



# Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 01:45 am BST

PDB ID : 4Y8R  
Title : Yeast 20S proteasome beta2-H116D mutant  
Authors : Huber, E.M.; Groll, M.  
Deposited on : 2015-02-16  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

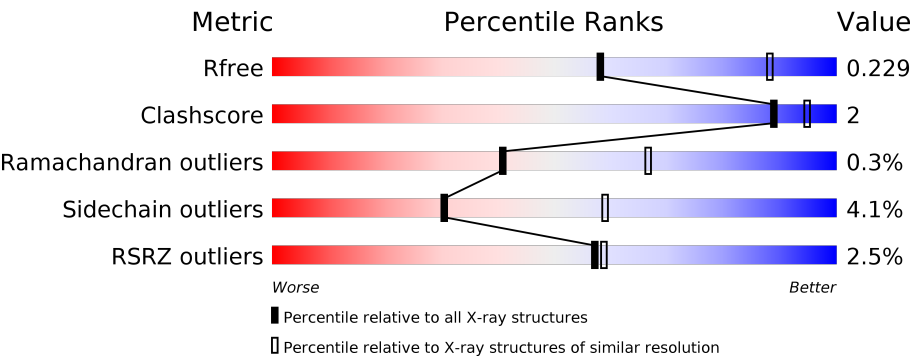
# 1 Overall quality at a glance i

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  $\geq 3$ , 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>4%</div><div>98%</div><div>•</div></div>
1	O	250	<div><div>4%</div><div>97%</div><div>•</div></div>
2	B	258	<div><div>4%</div><div>85%</div><div>8% • 5%</div></div>
2	P	258	<div><div>4%</div><div>85%</div><div>8% • 5%</div></div>
3	C	254	<div><div>5%</div><div>83%</div><div>9% • 6%</div></div>
3	Q	254	<div><div>8%</div><div>84%</div><div>9% • 6%</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	232	
8	V	232	
9	I	205	
9	W	205	
10	J	198	
10	X	198	
11	K	212	
11	Y	212	
12	L	222	
12	Z	222	
13	M	246	
13	a	246	
14	N	196	
14	b	196	

## 2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 50050 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
			1717	1080	296	334	7			
8	V	226	Total	C	N	O	S	0	0	0
			1717	1080	296	334	7			

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			
13	a	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			

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

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

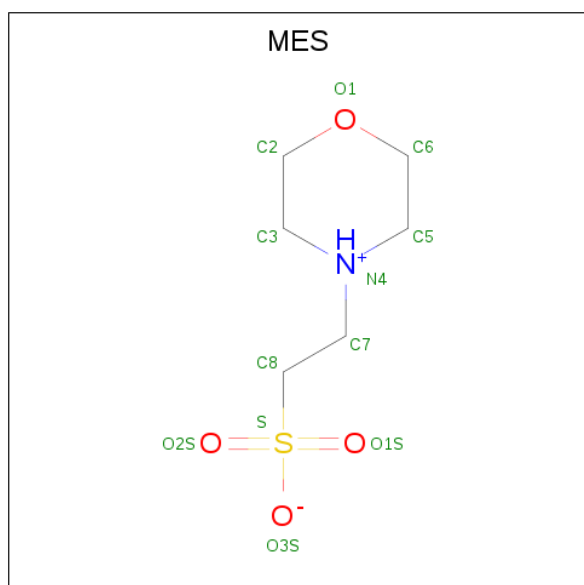
- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	G	1	Total 1 Mg 1	0	0
15	K	1	Total 1 Mg 1	0	0
15	I	1	Total 1 Mg 1	0	0
15	V	1	Total 1 Mg 1	0	0
15	W	1	Total 1 Mg 1	0	0
15	Z	1	Total 1 Mg 1	0	0
15	N	2	Total 2 Mg 2	0	0
15	Y	1	Total 1 Mg 1	0	0

- Molecule 16 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	G	1	Total 1 Cl 1	0	0
16	U	1	Total 1 Cl 1	0	0

- Molecule 17 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).



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

- Molecule 18 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	A	22	Total	O	0	0
			22	22		
18	B	18	Total	O	0	0
			18	18		
18	C	17	Total	O	0	0
			17	17		
18	D	22	Total	O	0	0
			22	22		
18	E	18	Total	O	0	0
			18	18		
18	F	16	Total	O	0	0
			16	16		
18	G	30	Total	O	0	0
			30	30		
18	H	37	Total	O	0	0
			37	37		
18	I	27	Total	O	0	0
			27	27		
18	J	30	Total	O	0	0
			30	30		
18	K	36	Total	O	0	0
			36	36		
18	L	42	Total	O	0	0
			42	42		
18	M	30	Total	O	0	0
			30	30		
18	N	18	Total	O	0	0
			18	18		
18	O	15	Total	O	0	0
			15	15		
18	P	16	Total	O	0	0
			16	16		
18	Q	14	Total	O	0	0
			14	14		
18	R	13	Total	O	0	0
			13	13		
18	S	13	Total	O	0	0
			13	13		

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	T	10	Total 10	O 10	0	0
18	U	28	Total 28	O 28	0	0
18	V	25	Total 25	O 25	0	0
18	W	25	Total 25	O 25	0	0
18	X	24	Total 24	O 24	0	0
18	Y	27	Total 27	O 27	0	0
18	Z	24	Total 24	O 24	0	0
18	a	38	Total 38	O 38	0	0
18	b	30	Total 30	O 30	0	0

### 3 Residue-property plots [i](#)

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

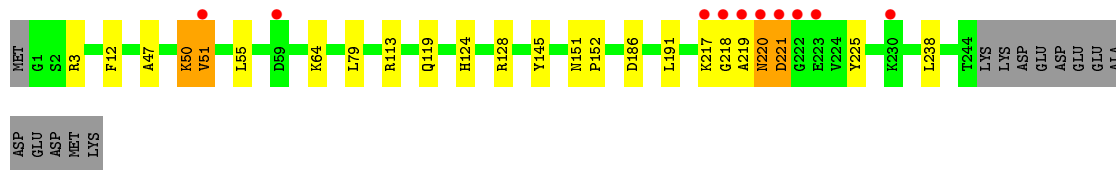
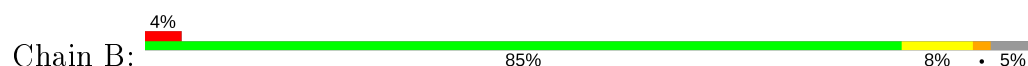
- Molecule 1: Proteasome subunit alpha type-2



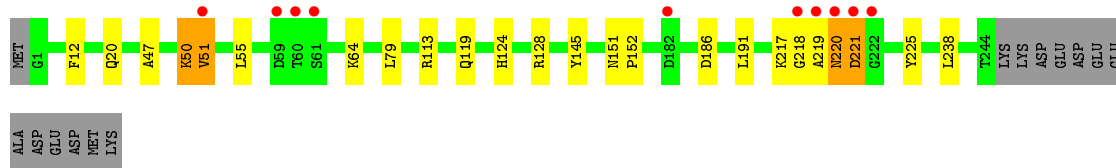
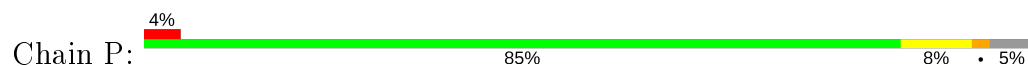
- Molecule 1: Proteasome subunit alpha type-2



