



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 06:03 PM UTC

PDB ID : 5LEY / pdb_00005ley
Title : Human 20S proteasome complex with Oprozomib at 1.9 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 : 1.90 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

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>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

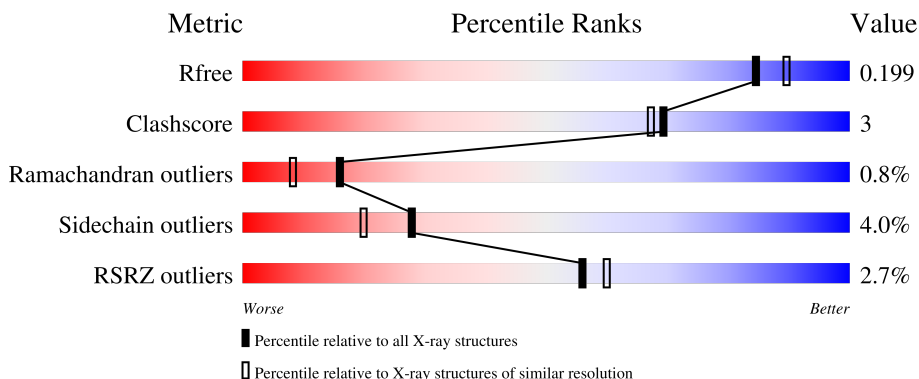
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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 ≥ 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	<p>3% 85% 11% . .</p>
1	O	234	<p>4% 89% 6% . .</p>
2	B	261	<p>3% 85% 9% . 5%</p>
2	P	261	<p>4% 82% 11% . 5%</p>
3	C	248	<p>5% 80% 12% . .</p>

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Mol	Chain	Length	Quality of chain
3	Q	248	11% 78% 16% . .
4	D	241	3% 87% 8% . .
4	R	241	3% 85% 10% . . .
5	E	263	3% 78% 10% . 11%
5	S	263	3% 77% 11% . 10%
6	F	255	2% 81% 11% . 6%
6	T	255	5% 78% 13% . 6%
7	G	246	2% 89% 8% . .
7	U	246	4% 82% 12% . .
8	H	234	% 82% 10% . 6%
8	V	234	4% 85% 7% . 6%
9	I	205	91% 7%
9	W	205	93% 5%
10	J	201	2% 78% 17% . .
10	X	201	87% 8% . . .
11	K	204	87% 10% . .
11	Y	204	% 85% 11% . .
12	L	213	91% 8%
12	Z	213	90% 9%
13	M	219	89% 9%
13	a	219	% 87% 11% . .
14	N	205	2% 92% 5%
14	b	205	2% 90% 8% . .
15	c	4	50% 50%
15	d	4	50% 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	YCM	U	137	-	-	X	-
7	6V1	U	47	X	-	-	-

2 Entry composition [i](#)

There are 20 unique types of molecules in this entry. The entry contains 51947 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	240	Total	C	N	O	S	0	0	0
			1825	1139	321	360	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	236	Total 1853	C 1160	N 335	O 347	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
			1545	974	269	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			

- Molecule 16 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	4	Total 4	Cl 4	0	0
16	B	2	Total 2	Cl 2	0	0
16	C	2	Total 2	Cl 2	0	0
16	D	2	Total 2	Cl 2	0	0
16	E	3	Total 3	Cl 3	0	0
16	F	1	Total 1	Cl 1	0	0
16	G	2	Total 2	Cl 2	0	0
16	H	2	Total 2	Cl 2	0	0
16	I	1	Total 1	Cl 1	0	0
16	K	4	Total 4	Cl 4	0	0
16	M	4	Total 4	Cl 4	0	0
16	N	3	Total 3	Cl 3	0	0
16	O	4	Total 4	Cl 4	0	0
16	P	1	Total 1	Cl 1	0	0
16	Q	2	Total 2	Cl 2	0	0
16	R	2	Total 2	Cl 2	0	0
16	S	3	Total 3	Cl 3	0	0
16	U	1	Total 1	Cl 1	0	0
16	V	2	Total 2	Cl 2	0	0
16	W	1	Total 1	Cl 1	0	0
16	Y	5	Total 5	Cl 5	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	a	3	Total Cl 3 3	0	0
16	b	4	Total Cl 4 4	0	0

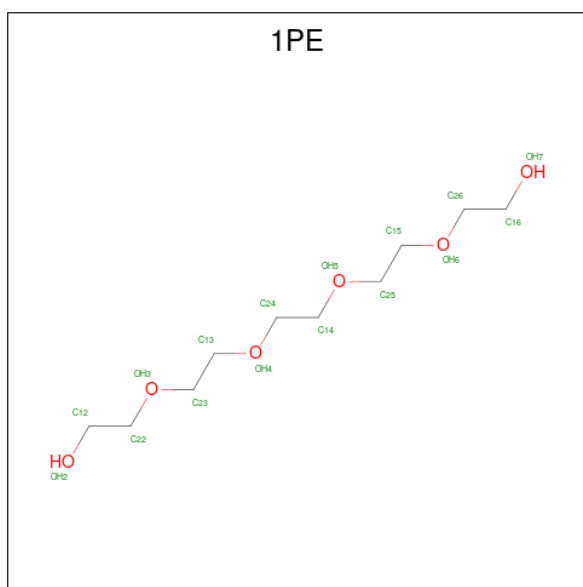
- Molecule 17 is POTASSIUM ION (CCD ID: K) (formula: K).

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

- Molecule 18 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 19 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: C₁₀H₂₂O₆).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	H	1	Total	C O	0	0
			16	10 6		
19	H	1	Total	C O	0	0
			16	10 6		
19	I	1	Total	C O	0	0
			16	10 6		
19	I	1	Total	C O	0	0
			16	10 6		
19	L	1	Total	C O	0	0
			16	10 6		
19	M	1	Total	C O	0	0
			16	10 6		
19	V	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		

- Molecule 20 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	A	109	Total	O	0	0
			109	109		
20	B	120	Total	O	0	0
			120	120		
20	C	76	Total	O	0	0
			76	76		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	D	93	Total O 93 93	0	0
20	E	137	Total O 137 137	0	0
20	F	180	Total O 180 180	0	0
20	G	187	Total O 187 187	0	0
20	H	157	Total O 157 157	0	0
20	I	155	Total O 155 155	0	0
20	J	133	Total O 133 133	0	0
20	K	98	Total O 98 98	0	0
20	L	124	Total O 124 124	0	0
20	M	148	Total O 148 148	0	0
20	N	168	Total O 168 168	0	0
20	O	89	Total O 89 89	0	0
20	P	117	Total O 117 117	0	0
20	Q	74	Total O 74 74	0	0
20	R	122	Total O 122 122	0	0
20	S	118	Total O 118 118	0	0
20	T	92	Total O 92 92	0	0
20	U	102	Total O 102 102	0	0
20	V	112	Total O 112 112	0	0
20	W	111	Total O 111 111	0	0
20	X	124	Total O 124 124	0	0

