



# wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 6, 2023 – 01:54 pm GMT

PDB ID : 5LEZ  
Title : Human 20S proteasome complex with Oprozomib in Mg-Acetate at 2.2 Angstrom  
Authors : Schrader, J.; Henneberg, F.; Mata, R.; Tittmann, K.; Schneider, T.R.; Stark, H.; Bourenkov, G.; Chari, A.  
Deposited on : 2016-06-30  
Resolution : 2.19 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 1.8.4, CSD as541be (2020)  
Xtrriage (Phenix) : 1.13  
EDS : 2.36  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

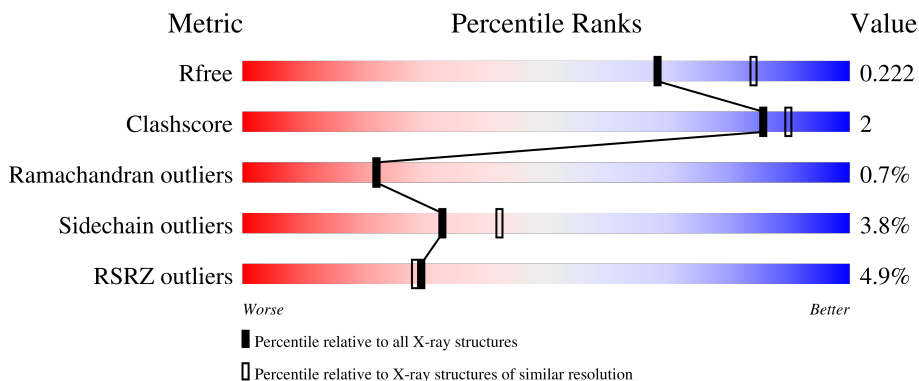
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.19 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))
$R_{free}$	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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	234	 2% 85% 12% ..
1	O	234	 13% 87% 9% ..
2	B	261	 7% 89% 6% 5%
2	P	261	 11% 84% 10% 5%
3	C	248	 12% 83% 9% ..



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Mol	Chain	Length	Quality of chain
3	Q	248	17% 83% 10% • 5%
4	D	241	8% 87% 9% •
4	R	241	2% 88% 7% • •
5	E	263	4% 80% 7% • 11%
5	S	263	2% 79% 10% • 10%
6	F	255	% 86% 7% • 6%
6	T	255	5% 85% 7% • 6%
7	G	246	4% 92% 5% • • •
7	U	246	15% 89% 7% • •
8	H	234	% 87% 7% 6%
8	V	234	3% 86% 7% • 6%
9	I	205	92% 7%
9	W	205	2% 95% • •
10	J	201	% 86% 10% • • •
10	X	201	% 86% 9% • •
11	K	204	2% 86% 11% • •
11	Y	204	% 87% 8% • •
12	L	213	93% 7%
12	Z	213	% 92% 7%
13	M	219	2% 93% 5% • •
13	a	219	% 94% 5% •
14	N	205	% 92% 6% •
14	b	205	5% 95% • •
15	c	4	50% 50%
15	d	4	75% 25%

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Mol	Chain	Length	Quality of chain	
15	e	4		50%
15	f	4		50%

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
7	6V1	U	47	X	-	-	-

## 2 Entry composition [i](#)

There are 20 unique types of molecules in this entry. The entry contains 52158 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
			Total	C	N	O	S			
1	A	230	Total	C	N	O	S	0	3	0
			1788	1145	301	336	6			
1	O	230	Total	C	N	O	S	0	0	0
			1741	1111	293	331	6			

- Molecule 2 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	248	Total	C	N	O	S	0	2	0
			1922	1217	331	363	11			
2	P	247	Total	C	N	O	S	0	2	0
			1898	1200	321	366	11			

- Molecule 3 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	237	Total	C	N	O	S	0	2	0
			1798	1121	320	352	5			
3	Q	235	Total	C	N	O	S	0	0	0
			1801	1126	316	354	5			

- Molecule 4 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	233	Total	C	N	O	S	0	1	0
			1762	1105	290	356	11			
4	R	233	Total	C	N	O	S	0	1	0
			1753	1103	293	346	11			

- Molecule 5 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	234	Total 1822	C 1144	N 325	O 342	S 11	0	1	0
5	S	238	Total 1875	C 1175	N 340	O 349	S 11	0	3	0

- Molecule 6 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	F	239	Total 1888	C 1198	N 325	O 353	S 12	0	4	0
6	T	240	Total 1856	C 1178	N 315	O 351	S 12	0	1	0

- Molecule 7 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	G	244	Total 1912	C 1214	N 321	O 364	S 13	0	2	0
7	U	238	Total 1815	C 1147	N 304	O 350	S 14	0	1	0

- Molecule 8 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	H	220	Total 1664	C 1047	N 284	O 320	S 13	0	2	0
8	V	220	Total 1622	C 1023	N 269	O 318	S 12	0	2	0

- Molecule 9 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
9	I	204	Total 1613	C 1028	N 270	O 295	S 20	0	3	0
9	W	204	Total 1599	C 1018	N 267	O 295	S 19	0	2	0

- Molecule 10 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	J	196	Total 1590	C 1021	N 271	O 288	S 10	0	3	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	X	196	Total	C	N	O	S	0	2	0
			1576	1012	267	287	10			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	200	Total	C	N	O	S	0	0	0
			1551	977	272	293	9			
11	Y	199	Total	C	N	O	S	0	3	0
			1570	991	278	291	10			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	213	Total	C	N	O	S	0	2	0
			1636	1038	277	310	11			
12	Z	213	Total	C	N	O	S	0	1	0
			1642	1041	280	310	11			

- Molecule 13 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	216	Total	C	N	O	S	0	1	0
			1692	1067	291	322	12			
13	a	216	Total	C	N	O	S	0	2	0
			1688	1064	291	321	12			

- Molecule 14 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	202	Total	C	N	O	S	0	1	0
			1519	953	258	295	13			
14	b	203	Total	C	N	O	S	0	1	0
			1524	956	259	296	13			

- Molecule 15 is a protein called bound Oprozomib.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	c	4	Total	C	N	O	S	0	0	0
			37	25	4	7	1			
15	d	4	Total	C	N	O	S	0	0	0
			37	25	4	7	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	e	4	Total	C	N	O	S	0	0	0
			37	25	4	7	1			
15	f	4	Total	C	N	O	S	0	0	0
			37	25	4	7	1			

- Molecule 16 is POTASSIUM ION (three-letter code: K) (formula: K).