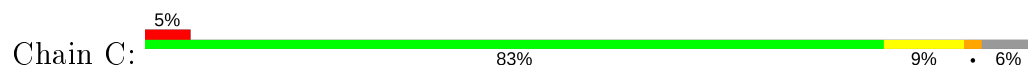
- Molecule 2: Proteasome subunit alpha type-3

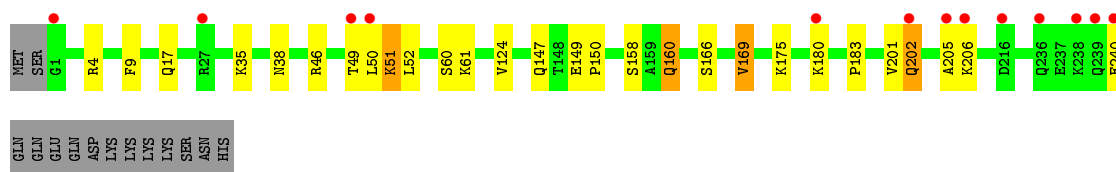


- Molecule 2: Proteasome subunit alpha type-3

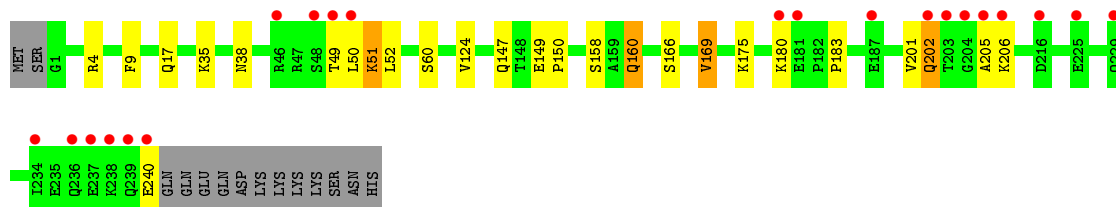
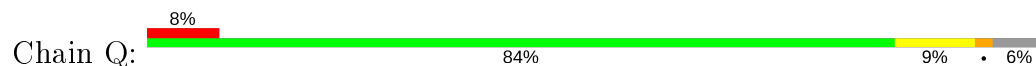


- Molecule 3: Proteasome subunit alpha type-4

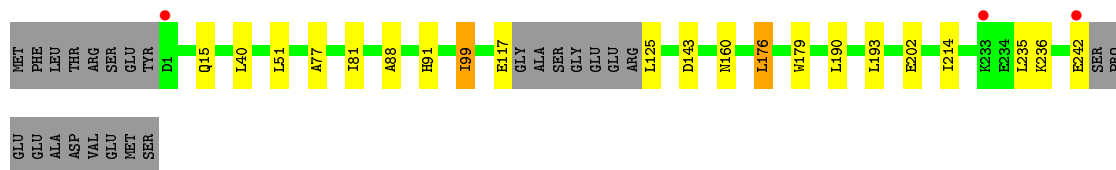
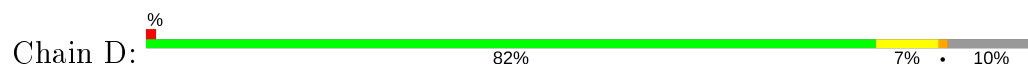




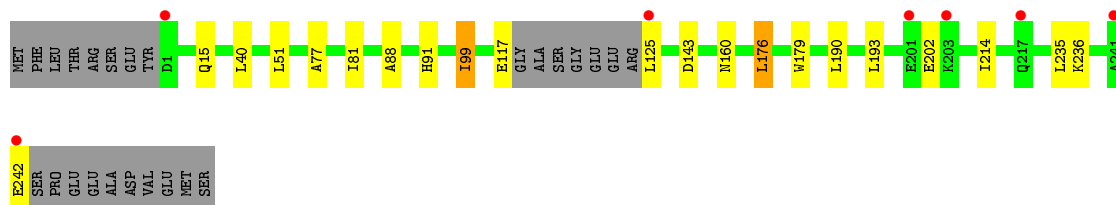
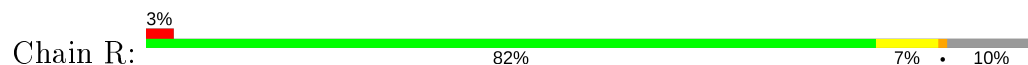
• Molecule 3: Proteasome subunit alpha type-4



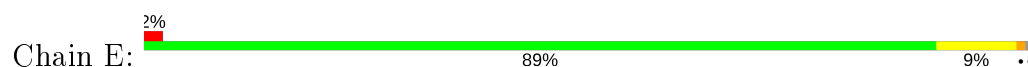
• Molecule 4: Proteasome subunit alpha type-5



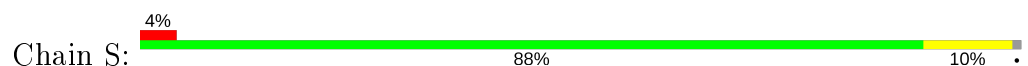
• Molecule 4: Proteasome subunit alpha type-5

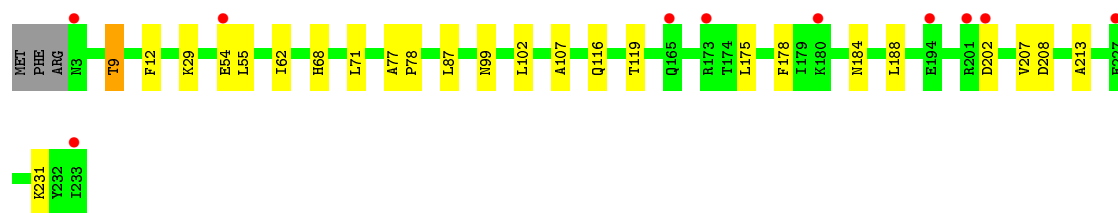


• Molecule 5: Proteasome subunit alpha type-6

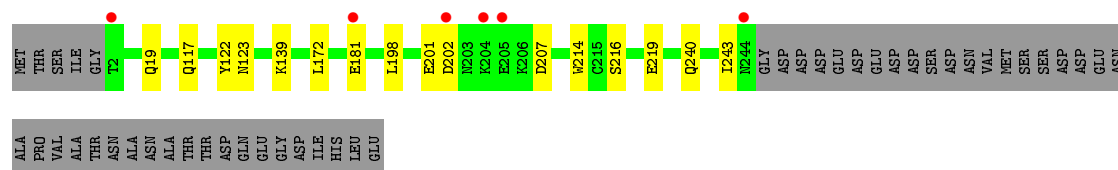
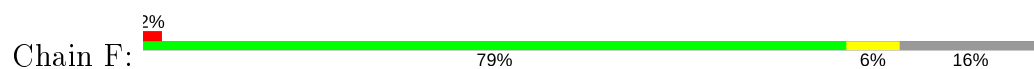


