



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 07:47 AM UTC

PDB ID : 5LF4 / pdb\_00005lf4  
Title : Human 20S proteasome complex with Delanzomib at 2.0 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 : 1.99 Å (reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
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

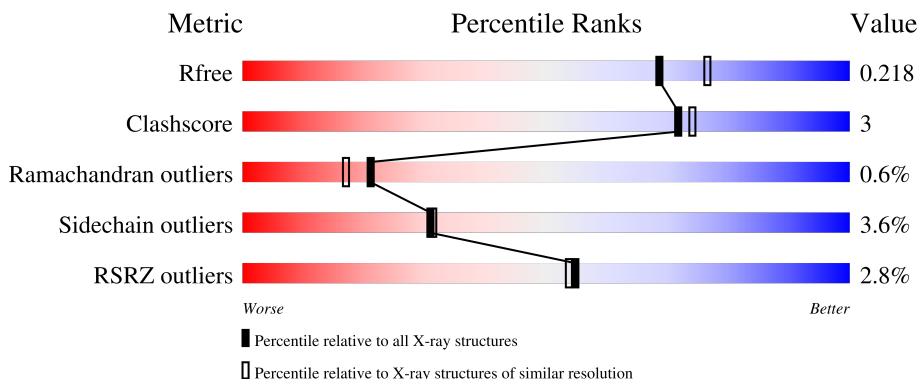
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.99 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.



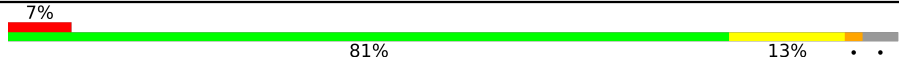

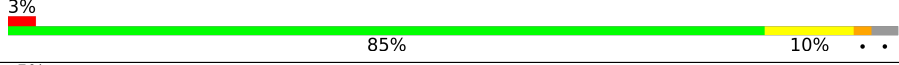



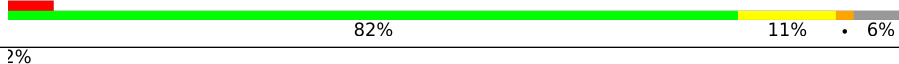

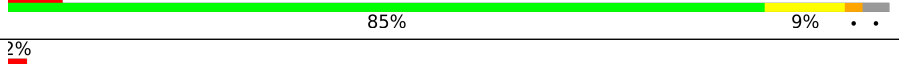


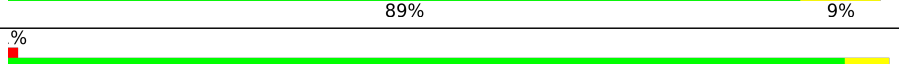
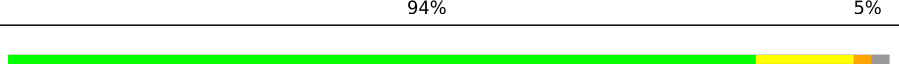
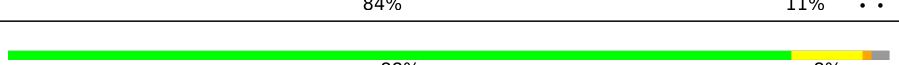
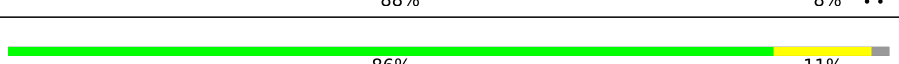
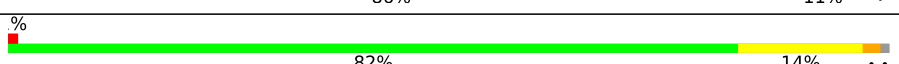
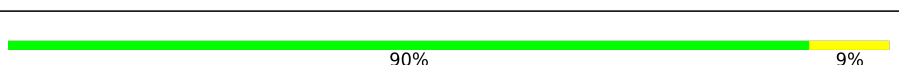
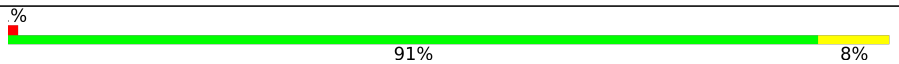
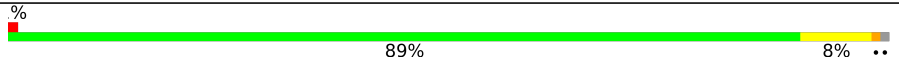

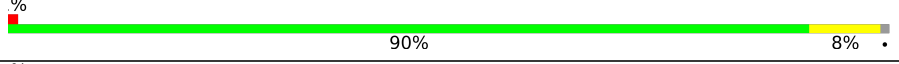
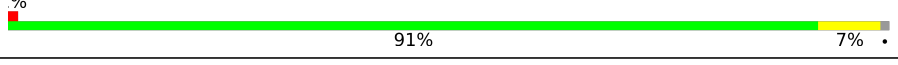

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	234	 3% 86% 10% ..
1	O	234	 3% 90% 6% ..
2	B	261	 3% 84% 10% . 5%
2	P	261	 6% 82% 11% .. 5%
3	C	248	 6% 80% 12% . .

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Mol	Chain	Length	Quality of chain
3	Q	248	 7% 81% 13% . .
4	D	241	 2% 86% 10% . .
4	R	241	 3% 85% 10% . .
5	E	263	 5% 80% 8% . 11%
5	S	263	 4% 77% 12% . 10%
6	F	255	 2% 80% 12% . 6%
6	T	255	 5% 82% 11% . 6%
7	G	246	 2% 85% 12% . .
7	U	246	 6% 85% 9% . .
8	H	234	 2% 80% 12% . 6%
8	V	234	 5% 85% 8% . 6%
9	I	205	 % 89% 9%
9	W	205	 % 94% 5%
10	J	201	 84% 11% . .
10	X	201	 88% 8% . .
11	K	204	 86% 11% .
11	Y	204	 % 82% 14% . .
12	L	213	 90% 9%
12	Z	213	 % 91% 8%
13	M	219	 % 89% 8% . .
13	a	219	 % 87% 10% . .
14	N	205	 % 90% 8% .
14	b	205	 % 91% 7% .

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:

<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
19	6V7	N	307	X	-	-	-
19	6V7	Y	306	X	-	-	-
7	6V1	U	47	X	-	-	-

## 2 Entry composition [i](#)

There are 20 unique types of molecules in this entry. The entry contains 52186 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
			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
			Total	C	N	O	S			
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
			Total	C	N	O	S			
4	D	233	Total	C	N	O	S	0	1	0
			1762	1105	290	356	11			
4	R	233	Total	C	N	O	S	0	1	0
			1753	1103	293	346	11			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	200	Total	C	N	O	S	0	1	0
			1550	978	269	293	10			
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			
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 CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	4	Total	Cl	0	0
			4	4		
15	B	2	Total	Cl	0	0
			2	2		

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

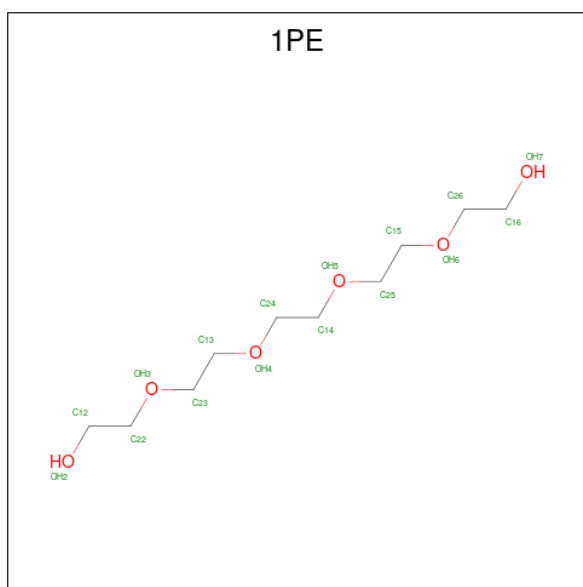
- Molecule 16 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	G	1	Total K 1 1	0	0
16	L	1	Total K 1 1	0	0
16	N	2	Total K 2 2	0	0
16	U	1	Total K 1 1	0	0
16	Z	1	Total K 1 1	0	0
16	b	2	Total K 2 2	0	0

- Molecule 17 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

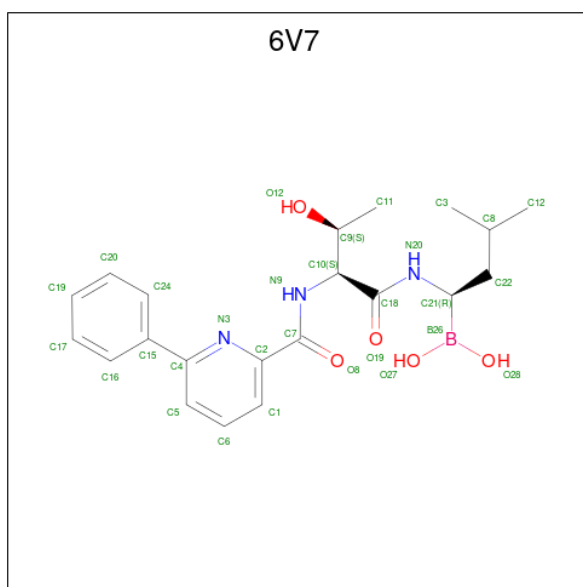
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	H	2	Total Mg 2 2	0	0
17	I	2	Total Mg 2 2	0	0
17	J	1	Total Mg 1 1	0	0
17	K	1	Total Mg 1 1	0	0
17	L	1	Total Mg 1 1	0	0
17	V	1	Total Mg 1 1	0	0
17	W	1	Total Mg 1 1	0	0
17	X	1	Total Mg 1 1	0	0

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



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

- Molecule 19 is [(1 {R})-3-methyl-1-[[[(2 {S},3 {S})-3-oxidanyl-2-[(6-phenylpyridin-2-yl)carbonylamino]butanoyl]amino]butyl]boronic acid (CCD ID: 6V7) (formula: C<sub>21</sub>H<sub>28</sub>BN<sub>3</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	B	C	N	O		
19	K	1	Total 30	B 1	C 21	N 3	O 5	0	0
19	N	1	Total 30	B 1	C 21	N 3	O 5	0	0
19	Y	1	Total 30	B 1	C 21	N 3	O 5	0	0
19	b	1	Total 30	B 1	C 21	N 3	O 5	0	0

