



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 5, 2016 – 06:01 PM EST

PDB ID : 5L64  
Title : Yeast 20S proteasome with human beta5c (1-138) and human beta6 (97-111; 118-133) in complex with epoxyketone inhibitor 18  
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.

---

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

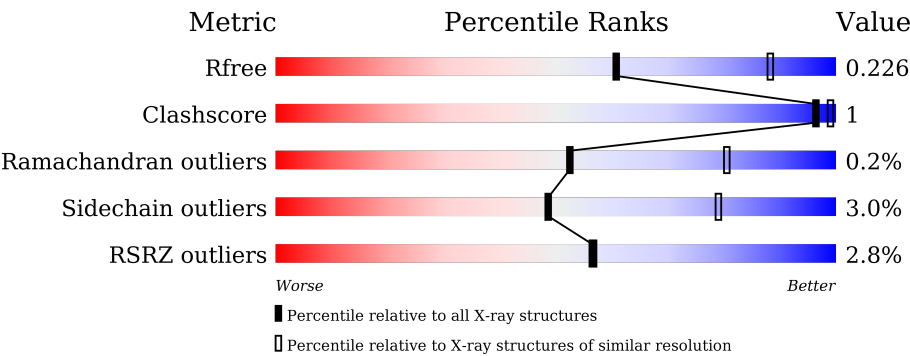
# 1 Overall quality at a glance i

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.



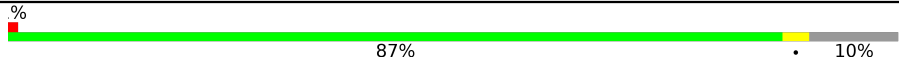

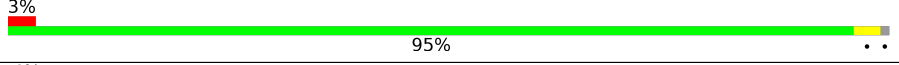
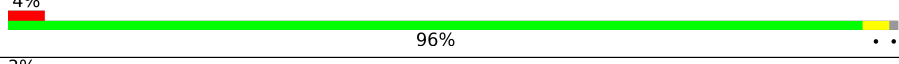
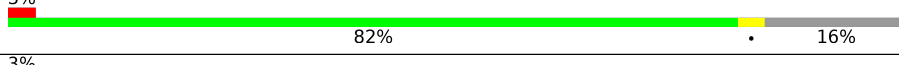
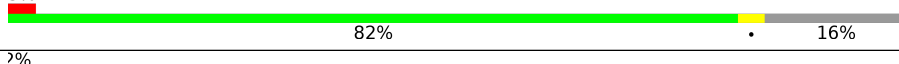
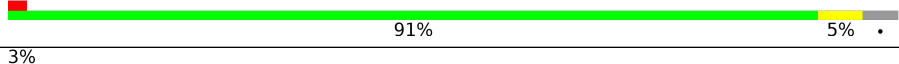
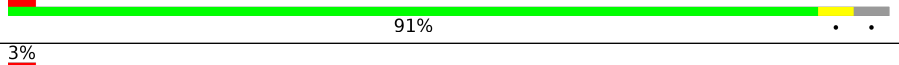
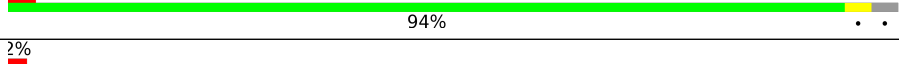
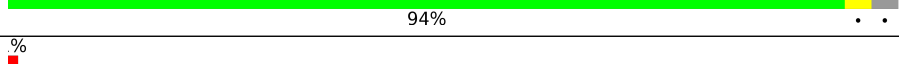
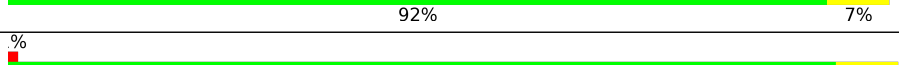
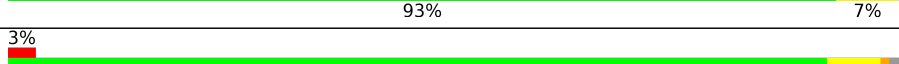
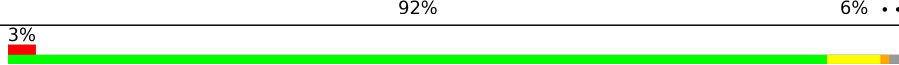
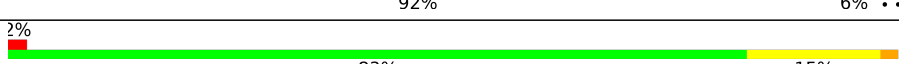

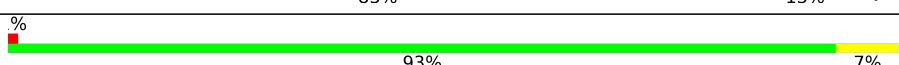
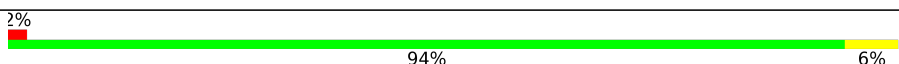
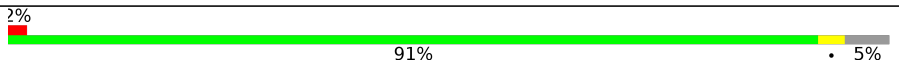
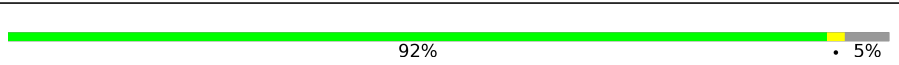
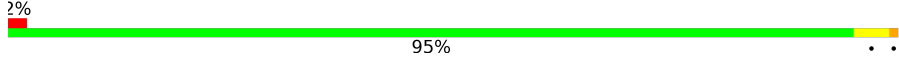
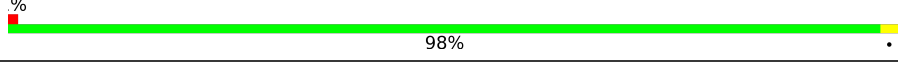

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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>4%</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>3%</div><div>91%</div><div>5%</div></div>
2	P	258	<div><div>3%</div><div>91%</div><div>5%</div></div>
3	C	254	<div><div>8%</div><div>87%</div><div>6% • 6%</div></div>
3	Q	254	<div><div>7%</div><div>87%</div><div>6% • 6%</div></div>

Continued on next page...

Continued from previous page...

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	I	301	-	-	-	X
15	MG	J	201	-	-	-	X
15	MG	N	201	-	-	-	X
17	MES	H	301	-	-	-	X
17	MES	K	304	-	-	-	X
17	MES	V	301	-	-	-	X
17	MES	X	201	-	-	-	X
18	6NV	K	301	-	-	-	X
18	6NV	Y	301	-	-	-	X

## 2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 49937 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	0	0
			1719	1082	298	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			

*Continued on next page...*

*Continued from previous page...*

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

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

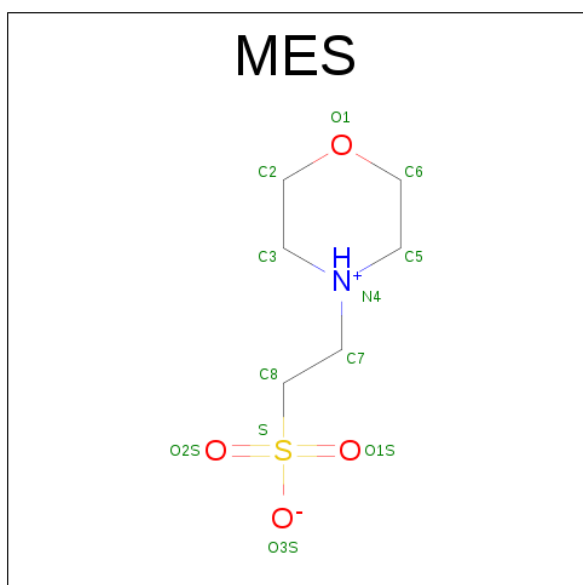
- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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	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

