



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 05:31 PM BST

PDB ID : 5LF4  
Title : Human 20S proteasome complex with Delanzomib at 2.0 Angstrom  
Authors : Schrader, J.; Henneberg, F.; Mata, R.; Tittmann, K.; Schneider, T.R.; Stark, H.; Bourenkov, G.; Chari, A.  
Deposited on : 2016-06-30  
Resolution : 1.99 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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

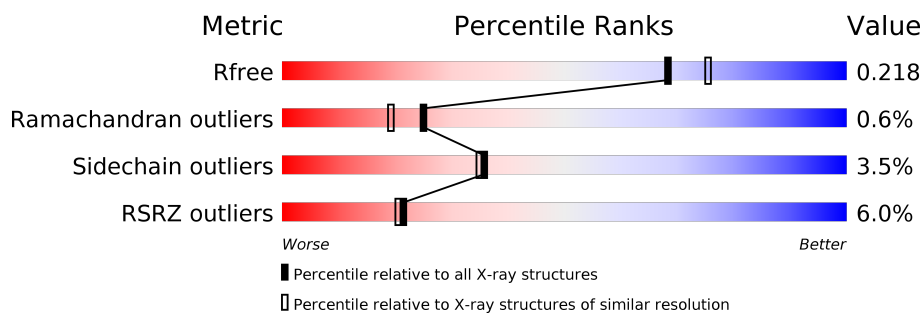
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.99 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	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>• •</div> </div>
1	O	234	<div> <div>17%</div> <div>92%</div> <div>5%</div> <div>• •</div> </div>
2	B	261	<div> <div>7%</div> <div>90%</div> <div>5%</div> <div>5%</div> </div>
2	P	261	<div> <div>19%</div> <div>89%</div> <div>6%</div> <div>• 5%</div> </div>
3	C	248	<div> <div>12%</div> <div>87%</div> <div>8%</div> <div>•</div> </div>
3	Q	248	<div> <div>21%</div> <div>86%</div> <div>9%</div> <div>• •</div> </div>
4	D	241	<div> <div>8%</div> <div>91%</div> <div>5%</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
19	6V7	N	307	X	-	-	-
19	6V7	Y	306	X	-	-	-

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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 52186 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	248	Total	C	N	O	S	0	2	0
			1926	1220	332	363	11			
2	P	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			

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	200	Total	C	N	O	S	0	1	0
			1550	978	269	293	10			
11	Y	201	Total	C	N	O	S	0	3	0
			1580	996	280	294	10			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	216	Total	C	N	O	S	0	1	0
			1692	1067	291	322	12			
13	a	216	Total	C	N	O	S	0	2	0
			1688	1064	291	321	12			

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

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

- Molecule 15 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

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



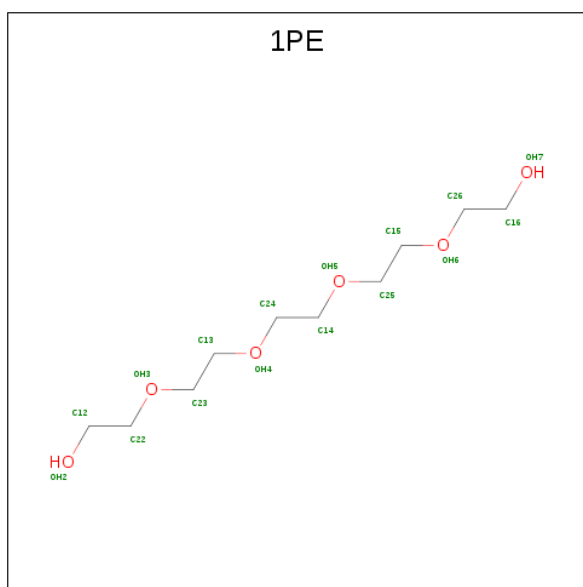
- Molecule 16 is POTASSIUM ION (three-letter code: K) (formula: K).

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

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

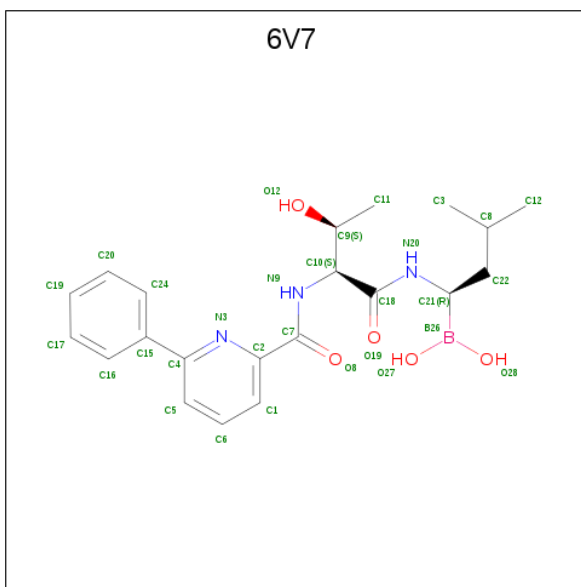
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	J	1	Total Mg 1 1	0	0
17	K	1	Total Mg 1 1	0	0
17	H	2	Total Mg 2 2	0	0
17	I	2	Total Mg 2 2	0	0
17	V	1	Total Mg 1 1	0	0
17	W	1	Total Mg 1 1	0	0
17	X	1	Total Mg 1 1	0	0
17	L	1	Total Mg 1 1	0	0

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



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

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



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

- Molecule 20 is water.

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

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

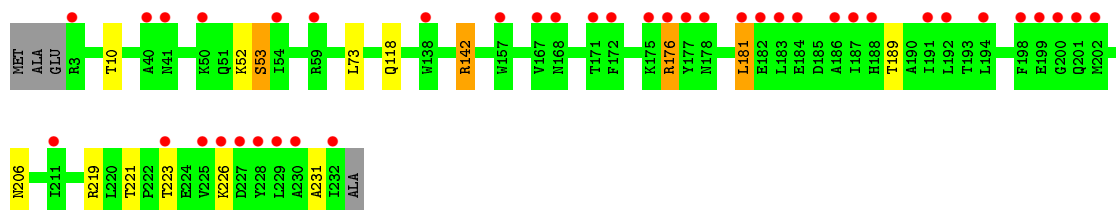
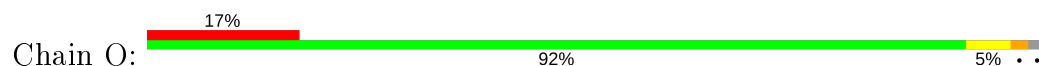
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

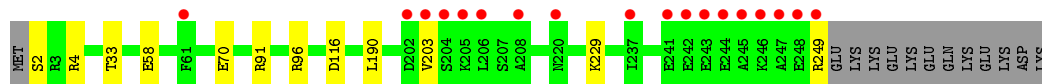
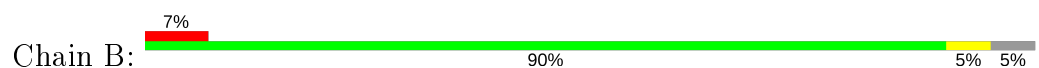
- Molecule 1: Proteasome subunit alpha type-2



