



Full wwPDB X-ray Structure Validation Report ⓘ

May 30, 2020 – 02:46 am BST

PDB ID : 6HTB
Title : Yeast 20S proteasome with human beta2c (S171G)
Authors : Huber, E.M.; Groll, M.
Deposited on : 2018-10-03
Resolution : 2.70 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

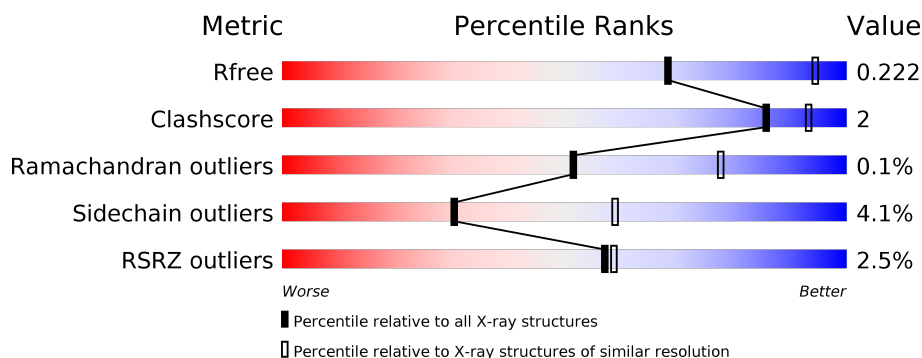
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	250	<div> <div>3%</div> <div> <div></div> <div>93%</div> <div>• • •</div> </div> </div>
1	O	250	<div> <div>3%</div> <div> <div></div> <div>90%</div> <div>• • •</div> </div> </div>
2	B	258	<div> <div>5%</div> <div> <div></div> <div>86%</div> <div>8% • 5%</div> </div> </div>
2	P	258	<div> <div>6%</div> <div> <div></div> <div>84%</div> <div>9% • 5%</div> </div> </div>
3	C	254	<div> <div>5%</div> <div> <div></div> <div>84%</div> <div>10% 6%</div> </div> </div>
3	Q	254	<div> <div>7%</div> <div> <div></div> <div>85%</div> <div>8% • 6%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
4	D	260	
4	R	260	
5	E	234	
5	S	234	
6	F	288	
6	T	288	
7	G	252	
7	U	252	
8	H	234	
8	V	234	
9	I	205	
9	W	205	
10	J	198	
10	X	198	
11	K	212	
11	Y	212	
12	L	222	
12	Z	222	
13	M	246	
13	a	246	
14	N	196	
14	b	196	

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 49877 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
1	A	240	Total	C	N	O	S	0	0	0
			1842	1171	305	362	4			
1	O	240	Total	C	N	O	S	0	0	0
			1842	1171	305	362	4			

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 8 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	219	Total	C	N	O	S	0	0	0
			1648	1038	282	316	12			
8	V	219	Total	C	N	O	S	0	0	0
			1648	1038	282	316	12			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	171	GLY	SER	engineered mutation	UNP Q99436
V	171	GLY	SER	engineered mutation	UNP Q99436

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	212	Total	C	N	O	S	0	0	0
			1644	1045	280	312	7			
11	Y	212	Total	C	N	O	S	0	0	0
			1644	1045	280	312	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	222	Total	C	N	O	S	0	0	0
			1757	1115	303	335	4			
12	Z	222	Total	C	N	O	S	0	0	0
			1757	1115	303	335	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	224	Total	C	N	O	S	0	0	0
			1753	1108	300	338	7			
13	a	224	Total	C	N	O	S	0	0	0
			1753	1108	300	338	7			

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

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

- 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	K	1	Total Mg 1 1	0	0
15	I	2	Total Mg 2 2	0	0
15	W	1	Total Mg 1 1	0	0
15	Z	1	Total Mg 1 1	0	0
15	N	1	Total Mg 1 1	0	0
15	L	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	1	Total Cl 1 1	0	0
16	U	1	Total Cl 1 1	0	0

- Molecule 17 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	35	Total O 35 35	0	0
17	B	34	Total O 34 34	0	0
17	C	34	Total O 34 34	0	0
17	D	31	Total O 31 31	0	0
17	E	20	Total O 20 20	0	0
17	F	25	Total O 25 25	0	0
17	G	40	Total O 40 40	0	0
17	H	27	Total O 27 27	0	0
17	I	36	Total O 36 36	0	0

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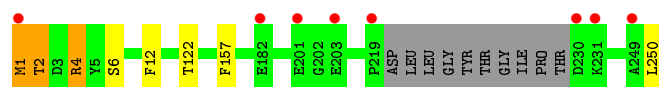
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	J	41	Total 41	O 41	0	0
17	K	54	Total 54	O 54	0	0
17	L	33	Total 33	O 33	0	0
17	M	36	Total 36	O 36	0	0
17	N	34	Total 34	O 34	0	0
17	O	17	Total 17	O 17	0	0
17	P	24	Total 24	O 24	0	0
17	Q	26	Total 26	O 26	0	0
17	R	25	Total 25	O 25	0	0
17	S	23	Total 23	O 23	0	0
17	T	29	Total 29	O 29	0	0
17	U	35	Total 35	O 35	0	0
17	V	26	Total 26	O 26	0	0
17	W	44	Total 44	O 44	0	0
17	X	45	Total 45	O 45	0	0
17	Y	41	Total 41	O 41	0	0
17	Z	41	Total 41	O 41	0	0
17	a	44	Total 44	O 44	0	0
17	b	31	Total 31	O 31	0	0

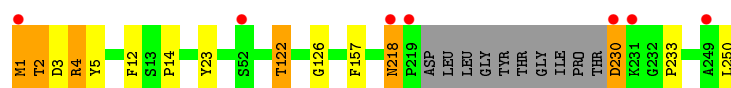
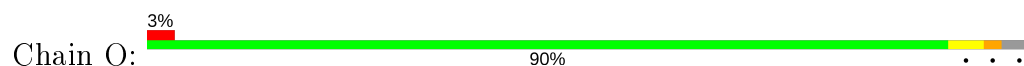
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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 ($\text{RSRZ} > 2$). 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.

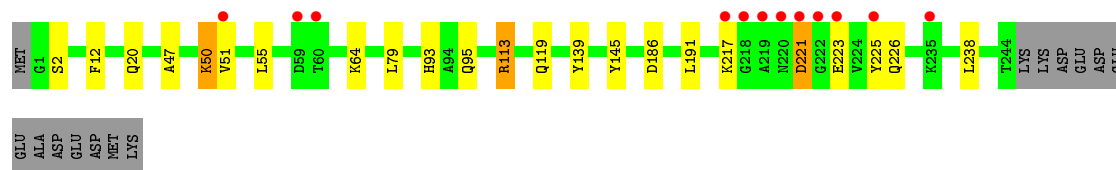
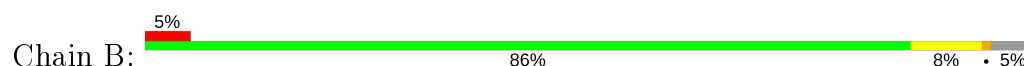
- Molecule 1: Proteasome subunit alpha type-2



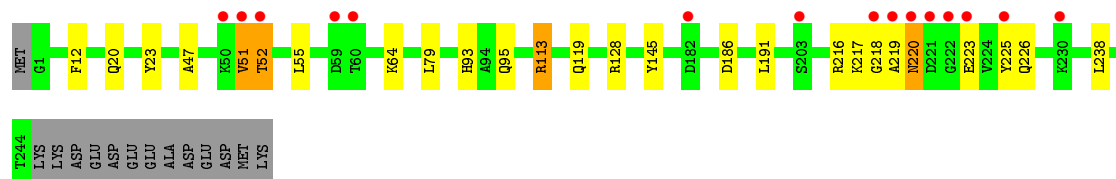
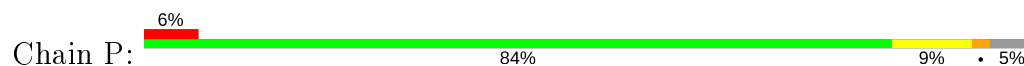
- Molecule 1: Proteasome subunit alpha type-2



