



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 13, 2016 – 01:42 AM EST

PDB ID : 5CZ9  
Title : Yeast 20S proteasome beta5-D17N mutant in complex with Carfilzomib;  
Propeptide expressed in trans  
Authors : Huber, E.M.; Groll, M.  
Deposited on : 2015-07-31  
Resolution : 2.90 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

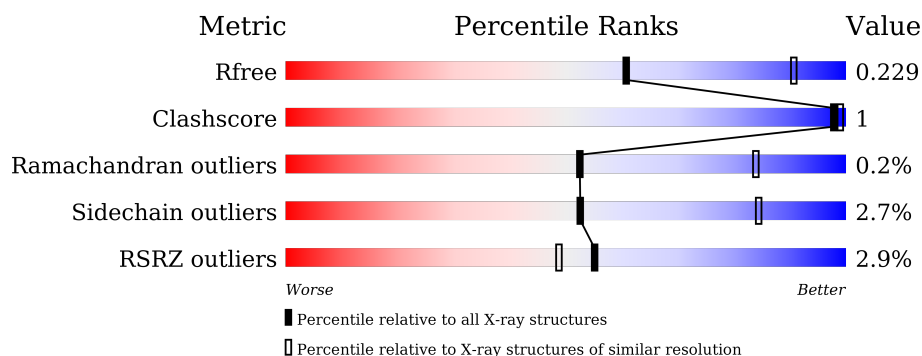
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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.



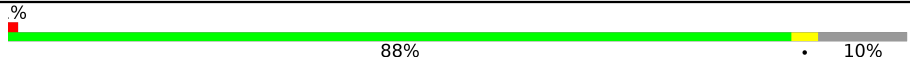

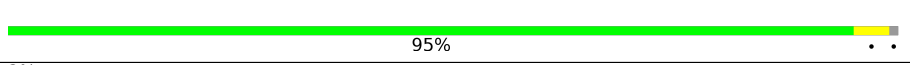
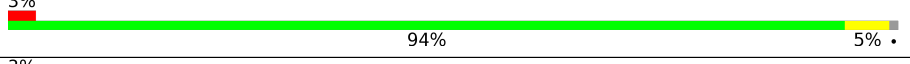
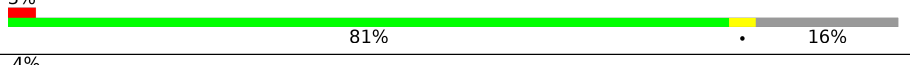
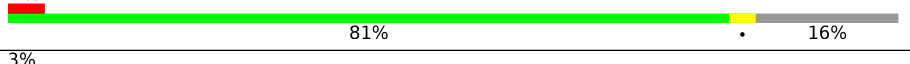
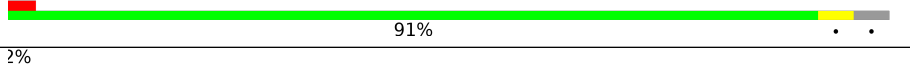
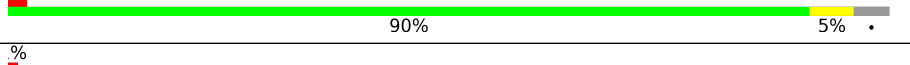
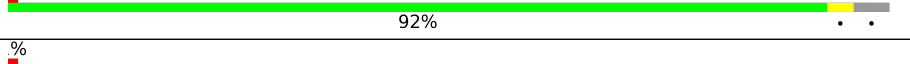
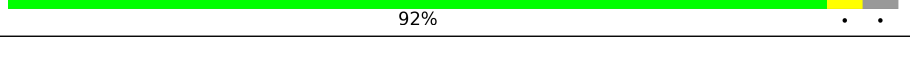
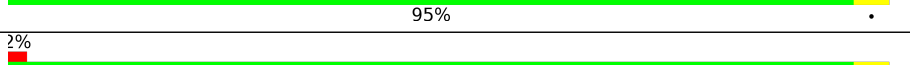


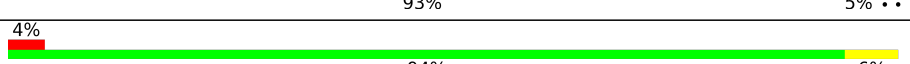
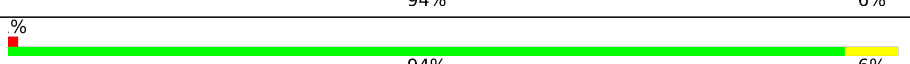
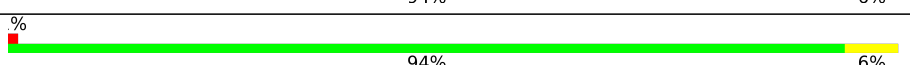
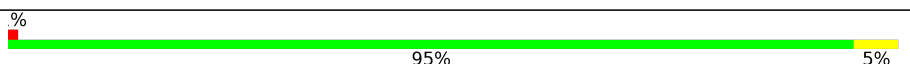
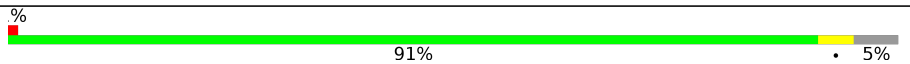
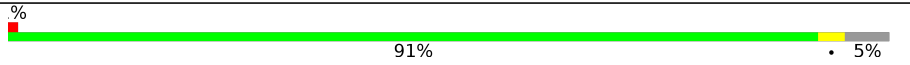
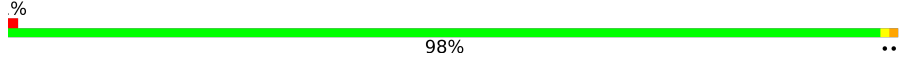
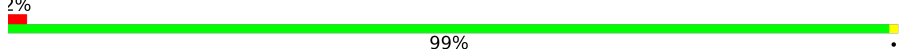
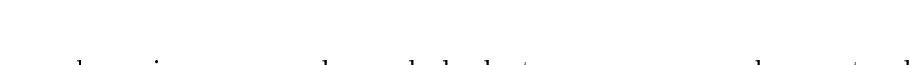
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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>2%</div> <div>99%</div> <div>•</div> </div>
1	O	250	<div> <div>3%</div> <div>98%</div> <div>•</div> </div>
2	B	258	<div> <div>6%</div> <div>90%</div> <div>• • 5%</div> </div>
2	P	258	<div> <div>5%</div> <div>91%</div> <div>• • 5%</div> </div>
3	C	254	<div> <div>8%</div> <div>90%</div> <div>• • 6%</div> </div>
3	Q	254	<div> <div>9%</div> <div>91%</div> <div>• • 6%</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	212	
11	Y	212	
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
17	3BV	H	301	-	-	-	X
17	3BV	K	301	-	-	-	X
17	3BV	N	201	-	-	-	X
17	3BV	V	301	-	-	-	X
17	3BV	Y	301	-	-	-	X
17	3BV	b	201	-	-	-	X
18	MES	H	302	-	-	-	X
18	MES	K	303	-	-	-	X
18	MES	V	303	-	-	-	X
18	MES	Y	303	-	-	-	X

## 2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 50013 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	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	17	ASN	ASP	engineered mutation	UNP P30656
Y	17	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	1	0
			1832	1159	315	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).

