



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 07:04 am BST

PDB ID : 5FG7
Title : Yeast 20S proteasome beta2-T1A mutant
Authors : Huber, E.M.; Groll, M.
Deposited on : 2015-12-20
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

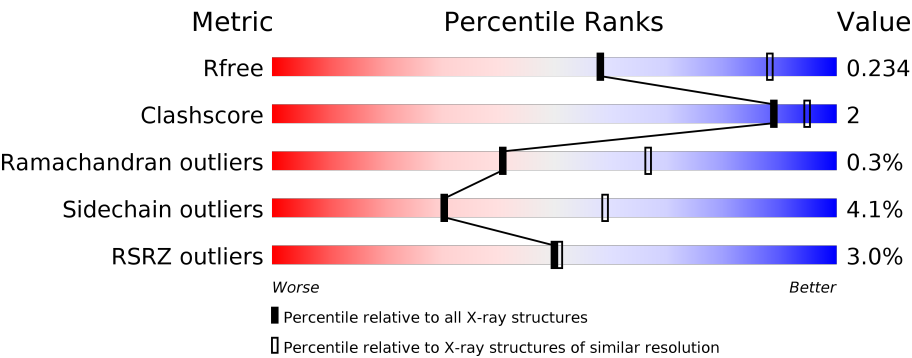
1 Overall quality at a glance i

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>5%</div><div><div></div><div>98%</div><div></div><div></div></div><div></div></div>
1	O	250	<div><div>6%</div><div><div></div><div>97%</div><div></div><div></div></div><div></div></div>
2	B	258	<div><div>3%</div><div><div></div><div>86%</div><div></div><div>8%</div><div>5%</div></div><div></div></div>
2	P	258	<div><div>5%</div><div><div></div><div>86%</div><div></div><div>7%</div><div>5%</div></div><div></div></div>
3	C	254	<div><div>5%</div><div><div></div><div>85%</div><div></div><div>8%</div><div>6%</div></div><div></div></div>
3	Q	254	<div><div>9%</div><div><div></div><div>85%</div><div></div><div>8%</div><div>6%</div></div><div></div></div>

Continued on next page...

Continued from previous page...

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	238	
8	V	238	
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 49981 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	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 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-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	228	Total	C	N	O	S	0	0	0
			1720	1082	300	331	7			
8	V	228	Total	C	N	O	S	0	0	0
			1720	1082	300	331	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	1	ALA	THR	engineered mutation	UNP P25043
V	1	ALA	THR	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	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.

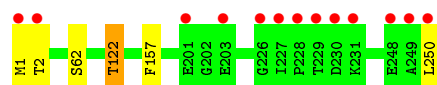
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	17	Total O 17 17	0	0
17	B	16	Total O 16 16	0	0
17	C	22	Total O 22 22	0	0
17	D	20	Total O 20 20	0	0
17	E	16	Total O 16 16	0	0
17	F	20	Total O 20 20	0	0
17	G	35	Total O 35 35	0	0
17	H	22	Total O 22 22	0	0
17	I	25	Total O 25 25	0	0

Continued on next page...

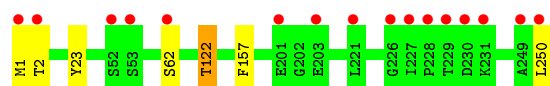
Continued from previous page...

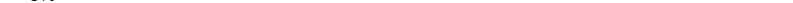
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	J	18	Total 18	O 18	0	0
17	K	23	Total 23	O 23	0	0
17	L	31	Total 31	O 31	0	0
17	M	28	Total 28	O 28	0	0
17	N	25	Total 25	O 25	0	0
17	O	17	Total 17	O 17	0	0
17	P	12	Total 12	O 12	0	0
17	Q	16	Total 16	O 16	0	0
17	R	11	Total 11	O 11	0	0
17	S	9	Total 9	O 9	0	0
17	T	20	Total 20	O 20	0	0
17	U	34	Total 34	O 34	0	0
17	V	21	Total 21	O 21	0	0
17	W	21	Total 21	O 21	0	0
17	X	19	Total 19	O 19	0	0
17	Y	22	Total 22	O 22	0	0
17	Z	23	Total 23	O 23	0	0
17	a	37	Total 37	O 37	0	0
17	b	23	Total 23	O 23	0	0