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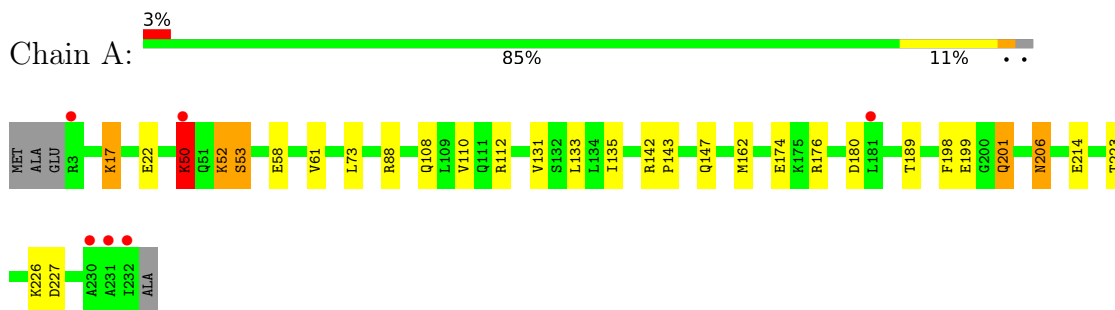
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	Y	137	Total 137	O 137	0	0
20	Z	164	Total 164	O 164	0	0
20	a	167	Total 167	O 167	0	0
20	b	126	Total 126	O 126	0	0
20	c	1	Total 1	O 1	0	0
20	d	1	Total 1	O 1	0	0

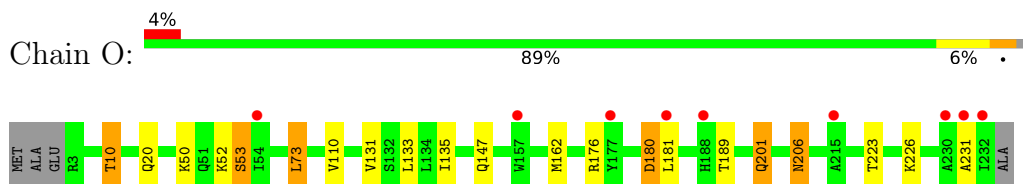
3 Residue-property plots [i](#)

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.

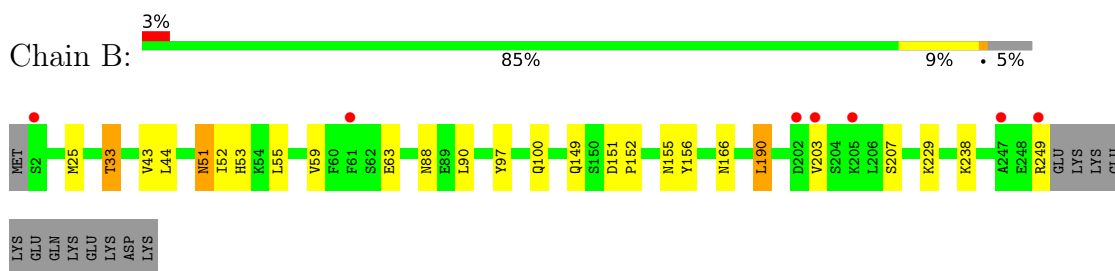
- Molecule 1: Proteasome subunit alpha type-2



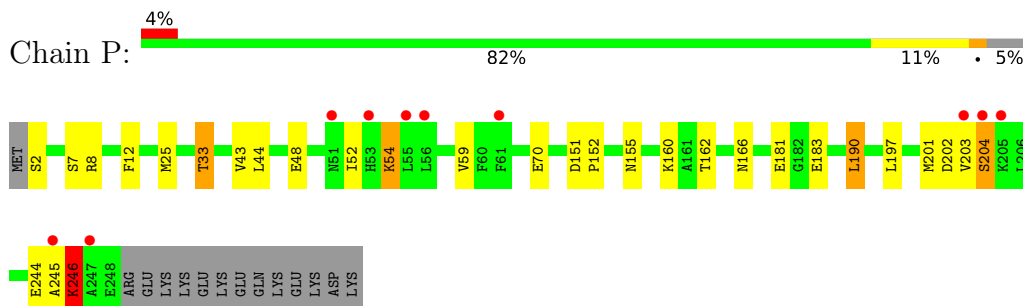
- Molecule 1: Proteasome subunit alpha type-2



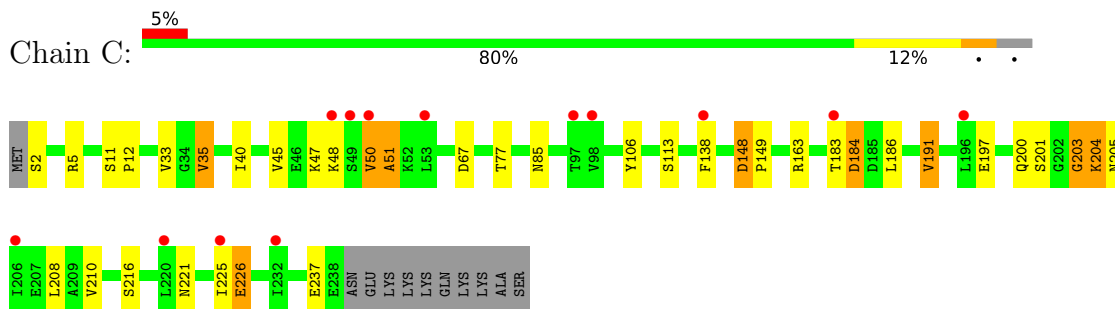
- Molecule 2: Proteasome subunit alpha type-4



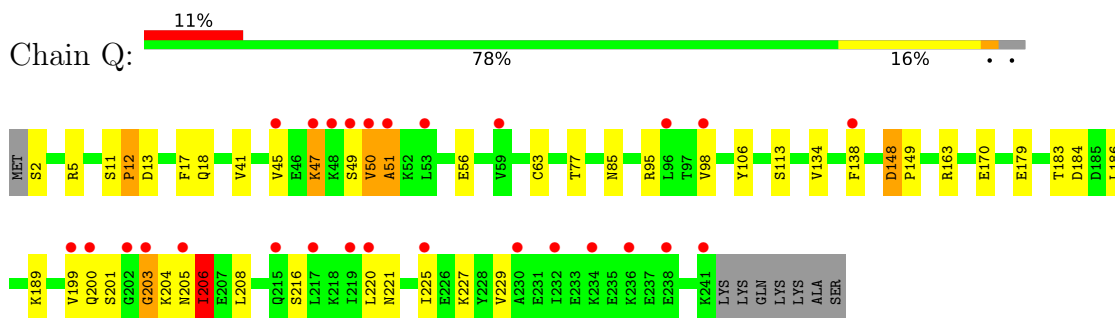
- Molecule 2: Proteasome subunit alpha type-4



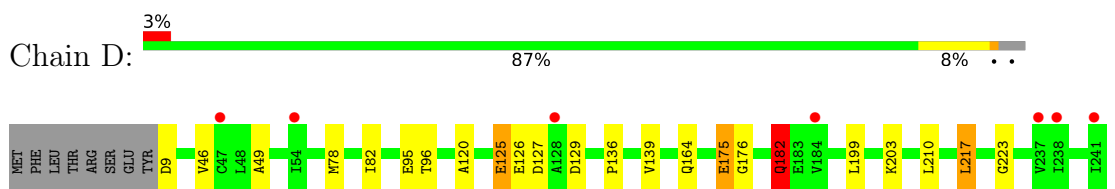
• Molecule 3: Proteasome subunit alpha type-7



