



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:52 PM UTC

PDB ID : 5FG9 / pdb_00005fg9
Title : Yeast 20S proteasome beta2-T(-2)V mutant
Authors : Huber, E.M.; Groll, M.
Deposited on : 2015-12-20
Resolution : 2.60 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

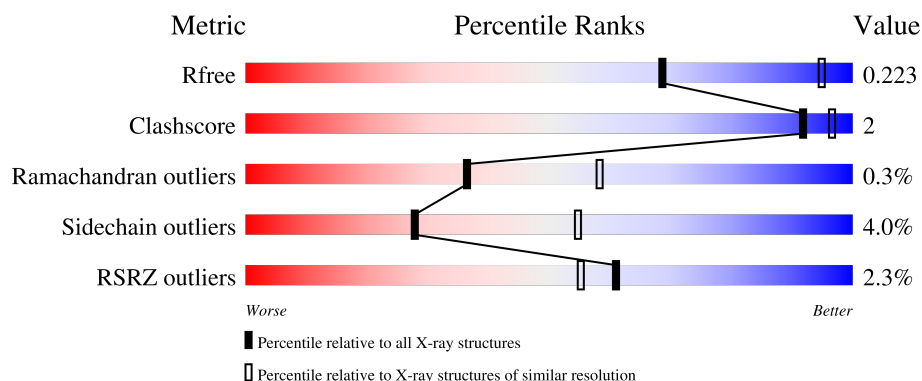
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

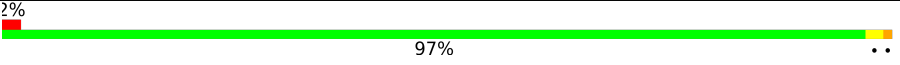
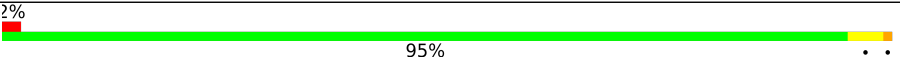
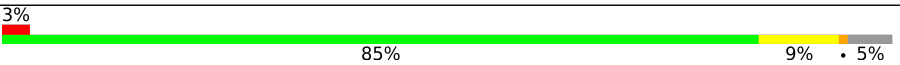
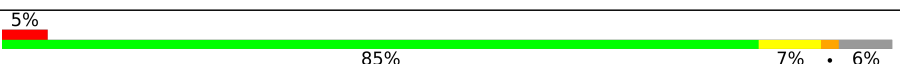
The reported resolution of this entry is 2.60 Å.

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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	
1	O	250	
2	B	258	
2	P	258	
3	C	254	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	Q	254	 7% 85% 7% • 6%
4	D	260	 2% 83% 7% • 10%
4	R	260	 2% 83% 7% 10%
5	E	234	 3% 91% 6% ••
5	S	234	 3% 93% 6% •
6	F	288	 % 80% 5% 16%
6	T	288	 2% 80% 5% 16%
7	G	252	 % 87% 8% ••
7	U	252	 3% 87% 8% ••
8	H	236	 3% 90% 7% •
8	V	236	 3% 90% 6% ••
9	I	205	 93% 6%
9	W	205	 % 93% 6%
10	J	198	 % 90% 8% ••
10	X	198	 2% 90% 8% ••
11	K	212	 % 91% 8% •
11	Y	212	 2% 91% 8% •
12	L	222	 % 95% ••
12	Z	222	 % 95% ••
13	M	246	 2% 91% • 5%
13	a	246	 2% 91% • 5%
14	N	196	 % 93% 6% •
14	b	196	 % 92% 7% •

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 50147 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	230	Total	C	N	O	S	0	0	0
			1743	1096	302	338	7			
8	V	230	Total	C	N	O	S	0	0	0
			1743	1096	302	338	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	-1	VAL	THR	engineered mutation	UNP P25043
V	-1	VAL	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 (CCD ID: MG) (formula: Mg).

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

- Molecule 16 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	A	34	Total O 34 34	0	0
16	B	18	Total O 18 18	0	0
16	C	21	Total O 21 21	0	0
16	D	20	Total O 20 20	0	0
16	E	17	Total O 17 17	0	0
16	F	22	Total O 22 22	0	0
16	G	42	Total O 42 42	0	0
16	H	25	Total O 25 25	0	0
16	I	31	Total O 31 31	0	0
16	J	29	Total O 29 29	0	0
16	K	37	Total O 37 37	0	0
16	L	38	Total O 38 38	0	0
16	M	36	Total O 36 36	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	N	19	Total 19	O 19	0	0
16	O	16	Total 16	O 16	0	0
16	P	16	Total 16	O 16	0	0
16	Q	24	Total 24	O 24	0	0
16	R	21	Total 21	O 21	0	0
16	S	10	Total 10	O 10	0	0
16	T	18	Total 18	O 18	0	0
16	U	33	Total 33	O 33	0	0
16	V	21	Total 21	O 21	0	0
16	W	33	Total 33	O 33	0	0
16	X	19	Total 19	O 19	0	0
16	Y	31	Total 31	O 31	0	0
16	Z	28	Total 28	O 28	0	0
16	a	37	Total 37	O 37	0	0
16	b	28	Total 28	O 28	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

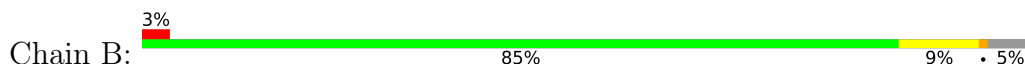
- Molecule 1: Proteasome subunit alpha type-2



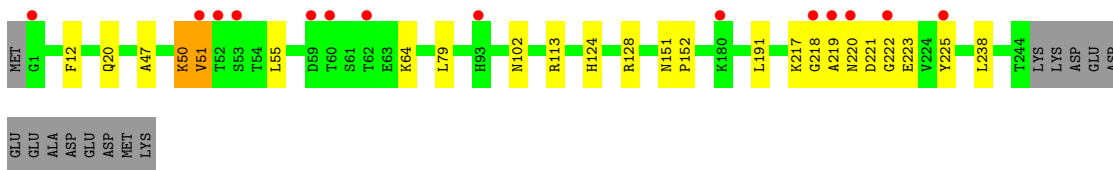
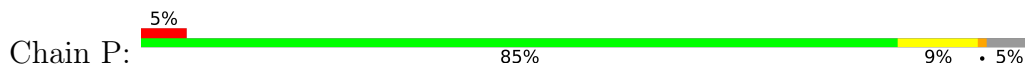
- Molecule 1: Proteasome subunit alpha type-2



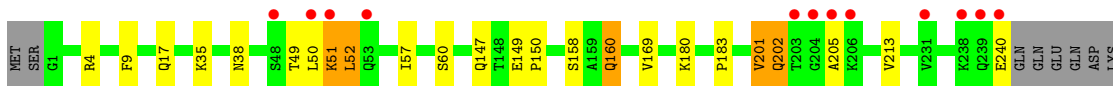
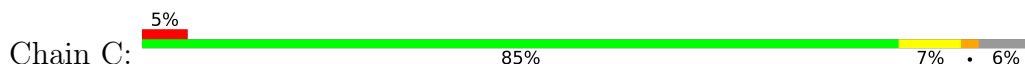
- Molecule 2: Proteasome subunit alpha type-3



