



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2026 – 09:21 AM UTC

PDB ID : 5LF1 / pdb\_00005lf1  
Title : Human 20S proteasome complex with Dihydroeponemycin 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

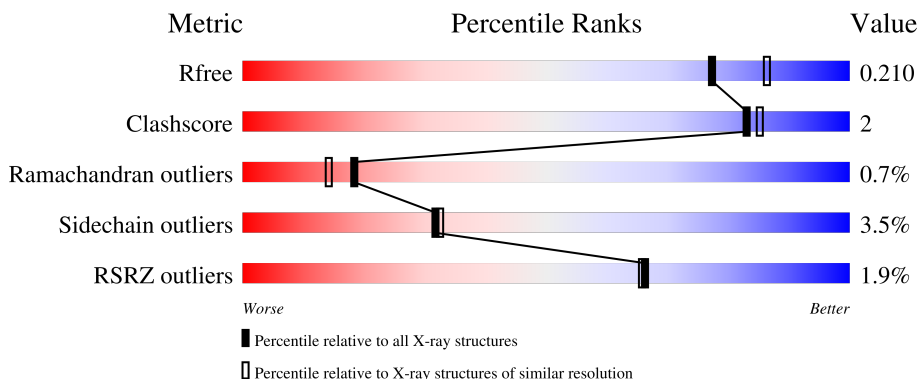
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	234	
1	O	234	
2	B	261	
2	P	261	
3	C	248	

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Mol	Chain	Length	Quality of chain
3	Q	248	4% 83% 11% . .
4	D	241	% 89% 7% . .
4	R	241	2% 91% 5% .
5	E	263	4% 83% 5% . 11%
5	S	263	3% 83% 7% . 10%
6	F	255	% 83% 10% . 6%
6	T	255	3% 82% 9% . 6%
7	G	246	2% 91% 7% . .
7	U	246	2% 88% 7% . .
8	H	234	% 86% 6% . 6%
8	V	234	3% 86% 7% . 6%
9	I	205	93% 6%
9	W	205	94% 5% .
10	J	201	87% 8% . .
10	X	201	90% 5% . .
11	K	204	87% 10% .
11	Y	204	% 86% 11% . .
12	L	213	92% 8%
12	Z	213	93% 7%
13	M	219	92% 6% .
13	a	219	% 93% 5% . .
14	N	205	2% 94% . . .
14	b	205	2% 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 52156 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	230	Total	C	N	O	S	0	3	0
			1788	1145	301	336	6			
1	O	230	Total	C	N	O	S	0	0	0
			1741	1111	293	331	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	248	Total	C	N	O	S	0	2	0
			1922	1217	331	363	11			
2	P	248	Total	C	N	O	S	0	2	0
			1909	1206	325	367	11			

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

There are 4 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	196	Total	C	N	O	S	0	3	0
			1590	1021	271	288	10			
10	X	196	Total	C	N	O	S	0	2	0
			1576	1012	267	287	10			

There are 2 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	200	Total	C	N	O	S	0	0	0
			1545	974	269	293	9			
11	Y	201	Total	C	N	O	S	0	3	0
			1580	996	280	294	10			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	216	Total	C	N	O	S	0	1	0
			1692	1067	291	322	12			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	a	216	Total	C	N	O	S	0	2	0
			1688	1064	291	321	12			

- Molecule 14 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	202	Total	C	N	O	S	0	1	0
			1519	953	258	295	13			
14	b	203	Total	C	N	O	S	0	1	0
			1524	956	259	296	13			

- Molecule 15 is 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		
15	C	2	Total	Cl	0	0
			2	2		
15	D	1	Total	Cl	0	0
			1	1		
15	E	4	Total	Cl	0	0
			4	4		
15	F	1	Total	Cl	0	0
			1	1		
15	G	2	Total	Cl	0	0
			2	2		
15	H	1	Total	Cl	0	0
			1	1		
15	I	1	Total	Cl	0	0
			1	1		
15	K	4	Total	Cl	0	0
			4	4		
15	M	3	Total	Cl	0	0
			3	3		
15	N	4	Total	Cl	0	0
			4	4		
15	O	4	Total	Cl	0	0
			4	4		
15	P	1	Total	Cl	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	Q	2	Total Cl 2 2	0	0
15	R	2	Total Cl 2 2	0	0
15	S	3	Total Cl 3 3	0	0
15	U	1	Total Cl 1 1	0	0
15	V	1	Total Cl 1 1	0	0
15	W	1	Total Cl 1 1	0	0
15	Y	5	Total Cl 5 5	0	0
15	a	3	Total Cl 3 3	0	0
15	b	4	Total Cl 4 4	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).

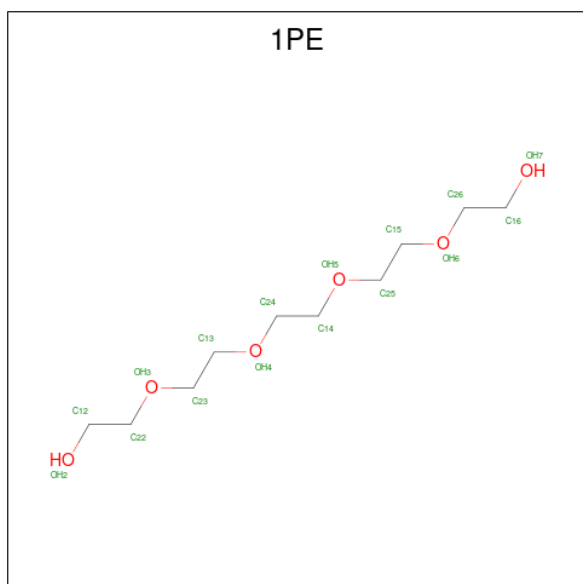
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	H	2	Total Mg 2 2	0	0
17	I	1	Total Mg 1 1	0	0

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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	V	2	Total Mg 2 2	0	0
17	W	1	Total Mg 1 1	0	0
17	X	1	Total Mg 1 1	0	0
17	Y	1	Total Mg 1 1	0	0

- Molecule 18 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula:  $C_{10}H_{22}O_6$ ).



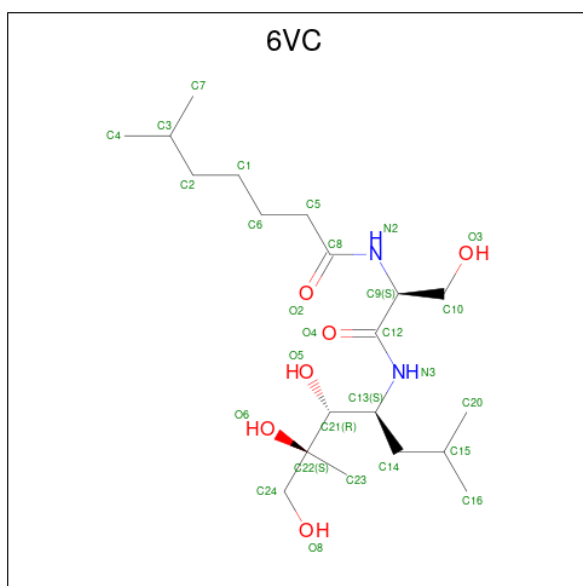
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	H	1	Total C O 16 10 6	0	0
18	I	1	Total C O 16 10 6	0	0
18	L	1	Total C O 16 10 6	0	0
18	M	1	Total C O 16 10 6	0	0
18	N	1	Total C O 16 10 6	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	U	1	Total	C	O	0	0
			16	10	6		
18	W	1	Total	C	O	0	0
			16	10	6		
18	Z	1	Total	C	O	0	0
			16	10	6		
18	a	1	Total	C	O	0	0
			16	10	6		

- Molecule 19 is {N}-[(2 {S})-1-[(2 {S},3 {R},4 {S})-2,6-dimethyl-1,2,3-tris(oxidanyl)heptan-4-yl]amino]-3-oxidanyl-1-oxidanylidene-propan-2-yl]-6-methyl-heptanamide (CCD ID: 6VC) (formula: C<sub>20</sub>H<sub>40</sub>N<sub>2</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
19	H	1	Total	C	N	O	0	0
			28	20	2	6		
19	K	1	Total	C	N	O	0	0
			28	20	2	6		
19	N	1	Total	C	N	O	0	0
			28	20	2	6		
19	V	1	Total	C	N	O	0	0
			28	20	2	6		
19	Y	1	Total	C	N	O	0	0
			28	20	2	6		
19	b	1	Total	C	N	O	0	0
			28	20	2	6		

- Molecule 20 is water.

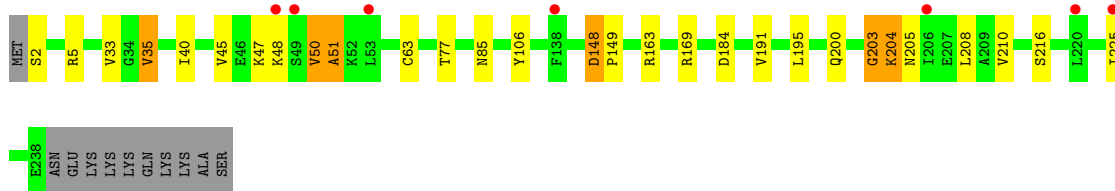
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	A	110	Total O 110 110	0	0
20	B	127	Total O 127 127	0	0
20	C	82	Total O 82 82	0	0
20	D	91	Total O 91 91	0	0
20	E	140	Total O 140 140	0	0
20	F	186	Total O 186 186	0	0
20	G	191	Total O 191 191	0	0
20	H	156	Total O 156 156	0	0
20	I	153	Total O 153 153	0	0
20	J	138	Total O 138 138	0	0
20	K	98	Total O 98 98	0	0
20	L	130	Total O 130 130	0	0
20	M	149	Total O 149 149	0	0
20	N	165	Total O 165 165	0	0
20	O	91	Total O 91 91	0	0
20	P	123	Total O 123 123	0	0
20	Q	75	Total O 75 75	0	0
20	R	127	Total O 127 127	0	0
20	S	122	Total O 122 122	0	0
20	T	93	Total O 93 93	0	0
20	U	112	Total O 112 112	0	0