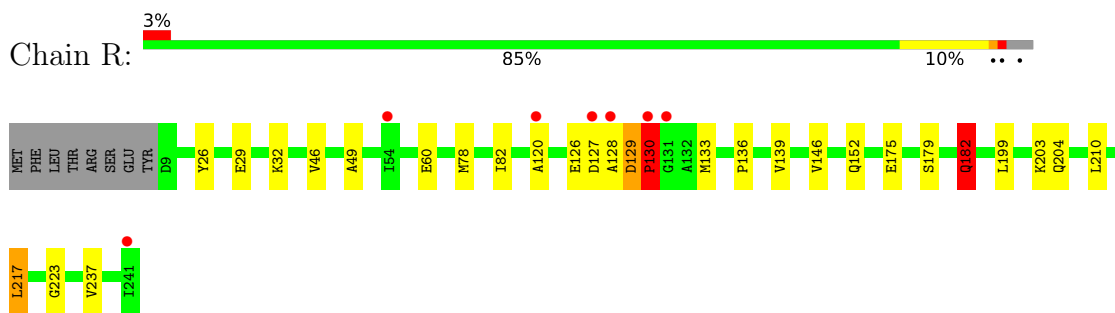
• Molecule 3: Proteasome subunit alpha type-7



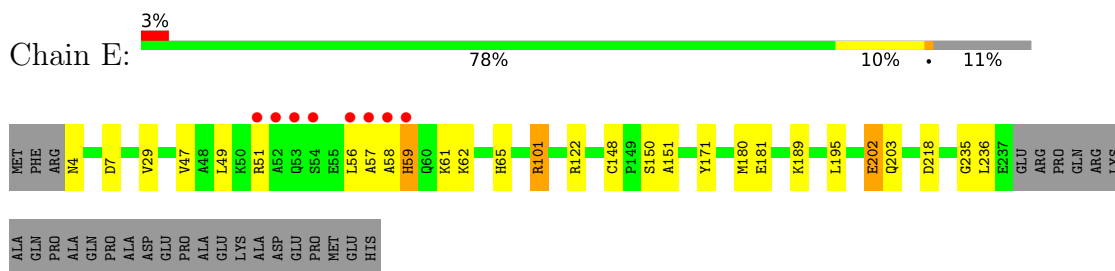
• Molecule 4: Proteasome subunit alpha type-5



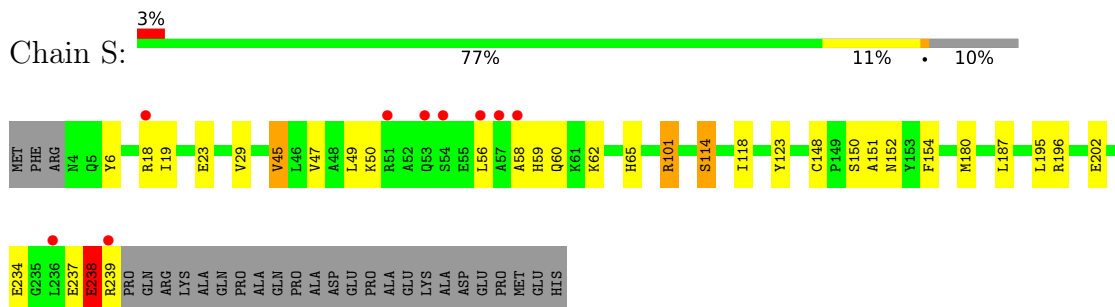
• Molecule 4: Proteasome subunit alpha type-5



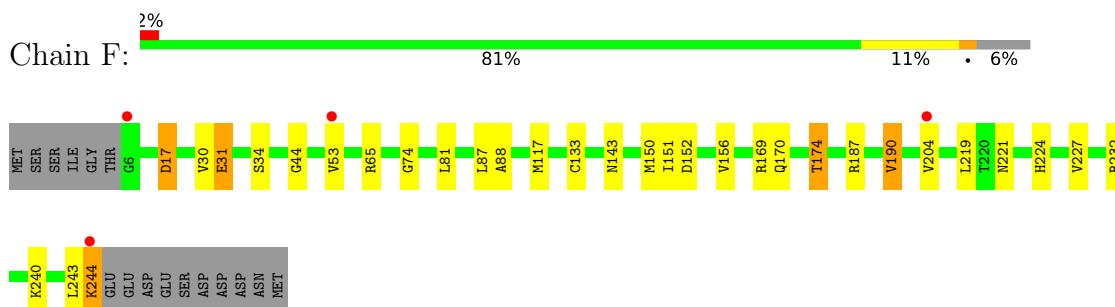
• Molecule 5: Proteasome subunit alpha type-1



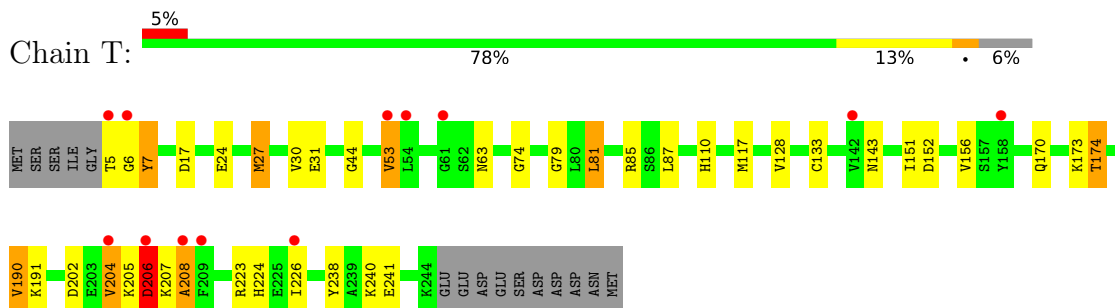
- Molecule 5: Proteasome subunit alpha type-1



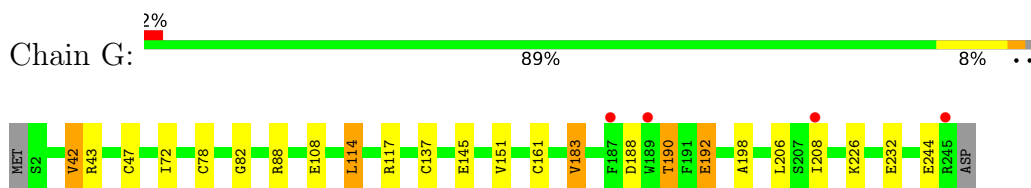
- Molecule 6: Proteasome subunit alpha type-3



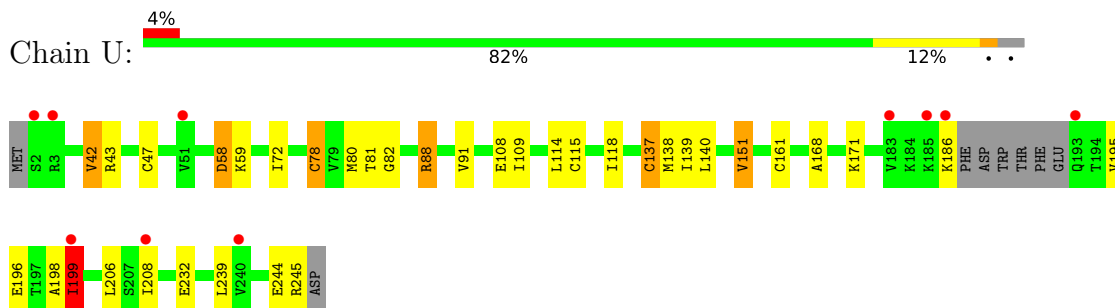
- Molecule 6: Proteasome subunit alpha type-3



