



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 12:54 am BST

PDB ID : 4Y9Y
Title : Yeast 20S proteasome beta2-H116E mutant
Authors : Huber, E.M.; Groll, M.
Deposited on : 2015-02-17
Resolution : 2.80 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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

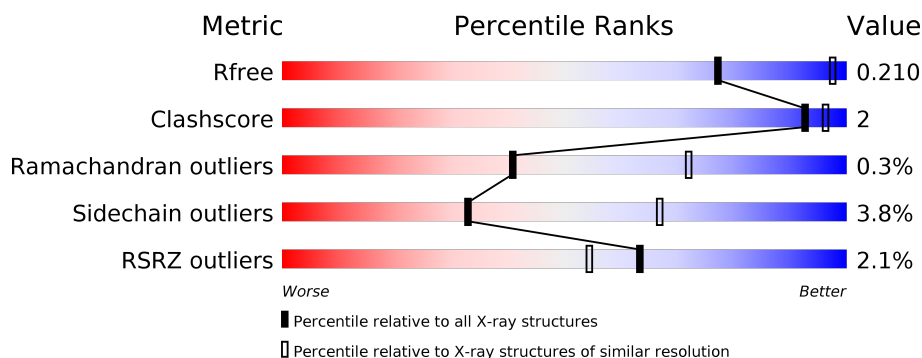
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



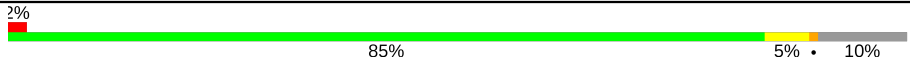

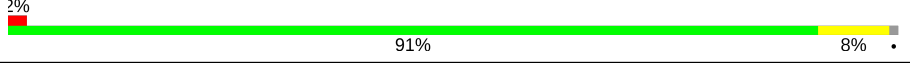
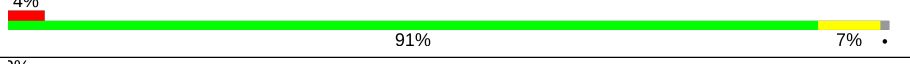
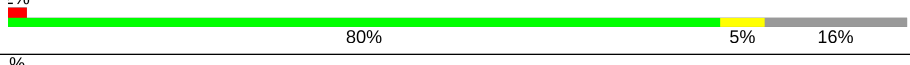
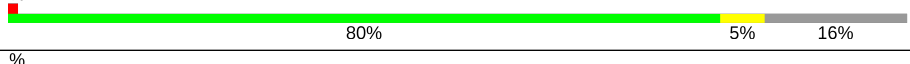
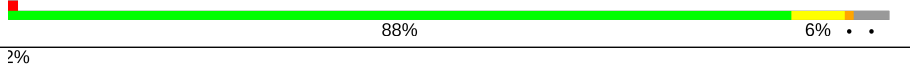

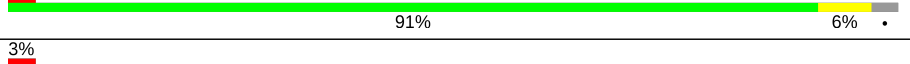
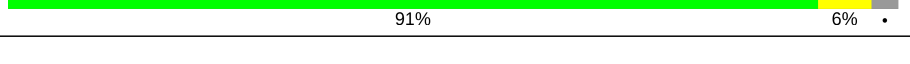
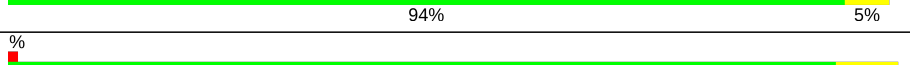
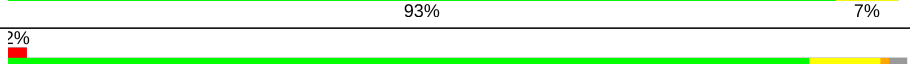
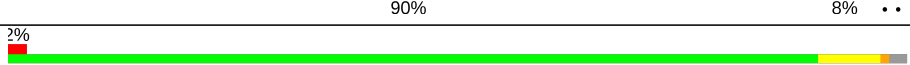
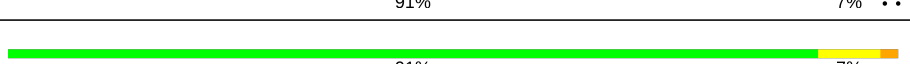
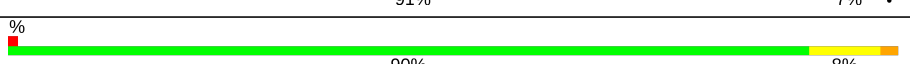
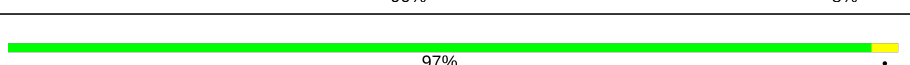
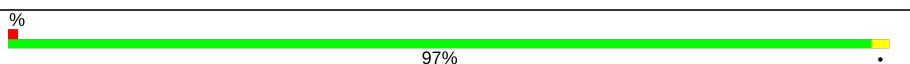
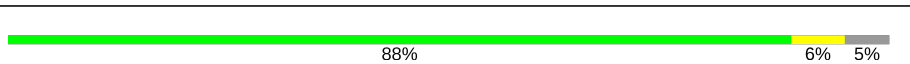
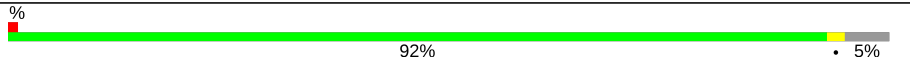
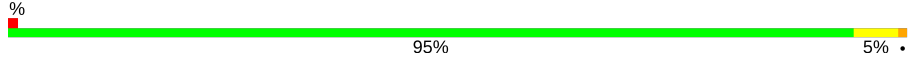
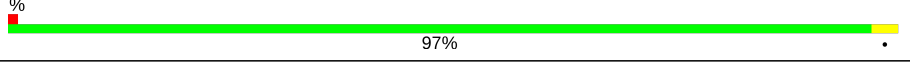
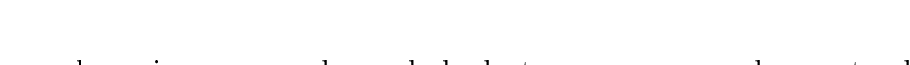
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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>2%</div> <div>98%</div> </div>
1	O	250	<div> <div>4%</div> <div>97%</div> </div>
2	B	258	<div> <div>3%</div> <div>86%</div> <div>8%</div> <div>5%</div> </div>
2	P	258	<div> <div>4%</div> <div>86%</div> <div>7%</div> <div>5%</div> </div>
3	C	254	<div> <div>4%</div> <div>86%</div> <div>7%</div> <div>6%</div> </div>
3	Q	254	<div> <div>5%</div> <div>86%</div> <div>7%</div> <div>6%</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	232	
8	V	232	
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	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	MES	N	202	-	-	X	-