• Molecule 5: Proteasome subunit alpha type-6

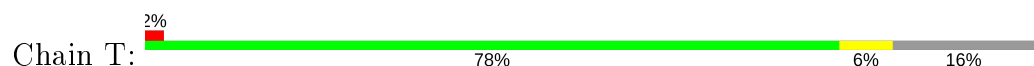




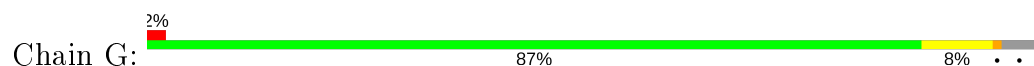
- Molecule 6: Probable proteasome subunit alpha type-7



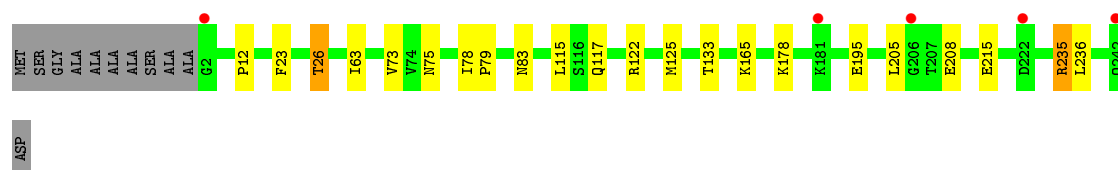
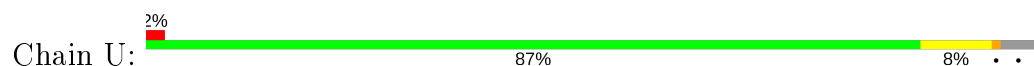
- Molecule 6: Probable proteasome subunit alpha type-7



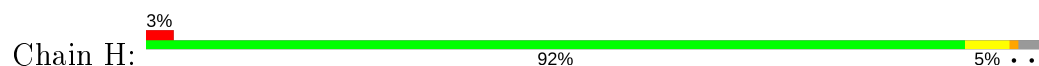
- Molecule 7: Proteasome subunit alpha type-1



- Molecule 7: Proteasome subunit alpha type-1

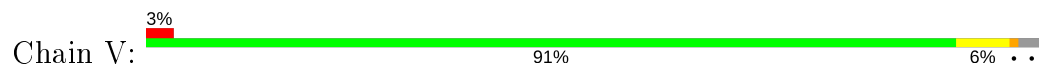


- Molecule 8: Proteasome subunit beta type-2

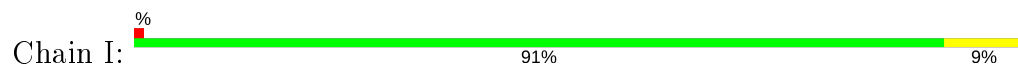




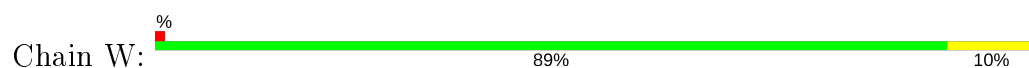
- Molecule 8: Proteasome subunit beta type-2



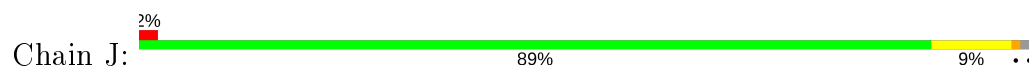
- Molecule 9: Proteasome subunit beta type-3



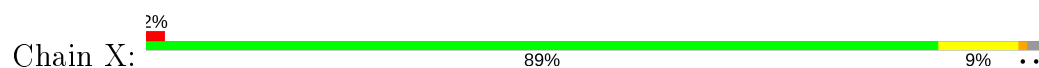
- Molecule 9: Proteasome subunit beta type-3



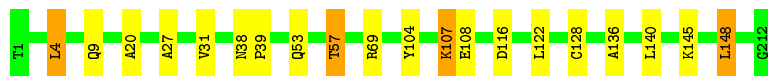
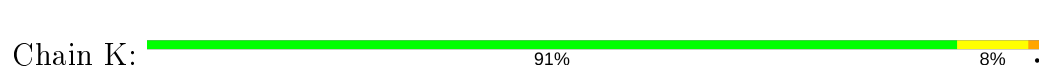
- Molecule 10: Proteasome subunit beta type-4



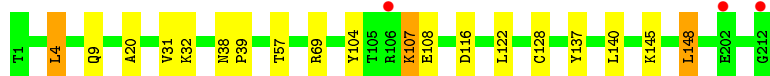
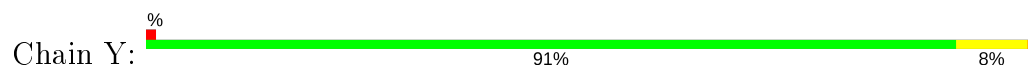
- Molecule 10: Proteasome subunit beta type-4



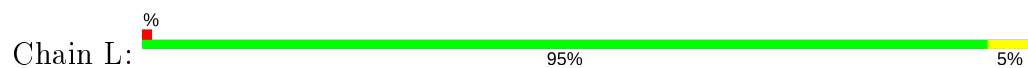
- Molecule 11: Proteasome subunit beta type-5



- Molecule 11: Proteasome subunit beta type-5



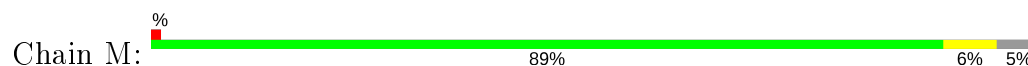
- Molecule 12: Proteasome subunit beta type-6



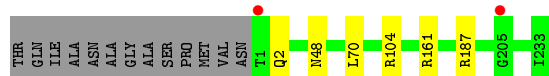
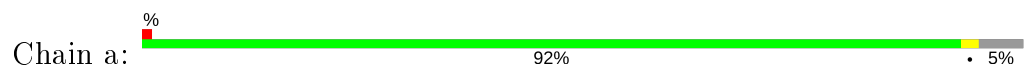
- Molecule 12: Proteasome subunit beta type-6



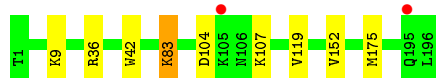
- Molecule 13: Proteasome subunit beta type-7



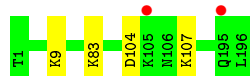
- Molecule 13: Proteasome subunit beta type-7