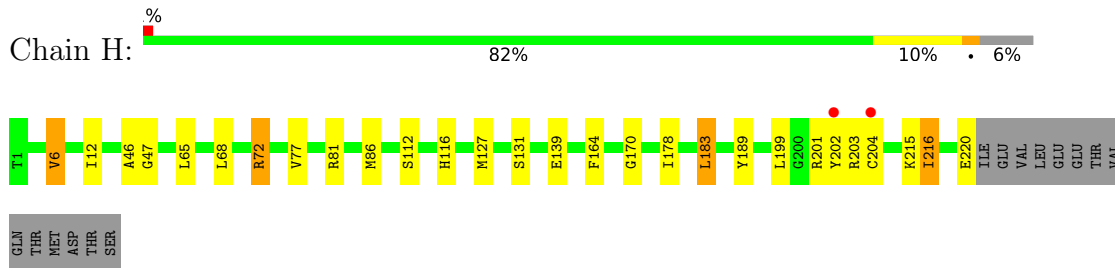
- Molecule 7: Proteasome subunit alpha type-6



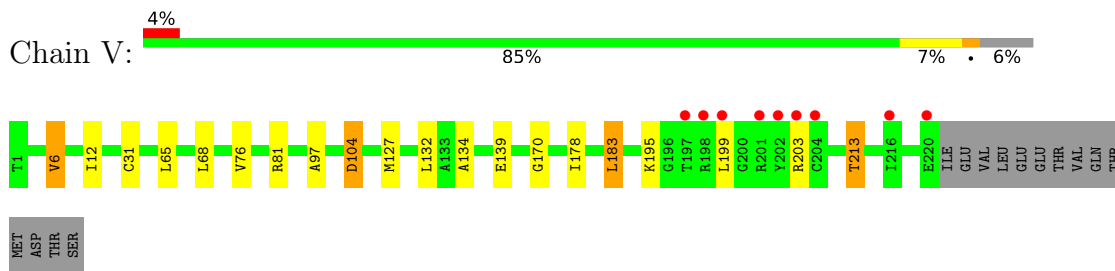
- Molecule 7: Proteasome subunit alpha type-6



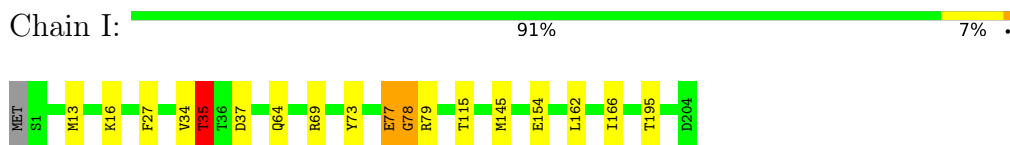
- Molecule 8: Proteasome subunit beta type-7



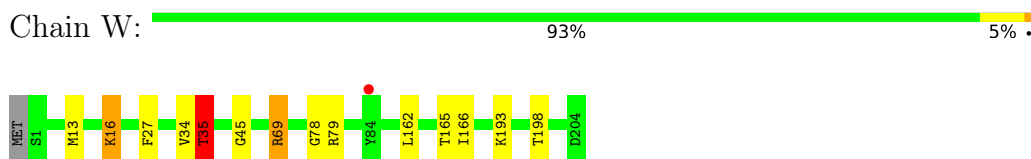
- Molecule 8: Proteasome subunit beta type-7



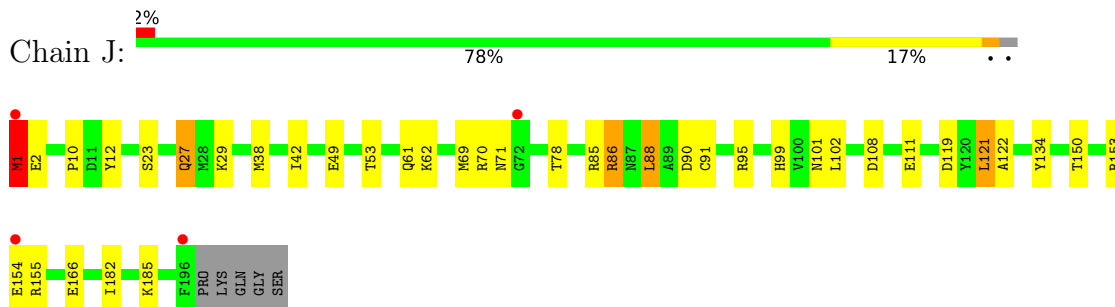
- Molecule 9: Proteasome subunit beta type-3



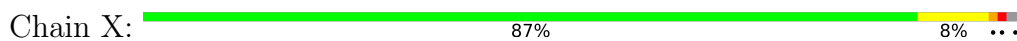
- Molecule 9: Proteasome subunit beta type-3



- Molecule 10: Proteasome subunit beta type-2



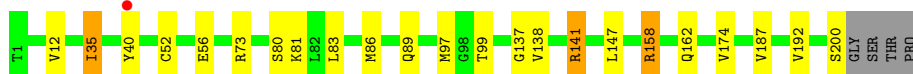
- Molecule 10: Proteasome subunit beta type-2





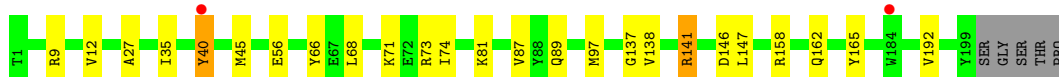
- Molecule 11: Proteasome subunit beta type-5

Chain K: 87% 10% ..



- Molecule 11: Proteasome subunit beta type-5

Chain Y: 85% 11% ..



- Molecule 12: Proteasome subunit beta type-1

Chain L: 91% 8% .



- Molecule 12: Proteasome subunit beta type-1

Chain Z: 90% 9% .



- Molecule 13: Proteasome subunit beta type-4

Chain M: 89% 9% .

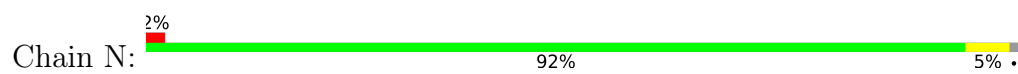


- Molecule 13: Proteasome subunit beta type-4

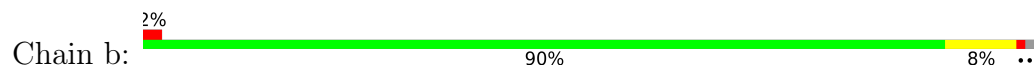
Chain a: 87% 11% ..