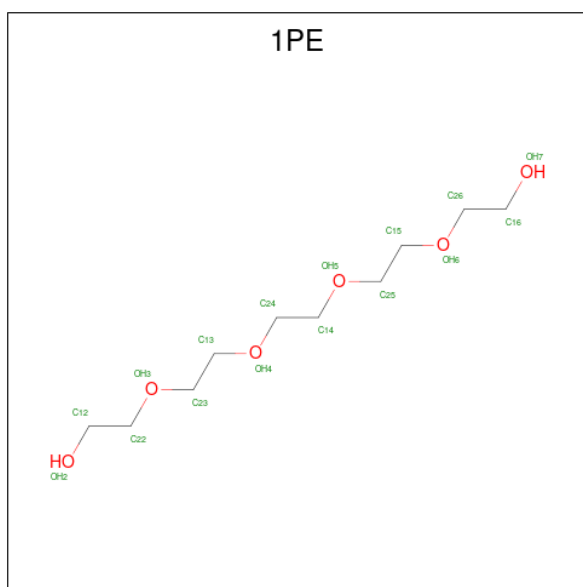
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	G	1	Total	K	0	0
			1	1		
16	L	1	Total	K	0	0
			1	1		
16	N	1	Total	K	0	0
			1	1		
16	U	1	Total	K	0	0
			1	1		
16	Z	1	Total	K	0	0
			1	1		
16	b	1	Total	K	0	0
			1	1		

- Molecule 17 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	H	2	Total	Mg	0	0
			2	2		
17	I	2	Total	Mg	0	0
			2	2		
17	J	1	Total	Mg	0	0
			1	1		
17	K	1	Total	Mg	0	0
			1	1		
17	L	1	Total	Mg	0	0
			1	1		
17	V	1	Total	Mg	0	0
			1	1		
17	W	1	Total	Mg	0	0
			1	1		
17	X	1	Total	Mg	0	0
			1	1		

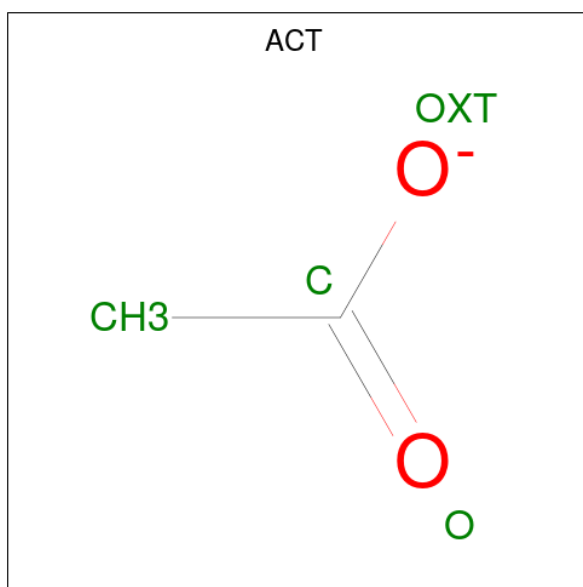
- Molecule 18 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: C<sub>10</sub>H<sub>22</sub>O<sub>6</sub>).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	H	1	Total	C	O	0	0
			16	10	6		
18	I	1	Total	C	O	0	0
			16	10	6		
18	K	1	Total	C	O	0	0
			16	10	6		
18	L	1	Total	C	O	0	0
			16	10	6		
18	N	1	Total	C	O	0	0
			16	10	6		
18	U	1	Total	C	O	0	0
			16	10	6		
18	W	1	Total	C	O	0	0
			16	10	6		
18	Y	1	Total	C	O	0	0
			16	10	6		
18	a	1	Total	C	O	0	0
			16	10	6		

- Molecule 19 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	c	1	Total C O 4 2 2	0	0
19	d	1	Total C O 4 2 2	0	0
19	e	1	Total C O 4 2 2	0	0
19	f	1	Total C O 4 2 2	0	0

- Molecule 20 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	A	120	Total O 120 120	0	0
20	B	130	Total O 130 130	0	0
20	C	80	Total O 80 80	0	0
20	D	99	Total O 99 99	0	0
20	E	147	Total O 147 147	0	0
20	F	185	Total O 185 185	0	0
20	G	196	Total O 196 196	0	0
20	H	156	Total O 156 156	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	I	161	Total 161	O 161	0	0
20	J	136	Total 136	O 136	0	0
20	K	106	Total 106	O 106	0	0
20	L	127	Total 127	O 127	0	0
20	M	155	Total 155	O 155	0	0
20	N	160	Total 160	O 160	0	0
20	O	94	Total 94	O 94	0	0
20	P	127	Total 127	O 127	0	0
20	Q	77	Total 77	O 77	0	0
20	R	133	Total 133	O 133	0	0
20	S	132	Total 132	O 132	0	0
20	T	95	Total 95	O 95	0	0
20	U	116	Total 116	O 116	0	0
20	V	114	Total 114	O 114	0	0
20	W	120	Total 120	O 120	0	0
20	X	129	Total 129	O 129	0	0
20	Y	149	Total 149	O 149	0	0
20	Z	168	Total 168	O 168	0	0
20	a	179	Total 179	O 179	0	0
20	b	118	Total 118	O 118	0	0
20	c	2	Total 2	O 2	0	0

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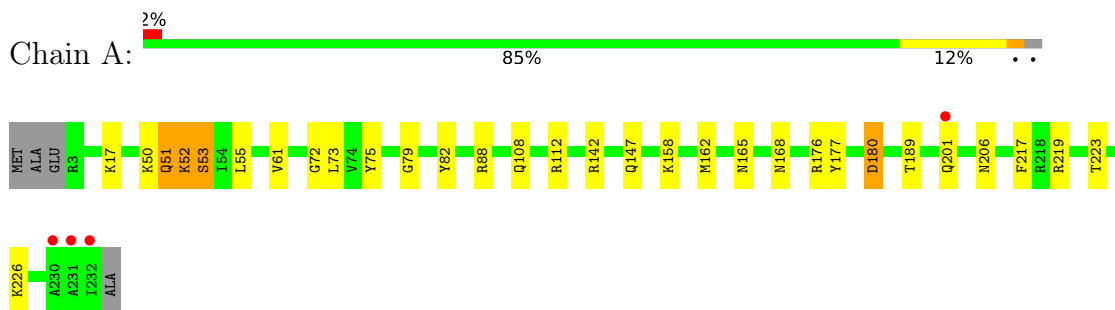
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>	<b>ZeroOcc</b>	<b>AltConf</b>
20	d	2	Total O 2 2	0	0
20	e	3	Total O 3 3	0	0
20	f	1	Total O 1 1	0	0

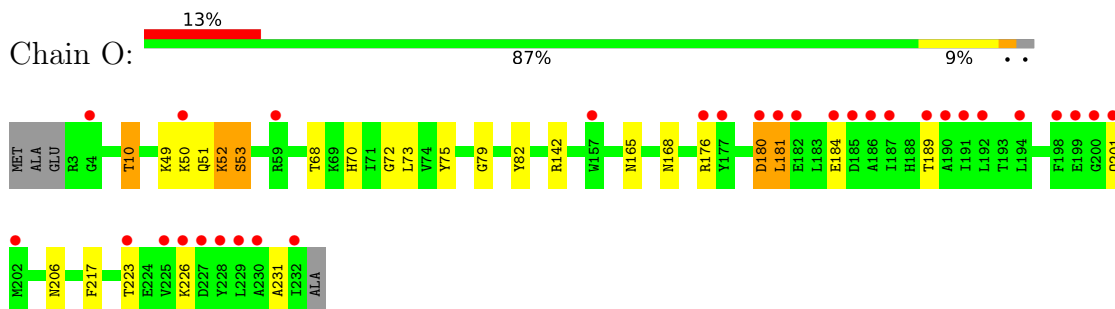
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

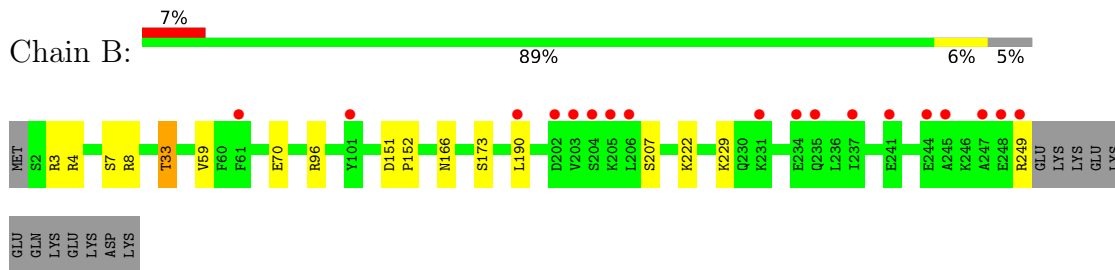
- Molecule 1: Proteasome subunit alpha type-2