- Molecule 1: Proteasome subunit alpha type-2



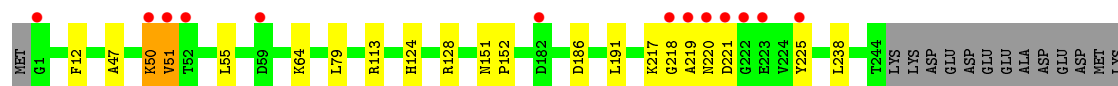
- Chain O:  6% 97%




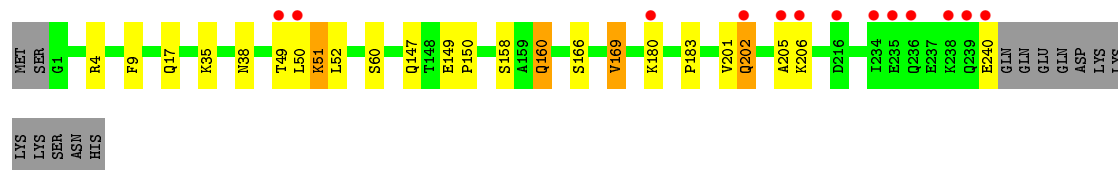
- Chain B:  3% 86% 8% 5%



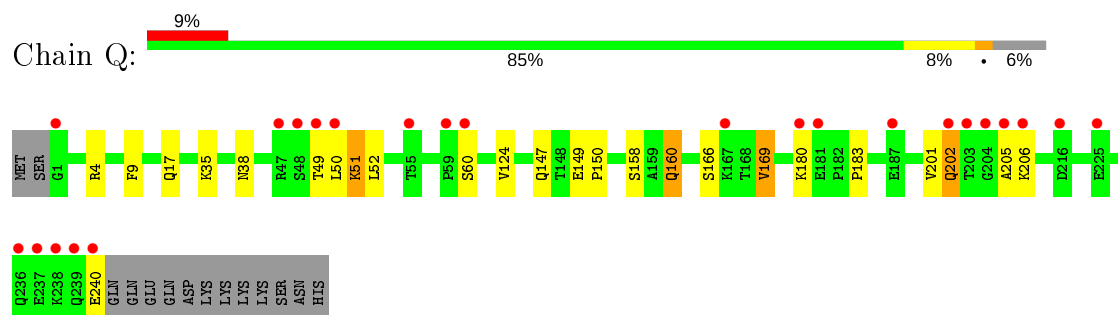
- Chain P: 5% 86% 7% • 5%



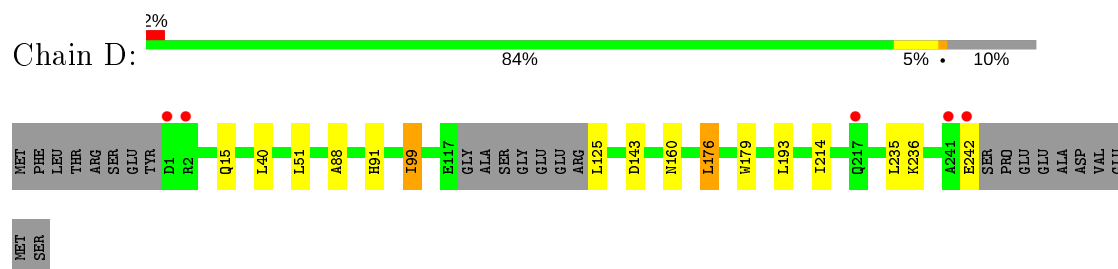
- Chain C:  5% 85% 8% 6%



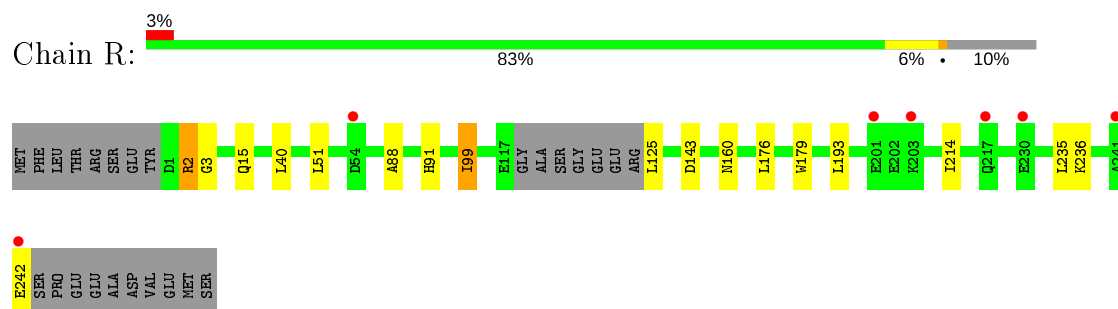
- Molecule 3: Proteasome subunit alpha type-4



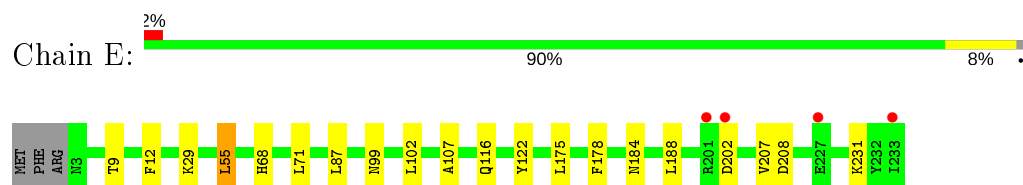
- Molecule 4: Proteasome subunit alpha type-5



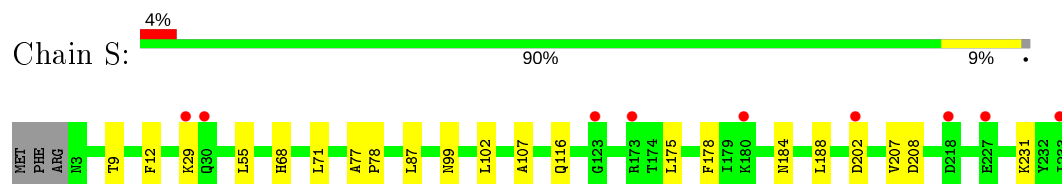
- Molecule 4: Proteasome subunit alpha type-5



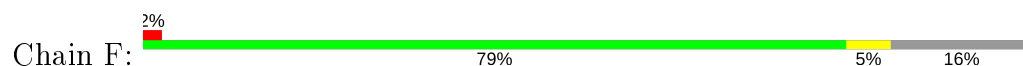
- Molecule 5: Proteasome subunit alpha type-6

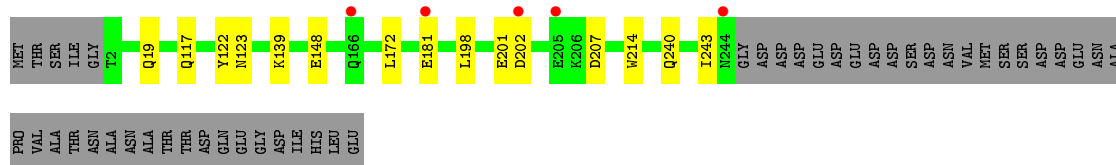


- Molecule 5: Proteasome subunit alpha type-6

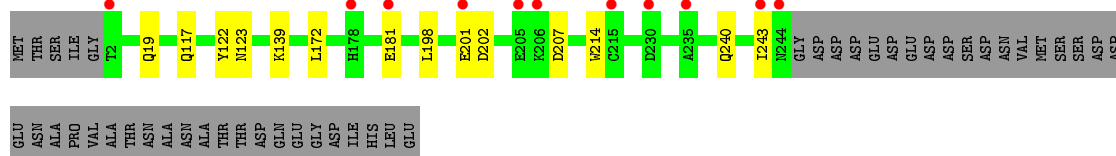
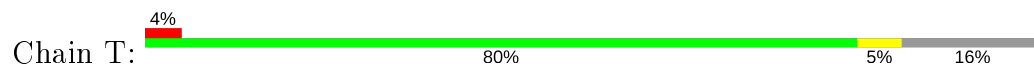


- Molecule 6: Probable proteasome subunit alpha type-7





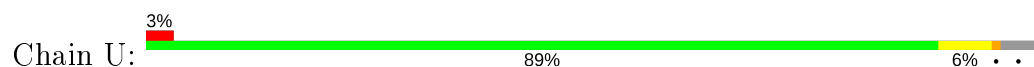
- Molecule 6: Probable proteasome subunit alpha type-7



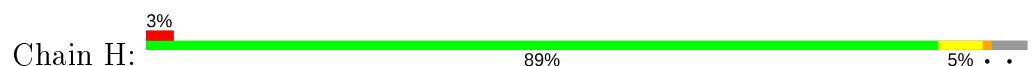
- Molecule 7: Proteasome subunit alpha type-1



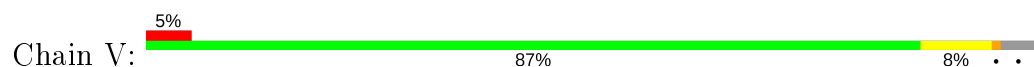
- Molecule 7: Proteasome subunit alpha type-1