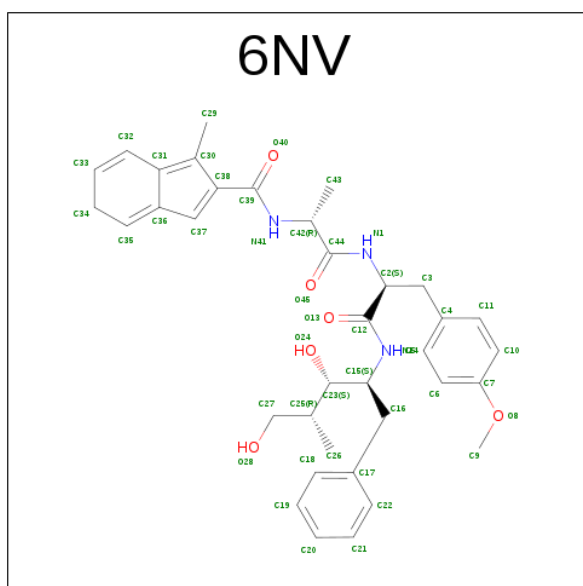
- Molecule 17 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	H	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
17	K	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
17	V	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
17	X	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 18 is {N}-(2 {R})-1-[(2 {S})-3-(4-methoxyphenyl)-1-[(2 {S},3 {S},4 {R})-4-methyl-3,5-bis(oxidanyl)-1-phenyl-pentan-2-yl]amino]-1-oxidanylidene-propan-2-yl]amino]-1-oxidanylidene-propan-2-yl]-1-methyl-5 {H}-indene-2-carboxamide (three-letter code: 6NV) (formula: C<sub>36</sub>H<sub>43</sub>N<sub>3</sub>O<sub>6</sub>).



*Continued from previous page...*

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	C	16	Total O 16 16	0	0
19	D	14	Total O 14 14	0	0
19	E	5	Total O 5 5	0	0
19	F	8	Total O 8 8	0	0
19	G	14	Total O 14 14	0	0
19	H	21	Total O 21 21	0	0
19	I	18	Total O 18 18	0	0
19	J	16	Total O 16 16	0	0
19	K	11	Total O 11 11	0	0
19	L	14	Total O 14 14	0	0
19	M	27	Total O 27 27	0	0
19	N	11	Total O 11 11	0	0
19	O	20	Total O 20 20	0	0
19	P	16	Total O 16 16	0	0
19	Q	7	Total O 7 7	0	0
19	R	15	Total O 15 15	0	0
19	S	7	Total O 7 7	0	0
19	T	12	Total O 12 12	0	0
19	U	22	Total O 22 22	0	0
19	V	15	Total O 15 15	0	0
19	W	14	Total O 14 14	0	0

*Continued on next page...*

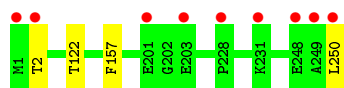
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	X	18	Total 18	O 18	0	0
19	Y	12	Total 12	O 12	0	0
19	Z	14	Total 14	O 14	0	0
19	a	27	Total 27	O 27	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.

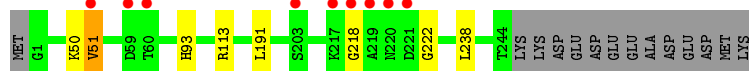
- Molecule 1: Proteasome subunit alpha type-2



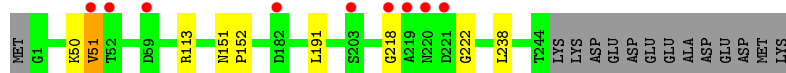
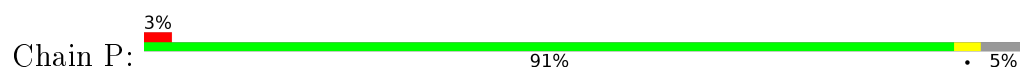
- Molecule 1: Proteasome subunit alpha type-2



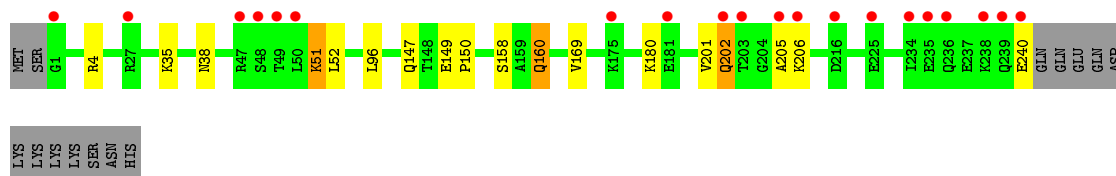
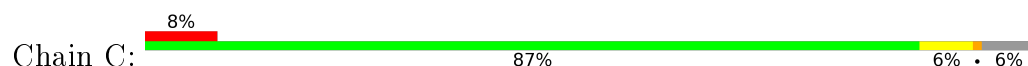
- Molecule 2: Proteasome subunit alpha type-3



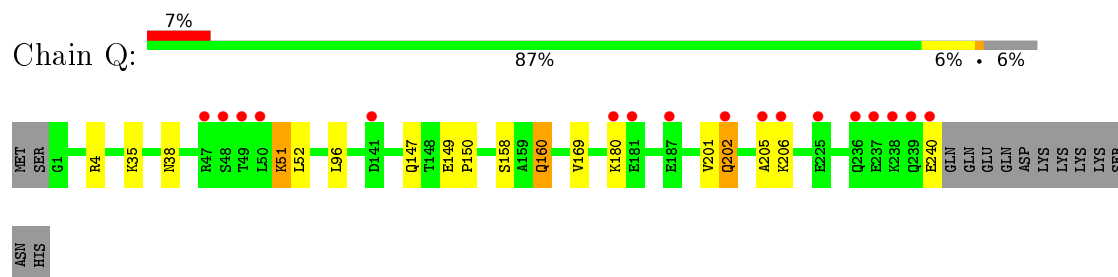
- Molecule 2: Proteasome subunit alpha type-3



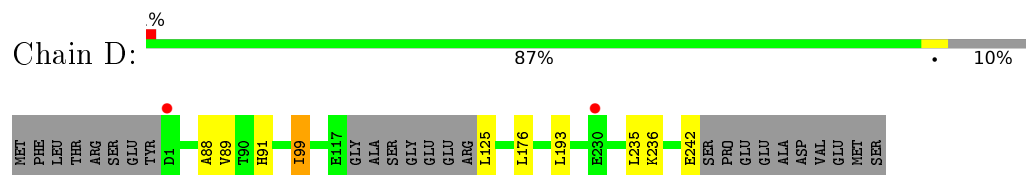
- Molecule 3: Proteasome subunit alpha type-4



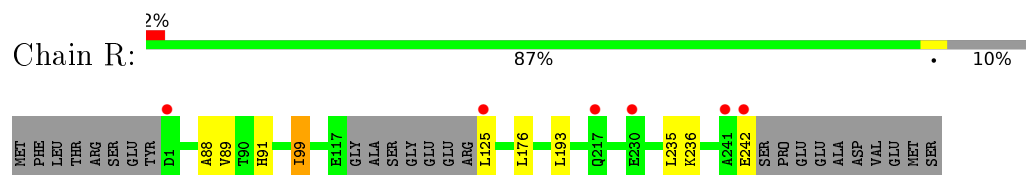
- Molecule 3: Proteasome subunit alpha type-4



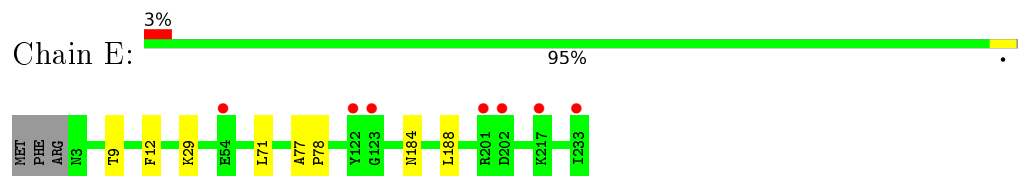
- Molecule 4: Proteasome subunit alpha type-5



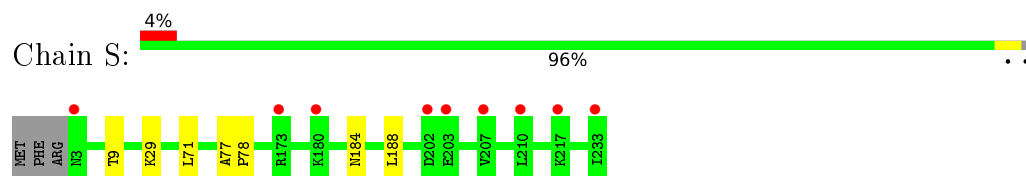
- Molecule 4: Proteasome subunit alpha type-5