- Molecule 14: Proteasome subunit beta type-6



- Molecule 14: Proteasome subunit beta type-6



- 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, α , β , γ	113.39Å 202.65Å 315.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	170.45 – 1.90 170.45 – 1.90	Depositor EDS
% Data completeness (in resolution range)	97.8 (170.45-1.90) 97.8 (170.45-1.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.26 (at 1.90Å)	Xtrriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.188 , 0.225 (Not available) , 0.199	Depositor DCC
R_{free} test set	27607 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	37.8	Xtrriage
Anisotropy	0.172	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 45.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	51947	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.81% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: YCM, 6V9, CL, MG, 1PE, 6VA, 6V1, K, OAS

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	1.18	2/1833 (0.1%)	1.10	0/2489
1	O	1.05	0/1778	1.06	1/2419 (0.0%)
2	B	1.28	4/1958 (0.2%)	1.16	3/2645 (0.1%)
2	P	1.12	1/1934 (0.1%)	1.09	1/2617 (0.0%)
3	C	1.27	1/1818 (0.1%)	1.23	5/2469 (0.2%)
3	Q	1.24	3/1839 (0.2%)	1.24	13/2497 (0.5%)
4	D	1.18	1/1789 (0.1%)	1.12	3/2424 (0.1%)
4	R	1.35	5/1780 (0.3%)	1.18	6/2408 (0.2%)
5	E	1.28	3/1842 (0.2%)	1.14	2/2493 (0.1%)
5	S	1.22	0/1878	1.12	8/2541 (0.3%)
6	F	1.36	3/1935 (0.2%)	1.21	5/2605 (0.2%)
6	T	1.25	4/1894 (0.2%)	1.23	11/2556 (0.4%)
7	G	1.35	3/1909 (0.2%)	1.16	5/2579 (0.2%)
7	U	1.20	6/1804 (0.3%)	1.08	2/2441 (0.1%)
8	H	1.37	4/1697 (0.2%)	1.19	10/2299 (0.4%)
8	V	1.17	1/1655 (0.1%)	1.10	3/2251 (0.1%)
9	I	1.32	7/1648 (0.4%)	1.21	9/2219 (0.4%)
9	W	1.09	0/1630	1.09	10/2197 (0.5%)
10	J	1.43	8/1613 (0.5%)	1.21	3/2180 (0.1%)
10	X	1.28	0/1599	1.16	5/2163 (0.2%)
11	K	1.24	3/1576 (0.2%)	1.17	2/2131 (0.1%)
11	Y	1.35	4/1610 (0.2%)	1.16	1/2172 (0.0%)
12	L	1.19	0/1672	1.09	5/2257 (0.2%)
12	Z	1.37	5/1675 (0.3%)	1.15	7/2257 (0.3%)
13	M	1.34	2/1728 (0.1%)	1.12	2/2339 (0.1%)
13	a	1.36	4/1724 (0.2%)	1.14	3/2336 (0.1%)
14	N	1.41	5/1548 (0.3%)	1.19	1/2095 (0.0%)
14	b	1.34	5/1554 (0.3%)	1.20	6/2104 (0.3%)
All	All	1.27	84/48920 (0.2%)	1.15	132/66183 (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	5
3	C	0	1
3	Q	0	2
4	D	0	5
4	R	0	2
5	E	0	1
6	T	0	1
7	U	1	0
9	I	0	1
9	W	0	1
10	J	0	2
10	X	0	2
12	L	0	1
12	Z	0	1
13	a	0	1
All	All	1	26

The worst 5 of 84 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	J	154	GLU	CA-C	8.68	1.64	1.52
13	M	3	ASN	C-O	-8.41	1.18	1.25
7	G	108	GLU	CD-OE1	8.15	1.40	1.25
10	J	153	ARG	NE-CZ	-7.84	1.24	1.33
3	C	12	PRO	CA-C	7.47	1.62	1.52

The worst 5 of 132 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	190	VAL	CB-CA-C	-11.63	96.80	112.04
10	X	86	ARG	NE-CZ-NH2	-10.72	109.55	119.20
10	J	86	ARG	NE-CZ-NH2	-10.63	109.63	119.20
6	T	190	VAL	CB-CA-C	-10.16	98.88	111.88
6	T	6	GLY	CA-C-N	9.54	138.87	121.70

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	U	47	6V1	C1

5 of 26 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	237	GLU	Peptide
4	D	127	ASP	Peptide
4	D	175[A]	GLU	Peptide
4	D	175[B]	GLU	Mainchain,Peptide
4	D	223	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	15	0
1	O	1741	0	1683	8	0
2	B	1922	0	1913	9	0
2	P	1898	0	1861	16	0
3	C	1798	0	1718	22	0
3	Q	1825	0	1751	17	0
4	D	1762	0	1709	9	0
4	R	1753	0	1726	12	0
5	E	1822	0	1779	13	0
5	S	1853	0	1796	25	0
6	F	1888	0	1882	13	0
6	T	1856	0	1816	15	0
7	G	1912	0	1882	7	0
7	U	1815	0	1748	24	0
8	H	1664	0	1681	12	0
8	V	1622	0	1595	7	0
9	I	1613	0	1646	10	0
9	W	1599	0	1621	8	0
10	J	1590	0	1581	24	0
10	X	1576	0	1561	15	0
11	K	1545	0	1495	7	0
11	Y	1570	0	1547	14	0
12	L	1636	0	1625	7	0
12	Z	1642	0	1635	7	0
13	M	1692	0	1670	12	0
13	a	1688	0	1658	15	0
14	N	1519	0	1496	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	b	1524	0	1496	11	0
15	c	37	0	6	0	0
15	d	37	0	6	0	0
16	A	4	0	0	0	0
16	B	2	0	0	1	0
16	C	2	0	0	1	0
16	D	2	0	0	0	0
16	E	3	0	0	0	0
16	F	1	0	0	0	0
16	G	2	0	0	0	0
16	H	2	0	0	1	0
16	I	1	0	0	0	0
16	K	4	0	0	0	0
16	M	4	0	0	1	0
16	N	3	0	0	0	0
16	O	4	0	0	0	0
16	P	1	0	0	0	0
16	Q	2	0	0	1	0
16	R	2	0	0	1	0
16	S	3	0	0	0	0
16	U	1	0	0	0	0
16	V	2	0	0	0	0
16	W	1	0	0	0	0
16	Y	5	0	0	0	0
16	a	3	0	0	1	0
16	b	4	0	0	1	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	32	0	44	0	0
19	I	32	0	44	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	L	16	0	22	0	0
19	M	16	0	22	1	0
19	V	16	0	22	1	0
19	W	16	0	22	0	0
19	Z	16	0	22	0	0
20	A	109	0	0	3	0
20	B	120	0	0	0	0
20	C	76	0	0	1	0
20	D	93	0	0	3	0
20	E	137	0	0	2	0
20	F	180	0	0	4	0
20	G	187	0	0	4	0
20	H	157	0	0	6	0
20	I	155	0	0	1	0
20	J	133	0	0	2	0
20	K	98	0	0	0	0
20	L	124	0	0	1	0
20	M	148	0	0	1	0
20	N	168	0	0	0	0
20	O	89	0	0	1	0
20	P	117	0	0	2	0
20	Q	74	0	0	1	0
20	R	122	0	0	2	0
20	S	118	0	0	5	0
20	T	92	0	0	2	0
20	U	102	0	0	1	0
20	V	112	0	0	2	0
20	W	111	0	0	2	0
20	X	124	0	0	3	0
20	Y	137	0	0	0	0
20	Z	164	0	0	0	0
20	a	167	0	0	2	0
20	b	126	0	0	0	0
20	c	1	0	0	0	0
20	d	1	0	0	0	0
All	All	51947	0	47542	334	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 3.

