Full wwPDB X-ray Structure Validation Report (i)

Jan 3, 2024 – 03:35 am GMT

PDB ID	:	5L5R
Title	:	Yeast 20S proteasome with human beta5i (1-138;V31M) and human beta6 (97-111; 118-133)
Authors	:	Groll, M.; Huber, E.M.
Deposited on	:	2016-05-28
Resolution	:	2.90 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:

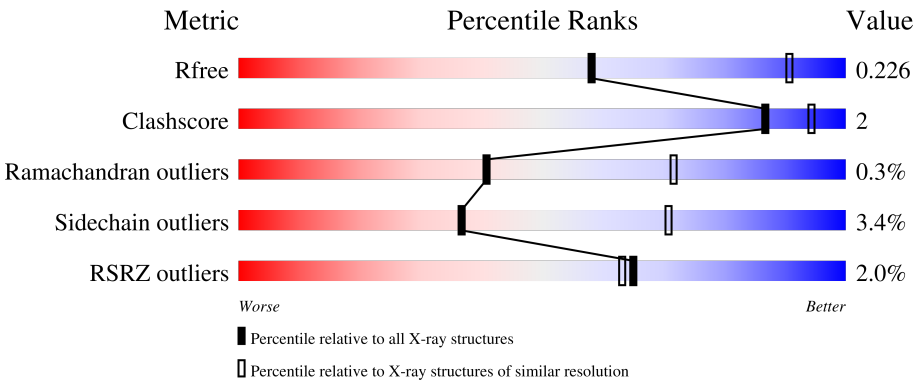
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	2% 97% •
1	O	250	3% 98% •
2	B	258	3% 87% 7% • 5%
2	P	258	3% 86% 7% • 5%
3	C	254	5% 86% 7% • 6%

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Mol	Chain	Length	Quality of chain
3	Q	254	5% 85% 7% 6%
4	D	260	85% 5% 10%
4	R	260	2% 85% 5% 10%
5	E	234	% 93% 6%
5	S	234	% 94% 5%
6	F	288	2% 80% 5% 16%
6	T	288	% 80% 5% 16%
7	G	252	% 88% 7%
7	U	252	% 88% 7%
8	H	232	3% 88% 8%
8	V	232	3% 89% 7%
9	I	205	% 94% 5%
9	W	205	2% 93% 7%
10	J	198	% 89% 7%
10	X	198	2% 88% 8%
11	K	211	% 86% 13%
11	Y	211	3% 84% 13%
12	L	222	% 93% 6%
12	Z	222	2% 93% 7%
13	M	246	87% 7% 5%
13	a	246	% 92% 5%
14	N	196	% 94% 5%
14	b	196	% 97%

2 Entry composition (i)

There are 17 unique types of molecules in this entry. The entry contains 49589 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	1726	1087	300	332	7	0	1	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	1641	1035	282	311	13	0	0	0
11	Y	211	1641	1035	282	311	13	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	31	MET	VAL	conflict	UNP P28062
Y	31	MET	VAL	conflict	UNP P28062

- 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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
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
			Total	Mg		
15	G	1	1	1	0	0
15	H	1	1	1	0	0
15	I	2	2	2	0	0
15	K	1	1	1	0	0
15	L	1	1	1	0	0
15	N	1	1	1	0	0
15	Z	1	1	1	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
16	G	1	1	1	0	0
16	U	1	1	1	0	0

- Molecule 17 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
17	A	5	5	5	0	0
17	B	6	6	6	0	0
17	C	6	6	6	0	0
17	D	10	10	10	0	0
17	E	4	4	4	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	F	7	Total O 7 7	0	0
17	G	6	Total O 6 6	0	0
17	H	5	Total O 5 5	0	0
17	I	9	Total O 9 9	0	0
17	J	8	Total O 8 8	0	0
17	K	5	Total O 5 5	0	0
17	L	8	Total O 8 8	0	0
17	M	6	Total O 6 6	0	0
17	N	9	Total O 9 9	0	0
17	O	3	Total O 3 3	0	0
17	P	9	Total O 9 9	0	0
17	Q	7	Total O 7 7	0	0
17	R	5	Total O 5 5	0	0
17	S	8	Total O 8 8	0	0
17	T	7	Total O 7 7	0	0
17	U	8	Total O 8 8	0	0
17	V	6	Total O 6 6	0	0
17	W	7	Total O 7 7	0	0
17	X	3	Total O 3 3	0	0
17	Y	7	Total O 7 7	0	0
17	Z	5	Total O 5 5	0	0

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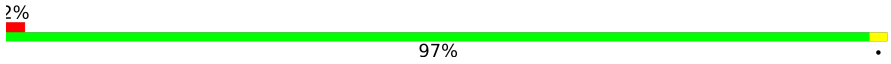
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
17	a	9	9	9	0	0
			Total	O		
17	b	9	9	9	0	0

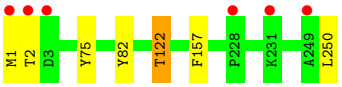
3 Residue-property plots (i)

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

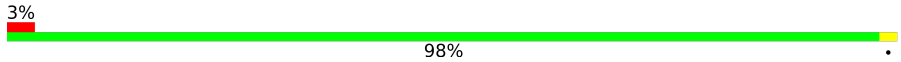
Chain A:

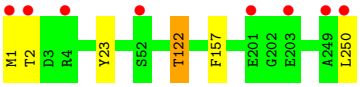




• Molecule 1: Proteasome subunit alpha type-2

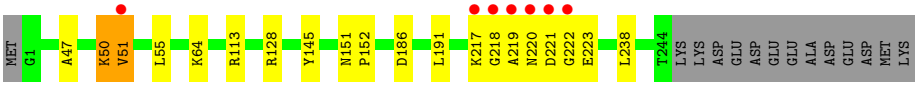
Chain O:





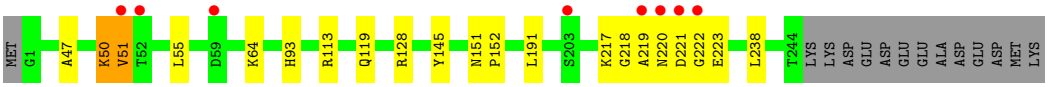
• Molecule 2: Proteasome subunit alpha type-3

Chain B:



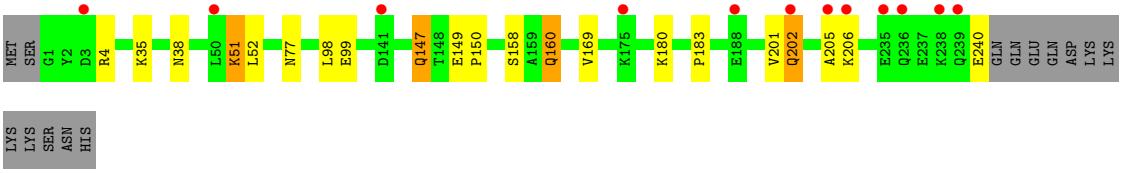
• Molecule 2: Proteasome subunit alpha type-3