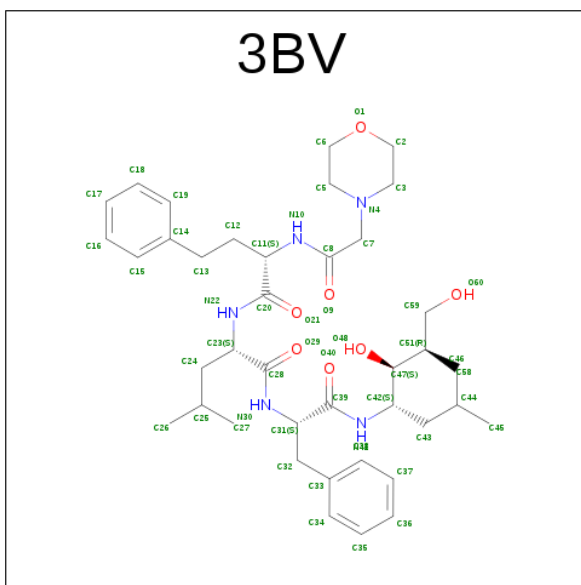
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	G	1	Total Mg 1 1	0	0
15	K	1	Total Mg 1 1	0	0
15	I	1	Total Mg 1 1	0	0
15	V	1	Total Mg 1 1	0	0
15	Z	1	Total Mg 1 1	0	0
15	N	1	Total Mg 1 1	0	0
15	Y	1	Total Mg 1 1	0	0

- 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

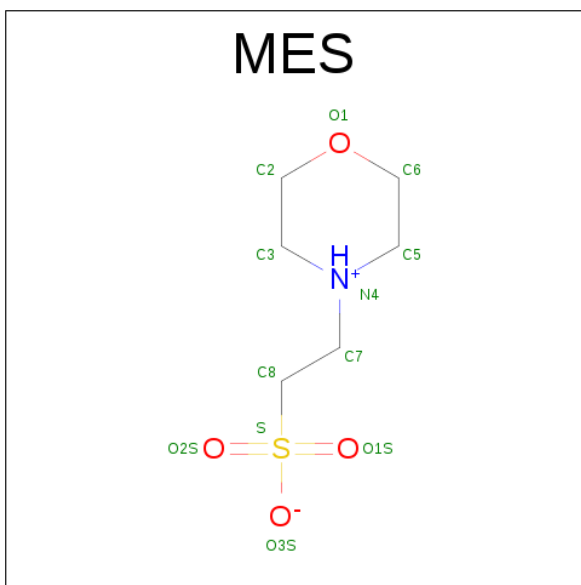
- Molecule 17 is N-[(2S)-2-[(morpholin-4-ylacetyl)amino]-4-phenylbutanoyl]-L-leucyl-N-[(2R,3S,4S)-1,3-dihydroxy-2,6-dimethylheptan-4-yl]-L-phenylalaninamide (three-letter code: 3BV) (formula: C<sub>40</sub>H<sub>61</sub>N<sub>5</sub>O<sub>7</sub>).





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	9	Total	O	0	0
			9	9		
19	B	17	Total	O	0	0
			17	17		
19	C	14	Total	O	0	0
			14	14		
19	D	5	Total	O	0	0
			5	5		
19	E	7	Total	O	0	0
			7	7		
19	F	24	Total	O	0	0
			24	24		
19	G	22	Total	O	0	0
			22	22		
19	H	12	Total	O	0	0
			12	12		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	I	9	Total 9	O 9	0	0
19	J	19	Total 19	O 19	0	0
19	K	6	Total 6	O 6	0	0
19	L	11	Total 11	O 11	0	0
19	M	18	Total 18	O 18	0	0
19	N	11	Total 11	O 11	0	0
19	O	5	Total 5	O 5	0	0
19	P	8	Total 8	O 8	0	0
19	Q	7	Total 7	O 7	0	0
19	R	6	Total 6	O 6	0	0
19	S	5	Total 5	O 5	0	0
19	T	19	Total 19	O 19	0	0
19	U	18	Total 18	O 18	0	0
19	V	17	Total 17	O 17	0	0
19	W	6	Total 6	O 6	0	0
19	X	11	Total 11	O 11	0	0
19	Y	9	Total 9	O 9	0	0
19	Z	16	Total 16	O 16	0	0
19	a	11	Total 11	O 11	0	0
19	b	17	Total 17	O 17	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.

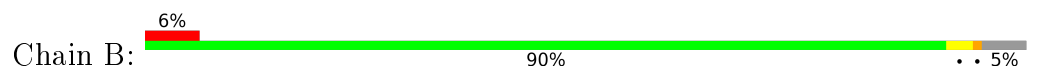
- Molecule 1: Proteasome subunit alpha type-2



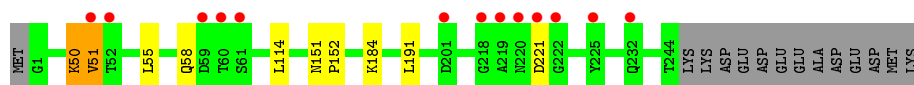
- Molecule 1: Proteasome subunit alpha type-2



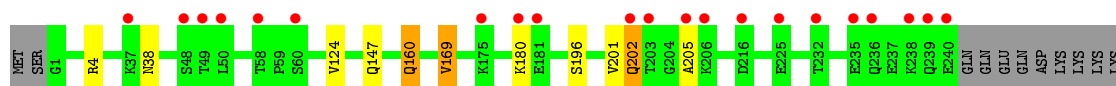
- Molecule 2: Proteasome subunit alpha type-3



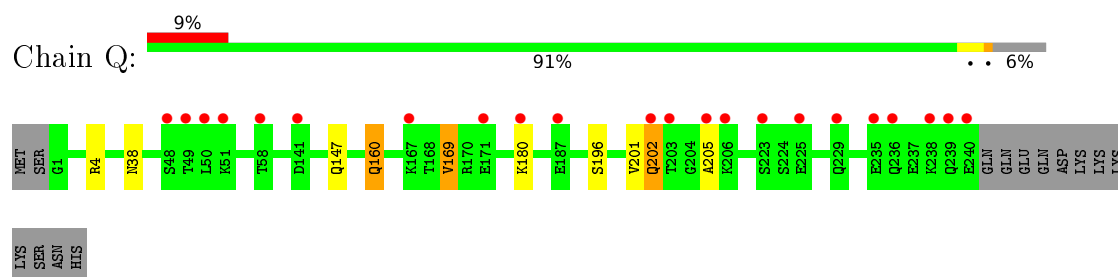
- Molecule 2: Proteasome subunit alpha type-3



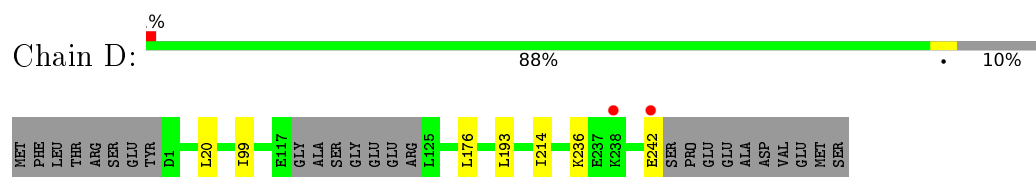
- Molecule 3: Proteasome subunit alpha type-4



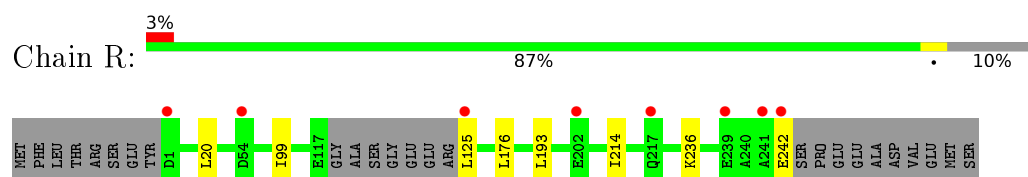
- Molecule 3: Proteasome subunit alpha type-4