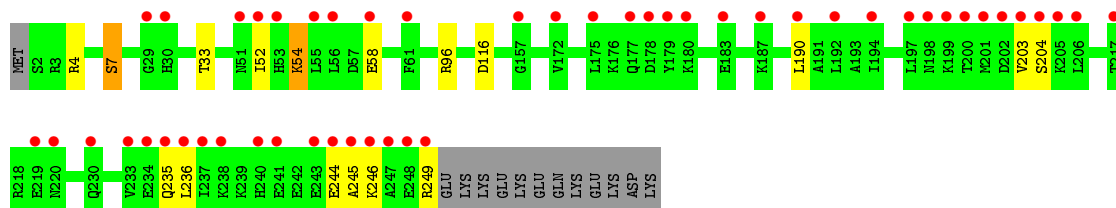
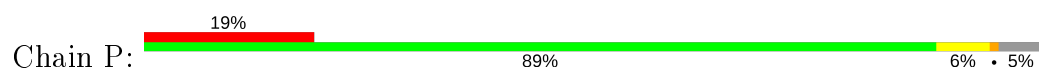
- Molecule 1: Proteasome subunit alpha type-2



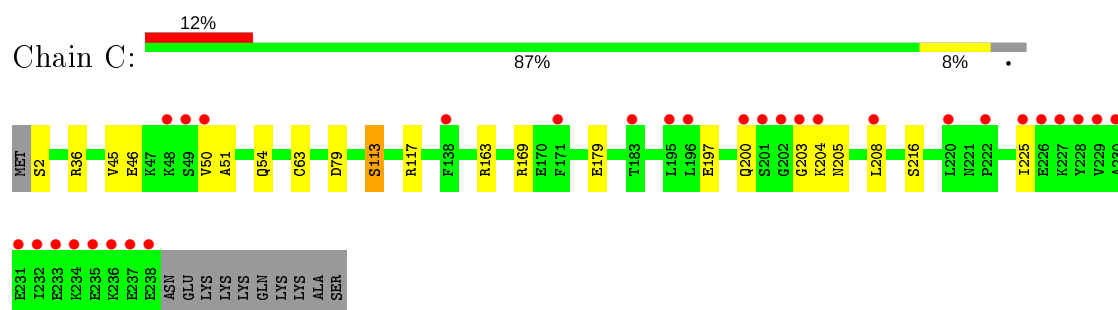
- Molecule 2: Proteasome subunit alpha type-4



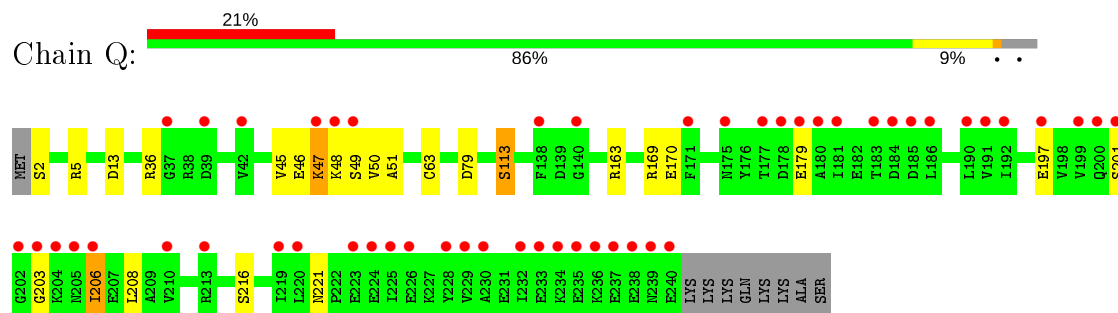
- Molecule 2: Proteasome subunit alpha type-4



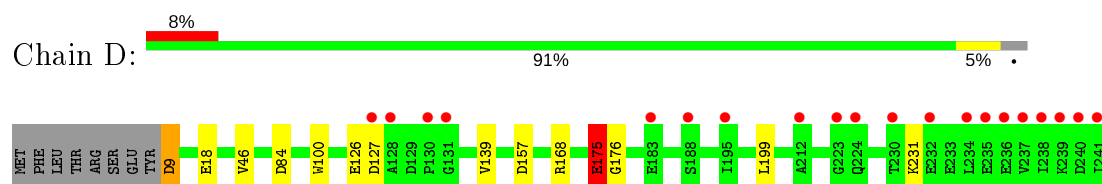
- Molecule 3: Proteasome subunit alpha type-7



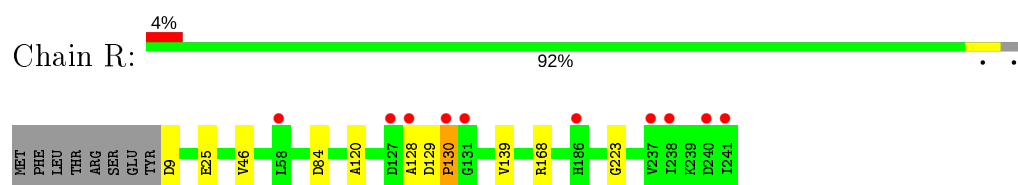
- Molecule 3: Proteasome subunit alpha type-7



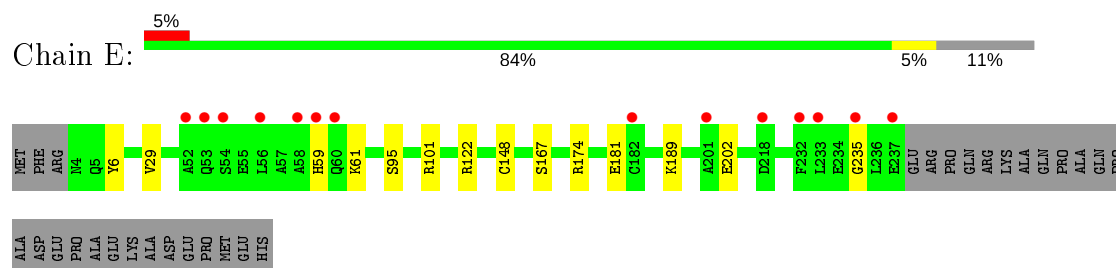
- Molecule 4: Proteasome subunit alpha type-5



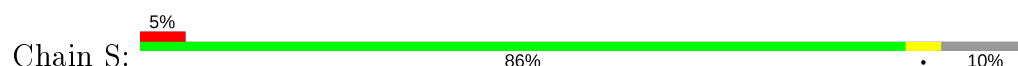
- Molecule 4: Proteasome subunit alpha type-5