The worst 5 of 334 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)
10:J:1[A]:MET:HE1	10:J:134:TYR:H	1.21	1.03
2:P:25[B]:MET:HE3	2:P:25[B]:MET:HA	1.41	1.03
10:X:1:MET:HE1	10:X:134:TYR:H	1.23	1.00
12:L:144:MET:HE1	12:L:185:ARG:HB2	1.55	0.88
5:S:65[A]:HIS:CE1	20:S:404:HOH:O	2.27	0.87

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	231/234 (99%)	219 (95%)	7 (3%)	5 (2%)	5 1
1	O	228/234 (97%)	217 (95%)	5 (2%)	6 (3%)	4 1
2	B	248/261 (95%)	238 (96%)	8 (3%)	2 (1%)	16 8
2	P	247/261 (95%)	232 (94%)	12 (5%)	3 (1%)	10 4
3	C	236/248 (95%)	220 (93%)	9 (4%)	7 (3%)	3 0
3	Q	237/248 (96%)	221 (93%)	6 (2%)	10 (4%)	2 0
4	D	232/241 (96%)	223 (96%)	6 (3%)	3 (1%)	9 3
4	R	232/241 (96%)	221 (95%)	7 (3%)	4 (2%)	7 2
5	E	232/263 (88%)	225 (97%)	6 (3%)	1 (0%)	30 22
5	S	236/263 (90%)	228 (97%)	7 (3%)	1 (0%)	30 22
6	F	241/255 (94%)	239 (99%)	2 (1%)	0	100 100
6	T	239/255 (94%)	232 (97%)	4 (2%)	3 (1%)	9 3
7	G	241/246 (98%)	237 (98%)	4 (2%)	0	100 100
7	U	232/246 (94%)	227 (98%)	4 (2%)	1 (0%)	30 22
8	H	220/234 (94%)	217 (99%)	3 (1%)	0	100 100
8	V	220/234 (94%)	216 (98%)	3 (1%)	1 (0%)	24 16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	I	205/205 (100%)	201 (98%)	4 (2%)	0	100	100
9	W	204/205 (100%)	198 (97%)	6 (3%)	0	100	100
10	J	195/201 (97%)	193 (99%)	2 (1%)	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	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%)	209 (97%)	6 (3%)	0	100	100
13	a	216/219 (99%)	208 (96%)	8 (4%)	0	100	100
14	N	201/205 (98%)	198 (98%)	2 (1%)	1 (0%)	24	16
14	b	202/205 (98%)	200 (99%)	1 (0%)	1 (0%)	24	16
All	All	6208/6458 (96%)	6025 (97%)	134 (2%)	49 (1%)	16	8

5 of 49 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	50	LYS
1	A	52	LYS
1	A	53	SER
3	C	50	VAL
3	C	216	SER

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%)	173 (94%)	12 (6%)	15	8
1	O	176/191 (92%)	166 (94%)	10 (6%)	18	11
2	B	199/221 (90%)	191 (96%)	8 (4%)	28	20
2	P	196/221 (89%)	183 (93%)	13 (7%)	15	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	179/210 (85%)	168 (94%)	11 (6%)	17	9
3	Q	184/210 (88%)	171 (93%)	13 (7%)	13	7
4	D	189/203 (93%)	181 (96%)	8 (4%)	26	19
4	R	187/203 (92%)	183 (98%)	4 (2%)	47	44
5	E	192/223 (86%)	184 (96%)	8 (4%)	26	19
5	S	195/223 (87%)	188 (96%)	7 (4%)	31	23
6	F	199/212 (94%)	189 (95%)	10 (5%)	22	14
6	T	192/212 (91%)	182 (95%)	10 (5%)	21	13
7	G	202/207 (98%)	193 (96%)	9 (4%)	24	17
7	U	186/207 (90%)	180 (97%)	6 (3%)	34	27
8	H	181/195 (93%)	174 (96%)	7 (4%)	28	21
8	V	172/195 (88%)	162 (94%)	10 (6%)	18	10
9	I	176/174 (101%)	174 (99%)	2 (1%)	65	67
9	W	173/174 (99%)	170 (98%)	3 (2%)	53	52
10	J	166/170 (98%)	157 (95%)	9 (5%)	20	12
10	X	165/170 (97%)	160 (97%)	5 (3%)	36	30
11	K	154/159 (97%)	143 (93%)	11 (7%)	13	7
11	Y	158/159 (99%)	150 (95%)	8 (5%)	21	13
12	L	175/178 (98%)	167 (95%)	8 (5%)	24	16
12	Z	175/178 (98%)	171 (98%)	4 (2%)	44	40
13	M	180/181 (99%)	177 (98%)	3 (2%)	53	52
13	a	178/181 (98%)	174 (98%)	4 (2%)	45	42
14	N	158/159 (99%)	156 (99%)	2 (1%)	61	61
14	b	158/159 (99%)	156 (99%)	2 (1%)	61	61
All	All	5030/5366 (94%)	4823 (96%)	207 (4%)	28	19

5 of 207 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	206	ASN
3	Q	227	LYS
12	Z	207	THR
2	P	7[B]	SER
2	P	246	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 63 such sidechains are listed below:

Mol	Chain	Res	Type
14	N	193	GLN
11	Y	119	ASN
2	P	142	HIS
11	Y	62	GLN
13	a	89	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](#)

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
7	6V1	G	47	7	13,15,16	2.72	5 (38%)	10,20,22	2.30	1 (10%)
7	YCM	G	137	7	7,9,10	2.21	3 (42%)	5,10,12	2.09	2 (40%)
5	6V1	E	148	5	13,15,16	1.73	2 (15%)	10,20,22	3.12	4 (40%)
3	YCM	C	63	3	7,9,10	0.92	0	5,10,12	1.02	0
7	6V1	U	47	7	13,15,16	2.05	4 (30%)	10,20,22	2.10	3 (30%)
7	6V1	G	161	7	13,15,16	1.71	3 (23%)	10,20,22	2.29	5 (50%)
5	6V1	S	148	5	13,15,16	1.98	5 (38%)	10,20,22	2.61	4 (40%)
10	6V1	J	91	10	13,15,16	1.90	3 (23%)	10,20,22	4.88	7 (70%)
7	6V1	U	161	7	13,15,16	1.90	4 (30%)	10,20,22	3.11	5 (50%)
15	6V9	d	1	15	7,8,9	1.12	1 (14%)	7,10,12	4.52	5 (71%)
15	OAS	c	3	15	5,6,9	0.88	0	2,6,11	0.41	0
3	YCM	Q	63	3	7,9,10	1.56	1 (14%)	5,10,12	3.30	3 (60%)
15	OAS	d	3	15	5,6,9	0.96	0	2,6,11	0.68	0
15	OAS	c	2	15	5,6,9	0.75	0	2,6,11	2.73	1 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	6V1	X	91	10	13,15,16	1.94	4 (30%)	10,20,22	5.13	7 (70%)
15	6V9	c	1	15	7,8,9	1.16	1 (14%)	7,10,12	3.38	5 (71%)
15	OAS	d	2	15	5,6,9	1.41	1 (20%)	2,6,11	4.70	2 (100%)
7	YCM	U	137	7	7,9,10	1.49	1 (14%)	5,10,12	3.18	3 (60%)

