



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 24, 2020 – 02:54 PM BST

PDB ID : 5LF7
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 Full wwPDB X-ray Structure Validation 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13

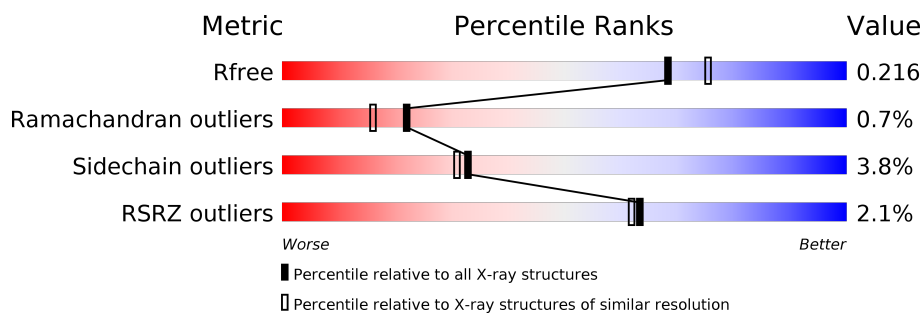
1 Overall quality at a glance

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}	130704	8085 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (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 on 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	<div> <div></div> <div>92% 5% ..</div> </div>
1	O	234	<div> <div>6%</div> <div>91% 6% ..</div> </div>
2	B	261	<div> <div>2%</div> <div>90% 5% 5%</div> </div>
2	P	261	<div> <div>5%</div> <div>87% 6% • 5%</div> </div>
3	C	248	<div> <div>6%</div> <div>87% 8% •</div> </div>
3	Q	248	<div> <div>7%</div> <div>85% 10% • •</div> </div>
4	D	241	<div> <div>2%</div> <div>92% 5% •</div> </div>

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Mol	Chain	Length	Quality of chain
4	R	241	
5	E	263	
5	S	263	
6	F	255	
6	T	255	
7	G	246	
7	U	246	
8	H	234	
8	V	234	
9	I	205	
9	W	205	
10	J	201	
10	X	201	
11	K	204	
11	Y	204	
12	L	213	
12	Z	213	
13	M	219	
13	a	219	
14	N	205	
14	b	205	

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

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
1	A	230	Total	C	N	O	S	0	3	0
			1788	1145	301	336	6			
1	O	230	Total	C	N	O	S	0	0	0
			1741	1111	293	331	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	248	Total	C	N	O	S	0	2	0
			1926	1220	332	363	11			
2	P	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
3	C	237	Total	C	N	O	S	0	2	0
			1798	1121	320	352	5			
3	Q	239	Total	C	N	O	S	0	0	0
			1820	1136	320	359	5			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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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 (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	P	1	Total	Cl	0	0
			1	1		
15	K	3	Total	Cl	0	0
			3	3		

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

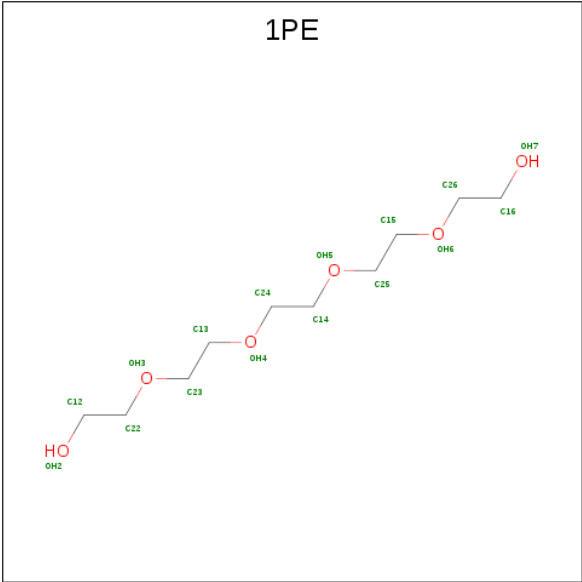
- Molecule 16 is POTASSIUM ION (three-letter code: K) (formula: K).

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

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

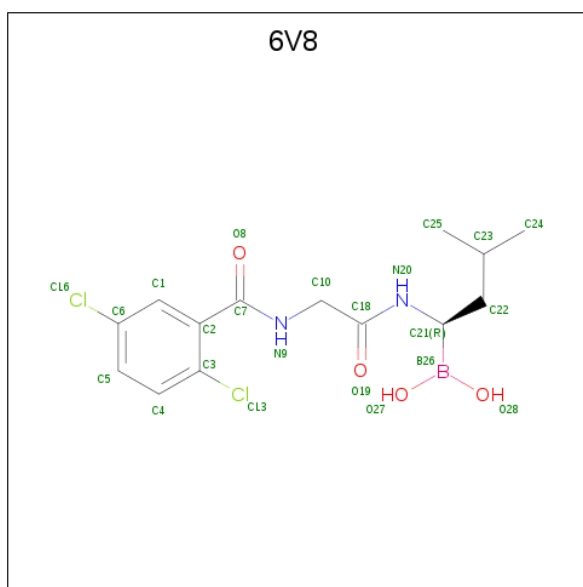
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	J	1	Total Mg 1 1	0	0
17	K	1	Total Mg 1 1	0	0
17	H	2	Total Mg 2 2	0	0
17	I	2	Total Mg 2 2	0	0
17	V	1	Total Mg 1 1	0	0
17	W	1	Total Mg 1 1	0	0
17	X	1	Total Mg 1 1	0	0
17	L	1	Total Mg 1 1	0	0

- Molecule 18 is PENTAETHYLENE GLYCOL (three-letter code: 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 (three-letter code: 6V8) (formula: C₁₄H₁₉BCl₂N₂O₄).



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

- Molecule 20 is water.

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

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

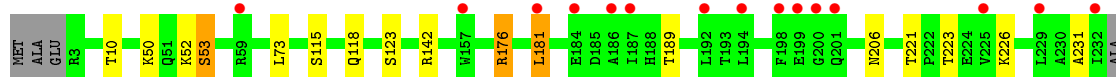
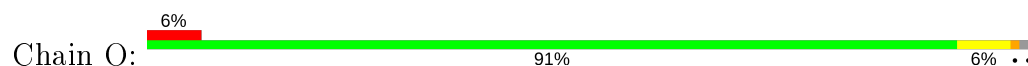
3 Residue-property plots [i](#)

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



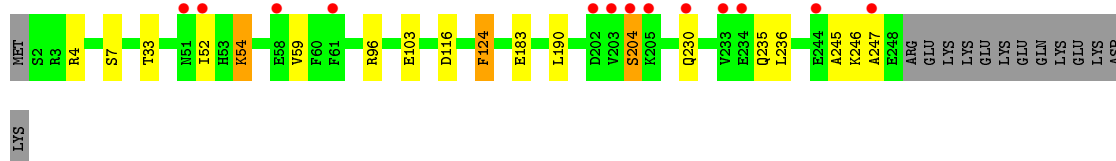
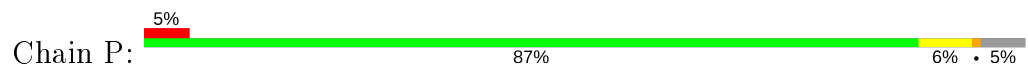
- Molecule 1: Proteasome subunit alpha type-2



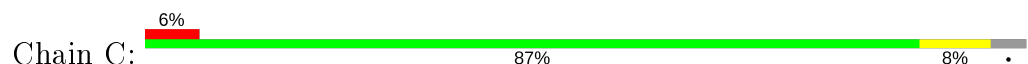
- Molecule 2: Proteasome subunit alpha type-4



- Molecule 2: Proteasome subunit alpha type-4



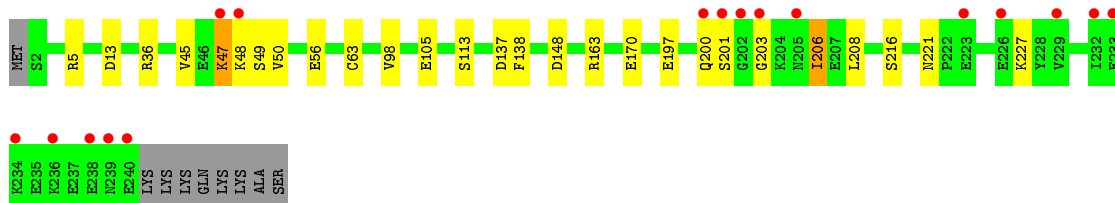
- Molecule 3: Proteasome subunit alpha type-7



LYS
GLN
LYS
LYS
ALA
SER

• Molecule 3: Proteasome subunit alpha type-7

Chain Q: 7% 85% 10% . .



• Molecule 4: Proteasome subunit alpha type-5

Chain D: 2% 92% 5% .



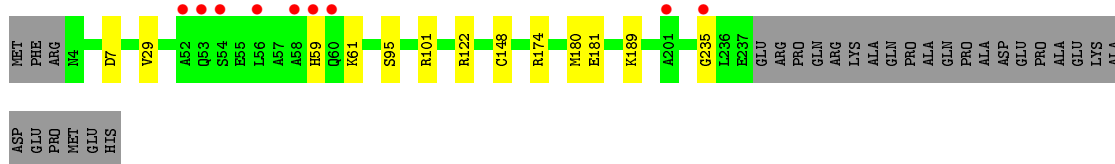
• Molecule 4: Proteasome subunit alpha type-5

Chain R: 2% 91% 5% .



• Molecule 5: Proteasome subunit alpha type-1

Chain E: 3% 84% 5% 11%



ASP
GLU
PRO
MET
GLU
HIS

• Molecule 5: Proteasome subunit alpha type-1

Chain S: 3% 86% 10% .

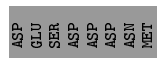
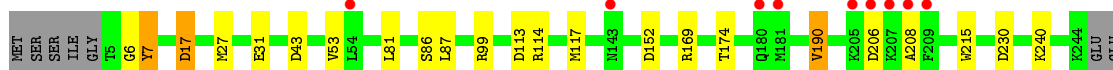
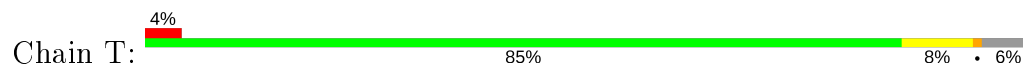


• Molecule 6: Proteasome subunit alpha type-3

Chain F: 87% 5% 6%



• Molecule 6: Proteasome subunit alpha type-3



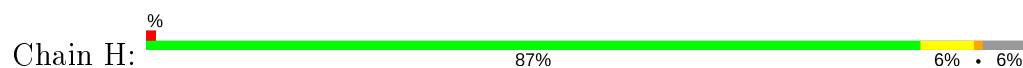
• Molecule 7: Proteasome subunit alpha type-6



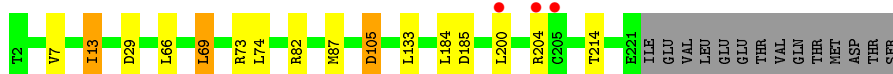
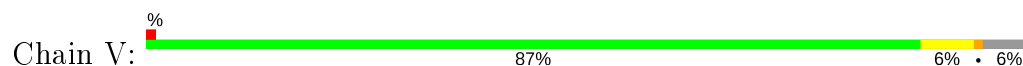
• Molecule 7: Proteasome subunit alpha type-6



• Molecule 8: Proteasome subunit beta type-7



• Molecule 8: Proteasome subunit beta type-7



• Molecule 9: Proteasome subunit beta type-3



- Molecule 9: Proteasome subunit beta type-3

Chain W:  94% 5%



- Molecule 10: Proteasome subunit beta type-2

Chain J:  91% 6% •



- Molecule 10: Proteasome subunit beta type-2

Chain X:  91% 6% •



- Molecule 11: Proteasome subunit beta type-5

Chain K:  92% 5% ••



- Molecule 11: Proteasome subunit beta type-5

Chain Y:  92% 6% •



- Molecule 12: Proteasome subunit beta type-1

Chain L:  95% ••



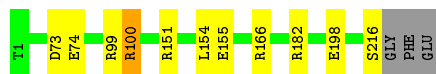
- Molecule 12: Proteasome subunit beta type-1

Chain Z:  94% 5% •



- Molecule 13: Proteasome subunit beta type-4

Chain M:  94% 5% •



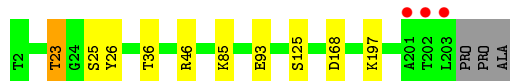
- Molecule 13: Proteasome subunit beta type-4

Chain a:  94% 5% •



- Molecule 14: Proteasome subunit beta type-6

Chain N:  94% • •



- Molecule 14: Proteasome subunit beta type-6

Chain b:  96% • • •



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 – 2.00 106.69 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.6 (170.33-2.00) 99.4 (106.69-2.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.08 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.175 , 0.213 0.181 , 0.216	Depositor DCC
R_{free} test set	24030 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	40.1	Xtriage
Anisotropy	0.156	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 51.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
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

Xtriage'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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 6V8, K, CL, 6V1, 1PE, YCM