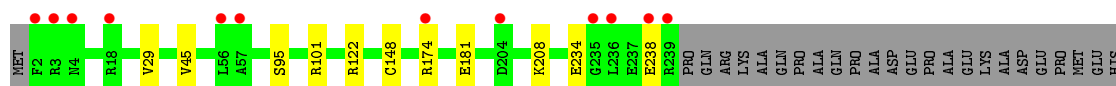


- Molecule 5: Proteasome subunit alpha type-1

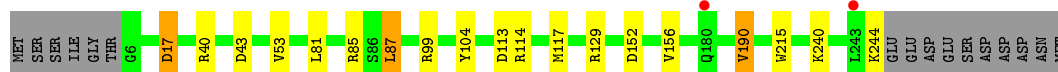
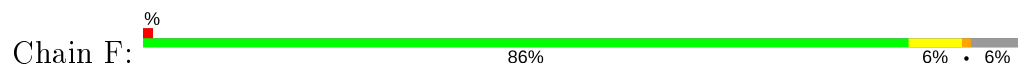


- Molecule 5: Proteasome subunit alpha type-1

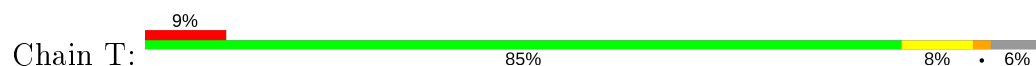




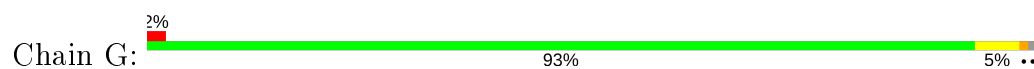
- Molecule 6: Proteasome subunit alpha type-3



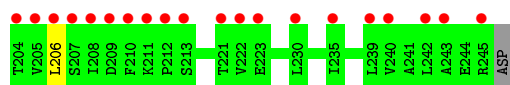
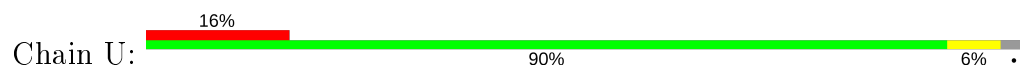
- Molecule 6: Proteasome subunit alpha type-3



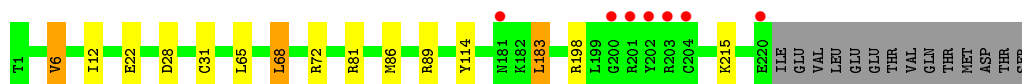
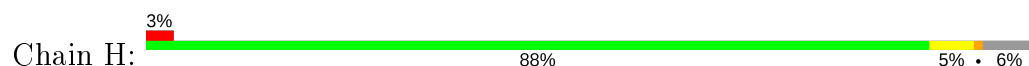
- Molecule 7: Proteasome subunit alpha type-6



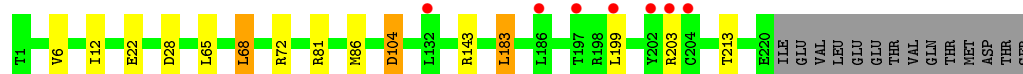
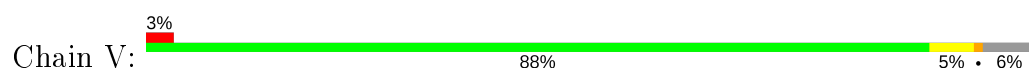
- Molecule 7: Proteasome subunit alpha type-6



- Molecule 8: Proteasome subunit beta type-7



- Molecule 8: Proteasome subunit beta type-7



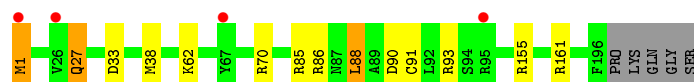
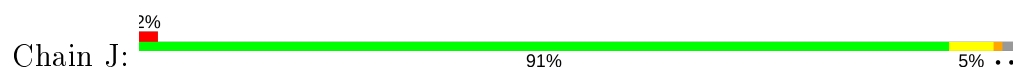
- Molecule 9: Proteasome subunit beta type-3



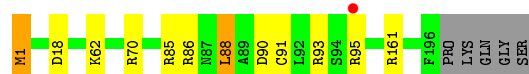
- Molecule 9: Proteasome subunit beta type-3



- Molecule 10: Proteasome subunit beta type-2



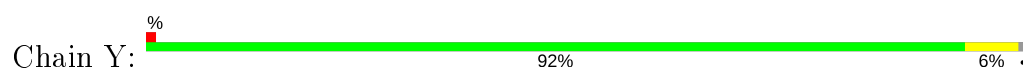
- Molecule 10: Proteasome subunit beta type-2



- Molecule 11: Proteasome subunit beta type-5



- Molecule 11: Proteasome subunit beta type-5





- Molecule 12: Proteasome subunit beta type-1

Chain L:  93% 5% .



- Molecule 12: Proteasome subunit beta type-1

Chain Z:  3% 92% 7% .



- Molecule 13: Proteasome subunit beta type-4

Chain M:  2% 94% 5% .



- Molecule 13: Proteasome subunit beta type-4

Chain a:  0% 92% 6% .



- Molecule 14: Proteasome subunit beta type-6

Chain N:  93% 5% .



- Molecule 14: Proteasome subunit beta type-6

Chain b:  3% 95% . . .



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	113.45Å 202.76Å 314.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	170.38 – 1.99 48.90 – 1.99	Depositor EDS
% Data completeness (in resolution range)	99.0 (170.38-1.99) 99.0 (48.90-1.99)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.47 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, $R_{free}$	0.181 , 0.216 0.187 , 0.218	Depositor DCC
$R_{free}$ test set	24259 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	35.9	Xtriage
Anisotropy	0.289	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 50.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	52186	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

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

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.93	2/1833 (0.1%)	0.95	7/2489 (0.3%)
1	O	0.77	0/1778	0.89	6/2419 (0.2%)
2	B	0.94	1/1962 (0.1%)	0.98	7/2649 (0.3%)
2	P	0.84	2/1945 (0.1%)	0.95	6/2631 (0.2%)
3	C	0.84	1/1818 (0.1%)	0.98	6/2469 (0.2%)
3	Q	0.81	2/1834 (0.1%)	0.97	8/2490 (0.3%)
4	D	0.89	4/1789 (0.2%)	0.93	6/2424 (0.2%)
4	R	0.98	1/1780 (0.1%)	1.01	4/2408 (0.2%)
5	E	0.96	2/1842 (0.1%)	0.98	3/2493 (0.1%)
5	S	0.88	0/1901	0.95	3/2571 (0.1%)
6	F	1.13	2/1935 (0.1%)	1.13	17/2605 (0.7%)
6	T	0.93	2/1894 (0.1%)	1.05	17/2556 (0.7%)
7	G	1.09	3/1909 (0.2%)	0.97	8/2579 (0.3%)
7	U	0.84	3/1804 (0.2%)	0.93	8/2441 (0.3%)
8	H	1.10	4/1697 (0.2%)	1.21	12/2299 (0.5%)
8	V	0.87	2/1655 (0.1%)	1.02	10/2251 (0.4%)
9	I	1.07	2/1648 (0.1%)	1.23	12/2219 (0.5%)
9	W	0.87	2/1630 (0.1%)	1.09	8/2197 (0.4%)
10	J	0.97	0/1613	1.23	14/2180 (0.6%)
10	X	0.93	0/1599	1.15	11/2163 (0.5%)
11	K	0.97	1/1584 (0.1%)	1.04	9/2141 (0.4%)
11	Y	1.11	2/1620 (0.1%)	1.15	12/2185 (0.5%)
12	L	0.97	4/1672 (0.2%)	0.98	6/2257 (0.3%)
12	Z	1.14	6/1675 (0.4%)	1.06	5/2257 (0.2%)
13	M	1.04	0/1728	1.09	8/2339 (0.3%)
13	a	1.12	3/1724 (0.2%)	1.10	5/2336 (0.2%)
14	N	1.17	5/1548 (0.3%)	1.03	4/2095 (0.2%)
14	b	1.05	4/1554 (0.3%)	1.02	3/2104 (0.1%)
All	All	0.97	60/48971 (0.1%)	1.04	225/66247 (0.3%)