- 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, $\alpha$ , $\beta$ , $\gamma$	134.36Å 300.59Å 143.85Å 90.00° 112.75° 90.00°	Depositor
Resolution (Å)	15.00 – 2.70 15.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	95.2 (15.00-2.70) 95.2 (15.00-2.70)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.63 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.203 , 0.222 0.208 , 0.229	Depositor DCC
$R_{free}$ test set	13579 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	51.4	Xtriage
Anisotropy	0.111	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 38.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	50050	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, 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	0.26	0/1952	0.47	0/2642
1	O	0.26	0/1952	0.47	0/2642
2	B	0.27	0/1934	0.50	0/2618
2	P	0.26	0/1934	0.51	0/2618
3	C	0.27	0/1910	0.51	0/2586
3	Q	0.26	0/1910	0.51	0/2586
4	D	0.26	0/1837	0.48	0/2475
4	R	0.26	0/1837	0.48	0/2475
5	E	0.26	0/1800	0.48	0/2433
5	S	0.26	0/1800	0.48	0/2433
6	F	0.26	0/1932	0.46	0/2609
6	T	0.26	0/1932	0.46	0/2609
7	G	0.26	0/1945	0.48	0/2634
7	U	0.26	0/1945	0.47	0/2634
8	H	0.29	0/1747	0.48	0/2369
8	V	0.25	0/1747	0.47	0/2369
9	I	0.27	0/1611	0.49	0/2174
9	W	0.26	0/1611	0.48	0/2174
10	J	0.25	0/1589	0.49	0/2142
10	X	0.25	0/1589	0.49	0/2142
11	K	0.26	0/1681	0.50	1/2274 (0.0%)
11	Y	0.28	0/1681	0.50	1/2274 (0.0%)
12	L	0.28	0/1795	0.49	0/2420
12	Z	0.29	0/1795	0.48	0/2420
13	M	0.27	0/1855	0.51	0/2514
13	a	0.27	0/1855	0.51	0/2514
14	N	0.26	0/1541	0.48	0/2087
14	b	0.25	0/1541	0.48	0/2087
All	All	0.26	0/50258	0.49	2/67954 (0.0%)

There are no bond length outliers.



All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	K	4	LEU	CA-CB-CG	5.28	127.44	115.30
11	Y	4	LEU	CA-CB-CG	5.27	127.42	115.30

