



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 16, 2018 – 10:07 PM EDT

PDB ID : 5D0S  
Title : Yeast 20S proteasome beta5-D166N mutant in complex with Carfilzomib  
Authors : Huber, E.M.; Groll, M.  
Deposited on : 2015-08-03  
Resolution : 2.50 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 : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : rb-20031633  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20031633

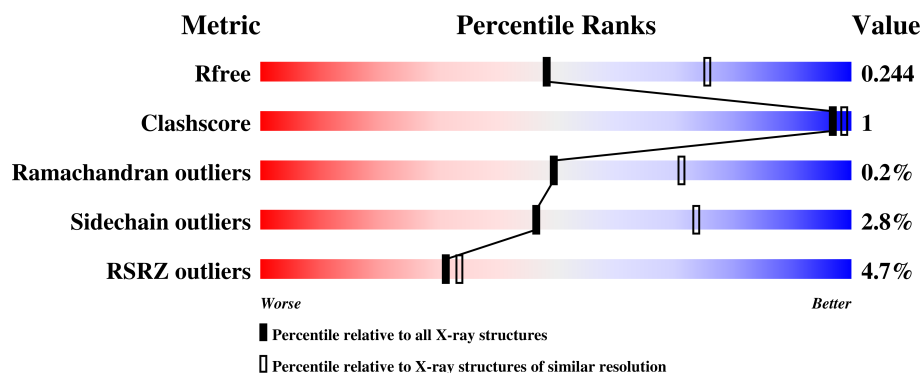
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
$R_{free}$	111664	4155 (2.50-2.50)
Clashscore	122126	4827 (2.50-2.50)
Ramachandran outliers	120053	4735 (2.50-2.50)
Sidechain outliers	120020	4737 (2.50-2.50)
RSRZ outliers	108989	4058 (2.50-2.50)

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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	250	<div> <div>5%</div> <div>98%</div> <div>.</div> </div>
1	O	250	<div> <div>6%</div> <div>98%</div> <div>.</div> </div>
2	B	258	<div> <div>8%</div> <div>90%</div> <div>.. 5%</div> </div>
2	P	258	<div> <div>8%</div> <div>91%</div> <div>.. 5%</div> </div>
3	C	254	<div> <div>12%</div> <div>90%</div> <div>.. 6%</div> </div>

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	Q	254	
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 19 unique types of molecules in this entry. The entry contains 50766 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
			1906	1214	320	364	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	222	Total	C	N	O	S	0	0	0
			1684	1061	293	323	7			
8	V	222	Total	C	N	O	S	0	0	0
			1684	1061	293	323	7			

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

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

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

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

*Continued on next page...*

*Continued from previous page...*

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	212	Total	C	N	O	S	0	0	0
			1644	1045	281	311	7			
11	Y	212	Total	C	N	O	S	0	0	0
			1644	1045	281	311	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	168	ASN	ASP	engineered mutation	UNP P30656
Y	168	ASN	ASP	engineered mutation	UNP P30656

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

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

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

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

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

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

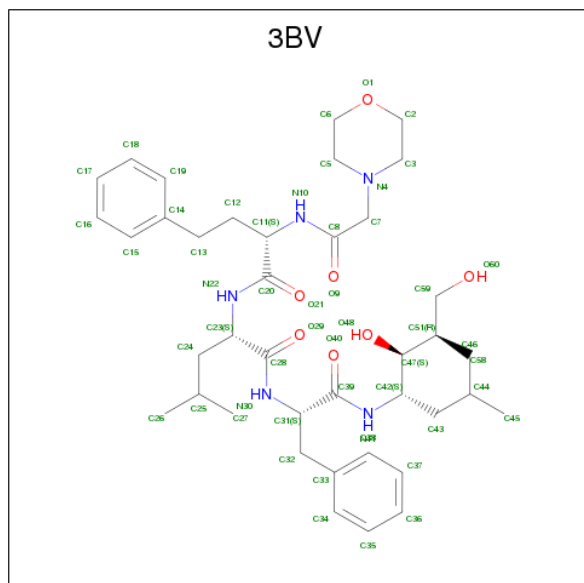
- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

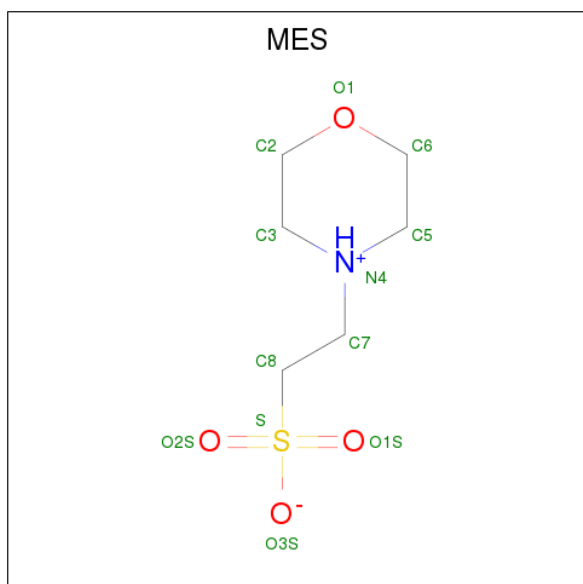
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	G	1	Total Cl 1 1	0	0
16	b	1	Total Cl 1 1	0	0
16	N	1	Total Cl 1 1	0	0
16	U	1	Total Cl 1 1	0	0

- Molecule 17 is N-{(2S)-2-[(morpholin-4-ylacetyl)amino]-4-phenylbutanoyl}-L-leucyl-N-[(2R,3S,4S)-1,3-dihydroxy-2,6-dimethylheptan-4-yl]-L-phenylalaninamide (three-letter code: 3BV) (formula: C<sub>40</sub>H<sub>61</sub>N<sub>5</sub>O<sub>7</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	H	1	Total	C	N	O	0	0
			52	40	5	7		
17	K	1	Total	C	N	O	0	0
			52	40	5	7		
17	N	1	Total	C	N	O	0	0
			52	40	5	7		
17	V	1	Total	C	N	O	0	0
			52	40	5	7		
17	Y	1	Total	C	N	O	0	0
			52	40	5	7		
17	b	1	Total	C	N	O	0	0
			52	40	5	7		

- Molecule 18 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
18	H	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
18	K	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
18	V	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
18	Y	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 19 is water.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	A	52	Total O 52 52	0	0
19	B	31	Total O 31 31	0	0
19	C	38	Total O 38 38	0	0
19	D	31	Total O 31 31	0	0
19	E	27	Total O 27 27	0	0
19	F	38	Total O 38 38	0	0
19	G	47	Total O 47 47	0	0
19	H	57	Total O 57 57	0	0
19	I	49	Total O 49 49	0	0
19	J	52	Total O 52 52	0	0
19	K	54	Total O 54 54	0	0
19	L	54	Total O 54 54	0	0
19	M	48	Total O 48 48	0	0
19	N	43	Total O 43 43	0	0
19	O	27	Total O 27 27	0	0
19	P	29	Total O 29 29	0	0
19	Q	15	Total O 15 15	0	0
19	R	18	Total O 18 18	0	0
19	S	11	Total O 11 11	0	0
19	T	28	Total O 28 28	0	0
19	U	44	Total O 44 44	0	0
19	V	42	Total O 42 42	0	0

*Continued on next page...*

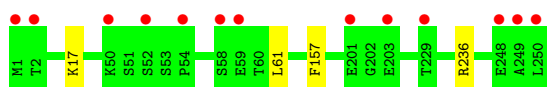
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	W	35	Total 35	O 35	0	0
19	X	47	Total 47	O 47	0	0
19	Y	35	Total 35	O 35	0	0
19	Z	47	Total 47	O 47	0	0
19	a	64	Total 64	O 64	0	0
19	b	37	Total 37	O 37	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.