Chain P:



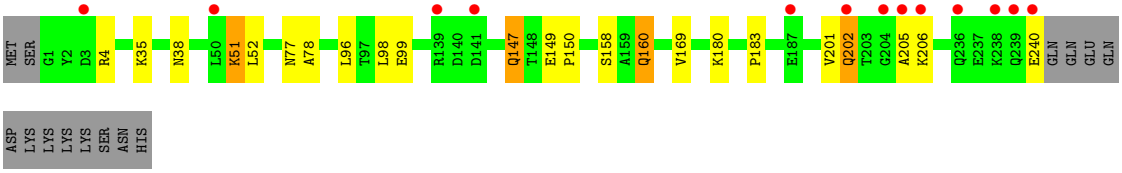
• Molecule 3: Proteasome subunit alpha type-4

Chain C:



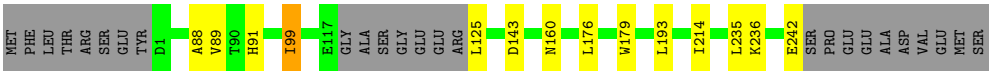
• Molecule 3: Proteasome subunit alpha type-4

Chain Q:



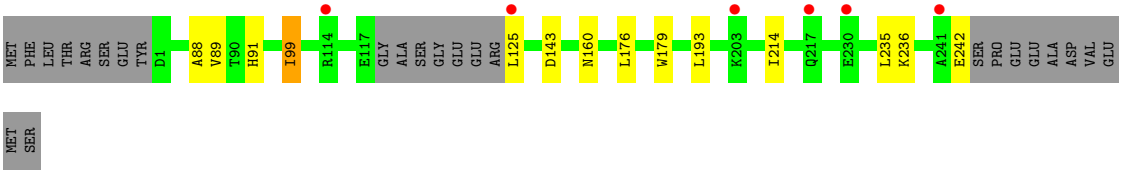
• Molecule 4: Proteasome subunit alpha type-5

Chain D:



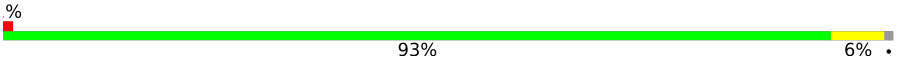
• Molecule 4: Proteasome subunit alpha type-5

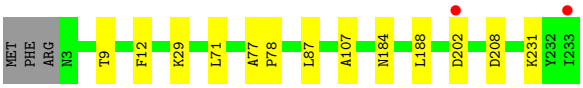
Chain R:



• Molecule 5: Proteasome subunit alpha type-6

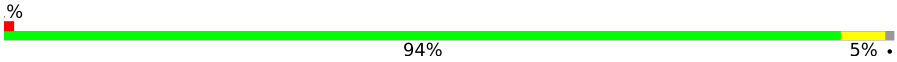
Chain E:

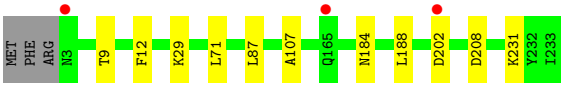




• Molecule 5: Proteasome subunit alpha type-6

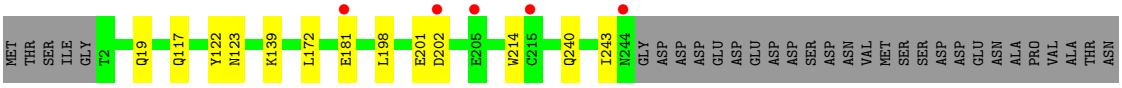
Chain S:

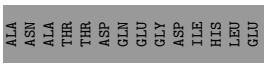




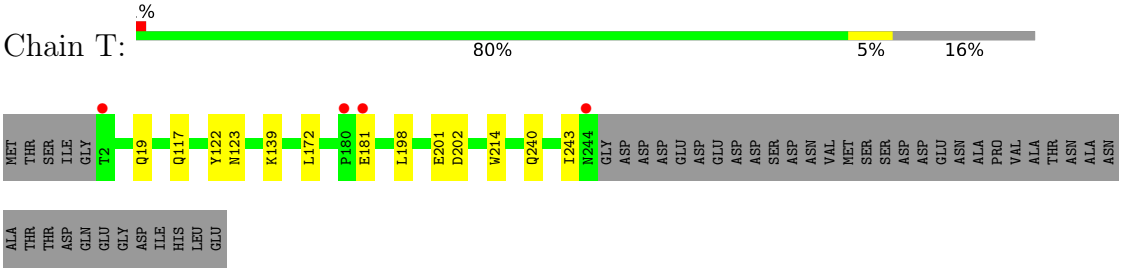
• Molecule 6: Probable proteasome subunit alpha type-7

Chain F:

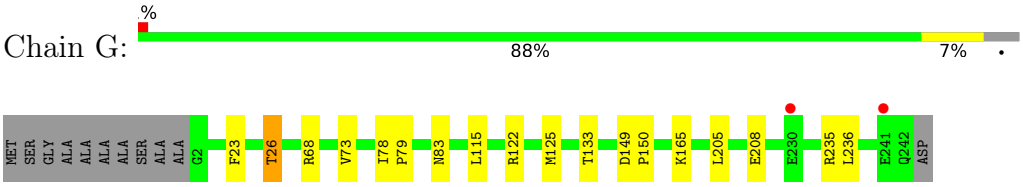




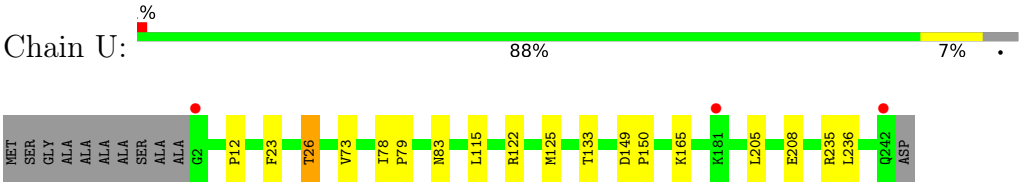
• Molecule 6: Probable proteasome subunit alpha type-7



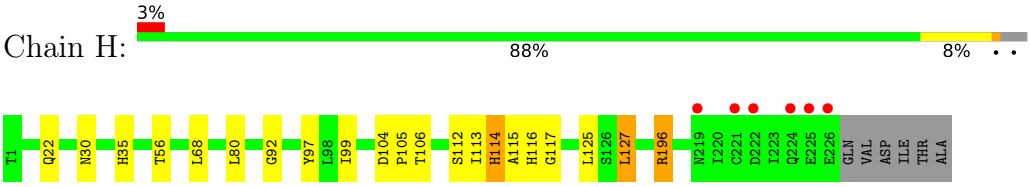
• Molecule 7: Proteasome subunit alpha type-1



