASN:C	1:K:173:ASN:HD22	2.23	0.46
1:A:115:LEU:HD21	1:A:190:MET:CE	2.45	0.46
1:B:98[B]:SER:CA	2:B:201:MPD:H11	2.46	0.46
1:E:34:SER:HA	3:F:308:HOH:O	2.15	0.46
1:I:119:GLU:HG2	3:I:409:HOH:O	2.15	0.46
1:B:20:ILE:HD12	1:B:21:TYR:N	2.31	0.45
1:B:115:LEU:HD21	1:B:190:MET:HE2	1.98	0.45
1:C:115:LEU:HD21	1:C:190:MET:CE	2.46	0.45
1:H:173:ASN:C	1:H:173:ASN:HD22	2.25	0.45
1:I:115:LEU:HD21	1:I:190:MET:CE	2.46	0.45
1:E:115[A]:LEU:HD21	1:E:190:MET:CE	2.47	0.45
1:I:173:ASN:ND2	3:I:302:HOH:O	2.48	0.45
1:M:115:LEU:HD21	1:M:190:MET:CE	2.46	0.45
1:A:33:GLY:O	1:B:42[B]:ASN:ND2	2.49	0.45
1:N:115:LEU:HD21	1:N:190:MET:CE	2.46	0.45
1:H:115:LEU:HD21	1:H:190:MET:CE	2.47	0.45
1:B:173:ASN:HD22	1:B:173:ASN:C	2.24	0.45
1:C:123:HIS:O	2:C:201:MPD:H11	2.17	0.45
1:L:3:LEU:C	1:L:4:ILE:O	2.57	0.45
1:C:95[B]:MET:HE1	1:C:121:MET:N	2.31	0.45
1:F:3:LEU:CD1	1:G:4:ILE:HD12	2.38	0.45
1:N:97:ALA:C	1:N:98[A]:SER:HG	2.24	0.45
1:B:15:GLU:O	1:B:16:ARG:CD	2.65	0.45
1:D:115:LEU:HD21	1:D:190:MET:CE	2.47	0.44
1:H:42[B]:ASN:ND2	1:I:33:GLY:O	2.50	0.44
1:B:98[A]:SER:HA	2:B:201:MPD:C1	2.47	0.44
1:E:173:ASN:C	1:E:173:ASN:HD22	2.25	0.44
1:A:95[B]:MET:HE2	1:A:97:ALA:CB	2.44	0.44
1:E:109:LYS:CE	3:E:330:HOH:O	2.67	0.43
1:F:8:ILE:HD12	1:G:18:TYR:CZ	2.53	0.43
1:J:117:ASN:ND2	3:J:304:HOH:O	2.51	0.43
1:K:95:MET:HG3	3:K:398:HOH:O	2.17	0.43
1:E:109:LYS:HE3	3:E:330:HOH:O	2.18	0.43
1:D:33:GLY:O	1:E:42:ASN:ND2	2.50	0.43
1:M:79:ASP:HB3	1:N:115:LEU:HD13	1.99	0.43
1:N:95[B]:MET:SD	1:N:119:GLU:OE2	2.76	0.43
1:B:3:LEU:HD23	1:B:4:ILE:N	2.33	0.43
1:G:20:ILE:HG23	1:G:21:TYR:N	2.33	0.43
1:G:54:GLN:HB3	3:G:442:HOH:O	2.19	0.43
1:L:173:ASN:HD22	1:L:173:ASN:C	2.25	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:115:LEU:HD21	1:F:190:MET:CE	2.48	0.42
1:G:31[A]:MET:HE2	1:G:63:ALA:O	2.19	0.42
1:H:20:ILE:H	1:H:20:ILE:HG13	1.66	0.42
1:N:107:GLY:O	1:N:157:ARG:NH2	2.52	0.42
1:B:15:GLU:O	1:B:16:ARG:HD2	2.19	0.42
1:H:22:SER:HB3	1:I:6:THR:O	2.18	0.42
1:J:173:ASN:C	1:J:173:ASN:HD22	2.26	0.42
1:C:20:ILE:HG23	1:C:21:TYR:N	2.33	0.42
1:G:115:LEU:HD21	1:G:190:MET:CE	2.49	0.42
1:I:42:ASN:ND2	1:J:33:GLY:HA3	2.34	0.42
1:L:83:HIS:HD2	3:M:336:HOH:O	2.02	0.42
