Full wwPDB X-ray Structure Validation Report (i)

Jan 4, 2024 – 09:52 pm GMT

PDB ID	:	5L5B
Title	:	Yeast 20S proteasome with human beta5i (1-138) and human beta6 (97-111; 118-133)
Authors	:	Groll, M.; Huber, E.M.
Deposited on	:	2016-05-28
Resolution	:	2.80 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:

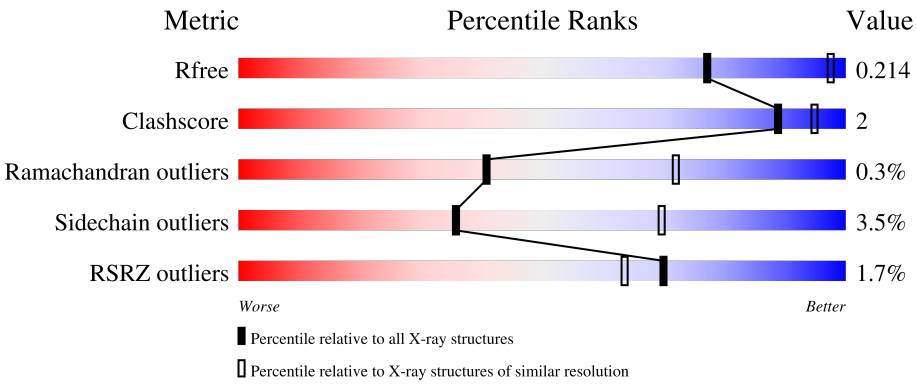
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	250	3%, 98%, •
1	O	250	2%, 98%, •
2	B	258	3%, 87%, 7%, • 5%
2	P	258	3%, 86%, 7%, • 5%
3	C	254	5%, 87%, 6%, • 6%

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Mol	Chain	Length	Quality of chain
3	Q	254	7% 86% 7% 6%
4	D	260	85% 5% 10%
4	R	260	2% 85% 5% 10%
5	E	234	93% 6%
5	S	234	% 93% 6%
6	F	288	% 80% 16%
6	T	288	% 80% 16%
7	G	252	% 89% 6%
7	U	252	2% 90% 5%
8	H	232	3% 91% 6%
8	V	232	3% 90% 6%
9	I	205	94% 6%
9	W	205	% 93% 6%
10	J	198	2% 86% 10%
10	X	198	% 88% 8%
11	K	211	88% 11%
11	Y	211	85% 13%
12	L	222	94% 6%
12	Z	222	94% 5%
13	M	246	89% 6% 5%
13	a	246	92% 5%
14	N	196	% 95% 5%
14	b	196	% 97%

2 Entry composition (i)

There are 17 unique types of molecules in this entry. The entry contains 49660 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 Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	250	1915	1219	315	377	4	0	0	0
1	O	250	1915	1219	315	377	4	0	0	0

- Molecule 2 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	244	1904	1201	321	379	3	0	0	0
2	P	244	1904	1201	321	379	3	0	0	0

- Molecule 3 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	240	1881	1176	329	372	4	0	0	0
3	Q	240	1881	1176	329	372	4	0	0	0

- Molecule 4 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	235	1813	1136	304	366	7	0	0	0
4	R	235	1813	1136	304	366	7	0	0	0

- Molecule 5 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	231	1773	1114	307	348	4	0	0	0
5	S	231	1773	1114	307	348	4	0	0	0

- Molecule 6 is a protein called Probable proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	F	243	1892	1203	329	356	4	0	0	0
6	T	243	1892	1203	329	356	4	0	0	0

- Molecule 7 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	G	241	1907	1214	320	365	8	0	0	0
7	U	241	1907	1214	320	365	8	0	0	0

- Molecule 8 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	H	226	1719	1082	298	332	7	0	0	0
8	V	226	1719	1082	298	332	7	0	0	0

- Molecule 9 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
9	I	204	1581	1010	258	305	8	0	0	0
9	W	204	1581	1010	258	305	8	0	0	0

- Molecule 10 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	J	195	1561	992	264	299	6	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	X	195	1561	992	264	299	6	0	0	0

- Molecule 11 is a protein called Proteasome subunit beta type-8,Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	K	211	1640	1035	282	311	12	0	0	0
11	Y	211	1640	1035	282	311	12	0	0	0

- Molecule 12 is a protein called Proteasome subunit beta type-6,Proteasome subunit beta type-1,Proteasome subunit beta type-6,Proteasome subunit beta type-1,Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	L	222	1764	1119	305	336	4	0	0	0
12	Z	222	1764	1119	305	336	4	0	0	0

- Molecule 13 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	M	233	1824	1154	312	351	7	0	0	0
13	a	233	1835	1160	316	352	7	0	1	0

- Molecule 14 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
14	N	196	1512	955	250	300	7	0	0	0
14	b	196	1512	955	250	300	7	0	0	0

- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	G	1	Total Mg 1 1	0	0
15	H	1	Total Mg 1 1	0	0
15	I	2	Total Mg 2 2	0	0
15	J	1	Total Mg 1 1	0	0
15	K	1	Total Mg 1 1	0	0
15	L	1	Total Mg 1 1	0	0
15	N	1	Total Mg 1 1	0	0
15	Z	1	Total Mg 1 1	0	0

- Molecule 16 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	G	2	Total Cl 2 2	0	0
16	U	2	Total Cl 2 2	0	0

- Molecule 17 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	5	Total O 5 5	0	0
17	B	6	Total O 6 6	0	0
17	C	7	Total O 7 7	0	0
17	D	6	Total O 6 6	0	0
17	E	6	Total O 6 6	0	0
17	F	6	Total O 6 6	0	0
17	G	11	Total O 11 11	0	0
17	H	12	Total O 12 12	0	0

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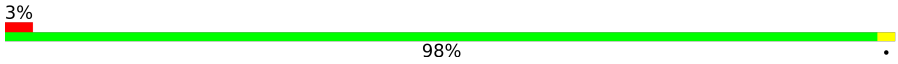
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	I	13	Total O 13 13	0	0
17	J	14	Total O 14 14	0	0
17	K	8	Total O 8 8	0	0
17	L	8	Total O 8 8	0	0
17	M	16	Total O 16 16	0	0
17	N	12	Total O 12 12	0	0
17	O	7	Total O 7 7	0	0
17	P	10	Total O 10 10	0	0
17	Q	9	Total O 9 9	0	0
17	R	5	Total O 5 5	0	0
17	S	7	Total O 7 7	0	0
17	T	4	Total O 4 4	0	0
17	U	16	Total O 16 16	0	0
17	V	10	Total O 10 10	0	0
17	W	13	Total O 13 13	0	0
17	X	7	Total O 7 7	0	0
17	Y	7	Total O 7 7	0	0
17	Z	7	Total O 7 7	0	0
17	a	21	Total O 21 21	0	0
17	b	11	Total O 11 11	0	0

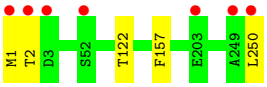
3 Residue-property plots (i)

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: Proteasome subunit alpha type-2

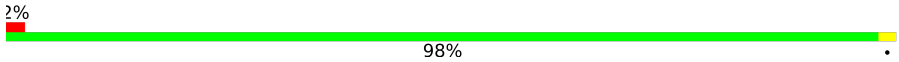
Chain A:





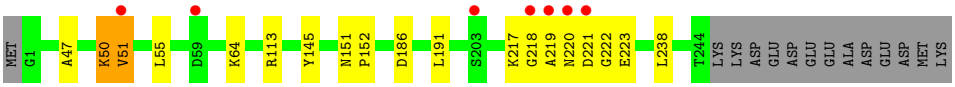
• Molecule 1: Proteasome subunit alpha type-2