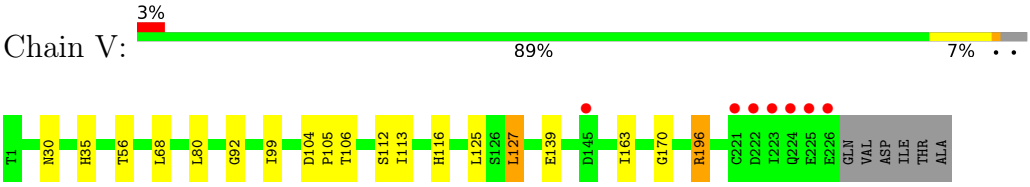
• Molecule 7: Proteasome subunit alpha type-1



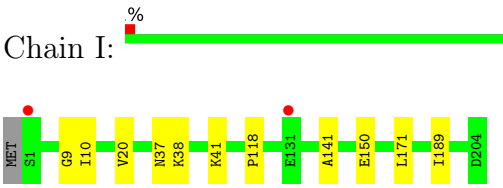
• Molecule 8: Proteasome subunit beta type-2



• Molecule 8: Proteasome subunit beta type-2

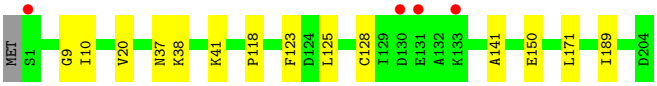


• Molecule 9: Proteasome subunit beta type-3



• Molecule 9: Proteasome subunit beta type-3

Chain W: 2% 93% 7%



• Molecule 10: Proteasome subunit beta type-4

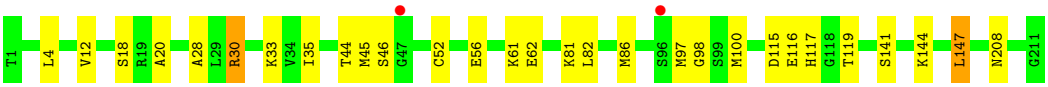
Chain J: % 89% 7% • •

• Molecule 10: Proteasome subunit beta type-4

Chain X: 2% 88% 8% • • •

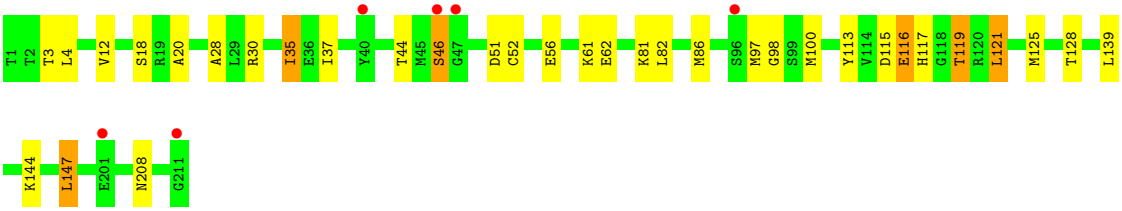
• Molecule 11: Proteasome subunit beta type-8,Proteasome subunit beta type-5

Chain K: % 86% 13% •



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

Chain Y: 3% 84% 13% •

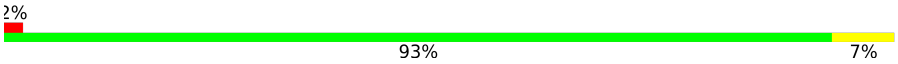


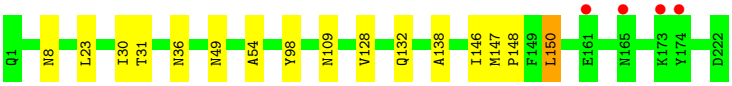
• Molecule 12: Proteasome subunit beta type-6,Proteasome subunit beta type-1,Proteasome subunit beta type-6,Proteasome subunit beta type-1,Proteasome subunit beta type-6

Chain L: % 93% 6%

• 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

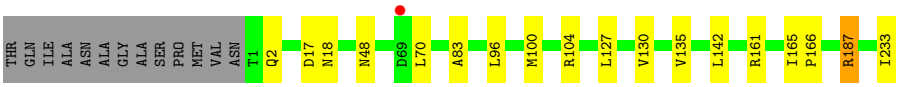
Chain Z:





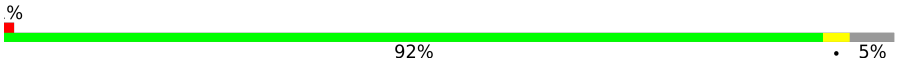
• Molecule 13: Proteasome subunit beta type-7

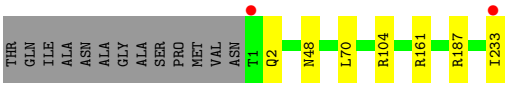
Chain M:



• Molecule 13: Proteasome subunit beta type-7

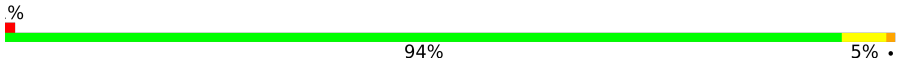
Chain a:

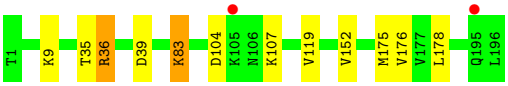




• Molecule 14: Proteasome subunit beta type-1

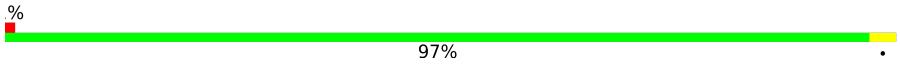
Chain N:

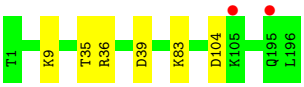




• Molecule 14: Proteasome subunit beta type-1

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	133.83Å 301.16Å 144.98Å 90.00° 112.67° 90.00°	Depositor
Resolution (Å)	15.00 – 2.90 15.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	97.3 (15.00-2.90) 97.3 (15.00-2.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.31 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.196 , 0.221 0.201 , 0.226	Depositor DCC
R_{free} test set	11263 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	64.0	Xtriage
Anisotropy	0.182	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 40.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	49589	wwPDB-VP
Average B, all atoms (Å^2)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.45% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.27	0/1952	0.47	0/2642
1	O	0.27	0/1952	0.46	0/2642
2	B	0.27	0/1934	0.49	0/2618
2	P	0.27	0/1934	0.50	0/2618
3	C	0.27	0/1910	0.51	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	0.26	0/1800	0.47	0/2433
6	F	0.27	0/1932	0.45	0/2609
6	T	0.27	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	0.37	2/1761 (0.1%)	0.62	4/2388 (0.2%)
8	V	0.26	0/1750	0.52	0/2373
9	I	0.30	0/1611	0.54	0/2174
9	W	0.32	0/1611	0.55	0/2174
10	J	0.27	0/1589	0.97	7/2142 (0.3%)
10	X	0.27	0/1589	0.95	6/2142 (0.3%)
11	K	0.30	0/1678	0.53	0/2263
11	Y	0.34	0/1678	0.54	0/2263
12	L	0.32	0/1802	0.53	0/2430
12	Z	0.34	0/1802	0.53	0/2430
13	M	0.29	0/1855	0.54	0/2514
13	a	0.29	0/1866	0.54	0/2528
14	N	0.27	0/1541	0.51	0/2087
14	b	0.27	0/1541	0.51	0/2087
All	All	0.29	2/50294 (0.0%)	0.54	17/67989 (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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	114[A]	HIS	CA-C	6.95	1.71	1.52
8	H	114[B]	HIS	CA-C	6.95	1.71	1.52