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.95	2/1833 (0.1%)	0.94	2/2489 (0.1%)
1	O	0.81	2/1778 (0.1%)	0.87	2/2419 (0.1%)
2	B	0.90	2/1962 (0.1%)	0.94	6/2649 (0.2%)
2	P	0.92	2/1934 (0.1%)	0.96	6/2617 (0.2%)
3	C	0.84	1/1818 (0.1%)	0.98	5/2469 (0.2%)
3	Q	0.87	2/1834 (0.1%)	0.96	5/2490 (0.2%)
4	D	0.87	1/1789 (0.1%)	0.91	3/2424 (0.1%)
4	R	0.98	3/1780 (0.2%)	0.98	5/2408 (0.2%)
5	E	0.94	1/1842 (0.1%)	0.98	2/2493 (0.1%)
5	S	0.85	0/1901	0.93	4/2571 (0.2%)
6	F	1.08	1/1935 (0.1%)	1.09	9/2605 (0.3%)
6	T	0.82	1/1894 (0.1%)	1.02	15/2556 (0.6%)
7	G	1.07	5/1909 (0.3%)	0.96	6/2579 (0.2%)
7	U	0.79	2/1804 (0.1%)	0.88	6/2441 (0.2%)
8	H	1.09	4/1697 (0.2%)	1.14	12/2299 (0.5%)
8	V	0.94	2/1655 (0.1%)	1.02	11/2251 (0.5%)
9	I	1.05	4/1648 (0.2%)	1.16	11/2219 (0.5%)
9	W	0.96	0/1630	1.10	11/2197 (0.5%)
10	J	0.94	1/1613 (0.1%)	1.14	10/2180 (0.5%)
10	X	0.99	2/1599 (0.1%)	1.14	8/2163 (0.4%)
11	K	1.04	3/1576 (0.2%)	1.04	6/2131 (0.3%)
11	Y	1.09	1/1620 (0.1%)	1.08	7/2185 (0.3%)
12	L	1.02	1/1672 (0.1%)	1.04	5/2257 (0.2%)
12	Z	1.11	3/1675 (0.2%)	1.09	7/2257 (0.3%)
13	M	1.01	1/1728 (0.1%)	1.04	7/2339 (0.3%)
13	a	1.01	3/1724 (0.2%)	1.01	3/2336 (0.1%)
14	N	1.06	5/1545 (0.3%)	0.98	4/2091 (0.2%)
14	b	0.92	1/1554 (0.1%)	0.99	4/2104 (0.2%)
All	All	0.96	56/48949 (0.1%)	1.01	182/66219 (0.3%)

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

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	108	GLU	CD-OE1	10.94	1.37	1.25
8	H	32	CYS	CB-SG	-9.11	1.66	1.82
12	Z	3	SER	CB-OG	9.01	1.53	1.42
2	P	103	GLU	CD-OE2	8.79	1.35	1.25
12	Z	142	SER	CB-OG	-7.82	1.32	1.42
1	O	123	SER	CB-OG	-7.69	1.32	1.42
2	B	103	GLU	CD-OE2	7.33	1.33	1.25
1	A	123	SER	CB-OG	-7.22	1.32	1.42
7	U	108	GLU	CD-OE1	7.06	1.33	1.25
10	X	86	ARG	CD-NE	-7.01	1.34	1.46
12	L	129	SER	CB-OG	-6.86	1.33	1.42
14	N	25	SER	CB-OG	-6.76	1.33	1.42
10	J	86	ARG	CD-NE	-6.75	1.34	1.46
8	V	105[A]	ASP	CB-CG	-6.67	1.37	1.51
8	V	105[B]	ASP	CB-CG	-6.67	1.37	1.51
8	H	132	SER	CB-OG	-6.47	1.33	1.42
9	I	105	GLU	CD-OE2	6.34	1.32	1.25
4	R	35	SER	CB-OG	-6.33	1.34	1.42
3	Q	13	ASP	CB-CG	6.25	1.64	1.51
6	F	17	ASP	CG-OD2	6.21	1.39	1.25
11	K	41	TYR	CG-CD1	6.19	1.47	1.39
3	Q	113	SER	CB-OG	-6.07	1.34	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	7	ASP	CB-CG	-5.87	1.39	1.51
11	K	54	SER	CB-OG	-5.76	1.34	1.42
1	O	115	SER	CB-OG	-5.76	1.34	1.42
13	M	74	GLU	CD-OE1	5.72	1.31	1.25
7	G	78	CYS	CB-SG	-5.68	1.72	1.81
2	B	103	GLU	CD-OE1	5.63	1.31	1.25
13	a	75	GLU	CG-CD	5.61	1.60	1.51
14	N	93	GLU	CD-OE1	5.60	1.31	1.25
8	H	7	VAL	CB-CG1	-5.59	1.41	1.52
14	N	93	GLU	CG-CD	5.58	1.60	1.51
11	Y	41	TYR	CG-CD1	5.50	1.46	1.39
4	R	25	GLU	CD-OE1	5.49	1.31	1.25
7	G	39	SER	CB-OG	5.48	1.49	1.42
13	a	119	GLU	CG-CD	5.47	1.60	1.51
1	A	97	TYR	CE1-CZ	5.46	1.45	1.38
13	a	82	SER	CB-OG	-5.44	1.35	1.42
7	G	108	GLU	CD-OE2	5.42	1.31	1.25
3	C	113	SER	CB-OG	-5.42	1.35	1.42
11	K	159	ARG	CZ-NH2	-5.40	1.26	1.33
12	Z	31	GLU	CD-OE2	5.36	1.31	1.25
14	N	26	TYR	CZ-OH	5.35	1.47	1.37
10	X	154	GLU	CG-CD	5.29	1.59	1.51
6	T	7	TYR	N-CA	5.28	1.56	1.46
4	R	216	GLU	CD-OE2	5.20	1.31	1.25
9	I	102	TYR	CG-CD2	5.18	1.45	1.39
7	G	101	TRP	CG-CD1	-5.14	1.29	1.36
9	I	16[A]	LYS	C-O	5.12	1.33	1.23
9	I	16[B]	LYS	C-O	5.12	1.33	1.23
4	D	25	GLU	CD-OE1	5.12	1.31	1.25
8	H	92	GLN	CG-CD	5.09	1.62	1.51
14	b	30	ARG	CD-NE	-5.07	1.37	1.46
2	P	124	PHE	CG-CD1	5.07	1.46	1.38
14	N	125	SER	CB-OG	-5.07	1.35	1.42
7	U	108	GLU	CD-OE2	5.00	1.31	1.25

All (182) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	X	86	ARG	NE-CZ-NH2	-18.15	111.23	120.30
10	J	86	ARG	NE-CZ-NH2	-17.76	111.42	120.30
9	I	69	ARG	NE-CZ-NH1	15.65	128.12	120.30
9	W	69	ARG	NE-CZ-NH1	13.79	127.20	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	J	86	ARG	NE-CZ-NH1	13.19	126.89	120.30
10	X	86	ARG	NE-CZ-NH1	12.78	126.69	120.30
8	H	73	ARG	NE-CZ-NH2	-12.55	114.03	120.30
14	b	30	ARG	NE-CZ-NH1	11.76	126.18	120.30
6	F	17	ASP	CB-CG-OD1	-10.77	108.60	118.30
2	P	124	PHE	CB-CG-CD1	-10.36	113.55	120.80
11	Y	158	ARG	NE-CZ-NH2	-10.11	115.25	120.30
2	P	124	PHE	CB-CG-CD2	9.80	127.66	120.80
12	Z	99	ARG	NE-CZ-NH2	-9.78	115.41	120.30
9	I	69	ARG	NE-CZ-NH2	-9.74	115.43	120.30
11	Y	158	ARG	NE-CZ-NH1	9.61	125.10	120.30
4	R	120[A]	ALA	C-N-CA	9.59	145.67	121.70
4	R	120[B]	ALA	C-N-CA	9.59	145.67	121.70
12	L	99	ARG	NE-CZ-NH1	9.23	124.92	120.30
9	I	25[A]	ARG	NE-CZ-NH1	8.93	124.77	120.30
9	I	25[B]	ARG	NE-CZ-NH1	8.93	124.77	120.30
12	L	99	ARG	NE-CZ-NH2	-8.67	115.97	120.30
7	G	117	ARG	NE-CZ-NH1	8.54	124.57	120.30
12	Z	99	ARG	NE-CZ-NH1	8.44	124.52	120.30
9	W	16[A]	LYS	C-N-CA	8.37	142.63	121.70
9	W	16[B]	LYS	C-N-CA	8.37	142.63	121.70
9	W	69	ARG	NE-CZ-NH2	-8.23	116.19	120.30
12	Z	172	MET	CG-SD-CE	-8.23	87.03	100.20
6	T	27	MET	CG-SD-CE	8.18	113.28	100.20
13	M	151	ARG	NE-CZ-NH1	8.04	124.32	120.30
6	F	206	ASP	CB-CG-OD1	-7.99	111.11	118.30
11	Y	159	ARG	NE-CZ-NH1	7.81	124.20	120.30
2	B	6	ASP	CB-CG-OD1	7.74	125.27	118.30
11	K	158	ARG	NE-CZ-NH1	7.67	124.14	120.30
11	Y	142[A]	ARG	NE-CZ-NH1	7.64	124.12	120.30
11	Y	142[B]	ARG	NE-CZ-NH1	7.64	124.12	120.30
8	H	73	ARG	NE-CZ-NH1	7.60	124.10	120.30
11	K	142	ARG	NE-CZ-NH1	7.56	124.08	120.30
11	K	155	ASP	CB-CG-OD2	7.54	125.08	118.30
11	Y	159	ARG	NE-CZ-NH2	-7.45	116.57	120.30
11	K	158	ARG	NE-CZ-NH2	-7.43	116.58	120.30
2	B	4	ARG	NE-CZ-NH1	7.42	124.01	120.30
2	B	4	ARG	NE-CZ-NH2	-7.39	116.60	120.30
12	L	172	MET	CG-SD-CE	-7.38	88.39	100.20
6	T	17	ASP	CB-CG-OD1	-7.35	111.68	118.30
7	G	86	ASP	CB-CG-OD1	7.29	124.86	118.30
7	U	117	ARG	NE-CZ-NH1	7.23	123.92	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	16[A]	LYS	C-N-CA	7.22	139.76	121.70
9	I	16[B]	LYS	C-N-CA	7.22	139.76	121.70
8	H	82	ARG	NE-CZ-NH2	-7.11	116.75	120.30
6	T	99	ARG	NE-CZ-NH1	7.10	123.85	120.30
13	M	100	ARG	NE-CZ-NH1	-7.00	116.80	120.30
12	Z	71	ARG	NE-CZ-NH2	6.98	123.79	120.30
7	U	88	ARG	NE-CZ-NH1	6.96	123.78	120.30
14	N	46	ARG	NE-CZ-NH2	-6.90	116.85	120.30
6	T	113	ASP	CB-CG-OD2	-6.90	112.09	118.30
3	Q	5	ARG	NE-CZ-NH2	-6.86	116.87	120.30
6	T	43	ASP	CB-CG-OD2	6.70	124.33	118.30
6	T	6	GLY	C-N-CA	6.68	138.41	121.70
10	X	184	ASP	CB-CG-OD1	6.68	124.31	118.30
7	U	80[A]	MET	CG-SD-CE	6.66	110.86	100.20
7	U	80[B]	MET	CG-SD-CE	6.66	110.86	100.20
14	b	30	ARG	NE-CZ-NH2	-6.64	116.98	120.30
10	J	70	ARG	NE-CZ-NH1	6.61	123.60	120.30
5	E	122	ARG	NE-CZ-NH2	-6.57	117.02	120.30
13	M	151	ARG	NE-CZ-NH2	-6.57	117.02	120.30
6	F	190	VAL	CB-CA-C	-6.55	98.96	111.40
6	F	113	ASP	CB-CG-OD2	-6.54	112.41	118.30
8	H	199	ARG	NE-CZ-NH2	-6.48	117.06	120.30
8	H	133	LEU	CB-CG-CD2	6.45	121.97	111.00
8	H	87	MET	CG-SD-CE	-6.44	89.90	100.20
10	X	70	ARG	NE-CZ-NH1	6.42	123.51	120.30
8	V	105[A]	ASP	CB-CG-OD1	-6.38	112.56	118.30
8	V	105[B]	ASP	CB-CG-OD1	-6.38	112.56	118.30
3	Q	5	ARG	NE-CZ-NH1	6.37	123.48	120.30
6	F	99	ARG	NE-CZ-NH1	6.33	123.47	120.30
10	J	184	ASP	CB-CG-OD1	6.33	123.99	118.30
6	F	156	VAL	CG1-CB-CG2	-6.25	100.90	110.90
13	a	151	ARG	NE-CZ-NH1	6.25	123.42	120.30
14	N	46	ARG	NE-CZ-NH1	6.24	123.42	120.30
7	G	183	VAL	CB-CA-C	-6.23	99.56	111.40
6	T	7	TYR	N-CA-CB	6.22	121.80	110.60
11	K	108	ARG	NE-CZ-NH1	6.21	123.41	120.30
6	F	87	LEU	CB-CG-CD1	6.15	121.46	111.00
1	O	181	LEU	CA-CB-CG	6.14	129.43	115.30
2	P	4	ARG	NE-CZ-NH1	6.14	123.37	120.30
10	X	52	ASP	CB-CG-OD2	-6.14	112.78	118.30
3	C	36	ARG	NE-CZ-NH1	6.13	123.36	120.30
9	I	158	ASP	CB-CG-OD1	6.11	123.80	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	88	ARG	NE-CZ-NH2	-6.11	117.25	120.30
4	R	157	ASP	CB-CG-OD1	6.02	123.72	118.30
3	C	5	ARG	NE-CZ-NH2	-6.01	117.29	120.30
11	K	167	ARG	NE-CZ-NH1	5.97	123.29	120.30
2	B	226	ARG	NE-CZ-NH2	-5.97	117.32	120.30
13	a	182	ARG	NE-CZ-NH1	5.96	123.28	120.30
9	W	25[A]	ARG	NE-CZ-NH1	5.96	123.28	120.30
9	W	25[B]	ARG	NE-CZ-NH1	5.96	123.28	120.30
9	I	192	ASP	CB-CG-OD1	5.95	123.66	118.30
4	D	175[A]	GLU	N-CA-C	-5.95	94.94	111.00
4	D	175[B]	GLU	N-CA-C	-5.95	94.94	111.00
13	M	73	ASP	CB-CG-OD2	-5.95	112.95	118.30
13	M	182	ARG	NE-CZ-NH1	5.93	123.27	120.30
6	T	190	VAL	CB-CA-C	-5.93	100.13	111.40
2	P	103	GLU	OE1-CD-OE2	5.90	130.38	123.30
9	W	158	ASP	CB-CG-OD1	5.89	123.61	118.30
8	V	73	ARG	NE-CZ-NH2	-5.89	117.35	120.30
8	V	185	ASP	CB-CG-OD1	-5.87	113.02	118.30
10	J	38	MET	CG-SD-CE	-5.87	90.81	100.20
8	V	87	MET	CG-SD-CE	-5.84	90.85	100.20
6	T	230	ASP	CB-CG-OD2	5.84	123.56	118.30
10	J	86	ARG	CD-NE-CZ	5.83	131.77	123.60
9	W	175	ASP	CB-CG-OD1	5.83	123.55	118.30
1	O	73	LEU	CB-CA-C	-5.82	99.13	110.20
8	V	133	LEU	CB-CG-CD2	5.81	120.88	111.00
5	S	155	ASP	CB-CG-OD2	5.81	123.53	118.30
9	W	77	GLU	C-N-CA	-5.80	110.11	122.30
4	D	157	ASP	CB-CG-OD1	5.80	123.52	118.30
12	Z	125	ASP	CB-CG-OD1	5.80	123.52	118.30
8	V	29	ASP	CB-CG-OD1	5.79	123.52	118.30
5	S	122	ARG	NE-CZ-NH2	-5.79	117.41	120.30
10	J	33	ASP	CB-CG-OD1	5.77	123.49	118.30
13	M	99	ARG	NE-CZ-NH1	5.75	123.17	120.30
2	B	96	ARG	NE-CZ-NH1	5.73	123.17	120.30
6	T	169	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	A	17	LYS	CD-CE-NZ	5.70	124.82	111.70
3	C	5	ARG	NE-CZ-NH1	5.70	123.15	120.30
7	U	11	ARG	NE-CZ-NH1	5.69	123.15	120.30
9	I	77	GLU	C-N-CA	-5.69	110.36	122.30
6	F	114	ARG	NE-CZ-NH2	-5.68	117.46	120.30
3	Q	137	ASP	CB-CG-OD2	-5.67	113.20	118.30
8	H	199	ARG	NE-CZ-NH1	5.65	123.13	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	V	73	ARG	NE-CZ-NH1	5.63	123.11	120.30
6	T	117	MET	CG-SD-CE	5.61	109.17	100.20
1	A	73	LEU	CB-CA-C	-5.61	99.55	110.20
9	I	47	ARG	NE-CZ-NH1	5.60	123.10	120.30
10	X	86	ARG	CD-NE-CZ	5.60	131.44	123.60
10	X	70	ARG	NE-CZ-NH2	-5.59	117.50	120.30
5	E	174	ARG	NE-CZ-NH1	5.57	123.09	120.30
8	H	69	LEU	CA-CB-CG	5.57	128.12	115.30
14	N	168	ASP	CB-CG-OD1	-5.56	113.29	118.30
12	Z	173	ARG	NE-CZ-NH1	5.56	123.08	120.30
10	J	70	ARG	NE-CZ-NH2	-5.54	117.53	120.30
7	G	226	LYS	CD-CE-NZ	5.54	124.44	111.70
13	M	166	ARG	NE-CZ-NH2	-5.54	117.53	120.30
8	V	82	ARG	NE-CZ-NH2	-5.50	117.55	120.30
7	U	88	ARG	NE-CZ-NH2	-5.49	117.56	120.30
3	Q	13	ASP	CB-CG-OD2	5.48	123.23	118.30
13	a	43	MET	CG-SD-CE	-5.40	91.56	100.20
9	I	175	ASP	CB-CG-OD2	-5.34	113.49	118.30
8	V	69	LEU	CB-CG-CD1	5.33	120.06	111.00
9	W	47	ARG	NE-CZ-NH1	5.33	122.96	120.30
2	P	116	ASP	CB-CG-OD1	5.29	123.06	118.30
5	S	7	ASP	CB-CG-OD1	-5.25	113.58	118.30
7	G	88	ARG	CG-CD-NE	-5.25	100.78	111.80
8	H	90	ARG	NE-CZ-NH1	5.24	122.92	120.30
6	T	114	ARG	NE-CZ-NH2	-5.23	117.69	120.30
14	b	23	THR	CB-CA-C	-5.22	97.51	111.60
8	H	73	ARG	CD-NE-CZ	5.21	130.89	123.60
6	F	230	ASP	CB-CG-OD1	-5.20	113.62	118.30
8	H	29	ASP	CB-CG-OD1	5.18	122.97	118.30
3	Q	36	ARG	NE-CZ-NH1	5.17	122.88	120.30
12	L	102	PHE	CB-CG-CD1	5.16	124.41	120.80
5	S	174	ARG	NE-CZ-NH1	5.16	122.88	120.30
14	N	23	THR	CB-CA-C	-5.15	97.69	111.60
8	V	13	ILE	CG1-CB-CG2	-5.15	100.07	111.40
14	b	168	ASP	CB-CG-OD1	-5.15	113.67	118.30
10	J	69	MET	CG-SD-CE	-5.14	91.97	100.20
9	W	192	ASP	CB-CG-OD1	5.14	122.92	118.30
6	T	17	ASP	CB-CG-OD2	5.13	122.92	118.30
2	P	96	ARG	NE-CZ-NH1	5.13	122.86	120.30
10	J	52	ASP	CB-CG-OD2	-5.12	113.69	118.30
10	X	69	MET	CG-SD-CE	-5.10	92.04	100.20
8	H	13	ILE	CG1-CB-CG2	-5.09	100.20	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	85[A]	ASN	CB-CA-C	5.07	120.54	110.40
3	C	85[B]	ASN	CB-CA-C	5.07	120.54	110.40
12	L	156	LYS	CD-CE-NZ	-5.06	100.06	111.70
6	T	113	ASP	CB-CG-OD1	5.05	122.85	118.30
6	T	152	ASP	CB-CG-OD1	5.03	122.83	118.30
12	Z	169	ASP	CB-CG-OD2	5.02	122.82	118.30
4	R	120[A]	ALA	N-CA-C	-5.02	97.46	111.00
4	R	120[B]	ALA	N-CA-C	-5.02	97.46	111.00
2	B	3	ARG	NE-CZ-NH2	-5.01	117.80	120.30
11	Y	108	ARG	NE-CZ-NH1	5.01	122.80	120.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	U	47	6V1	C1

