



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 10:15 AM UTC

PDB ID : 5LF7 / pdb_00005lf7
Title : Human 20S proteasome complex with Ixazomib 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 : 2.00 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)
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

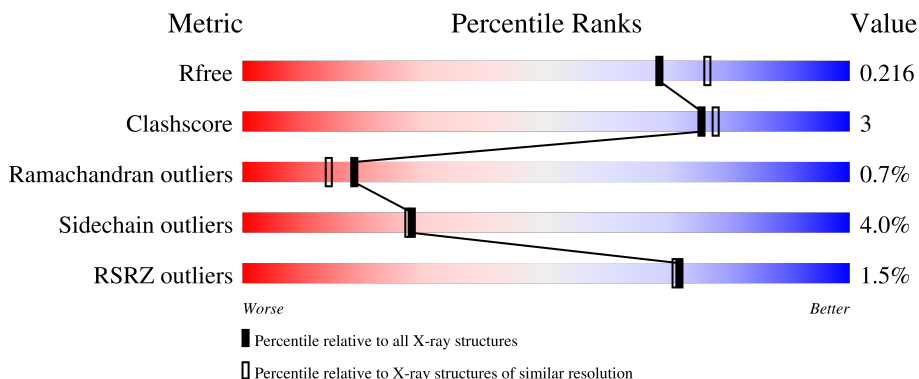
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

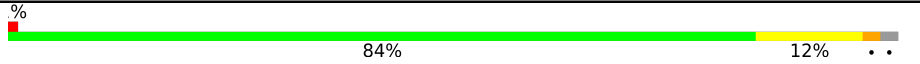
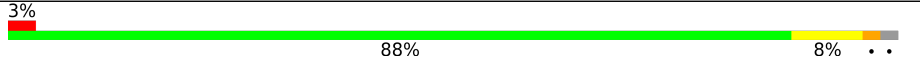



The reported resolution of this entry is 2.00 Å.

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 ≥ 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	 84% 12% . .
1	O	234	 88% 8% . .
2	B	261	 85% 9% . 5%
2	P	261	 83% 9% . . 5%
3	C	248	 81% 12% . .

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Mol	Chain	Length	Quality of chain
3	Q	248	4% 79% 15% . .
4	D	241	% 88% 7% . .
4	R	241	2% 89% 7% . .
5	E	263	2% 79% 9% . 11%
5	S	263	3% 80% 10% . 10%
6	F	255	% 82% 9% . 6%
6	T	255	3% 82% 9% . . 6%
7	G	246	% 90% 7% . .
7	U	246	% 87% 7% . .
8	H	234	% 82% 10% . 6%
8	V	234	3% 84% 9% 6%
9	I	205	90% 8%
9	W	205	90% 7% .
10	J	201	83% 13% . .
10	X	201	86% 10% . .
11	K	204	89% 6% . .
11	Y	204	% 86% 10% . .
12	L	213	93% 7%
12	Z	213	89% 10%
13	M	219	91% 7% .
13	a	219	% 89% 10% .
14	N	205	% 92% 6% .
14	b	205	% 93% 5% . .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	6V1	U	47	X	-	-	-

2 Entry composition [i](#)

There are 20 unique types of molecules in this entry. The entry contains 52085 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	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	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	0	0
			1545	974	269	293	9			
11	Y	201	Total	C	N	O	S	0	3	0
			1580	996	280	294	10			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	216	Total	C	N	O	S	0	1	0
			1692	1067	291	322	12			
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
			1516	950	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	1	Total 1	Cl 1	0	0
15	I	1	Total 1	Cl 1	0	0
15	K	3	Total 3	Cl 3	0	0
15	M	4	Total 4	Cl 4	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	1	Total 1	Cl 1	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

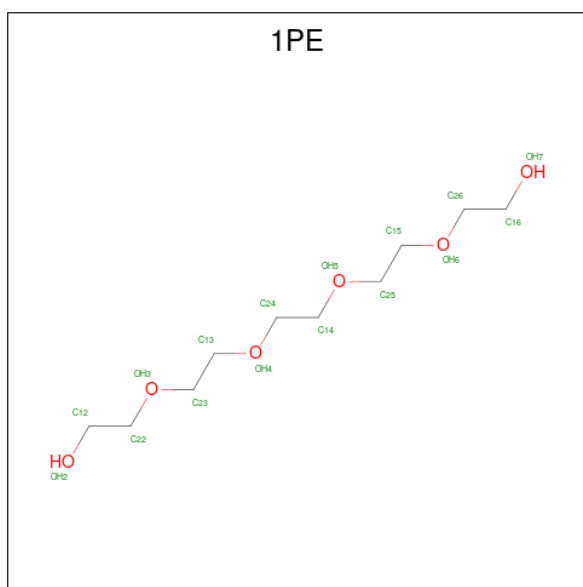
- Molecule 16 is POTASSIUM ION (CCD ID: K) (formula: K).

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	1	Total K 1 1	0	0
16	U	1	Total K 1 1	0	0
16	Z	1	Total K 1 1	0	0
16	b	1	Total K 1 1	0	0

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

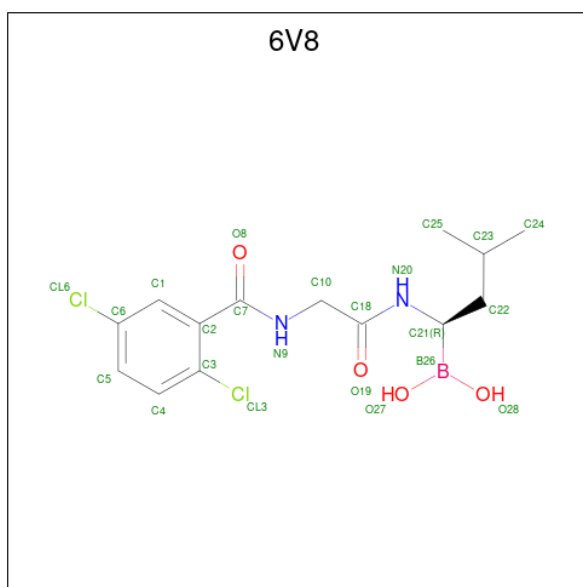
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	H	2	Total Mg 2 2	0	0
17	I	2	Total Mg 2 2	0	0
17	J	1	Total Mg 1 1	0	0
17	K	1	Total Mg 1 1	0	0
17	L	1	Total Mg 1 1	0	0
17	V	1	Total Mg 1 1	0	0
17	W	1	Total Mg 1 1	0	0
17	X	1	Total Mg 1 1	0	0

- Molecule 18 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: C₁₀H₂₂O₆).



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

- Molecule 19 is [(1 {R})-1-[2-[[2,5-bis(chloranyl)phenyl]carbonylamino]ethanoylamino]-3-methyl-butyl]boronic acid (CCD ID: 6V8) (formula: C₁₄H₁₉BCl₂N₂O₄).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	B	C	Cl	N			O
19	H	1	23	1	14	2	2	4	0	0
19	K	1	23	1	14	2	2	4	0	0
19	N	1	23	1	14	2	2	4	0	0
19	V	1	23	1	14	2	2	4	0	0
19	Y	1	23	1	14	2	2	4	0	0
19	b	1	23	1	14	2	2	4	0	0

- Molecule 20 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	A	110	Total 110	O 110	0	0
20	B	124	Total 124	O 124	0	0
20	C	76	Total 76	O 76	0	0
20	D	88	Total 88	O 88	0	0
20	E	143	Total 143	O 143	0	0
20	F	189	Total 189	O 189	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	G	190	Total 190	O 190	0	0
20	H	158	Total 158	O 158	0	0
20	I	153	Total 153	O 153	0	0
20	J	137	Total 137	O 137	0	0
20	K	100	Total 100	O 100	0	0
20	L	131	Total 131	O 131	0	0
20	M	146	Total 146	O 146	0	0
20	N	158	Total 158	O 158	0	0
20	O	92	Total 92	O 92	0	0
20	P	117	Total 117	O 117	0	0
20	Q	73	Total 73	O 73	0	0
20	R	124	Total 124	O 124	0	0
20	S	122	Total 122	O 122	0	0
20	T	89	Total 89	O 89	0	0
20	U	106	Total 106	O 106	0	0
20	V	114	Total 114	O 114	0	0
20	W	114	Total 114	O 114	0	0
20	X	128	Total 128	O 128	0	0
20	Y	150	Total 150	O 150	0	0
20	Z	169	Total 169	O 169	0	0
20	a	173	Total 173	O 173	0	0

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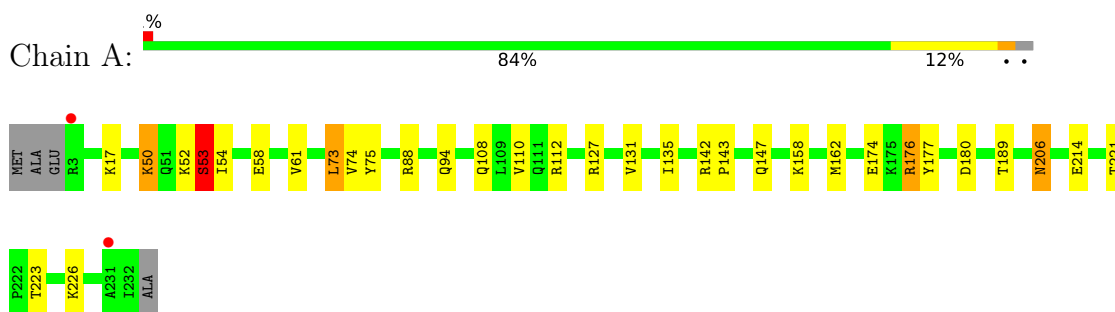
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	b	121	Total 121	O 121	0	0

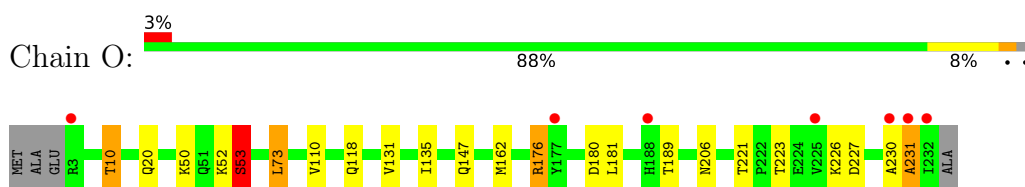
3 Residue-property plots [i](#)

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.