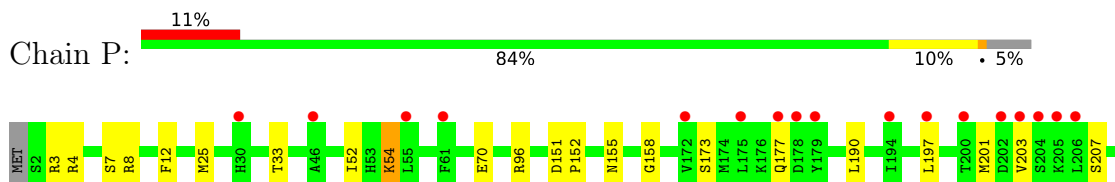
- Molecule 1: Proteasome subunit alpha type-2

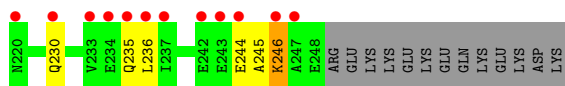


- Molecule 2: Proteasome subunit alpha type-4

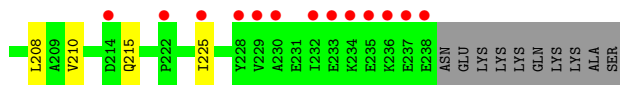
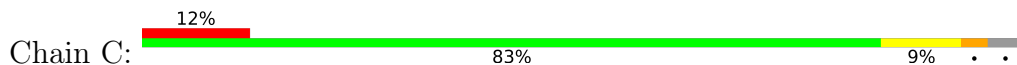


- Molecule 2: Proteasome subunit alpha type-4

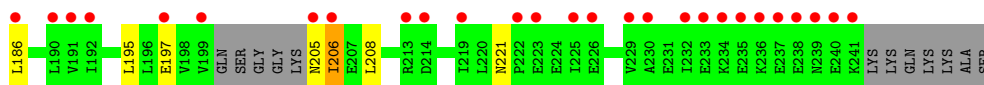
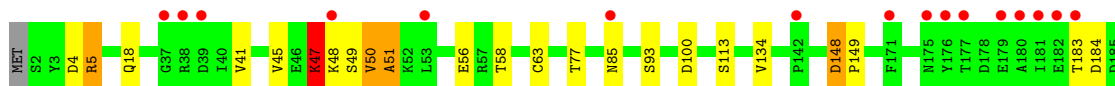
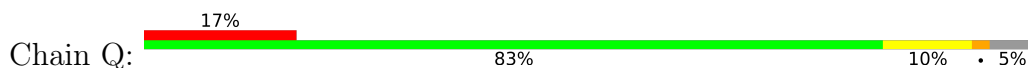




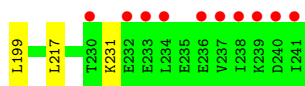
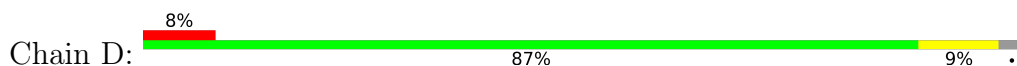
- Molecule 3: Proteasome subunit alpha type-7



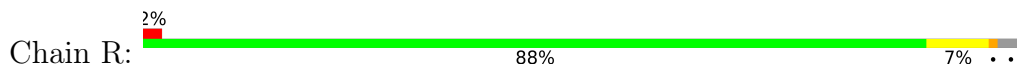
- Molecule 3: Proteasome subunit alpha type-7



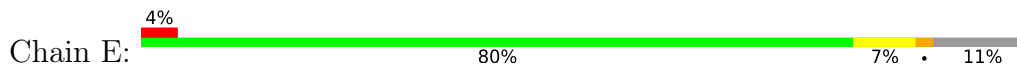
- Molecule 4: Proteasome subunit alpha type-5

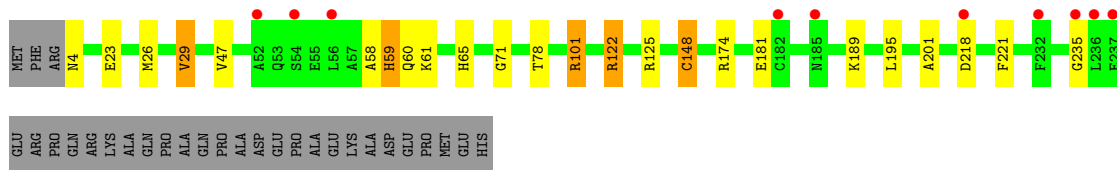


- Molecule 4: Proteasome subunit alpha type-5

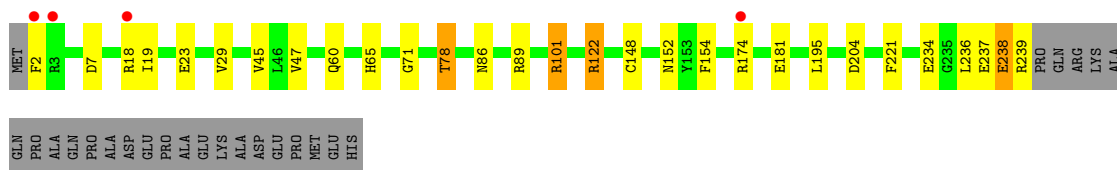
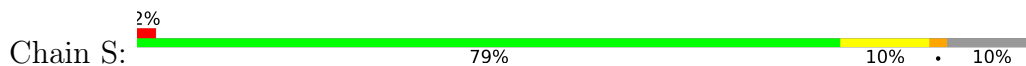


- Molecule 5: Proteasome subunit alpha type-1

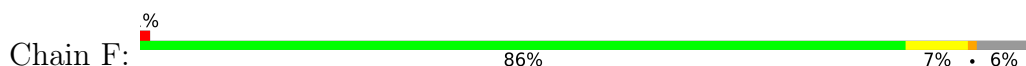




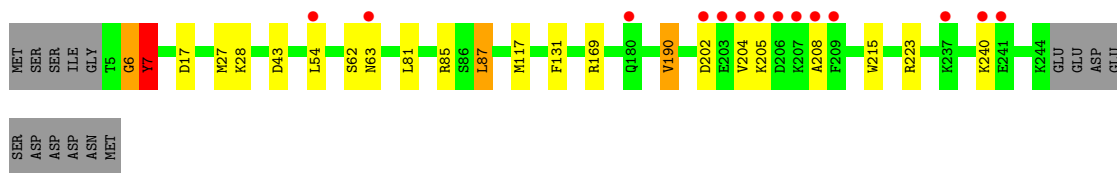
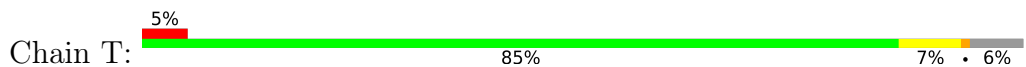
• Molecule 5: Proteasome subunit alpha type-1



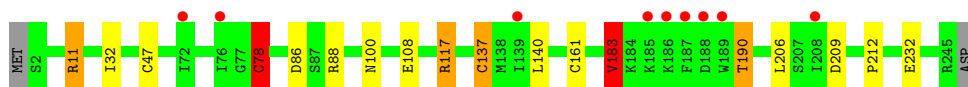
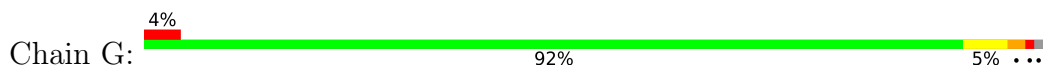
• Molecule 6: Proteasome subunit alpha type-3