- Molecule 20 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	A	115	Total 115	O 115	0	0
20	B	129	Total 129	O 129	0	0
20	C	78	Total 78	O 78	0	0
20	D	98	Total 98	O 98	0	0
20	E	143	Total 143	O 143	0	0
20	F	186	Total 186	O 186	0	0
20	G	195	Total 195	O 195	0	0
20	H	164	Total 164	O 164	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	I	155	Total 155	O 155	0	0
20	J	141	Total 141	O 141	0	0
20	K	102	Total 102	O 102	0	0
20	L	124	Total 124	O 124	0	0
20	M	148	Total 148	O 148	0	0
20	N	168	Total 168	O 168	0	0
20	O	95	Total 95	O 95	0	0
20	P	124	Total 124	O 124	0	0
20	Q	75	Total 75	O 75	0	0
20	R	129	Total 129	O 129	0	0
20	S	128	Total 128	O 128	0	0
20	T	96	Total 96	O 96	0	0
20	U	113	Total 113	O 113	0	0
20	V	117	Total 117	O 117	0	0
20	W	123	Total 123	O 123	0	0
20	X	128	Total 128	O 128	0	0
20	Y	149	Total 149	O 149	0	0
20	Z	171	Total 171	O 171	0	0
20	a	172	Total 172	O 172	0	0
20	b	126	Total 126	O 126	0	0

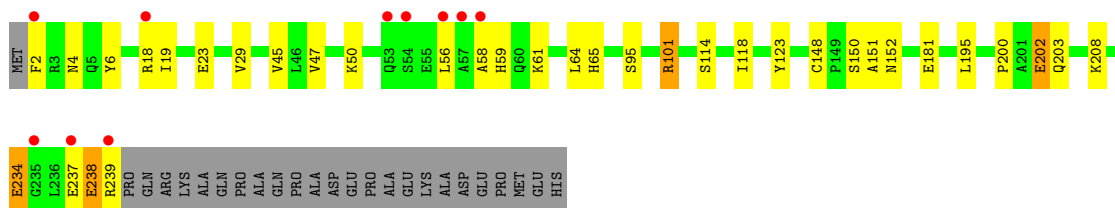




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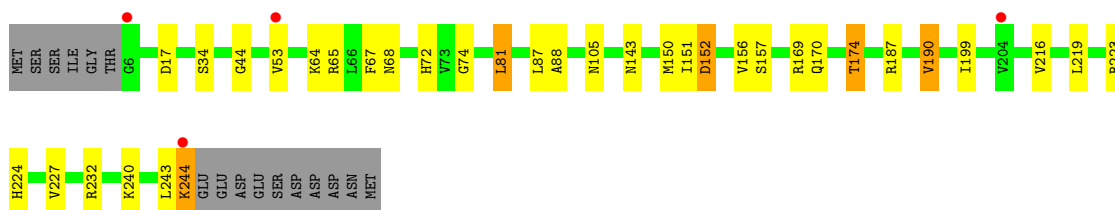
- Molecule 5: Proteasome subunit alpha type-1

Chain S: 4% 77% 12% 10%



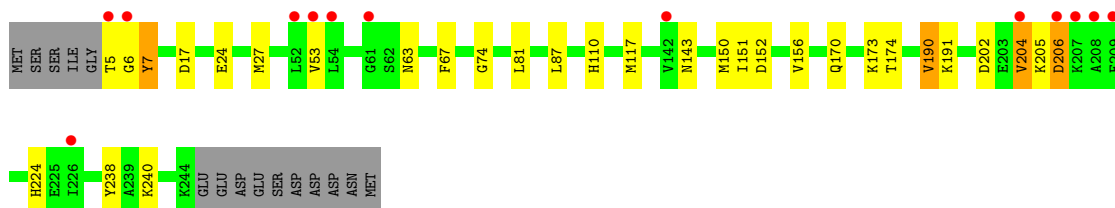
- Molecule 6: Proteasome subunit alpha type-3

Chain F: 2% 80% 12% 6%



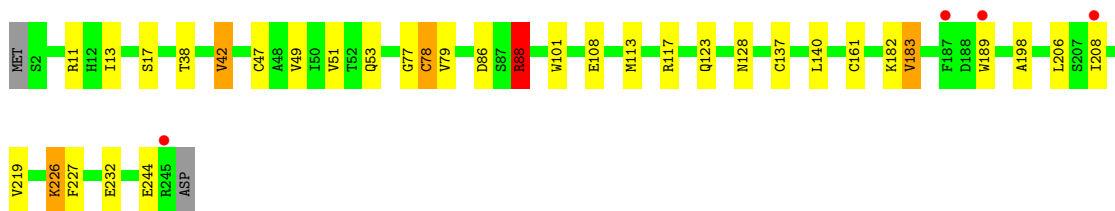
- Molecule 6: Proteasome subunit alpha type-3

Chain T: 5% 82% 11% 6%



- Molecule 7: Proteasome subunit alpha type-6

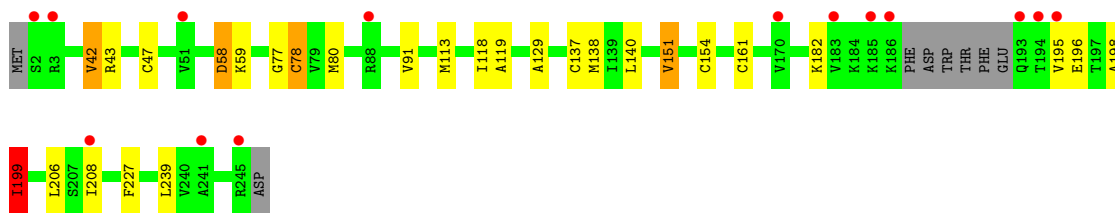
Chain G: 2% 85% 12% 2%



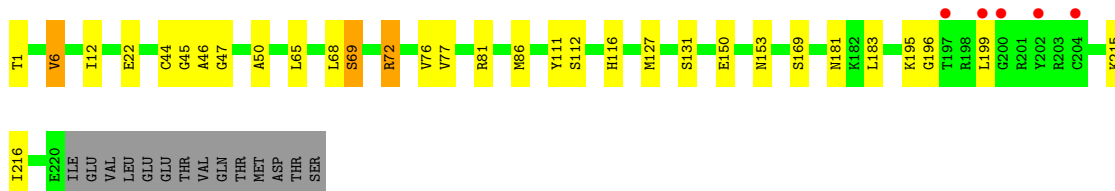
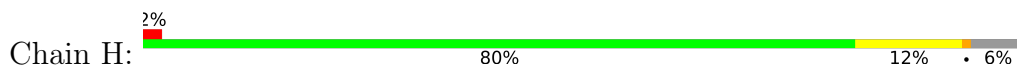
- Molecule 7: Proteasome subunit alpha type-6

Chain U: 6% 85% 9% 2%

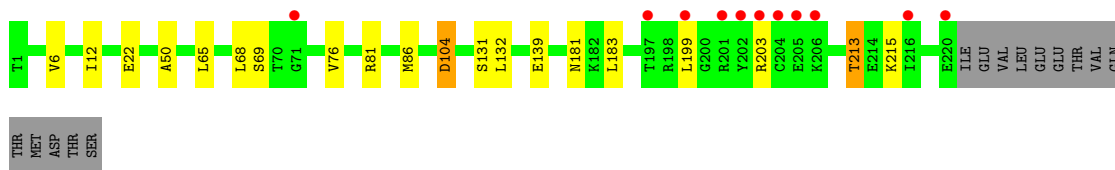
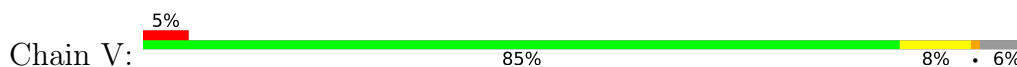




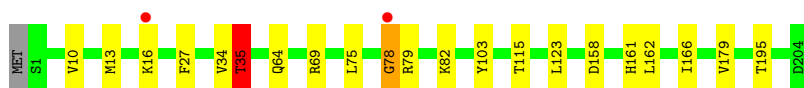
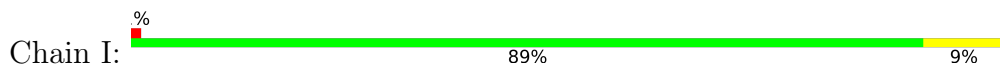
• Molecule 8: Proteasome subunit beta type-7



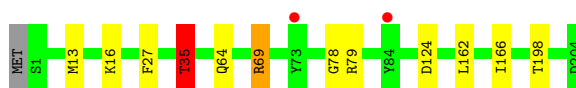
• Molecule 8: Proteasome subunit beta type-7



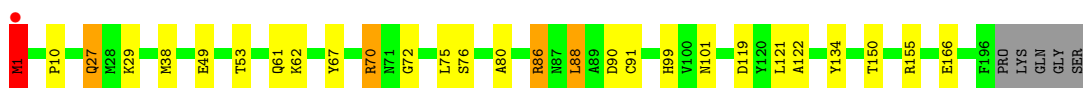
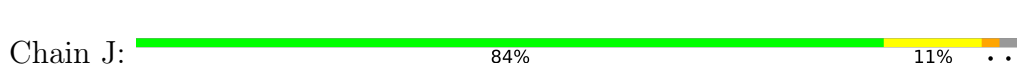
• Molecule 9: Proteasome subunit beta type-3



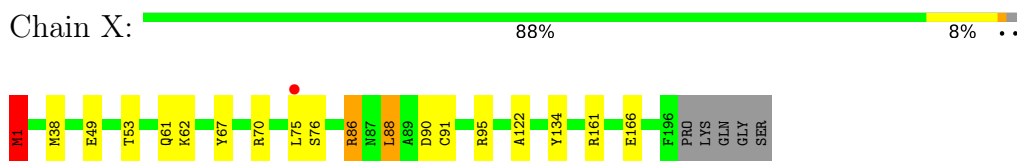
• Molecule 9: Proteasome subunit beta type-3