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	4	0
2	B	1904	0	1904	14	0
2	P	1904	0	1904	13	0
3	C	1881	0	1895	11	0
3	Q	1881	0	1895	9	0
4	D	1813	0	1797	7	0
4	R	1813	0	1797	7	0
5	E	1773	0	1775	8	0
5	S	1773	0	1775	8	0
6	F	1892	0	1883	4	0
6	T	1892	0	1883	5	0
7	G	1907	0	1901	7	0
7	U	1907	0	1901	7	0
8	H	1717	0	1716	7	0
8	V	1717	0	1716	11	0
9	I	1581	0	1574	9	0
9	W	1581	0	1574	13	0
10	J	1561	0	1569	12	0
10	X	1561	0	1569	12	0
11	K	1644	0	1595	8	0
11	Y	1644	0	1595	9	0
12	L	1757	0	1711	6	0
12	Z	1757	0	1711	4	0
13	M	1824	0	1832	4	0
13	a	1824	0	1832	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	N	1512	0	1481	4	0
14	b	1512	0	1481	0	0
15	G	1	0	0	0	0
15	I	1	0	0	0	0
15	K	1	0	0	0	0
15	N	2	0	0	0	0
15	V	1	0	0	0	0
15	W	1	0	0	0	0
15	Y	1	0	0	0	0
15	Z	1	0	0	0	0
16	G	1	0	0	0	0
16	U	1	0	0	0	0
17	K	12	0	13	0	0
18	A	22	0	0	0	0
18	B	18	0	0	0	0
18	C	17	0	0	2	0
18	D	22	0	0	0	0
18	E	18	0	0	0	0
18	F	16	0	0	0	0
18	G	30	0	0	0	0
18	H	37	0	0	0	0
18	I	27	0	0	0	0
18	J	30	0	0	0	0
18	K	36	0	0	2	0
18	L	42	0	0	0	0
18	M	30	0	0	0	0
18	N	18	0	0	0	0
18	O	15	0	0	0	0
18	P	16	0	0	0	0
18	Q	14	0	0	0	0
18	R	13	0	0	0	0
18	S	13	0	0	0	0
18	T	10	0	0	0	0
18	U	28	0	0	0	0
18	V	25	0	0	0	0
18	W	25	0	0	0	0
18	X	24	0	0	0	0
18	Y	27	0	0	0	0
18	Z	24	0	0	0	0
18	a	38	0	0	0	0
18	b	30	0	0	0	0
All	All	50050	0	49137	174	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 (174) 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:H:52:THR:O	8:H:56:THR:OG1	1.82	0.96
11:K:27:ALA:O	12:L:137:ARG:NH2	1.98	0.95
8:V:52:THR:O	8:V:56:THR:OG1	1.95	0.84
18:K:422:HOH:O	12:L:132:GLU:HG3	1.81	0.78
11:Y:128:CYS:HB2	11:Y:137:TYR:CZ	2.25	0.71
11:Y:128:CYS:HB2	11:Y:137:TYR:CE2	2.29	0.67
2:B:12:PHE:H	3:C:17:GLN:HE22	1.47	0.63
5:S:12:PHE:H	6:T:19:GLN:HE22	1.50	0.60
3:Q:51:LYS:O	3:Q:52:LEU:HB2	2.02	0.60
3:C:51:LYS:O	3:C:52:LEU:HB2	2.03	0.58
1:A:1:MET:HG3	6:F:122:TYR:CZ	2.38	0.58
7:G:68:ARG:HH12	14:N:36:ARG:HH22	1.50	0.58
2:B:3:ARG:HB3	5:E:122:TYR:OH	2.04	0.57
3:C:160:GLN:HE21	3:C:160:GLN:HA	1.70	0.57
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.87	0.56
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.88	0.56
3:Q:160:GLN:HE21	3:Q:160:GLN:HA	1.71	0.56
2:P:217:LYS:C	2:P:219:ALA:H	2.10	0.55
2:B:217:LYS:C	2:B:219:ALA:H	2.10	0.54
5:E:12:PHE:H	6:F:19:GLN:HE22	1.57	0.53
3:C:61:LYS:HD3	18:C:309:HOH:O	2.08	0.53
3:C:201:VAL:O	3:C:202:GLN:CB	2.56	0.53
9:I:9:GLY:HA3	9:I:41:LYS:HE2	1.91	0.53
2:B:47:ALA:HB1	2:B:64:LYS:HD2	1.91	0.52
2:P:47:ALA:HB1	2:P:64:LYS:HD2	1.91	0.52
14:N:83:LYS:HG3	14:N:119:VAL:CG2	2.39	0.52
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.57	0.52
18:K:422:HOH:O	12:L:132:GLU:CG	2.47	0.52
7:U:23:PHE:O	7:U:26:THR:HB	2.10	0.52
7:G:23:PHE:O	7:G:26:THR:HB	2.10	0.51
4:D:91:HIS:HB3	4:D:99:ILE:HG22	1.93	0.51
11:K:128:CYS:SG	11:K:136:ALA:HB3	2.51	0.51
4:R:91:HIS:HB3	4:R:99:ILE:HG22	1.93	0.51
9:W:9:GLY:HA3	9:W:41:LYS:HE2	1.93	0.50
3:C:35:LYS:HG2	3:C:158:SER:O	2.12	0.50
1:O:12:PHE:H	2:P:20:GLN:HE22	1.60	0.49
1:O:122:THR:HG22	2:P:128:ARG:HH21	1.77	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:21:VAL:HG11	11:Y:122:LEU:HD11	1.95	0.49
9:W:101:PRO:HB3	9:W:126:ILE:HD12	1.95	0.49
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.95	0.49
4:D:88:ALA:HA	4:D:99:ILE:HG21	1.96	0.48
10:J:21:VAL:HG11	11:K:122:LEU:HD11	1.95	0.48
7:G:73:VAL:HG12	7:G:133:THR:HB	1.94	0.48
1:O:1:MET:HG3	6:T:122:TYR:CZ	2.49	0.48
6:T:198:LEU:HD12	6:T:243:ILE:HG22	1.94	0.48
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.95	0.48
6:F:198:LEU:HD12	6:F:243:ILE:HG22	1.95	0.48
7:U:73:VAL:HG12	7:U:133:THR:HB	1.94	0.48
11:Y:20:ALA:HB2	11:Y:31:VAL:HG21	1.96	0.48
2:B:219:ALA:HB2	2:B:225:TYR:HB2	1.95	0.48
4:R:91:HIS:HB3	4:R:99:ILE:CG2	2.43	0.48
3:C:9:PHE:H	4:D:15:GLN:HE22	1.60	0.48
10:X:1:MET:HG2	10:X:34:LYS:HE3	1.96	0.48
11:Y:107:LYS:HG3	11:Y:108:GLU:HG3	1.95	0.48
11:Y:31:VAL:HA	12:Z:132:GLU:OE2	2.14	0.48
11:K:107:LYS:HG3	11:K:108:GLU:HG3	1.95	0.47
5:S:87:LEU:HD21	5:S:107:ALA:HB1	1.96	0.47
8:V:84:LYS:HA	8:V:113:ILE:HD11	1.96	0.47
3:Q:35:LYS:HG2	3:Q:158:SER:O	2.13	0.47
4:R:88:ALA:HA	4:R:99:ILE:HG21	1.96	0.47
4:D:91:HIS:HB3	4:D:99:ILE:CG2	2.44	0.47
2:B:151:ASN:HB2	2:B:152:PRO:CD	2.44	0.47
4:D:176:LEU:HD22	5:E:55:LEU:CD2	2.43	0.47
3:C:149:GLU:HB2	3:C:150:PRO:HD2	1.97	0.47
5:E:87:LEU:HD21	5:E:107:ALA:HB1	1.96	0.47
2:P:219:ALA:HB2	2:P:225:TYR:HB2	1.95	0.47
3:Q:149:GLU:HB2	3:Q:150:PRO:HD2	1.97	0.47
2:P:151:ASN:HB2	2:P:152:PRO:CD	2.45	0.47
8:H:84:LYS:HA	8:H:113:ILE:HD11	1.96	0.46
10:J:168:LEU:O	10:J:172:MET:HB2	2.15	0.46
10:J:1:MET:HG2	10:J:34:LYS:HE3	1.96	0.46
11:K:20:ALA:HB2	11:K:31:VAL:HG21	1.97	0.46
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.49	0.46
2:B:50:LYS:HA	2:B:50:LYS:HD2	1.80	0.46
10:X:168:LEU:O	10:X:172:MET:HB2	2.16	0.46
5:S:175:LEU:HA	5:S:178:PHE:CE2	2.51	0.45
10:J:3:ILE:HG23	10:J:18:SER:HB3	1.98	0.45
8:V:63:ILE:HG23	8:V:74:PRO:HB3	1.99	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:141:ALA:HB2	9:I:177:ASP:HB2	1.99	0.45
11:K:145:LYS:HB2	11:K:148:LEU:HD13	1.98	0.45
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.52	0.45
8:V:104:ASP:HB2	8:V:105:PRO:HD2	1.98	0.45
5:E:175:LEU:HA	5:E:178:PHE:CE2	2.52	0.45
13:M:27:LEU:HD21	13:M:34:LEU:HD22	1.99	0.45
10:X:3:ILE:HG23	10:X:18:SER:HB3	1.98	0.45
12:L:8:ASN:HA	12:L:30:ILE:O	2.17	0.45
14:N:36:ARG:HG3	14:N:42:TRP:CE2	2.51	0.45
11:Y:38:ASN:HB2	11:Y:39:PRO:CD	2.47	0.45
7:U:195:GLU:HG3	7:U:235:ARG:HG3	1.99	0.45
9:W:20:VAL:HG23	9:W:189:ILE:HB	1.99	0.45
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.52	0.45
10:X:1:MET:HB3	10:X:34:LYS:HE3	1.99	0.45
11:Y:145:LYS:HB2	11:Y:148:LEU:HD13	1.98	0.45
1:A:122:THR:HG22	2:B:128:ARG:HH21	1.81	0.44
8:H:63:ILE:HG23	8:H:74:PRO:HB3	1.98	0.44
10:J:1:MET:CB	10:J:34:LYS:HE3	2.47	0.44
10:J:1:MET:HB3	10:J:34:LYS:HE3	1.99	0.44
9:W:141:ALA:HB2	9:W:177:ASP:HB2	1.99	0.44
11:K:38:ASN:HB2	11:K:39:PRO:CD	2.47	0.44
2:P:151:ASN:HB2	2:P:152:PRO:HD2	2.00	0.44
10:X:119:ILE:HG12	10:X:125:LYS:HG3	1.99	0.44
10:X:1:MET:CB	10:X:34:LYS:HE3	2.47	0.44
11:Y:32:LYS:N	12:Z:132:GLU:OE2	2.38	0.44
9:I:94:LEU:HD11	9:I:106:PRO:HG2	2.00	0.44
10:J:119:ILE:HG12	10:J:125:LYS:HG3	1.99	0.44
7:G:195:GLU:HG3	7:G:235:ARG:HG3	1.99	0.44
8:H:104:ASP:HB2	8:H:105:PRO:HD2	1.99	0.44
12:L:137:ARG:HA	12:L:137:ARG:HD3	1.77	0.44
9:W:94:LEU:HD11	9:W:106:PRO:HG2	2.00	0.44
10:J:25:ILE:O	10:X:139:TYR:OH	2.36	0.44
13:M:127:LEU:HG	13:M:142:LEU:HD12	2.00	0.44
2:B:151:ASN:HB2	2:B:152:PRO:HD2	2.00	0.43
4:R:77:ALA:O	4:R:81:ILE:HG12	2.18	0.43
9:W:26:LEU:HD21	9:W:185:VAL:HG23	2.00	0.43
9:W:36:SER:HB2	10:X:126:VAL:HG11	2.00	0.43
8:V:35:HIS:HB2	8:V:56:THR:HG21	2.00	0.43
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.18	0.43
9:W:98:ARG:O	9:W:126:ILE:HD11	2.18	0.43
9:I:20:VAL:HG23	9:I:189:ILE:HB	1.99	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:78:ILE:N	7:U:79:PRO:CD	2.81	0.43
7:G:78:ILE:N	7:G:79:PRO:CD	2.81	0.43
9:I:36:SER:HB2	10:J:126:VAL:HG11	2.00	0.43
8:V:104:ASP:HB2	8:V:105:PRO:CD	2.49	0.43
3:C:46:ARG:HG2	18:C:309:HOH:O	2.18	0.43
9:I:20:VAL:HG13	9:I:118:PRO:HB3	2.00	0.42
9:W:20:VAL:HG13	9:W:118:PRO:HB3	2.00	0.42
5:S:68:HIS:HE1	5:S:102:LEU:O	2.01	0.42
2:B:145:TYR:OH	2:B:217:LYS:N	2.52	0.42
9:I:26:LEU:HD21	9:I:185:VAL:HG23	2.01	0.42
2:P:50:LYS:O	2:P:51:VAL:C	2.57	0.42
5:E:68:HIS:HE1	5:E:102:LEU:O	2.02	0.42
7:G:63:ILE:HD12	7:G:215:GLU:HG2	2.02	0.42
2:P:145:TYR:OH	2:P:217:LYS:N	2.52	0.42
2:P:124:HIS:HB3	3:Q:124:VAL:HG12	2.02	0.42
3:Q:166:SER:HA	3:Q:169:VAL:HG13	2.02	0.42
2:P:12:PHE:H	3:Q:17:GLN:HE22	1.66	0.42
7:U:165:LYS:HD2	7:U:205:LEU:HD22	2.02	0.42
4:D:77:ALA:O	4:D:81:ILE:HG12	2.19	0.42
12:Z:146:ILE:HG22	12:Z:150:LEU:HD22	2.02	0.42
8:H:104:ASP:HB2	8:H:105:PRO:CD	2.49	0.42
7:U:63:ILE:HD12	7:U:215:GLU:HG2	2.01	0.42
8:V:43:CYS:SG	8:V:56:THR:CG2	3.08	0.41
13:M:97:ALA:HA	13:M:130:VAL:HG21	2.02	0.41
14:N:152:VAL:HA	14:N:175:MET:HE1	2.01	0.41
5:S:9:THR:HG21	5:S:119:THR:HA	2.02	0.41
2:P:220:ASN:O	2:P:221:ASP:HB2	2.21	0.41
6:F:216:SER:HB3	6:F:219:GLU:HB2	2.02	0.41
6:T:216:SER:HB3	6:T:219:GLU:HB2	2.02	0.41
8:V:210:THR:HG21	9:W:167:SER:HB3	2.03	0.41
8:V:196:ARG:NH2	9:W:150:GLU:HG3	2.35	0.41
2:B:220:ASN:O	2:B:221:ASP:HB2	2.21	0.41
7:G:165:LYS:HD2	7:G:205:LEU:HD22	2.02	0.41
10:J:126:VAL:HG12	10:J:128:LEU:HG	2.03	0.41
10:J:139:TYR:OH	10:X:25:ILE:O	2.39	0.41
2:B:217:LYS:C	2:B:219:ALA:N	2.74	0.41
2:B:50:LYS:O	2:B:51:VAL:C	2.58	0.41
3:C:166:SER:HA	3:C:169:VAL:HG13	2.02	0.41
2:P:217:LYS:C	2:P:219:ALA:N	2.74	0.41
8:H:196:ARG:NH2	9:I:150:GLU:HG3	2.36	0.41
5:E:62:ILE:HG21	5:E:213:ALA:HB2	2.02	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:146:ILE:HG22	12:L:150:LEU:HD22	2.02	0.41
4:R:176:LEU:HD11	5:S:54:GLU:HB2	2.03	0.41
5:S:62:ILE:HG21	5:S:213:ALA:HB2	2.02	0.41
8:V:43:CYS:SG	8:V:56:THR:HG23	2.61	0.41
8:H:8:PHE:HB3	8:H:151:ALA:HB2	2.03	0.40
10:X:126:VAL:HG12	10:X:128:LEU:HG	2.02	0.40
2:B:124:HIS:HB3	3:C:124:VAL:HG12	2.03	0.40
5:S:77:ALA:N	5:S:78:PRO:CD	2.85	0.40
6:T:171:GLU:HB3	6:T:195:ILE:HG12	2.02	0.40
5:E:9:THR:HG21	5:E:119:THR:HA	2.02	0.40
13:M:165:ILE:HB	13:M:166:PRO:HD3	2.04	0.40
3:Q:9:PHE:H	4:R:15:GLN:HE22	1.67	0.40
11:K:53:GLN:O	11:K:57:THR:OG1	2.39	0.40
8:V:50:ALA:CB	9:W:126:ILE:HG23	2.51	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	248/250 (99%)	238 (96%)	9 (4%)	1 (0%)	34	60
1	O	248/250 (99%)	238 (96%)	9 (4%)	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%)	232 (98%)	3 (1%)	3 (1%)	12	30
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