1:N:95[B]:MET:HE3	1:N:119:GLU:O	2.19	0.42
1:A:7:VAL:HG22	1:B:18:TYR:CE1	2.55	0.42
1:G:173:ASN:C	1:G:173:ASN:HD22	2.26	0.42
1:E:93:ILE:HG22	1:E:115[B]:LEU:CD2	2.50	0.42
3:C:323:HOH:O	1:D:83:HIS:HD2	2.02	0.42
1:L:4:ILE:CB	1:L:5:PRO:HD3	2.49	0.42
1:A:6:THR:O	1:A:6:THR:HG22	2.16	0.42
1:F:31[A]:MET:HE2	1:F:63:ALA:O	2.19	0.42
1:H:20:ILE:HD12	1:H:21:TYR:N	2.34	0.42
3:K:338:HOH:O	1:L:95[B]:MET:HE1	2.19	0.42
1:H:42[B]:ASN:CG	1:I:31[B]:MET:HE1	2.45	0.41
1:G:109:LYS:HE3	3:G:344:HOH:O	2.20	0.41
1:J:115:LEU:HD21	1:J:190:MET:CE	2.50	0.41
1:A:132:GLN:NE2	3:A:2105:HOH:O	2.54	0.41
1:F:4:ILE:HD11	1:F:19:ASP:HB3	1.97	0.41
1:H:42[B]:ASN:CG	1:I:31[B]:MET:CE	2.93	0.41
1:K:42[B]:ASN:ND2	1:L:33:GLY:CA	2.80	0.41
1:C:166:GLN:HA	1:C:166:GLN:HE21	1.86	0.41
1:J:95:MET:HG3	3:J:406:HOH:O	2.21	0.41
1:N:153:ILE:O	1:N:157:ARG:HG2	2.20	0.41
1:D:4:ILE:CG2	3:E:318:HOH:O	2.65	0.41
1:G:109:LYS:CE	3:G:344:HOH:O	2.69	0.41
1:I:109:LYS:HE3	3:I:310:HOH:O	2.21	0.41
1:A:173:ASN:C	1:A:173:ASN:HD22	2.29	0.41
1:B:15:GLU:C	1:B:16:ARG:CD	2.94	0.41
1:M:173:ASN:C	1:M:173:ASN:HD22	2.26	0.41
1:N:123:HIS:CD2	1:N:123:HIS:C	2.99	0.41
1:A:149:LYS:HD2	1:G:117:ASN:HD22	1.86	0.41
1:L:76:ALA:HA	1:M:93:ILE:HG22	2.02	0.41
1:K:83:HIS:HD2	3:L:329:HOH:O	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:123:HIS:O	2:L:201:MPD:H11	2.22	0.40
3:A:2182:HOH:O	1:G:95:MET:HE3	2.20	0.40
1:M:93:ILE:CD1	1:M:115:LEU:HD12	2.40	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	179/195 (92%)	176 (98%)	3 (2%)	0	100	100
1	B	187/195 (96%)	183 (98%)	4 (2%)	0	100	100
1	C	184/195 (94%)	182 (99%)	2 (1%)	0	100	100
1	D	179/195 (92%)	176 (98%)	2 (1%)	1 (1%)	21	8
1	E	188/195 (96%)	186 (99%)	2 (1%)	0	100	100
1	F	185/195 (95%)	181 (98%)	4 (2%)	0	100	100
1	G	185/195 (95%)	183 (99%)	2 (1%)	0	100	100
1	H	178/195 (91%)	174 (98%)	4 (2%)	0	100	100
1	I	177/195 (91%)	175 (99%)	2 (1%)	0	100	100
1	J	184/195 (94%)	180 (98%)	4 (2%)	0	100	100
1	K	186/195 (95%)	182 (98%)	4 (2%)	0	100	100
1	L	181/195 (93%)	178 (98%)	2 (1%)	1 (1%)	21	8
1	M	180/195 (92%)	178 (99%)	2 (1%)	0	100	100
1	N	180/195 (92%)	178 (99%)	2 (1%)	0	100	100
All	All	2553/2730 (94%)	2512 (98%)	39 (2%)	2 (0%)	48	32

