



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 13, 2016 – 01:37 AM EST

PDB ID : 5FHS  
Title : Yeast 20S proteasome beta5-K33A mutant (propeptide expressed in trans) in complex with Carfilzomib  
Authors : Huber, E.M.; Groll, M.  
Deposited on : 2015-12-22  
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

<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

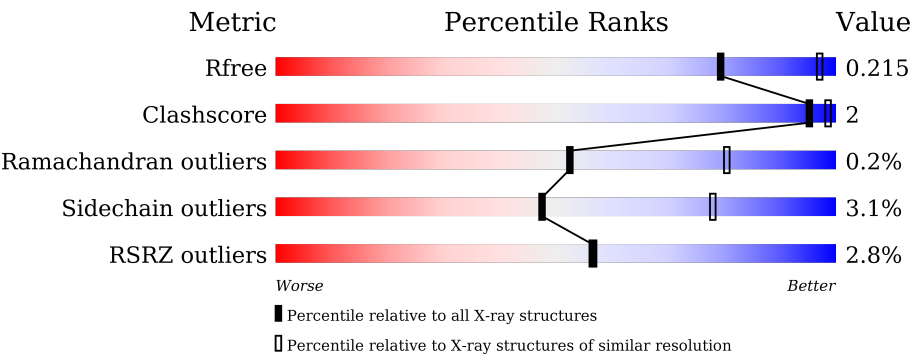
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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>98%</div><div>•</div></div>
1	O	250	<div><div>4%</div><div>98%</div><div>•</div></div>
2	B	258	<div><div>5%</div><div>89%</div><div>• • 5%</div></div>
2	P	258	<div><div>5%</div><div>90%</div><div>• • 5%</div></div>
3	C	254	<div><div>7%</div><div>89%</div><div>• • 6%</div></div>
3	Q	254	<div><div>6%</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
15	MG	I	301	-	-	-	X
15	MG	Z	301	-	-	-	X
17	3BV	H	301	-	-	-	X
17	3BV	K	301	-	-	-	X
17	3BV	N	201	-	-	-	X
17	3BV	V	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	302	-	-	-	X

## 2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 49920 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
			1640	1042	279	312	7			
11	Y	212	Total	C	N	O	S	0	0	0
			1640	1042	279	312	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	33	ALA	LYS	engineered mutation	UNP P30656
Y	33	ALA	LYS	engineered mutation	UNP P30656

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

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

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

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

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

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

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

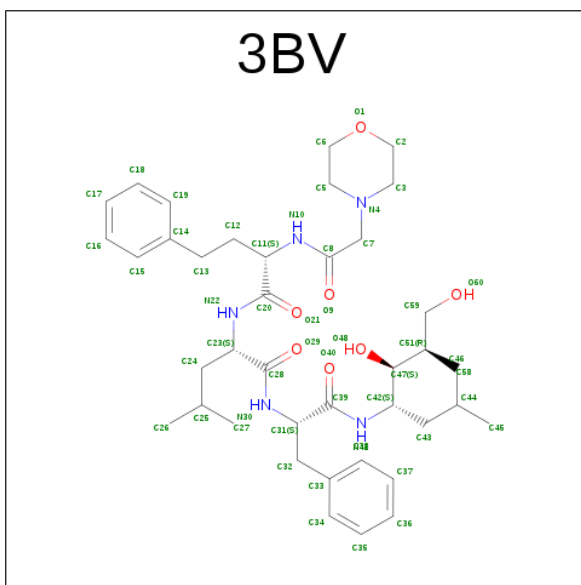
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	G	1	Total Mg 1 1	0	0
15	K	1	Total Mg 1 1	0	0
15	I	1	Total Mg 1 1	0	0
15	V	1	Total Mg 1 1	0	0
15	Z	1	Total Mg 1 1	0	0
15	N	1	Total Mg 1 1	0	0
15	Y	1	Total Mg 1 1	0	0

- 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

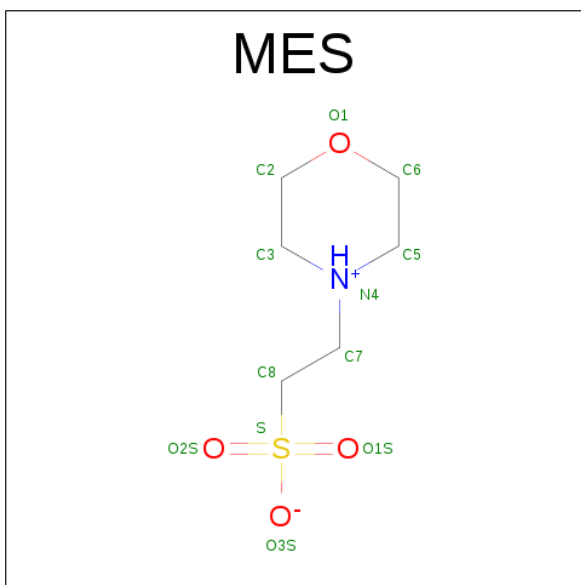
- Molecule 17 is N-[(2S)-2-[(morpholin-4-ylacetyl)amino]-4-phenylbutanoyl]-L-leucyl-N-[(2R,3S,4S)-1,3-dihydroxy-2,6-dimethylheptan-4-yl]-L-phenylalaninamide (three-letter code: 3BV) (formula: C<sub>40</sub>H<sub>61</sub>N<sub>5</sub>O<sub>7</sub>).





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

- Molecule 18 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula:  $\text{C}_6\text{H}_{13}\text{NO}_4\text{S}$ ).



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	11	Total	O	0	0
			11	11		
19	C	10	Total	O	0	0
			10	10		
19	D	6	Total	O	0	0
			6	6		
19	E	4	Total	O	0	0
			4	4		
19	F	15	Total	O	0	0
			15	15		
19	G	15	Total	O	0	0
			15	15		
19	H	15	Total	O	0	0
			15	15		

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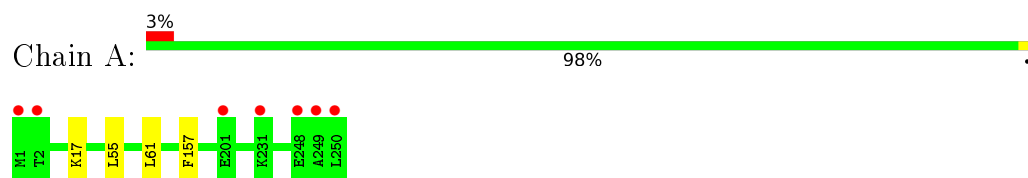
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	I	7	Total 7	O 7	0	0
19	J	13	Total 13	O 13	0	0
19	K	15	Total 15	O 15	0	0
19	L	16	Total 16	O 16	0	0
19	M	21	Total 21	O 21	0	0
19	N	13	Total 13	O 13	0	0
19	O	8	Total 8	O 8	0	0
19	P	7	Total 7	O 7	0	0
19	Q	6	Total 6	O 6	0	0
19	R	8	Total 8	O 8	0	0
19	S	4	Total 4	O 4	0	0
19	T	5	Total 5	O 5	0	0
19	U	13	Total 13	O 13	0	0
19	V	11	Total 11	O 11	0	0
19	W	10	Total 10	O 10	0	0
19	X	13	Total 13	O 13	0	0
19	Y	11	Total 11	O 11	0	0
19	Z	11	Total 11	O 11	0	0
19	a	18	Total 18	O 18	0	0
19	b	19	Total 19	O 19	0	0

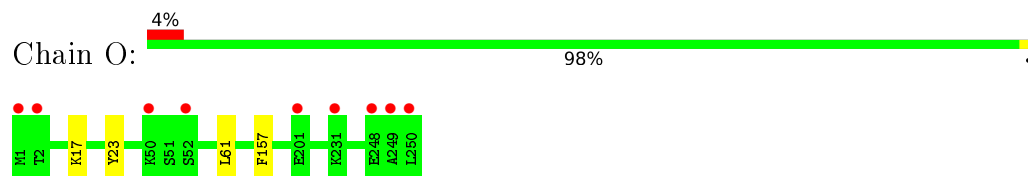
### 3 Residue-property plots [i](#)

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.

