



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 24, 2020 – 03:29 PM BST

PDB ID : 5LF1  
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.

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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

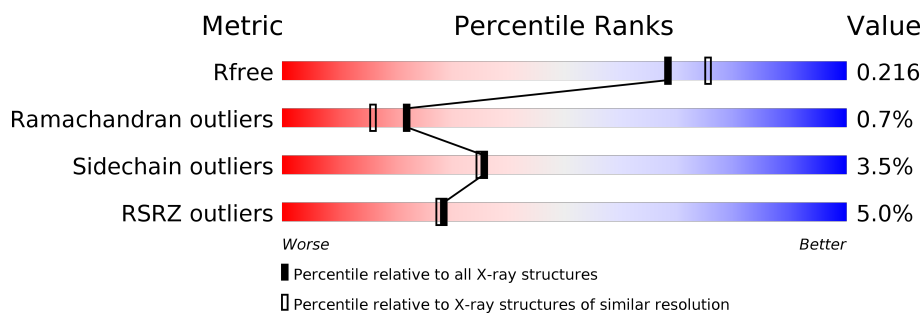
# 1 Overall quality at a glance ⓘ

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  $\geq 3$ , 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	<div> <div>3%</div> <div>91%</div> <div>6% ..</div> </div>
1	O	234	<div> <div>14%</div> <div>92%</div> <div>5% ..</div> </div>
2	B	261	<div> <div>5%</div> <div>91%</div> <div>5%</div> </div>
2	P	261	<div> <div>15%</div> <div>88%</div> <div>7% • 5%</div> </div>
3	C	248	<div> <div>11%</div> <div>90%</div> <div>5% •</div> </div>
3	Q	248	<div> <div>19%</div> <div>88%</div> <div>7% • •</div> </div>
4	D	241	<div> <div>7%</div> <div>92%</div> <div>• • •</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 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
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
			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
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			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	P	1	Total	Cl	0	0
			1	1		
15	K	4	Total	Cl	0	0
			4	4		
15	B	2	Total	Cl	0	0
			2	2		
15	W	1	Total	Cl	0	0
			1	1		
15	N	4	Total	Cl	0	0
			4	4		
15	S	3	Total	Cl	0	0
			3	3		
15	E	4	Total	Cl	0	0
			4	4		
15	b	4	Total	Cl	0	0
			4	4		
15	V	1	Total	Cl	0	0
			1	1		
15	A	4	Total	Cl	0	0
			4	4		
15	R	2	Total	Cl	0	0
			2	2		
15	M	3	Total	Cl	0	0
			3	3		
15	D	1	Total	Cl	0	0
			1	1		
15	I	1	Total	Cl	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	a	3	Total Cl 3 3	0	0
15	U	1	Total Cl 1 1	0	0
15	G	2	Total Cl 2 2	0	0
15	Q	2	Total Cl 2 2	0	0
15	H	1	Total Cl 1 1	0	0
15	C	2	Total Cl 2 2	0	0
15	O	4	Total Cl 4 4	0	0
15	Y	5	Total Cl 5 5	0	0
15	F	1	Total Cl 1 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

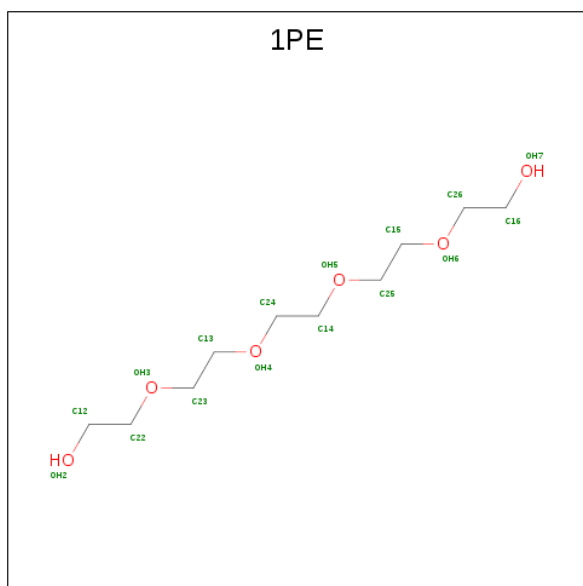
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	H	2	Total	Mg	0	0
			2	2		
17	I	2	Total	Mg	0	0
			2	2		
17	V	1	Total	Mg	0	0
			1	1		
17	W	1	Total	Mg	0	0
			1	1		
17	X	1	Total	Mg	0	0
			1	1		
17	L	1	Total	Mg	0	0
			1	1		

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



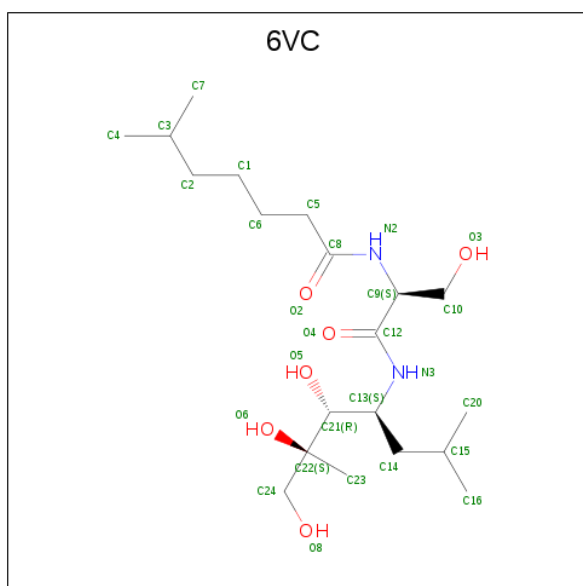
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	H	1	Total	C	O	0	0
			16	10	6		
18	I	1	Total	C	O	0	0
			16	10	6		
18	L	1	Total	C	O	0	0
			16	10	6		
18	M	1	Total	C	O	0	0
			16	10	6		
18	N	1	Total	C	O	0	0
			16	10	6		

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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 (three-letter code: 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.

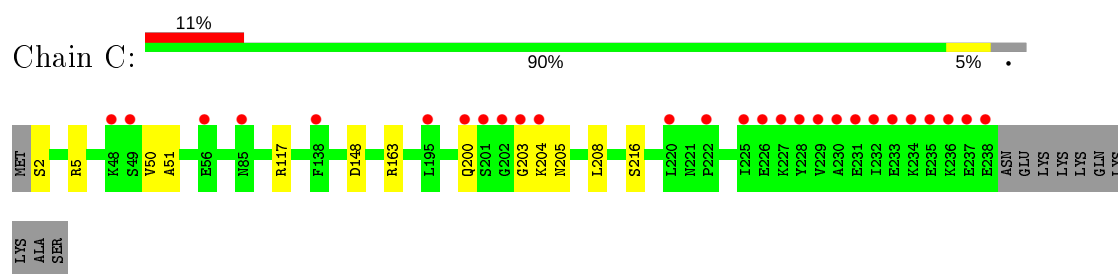
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	A	110	Total O 110 110	0	0
20	B	127	Total O 127 127	0	0
20	C	82	Total O 82 82	0	0
20	D	91	Total O 91 91	0	0
20	E	140	Total O 140 140	0	0
20	F	186	Total O 186 186	0	0
20	G	191	Total O 191 191	0	0
20	H	156	Total O 156 156	0	0
20	I	153	Total O 153 153	0	0
20	J	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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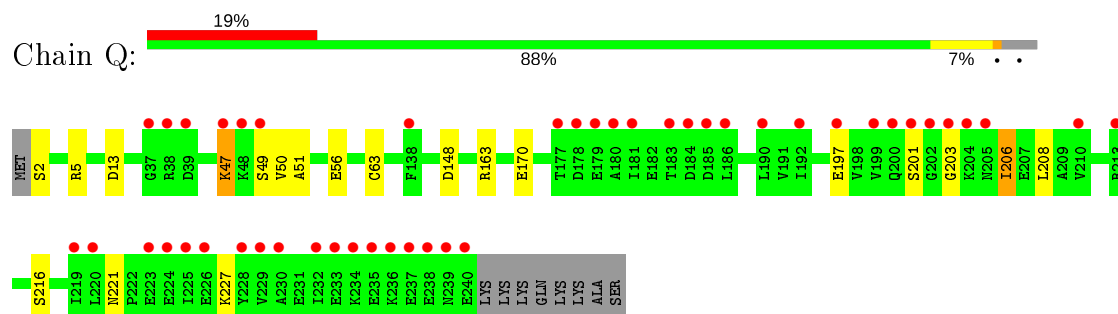
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	V	109	Total 109	O 109	0	0
20	W	116	Total 116	O 116	0	0
20	X	127	Total 127	O 127	0	0
20	Y	141	Total 141	O 141	0	0
20	Z	171	Total 171	O 171	0	0
20	a	174	Total 174	O 174	0	0
20	b	124	Total 124	O 124	0	0