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	4	ILE
1	D	4	ILE

5.3.2 Protein sidechains ⓘ

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	152/162 (94%)	149 (98%)	3 (2%)	48	29
1	B	159/162 (98%)	149 (94%)	10 (6%)	16	3
1	C	156/162 (96%)	151 (97%)	5 (3%)	34	14
1	D	151/162 (93%)	145 (96%)	6 (4%)	28	9
1	E	160/162 (99%)	156 (98%)	4 (2%)	42	22
1	F	157/162 (97%)	147 (94%)	10 (6%)	16	3
1	G	157/162 (97%)	149 (95%)	8 (5%)	21	5
1	H	151/162 (93%)	145 (96%)	6 (4%)	28	9
1	I	150/162 (93%)	146 (97%)	4 (3%)	39	19
1	J	156/162 (96%)	151 (97%)	5 (3%)	34	14
1	K	158/162 (98%)	151 (96%)	7 (4%)	25	7
1	L	153/162 (94%)	149 (97%)	4 (3%)	40	20
1	M	153/162 (94%)	146 (95%)	7 (5%)	24	6
1	N	153/162 (94%)	147 (96%)	6 (4%)	28	9
All	All	2166/2268 (96%)	2081 (96%)	85 (4%)	30	9

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	ILE
1	A	35	GLN
1	A	166	GLN
1	B	3	LEU
1	B	9	GLU
1	B	15	GLU

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Mol	Chain	Res	Type
1	B	16	ARG
1	B	20	ILE
1	B	95[A]	MET
1	B	95[B]	MET
1	B	154	LEU
1	B	166	GLN
1	B	175	LEU
1	C	95[A]	MET
1	C	95[B]	MET
1	C	109	LYS
1	C	154	LEU
1	C	166	GLN
1	D	4	ILE
1	D	6	THR
1	D	95	MET
1	D	154	LEU
1	D	166	GLN
1	D	175	LEU
1	E	3	LEU
1	E	95[A]	MET
1	E	95[B]	MET
1	E	166	GLN
1	F	4	ILE
1	F	9	GLU
1	F	15	GLU
1	F	16	ARG
1	F	31[A]	MET
1	F	31[B]	MET
1	F	95	MET
1	F	154	LEU
1	F	166	GLN
1	F	175	LEU
1	G	9	GLU
1	G	16	ARG
1	G	31[A]	MET
1	G	31[B]	MET
1	G	95	MET
1	G	154	LEU
1	G	166	GLN
1	G	175	LEU
1	H	20	ILE
1	H	23	ARG

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Mol	Chain	Res	Type
1	H	95	MET
1	H	154	LEU
1	H	166	GLN
1	H	175	LEU
1	I	20	ILE
1	I	95	MET
1	I	154	LEU
1	I	166	GLN
1	J	9	GLU
1	J	95	MET
1	J	109	LYS
1	J	154	LEU
1	J	166	GLN
1	K	4	ILE
1	K	9	GLU
1	K	95	MET
1	K	154	LEU
1	K	166	GLN
1	K	175	LEU
1	K	193	GLU
1	L	4	ILE
1	L	44	ILE
1	L	109	LYS
1	L	166	GLN
1	M	20	ILE
1	M	95	MET
1	M	154	LEU
1	M	166	GLN
1	M	175[A]	LEU
1	M	175[B]	LEU
1	M	193	GLU
1	N	20	ILE
1	N	95[A]	MET
1	N	95[B]	MET
1	N	154	LEU
1	N	156	GLU
1	N	166	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (101) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	ASN

