



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 13, 2016 – 03:59 AM EST

PDB ID : 5L63  
Title : Yeast 20S proteasome with human beta5c (1-138) and human beta6 (97-111; 118-133) in complex with epoxyketone inhibitor 17  
Authors : Groll, M.; Huber, E.M.  
Deposited on : 2016-05-28  
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

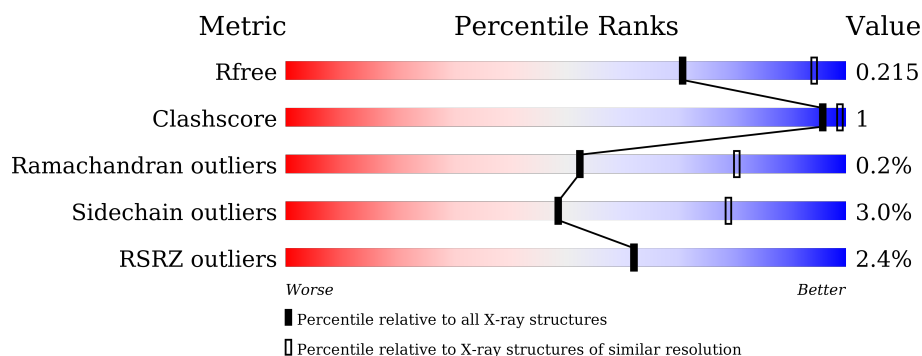
# 1 Overall quality at a glance

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.





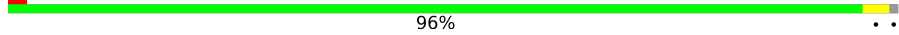
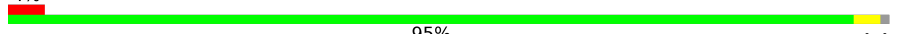






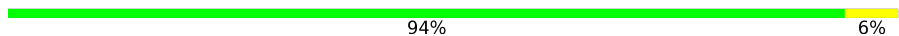





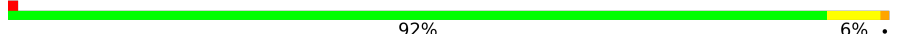



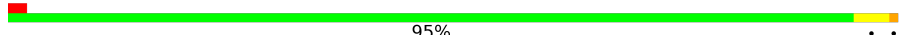

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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>2%</div> <div> <div></div> <div>98%</div> <div>.</div> </div> </div>
1	O	250	<div> <div>3%</div> <div> <div></div> <div>98%</div> <div>.</div> </div> </div>
2	B	258	<div> <div>3%</div> <div> <div></div> <div>90%</div> <div>5%</div> </div> </div>
2	P	258	<div> <div>3%</div> <div> <div></div> <div>90%</div> <div>5%</div> </div> </div>
3	C	254	<div> <div>6%</div> <div> <div></div> <div>87%</div> <div>6%</div> <div>6%</div> </div> </div>
3	Q	254	<div> <div>7%</div> <div> <div></div> <div>87%</div> <div>6%</div> <div>6%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
4	D	260	
4	R	260	
5	E	234	
5	S	234	
6	F	288	
6	T	288	
7	G	252	
7	U	252	
8	H	232	
8	V	232	
9	I	205	
9	W	205	
10	J	198	
10	X	198	
11	K	211	
11	Y	211	
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	A	301	-	-	-	X
17	04C	H	301	X	-	-	X
17	04C	K	301	X	-	-	-
17	04C	V	301	X	-	-	X
17	04C	Y	301	X	-	-	X
18	MES	H	302	-	-	-	X
18	MES	K	304	-	-	-	X
18	MES	V	302	-	-	-	X
18	MES	X	201	-	-	-	X

## 2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 49924 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
			1907	1214	320	365	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	226	Total	C	N	O	S	0	1	0
			1726	1087	300	332	7			
8	V	226	Total	C	N	O	S	0	0	0
			1719	1082	298	332	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,Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	211	Total	C	N	O	S	0	0	0
			1632	1036	282	306	8			
11	Y	211	Total	C	N	O	S	0	0	0
			1632	1036	282	306	8			

- Molecule 12 is a protein called Proteasome subunit beta type-6,Proteasome subunit beta type-1,Proteasome subunit beta type-6,Proteasome subunit beta type-1,Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	222	Total	C	N	O	S	0	0	0
			1764	1119	305	336	4			
12	Z	222	Total	C	N	O	S	0	0	0
			1764	1119	305	336	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).

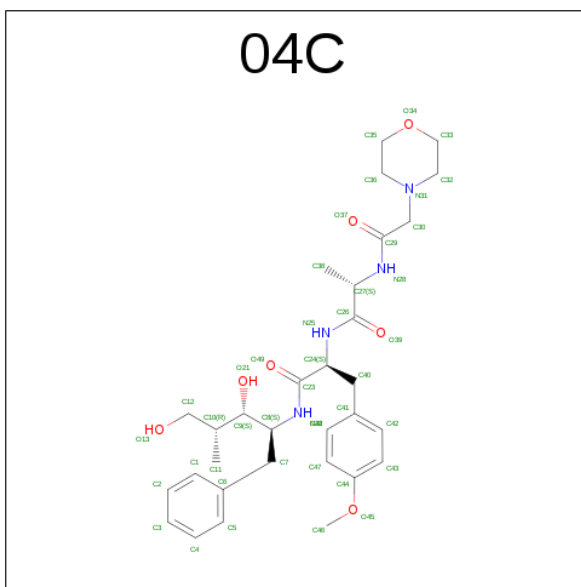
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	G	1	Total Mg 1 1	0	0
15	J	1	Total Mg 1 1	0	0
15	K	2	Total Mg 2 2	0	0
15	b	1	Total Mg 1 1	0	0
15	I	2	Total Mg 2 2	0	0
15	Z	1	Total Mg 1 1	0	0
15	A	1	Total Mg 1 1	0	0
15	N	1	Total Mg 1 1	0	0
15	L	1	Total Mg 1 1	0	0

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

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

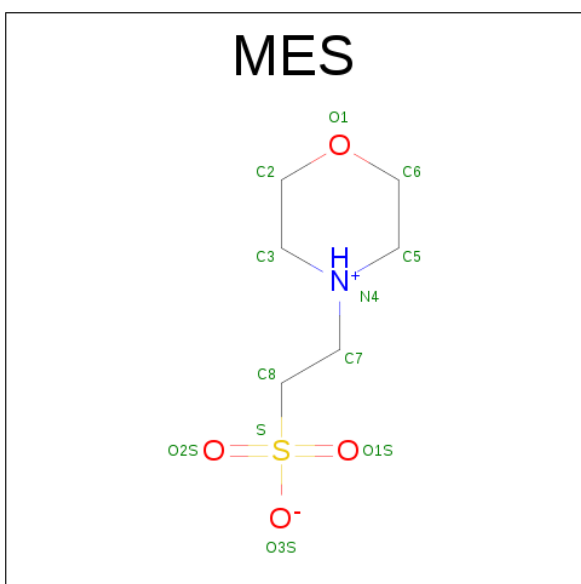
- Molecule 17 is 1,2,4-trideoxy-4-methyl-2- {[N-(morpholin-4-ylacetyl)-L-alanyl-O-methyl-L-tyrosyl]amino}-1-phenyl-D-xylitol (three-letter code: 04C) (formula: C<sub>31</sub>H<sub>44</sub>N<sub>4</sub>O<sub>7</sub>).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	H	1	Total	C	N	O	0	0
			42	31	4	7		
17	K	1	Total	C	N	O	0	0
			42	31	4	7		
17	V	1	Total	C	N	O	0	0
			42	31	4	7		
17	Y	1	Total	C	N	O	0	0
			42	31	4	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	X	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	18	Total	O	0	0
			18	18		
19	B	15	Total	O	0	0
			15	15		
19	C	8	Total	O	0	0
			8	8		
19	D	9	Total	O	0	0
			9	9		
19	E	7	Total	O	0	0
			7	7		
19	F	8	Total	O	0	0
			8	8		
19	G	16	Total	O	0	0
			16	16		
19	H	11	Total	O	0	0
			11	11		
19	I	10	Total	O	0	0
			10	10		
19	J	13	Total	O	0	0
			13	13		
19	K	7	Total	O	0	0
			7	7		
19	L	14	Total	O	0	0
			14	14		
19	M	23	Total	O	0	0
			23	23		
19	N	9	Total	O	0	0
			9	9		
19	O	9	Total	O	0	0
			9	9		
19	P	11	Total	O	0	0
			11	11		