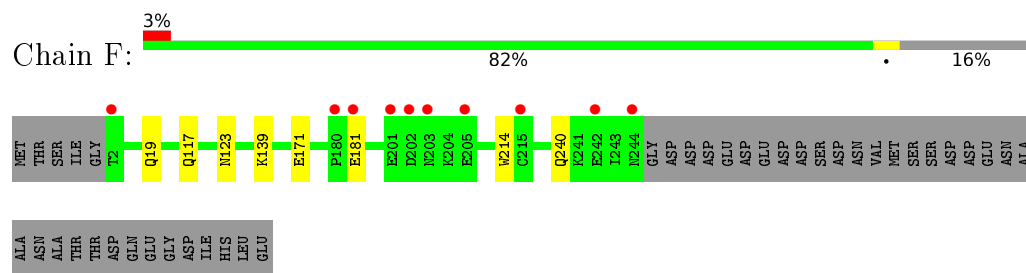
- Molecule 5: Proteasome subunit alpha type-6



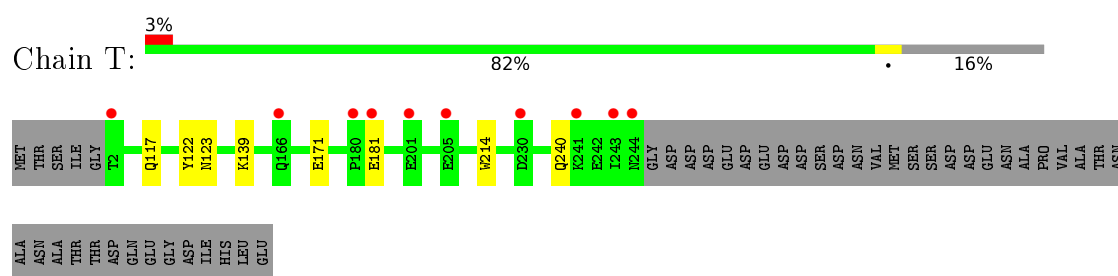
- Molecule 5: Proteasome subunit alpha type-6



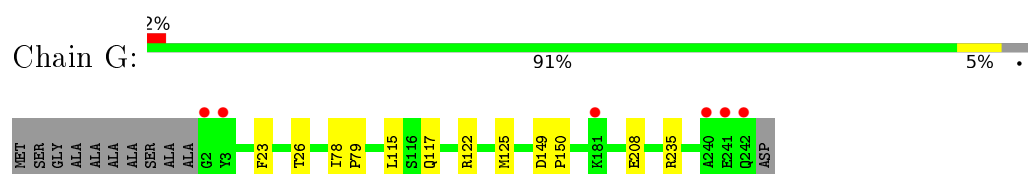
- Molecule 6: Probable proteasome subunit alpha type-7



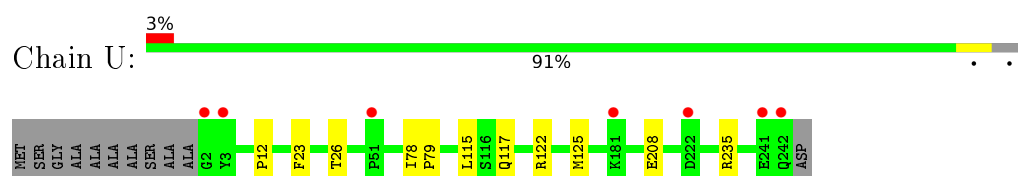
- Molecule 6: Probable proteasome subunit alpha type-7



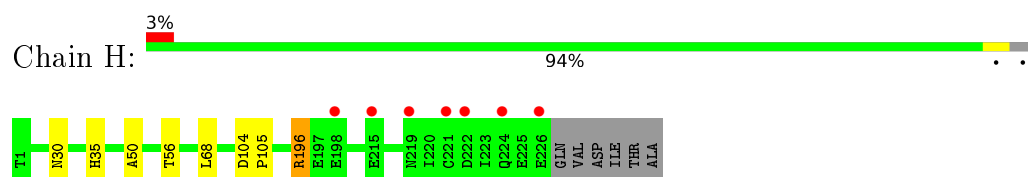
- Molecule 7: Proteasome subunit alpha type-1



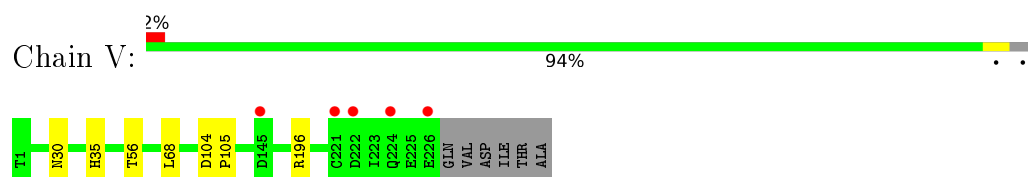
- Molecule 7: Proteasome subunit alpha type-1



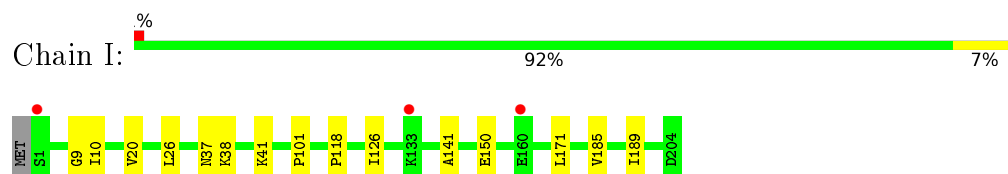
- Molecule 8: Proteasome subunit beta type-2



- Molecule 8: Proteasome subunit beta type-2

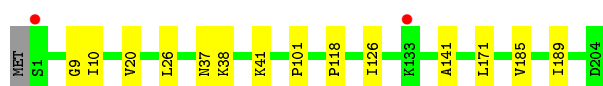


- Molecule 9: Proteasome subunit beta type-3

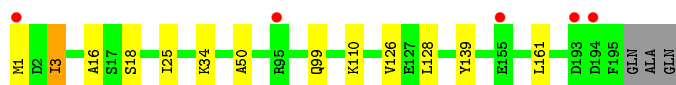
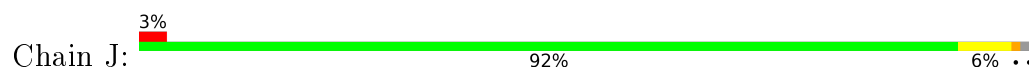


- Molecule 9: Proteasome subunit beta type-3

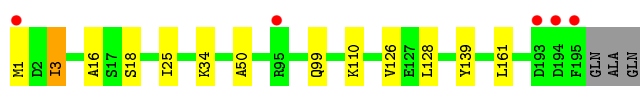




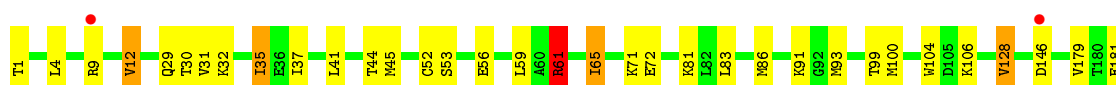
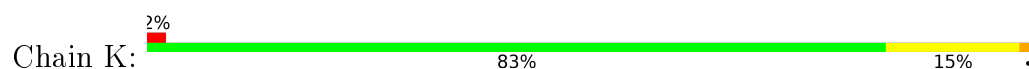
- Molecule 10: Proteasome subunit beta type-4



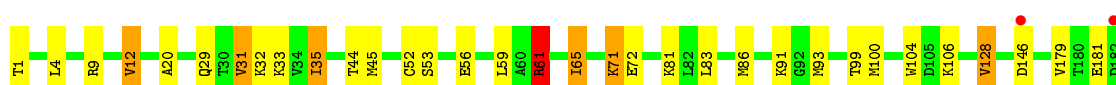
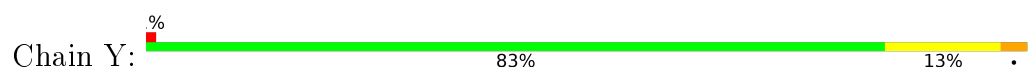
- Molecule 10: Proteasome subunit beta type-4