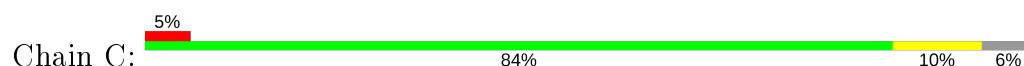
- Molecule 2: Proteasome subunit alpha type-3

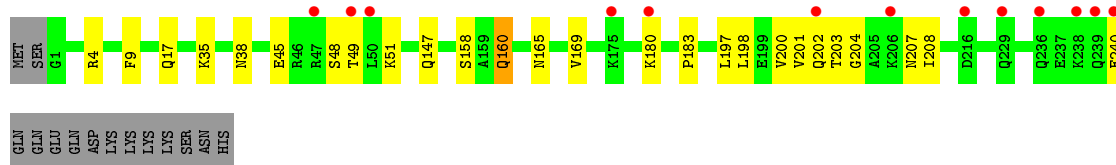


- Molecule 2: Proteasome subunit alpha type-3

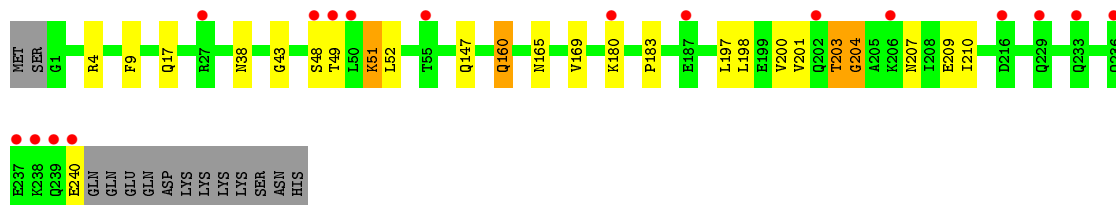
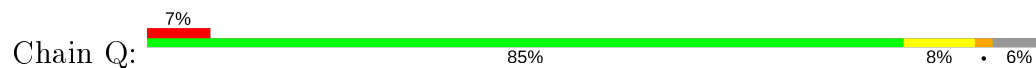


- Molecule 3: Proteasome subunit alpha type-4

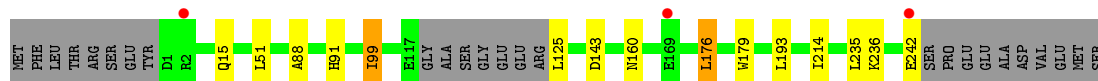
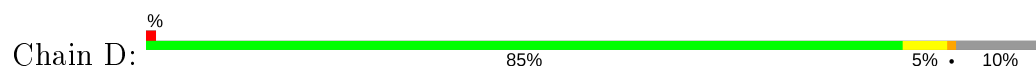




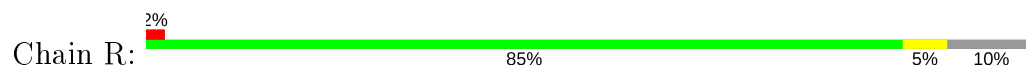
• Molecule 3: Proteasome subunit alpha type-4



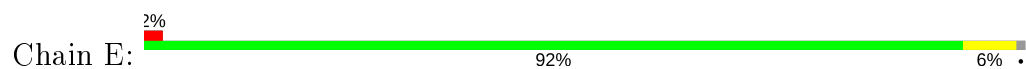
• Molecule 4: Proteasome subunit alpha type-5



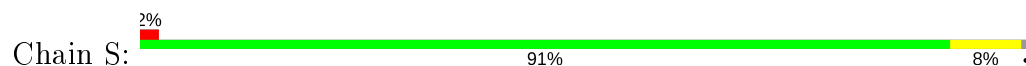
• Molecule 4: Proteasome subunit alpha type-5



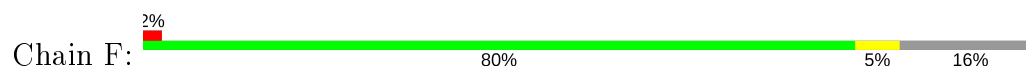
• Molecule 5: Proteasome subunit alpha type-6



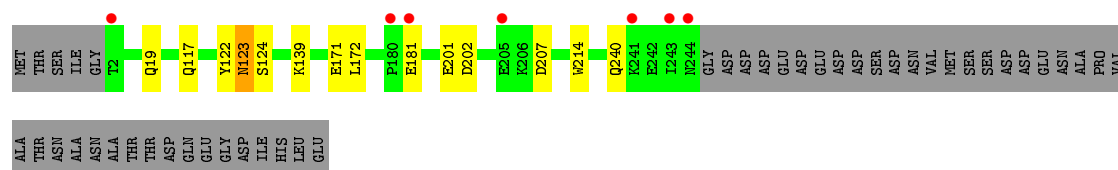
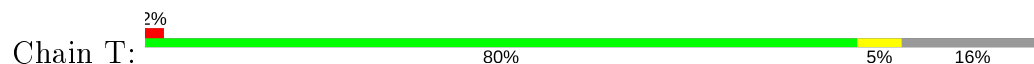
• Molecule 5: Proteasome subunit alpha type-6



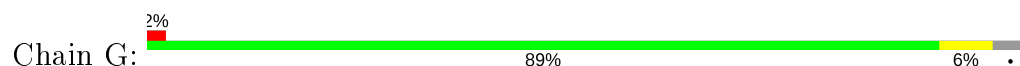
• Molecule 6: Probable proteasome subunit alpha type-7



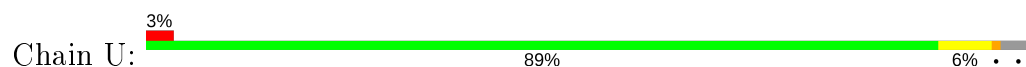
- Molecule 6: Probable proteasome subunit alpha type-7



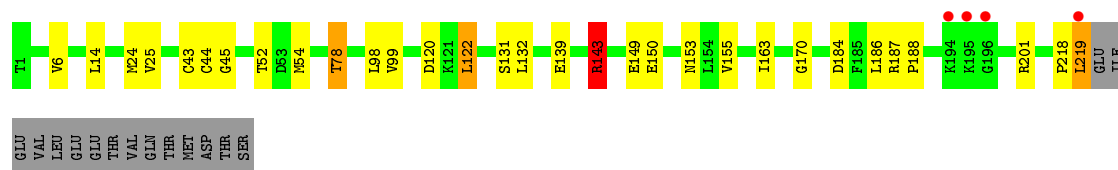
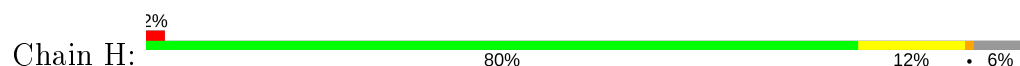
- Molecule 7: Proteasome subunit alpha type-1



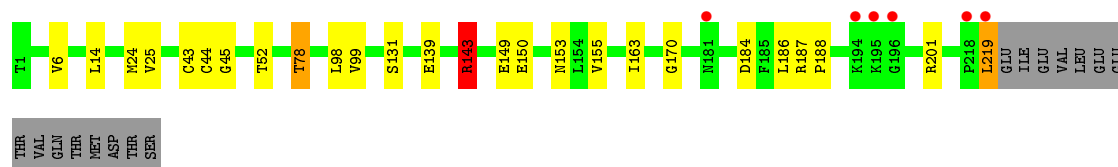
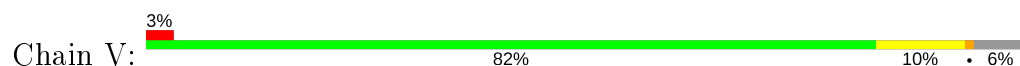
- Molecule 7: Proteasome subunit alpha type-1



- Molecule 8: Proteasome subunit beta type-7



- Molecule 8: Proteasome subunit beta type-7



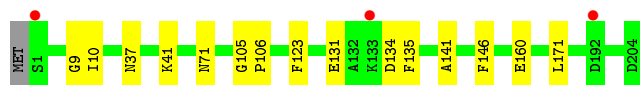
- Molecule 9: Proteasome subunit beta type-3

Chain I:  90% 9%



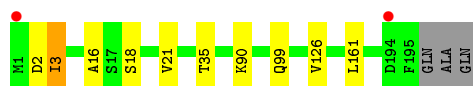
- Molecule 9: Proteasome subunit beta type-3

Chain W:  92% 7%



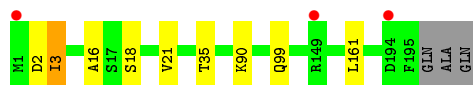
- Molecule 10: Proteasome subunit beta type-4

Chain J:  93% 5% ..