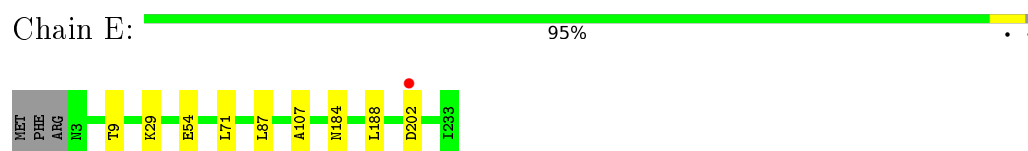
- Molecule 4: Proteasome subunit alpha type-5



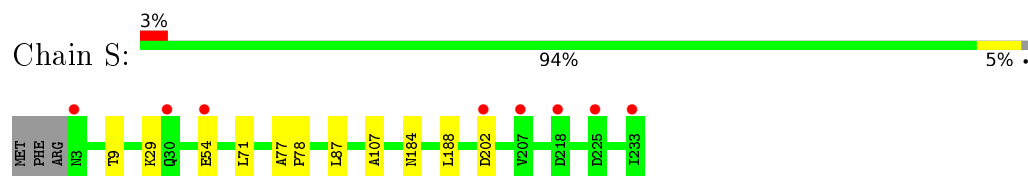
- Molecule 4: Proteasome subunit alpha type-5



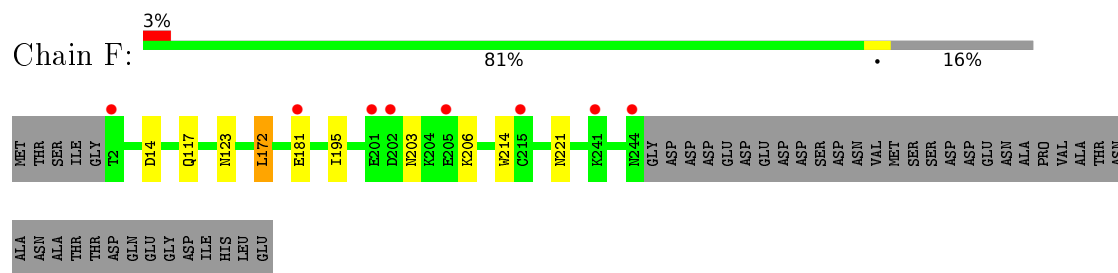
- Molecule 5: Proteasome subunit alpha type-6



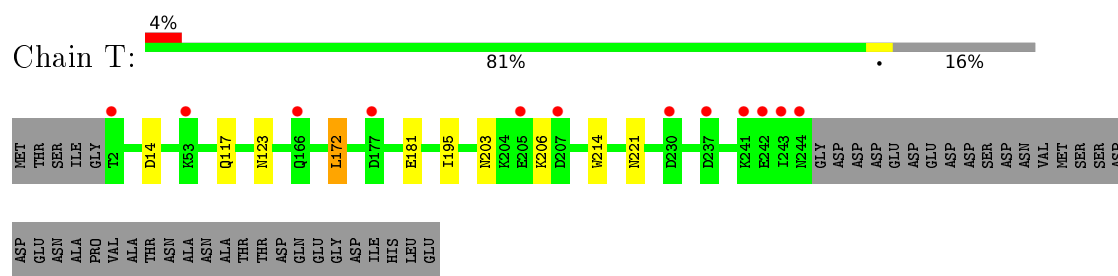
- Molecule 5: Proteasome subunit alpha type-6



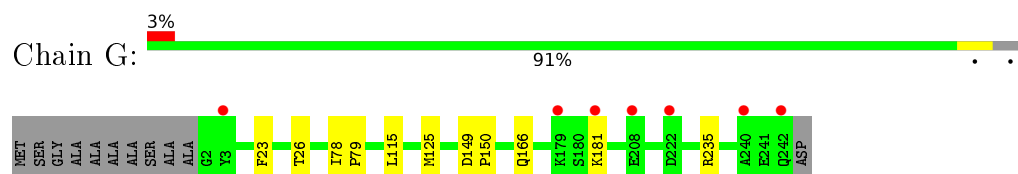
- Molecule 6: Probable proteasome subunit alpha type-7



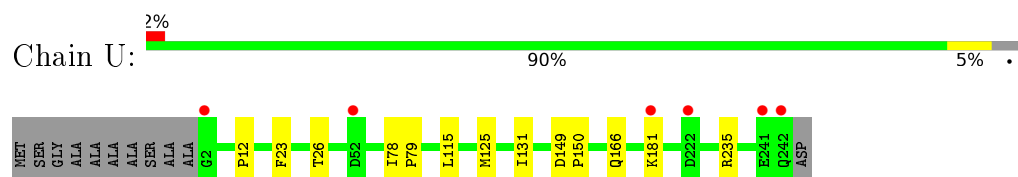
- Molecule 6: Probable proteasome subunit alpha type-7



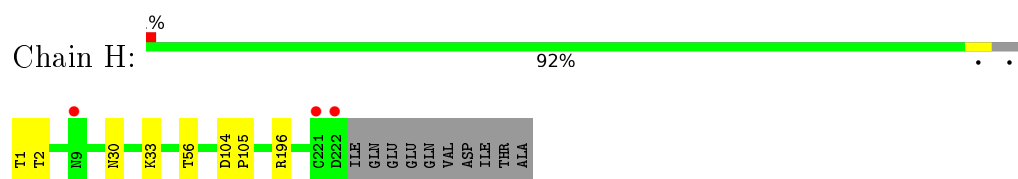
- Molecule 7: Proteasome subunit alpha type-1



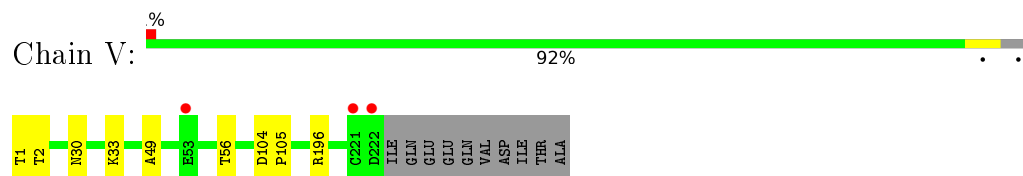
- Molecule 7: Proteasome subunit alpha type-1



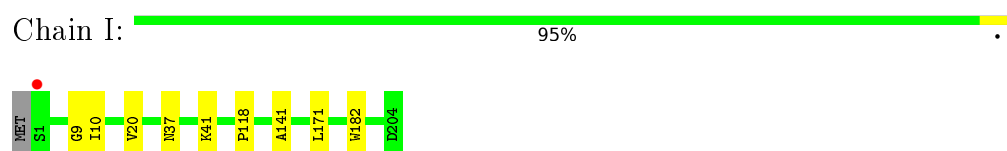
- Molecule 8: Proteasome subunit beta type-2



- Molecule 8: Proteasome subunit beta type-2

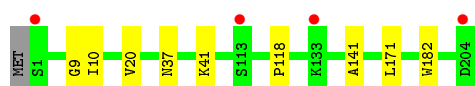


- Molecule 9: Proteasome subunit beta type-3

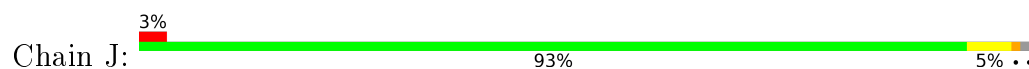


- Molecule 9: Proteasome subunit beta type-3

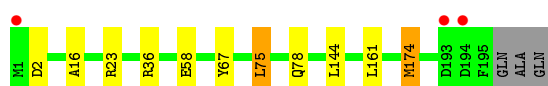
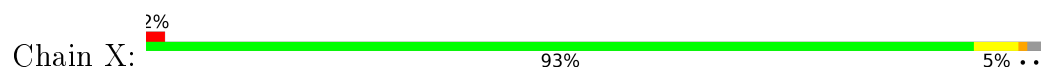