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



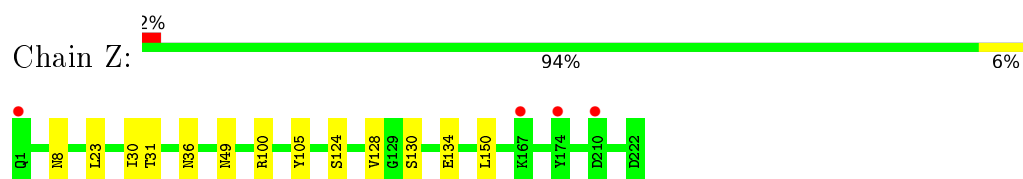
- Molecule 11: Proteasome subunit beta type-5, Proteasome subunit beta type-5



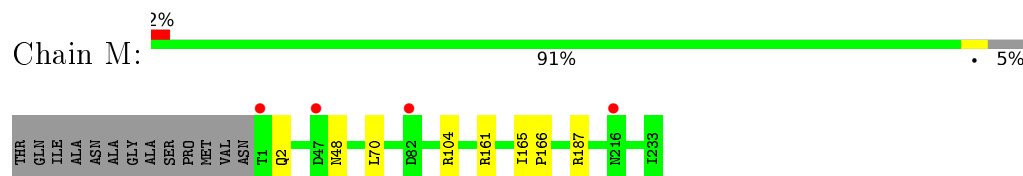
- Molecule 12: Proteasome subunit beta type-6, Proteasome subunit beta type-1, Proteasome subunit beta type-6, Proteasome subunit beta type-1, Proteasome subunit beta type-6



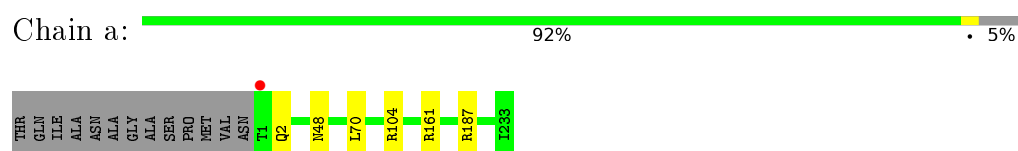
- Molecule 12: Proteasome subunit beta type-6, Proteasome subunit beta type-1, Proteasome subunit beta type-6, Proteasome subunit beta type-1, Proteasome subunit beta type-6



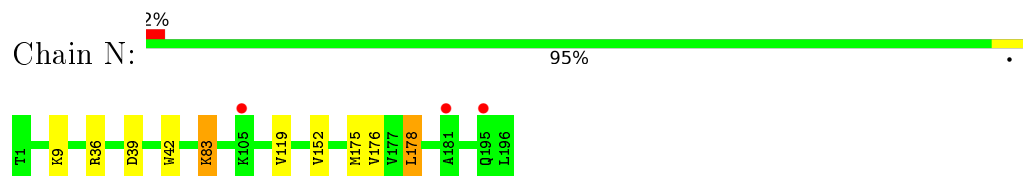
- Molecule 13: Proteasome subunit beta type-7



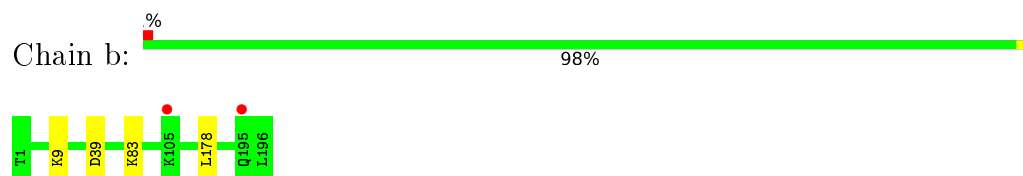
- Molecule 13: Proteasome subunit beta type-7



- 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, $\alpha$ , $\beta$ , $\gamma$	135.69Å 300.97Å 145.94Å 90.00° 113.08° 90.00°	Depositor
Resolution (Å)	15.00 – 2.70 15.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	96.4 (15.00-2.70) 96.4 (15.00-2.70)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.96 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.198 , 0.223 0.203 , 0.226	Depositor DCC
$R_{free}$ test set	14071 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	56.3	Xtriage
Anisotropy	0.144	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 31.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	49937	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.32% 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: 6NV, MG, 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	0.49	0/2586
3	Q	0.27	0/1910	0.49	0/2586
4	D	0.27	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	0.44	0/2609
7	G	0.27	0/1945	0.46	0/2634
7	U	0.27	0/1945	0.46	0/2634
8	H	0.25	0/1750	0.48	0/2373
8	V	0.25	0/1750	0.48	0/2373
9	I	0.27	0/1611	0.50	0/2174
9	W	0.27	0/1611	0.49	0/2174
10	J	0.26	0/1589	0.47	0/2142
10	X	0.26	0/1589	0.47	0/2142
11	K	0.31	0/1668	0.82	6/2253 (0.3%)
11	Y	0.33	0/1668	0.87	7/2253 (0.3%)
12	L	0.30	0/1802	0.49	0/2430
12	Z	0.30	0/1802	0.49	0/2430
13	M	0.27	0/1855	0.51	0/2514
13	a	0.26	0/1855	0.51	0/2514
14	N	0.25	0/1541	0.47	0/2087
14	b	0.25	0/1541	0.47	0/2087
All	All	0.27	0/50252	0.51	13/67940 (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
11	K	0	1
11	Y	0	1
All	All	0	2

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	Y	61	ARG	NE-CZ-NH2	19.30	129.95	120.30
11	K	61	ARG	NE-CZ-NH1	18.19	129.40	120.30
11	Y	61	ARG	NE-CZ-NH1	-17.61	111.50	120.30
11	K	61	ARG	NE-CZ-NH2	-15.47	112.56	120.30
11	Y	61	ARG	CB-CG-CD	8.89	134.71	111.60
11	Y	71	LYS	CD-CE-NZ	-8.80	91.47	111.70
11	K	61	ARG	CB-CG-CD	8.04	132.52	111.60
11	K	61	ARG	CD-NE-CZ	7.64	134.30	123.60
11	Y	61	ARG	CD-NE-CZ	7.50	134.11	123.60
11	Y	1	THR	N-CA-C	6.43	128.36	111.00
11	Y	71	LYS	CG-CD-CE	5.59	128.68	111.90
11	K	1	THR	N-CA-C	5.44	125.69	111.00
11	K	61	ARG	CA-CB-CG	5.41	125.31	113.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	K	61	ARG	Sidechain
11	Y	61	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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	O	1915	0	1929	2	0
2	B	1904	0	1904	3	0
2	P	1904	0	1904	2	0
3	C	1881	0	1895	7	0
3	Q	1881	0	1895	7	0
4	D	1813	0	1797	4	0
4	R	1813	0	1797	3	0
5	E	1773	0	1775	2	0
5	S	1773	0	1775	1	0
6	F	1892	0	1883	1	0
6	T	1892	0	1883	1	0
7	G	1907	0	1901	3	0
7	U	1907	0	1901	3	0
8	H	1719	0	1719	5	0
8	V	1719	0	1719	2	0
9	I	1581	0	1574	10	0
9	W	1581	0	1574	7	0
10	J	1561	0	1569	8	0
10	X	1561	0	1569	8	0
11	K	1632	0	1590	29	0
11	Y	1632	0	1590	26	0
12	L	1764	0	1716	5	0
12	Z	1764	0	1716	3	0
13	M	1824	0	1832	1	0
13	a	1824	0	1832	0	0
14	N	1512	0	1481	4	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
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
16	G	1	0	0	0	0
16	U	1	0	0	0	0
17	H	12	0	13	0	0
17	K	12	0	13	0	0
17	V	12	0	13	0	0
17	X	12	0	13	0	0
18	K	45	0	0	2	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	Y	45	0	0	3	0
19	A	21	0	0	0	0
19	B	17	0	0	1	0
19	C	16	0	0	0	0
19	D	14	0	0	0	0
19	E	5	0	0	0	0
19	F	8	0	0	0	0
19	G	14	0	0	0	0
19	H	21	0	0	0	0
19	I	18	0	0	0	0
19	J	16	0	0	0	0
19	K	11	0	0	0	0
19	L	14	0	0	0	0
19	M	27	0	0	0	0
19	N	11	0	0	0	0
19	O	20	0	0	0	0
19	P	16	0	0	0	0
19	Q	7	0	0	0	0
19	R	15	0	0	0	0
19	S	7	0	0	0	0
19	T	12	0	0	0	0
19	U	22	0	0	0	0
19	V	15	0	0	0	0
19	W	14	0	0	0	0
19	X	18	0	0	0	0
19	Y	12	0	0	0	0
19	Z	14	0	0	0	0
19	a	27	0	0	0	0
19	b	19	0	0	0	0
All	All	49937	0	49182	132	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 (132) 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:35:ILE:CG2	11:Y:45:MET:HE3	1.75	1.16
11:Y:35:ILE:HG21	11:Y:45:MET:CE	1.82	1.09
11:K:45:MET:HE2	11:K:53:SER:HA	1.40	1.03
11:K:35:ILE:HG21	11:K:45:MET:CE	1.89	1.01