- Molecule 8: Proteasome subunit beta type-2

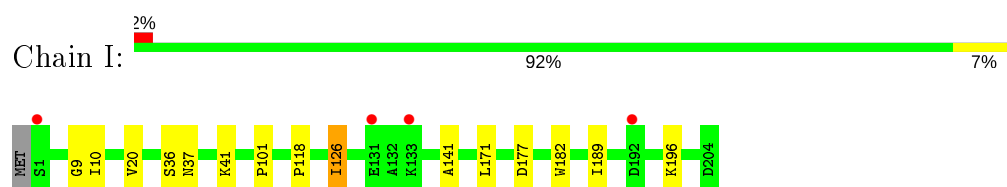


- Molecule 8: Proteasome subunit beta type-2

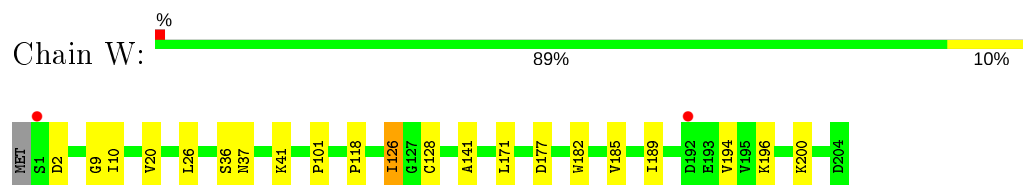


- Molecule 9: Proteasome subunit beta type-3

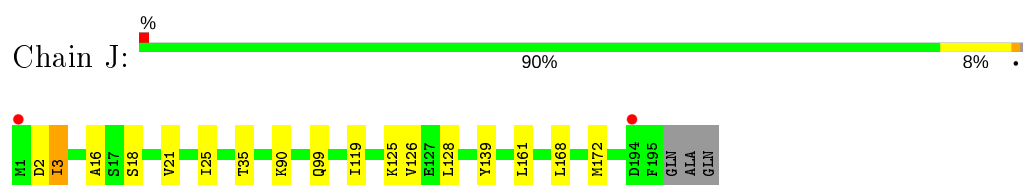




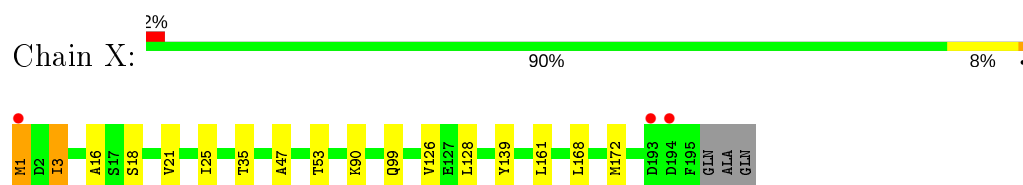
- Molecule 9: Proteasome subunit beta type-3



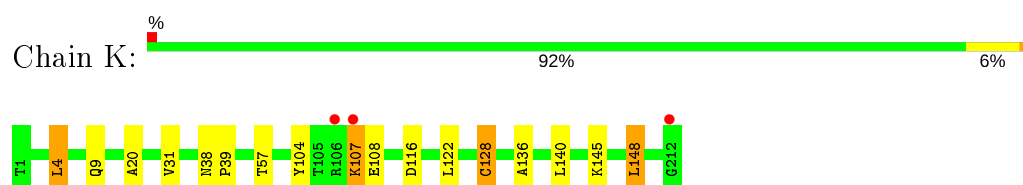
- Molecule 10: Proteasome subunit beta type-4



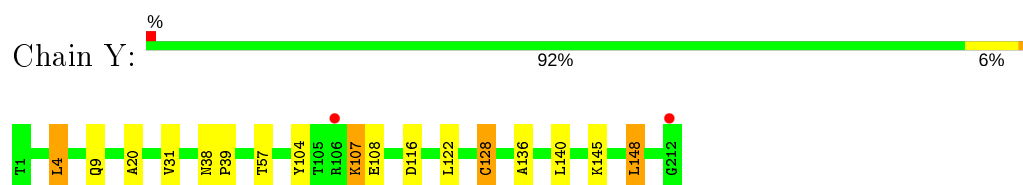
- Molecule 10: Proteasome subunit beta type-4



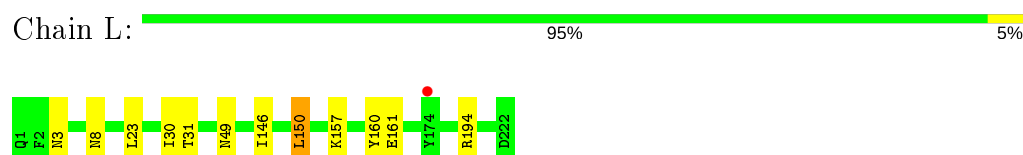
- Molecule 11: Proteasome subunit beta type-5



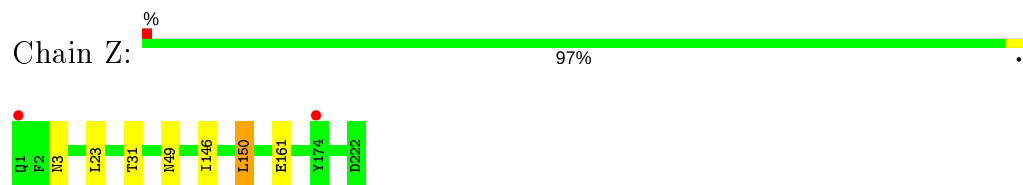
- Molecule 11: Proteasome subunit beta type-5



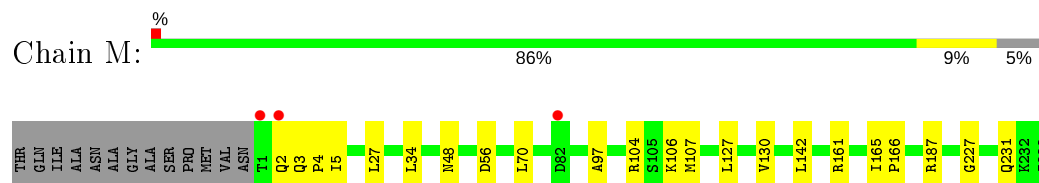
- Molecule 12: Proteasome subunit beta type-6



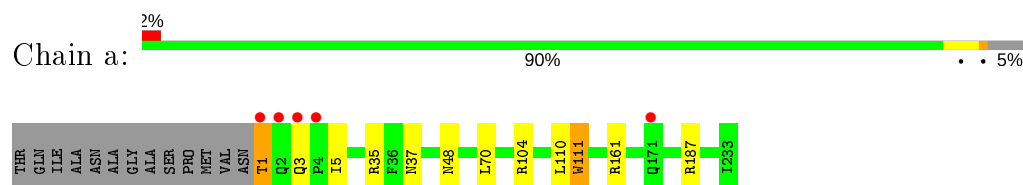
- Molecule 12: Proteasome subunit beta type-6



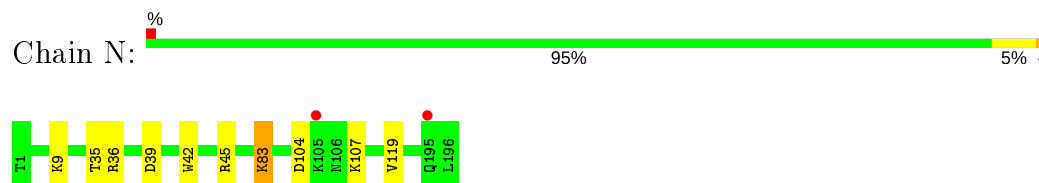
- Molecule 13: Proteasome subunit beta type-7