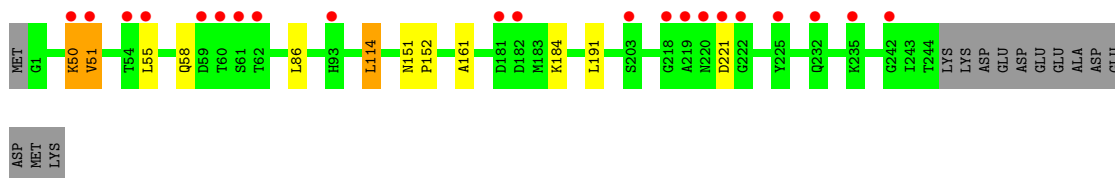
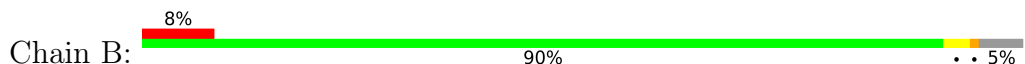
- Molecule 1: Proteasome subunit alpha type-2



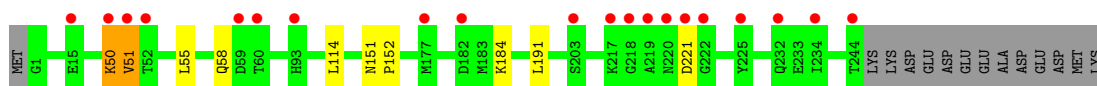
- Molecule 1: Proteasome subunit alpha type-2



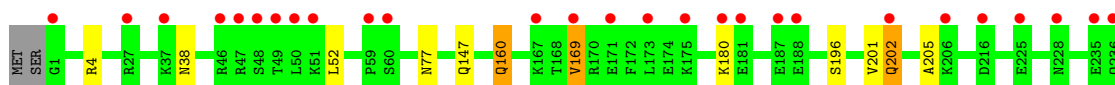
- Molecule 2: Proteasome subunit alpha type-3

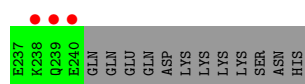


- Molecule 2: Proteasome subunit alpha type-3

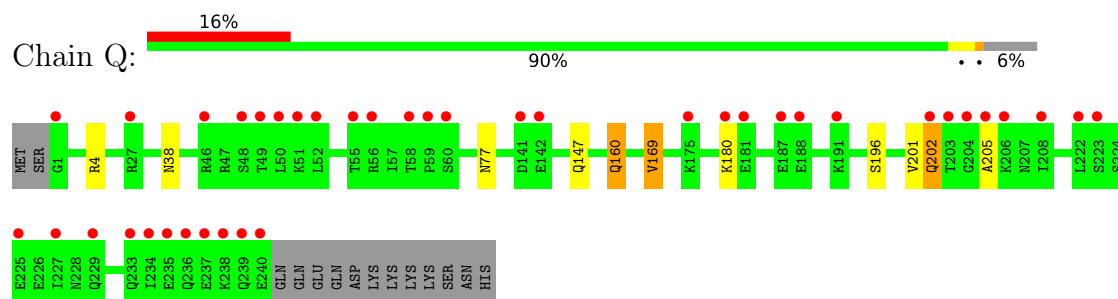


- Molecule 3: Proteasome subunit alpha type-4

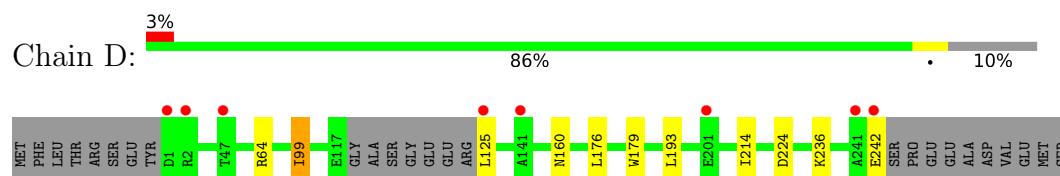




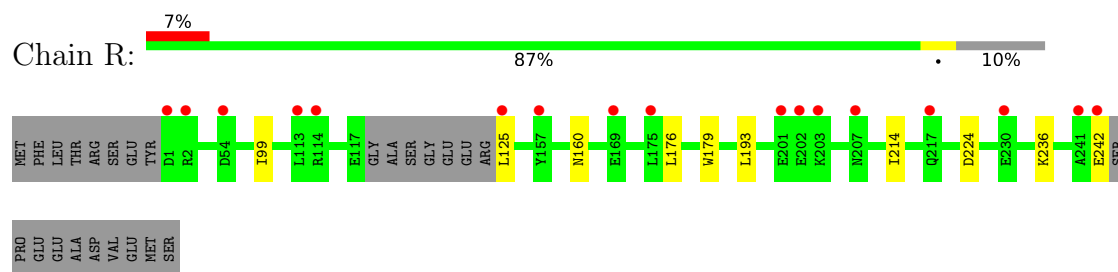
• Molecule 3: Proteasome subunit alpha type-4



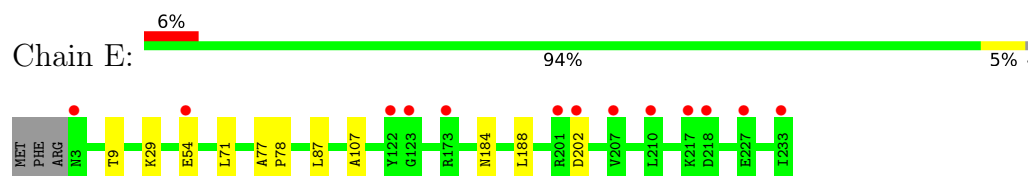
• Molecule 4: Proteasome subunit alpha type-5



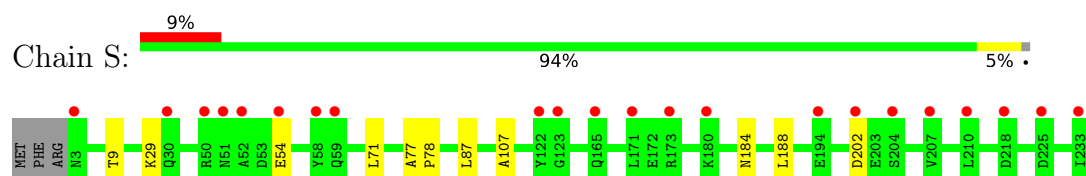
• Molecule 4: Proteasome subunit alpha type-5



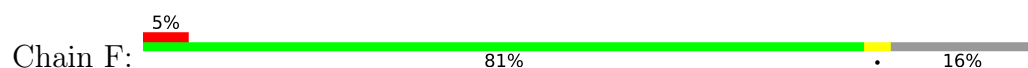
• Molecule 5: Proteasome subunit alpha type-6

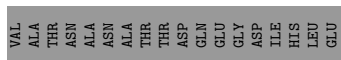


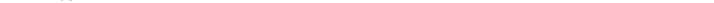
• Molecule 5: Proteasome subunit alpha type-6

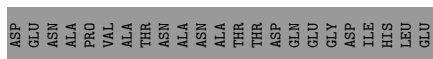


• Molecule 6: Probable proteasome subunit alpha type-7

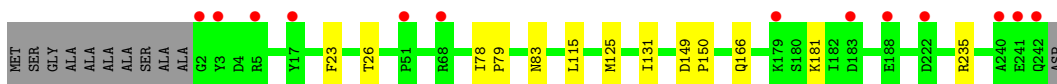


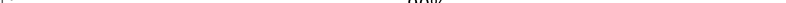


- Chain T:  4% 80% 16%

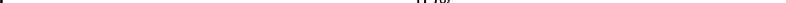


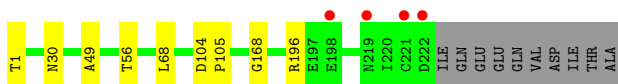
- Chain G:  5% 90% 5%



- Chain U:  4% 90% 5%



- Chain H:  2% 92%



- Chain V:  93% 2% . .



