



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 12, 2016 – 10:06 PM EST

PDB ID : 5FGE  
Title : Yeast 20S proteasome beta5-H(-2)T-T1A double mutant in complex with Carfilzomib  
Authors : Huber, E.M.; Groll, M.  
Deposited on : 2015-12-20  
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

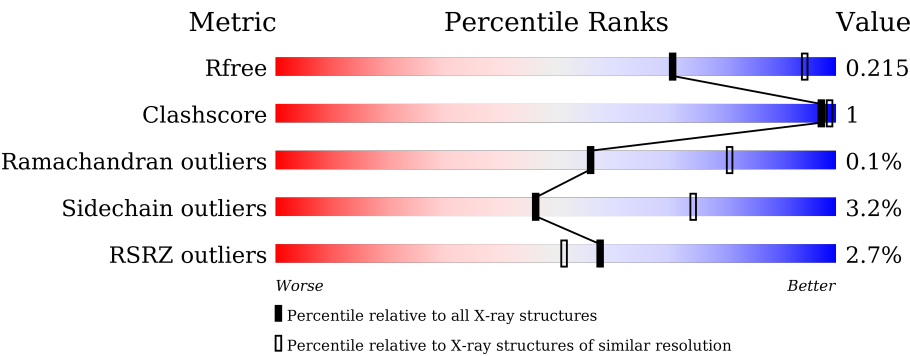
MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20028442  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20028442

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




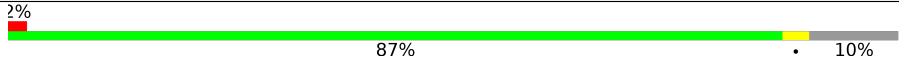
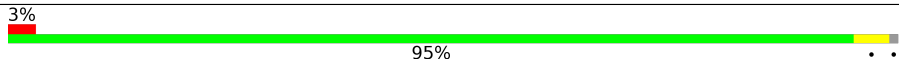
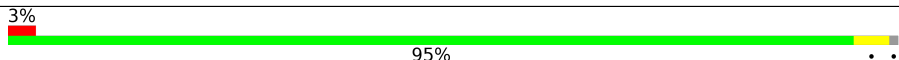
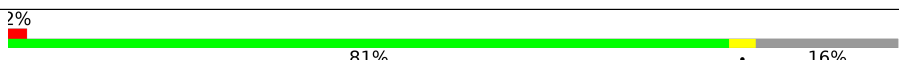
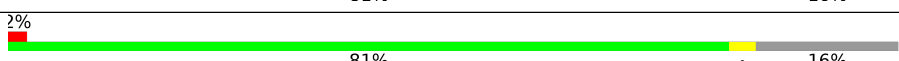
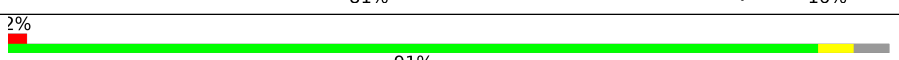
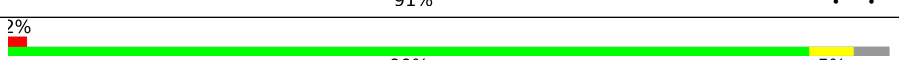
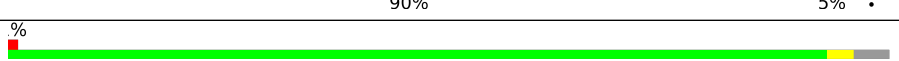
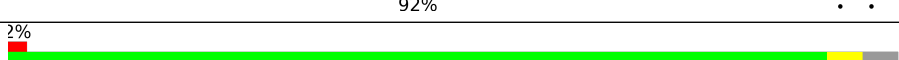
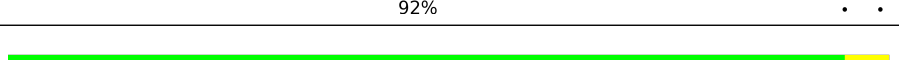
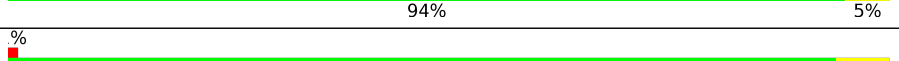
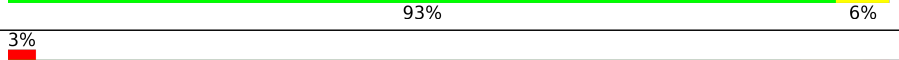
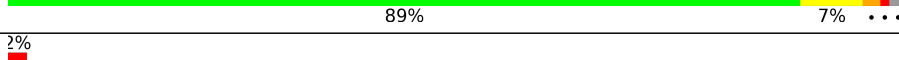
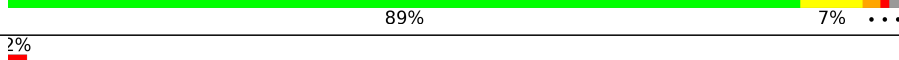
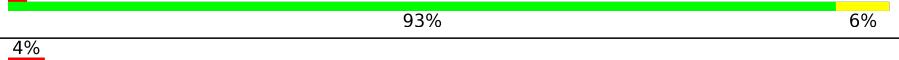
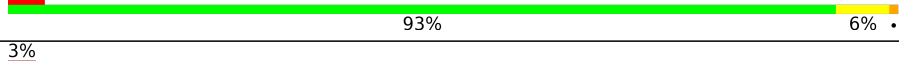
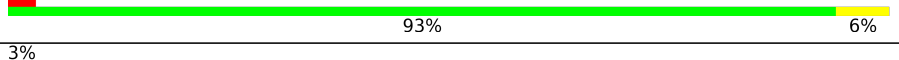
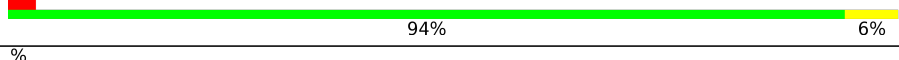
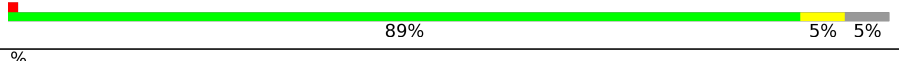
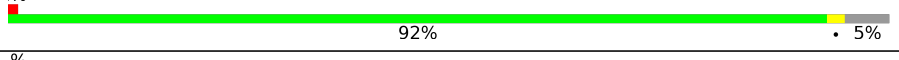
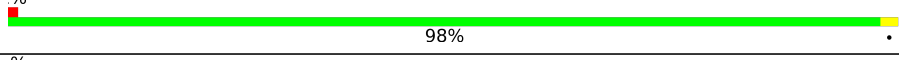
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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>3%</div><div><div></div><div>99%</div><div>.</div></div></div>
1	O	250	<div><div>4%</div><div><div></div><div>98%</div><div>.</div></div></div>
2	B	258	<div><div>5%</div><div><div></div><div>90%</div><div>. . 5%</div></div></div>
2	P	258	<div><div>5%</div><div><div></div><div>90%</div><div>. . 5%</div></div></div>
3	C	254	<div><div>7%</div><div><div></div><div>90%</div><div>. . 6%</div></div></div>
3	Q	254	<div><div>7%</div><div><div></div><div>91%</div><div>. . 6%</div></div></div>

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Mol	Chain	Length	Quality of chain
4	D	260	
4	R	260	
5	E	234	
5	S	234	
6	F	288	
6	T	288	
7	G	252	
7	U	252	
8	H	232	
8	V	232	
9	I	205	
9	W	205	
10	J	198	
10	X	198	
11	K	218	
11	Y	218	
12	L	222	
12	Z	222	
13	M	246	
13	a	246	
14	N	196	
14	b	196	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	MG	I	301	-	-	-	X
15	MG	Z	301	-	-	-	X
17	3BV	N	201	-	-	-	X
17	3BV	V	301	-	-	-	X
17	3BV	b	201	-	-	-	X
18	MES	H	302	-	-	-	X
18	MES	V	302	-	-	-	X