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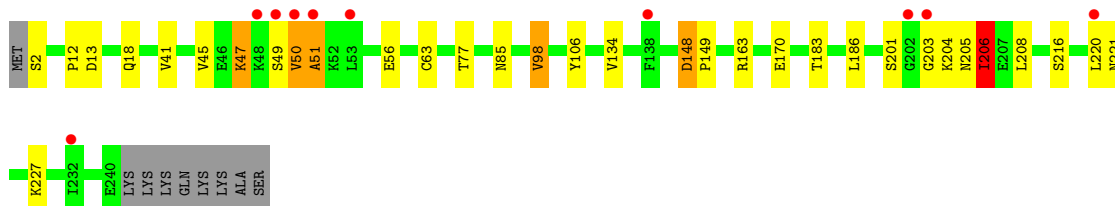
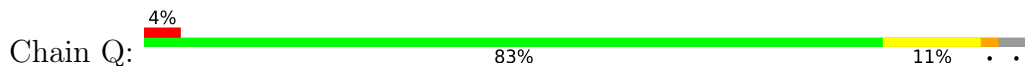
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
20	V	109	Total 109	O 109	0	0
20	W	116	Total 116	O 116	0	0
20	X	127	Total 127	O 127	0	0
20	Y	141	Total 141	O 141	0	0
20	Z	171	Total 171	O 171	0	0
20	a	174	Total 174	O 174	0	0
20	b	124	Total 124	O 124	0	0

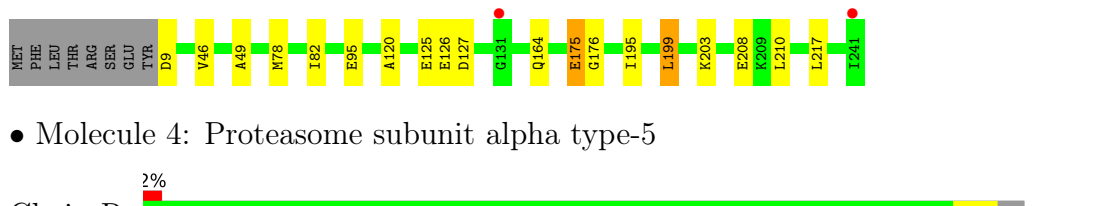
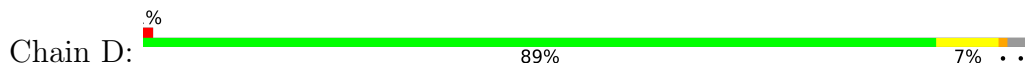




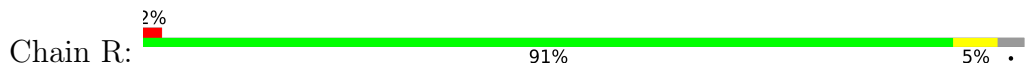
● Molecule 3: Proteasome subunit alpha type-7



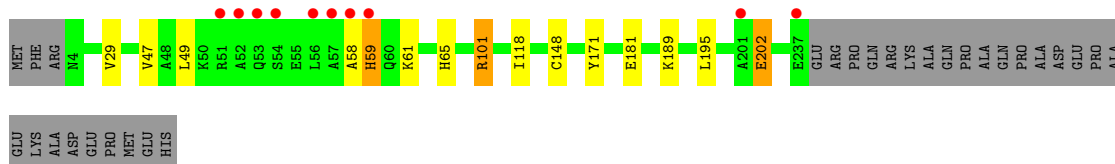
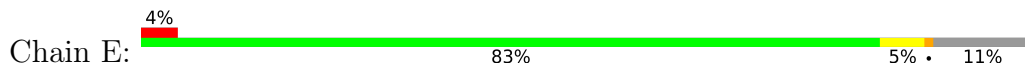
● Molecule 4: Proteasome subunit alpha type-5



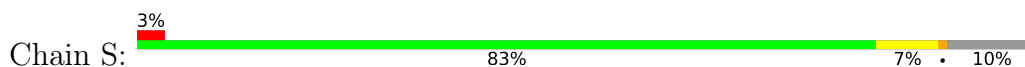
● Molecule 4: Proteasome subunit alpha type-5



● Molecule 5: Proteasome subunit alpha type-1



● Molecule 5: Proteasome subunit alpha type-1



PRO  
ALA  
GLU  
LYS  
ALA  
ASP  
GLU  
PRO  
MET  
GLU  
HIS

- Molecule 6: Proteasome subunit alpha type-3

Chain F: 83% 10% • 6%

MET SER SER SER ILE GLY THR G6 D17 E31 S34 G44 V53 R65 G74 L81 L87 N105 M117 N143 D152 V156 R169 Q170 T174 K182 R187 V190 D202 E203 V204 H224 V227 R232 K240 K244

GLU  
GLU  
ASP  
GLU  
SER  
ASP  
ASP  
ASN  
ASN  
MET

- Molecule 6: Proteasome subunit alpha type-3

Chain T: 82% 9% • 6%

MET SER SER ILE GLY T5 G6 Y7 D17 E24 M27 E31 S34 V53 G61 R65 G74 L81 L87 M117 V142 N143 D152 V156 Q170 T174 V190 K191 D202 E203 V204 K205 D206 K207 A208 R223 H224 Y238 A239

K240 E241 K244 GLU ASP SER ASP ASP ASN MET

- Molecule 7: Proteasome subunit alpha type-6

Chain G: 91% 7% •• 2%

MET S2 V42 C47 V51 I72 C78 R88 E108 M113 L114 R117 C137 C161 V183 F187 D188 H189 T190 A198 L206 S207 L208 K226 E232 E244 R245 ASP

- Molecule 7: Proteasome subunit alpha type-6

Chain U: 88% 7% ••• 2%

MET S2 V42 R43 C47 D58 K59 I72 C78 L114 I118 M138 I139 L140 V151 C161 V183 K184 K185 K186 PHE ASP TRP PHE GLU Q193 F194 V195 E196 T197 A198 I199 L206 L239 E244 R245 ASP

- Molecule 8: Proteasome subunit beta type-7

Chain H: 86% 6% • 6%

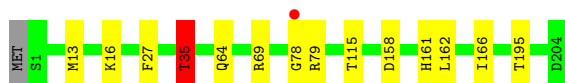
T1 V6 E22 E64 L65 L68 S69 R72 V77 R81 S112 M127 S131 L132 G170 L183 Y202 R203 C204 I216 E220 ILE GLU VAL LEU GLU THR VAL GLN THR MET ASP THR SER

- Molecule 8: Proteasome subunit beta type-7

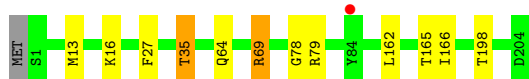
Chain V: 86% 7% • 6% 3%



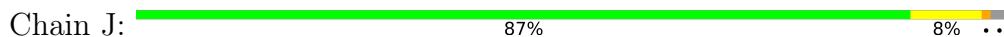
- Molecule 9: Proteasome subunit beta type-3



- Molecule 9: Proteasome subunit beta type-3



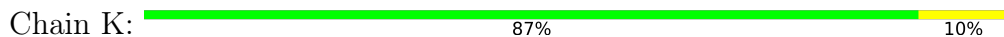
- Molecule 10: Proteasome subunit beta type-2



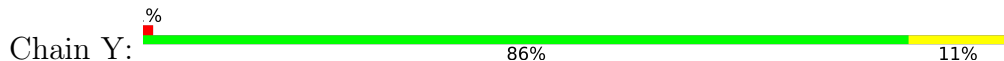
- Molecule 10: Proteasome subunit beta type-2



- Molecule 11: Proteasome subunit beta type-5

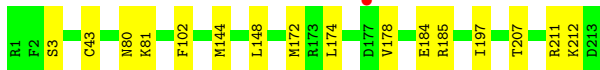


- Molecule 11: Proteasome subunit beta type-5



- Molecule 12: Proteasome subunit beta type-1

Chain L:  92% 8%



- Molecule 12: Proteasome subunit beta type-1

Chain Z:  93% 7%



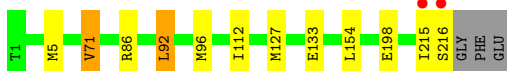
- Molecule 13: Proteasome subunit beta type-4

Chain M:  92% 6%



- Molecule 13: Proteasome subunit beta type-4

Chain a:  93% 5%

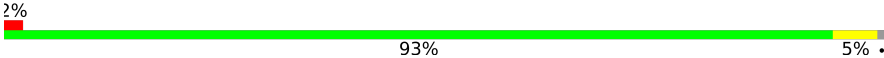


- Molecule 14: Proteasome subunit beta type-6

Chain N:  94% 5%



- 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, $\alpha$ , $\beta$ , $\gamma$	113.89Å 203.49Å 316.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	171.09 – 2.00 171.09 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.5 (171.09-2.00) 99.4 (171.09-2.00)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.40 (at 2.00Å)	Xtrriage
Refinement program	REFMAC 5.8.0103	Depositor
R, $R_{free}$	0.178 , 0.213 (Not available) , 0.210	Depositor DCC
$R_{free}$ test set	24379 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	39.6	Xtrriage
Anisotropy	0.246	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 41.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	52156	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.85% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: 1PE, CL, 6VC, K, MG, 6V1, 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	0.91	0/1833	0.97	0/2489
1	O	0.81	0/1778	0.94	0/2419
2	B	0.95	0/1958	0.98	1/2645 (0.0%)
2	P	0.85	1/1945 (0.1%)	0.97	1/2631 (0.0%)
3	C	0.93	0/1818	1.06	1/2469 (0.0%)
3	Q	0.92	1/1834 (0.1%)	1.08	10/2490 (0.4%)
4	D	0.90	0/1789	0.98	1/2424 (0.0%)
4	R	1.00	0/1780	1.03	2/2408 (0.1%)
5	E	0.94	1/1842 (0.1%)	1.00	0/2493
5	S	0.90	0/1901	0.97	1/2571 (0.0%)
6	F	1.00	1/1935 (0.1%)	1.05	4/2605 (0.2%)
6	T	0.95	1/1894 (0.1%)	1.06	9/2556 (0.4%)
7	G	1.00	2/1909 (0.1%)	1.00	4/2579 (0.2%)
7	U	0.90	0/1804	0.95	0/2441
8	H	1.01	0/1697	1.06	5/2299 (0.2%)
8	V	0.89	0/1655	0.98	2/2251 (0.1%)
9	I	0.98	1/1648 (0.1%)	1.10	7/2219 (0.3%)
9	W	0.84	0/1630	0.99	6/2197 (0.3%)
10	J	0.99	0/1613	0.99	2/2180 (0.1%)
10	X	0.94	0/1599	0.94	1/2163 (0.0%)
11	K	0.93	0/1576	1.03	1/2131 (0.0%)
11	Y	1.03	0/1620	1.05	2/2185 (0.1%)
12	L	0.89	1/1672 (0.1%)	0.94	1/2257 (0.0%)
12	Z	1.03	1/1675 (0.1%)	0.99	2/2257 (0.1%)
13	M	0.99	1/1728 (0.1%)	0.98	1/2339 (0.0%)
13	a	1.04	0/1724	1.01	1/2336 (0.0%)
14	N	1.09	1/1548 (0.1%)	1.08	1/2095 (0.0%)
14	b	1.00	0/1554	1.06	2/2104 (0.1%)
All	All	0.95	12/48959 (0.0%)	1.01	68/66233 (0.1%)