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

The worst 5 of 38 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	47	6V1	CB-SG	-6.62	1.75	1.82
7	U	47	6V1	CB-SG	-5.35	1.76	1.82
10	J	91	6V1	C1-SG	-5.33	1.77	1.83
7	U	161	6V1	CB-SG	-4.92	1.77	1.82
5	E	148	6V1	CB-SG	-4.55	1.77	1.82

The worst 5 of 57 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	d	1	6V9	S-C1-N	-9.40	108.24	114.63
10	J	91	6V1	C5-C4-N3	9.28	113.91	108.07
10	X	91	6V1	C5-C4-N3	8.51	113.43	108.07
10	X	91	6V1	O7-C2-N3	8.46	134.40	124.14
10	J	91	6V1	O7-C2-N3	7.29	132.99	124.14

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	U	47	6V1	C1

5 of 26 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	148	6V1	C3-C6-N3-C2
5	E	148	6V1	C3-C6-N3-C4
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.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	U	137	YCM	6	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	Z	301	-	15,15,15	0.64	0	14,14,14	0.58	0
19	1PE	H	306	-	15,15,15	0.60	0	14,14,14	0.48	0
19	1PE	I	303	-	15,15,15	0.55	0	14,14,14	0.99	1 (7%)
19	1PE	V	304	-	15,15,15	0.77	0	14,14,14	0.82	0
19	1PE	I	304	-	15,15,15	0.55	0	14,14,14	0.90	1 (7%)
19	1PE	W	303	-	15,15,15	0.66	0	14,14,14	0.46	0
19	1PE	M	305	-	15,15,15	0.57	0	14,14,14	0.37	0
19	1PE	L	301	-	15,15,15	0.62	0	14,14,14	0.76	0
19	1PE	H	305	-	15,15,15	0.59	0	14,14,14	0.65	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	Z	301	-	-	5/13/13/13	-
19	1PE	H	306	-	-	7/13/13/13	-
19	1PE	I	303	-	-	6/13/13/13	-
19	1PE	V	304	-	-	6/13/13/13	-
19	1PE	I	304	-	-	5/13/13/13	-
19	1PE	W	303	-	-	8/13/13/13	-
19	1PE	M	305	-	-	7/13/13/13	-
19	1PE	L	301	-	-	7/13/13/13	-
19	1PE	H	305	-	-	4/13/13/13	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	I	303	1PE	C25-OH5-C14	2.41	123.82	113.26
19	I	304	1PE	OH6-C15-C25	-2.23	100.20	110.35

There are no chirality outliers.

5 of 55 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	I	304	1PE	C24-C14-OH5-C25
19	I	303	1PE	C15-C25-OH5-C14
19	H	306	1PE	OH4-C13-C23-OH3
19	Z	301	1PE	C16-C26-OH6-C15
19	W	303	1PE	OH6-C15-C25-OH5

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	I	303	1PE	1	0
19	V	304	1PE	1	0
19	M	305	1PE	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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, 95th 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 ²)	Q<0.9
1	A	230/234 (98%)	0.10	6 (2%) 57 61	23, 46, 80, 96	3 (1%)
1	O	230/234 (98%)	0.60	9 (3%) 43 46	40, 62, 100, 123	0
2	B	248/261 (95%)	0.20	7 (2%) 55 59	21, 49, 89, 136	2 (0%)
2	P	247/261 (94%)	0.46	11 (4%) 38 40	32, 58, 99, 134	2 (0%)
3	C	236/248 (95%)	0.62	13 (5%) 30 32	23, 59, 102, 140	2 (0%)
3	Q	239/248 (96%)	0.77	27 (11%) 10 10	35, 63, 118, 149	0
4	D	233/241 (96%)	0.41	7 (3%) 52 56	29, 56, 86, 121	1 (0%)
4	R	233/241 (96%)	0.12	7 (3%) 52 56	20, 44, 67, 92	1 (0%)
5	E	233/263 (88%)	0.09	8 (3%) 48 51	25, 42, 87, 105	1 (0%)
5	S	235/263 (89%)	0.20	9 (3%) 44 47	22, 48, 81, 106	3 (1%)
6	F	239/255 (93%)	-0.17	4 (1%) 69 72	20, 36, 57, 75	4 (1%)
6	T	240/255 (94%)	0.42	12 (5%) 34 36	27, 51, 85, 110	1 (0%)
7	G	241/246 (97%)	-0.04	4 (1%) 69 72	19, 40, 74, 106	2 (0%)
7	U	235/246 (95%)	0.60	10 (4%) 40 42	29, 59, 93, 129	1 (0%)
8	H	220/234 (94%)	-0.12	2 (0%) 81 83	22, 37, 68, 100	2 (0%)
8	V	220/234 (94%)	0.27	9 (4%) 41 44	25, 49, 81, 103	2 (0%)
9	I	204/205 (99%)	-0.29	0 100 100	21, 36, 57, 73	3 (1%)
9	W	204/205 (99%)	0.15	1 (0%) 87 89	25, 49, 71, 78	2 (0%)
10	J	195/201 (97%)	-0.16	4 (2%) 63 67	16, 40, 57, 70	3 (1%)
10	X	195/201 (97%)	-0.03	1 (0%) 87 89	20, 42, 56, 69	2 (1%)
11	K	200/204 (98%)	-0.00	1 (0%) 87 89	33, 44, 68, 83	0
11	Y	199/204 (97%)	-0.26	2 (1%) 79 82	21, 36, 58, 69	3 (1%)
12	L	213/213 (100%)	0.12	0 100 100	25, 48, 70, 85	2 (0%)
12	Z	213/213 (100%)	-0.19	0 100 100	27, 38, 60, 74	1 (0%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	216/219 (98%)	-0.14	1 (0%) 87 89	27, 39, 61, 89	1 (0%)
13	a	216/219 (98%)	-0.18	2 (0%) 81 83	25, 39, 61, 81	2 (0%)
14	N	202/205 (98%)	-0.25	5 (2%) 58 62	21, 35, 55, 87	1 (0%)
14	b	203/205 (99%)	-0.06	4 (1%) 65 69	30, 40, 66, 96	1 (0%)
15	c	0/4	-	-	-	-
15	d	0/4	-	-	-	-
All	All	6219/6466 (96%)	0.13	166 (2%) 56 60	16, 45, 84, 149	48 (0%)

The worst 5 of 166 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
11	K	40	TYR	5.4
11	Y	40	TYR	5.3
4	R	241	ILE	4.8
5	E	54	SER	4.7
2	P	203	VAL	4.6