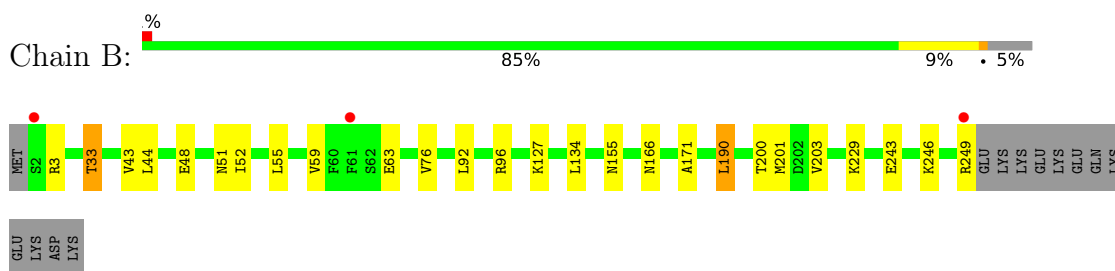
- Molecule 1: Proteasome subunit alpha type-2



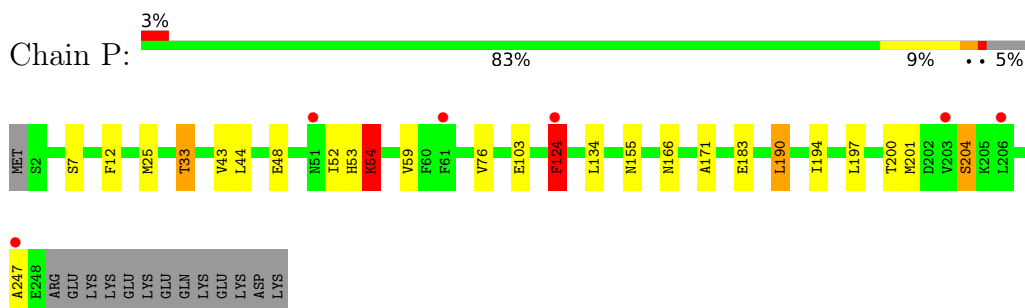
- Molecule 1: Proteasome subunit alpha type-2



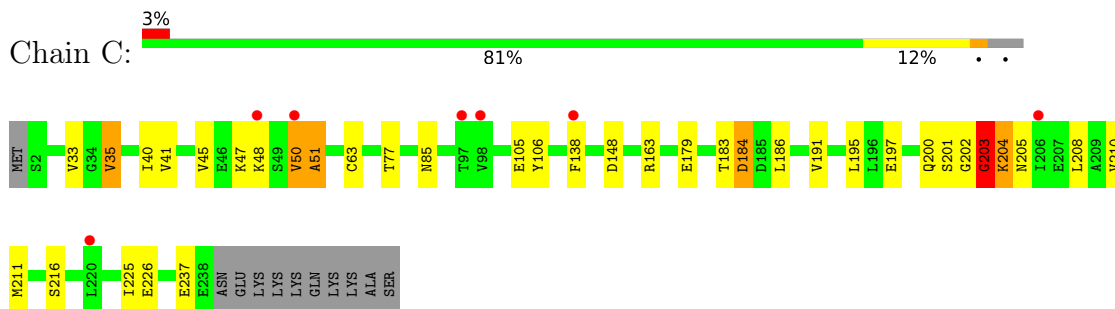
- Molecule 2: Proteasome subunit alpha type-4



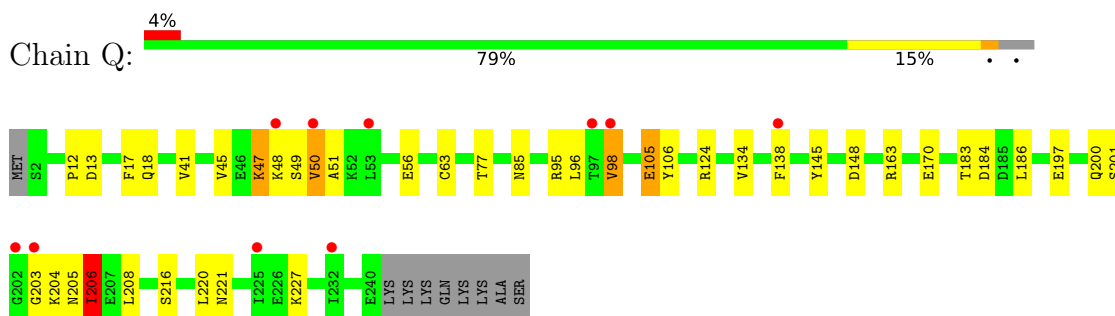
- Molecule 2: Proteasome subunit alpha type-4



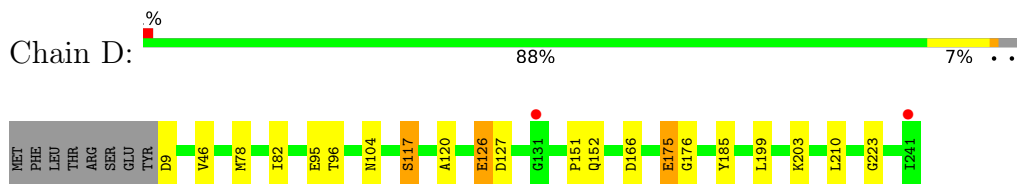
- Molecule 3: Proteasome subunit alpha type-7



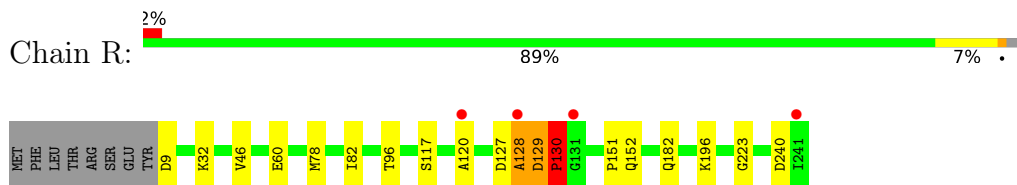
- Molecule 3: Proteasome subunit alpha type-7



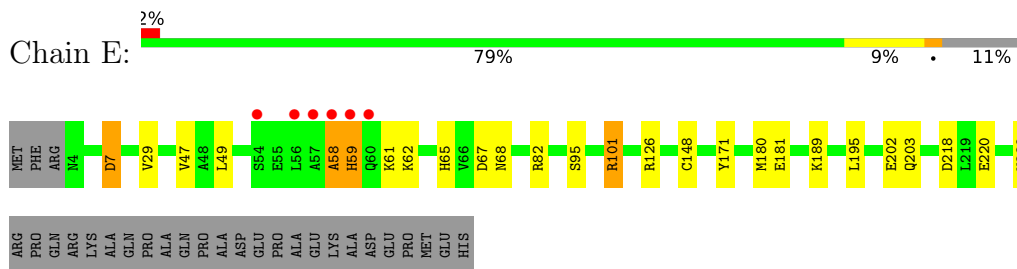
- Molecule 4: Proteasome subunit alpha type-5



- Molecule 4: Proteasome subunit alpha type-5



- Molecule 5: Proteasome subunit alpha type-1




- Molecule 5: Proteasome subunit alpha type-1



MET
ASP
THR
SER

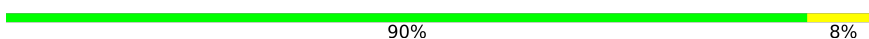
- Molecule 8: Proteasome subunit beta type-7

Chain V:  3% 84% 9% 6%



THR
SER

- Molecule 9: Proteasome subunit beta type-3

Chain I:  90% 8%




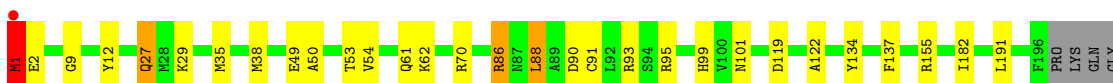
- Molecule 9: Proteasome subunit beta type-3

Chain W:  90% 7%



- Molecule 10: Proteasome subunit beta type-2

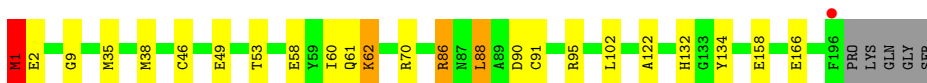
Chain J:  83% 13% ..




SER

- Molecule 10: Proteasome subunit beta type-2

Chain X:  86% 10% ..

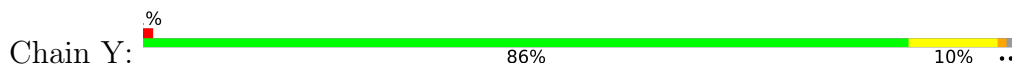


- Molecule 11: Proteasome subunit beta type-5

Chain K:  89% 6% ..