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	P	0	4
3	Q	0	2
4	D	0	4
4	R	0	2
7	U	1	0
9	I	0	1
9	W	0	1
10	J	0	2
10	X	0	1
13	a	0	1
All	All	1	18

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	Z	102	PHE	N-CA	7.68	1.55	1.46
6	F	44	GLY	N-CA	6.43	1.51	1.45
14	N	73	PRO	CA-C	6.06	1.55	1.51
13	M	3	ASN	C-O	-5.77	1.20	1.25
7	G	51	VAL	N-CA	5.72	1.53	1.46

The worst 5 of 68 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	190	VAL	CB-CA-C	-9.88	99.10	112.04
9	I	16[A]	LYS	CA-C-N	9.68	135.91	122.07
9	I	16[A]	LYS	C-N-CA	9.68	135.91	122.07
9	I	16[B]	LYS	CA-C-N	9.68	135.91	122.07
9	I	16[B]	LYS	C-N-CA	9.68	135.91	122.07

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	U	47	6V1	C1

5 of 18 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	127	ASP	Peptide

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Mol	Chain	Res	Type	Group
4	D	175[A]	GLU	Peptide
4	D	175[B]	GLU	Peptide,Mainchain
9	I	78	GLY	Peptide
10	J	1[A]	MET	Peptide

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1788	0	1761	7	0
1	O	1741	0	1683	4	0
2	B	1922	0	1913	8	0
2	P	1909	0	1874	13	1
3	C	1798	0	1718	18	0
3	Q	1820	0	1749	11	0
4	D	1762	0	1709	6	0
4	R	1753	0	1726	5	0
5	E	1822	0	1779	8	0
5	S	1875	0	1818	14	1
6	F	1888	0	1882	9	0
6	T	1856	0	1816	9	0
7	G	1912	0	1882	5	0
7	U	1815	0	1748	11	0
8	H	1664	0	1678	11	0
8	V	1622	0	1592	10	0
9	I	1613	0	1646	8	0
9	W	1599	0	1621	7	0
10	J	1590	0	1581	14	0
10	X	1576	0	1561	10	0
11	K	1545	0	1495	8	0
11	Y	1580	0	1555	15	0
12	L	1636	0	1625	8	0
12	Z	1642	0	1635	4	0
13	M	1692	0	1670	8	0
13	a	1688	0	1658	6	0
14	N	1519	0	1493	6	0
14	b	1524	0	1493	8	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	1	0	0	0	0
15	E	4	0	0	0	0
15	F	1	0	0	0	0
15	G	2	0	0	0	0
15	H	1	0	0	0	0
15	I	1	0	0	0	0
15	K	4	0	0	0	0
15	M	3	0	0	1	0
15	N	4	0	0	1	0
15	O	4	0	0	0	0
15	P	1	0	0	0	0
15	Q	2	0	0	0	0
15	R	2	0	0	1	0
15	S	3	0	0	0	0
15	U	1	0	0	0	0
15	V	1	0	0	0	0
15	W	1	0	0	0	0
15	Y	5	0	0	0	0
15	a	3	0	0	1	0
15	b	4	0	0	1	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	1	0	0	0	0
17	J	1	0	0	0	0
17	K	1	0	0	0	0
17	V	2	0	0	0	0
17	W	1	0	0	0	0
17	X	1	0	0	0	0
17	Y	1	0	0	0	0
18	H	16	0	22	0	0
18	I	16	0	22	0	0
18	L	16	0	22	0	0
18	M	16	0	22	0	0
18	N	16	0	22	0	0
18	U	16	0	22	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	W	16	0	22	0	0
18	Z	16	0	22	0	0
18	a	16	0	22	0	0
19	H	28	0	0	0	0
19	K	28	0	0	0	0
19	N	28	0	0	0	0
19	V	28	0	0	0	0
19	Y	28	0	0	0	0
19	b	28	0	0	2	0
20	A	110	0	0	0	0
20	B	127	0	0	0	0
20	C	82	0	0	1	0
20	D	91	0	0	0	0
20	E	140	0	0	3	0
20	F	186	0	0	3	0
20	G	191	0	0	2	0
20	H	156	0	0	3	0
20	I	153	0	0	1	0
20	J	138	0	0	2	0
20	K	98	0	0	0	0
20	L	130	0	0	2	0
20	M	149	0	0	0	0
20	N	165	0	0	0	0
20	O	91	0	0	1	0
20	P	123	0	0	0	0
20	Q	75	0	0	0	0
20	R	127	0	0	2	0
20	S	122	0	0	2	0
20	T	93	0	0	0	0
20	U	112	0	0	0	0
20	V	109	0	0	0	0
20	W	116	0	0	2	0
20	X	127	0	0	0	0
20	Y	141	0	0	0	0
20	Z	171	0	0	1	0
20	a	174	0	0	0	0
20	b	124	0	0	0	0
All	All	52156	0	47559	230	1

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

The worst 5 of 230 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:25[B]:MET:HE3	2:P:25[B]:MET:HA	1.36	1.06
10:J:1[A]:MET:HE1	10:J:134:TYR:H	1.31	0.91
10:X:1:MET:HE1	10:X:134:TYR:H	1.33	0.91
10:J:185:LYS:NZ	20:J:401:HOH:O	2.05	0.84
12:L:144:MET:HE1	12:L:185:ARG:HB2	1.60	0.83

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:241:GLU:OE1	5:S:234:GLU:OE2[1_455]	2.09	0.11

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	231/234 (99%)	221 (96%)	6 (3%)	4 (2%)	7 3
1	O	228/234 (97%)	217 (95%)	7 (3%)	4 (2%)	6 3
2	B	248/261 (95%)	238 (96%)	10 (4%)	0	100 100
2	P	248/261 (95%)	233 (94%)	11 (4%)	4 (2%)	7 3
3	C	236/248 (95%)	223 (94%)	7 (3%)	6 (2%)	4 1
3	Q	236/248 (95%)	221 (94%)	7 (3%)	8 (3%)	3 1
4	D	232/241 (96%)	223 (96%)	6 (3%)	3 (1%)	9 5
4	R	232/241 (96%)	223 (96%)	6 (3%)	3 (1%)	9 5
5	E	232/263 (88%)	226 (97%)	5 (2%)	1 (0%)	30 27
5	S	238/263 (90%)	231 (97%)	5 (2%)	2 (1%)	16 11
6	F	241/255 (94%)	239 (99%)	2 (1%)	0	100 100
6	T	239/255 (94%)	233 (98%)	3 (1%)	3 (1%)	9 5
7	G	241/246 (98%)	237 (98%)	4 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	U	232/246 (94%)	227 (98%)	3 (1%)	2 (1%)	14	9
8	H	220/234 (94%)	217 (99%)	3 (1%)	0	100	100
8	V	220/234 (94%)	216 (98%)	4 (2%)	0	100	100
9	I	205/205 (100%)	202 (98%)	3 (2%)	0	100	100
9	W	204/205 (100%)	199 (98%)	5 (2%)	0	100	100
10	J	195/201 (97%)	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%)	211 (99%)	2 (1%)	0	100	100
12	Z	212/213 (100%)	210 (99%)	2 (1%)	0	100	100
13	M	215/219 (98%)	208 (97%)	7 (3%)	0	100	100
13	a	216/219 (99%)	210 (97%)	6 (3%)	0	100	100
14	N	201/205 (98%)	198 (98%)	2 (1%)	1 (0%)	24	21
14	b	202/205 (98%)	198 (98%)	3 (2%)	1 (0%)	24	21
All	All	6212/6458 (96%)	6040 (97%)	129 (2%)	43 (1%)	18	14

5 of 43 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	52	LYS
3	C	204	LYS
4	D	176	GLY
1	O	52	LYS
2	P	54	LYS

### 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%)	174 (94%)	11 (6%)	18	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	O	176/191 (92%)	166 (94%)	10 (6%)	18	15
2	B	199/221 (90%)	191 (96%)	8 (4%)	28	27
2	P	197/221 (89%)	184 (93%)	13 (7%)	15	12
3	C	179/210 (85%)	171 (96%)	8 (4%)	24	23
3	Q	184/210 (88%)	174 (95%)	10 (5%)	20	17
4	D	189/203 (93%)	183 (97%)	6 (3%)	34	35
4	R	187/203 (92%)	184 (98%)	3 (2%)	55	62
5	E	192/223 (86%)	185 (96%)	7 (4%)	31	31
5	S	197/223 (88%)	193 (98%)	4 (2%)	48	54
6	F	199/212 (94%)	189 (95%)	10 (5%)	22	20
6	T	192/212 (91%)	182 (95%)	10 (5%)	21	18
7	G	202/207 (98%)	194 (96%)	8 (4%)	28	27
7	U	186/207 (90%)	181 (97%)	5 (3%)	39	42
8	H	181/195 (93%)	174 (96%)	7 (4%)	28	28
8	V	172/195 (88%)	164 (95%)	8 (5%)	23	22
9	I	176/174 (101%)	174 (99%)	2 (1%)	65	73
9	W	173/174 (99%)	171 (99%)	2 (1%)	63	70
10	J	166/170 (98%)	158 (95%)	8 (5%)	23	21
10	X	165/170 (97%)	160 (97%)	5 (3%)	36	38
11	K	154/159 (97%)	147 (96%)	7 (4%)	24	23
11	Y	159/159 (100%)	153 (96%)	6 (4%)	29	29
12	L	175/178 (98%)	170 (97%)	5 (3%)	37	40
12	Z	175/178 (98%)	171 (98%)	4 (2%)	44	49
13	M	180/181 (99%)	176 (98%)	4 (2%)	45	50
13	a	178/181 (98%)	173 (97%)	5 (3%)	38	41
14	N	158/159 (99%)	156 (99%)	2 (1%)	61	68
14	b	158/159 (99%)	154 (98%)	4 (2%)	42	45
All	All	5034/5366 (94%)	4852 (96%)	182 (4%)	32	31