## 2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 49996 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			

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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	218	Total	C	N	O	S	0	0	0
			1683	1071	287	318	7			
11	Y	218	Total	C	N	O	S	0	0	0
			1683	1071	287	318	7			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	-1	THR	HIS	engineered mutation	UNP P30656
K	1	ALA	THR	engineered mutation	UNP P30656
Y	-1	THR	HIS	engineered mutation	UNP P30656
Y	1	ALA	THR	engineered mutation	UNP P30656

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	222	Total	C	N	O	S	0	1	0
			1767	1121	306	336	4			
12	Z	222	Total	C	N	O	S	0	0	0
			1757	1115	303	335	4			

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

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

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

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

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

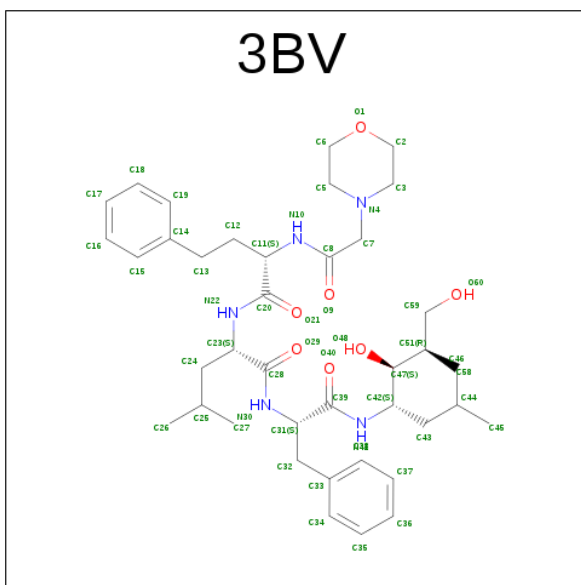
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	G	1	Total 1	Mg 1	0	0
15	K	1	Total 1	Mg 1	0	0
15	I	2	Total 2	Mg 2	0	0
15	Z	1	Total 1	Mg 1	0	0
15	N	1	Total 1	Mg 1	0	0
15	L	1	Total 1	Mg 1	0	0

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

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

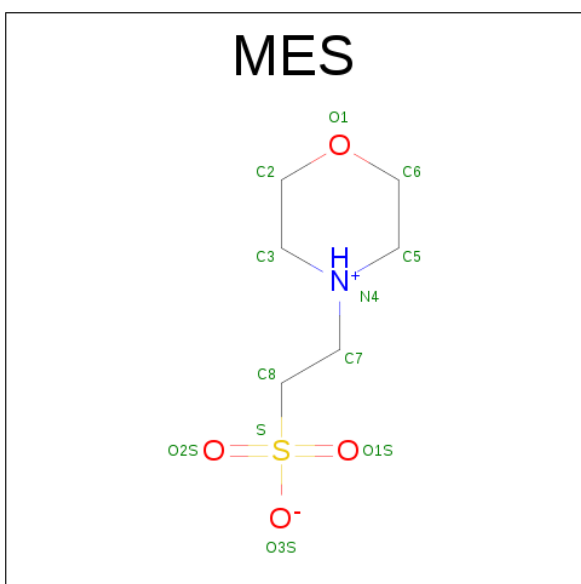
- Molecule 17 is N-{(2S)-2-[(morpholin-4-ylacetyl)amino]-4-phenylbutanoyl}-L-leucyl-N-[(2R,3S,4S)-1,3-dihydroxy-2,6-dimethylheptan-4-yl]-L-phenylalaninamide (three-letter code: 3BV) (formula: C<sub>40</sub>H<sub>61</sub>N<sub>5</sub>O<sub>7</sub>).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	H	1	Total	C	N	O	0	0
			52	40	5	7		
17	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	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	V	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	15	Total	O	0	0
			15	15		
19	B	15	Total	O	0	0
			15	15		
19	C	15	Total	O	0	0
			15	15		
19	D	4	Total	O	0	0
			4	4		
19	E	4	Total	O	0	0
			4	4		
19	F	10	Total	O	0	0
			10	10		
19	G	17	Total	O	0	0
			17	17		
19	H	22	Total	O	0	0
			22	22		
19	I	12	Total	O	0	0
			12	12		
19	J	14	Total	O	0	0
			14	14		
19	K	12	Total	O	0	0
			12	12		
19	L	20	Total	O	0	0
			20	20		
19	M	14	Total	O	0	0
			14	14		
19	N	16	Total	O	0	0
			16	16		
19	O	8	Total	O	0	0
			8	8		
19	P	13	Total	O	0	0
			13	13		
19	Q	12	Total	O	0	0
			12	12		
19	R	8	Total	O	0	0
			8	8		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	S	6	Total 6	O 6	0	0
19	T	9	Total 9	O 9	0	0
19	U	12	Total 12	O 12	0	0
19	V	15	Total 15	O 15	0	0
19	W	13	Total 13	O 13	0	0
19	X	10	Total 10	O 10	0	0
19	Y	14	Total 14	O 14	0	0
19	Z	18	Total 18	O 18	0	0
19	a	24	Total 24	O 24	0	0
19	b	18	Total 18	O 18	0	0

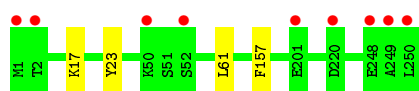
### 3 Residue-property plots [i](#)

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

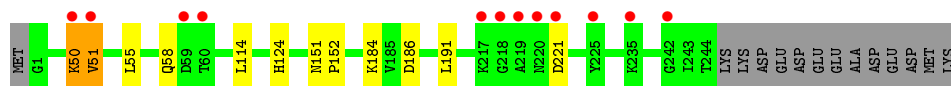
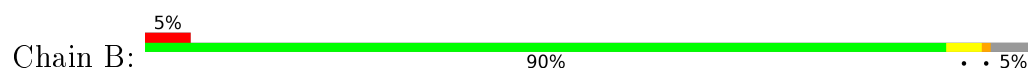
- Molecule 1: Proteasome subunit alpha type-2



- Molecule 1: Proteasome subunit alpha type-2



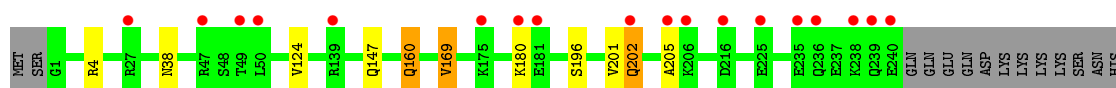
- Molecule 2: Proteasome subunit alpha type-3



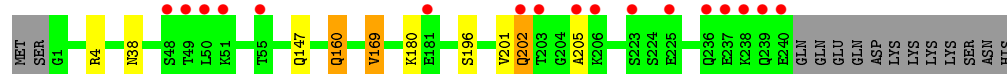
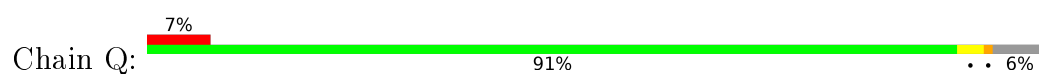
- Molecule 2: Proteasome subunit alpha type-3



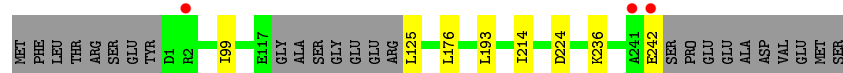
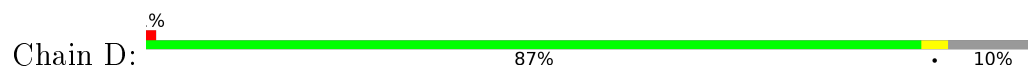
- Molecule 3: Proteasome subunit alpha type-4