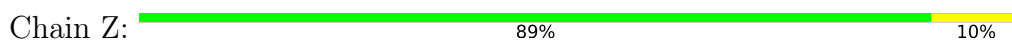
- Molecule 11: Proteasome subunit beta type-5



- Molecule 12: Proteasome subunit beta type-1



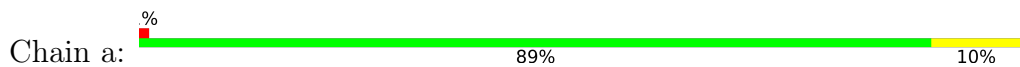
- Molecule 12: Proteasome subunit beta type-1



- Molecule 13: Proteasome subunit beta type-4



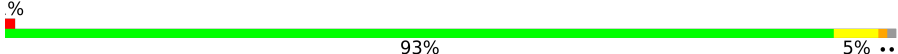
- Molecule 13: Proteasome subunit beta type-4



- Molecule 14: Proteasome subunit beta type-6



- Molecule 14: Proteasome subunit beta type-6

Chain b:  % 93% 5% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	113.41Å 202.61Å 314.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	170.33 – 2.00 170.33 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.6 (170.33-2.00) 99.6 (170.33-2.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.08 (at 2.00Å)	Xtrriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.175 , 0.213 0.182 , 0.216	Depositor DCC
R_{free} test set	24030 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	40.1	Xtrriage
Anisotropy	0.156	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 53.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	52085	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.87% 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, 6V8, MG, K, CL, 1PE, 6V1

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	1.24	1/1833 (0.1%)	1.11	3/2489 (0.1%)
1	O	1.06	0/1778	1.04	1/2419 (0.0%)
2	B	1.16	2/1962 (0.1%)	1.06	2/2649 (0.1%)
2	P	1.16	1/1934 (0.1%)	1.07	2/2617 (0.1%)
3	C	1.13	0/1818	1.16	2/2469 (0.1%)
3	Q	1.19	2/1834 (0.1%)	1.17	9/2490 (0.4%)
4	D	1.11	2/1789 (0.1%)	1.09	1/2424 (0.0%)
4	R	1.26	0/1780	1.16	3/2408 (0.1%)
5	E	1.27	1/1842 (0.1%)	1.14	3/2493 (0.1%)
5	S	1.15	0/1901	1.10	1/2571 (0.0%)
6	F	1.39	4/1935 (0.2%)	1.18	5/2605 (0.2%)
6	T	1.09	1/1894 (0.1%)	1.14	11/2556 (0.4%)
7	G	1.35	6/1909 (0.3%)	1.13	3/2579 (0.1%)
7	U	1.02	0/1804	1.00	1/2441 (0.0%)
8	H	1.47	8/1697 (0.5%)	1.21	6/2299 (0.3%)
8	V	1.24	1/1655 (0.1%)	1.12	5/2251 (0.2%)
9	I	1.32	6/1648 (0.4%)	1.26	10/2219 (0.5%)
9	W	1.26	4/1630 (0.2%)	1.18	9/2197 (0.4%)
10	J	1.27	3/1613 (0.2%)	1.08	4/2180 (0.2%)
10	X	1.31	4/1599 (0.3%)	1.11	4/2163 (0.2%)
11	K	1.28	4/1576 (0.3%)	1.11	2/2131 (0.1%)
11	Y	1.36	5/1620 (0.3%)	1.11	2/2185 (0.1%)
12	L	1.31	2/1672 (0.1%)	1.15	1/2257 (0.0%)
12	Z	1.42	8/1675 (0.5%)	1.18	6/2257 (0.3%)
13	M	1.27	1/1728 (0.1%)	1.12	3/2339 (0.1%)
13	a	1.30	6/1724 (0.3%)	1.11	3/2336 (0.1%)
14	N	1.35	5/1545 (0.3%)	1.15	2/2091 (0.1%)
14	b	1.21	2/1554 (0.1%)	1.11	1/2104 (0.0%)
All	All	1.25	79/48949 (0.2%)	1.13	105/66219 (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	2
3	C	0	2
3	Q	0	2
4	D	0	4
4	R	0	2
5	E	0	1
7	U	1	0
9	I	0	1
9	W	0	1
10	J	0	2
10	X	0	1
11	Y	0	1
13	a	0	1
All	All	1	20

The worst 5 of 79 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	X	86	ARG	CD-NE	-8.37	1.34	1.46
10	J	86	ARG	CD-NE	-8.05	1.34	1.46
6	F	17	ASP	CG-OD2	7.52	1.39	1.25
12	Z	171	ALA	N-CA	7.42	1.55	1.46
12	L	158	MET	N-CA	7.08	1.54	1.46

The worst 5 of 105 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	190	VAL	CB-CA-C	-9.76	98.96	112.14
7	G	183	VAL	CB-CA-C	-9.32	99.56	112.14
6	T	6	GLY	CA-C-N	9.29	138.41	121.70
6	T	6	GLY	C-N-CA	9.29	138.41	121.70
6	T	190	VAL	CB-CA-C	-9.09	100.13	112.04

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	U	47	6V1	C1

5 of 20 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	203	GLY	Peptide
3	C	237	GLU	Peptide
4	D	127	ASP	Peptide
4	D	175[A]	GLU	Peptide
4	D	175[B]	GLU	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	14	0
1	O	1741	0	1683	8	0
2	B	1926	0	1924	10	0
2	P	1898	0	1861	15	0
3	C	1798	0	1718	18	0
3	Q	1820	0	1749	14	0
4	D	1762	0	1709	6	0
4	R	1753	0	1726	9	0
5	E	1822	0	1779	13	0
5	S	1875	0	1818	18	0
6	F	1888	0	1882	13	0
6	T	1856	0	1816	11	0
7	G	1912	0	1882	9	0
7	U	1815	0	1748	13	0
8	H	1664	0	1677	11	0
8	V	1622	0	1591	7	0
9	I	1613	0	1646	9	0
9	W	1599	0	1621	11	0
10	J	1590	0	1581	18	0
10	X	1576	0	1561	15	0
11	K	1545	0	1494	7	0
11	Y	1580	0	1554	15	0
12	L	1636	0	1625	7	0
12	Z	1642	0	1635	6	0
13	M	1692	0	1670	7	0
13	a	1688	0	1658	8	0
14	N	1516	0	1483	7	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	1	0
15	G	2	0	0	0	0
15	H	1	0	0	0	0
15	I	1	0	0	0	0
15	K	3	0	0	0	0
15	M	4	0	0	1	0
15	N	2	0	0	0	0
15	O	4	0	0	0	0
15	P	1	0	0	0	0
15	Q	2	0	0	1	0
15	R	2	0	0	0	0
15	S	3	0	0	0	0
15	U	1	0	0	0	0
15	V	1	0	0	0	0
15	W	1	0	0	0	0
15	Y	4	0	0	0	0
15	a	4	0	0	2	0
15	b	1	0	0	0	0
16	G	1	0	0	0	0
16	L	1	0	0	0	0
16	N	1	0	0	0	0
16	U	1	0	0	0	0
16	Z	1	0	0	0	0
16	b	1	0	0	0	0
17	H	2	0	0	0	0
17	I	2	0	0	0	0
17	J	1	0	0	0	0
17	K	1	0	0	0	0
17	L	1	0	0	0	0
17	V	1	0	0	0	0
17	W	1	0	0	0	0
17	X	1	0	0	0	0
18	H	16	0	22	0	0
18	I	32	0	44	0	0
18	L	16	0	22	0	0
18	M	16	0	22	0	0
18	N	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
18	b	16	0	22	0	0
19	H	23	0	0	0	0
19	K	23	0	0	0	0
19	N	23	0	0	0	0
19	V	23	0	0	0	0
19	Y	23	0	0	0	0
19	b	23	0	0	0	0
20	A	110	0	0	2	0
20	B	124	0	0	0	0
20	C	76	0	0	0	0
20	D	88	0	0	1	0
20	E	143	0	0	2	0
20	F	189	0	0	5	0
20	G	190	0	0	2	0
20	H	158	0	0	5	0
20	I	153	0	0	1	0
20	J	137	0	0	2	0
20	K	100	0	0	0	0
20	L	131	0	0	0	0
20	M	146	0	0	1	0
20	N	158	0	0	1	0
20	O	92	0	0	2	0
20	P	117	0	0	0	0
20	Q	73	0	0	1	0
20	R	124	0	0	2	0
20	S	122	0	0	3	0
20	T	89	0	0	0	0
20	U	106	0	0	2	0
20	V	114	0	0	0	0
20	W	114	0	0	2	0
20	X	128	0	0	1	0
20	Y	150	0	0	2	0
20	Z	169	0	0	1	0
20	a	173	0	0	1	0
20	b	121	0	0	0	0
All	All	52085	0	47542	284	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 284 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	1.17	1.06
10:X:1:MET:HE1	10:X:134:TYR:H	1.22	1.03
11:Y:36:ILE:HD11	11:Y:46:MET:SD	2.12	0.90
8:H:78:VAL:HB	20:H:540:HOH:O	1.72	0.88
11:K:36:ILE:HD11	11:K:46:MET:SD	2.15	0.85

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%)	220 (95%)	7 (3%)	4 (2%)	7	3
1	O	228/234 (97%)	215 (94%)	8 (4%)	5 (2%)	5	2
2	B	248/261 (95%)	239 (96%)	8 (3%)	1 (0%)	30	27
2	P	247/261 (95%)	233 (94%)	10 (4%)	4 (2%)	7	3
3	C	236/248 (95%)	222 (94%)	7 (3%)	7 (3%)	3	1
3	Q	236/248 (95%)	219 (93%)	7 (3%)	10 (4%)	2	0
4	D	232/241 (96%)	224 (97%)	5 (2%)	3 (1%)	9	5
4	R	232/241 (96%)	225 (97%)	4 (2%)	3 (1%)	9	5
5	E	232/263 (88%)	228 (98%)	3 (1%)	1 (0%)	30	27
5	S	238/263 (90%)	232 (98%)	5 (2%)	1 (0%)	30	27
6	F	241/255 (94%)	237 (98%)	4 (2%)	0	100	100
6	T	239/255 (94%)	234 (98%)	2 (1%)	3 (1%)	9	5
7	G	241/246 (98%)	237 (98%)	4 (2%)	0	100	100
7	U	232/246 (94%)	228 (98%)	4 (2%)	0	100	100
8	H	220/234 (94%)	217 (99%)	2 (1%)	1 (0%)	24	21
8	V	220/234 (94%)	216 (98%)	3 (1%)	1 (0%)	24	21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	I	205/205 (100%)	200 (98%)	5 (2%)	0	100	100
9	W	204/205 (100%)	200 (98%)	4 (2%)	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	202/204 (99%)	198 (98%)	3 (2%)	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%)	210 (98%)	5 (2%)	0	100	100
13	a	216/219 (99%)	210 (97%)	6 (3%)	0	100	100
14	N	201/205 (98%)	198 (98%)	3 (2%)	0	100	100
14	b	202/205 (98%)	201 (100%)	1 (0%)	0	100	100
All	All	6211/6458 (96%)	6043 (97%)	123 (2%)	45 (1%)	18	14