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:35:ILE:CG2	11:Y:45:MET:CE	2.38	1.00
11:K:35:ILE:HG21	11:K:45:MET:HE1	1.45	0.98
11:K:35:ILE:CG2	11:K:45:MET:HE1	1.94	0.96
11:Y:35:ILE:HG22	11:Y:45:MET:HE3	1.47	0.93
11:Y:35:ILE:HG21	11:Y:45:MET:HE2	1.48	0.93
11:K:45:MET:HG2	11:K:52:CYS:HB3	1.53	0.88
11:K:35:ILE:CG2	11:K:45:MET:CE	2.55	0.79
11:K:44:THR:O	11:K:99:THR:HG22	1.86	0.76
11:Y:44:THR:O	11:Y:99:THR:HG22	1.86	0.75
11:Y:45:MET:HE1	11:Y:53:SER:HA	1.69	0.75
11:K:35:ILE:HG21	11:K:45:MET:HE3	1.71	0.73
11:K:45:MET:CE	11:K:53:SER:HA	2.18	0.72
11:K:9:ARG:NH2	11:K:146:ASP:OD1	2.24	0.70
11:Y:9:ARG:NH2	11:Y:146:ASP:OD1	2.25	0.70
11:K:45:MET:HE2	11:K:53:SER:CA	2.20	0.69
11:Y:56:GLU:OE2	11:Y:99:THR:HG21	1.96	0.66
11:K:45:MET:HG2	11:K:52:CYS:CB	2.25	0.65
11:K:56:GLU:OE2	11:K:99:THR:HG21	1.96	0.65
4:D:89:VAL:HG12	11:K:61:ARG:HD3	1.80	0.64
4:D:89:VAL:CG1	11:K:61:ARG:HD3	2.30	0.62
11:Y:35:ILE:HG22	11:Y:45:MET:CE	2.17	0.60
11:K:208:ASN:O	9:W:38:LYS:NZ	2.36	0.59
14:N:152:VAL:HA	14:N:175:MET:HE1	1.85	0.57
3:Q:96:LEU:O	11:Y:81:LYS:HE2	2.07	0.55
3:C:96:LEU:O	11:K:81:LYS:HE2	2.08	0.54
10:J:126:VAL:HG12	10:J:128:LEU:HG	1.90	0.54
18:K:301:6NV:N41	18:K:301:6NV:C29	2.72	0.53
2:B:93:HIS:HB3	19:B:301:HOH:O	2.09	0.53
10:J:25:ILE:O	10:X:139:TYR:OH	2.25	0.52
12:L:31:THR:HG23	12:L:36:ASN:HD21	1.74	0.52
10:X:126:VAL:HG12	10:X:128:LEU:HG	1.90	0.52
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.92	0.52
8:V:35:HIS:HB3	8:V:56:THR:HG21	1.92	0.51
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.92	0.51
9:I:38:LYS:NZ	11:Y:208:ASN:O	2.43	0.51
3:C:201:VAL:O	3:C:202:GLN:CB	2.58	0.51
8:H:35:HIS:HB3	8:H:56:THR:HG21	1.92	0.51
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.59	0.51
12:Z:31:THR:HG23	12:Z:36:ASN:HD21	1.74	0.50
9:W:20:VAL:HG23	9:W:189:ILE:HB	1.94	0.49
7:U:23:PHE:O	7:U:26:THR:HB	2.12	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:23:PHE:O	7:G:26:THR:HB	2.12	0.49
11:Y:12:VAL:HG13	11:Y:179:VAL:HB	1.94	0.49
9:I:20:VAL:HG23	9:I:189:ILE:HB	1.94	0.49
8:H:50:ALA:CB	9:I:126:ILE:HG23	2.43	0.49
11:Y:45:MET:CE	11:Y:53:SER:HA	2.42	0.48
11:K:30:THR:O	12:L:132:GLN:NE2	2.46	0.48
3:C:201:VAL:O	3:C:202:GLN:HB3	2.14	0.48
11:K:12:VAL:HG13	11:K:179:VAL:HB	1.94	0.48
11:K:35:ILE:HG22	11:K:45:MET:HE1	1.86	0.48
14:N:83:LYS:HG3	14:N:119:VAL:CG2	2.44	0.48
11:Y:45:MET:HG2	11:Y:52:CYS:HB3	1.96	0.48
3:Q:201:VAL:O	3:Q:202:GLN:HB3	2.14	0.47
3:C:160:GLN:HA	3:C:160:GLN:HE21	1.80	0.47
4:D:88:ALA:HA	4:D:99:ILE:HG21	1.97	0.47
11:K:72:GLU:OE1	11:K:106:LYS:NZ	2.40	0.47
10:X:50:ALA:O	11:Y:91:LYS:NZ	2.47	0.47
3:Q:160:GLN:HE21	3:Q:160:GLN:HA	1.81	0.46
11:K:61:ARG:O	11:K:65:ILE:HG13	2.15	0.46
4:R:89:VAL:HG12	11:Y:61:ARG:HD3	1.97	0.46
11:Y:33:LYS:HG2	18:Y:301:6NV:C18	2.46	0.46
14:N:176:VAL:HG12	14:N:178:LEU:HD13	1.97	0.46
9:W:9:GLY:HA3	9:W:41:LYS:HE2	1.97	0.46
11:K:35:ILE:HG22	11:K:45:MET:CE	2.41	0.46
9:I:9:GLY:HA3	9:I:41:LYS:HE2	1.98	0.45
10:J:1:MET:HG2	10:J:34:LYS:HE3	1.97	0.45
8:H:104:ASP:HB2	8:H:105:PRO:HD2	1.97	0.45
12:L:126:ASP:OD1	12:L:126:ASP:C	2.55	0.45
9:I:101:PRO:HB3	9:I:126:ILE:HD12	1.98	0.45
8:V:104:ASP:HB2	8:V:105:PRO:HD2	1.97	0.45
4:R:88:ALA:HA	4:R:99:ILE:HG21	1.97	0.45
10:X:1:MET:HB3	10:X:34:LYS:HE3	1.99	0.45
3:C:51:LYS:O	3:C:52:LEU:HB2	2.17	0.45
9:W:101:PRO:HB3	9:W:126:ILE:HD12	1.99	0.45
10:X:1:MET:HG2	10:X:34:LYS:HE3	1.97	0.45
11:K:61:ARG:O	11:K:65:ILE:CG1	2.64	0.45
10:J:50:ALA:O	11:K:91:LYS:NZ	2.50	0.44
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.99	0.44
3:Q:51:LYS:O	3:Q:52:LEU:HB2	2.17	0.44
3:C:35:LYS:HG2	3:C:158:SER:O	2.18	0.44
12:L:8:ASN:HA	12:L:30:ILE:O	2.18	0.44
18:Y:301:6NV:C29	18:Y:301:6NV:N41	2.79	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:61:ARG:O	11:Y:65:ILE:HG13	2.17	0.44
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.18	0.44
10:J:139:TYR:OH	10:X:25:ILE:O	2.30	0.44
2:B:50:LYS:O	2:B:51:VAL:C	2.56	0.44
5:E:12:PHE:H	6:F:19:GLN:HE22	1.65	0.44
11:K:35:ILE:HG22	11:K:45:MET:SD	2.58	0.44
7:G:78:ILE:N	7:G:79:PRO:CD	2.81	0.43
8:H:196:ARG:NH2	9:I:150:GLU:HG3	2.32	0.43
7:U:78:ILE:N	7:U:79:PRO:CD	2.81	0.43
10:J:1:MET:HB3	10:J:34:LYS:HE3	1.99	0.43
9:I:20:VAL:HG13	9:I:118:PRO:HB3	2.00	0.43
9:W:10:ILE:HG21	9:W:141:ALA:HB3	2.00	0.43
2:P:50:LYS:O	2:P:51:VAL:C	2.56	0.43
3:Q:35:LYS:HG2	3:Q:158:SER:O	2.19	0.43
9:I:26:LEU:HD21	9:I:185:VAL:HG23	2.01	0.43
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.53	0.43
12:Z:100:ARG:HD3	12:Z:105:TYR:CE2	2.54	0.43
3:C:149:GLU:HB2	3:C:150:PRO:HD2	2.01	0.43
9:W:20:VAL:HG13	9:W:118:PRO:HB3	2.00	0.43
3:Q:149:GLU:HB2	3:Q:150:PRO:HD2	2.00	0.42
1:O:1:MET:HG3	6:T:122:TYR:CZ	2.54	0.42
10:J:3:ILE:HG23	10:J:18:SER:HB3	2.01	0.42
2:B:50:LYS:HD3	2:B:50:LYS:HA	1.95	0.42
11:Y:100:MET:SD	11:Y:128:VAL:CG1	3.07	0.42
8:H:196:ARG:NH2	9:I:150:GLU:O	2.52	0.42
11:Y:61:ARG:O	11:Y:65:ILE:CG1	2.67	0.42
4:D:91:HIS:HB3	4:D:99:ILE:CG2	2.50	0.42
10:X:3:ILE:HG23	10:X:18:SER:HB3	2.01	0.42
11:K:100:MET:SD	11:K:128:VAL:CG1	3.08	0.42
9:W:26:LEU:HD21	9:W:185:VAL:HG23	2.01	0.42
11:Y:56:GLU:OE2	11:Y:99:THR:CG2	2.67	0.42
11:Y:72:GLU:OE1	11:Y:106:LYS:NZ	2.41	0.41
11:K:104:TRP:CE2	11:K:181:GLU:HB3	2.55	0.41
12:L:100:ARG:HD3	12:L:105:TYR:CE2	2.55	0.41
11:Y:104:TRP:CE2	11:Y:181:GLU:HB3	2.55	0.41
5:S:77:ALA:N	5:S:78:PRO:CD	2.84	0.41
4:R:91:HIS:HB3	4:R:99:ILE:CG2	2.50	0.41
14:N:36:ARG:HG3	14:N:42:TRP:CE2	2.55	0.41
11:Y:20:ALA:HB2	11:Y:31:VAL:HG11	2.02	0.41
5:E:77:ALA:N	5:E:78:PRO:CD	2.84	0.41
18:K:301:6NV:O40	18:K:301:6NV:C43	2.69	0.40