All (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
4	D	223	GLY	Peptide
5	E	235	GLY	Peptide
9	I	78	GLY	Peptide
10	J	1[A]	MET	Peptide
10	J	1[B]	MET	Peptide
2	P	245	ALA	Peptide
2	P	54	LYS	Peptide
3	Q	47	LYS	Peptide
3	Q	49	SER	Peptide
4	R	130	PRO	Peptide
4	R	223	GLY	Peptide
9	W	78	GLY	Peptide
10	X	1	MET	Peptide
11	Y	200	TYR	Peptide
13	a	215	ILE	Peptide

5.2 Too-close contacts ⓘ

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	231/234 (99%)	220 (95%)	7 (3%)	4 (2%)	9	4
1	O	228/234 (97%)	215 (94%)	8 (4%)	5 (2%)	6	2
2	B	248/261 (95%)	239 (96%)	8 (3%)	1 (0%)	34	30
2	P	247/261 (95%)	233 (94%)	10 (4%)	4 (2%)	9	4
3	C	236/248 (95%)	222 (94%)	7 (3%)	7 (3%)	4	1
3	Q	236/248 (95%)	219 (93%)	7 (3%)	10 (4%)	3	1
4	D	232/241 (96%)	224 (97%)	5 (2%)	3 (1%)	12	6
4	R	232/241 (96%)	225 (97%)	4 (2%)	3 (1%)	12	6
5	E	232/263 (88%)	228 (98%)	3 (1%)	1 (0%)	34	30
5	S	238/263 (90%)	232 (98%)	5 (2%)	1 (0%)	34	30
6	F	241/255 (94%)	237 (98%)	4 (2%)	0	100	100
6	T	239/255 (94%)	234 (98%)	2 (1%)	3 (1%)	12	6
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%)	29	23
8	V	220/234 (94%)	216 (98%)	3 (1%)	1 (0%)	29	23
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	Y	202/204 (99%)	198 (98%)	3 (2%)	1 (0%)	29	23
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%)	22	16

All (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
2	P	54	LYS
3	Q	47	LYS
3	Q	201	SER
3	Q	206	ILE
3	Q	221	ASN
4	R	128	ALA
4	R	129	ASP
4	R	130	PRO
5	S	238	GLU
6	T	7	TYR
8	V	204	ARG
11	Y	201	SER
1	A	50	LYS
3	C	200	GLN
4	D	176	GLY
1	O	176	ARG
1	O	231	ALA
2	P	204	SER
2	P	247	ALA
3	Q	138	PHE
3	Q	200	GLN
6	T	206	ASP
1	A	176	ARG

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Mol	Chain	Res	Type
2	B	203	VAL
3	C	50	VAL
3	C	138	PHE
8	H	204	ARG
1	O	50	LYS
3	Q	50	VAL
6	T	208	ALA
3	C	51	ALA
3	C	204	LYS
3	Q	48	LYS
3	C	203	GLY
3	C	216	SER
4	D	175[A]	GLU
4	D	175[B]	GLU
2	P	52	ILE
3	Q	216	SER
3	Q	203	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	185/191 (97%)	175 (95%)	10 (5%)	22	18
1	O	176/191 (92%)	165 (94%)	11 (6%)	18	13
2	B	200/221 (90%)	195 (98%)	5 (2%)	47	49
2	P	196/221 (89%)	184 (94%)	12 (6%)	18	14
3	C	179/210 (85%)	169 (94%)	10 (6%)	21	17
3	Q	184/210 (88%)	173 (94%)	11 (6%)	19	14
4	D	189/203 (93%)	183 (97%)	6 (3%)	39	38
4	R	187/203 (92%)	183 (98%)	4 (2%)	53	57
5	E	192/223 (86%)	184 (96%)	8 (4%)	30	27
5	S	197/223 (88%)	192 (98%)	5 (2%)	47	49
6	F	199/212 (94%)	188 (94%)	11 (6%)	21	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	T	192/212 (91%)	182 (95%)	10 (5%)	23	19
7	G	202/207 (98%)	195 (96%)	7 (4%)	36	35
7	U	186/207 (90%)	181 (97%)	5 (3%)	44	46
8	H	181/195 (93%)	175 (97%)	6 (3%)	38	37
8	V	172/195 (88%)	162 (94%)	10 (6%)	20	15
9	I	176/174 (101%)	174 (99%)	2 (1%)	73	78
9	W	173/174 (99%)	171 (99%)	2 (1%)	71	76
10	J	166/170 (98%)	158 (95%)	8 (5%)	25	22
10	X	165/170 (97%)	158 (96%)	7 (4%)	30	27
11	K	154/159 (97%)	147 (96%)	7 (4%)	27	24
11	Y	159/159 (100%)	150 (94%)	9 (6%)	20	16
12	L	175/178 (98%)	167 (95%)	8 (5%)	27	23
12	Z	175/178 (98%)	169 (97%)	6 (3%)	37	36
13	M	180/181 (99%)	175 (97%)	5 (3%)	43	44
13	a	178/181 (98%)	174 (98%)	4 (2%)	52	55
14	N	157/159 (99%)	153 (98%)	4 (2%)	47	49
14	b	158/159 (99%)	153 (97%)	5 (3%)	39	38
All	All	5033/5366 (94%)	4835 (96%)	198 (4%)	33	30

All (198) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LYS
1	A	53	SER
1	A	54	ILE
1	A	142	ARG
1	A	176	ARG
1	A	189	THR
1	A	206	ASN
1	A	223	THR
1	A	226	LYS
1	A	227	ASP
2	B	33	THR
2	B	59	VAL
2	B	190	LEU
2	B	229	LYS

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Mol	Chain	Res	Type
2	B	249	ARG
3	C	35	VAL
3	C	45	VAL
3	C	54	GLN
3	C	105	GLU
3	C	148	ASP
3	C	163	ARG
3	C	179	GLU
3	C	205	ASN
3	C	208	LEU
3	C	226	GLU
4	D	9	ASP
4	D	46	VAL
4	D	95	GLU
4	D	117	SER
4	D	126	GLU
4	D	199	LEU
5	E	29	VAL
5	E	61	LYS
5	E	95	SER
5	E	101[A]	ARG
5	E	101[B]	ARG
5	E	180	MET
5	E	181	GLU
5	E	189	LYS
6	F	17	ASP
6	F	31	GLU
6	F	53	VAL
6	F	81	LEU
6	F	86	SER
6	F	87	LEU
6	F	174	THR
6	F	190	VAL
6	F	215	TRP
6	F	240	LYS
6	F	244	LYS
7	G	42	VAL
7	G	78	CYS
7	G	88	ARG
7	G	183	VAL
7	G	190	THR
7	G	206	LEU