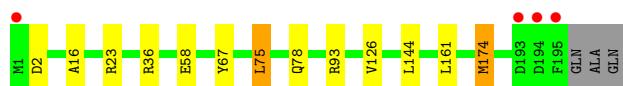
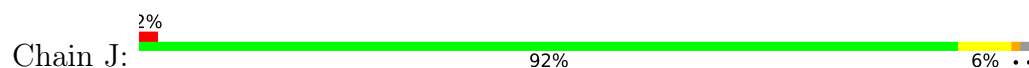
- Chain I:  95% 5%



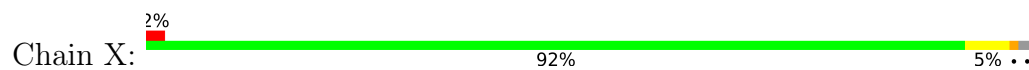
- Molecule 9: Proteasome subunit beta type-3



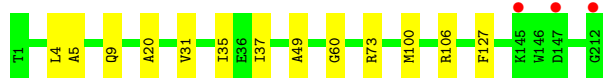
- Molecule 10: Proteasome subunit beta type-4



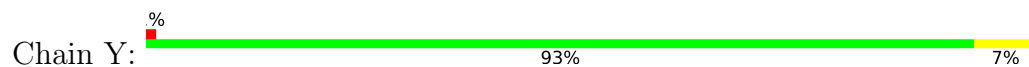
- Molecule 10: Proteasome subunit beta type-4



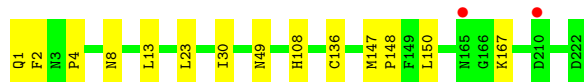
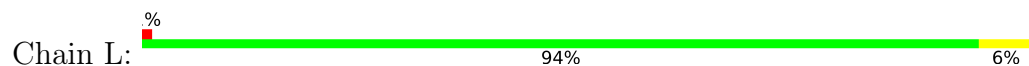
- Molecule 11: Proteasome subunit beta type-5



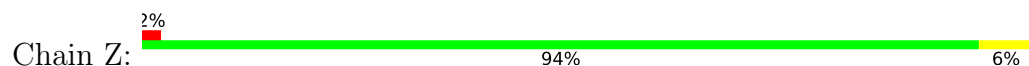
- Molecule 11: Proteasome subunit beta type-5



- Molecule 12: Proteasome subunit beta type-6

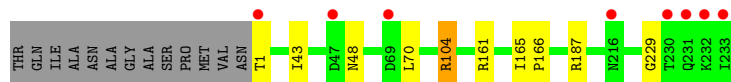
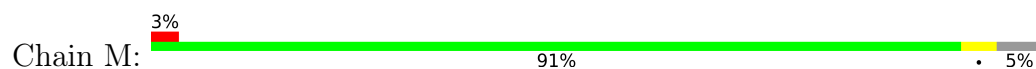


- Molecule 12: Proteasome subunit beta type-6

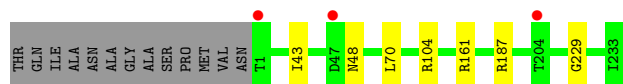
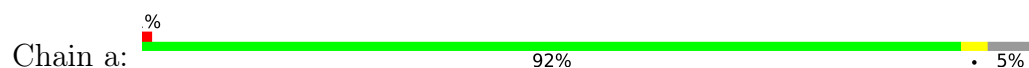




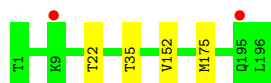
- Molecule 13: Proteasome subunit beta type-7



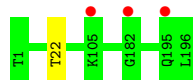
- Molecule 13: Proteasome subunit beta type-7



- 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, $\alpha$ , $\beta$ , $\gamma$	135.02Å 300.64Å 144.31Å 90.00° 113.02° 90.00°	Depositor
Resolution (Å)	15.00 – 2.50 15.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	96.4 (15.00-2.50) 96.4 (15.00-2.50)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.27 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.216 , 0.237 0.224 , 0.244	Depositor DCC
$R_{free}$ test set	17448 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	43.2	Xtriage
Anisotropy	0.088	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 37.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	50766	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.35% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 3BV, 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	0.27	0/1952	0.46	0/2642
1	O	0.27	0/1952	0.46	0/2642
2	B	0.27	0/1934	0.48	0/2618
2	P	0.26	0/1934	0.48	0/2618
3	C	0.27	0/1910	0.50	0/2586
3	Q	0.27	0/1910	0.49	0/2586
4	D	0.26	0/1837	0.46	0/2475
4	R	0.26	0/1837	0.46	0/2475
5	E	0.26	0/1800	0.46	0/2433
5	S	0.26	0/1800	0.46	0/2433
6	F	0.27	0/1932	0.45	0/2609
6	T	0.27	0/1932	0.45	0/2609
7	G	0.27	0/1945	0.47	0/2634
7	U	0.27	0/1944	0.46	0/2632
8	H	0.28	0/1715	0.47	1/2326 (0.0%)
8	V	0.28	0/1715	0.47	0/2326
9	I	0.27	0/1611	0.48	0/2174
9	W	0.27	0/1611	0.48	0/2174
10	J	0.26	0/1589	0.48	0/2142
10	X	0.26	0/1589	0.48	0/2142
11	K	0.33	0/1681	0.50	0/2274
11	Y	0.30	0/1681	0.49	0/2274
12	L	0.27	0/1795	0.47	0/2420
12	Z	0.27	0/1795	0.47	0/2420
13	M	0.27	0/1855	0.50	0/2514
13	a	0.27	0/1855	0.51	0/2514
14	N	0.27	0/1541	0.47	0/2087
14	b	0.27	0/1541	0.48	0/2087
All	All	0.27	0/50193	0.47	1/67866 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	1	THR	N-CA-C	5.50	125.85	111.00

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	1	0
1	O	1915	0	1929	1	0
2	B	1904	0	1904	4	0
2	P	1904	0	1904	2	0
3	C	1881	0	1895	5	0
3	Q	1881	0	1895	4	0
4	D	1813	0	1797	3	0
4	R	1813	0	1797	1	0
5	E	1773	0	1775	2	0
5	S	1773	0	1775	2	0
6	F	1892	0	1883	2	0
6	T	1892	0	1883	3	0
7	G	1907	0	1901	4	0
7	U	1906	0	1901	4	0
8	H	1684	0	1685	3	0
8	V	1684	0	1685	2	0
9	I	1581	0	1574	4	0
9	W	1581	0	1574	4	0
10	J	1561	0	1569	6	0
10	X	1561	0	1569	5	0
11	K	1644	0	1594	7	0
11	Y	1644	0	1594	8	0
12	L	1757	0	1711	8	0
12	Z	1757	0	1711	5	0
13	M	1824	0	1832	3	0
13	a	1824	0	1832	0	0
14	N	1512	0	1478	2	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	b	1512	0	1478	0	0
15	G	1	0	0	0	0
15	I	2	0	0	0	0
15	K	1	0	0	0	0
15	L	1	0	0	0	0
15	N	1	0	0	0	0
15	Z	1	0	0	0	0
16	G	1	0	0	0	0
16	N	1	0	0	0	0
16	U	1	0	0	0	0
16	b	1	0	0	0	0
17	H	52	0	59	2	0
17	K	52	0	58	4	0
17	N	52	0	58	1	0
17	V	52	0	58	4	0
17	Y	52	0	58	2	0
17	b	52	0	58	0	0
18	H	12	0	13	0	0
18	K	12	0	13	1	0
18	V	12	0	13	1	0
18	Y	12	0	13	0	0
19	A	52	0	0	1	0
19	B	31	0	0	0	0
19	C	38	0	0	0	0
19	D	31	0	0	2	0
19	E	27	0	0	0	0
19	F	38	0	0	1	0
19	G	47	0	0	0	0
19	H	57	0	0	0	0
19	I	49	0	0	0	0
19	J	52	0	0	1	0
19	K	54	0	0	0	0
19	L	54	0	0	2	0
19	M	48	0	0	0	0
19	N	43	0	0	1	0
19	O	27	0	0	0	0
19	P	29	0	0	0	0
19	Q	15	0	0	0	0
19	R	18	0	0	0	0
19	S	11	0	0	0	0
19	T	28	0	0	2	0
19	U	44	0	0	1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	V	42	0	0	0	0
19	W	35	0	0	0	0
19	X	47	0	0	1	0
19	Y	35	0	0	0	0
19	Z	47	0	0	0	0
19	a	64	0	0	0	0
19	b	37	0	0	0	0
All	All	50766	0	49455	95	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 1.

