



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 9, 2016 – 01:10 PM EDT

PDB ID : 5LF0  
Title : Human 20S proteasome complex with Epoxomicin at 2.4 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 : 2.41 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027939  
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-20027939

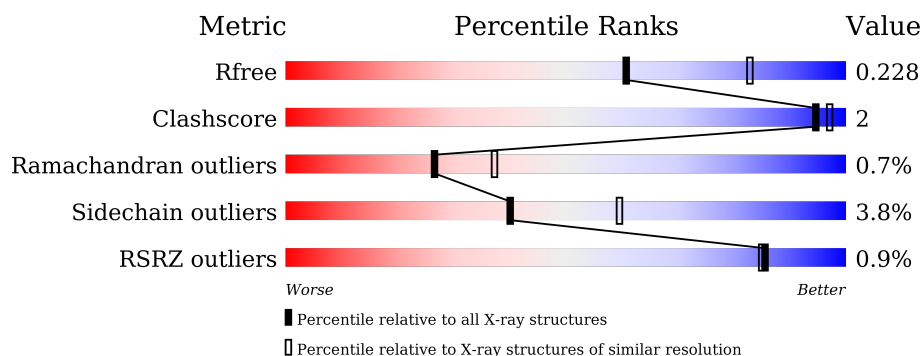
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.41 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.









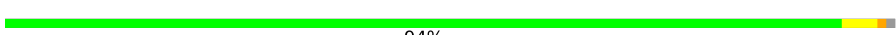




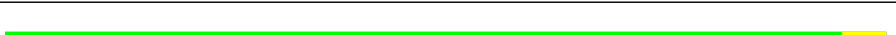

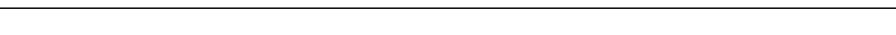
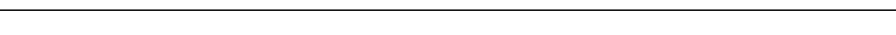
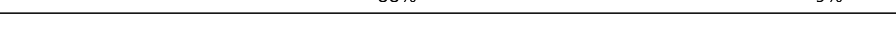

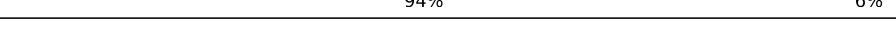
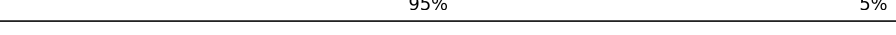
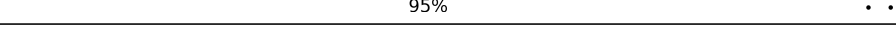
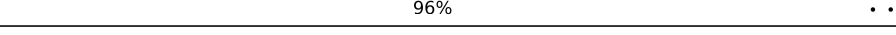
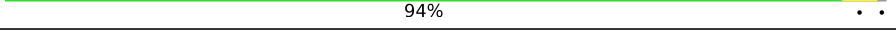
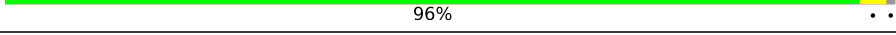


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	3386 (2.44-2.40)
Clashscore	102246	3897 (2.44-2.40)
Ramachandran outliers	100387	3837 (2.44-2.40)
Sidechain outliers	100360	3838 (2.44-2.40)
RSRZ outliers	91569	3396 (2.44-2.40)

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	234	<div> <div>88%</div> <div>10% .</div> </div>
1	O	234	<div> <div>2%</div> <div>90%</div> <div>7% ..</div> </div>
2	B	261	<div> <div>90%</div> <div>5% . 5%</div> </div>
2	P	261	<div> <div>3%</div> <div>85%</div> <div>7% . 5%</div> </div>
3	C	248	<div> <div>87%</div> <div>6% . .</div> </div>
3	Q	248	<div> <div>5%</div> <div>85%</div> <div>9% . .</div> </div>




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Mol	Chain	Length	Quality of chain
4	D	241	 92% 5% . .
4	R	241	 92% . . .
5	E	263	 2% 83% 5% . 11%
5	S	263	 2% 83% 7% . 10%
6	F	255	 86% 7% 6%
6	T	255	 4% 85% 8% . 6%
7	G	246	 94% . .
7	U	246	 1% 89% 6% . .
8	H	234	 1% 90% . 6%
8	V	234	 1% 88% 6% 6%
9	I	205	 94% 5%
9	W	205	 94% 5%
10	J	201	 90% 6% . .
10	X	201	 90% 5% . .
11	K	204	 88% 9% .
11	Y	204	 88% 9% . .
12	L	213	 94% 6%
12	Z	213	 95% 5%
13	M	219	 95% . .
13	a	219	 96% . .
14	N	205	 94% . .
14	b	205	 96% . .
15	c	5	 80% 20%
15	d	5	 60% 20% 20%
15	e	5	 80% 20%

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Mol	Chain	Length	Quality of chain
15	f	5	
15	g	5	
15	h	5	

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	IML	c	2	X	-	-	-
15	IML	d	2	X	-	-	-
15	IML	e	2	X	-	-	-
15	IML	f	2	X	-	-	-
15	IML	g	2	X	-	-	-
15	IML	h	2	X	-	-	-
16	CL	B	302	-	-	X	-
16	CL	D	301	-	-	-	X
16	CL	E	301	-	-	-	X
16	CL	G	301	-	-	-	X
16	CL	M	301	-	-	-	X
16	CL	Q	302	-	-	-	X
16	CL	S	301	-	-	-	X
16	CL	S	302	-	-	-	X
16	CL	S	303	-	-	-	X
16	CL	U	301	-	-	-	X
16	CL	b	302	-	-	-	X
18	MG	H	302	-	-	-	X
19	1PE	H	304	-	-	-	X
19	1PE	I	303	-	-	-	X
19	1PE	K	306	-	-	-	X
19	1PE	L	301	-	-	-	X
19	1PE	W	303	-	-	-	X
19	1PE	Z	301	-	-	-	X
19	1PE	a	304	-	-	-	X
19	1PE	b	305	-	-	-	X
7	6V1	U	47	X	-	-	-

## 2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 51776 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	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
2	B	248	Total	C	N	O	S	0	2	0
			1926	1220	332	363	11			
2	P	248	Total	C	N	O	S	0	2	0
			1909	1206	325	367	11			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	237	Total	C	N	O	S	0	2	0
			1798	1121	320	352	5			
3	Q	239	Total	C	N	O	S	0	0	0
			1820	1136	320	359	5			

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

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	148	6V1	CYS	modified residue	UNP P25786
S	148	6V1	CYS	modified residue	UNP P25786

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

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

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

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

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	47	6V1	CYS	modified residue	UNP P60900
G	161	6V1	CYS	modified residue	UNP P60900
U	47	6V1	CYS	modified residue	UNP P60900
U	161	6V1	CYS	modified residue	UNP P60900

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

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

- 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	3	0
			1613	1028	270	295	20			
9	W	204	Total	C	N	O	S	0	2	0
			1599	1018	267	295	19			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	196	Total	C	N	O	S	0	3	0
			1590	1021	271	288	10			
10	X	196	Total	C	N	O	S	0	2	0
			1572	1012	266	284	10			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	91	6V1	CYS	modified residue	UNP P49721
X	91	6V1	CYS	modified residue	UNP P49721