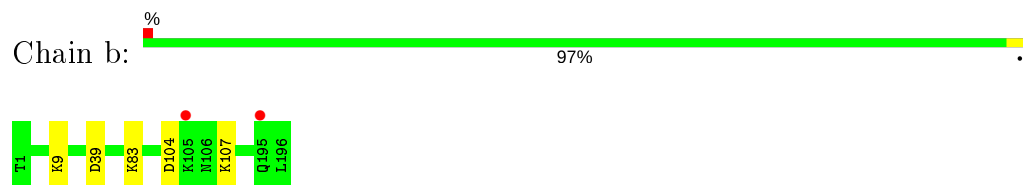
- Molecule 13: Proteasome subunit beta type-7



- 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	135.00Å 301.73Å 144.02Å 90.00° 113.06° 90.00°	Depositor
Resolution (Å)	15.00 – 2.70 14.99 – 2.70	Depositor EDS
% Data completeness (in resolution range)	94.8 (15.00-2.70) 94.8 (14.99-2.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.68 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.206 , 0.231 0.211 , 0.234	Depositor DCC
R_{free} test set	13629 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	50.0	Xtriage
Anisotropy	0.058	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 40.2	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	0.93	EDS
Total number of atoms	49981	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.38% 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	0.27	0/1952	0.47	0/2642
1	O	0.27	0/1952	0.47	0/2642
2	B	0.28	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	0.49	0/2475
5	E	0.27	0/1800	0.48	0/2433
5	S	0.27	0/1800	0.48	0/2433
6	F	0.27	0/1932	0.45	0/2609
6	T	0.27	0/1932	0.45	0/2609
7	G	0.27	0/1945	0.47	0/2634
7	U	0.27	0/1945	0.47	0/2634
8	H	0.40	0/1751	0.49	0/2374
8	V	0.37	0/1751	0.48	0/2374
9	I	0.28	0/1611	0.48	0/2174
9	W	0.28	0/1611	0.49	0/2174
10	J	0.28	0/1589	0.49	0/2142
10	X	0.27	0/1589	0.49	0/2142
11	K	0.28	0/1681	0.49	1/2274 (0.0%)
11	Y	0.30	0/1681	0.50	1/2274 (0.0%)
12	L	0.31	0/1795	0.49	0/2420
12	Z	0.28	0/1795	0.49	0/2420
13	M	0.40	0/1855	0.54	1/2514 (0.0%)
13	a	0.66	2/1855 (0.1%)	0.73	4/2514 (0.2%)
14	N	0.26	0/1541	0.48	0/2087
14	b	0.26	0/1541	0.48	0/2087
All	All	0.31	2/50266 (0.0%)	0.50	7/67964 (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
13	a	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	a	111	TRP	C-N	-19.51	0.89	1.34
13	a	110	LEU	C-N	-12.91	1.04	1.34

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	a	110	LEU	O-C-N	-15.83	97.37	122.70
13	a	110	LEU	C-N-CA	13.24	154.80	121.70
13	a	110	LEU	CA-C-N	11.10	141.62	117.20
13	a	3	GLN	C-N-CD	5.97	140.94	128.40
13	M	3	GLN	C-N-CD	5.39	139.72	128.40
11	K	4	LEU	CA-CB-CG	5.06	126.94	115.30
11	Y	4	LEU	CA-CB-CG	5.00	126.81	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	a	1	THR	Peptide

