



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 15, 2024 – 03:29 pm GMT

PDB ID : 6HV3  
Title : Yeast 20S proteasome with human beta2i (1-53)  
Authors : Huber, E.M.; Groll, M.  
Deposited on : 2018-10-10  
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 types of validation reports are described at

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

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

MolProbity : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

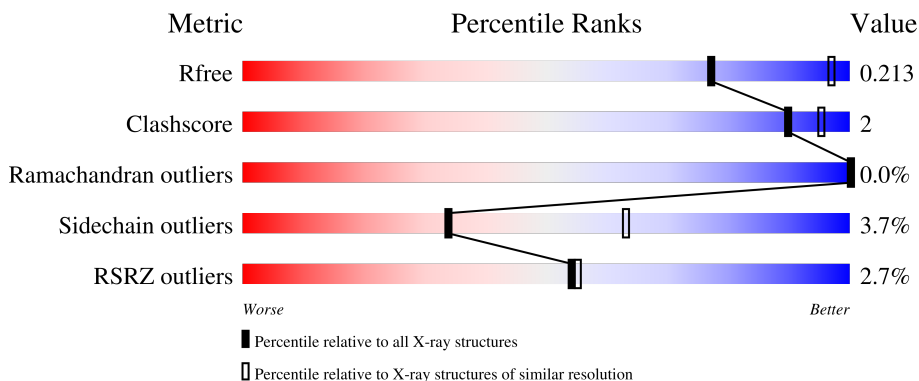
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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 of 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	 4% 98%
1	O	250	 4% 96%
2	B	258	 5% 86% 7% 5%
2	P	258	 6% 83% 11% 5%
3	C	254	 6% 87% 7% 6%

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Mol	Chain	Length	Quality of chain
3	Q	254	6% 85% 9% 6%
4	D	260	2% 86% 10%
4	R	260	3% 86% 10%
5	E	234	3% 92% 6%
5	S	234	3% 92% 6%
6	F	288	2% 80% 16%
6	T	288	3% 80% 5% 16%
7	G	252	3% 92% 10%
7	U	252	2% 91% 10%
8	H	226	4% 93% 5%
8	V	226	2% 93% 10%
9	I	205	95% 10%
9	W	205	2% 95% 10%
10	J	198	2% 95% 10%
10	X	198	2% 95% 10%
11	K	212	95% 5%
11	Y	212	95% 10%
12	L	222	94% 6%
12	Z	222	93% 7%
13	M	246	91% 5%
13	a	246	91% 5%
14	N	196	96% 10%
14	b	196	97% 10%

## 2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 49958 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
			Total	C	N	O	S			
1	A	250	Total 1915	C 1219	N 315	O 377	S 4	0	0	0
1	O	250	Total 1915	C 1219	N 315	O 377	S 4	0	0	0

- Molecule 2 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	244	Total 1904	C 1201	N 321	O 379	S 3	0	0	0
2	P	244	Total 1904	C 1201	N 321	O 379	S 3	0	0	0

- Molecule 3 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	240	Total 1881	C 1176	N 329	O 372	S 4	0	0	0
3	Q	240	Total 1881	C 1176	N 329	O 372	S 4	0	0	0

- Molecule 4 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	235	Total 1813	C 1136	N 304	O 366	S 7	0	0	0
4	R	235	Total 1813	C 1136	N 304	O 366	S 7	0	0	0

- Molecule 5 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	231	Total 1773	C 1114	N 307	O 348	S 4	0	0	0
5	S	231	Total 1773	C 1114	N 307	O 348	S 4	0	0	0

- Molecule 6 is a protein called Probable proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	F	243	Total 1892	C 1203	N 329	O 356	S 4	0	0	0
6	T	243	Total 1892	C 1203	N 329	O 356	S 4	0	0	0

- Molecule 7 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	G	241	Total 1907	C 1214	N 320	O 365	S 8	0	0	0
7	U	241	Total 1907	C 1214	N 320	O 365	S 8	0	0	0

- Molecule 8 is a protein called Proteasome subunit beta type-10, Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	H	226	Total 1716	C 1081	N 291	O 336	S 8	0	0	0
8	V	223	Total 1688	C 1066	N 287	O 327	S 8	0	0	0

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

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

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

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

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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
			1644	1045	280	312	7			
11	Y	212	Total	C	N	O	S	0	0	0
			1644	1045	280	312	7			

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	G	1	Total	Mg	0	0
			1	1		
15	I	1	Total	Mg	0	0
			1	1		

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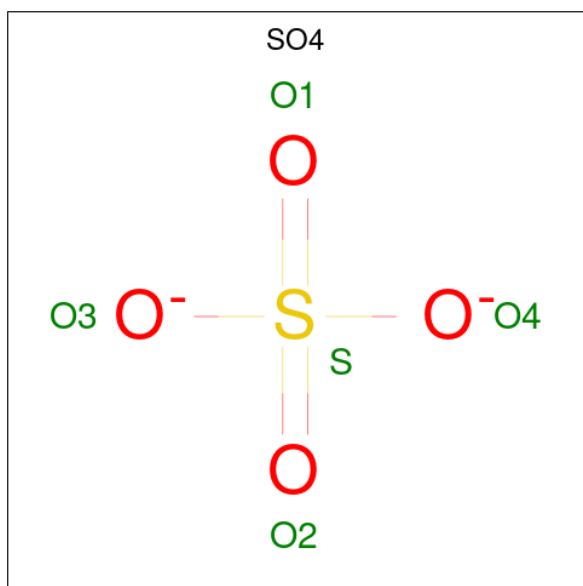
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	K	1	Total	Mg	0	0
			1	1		
15	N	1	Total	Mg	0	0
			1	1		
15	V	1	Total	Mg	0	0
			1	1		
15	W	1	Total	Mg	0	0
			1	1		
15	Y	1	Total	Mg	0	0
			1	1		
15	Z	1	Total	Mg	0	0
			1	1		

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

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

- Molecule 17 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
17	H	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
17	V	1	Total	O	S	0	0
			5	4	1		

- Molecule 18 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	A	27	Total	O	0	0
			27	27		
18	B	19	Total	O	0	0
			19	19		
18	C	13	Total	O	0	0
			13	13		
18	D	21	Total	O	0	0
			21	21		
18	E	14	Total	O	0	0
			14	14		
18	F	14	Total	O	0	0
			14	14		
18	G	25	Total	O	0	0
			25	25		
18	H	40	Total	O	0	0
			40	40		
18	I	19	Total	O	0	0
			19	19		
18	J	23	Total	O	0	0
			23	23		
18	K	23	Total	O	0	0
			23	23		
18	L	23	Total	O	0	0
			23	23		
18	M	27	Total	O	0	0
			27	27		
18	N	22	Total	O	0	0
			22	22		
18	O	12	Total	O	0	0
			12	12		
18	P	20	Total	O	0	0
			20	20		
18	Q	16	Total	O	0	0
			16	16		
18	R	19	Total	O	0	0
			19	19		