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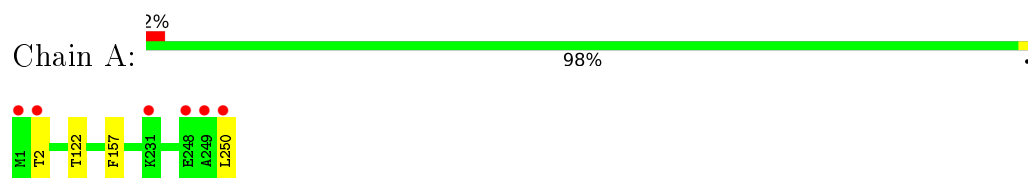
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	Q	8	Total 8	O 8	0	0
19	R	10	Total 10	O 10	0	0
19	S	7	Total 7	O 7	0	0
19	T	13	Total 13	O 13	0	0
19	U	20	Total 20	O 20	0	0
19	V	16	Total 16	O 16	0	0
19	W	10	Total 10	O 10	0	0
19	X	12	Total 12	O 12	0	0
19	Y	13	Total 13	O 13	0	0
19	Z	7	Total 7	O 7	0	0
19	a	19	Total 19	O 19	0	0
19	b	9	Total 9	O 9	0	0

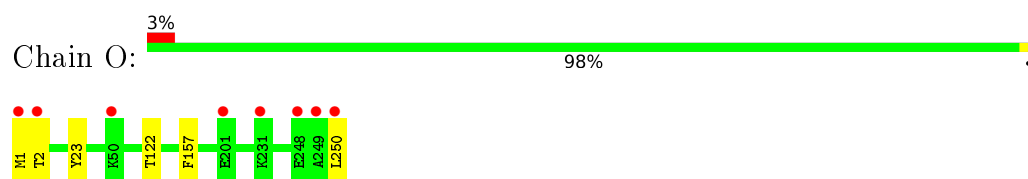
### 3 Residue-property plots [i](#)

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.

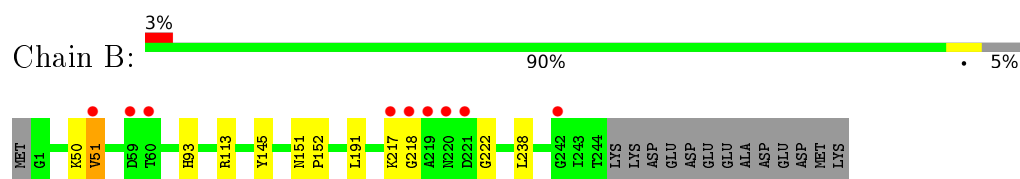
- Molecule 1: Proteasome subunit alpha type-2



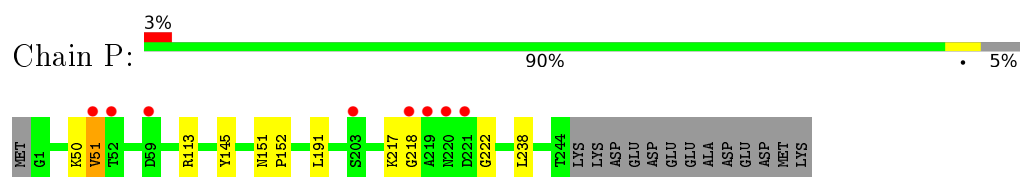
- Molecule 1: Proteasome subunit alpha type-2



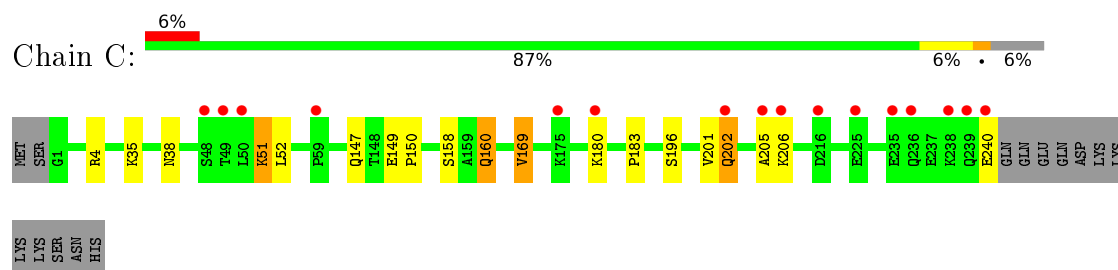
- Molecule 2: Proteasome subunit alpha type-3



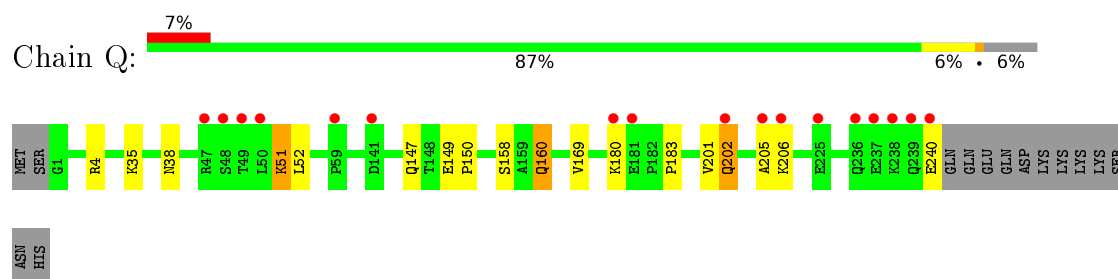
- Molecule 2: Proteasome subunit alpha type-3



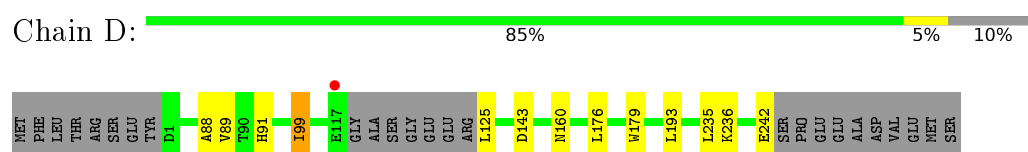
- Molecule 3: Proteasome subunit alpha type-4



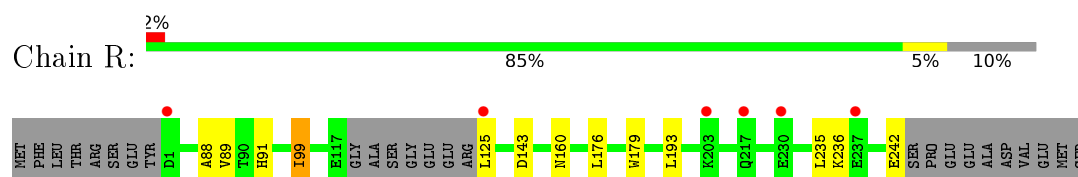
- Molecule 3: Proteasome subunit alpha type-4



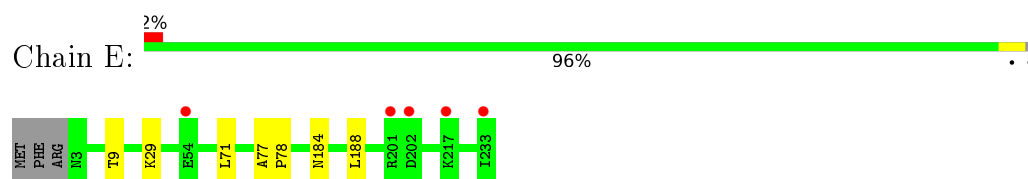
- Molecule 4: Proteasome subunit alpha type-5



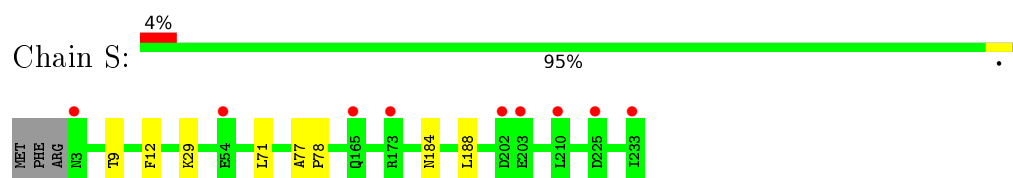
- Molecule 4: Proteasome subunit alpha type-5