5 of 45 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%)	171 (92%)	14 (8%)	12	9
1	O	176/191 (92%)	164 (93%)	12 (7%)	14	11
2	B	200/221 (90%)	194 (97%)	6 (3%)	36	38
2	P	196/221 (89%)	184 (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%)	183 (97%)	6 (3%)	34	35
4	R	187/203 (92%)	183 (98%)	4 (2%)	47	52
5	E	192/223 (86%)	183 (95%)	9 (5%)	23	22
5	S	197/223 (88%)	191 (97%)	6 (3%)	36	38
6	F	199/212 (94%)	187 (94%)	12 (6%)	17	14
6	T	192/212 (91%)	182 (95%)	10 (5%)	21	18
7	G	202/207 (98%)	195 (96%)	7 (4%)	32	32
7	U	186/207 (90%)	179 (96%)	7 (4%)	29	29
8	H	181/195 (93%)	173 (96%)	8 (4%)	25	24
8	V	172/195 (88%)	162 (94%)	10 (6%)	18	15
9	I	176/174 (101%)	173 (98%)	3 (2%)	53	60
9	W	173/174 (99%)	170 (98%)	3 (2%)	53	60
10	J	166/170 (98%)	158 (95%)	8 (5%)	23	21
10	X	165/170 (97%)	160 (97%)	5 (3%)	36	38
11	K	154/159 (97%)	146 (95%)	8 (5%)	21	18
11	Y	159/159 (100%)	152 (96%)	7 (4%)	25	24
12	L	175/178 (98%)	169 (97%)	6 (3%)	32	33
12	Z	175/178 (98%)	169 (97%)	6 (3%)	32	33
13	M	180/181 (99%)	174 (97%)	6 (3%)	33	34
13	a	178/181 (98%)	174 (98%)	4 (2%)	45	50
14	N	157/159 (99%)	155 (99%)	2 (1%)	61	68
14	b	158/159 (99%)	155 (98%)	3 (2%)	50	56
All	All	5033/5366 (94%)	4828 (96%)	205 (4%)	28	26

5 of 205 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	223	THR
4	R	117	SER
13	a	154	LEU
2	P	33	THR
3	Q	56	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 70 such sidechains are listed below:

Mol	Chain	Res	Type
9	W	168	GLN
10	X	61	GLN
12	Z	79	ASN
10	J	61	GLN
9	I	172	ASN

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
7	6V1	G	161	7	13,15,16	1.59	4 (30%)	10,20,22	3.11	7 (70%)
7	6V1	U	161	7	13,15,16	1.90	3 (23%)	10,20,22	2.73	4 (40%)
3	YCM	C	63	3	7,9,10	0.93	0	5,10,12	1.12	1 (20%)
7	YCM	G	137	7	7,9,10	2.27	3 (42%)	5,10,12	2.56	2 (40%)
7	YCM	U	137	7	7,9,10	1.01	0	5,10,12	1.82	1 (20%)
10	6V1	J	91	10	13,15,16	2.26	4 (30%)	10,20,22	5.44	7 (70%)
7	6V1	G	47	7	13,15,16	2.72	4 (30%)	10,20,22	1.50	2 (20%)
5	6V1	S	148	5	13,15,16	1.62	4 (30%)	10,20,22	2.86	4 (40%)
10	6V1	X	91	10	13,15,16	1.99	5 (38%)	10,20,22	5.82	7 (70%)
7	6V1	U	47	7	13,15,16	2.09	2 (15%)	10,20,22	1.98	3 (30%)
3	YCM	Q	63	3	7,9,10	1.10	1 (14%)	5,10,12	2.96	4 (80%)
5	6V1	E	148	5	13,15,16	1.67	3 (23%)	10,20,22	3.20	5 (50%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	6V1	G	161	7	-	2/6/25/27	0/1/1/1
7	6V1	U	161	7	-	1/6/25/27	0/1/1/1
3	YCM	C	63	3	-	1/6/8/10	-
7	YCM	G	137	7	-	3/6/8/10	-
7	YCM	U	137	7	-	1/6/8/10	-
10	6V1	J	91	10	-	2/6/25/27	0/1/1/1
7	6V1	G	47	7	-	0/6/25/27	0/1/1/1
5	6V1	S	148	5	-	2/6/25/27	0/1/1/1
10	6V1	X	91	10	-	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	Q	63	3	-	3/6/8/10	-
5	6V1	E	148	5	-	2/6/25/27	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	47	6V1	CB-SG	-7.29	1.74	1.82
7	U	47	6V1	CB-SG	-6.18	1.76	1.82
10	J	91	6V1	CB-SG	-5.88	1.76	1.82
10	X	91	6V1	CB-SG	-4.82	1.77	1.82
7	U	161	6V1	CB-SG	-4.45	1.77	1.82

The worst 5 of 47 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	X	91	6V1	C5-C4-N3	8.78	113.60	108.07
10	X	91	6V1	C2-N3-C4	-8.30	108.21	113.07
10	X	91	6V1	O7-C2-N3	8.21	134.10	124.14
10	J	91	6V1	C5-C4-N3	8.04	113.13	108.07
10	J	91	6V1	C6-N3-C2	8.03	132.78	123.37

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	U	47	6V1	C1

5 of 19 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	G	137	YCM	SG-CD-CE-OZ1
7	G	137	YCM	SG-CD-CE-NZ2
7	G	161	6V1	C3-C6-N3-C2
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 82 ligands modelled in this entry, 67 are monoatomic - leaving 15 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	6V8	K	305	11	19,23,23	1.64	3 (15%)	25,31,31	2.19	8 (32%)
18	1PE	M	305	-	15,15,15	0.51	0	14,14,14	0.43	0
19	6V8	Y	306	11	19,23,23	1.72	3 (15%)	25,31,31	2.80	9 (36%)
18	1PE	N	303	-	15,15,15	0.51	0	14,14,14	0.77	0
18	1PE	I	304	-	15,15,15	0.50	0	14,14,14	0.77	0
19	6V8	b	304	14	19,23,23	1.72	1 (5%)	25,31,31	1.62	5 (20%)
18	1PE	b	302	-	15,15,15	0.63	0	14,14,14	1.06	1 (7%)
18	1PE	W	303	-	15,15,15	0.58	0	14,14,14	0.47	0
18	1PE	H	304	-	15,15,15	0.44	0	14,14,14	0.46	0
18	1PE	I	303	-	15,15,15	0.57	0	14,14,14	0.89	0
18	1PE	L	301	-	15,15,15	0.61	0	14,14,14	0.75	0
19	6V8	H	305	8	19,23,23	2.44	3 (15%)	25,31,31	2.90	10 (40%)
19	6V8	V	303	8	19,23,23	2.78	3 (15%)	25,31,31	2.96	10 (40%)
19	6V8	N	305	14	19,23,23	1.35	2 (10%)	25,31,31	2.11	7 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	1PE	Y	305	-	15,15,15	0.57	0	14,14,14	0.54	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	6V8	K	305	11	-	0/16/21/21	0/1/1/1
18	1PE	M	305	-	-	7/13/13/13	-
19	6V8	Y	306	11	-	0/16/21/21	0/1/1/1
18	1PE	N	303	-	-	5/13/13/13	-
18	1PE	I	304	-	-	8/13/13/13	-
19	6V8	b	304	14	-	0/16/21/21	0/1/1/1
18	1PE	b	302	-	-	7/13/13/13	-
18	1PE	W	303	-	-	8/13/13/13	-
18	1PE	H	304	-	-	5/13/13/13	-
18	1PE	I	303	-	-	6/13/13/13	-
18	1PE	L	301	-	-	6/13/13/13	-
19	6V8	H	305	8	-	3/16/21/21	0/1/1/1
19	6V8	V	303	8	-	2/16/21/21	0/1/1/1
19	6V8	N	305	14	-	0/16/21/21	0/1/1/1
18	1PE	Y	305	-	-	6/13/13/13	-

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	V	303	6V8	C2-C3	10.68	1.54	1.39
19	H	305	6V8	C2-C3	9.00	1.52	1.39
19	b	304	6V8	C2-C3	6.73	1.48	1.39
19	K	305	6V8	C2-C3	5.30	1.46	1.39
19	Y	306	6V8	C1-C2	-4.98	1.32	1.39

The worst 5 of 50 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	V	303	6V8	C2-C3-CL3	7.74	132.44	121.01
19	V	303	6V8	C3-C2-C7	7.11	134.08	122.56
19	H	305	6V8	C2-C3-CL3	7.07	131.44	121.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	Y	306	6V8	C2-C3-CL3	-6.74	111.06	121.01
19	Y	306	6V8	C4-C3-C2	6.32	128.36	121.36

There are no chirality outliers.

5 of 63 torsion outliers are listed below:

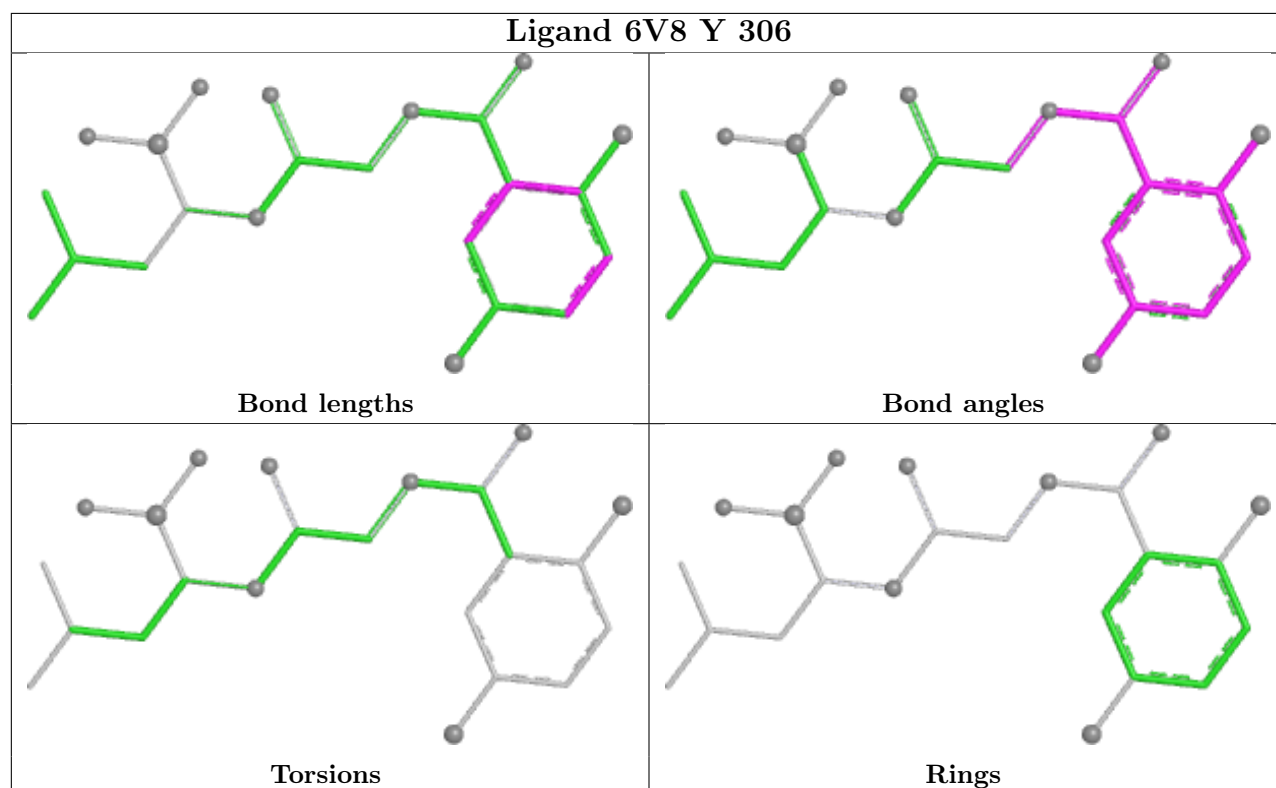
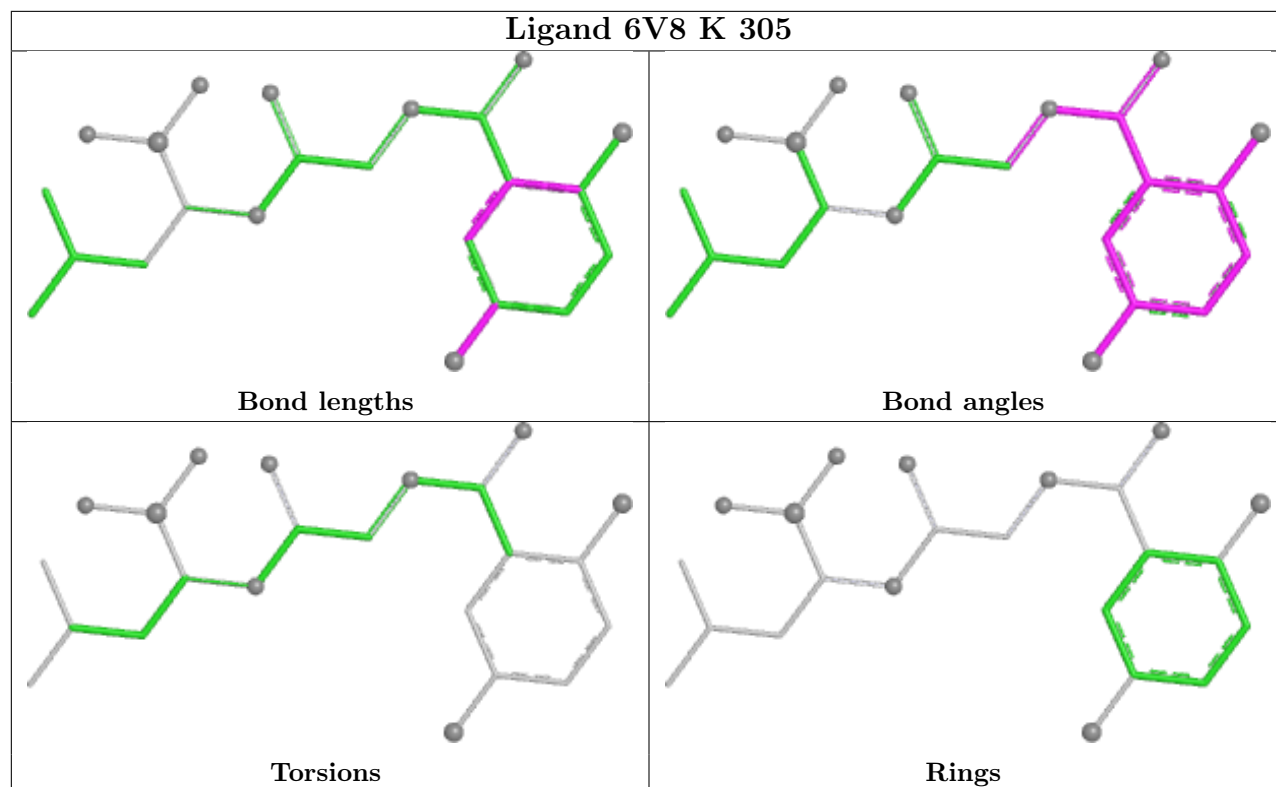
Mol	Chain	Res	Type	Atoms
18	b	302	1PE	C25-C15-OH6-C26
18	L	301	1PE	C16-C26-OH6-C15
18	N	303	1PE	C13-C23-OH3-C22
18	I	304	1PE	C24-C14-OH5-C25
18	I	303	1PE	OH6-C15-C25-OH5

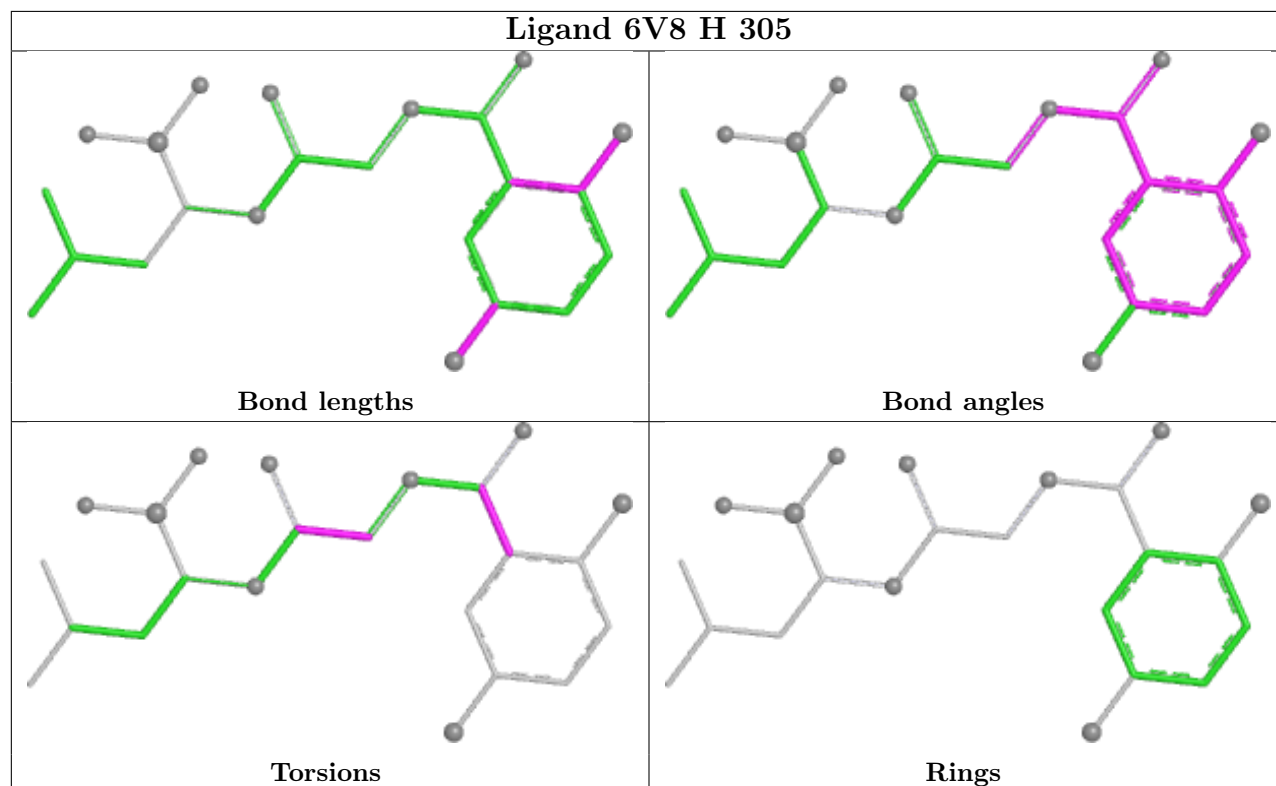
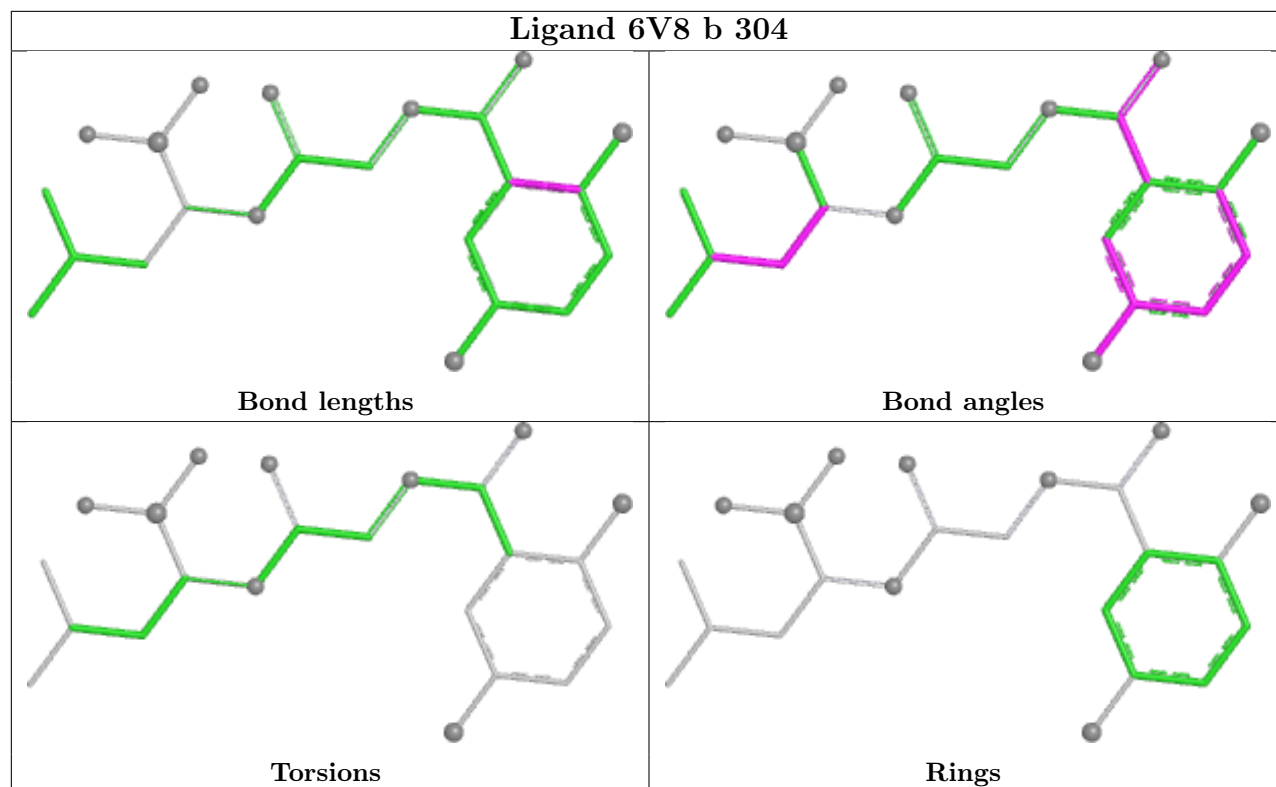
There are no ring outliers.