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Mol	Chain	Res	Type
7	G	209	ASP
8	H	7	VAL
8	H	13	ILE
8	H	66	LEU
8	H	69	LEU
8	H	74	LEU
8	H	184	LEU
9	I	35	THR
9	I	115	THR
10	J	1[A]	MET
10	J	1[B]	MET
10	J	27[A]	GLN
10	J	27[B]	GLN
10	J	62	LYS
10	J	88	LEU
10	J	95	ARG
10	J	155	ARG
11	K	13	VAL
11	K	139	VAL
11	K	142	ARG
11	K	148	LEU
11	K	159	ARG
11	K	175	VAL
11	K	188	VAL
12	L	3[A]	SER
12	L	3[B]	SER
12	L	102	PHE
12	L	163	HIS
12	L	169	ASP
12	L	172	MET
12	L	174	LEU
12	L	207	THR
13	M	100	ARG
13	M	154	LEU
13	M	155	GLU
13	M	198	GLU
13	M	216	SER
14	N	23	THR
14	N	36	THR
14	N	85	LYS
14	N	197	LYS
1	O	10	THR

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Mol	Chain	Res	Type
1	O	53	SER
1	O	118	GLN
1	O	142	ARG
1	O	176	ARG
1	O	181	LEU
1	O	189	THR
1	O	206	ASN
1	O	221	THR
1	O	223	THR
1	O	226	LYS
2	P	7[A]	SER
2	P	7[B]	SER
2	P	33	THR
2	P	59	VAL
2	P	124	PHE
2	P	183	GLU
2	P	190	LEU
2	P	204	SER
2	P	230	GLN
2	P	235	GLN
2	P	236	LEU
2	P	246	LYS
3	Q	45	VAL
3	Q	56	GLU
3	Q	98	VAL
3	Q	105	GLU
3	Q	148	ASP
3	Q	163	ARG
3	Q	170	GLU
3	Q	197	GLU
3	Q	206	ILE
3	Q	208	LEU
3	Q	227	LYS
4	R	9	ASP
4	R	32	LYS
4	R	46	VAL
4	R	117	SER
5	S	29	VAL
5	S	45	VAL
5	S	95	SER
5	S	101	ARG
5	S	180	MET

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Mol	Chain	Res	Type
6	T	17	ASP
6	T	31	GLU
6	T	53	VAL
6	T	81	LEU
6	T	86	SER
6	T	87	LEU
6	T	174	THR
6	T	190	VAL
6	T	215	TRP
6	T	240	LYS
7	U	42	VAL
7	U	78	CYS
7	U	196	GLU
7	U	199	ILE
7	U	206	LEU
8	V	7	VAL
8	V	13	ILE
8	V	66	LEU
8	V	69	LEU
8	V	74	LEU
8	V	105[A]	ASP
8	V	105[B]	ASP
8	V	184	LEU
8	V	200	LEU
8	V	214	THR
9	W	35	THR
9	W	193	LYS
10	X	1	MET
10	X	27	GLN
10	X	62	LYS
10	X	88	LEU
10	X	95	ARG
10	X	158	GLU
10	X	174	ASN
11	Y	9	PHE
11	Y	13	VAL
11	Y	107	LYS
11	Y	139	VAL
11	Y	142[A]	ARG
11	Y	142[B]	ARG
11	Y	148	LEU
11	Y	187[A]	ARG

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Mol	Chain	Res	Type
11	Y	187[B]	ARG
12	Z	102	PHE
12	Z	169	ASP
12	Z	172	MET
12	Z	174	LEU
12	Z	207	THR
12	Z	208	VAL
13	a	100	ARG
13	a	154	LEU
13	a	198	GLU
13	a	216	SER
14	b	23	THR
14	b	30	ARG
14	b	36	THR
14	b	85	LYS
14	b	197	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	GLN
1	A	108	GLN
1	A	206	ASN
2	B	40	ASN
2	B	109	GLN
3	C	175	ASN
5	E	65	HIS
6	F	143	ASN
8	H	117	HIS
8	H	154	ASN
9	I	161	HIS
10	J	101	ASN
10	J	132	HIS
11	K	163	GLN
12	L	157	ASN
13	M	162	GLN
14	N	194	GLN
1	O	62	HIS
1	O	118	GLN
1	O	206	ASN
2	P	40	ASN
2	P	146	GLN

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Mol	Chain	Res	Type
3	Q	18	GLN
3	Q	175	ASN
4	R	186	HIS
5	S	86	ASN
6	T	68	ASN
6	T	143	ASN
8	V	117	HIS
9	W	172	ASN
10	X	24	ASN
10	X	132	HIS
10	X	174	ASN
11	Y	163	GLN
12	Z	79	ASN
12	Z	157	ASN
13	a	89	HIS
13	a	162	GLN
14	b	194	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	1.07	1 (14%)	4,10,12	3.08	3 (75%)
7	6V1	G	47	7	12,15,16	2.62	4 (33%)	9,20,22	1.48	1 (11%)
5	6V1	E	148	5	12,15,16	1.57	3 (25%)	9,20,22	3.19	4 (44%)
10	6V1	J	91	10	12,15,16	2.23	4 (33%)	9,20,22	5.54	6 (66%)
3	YCM	C	63	3	7,9,10	0.90	0	4,10,12	0.74	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	6V1	G	161	7	12,15,16	1.58	4 (33%)	9,20,22	3.15	6 (66%)
7	6V1	U	47	7	12,15,16	2.01	2 (16%)	9,20,22	2.04	3 (33%)
7	YCM	U	137	7	7,9,10	0.97	0	4,10,12	2.18	1 (25%)
7	YCM	G	137	7	7,9,10	2.21	3 (42%)	4,10,12	2.99	2 (50%)
5	6V1	S	148	5	12,15,16	1.51	4 (33%)	9,20,22	2.89	3 (33%)
7	6V1	U	161	7	12,15,16	1.84	3 (25%)	9,20,22	2.87	4 (44%)
10	6V1	X	91	10	12,15,16	1.79	4 (33%)	9,20,22	5.90	6 (66%)

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

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

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	47	6V1	CB-SG	-6.71	1.74	1.82
7	U	47	6V1	CB-SG	-5.67	1.76	1.82
10	J	91	6V1	CB-SG	-5.40	1.76	1.82
10	X	91	6V1	CB-SG	-4.42	1.77	1.82
7	U	161	6V1	CB-SG	-4.07	1.77	1.82
7	G	137	YCM	CD-SG	3.82	1.91	1.81
7	G	47	6V1	C4-N3	-3.64	1.32	1.38
7	G	137	YCM	CE-NZ2	3.36	1.43	1.32
7	G	47	6V1	C1-SG	3.32	1.86	1.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	J	91	6V1	C1-SG	-3.25	1.79	1.83
7	U	161	6V1	C4-N3	-3.25	1.33	1.38
5	E	148	6V1	CB-SG	-3.18	1.78	1.82
5	S	148	6V1	CB-SG	-3.04	1.78	1.82
7	G	161	6V1	C2-N3	-2.98	1.34	1.38
10	J	91	6V1	C4-N3	-2.76	1.34	1.38
5	E	148	6V1	C4-N3	-2.73	1.34	1.38
7	G	47	6V1	C2-N3	-2.65	1.34	1.38
7	G	161	6V1	C4-N3	-2.63	1.34	1.38
5	E	148	6V1	C2-N3	-2.61	1.35	1.38
7	U	47	6V1	C4-N3	-2.52	1.34	1.38
7	G	161	6V1	CB-SG	2.49	1.84	1.82
7	U	161	6V1	C2-N3	-2.46	1.35	1.38
5	S	148	6V1	C4-N3	-2.41	1.34	1.38
10	X	91	6V1	C4-N3	-2.40	1.34	1.38
7	G	137	YCM	CB-SG	-2.29	1.71	1.80
10	J	91	6V1	O7-C2	2.29	1.26	1.22
10	X	91	6V1	C5-C4	2.23	1.54	1.50
5	S	148	6V1	C2-N3	-2.15	1.35	1.38
3	Q	63	YCM	CD-SG	-2.14	1.76	1.81
5	S	148	6V1	C5-C4	2.04	1.53	1.50
7	G	161	6V1	O-C	2.03	1.28	1.19
10	X	91	6V1	O7-C2	2.02	1.26	1.22

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	X	91	6V1	C5-C4-N3	9.28	113.60	108.13
10	J	91	6V1	C5-C4-N3	8.48	113.13	108.13
10	X	91	6V1	O7-C2-N3	8.14	134.10	124.14
10	X	91	6V1	C2-N3-C4	-8.14	108.21	113.04
10	J	91	6V1	O7-C2-N3	7.85	133.75	124.14
5	E	148	6V1	C2-N3-C4	-7.55	108.56	113.04
10	J	91	6V1	C6-N3-C2	7.43	132.78	123.36
10	X	91	6V1	C6-N3-C2	7.29	132.60	123.36
10	J	91	6V1	C2-N3-C4	-7.04	108.86	113.04
5	S	148	6V1	C5-C4-N3	5.73	111.51	108.13
7	U	161	6V1	C2-N3-C4	-5.40	109.84	113.04
5	S	148	6V1	C2-N3-C4	-5.38	109.85	113.04
7	U	161	6V1	C5-C4-N3	4.87	111.00	108.13
7	G	137	YCM	CE-CD-SG	4.74	127.54	113.59
7	G	161	6V1	C2-N3-C4	-4.67	110.27	113.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Q	63	YCM	CE-CD-SG	-4.61	100.03	113.59
7	G	161	6V1	O8-C4-N3	4.58	128.99	123.92
10	X	91	6V1	O8-C4-C5	-4.48	120.71	127.24
7	G	161	6V1	O8-C4-C5	-4.10	121.27	127.24
7	U	47	6V1	C2-N3-C4	-4.04	110.64	113.04
10	J	91	6V1	C6-N3-C4	-3.97	117.41	122.59
5	E	148	6V1	C5-C4-N3	3.92	110.44	108.13
10	X	91	6V1	C6-N3-C4	-3.89	117.52	122.59
10	J	91	6V1	O8-C4-C5	-3.84	121.64	127.24
7	U	137	YCM	CE-CD-SG	3.72	124.55	113.59
7	G	47	6V1	C2-N3-C4	-3.58	110.92	113.04
7	G	161	6V1	C6-N3-C2	3.50	127.80	123.36
7	U	47	6V1	C5-C4-N3	3.33	110.09	108.13
7	U	161	6V1	O8-C4-C5	-2.92	122.99	127.24
3	Q	63	YCM	CA-CB-SG	-2.84	103.33	113.74
7	U	47	6V1	C6-N3-C2	2.83	126.95	123.36
3	Q	63	YCM	CB-SG-CD	2.78	130.26	104.44
7	G	161	6V1	C5-C4-N3	2.73	109.74	108.13
5	E	148	6V1	C6-N3-C4	2.70	126.11	122.59
7	G	137	YCM	OZ1-CE-NZ2	-2.64	115.30	122.50
5	S	148	6V1	O8-C4-C5	-2.58	123.49	127.24
7	U	161	6V1	C6-N3-C2	2.45	126.47	123.36
7	G	161	6V1	O7-C2-N3	2.37	127.04	124.14
5	E	148	6V1	O8-C4-C5	-2.04	124.27	127.24

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	U	47	6V1	C1

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	Q	63	YCM	CE-CD-SG-CB
3	Q	63	YCM	SG-CD-CE-OZ1
3	Q	63	YCM	SG-CD-CE-NZ2
5	E	148	6V1	C3-C6-N3-C4
10	J	91	6V1	C3-C6-N3-C2
10	J	91	6V1	C3-C6-N3-C4
7	G	161	6V1	C3-C6-N3-C2
7	G	161	6V1	C3-C6-N3-C4
7	U	137	YCM	CE-CD-SG-CB