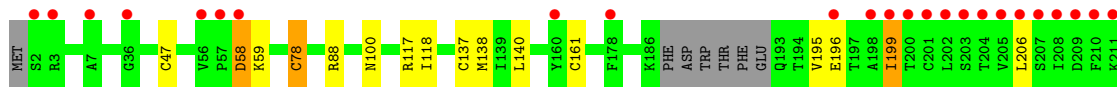
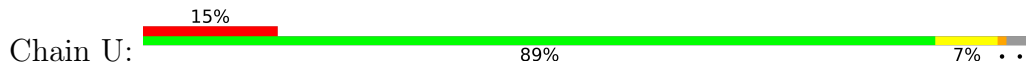
• Molecule 6: Proteasome subunit alpha type-3

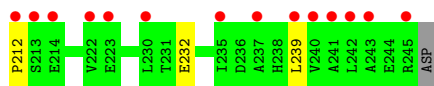


• Molecule 7: Proteasome subunit alpha type-6

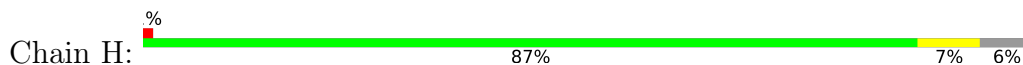


• Molecule 7: Proteasome subunit alpha type-6

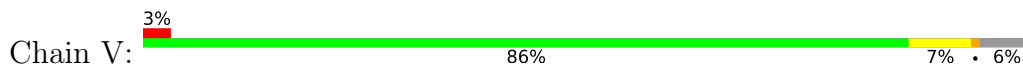




- Molecule 8: Proteasome subunit beta type-7



- Molecule 8: Proteasome subunit beta type-7



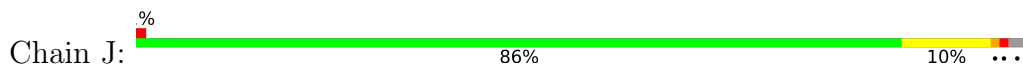
- Molecule 9: Proteasome subunit beta type-3



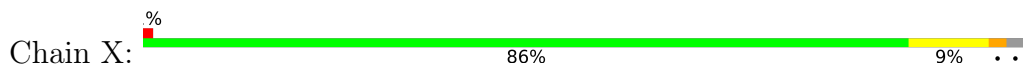
- Molecule 9: Proteasome subunit beta type-3



- Molecule 10: Proteasome subunit beta type-2

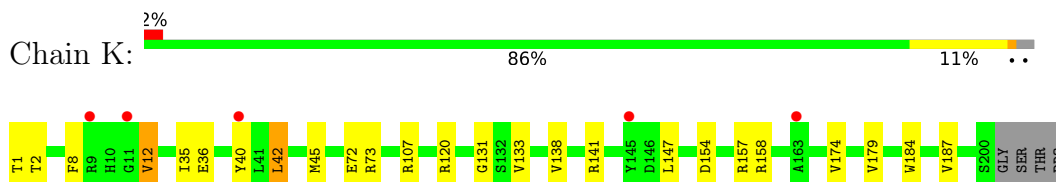


- Molecule 10: Proteasome subunit beta type-2

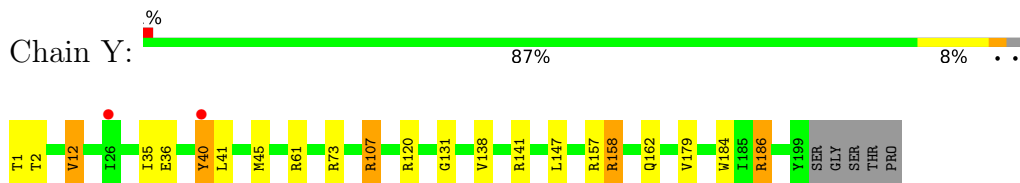


- Molecule 11: Proteasome subunit beta type-5

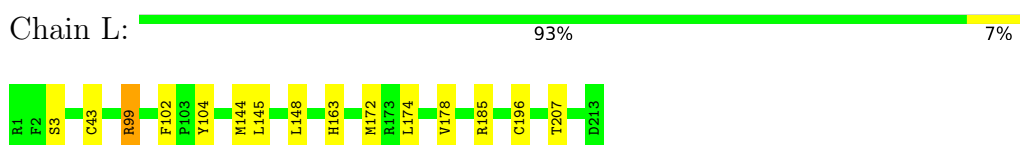




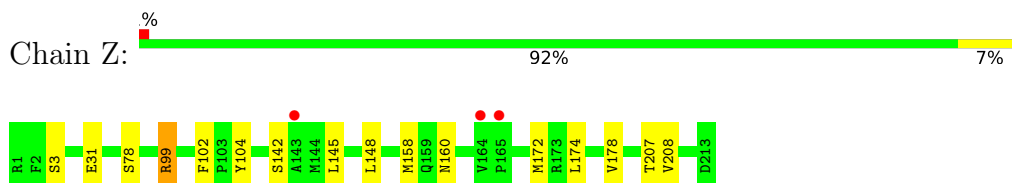
- Molecule 11: Proteasome subunit beta type-5



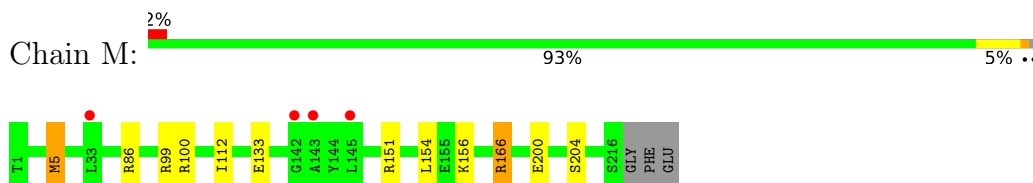
- Molecule 12: Proteasome subunit beta type-1



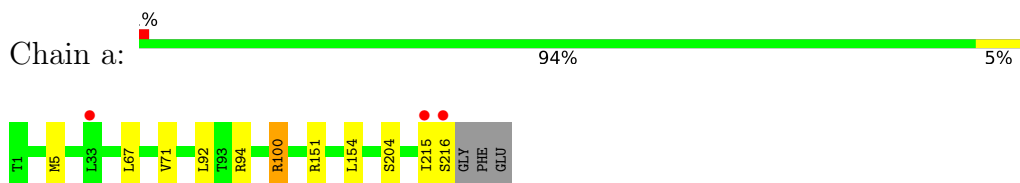
- Molecule 12: Proteasome subunit beta type-1



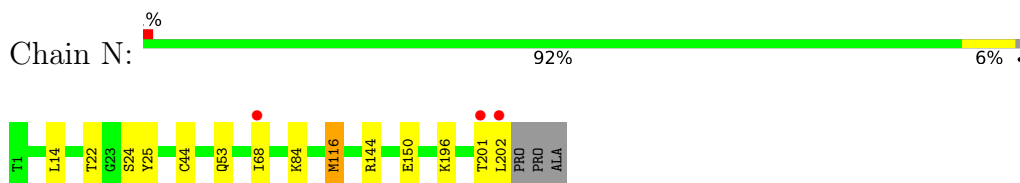
- Molecule 13: Proteasome subunit beta type-4