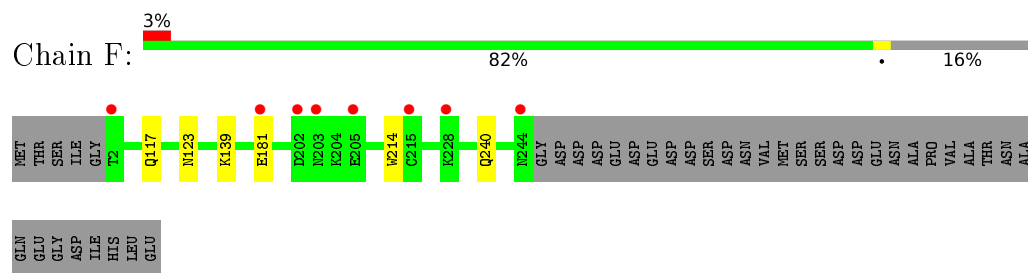
- Molecule 5: Proteasome subunit alpha type-6



- Molecule 5: Proteasome subunit alpha type-6



- Molecule 6: Probable proteasome subunit alpha type-7

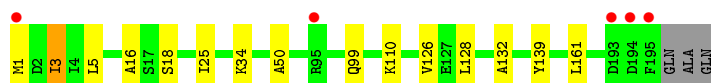
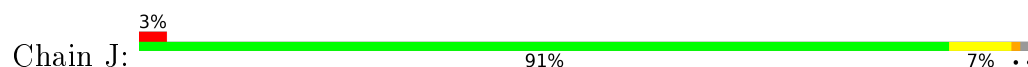


- Molecule 6: Probable proteasome subunit alpha type-7

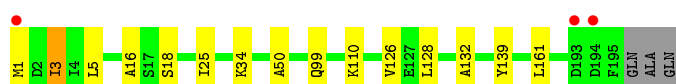




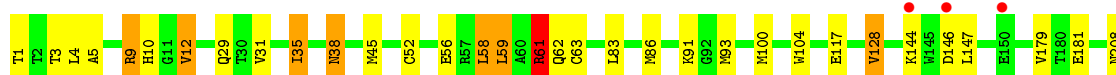
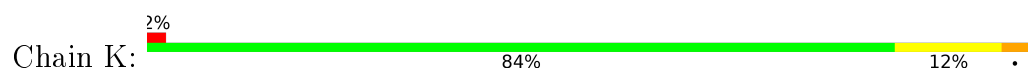
- Molecule 10: Proteasome subunit beta type-4



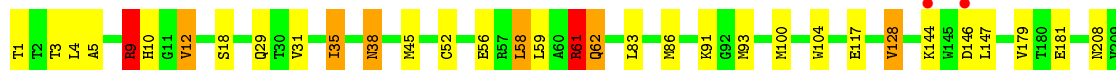
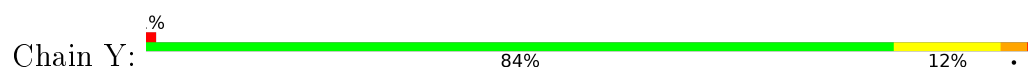
- Molecule 10: Proteasome subunit beta type-4



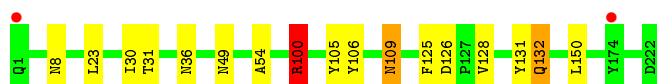
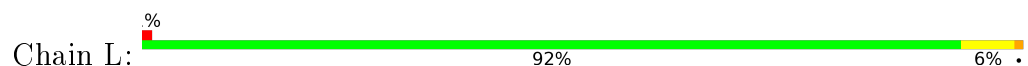
- Molecule 11: Proteasome subunit beta type-5, Proteasome subunit beta type-5



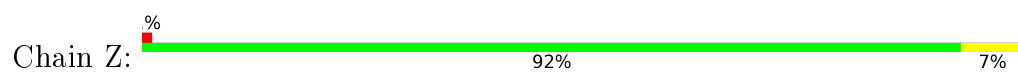
- Molecule 11: Proteasome subunit beta type-5, Proteasome subunit beta type-5



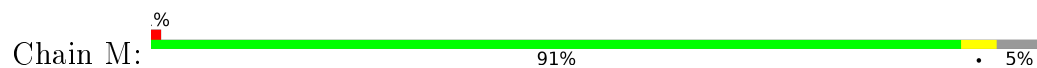
- Molecule 12: Proteasome subunit beta type-6, Proteasome subunit beta type-1, Proteasome subunit beta type-6, Proteasome subunit beta type-1, Proteasome subunit beta type-6



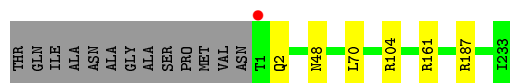
- Molecule 12: Proteasome subunit beta type-6, Proteasome subunit beta type-1, Proteasome subunit beta type-6, Proteasome subunit beta type-1, Proteasome subunit beta type-6



- 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, $\alpha$ , $\beta$ , $\gamma$	135.41Å 300.50Å 145.72Å 90.00° 112.82° 90.00°	Depositor
Resolution (Å)	15.00 – 2.70 15.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.1 (15.00-2.70) 98.1 (15.00-2.70)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.75 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.190 , 0.212 0.194 , 0.215	Depositor DCC
$R_{free}$ test set	14272 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	59.8	Xtriage
Anisotropy	0.078	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 32.9	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	49924	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.25% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 04C, 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	0.27	0/1910	0.50	0/2586
3	Q	0.27	0/1910	0.50	0/2586
4	D	0.26	0/1837	0.46	0/2475
4	R	0.26	0/1837	0.46	0/2475
5	E	0.27	0/1800	0.46	0/2433
5	S	0.27	0/1800	0.46	0/2433
6	F	0.27	0/1932	0.44	0/2609
6	T	0.27	0/1932	0.45	0/2609
7	G	0.27	0/1945	0.46	0/2634
7	U	0.27	0/1945	0.46	0/2634
8	H	0.26	0/1761	0.50	0/2388
8	V	0.26	0/1750	0.50	0/2373
9	I	0.27	0/1611	0.51	0/2174
9	W	0.27	0/1611	0.51	0/2174
10	J	0.26	0/1589	0.48	0/2142
10	X	0.26	0/1589	0.48	0/2142
11	K	0.31	0/1668	0.99	6/2253 (0.3%)
11	Y	0.31	0/1668	0.95	7/2253 (0.3%)
12	L	0.33	1/1802 (0.1%)	0.70	4/2430 (0.2%)
12	Z	0.34	1/1802 (0.1%)	0.72	4/2430 (0.2%)
13	M	0.26	0/1855	0.51	0/2514
13	a	0.26	0/1855	0.51	0/2514
14	N	0.25	0/1541	0.49	0/2087
14	b	0.25	0/1541	0.48	0/2087
All	All	0.27	2/50263 (0.0%)	0.55	21/67955 (0.0%)

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
12	L	0	1
12	Z	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	L	109	ASN	CG-ND2	-5.55	1.19	1.32
12	Z	109	ASN	CG-ND2	-5.17	1.20	1.32

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	K	9	ARG	NE-CZ-NH1	-21.51	109.55	120.30
11	Y	9	ARG	NE-CZ-NH2	-19.76	110.42	120.30
11	K	61	ARG	NE-CZ-NH2	-19.53	110.53	120.30
11	Y	61	ARG	NE-CZ-NH1	-18.97	110.82	120.30
11	K	9	ARG	NE-CZ-NH2	17.31	128.96	120.30
12	Z	100	ARG	NE-CZ-NH2	16.89	128.75	120.30
11	Y	61	ARG	NE-CZ-NH2	16.56	128.58	120.30
11	K	61	ARG	NE-CZ-NH1	16.48	128.54	120.30
12	L	100	ARG	NE-CZ-NH2	-16.31	112.15	120.30
12	Z	100	ARG	NE-CZ-NH1	-16.02	112.29	120.30
12	L	100	ARG	NE-CZ-NH1	14.99	127.79	120.30
11	Y	9	ARG	NE-CZ-NH1	13.08	126.84	120.30
11	K	9	ARG	CD-NE-CZ	8.49	135.48	123.60
11	Y	61	ARG	CD-NE-CZ	8.43	135.40	123.60
11	K	61	ARG	CD-NE-CZ	8.16	135.02	123.60
12	Z	100	ARG	CD-NE-CZ	7.92	134.69	123.60
12	L	100	ARG	CD-NE-CZ	7.85	134.59	123.60
11	Y	9	ARG	CD-NE-CZ	7.21	133.69	123.60
12	L	100	ARG	CG-CD-NE	-6.97	97.17	111.80
12	Z	100	ARG	CG-CD-NE	6.57	125.59	111.80
11	Y	9	ARG	CG-CD-NE	6.30	125.04	111.80