5 of 182 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	P	249	ARG

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Mol	Chain	Res	Type
7	U	42	VAL
3	Q	98	VAL
5	S	45	VAL
8	V	65	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 66 such sidechains are listed below:

Mol	Chain	Res	Type
10	X	174	ASN
11	Y	162	GLN
14	b	193	GLN
11	K	62	GLN
10	J	101	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	U	161	7	13,15,16	1.91	4 (30%)	10,20,22	2.77	4 (40%)
5	6V1	S	148	5	13,15,16	1.74	4 (30%)	10,20,22	3.00	6 (60%)
7	6V1	G	161	7	13,15,16	1.61	4 (30%)	10,20,22	2.44	4 (40%)
5	6V1	E	148	5	13,15,16	1.82	3 (23%)	10,20,22	3.73	4 (40%)
3	YCM	C	63	3	7,9,10	1.01	0	5,10,12	1.36	1 (20%)
7	YCM	U	137	7	7,9,10	0.99	0	5,10,12	1.13	0
7	6V1	U	47	7	13,15,16	1.93	3 (23%)	10,20,22	1.89	3 (30%)
10	6V1	X	91	10	13,15,16	1.73	3 (23%)	10,20,22	5.52	7 (70%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	YCM	G	137	7	7,9,10	1.79	3 (42%)	5,10,12	2.16	1 (20%)
10	6V1	J	91	10	13,15,16	1.76	3 (23%)	10,20,22	5.53	7 (70%)
3	YCM	Q	63	3	7,9,10	1.32	1 (14%)	5,10,12	3.04	4 (80%)
7	6V1	G	47	7	13,15,16	2.26	4 (30%)	10,20,22	2.13	2 (20%)

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

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

The worst 5 of 32 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	47	6V1	CB-SG	-5.93	1.76	1.82
7	U	47	6V1	CB-SG	-5.26	1.76	1.82
10	J	91	6V1	C1-SG	-5.16	1.77	1.83
10	X	91	6V1	C1-SG	-4.68	1.78	1.83
5	E	148	6V1	CB-SG	-4.45	1.77	1.82

The worst 5 of 43 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	J	91	6V1	C5-C4-N3	9.13	113.82	108.07
10	X	91	6V1	C6-N3-C2	8.54	133.38	123.37
10	J	91	6V1	C6-N3-C2	8.46	133.28	123.37
10	X	91	6V1	O7-C2-N3	8.10	133.96	124.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	X	91	6V1	C5-C4-N3	7.77	112.96	108.07

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	U	47	6V1	C1

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	G	137	YCM	SG-CD-CE-NZ2
3	Q	63	YCM	CE-CD-SG-CB
3	Q	63	YCM	SG-CD-CE-OZ1
3	Q	63	YCM	SG-CD-CE-NZ2
7	U	137	YCM	CE-CD-SG-CB

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 87 ligands modelled in this entry, 72 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	6VC	V	304	8	27,27,27	1.04	2 (7%)	34,36,36	1.33	5 (14%)
18	1PE	N	305	-	15,15,15	0.54	0	14,14,14	0.53	0
18	1PE	U	302	-	15,15,15	0.62	0	14,14,14	0.96	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
19	6VC	Y	307	11	27,27,27	1.28	4 (14%)	34,36,36	1.24	4 (11%)
18	1PE	M	304	-	15,15,15	0.63	0	14,14,14	0.35	0
18	1PE	H	304	-	15,15,15	0.60	0	14,14,14	0.58	0
18	1PE	a	304	-	15,15,15	0.70	0	14,14,14	0.46	0
19	6VC	H	305	8	27,27,27	1.02	2 (7%)	34,36,36	1.38	5 (14%)
19	6VC	N	307	14	27,27,27	1.19	1 (3%)	34,36,36	1.58	5 (14%)
18	1PE	Z	301	-	15,15,15	0.62	0	14,14,14	0.53	0
18	1PE	L	301	-	15,15,15	0.62	0	14,14,14	0.64	0
19	6VC	b	306	14	27,27,27	1.22	4 (14%)	34,36,36	1.93	10 (29%)
18	1PE	W	303	-	15,15,15	0.57	0	14,14,14	0.35	0
19	6VC	K	306	11	27,27,27	0.67	0	34,36,36	1.38	7 (20%)
18	1PE	I	303	-	15,15,15	0.57	0	14,14,14	0.84	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	6VC	V	304	8	-	5/38/38/38	-
18	1PE	N	305	-	-	4/13/13/13	-
18	1PE	U	302	-	-	8/13/13/13	-
19	6VC	Y	307	11	-	4/38/38/38	-
18	1PE	M	304	-	-	8/13/13/13	-
18	1PE	H	304	-	-	10/13/13/13	-
18	1PE	a	304	-	-	7/13/13/13	-
19	6VC	H	305	8	-	5/38/38/38	-
19	6VC	N	307	14	-	2/38/38/38	-
18	1PE	Z	301	-	-	8/13/13/13	-
18	1PE	L	301	-	-	7/13/13/13	-
19	6VC	b	306	14	-	5/38/38/38	-
18	1PE	W	303	-	-	7/13/13/13	-
19	6VC	K	306	11	-	5/38/38/38	-
18	1PE	I	303	-	-	6/13/13/13	-

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	N	307	6VC	C22-C21	4.53	1.60	1.55
19	Y	307	6VC	C22-C21	4.51	1.60	1.55
19	H	305	6VC	C23-C22	3.51	1.58	1.52
19	V	304	6VC	C22-C21	3.36	1.58	1.55
19	b	306	6VC	C22-C21	3.30	1.58	1.55

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	N	307	6VC	C10-C9-N2	-5.34	97.52	110.78
19	b	306	6VC	O3-C10-C9	-4.79	98.18	111.18
19	b	306	6VC	C1-C6-C5	-4.64	96.06	113.13
19	b	306	6VC	O2-C8-C5	-3.90	114.95	122.02
19	N	307	6VC	C10-C9-C12	3.63	119.30	110.12

There are no chirality outliers.

5 of 91 torsion outliers are listed below:

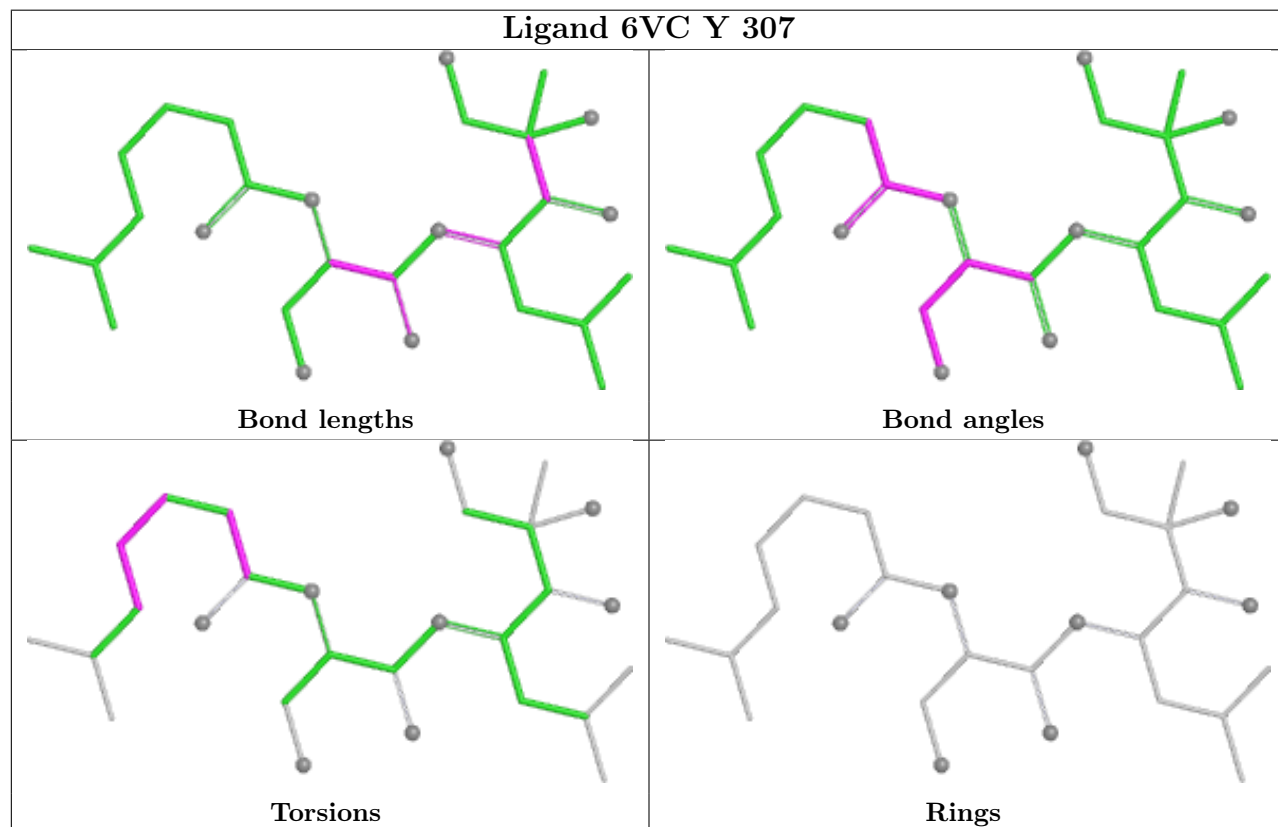
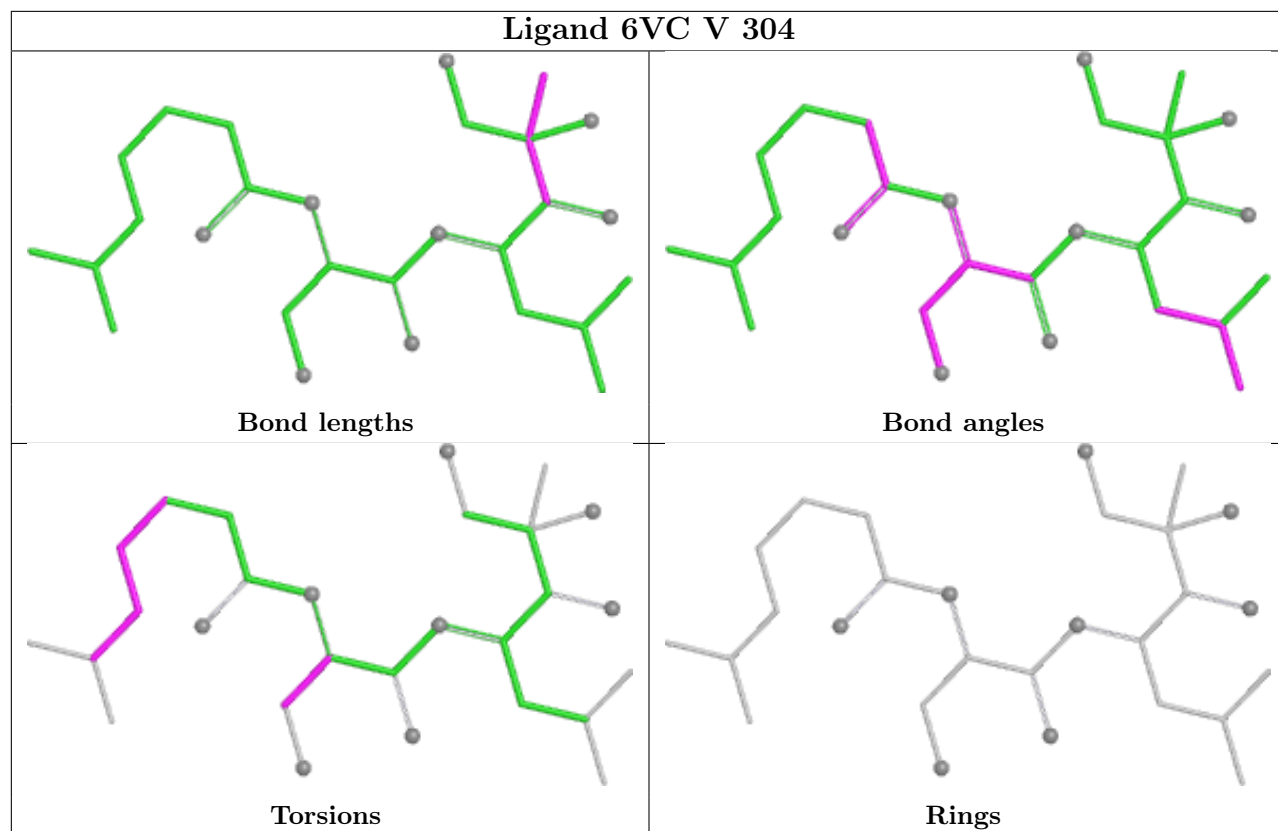
Mol	Chain	Res	Type	Atoms
19	b	306	6VC	O3-C10-C9-N2
18	U	302	1PE	C25-C15-OH6-C26
18	L	301	1PE	C16-C26-OH6-C15
18	U	302	1PE	OH4-C13-C23-OH3
18	a	304	1PE	OH4-C13-C23-OH3