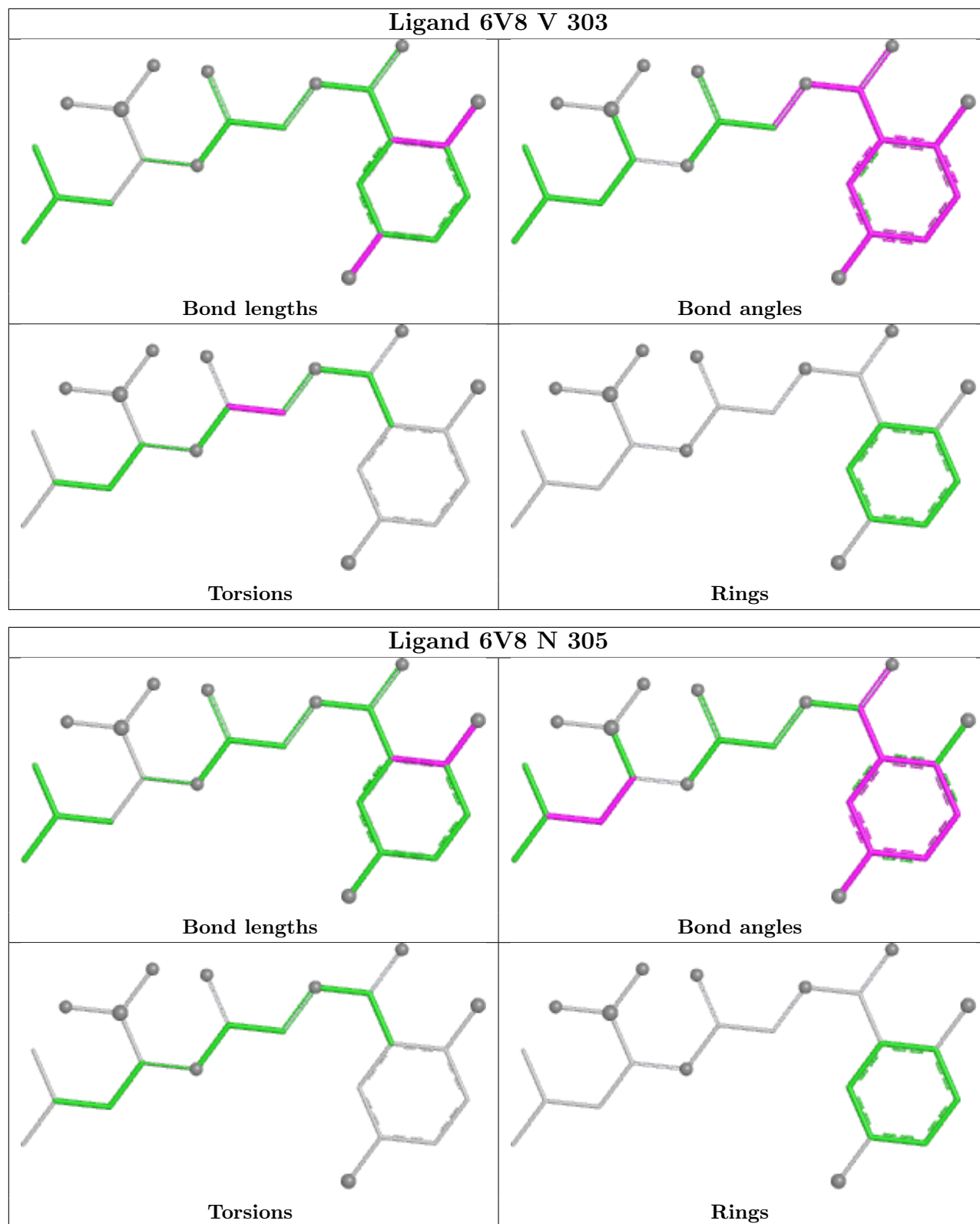
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	N	303	1PE	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

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%)	-0.17	2 (0%) 81 80	25, 45, 86, 98	3 (1%)
1	O	230/234 (98%)	0.34	7 (3%) 52 51	43, 67, 110, 149	0
2	B	248/261 (95%)	0.01	3 (1%) 76 76	21, 54, 98, 137	2 (0%)
2	P	247/261 (94%)	0.20	7 (2%) 55 54	34, 60, 107, 154	2 (0%)
3	C	236/248 (95%)	0.33	7 (2%) 52 51	27, 64, 106, 136	2 (0%)
3	Q	238/248 (95%)	0.44	10 (4%) 40 39	37, 66, 126, 160	0
4	D	233/241 (96%)	0.21	2 (0%) 81 80	33, 61, 91, 135	1 (0%)
4	R	233/241 (96%)	0.06	4 (1%) 69 68	23, 48, 76, 116	1 (0%)
5	E	233/263 (88%)	-0.13	6 (2%) 57 56	26, 43, 91, 112	1 (0%)
5	S	237/263 (90%)	0.10	7 (2%) 52 51	24, 53, 88, 113	3 (1%)
6	F	239/255 (93%)	-0.37	2 (0%) 82 82	21, 36, 60, 82	4 (1%)
6	T	240/255 (94%)	0.36	7 (2%) 53 52	34, 61, 96, 135	1 (0%)
7	G	241/246 (97%)	-0.30	3 (1%) 76 76	19, 40, 72, 110	2 (0%)
7	U	235/246 (95%)	0.32	3 (1%) 75 74	36, 70, 106, 140	1 (0%)
8	H	220/234 (94%)	-0.34	2 (0%) 81 80	22, 37, 75, 126	2 (0%)
8	V	220/234 (94%)	0.07	6 (2%) 56 55	26, 52, 83, 120	2 (0%)
9	I	204/205 (99%)	-0.39	1 (0%) 87 87	22, 38, 60, 77	3 (1%)
9	W	204/205 (99%)	-0.10	0 100 100	29, 50, 76, 88	2 (0%)
10	J	195/201 (97%)	-0.27	1 (0%) 87 87	18, 43, 62, 78	3 (1%)
10	X	195/201 (97%)	-0.23	1 (0%) 87 87	21, 44, 60, 81	2 (1%)
11	K	200/204 (98%)	-0.19	1 (0%) 87 87	33, 47, 76, 88	0
11	Y	201/204 (98%)	-0.33	3 (1%) 72 71	22, 39, 64, 84	3 (1%)
12	L	213/213 (100%)	-0.14	0 100 100	26, 48, 71, 91	2 (0%)
12	Z	213/213 (100%)	-0.33	1 (0%) 87 87	28, 39, 65, 81	1 (0%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	216/219 (98%)	-0.29	1 (0%) 87 87	28, 41, 67, 96	1 (0%)
13	a	216/219 (98%)	-0.26	2 (0%) 81 80	28, 43, 64, 86	2 (0%)
14	N	202/205 (98%)	-0.38	3 (1%) 72 71	20, 38, 60, 101	1 (0%)
14	b	203/205 (99%)	-0.16	3 (1%) 72 71	36, 47, 72, 111	1 (0%)
All	All	6222/6458 (96%)	-0.06	95 (1%) 72 71	18, 49, 91, 160	48 (0%)

The worst 5 of 95 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
11	K	41	TYR	5.0
14	N	203	LEU	4.9
5	S	57	ALA	4.6
11	Y	202	GLY	4.2
4	R	241	ILE	4.2

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	0.86	0.15	85,120,126,126	0
7	YCM	G	137	10/11	0.88	0.14	32,40,55,61	0
3	YCM	C	63	10/11	0.89	0.10	58,60,68,69	0
7	YCM	U	137	10/11	0.90	0.12	59,67,78,79	0
5	6V1	S	148	15/16	0.91	0.14	45,78,85,86	0
7	6V1	U	161	15/16	0.92	0.11	66,88,97,97	0
7	6V1	G	47	15/16	0.93	0.12	37,63,69,70	0
5	6V1	E	148	15/16	0.93	0.13	32,66,78,78	0
3	YCM	Q	63	10/11	0.94	0.09	56,59,73,73	0
10	6V1	X	91	15/16	0.94	0.14	37,67,74,80	0
7	6V1	G	161	15/16	0.95	0.10	33,53,59,61	0
10	6V1	J	91	15/16	0.95	0.12	35,59,70,71	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