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	L	100	ARG	Sidechain
12	Z	100	ARG	Sidechain

## 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	4	0
2	P	1904	0	1904	3	0
3	C	1881	0	1895	7	0
3	Q	1881	0	1895	6	0
4	D	1813	0	1797	5	0
4	R	1813	0	1797	4	0
5	E	1773	0	1775	1	0
5	S	1773	0	1775	2	0
6	F	1892	0	1883	0	0
6	T	1892	0	1883	2	0
7	G	1907	0	1901	3	0
7	U	1907	0	1901	4	0
8	H	1726	0	1723	12	0
8	V	1719	0	1716	8	0
9	I	1581	0	1574	8	0
9	W	1581	0	1574	7	0
10	J	1561	0	1569	9	0
10	X	1561	0	1569	9	0
11	K	1632	0	1591	20	0
11	Y	1632	0	1591	19	0
12	L	1764	0	1716	7	0
12	Z	1764	0	1716	5	0
13	M	1824	0	1832	3	0
13	a	1824	0	1832	0	0
14	N	1512	0	1481	3	0
14	b	1512	0	1481	0	0
15	A	1	0	0	0	0
15	G	1	0	0	0	0
15	I	2	0	0	0	0
15	J	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	K	2	0	0	0	0
15	L	1	0	0	0	0
15	N	1	0	0	0	0
15	Z	1	0	0	0	0
15	b	1	0	0	0	0
16	G	1	0	0	0	0
16	U	1	0	0	0	0
17	H	42	0	42	2	0
17	K	42	0	42	1	0
17	V	42	0	42	2	0
17	Y	42	0	42	1	0
18	H	12	0	13	1	0
18	K	12	0	13	0	0
18	V	12	0	13	1	0
18	X	12	0	13	0	0
19	A	18	0	0	0	0
19	B	15	0	0	1	0
19	C	8	0	0	0	0
19	D	9	0	0	0	0
19	E	7	0	0	0	0
19	F	8	0	0	0	0
19	G	16	0	0	0	0
19	H	11	0	0	0	0
19	I	10	0	0	0	0
19	J	13	0	0	0	0
19	K	7	0	0	1	0
19	L	14	0	0	0	0
19	M	23	0	0	1	0
19	N	9	0	0	0	0
19	O	9	0	0	0	0
19	P	11	0	0	0	0
19	Q	8	0	0	0	0
19	R	10	0	0	0	0
19	S	7	0	0	0	0
19	T	13	0	0	0	0
19	U	20	0	0	0	0
19	V	16	0	0	0	0
19	W	10	0	0	0	0
19	X	12	0	0	0	0
19	Y	13	0	0	0	0
19	Z	7	0	0	0	0
19	a	19	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	b	9	0	0	0	0
All	All	49924	0	49353	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 1.