- Molecule 10: Proteasome subunit beta type-4

Chain X:  94%



- Molecule 11: Proteasome subunit beta type-5

Chain K:  95% 5%



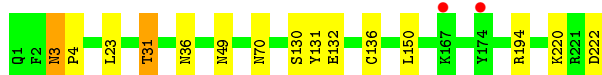
- Molecule 11: Proteasome subunit beta type-5

Chain Y:  95% 5%

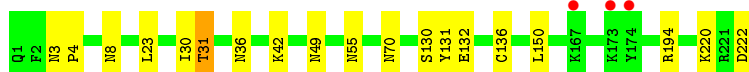


- Molecule 12: Proteasome subunit beta type-6

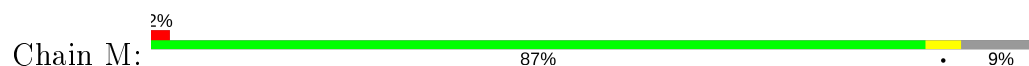
Chain L:  93% 6% .



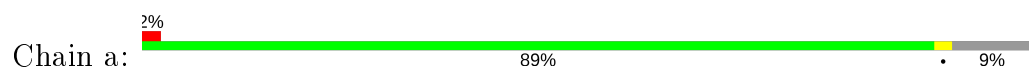
- Molecule 12: Proteasome subunit beta type-6



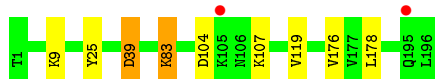
- Molecule 13: Proteasome subunit beta type-7



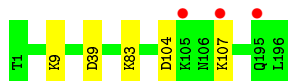
- Molecule 13: Proteasome subunit beta type-7



- Molecule 14: Proteasome subunit beta type-1



- Molecule 14: Proteasome subunit beta type-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	135.68Å 300.58Å 145.05Å 90.00° 113.06° 90.00°	Depositor
Resolution (Å)	15.00 – 2.70 15.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.2 (15.00-2.70) 98.8 (15.00-2.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.46 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.193 , 0.220 0.196 , 0.222	Depositor DCC
R_{free} test set	14322 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	47.8	Xtriage
Anisotropy	0.689	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 35.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	49877	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.32% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [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	0.44	0/1876	0.61	1/2535 (0.0%)
1	O	0.43	0/1876	0.63	3/2535 (0.1%)
2	B	0.42	0/1934	0.63	0/2618
2	P	0.41	0/1934	0.65	0/2618
3	C	0.39	0/1910	0.65	0/2586
3	Q	0.40	0/1910	0.66	1/2586 (0.0%)
4	D	0.35	0/1837	0.59	0/2475
4	R	0.35	0/1837	0.59	0/2475
5	E	0.35	0/1800	0.59	0/2433
5	S	0.35	0/1800	0.59	0/2433
6	F	0.36	0/1932	0.56	0/2609
6	T	0.36	0/1932	0.56	0/2609
7	G	0.39	0/1945	0.66	2/2634 (0.1%)
7	U	0.40	1/1945 (0.1%)	0.78	4/2634 (0.2%)
8	H	0.48	0/1675	0.98	4/2267 (0.2%)
8	V	0.36	0/1675	0.86	5/2267 (0.2%)
9	I	0.52	0/1611	0.66	1/2174 (0.0%)
9	W	0.45	0/1611	0.64	1/2174 (0.0%)
10	J	0.36	0/1589	0.62	0/2142
10	X	0.36	0/1589	0.62	0/2142
11	K	0.35	0/1681	0.61	2/2274 (0.1%)
11	Y	0.35	0/1681	0.61	2/2274 (0.1%)
12	L	0.36	0/1795	0.60	0/2420
12	Z	0.36	0/1795	0.60	0/2420
13	M	0.42	0/1783	0.64	0/2420
13	a	0.38	0/1783	0.64	0/2420
14	N	0.34	0/1541	0.59	0/2087
14	b	0.34	0/1541	0.59	0/2087
All	All	0.39	1/49818 (0.0%)	0.65	26/67348 (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
7	G	0	1
7	U	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	U	68	ARG	CZ-NH2	-5.85	1.25	1.33