- 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
			1545	974	269	293	9			
11	Y	201	Total	C	N	O	S	0	3	0
			1580	996	280	294	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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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 EPOXOMICIN (peptide inhibitor).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	c	5	Total	C	N	O	0	0	0
			39	28	4	7			
15	d	5	Total	C	N	O	0	0	0
			39	28	4	7			
15	e	5	Total	C	N	O	0	0	0
			39	28	4	7			
15	f	5	Total	C	N	O	0	0	0
			39	28	4	7			
15	g	5	Total	C	N	O	0	0	0
			39	28	4	7			
15	h	5	Total	C	N	O	0	0	0
			39	28	4	7			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	P	1	Total	Cl	0	0
			1	1		
16	K	4	Total	Cl	0	0
			4	4		
16	B	2	Total	Cl	0	0
			2	2		
16	c	1	Total	Cl	0	0
			1	1		
16	W	1	Total	Cl	0	0
			1	1		
16	N	4	Total	Cl	0	0
			4	4		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	S	3	Total 3	Cl 3	0	0
16	f	1	Total 1	Cl 1	0	0
16	E	4	Total 4	Cl 4	0	0
16	b	4	Total 4	Cl 4	0	0
16	V	1	Total 1	Cl 1	0	0
16	A	4	Total 4	Cl 4	0	0
16	R	2	Total 2	Cl 2	0	0
16	M	3	Total 3	Cl 3	0	0
16	D	1	Total 1	Cl 1	0	0
16	I	1	Total 1	Cl 1	0	0
16	a	3	Total 3	Cl 3	0	0
16	U	1	Total 1	Cl 1	0	0
16	G	2	Total 2	Cl 2	0	0
16	Q	2	Total 2	Cl 2	0	0
16	H	1	Total 1	Cl 1	0	0
16	C	2	Total 2	Cl 2	0	0
16	O	4	Total 4	Cl 4	0	0
16	Y	5	Total 5	Cl 5	0	0
16	F	1	Total 1	Cl 1	0	0

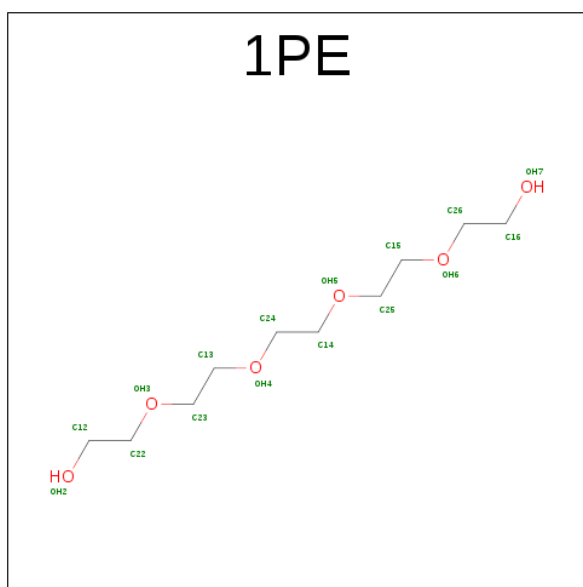
- Molecule 17 is POTASSIUM ION (three-letter code: K) (formula: K).

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

- Molecule 18 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 19 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
19	H	1	Total	C	O	0	0
			16	10	6		
19	I	1	Total	C	O	0	0
			16	10	6		
19	K	1	Total	C	O	0	0
			16	10	6		
19	L	1	Total	C	O	0	0
			16	10	6		
19	N	1	Total	C	O	0	0
			16	10	6		
19	W	1	Total	C	O	0	0
			16	10	6		
19	Z	1	Total	C	O	0	0
			16	10	6		
19	a	1	Total	C	O	0	0
			16	10	6		
19	b	1	Total	C	O	0	0
			16	10	6		

- Molecule 20 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	A	100	Total	O	0	0
			100	100		
20	B	116	Total	O	0	0
			116	116		
20	C	62	Total	O	0	0
			62	62		

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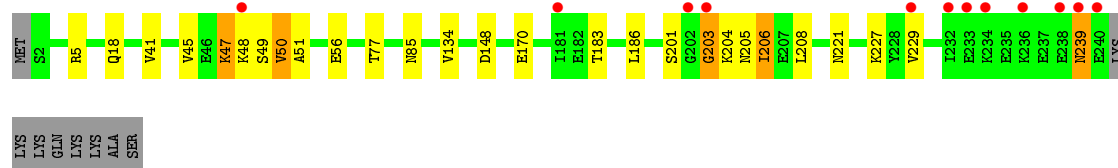
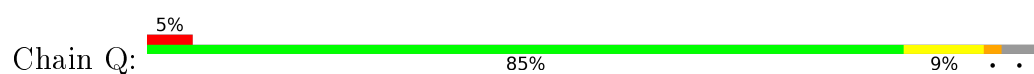
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	D	81	Total 81	O 81	0	0
20	E	127	Total 127	O 127	0	0
20	F	164	Total 164	O 164	0	0
20	G	172	Total 172	O 172	0	0
20	H	144	Total 144	O 144	0	0
20	I	142	Total 142	O 142	0	0
20	J	119	Total 119	O 119	0	0
20	K	95	Total 95	O 95	0	0
20	L	114	Total 114	O 114	0	0
20	M	141	Total 141	O 141	0	0
20	N	143	Total 143	O 143	0	0
20	O	71	Total 71	O 71	0	0
20	P	102	Total 102	O 102	0	0
20	Q	57	Total 57	O 57	0	0
20	R	109	Total 109	O 109	0	0
20	S	101	Total 101	O 101	0	0
20	T	73	Total 73	O 73	0	0
20	U	80	Total 80	O 80	0	0
20	V	104	Total 104	O 104	0	0
20	W	89	Total 89	O 89	0	0
20	X	109	Total 109	O 109	0	0

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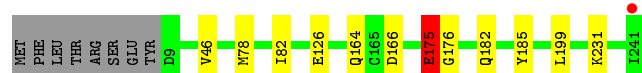
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	Y	135	Total 135	O 135	0	0
20	Z	155	Total 155	O 155	0	0
20	a	154	Total 154	O 154	0	0
20	b	110	Total 110	O 110	0	0
20	c	1	Total 1	O 1	0	0
20	d	1	Total 1	O 1	0	0
20	g	1	Total 1	O 1	0	0
20	h	1	Total 1	O 1	0	0

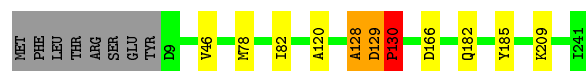




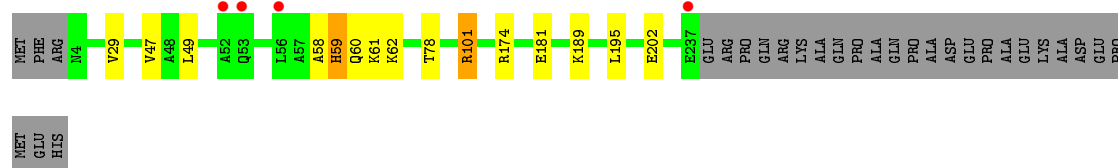
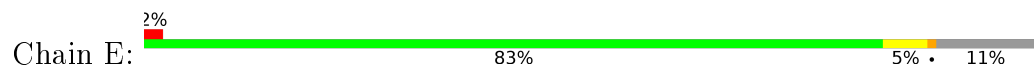
- Molecule 4: Proteasome subunit alpha type-5