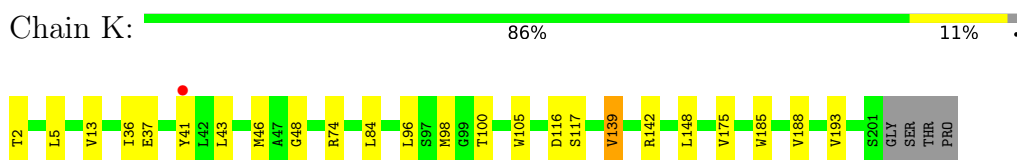
• Molecule 10: Proteasome subunit beta type-2



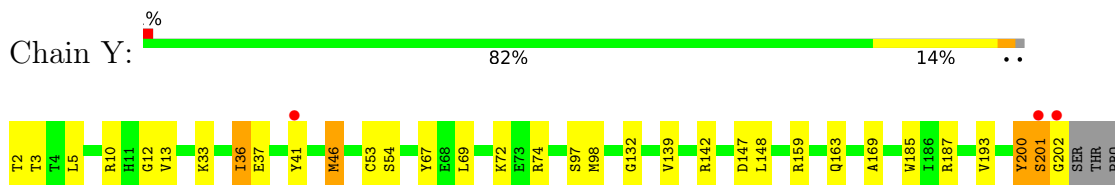
- Molecule 10: Proteasome subunit beta type-2



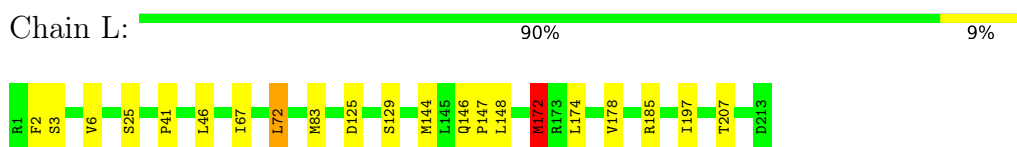
- Molecule 11: Proteasome subunit beta type-5



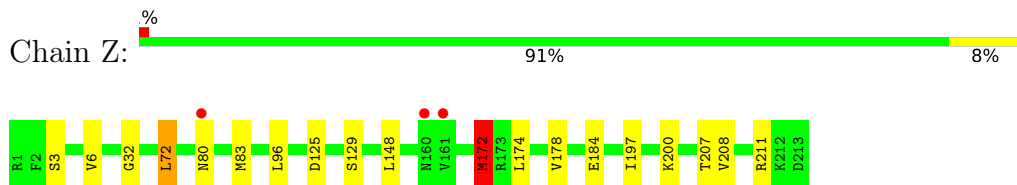
- Molecule 11: Proteasome subunit beta type-5



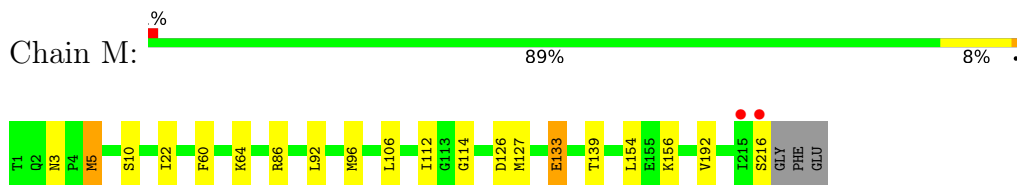
- Molecule 12: Proteasome subunit beta type-1



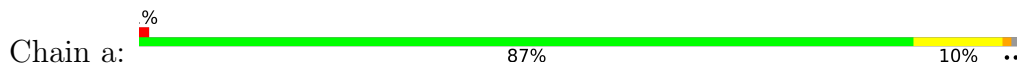
- Molecule 12: Proteasome subunit beta type-1



- Molecule 13: Proteasome subunit beta type-4

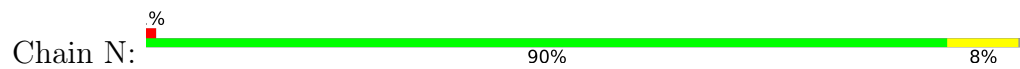


- Molecule 13: Proteasome subunit beta type-4

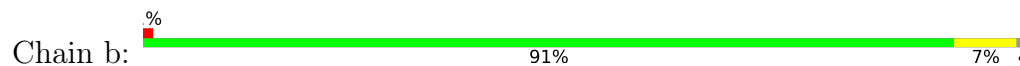




- Molecule 14: Proteasome subunit beta type-6



- Molecule 14: Proteasome subunit beta type-6



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	113.45Å 202.76Å 314.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	170.38 – 1.99 170.38 – 1.99	Depositor EDS
% Data completeness (in resolution range)	99.0 (170.38-1.99) 99.0 (170.38-1.99)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.47 (at 2.00Å)	Xtrriage
Refinement program	REFMAC 5.8.0103	Depositor
R, $R_{free}$	0.181 , 0.216 0.187 , 0.218	Depositor DCC
$R_{free}$ test set	24259 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	35.9	Xtrriage
Anisotropy	0.289	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 53.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	52186	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.84% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 6V7, CL, K, YCM, MG, 6V1, 1PE

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	1.19	0/1833	1.07	0/2489
1	O	1.01	1/1778 (0.1%)	1.03	1/2419 (0.0%)
2	B	1.23	6/1962 (0.3%)	1.10	4/2649 (0.2%)
2	P	1.08	2/1945 (0.1%)	1.07	3/2631 (0.1%)
3	C	1.13	2/1818 (0.1%)	1.15	1/2469 (0.0%)
3	Q	1.09	2/1834 (0.1%)	1.18	11/2490 (0.4%)
4	D	1.09	1/1789 (0.1%)	1.08	2/2424 (0.1%)
4	R	1.31	5/1780 (0.3%)	1.13	4/2408 (0.2%)
5	E	1.27	2/1842 (0.1%)	1.15	8/2493 (0.3%)
5	S	1.18	0/1901	1.16	9/2571 (0.4%)
6	F	1.44	9/1935 (0.5%)	1.22	3/2605 (0.1%)
6	T	1.18	2/1894 (0.1%)	1.18	10/2556 (0.4%)
7	G	1.36	13/1909 (0.7%)	1.15	5/2579 (0.2%)
7	U	1.10	2/1804 (0.1%)	1.06	2/2441 (0.1%)
8	H	1.43	8/1697 (0.5%)	1.22	10/2299 (0.4%)
8	V	1.17	0/1655	1.10	4/2251 (0.2%)
9	I	1.36	6/1648 (0.4%)	1.27	12/2219 (0.5%)
9	W	1.12	0/1630	1.11	7/2197 (0.3%)
10	J	1.29	2/1613 (0.1%)	1.17	6/2180 (0.3%)
10	X	1.20	1/1599 (0.1%)	1.08	3/2163 (0.1%)
11	K	1.21	2/1584 (0.1%)	1.11	1/2141 (0.0%)
11	Y	1.37	4/1620 (0.2%)	1.18	4/2185 (0.2%)
12	L	1.22	3/1672 (0.2%)	1.08	2/2257 (0.1%)
12	Z	1.43	5/1675 (0.3%)	1.13	2/2257 (0.1%)
13	M	1.35	3/1728 (0.2%)	1.13	3/2339 (0.1%)
13	a	1.45	6/1724 (0.3%)	1.17	1/2336 (0.0%)
14	N	1.48	6/1548 (0.4%)	1.23	3/2095 (0.1%)
14	b	1.34	6/1554 (0.4%)	1.18	2/2104 (0.1%)
All	All	1.26	99/48971 (0.2%)	1.14	123/66247 (0.2%)

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	P	0	3
3	C	0	1
3	Q	0	3
4	D	0	4
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	1
13	a	0	1
All	All	1	21

The worst 5 of 99 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	162	THR	C-N	8.74	1.44	1.33
6	F	44	GLY	N-CA	8.66	1.53	1.45
2	P	162	THR	C-N	8.22	1.44	1.33
14	b	87	MET	CA-C	7.72	1.62	1.52
7	G	108	GLU	CD-OE1	7.70	1.40	1.25

The worst 5 of 123 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	190	VAL	CB-CA-C	-11.30	97.24	112.04
6	T	190	VAL	CB-CA-C	-10.55	98.22	112.04
7	G	183	VAL	CB-CA-C	-9.84	98.65	112.22
10	J	86	ARG	NE-CZ-NH2	-9.45	110.70	119.20
9	I	16[A]	LYS	CA-C-N	8.86	135.11	122.08