All (95) 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)
11:Y:5:ALA:HB3	11:Y:100:MET:HE2	1.68	0.76
11:K:5:ALA:HB3	11:K:100:MET:HE2	1.69	0.75
6:T:19:GLN:NE2	19:T:301:HOH:O	2.23	0.72
14:N:35:THR:HG22	19:N:305:HOH:O	1.90	0.72
17:K:301:3BV:H16	12:L:108:HIS:NE2	2.10	0.67
12:Z:13:LEU:HD13	12:Z:150:LEU:HD21	1.77	0.66
12:L:13:LEU:HD13	12:L:150:LEU:HD21	1.78	0.65
17:N:201:3BV:H1	17:N:201:3BV:O9	1.98	0.63
17:K:301:3BV:H60	18:K:303:MES:O1S	2.05	0.56
6:F:215:CYS:HB3	19:F:304:HOH:O	2.06	0.56
8:H:49:ALA:HA	17:H:301:3BV:H50	1.88	0.56
10:J:67:TYR:CE1	10:J:75:LEU:HD13	2.44	0.52
10:X:67:TYR:CE1	10:X:75:LEU:HD13	2.44	0.52
11:K:5:ALA:HB3	11:K:100:MET:CE	2.40	0.52
17:K:301:3BV:H16	12:L:108:HIS:CE1	2.44	0.52
3:C:201:VAL:O	3:C:202:GLN:CB	2.58	0.51
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.91	0.51
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.59	0.51
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.91	0.51
11:Y:170:TYR:O	17:Y:301:3BV:H57	2.10	0.51
11:Y:5:ALA:HB3	11:Y:100:MET:CE	2.39	0.51
11:K:49:ALA:HA	17:K:301:3BV:H50	1.92	0.51
3:C:169:VAL:HG23	3:C:196:SER:HB2	1.94	0.50
14:N:152:VAL:HA	14:N:175:MET:HE1	1.92	0.50
11:Y:100:MET:HE3	11:Y:127:PHE:HB2	1.93	0.50
17:V:301:3BV:O60	18:V:302:MES:O1S	2.29	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:23:PHE:O	7:G:26:THR:HB	2.12	0.50
3:Q:169:VAL:HG23	3:Q:196:SER:HB2	1.94	0.50
4:D:99:ILE:HG23	19:D:321:HOH:O	2.12	0.49
11:K:100:MET:HE3	11:K:127:PHE:HB2	1.93	0.49
7:U:23:PHE:O	7:U:26:THR:HB	2.12	0.49
11:Y:49:ALA:HA	17:Y:301:3BV:H50	1.95	0.48
12:L:2:PHE:N	19:L:402:HOH:O	2.47	0.48
5:S:87:LEU:HD21	5:S:107:ALA:HB1	1.96	0.47
1:A:236:ARG:NH2	19:A:302:HOH:O	2.48	0.47
5:E:87:LEU:HD21	5:E:107:ALA:HB1	1.97	0.46
8:H:104:ASP:HB2	8:H:105:PRO:HD2	1.96	0.46
11:K:37:ILE:HG23	11:K:60:GLY:HA2	1.98	0.46
17:V:301:3BV:O9	17:V:301:3BV:H16	2.15	0.45
6:T:172:LEU:CD1	6:T:195:ILE:HD13	2.46	0.45
6:F:172:LEU:CD1	6:F:195:ILE:HD13	2.46	0.45
10:J:36:ARG:NH1	10:J:58:GLU:OE2	2.48	0.45
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.99	0.45
10:X:36:ARG:NH1	10:X:58:GLU:OE2	2.50	0.45
19:L:402:HOH:O	13:M:1:THR:HG23	2.16	0.45
3:Q:160:GLN:HA	3:Q:160:GLN:HE21	1.81	0.45
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.52	0.44
8:V:104:ASP:HB2	8:V:105:PRO:HD2	1.97	0.44
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.99	0.44
11:Y:37:ILE:HG23	11:Y:60:GLY:HA2	1.98	0.44
10:J:174:MET:HA	10:X:174:MET:HA	1.98	0.44
9:I:20:VAL:HG13	9:I:118:PRO:HB3	2.00	0.44
13:M:165:ILE:HB	13:M:166:PRO:HD3	2.00	0.44
3:C:201:VAL:HG13	3:C:202:GLN:N	2.33	0.43
9:W:20:VAL:HG13	9:W:118:PRO:HB3	2.00	0.43
3:C:160:GLN:HA	3:C:160:GLN:HE21	1.82	0.43
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.53	0.43
7:G:78:ILE:N	7:G:79:PRO:CD	2.82	0.43
12:L:13:LEU:CD1	12:L:150:LEU:HD21	2.48	0.43
3:Q:201:VAL:HG13	3:Q:202:GLN:N	2.33	0.43
12:L:4:PRO:O	13:M:104:ARG:NH1	2.46	0.43
12:L:8:ASN:HA	12:L:30:ILE:O	2.19	0.43
9:I:9:GLY:HA3	9:I:41:LYS:HE2	2.02	0.42
1:O:57:MET:HE1	19:U:407:HOH:O	2.19	0.42
7:U:78:ILE:N	7:U:79:PRO:CD	2.82	0.42
9:W:9:GLY:HA3	9:W:41:LYS:HE2	2.02	0.42
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.19	0.42

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:8:ASN:HB2	19:T:301:HOH:O	2.18	0.42
9:I:36:SER:HB2	10:J:126:VAL:HG11	2.01	0.42
2:P:50:LYS:O	2:P:51:VAL:C	2.58	0.42
2:B:161:ALA:HB3	3:C:52:LEU:HD23	2.02	0.41
7:G:149:ASP:HB2	7:G:150:PRO:CD	2.51	0.41
2:B:50:LYS:O	2:B:51:VAL:C	2.59	0.41
7:U:26:THR:HG21	7:U:131:ILE:HD12	2.02	0.41
12:Z:147:MET:N	12:Z:148:PRO:HD2	2.35	0.41
2:B:86:LEU:HB3	2:B:114:LEU:HD21	2.03	0.41
4:D:64:ARG:HG3	19:D:315:HOH:O	2.20	0.41
10:J:93:ARG:NH1	19:J:202:HOH:O	2.53	0.41
11:Y:20:ALA:HB2	11:Y:31:VAL:HG21	2.03	0.41
17:V:301:3BV:H17	9:W:125:LEU:HD22	2.03	0.41
10:X:55:GLN:NE2	19:X:202:HOH:O	2.52	0.41
8:H:168:GLY:O	17:H:301:3BV:H57	2.21	0.41
11:K:20:ALA:HB2	11:K:31:VAL:HG21	2.02	0.41
12:Z:125:PHE:CD2	12:Z:131:TYR:HB3	2.56	0.41
12:Z:13:LEU:CD1	12:Z:150:LEU:HD21	2.48	0.41
2:P:151:ASN:HB2	2:P:152:PRO:CD	2.51	0.41
7:U:149:ASP:HB2	7:U:150:PRO:CD	2.51	0.41
5:S:77:ALA:N	5:S:78:PRO:CD	2.84	0.41
2:B:151:ASN:HB2	2:B:152:PRO:CD	2.50	0.41
5:E:77:ALA:N	5:E:78:PRO:CD	2.84	0.40
7:G:26:THR:HG21	7:G:131:ILE:HD12	2.02	0.40
12:L:147:MET:N	12:L:148:PRO:HD2	2.36	0.40
11:Y:100:MET:CE	11:Y:127:PHE:HB2	2.52	0.40
11:K:100:MET:CE	11:K:127:PHE:HB2	2.52	0.40
8:V:168:GLY:O	17:V:301:3BV:H57	2.22	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%)	242 (98%)	6 (2%)	0	100	100
1	O	248/250 (99%)	242 (98%)	6 (2%)	0	100	100
2	B	242/258 (94%)	234 (97%)	6 (2%)	2 (1%)	21	37
2	P	242/258 (94%)	234 (97%)	6 (2%)	2 (1%)	21	37
3	C	238/254 (94%)	230 (97%)	6 (2%)	2 (1%)	21	37
3	Q	238/254 (94%)	231 (97%)	5 (2%)	2 (1%)	21	37
4	D	231/260 (89%)	226 (98%)	5 (2%)	0	100	100
4	R	231/260 (89%)	226 (98%)	5 (2%)	0	100	100
5	E	229/234 (98%)	223 (97%)	6 (3%)	0	100	100
5	S	229/234 (98%)	223 (97%)	6 (3%)	0	100	100
6	F	241/288 (84%)	236 (98%)	5 (2%)	0	100	100
6	T	241/288 (84%)	236 (98%)	5 (2%)	0	100	100
7	G	239/252 (95%)	235 (98%)	4 (2%)	0	100	100
7	U	239/252 (95%)	235 (98%)	4 (2%)	0	100	100
8	H	220/232 (95%)	214 (97%)	6 (3%)	0	100	100
8	V	220/232 (95%)	214 (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%)	3 (2%)	1 (0%)	31	51
10	X	193/198 (98%)	189 (98%)	3 (2%)	1 (0%)	31	51
11	K	210/212 (99%)	207 (99%)	3 (1%)	0	100	100
11	Y	210/212 (99%)	207 (99%)	3 (1%)	0	100	100
12	L	220/222 (99%)	217 (99%)	3 (1%)	0	100	100
12	Z	220/222 (99%)	217 (99%)	3 (1%)	0	100	100
13	M	231/246 (94%)	220 (95%)	10 (4%)	1 (0%)	36	57
13	a	231/246 (94%)	221 (96%)	9 (4%)	1 (0%)	36	57
14	N	194/196 (99%)	188 (97%)	6 (3%)	0	100	100
14	b	194/196 (99%)	188 (97%)	6 (3%)	0	100	100
All	All	6276/6614 (95%)	6114 (97%)	150 (2%)	12 (0%)	49	71