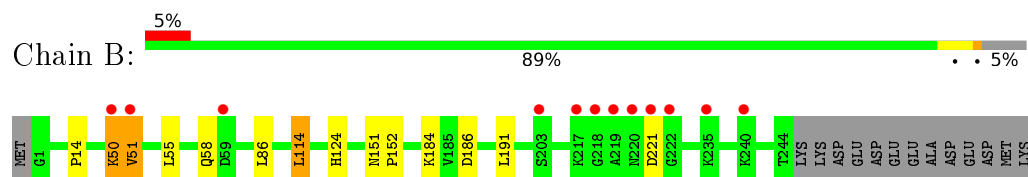
- Molecule 1: Proteasome subunit alpha type-2



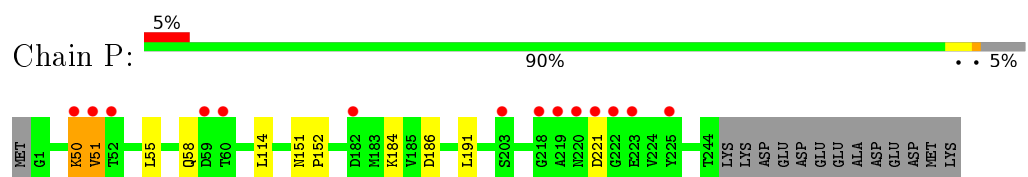
- Molecule 1: Proteasome subunit alpha type-2



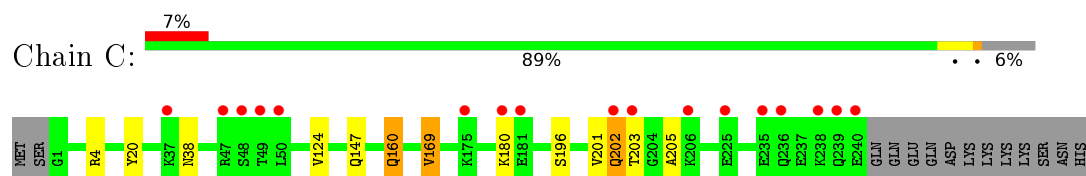
- Molecule 2: Proteasome subunit alpha type-3



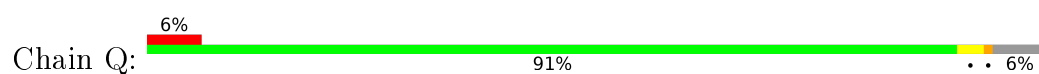
- Molecule 2: Proteasome subunit alpha type-3



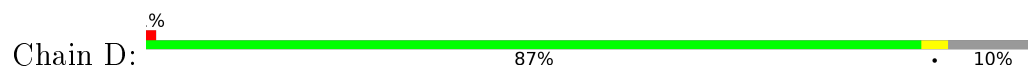
- Molecule 3: Proteasome subunit alpha type-4



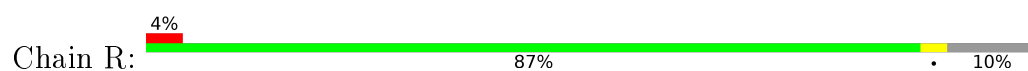
- Molecule 3: Proteasome subunit alpha type-4



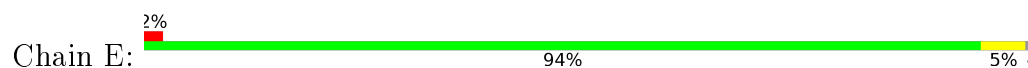
- Molecule 4: Proteasome subunit alpha type-5



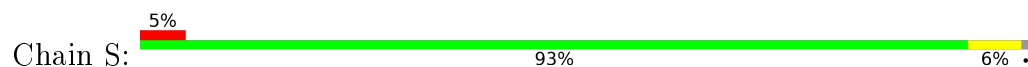
- Molecule 4: Proteasome subunit alpha type-5



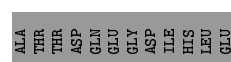
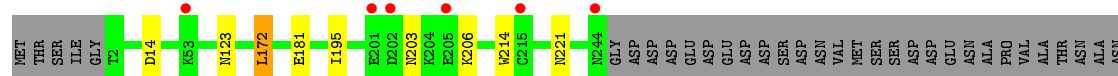
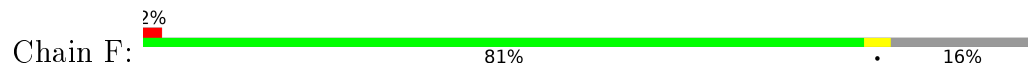
- Molecule 5: Proteasome subunit alpha type-6



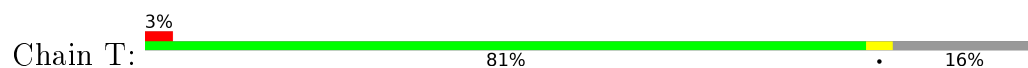
- Molecule 5: Proteasome subunit alpha type-6

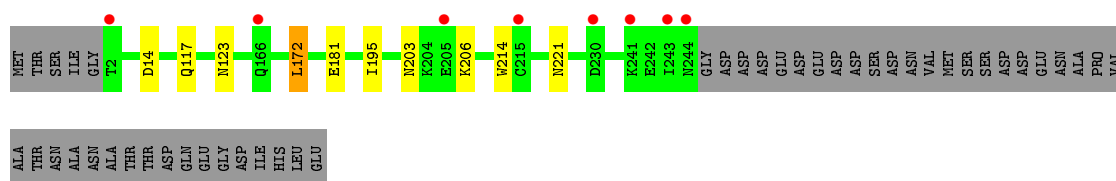


- Molecule 6: Probable proteasome subunit alpha type-7



- Molecule 6: Probable proteasome subunit alpha type-7

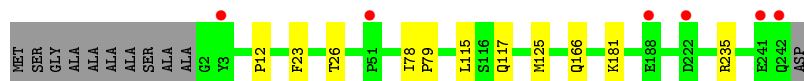




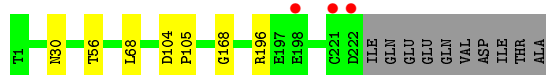
- Molecule 7: Proteasome subunit alpha type-1



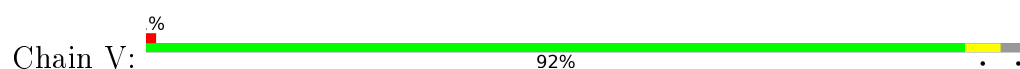
- Molecule 7: Proteasome subunit alpha type-1



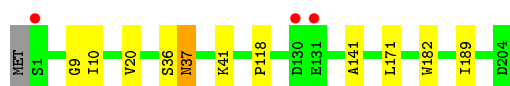
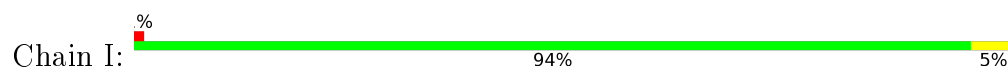
- Molecule 8: Proteasome subunit beta type-2



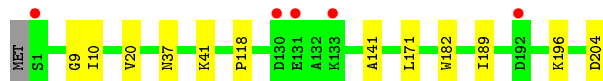
- Molecule 8: Proteasome subunit beta type-2