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 49702 atoms, of which 26 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	250	Total	C	N	O	S	0	0	0
			1915	1219	315	377	4			
1	O	250	Total	C	N	O	S	0	0	0
			1915	1219	315	377	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 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-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	226	Total	C	N	O	S	0	0	0
			1718	1081	296	334	7			
8	V	226	Total	C	N	O	S	0	0	0
			1718	1081	296	334	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	116	GLU	HIS	engineered mutation	UNP P25043
V	116	GLU	HIS	engineered mutation	UNP P25043

- 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	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			
13	a	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			

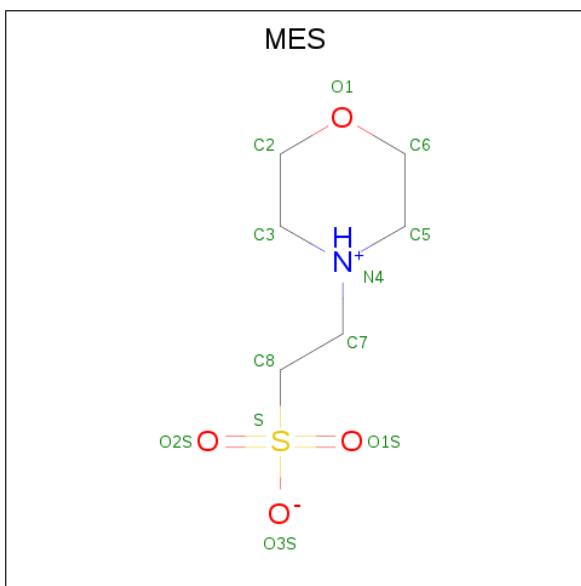
- Molecule 14 is a protein called Proteasome subunit beta type-1.

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	H	1	Total Mg 1 1	0	0
15	I	1	Total Mg 1 1	0	0
15	V	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	Y	1	Total Mg 1 1	0	0

- Molecule 16 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
16	N	1	Total	C	H	N	O	S	0	0
			25	6	13	1	4	1		
16	b	1	Total	C	H	N	O	S	0	0
			25	6	13	1	4	1		

- Molecule 17 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	1	Total O 1 1	0	0
17	B	10	Total O 10 10	0	0
17	C	7	Total O 7 7	0	0
17	D	4	Total O 4 4	0	0
17	E	7	Total O 7 7	0	0
17	F	11	Total O 11 11	0	0
17	G	11	Total O 11 11	0	0
17	H	17	Total O 17 17	0	0
17	I	10	Total O 10 10	0	0
17	J	7	Total O 7 7	0	0
17	K	11	Total O 11 11	0	0
17	L	15	Total O 15 15	0	0
17	M	22	Total O 22 22	0	0
17	N	17	Total O 17 17	0	0
17	O	2	Total O 2 2	0	0
17	P	9	Total O 9 9	0	0
17	Q	5	Total O 5 5	0	0
17	R	7	Total O 7 7	0	0
17	S	8	Total O 8 8	0	0
17	T	11	Total O 11 11	0	0
17	U	19	Total O 19 19	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	V	8	Total 8	O 8	0	0
17	W	5	Total 5	O 5	0	0
17	X	9	Total 9	O 9	0	0
17	Y	16	Total 16	O 16	0	0
17	Z	10	Total 10	O 10	0	0
17	a	11	Total 11	O 11	0	0
17	b	8	Total 8	O 8	0	0

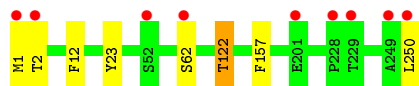
3 Residue-property plots [i](#)

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 ($RSRZ > 2$). 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.

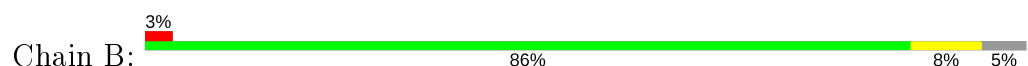
- Molecule 1: Proteasome subunit alpha type-2



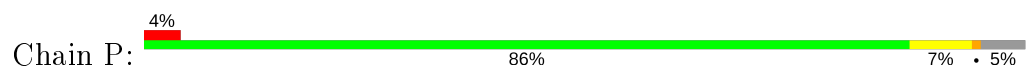
- Molecule 1: Proteasome subunit alpha type-2



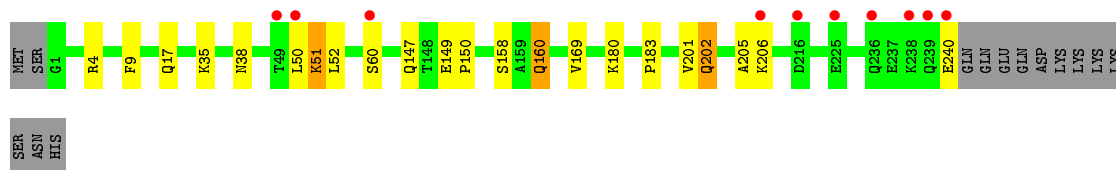
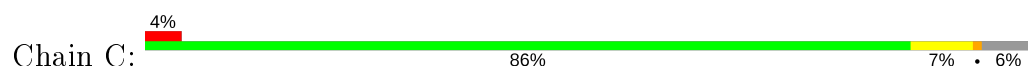
- Molecule 2: Proteasome subunit alpha type-3



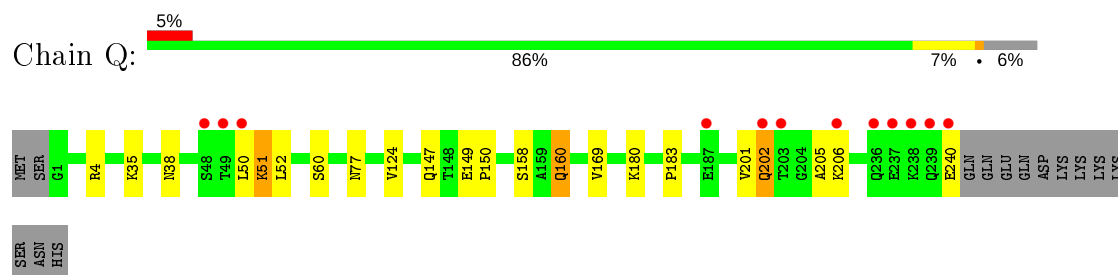
- Molecule 2: Proteasome subunit alpha type-3



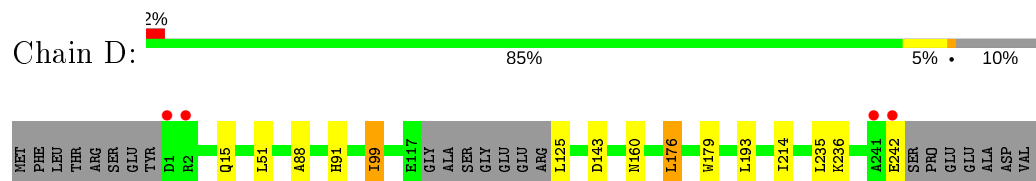
- Molecule 3: Proteasome subunit alpha type-4