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Mol	Chain	Res	Type
1	A	82	GLN
1	A	89	GLN
1	A	117	ASN
1	A	160	GLN
1	A	173	ASN
1	B	39	ASN
1	B	82	GLN
1	B	83	HIS
1	B	89	GLN
1	B	117	ASN
1	B	151	ASN
1	B	160	GLN
1	B	166	GLN
1	B	173	ASN
1	C	65	ASN
1	C	82	GLN
1	C	89	GLN
1	C	117	ASN
1	C	160	GLN
1	C	166	GLN
1	C	173	ASN
1	D	39	ASN
1	D	42	ASN
1	D	65	ASN
1	D	82	GLN
1	D	83	HIS
1	D	89	GLN
1	D	160	GLN
1	D	173	ASN
1	E	42	ASN
1	E	82	GLN
1	E	83	HIS
1	E	89	GLN
1	E	160	GLN
1	E	166	GLN
1	E	173	ASN
1	F	82	GLN
1	F	83	HIS
1	F	117	ASN
1	F	160	GLN
1	F	173	ASN
1	G	39	ASN

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Mol	Chain	Res	Type
1	G	54	GLN
1	G	65	ASN
1	G	82	GLN
1	G	83	HIS
1	G	89	GLN
1	G	117	ASN
1	G	151	ASN
1	G	160	GLN
1	G	166	GLN
1	G	173	ASN
1	H	82	GLN
1	H	83	HIS
1	H	89	GLN
1	H	160	GLN
1	H	173	ASN
1	I	39	ASN
1	I	42	ASN
1	I	82	GLN
1	I	83	HIS
1	I	89	GLN
1	I	160	GLN
1	I	173	ASN
1	J	35	GLN
1	J	39	ASN
1	J	65	ASN
1	J	82	GLN
1	J	83	HIS
1	J	89	GLN
1	J	173	ASN
1	K	82	GLN
1	K	83	HIS
1	K	117	ASN
1	K	160	GLN
1	K	173	ASN
1	L	39	ASN
1	L	42	ASN
1	L	82	GLN
1	L	83	HIS
1	L	89	GLN
1	L	117	ASN
1	L	151	ASN
1	L	160	GLN

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Mol	Chain	Res	Type
1	L	166	GLN
1	L	173	ASN
1	M	39	ASN
1	M	65	ASN
1	M	82	GLN
1	M	89	GLN
1	M	117	ASN
1	M	160	GLN
1	M	173	ASN
1	N	39	ASN
1	N	82	GLN
1	N	83	HIS
1	N	89	GLN
1	N	117	ASN
1	N	160	GLN
1	N	173	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

14 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	L	201	-	7,7,7	0.34	0	9,10,10	0.87	0
2	MPD	J	201	-	7,7,7	0.36	0	9,10,10	0.94	0
2	MPD	H	201	-	7,7,7	0.21	0	9,10,10	0.69	0
2	MPD	I	201	-	7,7,7	0.32	0	9,10,10	0.79	0
2	MPD	B	201	-	7,7,7	0.44	0	9,10,10	1.26	1 (11%)
2	MPD	K	201	-	7,7,7	0.33	0	9,10,10	0.65	0
2	MPD	C	201	-	7,7,7	0.38	0	9,10,10	0.75	0
2	MPD	F	201	-	7,7,7	0.42	0	9,10,10	0.83	0
2	MPD	D	201	-	7,7,7	0.22	0	9,10,10	0.44	0
2	MPD	N	201	-	7,7,7	0.30	0	9,10,10	0.58	0
2	MPD	G	201	-	7,7,7	0.32	0	9,10,10	0.56	0
2	MPD	A	2001	-	7,7,7	0.30	0	9,10,10	0.67	0
2	MPD	E	201	-	7,7,7	0.21	0	9,10,10	0.51	0
2	MPD	M	201	-	7,7,7	0.21	0	9,10,10	0.61	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	L	201	-	-	1/5/5/5	-
2	MPD	J	201	-	-	0/5/5/5	-
2	MPD	H	201	-	-	0/5/5/5	-
2	MPD	I	201	-	-	0/5/5/5	-
2	MPD	B	201	-	-	1/5/5/5	-
2	MPD	K	201	-	-	0/5/5/5	-
2	MPD	C	201	-	-	1/5/5/5	-
2	MPD	F	201	-	-	0/5/5/5	-
2	MPD	D	201	-	-	0/5/5/5	-
2	MPD	N	201	-	-	0/5/5/5	-
2	MPD	G	201	-	-	0/5/5/5	-
2	MPD	A	2001	-	-	0/5/5/5	-
2	MPD	E	201	-	-	0/5/5/5	-
2	MPD	M	201	-	-	0/5/5/5	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	201	MPD	CM-C2-C1	-2.89	104.16	110.63