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	51	VAL
3	C	202	GLN
2	P	51	VAL
3	Q	202	GLN
3	C	205	ALA
3	Q	205	ALA
2	B	221	ASP
10	J	2	ASP
2	P	221	ASP
10	X	2	ASP
13	M	229	GLY
13	a	229	GLY

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	209/209 (100%)	206 (99%)	3 (1%)	69	88
1	O	209/209 (100%)	206 (99%)	3 (1%)	69	88
2	B	203/216 (94%)	197 (97%)	6 (3%)	44	71
2	P	203/216 (94%)	197 (97%)	6 (3%)	44	71
3	C	212/226 (94%)	205 (97%)	7 (3%)	41	68
3	Q	212/226 (94%)	205 (97%)	7 (3%)	41	68
4	D	194/215 (90%)	186 (96%)	8 (4%)	33	59
4	R	194/215 (90%)	186 (96%)	8 (4%)	33	59
5	E	190/193 (98%)	183 (96%)	7 (4%)	37	64
5	S	190/193 (98%)	183 (96%)	7 (4%)	37	64
6	F	201/239 (84%)	193 (96%)	8 (4%)	34	60
6	T	201/239 (84%)	192 (96%)	9 (4%)	30	54
7	G	206/210 (98%)	200 (97%)	6 (3%)	45	72
7	U	206/210 (98%)	200 (97%)	6 (3%)	45	72
8	H	181/190 (95%)	177 (98%)	4 (2%)	55	80

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	V	181/190 (95%)	178 (98%)	3 (2%)	63	85
9	I	172/173 (99%)	169 (98%)	3 (2%)	63	85
9	W	172/173 (99%)	169 (98%)	3 (2%)	63	85
10	J	173/175 (99%)	168 (97%)	5 (3%)	45	72
10	X	173/175 (99%)	168 (97%)	5 (3%)	45	72
11	K	169/169 (100%)	164 (97%)	5 (3%)	44	71
11	Y	169/169 (100%)	164 (97%)	5 (3%)	44	71
12	L	185/185 (100%)	180 (97%)	5 (3%)	48	75
12	Z	185/185 (100%)	180 (97%)	5 (3%)	48	75
13	M	199/208 (96%)	193 (97%)	6 (3%)	44	71
13	a	199/208 (96%)	193 (97%)	6 (3%)	44	71
14	N	162/162 (100%)	161 (99%)	1 (1%)	87	96
14	b	162/162 (100%)	161 (99%)	1 (1%)	87	96
All	All	5312/5540 (96%)	5164 (97%)	148 (3%)	47	74

All (148) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LYS
1	A	61	LEU
1	A	157	PHE
2	B	50	LYS
2	B	55	LEU
2	B	58	GLN
2	B	114	LEU
2	B	184	LYS
2	B	191	LEU
3	C	4	ARG
3	C	38	ASN
3	C	77	ASN
3	C	147	GLN
3	C	160	GLN
3	C	169	VAL
3	C	180	LYS
4	D	99	ILE
4	D	125	LEU
4	D	176	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
4	D	193	LEU
4	D	214	ILE
4	D	224	ASP
4	D	236	LYS
4	D	242	GLU
5	E	9	THR
5	E	29	LYS
5	E	54	GLU
5	E	71	LEU
5	E	184	ASN
5	E	188	LEU
5	E	202	ASP
6	F	14	ASP
6	F	123	ASN
6	F	172	LEU
6	F	181	GLU
6	F	203	ASN
6	F	206	LYS
6	F	214	TRP
6	F	221	ASN
7	G	83	ASN
7	G	115	LEU
7	G	125	MET
7	G	166	GLN
7	G	181	LYS
7	G	235	ARG
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
10	J	23	ARG
10	J	75	LEU
10	J	78	GLN
10	J	144	LEU
10	J	174	MET
11	K	4	LEU
11	K	9	GLN
11	K	35	ILE
11	K	73	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
11	K	106	ARG
12	L	1	GLN
12	L	23	LEU
12	L	49	ASN
12	L	136	CYS
12	L	167	LYS
13	M	43	ILE
13	M	48	ASN
13	M	70	LEU
13	M	104	ARG
13	M	161	ARG
13	M	187	ARG
14	N	22	THR
1	O	17	LYS
1	O	61	LEU
1	O	157	PHE
2	P	50	LYS
2	P	55	LEU
2	P	58	GLN
2	P	114	LEU
2	P	184	LYS
2	P	191	LEU
3	Q	4	ARG
3	Q	38	ASN
3	Q	77	ASN
3	Q	147	GLN
3	Q	160	GLN
3	Q	169	VAL
3	Q	180	LYS
4	R	99	ILE
4	R	125	LEU
4	R	176	LEU
4	R	193	LEU
4	R	214	ILE
4	R	224	ASP
4	R	236	LYS
4	R	242	GLU
5	S	9	THR
5	S	29	LYS
5	S	54	GLU
5	S	71	LEU
5	S	184	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
5	S	188	LEU
5	S	202	ASP
6	T	14	ASP
6	T	117	GLN
6	T	123	ASN
6	T	172	LEU
6	T	181	GLU
6	T	203	ASN
6	T	206	LYS
6	T	214	TRP
6	T	221	ASN
7	U	83	ASN
7	U	115	LEU
7	U	125	MET
7	U	166	GLN
7	U	181	LYS
7	U	235	ARG
8	V	30	ASN
8	V	56	THR
8	V	196	ARG
9	W	37	ASN
9	W	171	LEU
9	W	182	TRP
10	X	23	ARG
10	X	75	LEU
10	X	78	GLN
10	X	144	LEU
10	X	174	MET
11	Y	4	LEU
11	Y	9	GLN
11	Y	35	ILE
11	Y	73	ARG
11	Y	106	ARG
12	Z	1	GLN
12	Z	23	LEU
12	Z	49	ASN
12	Z	136	CYS
12	Z	167	LYS
13	a	43	ILE
13	a	48	ASN
13	a	70	LEU
13	a	104	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
13	a	161	ARG
13	a	187	ARG
14	b	22	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (76) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	HIS
2	B	95	GLN
2	B	119	GLN
2	B	123	GLN
3	C	38	ASN
3	C	147	GLN
3	C	160	GLN
4	D	146	GLN
5	E	68	HIS
5	E	92	ASN
5	E	99	ASN
5	E	116	GLN
5	E	118	ASN
5	E	120	GLN
5	E	184	ASN
6	F	86	ASN
6	F	123	ASN
6	F	191	GLN
6	F	240	GLN
7	G	117	GLN
7	G	121	GLN
8	H	66	HIS
8	H	116	HIS
10	J	55	GLN
11	K	85	ASN
11	K	176	ASN
12	L	3	ASN
12	L	70	ASN
12	L	76	HIS
12	L	79	HIS
12	L	158	ASN
13	M	48	ASN
13	M	102	GLN
13	M	108	ASN
13	M	179	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
13	M	194	ASN
13	M	213	GLN
1	O	94	HIS
2	P	20	GLN
2	P	119	GLN
2	P	123	GLN
3	Q	38	ASN
3	Q	147	GLN
3	Q	160	GLN
4	R	91	HIS
4	R	146	GLN
5	S	68	HIS
5	S	92	ASN
5	S	99	ASN
5	S	116	GLN
5	S	118	ASN
5	S	120	GLN
5	S	184	ASN
6	T	86	ASN
6	T	117	GLN
6	T	123	ASN
6	T	191	GLN
6	T	240	GLN
7	U	83	ASN
7	U	117	GLN
7	U	121	GLN
8	V	116	HIS
9	W	203	GLN
10	X	55	GLN
11	Y	85	ASN
11	Y	176	ASN
12	Z	3	ASN
12	Z	70	ASN
12	Z	79	HIS
12	Z	158	ASN
13	a	48	ASN
13	a	102	GLN
13	a	108	ASN
13	a	179	ASN
13	a	194	ASN
13	a	213	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 21 ligands modelled in this entry, 11 are monoatomic - leaving 10 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	3BV	H	301	8	54,54,54	1.42	5 (9%)	67,71,71	1.71	9 (13%)
18	MES	H	302	-	12,12,12	2.17	1 (8%)	14,16,16	1.38	3 (21%)
17	3BV	K	301	11	54,54,54	1.85	6 (11%)	67,71,71	1.88	14 (20%)
18	MES	K	303	-	12,12,12	2.18	1 (8%)	14,16,16	1.26	1 (7%)
17	3BV	N	201	14	54,54,54	1.59	4 (7%)	67,71,71	1.54	7 (10%)
17	3BV	V	301	8	54,54,54	1.46	6 (11%)	67,71,71	1.49	5 (7%)
18	MES	V	302	-	12,12,12	2.18	1 (8%)	14,16,16	1.45	3 (21%)
17	3BV	Y	301	11	54,54,54	1.79	6 (11%)	67,71,71	1.81	10 (14%)
18	MES	Y	302	-	12,12,12	2.23	1 (8%)	14,16,16	1.33	1 (7%)
17	3BV	b	201	14	54,54,54	1.44	4 (7%)	67,71,71	1.65	9 (13%)