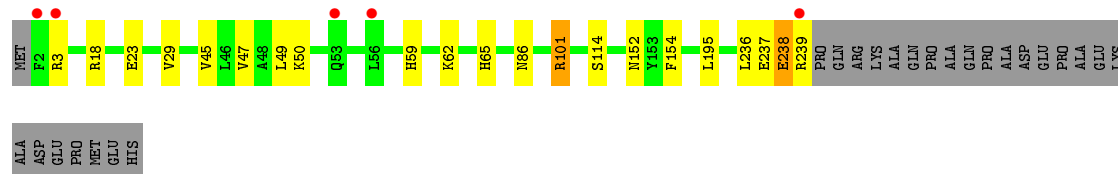
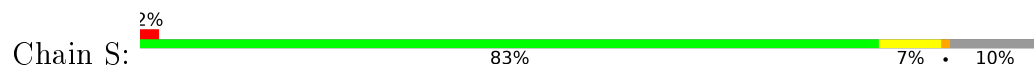
- Molecule 4: Proteasome subunit alpha type-5



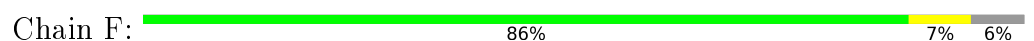
- Molecule 5: Proteasome subunit alpha type-1



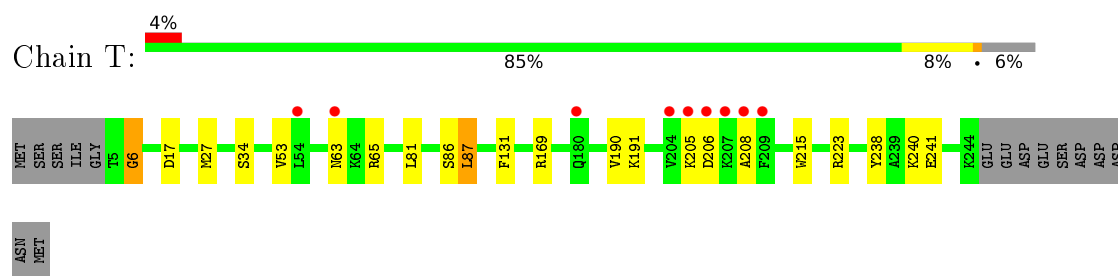
- Molecule 5: Proteasome subunit alpha type-1



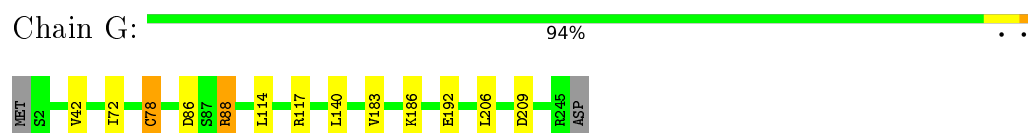
- Molecule 6: Proteasome subunit alpha type-3



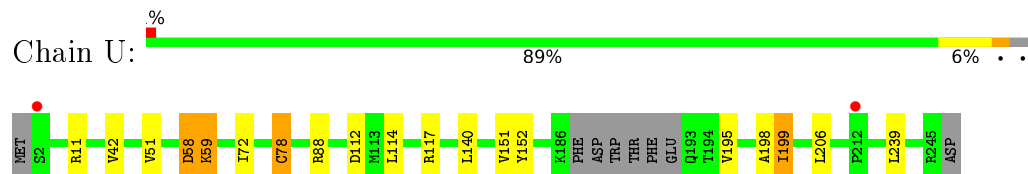
- Molecule 6: Proteasome subunit alpha type-3



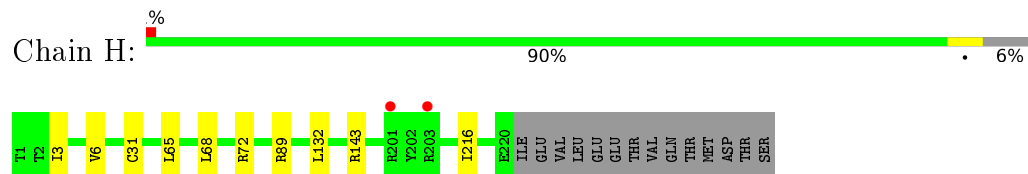
- Molecule 7: Proteasome subunit alpha type-6



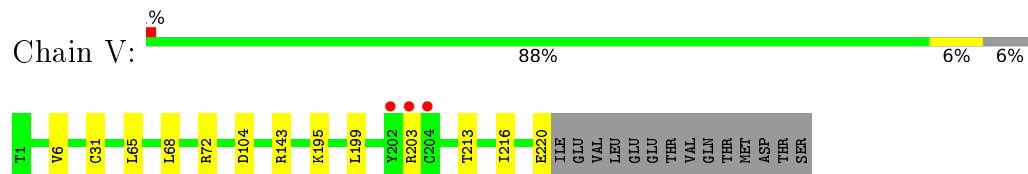
- Molecule 7: Proteasome subunit alpha type-6



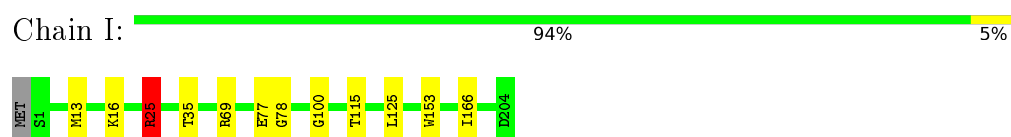
- Molecule 8: Proteasome subunit beta type-7



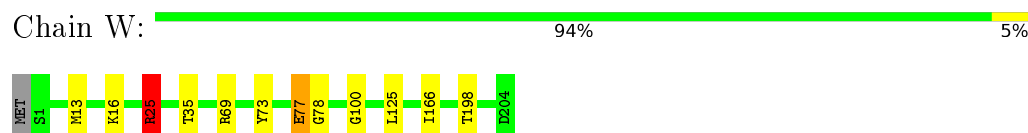
- Molecule 8: Proteasome subunit beta type-7



- Molecule 9: Proteasome subunit beta type-3

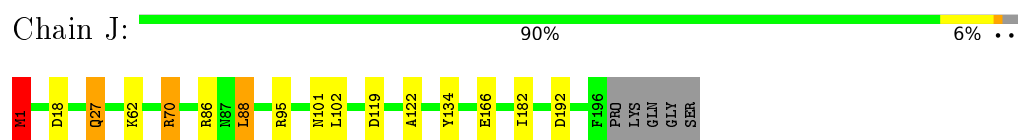


- Molecule 9: Proteasome subunit beta type-3

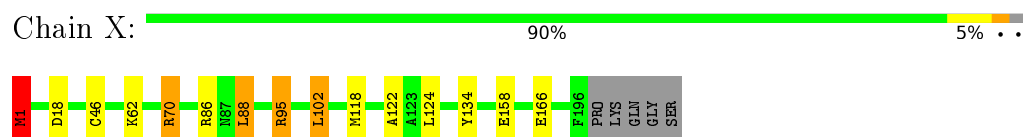




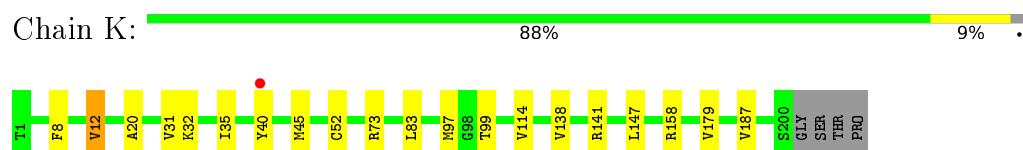
- Molecule 10: Proteasome subunit beta type-2