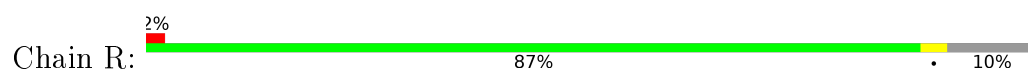
- Molecule 3: Proteasome subunit alpha type-4



- Molecule 4: Proteasome subunit alpha type-5



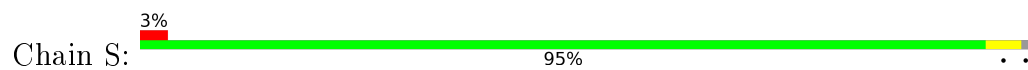
- Molecule 4: Proteasome subunit alpha type-5



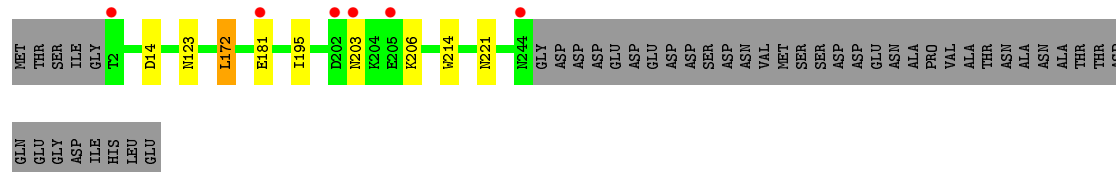
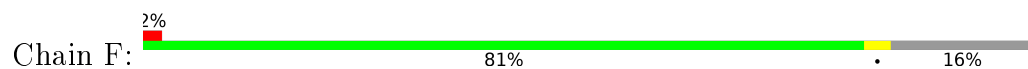
- Molecule 5: Proteasome subunit alpha type-6



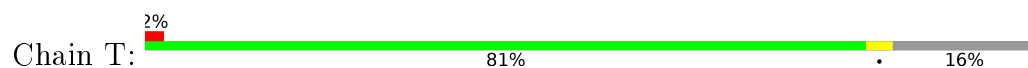
- Molecule 5: Proteasome subunit alpha type-6



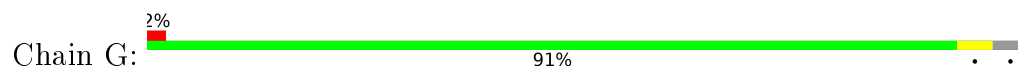
- Molecule 6: Probable proteasome subunit alpha type-7



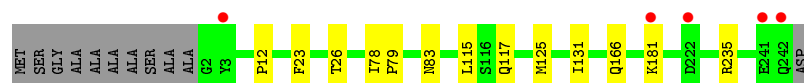
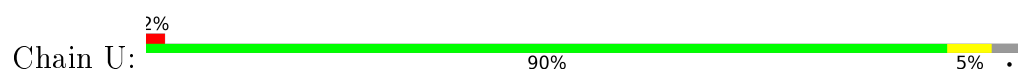
- Molecule 6: Probable proteasome subunit alpha type-7



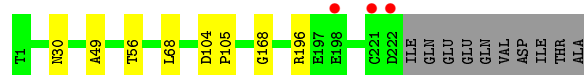
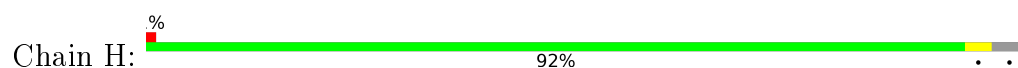
- Molecule 7: Proteasome subunit alpha type-1



- Molecule 7: Proteasome subunit alpha type-1



- Molecule 8: Proteasome subunit beta type-2



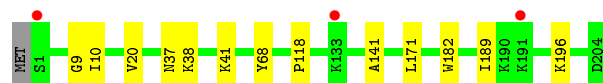
- Molecule 8: Proteasome subunit beta type-2



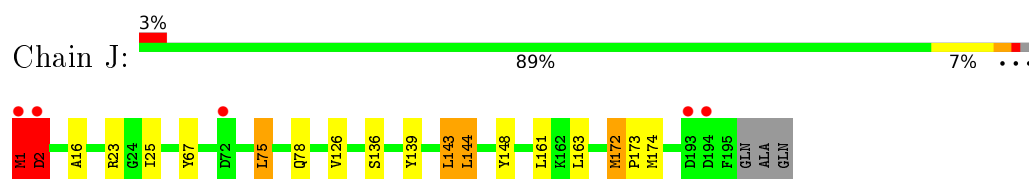
- Molecule 9: Proteasome subunit beta type-3



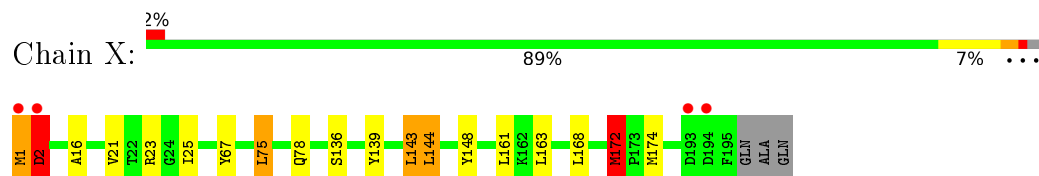
- Molecule 9: Proteasome subunit beta type-3



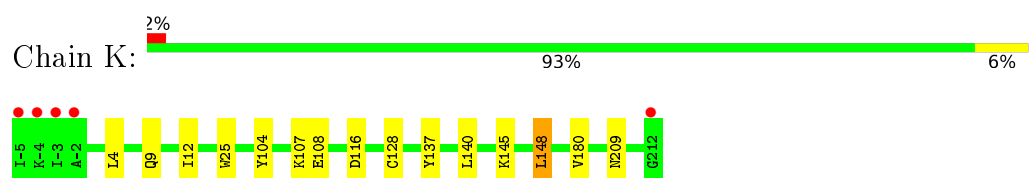
- Molecule 10: Proteasome subunit beta type-4



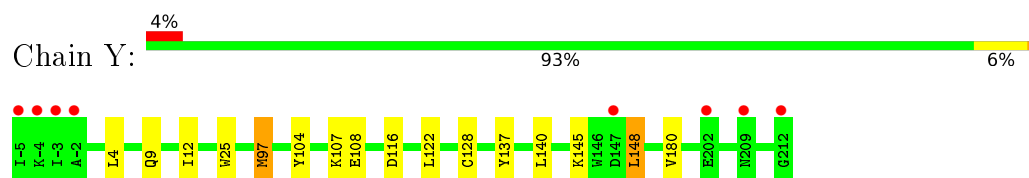
- Molecule 10: Proteasome subunit beta type-4



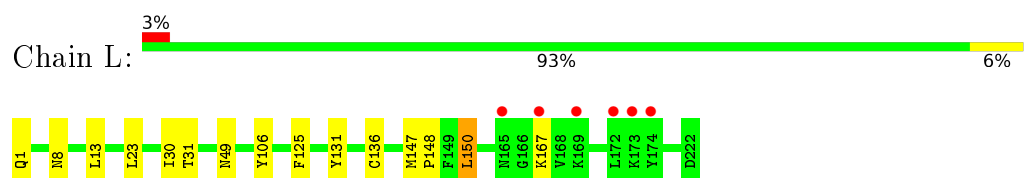
- Molecule 11: Proteasome subunit beta type-5



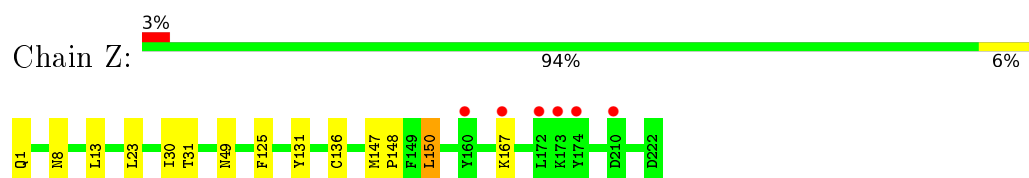
- Molecule 11: Proteasome subunit beta type-5