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	239 (100%)	0	0	100	100
7	U	239/252 (95%)	239 (100%)	0	0	100	100
8	H	224/232 (97%)	218 (97%)	6 (3%)	0	100	100
8	V	224/232 (97%)	218 (97%)	6 (3%)	0	100	100
9	I	202/205 (98%)	196 (97%)	6 (3%)	0	100	100
9	W	202/205 (98%)	196 (97%)	6 (3%)	0	100	100
10	J	193/198 (98%)	188 (97%)	5 (3%)	0	100	100
10	X	193/198 (98%)	188 (97%)	5 (3%)	0	100	100
11	K	210/212 (99%)	206 (98%)	4 (2%)	0	100	100
11	Y	210/212 (99%)	206 (98%)	4 (2%)	0	100	100
12	L	220/222 (99%)	216 (98%)	4 (2%)	0	100	100
12	Z	220/222 (99%)	216 (98%)	4 (2%)	0	100	100
13	M	231/246 (94%)	223 (96%)	8 (4%)	0	100	100
13	a	231/246 (94%)	223 (96%)	8 (4%)	0	100	100
14	N	194/196 (99%)	190 (98%)	4 (2%)	0	100	100
14	b	194/196 (99%)	190 (98%)	4 (2%)	0	100	100
All	All	6284/6614 (95%)	6141 (98%)	127 (2%)	16 (0%)	41	66

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	THR
2	B	51	VAL
2	B	221	ASP
3	C	202	GLN
1	O	2	THR
2	P	51	VAL
2	P	221	ASP
3	Q	202	GLN
2	B	218	GLY
2	B	220	ASN
2	P	218	GLY

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
2	P	220	ASN
3	C	205	ALA
3	Q	205	ALA
3	Q	183	PRO
3	C	183	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	209/209 (100%)	205 (98%)	4 (2%)	57	82
1	O	209/209 (100%)	205 (98%)	4 (2%)	57	82
2	B	203/216 (94%)	195 (96%)	8 (4%)	32	61
2	P	203/216 (94%)	195 (96%)	8 (4%)	32	61
3	C	212/226 (94%)	199 (94%)	13 (6%)	18	41
3	Q	212/226 (94%)	199 (94%)	13 (6%)	18	41
4	D	194/215 (90%)	180 (93%)	14 (7%)	14	34
4	R	194/215 (90%)	180 (93%)	14 (7%)	14	34
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
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%)	195 (95%)	11 (5%)	22	48
8	H	185/190 (97%)	181 (98%)	4 (2%)	52	79
8	V	185/190 (97%)	181 (98%)	4 (2%)	52	79
9	I	172/173 (99%)	168 (98%)	4 (2%)	50	78
9	W	172/173 (99%)	167 (97%)	5 (3%)	42	71
10	J	173/175 (99%)	169 (98%)	4 (2%)	50	78
10	X	173/175 (99%)	169 (98%)	4 (2%)	50	78

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	178 (96%)	7 (4%)	33	62
13	M	199/208 (96%)	193 (97%)	6 (3%)	41	70
13	a	199/208 (96%)	193 (97%)	6 (3%)	41	70
14	N	162/162 (100%)	158 (98%)	4 (2%)	47	76
14	b	162/162 (100%)	158 (98%)	4 (2%)	47	76
All	All	5320/5540 (96%)	5100 (96%)	220 (4%)	30	59