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	143	ARG	NE-CZ-NH1	-21.06	109.77	120.30
8	H	143	ARG	NE-CZ-NH2	20.26	130.43	120.30
7	U	68	ARG	NE-CZ-NH1	17.02	128.81	120.30
8	V	143	ARG	NE-CZ-NH2	-16.00	112.30	120.30
7	U	68	ARG	NE-CZ-NH2	-15.43	112.58	120.30
7	G	68	ARG	NE-CZ-NH2	13.46	127.03	120.30
8	V	143	ARG	NE-CZ-NH1	13.21	126.91	120.30
7	U	68	ARG	CG-CD-NE	-8.52	93.91	111.80
8	H	143	ARG	CD-NE-CZ	8.24	135.13	123.60
8	V	219	LEU	CD1-CG-CD2	-8.18	85.96	110.50
8	H	219	LEU	CD1-CG-CD2	-7.64	87.58	110.50
8	V	143	ARG	CD-NE-CZ	7.36	133.90	123.60
7	U	68	ARG	CD-NE-CZ	7.03	133.44	123.60
1	A	2	THR	N-CA-C	-6.42	93.67	111.00
8	V	219	LEU	CA-CB-CG	5.83	128.71	115.30
11	Y	4	LEU	CA-CB-CG	5.80	128.63	115.30
3	Q	204	GLY	N-CA-C	5.56	127.01	113.10
11	K	4	LEU	CA-CB-CG	5.56	128.08	115.30
1	O	218	ASN	C-N-CD	5.42	139.79	128.40
1	O	3	ASP	N-CA-C	-5.33	96.62	111.00
1	O	2	THR	N-CA-C	-5.24	96.86	111.00
11	Y	69	ARG	NE-CZ-NH1	5.15	122.87	120.30
9	I	127	GLY	N-CA-C	5.12	125.89	113.10
7	G	68	ARG	NE-CZ-NH1	-5.09	117.76	120.30
11	K	69	ARG	NE-CZ-NH1	5.06	122.83	120.30
9	W	105	GLY	C-N-CD	5.06	139.02	128.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	G	68	ARG	Sidechain
7	U	68	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1842	0	1855	8	0
1	O	1842	0	1855	19	0
2	B	1904	0	1904	23	0
2	P	1904	0	1904	24	0
3	C	1881	0	1895	17	0
3	Q	1881	0	1894	22	0
4	D	1813	0	1797	7	0
4	R	1813	0	1797	4	0
5	E	1773	0	1775	8	0
5	S	1773	0	1775	7	0
6	F	1892	0	1883	4	0
6	T	1892	0	1883	4	0
7	G	1907	0	1901	5	0
7	U	1907	0	1901	8	0
8	H	1648	0	1673	21	0
8	V	1648	0	1673	16	0
9	I	1581	0	1574	12	0
9	W	1581	0	1574	7	0
10	J	1561	0	1569	4	0
10	X	1561	0	1569	3	0
11	K	1644	0	1595	3	0
11	Y	1644	0	1595	3	0
12	L	1757	0	1711	9	0
12	Z	1757	0	1711	9	0
13	M	1753	0	1754	2	0
13	a	1753	0	1754	0	0
14	N	1512	0	1481	4	0
14	b	1512	0	1481	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	G	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	W	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
17	A	35	0	0	0	0
17	B	34	0	0	3	0
17	C	34	0	0	0	0
17	D	31	0	0	0	0
17	E	20	0	0	0	0
17	F	25	0	0	0	0
17	G	40	0	0	0	0
17	H	27	0	0	0	0
17	I	36	0	0	0	0
17	J	41	0	0	0	0
17	K	54	0	0	0	0
17	L	33	0	0	0	0
17	M	36	0	0	1	0
17	N	34	0	0	0	0
17	O	17	0	0	0	0
17	P	24	0	0	2	0
17	Q	26	0	0	0	0
17	R	25	0	0	0	0
17	S	23	0	0	1	0
17	T	29	0	0	0	0
17	U	35	0	0	0	0
17	V	26	0	0	0	0
17	W	44	0	0	0	0
17	X	45	0	0	0	0
17	Y	41	0	0	0	0
17	Z	41	0	0	0	0
17	a	44	0	0	0	0
17	b	31	0	0	0	0
All	All	49877	0	48733	206	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 (206) 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)
3:Q:197:LEU:O	3:Q:201:VAL:CG2	1.85	1.23
3:Q:197:LEU:O	3:Q:201:VAL:HG23	0.94	1.12
3:Q:203:THR:HG22	3:Q:204:GLY:H	1.22	1.02
3:Q:197:LEU:C	3:Q:201:VAL:HG23	1.84	0.95
3:Q:165:ASN:HB2	3:Q:200:VAL:HG11	1.50	0.94
2:B:145:TYR:OH	2:B:217:LYS:N	2.01	0.93
2:B:145:TYR:OH	2:B:217:LYS:HB2	1.69	0.91
3:C:203:THR:HG22	3:C:204:GLY:N	1.89	0.88
3:C:202:GLN:O	3:C:203:THR:OG1	1.93	0.87
3:C:203:THR:CG2	3:C:204:GLY:H	1.87	0.87
3:C:203:THR:HG22	3:C:204:GLY:H	1.39	0.85
1:A:4:ARG:HB2	2:B:2:SER:OG	1.77	0.85
3:Q:209:GLU:O	3:Q:210:ILE:HD13	1.77	0.84
3:Q:165:ASN:CB	3:Q:200:VAL:HG11	2.07	0.84
2:B:145:TYR:OH	2:B:217:LYS:CB	2.26	0.83
8:V:143:ARG:NH1	8:V:150:GLU:OE1	2.13	0.81
12:L:220:LYS:HE3	12:L:222:ASP:OD1	1.80	0.81
2:P:51:VAL:HG12	2:P:52:THR:H	1.45	0.81
12:Z:220:LYS:HE3	12:Z:222:ASP:OD1	1.83	0.79
2:P:219:ALA:HB3	2:P:223:GLU:O	1.82	0.78
3:Q:203:THR:HG22	3:Q:204:GLY:N	2.02	0.74
8:H:143:ARG:NH1	8:H:150:GLU:OE1	2.23	0.72
2:P:51:VAL:HG12	2:P:52:THR:N	2.03	0.71
8:H:149:GLU:O	8:H:153:ASN:ND2	2.20	0.71
1:A:4:ARG:CB	2:B:2:SER:OG	2.38	0.70
8:V:184:ASP:HB3	8:V:186:LEU:HD11	1.73	0.70
3:C:160:GLN:HA	3:C:160:GLN:HE21	1.56	0.70
8:H:184:ASP:HB3	8:H:186:LEU:HD11	1.76	0.68
3:Q:160:GLN:HA	3:Q:160:GLN:HE21	1.58	0.67
2:B:12:PHE:H	3:C:17:GLN:HE22	1.43	0.67
7:G:68:ARG:NH1	14:N:39:ASP:OD2	2.29	0.66
3:C:203:THR:CG2	3:C:204:GLY:N	2.48	0.65
2:B:221:ASP:C	17:B:301:HOH:O	2.22	0.64
3:C:48:SER:HB2	3:C:207:ASN:HD21	1.62	0.64
1:A:4:ARG:HD3	5:E:122:TYR:HD2	1.63	0.64
2:P:225:TYR:CE1	2:P:226:GLN:O	2.51	0.64
3:C:165:ASN:HB2	3:C:200:VAL:HG11	1.80	0.63
1:O:12:PHE:H	2:P:20:GLN:HE22	1.45	0.63
5:E:12:PHE:H	6:F:19:GLN:HE22	1.45	0.63
2:B:95:GLN:HE22	9:I:71:ASN:HD22	1.45	0.63
2:B:145:TYR:OH	2:B:217:LYS:CA	2.47	0.62
5:S:12:PHE:H	6:T:19:GLN:HE22	1.45	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:145:TYR:HH	2:B:217:LYS:H	1.43	0.62
1:A:4:ARG:HB2	2:B:2:SER:CB	2.28	0.61
3:C:202:GLN:O	3:C:202:GLN:HG3	1.99	0.61
3:Q:197:LEU:HB3	3:Q:201:VAL:HG21	1.82	0.61
8:H:219:LEU:HD11	9:I:194:VAL:HG23	1.82	0.61
7:G:23:PHE:O	7:G:26:THR:HB	2.01	0.60
8:H:132:LEU:HD22	14:N:25:TYR:CE1	2.37	0.59
2:B:51:VAL:O	2:B:51:VAL:HG22	2.02	0.59
1:O:230:ASP:N	1:O:230:ASP:OD1	2.36	0.59
1:A:12:PHE:H	2:B:20:GLN:HE22	1.50	0.59
3:Q:48:SER:HB2	3:Q:207:ASN:ND2	2.18	0.59
1:O:2:THR:OG1	1:O:4:ARG:HD2	2.03	0.58
2:P:95:GLN:HE22	9:W:71:ASN:HD22	1.49	0.58
3:Q:200:VAL:O	3:Q:200:VAL:HG12	2.02	0.58
2:B:139:TYR:OH	2:B:217:LYS:HE2	2.04	0.57
8:H:184:ASP:HB3	8:H:186:LEU:CD1	2.34	0.57
9:I:15:THR:HG23	9:I:120:ILE:HG12	1.86	0.57
7:G:99:TYR:O	8:H:78:THR:HB	2.04	0.57
8:V:184:ASP:HB3	8:V:186:LEU:CD1	2.34	0.57
12:Z:31:THR:CG2	12:Z:36:ASN:HD21	2.17	0.57
2:P:51:VAL:O	2:P:52:THR:HG23	2.04	0.57
8:V:163:ILE:HG23	8:V:170:GLY:HA2	1.87	0.57
3:Q:197:LEU:C	3:Q:201:VAL:CG2	2.56	0.57
2:P:93:HIS:HB3	17:P:301:HOH:O	2.04	0.56
7:U:23:PHE:O	7:U:26:THR:HB	2.04	0.56
2:B:50:LYS:O	2:B:51:VAL:HG12	2.06	0.56
8:H:45:GLY:HA3	8:H:52:THR:HG21	1.88	0.55
3:Q:203:THR:CG2	3:Q:204:GLY:H	2.03	0.55
1:O:1:MET:CE	7:U:124:TYR:HE2	2.18	0.55
8:H:163:ILE:HG23	8:H:170:GLY:HA2	1.88	0.55
2:B:145:TYR:HH	2:B:217:LYS:CB	2.19	0.55
9:I:120:ILE:HD12	9:I:136:ILE:HG12	1.88	0.55
12:L:31:THR:CG2	12:L:36:ASN:HD21	2.19	0.55
12:Z:31:THR:HG22	12:Z:36:ASN:HD21	1.73	0.54
8:H:218:PRO:C	8:H:219:LEU:HG	2.28	0.53
2:P:12:PHE:H	3:Q:17:GLN:HE22	1.55	0.53
2:P:216:ARG:HB3	2:P:218:GLY:H	1.73	0.53
3:Q:204:GLY:O	3:Q:207:ASN:N	2.41	0.53
12:L:31:THR:HG22	12:L:36:ASN:HD21	1.73	0.53
2:P:220:ASN:N	2:P:220:ASN:OD1	2.42	0.53
8:V:45:GLY:HA3	8:V:52:THR:HG21	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.92	0.52
8:V:186:LEU:HD12	8:V:186:LEU:N	2.24	0.52
6:T:123:ASN:HD22	6:T:124:SER:N	2.08	0.52
3:C:197:LEU:HD13	3:C:208:ILE:HG23	1.90	0.51
1:O:1:MET:HG3	6:T:122:TYR:CE1	2.45	0.51
8:H:186:LEU:HD12	8:H:186:LEU:N	2.26	0.51