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
19	6V8	V	303	23/23	0.79	0.15	60,69,96,114	0
15	CL	Q	301	1/1	0.83	0.12	92,92,92,92	0
18	1PE	I	304	16/16	0.84	0.17	60,79,98,99	0
19	6V8	H	305	23/23	0.84	0.14	47,57,91,103	0
15	CL	O	304	1/1	0.84	0.20	77,77,77,77	0
18	1PE	M	305	16/16	0.85	0.16	68,77,95,97	0
15	CL	D	301	1/1	0.87	0.18	84,84,84,84	0
15	CL	C	302	1/1	0.89	0.20	76,76,76,76	0
17	MG	V	301	1/1	0.89	0.09	75,75,75,75	0
18	1PE	W	303	16/16	0.89	0.13	62,71,82,82	0
18	1PE	H	304	16/16	0.89	0.14	59,66,97,97	0
18	1PE	I	303	16/16	0.89	0.12	54,61,77,87	0
15	CL	Y	304	1/1	0.90	0.21	77,77,77,77	0
18	1PE	Y	305	16/16	0.90	0.14	56,74,81,83	0
15	CL	K	303	1/1	0.90	0.16	78,78,78,78	0
15	CL	O	303	1/1	0.90	0.10	103,103,103,103	0
19	6V8	K	305	23/23	0.91	0.10	41,45,60,77	0
18	1PE	b	302	16/16	0.91	0.14	50,59,91,96	0
15	CL	K	302	1/1	0.92	0.12	80,80,80,80	0
15	CL	D	302	1/1	0.92	0.18	71,71,71,71	0
15	CL	Q	302	1/1	0.92	0.19	72,72,72,72	0
15	CL	E	303	1/1	0.92	0.13	62,62,62,62	0
18	1PE	L	301	16/16	0.92	0.13	59,76,84,85	0
17	MG	H	301	1/1	0.92	0.09	69,69,69,69	0
19	6V8	Y	306	23/23	0.92	0.10	35,37,53,63	0
16	K	L	302	1/1	0.93	0.16	57,57,57,57	0
16	K	Z	301	1/1	0.93	0.12	48,48,48,48	0
15	CL	B	302	1/1	0.93	0.20	64,64,64,64	0
15	CL	a	301	1/1	0.93	0.14	73,73,73,73	0
19	6V8	b	304	23/23	0.93	0.09	39,41,48,54	0
15	CL	M	301	1/1	0.94	0.27	70,70,70,70	0
18	1PE	N	303	16/16	0.94	0.10	43,48,66,68	0
15	CL	M	302	1/1	0.94	0.24	62,62,62,62	0
16	K	b	303	1/1	0.94	0.16	54,54,54,54	0
15	CL	R	302	1/1	0.94	0.22	69,69,69,69	0
15	CL	S	301	1/1	0.94	0.21	77,77,77,77	0
15	CL	Y	302	1/1	0.94	0.12	76,76,76,76	0

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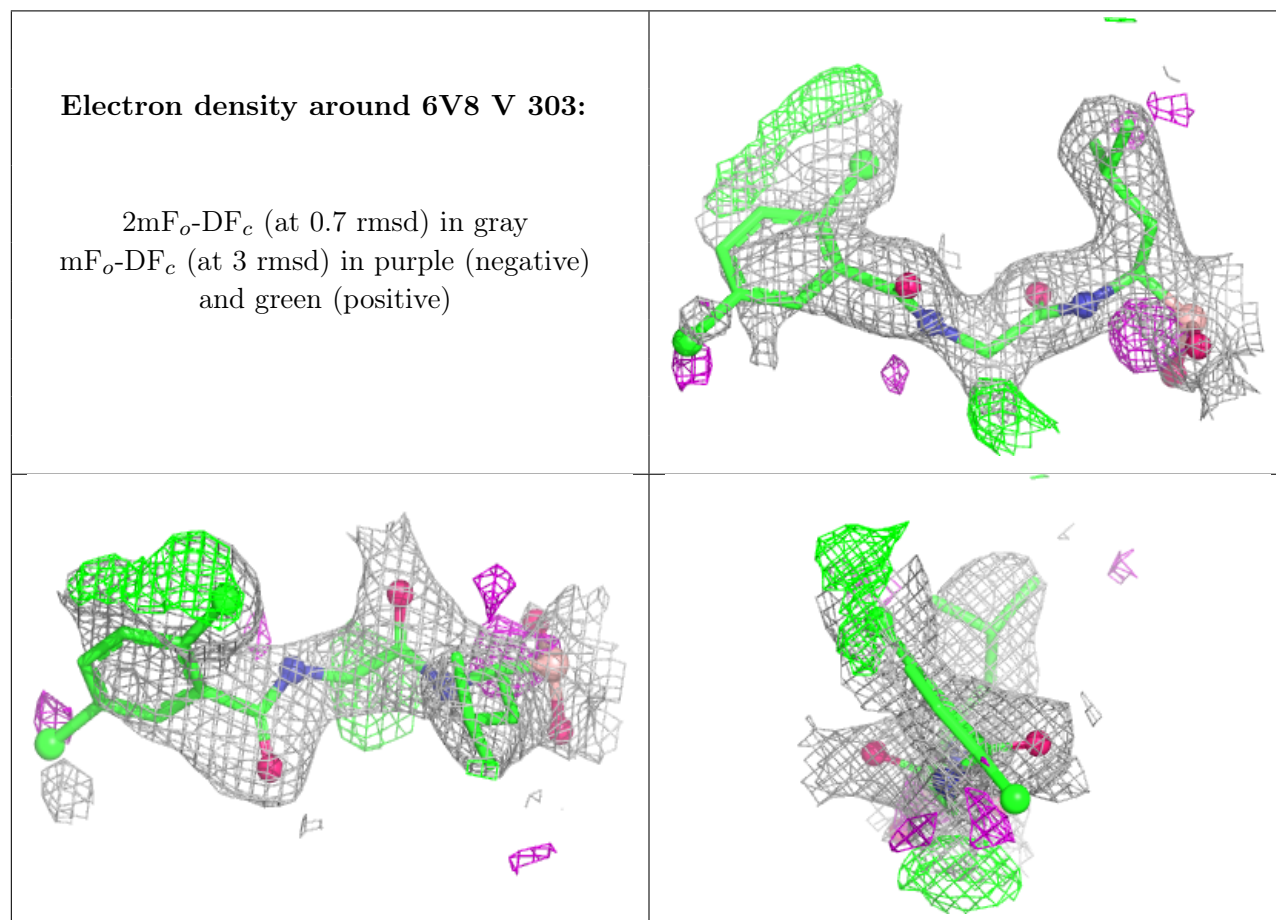
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
19	6V8	N	305	23/23	0.94	0.08	32,34,37,43	0
15	CL	Y	303	1/1	0.94	0.12	60,60,60,60	0
15	CL	C	301	1/1	0.94	0.10	72,72,72,72	0
15	CL	K	304	1/1	0.94	0.25	70,70,70,70	0
17	MG	H	302	1/1	0.95	0.13	34,34,34,34	0
17	MG	K	301	1/1	0.95	0.09	37,37,37,37	0
15	CL	F	301	1/1	0.95	0.14	58,58,58,58	0
15	CL	A	302	1/1	0.95	0.07	72,72,72,72	0
15	CL	a	304	1/1	0.95	0.09	68,68,68,68	0
15	CL	S	302	1/1	0.95	0.14	75,75,75,75	0
15	CL	V	302	1/1	0.95	0.15	66,66,66,66	0
15	CL	O	301	1/1	0.95	0.10	64,64,64,64	0
15	CL	O	302	1/1	0.95	0.10	67,67,67,67	0
15	CL	M	304	1/1	0.96	0.15	59,59,59,59	0
15	CL	E	301	1/1	0.96	0.12	69,69,69,69	0
15	CL	a	302	1/1	0.96	0.16	67,67,67,67	0
15	CL	E	302	1/1	0.96	0.10	57,57,57,57	0
15	CL	b	301	1/1	0.96	0.19	61,61,61,61	0
15	CL	A	304	1/1	0.96	0.15	68,68,68,68	0
15	CL	S	303	1/1	0.96	0.15	63,63,63,63	0
15	CL	A	301	1/1	0.96	0.11	50,50,50,50	0
15	CL	W	302	1/1	0.96	0.06	55,55,55,55	0
15	CL	Y	301	1/1	0.96	0.17	65,65,65,65	0
17	MG	I	305	1/1	0.96	0.09	33,33,33,33	0
15	CL	P	301	1/1	0.96	0.09	57,57,57,57	0
17	MG	L	303	1/1	0.96	0.13	42,42,42,42	0
15	CL	G	301	1/1	0.96	0.18	58,58,58,58	0
17	MG	W	301	1/1	0.96	0.10	38,38,38,38	0
15	CL	N	301	1/1	0.97	0.07	40,40,40,40	0
16	K	U	302	1/1	0.97	0.14	53,53,53,53	0
15	CL	U	301	1/1	0.97	0.08	68,68,68,68	0
15	CL	R	301	1/1	0.97	0.11	64,64,64,64	0
15	CL	N	302	1/1	0.97	0.22	58,58,58,58	0
15	CL	a	303	1/1	0.97	0.12	49,49,49,49	0
17	MG	I	301	1/1	0.97	0.11	34,34,34,34	0
15	CL	A	303	1/1	0.97	0.08	56,56,56,56	0
15	CL	G	302	1/1	0.97	0.07	64,64,64,64	0
15	CL	I	302	1/1	0.98	0.07	46,46,46,46	0
15	CL	B	301	1/1	0.98	0.11	44,44,44,44	0
15	CL	H	303	1/1	0.98	0.11	50,50,50,50	0
16	K	G	303	1/1	0.98	0.14	41,41,41,41	0
15	CL	M	303	1/1	0.98	0.14	45,45,45,45	0

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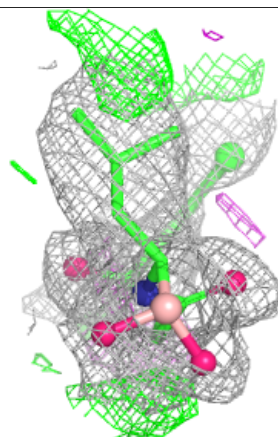
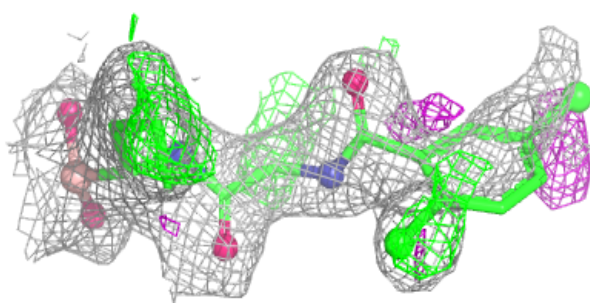
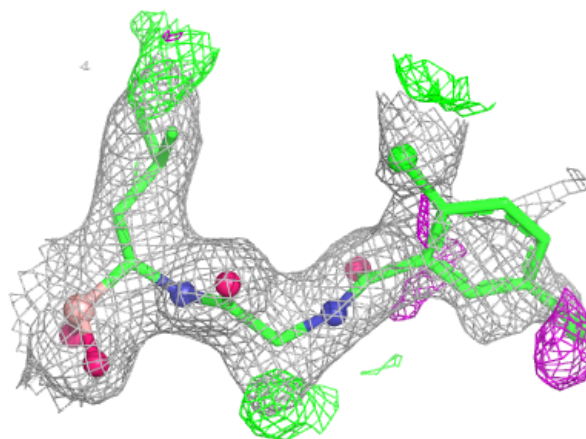
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
17	MG	X	301	1/1	0.98	0.04	49,49,49,49	0
16	K	N	304	1/1	0.98	0.12	49,49,49,49	0
17	MG	J	301	1/1	0.99	0.03	48,48,48,48	0

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.