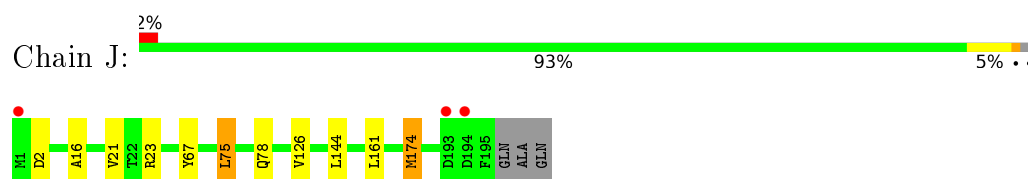
- Molecule 9: Proteasome subunit beta type-3



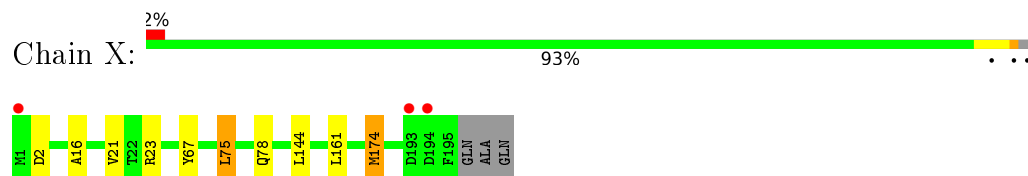
- Molecule 9: Proteasome subunit beta type-3



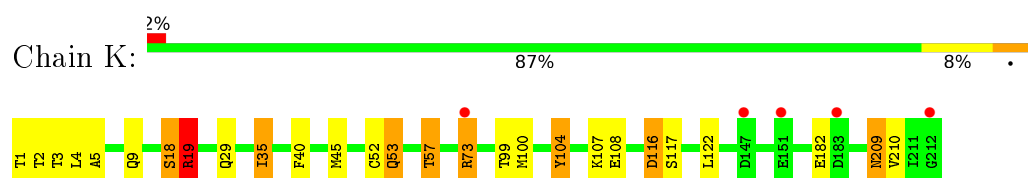
- Molecule 10: Proteasome subunit beta type-4



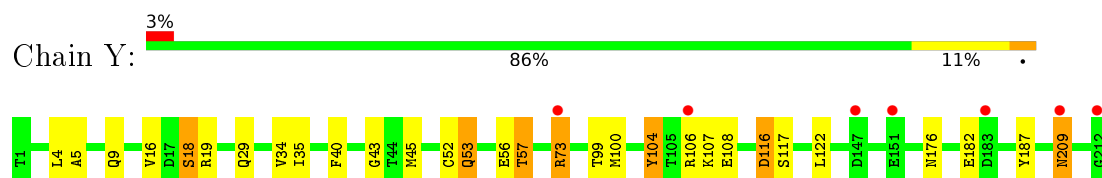
- Molecule 10: Proteasome subunit beta type-4



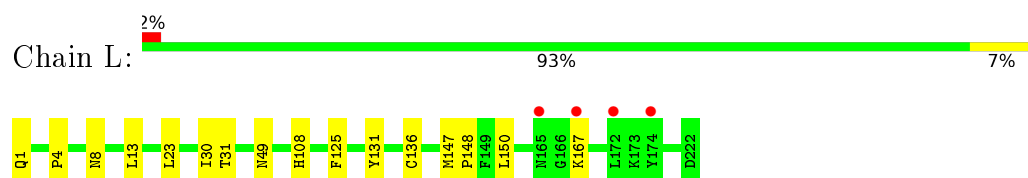
- Molecule 11: Proteasome subunit beta type-5



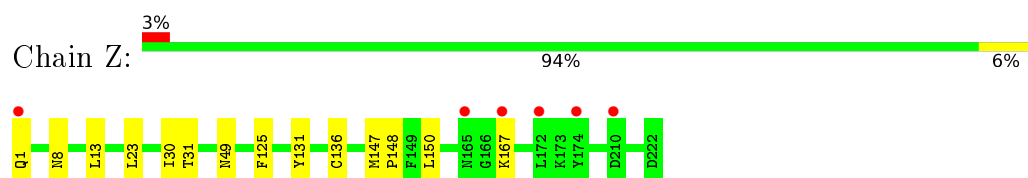
- Molecule 11: Proteasome subunit beta type-5



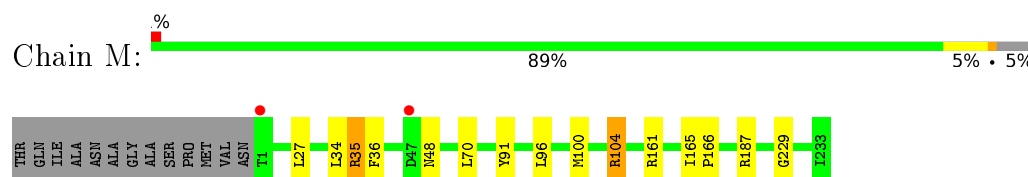
- Molecule 12: Proteasome subunit beta type-6



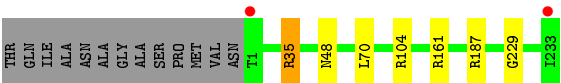
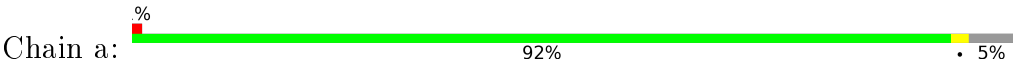
- Molecule 12: Proteasome subunit beta type-6



- Molecule 13: Proteasome subunit beta type-7



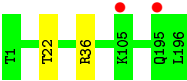
- Molecule 13: Proteasome subunit beta type-7



• 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, $\alpha$ , $\beta$ , $\gamma$	136.35Å 300.77Å 145.01Å 90.00° 113.16° 90.00°	Depositor
Resolution (Å)	15.00 – 2.70 14.99 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.5 (15.00-2.70) 98.5 (14.99-2.70)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.93 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.187 , 0.212 0.191 , 0.215	Depositor DCC
$R_{free}$ test set	14338 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	58.0	Xtriage
Anisotropy	0.022	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 39.2	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	49920	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 2.48% 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	0.47	0/2642
1	O	0.27	0/1952	0.47	0/2642
2	B	0.27	0/1934	0.48	0/2618
2	P	0.27	0/1934	0.48	0/2618
3	C	0.27	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	0.46	0/2475
5	E	0.27	0/1800	0.46	0/2433
5	S	0.27	0/1800	0.46	0/2433
6	F	0.27	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	0.25	0/1715	0.48	0/2326
8	V	0.25	0/1715	0.48	0/2326
9	I	0.26	0/1611	0.50	0/2174
9	W	0.27	0/1611	0.50	0/2174
10	J	0.26	0/1589	0.48	0/2142
10	X	0.26	0/1589	0.47	0/2142
11	K	0.42	1/1677 (0.1%)	0.73	5/2270 (0.2%)
11	Y	0.45	2/1677 (0.1%)	0.72	4/2270 (0.2%)
12	L	0.27	0/1795	0.49	0/2420
12	Z	0.27	0/1795	0.49	0/2420
13	M	0.34	1/1855 (0.1%)	0.81	2/2514 (0.1%)
13	a	0.35	1/1855 (0.1%)	0.80	3/2514 (0.1%)
14	N	0.25	0/1541	0.48	0/2087
14	b	0.25	0/1541	0.48	0/2087
All	All	0.29	5/50185 (0.0%)	0.53	14/67858 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	a	35	ARG	CZ-NH1	-9.64	1.20	1.33
13	M	35	ARG	CZ-NH1	-8.65	1.21	1.33
11	K	73	ARG	CZ-NH2	-7.77	1.23	1.33
11	Y	73	ARG	CZ-NH2	-7.17	1.23	1.33
11	Y	73	ARG	CZ-NH1	-6.31	1.24	1.33