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	P	0	3
3	C	0	1
3	Q	0	3
4	D	0	4
4	R	0	2
5	E	0	1
6	T	0	1
7	U	1	0
9	I	0	1
9	W	0	1
10	J	0	2
10	X	0	1
13	a	0	1
All	All	1	21

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	108	GLU	CD-OE1	13.03	1.40	1.25
7	G	108	GLU	CD-OE2	8.40	1.34	1.25
12	Z	3	SER	CB-OG	8.15	1.52	1.42
6	F	104	TYR	CE2-CZ	8.09	1.49	1.38
6	F	104	TYR	CG-CD1	7.99	1.49	1.39
12	L	129	SER	CB-OG	-7.77	1.32	1.42
11	K	89	TYR	CE1-CZ	7.70	1.48	1.38
7	U	108	GLU	CD-OE1	7.16	1.33	1.25
9	I	105	GLU	CD-OE2	7.12	1.33	1.25
9	W	77	GLU	CG-CD	7.05	1.62	1.51
13	a	75	GLU	CD-OE1	7.04	1.33	1.25
3	Q	13	ASP	CB-CG	6.95	1.66	1.51
4	D	175[A]	GLU	C-O	6.83	1.36	1.23
4	D	175[B]	GLU	C-O	6.83	1.36	1.23
14	N	25	SER	CB-OG	-6.74	1.33	1.42
12	Z	129	SER	CB-OG	-6.72	1.33	1.42
3	Q	113	SER	CB-OG	-6.66	1.33	1.42
7	G	78	CYS	CB-SG	-6.57	1.71	1.82
6	T	25	TYR	CG-CD1	6.53	1.47	1.39
14	b	36	THR	CB-CG2	-6.41	1.31	1.52
14	N	36	THR	CB-CG2	-6.35	1.31	1.52
8	H	31	CYS	CB-SG	-6.34	1.71	1.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	U	108	GLU	CD-OE2	6.33	1.32	1.25
12	Z	32	GLY	N-CA	6.29	1.55	1.46
13	a	10	SER	CB-OG	6.12	1.50	1.42
2	P	7[A]	SER	CB-OG	6.12	1.50	1.42
2	P	7[B]	SER	CB-OG	6.12	1.50	1.42
8	V	104[A]	ASP	CB-CG	-6.10	1.39	1.51
8	V	104[B]	ASP	CB-CG	-6.10	1.39	1.51
2	B	70	GLU	CD-OE1	6.07	1.32	1.25
8	H	6	VAL	CB-CG1	-5.96	1.40	1.52
14	N	89	TYR	CE1-CZ	5.93	1.46	1.38
14	b	25	SER	CB-OG	-5.89	1.34	1.42
11	Y	202	GLY	CA-C	5.83	1.61	1.51
12	Z	142	SER	CB-OG	-5.78	1.34	1.42
4	D	100	TRP	CE3-CZ3	5.78	1.48	1.38
14	b	134	SER	CB-OG	5.76	1.49	1.42
3	C	113	SER	CB-OG	-5.64	1.34	1.42
8	H	114	TYR	CG-CD2	5.62	1.46	1.39
1	A	212	CYS	CB-SG	-5.59	1.72	1.81
5	E	6	TYR	CG-CD1	5.56	1.46	1.39
12	L	122	TYR	CE1-CZ	5.52	1.45	1.38
4	R	25	GLU	CD-OE1	5.51	1.31	1.25
12	L	44	TYR	CE1-CZ	5.50	1.45	1.38
11	Y	202	GLY	C-O	5.34	1.32	1.23
7	U	78	CYS	CB-SG	-5.33	1.73	1.81
12	Z	78	SER	CB-OG	-5.30	1.35	1.42
14	N	26	TYR	CG-CD1	5.22	1.46	1.39
1	A	120	TYR	CG-CD1	5.19	1.46	1.39
9	I	77	GLU	CB-CG	5.16	1.61	1.52
6	T	7	TYR	N-CA	5.15	1.56	1.46
12	L	78	SER	CB-OG	-5.15	1.35	1.42
14	b	89	TYR	CE1-CZ	5.14	1.45	1.38
14	N	104	TRP	CE3-CZ3	5.13	1.47	1.38
12	Z	140	SER	CB-OG	-5.12	1.35	1.42
8	H	114	TYR	CE1-CZ	5.05	1.45	1.38
9	W	77	GLU	CB-CG	5.05	1.61	1.52
5	E	167	SER	CB-OG	-5.04	1.35	1.42
4	D	18	GLU	CD-OE1	5.02	1.31	1.25
13	a	119	GLU	CD-OE2	5.01	1.31	1.25