*Continued on next page...*



Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:151:ASN:HB2	2:P:152:PRO:CD	2.51	0.40
13:M:165:ILE:HB	13:M:166:PRO:HD3	2.04	0.40
7:G:149:ASP:HB2	7:G:150:PRO:CD	2.52	0.40
11:K:37:ILE:HB	11:K:41:LEU:HB3	2.03	0.40
11:Y:33:LYS:HE2	18:Y:301:6NV:C17	2.52	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%)	240 (97%)	7 (3%)	1 (0%)	39	69
1	O	248/250 (99%)	240 (97%)	7 (3%)	1 (0%)	39	69
2	B	242/258 (94%)	234 (97%)	5 (2%)	3 (1%)	16	39
2	P	242/258 (94%)	233 (96%)	6 (2%)	3 (1%)	16	39
3	C	238/254 (94%)	233 (98%)	3 (1%)	2 (1%)	24	51
3	Q	238/254 (94%)	233 (98%)	3 (1%)	2 (1%)	24	51
4	D	231/260 (89%)	227 (98%)	4 (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%)	236 (99%)	3 (1%)	0	100	100
7	U	239/252 (95%)	236 (99%)	3 (1%)	0	100	100
8	H	224/232 (97%)	218 (97%)	6 (3%)	0	100	100
8	V	224/232 (97%)	218 (97%)	6 (3%)	0	100	100

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	190 (98%)	3 (2%)	0	100	100
10	X	193/198 (98%)	190 (98%)	3 (2%)	0	100	100
11	K	209/211 (99%)	203 (97%)	6 (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%)	188 (97%)	6 (3%)	0	100	100
14	b	194/196 (99%)	188 (97%)	6 (3%)	0	100	100
All	All	6282/6612 (95%)	6124 (98%)	146 (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
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

### 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%)	187 (96%)	7 (4%)	42	73
4	R	194/215 (90%)	187 (96%)	7 (4%)	42	73
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%)	194 (96%)	7 (4%)	43	74
6	T	201/239 (84%)	194 (96%)	7 (4%)	43	74
7	G	206/210 (98%)	200 (97%)	6 (3%)	50	80
7	U	206/210 (98%)	200 (97%)	6 (3%)	50	80
8	H	185/190 (97%)	182 (98%)	3 (2%)	70	91
8	V	185/190 (97%)	182 (98%)	3 (2%)	70	91
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%)	150 (91%)	15 (9%)	12	26
12	L	186/186 (100%)	179 (96%)	7 (4%)	40	71
12	Z	186/186 (100%)	179 (96%)	7 (4%)	40	71
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%)	158 (98%)	4 (2%)	55	84
14	b	162/162 (100%)	158 (98%)	4 (2%)	55	84
All	All	5314/5534 (96%)	5154 (97%)	160 (3%)	48	79

All (160) 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	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	171	GLU
6	F	181	GLU
6	F	214	TRP
6	F	240	GLN
7	G	115	LEU
7	G	117	GLN
7	G	122	ARG
7	G	125	MET
7	G	208	GLU
7	G	235	ARG
8	H	30	ASN
8	H	68	LEU
8	H	196	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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	31	VAL
11	K	32	LYS
11	K	35	ILE
11	K	59	LEU
11	K	61	ARG
11	K	65	ILE
11	K	71	LYS
11	K	83	LEU
11	K	86	MET
11	K	93	MET
11	K	128	VAL
11	K	210	ILE
12	L	23	LEU
12	L	49	ASN
12	L	124	SER
12	L	128	VAL
12	L	130	SER
12	L	134	GLU
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	178	LEU
1	O	122	THR
1	O	157	PHE
1	O	250	LEU
2	P	113	ARG
2	P	191	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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	176	LEU
4	R	193	LEU
4	R	235	LEU
4	R	236	LYS
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	171	GLU
6	T	181	GLU
6	T	214	TRP
6	T	240	GLN
7	U	115	LEU
7	U	117	GLN
7	U	122	ARG
7	U	125	MET
7	U	208	GLU
7	U	235	ARG
8	V	30	ASN
8	V	68	LEU
8	V	196	ARG
9	W	37	ASN
9	W	171	LEU
10	X	3	ILE
10	X	99	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
10	X	110	LYS
11	Y	4	LEU
11	Y	12	VAL
11	Y	29	GLN
11	Y	31	VAL
11	Y	32	LYS
11	Y	35	ILE
11	Y	59	LEU
11	Y	61	ARG
11	Y	65	ILE
11	Y	71	LYS
11	Y	83	LEU
11	Y	86	MET
11	Y	93	MET
11	Y	128	VAL
11	Y	210	ILE
12	Z	23	LEU
12	Z	49	ASN
12	Z	124	SER
12	Z	128	VAL
12	Z	130	SER
12	Z	134	GLU
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	178	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (92) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	20	GLN
2	B	58	GLN
2	B	95	GLN
2	B	119	GLN
2	B	123	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
3	C	116	GLN
3	C	120	GLN
3	C	147	GLN
3	C	160	GLN
4	D	91	HIS
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	151	ASN
5	E	184	ASN
6	F	19	GLN
6	F	86	ASN
6	F	117	GLN
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
9	I	37	ASN
10	J	55	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	194	ASN
13	M	213	GLN
14	N	161	GLN
1	O	94	HIS
2	P	20	GLN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
2	P	58	GLN
2	P	95	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	15	GLN
4	R	91	HIS
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
5	S	151	ASN
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	35	HIS
9	W	37	ASN
10	X	55	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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
13	a	102	GLN
13	a	194	ASN
13	a	213	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 12 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
17	MES	H	301	-	12,12,12	2.12	1 (8%)	15,16,16	2.02	2 (13%)
18	6NV	K	301	11	48,48,48	1.77	12 (25%)	55,66,66	2.62	13 (23%)
17	MES	K	304	-	12,12,12	2.16	1 (8%)	15,16,16	1.79	4 (26%)
17	MES	V	301	-	12,12,12	2.16	1 (8%)	15,16,16	1.72	3 (20%)
17	MES	X	201	-	12,12,12	2.17	1 (8%)	15,16,16	1.89	4 (26%)
18	6NV	Y	301	11	48,48,48	1.82	13 (27%)	55,66,66	2.42	13 (23%)