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:9:ARG:HG2	11:Y:10:HIS:CD2	2.15	0.81
11:Y:35:ILE:HG13	11:Y:45:MET:CE	2.17	0.75
11:K:9:ARG:HG2	11:K:10:HIS:CD2	2.23	0.73
4:R:89:VAL:HG12	11:Y:61:ARG:HD3	1.70	0.73
11:Y:9:ARG:NH2	11:Y:146:ASP:OD1	2.27	0.67
4:D:89:VAL:HG12	11:K:61:ARG:HD2	1.76	0.67
11:K:9:ARG:NH2	11:K:146:ASP:OD1	2.29	0.65
11:Y:18:SER:O	11:Y:31:VAL:HG22	1.98	0.63
11:K:35:ILE:HG13	11:K:45:MET:CE	2.29	0.63
8:H:114[B]:HIS:HD2	8:H:116:HIS:H	1.48	0.61
11:K:208:ASN:O	9:W:38:LYS:NZ	2.35	0.60
11:K:31:VAL:HG12	12:L:132:GLN:NE2	2.19	0.58
11:K:52:CYS:O	11:K:56:GLU:HG3	2.04	0.58
11:Y:52:CYS:O	11:Y:56:GLU:HG3	2.03	0.57
14:N:152:VAL:HA	14:N:175:MET:HE1	1.85	0.57
10:J:25:ILE:O	10:X:139:TYR:OH	2.23	0.56
9:I:38:LYS:NZ	11:Y:208:ASN:O	2.39	0.56
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.89	0.55
12:Z:31:THR:HG23	12:Z:36:ASN:HD21	1.72	0.55
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.89	0.54
10:X:126:VAL:HG12	10:X:128:LEU:HG	1.89	0.54
10:J:126:VAL:HG12	10:J:128:LEU:HG	1.89	0.54
12:L:31:THR:HG23	12:L:36:ASN:HD21	1.71	0.54
8:V:53:GLU:O	8:V:57:GLN:HG2	2.09	0.52
11:Y:35:ILE:HG13	11:Y:45:MET:HE3	1.88	0.52
10:J:50:ALA:O	11:K:91:LYS:NZ	2.43	0.52
3:C:201:VAL:O	3:C:202:GLN:CB	2.58	0.51
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.58	0.51
13:M:2:GLN:NE2	19:M:301:HOH:O	2.43	0.51
7:U:23:PHE:O	7:U:26:THR:HB	2.10	0.51
10:J:139:TYR:OH	10:X:25:ILE:O	2.29	0.51
8:H:53:GLU:O	8:H:57:GLN:HG2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:93:HIS:HB3	19:B:301:HOH:O	2.11	0.50
7:G:23:PHE:O	7:G:26:THR:HB	2.11	0.50
14:N:83:LYS:HG3	14:N:119:VAL:CG2	2.42	0.50
10:X:50:ALA:O	11:Y:91:LYS:NZ	2.45	0.49
8:H:35:HIS:HB3	8:H:56:THR:HG21	1.93	0.49
10:J:1:MET:HG2	10:J:34:LYS:HE3	1.95	0.49
11:Y:12:VAL:HG13	11:Y:179:VAL:HB	1.94	0.49
8:V:35:HIS:HB3	8:V:56:THR:HG21	1.94	0.48
11:K:5:ALA:HB3	11:K:100:MET:HE2	1.95	0.48
17:V:301:04C:H37	18:V:302:MES:O1S	2.13	0.48
11:Y:58:LEU:O	11:Y:58:LEU:HD12	2.14	0.48
11:Y:5:ALA:HB3	11:Y:100:MET:HE2	1.94	0.48
8:H:196:ARG:NH2	9:I:150:GLU:O	2.46	0.48
11:K:12:VAL:HG13	11:K:179:VAL:HB	1.94	0.48
11:K:58:LEU:O	11:K:58:LEU:HD12	2.14	0.48
8:V:31:CYS:SG	17:V:301:04C:C4	3.02	0.48
12:L:54:ALA:HB2	12:L:109:ASN:OD1	2.13	0.48
12:Z:125:PHE:CD2	12:Z:131:TYR:HB3	2.49	0.47
3:C:160:GLN:HA	3:C:160:GLN:HE21	1.79	0.47
3:C:201:VAL:O	3:C:202:GLN:HB3	2.15	0.47
10:X:1:MET:HG2	10:X:34:LYS:HE3	1.95	0.46
11:Y:1:THR:CG2	11:Y:3:THR:HG23	2.45	0.46
8:H:35:HIS:CB	8:H:56:THR:HG21	2.45	0.46
12:L:125:PHE:CD2	12:L:131:TYR:HB3	2.50	0.46
9:I:26:LEU:HD21	9:I:185:VAL:HG23	1.98	0.46
3:Q:160:GLN:HE21	3:Q:160:GLN:HA	1.81	0.46
3:Q:201:VAL:O	3:Q:202:GLN:HB3	2.15	0.46
8:V:35:HIS:CB	8:V:56:THR:HG21	2.45	0.46
11:K:1:THR:CG2	11:K:3:THR:HG23	2.45	0.46
11:K:35:ILE:HG13	11:K:45:MET:HE3	1.96	0.46
9:W:26:LEU:HD21	9:W:185:VAL:HG23	1.97	0.46
11:K:100:MET:SD	11:K:128:VAL:CG1	3.04	0.46
9:W:20:VAL:HG23	9:W:189:ILE:HB	1.97	0.46
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.98	0.46
10:X:3:ILE:HG23	10:X:18:SER:HB3	1.98	0.46
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.98	0.45
8:H:196:ARG:NH2	9:I:150:GLU:HG3	2.31	0.45
9:I:20:VAL:HG23	9:I:189:ILE:HB	1.97	0.45
10:J:3:ILE:HG23	10:J:18:SER:HB3	1.98	0.45
2:P:50:LYS:O	2:P:51:VAL:C	2.54	0.45
8:H:104:ASP:HB2	8:H:105:PRO:HD2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:31:CYS:SG	17:H:301:04C:C4	3.04	0.45
2:B:50:LYS:O	2:B:51:VAL:C	2.55	0.45
17:H:301:04C:H37	18:H:302:MES:O3S	2.16	0.45
11:K:208:ASN:ND2	19:K:401:HOH:O	2.50	0.45
11:K:104:TRP:CE2	11:K:181:GLU:HB3	2.52	0.45
3:C:35:LYS:HG2	3:C:158:SER:O	2.17	0.45
11:Y:61:ARG:HG3	11:Y:62:GLN:N	2.31	0.45
3:C:51:LYS:O	3:C:52:LEU:HB2	2.17	0.45
8:H:1:THR:CG2	8:H:3:ILE:HG23	2.47	0.44
8:H:50:ALA:HB3	9:I:126:ILE:HD12	2.00	0.44
8:V:196:ARG:NH2	9:W:150:GLU:O	2.51	0.44
11:Y:104:TRP:CE2	11:Y:181:GLU:HB3	2.52	0.44
1:O:1:MET:HG3	6:T:122:TYR:CZ	2.52	0.44
11:Y:100:MET:SD	11:Y:128:VAL:CG1	3.05	0.44
9:I:20:VAL:HG13	9:I:118:PRO:HB3	1.99	0.44
8:V:104:ASP:HB2	8:V:105:PRO:HD2	1.99	0.44
8:V:1:THR:CG2	8:V:3:ILE:HG23	2.48	0.44
7:G:78:ILE:N	7:G:79:PRO:CD	2.81	0.43
14:N:176:VAL:HG12	14:N:178:LEU:HD13	1.99	0.43
3:Q:35:LYS:HG2	3:Q:158:SER:O	2.18	0.43
3:Q:51:LYS:O	3:Q:52:LEU:HB2	2.17	0.43
9:W:20:VAL:HG13	9:W:118:PRO:HB3	1.99	0.43
2:P:145:TYR:OH	2:P:217:LYS:N	2.52	0.43
17:Y:301:04C:H2	12:Z:126:ASP:HB3	2.00	0.43
8:H:22:GLN:HG3	8:H:27:ALA:HB2	2.01	0.43
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.53	0.43
8:V:22:GLN:HG3	8:V:27:ALA:HB2	2.00	0.43
2:B:145:TYR:OH	2:B:217:LYS:N	2.52	0.43
4:D:91:HIS:HB3	4:D:99:ILE:CG2	2.49	0.42
13:M:96:LEU:O	13:M:100:MET:HG2	2.19	0.42
7:U:78:ILE:N	7:U:79:PRO:CD	2.82	0.42
12:L:8:ASN:HA	12:L:30:ILE:O	2.20	0.42
3:C:149:GLU:HB2	3:C:150:PRO:HD2	2.01	0.42
3:Q:149:GLU:HB2	3:Q:150:PRO:HD2	2.01	0.42
13:M:165:ILE:HB	13:M:166:PRO:HD3	2.02	0.42
11:K:59:LEU:HD22	11:K:63:CYS:SG	2.61	0.41
4:R:91:HIS:HB3	4:R:99:ILE:CG2	2.49	0.41
7:U:149:ASP:HB2	7:U:150:PRO:CD	2.51	0.41
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.55	0.41
10:X:1:MET:HB3	10:X:34:LYS:HE3	2.03	0.41
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:149:ASP:HB2	7:G:150:PRO:CD	2.51	0.41
5:S:12:PHE:H	6:T:19:GLN:HE22	1.68	0.41
5:S:77:ALA:N	5:S:78:PRO:CD	2.84	0.41
5:E:77:ALA:N	5:E:78:PRO:CD	2.84	0.41
10:J:5:LEU:HD23	10:J:132:ALA:HB2	2.03	0.41
11:Y:38:ASN:OD1	11:Y:38:ASN:C	2.59	0.41
4:D:89:VAL:CG1	11:K:61:ARG:HD2	2.47	0.41
12:L:100:ARG:HD2	12:L:105:TYR:CZ	2.55	0.41
17:K:301:04C:H2	12:L:126:ASP:HB3	2.01	0.41
9:W:9:GLY:HA3	9:W:41:LYS:HE2	2.03	0.41
10:X:5:LEU:HD23	10:X:132:ALA:HB2	2.03	0.41
8:H:84:LYS:HA	8:H:113:ILE:HD11	2.04	0.40
11:K:144:LYS:HB2	11:K:147:LEU:HD13	2.03	0.40
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.56	0.40
2:B:151:ASN:HB2	2:B:152:PRO:CD	2.51	0.40
2:P:151:ASN:HB2	2:P:152:PRO:CD	2.51	0.40
11:K:38:ASN:C	11:K:38:ASN:OD1	2.59	0.40
11:Y:35:ILE:HG13	11:Y:45:MET:HE1	2.02	0.40
12:Z:138:ALA:HB3	12:Z:147:MET:HG2	2.03	0.40
10:J:1:MET:HB3	10:J:34:LYS:HE3	2.02	0.40
4:R:88:ALA:HA	4:R:99:ILE:HG21	2.02	0.40
3:C:169:VAL:HG23	3:C:196:SER:HB2	2.04	0.40
4:D:88:ALA:HA	4:D:99:ILE:HG21	2.02	0.40
11:Y:144:LYS:HB2	11:Y:147:LEU:HD13	2.03	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%)	239 (96%)	8 (3%)	1 (0%)	39 69

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	O	248/250 (99%)	239 (96%)	8 (3%)	1 (0%)	39	69
2	B	242/258 (94%)	232 (96%)	7 (3%)	3 (1%)	16	39
2	P	242/258 (94%)	232 (96%)	7 (3%)	3 (1%)	16	39
3	C	238/254 (94%)	233 (98%)	2 (1%)	3 (1%)	15	37
3	Q	238/254 (94%)	233 (98%)	2 (1%)	3 (1%)	15	37
4	D	231/260 (89%)	226 (98%)	5 (2%)	0	100	100
4	R	231/260 (89%)	226 (98%)	5 (2%)	0	100	100
5	E	229/234 (98%)	224 (98%)	5 (2%)	0	100	100
5	S	229/234 (98%)	224 (98%)	5 (2%)	0	100	100
6	F	241/288 (84%)	239 (99%)	2 (1%)	0	100	100
6	T	241/288 (84%)	239 (99%)	2 (1%)	0	100	100
7	G	239/252 (95%)	237 (99%)	2 (1%)	0	100	100
7	U	239/252 (95%)	237 (99%)	2 (1%)	0	100	100
8	H	225/232 (97%)	220 (98%)	5 (2%)	0	100	100
8	V	224/232 (97%)	219 (98%)	5 (2%)	0	100	100
9	I	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
9	W	202/205 (98%)	196 (97%)	6 (3%)	0	100	100
10	J	193/198 (98%)	190 (98%)	3 (2%)	0	100	100
10	X	193/198 (98%)	190 (98%)	3 (2%)	0	100	100
11	K	209/211 (99%)	202 (97%)	7 (3%)	0	100	100
11	Y	209/211 (99%)	203 (97%)	6 (3%)	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%)	221 (96%)	10 (4%)	0	100	100
13	a	231/246 (94%)	221 (96%)	10 (4%)	0	100	100
14	N	194/196 (99%)	187 (96%)	7 (4%)	0	100	100
14	b	194/196 (99%)	187 (96%)	7 (4%)	0	100	100
All	All	6283/6612 (95%)	6121 (97%)	148 (2%)	14 (0%)	52	80

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	51	VAL

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Mol	Chain	Res	Type
3	C	202	GLN
2	P	51	VAL
3	Q	202	GLN
1	A	2	THR
2	B	218	GLY
2	B	222	GLY
1	O	2	THR
2	P	218	GLY
2	P	222	GLY
3	C	205	ALA
3	Q	205	ALA
3	Q	183	PRO
3	C	183	PRO