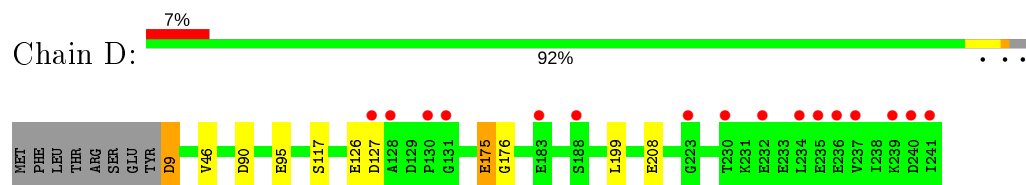




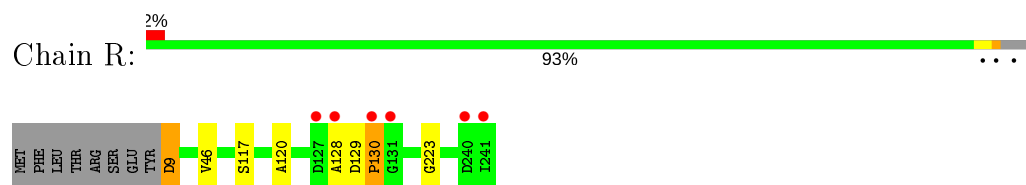
- Molecule 3: Proteasome subunit alpha type-7



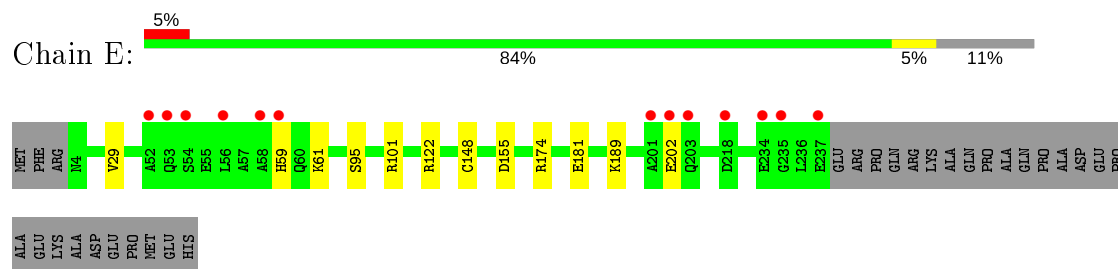
- Molecule 4: Proteasome subunit alpha type-5



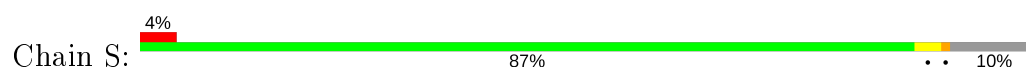
- Molecule 4: Proteasome subunit alpha type-5

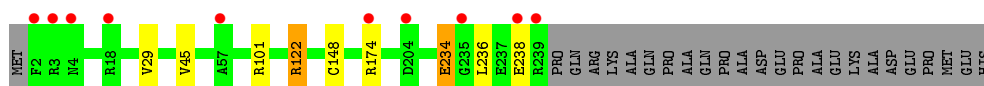


- Molecule 5: Proteasome subunit alpha type-1



- Molecule 5: Proteasome subunit alpha type-1





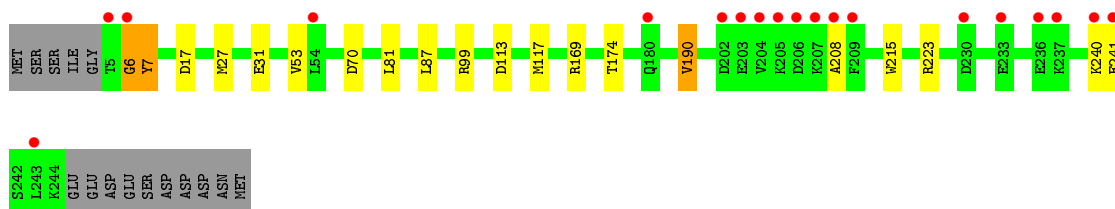
- Molecule 6: Proteasome subunit alpha type-3

Chain F: 87% 6% 6%



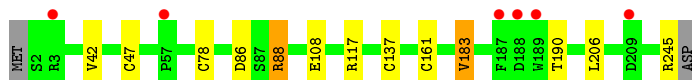
- Molecule 6: Proteasome subunit alpha type-3

Chain T: 7% 86% 7% 6%



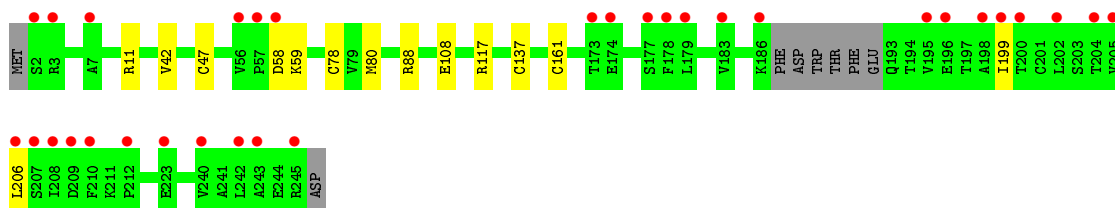
- Molecule 7: Proteasome subunit alpha type-6

Chain G: 2% 94% 2%



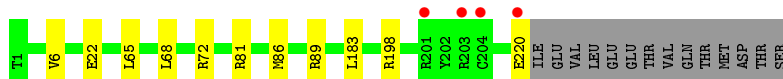
- Molecule 7: Proteasome subunit alpha type-6

Chain U: 13% 91% 6%



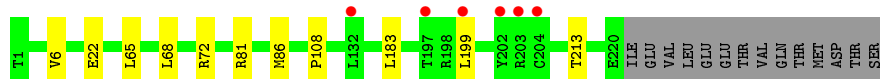
- Molecule 8: Proteasome subunit beta type-7

Chain H: 2% 89% 5% 6%



- Molecule 8: Proteasome subunit beta type-7

Chain V: 3% 89% 5% 6%



- Molecule 9: Proteasome subunit beta type-3

Chain I: 96%



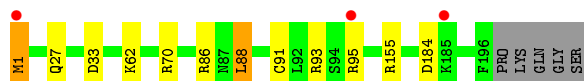
- Molecule 9: Proteasome subunit beta type-3

Chain W: 97%



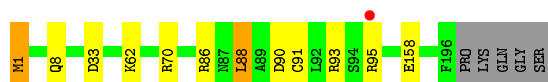
- Molecule 10: Proteasome subunit beta type-2

Chain J: 92%



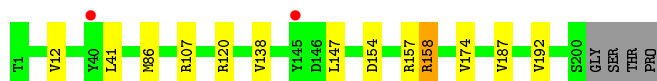
- Molecule 10: Proteasome subunit beta type-2

Chain X: 92%



- Molecule 11: Proteasome subunit beta type-5

Chain K: 92%



- Molecule 11: Proteasome subunit beta type-5

Chain Y: 92%



- Molecule 12: Proteasome subunit beta type-1

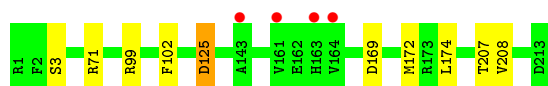


Chain L:  96% .



- Molecule 12: Proteasome subunit beta type-1

Chain Z:  95% .



- Molecule 13: Proteasome subunit beta type-4

Chain M:  95% ..



- Molecule 13: Proteasome subunit beta type-4

Chain a:  94% 5% .



- Molecule 14: Proteasome subunit beta type-6

Chain N:  95% ..



- 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, $\alpha$ , $\beta$ , $\gamma$	113.89Å 203.49Å 316.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	171.09 – 2.00 49.09 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.5 (171.09-2.00) 99.5 (49.09-2.00)	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)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, $R_{free}$	0.178 , 0.213 0.184 , 0.216	Depositor DCC
$R_{free}$ test set	24379 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	39.6	Xtriage
Anisotropy	0.246	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 44.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	52156	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtriage'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 ⓘ