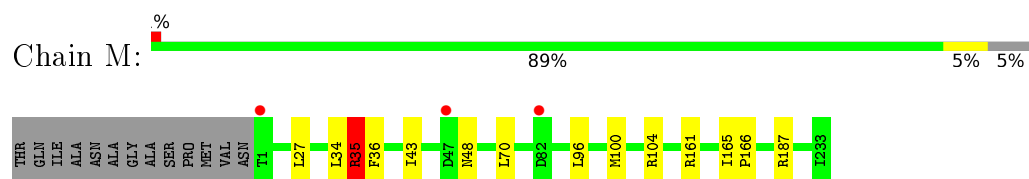
- Molecule 12: Proteasome subunit beta type-6



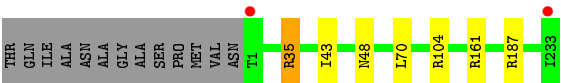
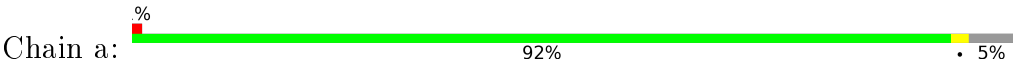
- Molecule 12: Proteasome subunit beta type-6



- Molecule 13: Proteasome subunit beta type-7



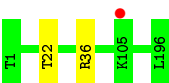
- Molecule 13: Proteasome subunit beta type-7



• Molecule 14: Proteasome subunit beta type-1



• Molecule 14: Proteasome subunit beta type-1





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	136.16Å 301.55Å 145.79Å 90.00° 113.20° 90.00°	Depositor
Resolution (Å)	15.00 – 2.60 15.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.7 (15.00-2.60) 98.7 (15.00-2.60)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.90 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.190 , 0.214 0.194 , 0.215	Depositor DCC
$R_{free}$ test set	16193 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	56.2	Xtriage
Anisotropy	0.068	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 41.5	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	0.95	EDS
Total number of atoms	49996	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.26% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 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	0.27	0/1934	0.48	0/2618
3	C	0.28	0/1910	0.50	0/2586
3	Q	0.28	0/1910	0.50	0/2586
4	D	0.27	0/1837	0.46	0/2475
4	R	0.27	0/1837	0.46	0/2475
5	E	0.27	0/1800	0.46	0/2433
5	S	0.27	0/1800	0.46	0/2433
6	F	0.28	0/1932	0.44	0/2609
6	T	0.27	0/1932	0.44	0/2609
7	G	0.27	0/1945	0.46	0/2634
7	U	0.28	0/1944	0.46	0/2632
8	H	0.26	0/1715	0.47	0/2326
8	V	0.26	0/1715	0.47	0/2326
9	I	0.27	0/1611	0.49	0/2174
9	W	0.27	0/1611	0.49	0/2174
10	J	0.43	2/1589 (0.1%)	0.68	6/2142 (0.3%)
10	X	0.53	5/1589 (0.3%)	0.82	6/2142 (0.3%)
11	K	0.26	0/1720	0.50	0/2326
11	Y	0.26	0/1720	0.51	1/2326 (0.0%)
12	L	0.27	0/1806	0.47	0/2435
12	Z	0.27	0/1795	0.47	0/2420
13	M	0.27	0/1855	0.74	3/2514 (0.1%)
13	a	0.27	0/1855	0.77	3/2514 (0.1%)
14	N	0.26	0/1541	0.48	0/2087
14	b	0.26	0/1541	0.48	0/2087
All	All	0.29	7/50282 (0.0%)	0.52	19/67985 (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
10	X	0	1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	X	1	MET	SD-CE	9.74	2.32	1.77
10	X	2	ASP	N-CA	-7.89	1.30	1.46
10	J	1	MET	CB-CG	-7.82	1.26	1.51
10	X	1	MET	CG-SD	6.77	1.98	1.81
10	J	2	ASP	N-CA	-6.54	1.33	1.46
10	X	1	MET	CB-CG	-5.81	1.32	1.51
10	X	1	MET	CA-C	-5.53	1.38	1.52

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	X	1	MET	CA-CB-CG	-22.15	75.64	113.30
13	a	35	ARG	NE-CZ-NH2	-19.49	110.56	120.30
13	a	35	ARG	NE-CZ-NH1	18.77	129.68	120.30
13	M	35	ARG	NE-CZ-NH1	-18.45	111.07	120.30
13	M	35	ARG	NE-CZ-NH2	17.41	129.01	120.30
10	X	2	ASP	N-CA-CB	-10.08	92.45	110.60
10	J	1	MET	CA-CB-CG	-9.65	96.90	113.30
10	X	172	MET	CB-CG-SD	-8.81	85.96	112.40
13	a	35	ARG	CD-NE-CZ	8.71	135.79	123.60
13	M	35	ARG	CD-NE-CZ	8.16	135.03	123.60
10	J	1	MET	N-CA-CB	-8.04	96.13	110.60
10	J	1	MET	CG-SD-CE	-7.71	87.86	100.20
10	X	1	MET	CB-CG-SD	-7.52	89.84	112.40
10	X	2	ASP	N-CA-C	6.68	129.03	111.00
10	J	2	ASP	CB-CG-OD1	-6.57	112.39	118.30
10	J	2	ASP	N-CA-CB	-6.54	98.84	110.60
10	X	1	MET	C-N-CA	-6.14	106.34	121.70
10	J	1	MET	CB-CG-SD	5.67	129.43	112.40
11	Y	97	MET	CB-CG-SD	5.03	127.50	112.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
10	X	2	ASP	Peptide