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	35	ARG	NE-CZ-NH1	-25.49	107.55	120.30
13	a	35	ARG	NE-CZ-NH1	-23.64	108.48	120.30
13	a	35	ARG	NE-CZ-NH2	18.05	129.32	120.30
13	M	35	ARG	NE-CZ-NH2	16.71	128.66	120.30
11	K	19	ARG	NE-CZ-NH1	-13.98	113.31	120.30
11	K	19	ARG	NE-CZ-NH2	13.54	127.07	120.30
11	Y	19	ARG	NE-CZ-NH2	-12.86	113.87	120.30
11	Y	19	ARG	NE-CZ-NH1	12.54	126.57	120.30
11	Y	73	ARG	CG-CD-NE	-12.20	86.18	111.80
11	K	73	ARG	CG-CD-NE	-9.11	92.67	111.80
11	K	73	ARG	NE-CZ-NH1	6.83	123.72	120.30
11	K	19	ARG	CG-CD-NE	5.66	123.69	111.80
11	Y	19	ARG	CG-CD-NE	5.54	123.44	111.80
13	a	35	ARG	CG-CD-NE	5.24	122.80	111.80

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1915	0	1929	1	0
1	O	1915	0	1929	1	0
2	B	1904	0	1904	5	0
2	P	1904	0	1904	2	0
3	C	1881	0	1895	6	0
3	Q	1881	0	1895	4	0
4	D	1813	0	1797	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	R	1813	0	1797	0	0
5	E	1773	0	1775	3	0
5	S	1773	0	1775	3	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	3	0
8	H	1684	0	1686	2	0
8	V	1684	0	1686	3	0
9	I	1581	0	1574	6	0
9	W	1581	0	1574	6	0
10	J	1561	0	1569	5	0
10	X	1561	0	1569	4	0
11	K	1640	0	1585	29	0
11	Y	1640	0	1587	31	0
12	L	1757	0	1711	7	0
12	Z	1757	0	1711	5	0
13	M	1824	0	1832	7	0
13	a	1824	0	1832	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	1	0
17	K	52	0	59	14	0
17	N	52	0	59	0	0
17	V	52	0	59	1	0
17	b	52	0	59	0	0
18	H	12	0	13	0	0
18	K	12	0	13	0	0
18	V	12	0	13	0	0
18	Y	12	0	13	0	0
19	A	9	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	B	11	0	0	0	0
19	C	10	0	0	0	0
19	D	6	0	0	0	0
19	E	4	0	0	0	0
19	F	15	0	0	0	0
19	G	15	0	0	0	0
19	H	15	0	0	0	0
19	I	7	0	0	0	0
19	J	13	0	0	0	0
19	K	15	0	0	1	0
19	L	16	0	0	0	0
19	M	21	0	0	0	0
19	N	13	0	0	0	0
19	O	8	0	0	0	0
19	P	7	0	0	0	0
19	Q	6	0	0	0	0
19	R	8	0	0	0	0
19	S	4	0	0	0	0
19	T	5	0	0	0	0
19	U	13	0	0	0	0
19	V	11	0	0	0	0
19	W	10	0	0	0	0
19	X	13	0	0	0	0
19	Y	11	0	0	0	0
19	Z	11	0	0	0	0
19	a	18	0	0	0	0
19	b	19	0	0	0	0
All	All	49920	0	49387	138	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (138) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:40:PHE:CD2	11:Y:73:ARG:NH2	2.08	1.22
11:K:40:PHE:CD2	11:K:73:ARG:NH2	2.06	1.22
11:K:35:ILE:CG2	11:K:45:MET:SD	2.32	1.18
11:K:35:ILE:HG21	11:K:45:MET:SD	1.87	1.15
11:Y:40:PHE:CG	11:Y:73:ARG:NH2	2.15	1.15
11:Y:45:MET:HG2	11:Y:52:CYS:HB3	1.47	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:40:PHE:CE2	11:K:73:ARG:NH2	2.39	0.89
11:Y:40:PHE:CD1	11:Y:73:ARG:NH1	2.41	0.87
17:K:301:3BV:C3	17:K:301:3BV:O9	2.24	0.85
11:Y:40:PHE:CB	11:Y:73:ARG:HH22	1.91	0.84
17:K:301:3BV:O48	17:K:301:3BV:O60	1.92	0.84
17:K:301:3BV:O9	17:K:301:3BV:H16	1.75	0.83
11:Y:40:PHE:CE1	11:Y:73:ARG:NH1	2.48	0.81
11:K:40:PHE:CG	11:K:73:ARG:NH1	2.48	0.80
11:K:35:ILE:HG22	11:K:45:MET:SD	2.21	0.80
11:K:209:ASN:C	11:K:209:ASN:OD1	2.21	0.79
11:K:40:PHE:CD1	11:K:73:ARG:NH1	2.49	0.78
11:K:45:MET:HG2	11:K:52:CYS:HB3	1.65	0.77
11:Y:53:GLN:O	11:Y:57:THR:OG1	2.02	0.77
17:K:301:3BV:O40	17:K:301:3BV:H53	1.85	0.77
11:Y:209:ASN:C	11:Y:209:ASN:OD1	2.23	0.76
11:K:53:GLN:O	11:K:57:THR:OG1	2.08	0.71
11:K:18:SER:OG	11:K:29:GLN:O	2.16	0.64
17:K:301:3BV:C46	17:K:301:3BV:C39	2.77	0.62
9:I:37:ASN:ND2	11:Y:209:ASN:OD1	2.28	0.62
11:Y:209:ASN:O	11:Y:209:ASN:OD1	2.18	0.62
11:Y:18:SER:OG	11:Y:29:GLN:O	2.20	0.59
11:Y:35:ILE:CG2	11:Y:56:GLU:OE1	2.51	0.58
11:K:40:PHE:CD2	11:K:73:ARG:CZ	2.84	0.57
11:K:73:ARG:NH1	19:K:401:HOH:O	2.23	0.57
11:Y:45:MET:HG2	11:Y:52:CYS:CB	2.30	0.57
17:K:301:3BV:C39	17:K:301:3BV:H53	2.35	0.56
14:N:152:VAL:HA	14:N:175:MET:HE1	1.87	0.56
11:Y:40:PHE:CG	11:Y:73:ARG:CZ	2.83	0.55
17:K:301:3BV:H52	17:K:301:3BV:C39	2.37	0.55
12:L:13:LEU:HD13	12:L:150:LEU:HD21	1.90	0.54
11:Y:35:ILE:HG21	11:Y:56:GLU:OE1	2.07	0.54
12:Z:13:LEU:HD13	12:Z:150:LEU:HD21	1.90	0.53
11:K:1:THR:CG2	11:K:3:THR:HG23	2.37	0.53
10:J:67:TYR:CE1	10:J:75:LEU:HD13	2.44	0.53
11:K:116:ASP:OD1	11:K:117:SER:N	2.42	0.53
11:Y:106:ARG:HG2	11:Y:182:GLU:OE1	2.09	0.52
11:K:40:PHE:CG	11:K:73:ARG:NH2	2.68	0.52
17:K:301:3BV:O40	17:K:301:3BV:C46	2.57	0.52
10:X:67:TYR:CE1	10:X:75:LEU:HD13	2.44	0.52
11:K:19:ARG:NH1	9:W:204:ASP:O	2.43	0.52
11:K:209:ASN:OD1	11:K:210:VAL:N	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:116:ASP:OD1	11:Y:117:SER:N	2.42	0.52
11:K:1:THR:HG22	11:K:2:THR:N	2.25	0.51
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.60	0.50
3:C:201:VAL:O	3:C:202:GLN:CB	2.59	0.50
9:I:20:VAL:HG13	9:I:118:PRO:HB3	1.94	0.50
11:K:40:PHE:CB	11:K:73:ARG:HH12	2.23	0.50
9:W:20:VAL:HG13	9:W:118:PRO:HB3	1.94	0.50
7:G:23:PHE:O	7:G:26:THR:HB	2.13	0.49
11:K:116:ASP:OD1	11:K:116:ASP:C	2.49	0.49
13:M:35:ARG:NE	14:N:135:TYR:OH	2.45	0.49
7:U:23:PHE:O	7:U:26:THR:HB	2.13	0.49
11:K:104:TYR:CD1	11:K:182:GLU:HG3	2.48	0.49
11:Y:107:LYS:HG3	11:Y:108:GLU:HG3	1.95	0.48
11:Y:40:PHE:CB	11:Y:73:ARG:NH2	2.64	0.48
3:C:169:VAL:HG23	3:C:196:SER:HB2	1.96	0.48