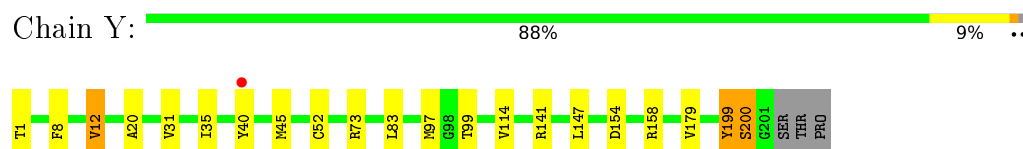
- Molecule 10: Proteasome subunit beta type-2



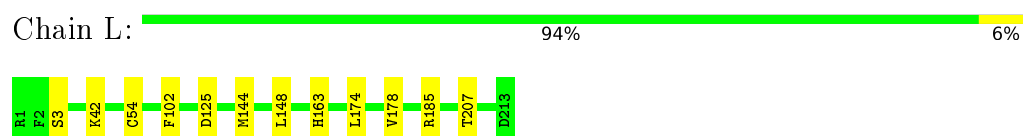
- Molecule 11: Proteasome subunit beta type-5



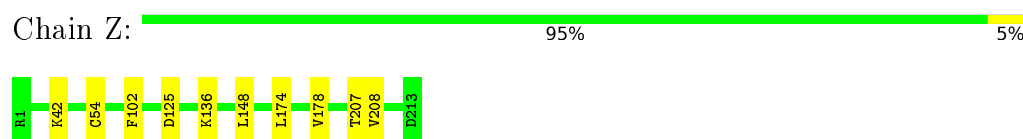
- Molecule 11: Proteasome subunit beta type-5



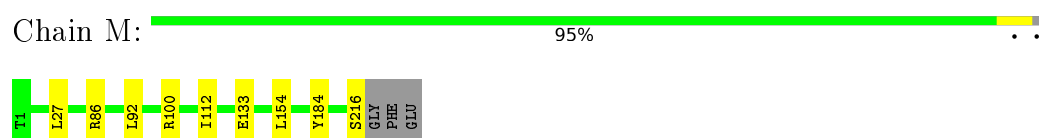
- Molecule 12: Proteasome subunit beta type-1



- Molecule 12: Proteasome subunit beta type-1



- Molecule 13: Proteasome subunit beta type-4



- Molecule 13: Proteasome subunit beta type-4

Chain a:  96% ..



- Molecule 14: Proteasome subunit beta type-6

Chain N:  94% ..




- Molecule 14: Proteasome subunit beta type-6

Chain b:  96% ..



- Molecule 15: EPOXOMICIN (peptide inhibitor)

Chain c:  80% 20%




- Molecule 15: EPOXOMICIN (peptide inhibitor)

Chain d:  60% 20% 20%




- Molecule 15: EPOXOMICIN (peptide inhibitor)

Chain e:  80% 20%



- Molecule 15: EPOXOMICIN (peptide inhibitor)

Chain f:  80% 20%



- Molecule 15: EPOXOMICIN (peptide inhibitor)

Chain g:  60% 40%



- Molecule 15: EPOXOMICIN (peptide inhibitor)



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	113.07Å 202.37Å 314.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	170.23 – 2.41 157.40 – 2.41	Depositor EDS
% Data completeness (in resolution range)	99.5 (170.23-2.41) 99.6 (157.40-2.41)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.24 (at 2.43Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, $R_{free}$	0.179 , 0.229 0.182 , 0.228	Depositor DCC
$R_{free}$ test set	13832 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	52.7	Xtriage
Anisotropy	0.278	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 43.6	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	0.96	EDS
Total number of atoms	51776	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.91% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ACE, CL, K, IML, 6V1, 1PE, 6VO, YCM

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	0.53	0/1833	0.71	0/2489
1	O	0.49	0/1778	0.72	1/2419 (0.0%)
2	B	0.54	0/1962	0.73	2/2649 (0.1%)
2	P	0.53	0/1945	0.74	2/2631 (0.1%)
3	C	0.54	0/1818	0.82	0/2469
3	Q	0.54	0/1834	0.79	0/2490
4	D	0.55	0/1789	0.75	2/2424 (0.1%)
4	R	0.56	0/1780	0.81	2/2408 (0.1%)
5	E	0.54	0/1842	0.75	1/2493 (0.0%)
5	S	0.52	0/1901	0.75	0/2571
6	F	0.55	0/1935	0.75	1/2605 (0.0%)
6	T	0.54	0/1894	0.80	4/2556 (0.2%)
7	G	0.56	0/1909	0.72	2/2579 (0.1%)
7	U	0.51	0/1804	0.73	3/2441 (0.1%)
8	H	0.54	0/1697	0.81	3/2299 (0.1%)
8	V	0.51	1/1655 (0.1%)	0.75	1/2251 (0.0%)
9	I	0.57	0/1648	0.87	6/2219 (0.3%)
9	W	0.57	2/1630 (0.1%)	0.84	5/2197 (0.2%)
10	J	0.53	0/1613	0.77	2/2180 (0.1%)
10	X	0.52	0/1595	0.75	2/2157 (0.1%)
11	K	0.55	0/1576	0.78	0/2131
11	Y	0.58	0/1620	0.83	4/2185 (0.2%)
12	L	0.51	0/1672	0.72	0/2257
12	Z	0.55	0/1675	0.75	0/2257
13	M	0.55	0/1728	0.78	0/2339
13	a	0.54	0/1724	0.77	0/2336
14	N	0.56	0/1548	0.76	1/2095 (0.0%)
14	b	0.52	0/1554	0.72	0/2104
15	c	0.60	0/14	1.73	0/18
15	d	0.45	0/14	1.86	1/18 (5.6%)
15	e	0.79	0/14	1.34	0/18
15	f	0.68	0/14	1.68	0/18

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
15	g	0.78	0/14	1.97	0/18
15	h	0.59	0/14	2.11	1/18 (5.6%)
All	All	0.54	3/49043 (0.0%)	0.77	46/66339 (0.1%)

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	4
3	C	0	1
3	Q	0	2
4	D	0	2
4	R	0	1
7	U	1	0
9	I	0	1
9	W	0	1
10	J	0	2
10	X	0	1
11	Y	0	1
13	a	0	1
15	c	1	0
15	d	2	0
15	e	1	0
15	f	1	0
15	g	2	0
15	h	2	0
All	All	10	17

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	W	77	GLU	CD-OE2	9.94	1.36	1.25
8	V	220	GLU	C-O	5.86	1.34	1.23
9	W	73	TYR	CG-CD1	5.13	1.45	1.39

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	R	120[A]	ALA	C-N-CA	10.29	147.42	121.70
4	R	120[B]	ALA	C-N-CA	10.29	147.42	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	W	16[A]	LYS	C-N-CA	9.36	145.11	121.70
9	W	16[B]	LYS	C-N-CA	9.36	145.11	121.70
6	T	6	GLY	N-CA-C	8.95	135.47	113.10

