



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 23, 2026 – 05:20 AM UTC

PDB ID : 5D0W / pdb_00005d0w
Title : Yeast 20S proteasome beta5-T1S mutant
Authors : Huber, E.M.; Groll, M.
Deposited on : 2015-08-03
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 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

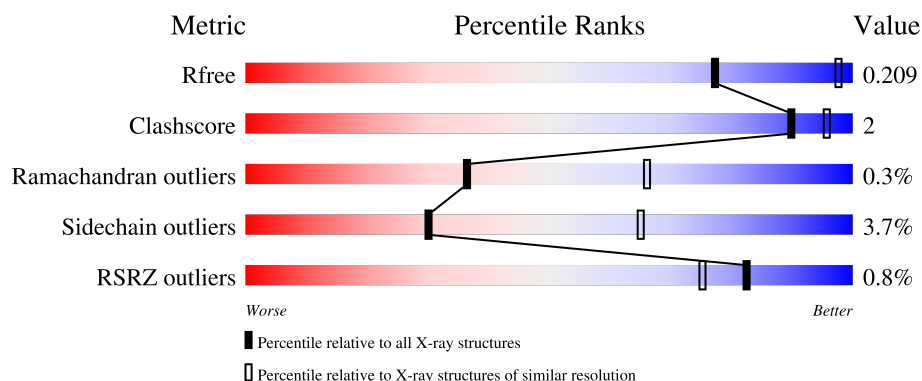
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

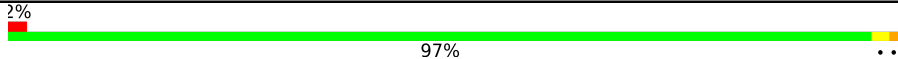
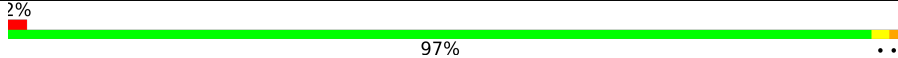
The reported resolution of this entry is 2.80 Å.

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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (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 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	 85% 7% 6%
4	D	260	 83% 7% 10%
4	R	260	 83% 7% 10%
5	E	234	 90% 8% ..
5	S	234	 89% 9% .
6	F	288	 80% . 16%
6	T	288	 80% 5% 16%
7	G	252	 88% 7% ..
7	U	252	 87% 8% ..
8	H	232	 92% 5% .
8	V	232	 91% 6% .
9	I	205	 92% 7%
9	W	205	 92% 7%
10	J	198	 88% 10% ..
10	X	198	 88% 10% ..
11	K	212	 92% 7% .
11	Y	212	 92% 8% .
12	L	222	 96% .
12	Z	222	 96% .
13	M	246	 90% . 5%
13	a	246	 89% 5% 5%
14	N	196	 93% 6% .
14	b	196	 93% 6% .

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 49864 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	226	Total	C	N	O	S	0	0	0
			1719	1082	298	332	7			
8	V	226	Total	C	N	O	S	0	0	0
			1719	1082	298	332	7			

- 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			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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
			1643	1044	280	312	7			
11	Y	212	Total	C	N	O	S	0	0	0
			1643	1044	280	312	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	1	SER	THR	engineered mutation	UNP P30656
Y	1	SER	THR	engineered mutation	UNP P30656

- 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			

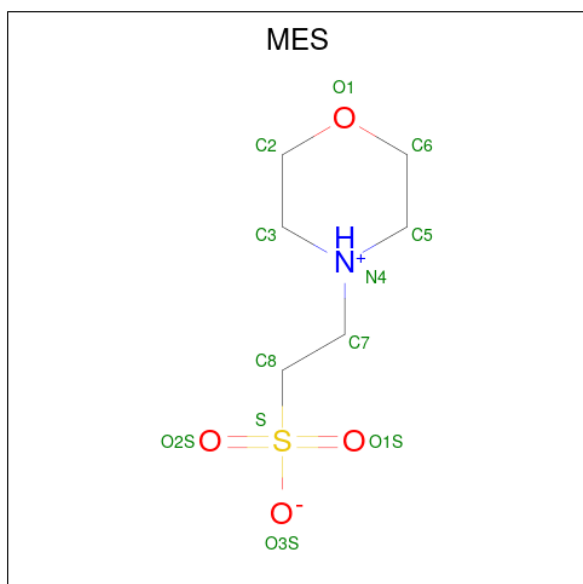
- Molecule 14 is a protein called Proteasome subunit beta type-1.

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	K	1	Total Mg 1 1	0	0
15	L	1	Total Mg 1 1	0	0
15	N	2	Total Mg 2 2	0	0
15	Z	1	Total Mg 1 1	0	0

- Molecule 16 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: C₆H₁₃NO₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	K	1	Total C N O S 12 6 1 4 1	0	0
16	Y	1	Total C N O S 12 6 1 4 1	0	0

- Molecule 17 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	11	Total O 11 11	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	B	13	Total 13	O 13	0	0
17	C	12	Total 12	O 12	0	0
17	D	12	Total 12	O 12	0	0
17	E	10	Total 10	O 10	0	0
17	F	14	Total 14	O 14	0	0
17	G	26	Total 26	O 26	0	0
17	H	16	Total 16	O 16	0	0
17	I	22	Total 22	O 22	0	0
17	J	24	Total 24	O 24	0	0
17	K	16	Total 16	O 16	0	0
17	L	23	Total 23	O 23	0	0
17	M	34	Total 34	O 34	0	0
17	N	19	Total 19	O 19	0	0
17	O	8	Total 8	O 8	0	0
17	P	13	Total 13	O 13	0	0
17	Q	12	Total 12	O 12	0	0
17	R	9	Total 9	O 9	0	0
17	S	6	Total 6	O 6	0	0
17	T	13	Total 13	O 13	0	0
17	U	14	Total 14	O 14	0	0
17	V	16	Total 16	O 16	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	W	15	Total 15	O 15	0	0
17	X	17	Total 17	O 17	0	0
17	Y	20	Total 20	O 20	0	0
17	Z	18	Total 18	O 18	0	0
17	a	28	Total 28	O 28	0	0
17	b	27	Total 27	O 27	0	0

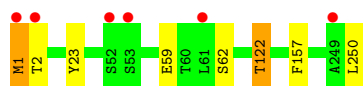
3 Residue-property plots

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.