Chain O:



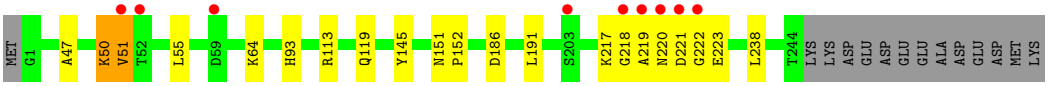
• Molecule 2: Proteasome subunit alpha type-3

Chain B:



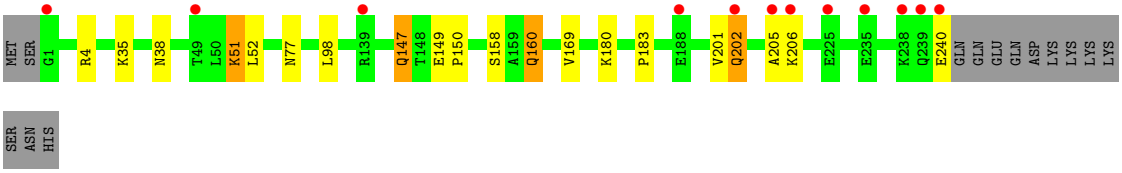
• Molecule 2: Proteasome subunit alpha type-3

Chain P:



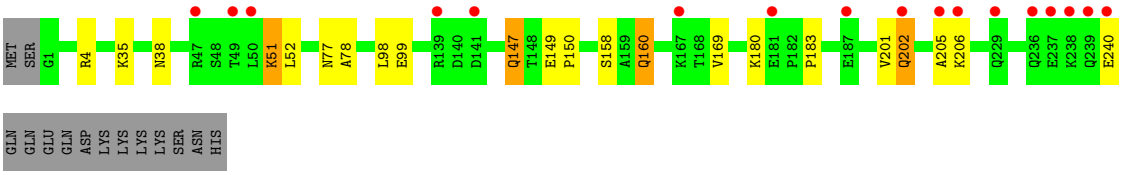
• Molecule 3: Proteasome subunit alpha type-4

Chain C:



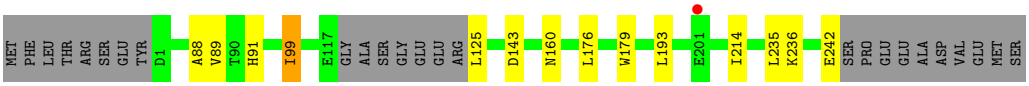
• Molecule 3: Proteasome subunit alpha type-4

Chain Q:



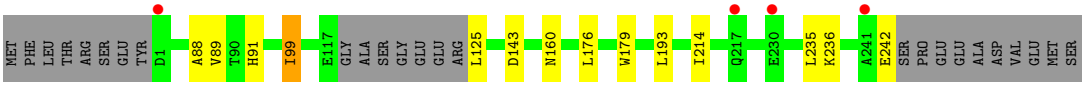
• Molecule 4: Proteasome subunit alpha type-5

Chain D:



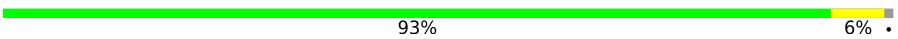
• Molecule 4: Proteasome subunit alpha type-5

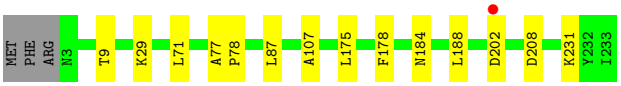
Chain R:



• Molecule 5: Proteasome subunit alpha type-6

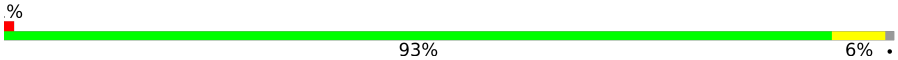
Chain E:

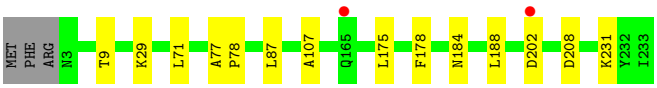




• Molecule 5: Proteasome subunit alpha type-6

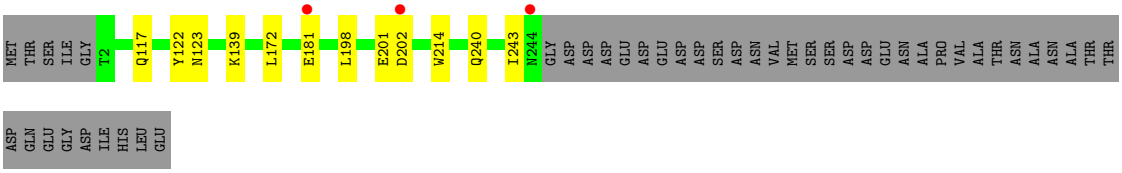
Chain S:





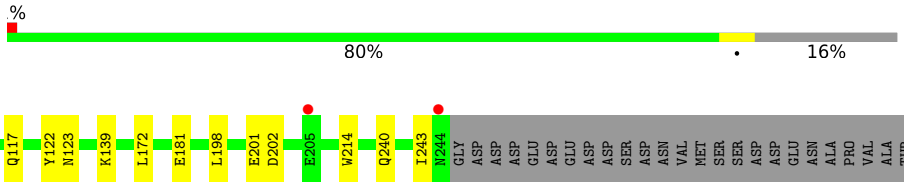
• Molecule 6: Probable proteasome subunit alpha type-7

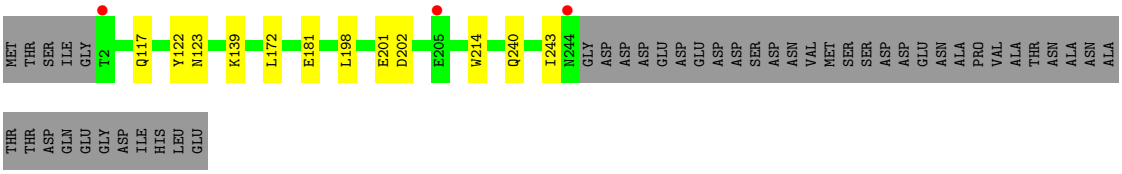
Chain F:



• Molecule 6: Probable proteasome subunit alpha type-7

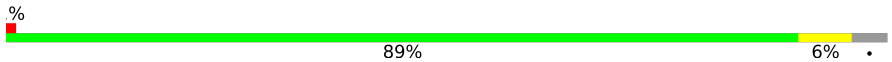
Chain T:





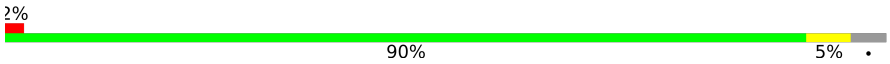
• Molecule 7: Proteasome subunit alpha type-1

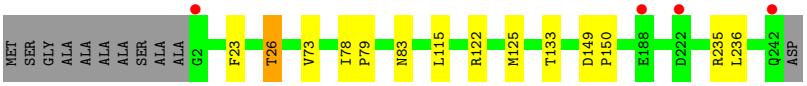
Chain G:



• Molecule 7: Proteasome subunit alpha type-1

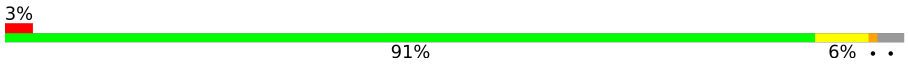
Chain U:





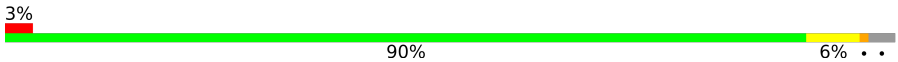
• Molecule 8: Proteasome subunit beta type-2