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, 95th 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 ²)	Q<0.9
7	6V1	U	47	15/16	0.88	0.15	73,107,113,116	0
7	YCM	U	137	10/11	0.88	0.18	51,60,74,76	0
3	YCM	C	63	10/11	0.90	0.11	52,53,61,61	0
7	6V1	U	161	15/16	0.91	0.12	53,71,79,80	0
7	YCM	G	137	10/11	0.92	0.10	31,40,53,56	0
5	6V1	E	148	15/16	0.93	0.12	33,49,59,60	0
7	6V1	G	47	15/16	0.93	0.12	38,57,61,61	0
10	6V1	X	91	15/16	0.93	0.13	35,54,58,65	0
5	6V1	S	148	15/16	0.94	0.11	37,61,67,67	0
3	YCM	Q	63	10/11	0.95	0.08	52,54,64,65	0
7	6V1	G	161	15/16	0.95	0.11	33,51,58,61	0
10	6V1	J	91	15/16	0.95	0.12	33,51,56,57	0
15	OAS	d	2	7/10	0.96	0.08	27,30,37,40	0
15	OAS	c	2	7/10	0.97	0.06	34,37,41,44	0
15	6V9	c	1	8/9	0.97	0.08	38,39,41,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
15	OAS	c	3	7/10	0.97	0.06	35,35,38,38	0
15	OAS	d	3	7/10	0.97	0.05	27,28,29,30	0
15	6V9	d	1	8/9	0.98	0.05	33,33,35,36	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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, 95th 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(\AA^2)	Q<0.9
19	1PE	I	304	16/16	0.80	0.16	53,62,77,81	0
19	1PE	M	305	16/16	0.82	0.17	70,73,87,90	0
19	1PE	H	306	16/16	0.86	0.15	55,66,88,88	0
16	CL	D	301	1/1	0.87	0.21	66,66,66,66	0
19	1PE	W	303	16/16	0.87	0.13	52,61,70,71	0
16	CL	O	303	1/1	0.88	0.11	85,85,85,85	0
19	1PE	L	301	16/16	0.89	0.12	53,64,70,71	0
16	CL	D	302	1/1	0.89	0.19	61,61,61,61	0
19	1PE	V	304	16/16	0.89	0.13	44,54,78,83	0
16	CL	V	302	1/1	0.89	0.15	56,56,56,56	0
19	1PE	I	303	16/16	0.90	0.12	50,55,61,67	0
16	CL	Y	305	1/1	0.90	0.26	59,59,59,59	0
16	CL	S	301	1/1	0.90	0.24	65,65,65,65	0
19	1PE	Z	301	16/16	0.90	0.12	53,61,66,66	0
16	CL	O	304	1/1	0.91	0.19	62,62,62,62	0
16	CL	C	302	1/1	0.91	0.19	62,62,62,62	0
16	CL	A	302	1/1	0.91	0.12	65,65,65,65	0
16	CL	Q	301	1/1	0.92	0.16	67,67,67,67	0
16	CL	H	303	1/1	0.92	0.16	53,53,53,53	0
16	CL	M	302	1/1	0.92	0.19	61,61,61,61	0
16	CL	M	304	1/1	0.92	0.12	54,54,54,54	0
16	CL	C	301	1/1	0.92	0.18	60,60,60,60	0
16	CL	B	302	1/1	0.92	0.20	57,57,57,57	0
16	CL	V	303	1/1	0.93	0.14	59,59,59,59	0
16	CL	Q	302	1/1	0.93	0.23	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
16	CL	a	301	1/1	0.93	0.18	60,60,60,60	0
19	1PE	H	305	16/16	0.93	0.10	39,53,62,62	0
16	CL	K	305	1/1	0.93	0.22	59,59,59,59	0
16	CL	K	303	1/1	0.93	0.12	69,69,69,69	0
16	CL	S	302	1/1	0.94	0.13	62,62,62,62	0
16	CL	K	304	1/1	0.94	0.20	60,60,60,60	0
16	CL	E	302	1/1	0.94	0.13	51,51,51,51	0
16	CL	Y	303	1/1	0.94	0.10	67,67,67,67	0
16	CL	R	301	1/1	0.94	0.14	57,57,57,57	0
16	CL	E	303	1/1	0.94	0.15	57,57,57,57	0
16	CL	a	303	1/1	0.94	0.12	56,56,56,56	0
16	CL	b	301	1/1	0.94	0.17	48,48,48,48	0
16	CL	b	302	1/1	0.94	0.19	62,62,62,62	0
16	CL	b	304	1/1	0.95	0.12	51,51,51,51	0
16	CL	O	302	1/1	0.95	0.11	59,59,59,59	0
16	CL	M	301	1/1	0.95	0.31	57,57,57,57	0
16	CL	A	304	1/1	0.95	0.17	56,56,56,56	0
16	CL	G	302	1/1	0.95	0.11	61,61,61,61	0
16	CL	b	303	1/1	0.96	0.13	51,51,51,51	0
16	CL	N	303	1/1	0.96	0.15	47,47,47,47	0
17	K	U	302	1/1	0.96	0.12	42,42,42,42	0
17	K	b	305	1/1	0.96	0.16	46,46,46,46	0
18	MG	I	301	1/1	0.96	0.09	34,34,34,34	0
16	CL	W	302	1/1	0.96	0.08	50,50,50,50	0
16	CL	B	301	1/1	0.96	0.10	41,41,41,41	0
16	CL	Y	304	1/1	0.96	0.10	56,56,56,56	0
16	CL	R	302	1/1	0.96	0.20	53,53,53,53	0
16	CL	F	301	1/1	0.96	0.12	51,51,51,51	0
16	CL	a	302	1/1	0.96	0.10	47,47,47,47	0
16	CL	I	302	1/1	0.96	0.11	44,44,44,44	0
16	CL	S	303	1/1	0.96	0.14	53,53,53,53	0
16	CL	N	302	1/1	0.96	0.11	47,47,47,47	0
16	CL	H	304	1/1	0.97	0.11	49,49,49,49	0
18	MG	I	305	1/1	0.97	0.12	30,30,30,30	0
16	CL	E	301	1/1	0.97	0.19	57,57,57,57	0
16	CL	G	301	1/1	0.97	0.22	46,46,46,46	0
16	CL	U	301	1/1	0.97	0.15	54,54,54,54	0
16	CL	P	301	1/1	0.97	0.09	52,52,52,52	0
16	CL	N	301	1/1	0.97	0.06	43,43,43,43	0
16	CL	A	303	1/1	0.97	0.11	49,49,49,49	0
16	CL	Y	302	1/1	0.97	0.20	59,59,59,59	0
16	CL	A	301	1/1	0.97	0.10	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
16	CL	O	301	1/1	0.97	0.11	55,55,55,55	0
18	MG	W	301	1/1	0.98	0.07	38,38,38,38	0
17	K	L	302	1/1	0.98	0.13	50,50,50,50	0
17	K	N	304	1/1	0.98	0.11	41,41,41,41	0
16	CL	Y	301	1/1	0.98	0.05	35,35,35,35	0
16	CL	K	302	1/1	0.98	0.10	38,38,38,38	0
18	MG	H	302	1/1	0.98	0.13	34,34,34,34	0
16	CL	M	303	1/1	0.98	0.12	44,44,44,44	0
17	K	G	303	1/1	0.98	0.10	35,35,35,35	0
18	MG	L	303	1/1	0.98	0.12	39,39,39,39	0
18	MG	V	301	1/1	0.98	0.06	53,53,53,53	0
18	MG	X	301	1/1	0.99	0.04	53,53,53,53	0
18	MG	K	301	1/1	0.99	0.07	35,35,35,35	0
18	MG	H	301	1/1	0.99	0.05	45,45,45,45	0
17	K	Z	302	1/1	0.99	0.09	42,42,42,42	0
18	MG	J	301	1/1	0.99	0.02	51,51,51,51	0

6.5 Other polymers [i](#)

There are no such residues in this entry.