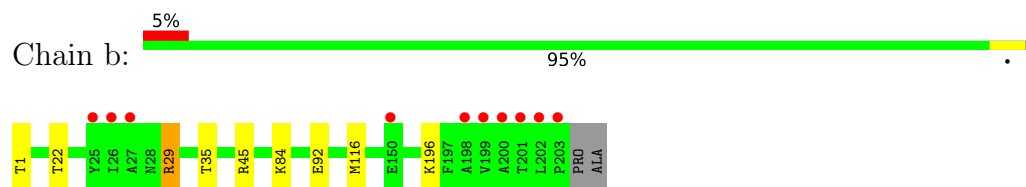
- Molecule 13: Proteasome subunit beta type-4



- Molecule 14: Proteasome subunit beta type-6



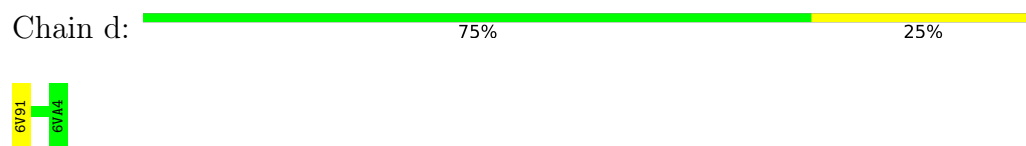
- Molecule 14: Proteasome subunit beta type-6



- Molecule 15: bound Oprozomib



- Molecule 15: bound Oprozomib



- Molecule 15: bound Oprozomib



- Molecule 15: bound Oprozomib



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	113.86Å 203.23Å 315.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	170.81 – 2.19 49.67 – 2.19	Depositor EDS
% Data completeness (in resolution range)	99.4 (170.81-2.19) 99.5 (49.67-2.19)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.50 (at 2.20Å)	Xtrriage
Refinement program	REFMAC 5.8.0103	Depositor
R, $R_{free}$	0.181 , 0.222 0.185 , 0.222	Depositor DCC
$R_{free}$ test set	18458 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	49.6	Xtrriage
Anisotropy	0.246	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 45.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	52158	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	64.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.76% 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: 6V9, 1PE, MG, OAS, 6VA, K, 6V1, YCM, ACT

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	0.70	0/1833	0.80	2/2489 (0.1%)
1	O	0.60	0/1778	0.79	1/2419 (0.0%)
2	B	0.73	0/1958	0.87	4/2645 (0.2%)
2	P	0.67	0/1934	0.86	3/2617 (0.1%)
3	C	0.77	1/1818 (0.1%)	0.94	8/2469 (0.3%)
3	Q	0.71	0/1814	0.88	2/2462 (0.1%)
4	D	0.70	0/1789	0.82	4/2424 (0.2%)
4	R	0.82	2/1780 (0.1%)	0.91	5/2408 (0.2%)
5	E	0.71	1/1842 (0.1%)	0.86	2/2493 (0.1%)
5	S	0.71	0/1901	0.89	5/2571 (0.2%)
6	F	0.78	0/1935	0.89	4/2605 (0.2%)
6	T	0.79	1/1894 (0.1%)	0.93	8/2556 (0.3%)
7	G	0.82	3/1909 (0.2%)	0.88	7/2579 (0.3%)
7	U	0.70	0/1804	0.82	2/2441 (0.1%)
8	H	0.81	1/1697 (0.1%)	0.97	5/2299 (0.2%)
8	V	0.68	2/1655 (0.1%)	0.88	4/2251 (0.2%)
9	I	0.76	0/1648	0.96	8/2219 (0.4%)
9	W	0.62	0/1630	0.89	6/2197 (0.3%)
10	J	0.82	0/1613	0.99	5/2180 (0.2%)
10	X	0.74	1/1599 (0.1%)	0.94	4/2163 (0.2%)
11	K	0.73	0/1582	0.97	9/2138 (0.4%)
11	Y	0.85	1/1610 (0.1%)	1.00	9/2172 (0.4%)
12	L	0.67	0/1672	0.85	3/2257 (0.1%)
12	Z	0.84	4/1675 (0.2%)	0.91	3/2257 (0.1%)
13	M	0.79	0/1728	0.93	5/2339 (0.2%)
13	a	0.83	0/1724	0.93	4/2336 (0.2%)
14	N	0.86	2/1548 (0.1%)	0.90	2/2095 (0.1%)
14	b	0.81	0/1554	0.90	4/2104 (0.2%)
All	All	0.75	19/48924 (0.0%)	0.90	128/66185 (0.2%)

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
2	P	0	3
3	Q	0	2
4	D	0	2
4	R	0	1
5	E	0	1
6	F	0	1
7	U	1	0
9	I	0	1
9	W	0	1
10	J	0	2
10	X	0	2
13	a	0	1
All	All	1	17

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	182	GLU	CD-OE2	8.46	1.34	1.25
7	G	108	GLU	CD-OE1	8.18	1.34	1.25
12	Z	3	SER	CB-OG	7.22	1.51	1.42
10	X	154	GLU	C-O	6.91	1.36	1.23
14	N	24	SER	CB-OG	-6.42	1.33	1.42

The worst 5 of 128 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	Z	99	ARG	NE-CZ-NH2	-11.67	114.46	120.30
10	J	86	ARG	NE-CZ-NH1	10.77	125.68	120.30
9	I	69	ARG	NE-CZ-NH1	10.36	125.48	120.30
4	R	120[A]	ALA	C-N-CA	9.90	146.45	121.70
4	R	120[B]	ALA	C-N-CA	9.90	146.45	121.70

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	U	47	6V1	C1

5 of 17 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	175[A]	GLU	Peptide
4	D	175[B]	GLU	Peptide
5	E	235	GLY	Peptide
6	F	206	ASP	Peptide
9	I	78	GLY	Peptide

## 5.2 Too-close contacts [i](#)

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	1788	0	1761	12	0
1	O	1741	0	1683	9	0
2	B	1922	0	1913	4	0
2	P	1898	0	1861	11	0
3	C	1798	0	1718	14	0
3	Q	1801	0	1735	14	0
4	D	1762	0	1709	10	0
4	R	1753	0	1726	10	0
5	E	1822	0	1779	11	0
5	S	1875	0	1818	15	0
6	F	1888	0	1882	4	0
6	T	1856	0	1816	4	0
7	G	1912	0	1882	7	0
7	U	1815	0	1748	6	0
8	H	1664	0	1681	6	0
8	V	1622	0	1595	8	0
9	I	1613	0	1646	5	0
9	W	1599	0	1621	4	0
10	J	1590	0	1581	14	0
10	X	1576	0	1561	16	0
11	K	1551	0	1506	9	0
11	Y	1570	0	1547	11	0
12	L	1636	0	1625	7	0
12	Z	1642	0	1635	6	0
13	M	1692	0	1670	4	0
13	a	1688	0	1658	0	0
14	N	1519	0	1493	6	0
14	b	1524	0	1493	0	0
15	c	37	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	d	37	0	6	0	0
15	e	37	0	6	0	0
15	f	37	0	6	0	0
16	G	1	0	0	0	0
16	L	1	0	0	0	0
16	N	1	0	0	0	0
16	U	1	0	0	0	0
16	Z	1	0	0	0	0
16	b	1	0	0	0	0
17	H	2	0	0	0	0
17	I	2	0	0	0	0
17	J	1	0	0	0	0
17	K	1	0	0	0	0
17	L	1	0	0	0	0
17	V	1	0	0	0	0
17	W	1	0	0	0	0
17	X	1	0	0	0	0
18	H	16	0	22	0	0
18	I	16	0	22	0	0
18	K	16	0	22	0	0
18	L	16	0	22	0	0
18	N	16	0	22	0	0
18	U	16	0	22	0	0
18	W	16	0	22	0	0
18	Y	16	0	22	0	0
18	a	16	0	22	0	0
19	c	4	0	3	0	0
19	d	4	0	3	0	0
19	e	4	0	3	0	0
19	f	4	0	3	0	0
20	A	120	0	0	2	0
20	B	130	0	0	1	0
20	C	80	0	0	1	0
20	D	99	0	0	1	0
20	E	147	0	0	3	0
20	F	185	0	0	1	1
20	G	196	0	0	2	1
20	H	156	0	0	1	0
20	I	161	0	0	1	0
20	J	136	0	0	2	0
20	K	106	0	0	1	0
20	L	127	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	M	155	0	0	0	0
20	N	160	0	0	0	0
20	O	94	0	0	1	0
20	P	127	0	0	2	0
20	Q	77	0	0	0	0
20	R	133	0	0	1	0
20	S	132	0	0	5	0
20	T	95	0	0	0	0
20	U	116	0	0	0	0
20	V	114	0	0	1	0
20	W	120	0	0	2	0
20	X	129	0	0	0	0
20	Y	149	0	0	1	0
20	Z	168	0	0	0	0
20	a	179	0	0	0	0
20	b	118	0	0	0	0
20	c	2	0	0	0	0
20	d	2	0	0	0	0
20	e	3	0	0	0	0
20	f	1	0	0	0	0
All	All	52158	0	47577	199	1