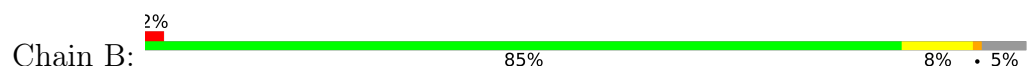
- Molecule 1: Proteasome subunit alpha type-2



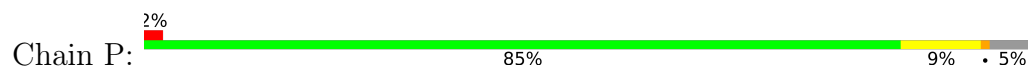
- Molecule 1: Proteasome subunit alpha type-2



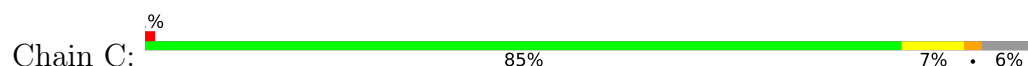
- Molecule 2: Proteasome subunit alpha type-3



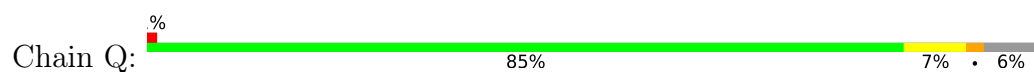
- Molecule 2: Proteasome subunit alpha type-3



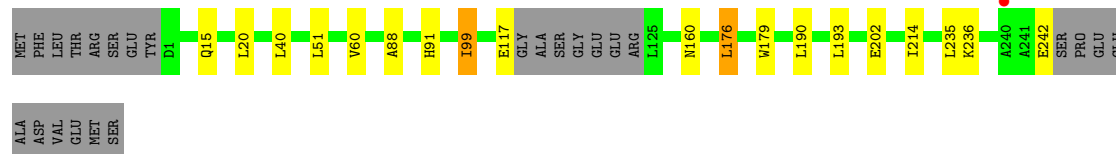
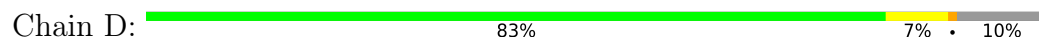
- Molecule 3: Proteasome subunit alpha type-4



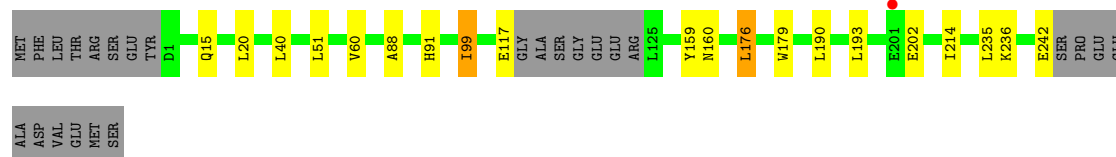
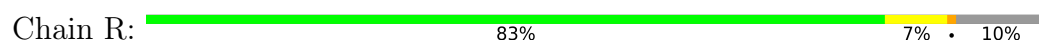
- Molecule 3: Proteasome subunit alpha type-4



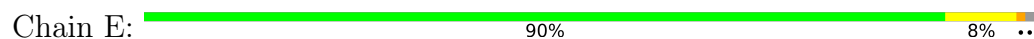
• Molecule 4: Proteasome subunit alpha type-5



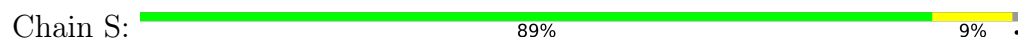
• Molecule 4: Proteasome subunit alpha type-5



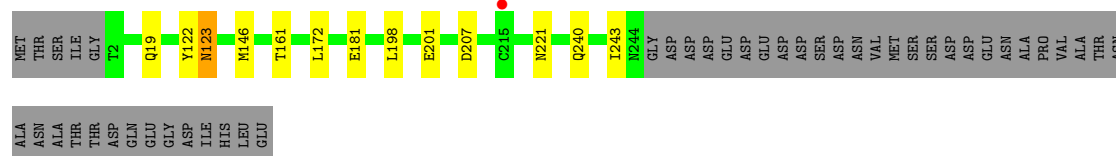
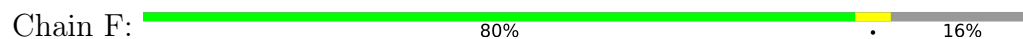
• Molecule 5: Proteasome subunit alpha type-6



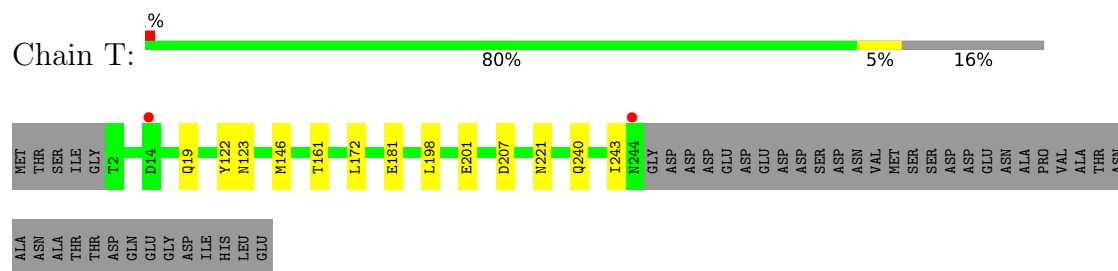
• Molecule 5: Proteasome subunit alpha type-6



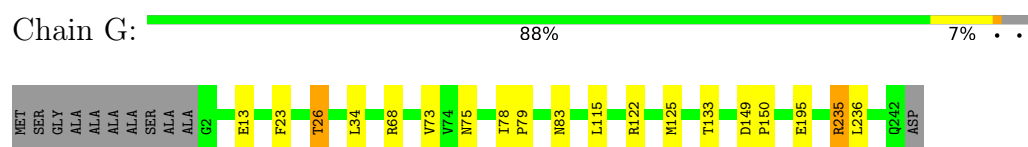
• Molecule 6: Probable proteasome subunit alpha type-7