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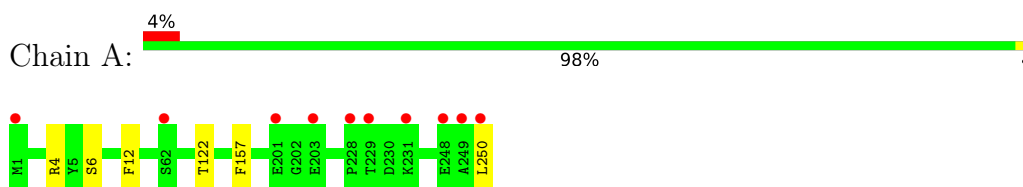
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>	<b>ZeroOcc</b>	<b>AltConf</b>
18	S	11	Total O 11 11	0	0
18	T	21	Total O 21 21	0	0
18	U	29	Total O 29 29	0	0
18	V	21	Total O 21 21	0	0
18	W	22	Total O 22 22	0	0
18	X	21	Total O 21 21	0	0
18	Y	31	Total O 31 31	0	0
18	Z	25	Total O 25 25	0	0
18	a	25	Total O 25 25	0	0
18	b	23	Total O 23 23	0	0

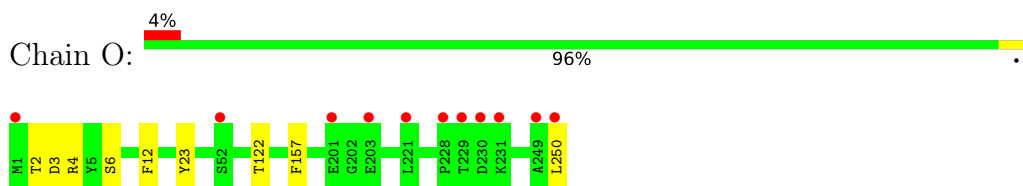
### 3 Residue-property plots [i](#)

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

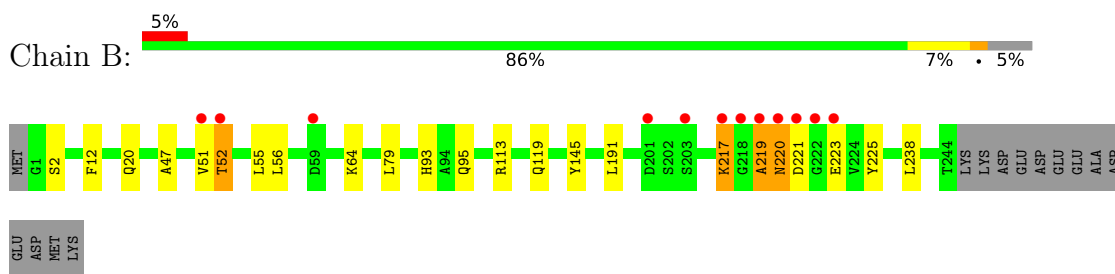
- Molecule 1: Proteasome subunit alpha type-2



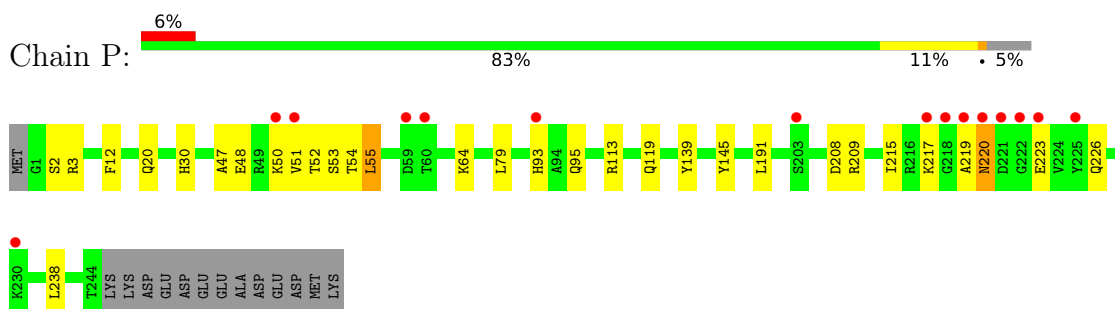
- Molecule 1: Proteasome subunit alpha type-2



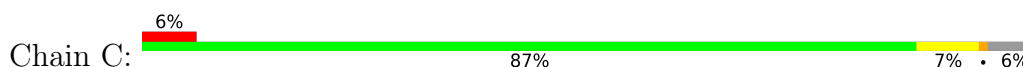
- Molecule 2: Proteasome subunit alpha type-3

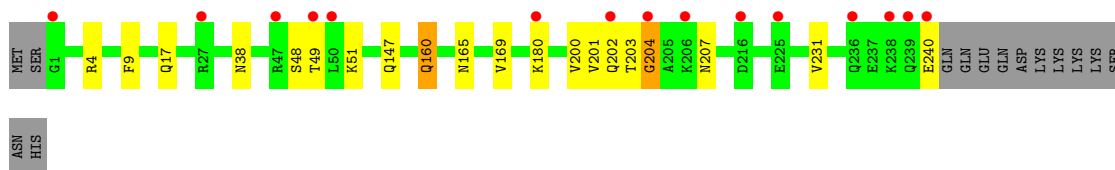


- Molecule 2: Proteasome subunit alpha type-3

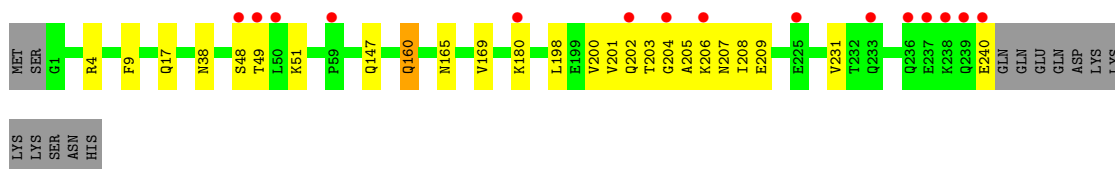
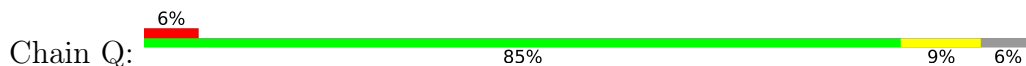


- Molecule 3: Proteasome subunit alpha type-4

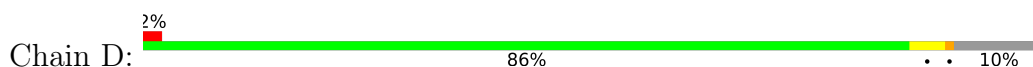




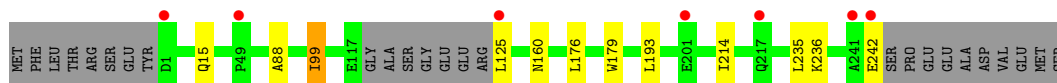
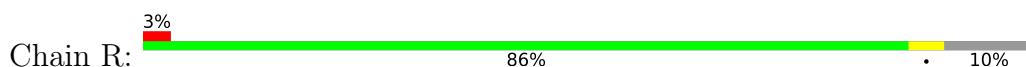
- Molecule 3: Proteasome subunit alpha type-4



- Molecule 4: Proteasome subunit alpha type-5



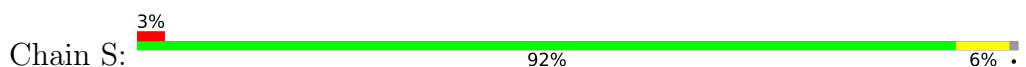
- Molecule 4: Proteasome subunit alpha type-5