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

The worst 5 of 199 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)
5:E:47:VAL:HG12	5:E:195:LEU:HD22	1.64	0.80
6:F:227:VAL:O	6:F:232[B]:ARG:NH1	2.14	0.80
5:S:18[B]:ARG:HG2	5:S:23:GLU:OE2	1.84	0.78
5:S:47:VAL:HG12	5:S:195:LEU:HD22	1.65	0.77
10:J:1[A]:MET:HE1	10:J:134:TYR:H	1.51	0.74

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:F:465:HOH:O	20:G:566:HOH:O[4_475]	2.06	0.14



## 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	231/234 (99%)	222 (96%)	4 (2%)	5 (2%)	6	4
1	O	228/234 (97%)	218 (96%)	4 (2%)	6 (3%)	5	3
2	B	248/261 (95%)	240 (97%)	8 (3%)	0	100	100
2	P	247/261 (95%)	233 (94%)	11 (4%)	3 (1%)	13	10
3	C	236/248 (95%)	217 (92%)	14 (6%)	5 (2%)	7	4
3	Q	230/248 (93%)	216 (94%)	8 (4%)	6 (3%)	5	3
4	D	232/241 (96%)	224 (97%)	5 (2%)	3 (1%)	12	9
4	R	232/241 (96%)	224 (97%)	4 (2%)	4 (2%)	9	6
5	E	232/263 (88%)	226 (97%)	5 (2%)	1 (0%)	34	37
5	S	238/263 (90%)	232 (98%)	4 (2%)	2 (1%)	19	19
6	F	241/255 (94%)	235 (98%)	5 (2%)	1 (0%)	34	37
6	T	239/255 (94%)	229 (96%)	6 (2%)	4 (2%)	9	6
7	G	241/246 (98%)	237 (98%)	4 (2%)	0	100	100
7	U	232/246 (94%)	227 (98%)	4 (2%)	1 (0%)	34	37
8	H	220/234 (94%)	217 (99%)	3 (1%)	0	100	100
8	V	220/234 (94%)	217 (99%)	3 (1%)	0	100	100
9	I	205/205 (100%)	202 (98%)	3 (2%)	0	100	100
9	W	204/205 (100%)	200 (98%)	2 (1%)	2 (1%)	15	14
10	J	195/201 (97%)	192 (98%)	3 (2%)	0	100	100
10	X	195/201 (97%)	191 (98%)	4 (2%)	0	100	100
11	K	198/204 (97%)	196 (99%)	2 (1%)	0	100	100
11	Y	200/204 (98%)	197 (98%)	3 (2%)	0	100	100
12	L	213/213 (100%)	211 (99%)	2 (1%)	0	100	100
12	Z	212/213 (100%)	210 (99%)	2 (1%)	0	100	100
13	M	215/219 (98%)	207 (96%)	8 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	a	216/219 (99%)	206 (95%)	10 (5%)	0	100	100
14	N	201/205 (98%)	198 (98%)	3 (2%)	0	100	100
14	b	202/205 (98%)	199 (98%)	3 (2%)	0	100	100
All	All	6203/6458 (96%)	6023 (97%)	137 (2%)	43 (1%)	22	22

5 of 43 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	50	LYS
1	A	53	SER
3	C	47	LYS
3	C	204	LYS
4	D	176	GLY

### 5.3.2 Protein sidechains [i](#)

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	185/191 (97%)	174 (94%)	11 (6%)	19	23
1	O	176/191 (92%)	165 (94%)	11 (6%)	18	20
2	B	199/221 (90%)	190 (96%)	9 (4%)	27	34
2	P	196/221 (89%)	184 (94%)	12 (6%)	18	21
3	C	179/210 (85%)	168 (94%)	11 (6%)	18	21
3	Q	183/210 (87%)	174 (95%)	9 (5%)	25	31
4	D	189/203 (93%)	185 (98%)	4 (2%)	53	67
4	R	187/203 (92%)	186 (100%)	1 (0%)	88	94
5	E	192/223 (86%)	184 (96%)	8 (4%)	30	38
5	S	197/223 (88%)	188 (95%)	9 (5%)	27	34
6	F	199/212 (94%)	189 (95%)	10 (5%)	24	30
6	T	192/212 (91%)	183 (95%)	9 (5%)	26	33
7	G	202/207 (98%)	195 (96%)	7 (4%)	36	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	U	186/207 (90%)	181 (97%)	5 (3%)	44	57
8	H	181/195 (93%)	173 (96%)	8 (4%)	28	35
8	V	172/195 (88%)	165 (96%)	7 (4%)	30	39
9	I	176/174 (101%)	173 (98%)	3 (2%)	60	74
9	W	173/174 (99%)	172 (99%)	1 (1%)	86	93
10	J	166/170 (98%)	158 (95%)	8 (5%)	25	32
10	X	165/170 (97%)	158 (96%)	7 (4%)	30	38
11	K	155/159 (98%)	146 (94%)	9 (6%)	20	23
11	Y	158/159 (99%)	152 (96%)	6 (4%)	33	42
12	L	175/178 (98%)	169 (97%)	6 (3%)	37	47
12	Z	175/178 (98%)	171 (98%)	4 (2%)	50	63
13	M	180/181 (99%)	176 (98%)	4 (2%)	52	65
13	a	178/181 (98%)	171 (96%)	7 (4%)	32	41
14	N	158/159 (99%)	154 (98%)	4 (2%)	47	60
14	b	158/159 (99%)	152 (96%)	6 (4%)	33	42
All	All	5032/5366 (94%)	4836 (96%)	196 (4%)	33	41

5 of 196 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	P	33	THR
5	S	234	GLU
2	P	190	LEU
3	Q	195	LEU
6	T	215	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
10	X	24	ASN
13	a	162	GLN
10	X	82	ASN
12	Z	157	ASN
11	K	10	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

24 non-standard protein/DNA/RNA residues are modelled in this entry.