### 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%)	200 (98%)	3 (2%)	72	91
2	P	203/216 (94%)	200 (98%)	3 (2%)	72	91
3	C	212/226 (94%)	203 (96%)	9 (4%)	36	68
3	Q	212/226 (94%)	203 (96%)	9 (4%)	36	68
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%)	185 (97%)	5 (3%)	54	83
5	S	190/193 (98%)	185 (97%)	5 (3%)	54	83
6	F	201/239 (84%)	195 (97%)	6 (3%)	48	79
6	T	201/239 (84%)	195 (97%)	6 (3%)	48	79
7	G	206/210 (98%)	201 (98%)	5 (2%)	57	85
7	U	206/210 (98%)	201 (98%)	5 (2%)	57	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	H	186/190 (98%)	182 (98%)	4 (2%)	60	86
8	V	185/190 (97%)	181 (98%)	4 (2%)	60	86
9	I	172/173 (99%)	170 (99%)	2 (1%)	78	93
9	W	172/173 (99%)	170 (99%)	2 (1%)	78	93
10	J	173/175 (99%)	170 (98%)	3 (2%)	68	90
10	X	173/175 (99%)	170 (98%)	3 (2%)	68	90
11	K	165/165 (100%)	150 (91%)	15 (9%)	12	26
11	Y	165/165 (100%)	149 (90%)	16 (10%)	10	23
12	L	186/186 (100%)	180 (97%)	6 (3%)	46	77
12	Z	186/186 (100%)	180 (97%)	6 (3%)	46	77
13	M	199/208 (96%)	193 (97%)	6 (3%)	48	79
13	a	199/208 (96%)	193 (97%)	6 (3%)	48	79
14	N	162/162 (100%)	157 (97%)	5 (3%)	47	78
14	b	162/162 (100%)	157 (97%)	5 (3%)	47	78
All	All	5315/5534 (96%)	5154 (97%)	161 (3%)	48	79

All (161) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	122	THR
1	A	157	PHE
1	A	250	LEU
2	B	113	ARG
2	B	191	LEU
2	B	238	LEU
3	C	4	ARG
3	C	38	ASN
3	C	51	LYS
3	C	147	GLN
3	C	160	GLN
3	C	169	VAL
3	C	180	LYS
3	C	206	LYS
3	C	240	GLU
4	D	99	ILE
4	D	125	LEU
4	D	143	ASP

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Mol	Chain	Res	Type
4	D	176	LEU
4	D	193	LEU
4	D	235	LEU
4	D	236	LYS
4	D	242	GLU
5	E	9	THR
5	E	29	LYS
5	E	71	LEU
5	E	184	ASN
5	E	188	LEU
6	F	117	GLN
6	F	123	ASN
6	F	139	LYS
6	F	181	GLU
6	F	214	TRP
6	F	240	GLN
7	G	115	LEU
7	G	122	ARG
7	G	125	MET
7	G	208	GLU
7	G	235	ARG
8	H	30	ASN
8	H	31	CYS
8	H	68	LEU
8	H	196	ARG
9	I	37	ASN
9	I	171	LEU
10	J	3	ILE
10	J	99	GLN
10	J	110	LYS
11	K	4	LEU
11	K	12	VAL
11	K	29	GLN
11	K	35	ILE
11	K	38	ASN
11	K	58	LEU
11	K	59	LEU
11	K	61	ARG
11	K	62	GLN
11	K	83	LEU
11	K	86	MET
11	K	93	MET

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Mol	Chain	Res	Type
11	K	117	GLU
11	K	128	VAL
11	K	210	ILE
12	L	23	LEU
12	L	49	ASN
12	L	106	TYR
12	L	128	VAL
12	L	132	GLN
12	L	150	LEU
13	M	2	GLN
13	M	48	ASN
13	M	70	LEU
13	M	104	ARG
13	M	161	ARG
13	M	187	ARG
14	N	9	LYS
14	N	39	ASP
14	N	83	LYS
14	N	104	ASP
14	N	178	LEU
1	O	122	THR
1	O	157	PHE
1	O	250	LEU
2	P	113	ARG
2	P	191	LEU
2	P	238	LEU
3	Q	4	ARG
3	Q	38	ASN
3	Q	51	LYS
3	Q	147	GLN
3	Q	160	GLN
3	Q	169	VAL
3	Q	180	LYS
3	Q	206	LYS
3	Q	240	GLU
4	R	99	ILE
4	R	125	LEU
4	R	143	ASP
4	R	176	LEU
4	R	193	LEU
4	R	235	LEU
4	R	236	LYS

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Mol	Chain	Res	Type
4	R	242	GLU
5	S	9	THR
5	S	29	LYS
5	S	71	LEU
5	S	184	ASN
5	S	188	LEU
6	T	117	GLN
6	T	123	ASN
6	T	139	LYS
6	T	181	GLU
6	T	214	TRP
6	T	240	GLN
7	U	115	LEU
7	U	122	ARG
7	U	125	MET
7	U	208	GLU
7	U	235	ARG
8	V	30	ASN
8	V	31	CYS
8	V	68	LEU
8	V	196	ARG
9	W	37	ASN
9	W	171	LEU
10	X	3	ILE
10	X	99	GLN
10	X	110	LYS
11	Y	4	LEU
11	Y	9	ARG
11	Y	12	VAL
11	Y	29	GLN
11	Y	35	ILE
11	Y	38	ASN
11	Y	58	LEU
11	Y	59	LEU
11	Y	61	ARG
11	Y	62	GLN
11	Y	83	LEU
11	Y	86	MET
11	Y	93	MET
11	Y	117	GLU
11	Y	128	VAL
11	Y	210	ILE

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Mol	Chain	Res	Type
12	Z	23	LEU
12	Z	49	ASN
12	Z	106	TYR
12	Z	128	VAL
12	Z	132	GLN
12	Z	150	LEU
13	a	2	GLN
13	a	48	ASN
13	a	70	LEU
13	a	104	ARG
13	a	161	ARG
13	a	187	ARG
14	b	9	LYS
14	b	39	ASP
14	b	83	LYS
14	b	104	ASP
14	b	178	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (91) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	58	GLN
2	B	119	GLN
2	B	123	GLN
3	C	116	GLN
3	C	120	GLN
3	C	147	GLN
3	C	160	GLN
4	D	91	HIS
4	D	146	GLN
4	D	210	GLN
4	D	225	ASN
5	E	68	HIS
5	E	92	ASN
5	E	99	ASN
5	E	116	GLN
5	E	118	ASN
5	E	120	GLN
5	E	184	ASN
6	F	19	GLN
6	F	86	ASN
6	F	117	GLN

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Mol	Chain	Res	Type
6	F	123	ASN
6	F	191	GLN
7	G	83	ASN
7	G	114	ASN
7	G	117	GLN
7	G	121	GLN
7	G	166	GLN
8	H	66	HIS
8	H	116	HIS
9	I	37	ASN
10	J	55	GLN
11	K	62	GLN
11	K	85	ASN
11	K	175	ASN
11	K	207	ASN
12	L	3	ASN
12	L	49	ASN
12	L	70	ASN
12	L	79	HIS
12	L	158	ASN
13	M	48	ASN
13	M	102	GLN
13	M	179	ASN
14	N	161	GLN
1	O	94	HIS
2	P	20	GLN
2	P	58	GLN
2	P	119	GLN
2	P	123	GLN
3	Q	116	GLN
3	Q	120	GLN
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	118	ASN
5	S	120	GLN

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Mol	Chain	Res	Type
5	S	184	ASN
6	T	19	GLN
6	T	86	ASN
6	T	117	GLN
6	T	123	ASN
6	T	191	GLN
7	U	83	ASN
7	U	114	ASN
7	U	117	GLN
7	U	121	GLN
7	U	166	GLN
8	V	116	HIS
9	W	37	ASN
10	X	55	GLN
11	Y	62	GLN
11	Y	85	ASN
11	Y	175	ASN
11	Y	207	ASN
12	Z	3	ASN
12	Z	49	ASN
12	Z	70	ASN
12	Z	79	HIS
12	Z	132	GLN
12	Z	158	ASN
13	a	48	ASN
13	a	102	GLN
13	a	179	ASN
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 21 ligands modelled in this entry, 13 are monoatomic - leaving 8 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	04C	H	301	8	44,44,44	1.37	4 (9%)	55,58,58	1.78	11 (20%)
18	MES	H	302	-	12,12,12	2.10	1 (8%)	15,16,16	2.44	2 (13%)
17	04C	K	301	11	44,44,44	1.21	3 (6%)	55,58,58	1.62	12 (21%)
18	MES	K	304	-	12,12,12	2.13	1 (8%)	15,16,16	1.83	4 (26%)
17	04C	V	301	8	44,44,44	1.35	3 (6%)	55,58,58	1.79	11 (20%)
18	MES	V	302	-	12,12,12	2.16	1 (8%)	15,16,16	1.52	2 (13%)
18	MES	X	201	-	12,12,12	2.14	1 (8%)	15,16,16	1.99	4 (26%)
17	04C	Y	301	11	44,44,44	1.22	3 (6%)	55,58,58	1.62	12 (21%)