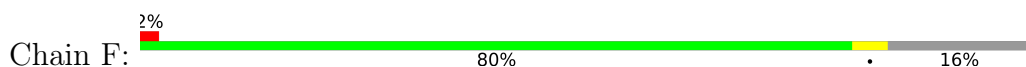
- Molecule 5: Proteasome subunit alpha type-6



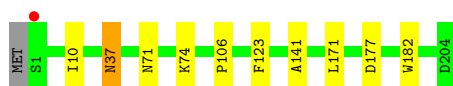
- Molecule 5: Proteasome subunit alpha type-6



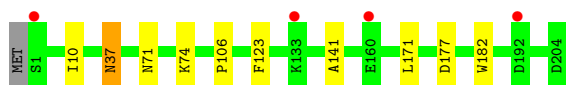
- Molecule 6: Probable proteasome subunit alpha type-7







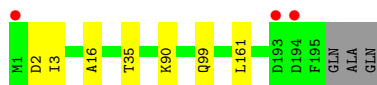
- Molecule 9: Proteasome subunit beta type-3



- Molecule 10: Proteasome subunit beta type-4



- Molecule 10: Proteasome subunit beta type-4



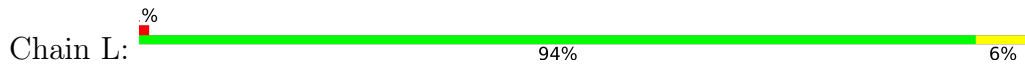
- Molecule 11: Proteasome subunit beta type-5



- Molecule 11: Proteasome subunit beta type-5



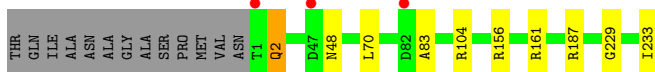
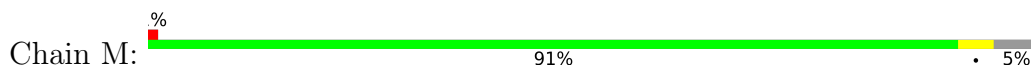
- Molecule 12: Proteasome subunit beta type-6



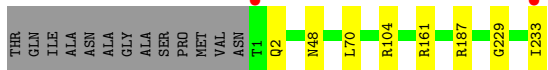
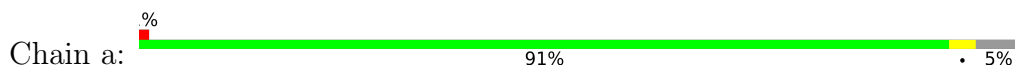
- Molecule 12: Proteasome subunit beta type-6



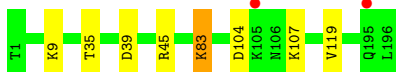
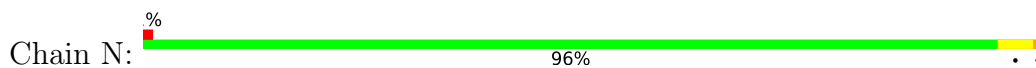
- Molecule 13: Proteasome subunit beta type-7



- 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, $\alpha$ , $\beta$ , $\gamma$	135.37Å 301.72Å 144.99Å 90.00° 113.12° 90.00°	Depositor
Resolution (Å)	15.00 – 2.70 15.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	96.5 (15.00-2.70) 97.1 (15.00-2.70)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.53 (at 2.69Å)	Xtrriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.177 , 0.209 0.182 , 0.213	Depositor DCC
$R_{free}$ test set	14073 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	55.9	Xtrriage
Anisotropy	0.385	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 37.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	49958	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	63.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.37% 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: CL, SO4, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.41	0/1952	0.57	0/2642
1	O	0.41	0/1952	0.58	0/2642
2	B	0.43	0/1934	0.66	2/2618 (0.1%)
2	P	0.45	0/1934	0.65	0/2618
3	C	0.39	0/1910	0.66	1/2586 (0.0%)
3	Q	0.40	0/1910	0.64	0/2586
4	D	0.37	0/1837	0.59	0/2475
4	R	0.37	0/1837	0.59	0/2475
5	E	0.37	0/1800	0.58	0/2433
5	S	0.40	0/1800	0.59	0/2433
6	F	0.37	0/1932	0.56	0/2609
6	T	0.37	0/1932	0.56	0/2609
7	G	0.37	0/1945	0.59	0/2634
7	U	0.37	0/1945	0.59	0/2634
8	H	0.41	0/1746	0.81	4/2365 (0.2%)
8	V	0.34	0/1718	0.83	4/2329 (0.2%)
9	I	0.41	0/1611	0.61	0/2174
9	W	0.43	0/1611	0.61	0/2174
10	J	0.37	0/1589	0.61	0/2142
10	X	0.37	0/1589	0.61	0/2142
11	K	0.36	0/1681	0.60	1/2274 (0.0%)
11	Y	0.35	0/1681	0.60	2/2274 (0.1%)
12	L	0.37	0/1795	0.59	0/2420
12	Z	0.37	0/1795	0.59	0/2420
13	M	0.38	0/1855	0.64	0/2514
13	a	0.47	0/1855	0.65	0/2514
14	N	0.35	0/1541	0.58	0/2087
14	b	0.35	0/1541	0.58	0/2087
All	All	0.39	0/50228	0.62	14/67910 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if



the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
8	H	0	1
8	V	0	1
All	All	0	2

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	V	188	ARG	NE-CZ-NH2	-21.14	109.73	120.30
8	H	188	ARG	NE-CZ-NH1	-19.04	110.78	120.30
8	V	188	ARG	NE-CZ-NH1	15.62	128.11	120.30
8	H	188	ARG	NE-CZ-NH2	15.48	128.04	120.30
8	V	188	ARG	CD-NE-CZ	9.70	137.18	123.60
8	H	188	ARG	CD-NE-CZ	8.74	135.84	123.60
2	B	217	LYS	N-CA-C	-7.26	91.39	111.00
2	B	219	ALA	N-CA-C	-6.86	92.47	111.00
3	C	204	GLY	N-CA-C	6.26	128.74	113.10
11	Y	4	LEU	CA-CB-CG	5.61	128.21	115.30
8	H	196	ARG	NE-CZ-NH1	5.58	123.09	120.30
11	K	4	LEU	CA-CB-CG	5.55	128.06	115.30
8	V	196	ARG	NE-CZ-NH1	5.35	122.98	120.30
11	Y	69	ARG	NE-CZ-NH1	5.17	122.89	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	H	188	ARG	Sidechain
8	V	188	ARG	Sidechain