- Molecule 2: Proteasome subunit alpha type-3



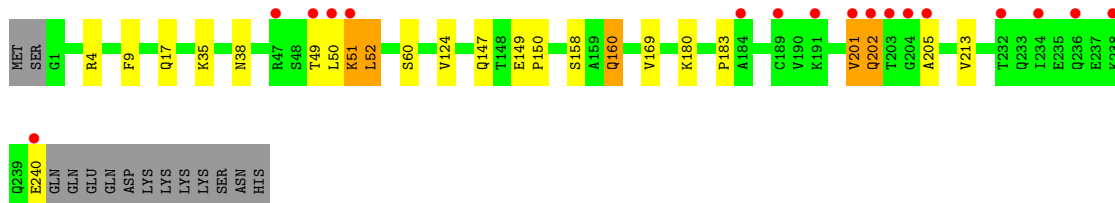
- Molecule 3: Proteasome subunit alpha type-4



LYS
LYS
LYS
SER
ASN
HIS

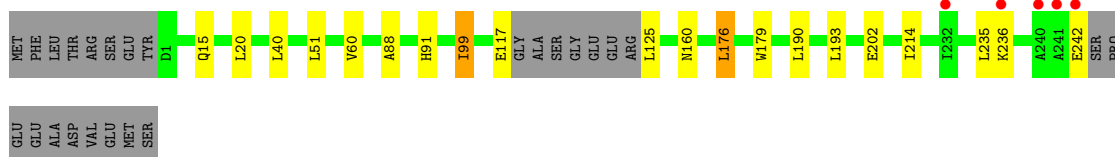
• Molecule 3: Proteasome subunit alpha type-4

Chain Q: 7% 85% 7% 6%



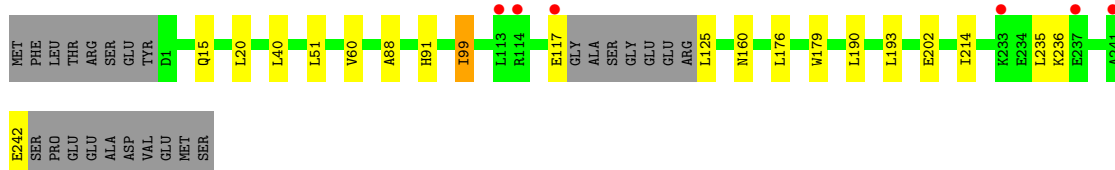
• Molecule 4: Proteasome subunit alpha type-5

Chain D: 2% 83% 7% 10%



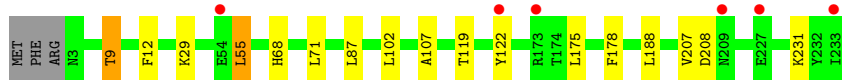
• Molecule 4: Proteasome subunit alpha type-5

Chain R: 2% 83% 7% 10%



• Molecule 5: Proteasome subunit alpha type-6

Chain E: 3% 91% 6% 2%

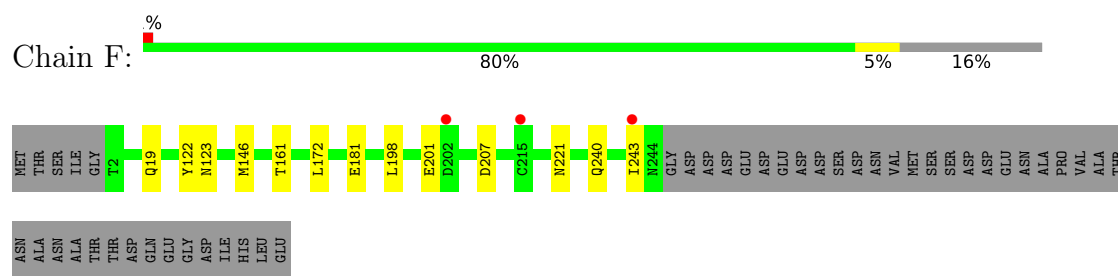


• Molecule 5: Proteasome subunit alpha type-6

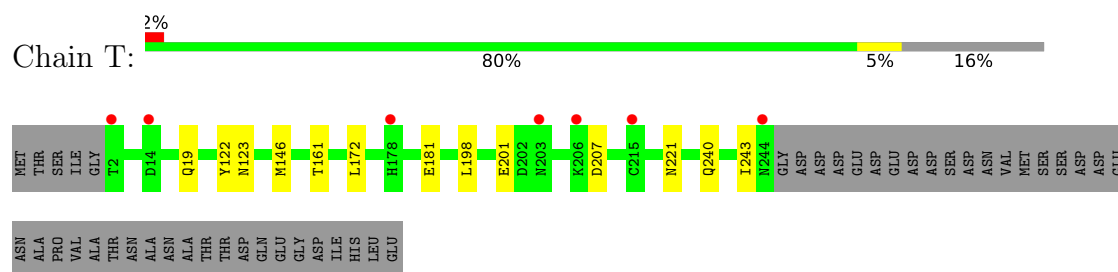
Chain S: 3% 93% 6% 2%



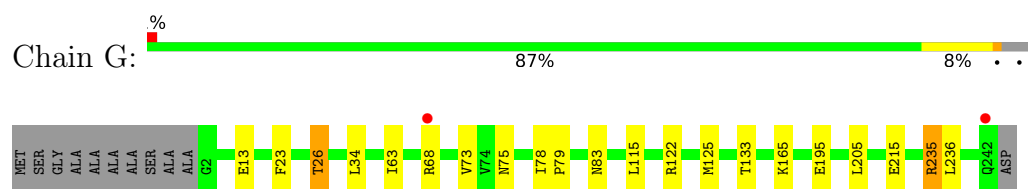
• Molecule 6: Probable proteasome subunit alpha type-7



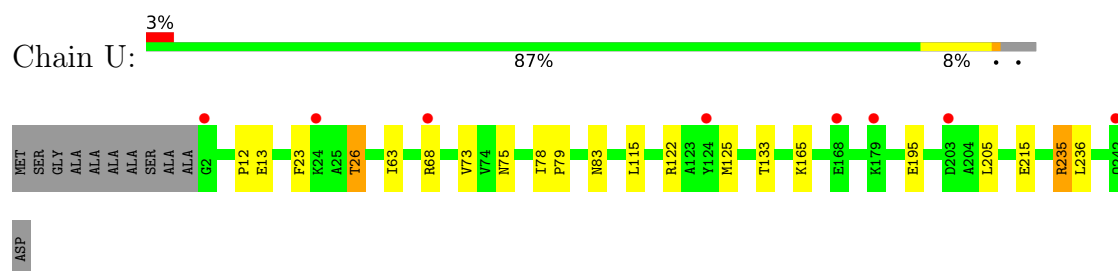
- Molecule 6: Probable proteasome subunit alpha type-7



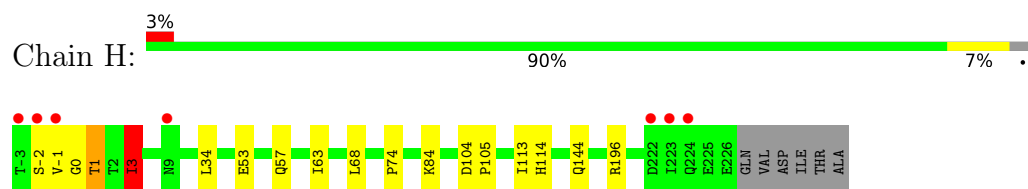
- Molecule 7: Proteasome subunit alpha type-1