All (225) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	J	86	ARG	NE-CZ-NH2	-19.20	110.70	120.30
10	J	86	ARG	NE-CZ-NH1	18.23	129.41	120.30
9	I	69	ARG	NE-CZ-NH1	18.08	129.34	120.30
8	H	72	ARG	NE-CZ-NH2	-17.59	111.50	120.30
10	X	86	ARG	NE-CZ-NH2	-17.59	111.50	120.30
9	W	69	ARG	NE-CZ-NH1	15.00	127.80	120.30
10	X	86	ARG	NE-CZ-NH1	14.42	127.51	120.30
8	H	72	ARG	NE-CZ-NH1	14.28	127.44	120.30
9	I	25[A]	ARG	NE-CZ-NH1	12.60	126.60	120.30
9	I	25[B]	ARG	NE-CZ-NH1	12.60	126.60	120.30
9	I	69	ARG	NE-CZ-NH2	-12.57	114.01	120.30
14	b	30	ARG	NE-CZ-NH1	12.23	126.42	120.30
13	M	151	ARG	NE-CZ-NH1	10.71	125.66	120.30
11	Y	158	ARG	NE-CZ-NH2	-10.60	115.00	120.30
13	a	151	ARG	NE-CZ-NH1	10.39	125.50	120.30
9	W	69	ARG	NE-CZ-NH2	-10.37	115.12	120.30
4	R	120[A]	ALA	C-N-CA	10.06	146.86	121.70
4	R	120[B]	ALA	C-N-CA	10.06	146.86	121.70
11	Y	158	ARG	NE-CZ-NH1	9.83	125.22	120.30
2	B	96	ARG	NE-CZ-NH1	9.37	124.99	120.30
2	P	96	ARG	NE-CZ-NH1	9.32	124.96	120.30
7	U	88	ARG	NE-CZ-NH1	9.19	124.89	120.30
10	X	90	ASP	CB-CG-OD1	9.19	126.57	118.30
12	Z	99	ARG	NE-CZ-NH2	-9.11	115.75	120.30
12	L	99	ARG	NE-CZ-NH2	-8.68	115.96	120.30
14	b	30	ARG	NE-CZ-NH2	-8.64	115.98	120.30
9	W	25[A]	ARG	NE-CZ-NH1	8.57	124.59	120.30
9	W	25[B]	ARG	NE-CZ-NH1	8.57	124.59	120.30
8	V	72	ARG	NE-CZ-NH2	-8.55	116.03	120.30
9	W	16[A]	LYS	C-N-CA	8.52	143.00	121.70
9	W	16[B]	LYS	C-N-CA	8.52	143.00	121.70
12	L	99	ARG	NE-CZ-NH1	8.51	124.56	120.30
8	H	86	MET	CG-SD-CE	-8.46	86.66	100.20
10	J	93	ARG	NE-CZ-NH1	8.35	124.47	120.30
11	Y	46	MET	CG-SD-CE	-8.30	86.92	100.20
1	A	219	ARG	NE-CZ-NH1	8.28	124.44	120.30
8	H	81	ARG	NE-CZ-NH2	-8.25	116.17	120.30
5	E	122	ARG	NE-CZ-NH2	-8.15	116.22	120.30
9	I	16[A]	LYS	C-N-CA	8.14	142.05	121.70
9	I	16[B]	LYS	C-N-CA	8.14	142.05	121.70
11	K	155	ASP	CB-CG-OD2	8.06	125.55	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	Z	172	MET	CG-SD-CE	-7.89	87.58	100.20
12	Z	99	ARG	NE-CZ-NH1	7.88	124.24	120.30
6	T	117	MET	CG-SD-CE	7.85	112.76	100.20
13	M	5	MET	CG-SD-CE	7.79	112.66	100.20
11	K	158	ARG	NE-CZ-NH2	-7.65	116.48	120.30
7	U	86	ASP	CB-CG-OD2	7.52	125.07	118.30
1	O	181	LEU	CA-CB-CG	7.49	132.53	115.30
7	U	88	ARG	NE-CZ-NH2	-7.47	116.56	120.30
6	F	190	VAL	CB-CA-C	-7.45	97.24	111.40
10	J	88	LEU	CB-CG-CD2	7.41	123.60	111.00
7	U	117	ARG	NE-CZ-NH1	7.33	123.97	120.30
9	I	25[A]	ARG	NE-CZ-NH2	-7.33	116.63	120.30
9	I	25[B]	ARG	NE-CZ-NH2	-7.33	116.63	120.30
11	Y	142[A]	ARG	NE-CZ-NH1	7.32	123.96	120.30
11	Y	142[B]	ARG	NE-CZ-NH1	7.32	123.96	120.30
13	M	151	ARG	NE-CZ-NH2	-7.28	116.66	120.30
10	J	93	ARG	NE-CZ-NH2	-7.27	116.67	120.30
10	J	86	ARG	CD-NE-CZ	7.25	133.75	123.60
12	L	172	MET	CG-SD-CE	-7.22	88.65	100.20
8	H	72	ARG	CD-NE-CZ	7.21	133.69	123.60
6	F	117	MET	CG-SD-CE	7.15	111.64	100.20
6	F	43	ASP	CB-CG-OD1	7.12	124.71	118.30
7	G	117	ARG	NE-CZ-NH1	7.11	123.85	120.30
8	V	86	MET	CG-SD-CE	-7.08	88.88	100.20
13	a	166	ARG	NE-CZ-NH2	-7.05	116.77	120.30
6	F	114	ARG	NE-CZ-NH2	-7.04	116.78	120.30
6	T	114	ARG	NE-CZ-NH2	-7.03	116.78	120.30
1	A	219	ARG	NE-CZ-NH2	-7.00	116.80	120.30
10	X	93	ARG	NE-CZ-NH1	6.94	123.77	120.30
6	T	190	VAL	CB-CA-C	-6.93	98.22	111.40
13	M	99	ARG	NE-CZ-NH1	6.89	123.75	120.30
11	Y	121	ARG	NE-CZ-NH1	6.84	123.72	120.30
8	V	72	ARG	NE-CZ-NH1	6.81	123.70	120.30
10	X	86	ARG	CD-NE-CZ	6.79	133.10	123.60
11	K	158	ARG	NE-CZ-NH1	6.76	123.68	120.30
6	T	114	ARG	NE-CZ-NH1	6.75	123.67	120.30
11	Y	159	ARG	NE-CZ-NH1	6.73	123.67	120.30
7	G	183	VAL	CB-CA-C	-6.71	98.65	111.40
10	X	93	ARG	NE-CZ-NH2	-6.71	116.94	120.30
2	B	4	ARG	NE-CZ-NH1	6.70	123.65	120.30
8	H	89	ARG	NE-CZ-NH1	6.69	123.65	120.30
13	a	5	MET	CG-SD-CE	6.61	110.78	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	J	70	ARG	NE-CZ-NH2	-6.55	117.03	120.30
2	P	116	ASP	CB-CG-OD1	6.52	124.17	118.30
4	R	84	ASP	CB-CG-OD1	6.52	124.17	118.30
10	X	88	LEU	CB-CG-CD2	6.50	122.05	111.00
6	F	114	ARG	NE-CZ-NH1	6.50	123.55	120.30
6	T	113	ASP	CB-CG-OD2	-6.49	112.46	118.30
7	G	78	CYS	CA-CB-SG	6.44	125.60	114.00
13	a	151	ARG	NE-CZ-NH2	-6.42	117.09	120.30
1	O	219	ARG	NE-CZ-NH1	6.36	123.48	120.30
6	F	87	LEU	CB-CG-CD1	6.33	121.76	111.00
2	P	4	ARG	NE-CZ-NH1	6.31	123.46	120.30
6	T	152	ASP	CB-CG-OD1	6.31	123.97	118.30
6	T	230	ASP	CB-CG-OD2	6.30	123.97	118.30
7	G	86	ASP	CB-CG-OD1	6.18	123.86	118.30
10	X	70	ARG	NE-CZ-NH2	-6.16	117.22	120.30
2	B	116	ASP	CB-CG-OD1	6.13	123.82	118.30
3	Q	36	ARG	NE-CZ-NH1	6.11	123.35	120.30
10	J	90	ASP	CB-CG-OD1	6.10	123.79	118.30
6	F	152	ASP	CB-CG-OD1	6.07	123.76	118.30
8	H	68	LEU	CB-CG-CD1	6.06	121.30	111.00
8	V	81	ARG	NE-CZ-NH2	-6.05	117.28	120.30
13	M	166	ARG	NE-CZ-NH2	-6.04	117.28	120.30
5	S	122	ARG	NE-CZ-NH2	-6.01	117.29	120.30
7	U	80[A]	MET	CG-SD-CE	6.01	109.82	100.20
7	U	80[B]	MET	CG-SD-CE	6.01	109.82	100.20
6	T	6	GLY	C-N-CA	5.95	136.59	121.70
11	K	142	ARG	NE-CZ-NH1	5.95	123.27	120.30
6	F	156	VAL	CG1-CB-CG2	-5.91	101.44	110.90
3	C	197	GLU	OE1-CD-OE2	5.91	130.39	123.30
5	E	122	ARG	NE-CZ-NH1	5.89	123.25	120.30