3:Q:48:SER:HB2	3:Q:207:ASN:HD21	1.76	0.51
5:E:92:ASN:HD21	12:L:70:ASN:HD21	1.58	0.51
1:O:2:THR:OG1	1:O:4:ARG:HG2	2.11	0.51
6:T:123:ASN:HD22	6:T:123:ASN:C	2.15	0.51
1:A:4:ARG:HD3	5:E:122:TYR:CD2	2.45	0.51
2:P:145:TYR:OH	2:P:217:LYS:HB2	2.11	0.51
1:O:218:ASN:O	1:O:233:PRO:HD2	2.11	0.50
2:P:51:VAL:C	2:P:52:THR:HG23	2.31	0.50
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.93	0.50
3:C:45:GLU:HG3	3:C:201:VAL:HG22	1.92	0.50
6:F:123:ASN:C	6:F:123:ASN:HD22	2.15	0.50
9:I:123:PHE:N	9:I:123:PHE:CD1	2.80	0.50
6:F:123:ASN:HD22	6:F:124:SER:N	2.10	0.50
11:K:128:CYS:HB2	11:K:137:TYR:CZ	2.47	0.49
8:H:143:ARG:NH1	8:H:150:GLU:CD	2.65	0.49
8:H:25:VAL:HG11	9:I:146:PHE:CD2	2.47	0.49
3:Q:197:LEU:HB3	3:Q:201:VAL:CG2	2.42	0.49
8:H:143:ARG:NH1	8:H:150:GLU:OE2	2.46	0.49
3:C:9:PHE:H	4:D:15:GLN:HE22	1.60	0.49
13:M:106:LYS:HE3	17:M:330:HOH:O	2.13	0.49
11:K:128:CYS:HB2	11:K:137:TYR:CE2	2.48	0.48
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.96	0.48
8:H:44:CYS:HB2	8:H:99:VAL:HB	1.95	0.48
11:Y:128:CYS:HB2	11:Y:137:TYR:CZ	2.49	0.48
8:H:120:ASP:HB3	8:H:122:LEU:HD22	1.96	0.47
2:B:95:GLN:NE2	9:I:71:ASN:HD22	2.11	0.47
8:V:44:CYS:HB2	8:V:99:VAL:HB	1.95	0.47
4:R:88:ALA:HA	4:R:99:ILE:HG21	1.96	0.47
8:V:143:ARG:NH1	8:V:150:GLU:CD	2.68	0.47
9:W:134:ASP:OD1	9:W:135:PHE:N	2.47	0.47
14:N:83:LYS:HG3	14:N:119:VAL:CG2	2.45	0.47
2:P:47:ALA:HB1	2:P:64:LYS:HD2	1.97	0.47
3:Q:198:LEU:HD23	3:Q:198:LEU:HA	1.74	0.47
1:O:5:TYR:HB3	1:O:126:GLY:CA	2.44	0.47
11:Y:128:CYS:HB2	11:Y:137:TYR:CE2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:113:ARG:NE	17:B:302:HOH:O	2.47	0.47
1:O:2:THR:OG1	1:O:4:ARG:CG	2.63	0.47
4:D:88:ALA:HA	4:D:99:ILE:HG21	1.97	0.46
12:Z:3:ASN:HD22	12:Z:4:PRO:HD2	1.81	0.46
2:B:47:ALA:HB1	2:B:64:LYS:HD2	1.97	0.46
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.97	0.46
8:V:25:VAL:HG11	9:W:146:PHE:CD2	2.50	0.46
2:B:145:TYR:CZ	2:B:217:LYS:HB2	2.49	0.46
8:V:187:ARG:HA	8:V:188:PRO:HA	1.78	0.46
3:Q:9:PHE:H	4:R:15:GLN:HE22	1.64	0.46
1:O:5:TYR:HB3	1:O:126:GLY:HA2	1.98	0.45
2:P:217:LYS:C	2:P:219:ALA:H	2.20	0.45
9:W:106:PRO:HD2	9:W:123:PHE:HB2	1.97	0.45
1:O:1:MET:HE3	7:U:124:TYR:HE2	1.79	0.45
12:L:3:ASN:HD22	12:L:4:PRO:HD2	1.81	0.45
2:B:225:TYR:CE1	2:B:226:GLN:O	2.69	0.45
8:H:6:VAL:HG22	8:H:155:VAL:CG2	2.47	0.45
2:P:217:LYS:O	2:P:219:ALA:N	2.40	0.45
3:C:203:THR:HG23	3:C:204:GLY:H	1.75	0.45
8:V:6:VAL:HG22	8:V:155:VAL:CG2	2.47	0.45
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.51	0.45
5:E:92:ASN:HD21	12:L:70:ASN:ND2	2.15	0.44
2:P:51:VAL:O	2:P:52:THR:OG1	2.22	0.44
5:S:147:GLN:NE2	17:S:302:HOH:O	2.50	0.44
2:P:95:GLN:NE2	9:W:71:ASN:HD22	2.14	0.44
1:A:1:MET:HG3	6:F:122:TYR:CE1	2.52	0.44
9:W:9:GLY:HA3	9:W:41:LYS:HE2	1.99	0.44
4:D:91:HIS:HB3	4:D:99:ILE:CG2	2.47	0.44
7:G:167:GLN:HE21	7:G:171:THR:HG23	1.83	0.43
4:D:176:LEU:HD22	5:E:55:LEU:CD2	2.49	0.43
2:P:220:ASN:O	2:P:223:GLU:HG2	2.18	0.43
7:U:99:TYR:O	8:V:78:THR:HB	2.19	0.43
5:E:92:ASN:ND2	12:L:70:ASN:HD21	2.16	0.43
9:I:9:GLY:HA3	9:I:41:LYS:HE2	1.99	0.43
1:O:1:MET:HE2	7:U:124:TYR:CE2	2.54	0.43
8:H:54:MET:HG3	9:I:95:TYR:CG	2.54	0.43
5:E:87:LEU:HD21	5:E:107:ALA:HB1	2.00	0.43
5:S:87:LEU:HD21	5:S:107:ALA:HB1	2.00	0.42
1:O:4:ARG:HD3	5:S:122:TYR:CD2	2.52	0.42
9:I:36:SER:HB2	10:J:126:VAL:HG11	2.01	0.42
7:U:167:GLN:HE21	7:U:171:THR:HG23	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.19	0.42
1:O:1:MET:HE2	7:U:124:TYR:HE2	1.84	0.42
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.55	0.42
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.55	0.42
8:V:153:ASN:HD22	8:V:153:ASN:N	2.17	0.42
4:R:91:HIS:HB3	4:R:99:ILE:CG2	2.48	0.42
8:V:149:GLU:O	8:V:153:ASN:ND2	2.53	0.42
3:C:198:LEU:HA	3:C:198:LEU:HD23	1.81	0.42
12:Z:131:TYR:O	12:Z:132:GLU:HG3	2.20	0.42
8:H:139:GLU:HA	8:H:139:GLU:OE2	2.20	0.41
12:L:194:ARG:O	8:V:25:VAL:HA	2.19	0.41
3:C:35:LYS:HG2	3:C:158:SER:O	2.20	0.41
3:C:48:SER:HB2	3:C:207:ASN:ND2	2.33	0.41
2:P:217:LYS:C	2:P:219:ALA:N	2.73	0.41
3:Q:43:GLY:HA2	3:Q:210:ILE:HD13	2.01	0.41
1:A:4:ARG:HB3	2:B:2:SER:OG	2.19	0.41
14:N:176:VAL:HG12	14:N:178:LEU:HD13	2.02	0.41
4:D:91:HIS:HB3	4:D:99:ILE:HG22	2.03	0.41
10:X:21:VAL:HG11	11:Y:122:LEU:HD11	2.03	0.41
2:B:93:HIS:HB3	17:B:302:HOH:O	2.20	0.41
9:I:141:ALA:HB2	9:I:177:ASP:HB2	2.03	0.41
8:H:25:VAL:HA	12:Z:194:ARG:O	2.20	0.41
1:O:4:ARG:HD3	5:S:122:TYR:HD2	1.86	0.41
8:H:187:ARG:HA	8:H:188:PRO:HA	1.80	0.41
12:L:131:TYR:O	12:L:132:GLU:HG3	2.21	0.41
10:J:3:ILE:HG23	10:J:18:SER:HB3	2.03	0.41
2:P:113:ARG:NE	17:P:301:HOH:O	2.43	0.41
13:M:97:ALA:HA	13:M:130:VAL:HG21	2.03	0.41
3:Q:51:LYS:O	3:Q:52:LEU:HB2	2.19	0.41
8:V:139:GLU:OE2	8:V:139:GLU:HA	2.20	0.41
12:Z:42:LYS:HD2	12:Z:55:ASN:HD22	1.86	0.41
1:O:14:PRO:HA	2:P:23:TYR:CD1	2.56	0.41
5:S:68:HIS:HE1	5:S:102:LEU:O	2.04	0.41
1:O:2:THR:OG1	1:O:4:ARG:CD	2.69	0.40
10:X:3:ILE:HG23	10:X:18:SER:HB3	2.03	0.40
1:O:122:THR:HG22	2:P:128:ARG:HH21	1.86	0.40
4:D:91:HIS:CD2	4:D:99:ILE:HG22	2.57	0.40
10:J:21:VAL:HG11	11:K:122:LEU:HD11	2.04	0.40
2:P:51:VAL:O	2:P:52:THR:CB	2.68	0.40
5:S:92:ASN:HD21	12:Z:70:ASN:HD21	1.69	0.40
7:G:165:LYS:HD2	7:G:205:LEU:HD22	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	236/250 (94%)	230 (98%)	6 (2%)	0	100	100
1	O	236/250 (94%)	229 (97%)	7 (3%)	0	100	100
2	B	242/258 (94%)	237 (98%)	5 (2%)	0	100	100
2	P	242/258 (94%)	237 (98%)	3 (1%)	2 (1%)	19	43
3	C	238/254 (94%)	236 (99%)	1 (0%)	1 (0%)	34	60
3	Q	238/254 (94%)	234 (98%)	2 (1%)	2 (1%)	19	43
4	D	231/260 (89%)	228 (99%)	3 (1%)	0	100	100
4	R	231/260 (89%)	227 (98%)	4 (2%)	0	100	100
5	E	229/234 (98%)	222 (97%)	7 (3%)	0	100	100
5	S	229/234 (98%)	222 (97%)	7 (3%)	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%)	238 (100%)	1 (0%)	0	100	100
7	U	239/252 (95%)	238 (100%)	1 (0%)	0	100	100
8	H	217/234 (93%)	215 (99%)	2 (1%)	0	100	100
8	V	217/234 (93%)	216 (100%)	1 (0%)	0	100	100
9	I	202/205 (98%)	196 (97%)	6 (3%)	0	100	100
9	W	202/205 (98%)	198 (98%)	4 (2%)	0	100	100
10	J	193/198 (98%)	189 (98%)	4 (2%)	0	100	100
10	X	193/198 (98%)	189 (98%)	4 (2%)	0	100	100
11	K	210/212 (99%)	205 (98%)	5 (2%)	0	100	100
11	Y	210/212 (99%)	205 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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	222/246 (90%)	215 (97%)	7 (3%)	0	100	100
13	a	222/246 (90%)	216 (97%)	6 (3%)	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	6228/6618 (94%)	6106 (98%)	117 (2%)	5 (0%)	51	78