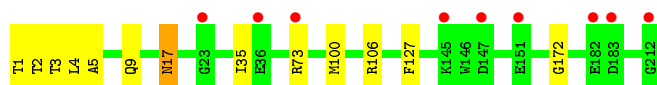
- Molecule 10: Proteasome subunit beta type-4



- Molecule 10: Proteasome subunit beta type-4



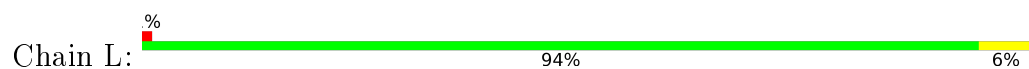
- Molecule 11: Proteasome subunit beta type-5



- Molecule 11: Proteasome subunit beta type-5



- Molecule 12: Proteasome subunit beta type-6

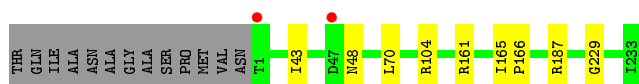


- Molecule 12: Proteasome subunit beta type-6

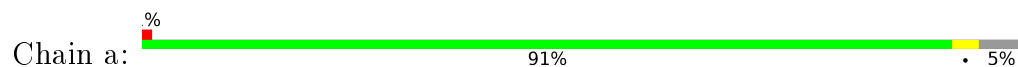


- Molecule 13: Proteasome subunit beta type-7





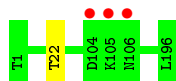
- Molecule 13: Proteasome subunit beta type-7



- 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, $\alpha$ , $\beta$ , $\gamma$	135.72Å 300.90Å 145.07Å 90.00° 112.94° 90.00°	Depositor
Resolution (Å)	15.00 – 2.90 15.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	94.7 (15.00-2.90) 94.8 (15.00-2.90)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.99 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.199 , 0.223 0.204 , 0.229	Depositor DCC
$R_{free}$ test set	11098 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	54.7	Xtriage
Anisotropy	0.034	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 33.7	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	0.92	EDS
Total number of atoms	50013	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.54% 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	0.27	0/1910	0.50	0/2586
4	D	0.27	0/1837	0.47	0/2475
4	R	0.27	0/1837	0.47	0/2475
5	E	0.26	0/1800	0.46	0/2433
5	S	0.27	0/1800	0.46	0/2433
6	F	0.27	0/1932	0.45	0/2609
6	T	0.27	0/1932	0.44	0/2609
7	G	0.27	0/1945	0.46	0/2634
7	U	0.27	0/1944	0.46	0/2632
8	H	0.27	0/1715	0.46	0/2326
8	V	0.27	0/1715	0.46	0/2326
9	I	0.27	0/1611	0.47	0/2174
9	W	0.27	0/1611	0.47	0/2174
10	J	0.27	0/1589	0.48	0/2142
10	X	0.26	0/1589	0.48	0/2142
11	K	0.28	0/1681	0.48	0/2274
11	Y	0.31	0/1681	0.48	0/2274
12	L	0.27	0/1795	0.46	0/2420
12	Z	0.27	0/1795	0.46	0/2420
13	M	0.27	0/1855	0.51	0/2514
13	a	0.41	2/1866 (0.1%)	0.58	4/2528 (0.2%)
14	N	0.27	0/1541	0.47	0/2087
14	b	0.26	0/1541	0.47	0/2087
All	All	0.28	2/50204 (0.0%)	0.48	4/67880 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	a	35[A]	ARG	CA-C	8.82	1.75	1.52
13	a	35[B]	ARG	CA-C	8.82	1.75	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	a	35[A]	ARG	CA-C-O	7.05	134.91	120.10
13	a	35[B]	ARG	CA-C-O	7.05	134.91	120.10
13	a	35[A]	ARG	CA-C-N	-5.40	105.32	117.20
13	a	35[B]	ARG	CA-C-N	-5.40	105.32	117.20