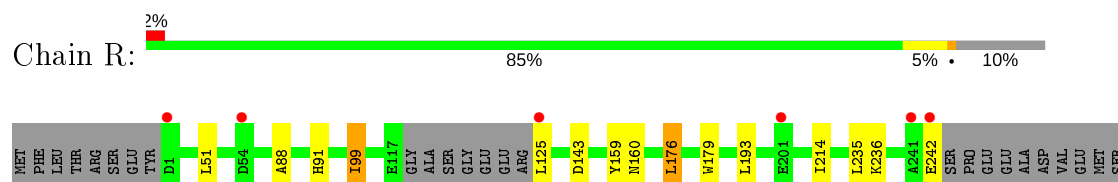
- Molecule 3: Proteasome subunit alpha type-4



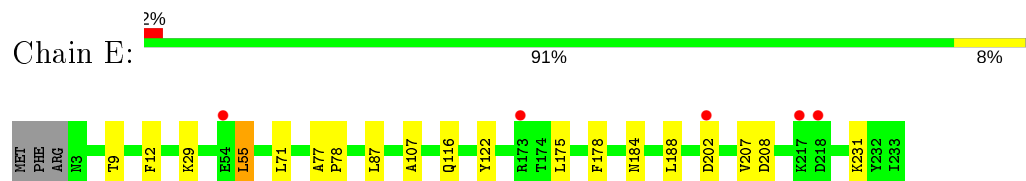
- Molecule 4: Proteasome subunit alpha type-5



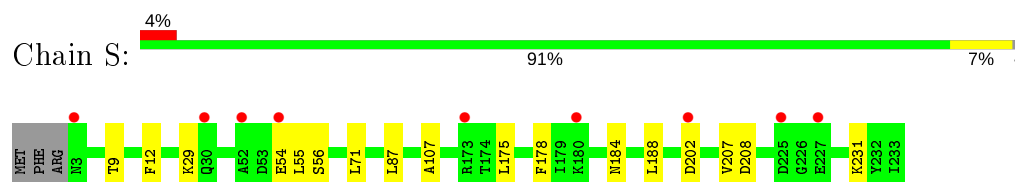
- Molecule 4: Proteasome subunit alpha type-5



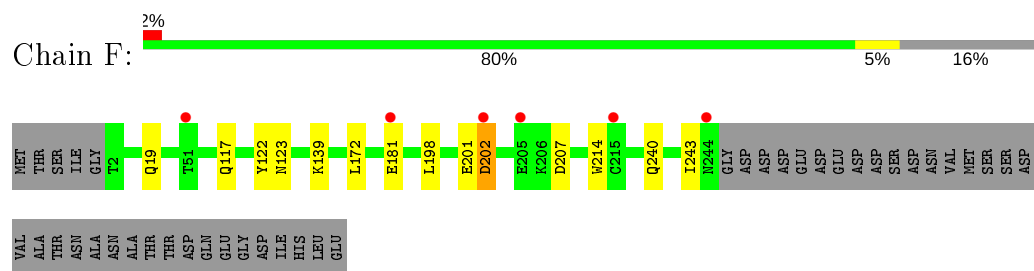
- Molecule 5: Proteasome subunit alpha type-6



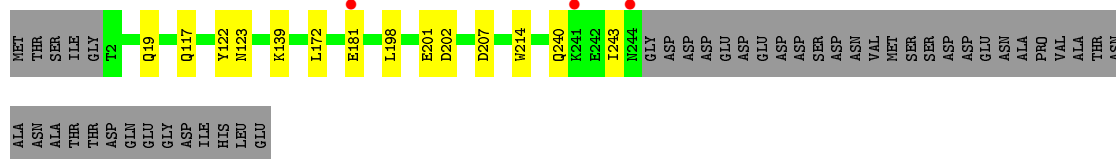
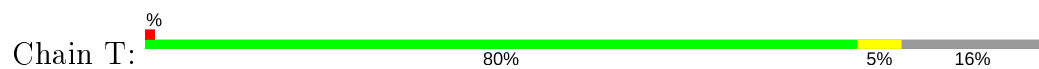
- Molecule 5: Proteasome subunit alpha type-6



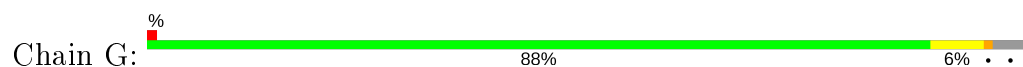
- Molecule 6: Proteasome subunit alpha type-7



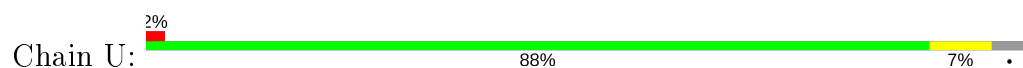
- Molecule 6: Proteasome subunit alpha type-7



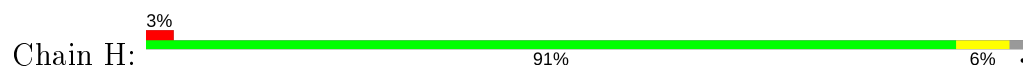
- Molecule 7: Proteasome subunit alpha type-1



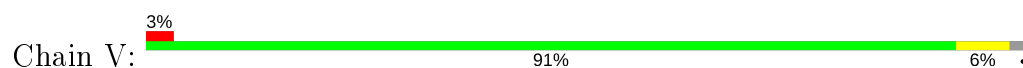
- Molecule 7: Proteasome subunit alpha type-1



- Molecule 8: Proteasome subunit beta type-2



- Molecule 8: Proteasome subunit beta type-2



- Molecule 9: Proteasome subunit beta type-3

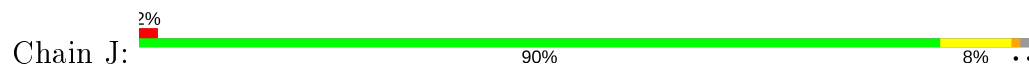


- Molecule 9: Proteasome subunit beta type-3

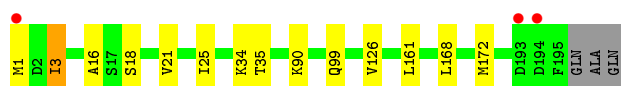
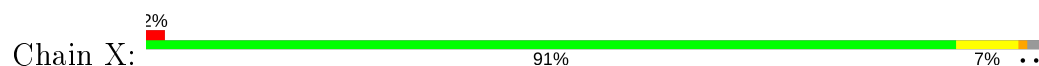




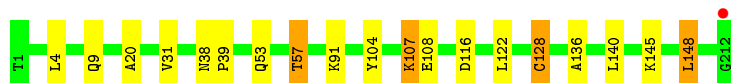
- Molecule 10: Proteasome subunit beta type-4



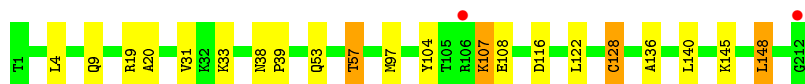
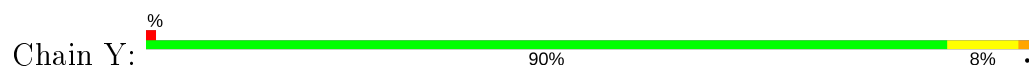
- Molecule 10: Proteasome subunit beta type-4



- Molecule 11: Proteasome subunit beta type-5



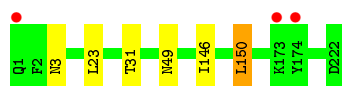
- Molecule 11: Proteasome subunit beta type-5