5 of 10 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	U	47	6V1	C1
15	c	2	IML	CB
15	d	2	IML	CB,CA
15	e	2	IML	CA
15	f	2	IML	CB

5 of 17 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	237	GLU	Peptide
4	D	175[A]	GLU	Peptide
4	D	175[B]	GLU	Peptide
9	I	78	GLY	Peptide
10	J	1[A]	MET	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	7	0
1	O	1741	0	1683	4	0
2	B	1926	0	1924	3	0
2	P	1909	0	1874	8	0
3	C	1798	0	1718	10	0
3	Q	1820	0	1749	12	0
4	D	1762	0	1709	3	0
4	R	1753	0	1726	5	0
5	E	1822	0	1779	7	0
5	S	1875	0	1818	13	0
6	F	1888	0	1882	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	T	1856	0	1816	5	0
7	G	1912	0	1882	4	0
7	U	1815	0	1748	7	0
8	H	1664	0	1678	4	0
8	V	1622	0	1592	2	0
9	I	1613	0	1646	3	0
9	W	1599	0	1621	4	0
10	J	1590	0	1581	9	0
10	X	1572	0	1559	9	0
11	K	1545	0	1495	10	0
11	Y	1580	0	1555	11	0
12	L	1636	0	1625	4	0
12	Z	1642	0	1635	3	0
13	M	1692	0	1670	3	0
13	a	1688	0	1658	0	0
14	N	1519	0	1493	5	0
14	b	1524	0	1493	0	0
15	c	39	0	34	0	0
15	d	39	0	34	0	0
15	e	39	0	34	0	0
15	f	39	0	34	0	0
15	g	39	0	34	0	0
15	h	39	0	34	0	0
16	A	4	0	0	1	0
16	B	2	0	0	2	0
16	C	2	0	0	0	0
16	D	1	0	0	0	0
16	E	4	0	0	0	0
16	F	1	0	0	0	0
16	G	2	0	0	1	0
16	H	1	0	0	0	0
16	I	1	0	0	0	0
16	K	4	0	0	1	0
16	M	3	0	0	0	0
16	N	4	0	0	0	0
16	O	4	0	0	0	0
16	P	1	0	0	0	0
16	Q	2	0	0	0	0
16	R	2	0	0	0	0
16	S	3	0	0	0	0
16	U	1	0	0	0	0
16	V	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	W	1	0	0	0	0
16	Y	5	0	0	0	0
16	a	3	0	0	0	0
16	b	4	0	0	0	0
16	c	1	0	0	0	0
16	f	1	0	0	0	0
17	G	1	0	0	0	0
17	L	1	0	0	0	0
17	N	1	0	0	0	0
17	U	1	0	0	0	0
17	Z	1	0	0	0	0
17	b	1	0	0	0	0
18	H	2	0	0	0	0
18	I	2	0	0	0	0
18	J	1	0	0	0	0
18	K	1	0	0	0	0
18	L	1	0	0	0	0
18	V	1	0	0	0	0
18	W	1	0	0	0	0
18	X	1	0	0	0	0
19	H	16	0	22	0	0
19	I	16	0	22	0	0
19	K	16	0	22	0	0
19	L	16	0	22	0	0
19	N	16	0	22	0	0
19	W	16	0	22	0	0
19	Z	16	0	22	0	0
19	a	16	0	22	0	0
19	b	16	0	22	0	0
20	A	100	0	0	2	0
20	B	116	0	0	0	0
20	C	62	0	0	0	0
20	D	81	0	0	0	0
20	E	127	0	0	1	0
20	F	164	0	0	3	0
20	G	172	0	0	0	0
20	H	144	0	0	0	0
20	I	142	0	0	0	0
20	J	119	0	0	1	0
20	K	95	0	0	0	0
20	L	114	0	0	1	0
20	M	141	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	N	143	0	0	0	0
20	O	71	0	0	1	0
20	P	102	0	0	0	0
20	Q	57	0	0	0	0
20	R	109	0	0	1	0
20	S	101	0	0	3	0
20	T	73	0	0	0	0
20	U	80	0	0	0	0
20	V	104	0	0	1	0
20	W	89	0	0	0	0
20	X	109	0	0	0	0
20	Y	135	0	0	0	0
20	Z	155	0	0	2	0
20	a	154	0	0	0	0
20	b	110	0	0	0	0
20	c	1	0	0	0	0
20	d	1	0	0	0	0
20	g	1	0	0	0	0
20	h	1	0	0	0	0
All	All	51776	0	47772	147	0

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

The worst 5 of 147 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)
6:F:105:ASN:ND2	20:F:401:HOH:O	2.16	0.77
11:K:35:ILE:HD11	11:K:45:MET:SD	2.33	0.69
2:P:12:PHE:H	3:Q:18:GLN:HE22	1.42	0.68
9:I:25[A]:ARG:HG2	9:I:25[A]:ARG:HH11	1.59	0.67
5:E:47:VAL:HG12	5:E:195:LEU:HD22	1.76	0.67

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	231/234 (99%)	220 (95%)	7 (3%)	4 (2%)	11	14
1	O	228/234 (97%)	217 (95%)	6 (3%)	5 (2%)	8	8
2	B	248/261 (95%)	236 (95%)	10 (4%)	2 (1%)	24	33
2	P	248/261 (95%)	233 (94%)	13 (5%)	2 (1%)	24	33
3	C	236/248 (95%)	223 (94%)	7 (3%)	6 (2%)	7	6
3	Q	236/248 (95%)	219 (93%)	10 (4%)	7 (3%)	5	4
4	D	232/241 (96%)	223 (96%)	6 (3%)	3 (1%)	15	20
4	R	232/241 (96%)	223 (96%)	6 (3%)	3 (1%)	15	20
5	E	232/263 (88%)	226 (97%)	5 (2%)	1 (0%)	39	54
5	S	238/263 (90%)	231 (97%)	5 (2%)	2 (1%)	24	33
6	F	241/255 (94%)	238 (99%)	3 (1%)	0	100	100
6	T	239/255 (94%)	232 (97%)	5 (2%)	2 (1%)	24	33
7	G	241/246 (98%)	236 (98%)	5 (2%)	0	100	100
7	U	232/246 (94%)	227 (98%)	3 (1%)	2 (1%)	21	29
8	H	220/234 (94%)	216 (98%)	4 (2%)	0	100	100
8	V	220/234 (94%)	217 (99%)	2 (1%)	1 (0%)	34	47
9	I	205/205 (100%)	201 (98%)	3 (2%)	1 (0%)	34	47
9	W	204/205 (100%)	196 (96%)	7 (3%)	1 (0%)	34	47
10	J	195/201 (97%)	191 (98%)	4 (2%)	0	100	100
10	X	195/201 (97%)	193 (99%)	2 (1%)	0	100	100
11	K	198/204 (97%)	195 (98%)	3 (2%)	0	100	100
11	Y	202/204 (99%)	198 (98%)	3 (2%)	1 (0%)	34	47
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%)	208 (96%)	8 (4%)	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
15	c	1/5 (20%)	1 (100%)	0	0	100	100
15	d	1/5 (20%)	1 (100%)	0	0	100	100
15	e	1/5 (20%)	1 (100%)	0	0	100	100
15	f	1/5 (20%)	1 (100%)	0	0	100	100
15	g	1/5 (20%)	1 (100%)	0	0	100	100
15	h	1/5 (20%)	1 (100%)	0	0	100	100
All	All	6218/6488 (96%)	6030 (97%)	145 (2%)	43 (1%)	26	37