11:K:107:LYS:HG3	11:K:108:GLU:HG3	1.96	0.48
5:S:87:LEU:HD21	5:S:107:ALA:HB1	1.96	0.48
12:L:13:LEU:CD1	12:L:150:LEU:HD21	2.44	0.48
3:Q:169:VAL:HG23	3:Q:196:SER:HB2	1.96	0.47
11:Y:40:PHE:CD2	11:Y:73:ARG:CZ	2.90	0.47
12:Z:13:LEU:CD1	12:Z:150:LEU:HD21	2.45	0.47
8:H:104:ASP:HB2	8:H:105:PRO:HD2	1.97	0.47
11:Y:40:PHE:HB2	11:Y:73:ARG:NH2	2.30	0.47
5:E:87:LEU:HD21	5:E:107:ALA:HB1	1.96	0.47
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.97	0.46
11:K:40:PHE:CG	11:K:73:ARG:CZ	2.98	0.46
8:V:104:ASP:HB2	8:V:105:PRO:HD2	1.97	0.46
9:W:20:VAL:HG23	9:W:189:ILE:HB	1.98	0.46
9:W:9:GLY:HA3	9:W:41:LYS:HE2	1.97	0.46
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.98	0.46
17:K:301:3BV:H18	12:L:108:HIS:HB2	1.97	0.46
17:K:301:3BV:H17	17:K:301:3BV:O9	2.12	0.46
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.97	0.46
11:K:5:ALA:HB3	11:K:100:MET:HE2	1.98	0.46
11:K:1:THR:CG2	11:K:2:THR:N	2.79	0.45
9:I:9:GLY:HA3	9:I:41:LYS:HE2	1.98	0.45
11:Y:104:TYR:CD1	11:Y:182:GLU:HG3	2.52	0.45
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.98	0.45
11:Y:40:PHE:CG	11:Y:73:ARG:NH1	2.80	0.45
12:Z:147:MET:N	12:Z:148:PRO:HD2	2.32	0.45
12:L:147:MET:N	12:L:148:PRO:HD2	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:174:MET:HA	10:X:174:MET:HA	1.98	0.44
11:Y:5:ALA:HB3	11:Y:100:MET:HE2	1.98	0.44
9:I:20:VAL:HG23	9:I:189:ILE:HB	1.98	0.44
17:K:301:3BV:C28	17:K:301:3BV:H38	2.47	0.44
6:F:172:LEU:CD1	6:F:195:ILE:HD13	2.48	0.44
8:V:218:VAL:CG2	9:W:196:LYS:HB2	2.48	0.44
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.17	0.43
12:L:8:ASN:HA	12:L:30:ILE:O	2.18	0.43
13:M:96:LEU:O	13:M:100:MET:HG2	2.19	0.43
6:T:172:LEU:CD1	6:T:195:ILE:HD13	2.48	0.43
10:J:21:VAL:HG11	11:K:122:LEU:HD11	1.99	0.43
11:Y:116:ASP:C	11:Y:116:ASP:OD1	2.57	0.43
11:Y:35:ILE:HG22	11:Y:43:GLY:O	2.18	0.43
10:X:21:VAL:HG11	11:Y:122:LEU:HD11	2.01	0.43
13:M:165:ILE:HB	13:M:166:PRO:HD3	2.01	0.43
3:Q:160:GLN:HA	3:Q:160:GLN:HE21	1.84	0.42
3:Q:201:VAL:HG13	3:Q:202:GLN:N	2.34	0.42
3:C:201:VAL:HG13	3:C:202:GLN:N	2.34	0.42
8:H:168:GLY:O	17:H:301:3BV:H57	2.20	0.42
7:G:78:ILE:N	7:G:79:PRO:CD	2.83	0.42
12:L:125:PHE:CD2	12:L:131:TYR:HB3	2.55	0.42
11:Y:40:PHE:CE2	11:Y:73:ARG:NH2	2.81	0.42
12:Z:125:PHE:CD2	12:Z:131:TYR:HB3	2.55	0.42
7:U:78:ILE:N	7:U:79:PRO:CD	2.82	0.42
9:I:36:SER:HB2	10:J:126:VAL:HG11	2.02	0.42
8:V:168:GLY:O	17:V:301:3BV:H57	2.19	0.42
11:K:19:ARG:O	17:K:301:3BV:H58	2.20	0.42
3:C:160:GLN:HA	3:C:160:GLN:HE21	1.84	0.41
13:M:27:LEU:HD21	13:M:34:LEU:HD22	2.01	0.41
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.54	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
17:K:301:3BV:C28	17:K:301:3BV:C38	2.99	0.41
11:Y:16:VAL:HG21	11:Y:34:VAL:HG23	2.01	0.41
2:B:14:PRO:HA	3:C:20:TYR:CE1	2.54	0.41
2:P:50:LYS:O	2:P:51:VAL:C	2.59	0.41
11:Y:18:SER:OG	11:Y:18:SER:O	2.38	0.41
1:A:55:LEU:HD12	7:G:170:THR:HG23	2.02	0.41
17:K:301:3BV:C46	17:K:301:3BV:N41	2.83	0.41
2:B:151:ASN:HB2	2:B:152:PRO:CD	2.50	0.41
5:E:175:LEU:HA	5:E:178:PHE:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:18:SER:OG	11:K:18:SER:O	2.38	0.41
5:E:98:PHE:O	13:M:91:TYR:HA	2.21	0.41
5:S:175:LEU:HA	5:S:178:PHE:CE2	2.55	0.40
5:S:77:ALA:N	5:S:78:PRO:CD	2.84	0.40
11:Y:176:ASN:ND2	11:Y:187:TYR:OH	2.54	0.40
2:B:50:LYS:O	2:B:51:VAL:C	2.60	0.40
2:B:86:LEU:HB3	2:B:114:LEU:HD21	2.04	0.40
13:M:35:ARG:HG2	13:M:36:PHE:CE2	2.56	0.40
12:L:4:PRO:O	13:M:104:ARG:NH1	2.50	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	248/250 (99%)	242 (98%)	6 (2%)	0	100	100
1	O	248/250 (99%)	242 (98%)	6 (2%)	0	100	100
2	B	242/258 (94%)	234 (97%)	6 (2%)	2 (1%)	24	51
2	P	242/258 (94%)	234 (97%)	6 (2%)	2 (1%)	24	51
3	C	238/254 (94%)	230 (97%)	6 (2%)	2 (1%)	24	51
3	Q	238/254 (94%)	230 (97%)	6 (2%)	2 (1%)	24	51
4	D	231/260 (89%)	225 (97%)	6 (3%)	0	100	100
4	R	231/260 (89%)	225 (97%)	6 (3%)	0	100	100
5	E	229/234 (98%)	223 (97%)	6 (3%)	0	100	100
5	S	229/234 (98%)	223 (97%)	6 (3%)	0	100	100
6	F	241/288 (84%)	236 (98%)	5 (2%)	0	100	100
6	T	241/288 (84%)	237 (98%)	4 (2%)	0	100	100
7	G	239/252 (95%)	235 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	U	239/252 (95%)	235 (98%)	4 (2%)	0	100	100
8	H	220/232 (95%)	214 (97%)	6 (3%)	0	100	100
8	V	220/232 (95%)	214 (97%)	6 (3%)	0	100	100
9	I	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
9	W	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
10	J	193/198 (98%)	189 (98%)	3 (2%)	1 (0%)	34	63
10	X	193/198 (98%)	189 (98%)	3 (2%)	1 (0%)	34	63
11	K	210/212 (99%)	205 (98%)	5 (2%)	0	100	100
11	Y	210/212 (99%)	205 (98%)	5 (2%)	0	100	100
12	L	220/222 (99%)	215 (98%)	5 (2%)	0	100	100
12	Z	220/222 (99%)	215 (98%)	5 (2%)	0	100	100
13	M	231/246 (94%)	222 (96%)	8 (4%)	1 (0%)	39	69
13	a	231/246 (94%)	222 (96%)	8 (4%)	1 (0%)	39	69
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	6276/6614 (95%)	6105 (97%)	159 (2%)	12 (0%)	52	80