7	U	11	ARG	NE-CZ-NH1	5.87	123.23	120.30
3	Q	5	ARG	NE-CZ-NH1	5.87	123.23	120.30
1	O	73	LEU	CB-CA-C	-5.84	99.11	110.20
3	C	36	ARG	NE-CZ-NH1	5.82	123.21	120.30
4	D	84	ASP	CB-CG-OD1	5.81	123.53	118.30
1	A	73	LEU	CA-CB-CG	5.78	128.59	115.30
8	H	12	ILE	CG1-CB-CG2	-5.78	98.69	111.40
12	L	114	ASP	CB-CG-OD1	5.75	123.48	118.30
3	Q	79	ASP	CB-CG-OD1	5.75	123.48	118.30
8	V	68	LEU	CB-CG-CD1	5.75	120.78	111.00
1	A	73	LEU	CB-CA-C	-5.75	99.28	110.20
10	J	38	MET	CG-SD-CE	-5.75	91.01	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	85	ARG	NE-CZ-NH1	5.73	123.17	120.30
6	F	40	ARG	NE-CZ-NH1	5.73	123.16	120.30
11	K	121	ARG	NE-CZ-NH1	5.71	123.16	120.30
7	G	245	ARG	NE-CZ-NH1	5.68	123.14	120.30
6	T	27	MET	CG-SD-CE	5.68	109.29	100.20
5	E	174	ARG	NE-CZ-NH1	5.67	123.14	120.30
8	V	12	ILE	CG1-CB-CG2	-5.67	98.94	111.40
6	F	99	ARG	NE-CZ-NH2	-5.66	117.47	120.30
3	C	79	ASP	CB-CG-OD2	-5.65	113.22	118.30
8	H	81	ARG	CB-CA-C	-5.64	99.11	110.40
11	Y	159	ARG	NE-CZ-NH2	-5.64	117.48	120.30
6	F	85	ARG	NE-CZ-NH2	-5.64	117.48	120.30
2	B	96	ARG	NE-CZ-NH2	-5.62	117.49	120.30
5	S	122	ARG	NE-CZ-NH1	5.62	123.11	120.30
11	Y	121	ARG	NE-CZ-NH2	-5.62	117.49	120.30
6	T	70	ASP	CB-CG-OD1	5.61	123.35	118.30
10	X	18	ASP	CB-CG-OD1	-5.61	113.25	118.30
7	U	138	MET	CG-SD-CE	-5.59	91.25	100.20
13	a	94	ARG	NE-CZ-NH1	5.59	123.10	120.30
4	D	9	ASP	CB-CG-OD1	5.58	123.33	118.30
3	Q	13	ASP	CB-CA-C	5.57	121.54	110.40
13	M	166	ARG	NE-CZ-NH1	5.55	123.08	120.30
7	G	88	ARG	NE-CZ-NH2	-5.53	117.54	120.30
6	F	17	ASP	CB-CG-OD1	-5.50	113.34	118.30
13	M	94	ARG	NE-CZ-NH1	5.50	123.05	120.30
3	Q	79	ASP	CB-CG-OD2	-5.49	113.36	118.30
1	O	219	ARG	NE-CZ-NH2	-5.48	117.56	120.30
4	D	157	ASP	CB-CG-OD1	5.46	123.21	118.30
13	M	182	ARG	NE-CZ-NH1	5.46	123.03	120.30
3	Q	169	ARG	NE-CZ-NH1	5.45	123.03	120.30
10	J	161	ARG	NE-CZ-NH2	-5.45	117.58	120.30
10	J	33	ASP	CB-CG-OD1	5.43	123.19	118.30
10	X	161	ARG	NE-CZ-NH2	-5.42	117.59	120.30
6	T	43	ASP	CB-CG-OD2	5.42	123.17	118.30
12	L	102	PHE	CB-CG-CD1	5.41	124.59	120.80
4	D	175[A]	GLU	N-CA-C	-5.41	96.41	111.00
4	D	175[B]	GLU	N-CA-C	-5.41	96.41	111.00
7	G	120	ASP	CB-CG-OD1	5.39	123.16	118.30
2	P	96	ARG	NE-CZ-NH2	-5.39	117.60	120.30
10	X	85	ARG	NE-CZ-NH2	-5.39	117.60	120.30
11	K	108	ARG	NE-CZ-NH1	5.39	122.99	120.30
9	I	25[A]	ARG	CD-NE-CZ	5.39	131.14	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	25[B]	ARG	CD-NE-CZ	5.39	131.14	123.60
3	C	79	ASP	CB-CG-OD1	5.38	123.14	118.30
11	Y	36	ILE	CA-CB-CG1	-5.37	100.80	111.00
1	A	142	ARG	NE-CZ-NH1	5.35	122.98	120.30
4	D	168	ARG	NE-CZ-NH1	5.35	122.98	120.30
14	N	123	ARG	NE-CZ-NH1	-5.35	117.62	120.30
1	A	17	LYS	CD-CE-NZ	5.35	124.00	111.70
14	N	46	ARG	NE-CZ-NH2	-5.34	117.63	120.30
11	K	43	LEU	CA-CB-CG	5.33	127.55	115.30
11	K	121	ARG	NE-CZ-NH2	-5.31	117.65	120.30
6	T	87	LEU	CB-CG-CD1	5.30	120.02	111.00
2	B	2	SER	N-CA-CB	5.29	118.44	110.50
6	F	113	ASP	CB-CG-OD2	-5.29	113.53	118.30
5	S	174	ARG	NE-CZ-NH1	5.28	122.94	120.30
14	N	23	THR	OG1-CB-CG2	-5.28	97.86	110.00
3	Q	36	ARG	NE-CZ-NH2	-5.27	117.66	120.30
11	Y	108	ARG	NE-CZ-NH1	5.26	122.93	120.30
8	V	28	ASP	CB-CG-OD1	5.25	123.03	118.30
12	Z	173	ARG	NE-CZ-NH2	-5.25	117.67	120.30
8	H	28	ASP	CB-CG-OD1	5.25	123.02	118.30
10	J	85	ARG	NE-CZ-NH2	-5.21	117.70	120.30
6	T	17	ASP	CB-CG-OD1	-5.21	113.61	118.30
8	V	143	ARG	NE-CZ-NH2	-5.21	117.70	120.30
8	V	81	ARG	CB-CA-C	-5.19	100.01	110.40
1	O	73	LEU	CA-CB-CG	5.19	127.23	115.30
8	V	183	LEU	CA-CB-CG	-5.18	103.38	115.30
6	T	7	TYR	N-CA-CB	5.18	119.93	110.60
12	Z	114	ASP	CB-CG-OD1	5.17	122.96	118.30
12	L	170	ARG	NE-CZ-NH2	-5.17	117.72	120.30
7	G	95	ARG	NE-CZ-NH2	-5.16	117.72	120.30
14	N	167	ARG	NE-CZ-NH2	-5.15	117.72	120.30
6	T	99	ARG	NE-CZ-NH1	5.15	122.87	120.30
2	P	7[A]	SER	N-CA-CB	-5.14	102.78	110.50
2	P	7[B]	SER	N-CA-CB	-5.14	102.78	110.50
6	T	71	ARG	NE-CZ-NH2	-5.14	117.73	120.30
9	W	25[A]	ARG	NE-CZ-NH2	-5.14	117.73	120.30
9	W	25[B]	ARG	NE-CZ-NH2	-5.14	117.73	120.30
4	R	168	ARG	NE-CZ-NH2	-5.14	117.73	120.30
8	H	198	ARG	NE-CZ-NH2	-5.13	117.74	120.30
10	J	27[A]	GLN	CA-CB-CG	5.13	124.68	113.40
10	J	27[B]	GLN	CA-CB-CG	5.13	124.68	113.40
3	Q	13	ASP	CB-CG-OD2	5.12	122.90	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	169	ARG	NE-CZ-NH1	5.11	122.86	120.30
14	b	30	ARG	CD-NE-CZ	5.11	130.75	123.60
6	F	40	ARG	NE-CZ-NH2	-5.09	117.76	120.30
3	C	117	ARG	NE-CZ-NH1	5.08	122.84	120.30
2	B	4	ARG	NE-CZ-NH2	-5.08	117.76	120.30
6	T	156	VAL	CG1-CB-CG2	-5.07	102.78	110.90
6	F	99	ARG	NE-CZ-NH1	5.07	122.83	120.30
11	K	167	ARG	NE-CZ-NH1	5.07	122.83	120.30
2	B	91	ARG	NE-CZ-NH1	5.05	122.83	120.30
8	H	183	LEU	CA-CB-CG	-5.05	103.68	115.30
11	Y	116	ASP	CB-CG-OD2	5.04	122.84	118.30
1	O	142	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	A	205	ASP	CB-CG-OD2	-5.03	113.77	118.30
9	I	69	ARG	CD-NE-CZ	5.02	130.63	123.60
6	F	129	ARG	CG-CD-NE	-5.01	101.28	111.80
9	I	35	THR	OG1-CB-CG2	5.01	121.51	110.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	U	47	6V1	C1