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	U	47	6V1	C1

5 of 21 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	46	GLU	Peptide
4	D	127	ASP	Peptide
4	D	175[A]	GLU	Peptide
4	D	175[B]	GLU	Mainchain,Peptide
5	E	235	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	16	0
1	O	1741	0	1683	7	0
2	B	1926	0	1924	12	0
2	P	1909	0	1874	18	0
3	C	1798	0	1718	24	0
3	Q	1820	0	1749	11	0
4	D	1762	0	1709	9	0
4	R	1753	0	1726	11	0
5	E	1822	0	1779	7	0
5	S	1875	0	1818	21	0
6	F	1888	0	1882	14	0
6	T	1856	0	1816	12	0
7	G	1912	0	1882	10	0
7	U	1815	0	1748	12	0
8	H	1664	0	1681	12	0
8	V	1622	0	1595	6	0
9	I	1613	0	1646	10	0
9	W	1599	0	1621	9	0
10	J	1590	0	1581	18	0
10	X	1576	0	1561	14	0
11	K	1550	0	1503	11	0
11	Y	1580	0	1554	30	0
12	L	1636	0	1625	10	0
12	Z	1642	0	1635	5	0
13	M	1692	0	1670	8	0
13	a	1688	0	1658	11	0
14	N	1519	0	1492	8	0
14	b	1524	0	1492	7	0
15	A	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	B	2	0	0	1	0
15	C	2	0	0	0	0
15	D	2	0	0	0	0
15	E	3	0	0	0	0
15	F	1	0	0	0	0
15	G	2	0	0	0	0
15	H	2	0	0	1	0
15	I	1	0	0	0	0
15	K	3	0	0	0	0
15	M	3	0	0	1	0
15	N	2	0	0	1	0
15	O	4	0	0	0	0
15	P	1	0	0	0	0
15	Q	2	0	0	0	0
15	R	2	0	0	1	0
15	S	3	0	0	0	0
15	U	1	0	0	0	0
15	V	2	0	0	0	0
15	W	1	0	0	0	0
15	Y	4	0	0	0	0
15	a	4	0	0	1	0
15	b	1	0	0	0	0
16	G	1	0	0	0	0
16	L	1	0	0	0	0
16	N	2	0	0	0	0
16	U	1	0	0	0	0
16	Z	1	0	0	0	0
16	b	2	0	0	0	0
17	H	2	0	0	0	0
17	I	2	0	0	0	0
17	J	1	0	0	0	0
17	K	1	0	0	0	0
17	L	1	0	0	0	0
17	V	1	0	0	0	0
17	W	1	0	0	0	0
17	X	1	0	0	0	0
18	H	16	0	22	0	0
18	I	16	0	22	0	0
18	L	32	0	44	0	0
18	N	32	0	44	0	0
18	U	16	0	22	1	0
18	W	16	0	22	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	Y	16	0	22	0	0
19	K	30	0	0	1	0
19	N	30	0	0	0	0
19	Y	30	0	0	1	0
19	b	30	0	0	0	0
20	A	115	0	0	3	0
20	B	129	0	0	2	0
20	C	78	0	0	2	0
20	D	98	0	0	1	0
20	E	143	0	0	1	0
20	F	186	0	0	4	0
20	G	195	0	0	3	0
20	H	164	0	0	5	0
20	I	155	0	0	1	0
20	J	141	0	0	1	0
20	K	102	0	0	0	0
20	L	124	0	0	2	0
20	M	148	0	0	0	0
20	N	168	0	0	1	0
20	O	95	0	0	1	0
20	P	124	0	0	0	0
20	Q	75	0	0	0	0
20	R	129	0	0	4	0
20	S	128	0	0	6	0
20	T	96	0	0	1	0
20	U	113	0	0	1	0
20	V	117	0	0	0	0
20	W	123	0	0	1	0
20	X	128	0	0	1	0
20	Y	149	0	0	0	0
20	Z	171	0	0	0	0
20	a	172	0	0	0	0
20	b	126	0	0	0	0
All	All	52186	0	47581	320	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 320 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)
2:P:25[B]:MET:HE3	2:P:25[B]:MET:HA	1.41	1.02
11:Y:46:MET:HE1	11:Y:54:SER:HA	1.45	0.99
10:J:1[A]:MET:HE1	10:J:134:TYR:H	1.28	0.96
10:X:1:MET:HE1	10:X:134:TYR:H	1.28	0.96
11:Y:36:ILE:HD12	11:Y:46:MET:HE3	1.52	0.92

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%)	221 (96%)	6 (3%)	4 (2%)	7 3
1	O	228/234 (97%)	217 (95%)	7 (3%)	4 (2%)	6 3
2	B	248/261 (95%)	238 (96%)	9 (4%)	1 (0%)	30 27
2	P	248/261 (95%)	235 (95%)	10 (4%)	3 (1%)	10 6
3	C	236/248 (95%)	223 (94%)	7 (3%)	6 (2%)	4 1
3	Q	236/248 (95%)	221 (94%)	6 (2%)	9 (4%)	2 1
4	D	232/241 (96%)	222 (96%)	7 (3%)	3 (1%)	9 5
4	R	232/241 (96%)	222 (96%)	7 (3%)	3 (1%)	9 5
5	E	232/263 (88%)	226 (97%)	5 (2%)	1 (0%)	30 27
5	S	238/263 (90%)	228 (96%)	9 (4%)	1 (0%)	30 27
6	F	241/255 (94%)	238 (99%)	3 (1%)	0	100 100
6	T	239/255 (94%)	233 (98%)	4 (2%)	2 (1%)	16 11
7	G	241/246 (98%)	235 (98%)	6 (2%)	0	100 100
7	U	232/246 (94%)	227 (98%)	4 (2%)	1 (0%)	30 27
8	H	220/234 (94%)	217 (99%)	3 (1%)	0	100 100
8	V	220/234 (94%)	217 (99%)	2 (1%)	1 (0%)	24 21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	I	205/205 (100%)	202 (98%)	3 (2%)	0	100	100
9	W	204/205 (100%)	199 (98%)	5 (2%)	0	100	100
10	J	195/201 (97%)	192 (98%)	3 (2%)	0	100	100
10	X	195/201 (97%)	193 (99%)	2 (1%)	0	100	100
11	K	199/204 (98%)	197 (99%)	2 (1%)	0	100	100
11	Y	202/204 (99%)	199 (98%)	2 (1%)	1 (0%)	24	21
12	L	213/213 (100%)	210 (99%)	3 (1%)	0	100	100
12	Z	212/213 (100%)	209 (99%)	3 (1%)	0	100	100
13	M	215/219 (98%)	209 (97%)	6 (3%)	0	100	100
13	a	216/219 (99%)	209 (97%)	7 (3%)	0	100	100
14	N	201/205 (98%)	199 (99%)	2 (1%)	0	100	100
14	b	202/205 (98%)	201 (100%)	1 (0%)	0	100	100
All	All	6213/6458 (96%)	6039 (97%)	134 (2%)	40 (1%)	21	17

5 of 40 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	52	LYS
1	A	53	SER
5	E	59	HIS
1	O	52	LYS
1	O	53	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%)	175 (95%)	10 (5%)	20	17
1	O	176/191 (92%)	166 (94%)	10 (6%)	18	15
2	B	200/221 (90%)	193 (96%)	7 (4%)	32	32
2	P	197/221 (89%)	185 (94%)	12 (6%)	17	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	179/210 (85%)	169 (94%)	10 (6%)	19	16
3	Q	184/210 (88%)	173 (94%)	11 (6%)	17	14
4	D	189/203 (93%)	182 (96%)	7 (4%)	30	30
4	R	187/203 (92%)	183 (98%)	4 (2%)	47	52
5	E	192/223 (86%)	184 (96%)	8 (4%)	26	25
5	S	197/223 (88%)	189 (96%)	8 (4%)	27	26
6	F	199/212 (94%)	190 (96%)	9 (4%)	24	23
6	T	192/212 (91%)	186 (97%)	6 (3%)	35	37
7	G	202/207 (98%)	194 (96%)	8 (4%)	28	27
7	U	186/207 (90%)	180 (97%)	6 (3%)	34	35
8	H	181/195 (93%)	173 (96%)	8 (4%)	25	24
8	V	172/195 (88%)	160 (93%)	12 (7%)	14	10
9	I	176/174 (101%)	174 (99%)	2 (1%)	65	73
9	W	173/174 (99%)	171 (99%)	2 (1%)	63	70
10	J	166/170 (98%)	159 (96%)	7 (4%)	26	25
10	X	165/170 (97%)	161 (98%)	4 (2%)	43	47
11	K	155/159 (98%)	148 (96%)	7 (4%)	24	23
11	Y	159/159 (100%)	155 (98%)	4 (2%)	42	45
12	L	175/178 (98%)	169 (97%)	6 (3%)	32	33
12	Z	175/178 (98%)	170 (97%)	5 (3%)	37	40
13	M	180/181 (99%)	176 (98%)	4 (2%)	45	50
13	a	178/181 (98%)	174 (98%)	4 (2%)	45	50
14	N	158/159 (99%)	156 (99%)	2 (1%)	61	68
14	b	158/159 (99%)	156 (99%)	2 (1%)	61	68
All	All	5036/5366 (94%)	4851 (96%)	185 (4%)	31	30

5 of 185 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	P	246	LYS
6	T	87	LEU
3	Q	98	VAL
4	R	139	VAL
7	U	199	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 78 such sidechains are listed below:

Mol	Chain	Res	Type
5	S	8	ASN
12	Z	79	ASN
6	T	68	ASN
10	X	24	ASN
13	a	162	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

12 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	Q	63	3	7,9,10	1.54	1 (14%)	5,10,12	3.02	4 (80%)
3	YCM	C	63	3	7,9,10	1.12	1 (14%)	5,10,12	1.55	2 (40%)
5	6V1	S	148	5	13,15,16	1.99	4 (30%)	10,20,22	2.93	5 (50%)
10	6V1	J	91	10	13,15,16	2.28	4 (30%)	10,20,22	4.48	7 (70%)
10	6V1	X	91	10	13,15,16	1.75	3 (23%)	10,20,22	4.83	7 (70%)
7	6V1	U	161	7	13,15,16	1.83	3 (23%)	10,20,22	3.27	5 (50%)
7	YCM	U	137	7	7,9,10	1.11	0	5,10,12	1.89	2 (40%)
5	6V1	E	148	5	13,15,16	2.13	2 (15%)	10,20,22	3.51	5 (50%)
7	6V1	G	161	7	13,15,16	1.38	3 (23%)	10,20,22	2.58	6 (60%)
7	6V1	U	47	7	13,15,16	2.22	4 (30%)	10,20,22	1.99	2 (20%)
7	YCM	G	137	7	7,9,10	1.96	3 (42%)	5,10,12	2.21	2 (40%)
7	6V1	G	47	7	13,15,16	2.06	3 (23%)	10,20,22	1.19	1 (10%)

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

The worst 5 of 31 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	J	91	6V1	C1-SG	-6.56	1.76	1.83
5	E	148	6V1	CB-SG	-5.80	1.76	1.82
7	U	47	6V1	CB-SG	-5.65	1.76	1.82
5	S	148	6V1	CB-SG	-4.90	1.77	1.82
7	G	47	6V1	CB-SG	-4.63	1.77	1.82

The worst 5 of 48 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	X	91	6V1	O7-C2-N3	7.77	133.57	124.14
10	J	91	6V1	O7-C2-N3	7.62	133.38	124.14
10	X	91	6V1	C5-C4-N3	7.20	112.60	108.07
5	E	148	6V1	C2-N3-C4	-7.18	108.86	113.07
10	J	91	6V1	C5-C4-N3	6.82	112.36	108.07