5 of 43 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	52	LYS
1	A	53	SER
3	C	47	LYS
4	D	176	GLY
5	E	59	HIS

### 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	185/191 (97%)	173 (94%)	12 (6%)	21	32
1	O	176/191 (92%)	165 (94%)	11 (6%)	22	34
2	B	200/221 (90%)	193 (96%)	7 (4%)	43	63
2	P	197/221 (89%)	185 (94%)	12 (6%)	23	35
3	C	179/210 (85%)	172 (96%)	7 (4%)	39	58
3	Q	184/210 (88%)	176 (96%)	8 (4%)	35	54
4	D	189/203 (93%)	184 (97%)	5 (3%)	54	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	R	187/203 (92%)	184 (98%)	3 (2%)	70	85
5	E	192/223 (86%)	185 (96%)	7 (4%)	42	62
5	S	197/223 (88%)	192 (98%)	5 (2%)	55	75
6	F	199/212 (94%)	189 (95%)	10 (5%)	30	47
6	T	192/212 (91%)	182 (95%)	10 (5%)	29	45
7	G	202/207 (98%)	195 (96%)	7 (4%)	43	63
7	U	186/207 (90%)	181 (97%)	5 (3%)	52	72
8	H	181/195 (93%)	175 (97%)	6 (3%)	45	65
8	V	172/195 (88%)	163 (95%)	9 (5%)	29	45
9	I	176/174 (101%)	171 (97%)	5 (3%)	51	71
9	W	173/174 (99%)	169 (98%)	4 (2%)	58	77
10	J	166/170 (98%)	155 (93%)	11 (7%)	21	31
10	X	163/170 (96%)	156 (96%)	7 (4%)	35	54
11	K	154/159 (97%)	148 (96%)	6 (4%)	39	58
11	Y	159/159 (100%)	156 (98%)	3 (2%)	65	82
12	L	175/178 (98%)	168 (96%)	7 (4%)	38	57
12	Z	175/178 (98%)	170 (97%)	5 (3%)	50	70
13	M	180/181 (99%)	177 (98%)	3 (2%)	68	84
13	a	178/181 (98%)	173 (97%)	5 (3%)	51	71
14	N	158/159 (99%)	154 (98%)	4 (2%)	55	75
14	b	158/159 (99%)	151 (96%)	7 (4%)	35	52
15	c	2/2 (100%)	1 (50%)	1 (50%)	0	0
15	d	2/2 (100%)	1 (50%)	1 (50%)	0	0
15	e	2/2 (100%)	1 (50%)	1 (50%)	0	0
15	f	2/2 (100%)	1 (50%)	1 (50%)	0	0
15	g	2/2 (100%)	1 (50%)	1 (50%)	0	0
15	h	2/2 (100%)	0	2 (100%)	0	0
All	All	5045/5378 (94%)	4847 (96%)	198 (4%)	40	58

5 of 198 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	L	207	THR

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Mol	Chain	Res	Type
2	P	43	VAL
13	a	154	LEU
13	M	216	SER
1	O	142	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
1	O	101	GLN
2	P	40	ASN
10	X	24	ASN
1	O	118	GLN
2	P	146	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

18 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
3	YCM	C	63	3	7,9,10	1.24	1 (14%)	5,10,12	1.35	0
5	6V1	E	148	5	11,15,16	1.59	3 (27%)	11,20,22	1.84	4 (36%)
7	YCM	G	137	7	7,9,10	1.71	1 (14%)	5,10,12	1.31	0
7	6V1	G	161	7	11,15,16	1.37	3 (27%)	11,20,22	2.71	4 (36%)
7	6V1	G	47	7	11,15,16	1.63	3 (27%)	11,20,22	3.32	4 (36%)
10	6V1	J	91	10	11,15,16	1.55	2 (18%)	11,20,22	3.51	7 (63%)
3	YCM	Q	63	3	7,9,10	1.38	1 (14%)	5,10,12	2.53	3 (60%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	6V1	S	148	5	11,15,16	1.37	2 (18%)	11,20,22	1.75	2 (18%)
7	YCM	U	137	7	7,9,10	1.18	1 (14%)	5,10,12	0.96	1 (20%)
7	6V1	U	161	7	11,15,16	1.39	3 (27%)	11,20,22	2.65	6 (54%)
7	6V1	U	47	7	11,15,16	1.30	2 (18%)	11,20,22	3.16	4 (36%)
10	6V1	X	91	10	11,15,16	1.36	2 (18%)	11,20,22	3.51	7 (63%)
15	IML	c	2	15	7,8,9	1.00	1 (14%)	7,9,11	1.52	2 (28%)
15	IML	d	2	15	7,8,9	1.07	1 (14%)	7,9,11	2.31	3 (42%)
15	IML	e	2	15	7,8,9	0.74	0	7,9,11	1.15	1 (14%)
15	IML	f	2	15	7,8,9	0.67	0	7,9,11	1.61	2 (28%)
15	IML	g	2	15	7,8,9	1.19	1 (14%)	7,9,11	2.41	3 (42%)
15	IML	h	2	15	7,8,9	0.42	0	7,9,11	1.89	2 (28%)

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
3	YCM	C	63	3	-	0/6/8/10	0/0/0/0
5	6V1	E	148	5	-	0/6/25/27	0/1/1/1
7	YCM	G	137	7	-	0/6/8/10	0/0/0/0
7	6V1	G	161	7	-	0/6/25/27	0/1/1/1
7	6V1	G	47	7	-	0/6/25/27	0/1/1/1
10	6V1	J	91	10	-	0/6/25/27	0/1/1/1
3	YCM	Q	63	3	-	0/6/8/10	0/0/0/0
5	6V1	S	148	5	-	0/6/25/27	0/1/1/1
7	YCM	U	137	7	-	0/6/8/10	0/0/0/0
7	6V1	U	161	7	-	0/6/25/27	0/1/1/1
7	6V1	U	47	7	1/1/5/6	0/6/25/27	0/1/1/1
10	6V1	X	91	10	-	0/6/25/27	0/1/1/1
15	IML	c	2	15	1/1/2/4	0/7/10/12	0/0/0/0
15	IML	d	2	15	2/2/2/4	0/7/10/12	0/0/0/0
15	IML	e	2	15	1/1/2/4	0/7/10/12	0/0/0/0
15	IML	f	2	15	1/1/2/4	0/7/10/12	0/0/0/0
15	IML	g	2	15	2/2/2/4	0/7/10/12	0/0/0/0
15	IML	h	2	15	2/2/2/4	0/7/10/12	0/0/0/0

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	137	YCM	CB-SG	-3.67	1.74	1.81
5	E	148	6V1	C1-SG	-3.63	1.78	1.83
10	J	91	6V1	C1-SG	-3.58	1.78	1.83
7	G	47	6V1	C4-N3	-3.39	1.32	1.38
7	G	47	6V1	C2-N3	-3.20	1.34	1.38