## 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	6	0
1	O	1915	0	1929	10	0
2	B	1904	0	1904	25	0
2	P	1904	0	1904	25	0
3	C	1881	0	1895	12	0
3	Q	1881	0	1895	29	0
4	D	1813	0	1797	4	0
4	R	1813	0	1797	3	0
5	E	1773	0	1775	9	0
5	S	1773	0	1775	10	0
6	F	1892	0	1883	4	0
6	T	1892	0	1883	4	0
7	G	1907	0	1901	1	0
7	U	1907	0	1901	2	0
8	H	1716	0	1703	11	0
8	V	1688	0	1683	6	0
9	I	1581	0	1574	7	0
9	W	1581	0	1574	7	0
10	J	1561	0	1569	1	0
10	X	1561	0	1569	1	0
11	K	1644	0	1595	3	0
11	Y	1644	0	1595	2	0
12	L	1757	0	1711	7	0
12	Z	1757	0	1711	8	0
13	M	1824	0	1832	2	0
13	a	1824	0	1832	0	0
14	N	1512	0	1481	2	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	1	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	H	5	0	0	0	0
17	V	5	0	0	0	0
18	A	27	0	0	0	0
18	B	19	0	0	1	0
18	C	13	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	D	21	0	0	0	0
18	E	14	0	0	0	0
18	F	14	0	0	0	0
18	G	25	0	0	0	0
18	H	40	0	0	0	0
18	I	19	0	0	0	0
18	J	23	0	0	0	0
18	K	23	0	0	0	0
18	L	23	0	0	0	0
18	M	27	0	0	1	0
18	N	22	0	0	0	0
18	O	12	0	0	0	0
18	P	20	0	0	1	0
18	Q	16	0	0	0	0
18	R	19	0	0	0	0
18	S	11	0	0	0	0
18	T	21	0	0	0	0
18	U	29	0	0	0	0
18	V	21	0	0	0	0
18	W	22	0	0	0	0
18	X	21	0	0	0	0
18	Y	31	0	0	0	0
18	Z	25	0	0	0	0
18	a	25	0	0	0	0
18	b	23	0	0	0	0
All	All	49958	0	49078	165	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 (165) 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:219:ALA:HB3	2:B:223:GLU:HG3	1.23	1.09
2:B:225:TYR:CE2	8:H:225:GLU:HB2	1.95	1.02
2:B:219:ALA:CB	2:B:223:GLU:HG3	1.93	0.98
1:O:4:ARG:HH11	1:O:4:ARG:HG2	1.33	0.92
3:Q:203:THR:HG22	3:Q:204:GLY:H	1.37	0.89
3:Q:203:THR:HB	3:Q:207:ASN:ND2	1.89	0.87
8:H:113:ILE:HG13	8:H:119:THR:HG22	1.56	0.85
8:V:113:ILE:HG13	8:V:119:THR:HG22	1.55	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:219:ALA:HB3	2:B:223:GLU:CG	2.08	0.84
2:B:145:TYR:OH	2:B:217:LYS:N	2.11	0.81
8:H:224:GLN:NE2	8:H:224:GLN:HA	1.94	0.80
2:P:219:ALA:HB3	2:P:223:GLU:O	1.82	0.80
2:B:145:TYR:OH	2:B:217:LYS:HB2	1.82	0.79
8:H:224:GLN:HA	8:H:224:GLN:HE21	1.47	0.78
3:Q:198:LEU:HA	3:Q:201:VAL:HG12	1.66	0.77
2:P:145:TYR:OH	2:P:217:LYS:HB2	1.85	0.75
2:P:48:GLU:OE2	2:P:209:ARG:NH1	2.17	0.75
2:P:54:THR:HG23	2:P:55:LEU:HD13	1.67	0.75
3:Q:165:ASN:HB2	3:Q:200:VAL:HG11	1.69	0.75
1:O:4:ARG:HB3	2:P:2:SER:OG	1.87	0.74
3:C:48:SER:HB2	3:C:207:ASN:HD21	1.54	0.72
3:Q:203:THR:HG22	3:Q:204:GLY:N	2.04	0.72
3:Q:202:GLN:O	3:Q:203:THR:OG1	2.06	0.72
2:B:51:VAL:HG13	2:B:52:THR:N	2.06	0.71
3:Q:203:THR:HB	3:Q:207:ASN:HD21	1.55	0.70
8:H:222:ASP:OD1	9:I:74:LYS:NZ	2.26	0.68
1:A:4:ARG:HB3	2:B:2:SER:OG	1.94	0.67
2:B:95:GLN:HE22	9:I:71:ASN:HD22	1.40	0.67
2:P:145:TYR:OH	2:P:217:LYS:N	2.29	0.66
3:Q:201:VAL:HG13	3:Q:202:GLN:N	2.10	0.66
3:C:204:GLY:O	3:C:231:VAL:HG21	1.97	0.64
2:B:12:PHE:H	3:C:17:GLN:HE22	1.45	0.64
3:C:160:GLN:HE21	3:C:160:GLN:HA	1.61	0.64
2:P:3:ARG:NH1	5:S:122:TYR:OH	2.32	0.63
3:Q:160:GLN:HE21	3:Q:160:GLN:HA	1.64	0.63
2:P:95:GLN:HE22	9:W:71:ASN:HD22	1.45	0.63
3:Q:198:LEU:HA	3:Q:201:VAL:CG1	2.28	0.63
2:P:3:ARG:CZ	5:S:122:TYR:OH	2.47	0.63
2:P:93:HIS:HB3	18:P:301:HOH:O	1.99	0.62
2:B:93:HIS:HB3	18:B:301:HOH:O	1.98	0.62
2:B:145:TYR:OH	2:B:217:LYS:CB	2.47	0.62
1:O:4:ARG:HG2	1:O:4:ARG:NH1	2.01	0.62
3:Q:205:ALA:HB2	3:Q:231:VAL:HG21	1.82	0.62
12:Z:31:THR:HG23	12:Z:36:ASN:HD21	1.66	0.60
3:Q:204:GLY:O	3:Q:207:ASN:ND2	2.34	0.60
2:P:51:VAL:HG12	2:P:52:THR:N	2.15	0.60
12:L:31:THR:HG23	12:L:36:ASN:HD21	1.66	0.59
3:C:165:ASN:HB2	3:C:200:VAL:HG11	1.83	0.59
1:A:4:ARG:HD3	5:E:122:TYR:CD2	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:203:THR:CG2	3:Q:204:GLY:H	2.10	0.59
3:Q:198:LEU:HD23	3:Q:201:VAL:HG11	1.85	0.58
1:A:4:ARG:CB	2:B:2:SER:OG	2.53	0.57
3:Q:203:THR:CB	3:Q:207:ASN:HD21	2.18	0.57
5:E:92:ASN:HD21	12:L:70:ASN:HD21	1.51	0.56
7:G:23:PHE:O	7:G:26:THR:HB	2.05	0.56
7:U:23:PHE:O	7:U:26:THR:HB	2.05	0.56
2:B:145:TYR:HH	2:B:217:LYS:N	2.02	0.56
3:C:201:VAL:O	3:C:202:GLN:HB3	2.05	0.55
1:A:4:ARG:CD	5:E:122:TYR:CD2	2.89	0.55
5:E:12:PHE:H	6:F:19:GLN:HE22	1.52	0.55
6:F:123:ASN:C	6:F:123:ASN:HD22	2.10	0.55
5:S:12:PHE:H	6:T:19:GLN:HE22	1.54	0.55
2:B:51:VAL:HG13	2:B:52:THR:H	1.72	0.54
1:A:4:ARG:CD	5:E:122:TYR:HD2	2.19	0.54
3:Q:48:SER:HB2	3:Q:207:ASN:OD1	2.08	0.54
2:B:51:VAL:HG21	2:B:56:LEU:HD22	1.89	0.54
2:B:145:TYR:HH	2:B:217:LYS:HB2	1.73	0.54
3:Q:206:LYS:HD2	3:Q:206:LYS:H	1.73	0.54
3:C:201:VAL:HG13	3:C:202:GLN:N	2.23	0.53
6:T:123:ASN:HD22	6:T:124:SER:N	2.06	0.53
5:S:92:ASN:HD21	12:Z:70:ASN:HD21	1.57	0.53
13:M:2:GLN:NE2	18:M:301:HOH:O	2.40	0.53
6:T:123:ASN:HD22	6:T:123:ASN:C	2.12	0.53
2:B:225:TYR:HE2	8:H:225:GLU:HB2	1.68	0.53
3:C:202:GLN:O	3:C:202:GLN:HG2	2.09	0.53
2:P:30:HIS:O	2:P:50:LYS:HE3	2.09	0.53
3:Q:201:VAL:CG1	3:Q:202:GLN:N	2.73	0.52
2:B:220:ASN:N	2:B:220:ASN:OD1	2.41	0.52
3:C:48:SER:HB2	3:C:207:ASN:ND2	2.22	0.52
6:F:123:ASN:HD22	6:F:124:SER:N	2.08	0.52
2:P:139:TYR:CZ	2:P:217:LYS:HE3	2.45	0.52
3:Q:203:THR:CG2	3:Q:204:GLY:N	2.72	0.51
2:B:51:VAL:CG1	2:B:52:THR:N	2.73	0.51
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.92	0.51
1:O:2:THR:HG22	1:O:3:ASP:N	2.25	0.51