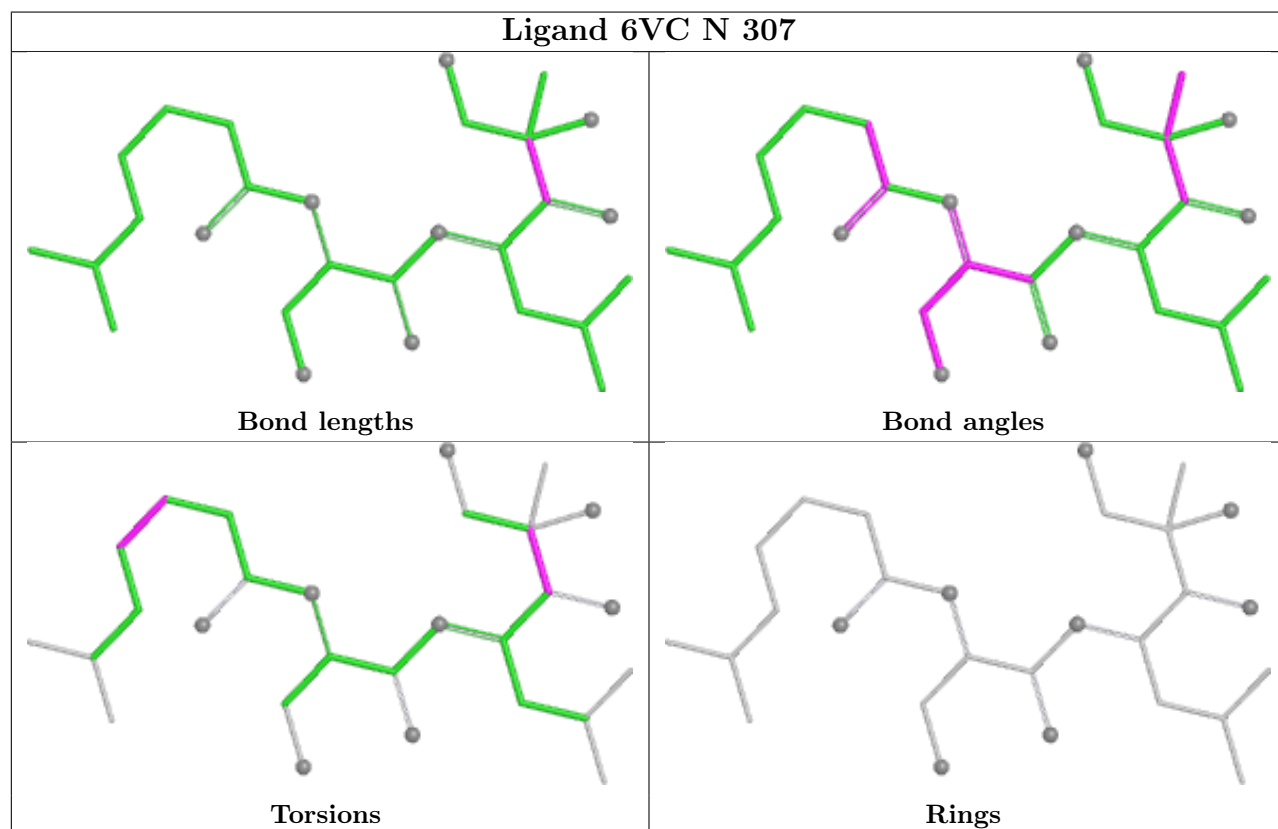
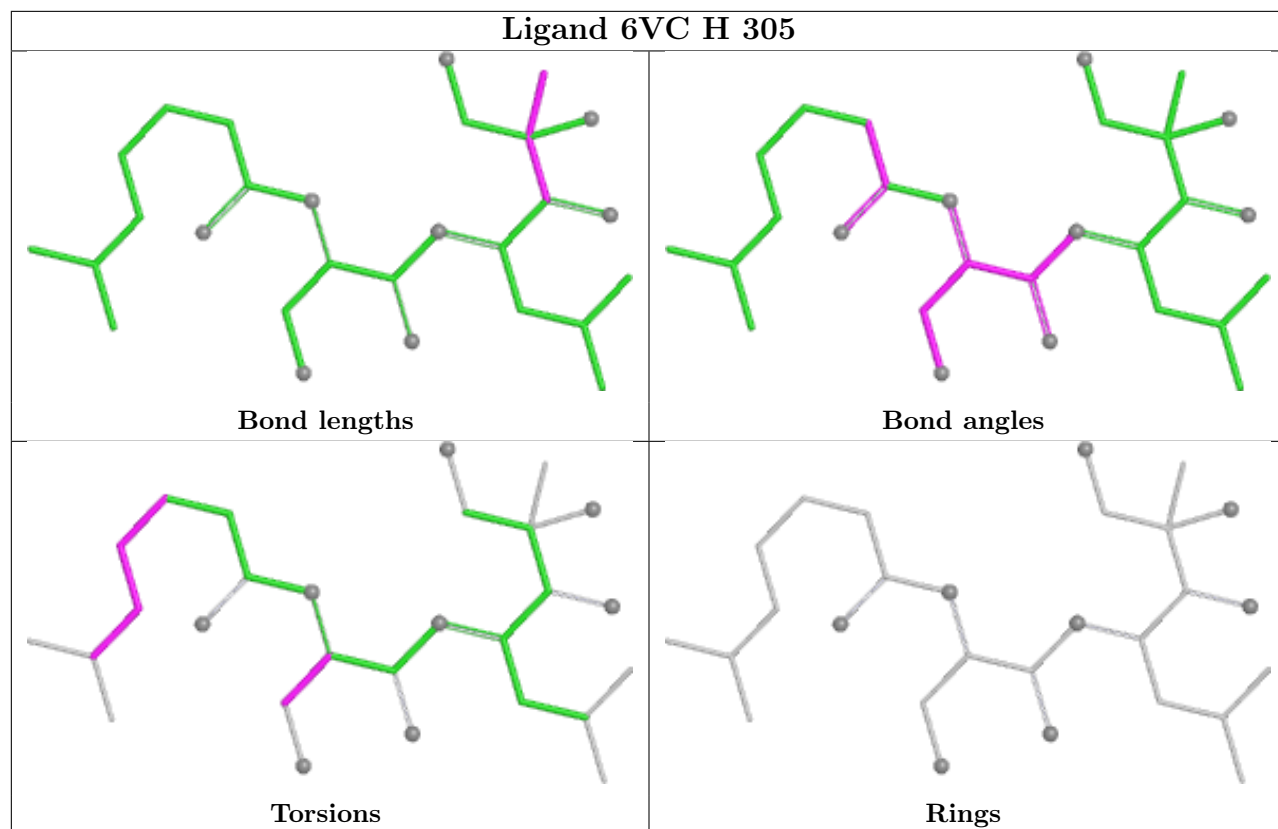
There are no ring outliers.