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	J	95	ARG	NE-CZ-NH2	-20.74	109.93	120.30
10	X	149	ARG	NE-CZ-NH2	-20.43	110.09	120.30
10	J	149	ARG	NE-CZ-NH1	-20.12	110.24	120.30
10	X	95	ARG	NE-CZ-NH1	-19.07	110.77	120.30
10	X	95	ARG	NE-CZ-NH2	15.93	128.26	120.30
10	J	149	ARG	NE-CZ-NH2	15.88	128.24	120.30
10	X	149	ARG	NE-CZ-NH1	14.77	127.68	120.30
10	J	95	ARG	NE-CZ-NH1	14.16	127.38	120.30
10	J	95	ARG	CD-NE-CZ	10.42	138.19	123.60
10	J	149	ARG	CD-NE-CZ	10.24	137.94	123.60
10	X	149	ARG	CD-NE-CZ	9.75	137.25	123.60
10	X	95	ARG	CD-NE-CZ	9.09	136.32	123.60
8	H	114[A]	HIS	CA-C-O	7.26	135.34	120.10
8	H	114[B]	HIS	CA-C-O	7.26	135.34	120.10
8	H	114[A]	HIS	CA-C-N	-5.91	104.20	117.20
8	H	114[B]	HIS	CA-C-N	-5.91	104.20	117.20
10	J	149	ARG	CG-CD-NE	-5.01	101.28	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	3	0
1	O	1915	0	1929	3	0
2	B	1904	0	1904	8	0
2	P	1904	0	1904	10	0
3	C	1881	0	1895	8	0
3	Q	1881	0	1895	13	0
4	D	1813	0	1797	5	0
4	R	1813	0	1797	6	0
5	E	1773	0	1775	3	0
5	S	1773	0	1775	2	0
6	F	1892	0	1883	3	0
6	T	1892	0	1883	3	0
7	G	1907	0	1901	6	0
7	U	1907	0	1901	6	0
8	H	1726	0	1726	18	0
8	V	1719	0	1719	12	0
9	I	1581	0	1574	7	0
9	W	1581	0	1574	9	0
10	J	1561	0	1569	12	0
10	X	1561	0	1569	17	0
11	K	1641	0	1581	26	0
11	Y	1641	0	1581	28	0
12	L	1764	0	1716	6	0
12	Z	1764	0	1716	7	0
13	M	1824	0	1832	6	0
13	a	1835	0	1844	0	0
14	N	1512	0	1481	4	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	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	1	0	0	0	0
16	U	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	A	5	0	0	0	0
17	B	6	0	0	0	0
17	C	6	0	0	0	0
17	D	10	0	0	0	0
17	E	4	0	0	0	0
17	F	7	0	0	0	0
17	G	6	0	0	0	0
17	H	5	0	0	0	0
17	I	9	0	0	0	0
17	J	8	0	0	0	0
17	K	5	0	0	2	0
17	L	8	0	0	0	0
17	M	6	0	0	0	0
17	N	9	0	0	0	0
17	O	3	0	0	0	0
17	P	9	0	0	1	0
17	Q	7	0	0	0	0
17	R	5	0	0	0	0
17	S	8	0	0	0	0
17	T	7	0	0	0	0
17	U	8	0	0	0	0
17	V	6	0	0	0	0
17	W	7	0	0	0	0
17	X	3	0	0	0	0
17	Y	7	0	0	0	0
17	Z	5	0	0	0	0
17	a	9	0	0	0	0
17	b	9	0	0	0	0
All	All	49589	0	49131	198	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 (198) 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)
11:K:35:ILE:HD12	11:K:56:GLU:OE1	1.58	1.03
8:H:97:TYR:HE2	8:H:114[B]:HIS:HD1	1.02	0.93
10:X:23:ARG:NH2	11:Y:119:THR:HG21	1.84	0.93
8:H:97:TYR:HE2	8:H:114[B]:HIS:ND1	1.67	0.92
11:Y:46:SER:HB2	11:Y:98:GLY:O	1.74	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:115:ASP:OD1	11:Y:117:HIS:HB2	1.77	0.85
8:H:97:TYR:CE2	8:H:114[B]:HIS:ND1	2.43	0.85
11:Y:116:GLU:OE1	11:Y:117:HIS:N	2.13	0.81
11:K:18:SER:OG	11:K:30:ARG:HA	1.81	0.81
11:K:115:ASP:OD1	11:K:119:THR:HB	1.85	0.77
11:Y:18:SER:OG	11:Y:30:ARG:HA	1.84	0.76
11:K:35:ILE:CD1	11:K:56:GLU:OE1	2.38	0.71
11:K:115:ASP:OD2	11:K:117:HIS:HB2	1.90	0.71
10:X:23:ARG:NH2	11:Y:119:THR:CG2	2.58	0.67
11:K:44:THR:HG1	11:K:100:MET:H	1.44	0.66
12:Z:31:THR:HG23	12:Z:36:ASN:HD21	1.62	0.65
12:L:31:THR:HG23	12:L:36:ASN:HD21	1.62	0.63
2:P:93:HIS:HB3	17:P:301:HOH:O	1.98	0.62
11:K:35:ILE:HD12	11:K:56:GLU:CD	2.21	0.61
11:K:20:ALA:HB3	11:K:28:ALA:HB3	1.83	0.61
7:G:23:PHE:O	7:G:26:THR:HB	2.01	0.60
11:Y:20:ALA:HB3	11:Y:28:ALA:HB3	1.84	0.59
11:K:144:LYS:HB2	11:K:147:LEU:HD13	1.85	0.58
8:H:97:TYR:HE2	8:H:114[B]:HIS:CE1	2.22	0.58
11:Y:44:THR:HG1	11:Y:100:MET:H	1.50	0.56
7:U:23:PHE:O	7:U:26:THR:HB	2.05	0.56
11:Y:144:LYS:HB2	11:Y:147:LEU:HD13	1.85	0.56
10:X:3:ILE:CD1	10:X:168:LEU:HD13	2.37	0.55
11:K:46:SER:HB2	11:K:98:GLY:O	2.06	0.55
14:N:152:VAL:HA	14:N:175:MET:HE1	1.88	0.55
10:J:3:ILE:CD1	10:J:168:LEU:HD13	2.37	0.55
1:O:1:MET:HG3	6:T:122:TYR:CZ	2.41	0.54
3:Q:51:LYS:O	3:Q:52:LEU:HB2	2.07	0.54
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.90	0.54
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.90	0.53
11:K:208:ASN:O	9:W:38:LYS:NZ	2.41	0.53
14:N:83:LYS:HG3	14:N:119:VAL:CG2	2.39	0.53
3:C:51:LYS:O	3:C:52:LEU:HB2	2.08	0.52
10:J:25:ILE:O	10:X:139:TYR:OH	2.23	0.52
10:J:23:ARG:NH2	11:K:119:THR:OG1	2.42	0.52
3:Q:99:GLU:HG3	11:Y:81:LYS:CD	2.40	0.52
3:C:201:VAL:O	3:C:202:GLN:CB	2.58	0.52
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.58	0.51
2:P:217:LYS:C	2:P:219:ALA:H	2.14	0.51
9:I:38:LYS:NZ	11:Y:208:ASN:O	2.44	0.51
8:H:196:ARG:NH2	9:I:150:GLU:O	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:116:GLU:OE2	11:K:116:GLU:N	2.44	0.50
2:B:217:LYS:C	2:B:219:ALA:H	2.14	0.50
10:J:139:TYR:OH	10:X:25:ILE:O	2.25	0.50
8:V:80:LEU:HD12	8:V:113:ILE:HD11	1.94	0.49
10:X:148:TYR:O	10:X:149:ARG:HD3	2.13	0.49
3:C:160:GLN:HE21	3:C:160:GLN:HA	1.78	0.49
3:Q:99:GLU:CG	11:Y:81:LYS:NZ	2.76	0.49
9:W:123:PHE:HA	9:W:128:CYS:O	2.12	0.48
8:H:80:LEU:HD12	8:H:113:ILE:HD11	1.94	0.48
11:K:115:ASP:OD1	11:K:119:THR:CB	2.58	0.48
2:B:47:ALA:HB1	2:B:64:LYS:HD2	1.96	0.48
11:Y:113:TYR:CD2	11:Y:121:LEU:HD12	2.49	0.48
10:X:168:LEU:O	10:X:172:MET:HB2	2.14	0.47
11:Y:113:TYR:HD2	11:Y:121:LEU:HD12	1.79	0.47
12:Z:146:ILE:HG22	12:Z:150:LEU:HD22	1.96	0.47
1:A:1:MET:HG3	6:F:122:TYR:CZ	2.49	0.47
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.49	0.47
2:P:47:ALA:HB1	2:P:64:LYS:HD2	1.96	0.47
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.97	0.47
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.97	0.47
9:W:9:GLY:HA3	9:W:41:LYS:HE2	1.96	0.47
2:B:221:ASP:O	2:B:223:GLU:N	2.48	0.47
10:J:168:LEU:O	10:J:172:MET:HB2	2.14	0.47
3:Q:160:GLN:HE21	3:Q:160:GLN:HA	1.78	0.47
9:I:20:VAL:HG13	9:I:118:PRO:HB3	1.96	0.47
11:K:44:THR:OG1	11:K:100:MET:N	2.35	0.46
8:V:35:HIS:CB	8:V:56:THR:HG21	2.45	0.46
2:P:221:ASP:O	2:P:223:GLU:N	2.48	0.46
11:K:35:ILE:HD12	11:K:56:GLU:HB2	1.97	0.46
8:H:35:HIS:CB	8:H:56:THR:HG21	2.46	0.46
11:K:35:ILE:HD12	11:K:56:GLU:CB	2.45	0.46
2:P:145:TYR:OH	2:P:217:LYS:N	2.48	0.46
9:W:20:VAL:HG13	9:W:118:PRO:HB3	1.96	0.46
9:I:20:VAL:HG23	9:I:189:ILE:HB	1.97	0.46
12:L:146:ILE:HG22	12:L:150:LEU:HD22	1.97	0.46
11:K:18:SER:HG	11:K:30:ARG:HA	1.79	0.46
3:Q:96:LEU:O	11:Y:81:LYS:HE2	2.15	0.46
4:D:91:HIS:HB3	4:D:99:ILE:CG2	2.46	0.46
4:R:91:HIS:HB3	4:R:99:ILE:CG2	2.46	0.46
8:V:104:ASP:HB2	8:V:105:PRO:HD2	1.97	0.45