1:O:12:PHE:H	2:P:20:GLN:HE22	1.57	0.51
3:Q:208:ILE:HG22	3:Q:209:GLU:N	2.27	0.50
12:Z:31:THR:CG2	12:Z:36:ASN:HD21	2.24	0.50
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.93	0.50
2:B:95:GLN:NE2	9:I:71:ASN:HD22	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:4:ARG:HE	5:S:122:TYR:HE2	1.61	0.49
12:L:31:THR:CG2	12:L:36:ASN:HD21	2.24	0.49
2:P:51:VAL:CG1	2:P:52:THR:N	2.75	0.49
8:V:98:LEU:HD12	8:V:113:ILE:HG21	1.95	0.49
3:Q:203:THR:CG2	3:Q:207:ASN:HD21	2.26	0.49
5:E:92:ASN:ND2	12:L:70:ASN:HD21	2.10	0.48
2:P:12:PHE:H	3:Q:17:GLN:HE22	1.62	0.48
5:E:92:ASN:HD21	12:L:70:ASN:ND2	2.11	0.48
8:H:98:LEU:HD12	8:H:113:ILE:HG21	1.95	0.48
13:M:156:ARG:HH11	8:V:165:ASN:HD22	1.62	0.47
3:Q:165:ASN:CB	3:Q:200:VAL:HG11	2.42	0.47
2:P:139:TYR:OH	2:P:217:LYS:HE3	2.14	0.47
2:P:3:ARG:NH2	5:S:122:TYR:OH	2.47	0.47
8:V:35:HIS:NE2	8:V:53:GLU:HG2	2.30	0.47
9:I:37:ASN:C	9:I:37:ASN:HD22	2.19	0.47
3:C:201:VAL:HG13	3:C:203:THR:H	1.80	0.46
9:W:37:ASN:C	9:W:37:ASN:HD22	2.18	0.46
12:L:3:ASN:HD22	12:L:4:PRO:HD2	1.80	0.46
1:A:12:PHE:H	2:B:20:GLN:HE22	1.63	0.46
8:H:224:GLN:HE21	8:H:224:GLN:CA	2.23	0.46
2:P:95:GLN:NE2	9:W:71:ASN:HD22	2.12	0.46
3:Q:200:VAL:HG12	3:Q:200:VAL:O	2.16	0.46
3:Q:208:ILE:CG2	3:Q:209:GLU:N	2.79	0.46
9:I:106:PRO:HD2	9:I:123:PHE:HB2	1.97	0.46
2:P:208:ASP:N	2:P:208:ASP:OD1	2.49	0.46
12:Z:3:ASN:HD22	12:Z:4:PRO:HD2	1.81	0.45
5:S:87:LEU:HD21	5:S:107:ALA:HB1	1.98	0.45
8:H:84:LYS:HE2	8:H:119:THR:HG23	1.99	0.45
5:E:87:LEU:HD21	5:E:107:ALA:HB1	1.98	0.44
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.53	0.44
11:K:128:CYS:HB2	11:K:137:TYR:CE2	2.53	0.44
14:N:83:LYS:HG3	14:N:119:VAL:CG2	2.48	0.44
2:P:47:ALA:HB1	2:P:64:LYS:HD2	2.00	0.44
5:S:92:ASN:ND2	12:Z:70:ASN:HD21	2.16	0.44
8:V:222:ASP:OD1	9:W:74:LYS:NZ	2.40	0.44
12:Z:42:LYS:HD2	12:Z:55:ASN:HD22	1.83	0.44
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.53	0.43
2:P:139:TYR:OH	2:P:217:LYS:CE	2.66	0.43
9:W:106:PRO:HD2	9:W:123:PHE:HB2	1.99	0.43
11:K:128:CYS:HB2	11:K:137:TYR:CZ	2.54	0.43
2:P:52:THR:HG22	2:P:53:SER:H	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:10:ILE:HG21	9:W:141:ALA:HB3	2.01	0.43
2:B:219:ALA:HB3	2:B:223:GLU:O	2.19	0.43
2:P:220:ASN:ND2	2:P:220:ASN:C	2.72	0.43
4:D:176:LEU:HD22	5:E:55:LEU:CD2	2.49	0.42
5:S:92:ASN:HD21	12:Z:70:ASN:ND2	2.15	0.42
3:C:9:PHE:H	4:D:15:GLN:HE22	1.67	0.42
3:Q:9:PHE:H	4:R:15:GLN:HE22	1.67	0.42
8:H:219:ASN:ND2	8:H:219:ASN:C	2.73	0.42
8:V:84:LYS:HE2	8:V:119:THR:HG23	2.02	0.42
9:I:10:ILE:HG21	9:I:141:ALA:HB3	2.02	0.42
3:C:200:VAL:HG12	3:C:200:VAL:O	2.19	0.42
11:Y:128:CYS:HB2	11:Y:137:TYR:CZ	2.55	0.42
12:L:42:LYS:HD2	12:L:55:ASN:HD22	1.83	0.42
11:K:176:ASN:ND2	11:K:190:ASN:HD22	2.18	0.41
14:N:35:THR:HG21	14:N:45:ARG:HE	1.84	0.41
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.55	0.41
4:D:88:ALA:HA	4:D:99:ILE:HG21	2.01	0.41
3:Q:203:THR:CB	3:Q:207:ASN:ND2	2.72	0.41
4:R:88:ALA:HA	4:R:99:ILE:HG21	2.02	0.41
6:T:198:LEU:HD12	6:T:243:ILE:HG22	2.03	0.41
2:B:47:ALA:HB1	2:B:64:LYS:HD2	2.02	0.41
2:B:51:VAL:CG1	2:B:52:THR:H	2.33	0.41
2:P:215:ILE:HG12	2:P:226:GLN:HG2	2.02	0.41
9:I:141:ALA:HB2	9:I:177:ASP:HB2	2.02	0.41
1:O:4:ARG:CD	5:S:122:TYR:CD2	3.04	0.41
1:O:4:ARG:HH11	1:O:4:ARG:CG	2.13	0.41
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.21	0.41
3:Q:201:VAL:CG1	3:Q:202:GLN:H	2.34	0.41
6:F:198:LEU:HD12	6:F:243:ILE:HG22	2.03	0.40
9:W:141:ALA:HB2	9:W:177:ASP:HB2	2.03	0.40
11:Y:128:CYS:HB2	11:Y:137:TYR:CE2	2.55	0.40
8:H:104:ASP:HB2	8:H:105:PRO:HD2	2.04	0.40
1:O:2:THR:CG2	1:O:3:ASP:N	2.84	0.40
3:Q:201:VAL:HG13	3:Q:202:GLN:H	1.83	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%)	242 (98%)	6 (2%)	0	100	100
1	O	248/250 (99%)	242 (98%)	6 (2%)	0	100	100
2	B	242/258 (94%)	238 (98%)	4 (2%)	0	100	100
2	P	242/258 (94%)	238 (98%)	4 (2%)	0	100	100
3	C	238/254 (94%)	234 (98%)	4 (2%)	0	100	100
3	Q	238/254 (94%)	234 (98%)	4 (2%)	0	100	100
4	D	231/260 (89%)	227 (98%)	4 (2%)	0	100	100
4	R	231/260 (89%)	227 (98%)	4 (2%)	0	100	100
5	E	229/234 (98%)	220 (96%)	9 (4%)	0	100	100
5	S	229/234 (98%)	221 (96%)	8 (4%)	0	100	100
6	F	241/288 (84%)	239 (99%)	2 (1%)	0	100	100
6	T	241/288 (84%)	237 (98%)	4 (2%)	0	100	100
7	G	239/252 (95%)	238 (100%)	1 (0%)	0	100	100
7	U	239/252 (95%)	238 (100%)	1 (0%)	0	100	100
8	H	224/226 (99%)	218 (97%)	6 (3%)	0	100	100
8	V	221/226 (98%)	215 (97%)	6 (3%)	0	100	100
9	I	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
9	W	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
10	J	193/198 (98%)	189 (98%)	4 (2%)	0	100	100
10	X	193/198 (98%)	189 (98%)	4 (2%)	0	100	100
11	K	210/212 (99%)	205 (98%)	5 (2%)	0	100	100
11	Y	210/212 (99%)	205 (98%)	5 (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%)	224 (97%)	5 (2%)	2 (1%)	17	40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	a	231/246 (94%)	224 (97%)	6 (3%)	1 (0%)	34	60
14	N	194/196 (99%)	190 (98%)	4 (2%)	0	100	100
14	b	194/196 (99%)	189 (97%)	5 (3%)	0	100	100
All	All	6281/6602 (95%)	6145 (98%)	133 (2%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	a	229	GLY
13	M	83	ALA
13	M	229	GLY