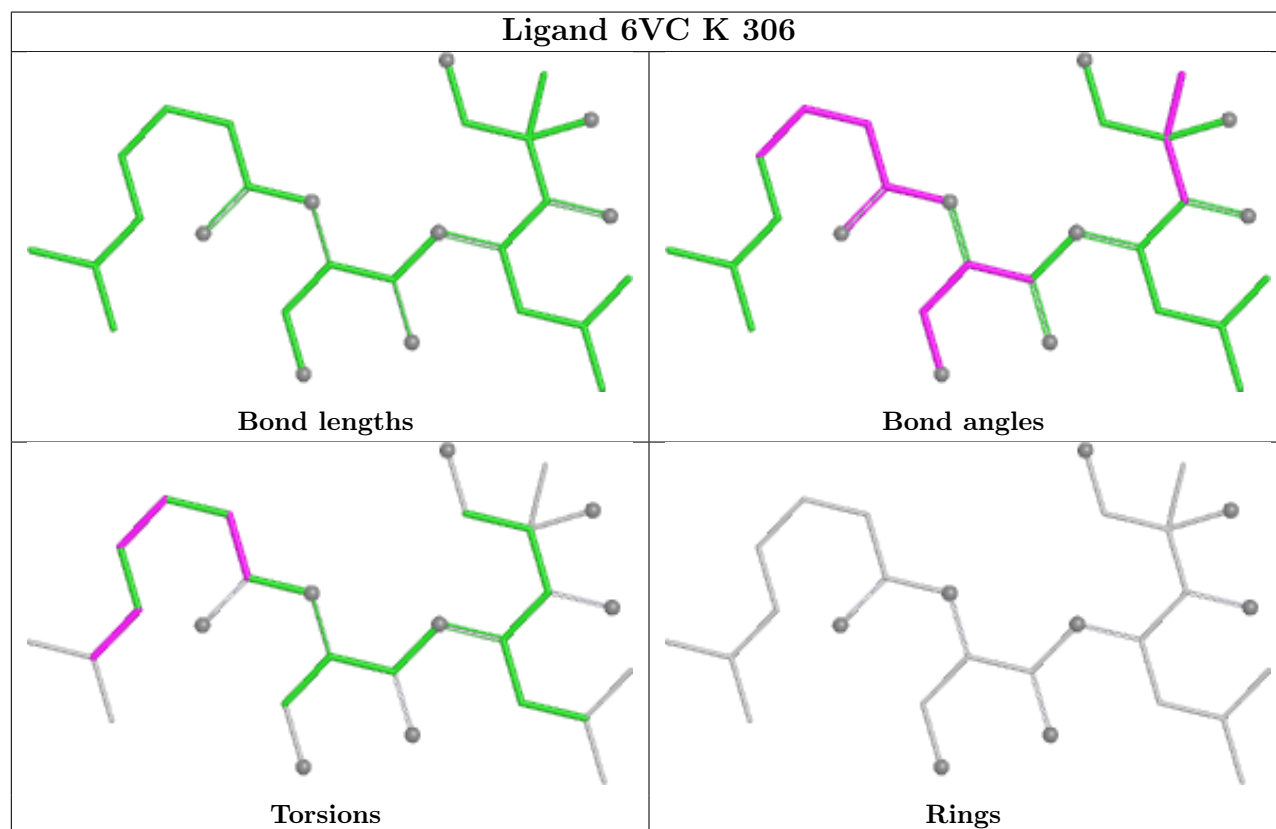
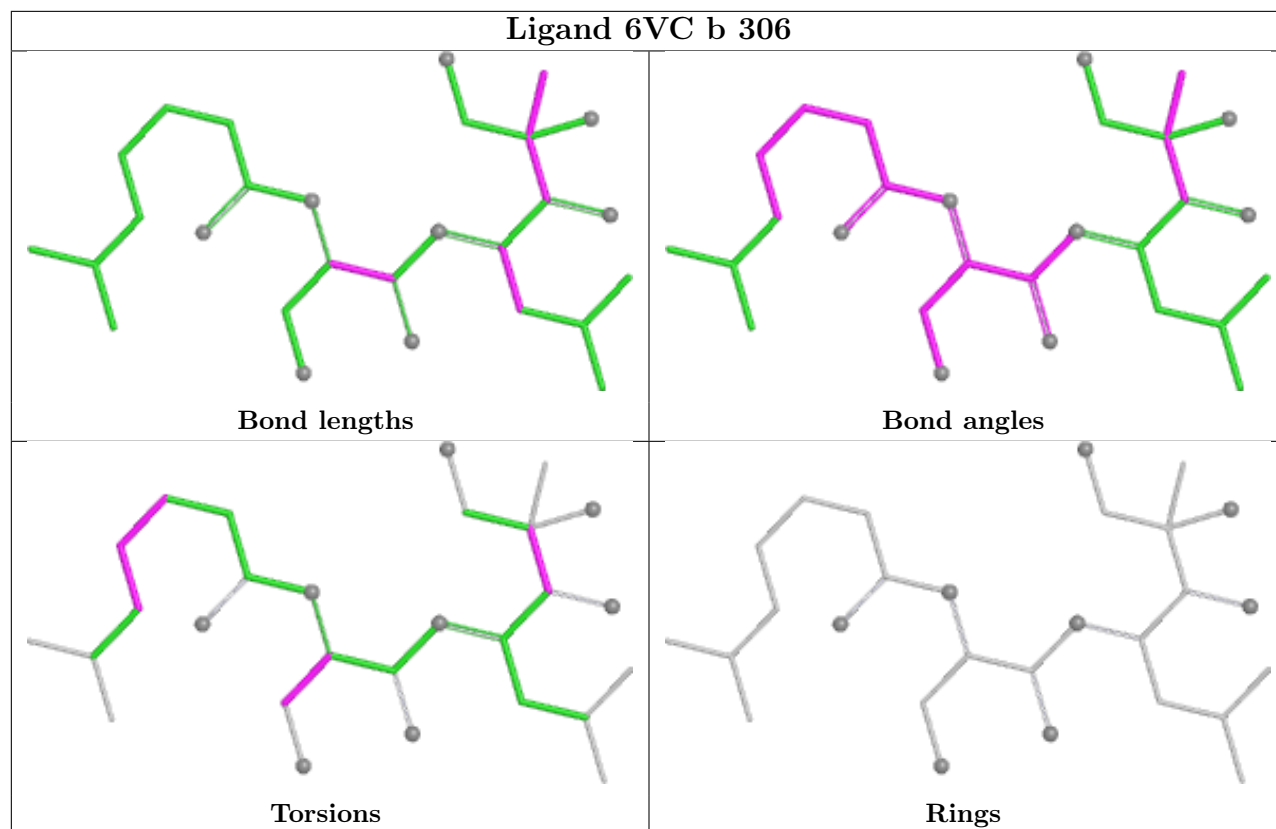
1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	b	306	6VC	2	0

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







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	230/234 (98%)	-0.05	5 (2%) 62 61	24, 46, 82, 92	3 (1%)
1	O	230/234 (98%)	0.43	7 (3%) 52 51	41, 63, 100, 120	0
2	B	248/261 (95%)	0.12	6 (2%) 59 59	21, 52, 89, 136	2 (0%)
2	P	248/261 (95%)	0.34	9 (3%) 46 45	32, 61, 106, 142	2 (0%)
3	C	236/248 (95%)	0.45	7 (2%) 52 51	27, 60, 100, 139	2 (0%)
3	Q	238/248 (95%)	0.42	10 (4%) 40 39	34, 61, 112, 149	0
4	D	233/241 (96%)	0.34	2 (0%) 81 80	31, 58, 88, 114	1 (0%)
4	R	233/241 (96%)	0.04	6 (2%) 57 56	20, 44, 71, 93	1 (0%)
5	E	233/263 (88%)	-0.00	10 (4%) 40 39	25, 43, 86, 100	1 (0%)
5	S	237/263 (90%)	0.09	9 (3%) 44 43	23, 47, 81, 104	3 (1%)
6	F	239/255 (93%)	-0.26	2 (0%) 82 82	20, 36, 58, 74	4 (1%)
6	T	240/255 (94%)	0.27	8 (3%) 49 48	28, 52, 85, 107	1 (0%)
7	G	241/246 (97%)	-0.16	5 (2%) 63 63	19, 40, 73, 101	2 (0%)
7	U	235/246 (95%)	0.33	4 (1%) 69 68	29, 60, 95, 124	1 (0%)
8	H	220/234 (94%)	-0.22	2 (0%) 81 80	21, 36, 66, 100	2 (0%)
8	V	220/234 (94%)	0.09	7 (3%) 50 49	25, 48, 84, 97	2 (0%)
9	I	204/205 (99%)	-0.34	1 (0%) 87 87	22, 37, 58, 74	3 (1%)
9	W	204/205 (99%)	-0.01	1 (0%) 87 87	29, 50, 73, 81	2 (0%)
10	J	195/201 (97%)	-0.22	1 (0%) 87 87	17, 42, 60, 76	3 (1%)
10	X	195/201 (97%)	-0.15	0 100 100	21, 44, 59, 74	2 (1%)
11	K	200/204 (98%)	-0.12	1 (0%) 87 87	36, 46, 71, 84	0
11	Y	201/204 (98%)	-0.31	3 (1%) 72 71	21, 37, 59, 70	3 (1%)
12	L	213/213 (100%)	0.00	1 (0%) 87 87	25, 49, 71, 85	2 (0%)
12	Z	213/213 (100%)	-0.24	0 100 100	26, 38, 60, 74	1 (0%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	M	216/219 (98%)	-0.28	1 (0%) 87 87	27, 39, 62, 95	1 (0%)
13	a	216/219 (98%)	-0.27	2 (0%) 81 80	25, 39, 60, 82	2 (0%)
14	N	202/205 (98%)	-0.37	4 (1%) 65 64	22, 35, 56, 94	1 (0%)
14	b	203/205 (99%)	-0.19	4 (1%) 65 64	32, 41, 66, 97	1 (0%)
All	All	6223/6458 (96%)	0.00	118 (1%) 66 66	17, 46, 84, 149	48 (0%)

The worst 5 of 118 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
11	K	40	TYR	5.1
5	S	2	PHE	4.7
13	a	216	SER	4.4
8	V	204	CYS	4.3
11	Y	40	TYR	4.3

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
7	6V1	U	47	15/16	0.83	0.17	72,103,109,110	0
7	YCM	U	137	10/11	0.86	0.14	51,59,75,76	0
7	YCM	G	137	10/11	0.87	0.14	33,39,51,53	0
5	6V1	E	148	15/16	0.88	0.16	32,54,64,65	0
3	YCM	C	63	10/11	0.89	0.11	55,56,63,64	0
7	6V1	G	47	15/16	0.90	0.15	39,61,64,65	0
5	6V1	S	148	15/16	0.90	0.15	37,63,68,70	0
10	6V1	X	91	15/16	0.91	0.15	36,54,57,61	0
7	6V1	U	161	15/16	0.92	0.11	53,73,78,78	0
10	6V1	J	91	15/16	0.93	0.13	33,53,58,59	0
3	YCM	Q	63	10/11	0.93	0.09	51,54,64,67	0
7	6V1	G	161	15/16	0.94	0.12	33,51,57,58	0