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$
7	6V1	U	161	7	12,15,16	2.30	3 (25%)	9,20,22	3.02	4 (44%)
15	6V9	d	1	15	6,8,9	1.34	2 (33%)	3,10,12	5.66	2 (66%)
15	OAS	e	3	15	5,6,9	0.50	0	2,6,11	0.71	0
10	6V1	X	91	10	12,15,16	1.63	5 (41%)	9,20,22	4.02	5 (55%)
15	OAS	e	2	15	5,6,9	1.03	1 (20%)	2,6,11	1.90	1 (50%)
7	YCM	G	137	7	7,9,10	1.67	2 (28%)	4,10,12	2.71	2 (50%)
3	YCM	Q	63	3	7,9,10	1.29	1 (14%)	4,10,12	2.80	2 (50%)
5	6V1	E	148	5	12,15,16	1.65	4 (33%)	9,20,22	2.49	3 (33%)
5	6V1	S	148	5	12,15,16	1.68	4 (33%)	9,20,22	2.58	4 (44%)
15	OAS	c	3	15	5,6,9	0.60	0	2,6,11	0.69	0
15	6V9	c	1	15	6,8,9	0.87	0	3,10,12	3.22	2 (66%)
15	OAS	f	2	15	5,6,9	0.55	0	2,6,11	1.56	1 (50%)
15	OAS	d	3	15	5,6,9	0.90	0	2,6,11	0.87	0
3	YCM	C	63	3	7,9,10	1.02	1 (14%)	4,10,12	1.27	1 (25%)
15	6V9	f	1	15	6,8,9	1.40	0	3,10,12	5.63	2 (66%)
15	OAS	d	2	15	5,6,9	0.55	0	2,6,11	1.64	0
7	6V1	G	47	7	12,15,16	1.77	3 (25%)	9,20,22	1.98	2 (22%)
10	6V1	J	91	10	12,15,16	1.71	4 (33%)	9,20,22	4.21	5 (55%)
7	6V1	G	161	7	12,15,16	1.57	4 (33%)	9,20,22	2.02	3 (33%)
15	OAS	f	3	15	5,6,9	0.99	0	2,6,11	1.13	0
7	YCM	U	137	7	7,9,10	1.00	0	4,10,12	3.22	1 (25%)
7	6V1	U	47	7	12,15,16	1.64	3 (25%)	9,20,22	2.02	2 (22%)
15	OAS	c	2	15	5,6,9	0.67	0	2,6,11	2.41	2 (100%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
15	6V9	e	1	15	6,8,9	0.78	0	3,10,12	2.95	2 (66%)

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
7	6V1	U	161	7	-	1/6/25/27	0/1/1/1
15	6V9	d	1	15	-	0/0/2/4	0/1/1/1
15	OAS	e	3	15	-	1/3/5/9	-
10	6V1	X	91	10	-	2/6/25/27	0/1/1/1
15	OAS	e	2	15	-	3/3/5/9	-
7	YCM	G	137	7	-	2/6/8/10	-
3	YCM	Q	63	3	-	3/6/8/10	-
5	6V1	E	148	5	-	2/6/25/27	0/1/1/1
5	6V1	S	148	5	-	0/6/25/27	0/1/1/1
15	OAS	c	3	15	-	1/3/5/9	-
15	6V9	c	1	15	-	0/0/2/4	0/1/1/1
15	OAS	f	2	15	-	0/3/5/9	-
15	OAS	d	3	15	-	0/3/5/9	-
3	YCM	C	63	3	-	0/6/8/10	-
15	6V9	f	1	15	-	0/0/2/4	0/1/1/1
15	OAS	d	2	15	-	0/3/5/9	-
7	6V1	G	47	7	-	0/6/25/27	0/1/1/1
10	6V1	J	91	10	-	2/6/25/27	0/1/1/1
7	6V1	G	161	7	-	0/6/25/27	0/1/1/1
15	OAS	f	3	15	-	1/3/5/9	-
7	YCM	U	137	7	-	1/6/8/10	-
7	6V1	U	47	7	1/1/5/6	1/6/25/27	0/1/1/1
15	OAS	c	2	15	-	3/3/5/9	-
15	6V9	e	1	15	-	0/0/2/4	0/1/1/1

The worst 5 of 37 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	U	161	6V1	C1-SG	-5.11	1.77	1.83
7	U	161	6V1	CB-SG	-4.69	1.77	1.82
7	G	47	6V1	CB-SG	-4.38	1.77	1.82
7	U	47	6V1	CB-SG	-4.04	1.77	1.82
10	J	91	6V1	C4-N3	-3.70	1.32	1.38

The worst 5 of 46 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	f	1	6V9	O-C-C3	-8.97	115.72	124.22
15	d	1	6V9	O-C-C3	-8.68	116.00	124.22
10	J	91	6V1	C6-N3-C2	6.60	131.74	123.36
10	X	91	6V1	C6-N3-C2	6.46	131.56	123.36
7	U	161	6V1	C5-C4-N3	6.35	111.87	108.13

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	U	47	6V1	C1

5 of 23 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	148	6V1	C3-C6-N3-C4
7	G	137	YCM	CE-CD-SG-CB
7	G	137	YCM	SG-CD-CE-NZ2
10	J	91	6V1	C3-C6-N3-C2
10	J	91	6V1	C3-C6-N3-C4

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	G	137	YCM	1	0
5	E	148	6V1	1	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 29 ligands modelled in this entry, 16 are monoatomic - leaving 13 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	$\# Z  > 2$
18	1PE	W	302	-	15,15,15	0.68	0	14,14,14	0.33	0
18	1PE	N	301	-	15,15,15	0.56	0	14,14,14	0.51	0
18	1PE	Y	301	-	15,15,15	0.63	0	14,14,14	0.62	0
18	1PE	K	302	-	15,15,15	0.70	0	14,14,14	0.75	0
19	ACT	c	101	-	3,3,3	0.75	0	3,3,3	0.98	0
18	1PE	I	302	-	15,15,15	0.73	0	14,14,14	0.84	0
18	1PE	U	301	-	15,15,15	0.65	0	14,14,14	0.68	0
18	1PE	a	301	-	15,15,15	0.59	0	14,14,14	0.39	0
19	ACT	f	101	-	3,3,3	0.96	0	3,3,3	0.70	0
19	ACT	e	101	-	3,3,3	0.83	0	3,3,3	0.41	0
19	ACT	d	101	-	3,3,3	0.68	0	3,3,3	0.87	0
18	1PE	L	301	-	15,15,15	0.59	0	14,14,14	0.46	0
18	1PE	H	303	-	15,15,15	0.64	0	14,14,14	0.76	0

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
18	1PE	W	302	-	-	5/13/13/13	-
18	1PE	N	301	-	-	5/13/13/13	-
18	1PE	Y	301	-	-	7/13/13/13	-
18	1PE	K	302	-	-	7/13/13/13	-
18	1PE	I	302	-	-	9/13/13/13	-
18	1PE	U	301	-	-	6/13/13/13	-
18	1PE	a	301	-	-	6/13/13/13	-
18	1PE	L	301	-	-	5/13/13/13	-
18	1PE	H	303	-	-	7/13/13/13	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 57 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	I	302	1PE	C15-C25-OH5-C14
18	H	303	1PE	C24-C14-OH5-C25
18	K	302	1PE	C16-C26-OH6-C15
18	Y	301	1PE	C16-C26-OH6-C15
18	H	303	1PE	OH4-C13-C23-OH3

There are no ring outliers.

No monomer is involved in short contacts.

## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	230/234 (98%)	-0.06	4 (1%) 70 68	42, 62, 99, 120	0
1	O	230/234 (98%)	0.61	31 (13%) 3 2	55, 82, 127, 151	0
2	B	248/261 (95%)	0.30	18 (7%) 15 14	47, 67, 118, 170	0
2	P	247/261 (94%)	0.55	29 (11%) 4 4	53, 80, 137, 171	0
3	C	236/248 (95%)	0.68	30 (12%) 3 3	48, 78, 130, 180	0
3	Q	234/248 (94%)	0.95	43 (18%) 1 1	44, 81, 152, 204	0
4	D	233/241 (96%)	0.28	19 (8%) 11 10	51, 76, 109, 141	0
4	R	233/241 (96%)	-0.03	5 (2%) 63 61	39, 55, 84, 118	0
5	E	233/263 (88%)	0.09	10 (4%) 35 33	40, 56, 99, 130	0
5	S	237/263 (90%)	-0.19	4 (1%) 70 68	41, 58, 94, 125	0
6	F	239/255 (93%)	-0.09	2 (0%) 86 85	39, 51, 77, 98	0
6	T	240/255 (94%)	0.17	14 (5%) 23 22	43, 63, 105, 134	0
7	G	241/246 (97%)	0.25	9 (3%) 41 39	38, 54, 99, 148	0
7	U	235/246 (95%)	0.68	38 (16%) 1 1	53, 74, 111, 148	0
8	H	220/234 (94%)	-0.15	3 (1%) 75 73	34, 48, 82, 112	0
8	V	220/234 (94%)	0.12	6 (2%) 54 52	45, 62, 106, 126	0
9	I	204/205 (99%)	0.04	1 (0%) 91 90	37, 49, 77, 96	0
9	W	204/205 (99%)	0.03	4 (1%) 65 63	48, 66, 98, 109	0
10	J	195/201 (97%)	-0.09	3 (1%) 73 72	38, 53, 74, 91	0
10	X	195/201 (97%)	-0.04	2 (1%) 82 81	44, 56, 77, 95	0
11	K	200/204 (98%)	0.16	5 (2%) 57 55	46, 60, 90, 109	0
11	Y	199/204 (97%)	0.08	2 (1%) 82 81	35, 47, 72, 83	0
12	L	213/213 (100%)	-0.07	0 100 100	43, 65, 91, 114	0
12	Z	213/213 (100%)	-0.03	3 (1%) 75 73	33, 48, 78, 99	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	M	216/219 (98%)	0.11	4 (1%) 66 65	35, 51, 77, 115	0
13	a	216/219 (98%)	0.03	3 (1%) 75 73	33, 47, 73, 107	0
14	N	202/205 (98%)	0.03	3 (1%) 73 72	35, 44, 70, 117	0
14	b	203/205 (99%)	0.23	10 (4%) 29 28	39, 50, 81, 131	0
15	c	0/4	-	-	-	-
15	d	0/4	-	-	-	-
15	e	0/4	-	-	-	-
15	f	0/4	-	-	-	-
All	All	6216/6474 (96%)	0.17	305 (4%) 29 28	33, 59, 107, 204	0

The worst 5 of 305 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	G	187	PHE	12.9
3	Q	232	ILE	11.9
1	O	232	ILE	9.3
14	b	203	PRO	9.2
2	P	204	SER	8.6

## 6.2 Non-standard residues in protein, DNA, RNA chains [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. 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	B-factors(Å <sup>2</sup> )	Q<0.9
7	YCM	U	137	10/11	0.84	0.18	60,70,87,87	0
7	6V1	U	47	15/16	0.87	0.33	94,131,141,141	0
5	6V1	S	148	15/16	0.88	0.16	44,74,82,83	0
5	6V1	E	148	15/16	0.89	0.17	47,68,74,76	0
7	6V1	U	161	15/16	0.91	0.12	70,89,97,99	0
15	OAS	f	2	7/10	0.91	0.11	53,56,58,60	0
7	6V1	G	161	15/16	0.92	0.17	46,69,77,78	0
7	6V1	G	47	15/16	0.92	0.16	53,79,84,85	0
10	6V1	X	91	15/16	0.92	0.17	48,69,76,76	0
15	6V9	f	1	8/9	0.92	0.13	61,63,68,68	0
7	YCM	G	137	10/11	0.92	0.15	46,53,68,69	0
3	YCM	Q	63	10/11	0.93	0.15	67,72,78,79	0
10	6V1	J	91	15/16	0.93	0.17	43,64,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	YCM	C	63	10/11	0.94	0.12	63,69,85,89	0
15	OAS	c	2	7/10	0.95	0.14	49,50,52,54	0
15	OAS	d	2	7/10	0.95	0.10	45,46,47,49	0
15	6V9	d	1	8/9	0.95	0.12	52,55,61,63	0
15	OAS	f	3	7/10	0.97	0.09	52,53,58,60	0
15	6V9	c	1	8/9	0.98	0.09	51,52,53,53	0
15	OAS	c	3	7/10	0.98	0.14	47,48,48,48	0
15	OAS	d	3	7/10	0.98	0.10	42,45,51,52	0
15	OAS	e	3	7/10	0.98	0.13	35,35,38,39	0
15	OAS	e	2	7/10	0.98	0.14	34,37,43,48	0
15	6V9	e	1	8/9	0.99	0.10	41,42,44,45	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides 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. 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	B-factors( $\text{\AA}^2$ )	Q<0.9
18	1PE	I	302	16/16	0.70	0.29	76,88,94,95	0
18	1PE	W	302	16/16	0.71	0.37	75,93,100,103	0
18	1PE	K	302	16/16	0.75	0.19	78,86,93,94	0
18	1PE	Y	301	16/16	0.77	0.18	64,80,88,91	0
17	MG	H	301	1/1	0.78	0.17	59,59,59,59	0
18	1PE	L	301	16/16	0.80	0.33	80,89,117,117	0
18	1PE	H	303	16/16	0.83	0.27	71,82,101,107	0
18	1PE	N	301	16/16	0.83	0.13	51,64,78,79	0
18	1PE	a	301	16/16	0.86	0.23	77,82,114,116	0
18	1PE	U	301	16/16	0.88	0.17	57,66,87,89	0
17	MG	K	301	1/1	0.89	0.07	50,50,50,50	0
17	MG	V	301	1/1	0.91	0.16	64,64,64,64	0
16	K	L	302	1/1	0.91	0.09	77,77,77,77	0
19	ACT	f	101	4/4	0.92	0.18	59,60,63,67	0
16	K	Z	301	1/1	0.93	0.04	67,67,67,67	0
17	MG	L	303	1/1	0.94	0.05	49,49,49,49	0
17	MG	I	303	1/1	0.95	0.09	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
17	MG	H	302	1/1	0.96	0.07	45,45,45,45	0
17	MG	X	301	1/1	0.96	0.07	65,65,65,65	0
17	MG	J	301	1/1	0.96	0.11	61,61,61,61	0
16	K	G	301	1/1	0.97	0.12	59,59,59,59	0
16	K	N	302	1/1	0.97	0.06	56,56,56,56	0
16	K	U	302	1/1	0.97	0.21	62,62,62,62	0
19	ACT	c	101	4/4	0.97	0.12	63,65,65,66	0
19	ACT	d	101	4/4	0.97	0.15	54,60,61,65	0
19	ACT	e	101	4/4	0.97	0.13	47,48,49,49	0
17	MG	I	301	1/1	0.97	0.09	43,43,43,43	0
16	K	b	301	1/1	0.98	0.05	60,60,60,60	0
17	MG	W	301	1/1	0.99	0.03	50,50,50,50	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.