### 5.1 Standard geometry ⓘ

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

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	0.68	0/1833	0.82	4/2489 (0.2%)
1	O	0.60	0/1778	0.80	3/2419 (0.1%)
2	B	0.73	1/1958 (0.1%)	0.83	4/2645 (0.2%)
2	P	0.66	0/1945	0.84	4/2631 (0.2%)
3	C	0.68	0/1818	0.90	2/2469 (0.1%)
3	Q	0.67	1/1834 (0.1%)	0.87	3/2490 (0.1%)
4	D	0.70	0/1789	0.83	2/2424 (0.1%)
4	R	0.76	0/1780	0.90	3/2408 (0.1%)
5	E	0.69	0/1842	0.85	4/2493 (0.2%)
5	S	0.67	0/1901	0.84	3/2571 (0.1%)
6	F	0.79	0/1935	0.94	7/2605 (0.3%)
6	T	0.73	1/1894 (0.1%)	0.93	9/2556 (0.4%)
7	G	0.79	2/1909 (0.1%)	0.83	6/2579 (0.2%)
7	U	0.68	1/1804 (0.1%)	0.82	7/2441 (0.3%)
8	H	0.76	0/1697	1.04	10/2299 (0.4%)
8	V	0.67	0/1655	0.91	4/2251 (0.2%)
9	I	0.76	1/1648 (0.1%)	1.06	9/2219 (0.4%)
9	W	0.64	0/1630	0.97	9/2197 (0.4%)
10	J	0.73	0/1613	1.01	9/2180 (0.4%)
10	X	0.70	0/1599	0.96	7/2163 (0.3%)
11	K	0.73	0/1576	0.95	8/2131 (0.4%)
11	Y	0.80	0/1620	1.02	9/2185 (0.4%)
12	L	0.69	0/1672	0.86	3/2257 (0.1%)
12	Z	0.80	1/1675 (0.1%)	0.91	5/2257 (0.2%)
13	M	0.77	0/1728	0.91	6/2339 (0.3%)
13	a	0.82	0/1724	0.94	4/2336 (0.2%)
14	N	0.85	1/1548 (0.1%)	0.89	5/2095 (0.2%)
14	b	0.79	2/1554 (0.1%)	0.89	3/2104 (0.1%)
All	All	0.73	11/48959 (0.0%)	0.90	152/66233 (0.2%)

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	P	0	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 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	108	GLU	CD-OE1	8.64	1.35	1.25
12	Z	3	SER	CB-OG	6.72	1.50	1.42
14	N	150	GLU	CG-CD	6.05	1.61	1.51
7	G	108	GLU	CD-OE2	5.77	1.31	1.25
3	Q	13	ASP	CB-CG	5.53	1.63	1.51

The worst 5 of 152 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	J	86	ARG	NE-CZ-NH2	-15.30	112.65	120.30
10	X	86	ARG	NE-CZ-NH2	-14.55	113.02	120.30
9	I	69	ARG	NE-CZ-NH1	14.17	127.39	120.30
10	J	86	ARG	NE-CZ-NH1	13.60	127.10	120.30
8	H	72	ARG	NE-CZ-NH2	-13.05	113.77	120.30

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	Mainchain,Peptide
9	I	78	GLY	Peptide
10	J	1[A]	MET	Peptide

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

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

## 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%)	9	4
1	O	228/234 (97%)	217 (95%)	7 (3%)	4 (2%)	8	3
2	B	248/261 (95%)	238 (96%)	10 (4%)	0	100	100
2	P	248/261 (95%)	233 (94%)	11 (4%)	4 (2%)	9	4
3	C	236/248 (95%)	223 (94%)	7 (3%)	6 (2%)	5	2
3	Q	236/248 (95%)	221 (94%)	7 (3%)	8 (3%)	3	1
4	D	232/241 (96%)	223 (96%)	6 (3%)	3 (1%)	12	6
4	R	232/241 (96%)	223 (96%)	6 (3%)	3 (1%)	12	6
5	E	232/263 (88%)	226 (97%)	5 (2%)	1 (0%)	34	30
5	S	238/263 (90%)	231 (97%)	5 (2%)	2 (1%)	19	13
6	F	241/255 (94%)	239 (99%)	2 (1%)	0	100	100
6	T	239/255 (94%)	233 (98%)	3 (1%)	3 (1%)	12	6
7	G	241/246 (98%)	237 (98%)	4 (2%)	0	100	100
7	U	232/246 (94%)	227 (98%)	3 (1%)	2 (1%)	17	11
8	H	220/234 (94%)	217 (99%)	3 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	29	23
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%)	29	23
14	b	202/205 (98%)	198 (98%)	3 (2%)	1 (0%)	29	23
All	All	6212/6458 (96%)	6040 (97%)	129 (2%)	43 (1%)	22	16

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 ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	185/191 (97%)	173 (94%)	12 (6%)	17	12
1	O	176/191 (92%)	164 (93%)	12 (7%)	16	11
2	B	199/221 (90%)	192 (96%)	7 (4%)	36	35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	P	197/221 (89%)	187 (95%)	10 (5%)	24	19
3	C	179/210 (85%)	174 (97%)	5 (3%)	43	44
3	Q	184/210 (88%)	175 (95%)	9 (5%)	25	21
4	D	189/203 (93%)	182 (96%)	7 (4%)	34	32
4	R	187/203 (92%)	184 (98%)	3 (2%)	62	67
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
6	T	192/212 (91%)	181 (94%)	11 (6%)	20	16
7	G	202/207 (98%)	196 (97%)	6 (3%)	41	41
7	U	186/207 (90%)	182 (98%)	4 (2%)	52	55
8	H	181/195 (93%)	175 (97%)	6 (3%)	38	37
8	V	172/195 (88%)	164 (95%)	8 (5%)	26	22
9	I	176/174 (101%)	175 (99%)	1 (1%)	86	90
9	W	173/174 (99%)	172 (99%)	1 (1%)	86	90
10	J	166/170 (98%)	158 (95%)	8 (5%)	25	22
10	X	165/170 (97%)	159 (96%)	6 (4%)	35	34
11	K	154/159 (97%)	146 (95%)	8 (5%)	23	19
11	Y	159/159 (100%)	153 (96%)	6 (4%)	33	31
12	L	175/178 (98%)	168 (96%)	7 (4%)	31	29
12	Z	175/178 (98%)	169 (97%)	6 (3%)	37	36
13	M	180/181 (99%)	178 (99%)	2 (1%)	73	78
13	a	178/181 (98%)	173 (97%)	5 (3%)	43	44
14	N	158/159 (99%)	155 (98%)	3 (2%)	57	61
14	b	158/159 (99%)	154 (98%)	4 (2%)	47	49
All	All	5034/5366 (94%)	4853 (96%)	181 (4%)	36	34

5 of 181 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	L	102	PHE
1	O	223	THR
12	Z	125	ASP

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Mol	Chain	Res	Type
12	L	174	LEU
1	O	10	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 41 such sidechains are listed below:

Mol	Chain	Res	Type
14	N	193	GLN
2	P	40	ASN
12	Z	157	ASN
1	O	101	GLN
1	O	118	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
7	YCM	G	137	7	7,9,10	1.75	3 (42%)	4,10,12	2.49	1 (25%)
3	YCM	Q	63	3	7,9,10	1.27	1 (14%)	4,10,12	3.17	3 (75%)
7	6V1	G	47	7	12,15,16	2.21	4 (33%)	9,20,22	2.07	1 (11%)
10	6V1	J	91	10	12,15,16	1.79	2 (16%)	9,20,22	5.68	6 (66%)
7	6V1	U	161	7	12,15,16	1.86	4 (33%)	9,20,22	2.89	4 (44%)
3	YCM	C	63	3	7,9,10	0.97	0	4,10,12	0.70	0
5	6V1	E	148	5	12,15,16	1.74	3 (25%)	9,20,22	3.87	3 (33%)
7	YCM	U	137	7	7,9,10	0.95	0	4,10,12	1.36	1 (25%)
7	6V1	U	47	7	12,15,16	1.76	2 (16%)	9,20,22	1.95	3 (33%)



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	1.59	4 (33%)	9,20,22	2.50	4 (44%)
10	6V1	X	91	10	12,15,16	1.75	3 (25%)	9,20,22	5.57	6 (66%)
5	6V1	S	148	5	12,15,16	1.66	3 (25%)	9,20,22	3.08	5 (55%)

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

The worst 5 of 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	47	6V1	CB-SG	-5.44	1.76	1.82
10	J	91	6V1	C1-SG	-5.12	1.77	1.83
7	U	47	6V1	CB-SG	-4.83	1.76	1.82
10	X	91	6V1	C1-SG	-4.63	1.78	1.83
5	E	148	6V1	CB-SG	-4.08	1.77	1.82

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	J	91	6V1	C5-C4-N3	9.65	113.82	108.13
10	X	91	6V1	C5-C4-N3	8.20	112.96	108.13
10	X	91	6V1	O7-C2-N3	8.03	133.96	124.14
10	X	91	6V1	C6-N3-C2	7.90	133.38	123.36
10	J	91	6V1	C6-N3-C2	7.82	133.28	123.36

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	U	47	6V1	C1

5 of 21 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	G	137	YCM	CE-CD-SG-CB
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