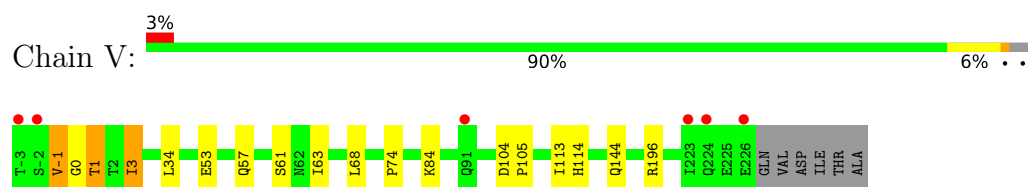
- Molecule 7: Proteasome subunit alpha type-1



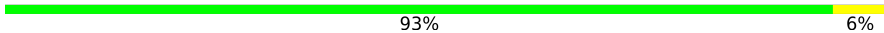
- Molecule 8: Proteasome subunit beta type-2



- Molecule 8: Proteasome subunit beta type-2

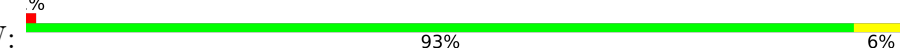


- Molecule 9: Proteasome subunit beta type-3

Chain I:  93% 6%

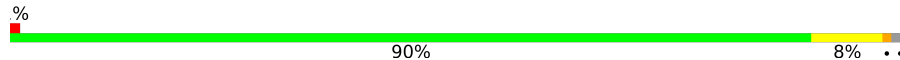


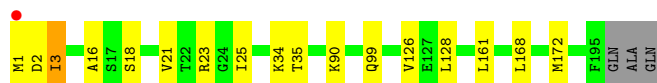
- Molecule 9: Proteasome subunit beta type-3

Chain W:  93% 6%

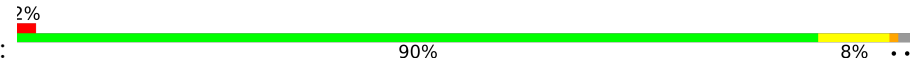


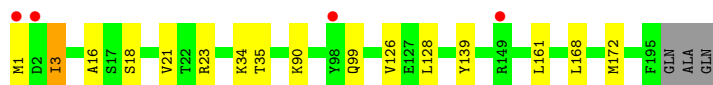
- Molecule 10: Proteasome subunit beta type-4

Chain J:  90% 8% ..

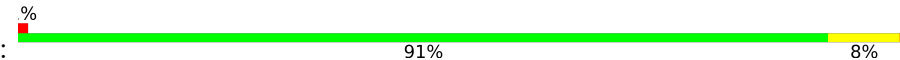


- Molecule 10: Proteasome subunit beta type-4

Chain X:  90% 8% ..

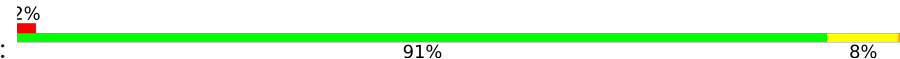


- Molecule 11: Proteasome subunit beta type-5

Chain K:  91% 8% .

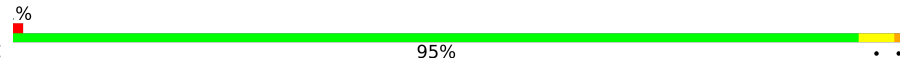


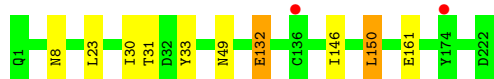
- Molecule 11: Proteasome subunit beta type-5

Chain Y:  91% 8% .



- Molecule 12: Proteasome subunit beta type-6

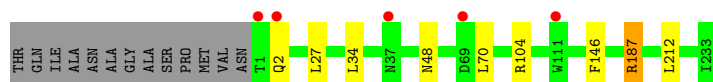
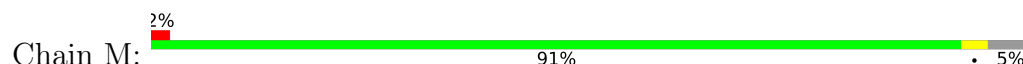
Chain L:  95% ..



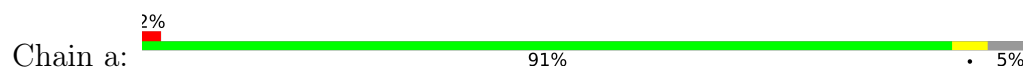
- Molecule 12: Proteasome subunit beta type-6



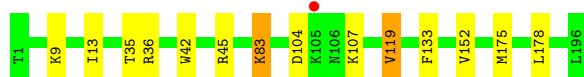
- Molecule 13: Proteasome subunit beta type-7



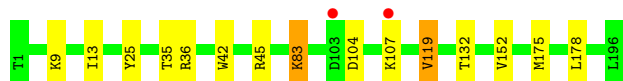
- Molecule 13: Proteasome subunit beta type-7



- 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	135.57Å 301.55Å 145.13Å 90.00° 113.36° 90.00°	Depositor
Resolution (Å)	15.00 – 2.60 15.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.2 (15.00-2.60) 96.7 (15.00-2.60)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.09 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.209 , 0.230 (Not available) , 0.223	Depositor DCC
R_{free} test set	15793 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	50.5	Xtriage
Anisotropy	0.066	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 52.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	50147	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 2.63% 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

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	0.40	0/1952	0.68	0/2642
1	O	0.41	0/1952	0.68	0/2642
2	B	0.42	0/1934	0.69	0/2618
2	P	0.42	0/1934	0.69	0/2618
3	C	0.41	0/1910	0.70	1/2586 (0.0%)
3	Q	0.41	0/1910	0.70	1/2586 (0.0%)
4	D	0.39	0/1837	0.67	0/2475
4	R	0.40	0/1837	0.67	0/2475
5	E	0.40	0/1800	0.65	0/2433
5	S	0.40	0/1800	0.65	0/2433
6	F	0.41	0/1932	0.69	0/2609
6	T	0.40	0/1932	0.69	0/2609
7	G	0.40	0/1945	0.68	0/2634
7	U	0.40	0/1945	0.68	0/2634
8	H	0.49	2/1774 (0.1%)	0.67	0/2406
8	V	0.48	1/1774 (0.1%)	0.67	0/2406
9	I	0.39	0/1611	0.68	0/2174
9	W	0.39	0/1611	0.68	0/2174
10	J	0.42	1/1589 (0.1%)	0.66	0/2142
10	X	0.42	0/1589	0.67	0/2142
11	K	0.39	0/1681	0.67	0/2274
11	Y	0.39	0/1681	0.67	0/2274
12	L	0.39	0/1795	0.67	0/2420
12	Z	0.41	0/1795	0.66	0/2420
13	M	0.44	0/1855	0.67	0/2514
13	a	0.41	0/1855	0.67	1/2514 (0.0%)
14	N	0.40	0/1541	0.67	0/2087
14	b	0.39	0/1541	0.67	0/2087
All	All	0.41	4/50312 (0.0%)	0.67	3/68028 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	114	HIS	CE1-NE2	6.41	1.39	1.32
8	H	3	ILE	C-O	-6.18	1.17	1.24
8	V	114	HIS	CE1-NE2	6.14	1.38	1.32
10	J	2	ASP	CA-C	5.02	1.54	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Q	201	VAL	N-CA-C	6.21	116.37	110.53
3	C	201	VAL	N-CA-C	6.17	116.33	110.53
13	a	10	SER	N-CA-C	5.00	117.29	110.24