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
18	1PE	M	304	16/16	0.80	0.19	78,83,97,98	0
18	1PE	H	304	16/16	0.81	0.15	58,69,77,79	0
18	1PE	a	304	16/16	0.81	0.17	66,70,86,87	0
18	1PE	W	303	16/16	0.85	0.13	59,64,71,74	0
15	CL	O	304	1/1	0.85	0.16	67,67,67,67	0
18	1PE	I	303	16/16	0.87	0.11	55,58,68,71	0
18	1PE	U	302	16/16	0.87	0.14	46,56,73,75	0
15	CL	D	301	1/1	0.88	0.26	69,69,69,69	0
18	1PE	L	301	16/16	0.88	0.13	60,70,74,76	0
18	1PE	Z	301	16/16	0.88	0.12	57,66,72,73	0
15	CL	O	303	1/1	0.88	0.11	87,87,87,87	0
15	CL	E	303	1/1	0.90	0.22	64,64,64,64	0
15	CL	K	303	1/1	0.90	0.14	69,69,69,69	0
19	6VC	V	304	28/28	0.90	0.11	42,45,60,61	0
15	CL	Y	306	1/1	0.91	0.26	63,63,63,63	0
15	CL	E	304	1/1	0.91	0.15	63,63,63,63	0
18	1PE	N	305	16/16	0.91	0.11	41,49,62,64	0
15	CL	C	302	1/1	0.91	0.20	71,71,71,71	0
15	CL	Q	301	1/1	0.92	0.17	67,67,67,67	0
15	CL	C	301	1/1	0.92	0.13	60,60,60,60	0
15	CL	B	302	1/1	0.92	0.23	57,57,57,57	0
15	CL	A	302	1/1	0.93	0.10	64,64,64,64	0
15	CL	Q	302	1/1	0.93	0.24	64,64,64,64	0
15	CL	K	305	1/1	0.93	0.24	65,65,65,65	0
15	CL	a	303	1/1	0.93	0.10	60,60,60,60	0
15	CL	M	303	1/1	0.93	0.14	59,59,59,59	0
15	CL	G	302	1/1	0.93	0.12	60,60,60,60	0
15	CL	I	302	1/1	0.93	0.12	48,48,48,48	0
15	CL	E	302	1/1	0.94	0.16	55,55,55,55	0
15	CL	S	301	1/1	0.94	0.30	64,64,64,64	0
15	CL	V	303	1/1	0.94	0.21	59,59,59,59	0
15	CL	K	304	1/1	0.94	0.16	60,60,60,60	0
19	6VC	H	305	28/28	0.94	0.10	33,37,55,60	0
15	CL	N	303	1/1	0.94	0.21	56,56,56,56	0
19	6VC	Y	307	28/28	0.94	0.09	27,29,51,56	0
15	CL	Y	304	1/1	0.95	0.09	64,64,64,64	0
15	CL	Y	305	1/1	0.95	0.12	57,57,57,57	0

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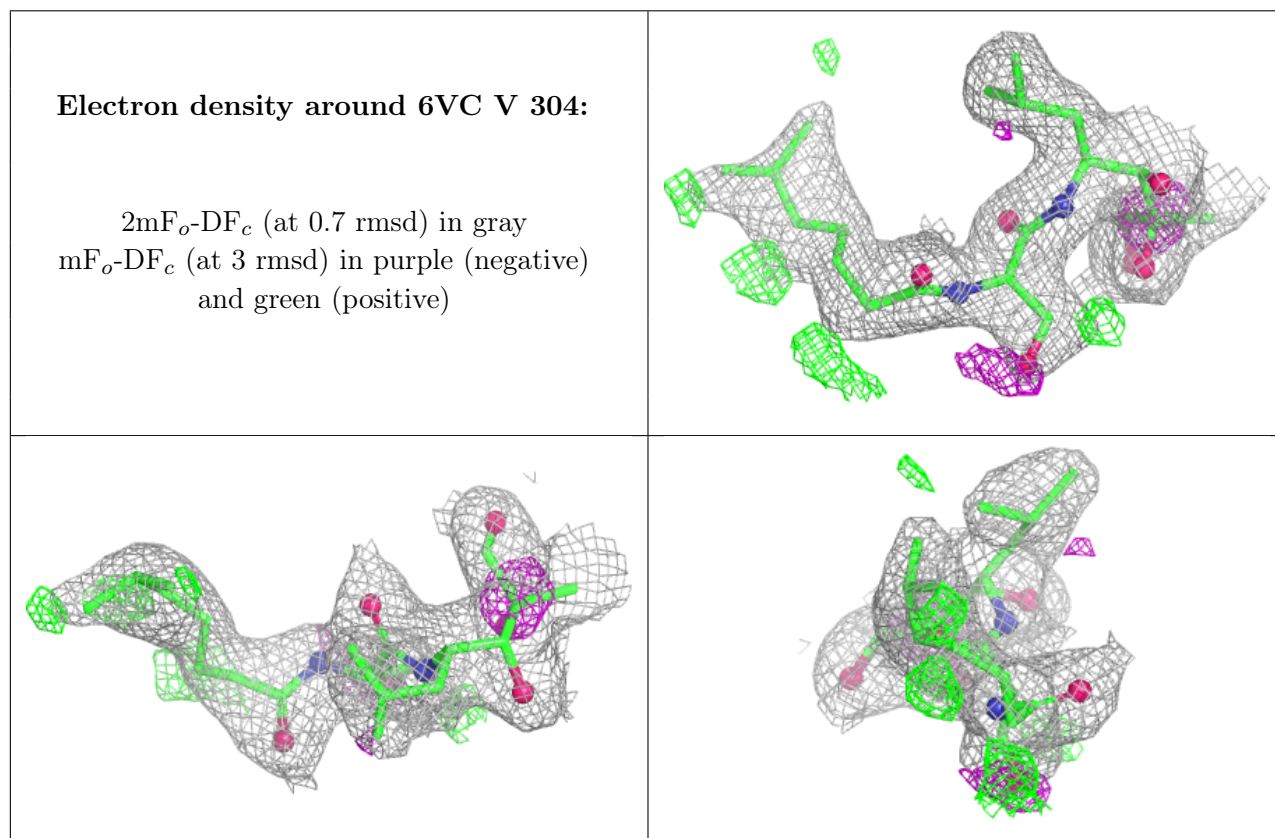
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
15	CL	M	301	1/1	0.95	0.33	56,56,56,56	0
15	CL	a	301	1/1	0.95	0.20	59,59,59,59	0
15	CL	R	301	1/1	0.95	0.14	58,58,58,58	0
16	K	b	305	1/1	0.95	0.12	41,41,41,41	0
15	CL	R	302	1/1	0.95	0.26	57,57,57,57	0
19	6VC	K	306	28/28	0.95	0.09	36,39,61,62	0
19	6VC	N	307	28/28	0.95	0.09	25,29,49,52	0
15	CL	N	304	1/1	0.95	0.26	52,52,52,52	0
15	CL	O	302	1/1	0.95	0.09	63,63,63,63	0
19	6VC	b	306	28/28	0.95	0.09	31,34,55,56	0
15	CL	W	302	1/1	0.96	0.09	54,54,54,54	0
15	CL	H	303	1/1	0.96	0.15	53,53,53,53	0
15	CL	F	301	1/1	0.96	0.15	51,51,51,51	0
15	CL	S	302	1/1	0.96	0.16	63,63,63,63	0
15	CL	S	303	1/1	0.96	0.13	55,55,55,55	0
15	CL	B	301	1/1	0.96	0.12	41,41,41,41	0
15	CL	b	302	1/1	0.96	0.16	55,55,55,55	0
15	CL	b	303	1/1	0.96	0.22	56,56,56,56	0
16	K	U	303	1/1	0.97	0.11	41,41,41,41	0
15	CL	Y	303	1/1	0.97	0.19	59,59,59,59	0
17	MG	I	301	1/1	0.97	0.10	33,33,33,33	0
17	MG	V	302	1/1	0.97	0.09	58,58,58,58	0
17	MG	Y	301	1/1	0.97	0.10	30,30,30,30	0
15	CL	a	302	1/1	0.97	0.09	43,43,43,43	0
15	CL	A	304	1/1	0.97	0.17	57,57,57,57	0
15	CL	A	303	1/1	0.97	0.08	50,50,50,50	0
15	CL	O	301	1/1	0.97	0.13	55,55,55,55	0
15	CL	b	304	1/1	0.97	0.08	42,42,42,42	0
15	CL	A	301	1/1	0.98	0.11	52,52,52,52	0
15	CL	b	301	1/1	0.98	0.15	45,45,45,45	0
15	CL	Y	302	1/1	0.98	0.08	38,38,38,38	0
15	CL	N	302	1/1	0.98	0.13	45,45,45,45	0
15	CL	E	301	1/1	0.98	0.15	61,61,61,61	0
16	K	G	303	1/1	0.98	0.11	33,33,33,33	0
16	K	L	302	1/1	0.98	0.13	47,47,47,47	0
16	K	N	306	1/1	0.98	0.08	38,38,38,38	0
15	CL	P	301	1/1	0.98	0.08	53,53,53,53	0
15	CL	G	301	1/1	0.98	0.30	48,48,48,48	0
17	MG	H	301	1/1	0.98	0.07	57,57,57,57	0
15	CL	U	301	1/1	0.98	0.18	54,54,54,54	0
17	MG	K	301	1/1	0.98	0.08	36,36,36,36	0
17	MG	V	301	1/1	0.98	0.10	37,37,37,37	0

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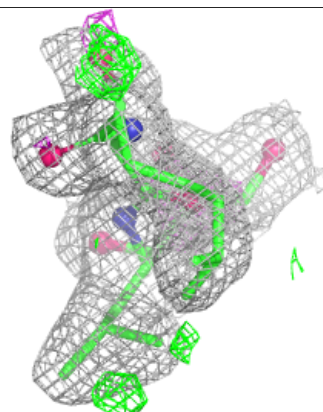
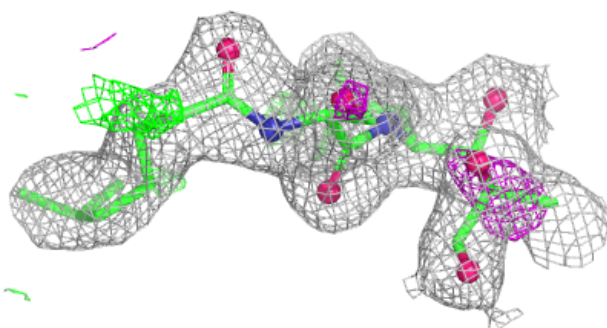
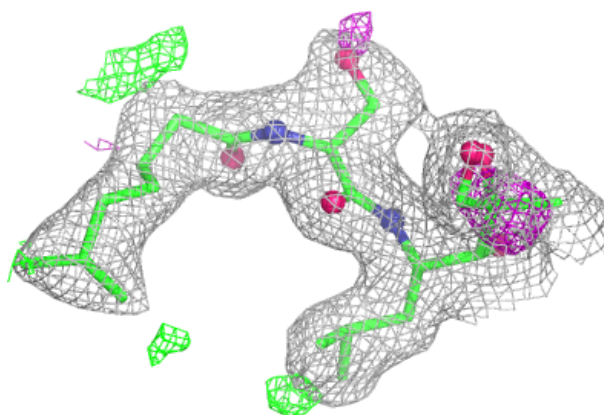
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
15	CL	K	302	1/1	0.98	0.10	42,42,42,42	0
17	MG	W	301	1/1	0.98	0.10	38,38,38,38	0
16	K	Z	302	1/1	0.99	0.08	39,39,39,39	0
17	MG	X	301	1/1	0.99	0.04	49,49,49,49	0
17	MG	J	301	1/1	0.99	0.02	48,48,48,48	0
15	CL	M	302	1/1	0.99	0.11	40,40,40,40	0
15	CL	N	301	1/1	0.99	0.04	35,35,35,35	0
17	MG	H	302	1/1	0.99	0.10	33,33,33,33	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.