All (220) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	SER
1	A	122	THR
1	A	157	PHE
1	A	250	LEU
2	B	50	LYS
2	B	55	LEU
2	B	79	LEU
2	B	113	ARG
2	B	119	GLN
2	B	186	ASP
2	B	191	LEU
2	B	238	LEU
3	C	4	ARG
3	C	38	ASN
3	C	49	THR
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	175	LYS
3	C	180	LYS
3	C	206	LYS
3	C	240	GLU
4	D	40	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
4	D	51	LEU
4	D	99	ILE
4	D	117	GLU
4	D	125	LEU
4	D	143	ASP
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	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
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	178	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
7	G	208	GLU
7	G	235	ARG
7	G	236	LEU
8	H	30	ASN
8	H	56	THR
8	H	68	LEU
8	H	196	ARG
9	I	37	ASN
9	I	171	LEU
9	I	182	TRP
9	I	192	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	69	ARG
11	K	104	TYR
11	K	107	LYS
11	K	116	ASP
11	K	140	LEU
11	K	148	LEU
12	L	3	ASN
12	L	23	LEU
12	L	31	THR
12	L	49	ASN
12	L	136	CYS
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	161	ARG
13	M	187	ARG
14	N	9	LYS
14	N	83	LYS
14	N	104	ASP
14	N	107	LYS
1	O	62	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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	119	GLN
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	175	LYS
3	Q	180	LYS
3	Q	206	LYS
3	Q	240	GLU
4	R	40	LEU
4	R	51	LEU
4	R	99	ILE
4	R	117	GLU
4	R	125	LEU
4	R	143	ASP
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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	178	LYS
7	U	208	GLU
7	U	235	ARG
7	U	236	LEU
8	V	30	ASN
8	V	56	THR
8	V	68	LEU
8	V	196	ARG
9	W	37	ASN
9	W	126	ILE
9	W	171	LEU
9	W	182	TRP
9	W	192	ASP
10	X	3	ILE
10	X	35	THR
10	X	90	LYS
10	X	99	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
11	Y	4	LEU
11	Y	9	GLN
11	Y	57	THR
11	Y	69	ARG
11	Y	104	TYR
11	Y	107	LYS
11	Y	116	ASP
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	136	CYS
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	161	ARG
13	a	187	ARG
14	b	9	LYS
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 (121) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	HIS
2	B	20	GLN
2	B	58	GLN
2	B	95	GLN
2	B	119	GLN
2	B	123	GLN
2	B	155	ASN
2	B	176	GLN
3	C	17	GLN
3	C	38	ASN
3	C	77	ASN
3	C	147	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
3	C	160	GLN
4	D	15	GLN
4	D	146	GLN
4	D	210	GLN
4	D	225	ASN
5	E	68	HIS
5	E	92	ASN
5	E	99	ASN
5	E	116	GLN
5	E	120	GLN
5	E	151	ASN
5	E	184	ASN
6	F	19	GLN
6	F	86	ASN
6	F	117	GLN
6	F	123	ASN
6	F	191	GLN
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	22	GLN
8	H	30	ASN
8	H	66	HIS
8	H	165	ASN
8	H	172	ASN
8	H	189	ASN
9	I	37	ASN
10	J	55	GLN
10	J	146	HIS
11	K	85	ASN
11	K	176	ASN
11	K	190	ASN
11	K	208	ASN
12	L	3	ASN
12	L	49	ASN
12	L	70	ASN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
12	L	158	ASN
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	100	ASN
4	R	146	GLN
4	R	225	ASN
5	S	68	HIS
5	S	92	ASN
5	S	99	ASN
5	S	116	GLN
5	S	120	GLN
5	S	151	ASN
5	S	184	ASN
6	T	19	GLN
6	T	86	ASN
6	T	117	GLN
6	T	123	ASN
6	T	191	GLN
6	T	240	GLN
7	U	30	ASN
7	U	83	ASN
7	U	114	ASN
7	U	117	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
7	U	121	GLN
7	U	166	GLN
7	U	167	GLN
7	U	175	ASN
8	V	22	GLN
8	V	66	HIS
8	V	165	ASN
9	W	37	ASN
10	X	55	GLN
10	X	86	GLN
10	X	146	HIS
11	Y	85	ASN
11	Y	176	ASN
11	Y	190	ASN
11	Y	208	ASN
12	Z	3	ASN
12	Z	49	ASN
12	Z	70	ASN
12	Z	158	ASN
13	a	18	ASN
13	a	48	ASN
13	a	102	GLN
13	a	194	ASN
13	a	213	GLN
14	b	161	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

Of 12 ligands modelled in this entry, 11 are monoatomic - leaving 1 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	$\# Z  > 2$
17	MES	K	302	-	12,12,12	2.10	1 (8%)	14,16,16	1.30	2 (14%)

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
17	MES	K	302	-	-	0/6/14/14	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	K	302	MES	C8-S	-6.91	1.67	1.77

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	K	302	MES	O3S-S-C8	2.84	110.35	105.77
17	K	302	MES	O2S-S-C8	2.47	109.89	106.92

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

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	250/250 (100%)	-0.35	9 (3%) 42 42	37, 50, 82, 121	0
1	O	250/250 (100%)	-0.24	11 (4%) 34 33	43, 58, 101, 129	0
2	B	244/258 (94%)	-0.20	10 (4%) 37 36	38, 56, 97, 146	0
2	P	244/258 (94%)	-0.19	10 (4%) 37 36	44, 60, 99, 145	0
3	C	240/254 (94%)	-0.11	13 (5%) 25 24	37, 60, 116, 144	0
3	Q	240/254 (94%)	0.16	21 (8%) 10 8	44, 72, 148, 170	0
4	D	235/260 (90%)	-0.30	3 (1%) 77 78	41, 60, 91, 131	0
4	R	235/260 (90%)	-0.24	7 (2%) 50 51	44, 64, 103, 138	0
5	E	231/234 (98%)	-0.20	5 (2%) 62 63	43, 62, 98, 144	0
5	S	231/234 (98%)	-0.09	10 (4%) 35 33	46, 71, 109, 153	0
6	F	243/288 (84%)	-0.36	6 (2%) 57 59	39, 56, 103, 131	0
6	T	243/288 (84%)	-0.23	6 (2%) 57 59	43, 66, 115, 142	0
7	G	241/252 (95%)	-0.38	5 (2%) 63 65	33, 53, 84, 133	0
7	U	241/252 (95%)	-0.28	5 (2%) 63 65	42, 57, 85, 127	0
8	H	226/232 (97%)	-0.28	7 (3%) 49 49	33, 49, 79, 143	0
8	V	226/232 (97%)	-0.22	7 (3%) 49 49	36, 52, 80, 153	0
9	I	204/205 (99%)	-0.58	3 (1%) 73 76	37, 46, 73, 96	0
9	W	204/205 (99%)	-0.54	2 (0%) 82 83	36, 48, 76, 98	0
10	J	195/198 (98%)	-0.38	4 (2%) 63 65	35, 50, 74, 130	0
10	X	195/198 (98%)	-0.33	3 (1%) 73 76	38, 52, 74, 136	0
11	K	212/212 (100%)	-0.41	0 100 100	33, 49, 70, 89	0
11	Y	212/212 (100%)	-0.45	3 (1%) 75 77	39, 50, 73, 93	0
12	L	222/222 (100%)	-0.47	2 (0%) 84 85	37, 51, 78, 114	0
12	Z	222/222 (100%)	-0.47	1 (0%) 91 92	36, 50, 79, 115	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	M	233/246 (94%)	-0.54	2 (0%) 84 85	34, 50, 72, 89	0
13	a	233/246 (94%)	-0.48	2 (0%) 84 85	34, 49, 68, 86	0
14	N	196/196 (100%)	-0.48	2 (1%) 82 83	34, 44, 70, 98	0
14	b	196/196 (100%)	-0.48	2 (1%) 82 83	35, 46, 71, 104	0
All	All	6344/6614 (95%)	-0.32	161 (2%) 57 59	33, 54, 96, 170	0