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 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	$\# Z  > 2$
18	1PE	W	303	-	15,15,15	0.57	0	14,14,14	0.36	0
18	1PE	H	304	-	15,15,15	0.60	0	14,14,14	0.59	0
19	6VC	Y	306	11	26,27,27	0.95	3 (11%)	30,36,36	1.30	4 (13%)
19	6VC	N	307	14	26,27,27	0.80	0	30,36,36	1.65	4 (13%)
18	1PE	U	302	-	15,15,15	0.62	0	14,14,14	0.96	1 (7%)
18	1PE	a	304	-	15,15,15	0.69	0	14,14,14	0.46	0
19	6VC	V	303	8	26,27,27	0.80	1 (3%)	30,36,36	1.38	5 (16%)
18	1PE	Z	301	-	15,15,15	0.61	0	14,14,14	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
19	6VC	H	305	8	26,27,27	0.91	1 (3%)	30,36,36	1.46	5 (16%)
18	1PE	M	304	-	15,15,15	0.62	0	14,14,14	0.35	0
18	1PE	L	301	-	15,15,15	0.62	0	14,14,14	0.64	0
19	6VC	K	306	11	26,27,27	0.64	0	30,36,36	1.41	6 (20%)
18	1PE	N	305	-	15,15,15	0.53	0	14,14,14	0.54	0
18	1PE	I	303	-	15,15,15	0.57	0	14,14,14	0.84	0
19	6VC	b	306	14	26,27,27	1.03	3 (11%)	30,36,36	2.04	9 (30%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	1PE	W	303	-	-	7/13/13/13	-
18	1PE	H	304	-	-	10/13/13/13	-
19	6VC	Y	306	11	-	4/38/38/38	-
19	6VC	N	307	14	-	2/38/38/38	-
18	1PE	U	302	-	-	8/13/13/13	-
18	1PE	a	304	-	-	7/13/13/13	-
19	6VC	V	303	8	-	6/38/38/38	-
18	1PE	Z	301	-	-	8/13/13/13	-
19	6VC	H	305	8	-	6/38/38/38	-
18	1PE	M	304	-	-	8/13/13/13	-
18	1PE	L	301	-	-	6/13/13/13	-
19	6VC	K	306	11	-	5/38/38/38	-
18	1PE	N	305	-	-	4/13/13/13	-
18	1PE	I	303	-	-	6/13/13/13	-
19	6VC	b	306	14	-	5/38/38/38	-

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	H	305	6VC	C23-C22	3.32	1.58	1.52
19	b	306	6VC	C23-C22	3.03	1.57	1.52
19	Y	306	6VC	C13-N3	-2.45	1.42	1.46
19	b	306	6VC	C14-C13	2.23	1.56	1.52
19	b	306	6VC	C9-C12	-2.16	1.47	1.52

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	N	307	6VC	C10-C9-N2	-5.79	97.52	110.56
19	b	306	6VC	O3-C10-C9	-5.14	98.18	111.03
19	b	306	6VC	C1-C6-C5	-4.76	96.06	113.19
19	b	306	6VC	O2-C8-C5	-3.86	114.95	122.02
19	H	305	6VC	O3-C10-C9	-3.83	101.47	111.03

There are no chirality outliers.

5 of 92 torsion outliers are listed below:

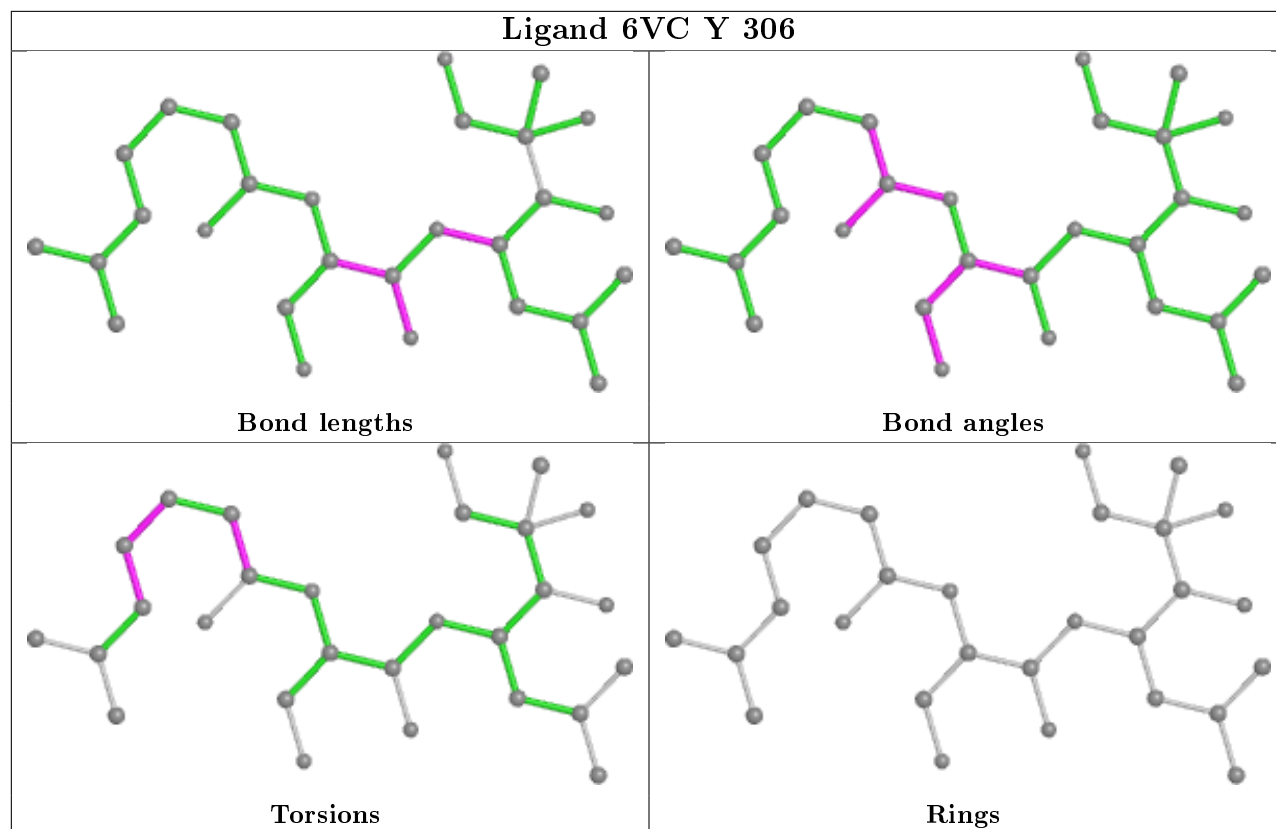
Mol	Chain	Res	Type	Atoms
19	b	306	6VC	O3-C10-C9-N2
18	U	302	1PE	C25-C15-OH6-C26
18	L	301	1PE	C16-C26-OH6-C15
18	I	303	1PE	C15-C25-OH5-C14
18	U	302	1PE	OH4-C13-C23-OH3

There are no ring outliers.

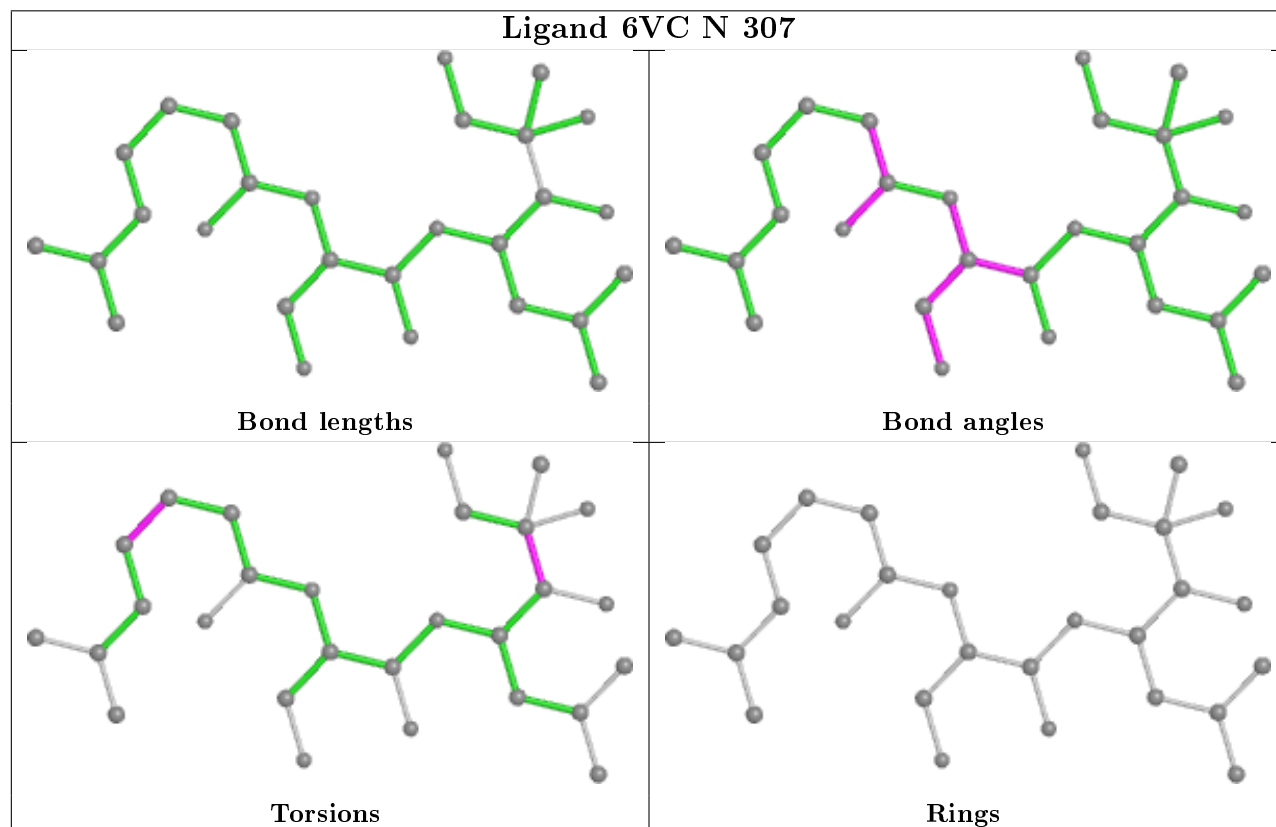
No monomer is involved in short contacts.