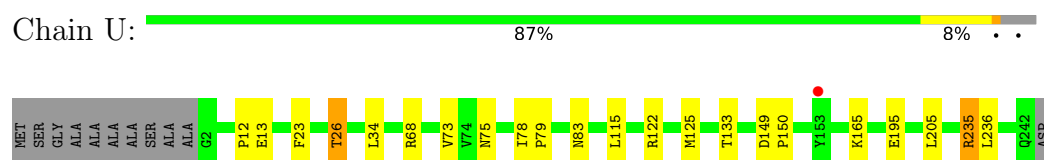
- Molecule 6: Probable proteasome subunit alpha type-7



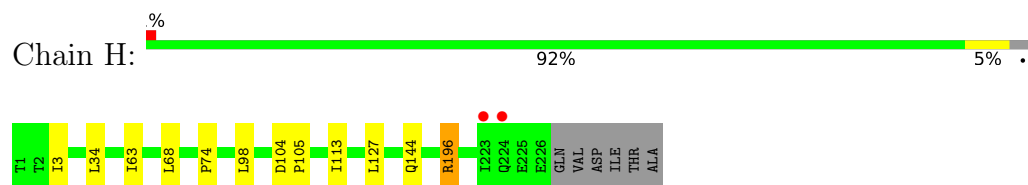
- Molecule 7: Proteasome subunit alpha type-1



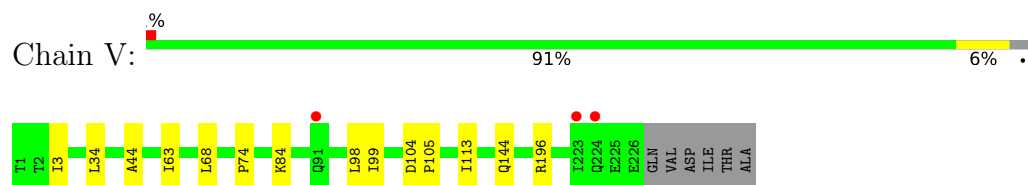
- Molecule 7: Proteasome subunit alpha type-1



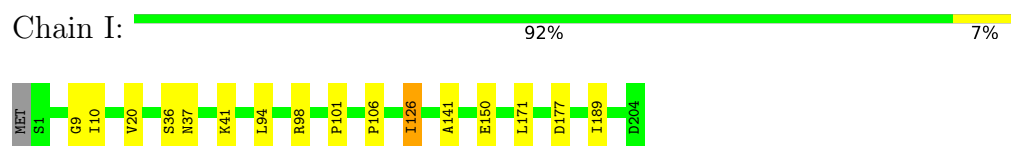
- Molecule 8: Proteasome subunit beta type-2



- Molecule 8: Proteasome subunit beta type-2



- Molecule 9: Proteasome subunit beta type-3

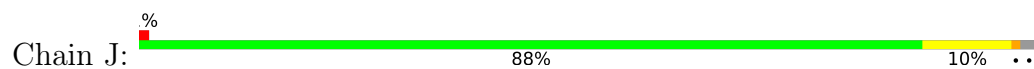


- Molecule 9: Proteasome subunit beta type-3

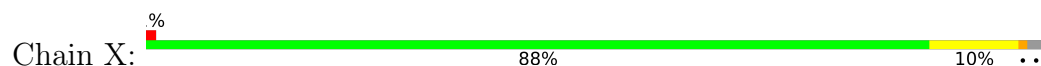




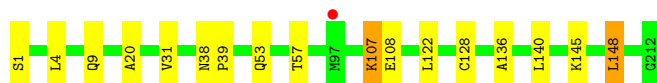
- Molecule 10: Proteasome subunit beta type-4



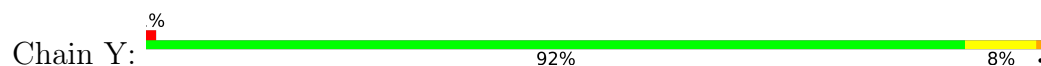
- Molecule 10: Proteasome subunit beta type-4



- Molecule 11: Proteasome subunit beta type-5



- Molecule 11: Proteasome subunit beta type-5



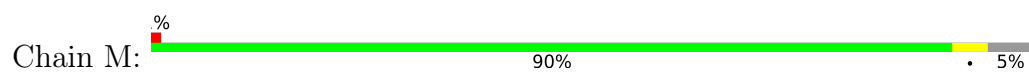
- Molecule 12: Proteasome subunit beta type-6



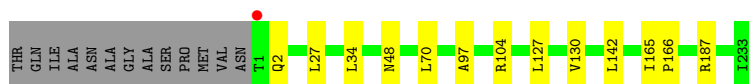
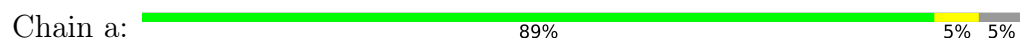
- Molecule 12: Proteasome subunit beta type-6



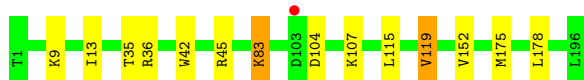
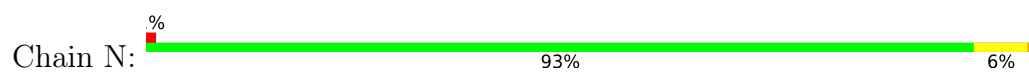
- Molecule 13: Proteasome subunit beta type-7



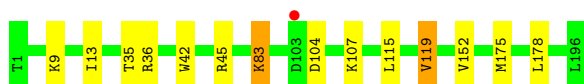
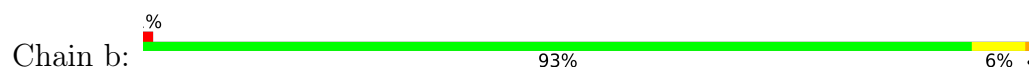
- Molecule 13: Proteasome subunit beta type-7