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Mol	Chain	Res	Type	Atoms
7	G	137	YCM	SG-CD-CE-OZ1
7	G	137	YCM	SG-CD-CE-NZ2
5	S	148	6V1	C3-C6-N3-C2
5	S	148	6V1	C3-C6-N3-C4
10	X	91	6V1	C3-C6-N3-C2
10	X	91	6V1	C3-C6-N3-C4
5	E	148	6V1	C3-C6-N3-C2
3	C	63	YCM	CE-CD-SG-CB
7	G	137	YCM	CE-CD-SG-CB
7	U	161	6V1	N-CA-CB-SG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides 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	$\# Z > 2$
18	1PE	I	303	-	15,15,15	0.56	0	14,14,14	0.90	0
18	1PE	L	301	-	15,15,15	0.60	0	14,14,14	0.76	0
18	1PE	Y	305	-	15,15,15	0.56	0	14,14,14	0.55	0
19	6V8	Y	306	11	19,23,23	1.70	5 (26%)	24,31,31	2.81	9 (37%)
18	1PE	N	303	-	15,15,15	0.51	0	14,14,14	0.78	0
19	6V8	b	304	14	19,23,23	1.73	1 (5%)	24,31,31	1.60	5 (20%)
18	1PE	b	302	-	15,15,15	0.63	0	14,14,14	1.07	1 (7%)
19	6V8	V	303	8	19,23,23	2.79	3 (15%)	24,31,31	3.00	10 (41%)
18	1PE	M	305	-	15,15,15	0.51	0	14,14,14	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	1PE	W	303	-	15,15,15	0.58	0	14,14,14	0.47	0
19	6V8	N	305	14	19,23,23	1.34	2 (10%)	24,31,31	2.11	8 (33%)
19	6V8	H	305	8	19,23,23	2.45	3 (15%)	24,31,31	2.93	10 (41%)
18	1PE	H	304	-	15,15,15	0.43	0	14,14,14	0.47	0
19	6V8	K	305	11	19,23,23	1.65	3 (15%)	24,31,31	2.20	8 (33%)
18	1PE	I	304	-	15,15,15	0.50	0	14,14,14	0.78	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	1PE	I	303	-	-	7/13/13/13	-
18	1PE	L	301	-	-	6/13/13/13	-
18	1PE	Y	305	-	-	7/13/13/13	-
19	6V8	Y	306	11	-	0/15/21/21	0/1/1/1
18	1PE	N	303	-	-	5/13/13/13	-
19	6V8	b	304	14	-	1/15/21/21	0/1/1/1
18	1PE	b	302	-	-	7/13/13/13	-
19	6V8	V	303	8	-	2/15/21/21	0/1/1/1
18	1PE	M	305	-	-	6/13/13/13	-
18	1PE	W	303	-	-	8/13/13/13	-
19	6V8	N	305	14	-	1/15/21/21	0/1/1/1
19	6V8	H	305	8	-	3/15/21/21	0/1/1/1
18	1PE	H	304	-	-	5/13/13/13	-
19	6V8	K	305	11	-	0/15/21/21	0/1/1/1
18	1PE	I	304	-	-	8/13/13/13	-

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	V	303	6V8	C2-C3	10.73	1.54	1.39
19	H	305	6V8	C2-C3	9.05	1.52	1.39
19	b	304	6V8	C2-C3	6.77	1.48	1.39
19	K	305	6V8	C2-C3	5.34	1.46	1.39
19	Y	306	6V8	C1-C2	-4.96	1.32	1.39
19	N	305	6V8	C2-C3	3.89	1.44	1.39
19	V	303	6V8	C3-CL3	3.67	1.82	1.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	H	305	6V8	C6-CL6	3.10	1.81	1.74
19	N	305	6V8	C3-CL3	3.07	1.80	1.73
19	H	305	6V8	C3-CL3	3.05	1.80	1.73
19	Y	306	6V8	C5-C4	-2.96	1.33	1.38
19	K	305	6V8	C1-C2	-2.67	1.35	1.39
19	V	303	6V8	C6-CL6	2.67	1.80	1.74
19	K	305	6V8	C6-CL6	2.54	1.80	1.74
19	Y	306	6V8	C2-C3	2.23	1.42	1.39
19	Y	306	6V8	O8-C7	-2.12	1.19	1.23
19	Y	306	6V8	C6-CL6	2.08	1.79	1.74

All (51) 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	121.00
19	V	303	6V8	C3-C2-C7	7.22	134.08	122.58
19	H	305	6V8	C2-C3-CL3	7.06	131.44	121.00
19	Y	306	6V8	C2-C3-CL3	-6.72	111.06	121.00
19	H	305	6V8	C3-C2-C7	6.20	132.45	122.58
19	Y	306	6V8	C4-C3-C2	6.07	128.36	121.36
19	Y	306	6V8	C1-C6-CL6	-5.91	111.77	119.15
19	K	305	6V8	C2-C3-CL3	-5.87	112.31	121.00
19	N	305	6V8	C5-C6-C1	5.39	128.69	121.53
19	H	305	6V8	O8-C7-C2	-5.06	111.77	121.01
19	K	305	6V8	C4-C3-C2	4.73	126.82	121.36
19	H	305	6V8	C4-C3-C2	-4.47	116.20	121.36
19	V	303	6V8	C4-C3-C2	-4.06	116.68	121.36
19	H	305	6V8	C10-N9-C7	4.02	130.88	121.33
19	Y	306	6V8	C1-C2-C3	-3.93	113.44	117.92
19	V	303	6V8	C1-C2-C7	-3.88	105.85	117.36
19	V	303	6V8	C4-C3-CL3	-3.75	110.88	118.41
19	N	305	6V8	C1-C6-CL6	-3.75	114.47	119.15
19	b	304	6V8	C5-C6-C1	3.74	126.50	121.53
19	V	303	6V8	C10-N9-C7	3.69	130.11	121.33
19	K	305	6V8	C5-C4-C3	-3.67	114.70	120.00
19	Y	306	6V8	C5-C6-C1	3.65	126.38	121.53
19	N	305	6V8	O8-C7-C2	-3.61	114.41	121.01
19	Y	306	6V8	C5-C4-C3	-3.51	114.93	120.00
19	H	305	6V8	C4-C5-C6	3.35	122.78	119.24
19	V	303	6V8	C4-C5-C6	3.20	122.62	119.24
19	K	305	6V8	C1-C6-CL6	-3.16	115.20	119.15
19	H	305	6V8	O8-C7-N9	3.11	128.81	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	b	302	1PE	C26-OH6-C15	3.08	126.63	113.29
19	H	305	6V8	C4-C3-CL3	-3.01	112.36	118.41
19	Y	306	6V8	C3-C2-C7	3.01	127.37	122.58
19	N	305	6V8	C2-C1-C6	-2.97	114.65	119.64
19	H	305	6V8	C1-C2-C7	-2.92	108.68	117.36
19	b	304	6V8	O8-C7-C2	-2.87	115.77	121.01
19	K	305	6V8	C10-N9-C7	2.80	127.99	121.33
19	K	305	6V8	C5-C6-C1	2.74	125.17	121.53
19	b	304	6V8	C21-C22-C23	2.70	118.79	115.39
19	N	305	6V8	C21-C22-C23	2.65	118.72	115.39
19	V	303	6V8	C1-C6-CL6	-2.63	115.86	119.15
19	Y	306	6V8	O8-C7-C2	-2.61	116.24	121.01
19	V	303	6V8	C5-C6-CL6	2.57	123.37	119.35
19	b	304	6V8	C1-C6-CL6	-2.56	115.96	119.15
19	N	305	6V8	C4-C5-C6	-2.52	116.59	119.24
19	Y	306	6V8	C10-N9-C7	2.38	126.98	121.33
19	V	303	6V8	O8-C7-C2	-2.24	116.91	121.01
19	N	305	6V8	C4-C3-C2	2.23	123.93	121.36
19	H	305	6V8	C5-C6-C1	-2.05	118.81	121.53
19	K	305	6V8	O8-C7-C2	-2.03	117.31	121.01
19	K	305	6V8	C1-C2-C3	-2.02	115.62	117.92
19	N	305	6V8	C10-N9-C7	2.02	126.12	121.33
19	b	304	6V8	C5-C4-C3	-2.00	117.10	120.00

There are no chirality outliers.

All (66) 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	M	305	1PE	OH5-C14-C24-OH4
18	I	303	1PE	OH6-C15-C25-OH5
18	I	304	1PE	OH4-C13-C23-OH3
18	Y	305	1PE	OH6-C15-C25-OH5
18	b	302	1PE	OH4-C13-C23-OH3
18	L	301	1PE	OH5-C14-C24-OH4
18	M	305	1PE	OH4-C13-C23-OH3
18	L	301	1PE	OH6-C15-C25-OH5
18	H	304	1PE	OH4-C13-C23-OH3
18	I	304	1PE	OH2-C12-C22-OH3

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Mol	Chain	Res	Type	Atoms
18	N	303	1PE	OH2-C12-C22-OH3
18	W	303	1PE	OH6-C15-C25-OH5
18	W	303	1PE	OH7-C16-C26-OH6
18	Y	305	1PE	C16-C26-OH6-C15
18	I	303	1PE	OH2-C12-C22-OH3
18	I	303	1PE	C15-C25-OH5-C14
18	M	305	1PE	OH6-C15-C25-OH5
18	I	304	1PE	OH7-C16-C26-OH6
18	N	303	1PE	OH7-C16-C26-OH6
18	Y	305	1PE	OH2-C12-C22-OH3
18	L	301	1PE	OH2-C12-C22-OH3
18	M	305	1PE	OH2-C12-C22-OH3
18	N	303	1PE	OH4-C13-C23-OH3
18	H	304	1PE	OH5-C14-C24-OH4
18	M	305	1PE	C23-C13-OH4-C24
18	W	303	1PE	C12-C22-OH3-C23
18	W	303	1PE	C13-C23-OH3-C22
18	I	304	1PE	C16-C26-OH6-C15
18	b	302	1PE	OH5-C14-C24-OH4
18	L	301	1PE	C13-C23-OH3-C22
18	Y	305	1PE	C15-C25-OH5-C14
18	H	304	1PE	OH6-C15-C25-OH5
18	H	304	1PE	OH2-C12-C22-OH3
18	b	302	1PE	OH2-C12-C22-OH3
18	I	303	1PE	C14-C24-OH4-C13
18	W	303	1PE	C14-C24-OH4-C13
19	b	304	6V8	C21-C22-C23-C25
18	Y	305	1PE	C12-C22-OH3-C23
18	W	303	1PE	C16-C26-OH6-C15
18	L	301	1PE	C25-C15-OH6-C26
18	W	303	1PE	C25-C15-OH6-C26
18	I	303	1PE	C12-C22-OH3-C23
18	I	303	1PE	C24-C14-OH5-C25
18	I	304	1PE	C23-C13-OH4-C24
18	b	302	1PE	C16-C26-OH6-C15
18	I	304	1PE	OH5-C14-C24-OH4
18	H	304	1PE	C25-C15-OH6-C26
18	I	304	1PE	OH6-C15-C25-OH5
18	W	303	1PE	C24-C14-OH5-C25
18	N	303	1PE	C23-C13-OH4-C24
18	b	302	1PE	OH6-C15-C25-OH5
18	M	305	1PE	C24-C14-OH5-C25