- Molecule 12: Proteasome subunit beta type-6



- Molecule 12: Proteasome subunit beta type-6



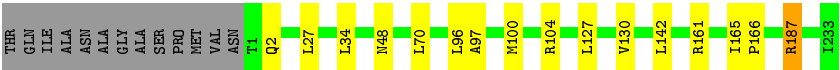
- Molecule 13: Proteasome subunit beta type-7

Chain M:

88%

6%

5%

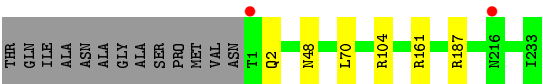


● Molecule 13: Proteasome subunit beta type-7

Chain a:

92%

5%

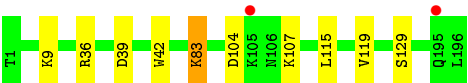


● Molecule 14: Proteasome subunit beta type-1

Chain N:

95%

5%

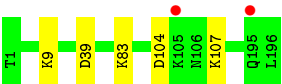


● Molecule 14: Proteasome subunit beta type-1

Chain b:

97%

5%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	135.01Å 300.43Å 144.37Å 90.00° 112.72° 90.00°	Depositor
Resolution (Å)	15.00 – 2.80 15.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.3 (15.00-2.80) 97.3 (15.00-2.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.34 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.176 , 0.203 0.183 , 0.210	Depositor DCC
R_{free} test set	12544 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	63.5	Xtriage
Anisotropy	0.021	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 49.3	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	0.95	EDS
Total number of atoms	49702	wwPDB-VP
Average B, all atoms (Å ²)	68.0	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.50	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	0.51	0/2586
4	D	0.27	0/1837	0.48	0/2475
4	R	0.27	0/1837	0.48	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	0.46	0/2609
7	G	0.27	0/1945	0.47	0/2634
7	U	0.27	0/1945	0.47	0/2634
8	H	0.30	0/1748	0.47	0/2370
8	V	0.33	0/1748	0.48	0/2370
9	I	0.28	0/1611	0.49	0/2174
9	W	0.28	0/1611	0.48	0/2174
10	J	0.26	0/1589	0.48	0/2142
10	X	0.26	0/1589	0.48	0/2142
11	K	0.27	0/1681	0.49	0/2274
11	Y	0.27	0/1681	0.50	0/2274
12	L	0.27	0/1795	0.48	0/2420
12	Z	0.27	0/1795	0.48	0/2420
13	M	0.27	0/1855	0.51	0/2514
13	a	0.27	0/1855	0.51	0/2514
14	N	0.27	0/1541	0.47	0/2087
14	b	0.26	0/1541	0.48	0/2087
All	All	0.27	0/50260	0.48	0/67956