- 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	133.97Å 300.92Å 143.87Å 90.00° 112.77° 90.00°	Depositor
Resolution (Å)	15.00 – 2.80 15.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.6 (15.00-2.80) 98.0 (15.00-2.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.88 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.179 , 0.203 0.186 , 0.209	Depositor DCC
R_{free} test set	12589 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	58.5	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 63.2	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	0.95	EDS
Total number of atoms	49864	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.06% 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, 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	0.39	0/1952	0.68	0/2642
1	O	0.38	0/1952	0.68	0/2642
2	B	0.39	0/1934	0.68	0/2618
2	P	0.39	0/1934	0.68	0/2618
3	C	0.39	0/1910	0.69	1/2586 (0.0%)
3	Q	0.39	0/1910	0.70	1/2586 (0.0%)
4	D	0.38	0/1837	0.66	0/2475
4	R	0.38	0/1837	0.66	0/2475
5	E	0.38	0/1800	0.66	0/2433
5	S	0.38	0/1800	0.66	0/2433
6	F	0.39	0/1932	0.68	0/2609
6	T	0.38	0/1932	0.69	0/2609
7	G	0.37	0/1945	0.67	0/2634
7	U	0.37	0/1945	0.67	0/2634
8	H	0.40	1/1750 (0.1%)	0.64	0/2373
8	V	0.38	0/1750	0.64	0/2373
9	I	0.36	0/1611	0.66	0/2174
9	W	0.36	0/1611	0.66	0/2174
10	J	0.40	0/1589	0.65	0/2142
10	X	0.40	0/1589	0.65	0/2142
11	K	0.36	0/1680	0.65	0/2272
11	Y	0.38	0/1680	0.66	0/2272
12	L	0.36	0/1795	0.65	0/2420
12	Z	0.37	0/1795	0.65	0/2420
13	M	0.38	0/1855	0.67	0/2514
13	a	0.38	0/1855	0.67	0/2514
14	N	0.39	0/1541	0.67	0/2087
14	b	0.38	0/1541	0.67	0/2087
All	All	0.38	1/50262 (0.0%)	0.67	2/67958 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	3	ILE	C-O	-5.28	1.18	1.24

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	201	VAL	N-CA-C	6.12	116.29	110.53
3	Q	201	VAL	N-CA-C	6.12	116.28	110.53