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	3BV	H	301	8	-	0/59/67/67	0/3/3/3
18	MES	H	302	-	-	0/6/14/14	0/1/1/1
17	3BV	K	301	11	-	0/59/67/67	0/3/3/3
18	MES	K	303	-	-	0/6/14/14	0/1/1/1
17	3BV	N	201	14	-	0/59/67/67	0/3/3/3
17	3BV	V	301	8	-	0/59/67/67	0/3/3/3
18	MES	V	302	-	-	0/6/14/14	0/1/1/1
17	3BV	Y	301	11	-	0/59/67/67	0/3/3/3
18	MES	Y	302	-	-	0/6/14/14	0/1/1/1
17	3BV	b	201	14	-	0/59/67/67	0/3/3/3

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	Y	302	MES	C8-S	-7.35	1.67	1.77
18	V	302	MES	C8-S	-7.25	1.67	1.77
18	H	302	MES	C8-S	-7.22	1.67	1.77
18	K	303	MES	C8-S	-7.21	1.67	1.77
17	K	301	3BV	C32-C33	-6.82	1.34	1.51
17	H	301	3BV	C32-C33	-6.46	1.35	1.51
17	N	201	3BV	C32-C33	-6.23	1.36	1.51
17	b	201	3BV	C32-C33	-5.96	1.36	1.51
17	Y	301	3BV	C32-C33	-5.91	1.37	1.51
17	V	301	3BV	C32-C33	-5.88	1.37	1.51
17	Y	301	3BV	C59-C51	-5.63	1.46	1.52
17	K	301	3BV	C59-C51	-5.59	1.46	1.52
17	b	201	3BV	C13-C14	-4.86	1.37	1.51
17	Y	301	3BV	C13-C14	-4.79	1.37	1.51
17	V	301	3BV	C13-C14	-4.41	1.38	1.51
17	K	301	3BV	C13-C14	-4.31	1.39	1.51
17	H	301	3BV	C13-C14	-4.27	1.39	1.51
17	N	201	3BV	C13-C14	-4.27	1.39	1.51
17	H	301	3BV	C59-C51	-3.64	1.48	1.52
17	K	301	3BV	O48-C47	-3.48	1.34	1.43
17	V	301	3BV	O48-C47	-3.36	1.34	1.43
17	V	301	3BV	C59-C51	-3.20	1.49	1.52
17	N	201	3BV	O48-C47	-2.93	1.35	1.43
17	b	201	3BV	O48-C47	-2.54	1.36	1.43
17	K	301	3BV	C23-C28	-2.45	1.46	1.52
17	Y	301	3BV	C39-N41	-2.17	1.29	1.34
17	H	301	3BV	O48-C47	-2.07	1.37	1.43
17	Y	301	3BV	O48-C47	-2.06	1.37	1.43
17	H	301	3BV	C8-N10	-2.04	1.29	1.34

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	V	301	3BV	C7-N4	2.04	1.51	1.47
17	V	301	3BV	C51-C47	2.86	1.58	1.53
17	b	201	3BV	C51-C47	4.14	1.61	1.53
17	Y	301	3BV	C51-C47	5.61	1.63	1.53
17	K	301	3BV	C51-C47	5.93	1.64	1.53
17	N	201	3BV	C51-C47	6.38	1.65	1.53

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	K	301	3BV	C43-C42-N41	-8.97	98.58	110.18
17	H	301	3BV	C58-C51-C59	-8.60	98.48	109.92
17	Y	301	3BV	C43-C42-N41	-8.57	99.10	110.18
17	N	201	3BV	C43-C42-N41	-7.24	100.82	110.18
17	V	301	3BV	C58-C51-C59	-7.01	100.61	109.92
17	H	301	3BV	C43-C42-N41	-6.92	101.24	110.18
17	b	201	3BV	C43-C42-N41	-6.87	101.30	110.18
17	N	201	3BV	C58-C51-C59	-6.03	101.91	109.92
17	K	301	3BV	C58-C51-C59	-5.80	102.21	109.92
17	V	301	3BV	C43-C42-N41	-5.57	102.98	110.18
17	Y	301	3BV	C58-C51-C59	-5.01	103.26	109.92
17	b	201	3BV	C7-N4-C3	-4.20	104.41	111.11
17	b	201	3BV	C7-N4-C5	-4.15	104.50	111.11
17	b	201	3BV	C58-C51-C59	-3.45	105.34	109.92
17	N	201	3BV	C20-C11-N10	-3.15	102.57	111.18
17	V	301	3BV	O48-C47-C42	-2.97	101.88	108.98
17	b	201	3BV	C20-C11-N10	-2.82	103.48	111.18
17	Y	301	3BV	O60-C59-C51	-2.80	105.70	111.39
17	K	301	3BV	C33-C32-C31	-2.80	105.61	113.41
17	H	301	3BV	O60-C59-C51	-2.80	105.71	111.39
17	K	301	3BV	O60-C59-C51	-2.66	105.99	111.39
17	b	201	3BV	C12-C13-C14	-2.50	104.25	113.19
17	K	301	3BV	C36-C37-C38	-2.42	116.88	120.20
17	K	301	3BV	C24-C23-C28	-2.40	104.78	110.59
17	K	301	3BV	O1-C2-C3	-2.29	106.79	111.81
17	N	201	3BV	C7-N4-C3	-2.26	107.50	111.11
17	N	201	3BV	O1-C2-C3	-2.26	106.85	111.81
17	Y	301	3BV	C25-C24-C23	-2.19	109.29	115.46
17	K	301	3BV	O48-C47-C42	-2.17	103.78	108.98
17	N	201	3BV	O1-C6-C5	-2.17	107.04	111.81
17	K	301	3BV	C25-C24-C23	-2.13	109.44	115.46
17	H	301	3BV	C12-C11-C20	-2.10	105.15	110.21