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	U	47	6V1	C1

5 of 21 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
7	G	161	6V1	C3-C6-N3-C4
10	J	91	6V1	C3-C6-N3-C2

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 83 ligands modelled in this entry, 70 are monoatomic - leaving 13 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
18	1PE	W	303	-	15,15,15	0.56	0	14,14,14	0.40	0
18	1PE	Y	305	-	15,15,15	0.53	0	14,14,14	0.52	0
18	1PE	L	301	-	15,15,15	0.55	0	14,14,14	0.69	0
18	1PE	U	302	-	15,15,15	0.57	0	14,14,14	0.84	0
18	1PE	N	304	-	15,15,15	0.53	0	14,14,14	0.38	0
18	1PE	N	303	-	15,15,15	0.50	0	14,14,14	0.73	0
18	1PE	L	302	-	15,15,15	0.52	0	14,14,14	0.41	0
19	6V7	b	304	14	27,31,31	0.97	1 (3%)	37,42,42	1.62	5 (13%)
19	6V7	K	305	11	27,31,31	1.45	4 (14%)	37,42,42	1.86	11 (29%)
18	1PE	H	305	-	15,15,15	0.46	0	14,14,14	0.57	0
18	1PE	I	303	-	15,15,15	0.55	0	14,14,14	1.10	2 (14%)
19	6V7	Y	306	11	27,31,31	1.09	1 (3%)	37,42,42	1.55	7 (18%)
19	6V7	N	307	14	27,31,31	0.96	1 (3%)	37,42,42	1.64	8 (21%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	1PE	W	303	-	-	6/13/13/13	-
18	1PE	Y	305	-	-	6/13/13/13	-
18	1PE	L	301	-	-	6/13/13/13	-
18	1PE	U	302	-	-	7/13/13/13	-
18	1PE	N	304	-	-	7/13/13/13	-
18	1PE	N	303	-	-	4/13/13/13	-
18	1PE	L	302	-	-	8/13/13/13	-
19	6V7	b	304	14	-	8/27/32/32	0/2/2/2
19	6V7	K	305	11	-	8/27/32/32	0/2/2/2
18	1PE	I	303	-	-	8/13/13/13	-
18	1PE	H	305	-	-	9/13/13/13	-
19	6V7	N	307	14	1/1/7/9	4/27/32/32	0/2/2/2
19	6V7	Y	306	11	1/1/7/9	5/27/32/32	0/2/2/2

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	K	305	6V7	C2-N3	4.16	1.40	1.34
19	Y	306	6V7	O12-C9	-3.52	1.33	1.43
19	K	305	6V7	C11-C9	-2.81	1.43	1.51
19	b	304	6V7	C10-C18	-2.25	1.47	1.52
19	K	305	6V7	C24-C15	2.10	1.43	1.39

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	b	304	6V7	C11-C9-C10	5.49	123.15	112.29
19	K	305	6V7	C6-C1-C2	-4.64	113.08	118.63
19	b	304	6V7	C2-C7-N9	4.07	123.00	115.19
19	K	305	6V7	C21-C22-C8	3.95	120.36	115.32
19	N	307	6V7	O12-C9-C10	3.84	116.81	109.07

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
19	N	307	6V7	C9
19	Y	306	6V7	C9

5 of 86 torsion outliers are listed below:

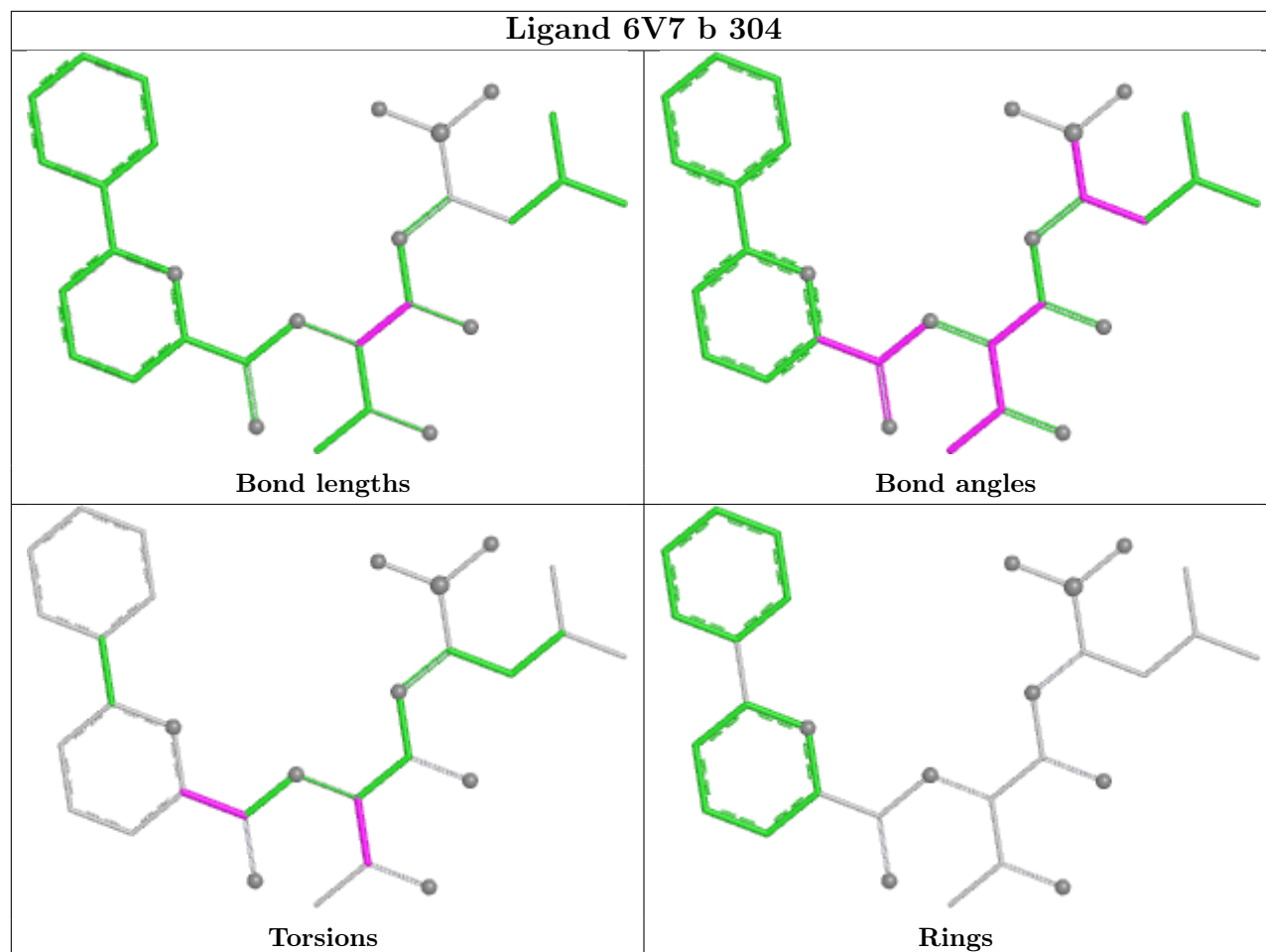
Mol	Chain	Res	Type	Atoms
19	K	305	6V7	C21-C22-C8-C12
19	Y	306	6V7	C21-C22-C8-C12
19	b	304	6V7	C18-C10-C9-C11
19	b	304	6V7	C18-C10-C9-O12
19	b	304	6V7	N9-C10-C9-C11

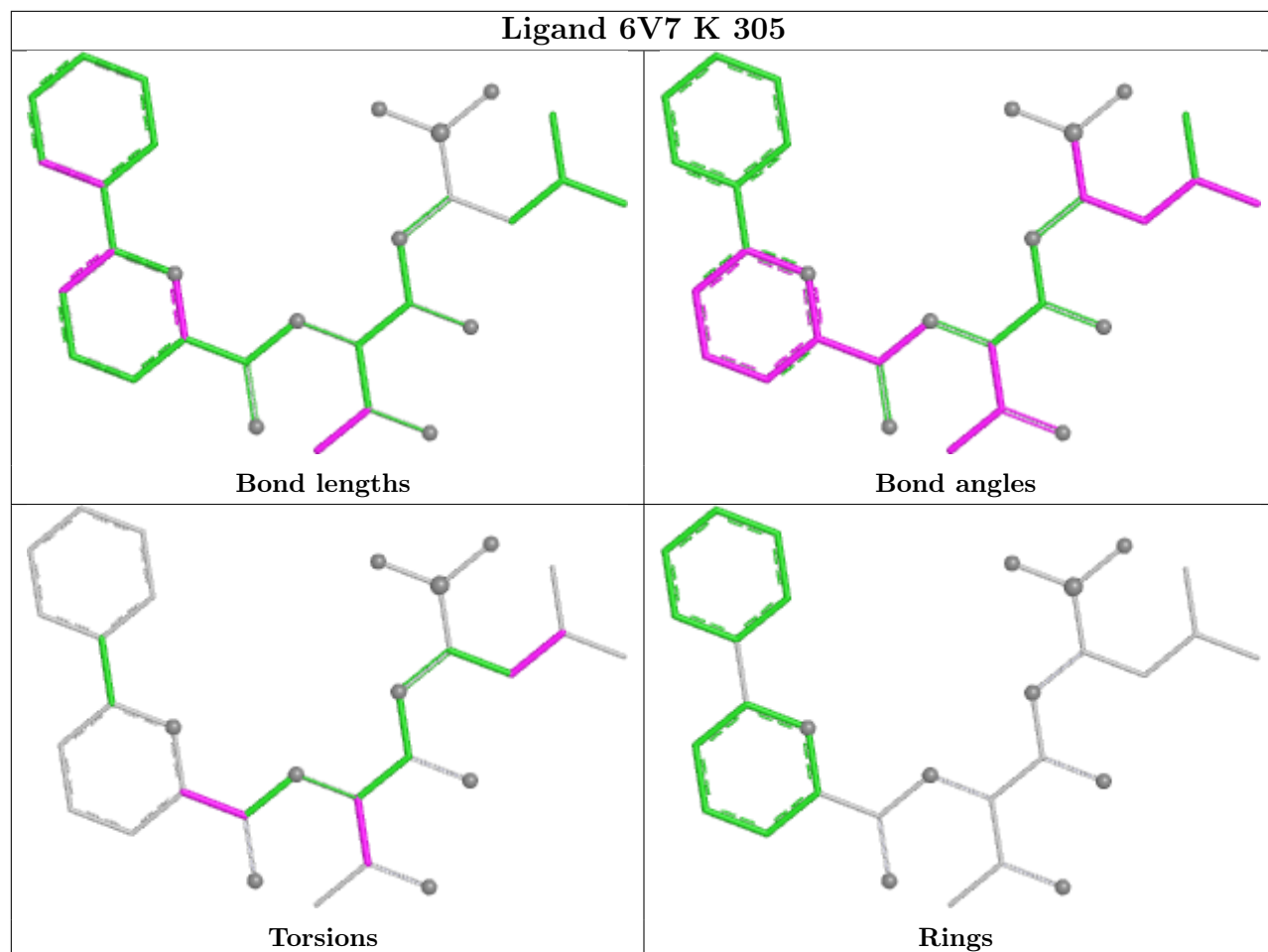
There are no ring outliers.