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1915	0	1929	1	0
1	O	1915	0	1929	4	0
2	B	1904	0	1904	9	0
2	P	1904	0	1904	9	0
3	C	1881	0	1895	7	0
3	Q	1881	0	1895	6	0
4	D	1813	0	1797	6	0
4	R	1813	0	1797	6	0
5	E	1773	0	1775	6	0
5	S	1773	0	1775	5	0
6	F	1892	0	1883	4	0
6	T	1892	0	1883	3	0
7	G	1907	0	1901	6	0
7	U	1907	0	1901	5	0
8	H	1718	0	1718	8	0
8	V	1718	0	1718	11	0
9	I	1581	0	1574	5	0
9	W	1581	0	1574	7	0
10	J	1561	0	1569	10	0
10	X	1561	0	1569	9	0
11	K	1644	0	1595	8	0
11	Y	1644	0	1595	8	0
12	L	1757	0	1711	2	0
12	Z	1757	0	1711	1	0
13	M	1824	0	1832	6	0
13	a	1824	0	1832	0	0
14	N	1512	0	1481	11	0
14	b	1512	0	1481	0	0
15	G	1	0	0	0	0
15	H	1	0	0	0	0
15	I	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	K	1	0	0	0	0
15	N	1	0	0	0	0
15	V	2	0	0	0	0
15	W	1	0	0	0	0
15	Y	1	0	0	0	0
15	Z	1	0	0	0	0
16	N	12	13	13	8	0
16	b	12	13	13	0	0
17	A	1	0	0	0	0
17	B	10	0	0	0	0
17	C	7	0	0	0	0
17	D	4	0	0	0	0
17	E	7	0	0	0	0
17	F	11	0	0	0	0
17	G	11	0	0	1	0
17	H	17	0	0	0	0
17	I	10	0	0	0	0
17	J	7	0	0	0	0
17	K	11	0	0	0	0
17	L	15	0	0	0	0
17	M	22	0	0	0	0
17	N	17	0	0	0	0
17	O	2	0	0	0	0
17	P	9	0	0	0	0
17	Q	5	0	0	0	0
17	R	7	0	0	0	0
17	S	8	0	0	0	0
17	T	11	0	0	0	0
17	U	19	0	0	0	0
17	V	8	0	0	1	0
17	W	5	0	0	0	0
17	X	9	0	0	0	0
17	Y	16	0	0	0	0
17	Z	10	0	0	0	0
17	a	11	0	0	0	0
17	b	8	0	0	0	0
All	All	49676	26	49154	141	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 (141) 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)
14:N:115:LEU:CD1	16:N:202:MES:H61	1.40	1.51
14:N:115:LEU:HD11	16:N:202:MES:C6	1.41	1.48
14:N:115:LEU:CD1	16:N:202:MES:C6	1.96	1.40
14:N:115:LEU:HD13	16:N:202:MES:H61	0.99	0.97
14:N:115:LEU:HD11	16:N:202:MES:H62	0.96	0.96
14:N:115:LEU:HD13	16:N:202:MES:C6	1.83	0.92
14:N:115:LEU:CD1	16:N:202:MES:H62	1.87	0.81
8:V:52:THR:O	8:V:56:THR:OG1	1.99	0.81
8:H:52:THR:O	8:H:56:THR:OG1	2.00	0.78
8:V:114:HIS:CD2	8:V:116:GLU:H	2.20	0.59
2:B:12:PHE:H	3:C:17:GLN:HE22	1.51	0.59
8:V:114:HIS:HD2	8:V:116:GLU:H	1.51	0.58
7:G:68:ARG:HH12	14:N:36:ARG:HH22	1.52	0.58
1:A:1:MET:HG3	6:F:122:TYR:CZ	2.40	0.57
8:V:126:SER:O	8:V:127:LEU:HD12	2.06	0.56
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.90	0.54
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.90	0.53
2:P:217:LYS:C	2:P:219:ALA:H	2.12	0.53
3:Q:51:LYS:O	3:Q:52:LEU:HB2	2.07	0.53
2:B:217:LYS:C	2:B:219:ALA:H	2.11	0.52
3:C:51:LYS:O	3:C:52:LEU:HB2	2.08	0.52
14:N:83:LYS:HG3	14:N:119:VAL:CG2	2.40	0.52
3:C:160:GLN:HA	3:C:160:GLN:HE21	1.75	0.51
7:G:23:PHE:O	7:G:26:THR:HB	2.10	0.51
3:C:201:VAL:O	3:C:202:GLN:CB	2.57	0.51
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.58	0.51
9:I:9:GLY:HA3	9:I:41:LYS:HE2	1.94	0.51
7:U:23:PHE:O	7:U:26:THR:HB	2.11	0.51
3:Q:160:GLN:HE21	3:Q:160:GLN:HA	1.76	0.49
11:Y:20:ALA:HB2	11:Y:31:VAL:HG21	1.94	0.49
8:V:114:HIS:CD2	8:V:116:GLU:HB2	2.47	0.49
7:G:122:ARG:HD2	17:G:404:HOH:O	2.12	0.49
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.95	0.49
9:W:9:GLY:HA3	9:W:41:LYS:HE2	1.94	0.48
11:K:53:GLN:O	11:K:57:THR:OG1	2.30	0.48
10:J:21:VAL:HG11	11:K:122:LEU:HD11	1.95	0.48
11:Y:53:GLN:O	11:Y:57:THR:OG1	2.30	0.48
11:K:128:CYS:SG	11:K:136:ALA:HB3	2.54	0.48
4:R:176:LEU:HD11	5:S:54:GLU:HB2	1.95	0.48
11:K:20:ALA:HB2	11:K:31:VAL:HG21	1.95	0.48
10:X:1:MET:HG2	10:X:34:LYS:HE3	1.96	0.48
2:P:47:ALA:HB1	2:P:64:LYS:HD2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:12:PHE:H	6:T:19:GLN:HE22	1.62	0.48
2:B:47:ALA:HB1	2:B:64:LYS:HD2	1.96	0.47
8:V:114:HIS:HB2	17:V:404:HOH:O	2.14	0.47
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.95	0.47
8:H:114:HIS:HD2	8:H:116:GLU:H	1.61	0.47
3:C:35:LYS:HG2	3:C:158:SER:O	2.15	0.47
8:H:50:ALA:HB3	9:I:126:ILE:HD12	1.96	0.47
3:Q:35:LYS:HG2	3:Q:158:SER:O	2.14	0.47
5:S:87:LEU:HD21	5:S:107:ALA:HB1	1.97	0.47
10:X:3:ILE:HG23	10:X:18:SER:HB3	1.97	0.46
5:E:87:LEU:HD21	5:E:107:ALA:HB1	1.97	0.46
10:J:3:ILE:HG23	10:J:18:SER:HB3	1.97	0.46
11:Y:128:CYS:SG	11:Y:136:ALA:HB3	2.55	0.46
4:D:88:ALA:HA	4:D:99:ILE:HG21	1.98	0.46
10:J:1:MET:HG2	10:J:34:LYS:HE3	1.96	0.46
10:X:1:MET:HB3	10:X:34:LYS:HE3	1.98	0.45
4:R:88:ALA:HA	4:R:99:ILE:HG21	1.99	0.45
7:G:73:VAL:HG12	7:G:133:THR:HB	1.97	0.45
10:J:1:MET:HB3	10:J:34:LYS:HE3	1.98	0.45
2:B:151:ASN:HB2	2:B:152:PRO:CD	2.46	0.45
2:B:3:ARG:HB3	5:E:122:TYR:OH	2.16	0.45
8:V:104:ASP:HB2	8:V:105:PRO:HD2	1.99	0.45
4:D:91:HIS:HB3	4:D:99:ILE:CG2	2.47	0.45
2:B:50:LYS:HD3	2:B:50:LYS:HA	1.86	0.44
4:R:91:HIS:HB3	4:R:99:ILE:CG2	2.47	0.44
10:X:21:VAL:HG11	11:Y:122:LEU:HD11	1.99	0.44
5:E:12:PHE:H	6:F:19:GLN:HE22	1.65	0.44
2:P:151:ASN:HB2	2:P:152:PRO:CD	2.47	0.44
4:R:91:HIS:HB3	4:R:99:ILE:HG22	2.00	0.44
7:U:73:VAL:HG12	7:U:133:THR:HB	1.98	0.44
8:H:104:ASP:HB2	8:H:105:PRO:HD2	1.99	0.44
4:D:91:HIS:HB3	4:D:99:ILE:HG22	2.00	0.44
1:O:122:THR:HG22	2:P:128:ARG:HH21	1.82	0.44
2:B:219:ALA:HB2	2:B:225:TYR:HB2	1.99	0.44
3:C:149:GLU:HB2	3:C:150:PRO:HD2	2.00	0.44
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.53	0.44
3:Q:149:GLU:HB2	3:Q:150:PRO:HD2	2.00	0.44
11:K:107:LYS:HG3	11:K:108:GLU:HG3	2.00	0.43
5:E:175:LEU:HA	5:E:178:PHE:CE2	2.54	0.43
11:K:38:ASN:HB2	11:K:39:PRO:CD	2.48	0.43
14:N:36:ARG:HG3	14:N:42:TRP:CE2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:114:HIS:HD2	8:V:116:GLU:HB2	1.82	0.43
5:S:175:LEU:HA	5:S:178:PHE:CE2	2.53	0.43
11:Y:38:ASN:HB2	11:Y:39:PRO:CD	2.48	0.43
13:M:127:LEU:HG	13:M:142:LEU:HD12	2.01	0.43
1:O:1:MET:HG3	6:T:122:TYR:CZ	2.54	0.43
6:T:198:LEU:HD12	6:T:243:ILE:HG22	1.99	0.43
6:F:198:LEU:HD12	6:F:243:ILE:HG22	2.00	0.43
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.54	0.43
10:J:139:TYR:OH	10:X:25:ILE:O	2.37	0.43
10:J:1:MET:CB	10:J:34:LYS:HE3	2.49	0.43
2:P:219:ALA:HB2	2:P:225:TYR:HB2	1.99	0.43
10:X:1:MET:CB	10:X:34:LYS:HE3	2.49	0.43
11:Y:107:LYS:HG3	11:Y:108:GLU:HG3	2.01	0.43
4:D:176:LEU:HD22	5:E:55:LEU:CD2	2.49	0.42
13:M:27:LEU:HD21	13:M:34:LEU:HD22	2.01	0.42
12:L:8:ASN:HA	12:L:30:ILE:O	2.20	0.42
9:I:141:ALA:HB2	9:I:177:ASP:HB2	2.02	0.42
11:K:145:LYS:HB2	11:K:148:LEU:HD13	2.02	0.42
7:U:78:ILE:N	7:U:79:PRO:CD	2.83	0.42
9:W:36:SER:HB2	10:X:126:VAL:HG11	2.02	0.42
11:Y:145:LYS:HB2	11:Y:148:LEU:HD13	2.01	0.42
9:W:101:PRO:HB3	9:W:126:ILE:HD12	2.02	0.42
12:Z:146:ILE:HG22	12:Z:150:LEU:HD22	2.02	0.42
8:V:63:ILE:HG23	8:V:74:PRO:HB3	2.02	0.42
8:V:104:ASP:HB2	8:V:105:PRO:CD	2.50	0.41
13:M:187:ARG:NH1	8:V:139:GLU:OE1	2.46	0.41
9:W:141:ALA:HB2	9:W:177:ASP:HB2	2.02	0.41
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.55	0.41
7:G:78:ILE:N	7:G:79:PRO:CD	2.83	0.41
3:C:9:PHE:H	4:D:15:GLN:HE22	1.67	0.41
10:J:168:LEU:O	10:J:172:MET:HB2	2.20	0.41
14:N:129:SER:N	16:N:202:MES:O3S	2.53	0.41
11:Y:19:ARG:O	11:Y:33:LYS:NZ	2.51	0.41
12:L:146:ILE:HG22	12:L:150:LEU:HD22	2.01	0.41
4:R:159:TYR:CE2	5:S:56:SER:HB3	2.56	0.41
7:G:149:ASP:HB2	7:G:150:PRO:CD	2.51	0.41
8:H:104:ASP:HB2	8:H:105:PRO:CD	2.50	0.41
8:H:63:ILE:HG23	8:H:74:PRO:HB3	2.02	0.41
9:W:20:VAL:HG23	9:W:189:ILE:HB	2.03	0.41
8:H:112:SER:HB3	8:H:125:LEU:HD13	2.02	0.41
2:P:151:ASN:HB2	2:P:152:PRO:HD2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:151:ASN:HB2	2:B:152:PRO:HD2	2.02	0.41
10:J:50:ALA:O	11:K:91:LYS:NZ	2.54	0.41
13:M:165:ILE:HB	13:M:166:PRO:HD3	2.03	0.41
2:P:124:HIS:HB3	3:Q:124:VAL:HG12	2.03	0.41
8:H:114:HIS:CD2	8:H:116:GLU:H	2.39	0.41
9:I:20:VAL:HG13	9:I:118:PRO:HB3	2.02	0.41
10:J:126:VAL:HG12	10:J:128:LEU:HG	2.04	0.40
7:U:149:ASP:HB2	7:U:150:PRO:CD	2.51	0.40
10:X:168:LEU:O	10:X:172:MET:HB2	2.21	0.40
5:E:77:ALA:N	5:E:78:PRO:CD	2.85	0.40
6:F:202:ASP:OD1	6:F:202:ASP:N	2.55	0.40
13:M:97:ALA:HA	13:M:130:VAL:HG21	2.04	0.40
13:M:96:LEU:O	13:M:100:MET:HG2	2.22	0.40
1:O:12:PHE:H	2:P:20:GLN:HE22	1.69	0.40
2:P:50:LYS:O	2:P:51:VAL:C	2.59	0.40
2:B:217:LYS:C	2:B:219:ALA:N	2.75	0.40
9:W:20:VAL:HG13	9:W:118:PRO:HB3	2.02	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	248/250 (99%)	238 (96%)	9 (4%)	1 (0%)	34	66
1	O	248/250 (99%)	238 (96%)	9 (4%)	1 (0%)	34	66
2	B	242/258 (94%)	235 (97%)	3 (1%)	4 (2%)	9	29
2	P	242/258 (94%)	235 (97%)	3 (1%)	4 (2%)	9	29
3	C	238/254 (94%)	232 (98%)	3 (1%)	3 (1%)	12	36
3	Q	238/254 (94%)	232 (98%)	3 (1%)	3 (1%)	12	36
4	D	231/260 (89%)	229 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	R	231/260 (89%)	229 (99%)	2 (1%)	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	224/232 (97%)	218 (97%)	6 (3%)	0	100	100
8	V	224/232 (97%)	218 (97%)	6 (3%)	0	100	100
9	I	202/205 (98%)	197 (98%)	5 (2%)	0	100	100
9	W	202/205 (98%)	197 (98%)	5 (2%)	0	100	100
10	J	193/198 (98%)	188 (97%)	5 (3%)	0	100	100
10	X	193/198 (98%)	188 (97%)	5 (3%)	0	100	100
11	K	210/212 (99%)	206 (98%)	4 (2%)	0	100	100
11	Y	210/212 (99%)	206 (98%)	4 (2%)	0	100	100
12	L	220/222 (99%)	216 (98%)	4 (2%)	0	100	100
12	Z	220/222 (99%)	216 (98%)	4 (2%)	0	100	100
13	M	231/246 (94%)	223 (96%)	8 (4%)	0	100	100
13	a	231/246 (94%)	223 (96%)	8 (4%)	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	6284/6614 (95%)	6138 (98%)	130 (2%)	16 (0%)	41	72