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	2	0
1	O	1915	0	1929	6	0
2	B	1904	0	1904	11	0
2	P	1904	0	1904	12	0
3	C	1881	0	1895	8	0
3	Q	1881	0	1895	8	0
4	D	1813	0	1797	6	0
4	R	1813	0	1797	5	0
5	E	1773	0	1775	7	0
5	S	1773	0	1775	4	0
6	F	1892	0	1883	4	0
6	T	1892	0	1883	4	0
7	G	1907	0	1901	8	0
7	U	1907	0	1901	8	0
8	H	1743	0	1743	8	0
8	V	1743	0	1743	10	0
9	I	1581	0	1574	7	0
9	W	1581	0	1574	7	0
10	J	1561	0	1569	10	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	5	0
12	Z	1757	0	1711	4	0
13	M	1824	0	1832	2	0
13	a	1824	0	1832	1	0
14	N	1512	0	1481	9	0
14	b	1512	0	1481	10	0
15	G	1	0	0	0	0
15	I	2	0	0	0	0
15	J	1	0	0	0	0
15	K	2	0	0	0	0
15	L	1	0	0	0	0
15	N	1	0	0	0	0
15	Z	1	0	0	0	0
16	A	34	0	0	0	0
16	B	18	0	0	0	0
16	C	21	0	0	0	0
16	D	20	0	0	0	0
16	E	17	0	0	0	0
16	F	22	0	0	0	0
16	G	42	0	0	0	0
16	H	25	0	0	0	0
16	I	31	0	0	0	0
16	J	29	0	0	0	0
16	K	37	0	0	0	0
16	L	38	0	0	0	0
16	M	36	0	0	0	0
16	N	19	0	0	0	0
16	O	16	0	0	0	0
16	P	16	0	0	0	0
16	Q	24	0	0	0	0
16	R	21	0	0	0	0
16	S	10	0	0	0	0
16	T	18	0	0	0	0
16	U	33	0	0	0	0
16	V	21	0	0	0	0
16	W	33	0	0	0	0
16	X	19	0	0	0	0
16	Y	31	0	0	0	0
16	Z	28	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	a	37	0	0	0	0
16	b	28	0	0	0	0
All	All	50147	0	49178	162	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 (162) 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)
12:L:33:TYR:CE2	8:V:-1:VAL:HG11	2.18	0.78
8:H:0:GLY:O	8:H:1:THR:HB	1.98	0.63
14:N:152:VAL:HA	14:N:175:MET:HE1	1.81	0.62
14:N:35:THR:HG21	14:N:45:ARG:HE	1.64	0.62
14:b:35:THR:HG21	14:b:45:ARG:HE	1.64	0.62
14:b:152:VAL:HA	14:b:175:MET:HE1	1.80	0.62
2:B:12:PHE:H	3:C:17:GLN:HE22	1.49	0.60
7:G:68:ARG:HH12	14:N:36:ARG:HH22	1.49	0.60
2:B:221:ASP:O	2:B:223:GLU:N	2.37	0.58
2:P:221:ASP:O	2:P:223:GLU:N	2.37	0.58
3:Q:51:LYS:O	3:Q:52:LEU:HB2	2.04	0.57
11:K:53:GLN:O	11:K:57:THR:HG23	2.05	0.57
11:Y:53:GLN:O	11:Y:57:THR:HG23	2.05	0.56
2:P:217:LYS:C	2:P:219:ALA:H	2.14	0.56
5:E:12:PHE:H	6:F:19:GLN:HE22	1.54	0.56
3:C:51:LYS:O	3:C:52:LEU:HB2	2.04	0.56
2:B:217:LYS:C	2:B:219:ALA:H	2.13	0.55
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
8:V:0:GLY:O	8:V:1:THR:HB	2.08	0.53
5:S:12:PHE:H	6:T:19:GLN:HE22	1.56	0.52
3:C:160:GLN:HE21	3:C:160:GLN:HA	1.75	0.52
3:C:201:VAL:O	3:C:202:GLN:CB	2.57	0.52
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.57	0.52
3:Q:160:GLN:HE21	3:Q:160:GLN:HA	1.75	0.51
2:P:47:ALA:HB1	2:P:64:LYS:HD2	1.93	0.51
7:G:23:PHE:O	7:G:26:THR:HB	2.11	0.51
7:U:23:PHE:O	7:U:26:THR:HB	2.10	0.51
2:B:47:ALA:HB1	2:B:64:LYS:HD2	1.93	0.51
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.46	0.50
10:X:21:VAL:HG11	11:Y:122:LEU:HD11	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:9:GLY:HA3	9:I:41:LYS:HE2	1.94	0.50
14:N:83:LYS:HG3	14:N:119:VAL:CG2	2.42	0.49
7:U:68:ARG:HH12	14:b:36:ARG:HH22	1.61	0.49
9:W:9:GLY:HA3	9:W:41:LYS:HE2	1.94	0.49
2:B:3:ARG:HB3	5:E:122:TYR:OH	2.13	0.49
10:X:1:MET:HG2	10:X:34:LYS:HE3	1.94	0.49
14:b:83:LYS:HG3	14:b:119:VAL:CG2	2.42	0.49
11:Y:20:ALA:HB2	11:Y:31:VAL:HG21	1.95	0.49
11:Y:32:LYS:N	12:Z:132:GLU:OE2	2.42	0.49
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.95	0.48
11:K:20:ALA:HB2	11:K:31:VAL:HG21	1.95	0.48
10:J:21:VAL:HG11	11:K:122:LEU:HD11	1.95	0.48
11:K:107:LYS:HG3	11:K:108:GLU:HG3	1.96	0.48
10:J:1:MET:HG2	10:J:34:LYS:HE3	1.95	0.47
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.95	0.47
10:J:3:ILE:HG23	10:J:18:SER:HB3	1.96	0.47
4:R:91:HIS:HB3	4:R:99:ILE:HG22	1.97	0.47
1:A:122:THR:HG22	2:B:128:ARG:HH21	1.80	0.47
3:C:35:LYS:HG2	3:C:158:SER:O	2.15	0.47
10:J:25:ILE:O	10:X:139:TYR:OH	2.33	0.47
14:N:13:ILE:HG21	14:N:175:MET:HE2	1.96	0.47
1:O:122:THR:HG22	2:P:128:ARG:HH21	1.78	0.47
11:K:128:CYS:SG	11:K:136:ALA:HB3	2.55	0.47
14:N:35:THR:CG2	14:N:45:ARG:HE	2.28	0.46
10:X:3:ILE:HG23	10:X:18:SER:HB3	1.97	0.46
4:D:91:HIS:HB3	4:D:99:ILE:HG22	1.97	0.46
9:I:36:SER:HB2	10:J:126:VAL:HG11	1.97	0.46
11:Y:107:LYS:HG3	11:Y:108:GLU:HG3	1.97	0.46
14:b:13:ILE:HG21	14:b:175:MET:HE2	1.97	0.46
11:Y:128:CYS:SG	11:Y:136:ALA:HB3	2.56	0.46
12:L:33:TYR:CE2	8:V:-1:VAL:CG1	2.97	0.46
4:D:176:LEU:HD22	5:E:55:LEU:CD2	2.45	0.45
3:Q:35:LYS:HG2	3:Q:158:SER:O	2.15	0.45
9:I:101:PRO:HB3	9:I:126:ILE:HD12	1.99	0.45
4:R:91:HIS:HB3	4:R:99:ILE:CG2	2.46	0.45
14:b:35:THR:CG2	14:b:45:ARG:HE	2.28	0.45
9:W:101:PRO:HB3	9:W:126:ILE:HD12	1.99	0.45
3:Q:149:GLU:HB2	3:Q:150:PRO:HD2	1.99	0.45
3:C:149:GLU:HB2	3:C:150:PRO:HD2	1.99	0.45
4:D:91:HIS:HB3	4:D:99:ILE:CG2	2.47	0.45
5:S:87:LEU:HD21	5:S:107:ALA:HB1	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:219:ALA:HB2	2:B:225:TYR:HB2	1.99	0.45
5:E:87:LEU:HD21	5:E:107:ALA:HB1	1.99	0.44
10:J:1:MET:CB	10:J:34:LYS:HE3	2.48	0.44
10:X:1:MET:CB	10:X:34:LYS:HE3	2.47	0.44
2:P:50:LYS:O	2:P:51:VAL:C	2.60	0.44