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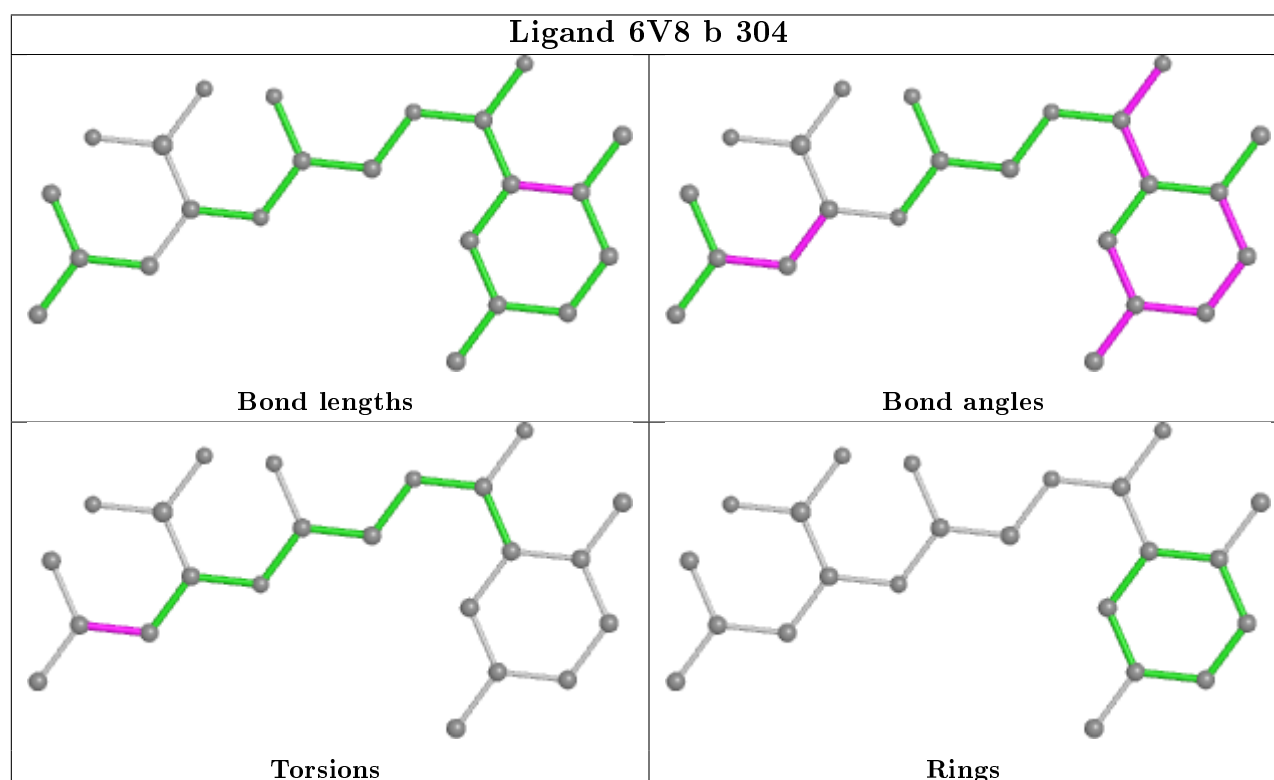
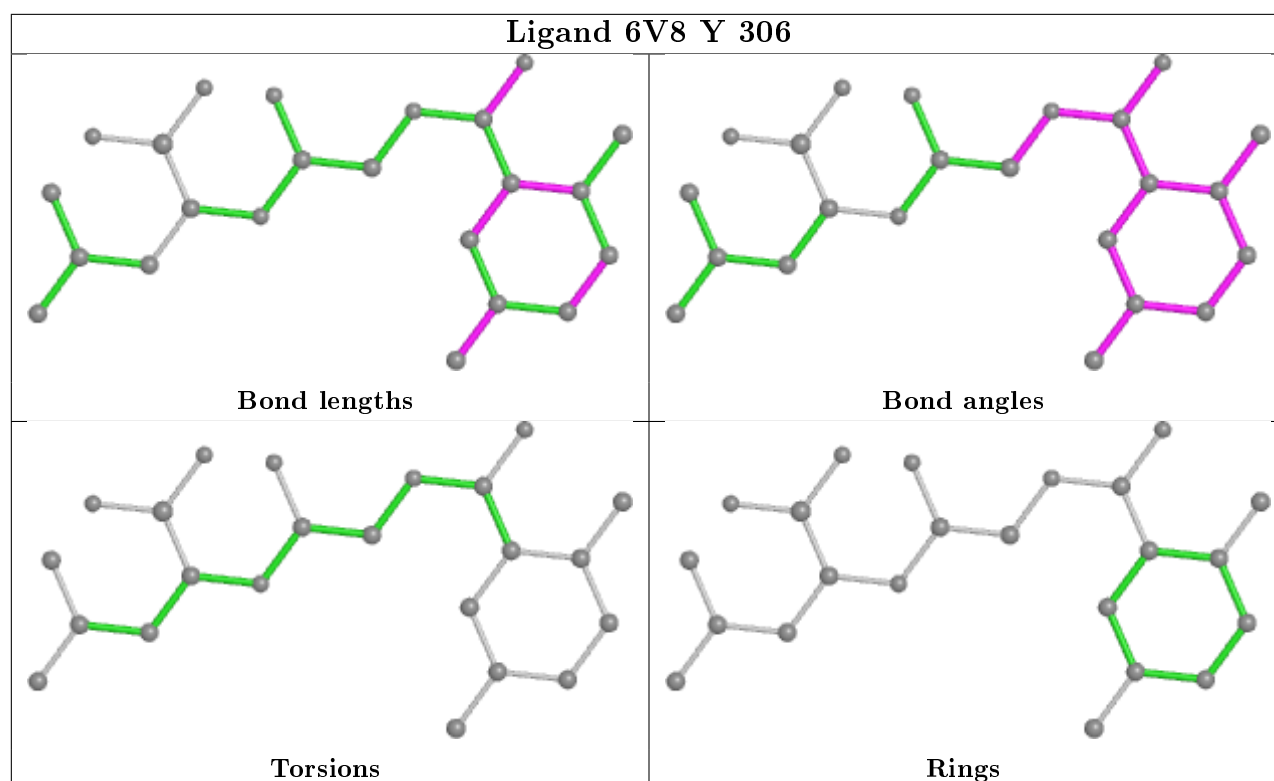
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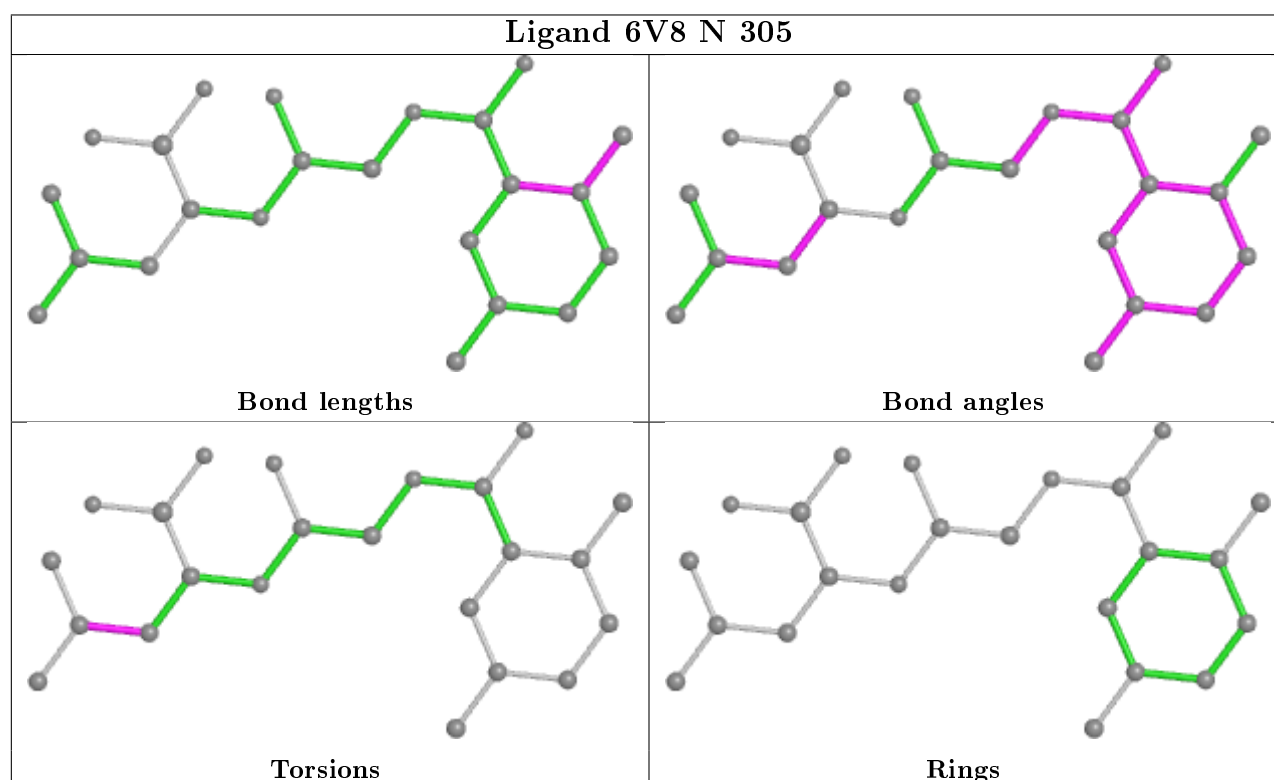
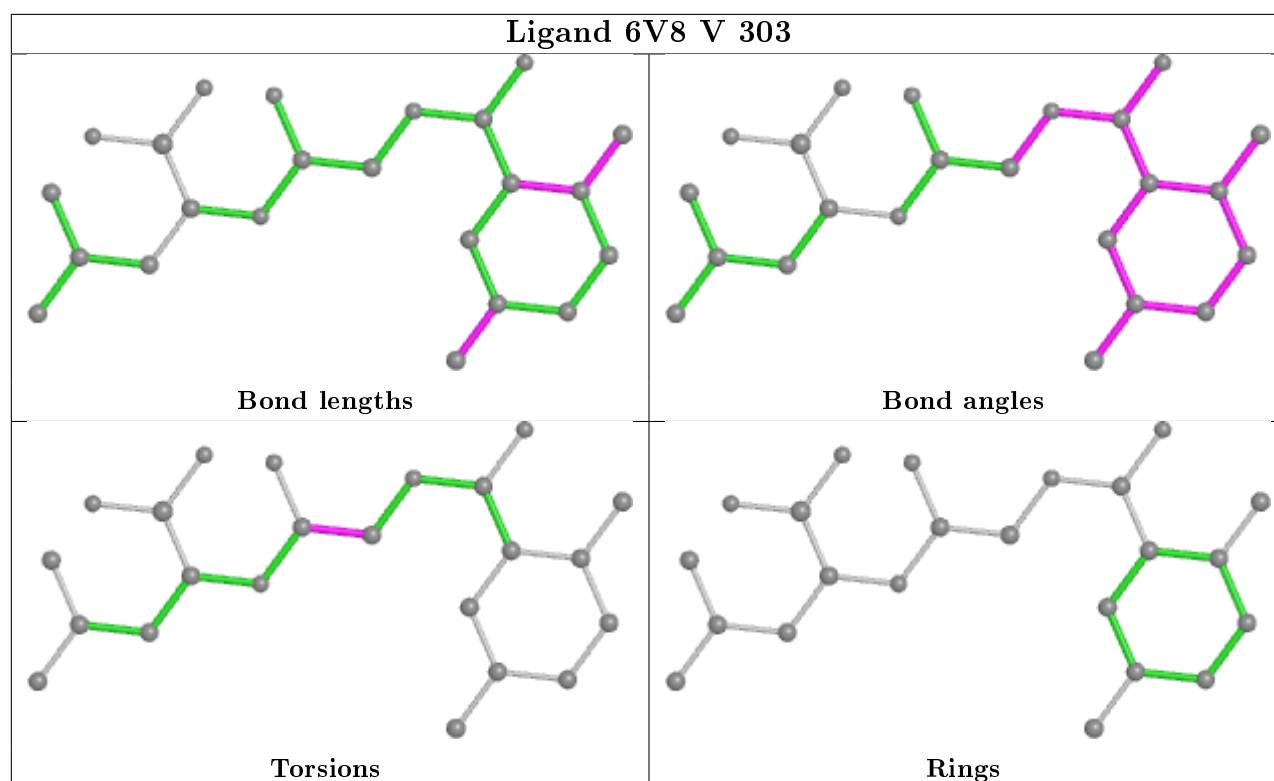
Mol	Chain	Res	Type	Atoms
18	b	302	1PE	C24-C14-OH5-C25
19	V	303	6V8	N9-C10-C18-N20
19	H	305	6V8	N9-C10-C18-N20
18	Y	305	1PE	C13-C23-OH3-C22
19	N	305	6V8	C21-C22-C23-C25
19	H	305	6V8	C1-C2-C7-N9
19	V	303	6V8	N9-C10-C18-O19
19	H	305	6V8	N9-C10-C18-O19
18	Y	305	1PE	OH4-C13-C23-OH3
18	I	303	1PE	OH5-C14-C24-OH4

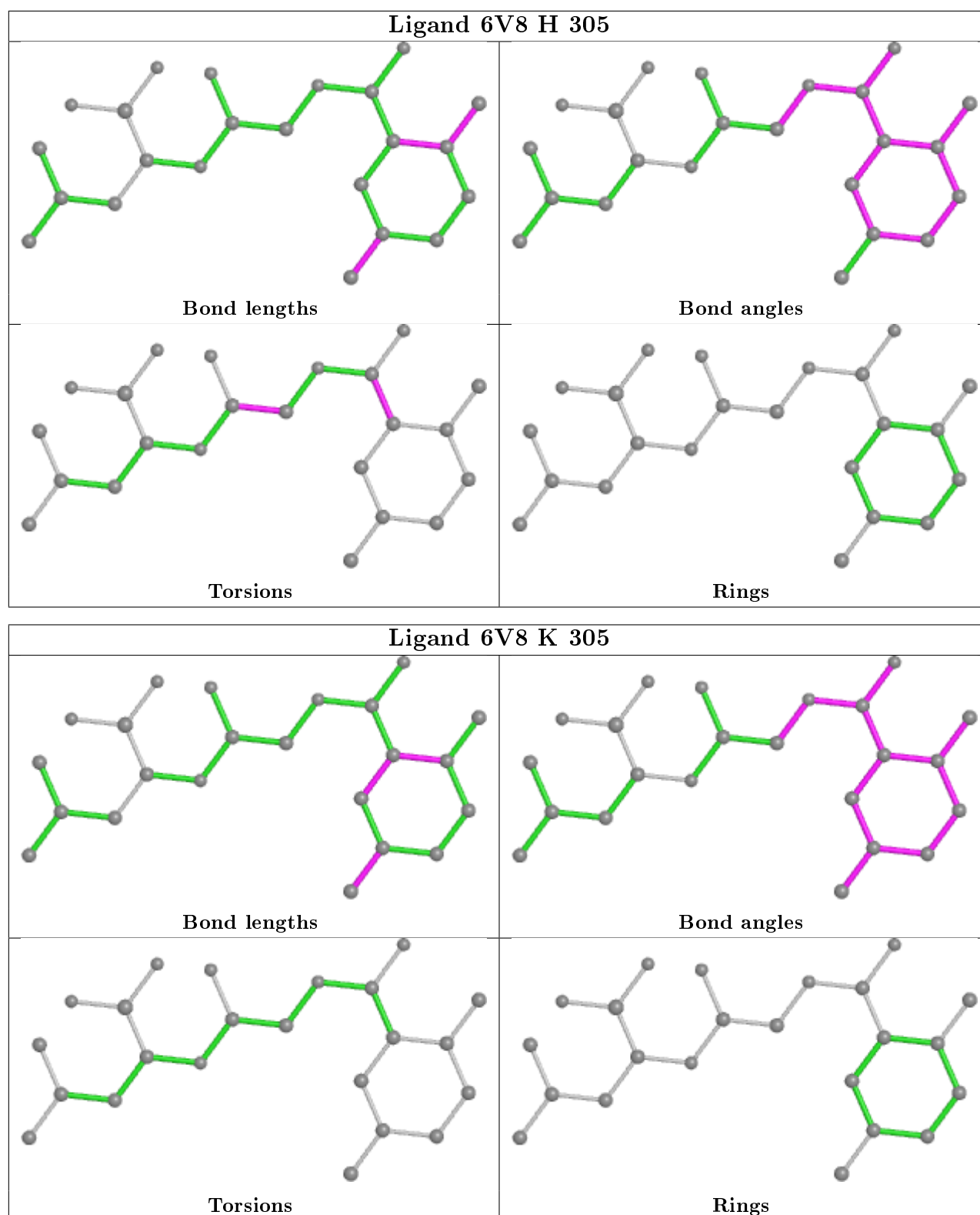
There are no ring outliers.