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	0	0
1	O	1915	0	1929	2	0
2	B	1904	0	1904	3	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	0	0
4	R	1813	0	1797	0	0
5	E	1773	0	1775	1	0
5	S	1773	0	1775	2	0
6	F	1892	0	1883	1	0
6	T	1892	0	1883	1	0
7	G	1907	0	1901	3	0
7	U	1906	0	1901	5	0
8	H	1684	0	1685	4	0
8	V	1684	0	1685	4	0
9	I	1581	0	1574	3	0
9	W	1581	0	1574	3	0
10	J	1561	0	1569	4	0
10	X	1561	0	1569	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	K	1644	0	1594	7	0
11	Y	1644	0	1595	11	0
12	L	1757	0	1711	4	0
12	Z	1757	0	1711	5	0
13	M	1824	0	1832	1	0
13	a	1832	0	1845	0	0
14	N	1512	0	1478	2	0
14	b	1512	0	1478	0	0
15	G	1	0	0	0	0
15	I	1	0	0	0	0
15	K	1	0	0	0	0
15	N	1	0	0	0	0
15	V	1	0	0	0	0
15	Y	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	6	0
17	K	52	0	59	9	0
17	N	52	0	59	1	0
17	V	52	0	59	4	0
17	Y	52	0	59	12	0
17	b	52	0	59	0	0
18	H	12	0	13	2	0
18	K	12	0	13	0	0
18	V	12	0	13	1	0
18	Y	12	0	13	1	0
19	A	9	0	0	0	0
19	B	17	0	0	0	0
19	C	14	0	0	0	0
19	D	5	0	0	0	0
19	E	7	0	0	0	0
19	F	24	0	0	0	0
19	G	22	0	0	0	0
19	H	12	0	0	0	0
19	I	9	0	0	0	0
19	J	19	0	0	0	0
19	K	6	0	0	4	0
19	L	11	0	0	0	0
19	M	18	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	N	11	0	0	0	0
19	O	5	0	0	0	0
19	P	8	0	0	0	0
19	Q	7	0	0	0	0
19	R	6	0	0	0	0
19	S	5	0	0	0	0
19	T	19	0	0	0	0
19	U	18	0	0	0	0
19	V	17	0	0	0	0
19	W	6	0	0	0	0
19	X	11	0	0	0	0
19	Y	9	0	0	0	0
19	Z	16	0	0	0	0
19	a	11	0	0	0	0
19	b	17	0	0	0	0
All	All	50013	0	49474	98	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 (98) 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)
17:V:301:3BV:O60	18:V:303:MES:O1S	1.77	1.02
17:H:301:3BV:O60	18:H:302:MES:O1S	1.83	0.96
11:K:17:ASN:ND2	11:K:172:GLY:H	1.83	0.76
11:Y:33:LYS:NZ	17:Y:301:3BV:H58	2.01	0.75
11:Y:27:ALA:CB	17:Y:301:3BV:H31	2.17	0.75
17:Y:301:3BV:H15	12:Z:126:ASP:HB3	1.70	0.73
17:H:301:3BV:O9	17:H:301:3BV:H2	1.93	0.68
17:K:301:3BV:O48	17:K:301:3BV:O60	2.11	0.68
11:K:17:ASN:HD22	11:K:172:GLY:H	1.43	0.64
17:Y:301:3BV:H2	17:Y:301:3BV:O9	1.96	0.64
14:N:22:THR:HG22	17:N:201:3BV:H17	1.78	0.64
11:Y:1:THR:HG22	11:Y:2:THR:N	2.12	0.64
17:H:301:3BV:O60	17:H:301:3BV:O48	2.13	0.63
17:H:301:3BV:O60	18:H:302:MES:S	2.54	0.61
11:Y:33:LYS:HZ1	17:Y:301:3BV:H58	1.65	0.60
12:Z:13:LEU:HD13	12:Z:150:LEU:HD21	1.84	0.60
12:L:13:LEU:HD13	12:L:150:LEU:HD21	1.84	0.60
11:K:1:THR:HG22	11:K:2:THR:N	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:1:THR:HG23	8:H:33:LYS:NZ	2.19	0.57
17:V:301:3BV:H2	17:V:301:3BV:O9	2.04	0.57
17:V:301:3BV:O60	17:V:301:3BV:O48	2.13	0.56
11:Y:27:ALA:HB3	17:Y:301:3BV:H31	1.87	0.56
11:Y:5:ALA:HB3	11:Y:100:MET:HE2	1.88	0.55
14:N:152:VAL:HA	14:N:175:MET:HE1	1.89	0.54
11:K:5:ALA:HB3	11:K:100:MET:HE2	1.91	0.53
17:K:301:3BV:H25	19:K:402:HOH:O	2.08	0.53
8:V:1:THR:HG22	8:V:2:THR:N	2.25	0.52
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.59	0.51
3:C:201:VAL:O	3:C:202:GLN:CB	2.59	0.51
17:K:301:3BV:H2	17:K:301:3BV:O9	2.11	0.51
17:Y:301:3BV:O48	18:Y:303:MES:O1S	2.28	0.51
10:J:67:TYR:CE1	10:J:75:LEU:HD13	2.46	0.51
10:X:67:TYR:CE1	10:X:75:LEU:HD13	2.46	0.50
11:Y:27:ALA:HB3	17:Y:301:3BV:C27	2.41	0.50
11:Y:33:LYS:HZ3	17:Y:301:3BV:H58	1.77	0.50
7:G:23:PHE:O	7:G:26:THR:HB	2.12	0.49
7:U:23:PHE:O	7:U:26:THR:HB	2.12	0.49
10:J:174:MET:HA	10:X:174:MET:HA	1.94	0.49
8:V:1:THR:HG23	8:V:33:LYS:NZ	2.28	0.48
8:V:49:ALA:HA	17:V:301:3BV:H50	1.95	0.48
17:K:301:3BV:N30	17:K:301:3BV:C38	2.73	0.48
17:K:301:3BV:C19	19:K:402:HOH:O	2.60	0.48
3:C:169:VAL:HG23	3:C:196:SER:HB2	1.97	0.47
17:H:301:3BV:O40	17:H:301:3BV:H53	2.14	0.47
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.96	0.47
11:K:100:MET:HE3	11:K:127:PHE:HB2	1.96	0.47
17:H:301:3BV:C36	17:H:301:3BV:H25	2.45	0.47
3:Q:169:VAL:HG23	3:Q:196:SER:HB2	1.97	0.47
8:H:1:THR:HG22	8:H:2:THR:N	2.29	0.47
5:S:87:LEU:HD21	5:S:107:ALA:HB1	1.97	0.46
5:E:87:LEU:HD21	5:E:107:ALA:HB1	1.97	0.46
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.97	0.46
11:K:1:THR:CG2	11:K:2:THR:N	2.78	0.46
8:H:104:ASP:HB2	8:H:105:PRO:HD2	1.98	0.45
17:Y:301:3BV:H59	17:Y:301:3BV:H44	1.62	0.45
17:K:301:3BV:O1	12:L:108:HIS:HE1	1.99	0.45
8:V:104:ASP:HB2	8:V:105:PRO:HD2	1.98	0.45
6:F:172:LEU:CD1	6:F:195:ILE:HD13	2.47	0.44
6:T:172:LEU:CD1	6:T:195:ILE:HD13	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:K:301:3BV:C18	19:K:402:HOH:O	2.66	0.43
11:Y:100:MET:HE3	11:Y:127:PHE:HB2	1.99	0.43
11:Y:27:ALA:HB1	17:Y:301:3BV:H31	1.97	0.43
17:K:301:3BV:H26	19:K:402:HOH:O	2.18	0.43
11:Y:1:THR:CG2	11:Y:2:THR:N	2.77	0.43
3:C:201:VAL:HG13	3:C:202:GLN:N	2.33	0.43
7:G:78:ILE:N	7:G:79:PRO:CD	2.82	0.43
3:Q:201:VAL:HG13	3:Q:202:GLN:N	2.33	0.43
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.53	0.43
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.19	0.43
12:L:8:ASN:HA	12:L:30:ILE:O	2.20	0.42
3:C:160:GLN:HA	3:C:160:GLN:HE21	1.83	0.42
9:I:20:VAL:HG13	9:I:118:PRO:HB3	2.02	0.42
9:I:9:GLY:HA3	9:I:41:LYS:HE2	2.02	0.42
7:U:78:ILE:N	7:U:79:PRO:CD	2.82	0.42
9:W:20:VAL:HG13	9:W:118:PRO:HB3	2.02	0.42
11:K:1:THR:CG2	11:K:3:THR:HG23	2.49	0.42
13:M:165:ILE:HB	13:M:166:PRO:HD3	2.02	0.42
9:W:9:GLY:HA3	9:W:41:LYS:HE2	2.02	0.42
10:J:36:ARG:NH1	10:J:58:GLU:OE2	2.51	0.42
3:Q:160:GLN:HA	3:Q:160:GLN:HE21	1.85	0.42
2:B:151:ASN:HB2	2:B:152:PRO:CD	2.50	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
7:U:149:ASP:HB2	7:U:150:PRO:CD	2.50	0.41
12:Z:147:MET:N	12:Z:148:PRO:HD2	2.35	0.41
7:G:149:ASP:HB2	7:G:150:PRO:CD	2.51	0.41
1:O:119:GLN:O	1:O:122:THR:HB	2.21	0.41
9:W:10:ILE:HG21	9:W:141:ALA:HB3	2.02	0.41
2:B:50:LYS:O	2:B:51:VAL:C	2.59	0.41
9:I:10:ILE:HG21	9:I:141:ALA:HB3	2.03	0.41
2:P:50:LYS:O	2:P:51:VAL:C	2.59	0.41
10:X:36:ARG:NH1	10:X:58:GLU:OE2	2.52	0.41
8:H:1:THR:HG23	8:H:33:LYS:HZ3	1.85	0.41
17:Y:301:3BV:H15	12:Z:126:ASP:CB	2.47	0.41
17:K:301:3BV:H55	17:K:301:3BV:H62	1.63	0.41
7:U:26:THR:HG21	7:U:131:ILE:HD12	2.03	0.40
5:S:77:ALA:N	5:S:78:PRO:CD	2.84	0.40
12:L:147:MET:N	12:L:148:PRO:HD2	2.36	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%)	241 (97%)	7 (3%)	0	100	100
1	O	248/250 (99%)	241 (97%)	7 (3%)	0	100	100
2	B	242/258 (94%)	235 (97%)	5 (2%)	2 (1%)	24	60
2	P	242/258 (94%)	234 (97%)	6 (2%)	2 (1%)	24	60
3	C	238/254 (94%)	231 (97%)	5 (2%)	2 (1%)	24	60
3	Q	238/254 (94%)	230 (97%)	6 (2%)	2 (1%)	24	60
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%)	234 (97%)	7 (3%)	0	100	100
6	T	241/288 (84%)	235 (98%)	6 (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%)	215 (98%)	5 (2%)	0	100	100
8	V	220/232 (95%)	215 (98%)	5 (2%)	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%)	34	71
10	X	193/198 (98%)	189 (98%)	3 (2%)	1 (0%)	34	71
11	K	210/212 (99%)	207 (99%)	3 (1%)	0	100	100
11	Y	210/212 (99%)	205 (98%)	5 (2%)	0	100	100
12	L	220/222 (99%)	216 (98%)	4 (2%)	0	100	100
12	Z	220/222 (99%)	216 (98%)	4 (2%)	0	100	100
13	M	231/246 (94%)	219 (95%)	11 (5%)	1 (0%)	39	74

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	a	232/246 (94%)	221 (95%)	10 (4%)	1 (0%)	39	74
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	6277/6614 (95%)	6111 (97%)	154 (2%)	12 (0%)	52	84