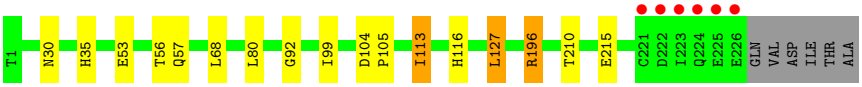
Chain H:



• Molecule 8: Proteasome subunit beta type-2

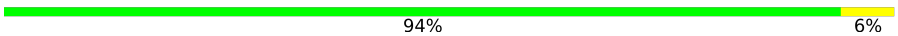
Chain V:





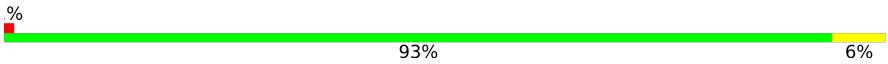
• Molecule 9: Proteasome subunit beta type-3

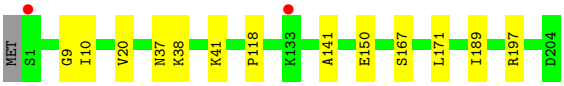
Chain I:



• Molecule 9: Proteasome subunit beta type-3

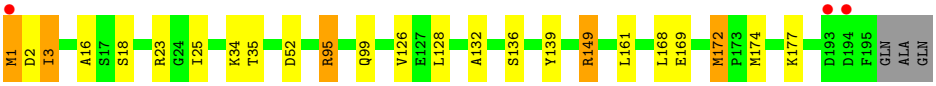
Chain W:





• Molecule 10: Proteasome subunit beta type-4

Chain J:



• Molecule 10: Proteasome subunit beta type-4

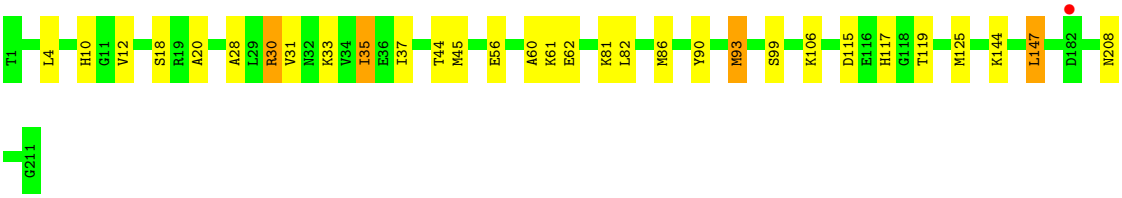
Chain X:

• Molecule 11: Proteasome subunit beta type-8,Proteasome subunit beta type-5

Chain K:

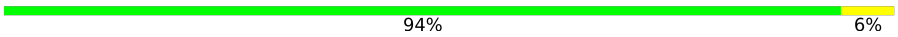
• Molecule 11: Proteasome subunit beta type-8,Proteasome subunit beta type-5

Chain Y:



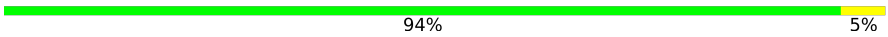
• Molecule 12: Proteasome subunit beta type-6,Proteasome subunit beta type-1,Proteasome subunit beta type-6,Proteasome subunit beta type-1,Proteasome subunit beta type-6

Chain L:



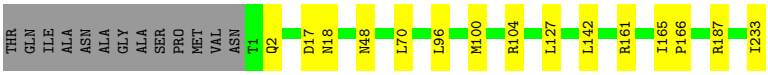
• Molecule 12: Proteasome subunit beta type-6,Proteasome subunit beta type-1,Proteasome subunit beta type-6,Proteasome subunit beta type-1,Proteasome subunit beta type-6

Chain Z:



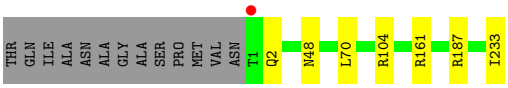
• Molecule 13: Proteasome subunit beta type-7

Chain M:



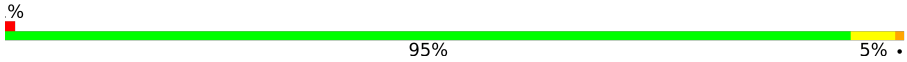
• Molecule 13: Proteasome subunit beta type-7

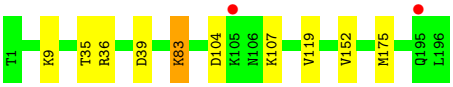
Chain a:



• Molecule 14: Proteasome subunit beta type-1

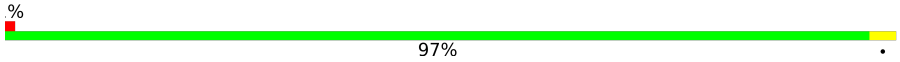
Chain N:

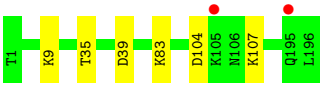




• Molecule 14: Proteasome subunit beta type-1

Chain b:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	134.05Å 301.90Å 144.45Å 90.00° 112.61° 90.00°	Depositor
Resolution (Å)	15.00 – 2.80 15.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.4 (15.00-2.80) 97.5 (15.00-2.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.61 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.187 , 0.211 0.193 , 0.214	Depositor DCC
R_{free} test set	12547 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	58.3	Xtriage
Anisotropy	0.073	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 42.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	49660	wwPDB-VP
Average B, all atoms (Å^2)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.34% 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: MG, CL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	A	0.26	0/1952	0.46	0/2642
1	O	0.26	0/1952	0.46	0/2642
2	B	0.26	0/1934	0.49	0/2618
2	P	0.26	0/1934	0.49	0/2618
3	C	0.26	0/1910	0.50	0/2586
3	Q	0.27	0/1910	0.50	0/2586
4	D	0.26	0/1837	0.47	0/2475
4	R	0.26	0/1837	0.47	0/2475
5	E	0.26	0/1800	0.47	0/2433
5	S	0.25	0/1800	0.47	0/2433
6	F	0.26	0/1932	0.45	0/2609
6	T	0.26	0/1932	0.45	0/2609
7	G	0.27	0/1945	0.47	0/2634
7	U	0.27	0/1945	0.47	0/2634
8	H	0.29	0/1750	0.51	0/2373
8	V	0.26	0/1750	0.50	0/2373
9	I	0.28	0/1611	0.52	0/2174
9	W	0.27	0/1611	0.52	0/2174
10	J	0.26	0/1589	0.98	7/2142 (0.3%)
10	X	0.26	0/1589	0.95	6/2142 (0.3%)
11	K	0.35	0/1677	0.54	0/2263
11	Y	0.35	0/1677	0.54	0/2263
12	L	0.35	0/1802	0.52	0/2430
12	Z	0.31	0/1802	0.51	0/2430
13	M	0.27	0/1855	0.53	0/2514
13	a	0.27	0/1866	0.53	0/2528
14	N	0.25	0/1541	0.50	0/2087
14	b	0.25	0/1541	0.50	0/2087
All	All	0.28	0/50281	0.54	13/67974 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if

the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
10	J	0	2
10	X	0	2
All	All	0	4