No monomer is involved in short contacts.

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 ⓘ

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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%)	-0.14	2 (0%) 84 83	31, 45, 86, 98	0
1	O	230/234 (98%)	0.29	15 (6%) 18 18	43, 67, 110, 149	0
2	B	248/261 (95%)	-0.00	4 (1%) 72 70	34, 54, 98, 137	0
2	P	247/261 (94%)	0.22	13 (5%) 26 25	39, 60, 107, 154	0
3	C	236/248 (95%)	0.24	14 (5%) 22 21	37, 65, 106, 136	0
3	Q	238/248 (95%)	0.33	17 (7%) 16 15	37, 66, 126, 160	0
4	D	233/241 (96%)	0.06	4 (1%) 70 68	38, 61, 91, 135	0
4	R	233/241 (96%)	-0.11	4 (1%) 70 68	32, 48, 76, 116	0
5	E	233/263 (88%)	-0.03	9 (3%) 39 38	27, 43, 91, 112	0
5	S	237/263 (90%)	0.02	8 (3%) 45 44	37, 53, 88, 113	0
6	F	239/255 (93%)	-0.18	0 100 100	26, 36, 60, 82	0
6	T	240/255 (94%)	0.17	9 (3%) 40 39	41, 61, 96, 135	0
7	G	241/246 (97%)	-0.14	3 (1%) 79 78	28, 40, 72, 110	0
7	U	235/246 (95%)	0.22	11 (4%) 31 30	48, 70, 106, 140	0
8	H	220/234 (94%)	-0.11	3 (1%) 75 74	27, 38, 75, 126	0
8	V	220/234 (94%)	-0.10	3 (1%) 75 74	39, 52, 83, 120	0
9	I	204/205 (99%)	-0.21	0 100 100	29, 38, 60, 77	0
9	W	204/205 (99%)	-0.12	0 100 100	33, 50, 78, 88	0
10	J	195/201 (97%)	-0.21	1 (0%) 91 90	33, 44, 62, 78	0
10	X	195/201 (97%)	-0.26	0 100 100	33, 44, 60, 81	0
11	K	200/204 (98%)	-0.20	1 (0%) 91 90	33, 47, 76, 88	0
11	Y	201/204 (98%)	-0.22	3 (1%) 73 72	29, 39, 64, 84	0
12	L	213/213 (100%)	-0.12	0 100 100	32, 48, 71, 91	0
12	Z	213/213 (100%)	-0.20	0 100 100	28, 39, 65, 81	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	216/219 (98%)	-0.15	0 100 100	28, 42, 67, 96	0
13	a	216/219 (98%)	-0.18	1 (0%) 91 90	31, 44, 64, 86	0
14	N	202/205 (98%)	-0.15	3 (1%) 73 72	28, 38, 60, 101	0
14	b	203/205 (99%)	-0.13	3 (1%) 73 72	36, 47, 72, 111	0
All	All	6222/6458 (96%)	-0.04	131 (2%) 63 62	26, 49, 91, 160	0

All (131) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	232	ILE	12.8
2	P	204	SER	12.2
4	D	241	ILE	8.7
3	Q	234	LYS	6.6
13	a	216	SER	6.5
2	P	203	VAL	6.1
11	K	41	TYR	5.9
3	C	49	SER	5.9
8	V	204	ARG	5.5
1	O	225	VAL	5.1
3	Q	202	GLY	5.1
8	H	205	CYS	5.1
3	Q	232	ILE	5.1
6	T	208	ALA	5.1
7	U	2	SER	5.0
5	E	54	SER	4.9
2	P	61	PHE	4.8
5	S	57	ALA	4.8
8	V	200	LEU	4.4
2	B	61	PHE	4.4
3	Q	238	GLU	4.3
5	E	52	ALA	4.3
3	C	138	PHE	4.2
7	U	206	LEU	4.2
8	H	204	ARG	4.0
3	Q	233	GLU	4.0
1	O	201	GLN	3.9
7	U	3	ARG	3.9
4	R	241	ILE	3.9
6	T	206	ASP	3.9
5	E	58	ALA	3.7
2	P	234	GLU	3.6

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Mol	Chain	Res	Type	RSRZ
3	Q	203	GLY	3.6
2	P	205	LYS	3.5
4	R	130	PRO	3.4
11	Y	41	TYR	3.4
5	E	201	ALA	3.4
5	E	53	GLN	3.4
5	S	2	PHE	3.3
3	Q	200	GLN	3.3
2	P	202	ASP	3.3
3	Q	229	VAL	3.3
3	Q	236	LYS	3.2
2	P	247	ALA	3.2
2	P	51	ASN	3.2
2	B	203	VAL	3.1
5	S	174	ARG	3.1
14	N	201	ALA	3.0
1	O	200	GLY	3.0
5	S	56	LEU	3.0
3	C	225	ILE	2.9
7	G	187	PHE	2.9
1	O	186	ALA	2.9
7	U	178	PHE	2.8
3	C	236	LYS	2.8
7	U	186	LYS	2.8
3	C	232	ILE	2.8
3	Q	240	GLU	2.8
5	S	54	SER	2.8
7	G	188	ASP	2.7
3	C	48	LYS	2.7
7	U	58	ASP	2.7
3	Q	48	LYS	2.6
1	A	232	ILE	2.6
3	Q	201	SER	2.6
11	Y	202	GLY	2.6
1	O	229	LEU	2.6
1	O	181	LEU	2.6
6	T	205	LYS	2.5
7	G	189	TRP	2.5
6	T	54	LEU	2.5
3	C	202	GLY	2.5
4	R	131	GLY	2.5
1	O	184	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	205	LYS	2.5
3	Q	223	GLU	2.4
3	C	200	GLN	2.4
14	b	204	PRO	2.4
3	C	98	VAL	2.4
5	S	239	ARG	2.4
1	A	231	ALA	2.4
2	P	233	VAL	2.4
1	O	157	TRP	2.4
3	Q	47	LYS	2.4
2	B	204	SER	2.4
3	C	203	GLY	2.4
3	Q	226	GLU	2.4
5	E	56	LEU	2.4
3	C	201	SER	2.4
5	S	51	ARG	2.4
4	R	128	ALA	2.4
4	D	131	GLY	2.4
2	P	244	GLU	2.3
14	N	203	LEU	2.3
3	C	229	VAL	2.3
7	U	7	ALA	2.3
1	O	198	PHE	2.3
14	b	201	ALA	2.3
2	P	230	GLN	2.3
7	U	50	ILE	2.3
11	Y	201	SER	2.3
3	Q	239	ASN	2.3
1	O	199	GLU	2.3
3	C	233	GLU	2.3
3	C	234	LYS	2.3
6	T	180	GLN	2.2
5	E	60	GLN	2.2
1	O	194	LEU	2.2
6	T	209	PHE	2.2
1	O	192	LEU	2.2
3	Q	205	ASN	2.2
7	U	208	ILE	2.2
10	J	1[A]	MET	2.2
8	V	205	CYS	2.1
8	H	202	ARG	2.1
7	U	204	THR	2.1

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Mol	Chain	Res	Type	RSRZ
6	T	207	LYS	2.1
5	S	53	GLN	2.1
7	U	240	VAL	2.1
4	D	240	ASP	2.1
2	P	58	GLU	2.1
2	P	52	ILE	2.1
14	b	200	VAL	2.1
1	O	59	ARG	2.0
1	O	187	ILE	2.0
5	E	59	HIS	2.0
6	T	181	MET	2.0
14	N	202	THR	2.0
4	D	183	GLU	2.0
5	E	235	GLY	2.0
6	T	143	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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	0.79	0.29	85,120,126,126	0
7	YCM	U	137	10/11	0.86	0.19	59,67,78,79	0
7	YCM	G	137	10/11	0.89	0.15	32,40,55,61	0
3	YCM	C	63	10/11	0.90	0.11	58,60,68,69	0
5	6V1	S	148	15/16	0.91	0.19	45,78,85,86	0
10	6V1	X	91	15/16	0.91	0.19	37,67,74,80	0
7	6V1	U	161	15/16	0.92	0.14	66,88,97,97	0
3	YCM	Q	63	10/11	0.92	0.12	56,59,73,73	0
10	6V1	J	91	15/16	0.93	0.17	35,59,70,71	0
7	6V1	G	47	15/16	0.94	0.18	37,63,69,70	0
5	6V1	E	148	15/16	0.94	0.13	32,66,78,78	0
7	6V1	G	161	15/16	0.94	0.15	33,53,59,61	0

6.3 Carbohydrates ⓘ

There are no monosaccharides 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
15	CL	O	303	1/1	0.69	0.17	103,103,103,103	0
17	MG	V	301	1/1	0.74	0.18	75,75,75,75	0
15	CL	Q	301	1/1	0.79	0.19	92,92,92,92	0
19	6V8	H	305	23/23	0.82	0.22	47,57,91,103	0
19	6V8	V	303	23/23	0.83	0.25	60,69,96,114	0
15	CL	A	302	1/1	0.84	0.10	72,72,72,72	0
18	1PE	I	304	16/16	0.84	0.23	60,79,98,99	0
18	1PE	L	301	16/16	0.85	0.20	59,76,84,85	0
18	1PE	M	305	16/16	0.86	0.19	68,77,95,97	0
15	CL	O	304	1/1	0.88	0.17	77,77,77,77	0
18	1PE	H	304	16/16	0.88	0.17	59,66,97,97	0
15	CL	K	303	1/1	0.88	0.18	78,78,78,78	0
18	1PE	Y	305	16/16	0.88	0.14	56,74,81,83	0
16	K	b	303	1/1	0.88	0.08	54,54,54,54	0
18	1PE	I	303	16/16	0.89	0.14	54,61,77,87	0
18	1PE	W	303	16/16	0.89	0.13	62,71,82,82	0
18	1PE	b	302	16/16	0.89	0.15	50,59,91,96	0
15	CL	C	302	1/1	0.90	0.17	76,76,76,76	0
16	K	L	302	1/1	0.92	0.08	57,57,57,57	0
19	6V8	K	305	23/23	0.92	0.14	41,45,60,77	0
15	CL	D	302	1/1	0.92	0.13	71,71,71,71	0
18	1PE	N	303	16/16	0.92	0.13	43,48,66,68	0
15	CL	a	302	1/1	0.92	0.11	67,67,67,67	0
15	CL	Q	302	1/1	0.92	0.16	72,72,72,72	0
15	CL	C	301	1/1	0.93	0.12	72,72,72,72	0
17	MG	K	301	1/1	0.93	0.08	37,37,37,37	0
15	CL	U	301	1/1	0.93	0.08	68,68,68,68	0
15	CL	R	302	1/1	0.93	0.27	69,69,69,69	0
19	6V8	Y	306	23/23	0.93	0.12	35,37,53,63	0
15	CL	V	302	1/1	0.93	0.09	66,66,66,66	0
15	CL	M	302	1/1	0.94	0.20	62,62,62,62	0
15	CL	K	304	1/1	0.94	0.22	70,70,70,70	0
17	MG	L	303	1/1	0.94	0.12	42,42,42,42	0
15	CL	O	302	1/1	0.94	0.11	67,67,67,67	0
15	CL	A	304	1/1	0.94	0.09	68,68,68,68	0
15	CL	S	301	1/1	0.94	0.29	77,77,77,77	0
17	MG	W	301	1/1	0.94	0.07	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
19	6V8	b	304	23/23	0.94	0.12	39,41,48,54	0
15	CL	M	304	1/1	0.94	0.08	59,59,59,59	0
15	CL	Y	304	1/1	0.94	0.18	77,77,77,77	0
19	6V8	N	305	23/23	0.94	0.10	32,34,37,43	0
15	CL	O	301	1/1	0.95	0.06	64,64,64,64	0
15	CL	D	301	1/1	0.95	0.25	84,84,84,84	0
15	CL	Y	303	1/1	0.95	0.08	60,60,60,60	0
15	CL	S	303	1/1	0.95	0.08	63,63,63,63	0
15	CL	N	302	1/1	0.96	0.14	58,58,58,58	0
17	MG	H	302	1/1	0.96	0.10	34,34,34,34	0
15	CL	B	302	1/1	0.96	0.20	64,64,64,64	0
17	MG	I	301	1/1	0.96	0.07	34,34,34,34	0
15	CL	A	301	1/1	0.96	0.09	50,50,50,50	0
15	CL	R	301	1/1	0.96	0.10	64,64,64,64	0
15	CL	a	303	1/1	0.96	0.09	49,49,49,49	0
17	MG	H	301	1/1	0.96	0.12	69,69,69,69	0
15	CL	a	301	1/1	0.96	0.11	73,73,73,73	0
16	K	N	304	1/1	0.96	0.06	49,49,49,49	0
17	MG	J	301	1/1	0.96	0.08	48,48,48,48	0
15	CL	E	301	1/1	0.96	0.10	69,69,69,69	0
15	CL	a	304	1/1	0.96	0.09	68,68,68,68	0
15	CL	E	303	1/1	0.97	0.09	62,62,62,62	0
15	CL	S	302	1/1	0.97	0.14	75,75,75,75	0
15	CL	W	302	1/1	0.97	0.07	55,55,55,55	0
15	CL	b	301	1/1	0.97	0.18	61,61,61,61	0
17	MG	I	305	1/1	0.97	0.08	33,33,33,33	0
15	CL	K	302	1/1	0.97	0.10	80,80,80,80	0
15	CL	E	302	1/1	0.97	0.07	57,57,57,57	0
16	K	Z	301	1/1	0.97	0.07	48,48,48,48	0
15	CL	F	301	1/1	0.97	0.12	58,58,58,58	0
15	CL	P	301	1/1	0.97	0.10	57,57,57,57	0
16	K	U	302	1/1	0.97	0.09	53,53,53,53	0
15	CL	Y	302	1/1	0.97	0.12	76,76,76,76	0
15	CL	Y	301	1/1	0.98	0.16	65,65,65,65	0
15	CL	G	301	1/1	0.98	0.11	58,58,58,58	0
15	CL	I	302	1/1	0.98	0.10	46,46,46,46	0
17	MG	X	301	1/1	0.98	0.07	49,49,49,49	0
15	CL	B	301	1/1	0.98	0.07	44,44,44,44	0
15	CL	M	303	1/1	0.98	0.06	45,45,45,45	0
15	CL	N	301	1/1	0.98	0.09	40,40,40,40	0
16	K	G	303	1/1	0.98	0.06	41,41,41,41	0
15	CL	M	301	1/1	0.98	0.27	70,70,70,70	0