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1915	0	1929	2	0
1	O	1915	0	1929	3	0
2	B	1904	0	1904	14	0
2	P	1904	0	1904	11	0
3	C	1881	0	1895	8	0
3	Q	1881	0	1895	9	0
4	D	1813	0	1797	6	0
4	R	1813	0	1797	7	0
5	E	1773	0	1775	8	0
5	S	1773	0	1775	9	0
6	F	1892	0	1883	5	0
6	T	1892	0	1883	4	0
7	G	1907	0	1901	7	0
7	U	1907	0	1901	9	0
8	H	1719	0	1719	5	0
8	V	1719	0	1719	7	0
9	I	1581	0	1574	9	0
9	W	1581	0	1574	8	0
10	J	1561	0	1569	12	0
10	X	1561	0	1569	11	0
11	K	1643	0	1593	8	0
11	Y	1643	0	1593	9	0
12	L	1757	0	1711	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	Z	1757	0	1711	2	0
13	M	1824	0	1832	3	0
13	a	1824	0	1832	4	0
14	N	1512	0	1481	8	0
14	b	1512	0	1481	9	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	2	0	0	0	0
15	Z	1	0	0	0	0
16	K	12	0	13	1	0
16	Y	12	0	13	0	0
17	A	11	0	0	0	0
17	B	13	0	0	2	0
17	C	12	0	0	0	0
17	D	12	0	0	0	0
17	E	10	0	0	0	0
17	F	14	0	0	0	0
17	G	26	0	0	0	0
17	H	16	0	0	0	0
17	I	22	0	0	0	0
17	J	24	0	0	0	0
17	K	16	0	0	0	0
17	L	23	0	0	0	0
17	M	34	0	0	0	0
17	N	19	0	0	0	0
17	O	8	0	0	0	0
17	P	13	0	0	0	0
17	Q	12	0	0	0	0
17	R	9	0	0	0	0
17	S	6	0	0	0	0
17	T	13	0	0	0	0
17	U	14	0	0	0	0
17	V	16	0	0	0	0
17	W	15	0	0	0	0
17	X	17	0	0	0	0
17	Y	20	0	0	0	0
17	Z	18	0	0	0	0
17	a	28	0	0	0	0
17	b	27	0	0	1	0
All	All	49864	0	49152	176	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 (176) 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)
2:B:93:HIS:HB3	17:B:301:HOH:O	1.93	0.67
14:N:152:VAL:HA	14:N:175:MET:HE1	1.81	0.63
14:b:152:VAL:HA	14:b:175:MET:HE1	1.79	0.63
3:Q:51:LYS:O	3:Q:52:LEU:HB2	2.01	0.61
3:C:51:LYS:O	3:C:52:LEU:HB2	2.01	0.60
14:b:35:THR:HG22	17:b:215:HOH:O	2.01	0.60
14:b:35:THR:HG21	14:b:45:ARG:HE	1.67	0.60
2:B:221:ASP:O	2:B:223:GLU:N	2.36	0.59
2:P:221:ASP:O	2:P:223:GLU:N	2.36	0.59
2:P:217:LYS:C	2:P:219:ALA:H	2.11	0.58
2:B:12:PHE:H	3:C:17:GLN:HE22	1.51	0.58
14:N:35:THR:HG21	14:N:45:ARG:HE	1.68	0.58
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.86	0.58
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.86	0.58
2:B:217:LYS:C	2:B:219:ALA:H	2.11	0.58
7:G:68:ARG:HH12	14:N:36:ARG:HH22	1.54	0.55
11:K:53:GLN:O	11:K:57:THR:HG23	2.07	0.55
3:C:160:GLN:HE21	3:C:160:GLN:HA	1.73	0.54
11:K:1:SER:HB3	16:K:302:MES:O2S	2.08	0.54
3:Q:160:GLN:HE21	3:Q:160:GLN:HA	1.73	0.53
11:Y:53:GLN:O	11:Y:57:THR:HG23	2.09	0.53
14:b:35:THR:CG2	14:b:45:ARG:HE	2.22	0.52
5:E:12:PHE:H	6:F:19:GLN:HE22	1.57	0.52
9:I:9:GLY:HA3	9:I:41:LYS:HE2	1.92	0.52
1:A:1:MET:HG3	6:F:122:TYR:CZ	2.45	0.52
3:C:201:VAL:O	3:C:202:GLN:CB	2.57	0.52
14:N:83:LYS:HG3	14:N:119:VAL:CG2	2.40	0.52
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.57	0.52
14:N:35:THR:CG2	14:N:45:ARG:HE	2.23	0.51
8:V:3:ILE:HG22	8:V:99:ILE:HD12	1.91	0.51
2:P:47:ALA:HB1	2:P:64:LYS:HD2	1.93	0.51
2:B:47:ALA:HB1	2:B:64:LYS:HD2	1.93	0.51
9:W:9:GLY:HA3	9:W:41:LYS:HE2	1.92	0.51
14:b:83:LYS:HG3	14:b:119:VAL:CG2	2.40	0.50
1:O:1:MET:HG3	6:T:122:TYR:CZ	2.46	0.50
5:S:12:PHE:H	6:T:19:GLN:HE22	1.59	0.50
7:U:23:PHE:O	7:U:26:THR:HB	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:3:ILE:HG23	10:X:18:SER:HB3	1.94	0.49
3:C:35:LYS:HG2	3:C:158:SER:O	2.13	0.49
2:B:113:ARG:NE	17:B:301:HOH:O	2.31	0.49
10:J:3:ILE:HG23	10:J:18:SER:HB3	1.94	0.48
10:J:25:ILE:O	10:X:139:TYR:OH	2.31	0.48
7:G:23:PHE:O	7:G:26:THR:HB	2.13	0.48
5:S:87:LEU:HD21	5:S:107:ALA:HB1	1.95	0.48
14:N:13:ILE:HG21	14:N:175:MET:HE2	1.95	0.48
11:K:128:CYS:SG	11:K:136:ALA:HB3	2.54	0.48
6:T:198:LEU:HD12	6:T:243:ILE:HG22	1.95	0.48
6:F:198:LEU:HD12	6:F:243:ILE:HG22	1.95	0.47
7:U:73:VAL:HG12	7:U:133:THR:HB	1.95	0.47
3:Q:35:LYS:HG2	3:Q:158:SER:O	2.14	0.47
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.96	0.47
5:E:87:LEU:HD21	5:E:107:ALA:HB1	1.96	0.47
10:J:1:MET:HB3	10:J:34:LYS:HE3	1.96	0.47
10:X:1:MET:HB3	10:X:34:LYS:HE3	1.96	0.47
2:B:219:ALA:HB2	2:B:225:TYR:HB2	1.96	0.47
7:G:73:VAL:HG12	7:G:133:THR:HB	1.95	0.47
10:X:1:MET:HG2	10:X:34:LYS:HE3	1.97	0.47
11:Y:107:LYS:HG3	11:Y:108:GLU:HG3	1.96	0.47
4:D:88:ALA:HA	4:D:99:ILE:HG21	1.97	0.47
8:V:104:ASP:HB2	8:V:105:PRO:HD2	1.97	0.47
11:Y:20:ALA:HB2	11:Y:31:VAL:HG21	1.97	0.47
11:Y:128:CYS:SG	11:Y:136:ALA:HB3	2.54	0.47
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.96	0.47
10:X:1:MET:CB	10:X:34:LYS:HE3	2.45	0.47
14:b:13:ILE:HG21	14:b:175:MET:HE2	1.97	0.46
4:R:91:HIS:HB3	4:R:99:ILE:HG22	1.98	0.46
10:J:1:MET:CB	10:J:34:LYS:HE3	2.45	0.46
4:D:91:HIS:HB3	4:D:99:ILE:HG22	1.98	0.46
11:K:107:LYS:HG3	11:K:108:GLU:HG3	1.97	0.46
2:P:219:ALA:HB2	2:P:225:TYR:HB2	1.96	0.46
10:J:1:MET:HG2	10:J:34:LYS:HE3	1.97	0.46
9:I:101:PRO:HB3	9:I:126:ILE:HD12	1.98	0.46
4:R:88:ALA:HA	4:R:99:ILE:HG21	1.98	0.46
8:H:104:ASP:HB2	8:H:105:PRO:HD2	1.97	0.45
4:R:91:HIS:HB3	4:R:99:ILE:CG2	2.46	0.45
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.51	0.45
2:B:151:ASN:HB2	2:B:152:PRO:CD	2.46	0.45
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:101:PRO:HB3	9:W:126:ILE:HD12	1.99	0.45
4:D:91:HIS:HB3	4:D:99:ILE:CG2	2.46	0.45
11:K:20:ALA:HB2	11:K:31:VAL:HG21	1.97	0.45
3:Q:9:PHE:H	4:R:15:GLN:HE22	1.63	0.45
9:I:94:LEU:HD11	9:I:106:PRO:HG2	1.99	0.45