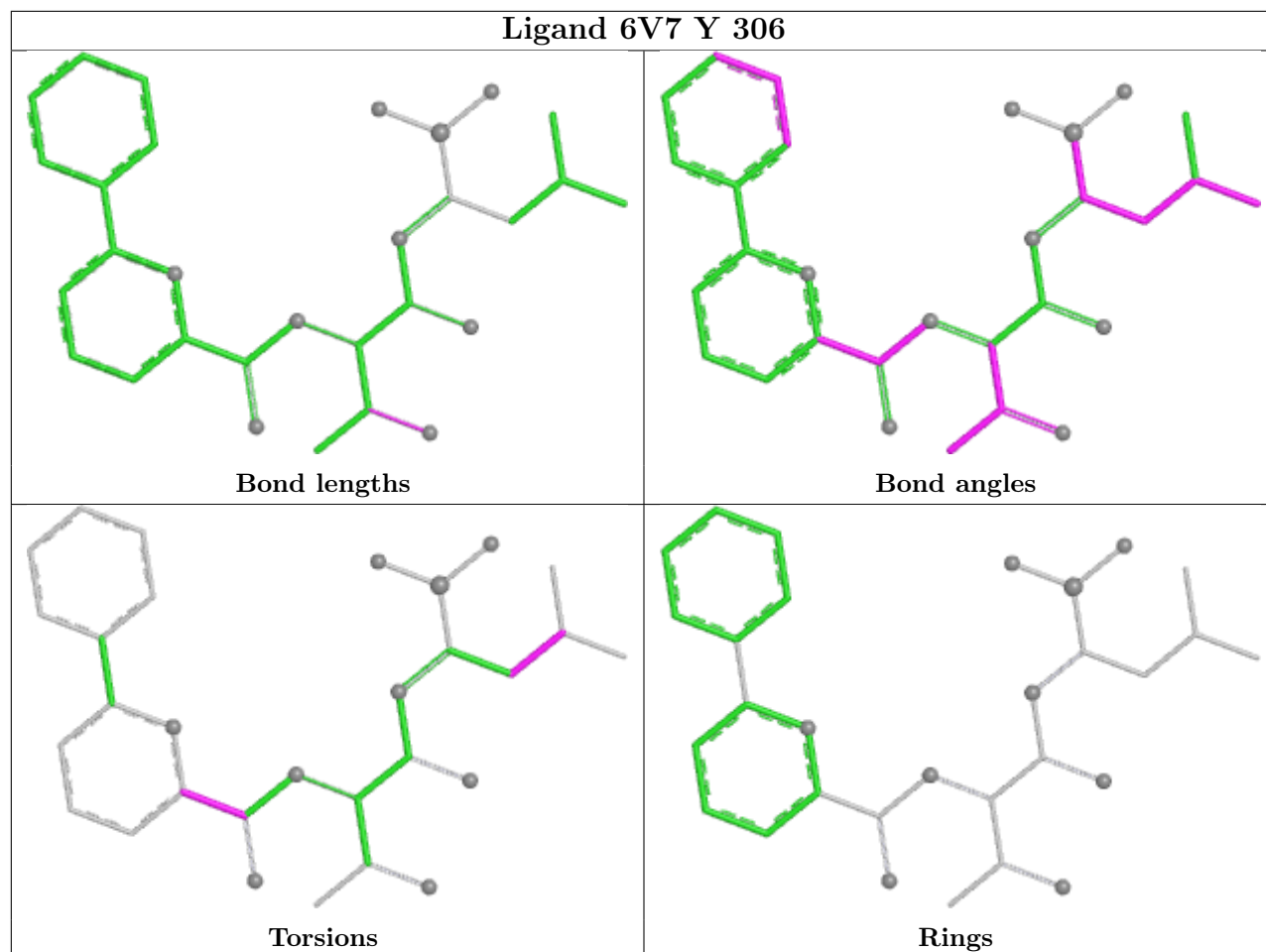
3 monomers are involved in 3 short contacts:

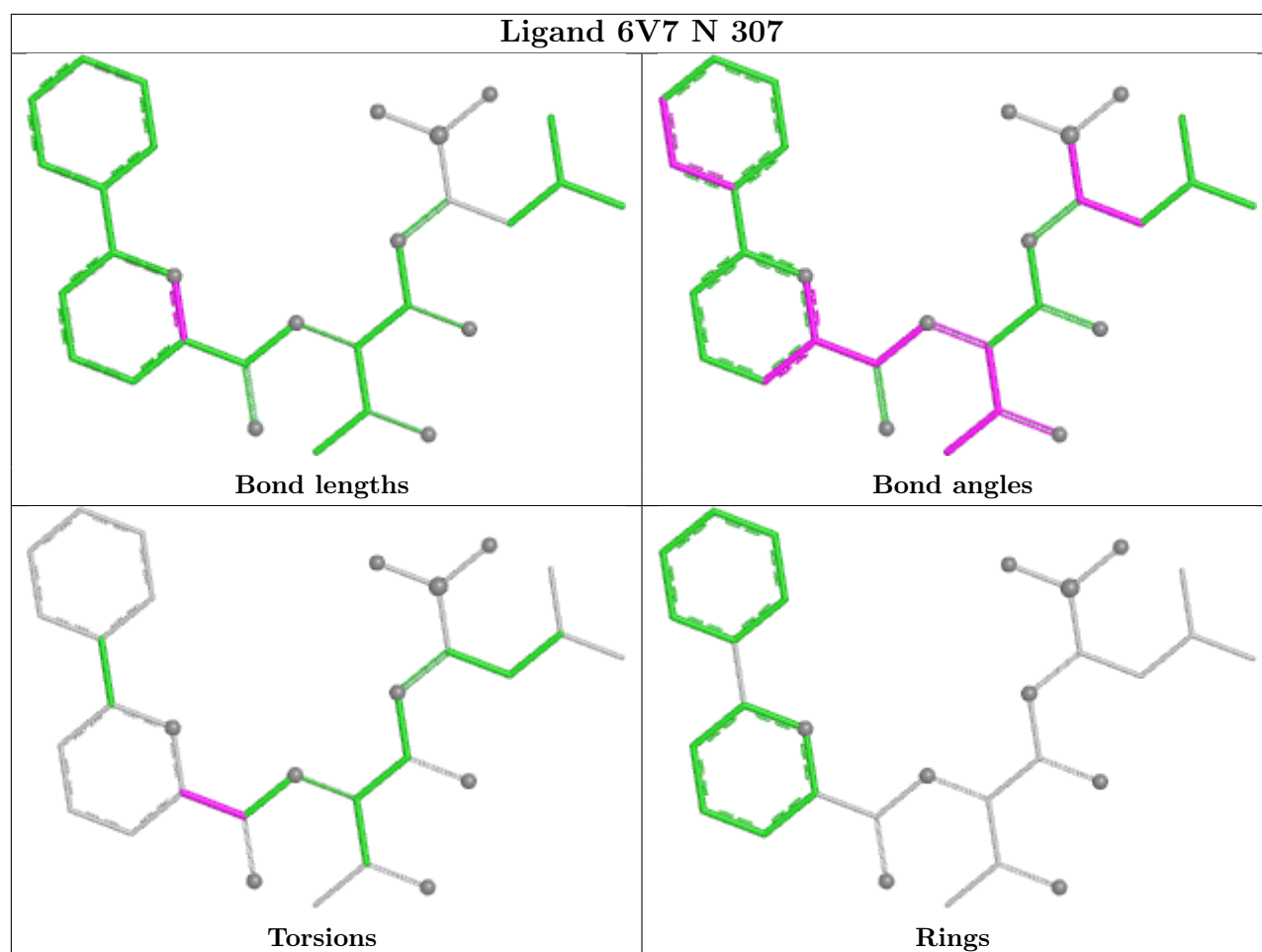
Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	U	302	1PE	1	0
19	K	305	6V7	1	0
19	Y	306	6V7	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	230/234 (98%)	0.06	6 (2%) 57 56	23, 46, 86, 102	3 (1%)
1	O	230/234 (98%)	0.51	7 (3%) 52 51	40, 68, 117, 148	0
2	B	248/261 (95%)	0.22	9 (3%) 46 45	20, 53, 98, 144	2 (0%)
2	P	248/261 (95%)	0.52	15 (6%) 27 26	32, 64, 127, 174	2 (0%)
3	C	236/248 (95%)	0.54	14 (5%) 28 27	27, 65, 112, 146	2 (0%)
3	Q	238/248 (95%)	0.68	17 (7%) 22 20	33, 66, 138, 175	0
4	D	233/241 (96%)	0.32	5 (2%) 63 63	33, 62, 95, 139	1 (0%)
4	R	233/241 (96%)	0.11	7 (3%) 52 51	19, 44, 75, 106	1 (0%)
5	E	233/263 (88%)	0.13	12 (5%) 33 31	24, 41, 92, 116	1 (0%)
5	S	237/263 (90%)	0.18	10 (4%) 40 39	22, 48, 86, 118	3 (1%)
6	F	239/255 (93%)	-0.21	4 (1%) 69 68	17, 33, 59, 77	4 (1%)
6	T	240/255 (94%)	0.39	13 (5%) 31 30	28, 57, 97, 137	1 (0%)
7	G	241/246 (97%)	-0.08	4 (1%) 69 68	17, 39, 73, 110	2 (0%)
7	U	235/246 (95%)	0.44	14 (5%) 27 26	33, 67, 107, 136	1 (0%)
8	H	220/234 (94%)	-0.17	5 (2%) 61 60	19, 35, 77, 133	2 (0%)
8	V	220/234 (94%)	0.23	11 (5%) 34 33	25, 50, 91, 130	2 (0%)
9	I	204/205 (99%)	-0.28	2 (0%) 79 79	22, 36, 61, 81	3 (1%)
9	W	204/205 (99%)	0.10	2 (0%) 79 79	30, 51, 80, 92	2 (0%)
10	J	195/201 (97%)	-0.15	1 (0%) 87 87	16, 43, 61, 84	3 (1%)
10	X	195/201 (97%)	-0.07	1 (0%) 87 87	19, 44, 60, 84	2 (1%)
11	K	200/204 (98%)	-0.03	1 (0%) 87 87	24, 47, 76, 97	1 (0%)
11	Y	201/204 (98%)	-0.25	3 (1%) 72 71	20, 35, 60, 81	3 (1%)
12	L	213/213 (100%)	0.03	0 100 100	22, 49, 75, 95	2 (0%)
12	Z	213/213 (100%)	-0.20	3 (1%) 73 73	22, 36, 63, 86	1 (0%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	M	216/219 (98%)	-0.21	2 (0%) 81 80	23, 37, 65, 98	1 (0%)
13	a	216/219 (98%)	-0.20	2 (0%) 81 80	24, 38, 60, 86	2 (0%)
14	N	202/205 (98%)	-0.33	3 (1%) 72 71	19, 32, 55, 81	1 (0%)
14	b	203/205 (99%)	-0.12	3 (1%) 72 71	29, 41, 69, 97	1 (0%)
All	All	6223/6458 (96%)	0.09	176 (2%) 55 54	16, 47, 93, 175	49 (0%)