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.

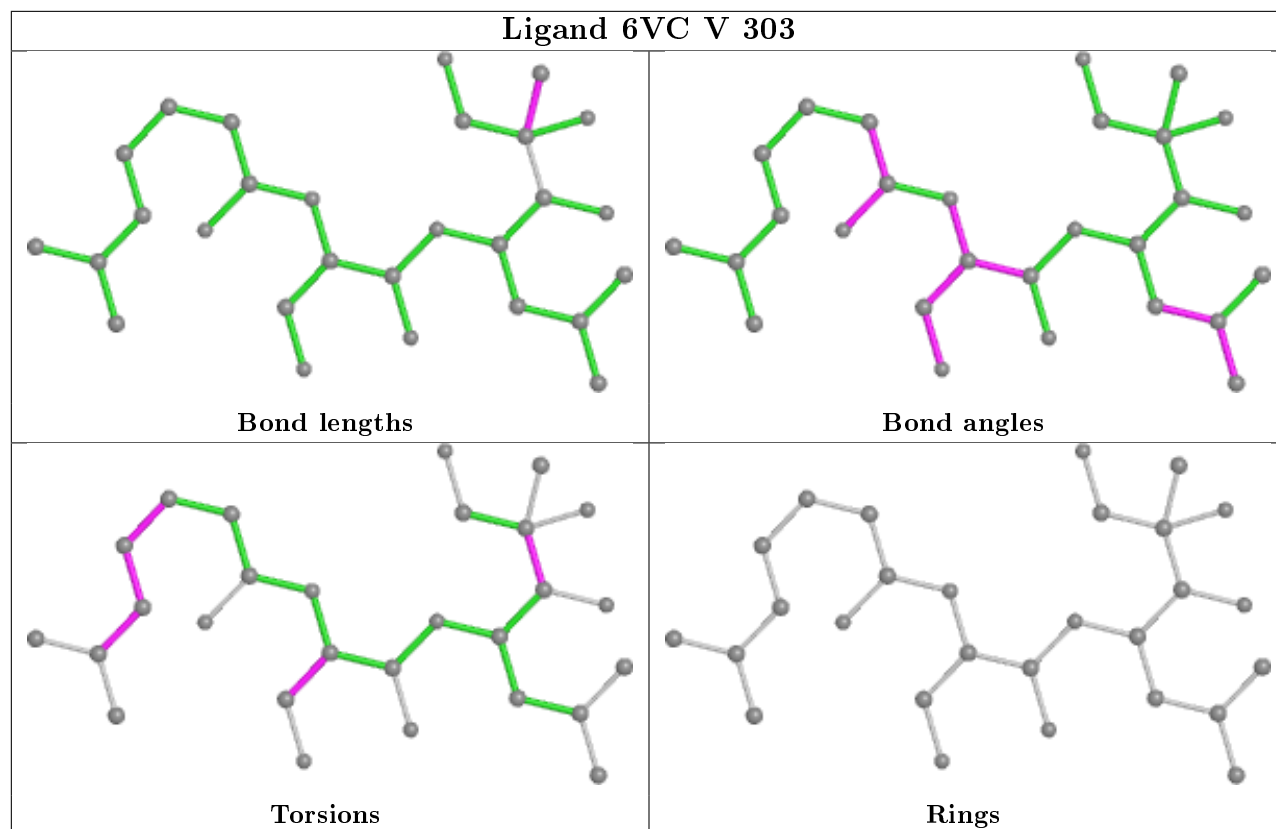
## Ligand 6VC Y 306



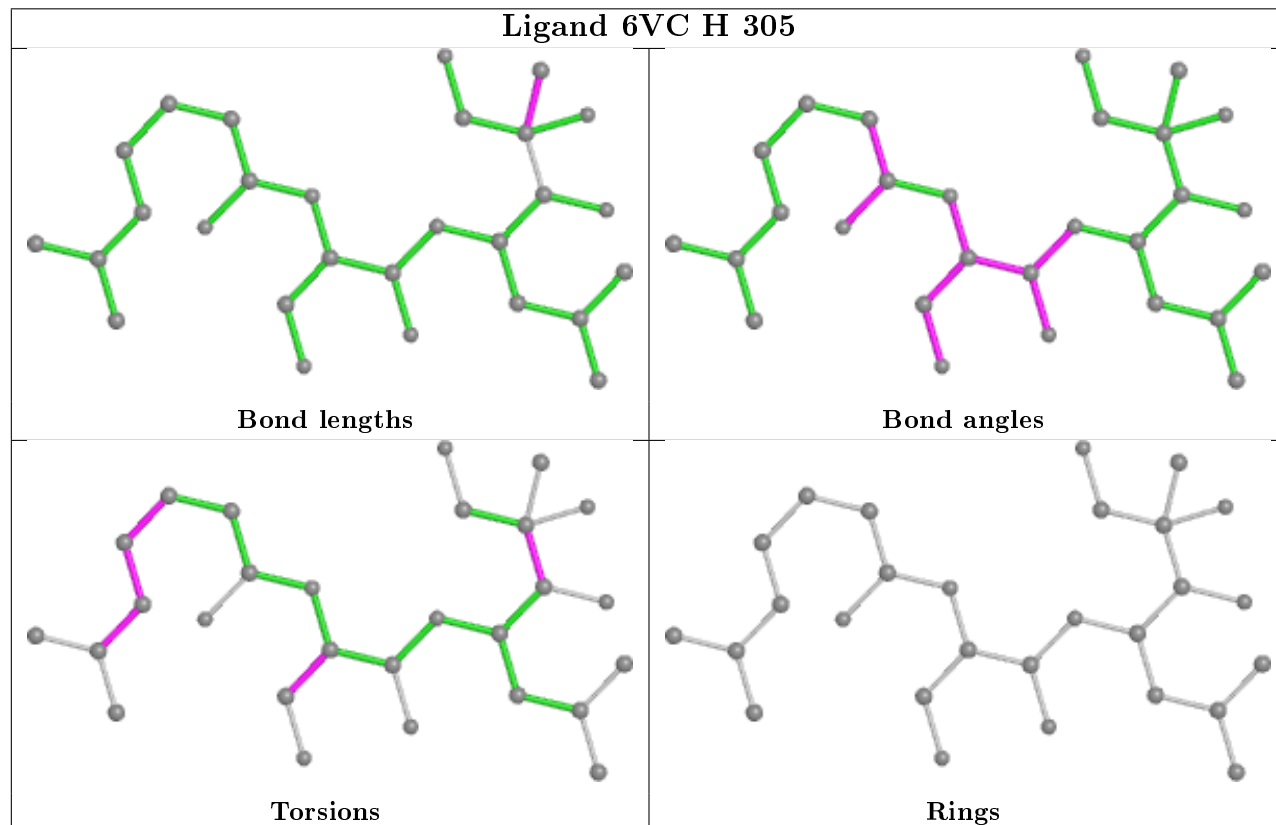
## Ligand 6VC N 307



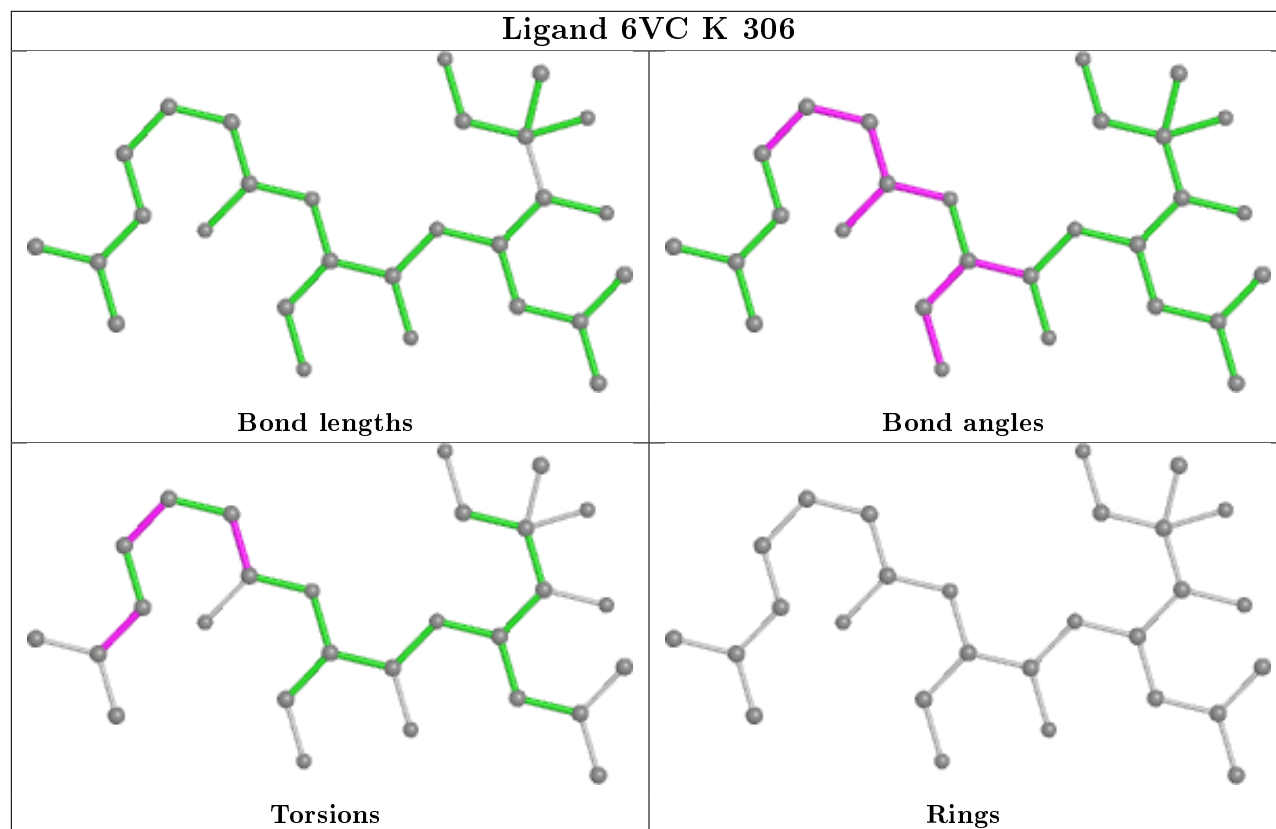
## Ligand 6VC V 303



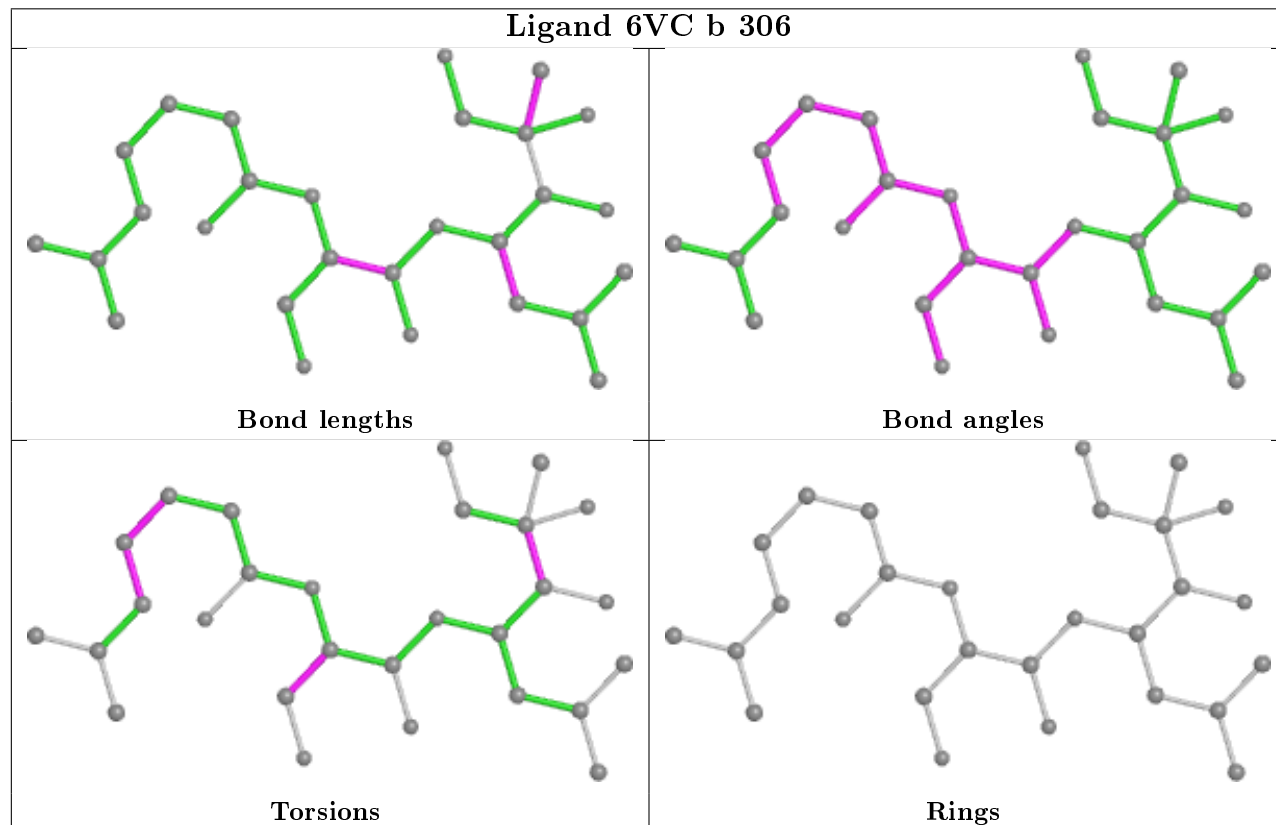
## Ligand 6VC H 305



## Ligand 6VC K 306



## Ligand 6VC b 306



## 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 ⓘ

### 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, 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%)	-0.03	7 (3%)	50	49	31, 46, 82, 92	0
1	O	230/234 (98%)	0.59	32 (13%)	2	2	41, 63, 100, 120	0
2	B	248/261 (95%)	0.30	14 (5%)	24	23	35, 52, 89, 136	0
2	P	248/261 (95%)	0.77	40 (16%)	1	1	40, 61, 106, 142	0
3	C	236/248 (95%)	0.57	27 (11%)	5	4	36, 61, 100, 139	0
3	Q	238/248 (95%)	0.85	46 (19%)	1	0	34, 61, 112, 149	0
4	D	233/241 (96%)	0.26	16 (6%)	16	16	39, 58, 88, 114	0
4	R	233/241 (96%)	0.06	6 (2%)	56	54	32, 44, 71, 93	0
5	E	233/263 (88%)	0.13	13 (5%)	24	23	29, 43, 86, 100	0
5	S	237/263 (90%)	0.08	10 (4%)	36	35	34, 47, 81, 104	0
6	F	239/255 (93%)	-0.08	0	100	100	27, 36, 58, 74	0
6	T	240/255 (94%)	0.27	19 (7%)	12	11	35, 52, 85, 107	0