1:O:122:THR:HG22	2:P:128:ARG:HH21	1.82	0.45
2:P:50:LYS:O	2:P:51:VAL:C	2.58	0.45
5:S:175:LEU:HA	5:S:178:PHE:CE2	2.52	0.45
5:E:175:LEU:HA	5:E:178:PHE:CE2	2.52	0.45
8:V:63:ILE:HG23	8:V:74:PRO:HB3	1.99	0.45
3:C:149:GLU:HB2	3:C:150:PRO:HD2	1.99	0.45
2:P:151:ASN:HB2	2:P:152:PRO:CD	2.47	0.44
7:U:68:ARG:HH12	14:b:36:ARG:HH22	1.64	0.44
9:W:94:LEU:HD11	9:W:106:PRO:HG2	1.99	0.44
2:B:50:LYS:O	2:B:51:VAL:C	2.59	0.44
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.52	0.44
3:Q:149:GLU:HB2	3:Q:150:PRO:HD2	1.99	0.44
2:B:217:LYS:C	2:B:219:ALA:N	2.75	0.44
9:I:141:ALA:HB2	9:I:177:ASP:HB2	2.00	0.44
14:b:36:ARG:HG3	14:b:42:TRP:CE2	2.53	0.44
14:N:36:ARG:HG3	14:N:42:TRP:CE2	2.52	0.44
11:Y:38:ASN:HB2	11:Y:39:PRO:CD	2.48	0.44
2:B:50:LYS:HD2	2:B:50:LYS:HA	1.82	0.44
8:H:63:ILE:HG23	8:H:74:PRO:HB3	1.99	0.44
10:J:139:TYR:OH	10:X:25:ILE:O	2.36	0.43
11:K:38:ASN:HB2	11:K:39:PRO:CD	2.48	0.43
10:J:168:LEU:O	10:J:172:MET:HB2	2.18	0.43
13:M:27:LEU:HD21	13:M:34:LEU:HD22	2.00	0.43
8:V:104:ASP:HB2	8:V:105:PRO:CD	2.48	0.43
12:Z:146:ILE:HG22	12:Z:150:LEU:HD22	2.00	0.43
2:P:151:ASN:HB2	2:P:152:PRO:HD2	2.01	0.43
7:U:78:ILE:N	7:U:79:PRO:CD	2.81	0.43
9:W:98:ARG:O	9:W:126:ILE:HD11	2.18	0.43
13:a:27:LEU:HD21	13:a:34:LEU:HD22	2.00	0.43
7:U:195:GLU:HG3	7:U:235:ARG:HG3	2.01	0.43
10:X:168:LEU:O	10:X:172:MET:HB2	2.18	0.43
9:W:20:VAL:HG23	9:W:189:ILE:HB	2.01	0.43
9:I:98:ARG:O	9:I:126:ILE:HD11	2.18	0.43
11:K:145:LYS:HB2	11:K:148:LEU:HD13	2.01	0.43
2:B:151:ASN:HB2	2:B:152:PRO:HD2	2.00	0.43
8:H:196:ARG:NH2	9:I:150:GLU:OE2	2.52	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:12:PHE:H	3:Q:17:GLN:HE22	1.67	0.43
11:Y:97:MET:HB2	11:Y:117:SER:HB3	2.00	0.43
5:E:68:HIS:HE1	5:E:102:LEU:O	2.02	0.42
13:M:127:LEU:HG	13:M:142:LEU:HD12	2.01	0.42
5:S:9:THR:HG21	5:S:119:THR:HA	2.01	0.42
4:D:176:LEU:HD22	5:E:55:LEU:CD2	2.48	0.42
9:W:141:ALA:HB2	9:W:177:ASP:HB2	2.01	0.42
11:Y:145:LYS:HB2	11:Y:148:LEU:HD13	2.01	0.42
3:C:9:PHE:H	4:D:15:GLN:HE22	1.66	0.42
7:G:195:GLU:HG3	7:G:235:ARG:HG3	2.01	0.42
7:G:34:LEU:C	7:G:34:LEU:HD23	2.44	0.42
8:H:104:ASP:HB2	8:H:105:PRO:CD	2.49	0.42
12:L:146:ILE:HG22	12:L:150:LEU:HD22	2.00	0.42
5:S:68:HIS:HE1	5:S:102:LEU:O	2.01	0.42
7:G:78:ILE:N	7:G:79:PRO:CD	2.82	0.42
13:a:127:LEU:HG	13:a:142:LEU:HD12	2.02	0.42
5:E:9:THR:HG21	5:E:119:THR:HA	2.01	0.42
14:N:83:LYS:HG3	14:N:119:VAL:HG22	2.01	0.42
6:F:146:MET:HE3	6:F:161:THR:HB	2.02	0.42
8:H:98:LEU:HB2	8:H:113:ILE:CG2	2.50	0.42
3:Q:166:SER:HA	3:Q:169:VAL:HG13	2.02	0.42
4:R:176:LEU:HD11	5:S:54:GLU:HB2	2.02	0.42
7:U:34:LEU:HD23	7:U:34:LEU:C	2.44	0.42
10:X:21:VAL:HG11	11:Y:122:LEU:HD11	2.02	0.42
9:I:36:SER:HB2	10:J:126:VAL:HG11	2.01	0.41
10:J:21:VAL:HG11	11:K:122:LEU:HD11	2.01	0.41
12:L:8:ASN:HA	12:L:30:ILE:O	2.20	0.41
2:P:145:TYR:OH	2:P:217:LYS:N	2.53	0.41
10:J:119:ILE:HG12	10:J:125:LYS:HG3	2.02	0.41
5:S:62:ILE:HG21	5:S:213:ALA:HB2	2.02	0.41
8:V:98:LEU:HB2	8:V:113:ILE:CG2	2.50	0.41
14:b:83:LYS:HG3	14:b:119:VAL:HG22	2.02	0.41
9:I:20:VAL:HG23	9:I:189:ILE:HB	2.01	0.41
6:T:146:MET:HE3	6:T:161:THR:HB	2.02	0.41
1:A:122:THR:HG22	2:B:128:ARG:HH21	1.85	0.41
5:E:62:ILE:HG21	5:E:213:ALA:HB2	2.02	0.41
4:R:159:TYR:CE2	5:S:56:SER:HB3	2.55	0.41
10:X:132:ALA:HB1	10:X:136:SER:HB2	2.02	0.41
5:E:77:ALA:N	5:E:78:PRO:CD	2.84	0.41
7:G:149:ASP:HB2	7:G:150:PRO:CD	2.51	0.41
9:W:26:LEU:HD21	9:W:185:VAL:HG23	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:166:SER:HA	3:C:169:VAL:HG13	2.02	0.41
13:M:165:ILE:HB	13:M:166:PRO:HD3	2.03	0.41
5:S:77:ALA:N	5:S:78:PRO:CD	2.84	0.41
7:U:165:LYS:HD2	7:U:205:LEU:HD22	2.03	0.41
10:X:119:ILE:HG12	10:X:125:LYS:HG3	2.02	0.41
13:a:165:ILE:HB	13:a:166:PRO:HD3	2.03	0.40
2:P:124:HIS:HB3	3:Q:124:VAL:HG12	2.03	0.40
8:V:84:LYS:HA	8:V:113:ILE:HD11	2.04	0.40
7:U:149:ASP:HB2	7:U:150:PRO:CD	2.51	0.40
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.20	0.40
2:B:145:TYR:OH	2:B:217:LYS:N	2.53	0.40
6:F:123:ASN:HD22	6:F:123:ASN:C	2.30	0.40
8:V:3:ILE:HG21	8:V:44:ALA:HB3	2.03	0.40
11:Y:97:MET:HE3	11:Y:97:MET:HB3	1.80	0.40
10:J:132:ALA:HB1	10:J:136:SER:HB2	2.02	0.40
13:a:97:ALA:HA	13:a:130:VAL:HG21	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%)	239 (96%)	8 (3%)	1 (0%)	30	60
1	O	248/250 (99%)	238 (96%)	9 (4%)	1 (0%)	30	60
2	B	242/258 (94%)	235 (97%)	3 (1%)	4 (2%)	7	25
2	P	242/258 (94%)	235 (97%)	3 (1%)	4 (2%)	7	25
3	C	238/254 (94%)	231 (97%)	4 (2%)	3 (1%)	9	31
3	Q	238/254 (94%)	231 (97%)	4 (2%)	3 (1%)	9	31
4	D	231/260 (89%)	229 (99%)	2 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	R	231/260 (89%)	229 (99%)	2 (1%)	0	100	100
5	E	229/234 (98%)	221 (96%)	8 (4%)	0	100	100
5	S	229/234 (98%)	220 (96%)	9 (4%)	0	100	100
6	F	241/288 (84%)	238 (99%)	3 (1%)	0	100	100
6	T	241/288 (84%)	238 (99%)	3 (1%)	0	100	100
7	G	239/252 (95%)	238 (100%)	1 (0%)	0	100	100
7	U	239/252 (95%)	237 (99%)	2 (1%)	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%)	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%)	3 (2%)	1 (0%)	24	55
10	X	193/198 (98%)	189 (98%)	3 (2%)	1 (0%)	24	55
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	6284/6614 (95%)	6133 (98%)	133 (2%)	18 (0%)	36	66