11:Y:52:CYS:SG	11:Y:97:MET:HG3	2.57	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:145:TYR:OH	2:B:217:LYS:N	2.49	0.45
8:H:97:TYR:CE2	8:H:114[B]:HIS:CE1	3.03	0.45
2:B:50:LYS:O	2:B:51:VAL:C	2.55	0.45
7:G:73:VAL:HG12	7:G:133:THR:HB	1.98	0.45
9:I:9:GLY:HA3	9:I:41:LYS:HE2	1.97	0.45
9:W:20:VAL:HG23	9:W:189:ILE:HB	1.97	0.45
10:J:132:ALA:HB1	10:J:136:SER:HB2	1.98	0.45
7:U:73:VAL:HG12	7:U:133:THR:HB	1.98	0.45
3:C:35:LYS:HG2	3:C:158:SER:O	2.17	0.44
3:C:99:GLU:HG3	11:K:81:LYS:CD	2.47	0.44
8:H:104:ASP:HB2	8:H:105:PRO:HD2	1.98	0.44
10:J:1:MET:HA	10:J:34:LYS:CE	2.47	0.44
10:X:1:MET:HA	10:X:34:LYS:CE	2.47	0.44
11:K:115:ASP:OD2	11:K:117:HIS:N	2.43	0.44
11:Y:82:LEU:O	11:Y:86:MET:HG3	2.18	0.44
2:P:50:LYS:O	2:P:51:VAL:C	2.55	0.44
11:Y:3:THR:HG1	11:Y:128:THR:HG1	1.65	0.44
10:X:23:ARG:HH22	11:Y:119:THR:HG21	1.78	0.44
13:M:96:LEU:O	13:M:100:MET:HG2	2.18	0.44
3:Q:99:GLU:HG3	11:Y:81:LYS:NZ	2.33	0.44
9:W:125:LEU:N	9:W:125:LEU:HD23	2.32	0.44
3:C:201:VAL:O	3:C:202:GLN:HB3	2.18	0.44
13:M:17:ASP:OD1	13:M:18:ASN:N	2.51	0.44
3:Q:35:LYS:HG2	3:Q:158:SER:O	2.18	0.44
12:Z:54:ALA:HA	12:Z:109:ASN:HD22	1.83	0.44
3:Q:201:VAL:O	3:Q:202:GLN:HB3	2.18	0.43
3:C:149:GLU:HB2	3:C:150:PRO:HD2	2.00	0.43
2:B:151:ASN:HB2	2:B:152:PRO:CD	2.48	0.43
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.53	0.43
7:G:78:ILE:N	7:G:79:PRO:CD	2.81	0.43
2:P:151:ASN:HB2	2:P:152:PRO:CD	2.48	0.43
7:U:78:ILE:N	7:U:79:PRO:CD	2.81	0.43
8:V:196:ARG:NH2	9:W:150:GLU:O	2.52	0.43
8:V:99:ILE:HG13	8:V:127:LEU:HD22	2.01	0.43
10:X:3:ILE:HG22	10:X:18:SER:HB3	2.00	0.43
4:D:91:HIS:HB3	4:D:99:ILE:HG22	2.01	0.43
2:P:119:GLN:CG	3:Q:78:ALA:HB1	2.48	0.43
3:Q:149:GLU:HB2	3:Q:150:PRO:HD2	2.00	0.43
5:S:87:LEU:HD21	5:S:107:ALA:HB1	2.00	0.43
10:X:132:ALA:HB1	10:X:136:SER:HB2	1.99	0.43
11:Y:35:ILE:HG21	11:Y:56:GLU:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:91:HIS:HB3	4:R:99:ILE:HG22	2.01	0.43
5:S:12:PHE:H	6:T:19:GLN:HE22	1.67	0.43
6:T:198:LEU:HD12	6:T:243:ILE:HG22	2.00	0.43
3:C:147:GLN:NE2	3:C:160:GLN:OE1	2.52	0.42
3:Q:99:GLU:HG3	11:Y:81:LYS:HD3	2.00	0.42
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.54	0.42
9:W:125:LEU:HD23	9:W:125:LEU:H	1.84	0.42
11:K:52:CYS:SG	11:K:97:MET:HG3	2.58	0.42
4:R:88:ALA:HA	4:R:99:ILE:HG21	2.02	0.42
8:V:112:SER:HB3	8:V:125:LEU:HD13	2.01	0.42
7:G:68:ARG:HH12	14:N:36:ARG:HH22	1.65	0.42
14:N:176:VAL:HG12	14:N:178:LEU:HD13	2.01	0.42
8:V:104:ASP:OD1	8:V:106:THR:HB	2.19	0.42
10:J:3:ILE:HG22	10:J:18:SER:HB3	2.00	0.42
4:D:88:ALA:HA	4:D:99:ILE:HG21	2.02	0.42
4:D:89:VAL:HG12	11:K:61:LYS:HG3	2.02	0.42
11:K:82:LEU:O	11:K:86:MET:HG3	2.19	0.42
11:K:117:HIS:CE1	17:K:402:HOH:O	2.73	0.42
8:V:92:GLY:HA3	8:V:116:HIS:ND1	2.34	0.42
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.20	0.42
7:G:149:ASP:HB2	7:G:150:PRO:CD	2.50	0.42
3:Q:147:GLN:NE2	3:Q:160:GLN:OE1	2.53	0.42
4:R:89:VAL:HG12	11:Y:61:LYS:HG3	2.00	0.42
11:Y:35:ILE:CG2	11:Y:37:ILE:HG13	2.50	0.42
8:H:92:GLY:HA3	8:H:116:HIS:ND1	2.35	0.42
8:H:99:ILE:HG13	8:H:127:LEU:HD22	2.02	0.42
7:U:149:ASP:HB2	7:U:150:PRO:CD	2.50	0.42
5:E:87:LEU:HD21	5:E:107:ALA:HB1	2.01	0.42
11:K:117:HIS:HE1	17:K:402:HOH:O	2.02	0.42
6:F:198:LEU:HD12	6:F:243:ILE:HG22	2.00	0.42
10:J:177:LYS:NZ	10:X:169:GLU:O	2.52	0.42
12:L:8:ASN:HA	12:L:30:ILE:O	2.20	0.41
10:X:1:MET:HE2	10:X:34:LYS:HG2	2.02	0.41
11:Y:125:MET:SD	11:Y:139:LEU:HB3	2.60	0.41
2:B:50:LYS:HD3	2:B:50:LYS:HA	1.81	0.41
8:H:112:SER:HB3	8:H:125:LEU:HD13	2.03	0.41
8:V:35:HIS:HB3	8:V:56:THR:HG21	2.02	0.41
5:E:77:ALA:N	5:E:78:PRO:CD	2.84	0.41
13:M:187:ARG:NH1	8:V:139:GLU:OE1	2.50	0.41
11:Y:51:ASP:OD1	12:Z:98:TYR:OH	2.30	0.41
8:H:104:ASP:OD1	8:H:106:THR:HB	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:169:GLU:O	10:X:177:LYS:NZ	2.53	0.41
11:K:33:LYS:O	11:K:45:MET:HG3	2.21	0.41
8:H:196:ARG:NH2	9:I:150:GLU:HG3	2.35	0.41
1:A:122:THR:HG22	2:B:128:ARG:HH21	1.85	0.41
5:E:12:PHE:H	6:F:19:GLN:HE22	1.69	0.41
13:M:130:VAL:HA	13:M:135:VAL:O	2.20	0.41
1:O:122:THR:HG22	2:P:128:ARG:HH21	1.85	0.41
10:J:1:MET:HE2	10:J:34:LYS:HG2	2.02	0.41
12:L:54:ALA:HA	12:L:109:ASN:HD22	1.85	0.41
13:M:165:ILE:HB	13:M:166:PRO:HD3	2.03	0.41
12:L:138:ALA:HB3	12:L:147:MET:HG2	2.03	0.41
4:R:91:HIS:CD2	4:R:99:ILE:HG22	2.56	0.40
8:V:163:ILE:HG23	8:V:170:GLY:HA2	2.02	0.40
12:Z:147:MET:N	12:Z:148:PRO:CD	2.84	0.40
7:G:165:LYS:HD2	7:G:205:LEU:HD22	2.03	0.40
12:L:147:MET:N	12:L:148:PRO:CD	2.84	0.40
10:X:23:ARG:HH21	11:Y:119:THR:HG21	1.76	0.40
13:M:127:LEU:HG	13:M:142:LEU:HD12	2.04	0.40
8:V:92:GLY:HA3	8:V:116:HIS:CE1	2.56	0.40
10:X:3:ILE:HG12	10:X:136:SER:OG	2.21	0.40
8:H:35:HIS:HB3	8:H:56:THR:HG21	2.03	0.40
2:P:50:LYS:HD3	2:P:50:LYS:HA	1.82	0.40
11:Y:115:ASP:CG	11:Y:119:THR:HG1	2.24	0.40
1:A:75:TYR:HB3	1:A:82:TYR:CD1	2.57	0.40
7:U:165:LYS:HD2	7:U:205:LEU:HD22	2.04	0.40
12:Z:138:ALA:HB3	12:Z:147:MET:HG2	2.04	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	31
2	P	242/258 (94%)	234 (97%)	4 (2%)	4 (2%)	9	31
3	C	238/254 (94%)	232 (98%)	3 (1%)	3 (1%)	12	37
3	Q	238/254 (94%)	232 (98%)	3 (1%)	3 (1%)	12	37
4	D	231/260 (89%)	226 (98%)	5 (2%)	0	100	100
4	R	231/260 (89%)	226 (98%)	5 (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%)	236 (98%)	5 (2%)	0	100	100
6	T	241/288 (84%)	236 (98%)	5 (2%)	0	100	100
7	G	239/252 (95%)	238 (100%)	1 (0%)	0	100	100
7	U	239/252 (95%)	238 (100%)	1 (0%)	0	100	100
8	H	225/232 (97%)	220 (98%)	5 (2%)	0	100	100
8	V	224/232 (97%)	219 (98%)	5 (2%)	0	100	100
9	I	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
9	W	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
10	J	193/198 (98%)	189 (98%)	4 (2%)	0	100	100
10	X	193/198 (98%)	190 (98%)	3 (2%)	0	100	100
11	K	209/211 (99%)	202 (97%)	7 (3%)	0	100	100
11	Y	209/211 (99%)	200 (96%)	9 (4%)	0	100	100
12	L	220/222 (99%)	213 (97%)	7 (3%)	0	100	100
12	Z	220/222 (99%)	214 (97%)	6 (3%)	0	100	100
13	M	231/246 (94%)	219 (95%)	11 (5%)	1 (0%)	34	66
13	a	232/246 (94%)	220 (95%)	12 (5%)	0	100	100
14	N	194/196 (99%)	188 (97%)	6 (3%)	0	100	100
14	b	194/196 (99%)	188 (97%)	6 (3%)	0	100	100
All	All	6284/6612 (95%)	6110 (97%)	157 (2%)	17 (0%)	41	71