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	J	95	ARG	NE-CZ-NH2	-20.82	109.89	120.30
10	J	149	ARG	NE-CZ-NH1	-20.48	110.06	120.30
10	X	149	ARG	NE-CZ-NH2	-20.05	110.27	120.30
10	X	95	ARG	NE-CZ-NH1	-19.12	110.74	120.30
10	J	149	ARG	NE-CZ-NH2	15.91	128.26	120.30
10	X	95	ARG	NE-CZ-NH2	15.79	128.19	120.30
10	X	149	ARG	NE-CZ-NH1	14.64	127.62	120.30
10	J	95	ARG	NE-CZ-NH1	13.91	127.25	120.30
10	J	149	ARG	CD-NE-CZ	10.58	138.41	123.60
10	J	95	ARG	CD-NE-CZ	10.44	138.22	123.60
10	X	149	ARG	CD-NE-CZ	9.71	137.19	123.60
10	X	95	ARG	CD-NE-CZ	9.18	136.44	123.60
10	J	149	ARG	CG-CD-NE	-5.36	100.54	111.80

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
10	J	149	ARG	Sidechain
10	J	95	ARG	Sidechain
10	X	149	ARG	Sidechain
10	X	95	ARG	Sidechain

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	1915	0	1929	1	0
1	O	1915	0	1929	1	0
2	B	1904	0	1904	8	0
2	P	1904	0	1904	9	0
3	C	1881	0	1895	7	0
3	Q	1881	0	1895	12	0
4	D	1813	0	1797	5	0
4	R	1813	0	1797	5	0
5	E	1773	0	1775	3	0
5	S	1773	0	1775	3	0
6	F	1892	0	1883	2	0
6	T	1892	0	1883	2	0
7	G	1907	0	1901	5	0
7	U	1907	0	1901	4	0
8	H	1719	0	1719	9	0
8	V	1719	0	1719	12	0
9	I	1581	0	1574	7	0
9	W	1581	0	1574	8	0
10	J	1561	0	1569	20	0
10	X	1561	0	1569	18	0
11	K	1640	0	1581	15	0
11	Y	1640	0	1581	31	0
12	L	1764	0	1716	6	0
12	Z	1764	0	1716	5	0
13	M	1824	0	1832	4	0
13	a	1835	0	1844	0	0
14	N	1512	0	1481	3	0
14	b	1512	0	1481	0	0
15	G	1	0	0	0	0
15	H	1	0	0	0	0
15	I	2	0	0	0	0
15	J	1	0	0	0	0
15	K	1	0	0	0	0
15	L	1	0	0	0	0
15	N	1	0	0	0	0
15	Z	1	0	0	0	0
16	G	2	0	0	0	0
16	U	2	0	0	0	0
17	A	5	0	0	0	0
17	B	6	0	0	0	0
17	C	7	0	0	0	0
17	D	6	0	0	0	0
17	E	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	F	6	0	0	0	0
17	G	11	0	0	0	0
17	H	12	0	0	0	0
17	I	13	0	0	0	0
17	J	14	0	0	0	0
17	K	8	0	0	0	0
17	L	8	0	0	0	0
17	M	16	0	0	0	0
17	N	12	0	0	0	0
17	O	7	0	0	0	0
17	P	10	0	0	1	0
17	Q	9	0	0	0	0
17	R	5	0	0	0	0
17	S	7	0	0	0	0
17	T	4	0	0	0	0
17	U	16	0	0	0	0
17	V	10	0	0	0	0
17	W	13	0	0	0	0
17	X	7	0	0	0	0
17	Y	7	0	0	0	0
17	Z	7	0	0	0	0
17	a	21	0	0	0	0
17	b	11	0	0	0	0
All	All	49660	0	49124	180	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 2.