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	220	ASN
3	C	205	ALA
2	P	218	GLY
2	P	220	ASN
3	Q	205	ALA
3	Q	183	PRO
3	C	183	PRO
10	J	24	GLY
10	X	24	GLY

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	73
1	O	209/209 (100%)	203 (97%)	6 (3%)	37	73
2	B	203/216 (94%)	196 (97%)	7 (3%)	32	68
2	P	203/216 (94%)	196 (97%)	7 (3%)	32	68
3	C	212/226 (94%)	199 (94%)	13 (6%)	17	46
3	Q	212/226 (94%)	199 (94%)	13 (6%)	17	46
4	D	194/215 (90%)	180 (93%)	14 (7%)	13	39
4	R	194/215 (90%)	180 (93%)	14 (7%)	13	39
5	E	190/193 (98%)	182 (96%)	8 (4%)	26	61
5	S	190/193 (98%)	182 (96%)	8 (4%)	26	61
6	F	201/239 (84%)	194 (96%)	7 (4%)	32	67
6	T	201/239 (84%)	194 (96%)	7 (4%)	32	67
7	G	206/210 (98%)	197 (96%)	9 (4%)	25	59
7	U	206/210 (98%)	197 (96%)	9 (4%)	25	59
8	H	185/190 (97%)	180 (97%)	5 (3%)	39	74
8	V	185/190 (97%)	181 (98%)	4 (2%)	45	78
9	I	172/173 (99%)	169 (98%)	3 (2%)	53	83

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	W	172/173 (99%)	169 (98%)	3 (2%)	53	83
10	J	173/175 (99%)	168 (97%)	5 (3%)	37	73
10	X	173/175 (99%)	168 (97%)	5 (3%)	37	73
11	K	169/169 (100%)	164 (97%)	5 (3%)	36	72
11	Y	169/169 (100%)	164 (97%)	5 (3%)	36	72
12	L	185/185 (100%)	180 (97%)	5 (3%)	39	74
12	Z	185/185 (100%)	180 (97%)	5 (3%)	39	74
13	M	199/208 (96%)	194 (98%)	5 (2%)	42	76
13	a	199/208 (96%)	194 (98%)	5 (2%)	42	76
14	N	162/162 (100%)	155 (96%)	7 (4%)	26	60
14	b	162/162 (100%)	155 (96%)	7 (4%)	26	60
All	All	5320/5540 (96%)	5123 (96%)	197 (4%)	30	65

All (197) 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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
4	D	99	ILE
4	D	117	GLU
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	H	34	LEU
8	H	68	LEU
8	H	127	LEU
8	H	144	GLN
8	H	196	ARG
9	I	37	ASN
9	I	126	ILE
9	I	171	LEU
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	107	LYS
11	K	140	LEU
11	K	148	LEU
12	L	23	LEU
12	L	31	THR
12	L	49	ASN
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	187	ARG
14	N	9	LYS
14	N	83	LYS
14	N	104	ASP
14	N	107	LYS
14	N	115	LEU
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	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
6	T	123	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	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
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	107	LYS
11	Y	140	LEU
11	Y	148	LEU
12	Z	23	LEU
12	Z	31	THR
12	Z	49	ASN
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
14	b	9	LYS
14	b	83	LYS
14	b	104	ASP
14	b	107	LYS
14	b	115	LEU
14	b	119	VAL
14	b	178	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (142) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	95	GLN
2	B	119	GLN
2	B	123	GLN
2	B	124	HIS
2	B	146	GLN
2	B	176	GLN
2	B	232	GLN
3	C	17	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	91	HIS
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
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	203	ASN

Continued on next page...

Continued from previous page...

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
7	G	175	ASN
8	H	66	HIS
8	H	194	ASN
9	I	37	ASN
9	I	63	ASN
9	I	88	GLN
9	I	203	GLN
10	J	10	GLN
10	J	55	GLN
10	J	63	ASN
11	K	9	GLN
11	K	85	ASN
11	K	143	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	197	GLN
13	M	48	ASN
13	M	102	GLN
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
2	P	95	GLN
2	P	119	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	P	123	GLN
2	P	124	HIS
2	P	146	GLN
2	P	176	GLN
2	P	232	GLN
3	Q	17	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	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	203	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
7	U	166	GLN
7	U	167	GLN
7	U	175	ASN
8	V	66	HIS
8	V	86	HIS
8	V	219	ASN
9	W	37	ASN
9	W	63	ASN
9	W	88	GLN
9	W	203	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
11	Y	209	ASN
12	Z	49	ASN
12	Z	70	ASN
12	Z	79	HIS
12	Z	153	GLN
12	Z	155	ASN
12	Z	158	ASN
12	Z	197	GLN
13	a	48	ASN
13	a	102	GLN
13	a	108	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 10 ligands modelled in this entry, 8 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	Y	301	-	12,12,12	2.15	1 (8%)	15,16,16	1.10	2 (13%)
16	MES	K	302	-	12,12,12	2.18	1 (8%)	15,16,16	1.14	1 (6%)