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	P	52	THR
3	Q	203	THR
2	P	51	VAL
3	Q	183	PRO
3	C	183	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	201/209 (96%)	194 (96%)	7 (4%)	36	65
1	O	201/209 (96%)	195 (97%)	6 (3%)	41	70
2	B	203/216 (94%)	193 (95%)	10 (5%)	25	52
2	P	203/216 (94%)	195 (96%)	8 (4%)	32	61
3	C	212/226 (94%)	203 (96%)	9 (4%)	30	58
3	Q	212/226 (94%)	203 (96%)	9 (4%)	30	58
4	D	194/215 (90%)	184 (95%)	10 (5%)	23	49
4	R	194/215 (90%)	185 (95%)	9 (5%)	27	54
5	E	190/193 (98%)	179 (94%)	11 (6%)	20	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	S	190/193 (98%)	179 (94%)	11 (6%)	20	43
6	F	201/239 (84%)	190 (94%)	11 (6%)	21	46
6	T	201/239 (84%)	190 (94%)	11 (6%)	21	46
7	G	206/210 (98%)	197 (96%)	9 (4%)	28	56
7	U	206/210 (98%)	196 (95%)	10 (5%)	25	52
8	H	179/194 (92%)	170 (95%)	9 (5%)	24	51
8	V	179/194 (92%)	170 (95%)	9 (5%)	24	51
9	I	172/173 (99%)	167 (97%)	5 (3%)	42	71
9	W	172/173 (99%)	168 (98%)	4 (2%)	50	78
10	J	173/175 (99%)	168 (97%)	5 (3%)	42	71
10	X	173/175 (99%)	168 (97%)	5 (3%)	42	71
11	K	169/169 (100%)	162 (96%)	7 (4%)	30	59
11	Y	169/169 (100%)	162 (96%)	7 (4%)	30	59
12	L	185/185 (100%)	178 (96%)	7 (4%)	33	62
12	Z	185/185 (100%)	179 (97%)	6 (3%)	39	68
13	M	192/208 (92%)	186 (97%)	6 (3%)	40	69
13	a	192/208 (92%)	186 (97%)	6 (3%)	40	69
14	N	162/162 (100%)	157 (97%)	5 (3%)	40	69
14	b	162/162 (100%)	157 (97%)	5 (3%)	40	69
All	All	5278/5548 (95%)	5061 (96%)	217 (4%)	30	59