All (21) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	46	GLU	Peptide
4	D	127	ASP	Peptide
4	D	175[A]	GLU	Peptide
4	D	175[B]	GLU	Mainchain,Peptide
5	E	235	GLY	Peptide
9	I	78	GLY	Peptide
10	J	1[A]	MET	Peptide
10	J	1[B]	MET	Peptide
2	P	203	VAL	Peptide
2	P	244	GLU	Peptide
2	P	245	ALA	Peptide
3	Q	46	GLU	Peptide
3	Q	47	LYS	Peptide
3	Q	49	SER	Peptide
4	R	130	PRO	Peptide
4	R	223	GLY	Peptide
6	T	5	THR	Peptide

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Mol	Chain	Res	Type	Group
9	W	78	GLY	Peptide
10	X	1	MET	Peptide
13	a	215	ILE	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%)	9 (4%)	1 (0%)	34	30
2	P	248/261 (95%)	235 (95%)	10 (4%)	3 (1%)	13	7
3	C	236/248 (95%)	223 (94%)	7 (3%)	6 (2%)	5	2
3	Q	236/248 (95%)	221 (94%)	6 (2%)	9 (4%)	3	1
4	D	232/241 (96%)	222 (96%)	7 (3%)	3 (1%)	12	6
4	R	232/241 (96%)	222 (96%)	7 (3%)	3 (1%)	12	6
5	E	232/263 (88%)	226 (97%)	5 (2%)	1 (0%)	34	30
5	S	238/263 (90%)	228 (96%)	9 (4%)	1 (0%)	34	30
6	F	241/255 (94%)	238 (99%)	3 (1%)	0	100	100
6	T	239/255 (94%)	233 (98%)	4 (2%)	2 (1%)	19	13
7	G	241/246 (98%)	235 (98%)	6 (2%)	0	100	100
7	U	232/246 (94%)	227 (98%)	4 (2%)	1 (0%)	34	30
8	H	220/234 (94%)	217 (99%)	3 (1%)	0	100	100
8	V	220/234 (94%)	217 (99%)	2 (1%)	1 (0%)	29	23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	I	205/205 (100%)	202 (98%)	3 (2%)	0	100	100
9	W	204/205 (100%)	199 (98%)	5 (2%)	0	100	100
10	J	195/201 (97%)	192 (98%)	3 (2%)	0	100	100
10	X	195/201 (97%)	193 (99%)	2 (1%)	0	100	100
11	K	199/204 (98%)	197 (99%)	2 (1%)	0	100	100
11	Y	202/204 (99%)	199 (98%)	2 (1%)	1 (0%)	29	23
12	L	213/213 (100%)	210 (99%)	3 (1%)	0	100	100
12	Z	212/213 (100%)	209 (99%)	3 (1%)	0	100	100
13	M	215/219 (98%)	209 (97%)	6 (3%)	0	100	100
13	a	216/219 (99%)	209 (97%)	7 (3%)	0	100	100
14	N	201/205 (98%)	199 (99%)	2 (1%)	0	100	100
14	b	202/205 (98%)	201 (100%)	1 (0%)	0	100	100
All	All	6213/6458 (96%)	6039 (97%)	134 (2%)	40 (1%)	25	19

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	52	LYS
1	A	53	SER
5	E	59	HIS
1	O	52	LYS
1	O	53	SER
1	O	231	ALA
2	P	52	ILE
2	P	54	LYS
3	Q	206	ILE
3	Q	221	ASN
4	R	128	ALA
4	R	130	PRO
5	S	238	GLU
11	Y	201	SER
1	A	176	ARG
2	B	203	VAL
3	C	50	VAL
3	C	200	GLN
3	C	204	LYS
3	C	216	SER
4	D	176	GLY

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Mol	Chain	Res	Type
1	O	176	ARG
3	Q	47	LYS
3	Q	50	VAL
3	Q	201	SER
3	Q	216	SER
6	T	7	TYR
6	T	206	ASP
8	V	203	ARG
3	C	51	ALA
4	D	175[A]	GLU
4	D	175[B]	GLU
4	R	129	ASP
7	U	58	ASP
1	A	50	LYS
3	Q	48	LYS
3	Q	51	ALA
3	C	203	GLY
3	Q	203	GLY
2	P	58	GLU