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	Y	301	-	-	1/6/14/14	0/1/1/1
16	MES	K	302	-	-	3/6/14/14	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	K	302	MES	C8-S	-7.19	1.67	1.77
16	Y	301	MES	C8-S	-7.07	1.67	1.77

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	K	302	MES	O3S-S-C8	2.52	110.94	106.00
16	Y	301	MES	O1S-S-C8	2.16	109.99	106.73
16	Y	301	MES	O3S-S-C8	2.08	110.08	106.00

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	K	302	MES	C7-C8-S-O3S
16	K	302	MES	C7-C8-S-O1S
16	Y	301	MES	C7-C8-S-O3S
16	K	302	MES	C7-C8-S-O2S

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	K	302	MES	1	0

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%)	-0.40	4 (1%) 70 61	42, 56, 95, 135	0
1	O	250/250 (100%)	-0.34	6 (2%) 59 49	47, 63, 110, 142	0
2	B	244/258 (94%)	-0.24	6 (2%) 58 48	42, 62, 106, 163	0
2	P	244/258 (94%)	-0.29	6 (2%) 58 48	47, 64, 107, 155	0
3	C	240/254 (94%)	-0.34	3 (1%) 75 66	42, 65, 123, 149	0
3	Q	240/254 (94%)	-0.06	3 (1%) 75 66	51, 80, 160, 185	0
4	D	235/260 (90%)	-0.35	1 (0%) 88 84	48, 68, 103, 141	0
4	R	235/260 (90%)	-0.24	1 (0%) 88 84	51, 73, 114, 145	0
5	E	231/234 (98%)	-0.26	1 (0%) 88 84	49, 70, 109, 155	0
5	S	231/234 (98%)	-0.13	0 100 100	52, 78, 119, 165	0
6	F	243/288 (84%)	-0.41	1 (0%) 88 84	45, 63, 114, 143	0
6	T	243/288 (84%)	-0.31	2 (0%) 82 75	48, 72, 123, 156	0
7	G	241/252 (95%)	-0.48	0 100 100	40, 58, 92, 145	0
7	U	241/252 (95%)	-0.40	1 (0%) 88 84	45, 61, 92, 138	0
8	H	226/232 (97%)	-0.38	2 (0%) 81 74	35, 55, 90, 161	0
8	V	226/232 (97%)	-0.40	3 (1%) 75 66	42, 57, 86, 171	0
9	I	204/205 (99%)	-0.66	0 100 100	39, 52, 80, 104	0
9	W	204/205 (99%)	-0.62	0 100 100	40, 53, 83, 110	0
10	J	195/198 (98%)	-0.56	1 (0%) 87 82	39, 55, 80, 136	0
10	X	195/198 (98%)	-0.53	1 (0%) 87 82	41, 55, 81, 140	0
11	K	212/212 (100%)	-0.43	1 (0%) 87 82	36, 54, 76, 98	0
11	Y	212/212 (100%)	-0.50	3 (1%) 73 64	44, 57, 81, 102	0
12	L	222/222 (100%)	-0.54	2 (0%) 81 74	38, 55, 87, 123	0
12	Z	222/222 (100%)	-0.54	0 100 100	39, 56, 87, 124	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%)	-0.63	2 (0%) 81 74	38, 53, 77, 96	0
13	a	233/246 (94%)	-0.63	1 (0%) 88 84	37, 54, 76, 94	0
14	N	196/196 (100%)	-0.64	1 (0%) 87 82	36, 49, 79, 106	0
14	b	196/196 (100%)	-0.62	1 (0%) 87 82	39, 50, 79, 112	0
All	All	6344/6614 (95%)	-0.42	53 (0%) 82 75	35, 60, 106, 185	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
8	V	223	ILE	6.2
8	H	223	ILE	5.9
3	Q	50	LEU	5.7
2	B	218	GLY	4.3
10	X	1	MET	4.1
2	B	219	ALA	4.1
3	Q	49	THR	3.7
2	B	51	VAL	3.4
2	B	1	GLY	3.3
4	D	240	ALA	3.3
8	H	224	GLN	3.3
2	P	219	ALA	3.3
10	J	1	MET	3.2
13	a	1	THR	3.2
7	U	153	TYR	2.7
14	b	103	ASP	2.7
3	Q	205	ALA	2.7
1	O	61	LEU	2.7
8	V	224	GLN	2.6
2	P	218	GLY	2.5
1	O	53	SER	2.5
11	Y	212	GLY	2.5
2	B	52	THR	2.5
1	A	1	MET	2.5
1	A	2	THR	2.4
1	O	2	THR	2.3
6	T	14	ASP	2.3
11	Y	116	ASP	2.3
11	K	97	MET	2.2
6	T	244	ASN	2.2
2	P	1	GLY	2.2
2	B	220	ASN	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	C	3	ASP	2.2
12	L	166	GLY	2.2
8	V	91	GLN	2.1
5	E	209	ASN	2.1
2	P	52	THR	2.1
13	M	1	THR	2.1
2	P	51	VAL	2.1
2	P	225	TYR	2.1
6	F	215	CYS	2.1
12	L	174	TYR	2.1
13	M	69	ASP	2.1
14	N	103	ASP	2.1
1	O	249	ALA	2.1
4	R	201	GLU	2.1
1	O	1	MET	2.0
1	O	52	SER	2.0
3	C	51	LYS	2.0
1	A	3	ASP	2.0
1	A	62	SER	2.0
11	Y	128	CYS	2.0
3	C	240	GLU	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 [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($\text{\AA}^2$)	Q<0.9
15	MG	Z	301	1/1	0.80	0.14	75,75,75,75	0
15	MG	N	202	1/1	0.86	0.23	66,66,66,66	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
16	MES	Y	301	12/12	0.91	0.19	49,50,68,72	0
16	MES	K	302	12/12	0.93	0.18	47,51,67,70	0
15	MG	I	301	1/1	0.95	0.10	65,65,65,65	0
15	MG	G	301	1/1	0.96	0.06	54,54,54,54	0
15	MG	N	201	1/1	0.96	0.07	54,54,54,54	0
15	MG	L	301	1/1	0.99	0.06	63,63,63,63	0
15	MG	I	302	1/1	0.99	0.07	53,53,53,53	0
15	MG	K	301	1/1	0.99	0.07	50,50,50,50	0

6.5 Other polymers [i](#)

There are no such residues in this entry.