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	201	MPD	C2-C3-C4-C5
2	C	201	MPD	O2-C2-C3-C4
2	L	201	MPD	O2-C2-C3-C4

There are no ring outliers.

3 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L	201	MPD	5	0
2	B	201	MPD	19	0
2	C	201	MPD	5	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, 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	179/195 (91%)	0.39	12 (6%)	24	28	11, 20, 43, 97	4 (2%)
1	B	187/195 (95%)	0.78	18 (9%)	13	16	16, 28, 47, 88	4 (2%)
1	C	182/195 (93%)	0.79	18 (9%)	13	15	16, 27, 45, 90	6 (3%)
1	D	180/195 (92%)	0.72	14 (7%)	19	22	15, 27, 44, 84	3 (1%)
1	E	186/195 (95%)	0.37	14 (7%)	20	23	10, 21, 41, 64	6 (3%)
1	F	186/195 (95%)	0.16	12 (6%)	25	29	11, 17, 39, 83	3 (1%)
1	G	186/195 (95%)	0.32	18 (9%)	13	15	9, 19, 43, 80	3 (1%)
1	H	179/195 (91%)	0.79	15 (8%)	17	20	16, 28, 49, 78	3 (1%)
1	I	179/195 (91%)	0.32	10 (5%)	30	34	13, 21, 39, 61	2 (1%)
1	J	185/195 (94%)	0.12	13 (7%)	22	26	11, 18, 39, 91	3 (1%)
1	K	186/195 (95%)	0.15	14 (7%)	20	23	11, 18, 38, 65	4 (2%)
1	L	182/195 (93%)	0.44	10 (5%)	30	35	13, 22, 42, 65	3 (1%)
1	M	180/195 (92%)	0.79	14 (7%)	19	22	16, 29, 46, 75	4 (2%)
1	N	181/195 (92%)	1.18	33 (18%)	3	4	17, 31, 50, 80	3 (1%)
All	All	2558/2730 (93%)	0.52	215 (8%)	17	20	9, 24, 47, 97	51 (1%)

All (215) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	7	VAL	11.7
1	L	4	ILE	9.4
1	A	8	ILE	9.1
1	D	4	ILE	8.5
1	K	3	LEU	8.1
1	G	17	ALA	8.0
1	D	6	THR	7.9
1	A	6	THR	7.7