### 5.3.2 Protein sidechains [i](#)

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%)	194 (96%)	9 (4%)	28	56
2	P	203/216 (94%)	196 (97%)	7 (3%)	37	66
3	C	212/226 (94%)	203 (96%)	9 (4%)	30	58
3	Q	212/226 (94%)	203 (96%)	9 (4%)	30	58
4	D	194/215 (90%)	186 (96%)	8 (4%)	30	59
4	R	194/215 (90%)	186 (96%)	8 (4%)	30	59
5	E	190/193 (98%)	180 (95%)	10 (5%)	22	48
5	S	190/193 (98%)	180 (95%)	10 (5%)	22	48
6	F	201/239 (84%)	192 (96%)	9 (4%)	27	55
6	T	201/239 (84%)	191 (95%)	10 (5%)	24	51
7	G	206/210 (98%)	198 (96%)	8 (4%)	32	61
7	U	206/210 (98%)	198 (96%)	8 (4%)	32	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	H	184/184 (100%)	176 (96%)	8 (4%)	29	57
8	V	181/184 (98%)	175 (97%)	6 (3%)	38	67
9	I	172/173 (99%)	169 (98%)	3 (2%)	60	84
9	W	172/173 (99%)	169 (98%)	3 (2%)	60	84
10	J	173/175 (99%)	168 (97%)	5 (3%)	42	71
10	X	173/175 (99%)	168 (97%)	5 (3%)	42	71
11	K	169/169 (100%)	162 (96%)	7 (4%)	30	59
11	Y	169/169 (100%)	162 (96%)	7 (4%)	30	59
12	L	185/185 (100%)	178 (96%)	7 (4%)	33	62
12	Z	185/185 (100%)	177 (96%)	8 (4%)	29	57
13	M	199/208 (96%)	192 (96%)	7 (4%)	36	65
13	a	199/208 (96%)	192 (96%)	7 (4%)	36	65
14	N	162/162 (100%)	157 (97%)	5 (3%)	40	69
14	b	162/162 (100%)	157 (97%)	5 (3%)	40	69
All	All	5315/5528 (96%)	5119 (96%)	196 (4%)	34	63