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	K	301	3BV	C39-C31-N30	-2.09	105.47	111.18
17	Y	301	3BV	O1-C2-C3	-2.08	107.24	111.81
17	Y	301	3BV	C39-C31-N30	-2.06	105.55	111.18
17	H	301	3BV	C33-C32-C31	-2.03	107.76	113.41
17	H	301	3BV	C12-C11-N10	-2.02	106.76	110.88
17	H	301	3BV	C7-N4-C5	2.05	114.37	111.11
18	H	302	MES	O3S-S-C8	2.08	109.13	105.77
17	H	301	3BV	C3-N4-C5	2.08	113.47	108.87
18	H	302	MES	O1S-S-C8	2.11	109.45	106.92
17	K	301	3BV	C44-C43-C42	2.21	120.72	115.85
18	V	302	MES	O2S-S-C8	2.28	109.66	106.92
18	V	302	MES	O3S-S-C8	2.31	109.50	105.77
17	Y	301	3BV	C23-N22-C20	2.34	126.72	121.66
17	b	201	3BV	C6-C5-N4	2.36	113.36	110.11
17	H	301	3BV	C7-N4-C3	2.53	115.15	111.11
17	b	201	3BV	C2-C3-N4	2.58	113.66	110.11
17	N	201	3BV	C44-C43-C42	2.74	121.91	115.85
17	Y	301	3BV	C3-N4-C5	2.77	114.99	108.87
17	Y	301	3BV	C12-C11-C20	2.82	116.99	110.21
18	Y	302	MES	O3S-S-C8	2.91	110.47	105.77
18	K	303	MES	O3S-S-C8	2.93	110.50	105.77
17	K	301	3BV	C3-N4-C5	2.99	115.48	108.87
17	K	301	3BV	C7-N4-C5	3.22	116.25	111.11
17	K	301	3BV	C12-C11-C20	3.26	118.05	110.21
18	H	302	MES	O2S-S-C8	3.43	111.05	106.92
18	V	302	MES	O1S-S-C8	3.47	111.09	106.92
17	V	301	3BV	C7-N4-C3	3.48	116.66	111.11
17	V	301	3BV	C6-C5-N4	3.49	114.92	110.11
17	b	201	3BV	C3-N4-C5	3.71	117.08	108.87
17	Y	301	3BV	C7-N4-C5	4.94	118.98	111.11

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	H	301	3BV	2	0
17	K	301	3BV	4	0
18	K	303	MES	1	0
17	N	201	3BV	1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	V	301	3BV	4	0
18	V	302	MES	1	0
17	Y	301	3BV	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.08	13 (5%)	27 29	29, 45, 85, 136	0
1	O	250/250 (100%)	0.18	16 (6%)	19 20	35, 54, 100, 140	0
2	B	244/258 (94%)	0.31	21 (8%)	10 10	30, 52, 99, 152	0
2	P	244/258 (94%)	0.33	20 (8%)	11 11	33, 55, 104, 153	0
3	C	240/254 (94%)	0.39	30 (12%)	4 3	30, 55, 120, 160	0
3	Q	240/254 (94%)	0.81	40 (16%)	1 1	38, 71, 163, 206	0
4	D	235/260 (90%)	0.12	8 (3%)	45 48	36, 56, 87, 140	0
4	R	235/260 (90%)	0.37	17 (7%)	15 16	44, 64, 106, 154	0
5	E	231/234 (98%)	0.22	13 (5%)	24 26	34, 57, 92, 130	0
5	S	231/234 (98%)	0.56	22 (9%)	8 8	40, 69, 121, 153	0
6	F	243/288 (84%)	0.04	14 (5%)	23 24	30, 51, 104, 129	0
6	T	243/288 (84%)	0.26	11 (4%)	33 36	34, 64, 123, 165	0
7	G	241/252 (95%)	0.06	13 (5%)	26 27	28, 48, 90, 141	0
7	U	241/252 (95%)	0.05	10 (4%)	37 40	30, 51, 85, 129	0
8	H	222/232 (95%)	-0.02	4 (1%)	68 71	30, 44, 80, 116	0
8	V	222/232 (95%)	0.07	5 (2%)	60 63	30, 49, 81, 120	0
9	I	204/205 (99%)	-0.34	1 (0%)	90 91	25, 41, 69, 95	0
9	W	204/205 (99%)	-0.23	3 (1%)	73 75	27, 43, 69, 96	0
10	J	195/198 (98%)	-0.18	4 (2%)	63 66	26, 42, 71, 110	0
10	X	195/198 (98%)	-0.09	4 (2%)	63 66	28, 45, 75, 121	0
11	K	212/212 (100%)	-0.21	3 (1%)	75 77	28, 43, 73, 90	0
11	Y	212/212 (100%)	-0.11	2 (0%)	84 85	30, 45, 76, 101	0
12	L	222/222 (100%)	-0.17	2 (0%)	84 85	25, 44, 75, 100	0
12	Z	222/222 (100%)	-0.15	4 (1%)	68 71	27, 45, 77, 100	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%)	-0.12	8 (3%) 45 48	24, 43, 71, 87	0
13	a	233/246 (94%)	-0.17	3 (1%) 77 78	24, 44, 69, 84	0
14	N	196/196 (100%)	-0.27	2 (1%) 82 84	25, 39, 71, 92	0
14	b	196/196 (100%)	-0.20	3 (1%) 73 75	28, 41, 72, 97	0
All	All	6336/6614 (95%)	0.07	296 (4%) 31 34	24, 49, 100, 206	0

All (296) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	219	ALA	14.4
2	P	51	VAL	10.2
1	A	1	MET	10.0
2	P	219	ALA	9.7
2	B	51	VAL	8.5
2	P	218	GLY	8.5
1	O	1	MET	8.3
3	Q	50	LEU	8.0
8	H	222	ASP	7.9
3	Q	238	LYS	7.9
8	V	222	ASP	7.9
8	H	221	CYS	7.8
3	Q	49	THR	7.6
2	B	221	ASP	7.5
3	Q	51	LYS	7.2
5	S	202	ASP	7.2
10	X	1	MET	7.2
2	B	220	ASN	7.0
11	Y	212	GLY	6.9
4	R	241	ALA	6.7
3	Q	48	SER	6.7
13	M	233	ILE	6.7
3	Q	206	LYS	6.6
3	Q	204	GLY	6.5
2	P	220	ASN	6.1
3	Q	202	GLN	5.9
8	V	221	CYS	5.8
2	B	218	GLY	5.8
6	F	205	GLU	5.7
4	D	242	GLU	5.6
10	J	1	MET	5.5
6	T	243	ILE	5.5

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	2	THR	5.4
3	Q	239	GLN	5.4
1	O	250	LEU	5.3
3	Q	205	ALA	5.3
1	O	52	SER	5.3
5	E	233	ILE	5.3
10	X	194	ASP	5.2
6	F	243	ILE	5.2
3	C	202	GLN	5.1
1	O	249	ALA	5.1
3	C	225	GLU	5.0
4	D	241	ALA	4.9
9	I	1	SER	4.8
13	a	1	THR	4.8
7	G	242	GLN	4.8
7	U	242	GLN	4.7
3	Q	223	SER	4.7
3	Q	240	GLU	4.6
2	P	221	ASP	4.6
7	U	222	ASP	4.6
5	S	233	ILE	4.5
3	C	238	LYS	4.5
4	R	242	GLU	4.4
3	C	240	GLU	4.4
7	U	2	GLY	4.3
10	J	194	ASP	4.3
2	P	222	GLY	4.2
7	G	240	ALA	4.2
3	C	48	SER	4.1
12	L	165	ASN	4.1
6	T	244	ASN	4.0
6	T	2	THR	3.9
5	S	173	ARG	3.9
5	E	201	ARG	3.9
13	M	1	THR	3.8
4	R	125	LEU	3.8
11	Y	106	ARG	3.8
1	A	250	LEU	3.8
2	P	59	ASP	3.8
6	F	2	THR	3.7
6	F	244	ASN	3.7
1	A	248	GLU	3.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	O	53	SER	3.7
10	X	193	ASP	3.6
5	S	225	ASP	3.6
9	W	1	SER	3.6
3	Q	225	GLU	3.6
7	G	188	GLU	3.6
3	C	236	GLN	3.6
3	C	180	LYS	3.6
5	S	51	ASN	3.6
3	Q	203	THR	3.5
5	S	180	LYS	3.5
13	M	232	LYS	3.5
3	C	50	LEU	3.5
6	T	178	HIS	3.5
10	J	193	ASP	3.5
2	P	52	THR	3.4
3	C	206	LYS	3.4
5	S	122	TYR	3.4
7	G	222	ASP	3.4
1	A	50	LYS	3.4
5	E	122	TYR	3.4
3	C	49	THR	3.4
3	C	239	GLN	3.4
13	a	47	ASP	3.4
6	F	215	CYS	3.3
6	T	215	CYS	3.3
3	Q	229	GLN	3.3
5	S	171	LEU	3.3
7	G	179	LYS	3.3
3	C	175	LYS	3.3
1	O	201	GLU	3.3
1	A	249	ALA	3.3
9	W	133	LYS	3.3
6	T	14	ASP	3.3
4	R	113	LEU	3.3
6	F	166	GLN	3.2
1	A	52	SER	3.2
5	S	210	LEU	3.2
3	Q	236	GLN	3.2
3	Q	55	THR	3.2
5	S	165	GLN	3.1
3	Q	180	LYS	3.1