All (17) 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
3	C	205	ALA
3	Q	205	ALA
2	B	220	ASN
13	M	83	ALA
2	P	220	ASN
3	Q	183	PRO
3	C	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	89
1	O	209/209 (100%)	206 (99%)	3 (1%)	67	89
2	B	203/216 (94%)	197 (97%)	6 (3%)	41	75
2	P	203/216 (94%)	198 (98%)	5 (2%)	47	78
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	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	T	201/239 (84%)	192 (96%)	9 (4%)	27	61
7	G	206/210 (98%)	198 (96%)	8 (4%)	32	66
7	U	206/210 (98%)	198 (96%)	8 (4%)	32	66
8	H	186/190 (98%)	181 (97%)	5 (3%)	44	77
8	V	185/190 (97%)	181 (98%)	4 (2%)	52	81
9	I	172/173 (99%)	170 (99%)	2 (1%)	71	91
9	W	172/173 (99%)	170 (99%)	2 (1%)	71	91
10	J	173/175 (99%)	168 (97%)	5 (3%)	42	76
10	X	173/175 (99%)	167 (96%)	6 (4%)	36	70
11	K	170/170 (100%)	164 (96%)	6 (4%)	36	70
11	Y	170/170 (100%)	161 (95%)	9 (5%)	22	54
12	L	186/186 (100%)	181 (97%)	5 (3%)	44	77
12	Z	186/186 (100%)	181 (97%)	5 (3%)	44	77
13	M	199/208 (96%)	192 (96%)	7 (4%)	36	70
13	a	200/208 (96%)	193 (96%)	7 (4%)	36	70
14	N	162/162 (100%)	155 (96%)	7 (4%)	29	62
14	b	162/162 (100%)	156 (96%)	6 (4%)	34	68
All	All	5326/5544 (96%)	5143 (97%)	183 (3%)	37	71