The worst 5 of 55 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	U	47	6V1	C5-C1-C2	-4.65	100.44	103.98
7	U	161	6V1	O8-C4-C5	-3.80	122.29	127.38
7	G	161	6V1	O8-C4-C5	-3.74	122.37	127.38
10	X	91	6V1	O7-C2-C1	-3.70	118.50	125.18
10	J	91	6V1	O8-C4-C5	-3.66	122.48	127.38

5 of 10 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
15	h	2	IML	CB
15	h	2	IML	CA
15	e	2	IML	CA
15	c	2	IML	CB
7	U	47	6V1	C1

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 83 ligands modelled in this entry, 74 are monoatomic - leaving 9 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected



value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
19	1PE	H	304	-	15,15,15	0.59	0	14,14,14	0.52	0
19	1PE	I	303	-	15,15,15	0.59	0	14,14,14	0.89	1 (7%)
19	1PE	K	306	-	15,15,15	0.58	0	14,14,14	0.62	0
19	1PE	L	301	-	15,15,15	0.57	0	14,14,14	0.34	0
19	1PE	N	305	-	15,15,15	0.54	0	14,14,14	0.33	0
19	1PE	W	303	-	15,15,15	0.65	0	14,14,14	0.49	0
19	1PE	Z	301	-	15,15,15	0.58	0	14,14,14	0.42	0
19	1PE	a	304	-	15,15,15	0.58	0	14,14,14	0.25	0
19	1PE	b	305	-	15,15,15	0.62	0	14,14,14	0.48	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
19	1PE	H	304	-	-	0/13/13/13	0/0/0/0
19	1PE	I	303	-	-	0/13/13/13	0/0/0/0
19	1PE	K	306	-	-	0/13/13/13	0/0/0/0
19	1PE	L	301	-	-	0/13/13/13	0/0/0/0
19	1PE	N	305	-	-	0/13/13/13	0/0/0/0
19	1PE	W	303	-	-	0/13/13/13	0/0/0/0
19	1PE	Z	301	-	-	0/13/13/13	0/0/0/0
19	1PE	a	304	-	-	0/13/13/13	0/0/0/0
19	1PE	b	305	-	-	0/13/13/13	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
19	I	303	1PE	C25-OH5-C14	2.20	122.72	113.31

There are no chirality outliers.

There are no torsion outliers.

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%)	-0.41	0 <b>100</b> <b>100</b>	41, 61, 99, 113	0
1	O	230/234 (98%)	-0.07	4 (1%) 73 72	56, 83, 125, 146	0
2	B	248/261 (95%)	-0.44	0 <b>100</b> <b>100</b>	48, 67, 117, 159	0
2	P	248/261 (95%)	-0.19	7 (2%) 56 55	54, 75, 126, 169	0
3	C	236/248 (95%)	-0.23	1 (0%) <b>93</b> <b>93</b>	47, 79, 125, 152	0
3	Q	238/248 (95%)	-0.01	12 (5%) 32 32	49, 80, 144, 184	0
4	D	233/241 (96%)	-0.24	1 (0%) <b>93</b> <b>93</b>	50, 72, 105, 135	0
4	R	233/241 (96%)	-0.37	0 <b>100</b> <b>100</b>	44, 59, 94, 124	0
5	E	233/263 (88%)	-0.28	4 (1%) 73 72	39, 56, 104, 129	0
5	S	237/263 (90%)	-0.16	5 (2%) 67 66	49, 65, 109, 124	0
6	F	239/255 (93%)	-0.33	0 <b>100</b> <b>100</b>	37, 48, 72, 93	0
6	T	240/255 (94%)	0.03	9 (3%) 44 44	53, 76, 112, 144	0
7	G	241/246 (97%)	-0.38	0 <b>100</b> <b>100</b>	39, 54, 93, 131	0
7	U	235/246 (95%)	-0.11	2 (0%) 85 85	60, 85, 119, 162	0
8	H	220/234 (94%)	-0.43	2 (0%) 85 85	38, 51, 85, 126	0
8	V	220/234 (94%)	-0.35	3 (1%) 78 77	49, 65, 100, 125	0
9	I	204/205 (99%)	-0.50	0 <b>100</b> <b>100</b>	40, 51, 76, 89	0
9	W	204/205 (99%)	-0.29	0 <b>100</b> <b>100</b>	47, 63, 93, 102	0
10	J	195/201 (97%)	-0.47	0 <b>100</b> <b>100</b>	43, 57, 78, 94	0
10	X	195/201 (97%)	-0.45	0 <b>100</b> <b>100</b>	42, 57, 74, 92	0
11	K	200/204 (98%)	-0.43	1 (0%) 91 91	44, 60, 87, 100	0
11	Y	201/204 (98%)	-0.47	1 (0%) 91 91	39, 51, 77, 95	0
12	L	213/213 (100%)	-0.39	0 <b>100</b> <b>100</b>	43, 60, 86, 108	0
12	Z	213/213 (100%)	-0.44	0 <b>100</b> <b>100</b>	40, 52, 79, 96	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	M	216/219 (98%)	-0.41	0 100 100	38, 53, 81, 112	0
13	a	216/219 (98%)	-0.44	1 (0%) 91 91	41, 56, 78, 101	0
14	N	202/205 (98%)	-0.46	0 100 100	38, 49, 77, 109	0
14	b	203/205 (99%)	-0.46	0 100 100	44, 59, 89, 127	0
15	c	2/5 (40%)	0.20	0 100 100	49, 49, 49, 55	0
15	d	2/5 (40%)	-0.11	0 100 100	51, 51, 51, 56	0
15	e	2/5 (40%)	-0.61	0 100 100	51, 51, 51, 51	0
15	f	2/5 (40%)	-0.14	0 100 100	62, 62, 62, 63	0
15	g	2/5 (40%)	-0.21	0 100 100	42, 42, 42, 49	0
15	h	2/5 (40%)	-0.16	0 100 100	59, 59, 59, 64	0
All	All	6235/6488 (96%)	-0.32	53 (0%) 85 85	37, 62, 108, 184	0

The worst 5 of 53 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	Q	234	LYS	9.4
3	Q	232	ILE	7.0
6	T	208	ALA	7.0
2	P	204	SER	6.9
1	O	232	ILE	6.4

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
15	IML	h	2	9/10	0.94	0.12	-	67,68,75,76	0
3	YCM	Q	63	10/11	0.91	0.14	-	67,70,76,77	0
5	6V1	S	148	15/16	0.91	0.19	-	56,86,92,92	0
3	YCM	C	63	10/11	0.93	0.09	-	69,74,80,82	0
15	IML	e	2	9/10	0.95	0.12	-	58,62,68,69	0
7	6V1	G	161	15/16	0.97	0.12	-	47,71,80,84	0
15	IML	c	2	9/10	0.95	0.24	-	52,59,59,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
7	6V1	U	47	15/16	0.87	0.33	-	103,127,131,132	0
15	IML	d	2	9/10	0.91	0.18	-	54,56,59,60	0
15	IML	g	2	9/10	0.91	0.17	-	55,57,60,64	0
5	6V1	E	148	15/16	0.95	0.15	-	44,70,77,81	0
7	YCM	U	137	10/11	0.89	0.15	-	75,84,96,96	0
10	6V1	X	91	15/16	0.93	0.16	-	55,73,77,77	0
7	6V1	U	161	15/16	0.95	0.09	-	78,92,98,101	0
7	6V1	G	47	15/16	0.94	0.17	-	54,68,71,72	0
10	6V1	J	91	15/16	0.95	0.17	-	50,71,74,78	0
15	IML	f	2	9/10	0.96	0.23	-	64,71,73,74	0
7	YCM	G	137	10/11	0.93	0.15	-	48,56,70,71	0