3:C:9:PHE:H	4:D:15:GLN:HE22	1.65	0.44
2:P:219:ALA:HB2	2:P:225:TYR:HB2	1.99	0.44
8:H:63:ILE:HG23	8:H:74:PRO:HB3	1.99	0.44
2:P:12:PHE:H	3:Q:17:GLN:HE22	1.66	0.43
2:P:151:ASN:HB2	2:P:152:PRO:CD	2.48	0.43
11:Y:38:ASN:HB2	11:Y:39:PRO:CD	2.48	0.43
1:A:1:MET:HG3	6:F:122:TYR:CZ	2.54	0.43
2:B:50:LYS:O	2:B:51:VAL:C	2.60	0.43
6:F:146:MET:HE3	6:F:161:THR:HB	2.00	0.43
9:I:98:ARG:O	9:I:126:ILE:HD11	2.18	0.43
11:K:38:ASN:HB2	11:K:39:PRO:CD	2.48	0.43
10:X:1:MET:HB3	10:X:34:LYS:HE3	2.00	0.43
2:B:151:ASN:HB2	2:B:152:PRO:CD	2.48	0.43
8:V:63:ILE:HG23	8:V:74:PRO:HB3	2.00	0.43
2:B:217:LYS:C	2:B:219:ALA:N	2.76	0.43
4:D:88:ALA:HA	4:D:99:ILE:HG21	2.01	0.43
9:I:20:VAL:HG13	9:I:118:PRO:HB3	2.00	0.43
8:V:104:ASP:HB2	8:V:105:PRO:HD2	2.00	0.43
12:L:8:ASN:HA	12:L:30:ILE:O	2.19	0.43
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.54	0.43
12:Z:213:ARG:NH1	16:Z:401:HOH:O	2.51	0.43
8:H:104:ASP:HB2	8:H:105:PRO:HD2	2.00	0.43
11:K:32:LYS:N	12:L:132:GLU:OE2	2.46	0.43
4:R:88:ALA:HA	4:R:99:ILE:HG21	2.01	0.43
6:F:198:LEU:HD12	6:F:243:ILE:HG22	2.00	0.43
1:O:1:MET:HG3	6:T:122:TYR:CZ	2.53	0.43
11:K:145:LYS:HB2	11:K:148:LEU:HD13	2.01	0.43
14:N:83:LYS:HG3	14:N:119:VAL:HG22	2.00	0.43
14:N:133:PHE:HA	14:b:132:THR:O	2.19	0.43
14:b:83:LYS:HG3	14:b:119:VAL:HG22	2.00	0.43
10:J:1:MET:HB3	10:J:34:LYS:HE3	2.00	0.42
6:T:198:LEU:HD12	6:T:243:ILE:HG22	2.00	0.42
1:O:12:PHE:H	2:P:20:GLN:HE22	1.67	0.42
11:Y:145:LYS:HB2	11:Y:148:LEU:HD13	2.00	0.42
14:b:36:ARG:HG3	14:b:42:TRP:CE2	2.54	0.42
7:G:63:ILE:HD12	7:G:215:GLU:HG2	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:36:ARG:HG3	14:N:42:TRP:CE2	2.54	0.42
5:S:175:LEU:HA	5:S:178:PHE:CE2	2.54	0.42
13:M:27:LEU:HD21	13:M:34:LEU:HD22	2.02	0.42
2:P:217:LYS:C	2:P:219:ALA:N	2.76	0.42
6:T:146:MET:HE3	6:T:161:THR:HB	2.00	0.42
9:W:98:ARG:O	9:W:126:ILE:HD11	2.19	0.42
2:B:146:GLN:HG2	3:C:57:ILE:HG21	2.02	0.42
7:G:73:VAL:HG12	7:G:133:THR:HB	2.00	0.42
9:W:20:VAL:HG13	9:W:118:PRO:HB3	2.00	0.42
13:a:27:LEU:HD21	13:a:34:LEU:HD22	2.02	0.42
5:E:175:LEU:HA	5:E:178:PHE:CE2	2.55	0.42
8:H:1:THR:CG2	8:H:3:ILE:HG23	2.50	0.42
7:U:73:VAL:HG12	7:U:133:THR:HB	2.01	0.42
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.55	0.42
10:X:126:VAL:HG12	10:X:128:LEU:HG	2.02	0.42
12:Z:146:ILE:HG22	12:Z:150:LEU:HD22	2.02	0.42
7:G:195:GLU:HG3	7:G:235:ARG:HG3	2.01	0.41
10:J:126:VAL:HG12	10:J:128:LEU:HG	2.02	0.41
3:Q:9:PHE:H	4:R:15:GLN:HE22	1.67	0.41
7:U:195:GLU:HG3	7:U:235:ARG:HG3	2.01	0.41
8:H:53:GLU:O	8:H:57:GLN:HG2	2.20	0.41
7:U:63:ILE:HD12	7:U:215:GLU:HG2	2.01	0.41
9:W:170:LEU:C	9:W:170:LEU:HD23	2.45	0.41
8:H:0:GLY:O	8:H:1:THR:CB	2.65	0.41
1:O:99:ARG:HE	8:V:61:SER:HG	1.68	0.41
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.20	0.41
5:S:9:THR:HG21	5:S:119:THR:HA	2.03	0.41
8:V:53:GLU:O	8:V:57:GLN:HG2	2.19	0.41
9:W:20:VAL:HG23	9:W:189:ILE:HB	2.03	0.41
5:E:68:HIS:HE1	5:E:102:LEU:O	2.03	0.41
7:G:78:ILE:N	7:G:79:PRO:CD	2.84	0.41
9:I:170:LEU:C	9:I:170:LEU:HD23	2.46	0.41
8:V:84:LYS:HA	8:V:113:ILE:HD11	2.02	0.41
13:M:187:ARG:HG3	14:b:25:TYR:CE1	2.55	0.41
7:U:78:ILE:N	7:U:79:PRO:CD	2.84	0.41
7:G:34:LEU:C	7:G:34:LEU:HD23	2.46	0.41
2:P:124:HIS:HB3	3:Q:124:VAL:HG12	2.03	0.40
5:E:9:THR:HG21	5:E:119:THR:HA	2.02	0.40
12:L:146:ILE:HG22	12:L:150:LEU:HD22	2.02	0.40
8:V:1:THR:CG2	8:V:3:ILE:HG23	2.51	0.40
8:V:104:ASP:HB2	8:V:105:PRO:CD	2.51	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:84:LYS:HA	8:H:113:ILE:HD11	2.02	0.40
8:H:104:ASP:HB2	8:H:105:PRO:CD	2.51	0.40
1:O:75:TYR:HB3	1:O:82:TYR:CD1	2.56	0.40
10:X:168:LEU:O	10:X:172:MET:HB2	2.21	0.40
10:J:168:LEU:O	10:J:172:MET:HB2	2.21	0.40
7:U:165:LYS:HD2	7:U:205:LEU:HD22	2.03	0.40
7:G:165:LYS:HD2	7:G:205:LEU:HD22	2.04	0.40
2:P:151:ASN:HB2	2:P:152:PRO:HD2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	248/250 (99%)	240 (97%)	7 (3%)	1 (0%)	30	51
1	O	248/250 (99%)	240 (97%)	7 (3%)	1 (0%)	30	51
2	B	242/258 (94%)	235 (97%)	3 (1%)	4 (2%)	7	15
2	P	242/258 (94%)	235 (97%)	3 (1%)	4 (2%)	7	15
3	C	238/254 (94%)	232 (98%)	3 (1%)	3 (1%)	9	21
3	Q	238/254 (94%)	232 (98%)	3 (1%)	3 (1%)	9	21
4	D	231/260 (89%)	229 (99%)	2 (1%)	0	100	100
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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	U	239/252 (95%)	238 (100%)	1 (0%)	0	100	100
8	H	228/236 (97%)	222 (97%)	5 (2%)	1 (0%)	30	51
8	V	228/236 (97%)	222 (97%)	5 (2%)	1 (0%)	30	51
9	I	202/205 (98%)	196 (97%)	6 (3%)	0	100	100
9	W	202/205 (98%)	196 (97%)	6 (3%)	0	100	100
10	J	193/198 (98%)	189 (98%)	4 (2%)	0	100	100
10	X	193/198 (98%)	189 (98%)	4 (2%)	0	100	100
11	K	210/212 (99%)	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%)	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	6292/6622 (95%)	6148 (98%)	126 (2%)	18 (0%)	36	58