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	2	0
1	O	1915	0	1929	3	0
2	B	1904	0	1904	9	0
2	P	1904	0	1904	9	0
3	C	1881	0	1895	8	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	Q	1881	0	1895	9	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	5	0
7	U	1907	0	1901	5	0
8	H	1720	0	1726	14	0
8	V	1720	0	1726	27	0
9	I	1581	0	1574	8	0
9	W	1581	0	1574	16	0
10	J	1561	0	1569	9	0
10	X	1561	0	1569	12	0
11	K	1644	0	1595	6	0
11	Y	1644	0	1595	6	0
12	L	1757	0	1711	4	0
12	Z	1757	0	1711	1	0
13	M	1824	0	1832	7	0
13	a	1824	0	1830	0	0
14	N	1512	0	1481	5	0
14	b	1512	0	1481	0	0
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	1	0
17	A	17	0	0	0	0
17	B	16	0	0	0	0
17	C	22	0	0	0	0
17	D	20	0	0	0	0
17	E	16	0	0	0	0
17	F	20	0	0	1	0
17	G	35	0	0	0	0
17	H	22	0	0	1	0
17	I	25	0	0	0	0
17	J	18	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	K	23	0	0	0	0
17	L	31	0	0	0	0
17	M	28	0	0	0	0
17	N	25	0	0	0	0
17	O	17	0	0	0	0
17	P	12	0	0	0	0
17	Q	16	0	0	0	0
17	R	11	0	0	0	0
17	S	9	0	0	0	0
17	T	20	0	0	0	0
17	U	34	0	0	0	0
17	V	21	0	0	0	0
17	W	21	0	0	1	0
17	X	19	0	0	0	0
17	Y	22	0	0	0	0
17	Z	23	0	0	0	0
17	a	37	0	0	0	0
17	b	23	0	0	0	0
All	All	49981	0	49142	163	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 (163) 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)
8:V:53:GLU:O	8:V:57:GLN:HG3	1.59	1.02
8:H:-5:LYS:HA	17:H:309:HOH:O	1.78	0.83
8:V:99:ILE:HG13	8:V:127:LEU:HD12	1.62	0.81
8:V:-5:LYS:HD2	17:W:420:HOH:O	1.83	0.78
10:X:1:MET:CE	10:X:53:THR:OG1	2.35	0.75
8:V:99:ILE:HG13	8:V:127:LEU:CD1	2.18	0.73
8:V:-5:LYS:NZ	9:W:2:ASP:OD1	2.22	0.72
8:V:3:ILE:CG2	8:V:44:ALA:HB1	2.21	0.71
8:V:3:ILE:HG21	8:V:44:ALA:HB1	1.74	0.68
8:H:46:ALA:HB3	8:H:127:LEU:HD23	1.75	0.66
10:X:1:MET:HE2	10:X:53:THR:OG1	1.95	0.66
10:X:1:MET:HE3	10:X:53:THR:OG1	1.97	0.64
8:H:46:ALA:HB3	8:H:127:LEU:CD2	2.28	0.62
8:H:-1:THR:OG1	8:H:20:SER:HA	2.00	0.61
6:F:148:GLU:HG2	17:F:301:HOH:O	2.02	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:35:THR:HG21	14:N:45:ARG:HE	1.67	0.59
12:L:160:TYR:CD1	8:V:211:ALA:HB2	2.38	0.59
8:H:218:VAL:CG2	9:I:196:LYS:HB2	2.33	0.59
7:G:68:ARG:HH12	14:N:36:ARG:HH22	1.50	0.58
8:V:213:LEU:HG	9:W:200:LYS:HB2	1.86	0.57
5:S:12:PHE:H	6:T:19:GLN:HE22	1.53	0.57
2:B:12:PHE:H	3:C:17:GLN:HE22	1.52	0.57
2:P:217:LYS:C	2:P:219:ALA:H	2.08	0.57
8:V:218:VAL:CG2	9:W:196:LYS:HB2	2.35	0.57
2:B:217:LYS:C	2:B:219:ALA:H	2.07	0.56
8:V:213:LEU:HD21	9:W:200:LYS:HD2	1.87	0.56
3:Q:51:LYS:O	3:Q:52:LEU:HB2	2.04	0.56
8:V:3:ILE:CG2	8:V:44:ALA:CB	2.85	0.55
10:X:21:VAL:HG11	11:Y:122:LEU:HD11	1.89	0.55
3:C:51:LYS:O	3:C:52:LEU:HB2	2.05	0.55
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.89	0.55
8:H:22:GLN:HG3	8:H:27:ALA:HB2	1.88	0.54
8:V:3:ILE:HG21	8:V:44:ALA:CB	2.35	0.54
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.89	0.54
13:M:4:PRO:HB3	13:M:56:ASP:HB2	1.90	0.53
10:J:25:ILE:O	10:X:139:TYR:OH	2.26	0.53
8:V:53:GLU:O	8:V:57:GLN:CG	2.47	0.53
3:C:160:GLN:HE21	3:C:160:GLN:HA	1.74	0.53
8:V:50:ALA:HB2	9:W:128:CYS:HB2	1.91	0.53
16:U:301:CL:CL	8:V:69:TYR:OH	2.51	0.52
8:H:3:ILE:CG2	8:H:44:ALA:HB1	2.39	0.52
8:V:97:TYR:HB3	8:V:127:LEU:CD2	2.40	0.52
3:C:201:VAL:O	3:C:202:GLN:CB	2.57	0.52
8:H:3:ILE:HG22	8:H:99:ILE:HD12	1.91	0.52
2:P:47:ALA:HB1	2:P:64:LYS:HD2	1.92	0.51
3:Q:160:GLN:HE21	3:Q:160:GLN:HA	1.74	0.51
2:B:47:ALA:HB1	2:B:64:LYS:HD2	1.92	0.51
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.57	0.51
8:V:99:ILE:CG1	8:V:127:LEU:HD12	2.39	0.51
8:V:-1:THR:OG1	8:V:20:SER:HA	2.11	0.51
14:N:83:LYS:HG3	14:N:119:VAL:CG2	2.41	0.51
8:H:46:ALA:CB	8:H:127:LEU:HD23	2.41	0.50
7:G:23:PHE:O	7:G:26:THR:HB	2.12	0.49
5:E:12:PHE:H	6:F:19:GLN:HE22	1.61	0.49
1:O:1:MET:HG3	6:T:122:TYR:CZ	2.49	0.48
2:P:124:HIS:HB3	3:Q:124:VAL:HG12	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:23:PHE:O	7:U:26:THR:HB	2.14	0.48
9:I:9:GLY:HA3	9:I:41:LYS:HE2	1.96	0.48
10:J:3:ILE:HG23	10:J:18:SER:HB3	1.96	0.48
9:I:101:PRO:HB3	9:I:126:ILE:HD12	1.96	0.47
10:X:3:ILE:HG23	10:X:18:SER:HB3	1.96	0.47
11:Y:107:LYS:HG3	11:Y:108:GLU:HG3	1.96	0.47
2:B:219:ALA:HB2	2:B:225:TYR:HB2	1.96	0.47
4:R:2:ARG:O	4:R:3:GLY:C	2.53	0.47
10:J:21:VAL:HG11	11:K:122:LEU:HD11	1.97	0.47
9:W:101:PRO:HB3	9:W:126:ILE:HD12	1.97	0.47
11:K:128:CYS:SG	11:K:136:ALA:HB3	2.55	0.47
3:C:35:LYS:HG2	3:C:158:SER:O	2.15	0.47
2:P:219:ALA:HB2	2:P:225:TYR:HB2	1.96	0.47
8:V:3:ILE:HG23	8:V:44:ALA:HB1	1.96	0.47
9:W:9:GLY:HA3	9:W:41:LYS:HE2	1.96	0.47
5:E:175:LEU:HA	5:E:178:PHE:CE2	2.51	0.46
8:V:97:TYR:HB3	8:V:127:LEU:HD22	1.96	0.46
2:B:151:ASN:HB2	2:B:152:PRO:CD	2.45	0.46
8:H:3:ILE:CG2	8:H:44:ALA:CB	2.94	0.46
11:K:107:LYS:HG3	11:K:108:GLU:HG3	1.96	0.46
4:D:88:ALA:HA	4:D:99:ILE:HG21	1.98	0.46
8:H:3:ILE:HG23	8:H:44:ALA:HB1	1.97	0.46
2:P:151:ASN:HB2	2:P:152:PRO:CD	2.45	0.46
4:D:176:LEU:HD22	5:E:55:LEU:CD2	2.45	0.46
1:A:1:MET:HG3	6:F:122:TYR:CZ	2.51	0.46
4:R:88:ALA:HA	4:R:99:ILE:HG21	1.98	0.46
5:S:175:LEU:HA	5:S:178:PHE:CE2	2.50	0.46
8:V:3:ILE:HD12	8:V:46:ALA:HB2	1.96	0.46
8:H:104:ASP:HB2	8:H:105:PRO:HD2	1.98	0.46
11:Y:128:CYS:SG	11:Y:136:ALA:HB3	2.56	0.46
4:R:91:HIS:HB3	4:R:99:ILE:HG22	1.98	0.46
5:S:87:LEU:HD21	5:S:107:ALA:HB1	1.98	0.45
5:E:87:LEU:HD21	5:E:107:ALA:HB1	1.98	0.45
14:N:35:THR:CG2	14:N:45:ARG:HE	2.30	0.45
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.98	0.45
8:V:104:ASP:HB2	8:V:105:PRO:HD2	1.98	0.45
4:D:91:HIS:HB3	4:D:99:ILE:HG22	1.99	0.45
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.99	0.45
13:M:106:LYS:O	13:M:107:MET:HB2	2.16	0.45
10:J:168:LEU:O	10:J:172:MET:HB2	2.17	0.45
3:Q:35:LYS:HG2	3:Q:158:SER:O	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:149:GLU:HB2	3:C:150:PRO:HD2	1.99	0.45
10:J:139:TYR:OH	10:X:25:ILE:O	2.35	0.45
2:P:12:PHE:H	3:Q:17:GLN:HE22	1.65	0.45
11:Y:20:ALA:HB2	11:Y:31:VAL:HG21	1.99	0.45
3:Q:9:PHE:H	4:R:15:GLN:HE22	1.65	0.44
6:F:198:LEU:HD12	6:F:243:ILE:HG22	1.98	0.44
6:T:198:LEU:HD12	6:T:243:ILE:HG22	1.98	0.44
9:W:36:SER:HB2	10:X:126:VAL:HG11	1.98	0.44
4:R:91:HIS:HB3	4:R:99:ILE:CG2	2.47	0.44
10:X:1:MET:HG3	10:X:47:ALA:HA	1.99	0.44
3:Q:149:GLU:HB2	3:Q:150:PRO:HD2	2.00	0.44
4:D:91:HIS:HB3	4:D:99:ILE:CG2	2.48	0.44
14:N:36:ARG:HG3	14:N:42:TRP:CE2	2.52	0.43
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.52	0.43
8:V:213:LEU:HD21	9:W:200:LYS:CD	2.48	0.43
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.53	0.43
7:G:73:VAL:HG12	7:G:133:THR:HB	1.99	0.43
11:K:20:ALA:HB2	11:K:31:VAL:HG21	2.00	0.43
7:U:73:VAL:HG12	7:U:133:THR:HB	2.00	0.43
5:E:68:HIS:HE1	5:E:102:LEU:O	2.02	0.43
11:K:145:LYS:HB2	11:K:148:LEU:HD13	2.01	0.43
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.54	0.42
10:X:168:LEU:O	10:X:172:MET:HB2	2.19	0.42
9:W:20:VAL:HG23	9:W:189:ILE:HB	2.01	0.42
11:Y:145:LYS:HB2	11:Y:148:LEU:HD13	2.00	0.42
2:P:151:ASN:HB2	2:P:152:PRO:HD2	2.01	0.42
7:U:78:ILE:N	7:U:79:PRO:CD	2.82	0.42
2:B:151:ASN:HB2	2:B:152:PRO:HD2	2.01	0.42
13:M:27:LEU:HD21	13:M:34:LEU:HD22	2.01	0.42
7:G:78:ILE:N	7:G:79:PRO:CD	2.82	0.42
9:I:141:ALA:HB2	9:I:177:ASP:HB2	2.02	0.42
10:J:126:VAL:HG12	10:J:128:LEU:HG	2.02	0.42
10:X:126:VAL:HG12	10:X:128:LEU:HG	2.02	0.42
9:I:36:SER:HB2	10:J:126:VAL:HG11	2.02	0.42
12:L:8:ASN:HA	12:L:30:ILE:O	2.20	0.42
11:Y:38:ASN:HB2	11:Y:39:PRO:CD	2.50	0.41
11:K:38:ASN:HB2	11:K:39:PRO:CD	2.50	0.41
13:M:127:LEU:HG	13:M:142:LEU:HD12	2.03	0.41
13:M:97:ALA:HA	13:M:130:VAL:HG21	2.02	0.41
12:Z:146:ILE:HG22	12:Z:150:LEU:HD22	2.02	0.41
7:G:195:GLU:HG3	7:G:235:ARG:HG3	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:220:ILE:HG21	9:W:194:VAL:HG21	2.02	0.41
1:A:122:THR:HG22	2:B:128:ARG:HH21	1.86	0.41
7:U:195:GLU:HG3	7:U:235:ARG:HG3	2.02	0.41
2:B:3:ARG:HB3	5:E:122:TYR:OH	2.21	0.41
9:I:20:VAL:HG13	9:I:118:PRO:HB3	2.02	0.41
13:M:227:GLY:HA3	13:M:231:GLN:HB3	2.03	0.41
9:W:141:ALA:HB2	9:W:177:ASP:HB2	2.02	0.41
8:V:213:LEU:HD11	9:W:200:LYS:HA	2.02	0.41
12:L:146:ILE:HG22	12:L:150:LEU:HD22	2.02	0.41
13:M:165:ILE:HB	13:M:166:PRO:HD3	2.03	0.41
9:W:26:LEU:HD21	9:W:185:VAL:HG23	2.03	0.41
10:J:119:ILE:HG12	10:J:125:LYS:HG3	2.03	0.41
3:C:9:PHE:H	4:D:15:GLN:HE22	1.68	0.41
1:O:122:THR:HG22	2:P:128:ARG:HH21	1.85	0.41
12:L:194:ARG:NH1	8:V:27:ALA:O	2.54	0.41
8:H:3:ILE:HG21	8:H:44:ALA:CB	2.51	0.40
5:S:77:ALA:N	5:S:78:PRO:CD	2.84	0.40
8:H:3:ILE:HG21	8:H:44:ALA:HB1	2.03	0.40
9:I:20:VAL:HG23	9:I:189:ILE:HB	2.01	0.40
3:Q:166:SER:HA	3:Q:169:VAL:HG13	2.03	0.40
5:S:68:HIS:HE1	5:S:102:LEU:O	2.03	0.40
3:C:166:SER:HA	3:C:169:VAL:HG13	2.02	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	2.74	0.40
9:W:20:VAL:HG13	9:W:118:PRO:HB3	2.03	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%)	239 (96%)	8 (3%)	1 (0%)	34 60