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
2	P	221	ASP
10	J	2	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%)	74	93
1	O	209/209 (100%)	206 (99%)	3 (1%)	74	93
2	B	203/216 (94%)	197 (97%)	6 (3%)	48	83
2	P	203/216 (94%)	197 (97%)	6 (3%)	48	83
3	C	212/226 (94%)	206 (97%)	6 (3%)	51	84
3	Q	212/226 (94%)	206 (97%)	6 (3%)	51	84
4	D	194/215 (90%)	187 (96%)	7 (4%)	42	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	R	194/215 (90%)	186 (96%)	8 (4%)	37	73
5	E	190/193 (98%)	183 (96%)	7 (4%)	41	77
5	S	190/193 (98%)	183 (96%)	7 (4%)	41	77
6	F	201/239 (84%)	192 (96%)	9 (4%)	34	70
6	T	201/239 (84%)	192 (96%)	9 (4%)	34	70
7	G	206/210 (98%)	201 (98%)	5 (2%)	57	86
7	U	206/210 (98%)	201 (98%)	5 (2%)	57	86
8	H	181/190 (95%)	178 (98%)	3 (2%)	68	91
8	V	181/190 (95%)	178 (98%)	3 (2%)	68	91
9	I	172/173 (99%)	169 (98%)	3 (2%)	68	91
9	W	172/173 (99%)	169 (98%)	3 (2%)	68	91
10	J	173/175 (99%)	168 (97%)	5 (3%)	50	83
10	X	173/175 (99%)	168 (97%)	5 (3%)	50	83
11	K	169/169 (100%)	163 (96%)	6 (4%)	42	78
11	Y	169/169 (100%)	164 (97%)	5 (3%)	48	83
12	L	185/185 (100%)	179 (97%)	6 (3%)	46	81
12	Z	185/185 (100%)	180 (97%)	5 (3%)	52	84
13	M	199/208 (96%)	193 (97%)	6 (3%)	48	83
13	a	200/208 (96%)	194 (97%)	6 (3%)	48	83
14	N	162/162 (100%)	161 (99%)	1 (1%)	90	97
14	b	162/162 (100%)	161 (99%)	1 (1%)	90	97
All	All	5313/5540 (96%)	5168 (97%)	145 (3%)	52	84

All (145) 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

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Mol	Chain	Res	Type
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	20	LEU
4	D	99	ILE
4	D	176	LEU
4	D	193	LEU
4	D	214	ILE
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	117	GLN
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	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	196	ARG
9	I	37	ASN
9	I	171	LEU
9	I	182	TRP
10	J	23	ARG
10	J	75	LEU

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Mol	Chain	Res	Type
10	J	78	GLN
10	J	144	LEU
10	J	174	MET
11	K	4	LEU
11	K	9	GLN
11	K	17	ASN
11	K	35	ILE
11	K	73	ARG
11	K	106	ARG
12	L	1	GLN
12	L	23	LEU
12	L	31	THR
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	147	GLN
3	Q	160	GLN
3	Q	169	VAL
3	Q	180	LYS
4	R	20	LEU
4	R	99	ILE
4	R	125	LEU
4	R	176	LEU
4	R	193	LEU

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Mol	Chain	Res	Type
4	R	214	ILE
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	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	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

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Mol	Chain	Res	Type
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
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 (69) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	HIS
2	B	119	GLN
2	B	123	GLN
3	C	38	ASN
3	C	147	GLN
3	C	160	GLN
4	D	15	GLN
4	D	91	HIS
4	D	146	GLN
4	D	225	ASN
5	E	68	HIS
5	E	92	ASN
5	E	99	ASN
5	E	116	GLN
5	E	120	GLN
5	E	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
10	J	55	GLN
11	K	85	ASN
11	K	176	ASN
12	L	3	ASN
12	L	70	ASN

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Mol	Chain	Res	Type
12	L	79	HIS
12	L	108	HIS
12	L	158	ASN
13	M	48	ASN
13	M	102	GLN
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
4	R	225	ASN
5	S	68	HIS
5	S	92	ASN
5	S	99	ASN
5	S	116	GLN
5	S	120	GLN
5	S	184	ASN
6	T	86	ASN
6	T	123	ASN
6	T	191	GLN
6	T	240	GLN
7	U	117	GLN
7	U	121	GLN
8	V	116	HIS
10	X	55	GLN
11	Y	62	GLN
11	Y	85	ASN
11	Y	176	ASN
12	Z	70	ASN
12	Z	108	HIS
12	Z	158	ASN
13	a	48	ASN
13	a	102	GLN
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	1.23	3 (5%)	67,71,71	1.43	7 (10%)
18	MES	H	302	-	12,12,12	2.05	1 (8%)	15,16,16	1.97	3 (20%)
17	3BV	K	301	11	54,54,54	1.14	2 (3%)	67,71,71	1.59	5 (7%)
18	MES	K	303	-	12,12,12	2.05	1 (8%)	15,16,16	1.60	3 (20%)
17	3BV	N	201	14	54,54,54	1.24	3 (5%)	67,71,71	1.37	6 (8%)
17	3BV	V	301	8	54,54,54	1.15	3 (5%)	67,71,71	1.35	6 (8%)
18	MES	V	303	-	12,12,12	2.03	1 (8%)	15,16,16	1.93	3 (20%)
17	3BV	Y	301	11	54,54,54	1.09	3 (5%)	67,71,71	1.60	9 (13%)
18	MES	Y	303	-	12,12,12	2.05	1 (8%)	15,16,16	1.65	3 (20%)
17	3BV	b	201	14	54,54,54	1.38	4 (7%)	67,71,71	1.48	12 (17%)

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	303	-	-	0/6/14/14	0/1/1/1
17	3BV	Y	301	11	-	0/59/67/67	0/3/3/3
18	MES	Y	303	-	-	0/6/14/14	0/1/1/1
17	3BV	b	201	14	-	0/59/67/67	0/3/3/3

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	H	302	MES	C8-S	-6.75	1.67	1.77
18	V	303	MES	C8-S	-6.66	1.67	1.77
18	K	303	MES	C8-S	-6.66	1.67	1.77
18	Y	303	MES	C8-S	-6.65	1.67	1.77
17	b	201	3BV	C32-C33	-6.27	1.35	1.51
17	K	301	3BV	C32-C33	-6.25	1.35	1.51
17	N	201	3BV	C32-C33	-5.99	1.36	1.51
17	H	301	3BV	C32-C33	-5.78	1.37	1.51
17	Y	301	3BV	C32-C33	-5.55	1.37	1.51
17	V	301	3BV	C32-C33	-5.25	1.38	1.51
17	b	201	3BV	C13-C14	-4.60	1.38	1.51
17	Y	301	3BV	C13-C14	-4.40	1.39	1.51
17	V	301	3BV	C13-C14	-4.34	1.39	1.51
17	K	301	3BV	C13-C14	-4.20	1.39	1.51
17	N	201	3BV	C13-C14	-3.87	1.40	1.51
17	H	301	3BV	C13-C14	-3.73	1.40	1.51
17	V	301	3BV	O48-C47	-2.48	1.37	1.43
17	H	301	3BV	O48-C47	-2.32	1.37	1.43
17	b	201	3BV	C59-C51	2.09	1.55	1.52
17	Y	301	3BV	C47-C42	2.11	1.57	1.53
17	b	201	3BV	C51-C47	2.91	1.59	1.53
17	N	201	3BV	C51-C47	3.79	1.60	1.53