All (18) Ramachandran outliers are listed below:

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	Q	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%)	203 (97%)	6 (3%)	37	65
1	O	209/209 (100%)	203 (97%)	6 (3%)	37	65
2	B	203/216 (94%)	196 (97%)	7 (3%)	32	60
2	P	203/216 (94%)	196 (97%)	7 (3%)	32	60
3	C	212/226 (94%)	199 (94%)	13 (6%)	17	37
3	Q	212/226 (94%)	199 (94%)	13 (6%)	17	37
4	D	194/215 (90%)	179 (92%)	15 (8%)	12	27
4	R	194/215 (90%)	179 (92%)	15 (8%)	12	27
5	E	190/193 (98%)	182 (96%)	8 (4%)	26	52
5	S	190/193 (98%)	182 (96%)	8 (4%)	26	52
6	F	201/239 (84%)	194 (96%)	7 (4%)	32	59
6	T	201/239 (84%)	194 (96%)	7 (4%)	32	59
7	G	206/210 (98%)	197 (96%)	9 (4%)	25	50
7	U	206/210 (98%)	197 (96%)	9 (4%)	25	50
8	H	188/193 (97%)	181 (96%)	7 (4%)	30	57
8	V	188/193 (97%)	182 (97%)	6 (3%)	34	62
9	I	172/173 (99%)	168 (98%)	4 (2%)	44	71
9	W	172/173 (99%)	168 (98%)	4 (2%)	44	71
10	J	173/175 (99%)	168 (97%)	5 (3%)	37	65
10	X	173/175 (99%)	168 (97%)	5 (3%)	37	65
11	K	169/169 (100%)	162 (96%)	7 (4%)	27	54
11	Y	169/169 (100%)	161 (95%)	8 (5%)	23	48
12	L	185/185 (100%)	179 (97%)	6 (3%)	34	62

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	Z	185/185 (100%)	179 (97%)	6 (3%)	34	62
13	M	199/208 (96%)	192 (96%)	7 (4%)	32	59
13	a	199/208 (96%)	193 (97%)	6 (3%)	36	64
14	N	162/162 (100%)	156 (96%)	6 (4%)	30	57
14	b	162/162 (100%)	156 (96%)	6 (4%)	30	57
All	All	5326/5546 (96%)	5113 (96%)	213 (4%)	28	55