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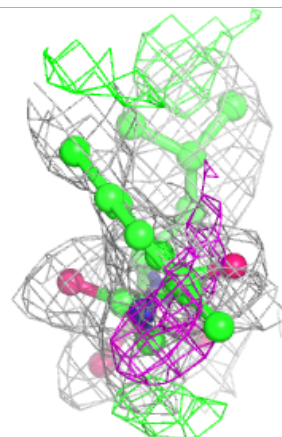
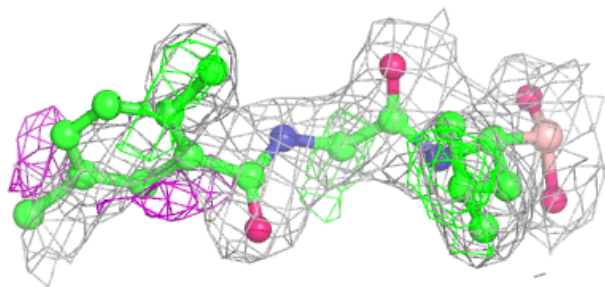
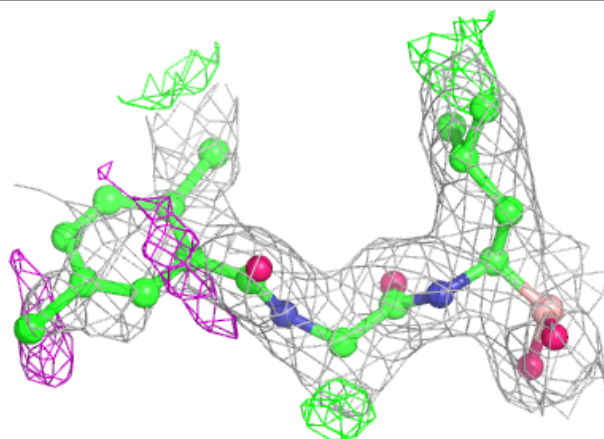
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
15	CL	A	303	1/1	0.99	0.08	56,56,56,56	0
15	CL	G	302	1/1	0.99	0.07	64,64,64,64	0
15	CL	H	303	1/1	0.99	0.09	50,50,50,50	0

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.

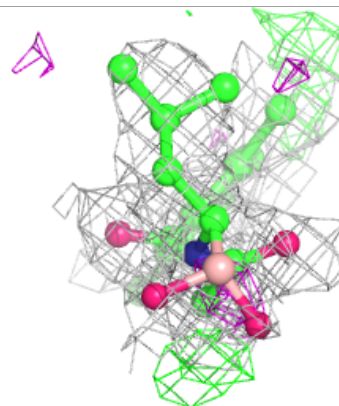
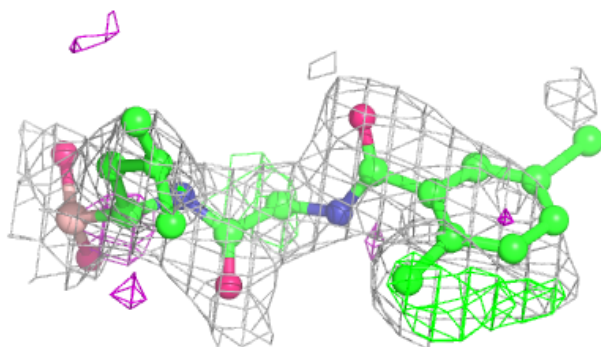
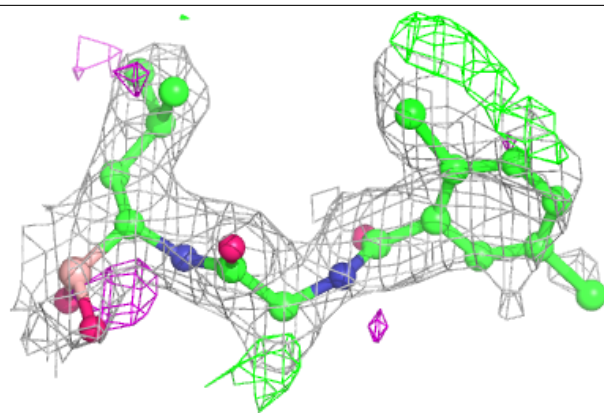
Electron density around 6V8 H 305:

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

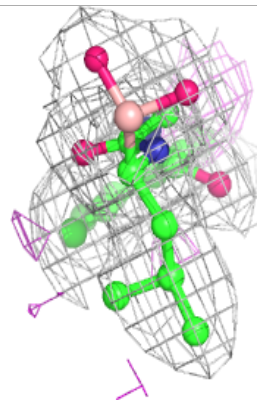
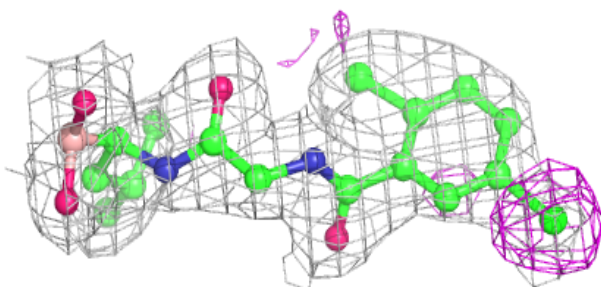
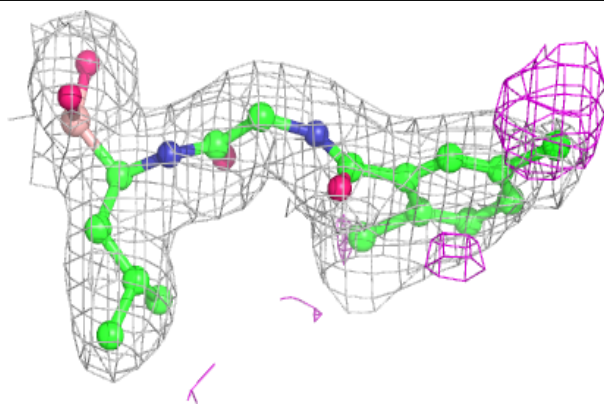


Electron density around 6V8 V 303:

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

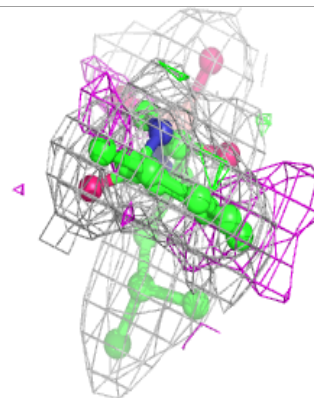
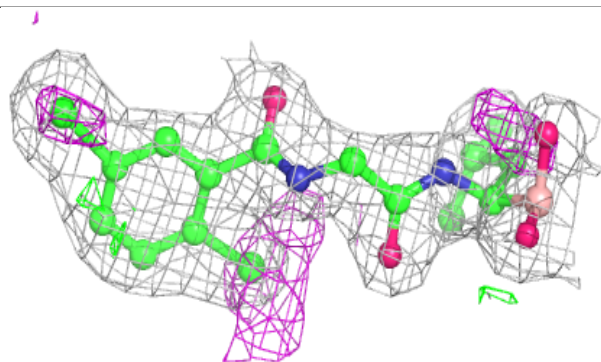
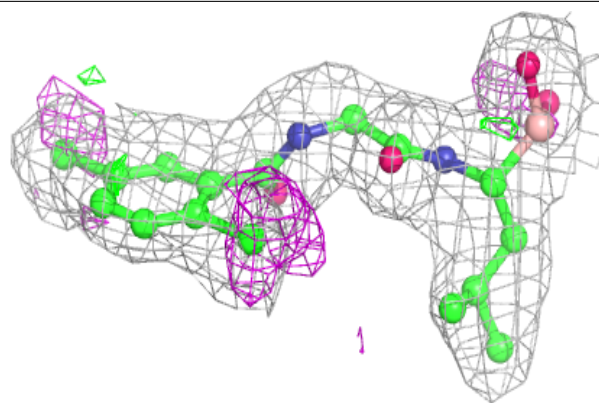
**Electron density around 6V8 K 305:**

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

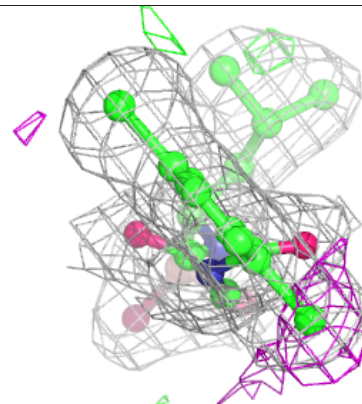
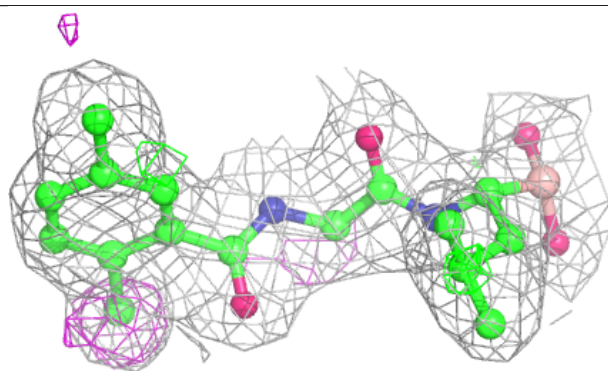
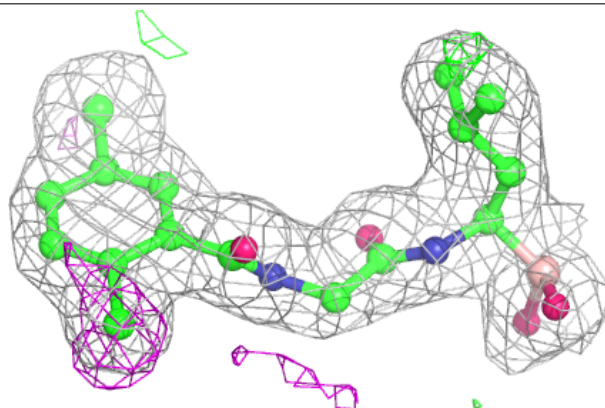


Electron density around 6V8 Y 306:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

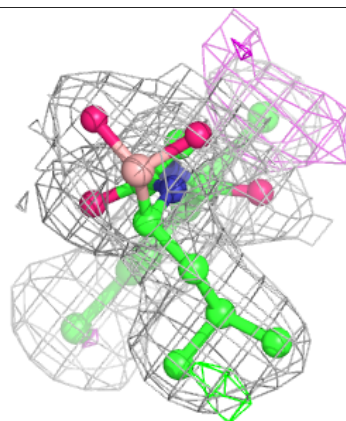
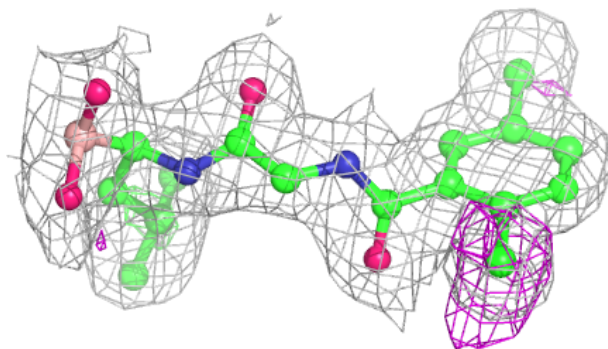
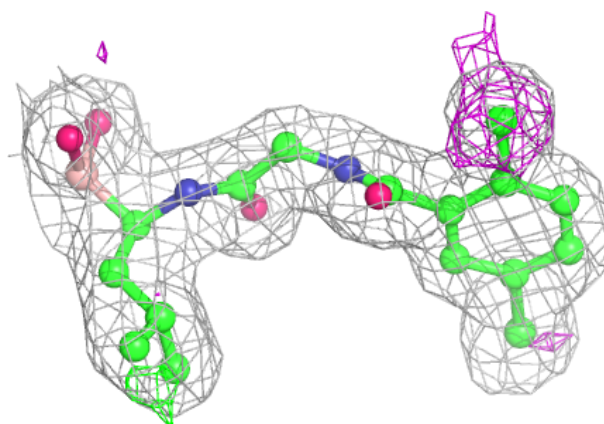
**Electron density around 6V8 b 304:**

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



Electron density around 6V8 N 305:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.