All (196) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	SER
1	A	122	THR
1	A	157	PHE
1	A	250	LEU
2	B	52	THR
2	B	55	LEU
2	B	79	LEU
2	B	113	ARG
2	B	119	GLN
2	B	191	LEU
2	B	220	ASN
2	B	221	ASP
2	B	238	LEU
3	C	4	ARG
3	C	38	ASN
3	C	49	THR
3	C	51	LYS
3	C	147	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	C	160	GLN
3	C	169	VAL
3	C	180	LYS
3	C	240	GLU
4	D	99	ILE
4	D	125	LEU
4	D	176	LEU
4	D	193	LEU
4	D	214	ILE
4	D	235	LEU
4	D	236	LYS
4	D	242	GLU
5	E	8	ASP
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	231	LYS
6	F	117	GLN
6	F	123	ASN
6	F	139	LYS
6	F	171	GLU
6	F	172	LEU
6	F	181	GLU
6	F	202	ASP
6	F	214	TRP
6	F	240	GLN
7	G	83	ASN
7	G	115	LEU
7	G	117	GLN
7	G	122	ARG
7	G	125	MET
7	G	208	GLU
7	G	235	ARG
7	G	236	LEU
8	H	9	GLN
8	H	68	LEU
8	H	113	ILE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
8	H	127	LEU
8	H	196	ARG
8	H	219	ASN
8	H	224	GLN
8	H	226	GLU
9	I	37	ASN
9	I	171	LEU
9	I	182	TRP
10	J	2	ASP
10	J	3	ILE
10	J	35	THR
10	J	90	LYS
10	J	99	GLN
11	K	4	LEU
11	K	9	GLN
11	K	104	TYR
11	K	107	LYS
11	K	116	ASP
11	K	140	LEU
11	K	148	LEU
12	L	18	GLU
12	L	23	LEU
12	L	49	ASN
12	L	108	HIS
12	L	130	SER
12	L	136	CYS
12	L	150	LEU
13	M	2	GLN
13	M	48	ASN
13	M	70	LEU
13	M	104	ARG
13	M	161	ARG
13	M	187	ARG
13	M	233	ILE
14	N	9	LYS
14	N	39	ASP
14	N	83	LYS
14	N	104	ASP
14	N	107	LYS
1	O	6	SER
1	O	122	THR
1	O	157	PHE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	O	250	LEU
2	P	55	LEU
2	P	79	LEU
2	P	113	ARG
2	P	119	GLN
2	P	191	LEU
2	P	220	ASN
2	P	238	LEU
3	Q	4	ARG
3	Q	38	ASN
3	Q	49	THR
3	Q	51	LYS
3	Q	147	GLN
3	Q	160	GLN
3	Q	169	VAL
3	Q	180	LYS
3	Q	240	GLU
4	R	99	ILE
4	R	125	LEU
4	R	176	LEU
4	R	193	LEU
4	R	214	ILE
4	R	235	LEU
4	R	236	LYS
4	R	242	GLU
5	S	8	ASP
5	S	9	THR
5	S	29	LYS
5	S	71	LEU
5	S	99	ASN
5	S	116	GLN
5	S	184	ASN
5	S	188	LEU
5	S	208	ASP
5	S	231	LYS
6	T	117	GLN
6	T	123	ASN
6	T	139	LYS
6	T	171	GLU
6	T	172	LEU
6	T	181	GLU
6	T	202	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
6	T	214	TRP
6	T	221	ASN
6	T	240	GLN
7	U	83	ASN
7	U	115	LEU
7	U	117	GLN
7	U	122	ARG
7	U	125	MET
7	U	208	GLU
7	U	235	ARG
7	U	236	LEU
8	V	9	GLN
8	V	53	GLU
8	V	68	LEU
8	V	113	ILE
8	V	188	ARG
8	V	196	ARG
9	W	37	ASN
9	W	171	LEU
9	W	182	TRP
10	X	2	ASP
10	X	3	ILE
10	X	35	THR
10	X	90	LYS
10	X	99	GLN
11	Y	4	LEU
11	Y	9	GLN
11	Y	104	TYR
11	Y	107	LYS
11	Y	116	ASP
11	Y	140	LEU
11	Y	148	LEU
12	Z	18	GLU
12	Z	23	LEU
12	Z	31	THR
12	Z	49	ASN
12	Z	108	HIS
12	Z	130	SER
12	Z	136	CYS
12	Z	150	LEU
13	a	2	GLN
13	a	48	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
13	a	70	LEU
13	a	104	ARG
13	a	161	ARG
13	a	187	ARG
13	a	233	ILE
14	b	9	LYS
14	b	39	ASP
14	b	83	LYS
14	b	104	ASP
14	b	107	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (121) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
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	116	GLN
3	C	120	GLN
3	C	147	GLN
3	C	160	GLN
3	C	207	ASN
4	D	15	GLN
4	D	100	ASN
4	D	160	ASN
4	D	225	ASN
5	E	68	HIS
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

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
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	ASN
8	H	165	ASN
8	H	172	ASN
8	H	224	GLN
9	I	37	ASN
10	J	55	GLN
11	K	85	ASN
11	K	176	ASN
12	L	3	ASN
12	L	49	ASN
12	L	55	ASN
12	L	70	ASN
12	L	80	ASN
12	L	158	ASN
13	M	18	ASN
13	M	48	ASN
13	M	102	GLN
13	M	179	ASN
13	M	194	ASN
13	M	213	GLN
14	N	161	GLN
2	P	20	GLN
2	P	58	GLN
2	P	95	GLN
2	P	119	GLN
2	P	123	GLN
2	P	155	ASN
2	P	176	GLN
2	P	220	ASN
3	Q	17	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	Q	38	ASN
3	Q	77	ASN
3	Q	116	GLN
3	Q	120	GLN
3	Q	147	GLN
3	Q	160	GLN
3	Q	207	ASN
4	R	15	GLN
4	R	91	HIS
4	R	100	ASN
4	R	160	ASN
4	R	225	ASN
5	S	68	HIS
5	S	99	ASN
5	S	116	GLN
5	S	118	ASN
5	S	120	GLN
5	S	151	ASN
5	S	184	ASN
6	T	19	GLN
6	T	86	ASN
6	T	117	GLN
6	T	123	ASN
6	T	191	GLN
6	T	240	GLN
7	U	30	ASN
7	U	83	ASN
7	U	114	ASN
7	U	117	GLN
7	U	121	GLN
7	U	166	GLN
7	U	167	GLN
7	U	175	ASN
8	V	165	ASN
8	V	172	ASN
9	W	37	ASN
10	X	55	GLN
10	X	86	GLN
11	Y	85	ASN
11	Y	176	ASN
12	Z	3	ASN
12	Z	49	ASN

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Mol	Chain	Res	Type
12	Z	55	ASN
12	Z	70	ASN
12	Z	80	ASN
12	Z	158	ASN
13	a	18	ASN
13	a	48	ASN
13	a	102	GLN
13	a	179	ASN
14	b	161	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
17	SO4	V	302	-	4,4,4	0.41	0	6,6,6	0.07	0
17	SO4	H	301	-	4,4,4	0.40	0	6,6,6	0.11	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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%)	-0.20	10 (4%) 38 37	46, 58, 85, 102	0
1	O	250/250 (100%)	-0.12	11 (4%) 34 33	51, 66, 96, 115	0
2	B	244/258 (94%)	-0.16	12 (4%) 29 28	47, 62, 90, 101	0
2	P	244/258 (94%)	-0.12	15 (6%) 21 20	51, 66, 94, 105	0
3	C	240/254 (94%)	-0.08	15 (6%) 20 19	46, 65, 104, 140	0
3	Q	240/254 (94%)	0.04	15 (6%) 20 19	52, 74, 122, 162	0
4	D	235/260 (90%)	-0.29	6 (2%) 56 57	51, 64, 86, 117	0
4	R	235/260 (90%)	-0.25	7 (2%) 50 51	53, 67, 89, 119	0
5	E	231/234 (98%)	-0.18	6 (2%) 56 57	54, 68, 93, 104	0
5	S	231/234 (98%)	-0.17	8 (3%) 44 44	56, 73, 102, 113	0
6	F	243/288 (84%)	-0.28	6 (2%) 57 59	44, 63, 95, 115	0
6	T	243/288 (84%)	-0.27	8 (3%) 46 46	47, 68, 104, 130	0
7	G	241/252 (95%)	-0.38	7 (2%) 51 52	45, 57, 80, 105	0
7	U	241/252 (95%)	-0.29	6 (2%) 57 59	50, 62, 83, 107	0
8	H	226/226 (100%)	-0.32	9 (3%) 38 37	47, 56, 81, 120	0
8	V	223/226 (98%)	-0.33	4 (1%) 68 70	49, 60, 82, 107	0
9	I	204/205 (99%)	-0.59	1 (0%) 91 92	43, 52, 69, 78	0
9	W	204/205 (99%)	-0.54	4 (1%) 65 67	45, 56, 73, 85	0
10	J	195/198 (98%)	-0.40	3 (1%) 73 76	45, 56, 71, 83	0
10	X	195/198 (98%)	-0.35	3 (1%) 73 76	49, 58, 71, 87	0
11	K	212/212 (100%)	-0.48	1 (0%) 91 92	45, 55, 70, 81	0
11	Y	212/212 (100%)	-0.49	0 100 100	47, 56, 71, 81	0
12	L	222/222 (100%)	-0.46	2 (0%) 84 85	47, 57, 78, 89	0
12	Z	222/222 (100%)	-0.41	2 (0%) 84 85	45, 57, 79, 88	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	M	233/246 (94%)	-0.51	3 (1%) 77 78	43, 55, 74, 85	0
13	a	233/246 (94%)	-0.49	2 (0%) 84 85	43, 54, 70, 81	0
14	N	196/196 (100%)	-0.57	2 (1%) 82 83	42, 51, 68, 80	0
14	b	196/196 (100%)	-0.49	2 (1%) 82 83	43, 53, 71, 82	0
All	All	6341/6602 (96%)	-0.32	170 (2%) 54 55	42, 60, 91, 162	0