All (12) Ramachandran outliers are listed below:

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

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	209/209 (100%)	206 (99%)	3 (1%)	74	92
1	O	209/209 (100%)	206 (99%)	3 (1%)	74	92
2	B	203/216 (94%)	196 (97%)	7 (3%)	44	75
2	P	203/216 (94%)	196 (97%)	7 (3%)	44	75
3	C	212/226 (94%)	205 (97%)	7 (3%)	45	76
3	Q	212/226 (94%)	206 (97%)	6 (3%)	51	81
4	D	194/215 (90%)	186 (96%)	8 (4%)	37	69
4	R	194/215 (90%)	186 (96%)	8 (4%)	37	69
5	E	190/193 (98%)	183 (96%)	7 (4%)	41	72
5	S	190/193 (98%)	183 (96%)	7 (4%)	41	72
6	F	201/239 (84%)	193 (96%)	8 (4%)	38	69
6	T	201/239 (84%)	192 (96%)	9 (4%)	34	65
7	G	206/210 (98%)	200 (97%)	6 (3%)	50	80
7	U	206/210 (98%)	200 (97%)	6 (3%)	50	80
8	H	181/190 (95%)	177 (98%)	4 (2%)	60	86
8	V	181/190 (95%)	176 (97%)	5 (3%)	51	81
9	I	172/173 (99%)	169 (98%)	3 (2%)	68	90
9	W	172/173 (99%)	169 (98%)	3 (2%)	68	90
10	J	173/175 (99%)	168 (97%)	5 (3%)	50	80
10	X	173/175 (99%)	168 (97%)	5 (3%)	50	80
11	K	168/168 (100%)	157 (94%)	11 (6%)	21	46
11	Y	168/168 (100%)	159 (95%)	9 (5%)	27	56
12	L	185/185 (100%)	179 (97%)	6 (3%)	46	77
12	Z	185/185 (100%)	179 (97%)	6 (3%)	46	77
13	M	199/208 (96%)	194 (98%)	5 (2%)	55	84
13	a	199/208 (96%)	193 (97%)	6 (3%)	48	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	N	162/162 (100%)	160 (99%)	2 (1%)	78	93
14	b	162/162 (100%)	160 (99%)	2 (1%)	78	93
All	All	5310/5538 (96%)	5146 (97%)	164 (3%)	47	78

All (164) 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
3	C	203	THR
4	D	99	ILE
4	D	125	LEU
4	D	176	LEU
4	D	193	LEU
4	D	214	ILE
4	D	224	ASP
4	D	236	LYS
4	D	242	GLU
5	E	9	THR
5	E	29	LYS
5	E	54	GLU
5	E	71	LEU
5	E	184	ASN
5	E	188	LEU
5	E	202	ASP
6	F	14	ASP
6	F	123	ASN

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Mol	Chain	Res	Type
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	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	23	ARG
10	J	75	LEU
10	J	78	GLN
10	J	144	LEU
10	J	174	MET
11	K	4	LEU
11	K	9	GLN
11	K	18	SER
11	K	19	ARG
11	K	35	ILE
11	K	53	GLN
11	K	57	THR
11	K	99	THR
11	K	104	TYR
11	K	116	ASP
11	K	209	ASN
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	48	ASN

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Mol	Chain	Res	Type
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
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	117	GLN
6	T	123	ASN
6	T	172	LEU
6	T	181	GLU

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Mol	Chain	Res	Type
6	T	203	ASN
6	T	206	LYS
6	T	214	TRP
6	T	221	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	31	CYS
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	144	LEU
10	X	174	MET
11	Y	4	LEU
11	Y	9	GLN
11	Y	18	SER
11	Y	53	GLN
11	Y	57	THR
11	Y	99	THR
11	Y	104	TYR
11	Y	116	ASP
11	Y	209	ASN
12	Z	1	GLN
12	Z	23	LEU
12	Z	31	THR
12	Z	49	ASN
12	Z	136	CYS
12	Z	167	LYS
13	a	35	ARG
13	a	48	ASN
13	a	70	LEU
13	a	104	ARG

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

Mol	Chain	Res	Type
1	A	94	HIS
2	B	119	GLN
2	B	123	GLN
2	B	155	ASN
3	C	38	ASN
3	C	147	GLN
3	C	160	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
10	J	55	GLN
11	K	85	ASN
11	K	176	ASN
11	K	190	ASN
12	L	3	ASN
12	L	70	ASN
12	L	108	HIS
12	L	158	ASN
12	L	159	GLN
13	M	48	ASN
13	M	102	GLN
13	M	179	ASN

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Mol	Chain	Res	Type
13	M	194	ASN
13	M	213	GLN
14	N	161	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	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
11	Y	190	ASN
12	Z	3	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
14	b	161	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 20 ligands modelled in this entry, 11 are monoatomic - leaving 9 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	1.16	3 (5%)	67,71,71	1.45	8 (11%)
18	MES	H	302	-	12,12,12	2.07	1 (8%)	15,16,16	1.94	3 (20%)
17	3BV	K	301	11	54,54,54	1.08	3 (5%)	67,71,71	1.81	14 (20%)
18	MES	K	303	-	12,12,12	2.15	1 (8%)	15,16,16	1.83	3 (20%)
17	3BV	N	201	14	54,54,54	1.33	3 (5%)	67,71,71	1.56	8 (11%)
17	3BV	V	301	8	54,54,54	1.14	3 (5%)	67,71,71	1.46	8 (11%)
18	MES	V	303	-	12,12,12	2.10	1 (8%)	15,16,16	1.86	3 (20%)
18	MES	Y	302	-	12,12,12	2.20	1 (8%)	15,16,16	1.66	3 (20%)
17	3BV	b	201	14	54,54,54	1.29	3 (5%)	67,71,71	1.55	8 (11%)

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
18	MES	Y	302	-	-	0/6/14/14	0/1/1/1
17	3BV	b	201	14	-	0/59/67/67	0/3/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	Y	302	MES	C8-S	-7.37	1.66	1.77
18	K	303	MES	C8-S	-7.19	1.66	1.77
18	V	303	MES	C8-S	-6.95	1.67	1.77
18	H	302	MES	C8-S	-6.85	1.67	1.77
17	K	301	3BV	C32-C33	-4.85	1.39	1.51
17	N	201	3BV	C32-C33	-4.30	1.40	1.51
17	b	201	3BV	C32-C33	-4.24	1.40	1.51
17	H	301	3BV	C32-C33	-4.19	1.41	1.51
17	V	301	3BV	C32-C33	-4.14	1.41	1.51
17	K	301	3BV	C13-C14	-3.82	1.40	1.51
17	N	201	3BV	C13-C14	-3.54	1.41	1.51
17	b	201	3BV	C13-C14	-3.54	1.41	1.51
17	H	301	3BV	C13-C14	-3.14	1.42	1.51
17	V	301	3BV	C13-C14	-3.13	1.42	1.51
17	K	301	3BV	C51-C47	3.40	1.60	1.53
17	V	301	3BV	C51-C47	4.56	1.62	1.53
17	H	301	3BV	C51-C47	4.73	1.62	1.53
17	b	201	3BV	C51-C47	5.96	1.64	1.53
17	N	201	3BV	C51-C47	6.38	1.65	1.53