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	THR
2	B	51	VAL
2	B	221	ASP
3	C	202	GLN
1	O	2	THR
2	P	51	VAL
2	P	221	ASP
3	Q	202	GLN
2	B	218	GLY

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Mol	Chain	Res	Type
2	B	220	ASN
2	P	218	GLY
2	P	220	ASN
3	C	205	ALA
3	Q	205	ALA
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	209/209 (100%)	205 (98%)	4 (2%)	57	85
1	O	209/209 (100%)	205 (98%)	4 (2%)	57	85
2	B	203/216 (94%)	195 (96%)	8 (4%)	32	66
2	P	203/216 (94%)	196 (97%)	7 (3%)	37	71
3	C	212/226 (94%)	201 (95%)	11 (5%)	23	55
3	Q	212/226 (94%)	200 (94%)	12 (6%)	20	50
4	D	194/215 (90%)	184 (95%)	10 (5%)	23	55
4	R	194/215 (90%)	184 (95%)	10 (5%)	23	55
5	E	190/193 (98%)	179 (94%)	11 (6%)	20	50
5	S	190/193 (98%)	180 (95%)	10 (5%)	22	54
6	F	201/239 (84%)	191 (95%)	10 (5%)	24	56
6	T	201/239 (84%)	191 (95%)	10 (5%)	24	56
7	G	206/210 (98%)	196 (95%)	10 (5%)	25	57
7	U	206/210 (98%)	196 (95%)	10 (5%)	25	57
8	H	185/190 (97%)	180 (97%)	5 (3%)	44	78
8	V	185/190 (97%)	180 (97%)	5 (3%)	44	78
9	I	172/173 (99%)	169 (98%)	3 (2%)	60	87
9	W	172/173 (99%)	169 (98%)	3 (2%)	60	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	J	173/175 (99%)	169 (98%)	4 (2%)	50	82
10	X	173/175 (99%)	169 (98%)	4 (2%)	50	82
11	K	169/169 (100%)	160 (95%)	9 (5%)	22	54
11	Y	169/169 (100%)	159 (94%)	10 (6%)	19	49
12	L	185/185 (100%)	181 (98%)	4 (2%)	52	83
12	Z	185/185 (100%)	180 (97%)	5 (3%)	44	78
13	M	199/208 (96%)	193 (97%)	6 (3%)	41	75
13	a	199/208 (96%)	193 (97%)	6 (3%)	41	75
14	N	162/162 (100%)	157 (97%)	5 (3%)	40	74
14	b	162/162 (100%)	157 (97%)	5 (3%)	40	74
All	All	5320/5540 (96%)	5119 (96%)	201 (4%)	33	67

All (201) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	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
2	B	119	GLN
2	B	186	ASP
2	B	191	LEU
2	B	238	LEU
3	C	4	ARG
3	C	38	ASN
3	C	50	LEU
3	C	51	LYS
3	C	60	SER
3	C	147	GLN
3	C	160	GLN
3	C	169	VAL
3	C	180	LYS
3	C	206	LYS
3	C	240	GLU