All (180) 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)
10:J:52:ASP:OD1	11:K:91:ARG:NH1	2.15	0.80
11:K:44:THR:O	11:K:99:SER:HB2	1.84	0.78
11:Y:18:SER:OG	11:Y:30:ARG:HA	1.83	0.78
11:K:18:SER:OG	11:K:30:ARG:HA	1.88	0.74
11:Y:35:ILE:HD12	11:Y:56:GLU:HB3	1.72	0.71
11:Y:35:ILE:HD13	11:Y:37:ILE:HG13	1.74	0.69
12:L:108:TYR:CE2	12:L:127:PRO:HD3	2.28	0.68
10:J:1:MET:CE	10:J:34:LYS:HG2	2.25	0.66
2:P:93:HIS:HB3	17:P:301:HOH:O	1.96	0.65
10:X:1:MET:HE2	10:X:34:LYS:HG2	1.76	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:23:ARG:NH2	11:K:119:THR:OG1	2.29	0.65
11:K:44:THR:O	11:K:99:SER:CB	2.45	0.64
10:X:1:MET:CE	10:X:34:LYS:HG2	2.27	0.64
10:X:23:ARG:NH2	11:Y:119:THR:OG1	2.30	0.64
11:Y:44:THR:O	11:Y:99:SER:HB2	1.99	0.62
10:X:3:ILE:CD1	10:X:168:LEU:HD13	2.31	0.60
10:J:174:MET:SD	10:X:174:MET:SD	3.00	0.60
11:Y:35:ILE:CG2	11:Y:56:GLU:OE1	2.50	0.60
10:J:25:ILE:O	10:X:139:TYR:OH	2.19	0.59
11:Y:35:ILE:HG23	11:Y:56:GLU:OE1	2.01	0.59
10:J:3:ILE:CD1	10:J:168:LEU:HD13	2.32	0.59
10:J:139:TYR:OH	10:X:25:ILE:O	2.21	0.59
12:Z:53:SER:O	12:Z:109:ASN:ND2	2.36	0.58
10:J:1:MET:HE1	10:J:34:LYS:HG2	1.88	0.56
11:Y:35:ILE:HD12	11:Y:56:GLU:OE1	2.06	0.56
8:H:92:GLY:HA3	8:H:116:HIS:ND1	2.22	0.55
11:K:82:LEU:O	11:K:86:MET:HG3	2.06	0.55
4:D:89:VAL:HG12	11:K:61:LYS:HG3	1.88	0.55
8:V:35:HIS:HB3	8:V:56:THR:HG21	1.88	0.55
11:Y:82:LEU:O	11:Y:86:MET:HG3	2.07	0.55
8:H:35:HIS:HB3	8:H:56:THR:HG21	1.87	0.55
10:X:3:ILE:HD11	10:X:168:LEU:HD13	1.88	0.55
11:K:144:LYS:HB2	11:K:147:LEU:HD13	1.88	0.55
8:V:92:GLY:HA3	8:V:116:HIS:CE1	2.42	0.55
8:H:92:GLY:HA3	8:H:116:HIS:CE1	2.42	0.55
10:J:1:MET:HE2	10:J:34:LYS:HG2	1.89	0.54
12:Z:31:THR:HG23	12:Z:36:ASN:HD21	1.72	0.54
12:L:31:THR:HG23	12:L:36:ASN:HD21	1.72	0.54
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.90	0.54
11:Y:144:LYS:HB2	11:Y:147:LEU:HD13	1.88	0.54
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.89	0.54
11:K:18:SER:HG	11:K:30:ARG:HA	1.73	0.54
3:Q:51:LYS:O	3:Q:52:LEU:HB2	2.08	0.53
11:Y:35:ILE:CD1	11:Y:37:ILE:HG13	2.36	0.53
14:N:83:LYS:HG3	14:N:119:VAL:CG2	2.39	0.53
11:Y:18:SER:HG	11:Y:30:ARG:HA	1.72	0.53
10:J:3:ILE:HD11	10:J:168:LEU:HD13	1.89	0.53
7:G:23:PHE:O	7:G:26:THR:HB	2.09	0.52
8:V:92:GLY:HA3	8:V:116:HIS:ND1	2.23	0.52
7:U:23:PHE:O	7:U:26:THR:HB	2.10	0.52
1:A:1:MET:HG3	6:F:122:TYR:CZ	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:160:GLN:HE21	3:C:160:GLN:HA	1.75	0.52
3:C:51:LYS:O	3:C:52:LEU:HB2	2.08	0.51
3:Q:99:GLU:HG3	11:Y:81:LYS:HD2	1.92	0.51
11:Y:20:ALA:HB3	11:Y:28:ALA:HB3	1.92	0.51
2:P:217:LYS:C	2:P:219:ALA:H	2.14	0.51
3:C:201:VAL:O	3:C:202:GLN:CB	2.58	0.51
11:K:20:ALA:HB3	11:K:28:ALA:HB3	1.93	0.51
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.58	0.51
10:X:1:MET:HA	10:X:34:LYS:CE	2.41	0.50
2:B:217:LYS:C	2:B:219:ALA:H	2.13	0.50
8:V:53:GLU:O	8:V:57:GLN:HG2	2.11	0.50
8:H:53:GLU:O	8:H:57:GLN:HG2	2.11	0.50
10:J:1:MET:HA	10:J:34:LYS:CE	2.41	0.50
11:Y:35:ILE:CD1	11:Y:56:GLU:HB3	2.40	0.50
4:R:89:VAL:HG12	11:Y:61:LYS:HG3	1.94	0.50
2:B:47:ALA:HB1	2:B:64:LYS:HD2	1.94	0.49
2:P:47:ALA:HB1	2:P:64:LYS:HD2	1.95	0.49
3:Q:160:GLN:HE21	3:Q:160:GLN:HA	1.76	0.49
10:X:3:ILE:HG12	10:X:136:SER:OG	2.12	0.49
10:J:3:ILE:HG12	10:J:136:SER:OG	2.13	0.49
10:X:148:TYR:O	10:X:149:ARG:HD3	2.13	0.49
10:X:168:LEU:O	10:X:172:MET:HB2	2.12	0.49
2:B:221:ASP:O	2:B:223:GLU:N	2.46	0.48
11:Y:90:TYR:HA	11:Y:93:MET:HG3	1.95	0.48
10:J:168:LEU:O	10:J:172:MET:HB2	2.13	0.48
2:P:221:ASP:O	2:P:223:GLU:N	2.47	0.48
3:Q:99:GLU:CG	11:Y:81:LYS:NZ	2.77	0.48
8:V:35:HIS:CB	8:V:56:THR:HG21	2.44	0.48
10:X:1:MET:HA	10:X:34:LYS:HE3	1.95	0.47
8:H:35:HIS:CB	8:H:56:THR:HG21	2.43	0.47
9:I:20:VAL:HG13	9:I:118:PRO:HB3	1.96	0.47
1:O:1:MET:HG3	6:T:122:TYR:CZ	2.49	0.47
9:W:20:VAL:HG13	9:W:118:PRO:HB3	1.96	0.47
7:G:68:ARG:HH12	14:N:36:ARG:HH22	1.62	0.46
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.98	0.46
4:R:91:HIS:HB3	4:R:99:ILE:CG2	2.45	0.46
10:J:1:MET:HA	10:J:34:LYS:HE3	1.96	0.46
9:W:9:GLY:HA3	9:W:41:LYS:HE2	1.96	0.46
9:I:9:GLY:HA3	9:I:41:LYS:HE2	1.97	0.46
4:D:91:HIS:HB3	4:D:99:ILE:CG2	2.46	0.46
11:Y:44:THR:O	11:Y:99:SER:CB	2.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:38:LYS:NZ	11:Y:208:ASN:O	2.49	0.46
9:I:20:VAL:HG23	9:I:189:ILE:HB	1.97	0.46
9:W:20:VAL:HG23	9:W:189:ILE:HB	1.97	0.46
4:R:91:HIS:HB3	4:R:99:ILE:HG22	1.99	0.45
12:Z:146:ILE:HG22	12:Z:150:LEU:HD22	1.99	0.45
8:V:104:ASP:HB2	8:V:105:PRO:HD2	1.98	0.45
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.97	0.45
3:C:149:GLU:HB2	3:C:150:PRO:HD2	1.99	0.45
7:G:73:VAL:HG12	7:G:133:THR:HB	1.97	0.45
2:B:50:LYS:O	2:B:51:VAL:C	2.55	0.45
11:K:208:ASN:O	9:W:38:LYS:NZ	2.49	0.45
4:D:91:HIS:HB3	4:D:99:ILE:HG22	1.99	0.45
5:S:87:LEU:HD21	5:S:107:ALA:HB1	1.98	0.45
7:U:73:VAL:HG12	7:U:133:THR:HB	1.98	0.44
2:B:145:TYR:OH	2:B:217:LYS:N	2.50	0.44
8:H:104:ASP:HB2	8:H:105:PRO:HD2	1.98	0.44
3:Q:35:LYS:HG2	3:Q:158:SER:O	2.17	0.44
3:Q:149:GLU:HB2	3:Q:150:PRO:HD2	1.99	0.44
2:B:151:ASN:HB2	2:B:152:PRO:CD	2.47	0.44
3:C:35:LYS:HG2	3:C:158:SER:O	2.17	0.44
4:D:88:ALA:HA	4:D:99:ILE:HG21	2.00	0.44
13:M:96:LEU:O	13:M:100:MET:HG2	2.18	0.44
4:R:88:ALA:HA	4:R:99:ILE:HG21	2.00	0.44
11:Y:35:ILE:CD1	11:Y:37:ILE:CG1	2.95	0.44
10:X:3:ILE:HG22	10:X:18:SER:HB3	1.98	0.44
2:P:50:LYS:O	2:P:51:VAL:C	2.55	0.44
2:P:145:TYR:OH	2:P:217:LYS:N	2.50	0.44
6:T:198:LEU:HD12	6:T:243:ILE:HG22	1.99	0.44
5:E:87:LEU:HD21	5:E:107:ALA:HB1	1.99	0.44
2:P:151:ASN:HB2	2:P:152:PRO:CD	2.47	0.44
7:G:78:ILE:N	7:G:79:PRO:CD	2.81	0.43
12:L:146:ILE:HG22	12:L:150:LEU:HD22	1.99	0.43
3:Q:99:GLU:HG3	11:Y:81:LYS:CD	2.48	0.43
7:U:78:ILE:N	7:U:79:PRO:CD	2.81	0.43
2:B:50:LYS:HD3	2:B:50:LYS:HA	1.83	0.43
8:H:196:ARG:NH2	9:I:150:GLU:HG3	2.34	0.43
6:F:198:LEU:HD12	6:F:243:ILE:HG22	1.99	0.43
10:J:177:LYS:NZ	10:X:169:GLU:O	2.50	0.43
10:X:1:MET:HE2	10:X:34:LYS:CG	2.46	0.43
8:V:196:ARG:NH2	9:W:150:GLU:HG3	2.34	0.43
11:K:35:ILE:CG2	11:K:37:ILE:HG13	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:147:GLN:NE2	3:Q:160:GLN:OE1	2.52	0.43
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.54	0.43
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.54	0.43
10:J:169:GLU:O	10:X:177:LYS:NZ	2.52	0.43
3:Q:99:GLU:HG3	11:Y:81:LYS:NZ	2.34	0.42
11:Y:31:VAL:CG2	11:Y:33:LYS:HE3	2.49	0.42
7:G:149:ASP:HB2	7:G:150:PRO:CD	2.49	0.42
10:J:3:ILE:HG22	10:J:18:SER:HB3	2.00	0.42
2:P:119:GLN:CG	3:Q:78:ALA:HB1	2.49	0.42
12:L:8:ASN:HA	12:L:30:ILE:O	2.20	0.42
3:C:147:GLN:NE2	3:C:160:GLN:OE1	2.53	0.42
5:E:175:LEU:HA	5:E:178:PHE:CE2	2.55	0.42
11:Y:90:TYR:CA	11:Y:93:MET:HG3	2.49	0.42
2:P:151:ASN:HB2	2:P:152:PRO:HD2	2.02	0.42
8:V:210:THR:HG21	9:W:167:SER:HB3	2.02	0.42
12:Z:138:ALA:HB3	12:Z:147:MET:HG2	2.02	0.42
13:M:17:ASP:OD1	13:M:18:ASN:N	2.53	0.42
13:M:165:ILE:HB	13:M:166:PRO:HD3	2.02	0.42
8:H:80:LEU:HD12	8:H:113:ILE:HD11	2.02	0.42
5:S:175:LEU:HA	5:S:178:PHE:CE2	2.54	0.42
11:K:31:VAL:CG2	11:K:33:LYS:HE3	2.49	0.41
13:M:127:LEU:HG	13:M:142:LEU:HD12	2.02	0.41
3:Q:201:VAL:O	3:Q:202:GLN:HB3	2.20	0.41
7:U:149:ASP:HB2	7:U:150:PRO:CD	2.50	0.41
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.20	0.41
11:K:33:LYS:O	11:K:45:MET:HG3	2.20	0.41
11:Y:37:ILE:HG23	11:Y:60:ALA:HB2	2.03	0.41
3:C:201:VAL:O	3:C:202:GLN:HB3	2.19	0.41
8:V:80:LEU:HD12	8:V:113:ILE:HD11	2.01	0.41
11:K:37:ILE:HG23	11:K:60:ALA:HB2	2.02	0.41
8:V:104:ASP:HB2	8:V:105:PRO:CD	2.51	0.41
12:L:108:TYR:CZ	12:L:127:PRO:HD3	2.54	0.41
12:L:138:ALA:HB3	12:L:147:MET:HG2	2.02	0.41
11:Y:35:ILE:HG21	11:Y:56:GLU:OE1	2.17	0.41
14:N:152:VAL:HA	14:N:175:MET:HE1	2.02	0.41
10:J:132:ALA:HB1	10:J:136:SER:HB2	2.02	0.41
5:S:77:ALA:N	5:S:78:PRO:CD	2.84	0.41
5:E:77:ALA:N	5:E:78:PRO:CD	2.84	0.40
8:V:99:ILE:HG13	8:V:127:LEU:HD22	2.03	0.40
11:Y:10:HIS:CD2	11:Y:10:HIS:N	2.89	0.40
2:B:151:ASN:HB2	2:B:152:PRO:HD2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:126:VAL:HG12	10:J:128:LEU:HG	2.04	0.40
11:Y:33:LYS:O	11:Y:45:MET:HG3	2.21	0.40
11:Y:35:ILE:HD11	11:Y:37:ILE:HG12	2.04	0.40
8:V:215:GLU:HG2	9:W:197:ARG:HG2	2.02	0.40
8:H:210:THR:HG21	9:I:167:SER:HB3	2.03	0.40
11:Y:115:ASP:OD1	11:Y:117:HIS:HB2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	248/250 (99%)	239 (96%)	8 (3%)	1 (0%)	34	66
1	O	248/250 (99%)	239 (96%)	8 (3%)	1 (0%)	34	66
2	B	242/258 (94%)	234 (97%)	4 (2%)	4 (2%)	9	29
2	P	242/258 (94%)	234 (97%)	4 (2%)	4 (2%)	9	29
3	C	238/254 (94%)	232 (98%)	3 (1%)	3 (1%)	12	36
3	Q	238/254 (94%)	232 (98%)	3 (1%)	3 (1%)	12	36
4	D	231/260 (89%)	227 (98%)	4 (2%)	0	100	100
4	R	231/260 (89%)	227 (98%)	4 (2%)	0	100	100
5	E	229/234 (98%)	224 (98%)	5 (2%)	0	100	100
5	S	229/234 (98%)	224 (98%)	5 (2%)	0	100	100
6	F	241/288 (84%)	237 (98%)	4 (2%)	0	100	100
6	T	241/288 (84%)	237 (98%)	4 (2%)	0	100	100
7	G	239/252 (95%)	237 (99%)	2 (1%)	0	100	100
7	U	239/252 (95%)	237 (99%)	2 (1%)	0	100	100
8	H	224/232 (97%)	219 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	V	224/232 (97%)	218 (97%)	6 (3%)	0	100	100
9	I	202/205 (98%)	196 (97%)	6 (3%)	0	100	100
9	W	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
10	J	193/198 (98%)	191 (99%)	2 (1%)	0	100	100
10	X	193/198 (98%)	191 (99%)	2 (1%)	0	100	100
11	K	209/211 (99%)	199 (95%)	10 (5%)	0	100	100
11	Y	209/211 (99%)	198 (95%)	11 (5%)	0	100	100
12	L	220/222 (99%)	215 (98%)	5 (2%)	0	100	100
12	Z	220/222 (99%)	215 (98%)	5 (2%)	0	100	100
13	M	231/246 (94%)	220 (95%)	11 (5%)	0	100	100
13	a	232/246 (94%)	221 (95%)	11 (5%)	0	100	100
14	N	194/196 (99%)	190 (98%)	4 (2%)	0	100	100
14	b	194/196 (99%)	190 (98%)	4 (2%)	0	100	100
All	All	6283/6612 (95%)	6118 (97%)	149 (2%)	16 (0%)	41	72