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	O	248/250 (99%)	240 (97%)	7 (3%)	1 (0%)	34	60
2	B	242/258 (94%)	236 (98%)	2 (1%)	4 (2%)	9	23
2	P	242/258 (94%)	236 (98%)	2 (1%)	4 (2%)	9	23
3	C	238/254 (94%)	233 (98%)	2 (1%)	3 (1%)	12	30
3	Q	238/254 (94%)	233 (98%)	2 (1%)	3 (1%)	12	30
4	D	231/260 (89%)	229 (99%)	2 (1%)	0	100	100
4	R	231/260 (89%)	228 (99%)	3 (1%)	0	100	100
5	E	229/234 (98%)	222 (97%)	7 (3%)	0	100	100
5	S	229/234 (98%)	221 (96%)	8 (4%)	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	226/238 (95%)	221 (98%)	5 (2%)	0	100	100
8	V	226/238 (95%)	220 (97%)	6 (3%)	0	100	100
9	I	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
9	W	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
10	J	193/198 (98%)	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%)	215 (98%)	5 (2%)	0	100	100
12	Z	220/222 (99%)	215 (98%)	5 (2%)	0	100	100
13	M	231/246 (94%)	224 (97%)	7 (3%)	0	100	100
13	a	231/246 (94%)	223 (96%)	6 (3%)	2 (1%)	17	40
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	6288/6626 (95%)	6143 (98%)	127 (2%)	18 (0%)	41	66

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
13	a	111	TRP
2	B	220	ASN
2	P	220	ASN
2	B	218	GLY
3	C	205	ALA
2	P	218	GLY
3	Q	205	ALA
3	C	183	PRO
3	Q	183	PRO
13	a	5	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	209/209 (100%)	205 (98%)	4 (2%)	57	82
1	O	209/209 (100%)	205 (98%)	4 (2%)	57	82
2	B	203/216 (94%)	196 (97%)	7 (3%)	37	66
2	P	203/216 (94%)	196 (97%)	7 (3%)	37	66
3	C	212/226 (94%)	200 (94%)	12 (6%)	20	44
3	Q	212/226 (94%)	200 (94%)	12 (6%)	20	44
4	D	194/215 (90%)	183 (94%)	11 (6%)	20	44
4	R	194/215 (90%)	182 (94%)	12 (6%)	18	40
5	E	190/193 (98%)	178 (94%)	12 (6%)	18	40
5	S	190/193 (98%)	178 (94%)	12 (6%)	18	40
6	F	201/239 (84%)	191 (95%)	10 (5%)	24	51