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	V	301	3BV	C43-C42-N41	-6.95	100.46	109.98
17	H	301	3BV	C43-C42-N41	-6.86	100.59	109.98
17	K	301	3BV	C43-C42-N41	-6.48	101.10	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	Y	301	3BV	C43-C42-N41	-6.08	101.66	109.98
17	N	201	3BV	C58-C51-C59	-4.71	103.53	109.73
17	N	201	3BV	C43-C42-N41	-4.68	103.58	109.98
17	K	301	3BV	C33-C32-C31	-4.51	100.13	113.44
17	b	201	3BV	C43-C42-N41	-4.49	103.83	109.98
17	Y	301	3BV	C25-C24-C23	-3.66	104.50	115.49
17	Y	301	3BV	C58-C51-C59	-3.64	104.94	109.73
17	b	201	3BV	C12-C11-C20	-3.29	102.28	110.34
17	K	301	3BV	C39-C31-N30	-3.27	102.03	111.28
17	N	201	3BV	C20-C11-N10	-3.09	102.54	111.28
17	Y	301	3BV	C33-C32-C31	-2.80	105.17	113.44
17	V	301	3BV	C20-C11-N10	-2.75	103.50	111.28
17	b	201	3BV	C33-C32-C31	-2.64	105.64	113.44
17	b	201	3BV	C7-N4-C3	-2.39	107.62	111.14
17	b	201	3BV	C8-C7-N4	-2.34	107.40	113.26
17	H	301	3BV	C12-C11-C20	-2.33	104.64	110.34
17	Y	301	3BV	C24-C23-N22	-2.30	104.69	110.47
17	V	301	3BV	C12-C11-N10	-2.22	106.61	110.81
17	b	201	3BV	O1-C2-C3	-2.15	106.87	111.83
17	N	201	3BV	C7-N4-C5	-2.14	107.99	111.14
17	Y	301	3BV	O1-C6-C5	-2.10	106.97	111.83
17	H	301	3BV	C25-C24-C23	-2.08	109.25	115.49
17	N	201	3BV	C8-C7-N4	-2.06	108.11	113.26
17	b	201	3BV	C24-C23-C28	-2.00	105.43	110.58
18	H	302	MES	O3S-S-C8	2.06	109.26	104.99
17	V	301	3BV	C2-C3-N4	2.10	113.33	110.11
17	b	201	3BV	C42-N41-C39	2.11	127.11	123.15
17	b	201	3BV	C23-N22-C20	2.18	126.53	121.66
17	N	201	3BV	C23-N22-C20	2.20	126.58	121.66
17	b	201	3BV	C11-N10-C8	2.28	126.67	121.72
18	V	303	MES	O3S-S-C8	2.42	110.01	104.99
17	H	301	3BV	C7-N4-C5	2.47	114.76	111.14
17	b	201	3BV	C3-N4-C5	2.50	114.46	108.87
17	H	301	3BV	C6-C5-N4	2.52	113.97	110.11
17	H	301	3BV	C47-C42-N41	2.53	115.49	110.06
18	Y	303	MES	O3S-S-C8	2.53	110.25	104.99
18	K	303	MES	O3S-S-C8	2.58	110.34	104.99
17	H	301	3BV	C3-N4-C5	2.59	114.68	108.87
17	b	201	3BV	O9-C8-N10	2.88	127.80	122.96
18	Y	303	MES	O1S-S-C8	2.88	108.91	106.87
17	V	301	3BV	C47-C42-N41	2.92	116.32	110.06
17	V	301	3BV	C3-N4-C5	3.02	115.63	108.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	K	301	3BV	C3-N4-C5	3.03	115.66	108.87
17	Y	301	3BV	C47-C42-N41	3.10	116.72	110.06
18	K	303	MES	O1S-S-C8	3.16	109.10	106.87
18	K	303	MES	O2S-S-C8	3.74	109.51	106.87
18	V	303	MES	O2S-S-C8	3.86	109.60	106.87
18	H	302	MES	O1S-S-C8	3.94	109.66	106.87
18	Y	303	MES	O2S-S-C8	4.07	109.74	106.87
17	Y	301	3BV	C7-N4-C5	4.12	117.19	111.14
17	Y	301	3BV	C3-N4-C5	4.73	119.45	108.87
18	V	303	MES	O1S-S-C8	5.24	110.57	106.87
17	K	301	3BV	C7-N4-C5	5.28	118.88	111.14
18	H	302	MES	O2S-S-C8	5.52	110.77	106.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	H	301	3BV	6	0
18	H	302	MES	2	0
17	K	301	3BV	9	0
17	N	201	3BV	1	0
17	V	301	3BV	4	0
18	V	303	MES	1	0
17	Y	301	3BV	12	0
18	Y	303	MES	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	-0.23	5 (2%) 68 64	33, 48, 84, 142	0
1	O	250/250 (100%)	-0.22	7 (2%) 56 50	34, 53, 97, 141	0
2	B	244/258 (94%)	-0.11	16 (6%) 22 16	31, 53, 100, 152	0
2	P	244/258 (94%)	-0.12	13 (5%) 30 23	35, 56, 102, 150	0
3	C	240/254 (94%)	0.01	21 (8%) 12 8	32, 57, 126, 165	0
3	Q	240/254 (94%)	0.16	22 (9%) 11 7	36, 66, 142, 183	0
4	D	235/260 (90%)	-0.26	2 (0%) 85 84	36, 58, 86, 128	0
4	R	235/260 (90%)	-0.08	8 (3%) 49 41	44, 64, 102, 143	0
5	E	231/234 (98%)	-0.11	1 (0%) 93 92	39, 62, 94, 133	0
5	S	231/234 (98%)	-0.03	8 (3%) 48 40	40, 64, 106, 138	0
6	F	243/288 (84%)	-0.27	8 (3%) 50 42	33, 54, 103, 133	0
6	T	243/288 (84%)	-0.19	12 (4%) 33 27	32, 61, 115, 157	0
7	G	241/252 (95%)	-0.29	7 (2%) 55 49	28, 48, 90, 144	0
7	U	241/252 (95%)	-0.33	6 (2%) 61 55	29, 49, 82, 124	0
8	H	222/232 (95%)	-0.32	3 (1%) 78 76	35, 48, 86, 121	0
8	V	222/232 (95%)	-0.31	3 (1%) 78 76	32, 49, 90, 129	0
9	I	204/205 (99%)	-0.46	1 (0%) 91 90	31, 48, 79, 99	0
9	W	204/205 (99%)	-0.42	4 (1%) 68 64	32, 50, 77, 102	0
10	J	195/198 (98%)	-0.34	5 (2%) 59 54	30, 50, 81, 119	0
10	X	195/198 (98%)	-0.36	3 (1%) 76 74	32, 51, 78, 124	0
11	K	212/212 (100%)	-0.08	9 (4%) 40 33	39, 60, 92, 114	0
11	Y	212/212 (100%)	-0.12	3 (1%) 78 76	38, 59, 92, 113	0
12	L	222/222 (100%)	-0.32	3 (1%) 78 76	29, 50, 84, 118	0
12	Z	222/222 (100%)	-0.34	3 (1%) 78 76	32, 50, 84, 113	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
13	M	233/246 (94%)	-0.44	2 (0%)	85 84	28, 45, 70, 81	0
13	a	233/246 (94%)	-0.46	2 (0%)	85 84	27, 45, 69, 82	0
14	N	196/196 (100%)	-0.50	1 (0%)	91 90	26, 42, 74, 98	0
14	b	196/196 (100%)	-0.50	3 (1%)	76 74	28, 41, 72, 97	0
All	All	6336/6614 (95%)	-0.25	181 (2%)	55 49	26, 53, 97, 183	0