All (217) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	2	THR
1	A	4	ARG
1	A	6	SER
1	A	122	THR
1	A	157	PHE
1	A	250	LEU
2	B	50	LYS
2	B	55	LEU
2	B	79	LEU
2	B	113	ARG

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Mol	Chain	Res	Type
2	B	119	GLN
2	B	186	ASP
2	B	191	LEU
2	B	221	ASP
2	B	223	GLU
2	B	238	LEU
3	C	4	ARG
3	C	38	ASN
3	C	49	THR
3	C	51	LYS
3	C	147	GLN
3	C	160	GLN
3	C	169	VAL
3	C	180	LYS
3	C	240	GLU
4	D	51	LEU
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	55	LEU
5	E	71	LEU
5	E	99	ASN
5	E	116	GLN
5	E	184	ASN
5	E	188	LEU
5	E	202	ASP
5	E	207	VAL
5	E	231	LYS
6	F	117	GLN
6	F	123	ASN
6	F	139	LYS
6	F	171	GLU
6	F	172	LEU
6	F	181	GLU

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Mol	Chain	Res	Type
6	F	201	GLU
6	F	202	ASP
6	F	207	ASP
6	F	214	TRP
6	F	240	GLN
7	G	13	GLU
7	G	83	ASN
7	G	115	LEU
7	G	117	GLN
7	G	122	ARG
7	G	125	MET
7	G	208	GLU
7	G	235	ARG
7	G	236	LEU
8	H	14	LEU
8	H	24	MET
8	H	43	CYS
8	H	78	THR
8	H	98	LEU
8	H	122	LEU
8	H	131	SER
8	H	143	ARG
8	H	201	ARG
9	I	37	ASN
9	I	123	PHE
9	I	131	GLU
9	I	160	GLU
9	I	171	LEU
10	J	2	ASP
10	J	3	ILE
10	J	35	THR
10	J	90	LYS
10	J	99	GLN
11	K	4	LEU
11	K	9	GLN
11	K	104	TYR
11	K	107	LYS
11	K	116	ASP
11	K	140	LEU
11	K	148	LEU
12	L	3	ASN
12	L	23	LEU

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Mol	Chain	Res	Type
12	L	31	THR
12	L	49	ASN
12	L	130	SER
12	L	136	CYS
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
14	N	9	LYS
14	N	39	ASP
14	N	83	LYS
14	N	104	ASP
14	N	107	LYS
1	O	1	MET
1	O	4	ARG
1	O	122	THR
1	O	157	PHE
1	O	230	ASP
1	O	250	LEU
2	P	55	LEU
2	P	79	LEU
2	P	113	ARG
2	P	119	GLN
2	P	186	ASP
2	P	191	LEU
2	P	220	ASN
2	P	238	LEU
3	Q	4	ARG
3	Q	38	ASN
3	Q	49	THR
3	Q	51	LYS
3	Q	147	GLN
3	Q	160	GLN
3	Q	169	VAL
3	Q	180	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	55	LEU
5	S	71	LEU
5	S	99	ASN
5	S	116	GLN
5	S	184	ASN
5	S	188	LEU
5	S	202	ASP
5	S	207	VAL
5	S	231	LYS
6	T	117	GLN
6	T	123	ASN
6	T	139	LYS
6	T	171	GLU
6	T	172	LEU
6	T	181	GLU
6	T	201	GLU
6	T	202	ASP
6	T	207	ASP
6	T	214	TRP
6	T	240	GLN
7	U	13	GLU
7	U	26	THR
7	U	83	ASN
7	U	115	LEU
7	U	117	GLN
7	U	122	ARG
7	U	125	MET
7	U	208	GLU
7	U	235	ARG
7	U	236	LEU
8	V	14	LEU
8	V	24	MET
8	V	43	CYS
8	V	78	THR

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Mol	Chain	Res	Type
8	V	98	LEU
8	V	131	SER
8	V	143	ARG
8	V	201	ARG
8	V	219	LEU
9	W	37	ASN
9	W	131	GLU
9	W	160	GLU
9	W	171	LEU
10	X	2	ASP
10	X	3	ILE
10	X	35	THR
10	X	90	LYS
10	X	99	GLN
11	Y	4	LEU
11	Y	9	GLN
11	Y	104	TYR
11	Y	107	LYS
11	Y	116	ASP
11	Y	140	LEU
11	Y	148	LEU
12	Z	23	LEU
12	Z	31	THR
12	Z	49	ASN
12	Z	130	SER
12	Z	136	CYS
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
14	b	9	LYS
14	b	39	ASP
14	b	83	LYS
14	b	104	ASP
14	b	107	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (123) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	20	GLN
2	B	58	GLN
2	B	95	GLN
2	B	119	GLN
2	B	123	GLN
2	B	155	ASN
2	B	176	GLN
3	C	17	GLN
3	C	38	ASN
3	C	77	ASN
3	C	116	GLN
3	C	120	GLN
3	C	147	GLN
3	C	160	GLN
3	C	207	ASN
4	D	15	GLN
4	D	100	ASN
4	D	160	ASN
4	D	225	ASN
5	E	68	HIS
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	30	ASN
7	G	83	ASN
7	G	114	ASN
7	G	117	GLN
7	G	121	GLN
7	G	166	GLN
7	G	167	GLN
7	G	175	ASN
9	I	37	ASN
10	J	55	GLN
11	K	85	ASN

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Mol	Chain	Res	Type
11	K	176	ASN
12	L	3	ASN
12	L	49	ASN
12	L	55	ASN
12	L	70	ASN
12	L	80	ASN
12	L	158	ASN
12	L	159	GLN
13	M	18	ASN
13	M	48	ASN
13	M	102	GLN
13	M	179	ASN
13	M	194	ASN
13	M	213	GLN
14	N	69	GLN
14	N	161	GLN
1	O	218	ASN
2	P	20	GLN
2	P	58	GLN
2	P	95	GLN
2	P	119	GLN
2	P	123	GLN
2	P	176	GLN
3	Q	17	GLN
3	Q	38	ASN
3	Q	77	ASN
3	Q	116	GLN
3	Q	120	GLN
3	Q	147	GLN
3	Q	160	GLN
3	Q	202	GLN
4	R	15	GLN
4	R	91	HIS
4	R	100	ASN
4	R	146	GLN
4	R	160	ASN
4	R	225	ASN
5	S	68	HIS
5	S	92	ASN
5	S	99	ASN
5	S	116	GLN
5	S	118	ASN

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Mol	Chain	Res	Type
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	30	ASN
7	U	83	ASN
7	U	114	ASN
7	U	117	GLN
7	U	121	GLN
7	U	166	GLN
7	U	167	GLN
7	U	175	ASN
8	V	153	ASN
9	W	37	ASN
10	X	55	GLN
10	X	86	GLN
10	X	118	GLN
11	Y	85	ASN
11	Y	176	ASN
12	Z	3	ASN
12	Z	49	ASN
12	Z	55	ASN
12	Z	70	ASN
12	Z	80	ASN
12	Z	158	ASN
12	Z	159	GLN
13	a	18	ASN
13	a	48	ASN
13	a	102	GLN
13	a	194	ASN
13	a	213	GLN
14	b	69	GLN
14	b	161	GLN