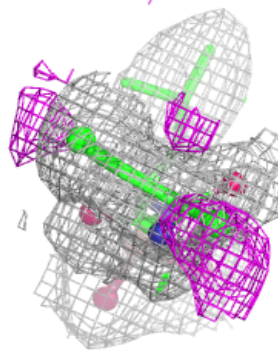
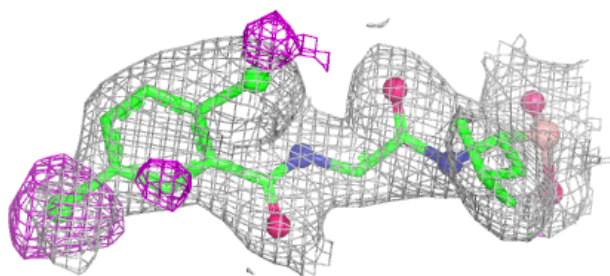
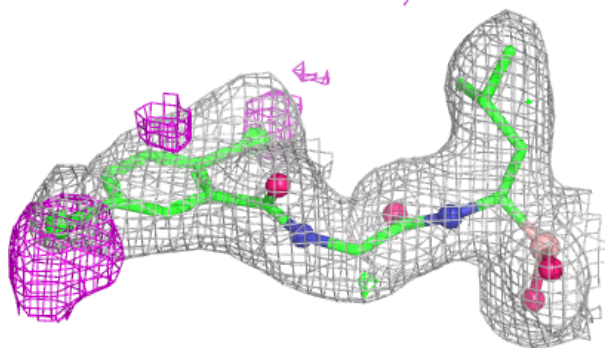


Electron density around 6V8 H 305:

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

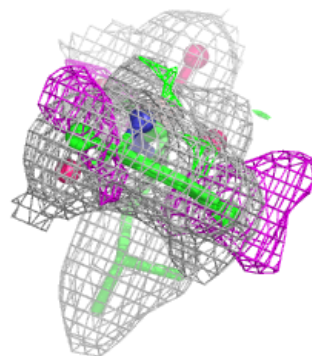
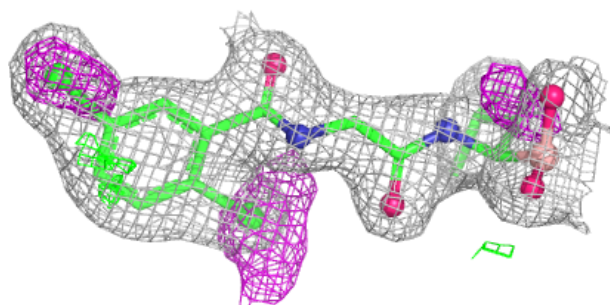
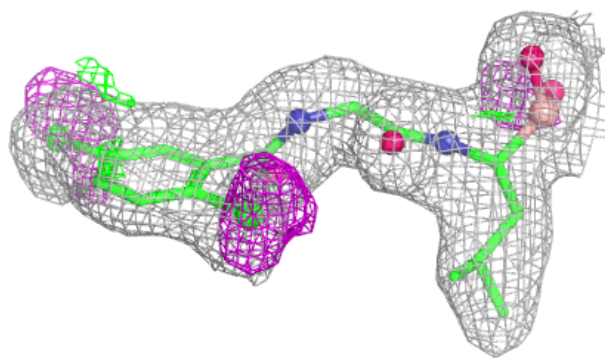
**Electron density around 6V8 K 305:**

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

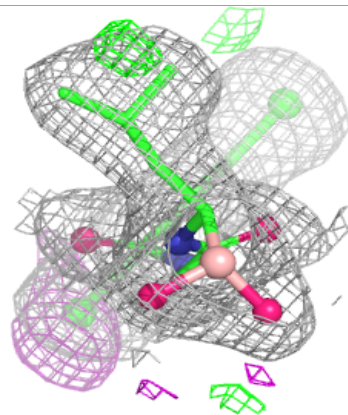
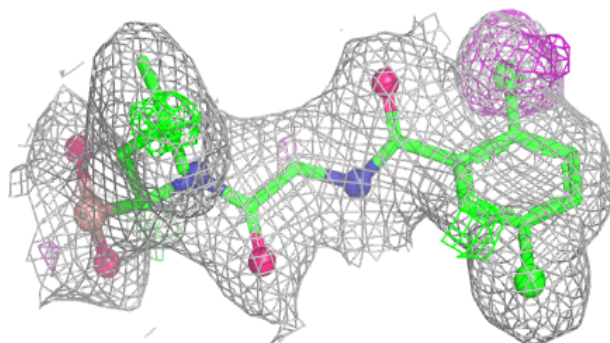
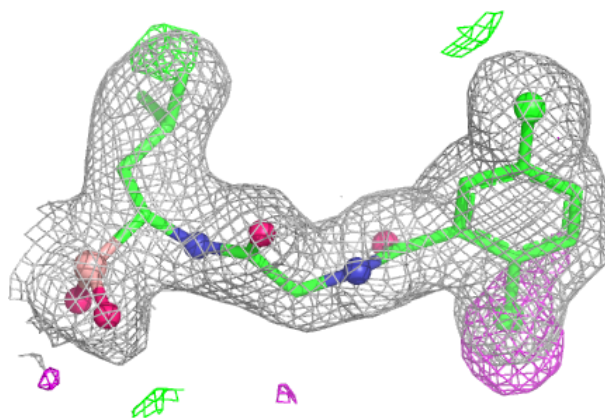


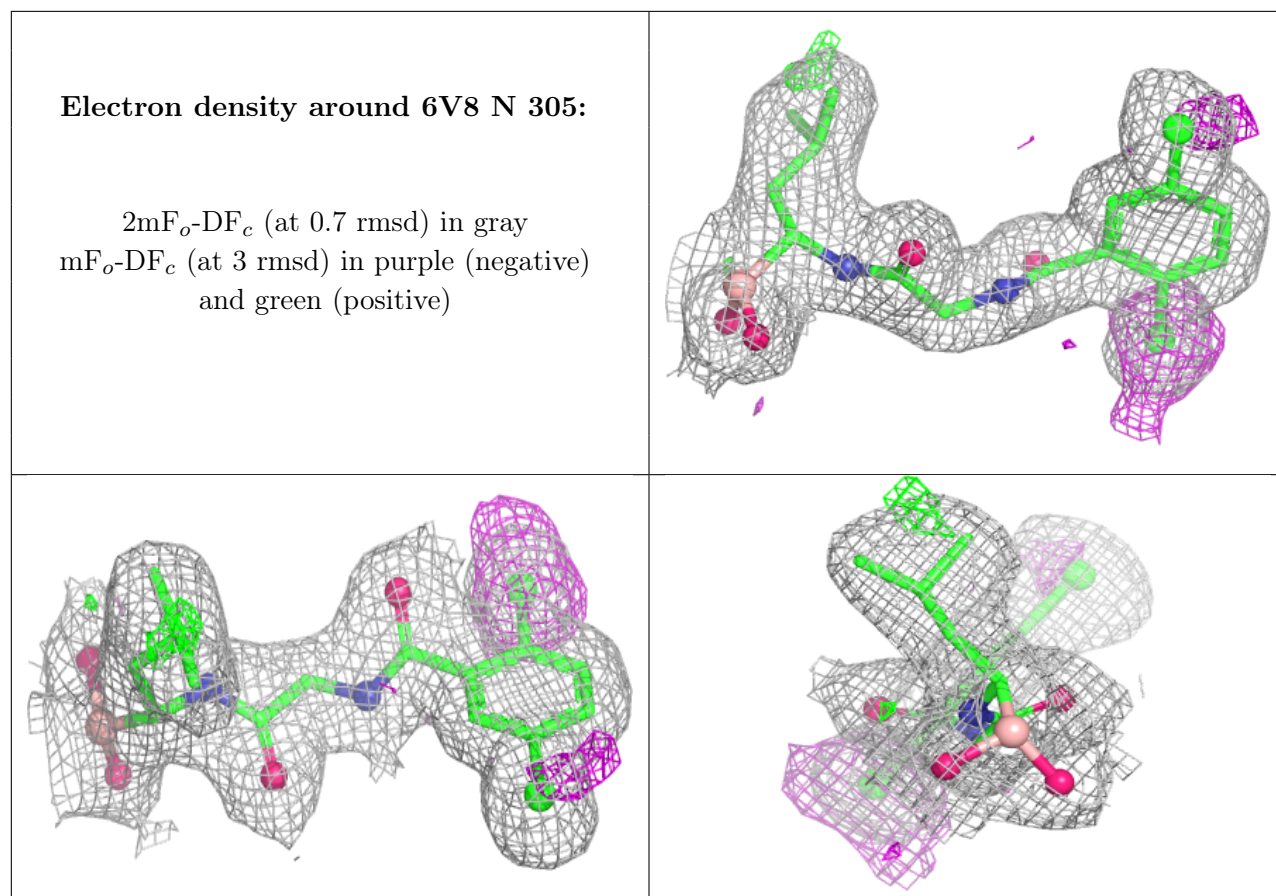
Electron density around 6V8 Y 306:

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

**Electron density around 6V8 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.