7	G	241/246 (97%)	0.15	6 (2%)	57	56	27, 40, 73, 101	0
7	U	235/246 (95%)	0.61	32 (13%)	3	2	42, 60, 95, 124	0
8	H	220/234 (94%)	-0.07	4 (1%)	68	66	27, 36, 66, 100	0
8	V	220/234 (94%)	0.12	6 (2%)	54	53	36, 48, 84, 97	0
9	I	204/205 (99%)	0.03	1 (0%)	91	90	29, 38, 58, 74	0
9	W	204/205 (99%)	0.08	3 (1%)	73	72	36, 50, 73, 81	0
10	J	195/201 (97%)	-0.12	3 (1%)	73	72	32, 42, 60, 76	0
10	X	195/201 (97%)	-0.06	1 (0%)	91	90	34, 44, 59, 74	0
11	K	200/204 (98%)	0.07	2 (1%)	82	81	36, 46, 71, 84	0
11	Y	201/204 (98%)	0.03	4 (1%)	65	63	28, 37, 59, 70	0
12	L	213/213 (100%)	-0.09	0	100	100	34, 49, 71, 85	0
12	Z	213/213 (100%)	0.07	4 (1%)	66	65	27, 38, 60, 74	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	M	216/219 (98%)	0.12	3 (1%) 75 74	27, 39, 62, 95	0
13	a	216/219 (98%)	-0.05	3 (1%) 75 74	27, 39, 60, 82	0
14	N	202/205 (98%)	-0.05	0 100 100	27, 35, 56, 94	0
14	b	203/205 (99%)	0.15	8 (3%) 39 38	32, 41, 66, 97	0
All	All	6223/6458 (96%)	0.18	310 (4%) 28 28	27, 46, 85, 149	0

The worst 5 of 310 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	P	204	SER	14.1
1	O	232	ILE	11.1
4	D	241	ILE	9.9
2	P	203	VAL	8.8
3	Q	232	ILE	7.8