5.3.3 RNA ⓘ

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 carbohydrates 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	240/250 (96%)	-0.25	8 (3%) 46 46	40, 58, 95, 134	0
1	O	240/250 (96%)	-0.14	7 (2%) 51 52	44, 65, 111, 144	0
2	B	244/258 (94%)	-0.16	12 (4%) 29 28	38, 58, 105, 154	0
2	P	244/258 (94%)	-0.21	15 (6%) 21 20	42, 59, 103, 153	0
3	C	240/254 (94%)	-0.20	13 (5%) 25 24	37, 60, 120, 152	0
3	Q	240/254 (94%)	-0.07	17 (7%) 16 14	42, 69, 147, 174	0
4	D	235/260 (90%)	-0.43	3 (1%) 77 78	42, 59, 91, 134	0
4	R	235/260 (90%)	-0.31	6 (2%) 56 57	46, 65, 103, 134	0
5	E	231/234 (98%)	-0.30	4 (1%) 70 72	44, 61, 98, 138	0
5	S	231/234 (98%)	-0.20	5 (2%) 62 63	44, 66, 102, 142	0
6	F	243/288 (84%)	-0.36	6 (2%) 57 59	38, 55, 105, 133	0
6	T	243/288 (84%)	-0.36	7 (2%) 51 52	38, 62, 114, 144	0
7	G	241/252 (95%)	-0.45	6 (2%) 57 59	36, 51, 86, 135	0
7	U	241/252 (95%)	-0.36	8 (3%) 46 46	40, 55, 86, 128	0
8	H	219/234 (93%)	-0.40	4 (1%) 68 70	32, 51, 101, 114	0
8	V	219/234 (93%)	-0.34	6 (2%) 54 55	37, 55, 110, 127	0
9	I	204/205 (99%)	-0.71	1 (0%) 91 92	33, 47, 72, 93	0
9	W	204/205 (99%)	-0.67	3 (1%) 73 76	36, 48, 79, 102	0
10	J	195/198 (98%)	-0.53	2 (1%) 82 83	36, 50, 75, 128	0
10	X	195/198 (98%)	-0.48	3 (1%) 73 76	36, 52, 77, 138	0
11	K	212/212 (100%)	-0.63	0 100 100	31, 48, 70, 91	0
11	Y	212/212 (100%)	-0.60	1 (0%) 91 92	37, 49, 72, 93	0
12	L	222/222 (100%)	-0.50	2 (0%) 84 85	36, 51, 84, 115	0
12	Z	222/222 (100%)	-0.53	3 (1%) 75 77	37, 51, 85, 119	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
13	M	224/246 (91%)	-0.44	5 (2%)	62 63	35, 54, 80, 112	0
13	a	224/246 (91%)	-0.40	5 (2%)	62 63	35, 51, 75, 107	0
14	N	196/196 (100%)	-0.56	2 (1%)	82 83	33, 46, 75, 104	0
14	b	196/196 (100%)	-0.55	3 (1%)	73 76	34, 47, 74, 110	0
All	All	6292/6618 (95%)	-0.39	157 (2%)	57 59	31, 55, 98, 174	0

All (157) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	P	221	ASP	8.7
3	Q	50	LEU	7.6
2	P	219	ALA	7.5
2	B	221	ASP	7.0
2	B	220	ASN	6.7
2	B	219	ALA	6.3
1	O	230	ASP	6.0
10	X	1	MET	5.8
13	a	1	THR	5.8
2	B	51	VAL	5.7
9	W	1	SER	5.5
13	M	216	ASN	5.4
1	O	249	ALA	5.3
2	P	222	GLY	5.3
13	a	216	ASN	5.3
1	A	1	MET	5.2
3	Q	240	GLU	5.1
10	X	194	ASP	4.8
3	Q	49	THR	4.8
5	E	202	ASP	4.8
3	Q	239	GLN	4.7
1	A	230	ASP	4.7
3	C	202	GLN	4.6
2	P	59	ASP	4.5
3	C	239	GLN	4.4
13	a	224	ASP	4.3
1	A	249	ALA	4.3
3	Q	236	GLN	4.3
13	M	1	THR	4.3
3	Q	238	LYS	4.2
2	P	51	VAL	4.2
3	C	50	LEU	4.1

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Mol	Chain	Res	Type	RSRZ
5	S	202	ASP	4.1
3	C	238	LYS	4.0
12	L	174	TYR	4.0
2	B	217	LYS	3.9
5	S	180	LYS	3.9
14	b	195	GLN	3.9
9	I	1	SER	3.9
14	N	105	LYS	3.8
2	B	218	GLY	3.8
8	H	196	GLY	3.8
3	C	49	THR	3.8
2	P	225	TYR	3.8
2	B	223	GLU	3.7
1	A	219	PRO	3.7
2	B	59	ASP	3.6
14	N	195	GLN	3.6
3	C	236	GLN	3.5
6	T	244	ASN	3.5
1	A	201	GLU	3.5
7	U	242	GLN	3.4
10	J	1	MET	3.4
12	Z	174	TYR	3.4
3	C	180	LYS	3.3
7	U	222	ASP	3.3
1	O	231	LYS	3.3
13	a	220	ASP	3.3
6	F	181	GLU	3.3
13	a	215	GLU	3.3
1	O	1	MET	3.2
4	R	1	ASP	3.1
8	V	181	ASN	3.1
4	R	241	ALA	3.1
2	B	222	GLY	3.1
6	F	205	GLU	3.1
6	T	243	ILE	3.1
4	D	242	GLU	3.1
8	V	194	LYS	3.0
7	U	51	PRO	3.0
6	T	2	THR	3.0
6	F	241	LYS	3.0
4	R	230	GLU	3.0
2	P	223	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
6	F	202	ASP	3.0
7	G	222	ASP	3.0
7	G	241	GLU	2.9
13	M	47	ASP	2.9
8	V	196	GLY	2.9
2	P	218	GLY	2.9
8	V	219	LEU	2.9
2	P	220	ASN	2.9
10	J	194	ASP	2.9
8	H	194	LYS	2.8
1	O	219	PRO	2.8
7	G	2	GLY	2.8
3	Q	206	LYS	2.7
4	R	125	LEU	2.7
6	F	244	ASN	2.7
3	Q	180	LYS	2.7
8	H	219	LEU	2.7
2	B	225	TYR	2.7
5	S	203	GLU	2.6
9	W	133	LYS	2.6
14	b	105	LYS	2.6
9	W	192	ASP	2.6
3	Q	237	GLU	2.6
6	T	241	LYS	2.6
6	T	205	GLU	2.6
7	U	206	GLY	2.6
6	T	181	GLU	2.6
2	P	60	THR	2.5
3	Q	233	GLN	2.5
5	E	217	LYS	2.5
4	R	242	GLU	2.5
3	C	240	GLU	2.5
2	B	60	THR	2.5
13	M	224	ASP	2.5
12	Z	173	LYS	2.5
7	U	2	GLY	2.5
2	P	52	THR	2.5
4	R	217	GLN	2.5
3	Q	187	GLU	2.5
2	P	230	LYS	2.4
12	L	167	LYS	2.4
3	C	206	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
3	Q	48	SER	2.4
3	Q	229	GLN	2.4
3	Q	27	ARG	2.4
12	Z	167	LYS	2.4
2	P	50	LYS	2.3
3	C	47	ARG	2.3
6	F	180	PRO	2.3
1	O	52	SER	2.3
5	S	173	ARG	2.3
7	G	68	ARG	2.3
11	Y	106	ARG	2.3
3	C	216	ASP	2.3
8	H	195	LYS	2.3
5	E	201	ARG	2.3
7	U	181	LYS	2.2
3	C	175	LYS	2.2
8	V	218	PRO	2.2
13	M	215	GLU	2.2
7	G	3	TYR	2.2
3	Q	202	GLN	2.2
2	P	203	SER	2.2
4	D	169	GLU	2.1
7	U	3	TYR	2.1
6	T	180	PRO	2.1
4	D	2	ARG	2.1
3	Q	55	THR	2.1
7	U	183	ASP	2.1
1	A	203	GLU	2.1
14	b	107	LYS	2.1
3	C	229	GLN	2.0
2	P	182	ASP	2.0
3	Q	216	ASP	2.0
5	S	218	ASP	2.0
1	A	231	LYS	2.0
1	A	182	GLU	2.0
1	O	218	ASN	2.0
5	E	173	ARG	2.0
7	G	188	GLU	2.0
10	X	149	ARG	2.0
2	B	235	LYS	2.0
8	V	195	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates 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(\AA^2)	Q<0.9
15	MG	Z	301	1/1	0.85	0.47	70,70,70,70	0
15	MG	I	301	1/1	0.90	0.41	69,69,69,69	0
15	MG	N	201	1/1	0.92	0.13	64,64,64,64	0
15	MG	G	301	1/1	0.94	0.09	58,58,58,58	0
15	MG	K	301	1/1	0.98	0.08	57,57,57,57	0
16	CL	G	302	1/1	0.98	0.25	66,66,66,66	0
15	MG	W	301	1/1	0.98	0.29	64,64,64,64	0
15	MG	I	302	1/1	0.99	0.12	59,59,59,59	0
16	CL	U	301	1/1	0.99	0.37	66,66,66,66	0
15	MG	L	301	1/1	0.99	0.10	72,72,72,72	0

6.5 Other polymers [i](#)

There are no such residues in this entry.