### 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
19	1PE	H	304	16/16	0.83	0.30	11.49	85,100,110,110	0
16	CL	S	301	1/1	0.90	0.40	8.95	95,95,95,95	0
16	CL	b	302	1/1	0.93	0.24	7.38	91,91,91,91	0
16	CL	G	301	1/1	0.98	0.26	7.35	65,65,65,65	0
19	1PE	a	304	16/16	0.86	0.23	5.81	82,88,121,123	0
16	CL	M	301	1/1	0.99	0.18	5.60	86,86,86,86	0
19	1PE	L	301	16/16	0.79	0.24	5.32	95,101,126,127	0
16	CL	D	301	1/1	0.91	0.37	5.31	90,90,90,90	0
16	CL	Q	302	1/1	0.93	0.37	4.91	89,89,89,89	0
19	1PE	I	303	16/16	0.84	0.18	3.22	68,81,97,102	0
18	MG	H	302	1/1	0.98	0.18	2.90	63,63,63,63	0
19	1PE	b	305	16/16	0.89	0.19	2.88	67,72,100,102	0
16	CL	E	301	1/1	0.95	0.17	2.73	85,85,85,85	0
19	1PE	Z	301	16/16	0.82	0.17	2.62	74,89,98,101	0
16	CL	S	303	1/1	0.96	0.19	2.57	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
19	1PE	K	306	16/16	0.88	0.16	2.41	75,87,95,97	0
16	CL	U	301	1/1	0.92	0.23	2.36	79,79,79,79	0
16	CL	S	302	1/1	0.82	0.24	2.21	95,95,95,95	0
19	1PE	W	303	16/16	0.87	0.16	2.05	78,85,94,95	0
16	CL	N	303	1/1	0.94	0.16	2.00	87,87,87,87	0
16	CL	N	304	1/1	0.94	0.16	1.68	72,72,72,72	0
16	CL	B	302	1/1	0.93	0.17	1.32	80,80,80,80	0
16	CL	F	301	1/1	0.99	0.17	0.34	79,79,79,79	0
16	CL	A	304	1/1	0.95	0.13	0.18	77,77,77,77	0
16	CL	E	304	1/1	0.96	0.12	-0.28	81,81,81,81	0
19	1PE	N	305	16/16	0.95	0.13	-0.44	55,61,82,83	0
16	CL	b	303	1/1	0.95	0.13	-0.47	82,82,82,82	0
16	CL	C	301	1/1	0.88	0.13	-0.81	82,82,82,82	0
16	CL	O	301	1/1	0.97	0.10	-0.87	80,80,80,80	0
17	K	Z	302	1/1	0.88	0.10	-1.33	63,63,63,63	0
16	CL	Y	303	1/1	0.95	0.10	-1.35	77,77,77,77	0
17	K	L	302	1/1	0.88	0.09	-1.63	78,78,78,78	0
18	MG	K	301	1/1	0.98	0.09	-1.64	52,52,52,52	0
18	MG	I	301	1/1	0.97	0.07	-1.86	60,60,60,60	0
16	CL	Y	304	1/1	0.96	0.09	-1.90	84,84,84,84	0
18	MG	I	304	1/1	0.97	0.08	-2.00	47,47,47,47	0
16	CL	K	303	1/1	0.87	0.06	-2.50	84,84,84,84	0
17	K	G	303	1/1	0.97	0.09	-2.51	56,56,56,56	0
16	CL	a	301	1/1	0.96	0.06	-2.57	88,88,88,88	0
16	CL	A	301	1/1	0.95	0.08	-2.60	64,64,64,64	0
17	K	N	306	1/1	0.90	0.08	-2.63	65,65,65,65	0
17	K	b	306	1/1	0.93	0.06	-2.65	73,73,73,73	0
16	CL	N	301	1/1	0.98	0.10	-2.74	47,47,47,47	0
18	MG	W	301	1/1	0.92	0.08	-2.95	56,56,56,56	0
18	MG	L	303	1/1	0.98	0.08	-3.05	55,55,55,55	0
16	CL	G	302	1/1	0.95	0.06	-3.25	79,79,79,79	0
17	K	U	302	1/1	0.96	0.07	-3.32	72,72,72,72	0
16	CL	b	304	1/1	0.98	0.05	-3.38	55,55,55,55	0
16	CL	M	303	1/1	0.97	0.09	-	72,72,72,72	0
18	MG	X	301	1/1	0.99	0.04	-	54,54,54,54	0
16	CL	K	305	1/1	0.95	0.18	-	80,80,80,80	0
16	CL	O	303	1/1	0.92	0.15	-	101,101,101,101	0
16	CL	Q	301	1/1	0.98	0.11	-	97,97,97,97	0
16	CL	Y	305	1/1	0.95	0.43	-	90,90,90,90	0
16	CL	W	302	1/1	0.98	0.06	-	70,70,70,70	0
16	CL	b	301	1/1	0.97	0.07	-	62,62,62,62	0
16	CL	B	301	1/1	0.98	0.07	-	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
16	CL	M	302	1/1	0.98	0.07	-	59,59,59,59	0
16	CL	c	101	1/1	0.96	0.11	-	63,63,63,63	0
16	CL	A	302	1/1	0.96	0.06	-	80,80,80,80	0
16	CL	R	302	1/1	0.94	0.44	-	81,81,81,81	0
16	CL	C	302	1/1	0.89	0.22	-	86,86,86,86	0
16	CL	a	303	1/1	0.90	0.12	-	84,84,84,84	0
16	CL	E	302	1/1	0.96	0.13	-	79,79,79,79	0
18	MG	J	301	1/1	0.93	0.04	-	66,66,66,66	0
16	CL	P	301	1/1	0.96	0.09	-	67,67,67,67	0
16	CL	R	301	1/1	0.93	0.16	-	84,84,84,84	0
16	CL	E	303	1/1	0.97	0.26	-	91,91,91,91	0
16	CL	N	302	1/1	0.97	0.07	-	53,53,53,53	0
18	MG	H	301	1/1	0.97	0.05	-	64,64,64,64	0
16	CL	K	304	1/1	0.91	0.17	-	89,89,89,89	0
16	CL	V	302	1/1	0.89	0.13	-	75,75,75,75	0
16	CL	O	302	1/1	0.87	0.15	-	79,79,79,79	0
16	CL	H	303	1/1	0.98	0.11	-	70,70,70,70	0
16	CL	A	303	1/1	0.94	0.08	-	72,72,72,72	0
16	CL	I	302	1/1	0.94	0.07	-	64,64,64,64	0
16	CL	O	304	1/1	0.94	0.27	-	91,91,91,91	0
16	CL	K	302	1/1	0.99	0.07	-	54,54,54,54	0
16	CL	Y	301	1/1	0.99	0.07	-	49,49,49,49	0
16	CL	f	101	1/1	0.98	0.07	-	64,64,64,64	0
16	CL	Y	302	1/1	0.93	0.29	-	89,89,89,89	0
16	CL	a	302	1/1	0.96	0.07	-	64,64,64,64	0
18	MG	V	301	1/1	0.98	0.04	-	72,72,72,72	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.