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	THR
2	B	51	VAL
2	B	222	GLY
3	C	202	GLN
1	O	2	THR
2	P	51	VAL
2	P	222	GLY
3	Q	202	GLN
2	B	218	GLY
2	P	218	GLY
2	B	220	ASN
3	C	205	ALA
2	P	220	ASN
3	Q	205	ALA
3	C	183	PRO
3	Q	183	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	209/209 (100%)	206 (99%)	3 (1%)	67	90
1	O	209/209 (100%)	206 (99%)	3 (1%)	67	90
2	B	203/216 (94%)	197 (97%)	6 (3%)	41	75
2	P	203/216 (94%)	197 (97%)	6 (3%)	41	75
3	C	212/226 (94%)	201 (95%)	11 (5%)	23	55
3	Q	212/226 (94%)	201 (95%)	11 (5%)	23	55
4	D	194/215 (90%)	185 (95%)	9 (5%)	27	60
4	R	194/215 (90%)	185 (95%)	9 (5%)	27	60
5	E	190/193 (98%)	182 (96%)	8 (4%)	30	63
5	S	190/193 (98%)	182 (96%)	8 (4%)	30	63
6	F	201/239 (84%)	192 (96%)	9 (4%)	27	60
6	T	201/239 (84%)	192 (96%)	9 (4%)	27	60
7	G	206/210 (98%)	198 (96%)	8 (4%)	32	66
7	U	206/210 (98%)	199 (97%)	7 (3%)	37	71
8	H	185/190 (97%)	179 (97%)	6 (3%)	39	73
8	V	185/190 (97%)	180 (97%)	5 (3%)	44	78
9	I	172/173 (99%)	170 (99%)	2 (1%)	71	92
9	W	172/173 (99%)	170 (99%)	2 (1%)	71	92
10	J	173/175 (99%)	167 (96%)	6 (4%)	36	70
10	X	173/175 (99%)	167 (96%)	6 (4%)	36	70
11	K	170/170 (100%)	161 (95%)	9 (5%)	22	54
11	Y	170/170 (100%)	161 (95%)	9 (5%)	22	54
12	L	186/186 (100%)	181 (97%)	5 (3%)	44	78
12	Z	186/186 (100%)	182 (98%)	4 (2%)	52	83
13	M	199/208 (96%)	192 (96%)	7 (4%)	36	70
13	a	200/208 (96%)	193 (96%)	7 (4%)	36	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	N	162/162 (100%)	156 (96%)	6 (4%)	34	68
14	b	162/162 (100%)	156 (96%)	6 (4%)	34	68
All	All	5325/5544 (96%)	5138 (96%)	187 (4%)	36	70