All (181) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
8	H	221	CYS	6.9
1	A	1	MET	6.7
10	J	1	MET	5.7
3	C	206	LYS	5.5
8	V	221	CYS	5.4
3	Q	49	THR	5.4
2	B	218	GLY	5.3
9	I	1	SER	5.1
3	C	240	GLU	5.1
1	O	249	ALA	5.0
3	Q	236	GLN	5.0
9	W	1	SER	5.0
2	B	220	ASN	4.9
2	P	218	GLY	4.9
3	C	239	GLN	4.8
5	S	202	ASP	4.8
1	O	1	MET	4.8
10	X	194	ASP	4.8
3	Q	238	LYS	4.7
2	P	219	ALA	4.7
10	X	1	MET	4.5
2	B	219	ALA	4.5
3	Q	48	SER	4.5
3	Q	180	LYS	4.4
2	B	222	GLY	4.4
11	Y	212	GLY	4.4
2	P	51	VAL	4.3
3	C	49	THR	4.3
3	C	50	LEU	4.2
3	Q	223	SER	4.2
3	C	238	LYS	4.1
11	K	212	GLY	4.1

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Mol	Chain	Res	Type	RSRZ
3	Q	202	GLN	4.1
3	C	225	GLU	4.0
7	G	242	GLN	4.0
4	R	242	GLU	3.9
2	B	221	ASP	3.7
8	V	222	ASP	3.7
8	H	222	ASP	3.6
1	O	250	LEU	3.6
3	Q	51	LYS	3.6
11	Y	147	ASP	3.6
6	T	166	GLN	3.6
2	P	220	ASN	3.6
5	S	225	ASP	3.5
6	F	244	ASN	3.5
6	T	237	ASP	3.5
2	P	221	ASP	3.5
4	R	241	ALA	3.5
5	S	233	ILE	3.5
12	Z	1	GLN	3.5
3	C	235	GLU	3.4
13	M	1	THR	3.4
3	Q	206	LYS	3.4
3	Q	239	GLN	3.3
10	X	193	ASP	3.3
6	F	202	ASP	3.3
2	B	182	ASP	3.2
3	Q	50	LEU	3.2
1	A	2	THR	3.2
10	J	194	ASP	3.2
3	C	216	ASP	3.2
1	O	52	SER	3.2
5	S	54	GLU	3.1
13	a	1	THR	3.1
2	P	222	GLY	3.1
3	C	180	LYS	3.1
7	U	242	GLN	3.1
3	Q	225	GLU	3.1
14	b	105	LYS	3.0
6	F	205	GLU	3.0
3	Q	240	GLU	3.0
5	S	218	ASP	3.0
5	E	202	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	249	ALA	2.9
11	K	182	GLU	2.9
6	T	205	GLU	2.9
3	C	232	THR	2.9
2	P	232	GLN	2.9
9	W	133	LYS	2.9
2	B	51	VAL	2.9
3	C	181	GLU	2.9
11	K	36	GLU	2.9
5	S	207	VAL	2.9
2	P	59	ASP	2.8
4	R	217	GLN	2.8
2	B	59	ASP	2.8
3	C	236	GLN	2.8
2	B	60	THR	2.8
12	L	172	LEU	2.8
2	P	225	TYR	2.8
7	G	208	GLU	2.7
3	Q	141	ASP	2.7
4	R	1	ASP	2.7
2	B	203	SER	2.7
2	B	242	GLY	2.7
1	O	2	THR	2.7
2	B	181	ASP	2.7
6	T	243	ILE	2.7
11	K	73	ARG	2.7
1	O	201	GLU	2.6
8	V	53	GLU	2.6
6	F	241	LYS	2.6
10	J	95	ARG	2.6
12	L	165	ASN	2.6
7	G	240	ALA	2.6
3	C	60	SER	2.6
3	Q	187	GLU	2.6
6	F	201	GLU	2.6
7	G	179	LYS	2.6
6	T	242	GLU	2.6
12	Z	210	ASP	2.6
3	C	48	SER	2.6
1	O	231	LYS	2.5
12	Z	165	ASN	2.5
14	N	104	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
2	P	60	THR	2.5
4	D	242	GLU	2.5
7	U	241	GLU	2.4
11	K	151	GLU	2.4
3	Q	205	ALA	2.4
3	Q	229	GLN	2.4
6	F	181	GLU	2.4
11	K	183	ASP	2.4
4	R	125	LEU	2.4
4	D	238	LYS	2.4
3	Q	171	GLU	2.4
3	Q	167	LYS	2.4
7	U	222	ASP	2.4
13	M	47	ASP	2.4
7	U	52	ASP	2.4
6	T	53	LYS	2.4
5	S	3	ASN	2.3
6	T	177	ASP	2.3
3	Q	235	GLU	2.3
6	T	230	ASP	2.3
3	Q	58	THR	2.3
7	U	2	GLY	2.3
5	S	30	GLN	2.3
11	Y	202	GLU	2.3
3	C	205	ALA	2.3
9	W	113	SER	2.3
11	K	147	ASP	2.2
7	G	3	TYR	2.2
2	P	61	SER	2.2
6	F	215	CYS	2.2
3	C	37	LYS	2.2
7	G	181	LYS	2.2
4	R	54	ASP	2.2
11	K	23	GLY	2.2
14	b	104	ASP	2.2
3	Q	203	THR	2.2
7	G	222	ASP	2.2
10	J	30	ASP	2.2
3	C	202	GLN	2.2
6	T	241	LYS	2.2
2	B	232	GLN	2.2
14	b	106	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
6	T	207	ASP	2.2
1	A	248	GLU	2.2
6	F	2	THR	2.1
7	U	181	LYS	2.1
10	J	10	GLN	2.1
6	T	2	THR	2.1
4	R	202	GLU	2.1
4	R	239	GLU	2.1
13	a	121	SER	2.1
2	P	52	THR	2.1
3	C	58	THR	2.1
8	H	9	ASN	2.1
2	B	3	ARG	2.1
1	A	230	ASP	2.1
6	T	244	ASN	2.1
2	B	169	SER	2.1
3	C	203	THR	2.0
12	L	210	ASP	2.0
3	C	175	LYS	2.0
2	P	201	ASP	2.0
11	K	145	LYS	2.0
9	W	204	ASP	2.0
2	B	244	THR	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. 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( $\text{\AA}^2$ )	Q<0.9
18	MES	K	303	12/12	0.89	0.57	9.98	41,44,89,91	0
18	MES	V	303	12/12	0.86	0.39	7.80	68,74,91,99	0
18	MES	H	302	12/12	0.88	0.39	7.65	67,71,85,95	0
18	MES	Y	303	12/12	0.90	0.52	6.80	40,43,80,84	0
17	3BV	K	301	52/52	0.72	0.40	5.49	38,48,102,106	48
17	3BV	Y	301	52/52	0.75	0.36	4.76	36,47,101,104	48
17	3BV	N	201	52/52	0.85	0.26	3.95	35,50,128,131	0
17	3BV	b	201	52/52	0.88	0.24	3.88	36,50,127,131	0
17	3BV	V	301	52/52	0.86	0.27	2.75	51,58,104,108	0
17	3BV	H	301	52/52	0.87	0.25	2.31	49,57,107,110	0
15	MG	I	301	1/1	0.92	0.26	1.34	48,48,48,48	0
15	MG	Y	302	1/1	0.95	0.26	1.31	47,47,47,47	0
15	MG	N	202	1/1	0.90	0.17	0.72	44,44,44,44	0
15	MG	Z	301	1/1	0.92	0.15	-0.17	50,50,50,50	0
15	MG	G	301	1/1	0.96	0.10	-0.74	41,41,41,41	0
16	CL	N	203	1/1	0.97	0.12	-0.85	53,53,53,53	0
15	MG	V	302	1/1	0.83	0.13	-1.10	61,61,61,61	0
15	MG	K	302	1/1	0.99	0.07	-1.37	41,41,41,41	0
16	CL	b	202	1/1	0.96	0.08	-2.60	49,49,49,49	0
16	CL	G	302	1/1	0.99	0.14	-	34,34,34,34	0
16	CL	U	301	1/1	0.98	0.11	-	37,37,37,37	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.