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	N	201	3BV	C43-C42-N41	-6.71	100.80	109.98
17	b	201	3BV	C43-C42-N41	-6.66	100.86	109.98
17	K	301	3BV	C2-C3-N4	-6.08	100.80	110.11
17	V	301	3BV	C43-C42-N41	-5.95	101.83	109.98
17	H	301	3BV	C43-C42-N41	-5.89	101.92	109.98
17	N	201	3BV	C58-C51-C59	-5.70	102.23	109.73
17	K	301	3BV	C7-N4-C5	-5.69	102.78	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	b	201	3BV	C58-C51-C59	-5.46	102.55	109.73
17	V	301	3BV	C58-C51-C59	-4.36	104.00	109.73
17	H	301	3BV	C58-C51-C59	-4.16	104.27	109.73
17	K	301	3BV	C44-C43-C42	-3.89	107.53	115.64
17	V	301	3BV	O1-C6-C5	-3.88	102.87	111.83
17	H	301	3BV	O1-C6-C5	-3.87	102.88	111.83
17	K	301	3BV	C33-C32-C31	-3.61	102.79	113.44
17	K	301	3BV	C6-C5-N4	-3.50	104.76	110.11
17	K	301	3BV	C25-C24-C23	-3.50	104.99	115.49
17	K	301	3BV	O1-C6-C5	-3.47	103.82	111.83
17	b	201	3BV	C33-C32-C31	-3.22	103.93	113.44
17	K	301	3BV	O60-C59-C51	-3.17	104.54	111.16
17	N	201	3BV	C33-C32-C31	-3.16	104.10	113.44
17	H	301	3BV	C25-C24-C23	-3.12	106.11	115.49
17	V	301	3BV	C25-C24-C23	-3.10	106.18	115.49
17	K	301	3BV	C58-C51-C59	-3.03	105.75	109.73
17	N	201	3BV	O1-C6-C5	-2.97	104.98	111.83
17	K	301	3BV	C43-C42-N41	-2.93	105.97	109.98
17	b	201	3BV	O1-C6-C5	-2.93	105.06	111.83
17	V	301	3BV	C33-C32-C31	-2.86	105.00	113.44
17	H	301	3BV	C6-C5-N4	-2.82	105.80	110.11
17	H	301	3BV	C33-C32-C31	-2.82	105.12	113.44
17	b	201	3BV	O1-C2-C3	-2.81	105.35	111.83
17	N	201	3BV	O1-C2-C3	-2.80	105.35	111.83
17	b	201	3BV	C12-C11-C20	-2.79	103.49	110.34
17	N	201	3BV	C12-C11-C20	-2.78	103.52	110.34
17	V	301	3BV	C6-C5-N4	-2.76	105.89	110.11
17	V	301	3BV	O60-C59-C51	-2.69	105.54	111.16
17	b	201	3BV	C12-C13-C14	-2.68	103.29	113.18
17	N	201	3BV	C12-C13-C14	-2.67	103.33	113.18
17	K	301	3BV	O1-C2-C3	-2.63	105.75	111.83
17	H	301	3BV	O60-C59-C51	-2.55	105.83	111.16
17	K	301	3BV	C12-C13-C14	-2.21	105.00	113.18
17	K	301	3BV	C23-C28-N30	-2.09	111.91	116.80
17	K	301	3BV	C39-C31-N30	-2.07	105.41	111.28
17	H	301	3BV	C7-N4-C5	2.08	114.18	111.14
17	V	301	3BV	C7-N4-C5	2.09	114.20	111.14
18	H	302	MES	O3S-S-C8	2.10	109.36	104.99
18	Y	302	MES	O3S-S-C8	2.15	109.45	104.99
17	N	201	3BV	C24-C23-N22	2.28	116.21	110.47
18	K	303	MES	O3S-S-C8	2.29	109.74	104.99
18	V	303	MES	O3S-S-C8	2.32	109.81	104.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	b	201	3BV	C24-C23-N22	2.33	116.34	110.47
18	K	303	MES	O2S-S-C8	3.38	109.26	106.87
18	V	303	MES	O2S-S-C8	3.44	109.30	106.87
18	H	302	MES	O1S-S-C8	3.53	109.36	106.87
18	Y	302	MES	O2S-S-C8	3.60	109.42	106.87
18	Y	302	MES	O1S-S-C8	3.64	109.44	106.87
18	K	303	MES	O1S-S-C8	4.51	110.05	106.87
18	V	303	MES	O1S-S-C8	5.20	110.54	106.87
18	H	302	MES	O2S-S-C8	5.61	110.83	106.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	H	301	3BV	1	0
17	K	301	3BV	14	0
17	V	301	3BV	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%)	-0.31	7 (2%) 56 57	39, 54, 92, 145	0
1	O	250/250 (100%)	-0.17	9 (3%) 46 46	45, 64, 108, 148	0
2	B	244/258 (94%)	-0.10	12 (4%) 33 32	40, 62, 109, 165	0
2	P	244/258 (94%)	-0.07	14 (5%) 27 26	46, 66, 113, 164	0
3	C	240/254 (94%)	-0.02	17 (7%) 19 17	44, 66, 131, 165	0
3	Q	240/254 (94%)	0.14	16 (6%) 21 19	50, 80, 157, 193	0
4	D	235/260 (90%)	-0.31	2 (0%) 85 86	44, 66, 98, 145	0
4	R	235/260 (90%)	-0.13	10 (4%) 39 38	52, 73, 114, 157	0
5	E	231/234 (98%)	-0.13	5 (2%) 65 66	45, 68, 103, 143	0
5	S	231/234 (98%)	-0.07	11 (4%) 34 33	50, 74, 116, 152	0
6	F	243/288 (84%)	-0.32	6 (2%) 61 61	40, 60, 112, 140	0
6	T	243/288 (84%)	-0.22	8 (3%) 50 50	38, 68, 121, 161	0
7	G	241/252 (95%)	-0.35	6 (2%) 61 61	39, 56, 97, 149	0
7	U	241/252 (95%)	-0.33	6 (2%) 61 61	38, 59, 92, 134	0
8	H	222/232 (95%)	-0.36	3 (1%) 78 77	41, 54, 93, 131	0
8	V	222/232 (95%)	-0.33	2 (0%) 85 86	41, 57, 93, 138	0
9	I	204/205 (99%)	-0.51	3 (1%) 76 76	40, 55, 85, 107	0
9	W	204/205 (99%)	-0.41	5 (2%) 61 61	41, 58, 87, 114	0
10	J	195/198 (98%)	-0.34	3 (1%) 76 76	38, 58, 88, 123	0
10	X	195/198 (98%)	-0.39	3 (1%) 76 76	42, 60, 87, 137	0
11	K	212/212 (100%)	-0.28	5 (2%) 62 62	45, 62, 96, 111	0
11	Y	212/212 (100%)	-0.21	7 (3%) 50 50	49, 62, 91, 113	0
12	L	222/222 (100%)	-0.40	4 (1%) 71 72	35, 57, 94, 127	0
12	Z	222/222 (100%)	-0.33	6 (2%) 58 58	38, 57, 94, 121	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	M	233/246 (94%)	-0.56	2 (0%) 85 86	34, 52, 77, 86	0
13	a	233/246 (94%)	-0.50	2 (0%) 85 86	36, 52, 75, 86	0
14	N	196/196 (100%)	-0.56	0 100 100	34, 48, 79, 102	0
14	b	196/196 (100%)	-0.55	2 (1%) 84 85	36, 49, 79, 102	0
All	All	6336/6614 (95%)	-0.28	176 (2%) 56 57	34, 61, 107, 193	0