All (187) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	122	THR
1	A	157	PHE
1	A	250	LEU
2	B	50	LYS
2	B	55	LEU
2	B	113	ARG
2	B	186	ASP
2	B	191	LEU
2	B	238	LEU
3	C	4	ARG
3	C	38	ASN
3	C	51	LYS
3	C	77	ASN
3	C	98	LEU
3	C	147	GLN
3	C	160	GLN
3	C	169	VAL
3	C	180	LYS
3	C	206	LYS
3	C	240	GLU
4	D	99	ILE
4	D	125	LEU
4	D	143	ASP
4	D	176	LEU
4	D	193	LEU
4	D	214	ILE
4	D	235	LEU
4	D	236	LYS
4	D	242	GLU
5	E	9	THR
5	E	29	LYS
5	E	71	LEU
5	E	184	ASN
5	E	188	LEU

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Mol	Chain	Res	Type
5	E	202	ASP
5	E	208	ASP
5	E	231	LYS
6	F	117	GLN
6	F	123	ASN
6	F	139	LYS
6	F	172	LEU
6	F	181	GLU
6	F	201	GLU
6	F	202	ASP
6	F	214	TRP
6	F	240	GLN
7	G	26	THR
7	G	83	ASN
7	G	115	LEU
7	G	122	ARG
7	G	125	MET
7	G	208	GLU
7	G	235	ARG
7	G	236	LEU
8	H	22	GLN
8	H	30	ASN
8	H	68	LEU
8	H	113	ILE
8	H	127	LEU
8	H	196	ARG
9	I	37	ASN
9	I	171	LEU
10	J	1	MET
10	J	2	ASP
10	J	3	ILE
10	J	35	THR
10	J	99	GLN
10	J	172	MET
11	K	4	LEU
11	K	12	VAL
11	K	30	ARG
11	K	35	ILE
11	K	46	SER
11	K	62	GLU
11	K	107	LYS
11	K	125	MET

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Mol	Chain	Res	Type
11	K	147	LEU
12	L	23	LEU
12	L	49	ASN
12	L	106	TYR
12	L	128	VAL
12	L	150	LEU
13	M	2	GLN
13	M	48	ASN
13	M	70	LEU
13	M	104	ARG
13	M	161	ARG
13	M	187	ARG
13	M	233	ILE
14	N	9	LYS
14	N	35	THR
14	N	39	ASP
14	N	83	LYS
14	N	104	ASP
14	N	107	LYS
1	O	122	THR
1	O	157	PHE
1	O	250	LEU
2	P	50	LYS
2	P	55	LEU
2	P	113	ARG
2	P	186	ASP
2	P	191	LEU
2	P	238	LEU
3	Q	4	ARG
3	Q	38	ASN
3	Q	51	LYS
3	Q	77	ASN
3	Q	98	LEU
3	Q	147	GLN
3	Q	160	GLN
3	Q	169	VAL
3	Q	180	LYS
3	Q	206	LYS
3	Q	240	GLU
4	R	99	ILE
4	R	125	LEU
4	R	143	ASP

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Mol	Chain	Res	Type
4	R	176	LEU
4	R	193	LEU
4	R	214	ILE
4	R	235	LEU
4	R	236	LYS
4	R	242	GLU
5	S	9	THR
5	S	29	LYS
5	S	71	LEU
5	S	184	ASN
5	S	188	LEU
5	S	202	ASP
5	S	208	ASP
5	S	231	LYS
6	T	117	GLN
6	T	123	ASN
6	T	139	LYS
6	T	172	LEU
6	T	181	GLU
6	T	201	GLU
6	T	202	ASP
6	T	214	TRP
6	T	240	GLN
7	U	26	THR
7	U	83	ASN
7	U	115	LEU
7	U	122	ARG
7	U	125	MET
7	U	235	ARG
7	U	236	LEU
8	V	30	ASN
8	V	68	LEU
8	V	113	ILE
8	V	127	LEU
8	V	196	ARG
9	W	37	ASN
9	W	171	LEU
10	X	1	MET
10	X	2	ASP
10	X	3	ILE
10	X	35	THR
10	X	99	GLN

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Mol	Chain	Res	Type
10	X	172	MET
11	Y	4	LEU
11	Y	12	VAL
11	Y	30	ARG
11	Y	35	ILE
11	Y	62	GLU
11	Y	93	MET
11	Y	106	LYS
11	Y	125	MET
11	Y	147	LEU
12	Z	23	LEU
12	Z	49	ASN
12	Z	128	VAL
12	Z	150	LEU
13	a	2	GLN
13	a	48	ASN
13	a	70	LEU
13	a	104	ARG
13	a	161	ARG
13	a	187	ARG
13	a	233	ILE
14	b	9	LYS
14	b	35	THR
14	b	39	ASP
14	b	83	LYS
14	b	104	ASP
14	b	107	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (102) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	HIS
2	B	58	GLN
2	B	95	GLN
2	B	119	GLN
2	B	123	GLN
3	C	17	GLN
3	C	77	ASN
3	C	147	GLN
3	C	160	GLN
4	D	15	GLN
4	D	100	ASN

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Mol	Chain	Res	Type
4	D	146	GLN
4	D	225	ASN
5	E	68	HIS
5	E	92	ASN
5	E	99	ASN
5	E	116	GLN
5	E	118	ASN
5	E	120	GLN
5	E	151	ASN
5	E	184	ASN
6	F	19	GLN
6	F	86	ASN
6	F	117	GLN
6	F	123	ASN
6	F	191	GLN
6	F	240	GLN
7	G	83	ASN
7	G	114	ASN
7	G	117	GLN
7	G	121	GLN
7	G	166	GLN
8	H	66	HIS
8	H	165	ASN
9	I	37	ASN
10	J	55	GLN
10	J	146	HIS
11	K	10	HIS
11	K	89	GLN
11	K	175	ASN
11	K	207	ASN
12	L	3	ASN
12	L	49	ASN
12	L	70	ASN
12	L	158	ASN
13	M	48	ASN
13	M	102	GLN
13	M	194	ASN
13	M	213	GLN
14	N	161	GLN
1	O	94	HIS
2	P	20	GLN
2	P	58	GLN

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Mol	Chain	Res	Type
2	P	95	GLN
2	P	119	GLN
2	P	123	GLN
3	Q	77	ASN
3	Q	116	GLN
3	Q	120	GLN
3	Q	147	GLN
3	Q	160	GLN
4	R	15	GLN
4	R	91	HIS
4	R	100	ASN
4	R	146	GLN
4	R	225	ASN
5	S	68	HIS
5	S	92	ASN
5	S	99	ASN
5	S	116	GLN
5	S	120	GLN
5	S	151	ASN
5	S	184	ASN
6	T	19	GLN
6	T	86	ASN
6	T	117	GLN
6	T	123	ASN
6	T	191	GLN
6	T	240	GLN
7	U	83	ASN
7	U	114	ASN
7	U	117	GLN
7	U	121	GLN
7	U	166	GLN
8	V	165	ASN
9	W	37	ASN
10	X	55	GLN
11	Y	10	HIS
11	Y	85	ASN
11	Y	89	GLN
11	Y	175	ASN
11	Y	207	ASN
12	Z	3	ASN
12	Z	49	ASN
12	Z	70	ASN

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Mol	Chain	Res	Type
12	Z	109	ASN
12	Z	158	ASN
13	a	48	ASN
13	a	102	GLN
13	a	194	ASN
13	a	213	GLN
14	b	161	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)