All (213) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	59	GLU
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	102	ASN
2	B	113	ARG
2	B	191	LEU
2	B	238	LEU
3	C	4	ARG
3	C	38	ASN
3	C	49	THR
3	C	50	LEU
3	C	51	LYS
3	C	52	LEU
3	C	60	SER
3	C	147	GLN
3	C	160	GLN
3	C	169	VAL
3	C	180	LYS
3	C	213	VAL
3	C	240	GLU
4	D	20	LEU
4	D	40	LEU
4	D	51	LEU
4	D	60	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	D	99	ILE
4	D	117	GLU
4	D	125	LEU
4	D	176	LEU
4	D	190	LEU
4	D	193	LEU
4	D	202	GLU
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	188	LEU
5	E	207	VAL
5	E	208	ASP
5	E	231	LYS
6	F	123	ASN
6	F	172	LEU
6	F	181	GLU
6	F	201	GLU
6	F	207	ASP
6	F	221	ASN
6	F	240	GLN
7	G	13	GLU
7	G	26	THR
7	G	75	ASN
7	G	83	ASN
7	G	115	LEU
7	G	122	ARG
7	G	125	MET
7	G	235	ARG
7	G	236	LEU
8	H	-2	SER
8	H	-1	VAL
8	H	3	ILE
8	H	34	LEU
8	H	68	LEU
8	H	144	GLN
8	H	196	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	I	37	ASN
9	I	126	ILE
9	I	171	LEU
9	I	192	ASP
10	J	3	ILE
10	J	23	ARG
10	J	35	THR
10	J	90	LYS
10	J	99	GLN
11	K	4	LEU
11	K	9	GLN
11	K	45	MET
11	K	69	ARG
11	K	107	LYS
11	K	140	LEU
11	K	148	LEU
12	L	23	LEU
12	L	31	THR
12	L	49	ASN
12	L	132	GLU
12	L	150	LEU
12	L	161	GLU
13	M	2	GLN
13	M	48	ASN
13	M	70	LEU
13	M	104	ARG
13	M	146	PHE
13	M	187	ARG
13	M	212	LEU
14	N	9	LYS
14	N	83	LYS
14	N	104	ASP
14	N	107	LYS
14	N	119	VAL
14	N	178	LEU
1	O	1	MET
1	O	59	GLU
1	O	62	SER
1	O	122	THR
1	O	157	PHE
1	O	250	LEU
2	P	50	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	P	55	LEU
2	P	79	LEU
2	P	102	ASN
2	P	113	ARG
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	52	LEU
3	Q	60	SER
3	Q	147	GLN
3	Q	160	GLN
3	Q	169	VAL
3	Q	180	LYS
3	Q	213	VAL
3	Q	240	GLU
4	R	20	LEU
4	R	40	LEU
4	R	51	LEU
4	R	60	VAL
4	R	99	ILE
4	R	117	GLU
4	R	125	LEU
4	R	176	LEU
4	R	190	LEU
4	R	193	LEU
4	R	202	GLU
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	188	LEU
5	S	207	VAL
5	S	208	ASP
5	S	231	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	T	123	ASN
6	T	172	LEU
6	T	181	GLU
6	T	201	GLU
6	T	207	ASP
6	T	221	ASN
6	T	240	GLN
7	U	13	GLU
7	U	26	THR
7	U	75	ASN
7	U	83	ASN
7	U	115	LEU
7	U	122	ARG
7	U	125	MET
7	U	235	ARG
7	U	236	LEU
8	V	-1	VAL
8	V	3	ILE
8	V	34	LEU
8	V	68	LEU
8	V	144	GLN
8	V	196	ARG
9	W	37	ASN
9	W	126	ILE
9	W	171	LEU
9	W	192	ASP
10	X	3	ILE
10	X	23	ARG
10	X	35	THR
10	X	90	LYS
10	X	99	GLN
11	Y	4	LEU
11	Y	9	GLN
11	Y	45	MET
11	Y	69	ARG
11	Y	107	LYS
11	Y	128	CYS
11	Y	140	LEU
11	Y	148	LEU
12	Z	23	LEU
12	Z	31	THR
12	Z	49	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	Z	132	GLU
12	Z	150	LEU
12	Z	161	GLU
13	a	2	GLN
13	a	48	ASN
13	a	70	LEU
13	a	104	ARG
13	a	187	ARG
13	a	212	LEU
14	b	9	LYS
14	b	83	LYS
14	b	104	ASP
14	b	107	LYS
14	b	119	VAL
14	b	178	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (141) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	HIS
2	B	20	GLN
2	B	95	GLN
2	B	119	GLN
2	B	123	GLN
2	B	124	HIS
2	B	176	GLN
2	B	232	GLN
3	C	17	GLN
3	C	115	GLN
3	C	116	GLN
3	C	120	GLN
3	C	147	GLN
3	C	160	GLN
3	C	233	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	118	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	E	120	GLN
5	E	184	ASN
6	F	19	GLN
6	F	86	ASN
6	F	117	GLN
6	F	123	ASN
6	F	240	GLN
7	G	30	ASN
7	G	83	ASN
7	G	114	ASN
7	G	117	GLN
7	G	121	GLN
7	G	166	GLN
7	G	167	GLN
7	G	175	ASN
8	H	66	HIS
8	H	116	HIS
8	H	165	ASN
8	H	194	ASN
9	I	37	ASN
9	I	63	ASN
9	I	88	GLN
9	I	203	GLN
10	J	55	GLN
10	J	63	ASN
10	J	146	HIS
10	J	147	HIS
11	K	9	GLN
11	K	85	ASN
11	K	176	ASN
11	K	208	ASN
12	L	49	ASN
12	L	70	ASN
12	L	79	HIS
12	L	80	ASN
12	L	153	GLN
12	L	155	ASN
12	L	158	ASN
12	L	165	ASN
12	L	197	GLN
13	M	48	ASN
13	M	102	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	M	108	ASN
13	M	149	HIS
13	M	194	ASN
13	M	213	GLN
14	N	38	HIS
14	N	141	ASN
14	N	161	GLN
1	O	94	HIS
2	P	20	GLN
2	P	95	GLN
2	P	119	GLN
2	P	123	GLN
2	P	124	HIS
2	P	176	GLN
2	P	232	GLN
3	Q	17	GLN
3	Q	115	GLN
3	Q	116	GLN
3	Q	120	GLN
3	Q	147	GLN
3	Q	160	GLN
3	Q	233	GLN
4	R	15	GLN
4	R	91	HIS
4	R	100	ASN
4	R	225	ASN
5	S	68	HIS
5	S	92	ASN
5	S	99	ASN
5	S	118	ASN
5	S	120	GLN
5	S	184	ASN
6	T	19	GLN
6	T	86	ASN
6	T	117	GLN
6	T	123	ASN
6	T	240	GLN
7	U	30	ASN
7	U	83	ASN
7	U	114	ASN
7	U	117	GLN
7	U	121	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	U	166	GLN
7	U	167	GLN
7	U	175	ASN
8	V	66	HIS
8	V	86	HIS
8	V	194	ASN
9	W	37	ASN
9	W	44	HIS
9	W	63	ASN
9	W	88	GLN
9	W	203	GLN
10	X	10	GLN
10	X	55	GLN
10	X	61	GLN
10	X	63	ASN
10	X	146	HIS
10	X	147	HIS
11	Y	9	GLN
11	Y	85	ASN
11	Y	176	ASN
11	Y	208	ASN
12	Z	49	ASN
12	Z	70	ASN
12	Z	80	ASN
12	Z	153	GLN
12	Z	155	ASN
12	Z	197	GLN
13	a	48	ASN
13	a	149	HIS
13	a	194	ASN
13	a	213	GLN
14	b	38	HIS
14	b	141	ASN
14	b	161	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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%)	-0.16	4 (1%) 70 66	33, 45, 78, 113	0
1	O	250/250 (100%)	-0.06	5 (2%) 65 60	37, 53, 95, 122	0
2	B	244/258 (94%)	0.07	8 (3%) 49 43	36, 55, 94, 143	0
2	P	244/258 (94%)	0.15	14 (5%) 29 24	40, 56, 98, 146	0
3	C	240/254 (94%)	0.13	12 (5%) 34 28	36, 58, 115, 143	0
3	Q	240/254 (94%)	0.40	17 (7%) 22 17	39, 68, 144, 170	0
4	D	235/260 (90%)	0.03	5 (2%) 63 58	40, 58, 91, 134	0
4	R	235/260 (90%)	0.11	6 (2%) 57 51	42, 62, 101, 133	0
5	E	231/234 (98%)	0.14	6 (2%) 57 51	39, 60, 98, 144	0
5	S	231/234 (98%)	0.28	8 (3%) 47 41	43, 68, 105, 150	0
6	F	243/288 (84%)	-0.08	3 (1%) 76 73	34, 51, 100, 130	0
6	T	243/288 (84%)	0.15	7 (2%) 53 48	38, 62, 113, 143	0
7	G	241/252 (95%)	-0.20	2 (0%) 82 80	27, 46, 78, 131	0
7	U	241/252 (95%)	-0.02	8 (3%) 49 43	38, 52, 81, 125	0
8	H	230/236 (97%)	-0.12	7 (3%) 52 47	31, 47, 77, 140	0
8	V	230/236 (97%)	-0.05	6 (2%) 57 51	36, 50, 76, 148	0
9	I	204/205 (99%)	-0.34	0 100 100	32, 43, 69, 95	0
9	W	204/205 (99%)	-0.32	2 (0%) 79 76	34, 45, 73, 97	0
10	J	195/198 (98%)	-0.18	1 (0%) 87 85	34, 49, 72, 126	0
10	X	195/198 (98%)	-0.13	4 (2%) 63 58	34, 48, 72, 134	0
11	K	212/212 (100%)	-0.27	2 (0%) 81 78	30, 46, 67, 88	0
11	Y	212/212 (100%)	-0.17	4 (1%) 66 61	36, 48, 70, 88	0
12	L	222/222 (100%)	-0.15	2 (0%) 81 78	33, 48, 81, 117	0
12	Z	222/222 (100%)	-0.21	2 (0%) 81 78	31, 48, 80, 115	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%)	-0.21	5 (2%) 63 58	32, 47, 69, 88	0
13	a	233/246 (94%)	-0.18	4 (1%) 69 64	33, 46, 65, 84	0
14	N	196/196 (100%)	-0.32	1 (0%) 87 85	29, 42, 68, 96	0
14	b	196/196 (100%)	-0.26	2 (1%) 79 76	32, 43, 72, 105	0
All	All	6352/6622 (95%)	-0.06	147 (2%) 61 55	27, 51, 94, 170	0