All (170) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	228	PRO	8.9
3	Q	50	LEU	8.1
2	P	219	ALA	7.4
10	X	1	MET	6.1
2	P	221	ASP	6.1
2	B	221	ASP	6.0
2	B	219	ALA	5.9
1	A	229	THR	5.7
9	W	1	SER	5.4
10	J	1	MET	5.3
2	P	220	ASN	5.3
1	O	249	ALA	5.3
1	O	229	THR	5.2
1	O	228	PRO	5.2
3	Q	49	THR	5.1
8	H	226	GLU	5.1
8	V	223	ILE	4.7
2	B	217	LYS	4.6
8	V	222	ASP	4.6
3	Q	204	GLY	4.6
14	b	195	GLN	4.5
2	B	220	ASN	4.5
2	P	51	VAL	4.5
1	A	249	ALA	4.4
10	X	194	ASP	4.3
1	O	231	LYS	4.3
3	Q	238	LYS	4.2
6	F	181	GLU	4.2
4	R	241	ALA	4.0
3	Q	202	GLN	4.0
2	P	59	ASP	4.0
5	E	202	ASP	4.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
8	V	221	CYS	4.0
5	S	202	ASP	3.9
3	Q	237	GLU	3.9
1	O	1	MET	3.9
8	H	221	CYS	3.8
14	N	105	LYS	3.7
1	O	250	LEU	3.7
1	A	231	LYS	3.7
3	C	206	LYS	3.7
12	Z	174	TYR	3.7
10	J	194	ASP	3.6
3	C	50	LEU	3.6
14	N	195	GLN	3.5
7	U	2	GLY	3.5
8	H	222	ASP	3.5
3	Q	240	GLU	3.5
6	F	205	GLU	3.5
3	C	202	GLN	3.5
7	U	242	GLN	3.5
12	L	174	TYR	3.4
3	Q	239	GLN	3.4
1	O	201	GLU	3.4
2	B	222	GLY	3.4
6	T	181	GLU	3.4
2	B	59	ASP	3.4
3	C	236	GLN	3.3
5	S	201	ARG	3.3
7	G	188	GLU	3.3
8	H	223	ILE	3.2
3	C	49	THR	3.2
3	C	238	LYS	3.2
4	R	201	GLU	3.2
2	B	218	GLY	3.2
3	C	239	GLN	3.2
6	T	244	ASN	3.1
3	Q	236	GLN	3.1
13	a	1	THR	3.1
6	F	244	ASN	3.1
8	H	224	GLN	3.0
13	a	233	ILE	3.0
4	D	242	GLU	3.0
6	T	243	ILE	3.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
8	H	225	GLU	3.0
1	A	248	GLU	3.0
9	W	192	ASP	3.0
9	I	1	SER	3.0
14	b	105	LYS	2.9
2	B	51	VAL	2.9
5	E	233	ILE	2.9
4	R	217	GLN	2.9
2	P	223	GLU	2.9
6	T	180	PRO	2.9
10	X	193	ASP	2.9
4	R	242	GLU	2.9
2	P	222	GLY	2.8
10	J	193	ASP	2.8
11	K	212	GLY	2.8
2	P	230	LYS	2.8
6	T	230	ASP	2.8
1	A	250	LEU	2.8
8	H	198	GLU	2.7
1	O	221	LEU	2.7
3	C	1	GLY	2.7
3	Q	180	LYS	2.7
1	A	201	GLU	2.7
7	U	222	ASP	2.7
3	C	204	GLY	2.6
7	G	241	GLU	2.6
3	C	180	LYS	2.6
1	A	1	MET	2.6
5	E	201	ARG	2.6
3	C	240	GLU	2.6
1	O	52	SER	2.6
2	B	201	ASP	2.5
4	R	125	LEU	2.5
7	U	188	GLU	2.5
13	M	47	ASP	2.5
5	S	54	GLU	2.5
2	B	203	SER	2.5
7	G	242	GLN	2.5
2	P	60	THR	2.5
2	P	50	LYS	2.5
4	D	241	ALA	2.5
13	M	1	THR	2.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
6	T	58	GLN	2.4
6	F	202	ASP	2.4
3	Q	48	SER	2.4
3	C	216	ASP	2.4
1	O	203	GLU	2.4
9	W	160	GLU	2.4
3	Q	233	GLN	2.4
5	E	54	GLU	2.4
4	R	1	ASP	2.3
1	A	203	GLU	2.3
3	C	225	GLU	2.3
5	E	218	ASP	2.3
5	E	173	ARG	2.3
7	G	240	ALA	2.3
4	D	238	LYS	2.3
7	G	222	ASP	2.3
4	D	2	ARG	2.3
2	B	223	GLU	2.3
3	Q	225	GLU	2.3
1	O	230	ASP	2.3
5	S	225	ASP	2.3
4	D	217	GLN	2.2
7	U	230	GLU	2.2
5	S	203	GLU	2.2
6	T	201	GLU	2.2
7	G	179	LYS	2.2
5	S	165	GLN	2.2
5	S	180	LYS	2.2
2	P	217	LYS	2.2
2	P	218	GLY	2.2
5	S	218	ASP	2.2
13	M	82	ASP	2.2
7	G	68	ARG	2.2
3	Q	206	LYS	2.2
12	Z	173	LYS	2.2
12	L	166	GLY	2.2
2	P	203	SER	2.1
7	U	241	GLU	2.1
8	V	145	ASP	2.1
2	B	52	THR	2.1
6	F	204	LYS	2.1
3	C	27	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
3	C	47	ARG	2.1
8	H	10	ASP	2.1
6	T	207	ASP	2.1
9	W	133	LYS	2.1
2	P	225	TYR	2.1
8	H	22	ASN	2.1
6	F	241	LYS	2.0
4	R	49	PRO	2.0
1	A	62	SER	2.0
2	P	93	HIS	2.0
3	Q	59	PRO	2.0
4	D	224	ASP	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 monosaccharides 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
15	MG	G	301	1/1	0.97	0.07	43,43,43,43	0
15	MG	Z	301	1/1	0.97	0.31	57,57,57,57	0
15	MG	K	301	1/1	0.98	0.08	63,63,63,63	0
15	MG	I	301	1/1	0.98	0.22	62,62,62,62	0
17	SO4	V	302	5/5	0.98	0.20	54,57,58,62	0
15	MG	W	301	1/1	0.99	0.34	71,71,71,71	0
15	MG	Y	301	1/1	0.99	0.08	64,64,64,64	0
15	MG	N	201	1/1	0.99	0.07	39,39,39,39	0
16	CL	U	301	1/1	0.99	0.13	55,55,55,55	0
17	SO4	H	301	5/5	0.99	0.18	55,58,59,65	0
15	MG	V	301	1/1	0.99	0.14	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
16	CL	G	302	1/1	1.00	0.05	48,48,48,48	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.