The worst 5 of 176 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
8	V	204	CYS	5.5
11	K	41	TYR	5.0
5	S	2	PHE	4.9
11	Y	202	GLY	4.4
4	R	241	ILE	4.4

## 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. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
7	YCM	G	137	10/11	0.87	0.14	27,36,52,53	0
7	6V1	U	47	15/16	0.90	0.14	81,117,124,127	0
7	YCM	U	137	10/11	0.91	0.12	54,64,77,80	0
3	YCM	C	63	10/11	0.92	0.10	58,62,76,78	0
5	6V1	S	148	15/16	0.92	0.13	38,70,77,78	0
5	6V1	E	148	15/16	0.92	0.13	31,59,70,71	0
7	6V1	G	47	15/16	0.92	0.12	39,60,67,69	0
10	6V1	X	91	15/16	0.94	0.13	34,57,64,68	0
10	6V1	J	91	15/16	0.95	0.11	32,51,60,60	0
7	6V1	U	161	15/16	0.95	0.09	58,74,81,82	0
3	YCM	Q	63	10/11	0.95	0.08	53,58,69,69	0
7	6V1	G	161	15/16	0.96	0.10	32,53,59,62	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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
15	CL	O	304	1/1	0.79	0.20	77,77,77,77	0
18	1PE	H	305	16/16	0.81	0.17	60,83,112,113	0
15	CL	Q	301	1/1	0.84	0.15	84,84,84,84	0
15	CL	D	301	1/1	0.85	0.22	81,81,81,81	0
15	CL	O	303	1/1	0.86	0.12	99,99,99,99	0
18	1PE	W	303	16/16	0.86	0.13	65,69,85,87	0
18	1PE	L	302	16/16	0.87	0.18	75,84,119,120	0
15	CL	M	303	1/1	0.88	0.15	65,65,65,65	0
18	1PE	L	301	16/16	0.88	0.14	60,77,83,91	0
15	CL	C	302	1/1	0.88	0.18	76,76,76,76	0
18	1PE	N	304	16/16	0.88	0.18	72,74,112,114	0
15	CL	Q	302	1/1	0.88	0.21	72,72,72,72	0
18	1PE	Y	305	16/16	0.88	0.14	59,75,81,84	0
15	CL	E	303	1/1	0.89	0.17	74,74,74,74	0
18	1PE	U	302	16/16	0.90	0.14	50,57,92,92	0
18	1PE	I	303	16/16	0.90	0.12	60,62,82,83	0
15	CL	S	301	1/1	0.90	0.18	81,81,81,81	0
15	CL	D	302	1/1	0.91	0.21	72,72,72,72	0
15	CL	Y	304	1/1	0.91	0.27	75,75,75,75	0
15	CL	a	304	1/1	0.91	0.12	67,67,67,67	0
17	MG	V	301	1/1	0.91	0.06	85,85,85,85	0
15	CL	K	302	1/1	0.92	0.12	84,84,84,84	0
15	CL	a	302	1/1	0.92	0.23	69,69,69,69	0
18	1PE	N	303	16/16	0.92	0.11	39,48,65,68	0
15	CL	K	304	1/1	0.92	0.23	80,80,80,80	0
15	CL	B	302	1/1	0.92	0.22	64,64,64,64	0
15	CL	C	301	1/1	0.92	0.14	76,76,76,76	0
15	CL	S	302	1/1	0.92	0.13	72,72,72,72	0
15	CL	U	301	1/1	0.93	0.16	67,67,67,67	0
15	CL	V	302	1/1	0.93	0.12	68,68,68,68	0
15	CL	V	303	1/1	0.93	0.20	62,62,62,62	0
15	CL	Y	301	1/1	0.93	0.19	69,69,69,69	0
15	CL	K	303	1/1	0.93	0.16	74,74,74,74	0
15	CL	a	301	1/1	0.93	0.20	74,74,74,74	0
15	CL	R	301	1/1	0.93	0.13	67,67,67,67	0
15	CL	H	303	1/1	0.93	0.15	63,63,63,63	0
15	CL	B	301	1/1	0.93	0.11	44,44,44,44	0

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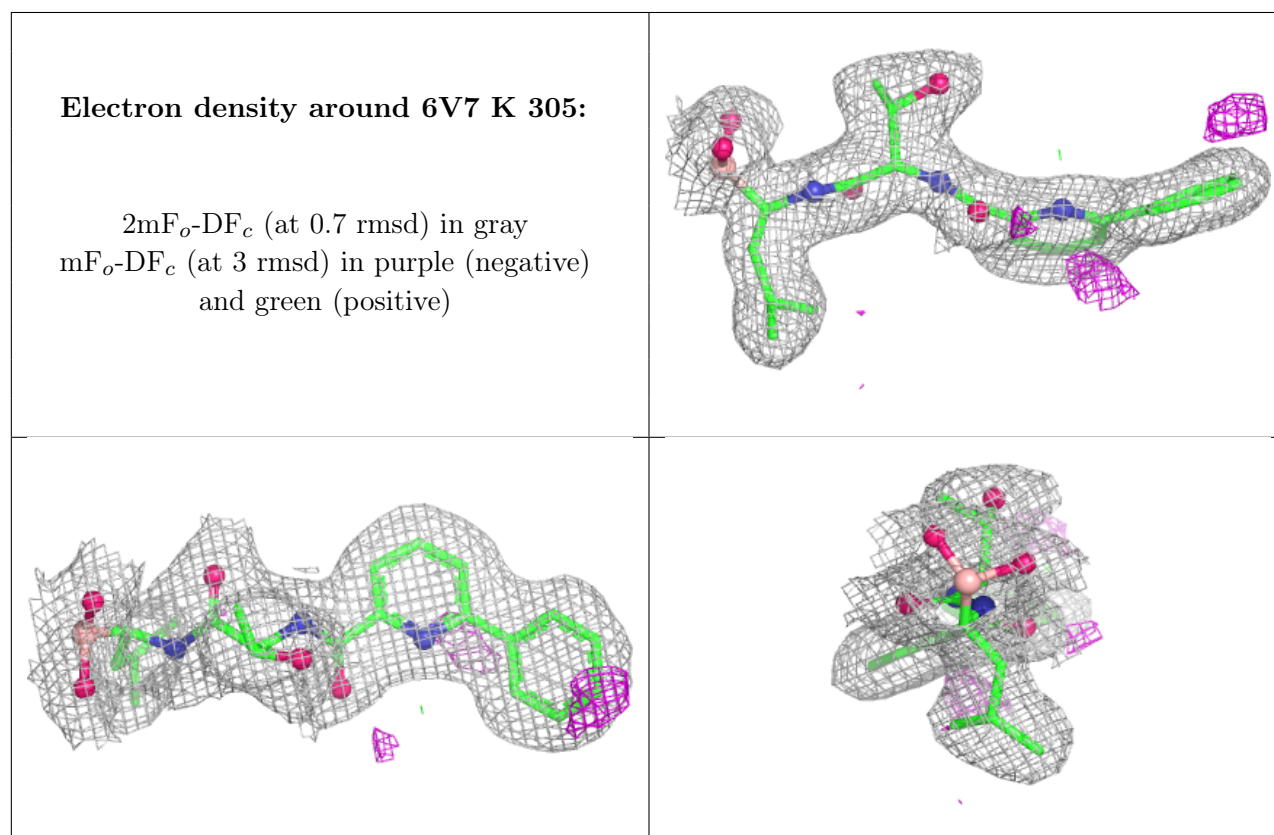
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
15	CL	R	302	1/1	0.94	0.23	61,61,61,61	0
15	CL	E	302	1/1	0.94	0.15	62,62,62,62	0
15	CL	G	301	1/1	0.94	0.24	53,53,53,53	0
15	CL	S	303	1/1	0.94	0.14	59,59,59,59	0
15	CL	b	301	1/1	0.94	0.19	69,69,69,69	0
16	K	N	305	1/1	0.95	0.09	41,41,41,41	0
16	K	b	302	1/1	0.95	0.11	43,43,43,43	0
15	CL	A	304	1/1	0.95	0.12	63,63,63,63	0
15	CL	G	302	1/1	0.95	0.09	68,68,68,68	0
15	CL	M	301	1/1	0.95	0.35	62,62,62,62	0
15	CL	Y	303	1/1	0.95	0.10	68,68,68,68	0
15	CL	A	302	1/1	0.95	0.10	72,72,72,72	0
15	CL	N	301	1/1	0.95	0.20	68,68,68,68	0
15	CL	O	302	1/1	0.95	0.09	72,72,72,72	0
15	CL	a	303	1/1	0.95	0.10	46,46,46,46	0
15	CL	I	302	1/1	0.95	0.10	51,51,51,51	0
15	CL	A	303	1/1	0.95	0.11	57,57,57,57	0
19	6V7	K	305	30/30	0.95	0.07	34,37,46,49	0
19	6V7	Y	306	30/30	0.95	0.07	24,28,34,37	0
15	CL	A	301	1/1	0.96	0.10	55,55,55,55	0
15	CL	F	301	1/1	0.96	0.11	61,61,61,61	0
16	K	U	303	1/1	0.96	0.10	46,46,46,46	0
15	CL	O	301	1/1	0.96	0.14	61,61,61,61	0
16	K	b	303	1/1	0.96	0.10	48,48,48,48	0
17	MG	H	301	1/1	0.96	0.05	71,71,71,71	0
17	MG	I	301	1/1	0.96	0.08	33,33,33,33	0
17	MG	I	304	1/1	0.96	0.09	29,29,29,29	0
15	CL	Y	302	1/1	0.96	0.09	68,68,68,68	0
15	CL	P	301	1/1	0.96	0.09	56,56,56,56	0
19	6V7	b	304	30/30	0.96	0.07	32,36,44,45	0
16	K	N	306	1/1	0.97	0.05	40,40,40,40	0
15	CL	H	304	1/1	0.97	0.10	50,50,50,50	0
17	MG	K	301	1/1	0.97	0.08	37,37,37,37	0
17	MG	L	304	1/1	0.97	0.12	39,39,39,39	0
15	CL	W	302	1/1	0.97	0.06	61,61,61,61	0
17	MG	W	301	1/1	0.97	0.06	37,37,37,37	0
16	K	L	303	1/1	0.97	0.09	53,53,53,53	0
19	6V7	N	307	30/30	0.97	0.06	25,26,37,38	0
15	CL	E	301	1/1	0.97	0.10	68,68,68,68	0
17	MG	H	302	1/1	0.97	0.11	32,32,32,32	0
16	K	Z	301	1/1	0.98	0.07	41,41,41,41	0
15	CL	N	302	1/1	0.98	0.14	59,59,59,59	0