All (183) 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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
8	H	68	LEU
8	H	127	LEU
8	H	196	ARG
9	I	37	ASN
9	I	171	LEU
10	J	1	MET
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	62	GLU
11	K	141	SER
11	K	147	LEU
12	L	23	LEU
12	L	49	ASN
12	L	128	VAL
12	L	132	GLN
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	36	ARG
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	191	LEU

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
7	U	125	MET
7	U	208	GLU
7	U	235	ARG
7	U	236	LEU
8	V	30	ASN
8	V	68	LEU
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
10	X	172	MET
11	Y	4	LEU
11	Y	12	VAL
11	Y	35	ILE
11	Y	46	SER
11	Y	62	GLU
11	Y	116	GLU
11	Y	119	THR
11	Y	121	LEU
11	Y	147	LEU
12	Z	23	LEU
12	Z	49	ASN
12	Z	128	VAL
12	Z	132	GLN
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	36	ARG
14	b	39	ASP
14	b	83	LYS

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Mol	Chain	Res	Type
14	b	104	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (100) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	HIS
2	B	20	GLN
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	91	HIS
4	D	100	ASN
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	22	GLN
8	H	66	HIS
8	H	165	ASN

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Mol	Chain	Res	Type
9	I	37	ASN
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	79	HIS
12	L	109	ASN
12	L	158	ASN
13	M	48	ASN
13	M	102	GLN
13	M	179	ASN
13	M	194	ASN
13	M	213	GLN
14	N	161	GLN
1	O	94	HIS
2	P	20	GLN
2	P	58	GLN
2	P	95	GLN
2	P	119	GLN
2	P	123	GLN
3	Q	77	ASN
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	118	ASN
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

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Mol	Chain	Res	Type
6	T	191	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	175	ASN
12	Z	3	ASN
12	Z	49	ASN
12	Z	70	ASN
12	Z	109	ASN
12	Z	158	ASN
13	a	18	ASN
13	a	48	ASN
13	a	102	GLN
13	a	179	ASN
13	a	194	ASN
13	a	213	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 10 ligands modelled in this entry, 10 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%)	-0.32	6 (2%)	59	56	47, 62, 102, 140	0
1	O	250/250 (100%)	-0.30	8 (3%)	47	43	51, 68, 117, 151	0
2	B	244/258 (94%)	-0.22	7 (2%)	51	47	49, 70, 114, 171	0
2	P	244/258 (94%)	-0.28	8 (3%)	46	41	53, 71, 113, 166	0
3	C	240/254 (94%)	0.04	12 (5%)	28	25	51, 79, 146, 187	0
3	Q	240/254 (94%)	-0.03	13 (5%)	25	22	40, 82, 153, 197	0
4	D	235/260 (90%)	-0.28	0	100	100	55, 75, 109, 143	0
4	R	235/260 (90%)	-0.23	6 (2%)	56	52	64, 80, 117, 145	0
5	E	231/234 (98%)	-0.29	2 (0%)	84	84	54, 73, 111, 153	0
5	S	231/234 (98%)	-0.27	3 (1%)	77	77	55, 78, 116, 161	0
6	F	243/288 (84%)	-0.38	5 (2%)	63	61	49, 68, 118, 144	0
6	T	243/288 (84%)	-0.37	4 (1%)	72	71	50, 75, 129, 154	0
7	G	241/252 (95%)	-0.41	2 (0%)	86	86	46, 63, 98, 149	0
7	U	241/252 (95%)	-0.34	3 (1%)	79	79	51, 67, 101, 144	0
8	H	226/232 (97%)	-0.30	6 (2%)	54	50	46, 62, 97, 161	0
8	V	226/232 (97%)	-0.31	7 (3%)	49	44	48, 62, 98, 171	0
9	I	204/205 (99%)	-0.49	2 (0%)	82	82	50, 63, 93, 117	0
9	W	204/205 (99%)	-0.46	4 (1%)	65	63	51, 64, 95, 119	0
10	J	195/198 (98%)	-0.43	2 (1%)	82	82	46, 65, 90, 137	0
10	X	195/198 (98%)	-0.38	3 (1%)	73	73	46, 65, 91, 145	0
11	K	211/211 (100%)	-0.15	2 (0%)	84	84	58, 78, 104, 123	0
11	Y	211/211 (100%)	-0.15	6 (2%)	53	49	58, 79, 107, 127	0
12	L	222/222 (100%)	-0.38	3 (1%)	75	75	49, 70, 111, 144	0
12	Z	222/222 (100%)	-0.33	4 (1%)	68	67	51, 71, 114, 145	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
13	M	233/246 (94%)	-0.53	1 (0%)	92	93	46, 62, 85, 104	0
13	a	233/246 (94%)	-0.51	2 (0%)	84	84	48, 63, 84, 103	0
14	N	196/196 (100%)	-0.55	2 (1%)	82	82	43, 57, 86, 115	0
14	b	196/196 (100%)	-0.54	2 (1%)	82	82	47, 58, 87, 118	0
All	All	6342/6612 (95%)	-0.32	125 (1%)	65	63	40, 69, 112, 197	0