Of 13 ligands modelled in this entry, 13 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	250/250 (100%)	-0.37	7 (2%)	53	43	39, 53, 91, 134	0
1	O	250/250 (100%)	-0.38	5 (2%)	65	56	44, 61, 109, 142	0
2	B	244/258 (94%)	-0.32	7 (2%)	51	41	40, 60, 105, 157	0
2	P	244/258 (94%)	-0.29	9 (3%)	41	31	45, 63, 106, 155	0
3	C	240/254 (94%)	-0.04	12 (5%)	28	19	42, 69, 136, 177	0
3	Q	240/254 (94%)	-0.01	17 (7%)	16	9	34, 75, 153, 197	0
4	D	235/260 (90%)	-0.32	1 (0%)	92	91	49, 66, 102, 141	0
4	R	235/260 (90%)	-0.26	4 (1%)	70	63	55, 73, 112, 149	0
5	E	231/234 (98%)	-0.34	1 (0%)	92	91	46, 67, 109, 154	0
5	S	231/234 (98%)	-0.26	2 (0%)	84	80	49, 73, 114, 159	0
6	F	243/288 (84%)	-0.47	3 (1%)	79	73	40, 60, 112, 138	0
6	T	243/288 (84%)	-0.38	3 (1%)	79	73	42, 68, 124, 151	0
7	G	241/252 (95%)	-0.53	2 (0%)	86	81	35, 54, 88, 139	0
7	U	241/252 (95%)	-0.43	4 (1%)	70	63	42, 58, 90, 135	0
8	H	226/232 (97%)	-0.46	6 (2%)	54	44	35, 50, 86, 150	1 (0%)
8	V	226/232 (97%)	-0.41	6 (2%)	54	44	38, 53, 89, 164	0
9	I	204/205 (99%)	-0.74	1 (0%)	91	88	37, 50, 78, 101	0
9	W	204/205 (99%)	-0.66	2 (0%)	82	77	38, 51, 83, 105	0
10	J	195/198 (98%)	-0.49	3 (1%)	73	68	38, 56, 81, 130	0
10	X	195/198 (98%)	-0.52	2 (1%)	82	77	37, 55, 81, 138	0
11	K	211/211 (100%)	-0.33	0	100	100	45, 63, 92, 114	0
11	Y	211/211 (100%)	-0.36	1 (0%)	91	88	47, 63, 92, 118	0
12	L	222/222 (100%)	-0.46	1 (0%)	91	88	41, 60, 104, 134	0
12	Z	222/222 (100%)	-0.45	1 (0%)	91	88	40, 60, 103, 137	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	M	233/246 (94%)	-0.68	0 100 100	34, 51, 73, 91	0
13	a	233/246 (94%)	-0.64	1 (0%) 92 91	37, 52, 72, 90	0
14	N	196/196 (100%)	-0.64	2 (1%) 82 77	31, 47, 75, 105	0
14	b	196/196 (100%)	-0.64	2 (1%) 82 77	36, 48, 76, 109	0
All	All	6342/6612 (95%)	-0.42	105 (1%) 70 63	31, 59, 105, 197	1 (0%)

All (105) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
8	V	224	GLN	6.6
2	P	220	ASN	6.3
2	B	221	ASP	5.8
8	V	222	ASP	5.6
8	H	224	GLN	5.6
2	P	219	ALA	5.3
2	P	222	GLY	5.3
2	P	51	VAL	5.1
9	W	1	SER	5.1
8	V	226	GLU	5.0
2	B	51	VAL	5.0
1	A	2	THR	4.9
1	O	2	THR	4.9
1	A	1	MET	4.7
5	S	202	ASP	4.6
8	H	226	GLU	4.6
5	E	202	ASP	4.6
2	B	220	ASN	4.5
12	L	174	TYR	4.4
8	V	221	CYS	4.3
1	O	249	ALA	4.2
3	C	238	LYS	4.1
3	C	202	GLN	4.1
3	Q	202	GLN	3.9
8	V	223	ILE	3.9
2	P	221	ASP	3.8
10	X	1	MET	3.8
3	Q	206	LYS	3.8
3	C	206	LYS	3.8
3	C	239	GLN	3.7
12	Z	174	TYR	3.7
8	H	225	GLU	3.7

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Mol	Chain	Res	Type	RSRZ
3	Q	238	LYS	3.7
10	J	1	MET	3.6
6	F	181	GLU	3.6
8	H	222	ASP	3.6
8	H	221	CYS	3.5
1	O	1	MET	3.5
6	F	244	ASN	3.4
3	Q	237	GLU	3.4
3	C	235	GLU	3.4
13	a	1	THR	3.3
8	V	225	GLU	3.3
3	Q	49	THR	3.3
1	A	249	ALA	3.3
3	Q	240	GLU	3.2
9	I	1	SER	3.2
14	b	105	LYS	3.2
2	B	219	ALA	3.1
14	N	195	GLN	3.0
3	Q	50	LEU	3.0
4	R	241	ALA	2.9
14	b	195	GLN	2.9
4	R	230	GLU	2.9
4	R	217	GLN	2.8
1	A	203	GLU	2.8
2	P	59	ASP	2.8
7	U	242	GLN	2.7
8	H	223	ILE	2.7
7	U	2	GLY	2.7
3	C	188	GLU	2.7
3	Q	187	GLU	2.7
1	A	3	ASP	2.6
5	S	165	GLN	2.6
10	X	194	ASP	2.6
3	Q	236	GLN	2.6
2	P	52	THR	2.6
3	C	139	ARG	2.6
3	Q	239	GLN	2.5
6	T	244	ASN	2.5
2	B	59	ASP	2.5
4	R	1	ASP	2.5
2	P	218	GLY	2.5
3	Q	139	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
6	T	2	THR	2.5
1	O	201	GLU	2.4
10	J	194	ASP	2.4
1	O	52	SER	2.4
3	Q	205	ALA	2.4
9	W	133	LYS	2.4
6	T	205	GLU	2.3
3	C	240	GLU	2.3
7	U	188	GLU	2.3
3	C	225	GLU	2.3
14	N	105	LYS	2.3
6	F	202	ASP	2.3
7	G	242	GLN	2.2
3	Q	167	LYS	2.2
3	Q	141	ASP	2.2
7	U	222	ASP	2.2
3	C	205	ALA	2.2
1	A	52	SER	2.2
7	G	40	ASP	2.2
10	J	193	ASP	2.2
3	Q	47	ARG	2.2
2	B	203	SER	2.2
2	B	218	GLY	2.1
3	C	49	THR	2.1
4	D	201	GLU	2.1
1	A	250	LEU	2.1
11	Y	182	ASP	2.1
3	Q	181	GLU	2.1
2	P	203	SER	2.1
3	Q	229	GLN	2.0
3	C	1	GLY	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
15	MG	G	301	1/1	0.92	0.10	59,59,59,59	0
15	MG	H	301	1/1	0.93	0.22	55,55,55,55	0
15	MG	N	201	1/1	0.94	0.13	50,50,50,50	0
15	MG	I	301	1/1	0.95	0.13	54,54,54,54	0
15	MG	Z	301	1/1	0.95	0.40	72,72,72,72	0
15	MG	J	201	1/1	0.96	0.32	65,65,65,65	0
15	MG	I	302	1/1	0.97	0.09	49,49,49,49	0
15	MG	K	301	1/1	0.98	0.19	47,47,47,47	0
16	CL	G	303	1/1	0.98	0.18	30,30,30,30	0
16	CL	U	301	1/1	0.98	0.18	46,46,46,46	0
16	CL	U	302	1/1	0.98	0.20	30,30,30,30	0
15	MG	L	301	1/1	0.99	0.03	60,60,60,60	0
16	CL	G	302	1/1	1.00	0.12	41,41,41,41	0

6.5 Other polymers (i)

There are no such residues in this entry.