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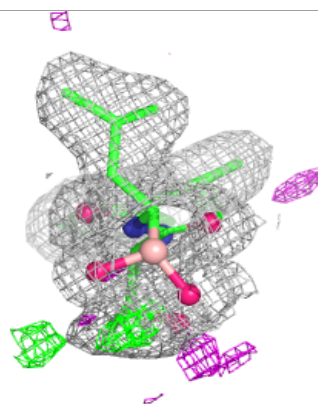
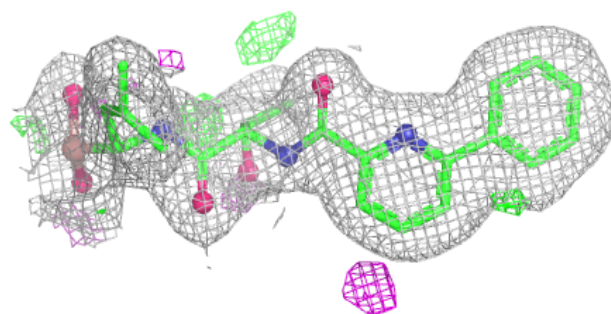
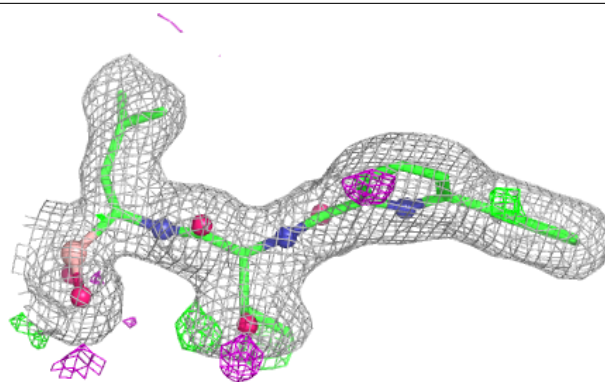
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
15	CL	M	302	1/1	0.98	0.07	42,42,42,42	0
17	MG	J	301	1/1	0.99	0.06	59,59,59,59	0
17	MG	X	301	1/1	0.99	0.03	58,58,58,58	0
16	K	G	303	1/1	0.99	0.07	36,36,36,36	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

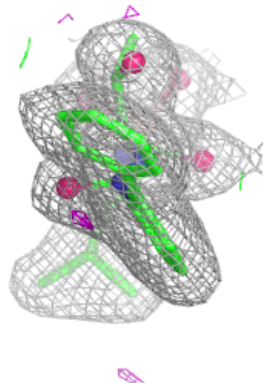
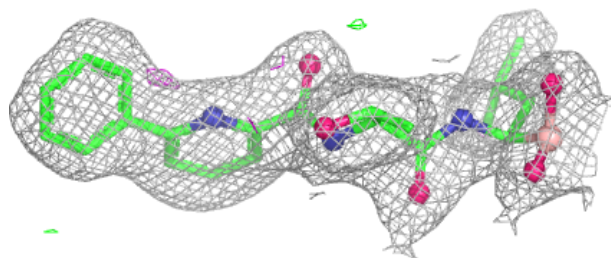
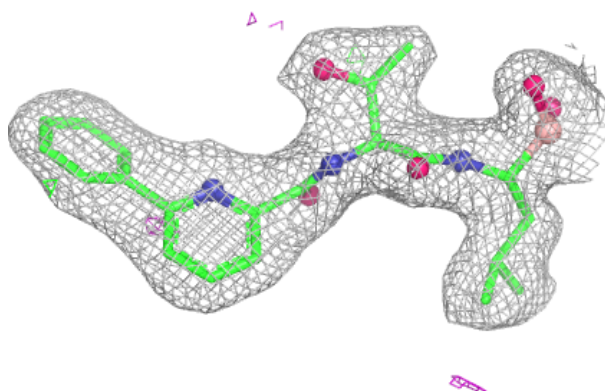


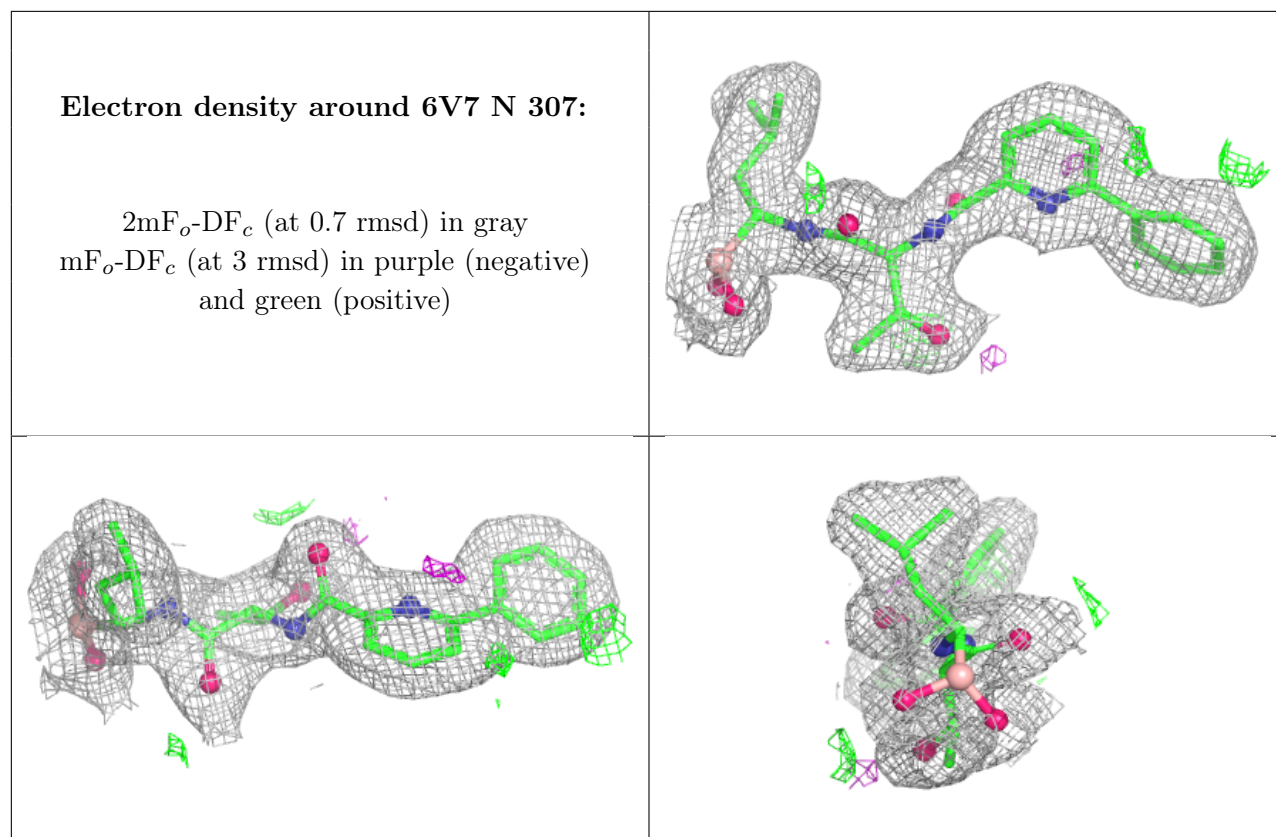
**Electron density around 6V7 Y 306:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around 6V7 b 304:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.