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	MES	H	301	-	-	0/6/14/14	0/1/1/1
18	6NV	K	301	11	-	0/44/67/67	0/4/4/4
17	MES	K	304	-	-	0/6/14/14	0/1/1/1
17	MES	V	301	-	-	0/6/14/14	0/1/1/1
17	MES	X	201	-	-	0/6/14/14	0/1/1/1
18	6NV	Y	301	11	-	0/44/67/67	0/4/4/4

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	X	201	MES	C8-S	-7.19	1.66	1.77
17	K	304	MES	C8-S	-7.18	1.66	1.77
17	V	301	MES	C8-S	-7.15	1.66	1.77
17	H	301	MES	C8-S	-6.99	1.67	1.77
18	Y	301	6NV	C3-C4	-5.03	1.38	1.51
18	K	301	6NV	C16-C17	-4.96	1.39	1.51
18	K	301	6NV	C3-C4	-4.95	1.39	1.51
18	K	301	6NV	C38-C39	-4.49	1.33	1.50
18	Y	301	6NV	C31-C36	-4.23	1.32	1.46
18	Y	301	6NV	C16-C17	-4.15	1.41	1.51
18	Y	301	6NV	C38-C39	-4.09	1.35	1.50
18	K	301	6NV	C31-C36	-4.03	1.33	1.46
18	K	301	6NV	C34-C35	-3.14	1.38	1.49
18	Y	301	6NV	C32-C31	-3.11	1.32	1.40
18	Y	301	6NV	C34-C35	-3.07	1.39	1.49
18	K	301	6NV	C32-C31	-2.73	1.33	1.40
18	K	301	6NV	C35-C36	-2.45	1.32	1.34
18	K	301	6NV	C31-C30	-2.44	1.32	1.37
18	Y	301	6NV	C31-C30	-2.14	1.33	1.37
18	K	301	6NV	C38-C30	-2.12	1.32	1.41
18	Y	301	6NV	C34-C33	-2.10	1.37	1.47
18	Y	301	6NV	C38-C30	-2.05	1.32	1.41
18	K	301	6NV	C34-C33	-2.05	1.37	1.47
18	Y	301	6NV	C35-C36	-2.01	1.32	1.34
18	Y	301	6NV	C42-N41	2.06	1.50	1.46
18	K	301	6NV	C32-C33	2.46	1.38	1.32
18	Y	301	6NV	C32-C33	2.61	1.38	1.32
18	K	301	6NV	C25-C23	3.11	1.59	1.53
18	Y	301	6NV	C25-C23	4.32	1.61	1.53

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	K	301	6NV	C34-C33-C32	-12.42	117.06	123.52
18	Y	301	6NV	C34-C33-C32	-11.89	117.34	123.52
18	K	301	6NV	C16-C15-N14	-10.02	99.09	110.17
18	Y	301	6NV	C16-C15-N14	-8.85	100.38	110.17
18	Y	301	6NV	C9-O8-C7	-2.96	110.66	117.51
18	K	301	6NV	C29-C30-C31	-2.87	121.70	128.58
18	K	301	6NV	C4-C3-C2	-2.63	105.68	113.44
18	Y	301	6NV	C20-C19-C18	-2.48	116.75	120.20
18	Y	301	6NV	C4-C3-C2	-2.42	106.30	113.44
18	Y	301	6NV	C29-C30-C31	-2.37	122.90	128.58
18	Y	301	6NV	O24-C23-C15	-2.30	105.08	109.59
18	K	301	6NV	C26-C25-C23	-2.25	107.22	111.42
18	K	301	6NV	C44-C42-N41	-2.03	106.54	111.63
18	K	301	6NV	C12-C2-N1	-2.00	105.62	111.28
17	V	301	MES	O3S-S-C8	2.05	109.26	104.99
17	K	304	MES	O3S-S-C8	2.14	109.44	104.99
18	Y	301	6NV	O28-C27-C25	2.15	115.65	111.16
18	K	301	6NV	C17-C16-C15	2.16	116.85	113.40
18	Y	301	6NV	C19-C18-C17	2.17	123.95	120.65
18	K	301	6NV	C26-C25-C27	2.23	112.66	109.73
18	Y	301	6NV	C23-C15-N14	2.30	115.00	110.06
17	X	201	MES	O3S-S-C8	2.33	109.82	104.99
18	Y	301	6NV	C35-C34-C33	2.43	118.17	113.73
17	K	304	MES	C6-C5-N4	2.46	113.87	110.11
18	K	301	6NV	C43-C42-N41	2.50	115.03	110.27
18	Y	301	6NV	C17-C16-C15	2.96	118.14	113.40
17	X	201	MES	C6-C5-N4	3.09	114.84	110.11
17	K	304	MES	O1S-S-C8	3.12	109.07	106.87
17	V	301	MES	O2S-S-C8	3.15	109.09	106.87
17	H	301	MES	O1S-S-C8	3.15	109.09	106.87
18	K	301	6NV	C35-C34-C33	3.19	119.56	113.73
18	K	301	6NV	C23-C15-N14	3.38	117.31	110.06
17	X	201	MES	O2S-S-C8	3.42	109.28	106.87
17	X	201	MES	O1S-S-C8	3.45	109.31	106.87
17	K	304	MES	O2S-S-C8	3.86	109.60	106.87
18	K	301	6NV	C42-N41-C39	3.93	127.43	121.48
18	Y	301	6NV	C42-N41-C39	4.03	127.58	121.48
17	V	301	MES	O1S-S-C8	4.63	110.14	106.87
17	H	301	MES	O2S-S-C8	6.09	111.17	106.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	K	301	6NV	2	0
18	Y	301	6NV	3	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%)	-0.28	9 (3%)	46 46	30, 49, 85, 121	0
1	O	250/250 (100%)	-0.21	9 (3%)	46 46	36, 52, 98, 134	0
2	B	244/258 (94%)	-0.15	9 (3%)	45 45	35, 55, 97, 150	0
2	P	244/258 (94%)	-0.15	9 (3%)	45 45	37, 55, 100, 150	0
3	C	240/254 (94%)	0.08	20 (8%)	14 11	34, 61, 127, 161	0
3	Q	240/254 (94%)	0.15	17 (7%)	19 17	38, 66, 144, 183	0
4	D	235/260 (90%)	-0.25	2 (0%)	85 86	38, 57, 88, 125	0
4	R	235/260 (90%)	-0.10	6 (2%)	59 59	47, 64, 107, 137	0
5	E	231/234 (98%)	-0.13	7 (3%)	54 54	40, 60, 97, 141	0
5	S	231/234 (98%)	-0.02	9 (3%)	43 43	44, 65, 105, 138	0
6	F	243/288 (84%)	-0.23	10 (4%)	41 41	34, 55, 106, 131	0
6	T	243/288 (84%)	-0.18	10 (4%)	41 41	36, 60, 117, 151	0
7	G	241/252 (95%)	-0.27	6 (2%)	61 61	32, 51, 91, 148	0
7	U	241/252 (95%)	-0.25	7 (2%)	55 55	33, 51, 89, 129	0
8	H	226/232 (97%)	-0.28	7 (3%)	52 52	33, 48, 84, 144	0
8	V	226/232 (97%)	-0.23	5 (2%)	65 66	35, 50, 82, 154	0
9	I	204/205 (99%)	-0.54	3 (1%)	76 76	32, 46, 76, 97	0
9	W	204/205 (99%)	-0.51	2 (0%)	84 85	27, 47, 77, 97	0
10	J	195/198 (98%)	-0.30	5 (2%)	59 59	33, 53, 82, 120	0
10	X	195/198 (98%)	-0.30	5 (2%)	59 59	34, 53, 82, 128	0
11	K	211/211 (100%)	-0.17	4 (1%)	70 70	32, 57, 89, 115	0
11	Y	211/211 (100%)	-0.15	2 (0%)	85 86	33, 58, 88, 114	0
12	L	222/222 (100%)	-0.28	3 (1%)	78 77	41, 54, 96, 126	0
12	Z	222/222 (100%)	-0.20	4 (1%)	71 72	36, 56, 99, 131	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
13	M	233/246 (94%)	-0.40	4 (1%)	73 74	32, 51, 80, 103	0
13	a	233/246 (94%)	-0.34	1 (0%)	93 94	29, 52, 79, 107	0
14	N	196/196 (100%)	-0.43	3 (1%)	76 76	31, 45, 74, 101	0
14	b	196/196 (100%)	-0.46	2 (1%)	84 85	31, 45, 75, 102	0
All	All	6342/6612 (95%)	-0.23	180 (2%)	56 57	27, 54, 98, 183	0