## 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, 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	0.78	0.38	72,103,109,110	0
7	YCM	U	137	10/11	0.82	0.18	51,59,75,76	0
5	6V1	S	148	15/16	0.87	0.20	37,63,68,70	0
3	YCM	C	63	10/11	0.88	0.12	55,56,63,64	0
7	YCM	G	137	10/11	0.88	0.16	33,39,51,53	0
5	6V1	E	148	15/16	0.90	0.17	32,54,64,65	0
7	6V1	G	47	15/16	0.90	0.20	39,61,64,65	0
10	6V1	J	91	15/16	0.91	0.20	33,53,58,59	0
10	6V1	X	91	15/16	0.91	0.22	36,54,57,61	0
3	YCM	Q	63	10/11	0.91	0.13	51,54,64,67	0
7	6V1	U	161	15/16	0.92	0.12	53,73,78,78	0
7	6V1	G	161	15/16	0.92	0.17	33,51,57,58	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, 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	0.66	0.34	78,83,97,98	0
18	1PE	a	304	16/16	0.71	0.26	66,70,86,87	0
18	1PE	L	301	16/16	0.75	0.21	60,70,74,76	0
18	1PE	H	304	16/16	0.77	0.28	58,69,77,79	0
18	1PE	W	303	16/16	0.81	0.25	59,64,71,74	0
15	CL	O	303	1/1	0.82	0.25	87,87,87,87	0
18	1PE	Z	301	16/16	0.83	0.20	57,66,72,73	0
18	1PE	I	303	16/16	0.88	0.21	55,58,68,71	0
18	1PE	U	302	16/16	0.88	0.17	46,56,73,75	0
15	CL	M	303	1/1	0.90	0.10	59,59,59,59	0
15	CL	O	304	1/1	0.90	0.07	67,67,67,67	0
15	CL	Q	302	1/1	0.90	0.23	64,64,64,64	0
15	CL	E	303	1/1	0.90	0.16	64,64,64,64	0
15	CL	B	302	1/1	0.91	0.11	57,57,57,57	0
15	CL	D	301	1/1	0.91	0.22	69,69,69,69	0
15	CL	Y	305	1/1	0.91	0.23	63,63,63,63	0
18	1PE	N	305	16/16	0.91	0.15	41,49,62,64	0
15	CL	I	302	1/1	0.91	0.08	48,48,48,48	0
19	6VC	V	303	28/28	0.92	0.14	42,45,60,61	0
15	CL	R	301	1/1	0.92	0.09	58,58,58,58	0
15	CL	V	302	1/1	0.93	0.10	59,59,59,59	0
17	MG	V	301	1/1	0.93	0.24	58,58,58,58	0
15	CL	K	304	1/1	0.93	0.16	60,60,60,60	0
15	CL	Q	301	1/1	0.93	0.17	67,67,67,67	0
15	CL	E	304	1/1	0.94	0.09	63,63,63,63	0
15	CL	A	302	1/1	0.94	0.10	64,64,64,64	0
15	CL	C	301	1/1	0.94	0.10	60,60,60,60	0
15	CL	K	303	1/1	0.94	0.07	69,69,69,69	0
19	6VC	H	305	28/28	0.95	0.11	33,37,55,60	0
17	MG	H	301	1/1	0.95	0.17	57,57,57,57	0
15	CL	K	305	1/1	0.95	0.23	65,65,65,65	0
15	CL	M	301	1/1	0.95	0.22	56,56,56,56	0
15	CL	Y	303	1/1	0.95	0.09	64,64,64,64	0
15	CL	O	302	1/1	0.95	0.09	63,63,63,63	0
19	6VC	N	307	28/28	0.95	0.17	25,29,49,52	0
15	CL	a	303	1/1	0.95	0.08	60,60,60,60	0
15	CL	C	302	1/1	0.95	0.16	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
15	CL	B	301	1/1	0.96	0.07	41,41,41,41	0
15	CL	Y	304	1/1	0.96	0.08	57,57,57,57	0
19	6VC	Y	306	28/28	0.96	0.15	27,29,51,56	0
17	MG	W	301	1/1	0.96	0.06	38,38,38,38	0
15	CL	S	303	1/1	0.96	0.06	55,55,55,55	0
19	6VC	K	306	28/28	0.96	0.14	36,39,61,62	0
16	K	b	305	1/1	0.96	0.07	41,41,41,41	0
15	CL	R	302	1/1	0.96	0.17	57,57,57,57	0
16	K	L	302	1/1	0.96	0.04	47,47,47,47	0
17	MG	I	301	1/1	0.96	0.08	33,33,33,33	0
15	CL	b	302	1/1	0.96	0.09	55,55,55,55	0
19	6VC	b	306	28/28	0.96	0.15	31,34,55,56	0
15	CL	O	301	1/1	0.96	0.10	55,55,55,55	0
17	MG	L	303	1/1	0.97	0.04	37,37,37,37	0
15	CL	K	302	1/1	0.97	0.07	42,42,42,42	0
15	CL	F	301	1/1	0.97	0.11	51,51,51,51	0
17	MG	J	301	1/1	0.97	0.05	48,48,48,48	0
15	CL	b	303	1/1	0.97	0.08	56,56,56,56	0
15	CL	N	304	1/1	0.97	0.12	52,52,52,52	0
15	CL	G	302	1/1	0.97	0.11	60,60,60,60	0
17	MG	I	304	1/1	0.97	0.07	30,30,30,30	0
15	CL	A	304	1/1	0.97	0.14	57,57,57,57	0
15	CL	E	302	1/1	0.97	0.05	55,55,55,55	0
15	CL	a	301	1/1	0.97	0.13	59,59,59,59	0
15	CL	H	303	1/1	0.97	0.07	53,53,53,53	0
15	CL	W	302	1/1	0.97	0.07	54,54,54,54	0
15	CL	A	303	1/1	0.97	0.08	50,50,50,50	0
15	CL	U	301	1/1	0.98	0.12	54,54,54,54	0
15	CL	b	304	1/1	0.98	0.11	42,42,42,42	0
15	CL	a	302	1/1	0.98	0.08	43,43,43,43	0
17	MG	H	302	1/1	0.98	0.05	33,33,33,33	0
15	CL	G	301	1/1	0.98	0.18	48,48,48,48	0
15	CL	P	301	1/1	0.98	0.07	53,53,53,53	0
15	CL	E	301	1/1	0.98	0.05	61,61,61,61	0
15	CL	Y	302	1/1	0.98	0.15	59,59,59,59	0
17	MG	K	301	1/1	0.98	0.08	36,36,36,36	0
15	CL	S	301	1/1	0.98	0.31	64,64,64,64	0
15	CL	N	303	1/1	0.98	0.11	56,56,56,56	0
16	K	G	303	1/1	0.98	0.05	33,33,33,33	0
17	MG	X	301	1/1	0.98	0.11	49,49,49,49	0
16	K	U	303	1/1	0.98	0.06	41,41,41,41	0
15	CL	b	301	1/1	0.98	0.06	45,45,45,45	0

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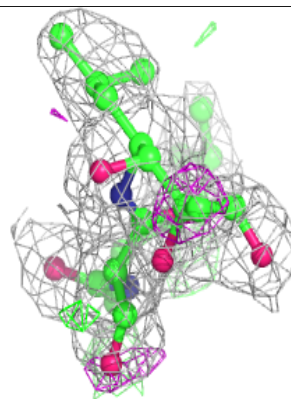
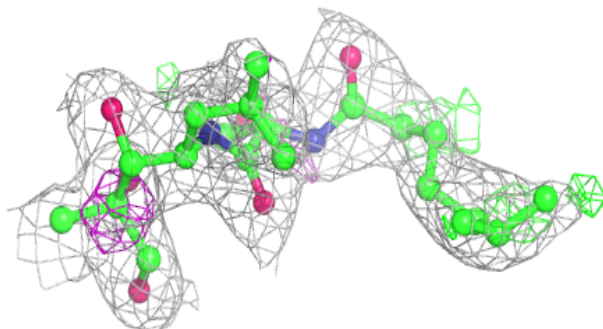
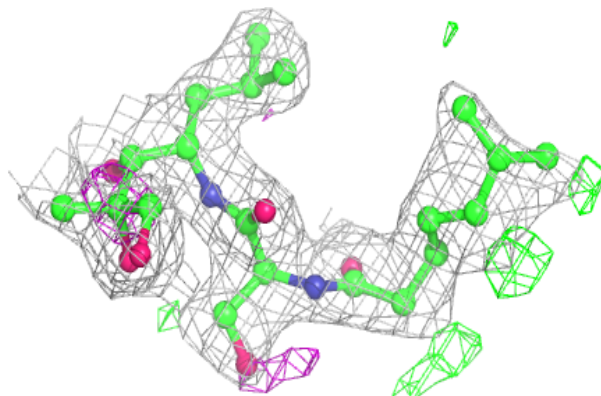
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
15	CL	M	302	1/1	0.99	0.07	40,40,40,40	0
15	CL	A	301	1/1	0.99	0.11	52,52,52,52	0
15	CL	N	301	1/1	0.99	0.15	35,35,35,35	0
15	CL	N	302	1/1	0.99	0.06	45,45,45,45	0
16	K	N	306	1/1	0.99	0.08	38,38,38,38	0
15	CL	S	302	1/1	0.99	0.13	63,63,63,63	0
16	K	Z	302	1/1	0.99	0.08	39,39,39,39	0
15	CL	Y	301	1/1	1.00	0.08	38,38,38,38	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.