All (125) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	221	ASP	6.8
8	V	224	GLN	5.8
8	V	222	ASP	5.7
2	B	219	ALA	5.6
2	P	219	ALA	5.6
8	V	226	GLU	5.5
2	P	51	VAL	5.1
8	V	221	CYS	5.1
8	H	226	GLU	5.0
8	H	224	GLN	4.8
5	E	202	ASP	4.6
1	A	2	THR	4.6
9	W	1	SER	4.5
8	H	221	CYS	4.4
3	Q	238	LYS	4.3
2	B	220	ASN	4.3
2	P	220	ASN	4.2
2	B	51	VAL	4.2
3	Q	202	GLN	4.1
1	O	2	THR	4.0
10	X	1	MET	4.0
12	L	174	TYR	4.0
10	J	1	MET	4.0
3	C	202	GLN	3.9
2	P	221	ASP	3.8
3	Q	239	GLN	3.8
12	Z	174	TYR	3.8
6	F	181	GLU	3.8
3	Q	236	GLN	3.7
1	O	1	MET	3.6
2	P	59	ASP	3.6
8	H	225	GLU	3.6

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Mol	Chain	Res	Type	RSRZ
5	S	202	ASP	3.5
3	C	235	GLU	3.5
9	I	1	SER	3.5
3	Q	240	GLU	3.4
14	b	195	GLN	3.4
1	A	1	MET	3.3
3	C	206	LYS	3.3
1	O	249	ALA	3.3
3	C	239	GLN	3.3
6	F	202	ASP	3.3
2	P	222	GLY	3.2
3	Q	141	ASP	3.2
6	F	244	ASN	3.2
3	Q	50	LEU	3.2
11	K	47	GLY	3.1
7	U	242	GLN	3.1
3	C	205	ALA	3.1
3	C	238	LYS	3.1
11	Y	47	GLY	3.0
3	Q	206	LYS	3.0
8	H	222	ASP	3.0
4	R	217	GLN	2.9
4	R	241	ALA	2.9
13	a	1	THR	2.8
1	A	249	ALA	2.8
8	V	225	GLU	2.8
1	O	52	SER	2.8
9	I	131	GLU	2.8
4	R	125	LEU	2.8
14	b	105	LYS	2.8
7	U	2	GLY	2.8
3	C	236	GLN	2.7
14	N	105	LYS	2.7
14	N	195	GLN	2.7
2	B	217	LYS	2.7
1	A	3	ASP	2.6
3	C	3	ASP	2.6
4	R	230	GLU	2.6
3	C	50	LEU	2.6
3	Q	204	GLY	2.6
8	V	145	ASP	2.6
11	K	96	SER	2.6

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Mol	Chain	Res	Type	RSRZ
10	X	96	ARG	2.6
1	O	250	LEU	2.5
6	F	215	CYS	2.5
6	T	2	THR	2.5
3	Q	139	ARG	2.5
5	E	233	ILE	2.5
10	J	194	ASP	2.4
5	S	3	ASN	2.4
10	X	194	ASP	2.4
3	C	141	ASP	2.4
6	T	244	ASN	2.3
5	S	165	GLN	2.3
12	Z	173	LYS	2.3
9	W	133	LYS	2.3
4	R	203	LYS	2.3
1	O	4	ARG	2.3
7	G	230	GLU	2.3
11	Y	211	GLY	2.3
3	Q	3	ASP	2.3
9	W	131	GLU	2.3
2	B	222	GLY	2.3
1	O	203	GLU	2.3
11	Y	46	SER	2.3
6	F	205	GLU	2.2
12	L	166	GLY	2.2
11	Y	201	GLU	2.2
12	Z	165	ASN	2.2
2	P	203	SER	2.2
11	Y	96	SER	2.2
8	V	223	ILE	2.1
2	P	52	THR	2.1
11	Y	40	TYR	2.1
12	Z	161	GLU	2.1
1	A	228	PRO	2.1
4	R	114	ARG	2.1
3	Q	205	ALA	2.1
3	C	175	LYS	2.1
7	U	181	LYS	2.1
2	B	218	GLY	2.1
8	H	219	ASN	2.1
3	Q	187	GLU	2.1
13	M	69	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
13	a	233	ILE	2.1
7	G	241	GLU	2.1
12	L	1	GLN	2.0
9	W	130	ASP	2.0
3	C	188	GLU	2.0
6	T	181	GLU	2.0
1	A	231	LYS	2.0
1	O	201	GLU	2.0
6	T	180	PRO	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	H	301	1/1	0.93	0.14	51,51,51,51	0
15	MG	I	301	1/1	0.95	0.15	63,63,63,63	0
15	MG	G	301	1/1	0.96	0.11	67,67,67,67	0
15	MG	K	301	1/1	0.96	0.15	45,45,45,45	0
15	MG	N	201	1/1	0.96	0.09	50,50,50,50	0
15	MG	I	302	1/1	0.97	0.10	51,51,51,51	0
15	MG	Z	301	1/1	0.97	0.24	66,66,66,66	0
15	MG	L	301	1/1	0.99	0.07	67,67,67,67	0
16	CL	G	302	1/1	0.99	0.09	42,42,42,42	0
16	CL	U	301	1/1	0.99	0.16	50,50,50,50	0

6.5 Other polymers (i)

There are no such residues in this entry.