## 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	0	0
1	O	1915	0	1929	1	0
2	B	1904	0	1904	3	0
2	P	1904	0	1904	3	0
3	C	1881	0	1895	5	0
3	Q	1881	0	1895	4	0
4	D	1813	0	1797	0	0
4	R	1813	0	1797	0	0
5	E	1773	0	1775	1	0
5	S	1773	0	1775	1	0
6	F	1892	0	1883	1	0
6	T	1892	0	1883	1	0
7	G	1907	0	1901	2	0
7	U	1906	0	1901	4	0
8	H	1684	0	1686	3	0
8	V	1684	0	1685	4	0
9	I	1581	0	1574	5	0
9	W	1581	0	1574	7	0
10	J	1561	0	1568	13	0
10	X	1561	0	1569	30	0
11	K	1683	0	1643	7	0
11	Y	1683	0	1643	7	0
12	L	1767	0	1717	6	0
12	Z	1757	0	1711	5	0
13	M	1824	0	1832	4	0
13	a	1824	0	1832	0	0
14	N	1512	0	1478	1	0
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	N	52	0	59	0	0
17	V	52	0	59	2	0
17	b	52	0	59	0	0
18	H	12	0	13	0	0
18	V	12	0	13	0	0
19	A	15	0	0	0	0
19	B	15	0	0	0	0
19	C	15	0	0	0	0
19	D	4	0	0	0	0
19	E	4	0	0	0	0
19	F	10	0	0	0	0
19	G	17	0	0	0	0
19	H	22	0	0	0	0
19	I	12	0	0	0	0
19	J	14	0	0	0	0
19	K	12	0	0	0	0
19	L	20	0	0	0	0
19	M	14	0	0	0	0
19	N	16	0	0	0	0
19	O	8	0	0	0	0
19	P	13	0	0	0	0
19	Q	12	0	0	0	0
19	R	8	0	0	0	0
19	S	6	0	0	0	0
19	T	9	0	0	0	0
19	U	12	0	0	0	0
19	V	15	0	0	0	0
19	W	13	0	0	0	0
19	X	10	0	0	1	0
19	Y	14	0	0	0	0
19	Z	18	0	0	0	0
19	a	24	0	0	0	0
19	b	18	0	0	0	0
All	All	49996	0	49420	106	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 (106) 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)
10:X:1:MET:CE	10:X:2:ASP:N	2.00	1.24
10:J:174:MET:SD	10:X:174:MET:SD	2.38	1.22
10:X:1:MET:SD	10:X:1:MET:CE	2.32	1.17
10:X:1:MET:HA	10:X:1:MET:CE	1.81	1.10
10:J:25:ILE:O	10:X:139:TYR:OH	1.70	1.09
10:X:1:MET:CA	10:X:1:MET:CE	2.36	1.03
10:X:1:MET:C	10:X:1:MET:CE	2.29	1.01
10:J:139:TYR:OH	10:X:25:ILE:O	1.83	0.96
10:X:1:MET:C	10:X:1:MET:HE2	1.91	0.91
10:X:1:MET:CE	10:X:2:ASP:HB2	2.04	0.86
10:X:1:MET:HE2	10:X:2:ASP:HB2	1.59	0.83
10:J:1:MET:O	10:J:2:ASP:OD2	1.88	0.81
10:X:1:MET:HE1	10:X:2:ASP:N	1.96	0.80
10:X:1:MET:CE	10:X:2:ASP:CB	2.60	0.80
10:X:1:MET:HE2	10:X:2:ASP:CB	2.12	0.80
10:X:1:MET:HE2	10:X:1:MET:CA	2.12	0.76
10:X:1:MET:CE	10:X:2:ASP:H	2.00	0.70
10:X:1:MET:HB3	19:X:209:HOH:O	1.91	0.69
10:J:1:MET:HE1	10:J:2:ASP:HA	1.78	0.66
10:X:1:MET:HE1	10:X:2:ASP:HB2	1.77	0.65
10:X:1:MET:HE2	10:X:2:ASP:CG	2.17	0.65
10:J:1:MET:CE	10:J:2:ASP:HA	2.32	0.59
10:J:1:MET:CE	10:J:2:ASP:CA	2.76	0.56
14:N:152:VAL:HA	14:N:175:MET:HE1	1.86	0.56
8:V:218:VAL:CG2	9:W:196:LYS:HB2	2.36	0.55
10:X:1:MET:CE	10:X:2:ASP:CA	2.81	0.55
10:X:67:TYR:CE1	10:X:75:LEU:HD13	2.43	0.54
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.90	0.54
10:X:1:MET:HE2	10:X:1:MET:N	2.23	0.53
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.90	0.53
8:H:168:GLY:O	17:H:301:3BV:H57	2.09	0.53
11:K:128:CYS:HB2	11:K:137:TYR:CZ	2.44	0.53
10:J:67:TYR:CE1	10:J:75:LEU:HD13	2.44	0.53
10:X:1:MET:HE1	10:X:2:ASP:CA	2.39	0.52
11:Y:128:CYS:HB2	11:Y:137:TYR:CZ	2.45	0.52
8:V:168:GLY:O	17:V:301:3BV:H57	2.09	0.52
3:C:201:VAL:O	3:C:202:GLN:CB	2.59	0.51
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.59	0.51
10:X:1:MET:N	10:X:1:MET:CE	2.73	0.50
10:X:21:VAL:HG11	11:Y:122:LEU:HD11	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:128:CYS:HB2	11:K:137:TYR:CE2	2.48	0.48
3:C:169:VAL:HG23	3:C:196:SER:HB2	1.96	0.48
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.96	0.48
9:I:9:GLY:HA3	9:I:41:LYS:HE2	1.96	0.47
3:Q:169:VAL:HG23	3:Q:196:SER:HB2	1.96	0.47
7:G:23:PHE:O	7:G:26:THR:HB	2.15	0.47
10:X:168:LEU:O	10:X:172:MET:HB2	2.14	0.47
11:Y:128:CYS:HB2	11:Y:137:TYR:CE2	2.49	0.47
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.96	0.47
11:Y:107:LYS:HG3	11:Y:108:GLU:HG3	1.97	0.47
9:W:9:GLY:HA3	9:W:41:LYS:HE2	1.96	0.47
9:I:20:VAL:HG13	9:I:118:PRO:HB3	1.97	0.47
13:M:35:ARG:HG2	13:M:36:PHE:CE2	2.50	0.47
10:X:1:MET:HE1	10:X:2:ASP:CB	2.38	0.46
9:W:20:VAL:HG13	9:W:118:PRO:HB3	1.96	0.46
11:Y:25:TRP:HH2	12:Z:147:MET:HB3	1.80	0.46
11:K:107:LYS:HG3	11:K:108:GLU:HG3	1.97	0.46
11:K:25:TRP:HH2	12:L:147:MET:HB3	1.81	0.46
10:X:143:LEU:HD21	10:X:163:LEU:HG	1.97	0.46
7:U:23:PHE:O	7:U:26:THR:HB	2.15	0.46
10:J:143:LEU:HD21	10:J:163:LEU:HG	1.97	0.46
5:S:87:LEU:HD21	5:S:107:ALA:HB1	1.97	0.45
2:P:95:GLN:HB3	9:W:68:TYR:CD2	2.52	0.44
5:E:87:LEU:HD21	5:E:107:ALA:HB1	1.98	0.44
6:F:172:LEU:CD1	6:F:195:ILE:HD13	2.47	0.44
9:I:36:SER:HB2	10:J:126:VAL:HG11	2.00	0.44
8:V:104:ASP:HB2	8:V:105:PRO:HD2	1.99	0.44
6:T:172:LEU:CD1	6:T:195:ILE:HD13	2.47	0.44
12:Z:147:MET:N	12:Z:148:PRO:HD2	2.33	0.44
8:H:104:ASP:HB2	8:H:105:PRO:HD2	1.99	0.44
11:Y:145:LYS:HB2	11:Y:148:LEU:HD13	1.99	0.43
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.53	0.43
13:M:96:LEU:O	13:M:100:MET:HG2	2.19	0.43
9:W:20:VAL:HG23	9:W:189:ILE:HB	2.01	0.43
12:L:147:MET:N	12:L:148:PRO:HD2	2.33	0.42
7:G:78:ILE:N	7:G:79:PRO:CD	2.82	0.42
11:K:209:ASN:O	9:W:38:LYS:NZ	2.52	0.42
9:I:20:VAL:HG23	9:I:189:ILE:HB	2.00	0.42
11:K:145:LYS:HB2	11:K:148:LEU:HD13	2.00	0.42
3:C:201:VAL:HG13	3:C:202:GLN:N	2.34	0.42
7:U:78:ILE:N	7:U:79:PRO:CD	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:27:LEU:HD21	13:M:34:LEU:HD22	2.01	0.42
3:Q:201:VAL:HG13	3:Q:202:GLN:N	2.34	0.42
10:J:144:LEU:O	10:J:148:TYR:HB3	2.20	0.42
8:V:49:ALA:HA	17:V:301:3BV:H50	2.02	0.42
8:H:49:ALA:HA	17:H:301:3BV:H50	2.02	0.41
12:L:8:ASN:HA	12:L:30:ILE:O	2.20	0.41
2:B:124:HIS:HB3	3:C:124:VAL:HG12	2.02	0.41
2:P:151:ASN:HB2	2:P:152:PRO:CD	2.50	0.41
10:X:144:LEU:O	10:X:148:TYR:HB3	2.19	0.41
12:L:13:LEU:CD1	12:L:150:LEU:HD21	2.50	0.41
12:Z:13:LEU:CD1	12:Z:150:LEU:HD21	2.51	0.41
2:B:151:ASN:HB2	2:B:152:PRO:CD	2.50	0.41
13:M:165:ILE:HB	13:M:166:PRO:HD3	2.03	0.41
7:U:26:THR:HG21	7:U:131:ILE:HD12	2.03	0.41
10:J:172:MET:HA	10:J:173:PRO:HD3	1.93	0.41
12:Z:125:PHE:CD2	12:Z:131:TYR:HB3	2.56	0.41
3:C:160:GLN:HA	3:C:160:GLN:HE21	1.85	0.41
12:L:125:PHE:CD2	12:L:131:TYR:HB3	2.56	0.41
3:Q:160:GLN:HA	3:Q:160:GLN:HE21	1.85	0.41
2:B:50:LYS:O	2:B:51:VAL:C	2.59	0.41
2:P:50:LYS:O	2:P:51:VAL:C	2.59	0.41
11:Y:12:ILE:HB	11:Y:180:VAL:HB	2.03	0.41
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.20	0.40
12:L:13:LEU:HD13	12:L:150:LEU:HD21	2.04	0.40
11:K:12:ILE:HB	11:K:180:VAL:HB	2.03	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	O	248/250 (99%)	242 (98%)	6 (2%)	0	100	100
2	B	242/258 (94%)	235 (97%)	5 (2%)	2 (1%)	24	46
2	P	242/258 (94%)	235 (97%)	5 (2%)	2 (1%)	24	46
3	C	238/254 (94%)	229 (96%)	7 (3%)	2 (1%)	24	46
3	Q	238/254 (94%)	229 (96%)	7 (3%)	2 (1%)	24	46
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%)	224 (98%)	5 (2%)	0	100	100
5	S	229/234 (98%)	224 (98%)	5 (2%)	0	100	100
6	F	241/288 (84%)	235 (98%)	6 (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%)	213 (97%)	7 (3%)	0	100	100
8	V	220/232 (95%)	213 (97%)	7 (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%)	3 (2%)	1 (0%)	34	60
11	K	216/218 (99%)	210 (97%)	6 (3%)	0	100	100
11	Y	216/218 (99%)	211 (98%)	5 (2%)	0	100	100
12	L	221/222 (100%)	218 (99%)	3 (1%)	0	100	100
12	Z	220/222 (99%)	217 (99%)	3 (1%)	0	100	100
13	M	231/246 (94%)	221 (96%)	10 (4%)	0	100	100
13	a	231/246 (94%)	221 (96%)	10 (4%)	0	100	100
14	N	194/196 (99%)	187 (96%)	7 (4%)	0	100	100
14	b	194/196 (99%)	187 (96%)	7 (4%)	0	100	100
All	All	6289/6626 (95%)	6121 (97%)	159 (2%)	9 (0%)	56	81