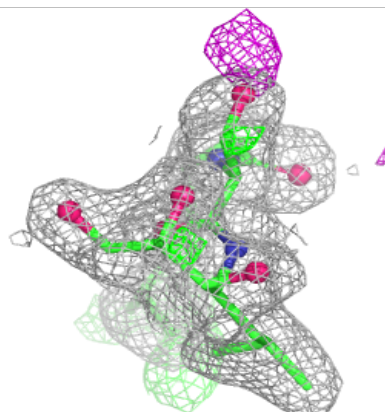
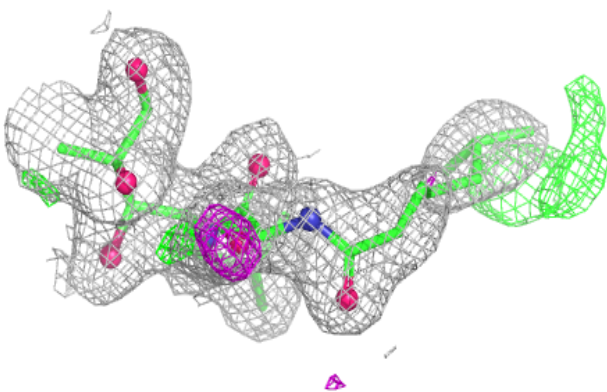
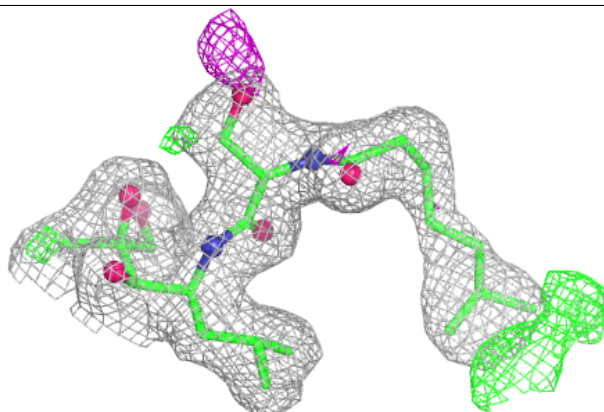


**Electron density around 6VC H 305:**

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

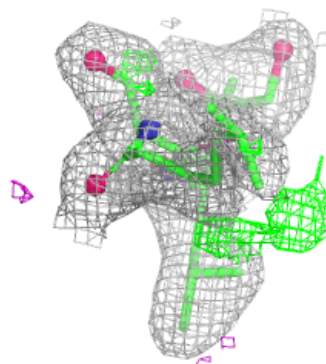
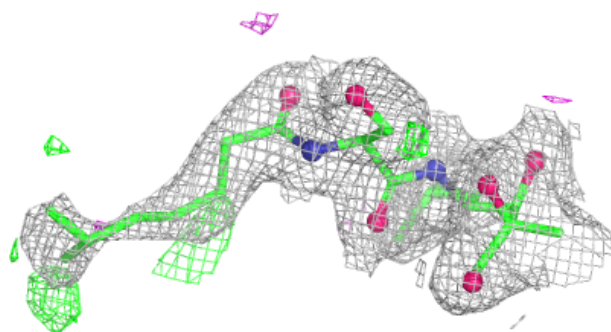
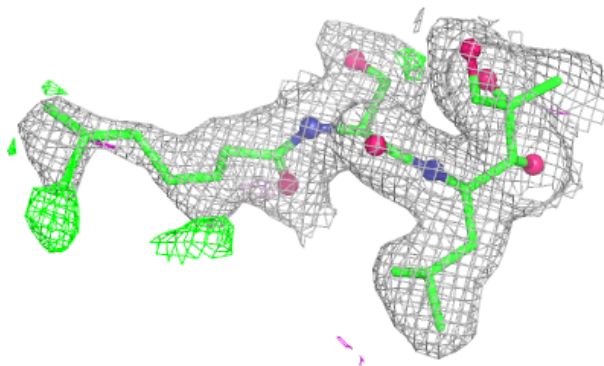
**Electron density around 6VC Y 307:**

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

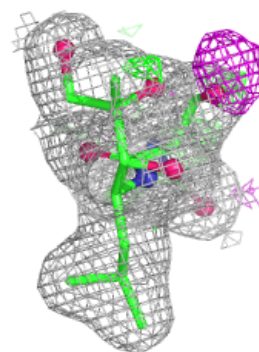
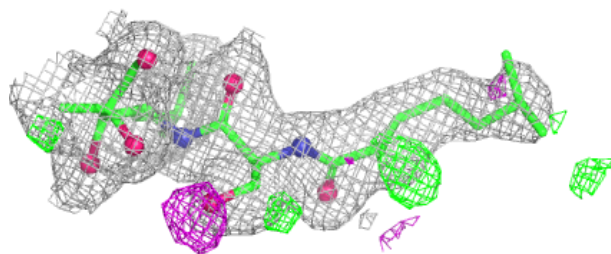
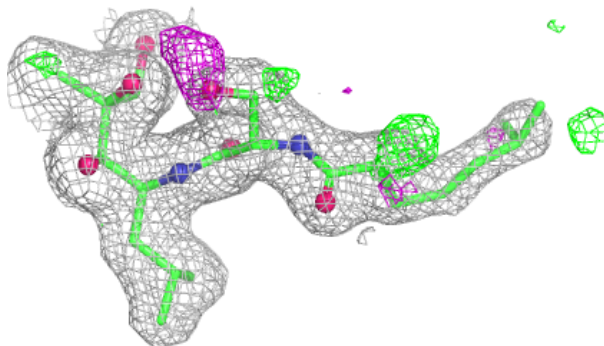


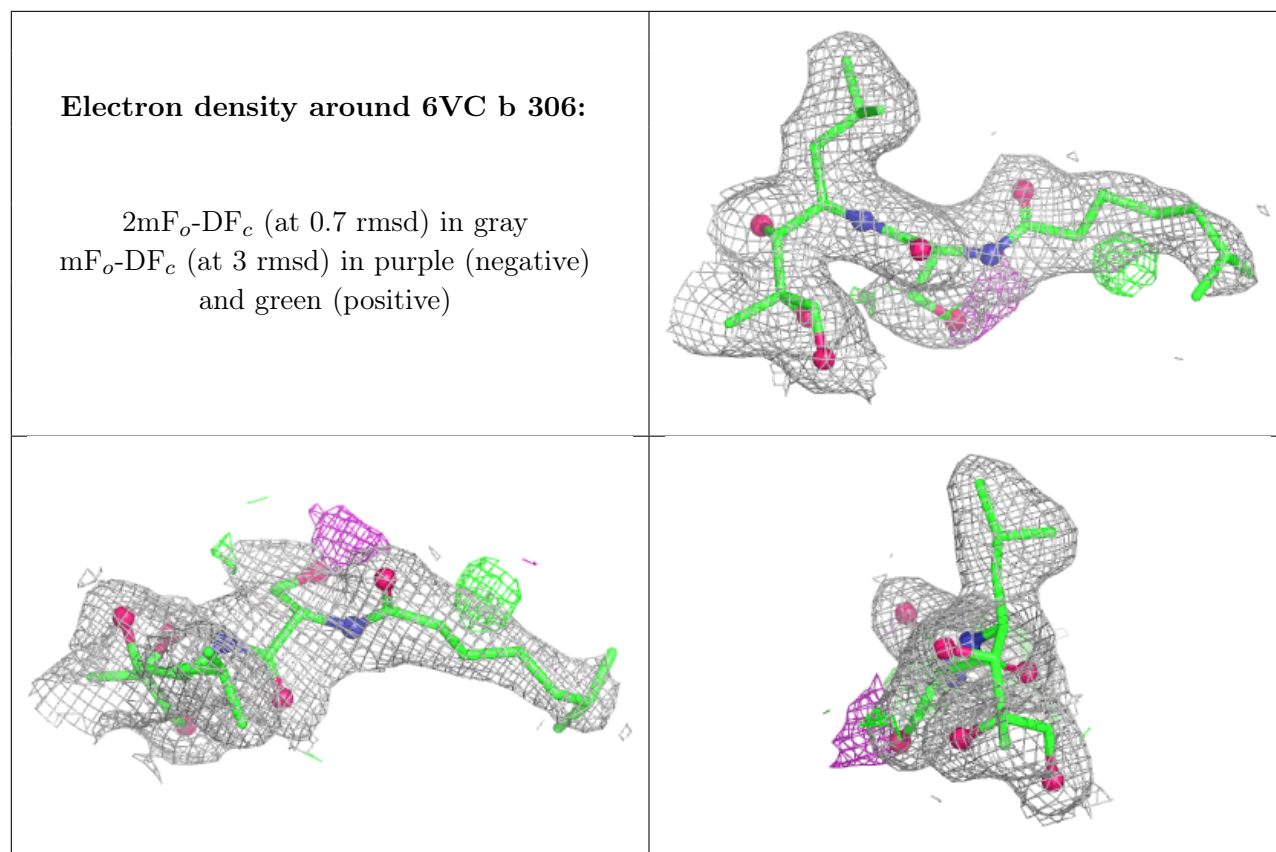
**Electron density around 6VC K 306:**

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

**Electron density around 6VC N 307:**

$2mF_o-DF_c$  (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.