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
14	b	105	LYS	3.1
3	Q	58	THR	3.1
5	E	202	ASP	3.1
13	M	47	ASP	3.1
3	Q	59	PRO	3.1
7	G	3	TYR	3.1
5	S	54	GLU	3.1
6	F	181	GLU	3.0
3	Q	234	ILE	3.0
4	R	201	GLU	3.0
13	M	231	GLN	3.0
2	P	182	ASP	3.0
3	Q	46	ARG	3.0
3	Q	60	SER	3.0
3	C	235	GLU	3.0
4	D	47	THR	3.0
12	Z	165	ASN	3.0
2	B	232	GLN	3.0
3	Q	52	LEU	3.0
3	C	60	SER	3.0
2	B	222	GLY	3.0
5	S	3	ASN	3.0
3	Q	181	GLU	2.9
2	B	203	SER	2.9
6	T	181	GLU	2.9
3	Q	141	ASP	2.9
1	A	201	GLU	2.9
2	B	182	ASP	2.9
2	P	244	THR	2.9
1	O	169	VAL	2.8
2	B	242	GLY	2.8
3	C	1	GLY	2.8
13	M	216	ASN	2.8
1	O	203	GLU	2.8
3	Q	237	GLU	2.8
3	C	228	ASN	2.8
7	U	241	GLU	2.8
3	Q	191	LYS	2.8
7	U	203	ASP	2.8
2	B	225	TYR	2.8
1	A	54	PRO	2.8
8	H	198	GLU	2.7

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
4	R	169	GLU	2.7
12	Z	1	GLN	2.7
6	F	201	GLU	2.7
2	P	217	LYS	2.7
2	B	59	ASP	2.7
6	T	241	LYS	2.7
2	B	61	SER	2.7
7	U	188	GLU	2.7
3	Q	27	ARG	2.7
14	N	195	GLN	2.7
14	b	195	GLN	2.6
5	S	50	ARG	2.6
5	S	123	GLY	2.6
13	a	204	THR	2.6
14	b	182	GLY	2.6
3	C	47	ARG	2.6
4	R	2	ARG	2.6
2	P	203	SER	2.6
2	B	62	THR	2.6
2	P	225	TYR	2.6
5	E	54	GLU	2.6
5	S	58	TYR	2.6
3	C	216	ASP	2.6
4	D	1	ASP	2.6
4	R	230	GLU	2.6
11	K	145	LYS	2.6
2	P	234	ILE	2.5
2	B	60	THR	2.5
4	D	125	LEU	2.5
4	R	54	ASP	2.5
7	G	241	GLU	2.5
3	Q	208	ILE	2.5
4	R	207	ASN	2.5
11	K	212	GLY	2.5
2	P	60	THR	2.5
12	Z	106	TYR	2.5
4	D	141	ALA	2.5
2	B	54	THR	2.5
7	G	2	GLY	2.5
3	C	27	ARG	2.4
4	D	2	ARG	2.4
5	E	210	LEU	2.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	O	29	LYS	2.4
3	C	181	GLU	2.4
7	U	3	TYR	2.4
7	G	68	ARG	2.4
3	Q	1	GLY	2.4
3	Q	227	ILE	2.4
5	E	123	GLY	2.4
6	F	202	ASP	2.4
7	U	183	ASP	2.4
6	T	205	GLU	2.4
3	C	167	LYS	2.4
5	E	173	ARG	2.4
7	G	183	ASP	2.4
6	T	53	LYS	2.3
2	P	177	MET	2.3
12	Z	210	ASP	2.3
13	M	69	ASP	2.3
4	R	157	TYR	2.3
3	Q	235	GLU	2.3
1	A	203	GLU	2.3
5	E	218	ASP	2.3
5	S	59	GLN	2.3
2	P	50	LYS	2.3
3	Q	187	GLU	2.3
2	B	235	LYS	2.3
6	F	204	LYS	2.3
8	H	219	ASN	2.3
6	F	229	GLY	2.3
1	O	231	LYS	2.3
3	C	173	LEU	2.3
6	F	241	LYS	2.3
7	U	237	VAL	2.3
3	C	188	GLU	2.3
5	E	227	GLU	2.3
3	C	46	ARG	2.3
8	V	219	ASN	2.3
9	W	191	LYS	2.3
3	C	169	VAL	2.3
5	E	217	LYS	2.3
4	R	1	ASP	2.3
6	F	230	ASP	2.3
10	X	151	ASP	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	59	GLU	2.3
3	C	187	GLU	2.3
3	C	37	LYS	2.2
1	A	229	THR	2.2
4	R	203	LYS	2.2
5	S	207	VAL	2.2
6	T	230	ASP	2.2
3	Q	188	GLU	2.2
2	B	50	LYS	2.2
13	M	230	THR	2.2
1	O	50	LYS	2.2
5	E	207	VAL	2.2
3	Q	175	LYS	2.2
7	U	153	TYR	2.2
4	D	201	GLU	2.2
5	E	3	ASN	2.2
5	S	194	GLU	2.2
3	C	51	LYS	2.2
5	S	52	ALA	2.2
12	L	210	ASP	2.2
3	Q	142	GLU	2.2
11	K	147	ASP	2.1
4	R	114	ARG	2.1
8	V	9	ASN	2.1
3	C	59	PRO	2.1
7	G	17	TYR	2.1
2	P	15	GLU	2.1
7	G	51	PRO	2.1
3	Q	222	LEU	2.1
4	R	217	GLN	2.1
1	O	2	THR	2.1
1	O	229	THR	2.1
7	G	5	ARG	2.1
1	O	40	THR	2.1
1	O	62	SER	2.1
5	S	204	SER	2.1
1	O	61	LEU	2.1
8	V	173	VAL	2.1
2	P	93	HIS	2.1
1	A	58	SER	2.1
4	R	175	LEU	2.1
6	F	206	LYS	2.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	B	181	ASP	2.0
2	B	55	LEU	2.0
3	Q	56	ARG	2.0
2	B	93	HIS	2.0
2	P	232	GLN	2.0
3	Q	233	GLN	2.0
14	N	9	LYS	2.0
10	J	195	PHE	2.0
3	C	171	GLU	2.0
4	R	202	GLU	2.0
5	S	218	ASP	2.0
5	S	30	GLN	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no 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	3BV	N	201	52/52	0.83	0.25	28,43,124,130	0
18	MES	V	302	12/12	0.83	0.36	63,66,82,97	0
17	3BV	b	201	52/52	0.85	0.22	30,44,121,126	0
15	MG	Z	301	1/1	0.87	0.37	58,58,58,58	0
17	3BV	V	301	52/52	0.87	0.22	43,51,94,99	0
15	MG	G	301	1/1	0.88	0.13	49,49,49,49	0
18	MES	H	302	12/12	0.88	0.32	61,63,70,82	0
17	3BV	H	301	52/52	0.88	0.19	41,49,95,99	0
15	MG	L	301	1/1	0.89	0.10	39,39,39,39	0
17	3BV	K	301	52/52	0.89	0.18	29,39,91,97	0
17	3BV	Y	301	52/52	0.91	0.17	31,40,92,97	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
18	MES	K	303	12/12	0.93	0.32	34,37,53,56	0
18	MES	Y	302	12/12	0.94	0.30	33,36,53,56	0
15	MG	I	302	1/1	0.95	0.05	48,48,48,48	0
15	MG	I	301	1/1	0.95	0.18	48,48,48,48	0
16	CL	N	203	1/1	0.97	0.07	50,50,50,50	0
16	CL	b	202	1/1	0.97	0.09	60,60,60,60	0
15	MG	N	202	1/1	0.97	0.12	37,37,37,37	0
16	CL	U	301	1/1	0.99	0.09	37,37,37,37	0
15	MG	K	302	1/1	0.99	0.11	32,32,32,32	0
16	CL	G	302	1/1	0.99	0.03	35,35,35,35	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.