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	51	VAL

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Mol	Chain	Res	Type
3	C	202	GLN
2	P	51	VAL
3	Q	202	GLN
10	X	2	ASP
2	B	221	ASP
3	C	205	ALA
2	P	221	ASP
3	Q	205	ALA

### 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%)	74	90
1	O	209/209 (100%)	206 (99%)	3 (1%)	74	90
2	B	203/216 (94%)	196 (97%)	7 (3%)	44	72
2	P	203/216 (94%)	196 (97%)	7 (3%)	44	72
3	C	212/226 (94%)	206 (97%)	6 (3%)	51	78
3	Q	212/226 (94%)	206 (97%)	6 (3%)	51	78
4	D	194/215 (90%)	186 (96%)	8 (4%)	37	66
4	R	194/215 (90%)	186 (96%)	8 (4%)	37	66
5	E	190/193 (98%)	183 (96%)	7 (4%)	41	69
5	S	190/193 (98%)	183 (96%)	7 (4%)	41	69
6	F	201/239 (84%)	193 (96%)	8 (4%)	38	67
6	T	201/239 (84%)	193 (96%)	8 (4%)	38	67
7	G	206/210 (98%)	199 (97%)	7 (3%)	44	72
7	U	206/210 (98%)	199 (97%)	7 (3%)	44	72
8	H	181/190 (95%)	177 (98%)	4 (2%)	60	83
8	V	181/190 (95%)	177 (98%)	4 (2%)	60	83
9	I	172/173 (99%)	169 (98%)	3 (2%)	68	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	W	172/173 (99%)	169 (98%)	3 (2%)	68	88
10	J	173/175 (99%)	164 (95%)	9 (5%)	29	54
10	X	173/175 (99%)	166 (96%)	7 (4%)	38	67
11	K	172/172 (100%)	166 (96%)	6 (4%)	43	71
11	Y	172/172 (100%)	165 (96%)	7 (4%)	37	66
12	L	186/185 (100%)	178 (96%)	8 (4%)	35	64
12	Z	185/185 (100%)	178 (96%)	7 (4%)	40	68
13	M	199/208 (96%)	192 (96%)	7 (4%)	43	71
13	a	199/208 (96%)	192 (96%)	7 (4%)	43	71
14	N	162/162 (100%)	160 (99%)	2 (1%)	78	92
14	b	162/162 (100%)	160 (99%)	2 (1%)	78	92
All	All	5319/5546 (96%)	5151 (97%)	168 (3%)	46	74

All (168) 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	186	ASP
2	B	191	LEU
3	C	4	ARG
3	C	38	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
4	D	193	LEU
4	D	214	ILE
4	D	224	ASP

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Mol	Chain	Res	Type
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	117	GLN
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	1	MET
10	J	2	ASP
10	J	23	ARG
10	J	75	LEU
10	J	78	GLN
10	J	136	SER
10	J	143	LEU
10	J	144	LEU
10	J	172	MET
11	K	4	LEU
11	K	9	GLN

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Mol	Chain	Res	Type
11	K	104	TYR
11	K	116	ASP
11	K	140	LEU
11	K	148	LEU
12	L	1	GLN
12	L	23	LEU
12	L	31	THR
12	L	49	ASN
12	L	106	TYR
12	L	136	CYS
12	L	150	LEU
12	L	167	LYS
13	M	35	ARG
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
14	N	36	ARG
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	186	ASP
2	P	191	LEU
3	Q	4	ARG
3	Q	38	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

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Mol	Chain	Res	Type
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
5	S	188	LEU
5	S	202	ASP
6	T	14	ASP
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	117	GLN
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	68	LEU
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	136	SER
10	X	143	LEU
10	X	144	LEU
10	X	172	MET
11	Y	4	LEU
11	Y	9	GLN
11	Y	97	MET

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Mol	Chain	Res	Type
11	Y	104	TYR
11	Y	116	ASP
11	Y	140	LEU
11	Y	148	LEU
12	Z	1	GLN
12	Z	23	LEU
12	Z	31	THR
12	Z	49	ASN
12	Z	136	CYS
12	Z	150	LEU
12	Z	167	LYS
13	a	35	ARG
13	a	43	ILE
13	a	48	ASN
13	a	70	LEU
13	a	104	ARG
13	a	161	ARG
13	a	187	ARG
14	b	22	THR
14	b	36	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) 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	92	GLN
3	C	147	GLN
3	C	160	GLN
4	D	91	HIS
5	E	68	HIS
5	E	92	ASN
5	E	99	ASN
5	E	116	GLN
5	E	120	GLN
5	E	184	ASN
6	F	117	GLN
6	F	123	ASN
6	F	191	GLN

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Mol	Chain	Res	Type
6	F	240	GLN
7	G	83	ASN
7	G	117	GLN
7	G	121	GLN
9	I	203	GLN
10	J	55	GLN
11	K	85	ASN
11	K	176	ASN
12	L	3	ASN
12	L	70	ASN
12	L	158	ASN
12	L	159	GLN
13	M	48	ASN
13	M	102	GLN
13	M	179	ASN
1	O	94	HIS
2	P	20	GLN
2	P	95	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	100	ASN
4	R	146	GLN
5	S	68	HIS
5	S	99	ASN
5	S	116	GLN
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
10	X	55	GLN
11	Y	85	ASN
11	Y	176	ASN