All (147) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
10	X	1	MET	6.8
13	M	1	THR	6.7
3	Q	50	LEU	5.7
13	a	1	THR	5.2
2	B	219	ALA	4.9
2	P	219	ALA	4.9
10	J	1	MET	4.8
8	V	223	ILE	4.6
13	M	2	GLN	4.5
3	Q	205	ALA	4.3
13	a	2	GLN	4.3
12	L	174	TYR	4.2
1	A	2	THR	4.0
8	H	-2	SER	4.0
3	C	205	ALA	3.9
2	P	218	GLY	3.9
2	B	51	VAL	3.8
5	S	207	VAL	3.6
1	O	53	SER	3.5
8	V	-2	SER	3.5
2	P	51	VAL	3.5
8	V	-3	THR	3.4
2	P	1	GLY	3.4
4	D	241	ALA	3.4
2	P	222	GLY	3.3
2	P	52	THR	3.3
12	Z	174	TYR	3.3
4	D	240	ALA	3.3
3	Q	49	THR	3.1
8	H	223	ILE	3.1
10	X	98	TYR	3.1
8	H	-3	THR	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
5	E	54	GLU	3.0
6	T	206	LYS	3.0
5	S	173	ARG	3.0
4	D	242	GLU	3.0
3	C	50	LEU	3.0
2	B	220	ASN	3.0
7	U	242	GLN	2.9
5	S	233	ILE	2.9
4	R	113	LEU	2.9
14	b	103	ASP	2.8
2	B	93	HIS	2.8
1	O	1	MET	2.8
3	Q	204	GLY	2.8
5	E	209	ASN	2.8
13	a	69	ASP	2.8
8	H	-1	VAL	2.8
6	T	178	HIS	2.7
6	T	203	ASN	2.7
13	M	111	TRP	2.7
8	V	226	GLU	2.7
3	Q	232	THR	2.7
3	C	51	LYS	2.7
1	O	2	THR	2.7
7	G	242	GLN	2.6
3	Q	234	ILE	2.6
2	B	218	GLY	2.6
10	X	2	ASP	2.6
5	S	122	TYR	2.6
7	U	68	ARG	2.6
2	P	220	ASN	2.6
5	E	233	ILE	2.6
5	S	52	ALA	2.5
4	R	233	LYS	2.5
3	Q	202	GLN	2.5
11	Y	208	ASN	2.5
13	M	37	ASN	2.5
1	A	1	MET	2.5
3	Q	184	ALA	2.5
6	F	215	CYS	2.5
13	M	69	ASP	2.5
3	Q	240	GLU	2.5
5	E	122	TYR	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	P	53	SER	2.4
9	W	1	SER	2.4
2	P	93	HIS	2.4
7	U	2	GLY	2.4
1	O	50	LYS	2.4
6	T	244	ASN	2.4
7	U	203	ASP	2.4
8	V	91	GLN	2.4
2	P	59	ASP	2.4
4	R	117	GLU	2.4
6	F	202	ASP	2.4
6	T	14	ASP	2.4
13	a	111	TRP	2.4
8	V	224	GLN	2.4
7	U	179	LYS	2.4
7	U	24	LYS	2.3
1	O	249	ALA	2.3
6	T	215	CYS	2.3
14	b	107	LYS	2.3
5	S	209	ASN	2.3
10	X	149	ARG	2.3
3	C	204	GLY	2.3
7	U	168	GLU	2.2
3	Q	51	LYS	2.2
9	W	133	LYS	2.2
6	T	2	THR	2.2
11	K	208	ASN	2.2
8	H	222	ASP	2.2
3	C	206	LYS	2.2
3	Q	191	LYS	2.2
3	Q	201	VAL	2.2
3	Q	238	LYS	2.2
4	R	241	ALA	2.2
3	C	53	GLN	2.2
1	A	231	LYS	2.2
11	Y	116	ASP	2.2
7	G	68	ARG	2.2
12	L	136	CYS	2.2
2	P	180	LYS	2.2
2	B	222	GLY	2.2
4	D	232	ILE	2.2
4	R	237	GLU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
5	E	227	GLU	2.1
2	P	60	THR	2.1
5	E	173	ARG	2.1
3	C	238	LYS	2.1
12	Z	165	ASN	2.1
7	U	124	TYR	2.1
3	C	231	VAL	2.1
2	B	52	THR	2.1
3	Q	236	GLN	2.1
11	K	128	CYS	2.1
2	P	225	TYR	2.1
3	C	48	SER	2.1
3	C	203	THR	2.1
14	N	105	LYS	2.1
3	Q	189	CYS	2.1
3	C	240	GLU	2.1
2	P	62	THR	2.1
5	S	55	LEU	2.1
8	H	9	ASN	2.1
2	B	1	GLY	2.1
11	Y	128	CYS	2.1
6	F	243	ILE	2.1
1	A	62	SER	2.0
11	Y	18	SER	2.0
3	Q	203	THR	2.0
3	C	239	GLN	2.0
3	Q	47	ARG	2.0
4	R	114	ARG	2.0
5	S	54	GLU	2.0
4	D	236	LYS	2.0
8	H	224	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 oligosaccharides in this entry.

6.4 Ligands

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	I	302	1/1	0.79	0.14	40,40,40,40	0
15	MG	Z	301	1/1	0.88	0.12	59,59,59,59	0
15	MG	I	301	1/1	0.90	0.09	56,56,56,56	0
15	MG	J	201	1/1	0.92	0.15	54,54,54,54	0
15	MG	K	302	1/1	0.93	0.20	46,46,46,46	0
15	MG	G	301	1/1	0.93	0.06	47,47,47,47	0
15	MG	L	301	1/1	0.96	0.09	52,52,52,52	0
15	MG	K	301	1/1	0.97	0.05	41,41,41,41	0
15	MG	N	201	1/1	0.98	0.03	40,40,40,40	0

6.5 Other polymers

There are no such residues in this entry.