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Mol	Chain	Res	Type
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	116	GLN
5	E	184	ASN
5	E	188	LEU
5	E	202	ASP
5	E	207	VAL
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	207	ASP
6	F	214	TRP
6	F	240	GLN
7	G	26	THR
7	G	75	ASN
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	30	ASN

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Mol	Chain	Res	Type
8	H	56	THR
8	H	68	LEU
8	H	120	ASP
8	H	196	ARG
9	I	37	ASN
9	I	171	LEU
9	I	182	TRP
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	57	THR
11	K	104	TYR
11	K	107	LYS
11	K	116	ASP
11	K	128	CYS
11	K	140	LEU
11	K	148	LEU
12	L	3	ASN
12	L	23	LEU
12	L	31	THR
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	62	SER
1	O	122	THR
1	O	157	PHE
1	O	250	LEU
2	P	50	LYS
2	P	55	LEU
2	P	79	LEU

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Mol	Chain	Res	Type
2	P	113	ARG
2	P	186	ASP
2	P	191	LEU
2	P	238	LEU
3	Q	4	ARG
3	Q	38	ASN
3	Q	50	LEU
3	Q	51	LYS
3	Q	60	SER
3	Q	77	ASN
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	51	LEU
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	55	LEU
5	S	71	LEU
5	S	184	ASN
5	S	188	LEU
5	S	202	ASP
5	S	207	VAL
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

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Mol	Chain	Res	Type
6	T	202	ASP
6	T	207	ASP
6	T	214	TRP
6	T	240	GLN
7	U	26	THR
7	U	75	ASN
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	30	ASN
8	V	56	THR
8	V	68	LEU
8	V	120	ASP
8	V	196	ARG
9	W	37	ASN
9	W	171	LEU
9	W	182	TRP
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	57	THR
11	Y	97	MET
11	Y	104	TYR
11	Y	107	LYS
11	Y	116	ASP
11	Y	128	CYS
11	Y	140	LEU
11	Y	148	LEU
12	Z	3	ASN
12	Z	23	LEU
12	Z	31	THR
12	Z	49	ASN
12	Z	150	LEU
13	a	2	GLN

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Mol	Chain	Res	Type
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 (115) 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
2	B	155	ASN
2	B	176	GLN
3	C	17	GLN
3	C	38	ASN
3	C	77	ASN
3	C	147	GLN
3	C	160	GLN
4	D	15	GLN
4	D	100	ASN
4	D	225	ASN
5	E	68	HIS
5	E	92	ASN
5	E	99	ASN
5	E	116	GLN
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

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Mol	Chain	Res	Type
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
8	H	66	HIS
8	H	114	HIS
9	I	37	ASN
10	J	55	GLN
10	J	63	ASN
10	J	146	HIS
11	K	85	ASN
11	K	176	ASN
11	K	190	ASN
11	K	208	ASN
12	L	3	ASN
12	L	49	ASN
12	L	70	ASN
12	L	158	ASN
13	M	18	ASN
13	M	48	ASN
13	M	102	GLN
13	M	179	ASN
13	M	194	ASN
13	M	213	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
2	P	176	GLN
3	Q	17	GLN
3	Q	38	ASN
3	Q	77	ASN
3	Q	147	GLN
3	Q	160	GLN
4	R	15	GLN
4	R	100	ASN

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Mol	Chain	Res	Type
4	R	225	ASN
5	S	68	HIS
5	S	92	ASN
5	S	99	ASN
5	S	116	GLN
5	S	120	GLN
5	S	151	ASN
5	S	184	ASN
6	T	19	GLN
6	T	86	ASN
6	T	117	GLN
6	T	123	ASN
6	T	191	GLN
6	T	240	GLN
7	U	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
8	V	22	GLN
8	V	66	HIS
8	V	114	HIS
8	V	165	ASN
9	W	37	ASN
10	X	55	GLN
10	X	63	ASN
10	X	86	GLN
10	X	146	HIS
11	Y	85	ASN
11	Y	176	ASN
11	Y	190	ASN
11	Y	208	ASN
12	Z	3	ASN
12	Z	49	ASN
12	Z	70	ASN
12	Z	158	ASN
13	a	18	ASN
13	a	48	ASN
13	a	102	GLN
13	a	179	ASN

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Mol	Chain	Res	Type
13	a	194	ASN
13	a	213	GLN
14	b	161	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 10 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
16	MES	b	201	-	12,12,12	2.95	1 (8%)	14,16,16	1.92	5 (35%)
16	MES	N	202	-	12,12,12	3.02	1 (8%)	14,16,16	1.77	5 (35%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	MES	b	201	-	-	4/6/14/14	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	MES	N	202	-	-	0/6/14/14	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	N	202	MES	C8-S	-10.37	1.62	1.77
16	b	201	MES	C8-S	-10.11	1.63	1.77

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	b	201	MES	C6-C5-N4	-3.52	104.77	110.10
16	N	202	MES	C5-N4-C3	3.36	116.40	108.83
16	b	201	MES	C2-C3-N4	-3.11	105.39	110.10
16	b	201	MES	O3S-S-C8	2.69	110.12	105.77
16	b	201	MES	O2S-S-C8	2.63	110.08	106.92
16	N	202	MES	O1-C2-C3	-2.60	106.08	111.80
16	b	201	MES	C6-O1-C2	2.54	118.39	109.89
16	N	202	MES	C7-N4-C3	-2.24	105.50	111.23
16	N	202	MES	O1-C6-C5	-2.18	106.99	111.80
16	N	202	MES	O2S-S-C8	2.11	109.46	106.92

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	b	201	MES	N4-C7-C8-S
16	b	201	MES	C7-C8-S-O1S
16	b	201	MES	C7-C8-S-O2S
16	b	201	MES	C7-C8-S-O3S

There are no ring outliers.