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Mol	Chain	Res	Type	RSRZ
1	A	5	PRO	7.4
1	F	3	LEU	7.2
1	N	8	ILE	7.0
1	I	7	VAL	6.9
1	E	3	LEU	6.7
1	C	7	VAL	6.6
1	D	3	LEU	6.6
1	A	18	TYR	6.6
1	H	6	THR	6.5
1	L	6	THR	6.4
1	L	3	LEU	6.3
1	D	18	TYR	6.2
1	I	4	ILE	6.2
1	L	17	ALA	6.1
1	G	8	ILE	6.1
1	J	17	ALA	6.1
1	F	9	GLU	6.0
1	C	3	LEU	5.8
1	H	18	TYR	5.8
1	M	93	ILE	5.8
1	L	18	TYR	5.8
1	G	6	THR	5.8
1	B	3	LEU	5.7
1	B	193	GLU	5.5
1	H	4	ILE	5.4
1	H	7	VAL	5.3
1	B	8	ILE	5.3
1	M	7	VAL	5.1
1	I	18	TYR	5.0
1	L	5	PRO	5.0
1	E	8	ILE	5.0
1	B	17	ALA	4.9
1	F	8	ILE	4.9
1	M	4	ILE	4.9
1	D	5	PRO	4.8
1	J	10	THR	4.8
1	E	17	ALA	4.8
1	N	4	ILE	4.8
1	D	17	ALA	4.7
1	F	4	ILE	4.7
1	K	4	ILE	4.6
1	J	191	VAL	4.5