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	T	201/239 (84%)	191 (95%)	10 (5%)	24	51
7	G	206/210 (98%)	196 (95%)	10 (5%)	25	52
7	U	206/210 (98%)	196 (95%)	10 (5%)	25	52
8	H	184/193 (95%)	180 (98%)	4 (2%)	52	79
8	V	184/193 (95%)	179 (97%)	5 (3%)	44	74
9	I	172/173 (99%)	168 (98%)	4 (2%)	50	78
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%)	160 (95%)	9 (5%)	22	48
11	Y	169/169 (100%)	160 (95%)	9 (5%)	22	48
12	L	185/185 (100%)	178 (96%)	7 (4%)	33	62
12	Z	185/185 (100%)	179 (97%)	6 (3%)	39	68
13	M	199/208 (96%)	192 (96%)	7 (4%)	36	65
13	a	199/208 (96%)	191 (96%)	8 (4%)	31	60
14	N	162/162 (100%)	157 (97%)	5 (3%)	40	69
14	b	162/162 (100%)	157 (97%)	5 (3%)	40	69
All	All	5318/5546 (96%)	5102 (96%)	216 (4%)	30	59

All (216) 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	186	ASP
2	B	191	LEU
2	B	238	LEU
3	C	4	ARG
3	C	38	ASN
3	C	49	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
4	D	40	LEU
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	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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	-5	LYS
8	H	30	ASN
8	H	127	LEU
8	H	196	ARG
9	I	37	ASN
9	I	126	ILE
9	I	171	LEU
9	I	182	TRP
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	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	49	ASN
12	L	150	LEU
12	L	157	LYS
12	L	161	GLU
13	M	2	GLN
13	M	5	ILE
13	M	48	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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	49	THR
3	Q	50	LEU
3	Q	51	LYS
3	Q	60	SER
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	2	ARG
4	R	40	LEU
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	208	ASP
5	S	231	LYS
6	T	117	GLN
6	T	123	ASN
6	T	139	LYS
6	T	172	LEU
6	T	181	GLU
6	T	201	GLU
6	T	202	ASP
6	T	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	-5	LYS
8	V	30	ASN
8	V	53	GLU
8	V	127	LEU
8	V	196	ARG
9	W	37	ASN
9	W	126	ILE
9	W	171	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	W	182	TRP
10	X	1	MET
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	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
12	Z	161	GLU
13	a	1	THR
13	a	35	ARG
13	a	37	ASN
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 (117) 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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	92	GLN
3	C	116	GLN
3	C	120	GLN
3	C	147	GLN
3	C	160	GLN
4	D	15	GLN
4	D	146	GLN
4	D	225	ASN
5	E	68	HIS
5	E	92	ASN
5	E	99	ASN
5	E	116	GLN
5	E	118	ASN
5	E	120	GLN
5	E	151	ASN
5	E	184	ASN
6	F	19	GLN
6	F	86	ASN
6	F	117	GLN
6	F	123	ASN
6	F	191	GLN
6	F	240	GLN
7	G	30	ASN
7	G	83	ASN
7	G	117	GLN
7	G	121	GLN
7	G	166	GLN
7	G	167	GLN
7	G	175	ASN
8	H	66	HIS
8	H	116	HIS
9	I	37	ASN
9	I	203	GLN
10	J	55	GLN
10	J	146	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	K	85	ASN
11	K	176	ASN
12	L	3	ASN
12	L	49	ASN
12	L	70	ASN
12	L	158	ASN
12	L	159	GLN
12	L	165	ASN
13	M	3	GLN
13	M	18	ASN
13	M	48	ASN
13	M	102	GLN
13	M	194	ASN
13	M	213	GLN
14	N	161	GLN
1	O	94	HIS
2	P	20	GLN
2	P	58	GLN
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
4	R	15	GLN
4	R	146	GLN
4	R	210	GLN
4	R	225	ASN
5	S	68	HIS
5	S	92	ASN
5	S	99	ASN
5	S	116	GLN
5	S	118	ASN
5	S	120	GLN
5	S	151	ASN
5	S	184	ASN
6	T	19	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	117	GLN
7	U	121	GLN
7	U	166	GLN
7	U	167	GLN
7	U	175	ASN
8	V	116	HIS
9	W	37	ASN
10	X	55	GLN
11	Y	85	ASN
11	Y	176	ASN
11	Y	208	ASN
12	Z	1	GLN
12	Z	3	ASN
12	Z	49	ASN
12	Z	70	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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
13	a	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	a	110:LEU	C	111:TRP	N	1.04
1	a	111:TRP	C	112:ASN	N	0.89

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%)	-0.18	13 (5%)	27 25	33, 46, 82, 120	0
1	O	250/250 (100%)	-0.05	16 (6%)	19 18	39, 55, 98, 128	0
2	B	244/258 (94%)	-0.14	8 (3%)	46 46	35, 53, 92, 143	0
2	P	244/258 (94%)	-0.09	13 (5%)	26 25	41, 56, 95, 140	0
3	C	240/254 (94%)	-0.09	13 (5%)	25 24	35, 57, 111, 140	0
3	Q	240/254 (94%)	0.19	24 (10%)	7 5	38, 66, 145, 171	0
4	D	235/260 (90%)	-0.30	5 (2%)	63 65	36, 56, 86, 127	0
4	R	235/260 (90%)	-0.18	7 (2%)	50 51	37, 59, 99, 131	0
5	E	231/234 (98%)	-0.20	4 (1%)	70 72	35, 56, 91, 133	0
5	S	231/234 (98%)	-0.11	9 (3%)	39 38	43, 66, 101, 145	0
6	F	243/288 (84%)	-0.34	5 (2%)	63 65	35, 52, 101, 127	0
6	T	243/288 (84%)	-0.23	11 (4%)	33 31	36, 61, 108, 135	0
7	G	241/252 (95%)	-0.40	3 (1%)	79 80	30, 48, 78, 130	0
7	U	241/252 (95%)	-0.28	7 (2%)	51 52	38, 52, 81, 124	0
8	H	228/238 (95%)	0.03	6 (2%)	56 57	33, 49, 90, 121	0
8	V	228/238 (95%)	0.16	13 (5%)	23 22	34, 55, 100, 139	0
9	I	204/205 (99%)	-0.53	4 (1%)	65 67	31, 42, 69, 93	0
9	W	204/205 (99%)	-0.53	2 (0%)	82 83	32, 44, 70, 94	0
10	J	195/198 (98%)	-0.43	2 (1%)	82 83	33, 46, 72, 128	0
10	X	195/198 (98%)	-0.27	3 (1%)	73 76	35, 49, 73, 134	0
11	K	212/212 (100%)	-0.42	3 (1%)	75 77	27, 44, 63, 85	0
11	Y	212/212 (100%)	-0.46	2 (0%)	84 85	33, 47, 69, 91	0
12	L	222/222 (100%)	-0.38	1 (0%)	91 92	31, 45, 74, 111	0
12	Z	222/222 (100%)	-0.42	2 (0%)	84 85	33, 46, 76, 111	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
13	M	233/246 (94%)	-0.51	3 (1%)	77	78	31, 46, 67, 83	0
13	a	233/246 (94%)	-0.37	5 (2%)	63	65	24, 45, 65, 84	0
14	N	196/196 (100%)	-0.49	2 (1%)	82	83	30, 41, 69, 94	0
14	b	196/196 (100%)	-0.44	2 (1%)	82	83	32, 43, 70, 100	0
All	All	6348/6626 (95%)	-0.26	188 (2%)	50	51	24, 51, 93, 171	0