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Mol	Chain	Res	Type
12	Z	3	ASN
12	Z	108	HIS
12	Z	158	ASN
13	a	48	ASN
13	a	102	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 11 are monoatomic - leaving 6 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	1.11	3 (5%)	67,71,71	1.42	7 (10%)
18	MES	H	302	-	12,12,12	2.05	1 (8%)	15,16,16	2.02	2 (13%)
17	3BV	N	201	14	54,54,54	1.29	3 (5%)	67,71,71	1.44	11 (16%)
17	3BV	V	301	8	54,54,54	1.10	3 (5%)	67,71,71	1.42	7 (10%)
18	MES	V	302	-	12,12,12	2.10	1 (8%)	15,16,16	1.89	3 (20%)
17	3BV	b	201	14	54,54,54	1.26	3 (5%)	67,71,71	1.45	10 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	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	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	b	201	14	-	0/59/67/67	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	V	302	MES	C8-S	-6.95	1.67	1.77
18	H	302	MES	C8-S	-6.78	1.67	1.77
17	H	301	3BV	C32-C33	-4.55	1.40	1.51
17	N	201	3BV	C32-C33	-4.39	1.40	1.51
17	V	301	3BV	C32-C33	-4.35	1.40	1.51
17	b	201	3BV	C32-C33	-4.29	1.40	1.51
17	N	201	3BV	C13-C14	-3.80	1.40	1.51
17	b	201	3BV	C13-C14	-3.74	1.40	1.51
17	H	301	3BV	C13-C14	-3.38	1.41	1.51
17	V	301	3BV	C13-C14	-3.29	1.42	1.51
17	V	301	3BV	C51-C47	3.99	1.61	1.53
17	H	301	3BV	C51-C47	4.00	1.61	1.53
17	b	201	3BV	C51-C47	5.69	1.64	1.53
17	N	201	3BV	C51-C47	6.05	1.64	1.53

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	H	301	3BV	C43-C42-N41	-5.51	102.44	109.98
17	V	301	3BV	C43-C42-N41	-5.39	102.60	109.98
17	b	201	3BV	C43-C42-N41	-5.18	102.89	109.98
17	N	201	3BV	C43-C42-N41	-5.13	102.96	109.98
17	b	201	3BV	C58-C51-C59	-5.12	103.00	109.73
17	N	201	3BV	C58-C51-C59	-5.05	103.09	109.73
17	V	301	3BV	C58-C51-C59	-4.63	103.64	109.73
17	H	301	3BV	C58-C51-C59	-4.51	103.80	109.73
17	H	301	3BV	O1-C6-C5	-3.84	102.96	111.83
17	V	301	3BV	O1-C6-C5	-3.84	102.97	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	H	301	3BV	C25-C24-C23	-3.15	106.03	115.49
17	V	301	3BV	C25-C24-C23	-3.13	106.08	115.49
17	N	201	3BV	O1-C6-C5	-3.12	104.62	111.83
17	b	201	3BV	O1-C6-C5	-3.02	104.84	111.83
17	V	301	3BV	C33-C32-C31	-2.98	104.65	113.44
17	H	301	3BV	C33-C32-C31	-2.94	104.75	113.44
17	b	201	3BV	O1-C2-C3	-2.89	105.15	111.83
17	N	201	3BV	O1-C2-C3	-2.80	105.35	111.83
17	b	201	3BV	C33-C32-C31	-2.79	105.20	113.44
17	N	201	3BV	C33-C32-C31	-2.69	105.50	113.44
17	b	201	3BV	C12-C13-C14	-2.67	103.32	113.18
17	b	201	3BV	C7-N4-C3	-2.65	107.25	111.14
17	N	201	3BV	C12-C13-C14	-2.62	103.49	113.18
17	N	201	3BV	C7-N4-C3	-2.62	107.29	111.14
17	b	201	3BV	C25-C24-C23	-2.24	108.75	115.49
17	H	301	3BV	O60-C59-C51	-2.22	106.51	111.16
17	N	201	3BV	C25-C24-C23	-2.22	108.83	115.49
17	V	301	3BV	O60-C59-C51	-2.21	106.54	111.16
17	b	201	3BV	C12-C11-C20	-2.11	105.16	110.34
17	V	301	3BV	C6-C5-N4	-2.09	106.92	110.11
17	H	301	3BV	C6-C5-N4	-2.08	106.92	110.11
17	N	201	3BV	C12-C11-C20	-2.07	105.26	110.34
17	N	201	3BV	O60-C59-C51	-2.02	106.93	111.16
18	V	302	MES	O3S-S-C8	2.20	109.56	104.99
17	N	201	3BV	C3-N4-C5	2.35	114.12	108.87
17	b	201	3BV	C3-N4-C5	2.41	114.27	108.87
18	V	302	MES	O2S-S-C8	3.92	109.64	106.87
18	H	302	MES	O1S-S-C8	3.96	109.67	106.87
18	V	302	MES	O1S-S-C8	5.07	110.45	106.87
18	H	302	MES	O2S-S-C8	5.80	110.97	106.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	H	301	3BV	2	0
17	V	301	3BV	2	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	250/250 (100%)	-0.33	7 (2%) 56 49	39, 55, 92, 146	0
1	O	250/250 (100%)	-0.26	9 (3%) 46 38	45, 63, 108, 148	0
2	B	244/258 (94%)	-0.16	12 (4%) 33 26	41, 60, 108, 162	0
2	P	244/258 (94%)	-0.09	13 (5%) 30 23	45, 64, 112, 165	0
3	C	240/254 (94%)	-0.03	18 (7%) 17 12	42, 66, 137, 175	0
3	Q	240/254 (94%)	0.08	17 (7%) 19 13	48, 75, 158, 191	0
4	D	235/260 (90%)	-0.32	3 (1%) 79 75	46, 68, 101, 149	0
4	R	235/260 (90%)	-0.19	5 (2%) 67 61	49, 70, 111, 153	0
5	E	231/234 (98%)	-0.19	7 (3%) 54 47	45, 69, 105, 149	0
5	S	231/234 (98%)	-0.11	7 (3%) 54 47	50, 76, 121, 158	0
6	F	243/288 (84%)	-0.32	6 (2%) 61 54	42, 63, 113, 145	0
6	T	243/288 (84%)	-0.25	6 (2%) 61 54	39, 71, 131, 170	0
7	G	241/252 (95%)	-0.37	5 (2%) 67 61	38, 56, 98, 145	0
7	U	241/252 (95%)	-0.34	5 (2%) 67 61	35, 60, 93, 139	0
8	H	222/232 (95%)	-0.49	3 (1%) 78 74	39, 51, 87, 128	0
8	V	222/232 (95%)	-0.37	4 (1%) 71 66	39, 56, 94, 138	0
9	I	204/205 (99%)	-0.65	1 (0%) 91 90	36, 51, 82, 102	0
9	W	204/205 (99%)	-0.57	3 (1%) 76 71	37, 54, 84, 112	0
10	J	195/198 (98%)	-0.34	5 (2%) 59 53	36, 57, 85, 124	0
10	X	195/198 (98%)	-0.40	4 (2%) 67 61	40, 58, 87, 135	0
11	K	218/218 (100%)	-0.38	5 (2%) 64 57	40, 56, 83, 104	4 (1%)
11	Y	218/218 (100%)	-0.28	8 (3%) 45 37	41, 56, 86, 110	0
12	L	222/222 (100%)	-0.31	6 (2%) 58 51	36, 58, 107, 149	0
12	Z	222/222 (100%)	-0.32	6 (2%) 58 51	35, 57, 102, 134	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
13	M	233/246 (94%)	-0.60	3 (1%)	79	75	35, 54, 78, 89	0
13	a	233/246 (94%)	-0.58	2 (0%)	85	83	37, 52, 77, 87	0
14	N	196/196 (100%)	-0.56	1 (0%)	91	90	32, 49, 81, 105	0
14	b	196/196 (100%)	-0.58	1 (0%)	91	90	38, 50, 83, 106	0
All	All	6348/6626 (95%)	-0.33	172 (2%)	58	51	32, 60, 108, 191	4 (0%)