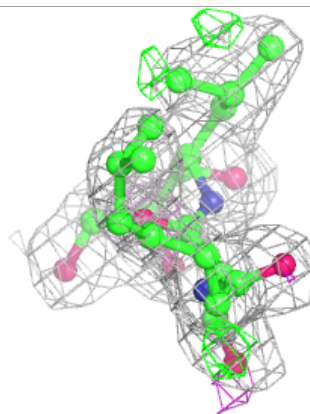
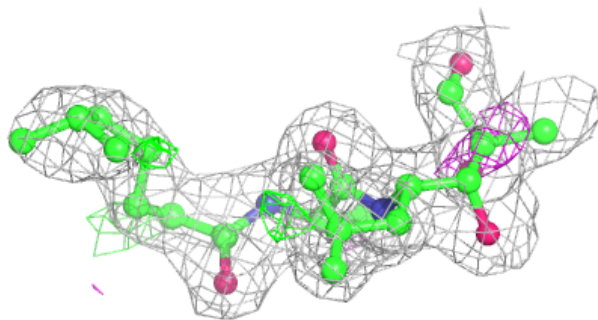
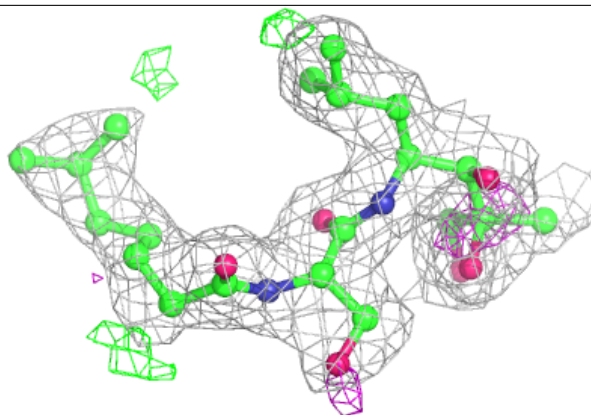
**Electron density around 6VC V 303:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

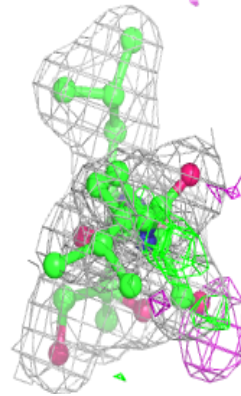
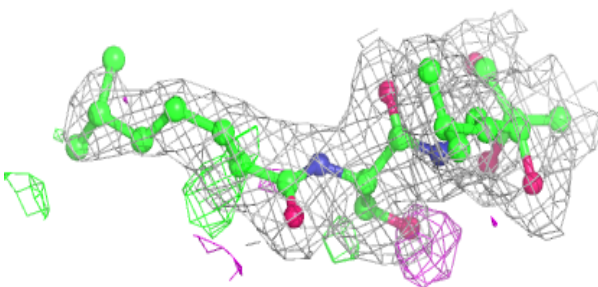
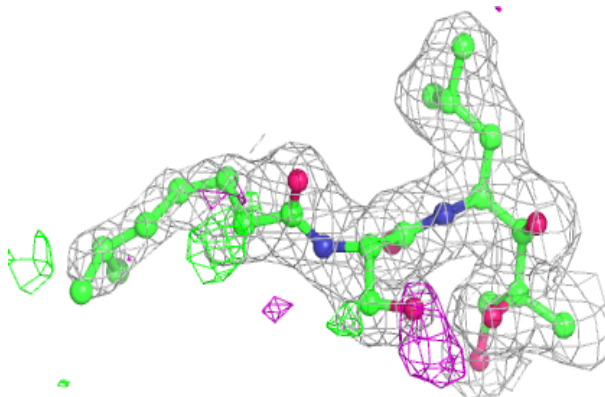


**Electron density around 6VC H 305:**

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

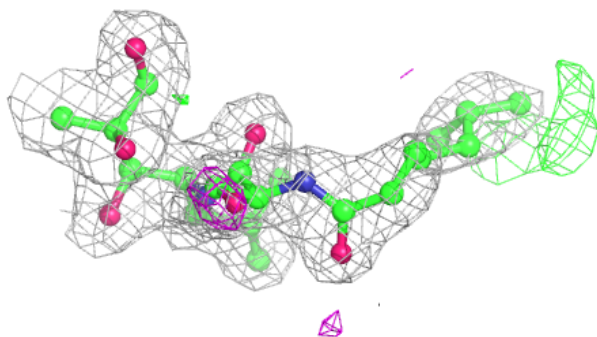
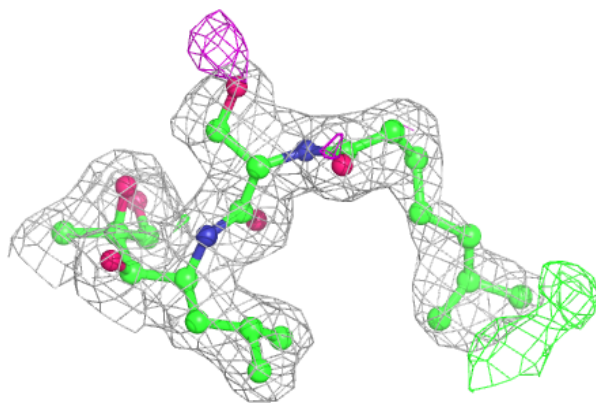
**Electron density around 6VC N 307:**

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

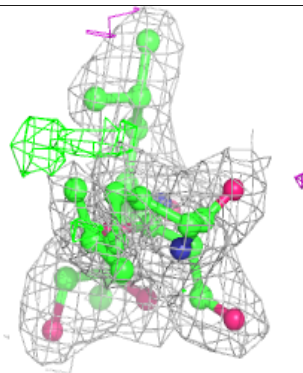
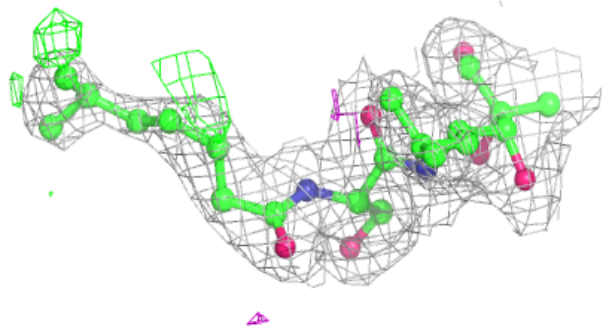
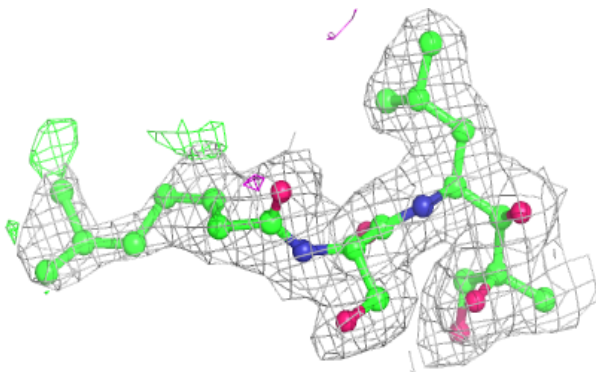


**Electron density around 6VC Y 306:**

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

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

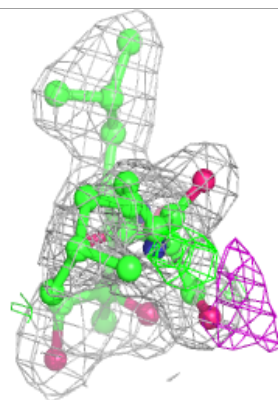
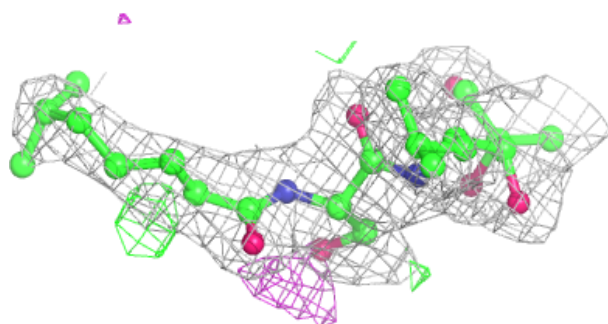
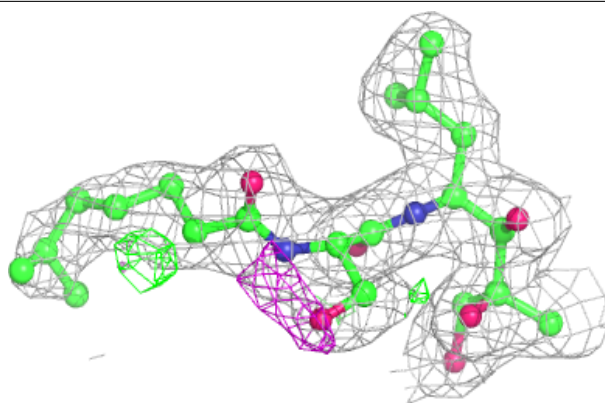
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





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

$2mF_o-DF_c$  (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.