All (188) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	220	ASN	7.6
3	Q	50	LEU	7.5
2	B	219	ALA	6.9
2	B	51	VAL	6.8
12	L	174	TYR	6.4
2	B	221	ASP	6.0
8	V	222	ASP	5.7
1	O	231	LYS	5.6
2	P	51	VAL	5.6
2	P	220	ASN	5.6
3	Q	49	THR	5.5
2	P	221	ASP	5.4
3	Q	236	GLN	5.2
13	a	2	GLN	5.2
1	A	231	LYS	5.2
5	S	202	ASP	5.1
13	a	1	THR	5.1
8	H	222	ASP	4.9
3	Q	240	GLU	4.8
1	A	2	THR	4.7
4	R	241	ALA	4.7
2	P	219	ALA	4.6
1	A	229	THR	4.6
5	E	202	ASP	4.5
1	O	249	ALA	4.5
13	M	1	THR	4.5
3	C	49	THR	4.4
3	C	206	LYS	4.4
1	O	1	MET	4.2
1	O	2	THR	4.2
10	X	194	ASP	4.1
3	C	205	ALA	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	O	229	THR	4.0
5	S	173	ARG	4.0
1	A	1	MET	4.0
2	P	59	ASP	4.0
3	Q	206	LYS	4.0
9	W	1	SER	3.9
8	V	204	LYS	3.8
3	Q	205	ALA	3.8
3	Q	225	GLU	3.7
12	Z	174	TYR	3.7
1	O	52	SER	3.7
7	U	242	GLN	3.6
8	H	221	CYS	3.6
1	A	226	GLY	3.5
3	C	239	GLN	3.5
14	b	195	GLN	3.5
1	O	228	PRO	3.5
8	V	207	ARG	3.5
1	O	201	GLU	3.5
1	A	250	LEU	3.5
2	P	225	TYR	3.5
14	b	105	LYS	3.5
3	Q	180	LYS	3.5
8	V	221	CYS	3.4
3	Q	238	LYS	3.4
3	C	240	GLU	3.4
3	Q	237	GLU	3.4
6	F	181	GLU	3.4
1	O	53	SER	3.3
8	H	198	GLU	3.3
3	C	238	LYS	3.3
2	P	222	GLY	3.3
3	C	235	GLU	3.3
10	J	194	ASP	3.3
10	X	1	MET	3.2
3	Q	48	SER	3.2
2	B	218	GLY	3.2
14	N	195	GLN	3.2
1	O	227	ILE	3.2
4	D	242	GLU	3.1
3	C	180	LYS	3.1
6	T	244	ASN	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	O	250	LEU	3.0
3	C	236	GLN	3.0
13	a	3	GLN	3.0
3	Q	187	GLU	3.0
1	A	249	ALA	3.0
1	A	203	GLU	3.0
9	I	133	LYS	3.0
2	P	218	GLY	3.0
1	A	230	ASP	3.0
6	T	243	ILE	2.9
4	D	1	ASP	2.9
9	I	1	SER	2.9
1	O	226	GLY	2.9
5	E	233	ILE	2.9
6	T	2	THR	2.9
8	V	198	GLU	2.8
8	V	205	PHE	2.8
14	N	105	LYS	2.8
6	T	178	HIS	2.8
3	C	50	LEU	2.8
13	M	2	GLN	2.8
8	V	206	PRO	2.8
4	R	203	LYS	2.8
1	O	62	SER	2.8
5	S	227	GLU	2.8
5	S	233	ILE	2.7
3	Q	204	GLY	2.7
3	Q	239	GLN	2.7
8	V	212	VAL	2.7
13	M	82	ASP	2.7
1	O	230	ASP	2.7
6	F	202	ASP	2.7
1	A	228	PRO	2.6
4	D	217	GLN	2.6
1	A	201	GLU	2.6
1	A	248	GLU	2.6
8	V	196	ARG	2.6
7	G	242	GLN	2.6
7	U	183	ASP	2.6
4	R	217	GLN	2.6
6	T	205	GLU	2.6
5	E	201	ARG	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	R	201	GLU	2.6
7	U	188	GLU	2.6
4	D	241	ALA	2.5
6	T	206	LYS	2.5
1	A	227	ILE	2.5
1	O	203	GLU	2.5
2	P	52	THR	2.5
8	V	208	GLY	2.5
10	X	193	ASP	2.5
4	R	54	ASP	2.5
2	B	217	LYS	2.4
11	Y	106	ARG	2.4
9	I	131	GLU	2.4
3	Q	181	GLU	2.4
3	C	216	ASP	2.4
6	T	215	CYS	2.4
12	Z	1	GLN	2.4
10	J	1	MET	2.4
6	F	244	ASN	2.4
3	Q	47	ARG	2.4
8	V	218	VAL	2.4
5	E	227	GLU	2.3
7	G	68	ARG	2.3
5	S	180	LYS	2.3
1	O	221	LEU	2.3
7	U	181	LYS	2.3
9	W	192	ASP	2.3
8	H	196	ARG	2.3
2	P	182	ASP	2.3
11	Y	212	GLY	2.2
3	Q	59	PRO	2.2
2	B	59	ASP	2.2
7	U	222	ASP	2.2
7	U	241	GLU	2.2
13	a	171	GLN	2.2
4	R	242	GLU	2.2
6	T	201	GLU	2.2
3	Q	55	THR	2.2
6	T	181	GLU	2.2
6	F	205	GLU	2.2
3	Q	1	GLY	2.2
6	T	230	ASP	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
9	I	192	ASP	2.2
11	K	212	GLY	2.2
6	F	166	GLN	2.1
8	V	200	GLN	2.1
13	a	4	PRO	2.1
2	P	1	GLY	2.1
5	S	123	GLY	2.1
7	U	206	GLY	2.1
11	K	107	LYS	2.1
2	P	223	GLU	2.1
8	H	21	THR	2.1
5	S	218	ASP	2.1
5	S	30	GLN	2.1
3	Q	202	GLN	2.1
3	C	234	ILE	2.1
3	C	202	GLN	2.1
3	Q	203	THR	2.1
4	D	2	ARG	2.0
4	R	230	GLU	2.0
6	T	235	ALA	2.0
8	H	188	ARG	2.0
2	B	244	THR	2.0
3	Q	216	ASP	2.0
3	Q	167	LYS	2.0
5	S	29	LYS	2.0
2	P	50	LYS	2.0
3	Q	60	SER	2.0
8	V	214	LYS	2.0
7	G	241	GLU	2.0
11	K	106	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

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	G	301	1/1	0.90	0.09	44,44,44,44	0
15	MG	W	301	1/1	0.96	0.29	70,70,70,70	0
16	CL	U	301	1/1	0.96	0.23	30,30,30,30	0
15	MG	I	301	1/1	0.97	0.16	54,54,54,54	0
15	MG	Z	301	1/1	0.97	0.24	56,56,56,56	0
15	MG	I	302	1/1	0.98	0.08	47,47,47,47	0
15	MG	K	301	1/1	0.98	0.07	45,45,45,45	0
15	MG	N	201	1/1	0.99	0.04	44,44,44,44	0
15	MG	L	301	1/1	0.99	0.04	46,46,46,46	0
16	CL	G	302	1/1	0.99	0.10	30,30,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.