All (172) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	MET	8.4
3	C	206	LYS	8.1
1	O	1	MET	8.0
2	P	219	ALA	7.6
3	Q	50	LEU	7.6
2	B	218	GLY	7.1
3	Q	49	THR	7.0
10	J	1	MET	7.0
2	P	218	GLY	6.9
10	X	1	MET	6.7
3	Q	206	LYS	6.6
2	B	220	ASN	6.0
2	B	221	ASP	5.9
5	E	202	ASP	5.7
3	C	49	THR	5.3
9	W	1	SER	5.2
12	Z	174	TYR	5.2
2	P	59	ASP	5.1
8	V	222	ASP	5.1
2	B	219	ALA	5.1
4	R	241	ALA	5.0
8	H	221	CYS	5.0
11	Y	-2	ALA	5.0
3	C	50	LEU	4.9
5	S	233	ILE	4.9
5	S	202	ASP	4.8
12	L	174	TYR	4.7
2	P	52	THR	4.7
8	V	221	CYS	4.6
2	P	220	ASN	4.6
9	I	1	SER	4.3
2	P	221	ASP	4.3

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Mol	Chain	Res	Type	RSRZ
13	a	1	THR	4.3
3	Q	238	LYS	4.2
4	D	241	ALA	4.2
2	P	51	VAL	4.0
10	X	194	ASP	3.9
2	B	51	VAL	3.9
3	C	239	GLN	3.7
3	Q	239	GLN	3.7
3	C	238	LYS	3.6
3	C	202	GLN	3.6
12	L	172	LEU	3.5
3	Q	240	GLU	3.5
11	Y	-4	LYS	3.4
3	Q	236	GLN	3.4
6	T	243	ILE	3.4
12	L	167	LYS	3.4
3	C	225	GLU	3.4
11	K	212	GLY	3.4
4	R	242	GLU	3.4
3	C	236	GLN	3.4
12	Z	167	LYS	3.3
10	J	2	ASP	3.3
12	Z	172	LEU	3.3
3	C	205	ALA	3.3
3	Q	205	ALA	3.3
7	U	242	GLN	3.3
12	L	165	ASN	3.3
1	O	250	LEU	3.3
6	F	202	ASP	3.2
2	B	59	ASP	3.2
2	B	217	LYS	3.2
11	K	-4	LYS	3.2
13	M	1	THR	3.2
8	H	222	ASP	3.2
2	P	203	SER	3.2
11	K	-3	ILE	3.1
2	P	60	THR	3.1
11	Y	212	GLY	3.1
13	M	47	ASP	3.1
1	A	250	LEU	3.0
11	Y	-5	ILE	3.0
1	O	201	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
3	C	181	GLU	3.0
11	K	-2	ALA	3.0
6	F	205	GLU	3.0
10	X	2	ASP	3.0
4	D	242	GLU	3.0
6	T	2	THR	2.9
3	Q	51	LYS	2.8
6	F	2	THR	2.8
12	Z	210	ASP	2.8
2	B	60	THR	2.8
3	C	27	ARG	2.8
7	G	179	LYS	2.8
7	G	222	ASP	2.8
3	Q	48	SER	2.8
1	A	2	THR	2.8
4	R	217	GLN	2.8
7	U	3	TYR	2.8
1	O	249	ALA	2.7
5	E	54	GLU	2.7
1	A	201	GLU	2.6
1	A	248	GLU	2.6
3	C	235	GLU	2.6
2	P	222	GLY	2.6
5	E	233	ILE	2.6
9	W	133	LYS	2.6
10	J	194	ASP	2.6
10	J	193	ASP	2.6
1	A	249	ALA	2.6
5	E	217	LYS	2.5
11	K	-5	ILE	2.5
2	B	242	GLY	2.5
5	E	201	ARG	2.5
1	O	248	GLU	2.5
6	T	244	ASN	2.5
10	X	193	ASP	2.5
4	R	125	LEU	2.5
7	G	3	TYR	2.5
3	C	240	GLU	2.5
3	Q	55	THR	2.5
7	U	222	ASP	2.5
11	Y	209	ASN	2.5
7	G	240	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
5	S	207	VAL	2.5
7	G	181	LYS	2.5
1	O	2	THR	2.5
13	a	233	ILE	2.5
3	Q	225	GLU	2.5
5	S	54	GLU	2.5
11	Y	-3	ILE	2.5
6	F	244	ASN	2.4
3	C	47	ARG	2.4
8	V	145	ASP	2.4
2	B	50	LYS	2.4
3	Q	203	THR	2.4
1	O	52	SER	2.4
2	P	50	LYS	2.4
6	T	181	GLU	2.4
5	E	218	ASP	2.4
3	C	180	LYS	2.4
3	C	216	ASP	2.4
3	Q	237	GLU	2.4
3	Q	223	SER	2.3
5	S	225	ASP	2.3
11	Y	147	ASP	2.3
12	Z	173	LYS	2.3
7	U	241	GLU	2.2
1	O	220	ASP	2.2
14	N	195	GLN	2.2
12	L	169	LYS	2.2
4	D	2	ARG	2.2
3	C	139	ARG	2.2
2	P	182	ASP	2.2
6	T	205	GLU	2.2
2	P	225	TYR	2.1
5	S	3	ASN	2.1
6	F	203	ASN	2.1
13	M	82	ASP	2.1
3	C	175	LYS	2.1
11	Y	202	GLU	2.1
4	R	1	ASP	2.1
8	V	215	GLU	2.1
5	S	210	LEU	2.1
6	F	181	GLU	2.1
12	Z	160	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
7	U	181	LYS	2.1
12	L	173	LYS	2.1
10	J	72	ASP	2.1
3	Q	181	GLU	2.0
6	T	201	GLU	2.0
9	W	191	LYS	2.0
2	B	225	TYR	2.0
8	H	198	GLU	2.0
1	A	229	THR	2.0
3	Q	202	GLN	2.0
5	E	227	GLU	2.0
1	O	50	LYS	2.0
2	B	235	LYS	2.0
14	b	105	LYS	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
18	MES	V	302	12/12	0.85	0.38	9.74	80,82,98,110	0
15	MG	I	301	1/1	0.95	0.42	9.06	74,74,74,74	0
18	MES	H	302	12/12	0.92	0.33	8.31	76,80,88,98	0
15	MG	Z	301	1/1	0.87	0.31	6.96	69,69,69,69	0
17	3BV	b	201	52/52	0.88	0.22	4.99	39,55,133,136	0
17	3BV	N	201	52/52	0.87	0.22	4.59	38,52,133,136	0
17	3BV	V	301	52/52	0.90	0.20	2.41	46,58,106,110	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
17	3BV	H	301	52/52	0.91	0.20	1.97	44,56,103,106	0
15	MG	G	301	1/1	0.94	0.16	0.61	58,58,58,58	0
15	MG	N	202	1/1	0.98	0.08	-1.48	51,51,51,51	0
15	MG	K	301	1/1	0.98	0.08	-1.61	65,65,65,65	0
16	CL	b	202	1/1	0.99	0.06	-1.97	53,53,53,53	0
16	CL	N	203	1/1	0.99	0.06	-2.04	49,49,49,49	0
15	MG	I	302	1/1	0.97	0.07	-4.28	52,52,52,52	0
15	MG	L	301	1/1	0.98	0.05	-4.54	60,60,60,60	0
16	CL	U	301	1/1	0.99	0.13	-	47,47,47,47	0
16	CL	G	302	1/1	0.99	0.09	-	49,49,49,49	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.