All (180) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	P	51	VAL	7.1
2	P	219	ALA	7.0
10	X	1	MET	6.8
1	O	1	MET	6.3
2	B	221	ASP	6.1
3	Q	206	LYS	6.0
3	C	238	LYS	5.9
9	W	1	SER	5.8
2	B	218	GLY	5.5
5	S	202	ASP	5.5
12	Z	174	TYR	5.5
10	J	1	MET	5.3
5	E	202	ASP	5.3
3	Q	240	GLU	5.2
3	Q	202	GLN	4.9
3	Q	49	THR	4.8
3	Q	48	SER	4.6
9	I	1	SER	4.6
2	P	221	ASP	4.6
3	C	206	LYS	4.5
6	F	181	GLU	4.5
10	X	194	ASP	4.4
12	L	174	TYR	4.4
3	C	205	ALA	4.4
13	a	1	THR	4.4
3	C	202	GLN	4.3
4	R	1	ASP	4.3
3	Q	205	ALA	4.2
2	B	51	VAL	4.2
1	O	2	THR	4.2
1	A	1	MET	4.2
8	H	226	GLU	4.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
8	V	226	GLU	4.2
2	P	218	GLY	4.0
3	C	50	LEU	4.0
1	O	249	ALA	4.0
3	Q	238	LYS	4.0
4	R	217	GLN	3.9
3	C	48	SER	3.8
6	F	205	GLU	3.7
8	V	222	ASP	3.7
3	C	49	THR	3.7
3	Q	50	LEU	3.6
2	P	220	ASN	3.6
3	Q	236	GLN	3.6
4	R	241	ALA	3.5
8	V	221	CYS	3.5
1	A	249	ALA	3.4
3	C	239	GLN	3.4
5	S	3	ASN	3.4
4	R	230	GLU	3.4
3	C	236	GLN	3.3
7	G	3	TYR	3.3
3	Q	239	GLN	3.3
7	G	241	GLU	3.3
3	C	235	GLU	3.2
11	K	146	ASP	3.2
6	T	181	GLU	3.2
3	Q	141	ASP	3.2
3	Q	225	GLU	3.2
6	T	205	GLU	3.1
8	V	224	GLN	3.1
2	B	220	ASN	3.1
10	X	193	ASP	3.1
3	C	240	GLU	3.1
3	C	216	ASP	3.1
5	S	180	LYS	3.1
5	E	217	LYS	3.0
7	G	2	GLY	3.0
1	O	201	GLU	3.0
5	E	233	ILE	3.0
6	T	2	THR	3.0
3	Q	181	GLU	3.0
6	T	243	ILE	2.9

*Continued on next page...*



*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
10	J	194	ASP	2.9
14	N	195	GLN	2.9
1	A	201	GLU	2.9
8	V	145	ASP	2.9
7	U	242	GLN	2.9
5	E	54	GLU	2.9
11	Y	182	ASP	2.9
7	U	2	GLY	2.9
2	B	217	LYS	2.9
10	X	95	ARG	2.9
1	O	231	LYS	2.8
1	A	250	LEU	2.8
13	M	47	ASP	2.8
2	B	59	ASP	2.8
6	F	244	ASN	2.8
11	K	211	GLY	2.8
3	C	175	LYS	2.7
2	P	59	ASP	2.7
1	A	2	THR	2.7
6	F	2	THR	2.7
7	U	222	ASP	2.7
5	S	173	ARG	2.7
6	F	202	ASP	2.7
6	F	180	PRO	2.7
14	N	181	ALA	2.6
5	E	122	TYR	2.6
8	H	221	CYS	2.6
5	S	210	LEU	2.6
3	C	203	THR	2.6
4	R	125	LEU	2.6
4	D	1	ASP	2.6
14	b	195	GLN	2.6
5	S	203	GLU	2.6
1	O	250	LEU	2.6
3	Q	180	LYS	2.6
3	Q	187	GLU	2.6
7	U	241	GLU	2.6
13	M	1	THR	2.6
12	L	173	LYS	2.6
3	Q	237	GLU	2.6
12	Z	1	GLN	2.6
11	Y	146	ASP	2.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	P	203	SER	2.5
9	W	133	LYS	2.5
8	H	222	ASP	2.5
1	A	248	GLU	2.5
7	G	242	GLN	2.5
13	M	82	ASP	2.5
6	T	241	LYS	2.4
5	E	123	GLY	2.4
2	P	52	THR	2.4
12	Z	210	ASP	2.4
3	C	47	ARG	2.4
1	O	52	SER	2.4
8	H	219	ASN	2.4
5	S	233	ILE	2.4
6	T	244	ASN	2.4
1	O	248	GLU	2.4
7	G	240	ALA	2.3
7	U	181	LYS	2.3
8	H	198	GLU	2.3
6	T	166	GLN	2.3
6	T	201	GLU	2.3
9	I	160	GLU	2.3
3	C	181	GLU	2.3
11	K	9	ARG	2.3
3	C	1	GLY	2.3
9	I	133	LYS	2.3
8	H	224	GLN	2.2
6	T	180	PRO	2.2
3	C	225	GLU	2.2
4	R	242	GLU	2.2
12	Z	167	LYS	2.2
2	B	60	THR	2.2
5	S	207	VAL	2.2
5	S	217	LYS	2.2
1	O	53	SER	2.2
11	K	182	ASP	2.2
3	C	27	ARG	2.2
10	X	195	PHE	2.2
13	M	216	ASN	2.2
6	F	201	GLU	2.2
7	U	51	PRO	2.2
10	J	193	ASP	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	B	219	ALA	2.2
6	F	215	CYS	2.2
1	A	228	PRO	2.1
4	D	230	GLU	2.1
10	J	95	ARG	2.1
1	A	203	GLU	2.1
2	P	182	ASP	2.1
7	U	3	TYR	2.1
1	A	231	LYS	2.1
6	F	242	GLU	2.1
2	B	203	SER	2.1
5	E	201	ARG	2.1
7	G	181	LYS	2.1
14	N	105	LYS	2.1
14	b	105	LYS	2.1
12	L	1	GLN	2.0
6	T	230	ASP	2.0
3	Q	47	ARG	2.0
6	F	203	ASN	2.0
3	C	234	ILE	2.0
8	H	215	GLU	2.0
10	J	155	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( $\text{\AA}^2$ )	Q<0.9
17	MES	H	301	12/12	0.74	0.50	14.72	67,70,92,92	0
17	MES	V	301	12/12	0.85	0.46	9.46	66,70,86,97	0
17	MES	X	201	12/12	0.88	0.33	3.36	47,49,61,70	12
17	MES	K	304	12/12	0.85	0.39	3.24	44,47,61,67	12
15	MG	J	201	1/1	0.98	0.19	2.92	50,50,50,50	0
15	MG	I	301	1/1	0.93	0.27	2.84	66,66,66,66	0
18	6NV	Y	301	45/45	0.84	0.28	2.64	33,50,65,71	45
15	MG	N	201	1/1	0.88	0.17	2.10	55,55,55,55	0
18	6NV	K	301	45/45	0.86	0.25	2.05	32,48,64,69	45
15	MG	G	301	1/1	0.95	0.09	-0.90	42,42,42,42	0
15	MG	Z	301	1/1	0.94	0.13	-1.28	65,65,65,65	0
15	MG	I	302	1/1	0.97	0.08	-1.88	57,57,57,57	0
15	MG	A	301	1/1	0.95	0.10	-2.13	45,45,45,45	0
15	MG	K	302	1/1	0.98	0.05	-2.46	52,52,52,52	0
15	MG	L	301	1/1	0.99	0.04	-3.55	57,57,57,57	0
16	CL	G	302	1/1	0.99	0.09	-	37,37,37,37	0
15	MG	K	303	1/1	0.93	0.41	-	58,58,58,58	0
16	CL	U	301	1/1	0.99	0.13	-	40,40,40,40	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.