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	04C	H	301	8	1/1/9/12	0/44/52/52	0/3/3/3
18	MES	H	302	-	-	0/6/14/14	0/1/1/1
17	04C	K	301	11	1/1/9/12	0/44/52/52	0/3/3/3
18	MES	K	304	-	-	0/6/14/14	0/1/1/1
17	04C	V	301	8	1/1/9/12	0/44/52/52	0/3/3/3
18	MES	V	302	-	-	0/6/14/14	0/1/1/1
18	MES	X	201	-	-	0/6/14/14	0/1/1/1
17	04C	Y	301	11	1/1/9/12	0/44/52/52	0/3/3/3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	V	302	MES	C8-S	-7.23	1.66	1.77
18	X	201	MES	C8-S	-7.07	1.66	1.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	K	304	MES	C8-S	-7.02	1.67	1.77
18	H	302	MES	C8-S	-6.99	1.67	1.77
17	K	301	04C	C40-C41	-4.61	1.39	1.51
17	Y	301	04C	C40-C41	-4.44	1.40	1.51
17	H	301	04C	C40-C41	-4.27	1.40	1.51
17	V	301	04C	C40-C41	-4.22	1.40	1.51
17	Y	301	04C	C7-C6	-3.92	1.41	1.51
17	H	301	04C	C7-C6	-3.91	1.41	1.51
17	K	301	04C	C7-C6	-3.90	1.41	1.51
17	V	301	04C	C7-C6	-3.76	1.42	1.51
17	H	301	04C	C12-C10	2.13	1.55	1.52
17	K	301	04C	C10-C9	3.97	1.61	1.53
17	Y	301	04C	C10-C9	4.28	1.61	1.53
17	V	301	04C	C10-C9	4.73	1.62	1.53
17	H	301	04C	C10-C9	4.75	1.62	1.53

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	V	301	04C	C30-N31-C32	-7.12	100.69	111.14
17	H	301	04C	C30-N31-C32	-6.99	100.88	111.14
17	Y	301	04C	C30-N31-C32	-5.95	102.41	111.14
17	K	301	04C	C30-N31-C32	-5.89	102.50	111.14
17	V	301	04C	C30-N31-C36	-5.14	103.59	111.14
17	H	301	04C	C30-N31-C36	-5.06	103.71	111.14
17	Y	301	04C	C11-C10-C12	-4.25	104.15	109.73
17	K	301	04C	C11-C10-C12	-4.24	104.16	109.73
17	Y	301	04C	C41-C40-C24	-3.34	103.56	113.44
17	K	301	04C	C41-C40-C24	-3.32	103.62	113.44
17	H	301	04C	C41-C40-C24	-3.00	104.58	113.44
17	V	301	04C	C41-C40-C24	-2.99	104.59	113.44
17	K	301	04C	O13-C12-C10	-2.81	105.28	111.16
17	K	301	04C	O34-C33-C32	-2.77	105.42	111.83
17	Y	301	04C	O34-C33-C32	-2.70	105.59	111.83
17	Y	301	04C	C46-O45-C44	-2.69	111.29	117.51
17	Y	301	04C	O13-C12-C10	-2.64	105.63	111.16
17	Y	301	04C	C7-C6-C1	-2.62	115.62	120.91
17	K	301	04C	C46-O45-C44	-2.61	111.48	117.51
17	V	301	04C	C29-C30-N31	-2.60	106.77	113.26
17	H	301	04C	C29-C30-N31	-2.58	106.80	113.26
17	K	301	04C	C7-C6-C1	-2.55	115.75	120.91
17	V	301	04C	C7-C6-C1	-2.42	116.02	120.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	K	301	04C	C7-C8-N22	-2.40	107.52	110.17
17	H	301	04C	C7-C8-N22	-2.37	107.55	110.17
17	V	301	04C	C46-O45-C44	-2.36	112.05	117.51
17	H	301	04C	C46-O45-C44	-2.36	112.06	117.51
17	H	301	04C	C7-C6-C1	-2.36	116.15	120.91
17	Y	301	04C	C7-C8-N22	-2.35	107.57	110.17
17	V	301	04C	C7-C8-N22	-2.33	107.59	110.17
18	K	304	MES	O1S-S-C8	2.23	108.44	106.87
17	K	301	04C	C32-N31-C36	2.27	113.96	108.87
17	Y	301	04C	C32-N31-C36	2.28	113.98	108.87
17	H	301	04C	C7-C6-C5	2.34	125.64	120.91
17	V	301	04C	C7-C6-C5	2.42	125.79	120.91
18	X	201	MES	O3S-S-C8	2.42	110.02	104.99
17	K	301	04C	C7-C6-C5	2.51	125.98	120.91
17	Y	301	04C	C7-C6-C5	2.55	126.06	120.91
18	K	304	MES	O3S-S-C8	2.64	110.48	104.99
17	H	301	04C	C33-O34-C35	2.88	119.72	109.89
17	K	301	04C	C30-N31-C36	2.90	115.39	111.14
17	Y	301	04C	C30-N31-C36	2.90	115.39	111.14
18	K	304	MES	C6-C5-N4	2.90	114.55	110.11
17	Y	301	04C	C33-C32-N31	3.03	114.74	110.11
17	V	301	04C	C38-C27-C26	3.03	116.27	110.20
17	V	301	04C	C33-O34-C35	3.03	120.23	109.89
17	H	301	04C	C38-C27-C26	3.05	116.31	110.20
17	K	301	04C	C33-C32-N31	3.14	114.91	110.11
18	X	201	MES	C6-C5-N4	3.25	115.08	110.11
18	V	302	MES	O3S-S-C8	3.26	111.76	104.99
18	X	201	MES	O1S-S-C8	3.29	109.19	106.87
18	V	302	MES	O2S-S-C8	3.76	109.53	106.87
17	H	301	04C	C32-N31-C36	3.78	117.33	108.87
17	V	301	04C	C32-N31-C36	3.83	117.44	108.87
18	X	201	MES	O2S-S-C8	4.04	109.73	106.87
18	K	304	MES	O2S-S-C8	4.28	109.89	106.87
18	H	302	MES	O1S-S-C8	4.44	110.00	106.87
18	H	302	MES	O2S-S-C8	7.64	112.26	106.87

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
17	K	301	04C	C27
17	V	301	04C	C27
17	H	301	04C	C27

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Mol	Chain	Res	Type	Atom
17	Y	301	04C	C27

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	H	301	04C	2	0
18	H	302	MES	1	0
17	K	301	04C	1	0
17	V	301	04C	2	0
18	V	302	MES	1	0
17	Y	301	04C	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%)	-0.33	6 (2%) 62 62	36, 54, 91, 129	0
1	O	250/250 (100%)	-0.32	8 (3%) 51 51	41, 58, 103, 140	0
2	B	244/258 (94%)	-0.23	9 (3%) 45 45	41, 60, 106, 157	0
2	P	244/258 (94%)	-0.22	8 (3%) 50 50	43, 61, 103, 156	0
3	C	240/254 (94%)	-0.03	16 (6%) 21 19	38, 67, 137, 172	0
3	Q	240/254 (94%)	0.06	17 (7%) 19 17	43, 75, 155, 199	0
4	D	235/260 (90%)	-0.37	1 (0%) 93 94	43, 62, 94, 130	0
4	R	235/260 (90%)	-0.20	6 (2%) 59 59	53, 71, 114, 141	0
5	E	231/234 (98%)	-0.22	5 (2%) 65 66	44, 65, 105, 150	0
5	S	231/234 (98%)	-0.19	9 (3%) 43 43	48, 69, 113, 150	0
6	F	243/288 (84%)	-0.38	8 (3%) 50 50	38, 59, 108, 136	0
6	T	243/288 (84%)	-0.33	7 (2%) 55 55	40, 64, 120, 155	0
7	G	241/252 (95%)	-0.41	6 (2%) 61 61	38, 56, 98, 157	0
7	U	241/252 (95%)	-0.40	6 (2%) 61 61	36, 55, 92, 133	0
8	H	226/232 (97%)	-0.41	3 (1%) 79 79	38, 54, 91, 145	0
8	V	226/232 (97%)	-0.39	5 (2%) 65 66	40, 54, 88, 159	0
9	I	204/205 (99%)	-0.60	1 (0%) 91 93	37, 52, 83, 106	0
9	W	204/205 (99%)	-0.58	2 (0%) 84 85	38, 54, 85, 108	0
10	J	195/198 (98%)	-0.40	5 (2%) 59 59	38, 59, 90, 132	0
10	X	195/198 (98%)	-0.36	3 (1%) 76 76	41, 61, 90, 137	0
11	K	211/211 (100%)	-0.24	4 (1%) 70 70	44, 65, 97, 125	0
11	Y	211/211 (100%)	-0.27	2 (0%) 85 86	44, 65, 97, 128	0
12	L	222/222 (100%)	-0.28	2 (0%) 85 86	46, 62, 106, 135	0
12	Z	222/222 (100%)	-0.29	3 (1%) 78 77	47, 63, 106, 136	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	M	233/246 (94%)	-0.50	3 (1%) 79 79	37, 56, 84, 101	0
13	a	233/246 (94%)	-0.49	1 (0%) 93 94	35, 56, 82, 99	0
14	N	196/196 (100%)	-0.53	3 (1%) 76 76	36, 50, 83, 107	0
14	b	196/196 (100%)	-0.58	1 (0%) 91 93	36, 50, 81, 106	0
All	All	6342/6612 (95%)	-0.33	150 (2%) 62 62	35, 60, 105, 199	0