All (176) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	1	MET	9.3
1	A	1	MET	7.3
2	B	219	ALA	7.0
2	P	219	ALA	7.0
2	B	220	ASN	6.5
3	Q	50	LEU	6.2
10	X	1	MET	6.1
3	Q	49	THR	6.1
5	E	202	ASP	5.9
3	Q	238	LYS	5.7
8	H	221	CYS	5.5
2	P	51	VAL	5.4
3	C	238	LYS	5.4
5	S	202	ASP	5.3
10	J	1	MET	5.3
3	C	206	LYS	5.0
2	B	218	GLY	4.9
9	W	1	SER	4.9
3	Q	206	LYS	4.8
8	V	222	ASP	4.7
2	B	51	VAL	4.7
2	B	221	ASP	4.6
2	P	59	ASP	4.6
4	R	241	ALA	4.6
2	P	221	ASP	4.5
1	O	249	ALA	4.5
13	a	1	THR	4.5
3	C	49	THR	4.5
3	Q	236	GLN	4.4
9	I	1	SER	4.3
11	Y	212	GLY	4.2
2	P	220	ASN	4.2

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Mol	Chain	Res	Type	RSRZ
2	P	222	GLY	4.2
12	Z	174	TYR	4.1
10	X	194	ASP	4.0
8	V	221	CYS	4.0
11	Y	147	ASP	4.0
13	M	1	THR	4.0
3	Q	239	GLN	4.0
4	D	241	ALA	4.0
3	C	202	GLN	3.8
12	L	172	LEU	3.7
1	O	201	GLU	3.7
6	T	243	ILE	3.6
1	O	250	LEU	3.6
3	Q	205	ALA	3.5
5	E	233	ILE	3.5
8	H	222	ASP	3.5
5	S	233	ILE	3.5
2	P	218	GLY	3.4
3	C	239	GLN	3.4
4	R	242	GLU	3.3
10	J	193	ASP	3.3
3	Q	51	LYS	3.3
10	X	193	ASP	3.3
3	C	225	GLU	3.3
3	Q	48	SER	3.2
3	C	236	GLN	3.2
2	P	52	THR	3.2
1	A	2	THR	3.1
6	T	2	THR	3.1
3	Q	240	GLU	3.1
1	A	248	GLU	3.0
4	R	230	GLU	3.0
9	W	131	GLU	3.0
10	J	194	ASP	3.0
3	C	240	GLU	3.0
1	O	231	LYS	3.0
4	D	242	GLU	3.0
3	C	235	GLU	3.0
11	K	183	ASP	2.9
1	O	50	LYS	2.9
5	S	54	GLU	2.9
11	Y	183	ASP	2.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
13	a	233	ILE	2.9
1	A	250	LEU	2.9
12	Z	210	ASP	2.8
4	R	125	LEU	2.8
7	G	3	TYR	2.8
9	W	130	ASP	2.7
11	K	147	ASP	2.7
3	C	181	GLU	2.7
3	Q	202	GLN	2.7
1	O	2	THR	2.7
2	B	59	ASP	2.7
6	F	205	GLU	2.7
4	R	201	GLU	2.7
2	P	225	TYR	2.7
12	L	165	ASN	2.7
11	Y	209	ASN	2.6
12	Z	165	ASN	2.6
9	W	133	LYS	2.6
1	A	249	ALA	2.6
3	C	50	LEU	2.6
4	R	1	ASP	2.6
3	C	47	ARG	2.6
12	L	174	TYR	2.6
5	S	225	ASP	2.6
1	A	201	GLU	2.5
3	Q	141	ASP	2.5
7	U	222	ASP	2.5
5	S	30	GLN	2.5
9	I	131	GLU	2.5
5	E	54	GLU	2.5
7	U	51	PRO	2.5
5	E	227	GLU	2.5
1	O	52	SER	2.5
2	B	217	LYS	2.5
13	M	47	ASP	2.5
2	B	235	LYS	2.5
6	F	53	LYS	2.5
12	Z	167	LYS	2.5
2	P	203	SER	2.4
2	B	50	LYS	2.4
6	T	241	LYS	2.4
7	G	242	GLN	2.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	P	182	ASP	2.4
7	U	242	GLN	2.4
1	O	248	GLU	2.4
14	b	105	LYS	2.4
9	I	130	ASP	2.4
5	E	201	ARG	2.4
5	S	173	ARG	2.4
3	Q	187	GLU	2.4
7	G	179	LYS	2.4
12	Z	172	LEU	2.4
14	b	195	GLN	2.4
7	G	222	ASP	2.3
3	C	175	LYS	2.3
2	P	223	GLU	2.3
6	T	244	ASN	2.3
7	U	188	GLU	2.3
6	T	230	ASP	2.3
4	R	116	GLY	2.3
11	Y	106	ARG	2.3
7	U	241	GLU	2.3
11	K	73	ARG	2.3
12	Z	1	GLN	2.3
11	Y	151	GLU	2.3
1	A	231	LYS	2.3
3	C	180	LYS	2.3
2	P	50	LYS	2.3
6	F	215	CYS	2.3
5	S	122	TYR	2.2
7	U	3	TYR	2.2
2	B	222	GLY	2.2
7	G	241	GLU	2.2
6	F	202	ASP	2.2
11	K	212	GLY	2.2
5	S	180	LYS	2.2
7	G	181	LYS	2.2
3	C	203	THR	2.2
9	W	192	ASP	2.2
4	R	239	GLU	2.1
3	Q	223	SER	2.1
6	F	201	GLU	2.1
5	S	207	VAL	2.1
2	P	60	THR	2.1

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Mol	Chain	Res	Type	RSRZ
6	F	244	ASN	2.1
6	T	166	GLN	2.1
5	S	218	ASP	2.1
4	R	217	GLN	2.1
2	B	240	LYS	2.1
3	Q	180	LYS	2.1
4	R	54	ASP	2.1
2	B	203	SER	2.1
3	Q	204	GLY	2.1
6	T	205	GLU	2.1
11	Y	73	ARG	2.1
3	C	48	SER	2.1
3	C	37	LYS	2.0
8	H	198	GLU	2.0
5	S	3	ASN	2.0
6	T	215	CYS	2.0
12	L	167	LYS	2.0
11	K	151	GLU	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(Å <sup>2</sup> )	Q<0.9
18	MES	K	303	12/12	0.70	0.47	10.65	48,50,69,72	12
18	MES	Y	302	12/12	0.65	0.50	10.38	49,50,68,68	12
18	MES	V	303	12/12	0.88	0.45	8.68	81,84,112,118	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
15	MG	I	301	1/1	0.95	0.44	7.98	74,74,74,74	0
17	3BV	N	201	52/52	0.84	0.25	6.80	37,51,131,136	0
18	MES	H	302	12/12	0.91	0.36	6.56	77,81,93,98	0
17	3BV	K	301	52/52	0.71	0.35	5.90	46,59,114,117	52
17	3BV	b	201	52/52	0.87	0.22	4.54	40,54,133,136	0
17	3BV	V	301	52/52	0.85	0.29	2.70	57,64,111,117	0
17	3BV	H	301	52/52	0.87	0.28	2.48	54,63,112,116	0
15	MG	Z	301	1/1	0.95	0.22	2.27	74,74,74,74	0
15	MG	G	301	1/1	0.94	0.13	-0.34	64,64,64,64	0
15	MG	N	202	1/1	0.99	0.08	-1.40	46,46,46,46	0
16	CL	b	202	1/1	0.99	0.06	-1.81	56,56,56,56	0
15	MG	K	302	1/1	0.99	0.06	-2.52	64,64,64,64	0
15	MG	Y	301	1/1	0.95	0.07	-3.00	61,61,61,61	0
16	CL	N	203	1/1	0.98	0.05	-3.08	52,52,52,52	0
15	MG	V	302	1/1	0.96	0.07	-4.35	69,69,69,69	0
16	CL	G	302	1/1	0.99	0.08	-	44,44,44,44	0
16	CL	U	301	1/1	0.99	0.15	-	45,45,45,45	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.