All (161) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
8	V	224	GLN	8.5
2	B	221	ASP	8.1
3	Q	50	LEU	7.6
3	Q	49	THR	7.0
8	V	223	ILE	6.3
2	B	51	VAL	5.8
2	P	221	ASP	5.7
2	P	51	VAL	5.7
3	Q	206	LYS	5.4
8	V	222	ASP	5.3
3	Q	236	GLN	5.3
10	X	1	MET	5.1
1	O	2	THR	5.1
8	V	226	GLU	4.7
1	A	2	THR	4.6
5	E	202	ASP	4.6
2	P	220	ASN	4.6
14	N	105	LYS	4.6
14	b	195	GLN	4.5
12	Z	174	TYR	4.5
12	L	174	TYR	4.5
5	S	202	ASP	4.5
8	H	222	ASP	4.4
14	b	105	LYS	4.4
10	X	194	ASP	4.3
9	W	1	SER	4.2
2	B	220	ASN	4.2
8	H	224	GLN	4.2
3	Q	204	GLY	4.1
14	N	195	GLN	4.1
2	P	59	ASP	4.1
3	C	206	LYS	4.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	O	1	MET	4.0
3	C	238	LYS	4.0
4	R	241	ALA	4.0
10	J	1	MET	3.9
6	F	2	THR	3.8
7	U	206	GLY	3.8
7	U	242	GLN	3.7
1	O	62	SER	3.7
3	Q	240	GLU	3.7
2	P	218	GLY	3.5
3	Q	239	GLN	3.5
8	H	226	GLU	3.5
8	V	225	GLU	3.4
7	G	240	ALA	3.4
1	A	1	MET	3.3
6	T	244	ASN	3.3
3	C	239	GLN	3.3
5	S	173	ARG	3.3
2	P	222	GLY	3.3
3	Q	229	GLN	3.3
3	Q	48	SER	3.3
3	C	50	LEU	3.2
8	V	221	CYS	3.2
3	C	49	THR	3.1
4	R	242	GLU	3.1
2	P	219	ALA	3.1
8	H	221	CYS	3.1
13	a	1	THR	3.0
1	O	249	ALA	3.0
10	X	193	ASP	3.0
8	H	223	ILE	3.0
8	H	198	GLU	2.9
6	T	243	ILE	2.9
2	B	219	ALA	2.9
3	Q	238	LYS	2.9
5	S	227	GLU	2.8
8	H	225	GLU	2.8
3	Q	202	GLN	2.8
9	I	1	SER	2.8
4	R	125	LEU	2.8
3	Q	187	GLU	2.7
3	Q	203	THR	2.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
6	F	181	GLU	2.7
6	T	178	HIS	2.7
1	A	249	ALA	2.7
10	J	24	GLY	2.7
6	F	205	GLU	2.7
5	E	122	TYR	2.6
1	A	201	GLU	2.6
3	C	180	LYS	2.6
10	J	193	ASP	2.6
13	M	1	THR	2.5
3	Q	237	GLU	2.5
3	Q	46	ARG	2.5
3	C	240	GLU	2.5
11	Y	212	GLY	2.5
4	D	242	GLU	2.5
5	S	3	ASN	2.5
4	D	1	ASP	2.5
1	A	228	PRO	2.5
1	A	229	THR	2.5
6	F	202	ASP	2.5
3	C	205	ALA	2.5
7	U	2	GLY	2.4
3	C	216	ASP	2.4
5	S	54	GLU	2.4
1	O	201	GLU	2.4
7	G	241	GLU	2.4
1	O	231	LYS	2.4
3	Q	181	GLU	2.4
10	J	194	ASP	2.4
2	B	218	GLY	2.4
5	E	201	ARG	2.4
1	A	203	GLU	2.4
3	Q	180	LYS	2.4
1	O	52	SER	2.4
7	G	68	ARG	2.4
3	Q	205	ALA	2.3
6	T	180	PRO	2.3
5	S	194	GLU	2.3
12	L	166	GLY	2.3
3	Q	225	GLU	2.3
5	S	201	ARG	2.3
4	D	233	LYS	2.3

*Continued on next page...*



*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
7	U	222	ASP	2.3
13	M	47	ASP	2.3
3	C	202	GLN	2.3
2	B	217	LYS	2.3
5	S	180	LYS	2.2
2	B	59	ASP	2.2
4	R	201	GLU	2.2
6	F	244	ASN	2.2
2	B	230	LYS	2.2
5	S	165	GLN	2.2
3	C	236	GLN	2.2
4	R	1	ASP	2.2
13	a	205	GLY	2.2
9	W	133	LYS	2.1
5	S	233	ILE	2.1
2	B	222	GLY	2.1
5	E	173	ARG	2.1
3	C	27	ARG	2.1
1	O	50	LYS	2.1
4	R	217	GLN	2.1
1	A	54	PRO	2.1
2	P	182	ASP	2.1
9	I	192	ASP	2.1
6	T	2	THR	2.1
3	Q	234	ILE	2.1
8	V	145	ASP	2.1
7	U	181	LYS	2.1
3	Q	216	ASP	2.1
1	A	182	GLU	2.1
5	E	217	LYS	2.1
2	P	61	SER	2.1
11	Y	106	ARG	2.1
7	G	188	GLU	2.1
6	F	204	LYS	2.0
2	P	60	THR	2.0
3	C	1	GLY	2.0
6	T	229	GLY	2.0
2	B	223	GLU	2.0
7	G	242	GLN	2.0
1	O	198	GLU	2.0
1	O	203	GLU	2.0
4	R	203	LYS	2.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
9	I	160	GLU	2.0
11	Y	202	GLU	2.0
1	O	228	PRO	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
17	MES	K	302	12/12	0.81	0.29	79,97,100,100	0
15	MG	I	301	1/1	0.91	0.10	52,52,52,52	0
15	MG	W	301	1/1	0.91	0.18	59,59,59,59	0
15	MG	N	202	1/1	0.95	0.11	43,43,43,43	0
15	MG	Z	301	1/1	0.97	0.22	55,55,55,55	0
15	MG	V	301	1/1	0.98	0.04	52,52,52,52	0
16	CL	U	301	1/1	0.98	0.25	30,30,30,30	0
16	CL	G	302	1/1	0.98	0.16	30,30,30,30	0
15	MG	G	301	1/1	0.99	0.09	48,48,48,48	0
15	MG	N	201	1/1	0.99	0.07	48,48,48,48	0
15	MG	K	301	1/1	0.99	0.08	40,40,40,40	0
15	MG	Y	301	1/1	0.99	0.06	45,45,45,45	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.