All (150) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
10	X	1	MET	8.4
10	J	1	MET	7.1
9	W	1	SER	6.5
2	P	51	VAL	6.2
2	P	219	ALA	5.4
5	E	202	ASP	5.4
3	Q	206	LYS	5.3
2	B	218	GLY	5.3
1	O	1	MET	5.0
2	B	51	VAL	5.0
2	B	221	ASP	4.9
3	C	206	LYS	4.9
3	C	50	LEU	4.7
3	C	202	GLN	4.7
3	Q	240	GLU	4.7
1	O	249	ALA	4.5
8	V	222	ASP	4.2
1	A	1	MET	4.2
2	P	221	ASP	4.2
3	Q	49	THR	4.2
3	C	238	LYS	4.2
12	Z	174	TYR	4.0
3	Q	238	LYS	4.0
13	a	1	THR	3.9
3	Q	202	GLN	3.8
1	A	249	ALA	3.8
3	Q	50	LEU	3.8
5	S	3	ASN	3.7
12	L	174	TYR	3.7
10	X	194	ASP	3.7
3	Q	225	GLU	3.6
3	C	49	THR	3.6

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Mol	Chain	Res	Type	RSRZ
2	B	217	LYS	3.6
4	R	1	ASP	3.6
3	Q	239	GLN	3.6
3	C	205	ALA	3.6
8	V	226	GLU	3.6
3	Q	236	GLN	3.5
2	B	220	ASN	3.5
8	H	226	GLU	3.5
5	S	202	ASP	3.5
7	G	3	TYR	3.4
10	J	194	ASP	3.4
3	Q	205	ALA	3.4
5	S	173	ARG	3.4
9	I	1	SER	3.3
3	C	240	GLU	3.3
3	C	239	GLN	3.3
8	V	224	GLN	3.2
11	K	146	ASP	3.2
3	C	48	SER	3.2
6	F	205	GLU	3.2
1	O	2	THR	3.1
2	P	218	GLY	3.0
3	Q	237	GLU	3.0
6	F	181	GLU	3.0
10	X	193	ASP	2.9
5	E	217	LYS	2.9
4	R	217	GLN	2.8
7	G	2	GLY	2.8
1	A	231	LYS	2.8
5	E	201	ARG	2.8
8	H	224	GLN	2.8
5	S	210	LEU	2.8
12	Z	167	LYS	2.8
4	R	230	GLU	2.8
2	P	59	ASP	2.8
8	V	145	ASP	2.8
1	A	250	LEU	2.8
7	U	242	GLN	2.7
2	P	52	THR	2.7
12	L	1	GLN	2.7
3	C	175	LYS	2.7
6	F	244	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
14	N	105	LYS	2.7
6	F	202	ASP	2.7
2	B	59	ASP	2.7
5	E	233	ILE	2.7
11	Y	146	ASP	2.6
3	C	225	GLU	2.6
3	Q	48	SER	2.6
5	S	165	GLN	2.6
14	N	181	ALA	2.6
3	Q	180	LYS	2.6
6	F	215	CYS	2.6
7	G	242	GLN	2.6
8	V	9	ASN	2.6
3	Q	141	ASP	2.6
7	U	222	ASP	2.6
11	K	211	GLY	2.6
3	Q	181	GLU	2.5
5	S	225	ASP	2.5
1	O	201	GLU	2.5
14	N	195	GLN	2.5
6	T	2	THR	2.5
2	P	203	SER	2.5
3	C	235	GLU	2.5
6	T	205	GLU	2.4
14	b	195	GLN	2.4
5	E	54	GLU	2.4
1	O	250	LEU	2.4
2	B	219	ALA	2.4
6	T	243	ILE	2.4
2	P	220	ASN	2.4
11	Y	144	LYS	2.4
1	A	248	GLU	2.4
6	T	201	GLU	2.4
6	F	2	THR	2.4
3	C	180	LYS	2.4
3	C	236	GLN	2.3
13	M	1	THR	2.3
6	T	181	GLU	2.3
4	R	203	LYS	2.3
4	R	125	LEU	2.3
10	J	195	PHE	2.3
4	D	117	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
13	M	47	ASP	2.3
2	B	60	THR	2.3
11	K	150	GLU	2.2
7	U	181	LYS	2.2
7	U	2	GLY	2.2
1	O	231	LYS	2.2
3	C	216	ASP	2.2
7	U	3	TYR	2.2
6	T	244	ASN	2.2
1	A	2	THR	2.2
8	H	222	ASP	2.2
12	Z	210	ASP	2.2
10	J	95	ARG	2.2
5	S	203	GLU	2.1
3	C	59	PRO	2.1
7	G	230	GLU	2.1
2	B	242	GLY	2.1
9	W	192	ASP	2.1
4	R	237	GLU	2.1
7	G	240	ALA	2.1
7	G	241	GLU	2.1
3	Q	47	ARG	2.1
11	K	144	LYS	2.1
10	J	193	ASP	2.1
5	S	54	GLU	2.1
6	T	241	LYS	2.0
5	S	233	ILE	2.0
6	F	203	ASN	2.0
13	M	216	ASN	2.0
1	O	248	GLU	2.0
3	Q	59	PRO	2.0
7	U	241	GLU	2.0
1	O	50	LYS	2.0
6	F	228	LYS	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
18	MES	V	302	12/12	0.90	0.30	4.91	66,71,85,91	12
15	MG	A	301	1/1	0.97	0.21	4.82	47,47,47,47	0
17	04C	V	301	42/42	0.84	0.28	4.77	37,58,85,88	42
17	04C	H	301	42/42	0.85	0.28	4.02	41,57,86,88	0
18	MES	X	201	12/12	0.91	0.33	3.95	56,58,75,86	12
18	MES	K	304	12/12	0.89	0.39	3.40	53,59,77,87	12
18	MES	H	302	12/12	0.92	0.23	3.03	68,75,86,91	12
17	04C	Y	301	42/42	0.85	0.25	2.03	61,67,97,102	0
15	MG	Z	301	1/1	0.95	0.22	1.86	72,72,72,72	0
17	04C	K	301	42/42	0.86	0.22	1.25	48,67,98,100	0
15	MG	I	301	1/1	0.93	0.18	0.79	66,66,66,66	0
15	MG	J	201	1/1	0.98	0.13	0.57	59,59,59,59	0
15	MG	G	301	1/1	0.91	0.13	0.12	54,54,54,54	0
15	MG	b	201	1/1	0.97	0.10	-0.23	46,46,46,46	0
15	MG	K	302	1/1	0.99	0.09	-1.38	57,57,57,57	0
15	MG	N	201	1/1	0.98	0.08	-1.78	53,53,53,53	0
15	MG	I	302	1/1	1.00	0.04	-2.32	58,58,58,58	0
15	MG	L	301	1/1	0.99	0.05	-3.23	66,66,66,66	0
16	CL	G	302	1/1	0.99	0.14	-	46,46,46,46	0
15	MG	K	303	1/1	0.93	0.40	-	63,63,63,63	0
16	CL	U	301	1/1	0.99	0.16	-	47,47,47,47	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.