1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	N	202	MES	8	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	250/250 (100%)	-0.36	5 (2%) 65 56	48, 60, 95, 133	0
1	O	250/250 (100%)	-0.31	9 (3%) 42 32	51, 67, 111, 141	0
2	B	244/258 (94%)	-0.27	7 (2%) 51 41	46, 65, 106, 163	0
2	P	244/258 (94%)	-0.24	10 (4%) 37 27	52, 68, 110, 157	0
3	C	240/254 (94%)	-0.25	10 (4%) 36 26	47, 69, 124, 149	0
3	Q	240/254 (94%)	-0.01	12 (5%) 28 19	51, 80, 158, 187	0
4	D	235/260 (90%)	-0.40	4 (1%) 70 63	49, 69, 101, 139	0
4	R	235/260 (90%)	-0.28	6 (2%) 56 46	52, 75, 115, 149	0
5	E	231/234 (98%)	-0.32	5 (2%) 62 52	51, 72, 109, 151	0
5	S	231/234 (98%)	-0.12	9 (3%) 39 29	56, 82, 125, 172	0
6	F	243/288 (84%)	-0.45	6 (2%) 57 47	49, 66, 113, 139	0
6	T	243/288 (84%)	-0.36	3 (1%) 79 73	51, 76, 127, 156	0
7	G	241/252 (95%)	-0.46	3 (1%) 79 73	41, 61, 93, 143	0
7	U	241/252 (95%)	-0.38	5 (2%) 63 54	50, 66, 96, 142	0
8	H	226/232 (97%)	-0.32	7 (3%) 49 39	39, 58, 87, 154	0
8	V	226/232 (97%)	-0.26	7 (3%) 49 39	46, 60, 89, 169	0
9	I	204/205 (99%)	-0.63	1 (0%) 91 88	42, 55, 81, 107	0
9	W	204/205 (99%)	-0.59	3 (1%) 73 68	45, 57, 85, 110	0
10	J	195/198 (98%)	-0.49	3 (1%) 73 68	43, 58, 83, 135	0
10	X	195/198 (98%)	-0.49	3 (1%) 73 68	44, 59, 84, 143	0
11	K	212/212 (100%)	-0.54	1 (0%) 91 88	39, 57, 78, 99	0
11	Y	212/212 (100%)	-0.51	2 (0%) 84 80	45, 58, 81, 102	0
12	L	222/222 (100%)	-0.56	1 (0%) 91 88	43, 59, 86, 121	0
12	Z	222/222 (100%)	-0.54	3 (1%) 75 70	44, 59, 89, 124	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
13	M	233/246 (94%)	-0.61	0	100	100	41, 57, 78, 96	0
13	a	233/246 (94%)	-0.59	2 (0%)	84	80	42, 57, 77, 95	0
14	N	196/196 (100%)	-0.63	2 (1%)	82	77	42, 52, 79, 106	0
14	b	196/196 (100%)	-0.60	2 (1%)	82	77	42, 54, 81, 112	0
All	All	6344/6614 (95%)	-0.41	131 (2%)	63	54	39, 63, 108, 187	0

All (131) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
8	V	224	GLN	9.2
3	Q	49	THR	7.2
2	B	221	ASP	7.0
3	Q	50	LEU	6.3
5	S	202	ASP	6.2
8	V	226	GLU	6.2
2	P	219	ALA	6.0
8	V	222	ASP	5.9
2	B	220	ASN	5.6
8	H	224	GLN	5.4
2	P	221	ASP	5.3
8	V	223	ILE	5.2
4	R	241	ALA	5.1
8	H	222	ASP	5.1
8	V	221	CYS	5.0
2	P	220	ASN	4.8
1	A	2	THR	4.8
8	H	226	GLU	4.8
2	P	51	VAL	4.7
3	Q	236	GLN	4.7
2	B	51	VAL	4.6
8	H	221	CYS	4.3
8	H	223	ILE	4.3
7	U	242	GLN	4.3
1	O	2	THR	4.2
8	V	225	GLU	4.1
2	P	59	ASP	4.1
3	C	206	LYS	4.1
10	X	1	MET	4.0
11	Y	212	GLY	4.0
3	C	49	THR	3.9
8	H	225	GLU	3.9

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Mol	Chain	Res	Type	RSRZ
3	Q	238	LYS	3.8
12	L	174	TYR	3.7
1	O	249	ALA	3.6
9	W	1	SER	3.5
10	J	1	MET	3.4
5	E	202	ASP	3.4
14	b	195	GLN	3.4
3	C	50	LEU	3.3
3	Q	240	GLU	3.3
4	R	1	ASP	3.3
3	Q	202	GLN	3.3
6	T	244	ASN	3.2
3	Q	239	GLN	3.2
1	O	201	GLU	3.1
9	I	1	SER	3.1
7	G	242	GLN	3.1
6	F	244	ASN	3.1
2	P	218	GLY	3.1
10	J	193	ASP	3.0
3	Q	203	THR	3.0
3	Q	206	LYS	3.0
10	X	194	ASP	2.9
3	Q	187	GLU	2.9
14	b	105	LYS	2.9
11	K	212	GLY	2.9
2	B	219	ALA	2.9
13	a	1	THR	2.8
6	F	205	GLU	2.8
7	U	222	ASP	2.8
3	C	236	GLN	2.8
7	G	240	ALA	2.8
1	O	250	LEU	2.8
8	V	219	ASN	2.8
14	N	105	LYS	2.8
3	C	238	LYS	2.7
3	C	60	SER	2.7
5	E	54	GLU	2.7
3	Q	237	GLU	2.7
5	S	227	GLU	2.7
6	F	215	CYS	2.6
10	J	194	ASP	2.6
10	X	193	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
6	F	202	ASP	2.5
1	A	203	GLU	2.5
5	S	3	ASN	2.5
1	O	1	MET	2.5
4	R	242	GLU	2.5
3	C	239	GLN	2.5
12	Z	174	TYR	2.5
1	A	1	MET	2.5
14	N	195	GLN	2.5
4	D	242	GLU	2.5
6	T	181	GLU	2.5
4	D	1	ASP	2.4
5	S	225	ASP	2.4
2	P	52	THR	2.4
5	S	173	ARG	2.4
2	B	203	SER	2.4
5	S	52	ALA	2.4
1	O	229	THR	2.4
3	C	216	ASP	2.4
13	a	216	ASN	2.4
1	O	228	PRO	2.3
7	U	203	ASP	2.3
2	P	222	GLY	2.3
3	C	240	GLU	2.3
3	Q	48	SER	2.3
8	H	198	GLU	2.3
5	S	54	GLU	2.3
2	B	59	ASP	2.3
9	W	192	ASP	2.3
3	C	225	GLU	2.2
1	O	52	SER	2.2
9	W	133	LYS	2.2
12	Z	173	LYS	2.2
6	F	181	GLU	2.2
2	P	60	THR	2.2
5	E	217	LYS	2.2
6	T	241	LYS	2.2
1	O	62	SER	2.2
2	P	203	SER	2.2
7	U	206	GLY	2.1
4	D	241	ALA	2.1
12	Z	1	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
11	Y	106	ARG	2.1
1	A	229	THR	2.1
4	R	125	LEU	2.1
1	A	248	GLU	2.1
5	E	173	ARG	2.1
6	F	51	THR	2.1
4	R	54	ASP	2.1
5	E	218	ASP	2.1
7	G	230	GLU	2.1
7	U	188	GLU	2.1
4	R	201	GLU	2.0
5	S	180	LYS	2.0
2	B	169	SER	2.0
4	D	2	ARG	2.0
5	S	30	GLN	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(Å ²)	Q<0.9
15	MG	Z	301	1/1	0.90	0.37	67,67,67,67	0
15	MG	I	301	1/1	0.93	0.45	77,77,77,77	0
16	MES	N	202	12/12	0.94	0.56	20,20,20,20	0
16	MES	b	201	12/12	0.95	0.55	20,20,20,20	0
15	MG	N	201	1/1	0.95	0.11	65,65,65,65	0
15	MG	V	302	1/1	0.96	0.09	30,30,30,30	0
15	MG	H	301	1/1	0.96	0.13	53,53,53,53	0
15	MG	G	301	1/1	0.96	0.05	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
15	MG	K	301	1/1	0.97	0.09	60,60,60,60	0
15	MG	V	301	1/1	0.98	0.07	77,77,77,77	0
15	MG	W	301	1/1	0.99	0.58	67,67,67,67	0
15	MG	Y	301	1/1	0.99	0.08	63,63,63,63	0

6.5 Other polymers [i](#)

There are no such residues in this entry.