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Mol	Chain	Res	Type	RSRZ
1	M	18	TYR	4.5
1	G	18	TYR	4.5
1	L	7	VAL	4.4
1	J	8	ILE	4.4
1	B	10	THR	4.3
1	H	57	GLU	4.3
1	A	191	VAL	4.3
1	F	7	VAL	4.3
1	G	7	VAL	4.3
1	G	4	ILE	4.3
1	E	194	THR	4.3
1	C	17	ALA	4.2
1	N	7	VAL	4.2
1	I	6	THR	4.1
1	G	10	THR	4.0
1	F	16	ARG	4.0
1	G	9	GLU	4.0
1	J	9	GLU	3.9
1	F	15	GLU	3.9
1	B	20	ILE	3.9
1	C	4	ILE	3.9
1	K	15	GLU	3.8
1	M	191	VAL	3.8
1	N	18	TYR	3.8
1	E	32	LEU	3.8
1	N	162	ILE	3.7
1	F	191	VAL	3.7
1	K	8	ILE	3.7
1	B	16	ARG	3.7
1	E	4	ILE	3.7
1	E	9	GLU	3.7
1	K	193	GLU	3.7
1	F	17	ALA	3.7
1	C	191	VAL	3.6
1	N	191	VAL	3.6
1	B	18	TYR	3.6
1	E	18	TYR	3.6
1	B	4	ILE	3.6
1	G	16	ARG	3.6
1	K	9	GLU	3.6
1	N	156	GLU	3.5
1	C	57	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
1	G	11	THR	3.5
1	C	18	TYR	3.5
1	F	130	GLN	3.4
1	I	191	VAL	3.4
1	F	193	GLU	3.3
1	M	20	ILE	3.3
1	C	130	GLN	3.2
1	L	19	ASP	3.2
1	C	95[A]	MET	3.2
1	F	18	TYR	3.2
1	K	130	GLN	3.2
1	N	54	GLN	3.2
1	B	15	GLU	3.2
1	B	191	VAL	3.2
1	H	20	ILE	3.1
1	J	15	GLU	3.1
1	K	18	TYR	3.1
1	M	31[A]	MET	3.1
1	N	95[A]	MET	3.1
1	N	130	GLN	3.1
1	G	191	VAL	3.0
1	N	159	GLY	3.0
1	H	167	LYS	3.0
1	H	5	PRO	3.0
1	D	191	VAL	2.9
1	H	191	VAL	2.9
1	N	155	SER	2.9
1	H	182	GLU	2.9
1	G	130	GLN	2.9
1	B	57	GLU	2.9
1	I	5	PRO	2.9
1	G	54	GLN	2.8
1	H	130	GLN	2.8
1	E	193	GLU	2.8
1	J	130	GLN	2.8
1	A	19	ASP	2.8
1	E	16	ARG	2.8
1	J	16	ARG	2.8
1	M	54	GLN	2.8
1	L	130	GLN	2.8
1	I	19	ASP	2.8
1	E	119	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	N	182	GLU	2.7
1	B	130	GLN	2.7
1	N	6	THR	2.7
1	G	15	GLU	2.7
1	D	130	GLN	2.7
1	E	130	GLN	2.7
1	J	4	ILE	2.7
1	C	19	ASP	2.7
1	M	193	GLU	2.6
1	H	95	MET	2.6
1	C	93	ILE	2.6
1	M	162	ILE	2.6
1	N	85	LYS	2.6
1	N	31	MET	2.6
1	N	189	VAL	2.6
1	N	20	ILE	2.6
1	I	130	GLN	2.5
1	D	109	LYS	2.5
1	E	35	GLN	2.5
1	K	16	ARG	2.5
1	A	130	GLN	2.5
1	A	20	ILE	2.5
1	B	9	GLU	2.5
1	N	57	GLU	2.5
1	J	192	PRO	2.5
1	B	109	LYS	2.4
1	N	109	LYS	2.4
1	C	31[A]	MET	2.4
1	C	6	THR	2.4
1	C	20	ILE	2.4
1	M	29	ILE	2.4
1	A	192	PRO	2.4
1	D	22	SER	2.4
1	I	20	ILE	2.4
1	K	7	VAL	2.4
1	B	19	ASP	2.4
1	N	58	LYS	2.4
1	H	190	MET	2.4
1	M	110	GLY	2.4
1	N	154	LEU	2.4
1	D	53	ALA	2.4
1	C	16	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	I	95	MET	2.3
1	J	93	ILE	2.3
1	A	22	SER	2.3
1	N	192	PRO	2.3
1	B	7	VAL	2.3
1	E	7	VAL	2.3
1	N	152	ARG	2.3
1	G	192	PRO	2.2
1	H	23	ARG	2.2
1	B	95[A]	MET	2.2
1	H	192	PRO	2.2
1	K	17	ALA	2.2
1	J	6	THR	2.2
1	N	42[A]	ASN	2.2
1	M	130	GLN	2.2
1	N	188	GLU	2.2
1	A	32	LEU	2.2
1	J	18	TYR	2.2
1	C	5	PRO	2.2
1	N	51	LEU	2.1
1	C	167	LYS	2.1
1	N	56	SER	2.1
1	G	93	ILE	2.1
1	N	175	LEU	2.1
1	D	190	MET	2.1
1	C	54	GLN	2.1
1	D	19	ASP	2.1
1	N	21	TYR	2.1
1	M	184	GLY	2.1
1	N	119	GLU	2.1
1	G	35	GLN	2.1
1	L	55	ASP	2.1
1	D	192	PRO	2.1
1	N	93	ILE	2.1
1	N	193	GLU	2.0
1	K	19	ASP	2.0
1	K	191	VAL	2.0
1	G	109	LYS	2.0
1	K	109	LYS	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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
2	MPD	B	201	8/8	0.69	0.16	25,27,28,29	0
2	MPD	D	201	8/8	0.83	0.15	33,34,38,39	0
2	MPD	C	201	8/8	0.86	0.14	32,35,38,42	0
2	MPD	L	201	8/8	0.86	0.13	23,29,33,34	0
2	MPD	E	201	8/8	0.87	0.12	27,31,33,34	0
2	MPD	A	2001	8/8	0.87	0.13	28,30,34,35	0
2	MPD	N	201	8/8	0.87	0.13	33,37,41,41	0
2	MPD	I	201	8/8	0.88	0.12	25,28,30,30	0
2	MPD	F	201	8/8	0.89	0.10	22,24,26,27	0
2	MPD	M	201	8/8	0.90	0.12	33,35,38,41	0
2	MPD	J	201	8/8	0.91	0.11	22,25,28,30	0
2	MPD	H	201	8/8	0.92	0.11	31,34,36,38	0
2	MPD	K	201	8/8	0.93	0.09	26,28,29,31	0
2	MPD	G	201	8/8	0.94	0.09	25,27,28,31	0

6.5 Other polymers [i](#)

There are no such residues in this entry.