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	185/191 (97%)	175 (95%)	10 (5%)	22	18
1	O	176/191 (92%)	165 (94%)	11 (6%)	18	13
2	B	200/221 (90%)	195 (98%)	5 (2%)	47	49
2	P	197/221 (89%)	187 (95%)	10 (5%)	24	19
3	C	179/210 (85%)	170 (95%)	9 (5%)	24	20
3	Q	184/210 (88%)	175 (95%)	9 (5%)	25	21
4	D	189/203 (93%)	183 (97%)	6 (3%)	39	38
4	R	187/203 (92%)	184 (98%)	3 (2%)	62	67
5	E	192/223 (86%)	184 (96%)	8 (4%)	30	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	S	197/223 (88%)	190 (96%)	7 (4%)	35	34
6	F	199/212 (94%)	191 (96%)	8 (4%)	31	29
6	T	192/212 (91%)	184 (96%)	8 (4%)	30	27
7	G	202/207 (98%)	195 (96%)	7 (4%)	36	35
7	U	186/207 (90%)	181 (97%)	5 (3%)	44	46
8	H	181/195 (93%)	175 (97%)	6 (3%)	38	37
8	V	172/195 (88%)	163 (95%)	9 (5%)	23	19
9	I	176/174 (101%)	174 (99%)	2 (1%)	73	78
9	W	173/174 (99%)	172 (99%)	1 (1%)	86	90
10	J	166/170 (98%)	159 (96%)	7 (4%)	30	27
10	X	165/170 (97%)	161 (98%)	4 (2%)	49	51
11	K	155/159 (98%)	148 (96%)	7 (4%)	27	24
11	Y	159/159 (100%)	156 (98%)	3 (2%)	57	61
12	L	175/178 (98%)	166 (95%)	9 (5%)	24	19
12	Z	175/178 (98%)	167 (95%)	8 (5%)	27	23
13	M	180/181 (99%)	175 (97%)	5 (3%)	43	44
13	a	178/181 (98%)	172 (97%)	6 (3%)	37	36
14	N	158/159 (99%)	154 (98%)	4 (2%)	47	49
14	b	158/159 (99%)	153 (97%)	5 (3%)	39	38
All	All	5036/5366 (94%)	4854 (96%)	182 (4%)	36	34

All (182) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LYS
1	A	53	SER
1	A	61	VAL
1	A	142	ARG
1	A	176	ARG
1	A	189	THR
1	A	206	ASN
1	A	223	THR
1	A	226	LYS
1	A	227	ASP
2	B	33	THR

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Mol	Chain	Res	Type
2	B	58	GLU
2	B	190	LEU
2	B	229	LYS
2	B	249	ARG
3	C	2	SER
3	C	45	VAL
3	C	54	GLN
3	C	113	SER
3	C	163	ARG
3	C	179	GLU
3	C	205	ASN
3	C	208	LEU
3	C	225	ILE
4	D	9	ASP
4	D	46	VAL
4	D	126	GLU
4	D	139	VAL
4	D	199	LEU
4	D	231	LYS
5	E	29	VAL
5	E	61	LYS
5	E	95	SER
5	E	101[A]	ARG
5	E	101[B]	ARG
5	E	181	GLU
5	E	189	LYS
5	E	202	GLU
6	F	17	ASP
6	F	53	VAL
6	F	81	LEU
6	F	87	LEU
6	F	190	VAL
6	F	215	TRP
6	F	240	LYS
6	F	244	LYS
7	G	42	VAL
7	G	78	CYS
7	G	88	ARG
7	G	182	LYS
7	G	183	VAL
7	G	206	LEU
7	G	209	ASP

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Mol	Chain	Res	Type
8	H	6	VAL
8	H	22	GLU
8	H	65	LEU
8	H	68	LEU
8	H	183	LEU
8	H	215	LYS
9	I	35	THR
9	I	115	THR
10	J	1[A]	MET
10	J	1[B]	MET
10	J	27[A]	GLN
10	J	27[B]	GLN
10	J	62	LYS
10	J	88	LEU
10	J	155	ARG
11	K	9	PHE
11	K	13	VAL
11	K	43	LEU
11	K	148	LEU
11	K	159	ARG
11	K	175	VAL
11	K	188	VAL
12	L	3[A]	SER
12	L	3[B]	SER
12	L	72	LEU
12	L	78	SER
12	L	102	PHE
12	L	163	HIS
12	L	172	MET
12	L	174	LEU
12	L	207	THR
13	M	100	ARG
13	M	154	LEU
13	M	155	GLU
13	M	156	LYS
13	M	216	SER
14	N	36	THR
14	N	85	LYS
14	N	146	GLU
14	N	197	LYS
1	O	10	THR
1	O	53	SER

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Mol	Chain	Res	Type
1	O	118	GLN
1	O	142	ARG
1	O	176	ARG
1	O	181	LEU
1	O	189	THR
1	O	206	ASN
1	O	221	THR
1	O	223	THR
1	O	226	LYS
2	P	7[A]	SER
2	P	7[B]	SER
2	P	33	THR
2	P	54	LYS
2	P	190	LEU
2	P	204	SER
2	P	235	GLN
2	P	236	LEU
2	P	246	LYS
2	P	249	ARG
3	Q	2	SER
3	Q	45	VAL
3	Q	113	SER
3	Q	163	ARG
3	Q	170	GLU
3	Q	179	GLU
3	Q	197	GLU
3	Q	206	ILE
3	Q	208	LEU
4	R	9	ASP
4	R	46	VAL
4	R	139	VAL
5	S	29	VAL
5	S	45	VAL
5	S	95	SER
5	S	101	ARG
5	S	181	GLU
5	S	208	LYS
5	S	234	GLU
6	T	17	ASP
6	T	53	VAL
6	T	81	LEU
6	T	87	LEU

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Mol	Chain	Res	Type
6	T	190	VAL
6	T	215	TRP
6	T	223	ARG
6	T	240	LYS
7	U	42	VAL
7	U	78	CYS
7	U	182	LYS
7	U	199	ILE
7	U	206	LEU
8	V	6	VAL
8	V	22	GLU
8	V	65	LEU
8	V	68	LEU
8	V	104[A]	ASP
8	V	104[B]	ASP
8	V	183	LEU
8	V	199	LEU
8	V	213	THR
9	W	35	THR
10	X	1	MET
10	X	62	LYS
10	X	88	LEU
10	X	95	ARG
11	Y	9	PHE
11	Y	13	VAL
11	Y	148	LEU
12	Z	72	LEU
12	Z	78	SER
12	Z	102	PHE
12	Z	172	MET
12	Z	174	LEU
12	Z	200	LYS
12	Z	207	THR
12	Z	208	VAL
13	a	71	VAL
13	a	92	LEU
13	a	100	ARG
13	a	154	LEU
13	a	198	GLU
13	a	216	SER
14	b	30	ARG
14	b	36	THR

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Mol	Chain	Res	Type
14	b	85	LYS
14	b	93	GLU
14	b	197	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	GLN
1	A	108	GLN
1	A	206	ASN
2	B	40	ASN
3	C	175	ASN
4	D	227	HIS
5	E	65	HIS
6	F	143	ASN
8	H	116	HIS
8	H	153	ASN
9	I	161	HIS
10	J	101	ASN
10	J	132	HIS
12	L	157	ASN
13	M	162	GLN
14	N	194	GLN
1	O	118	GLN
1	O	206	ASN
2	P	40	ASN
2	P	146	GLN
3	Q	18	GLN
3	Q	175	ASN
4	R	186	HIS
4	R	227	HIS
5	S	86	ASN
6	T	68	ASN
6	T	143	ASN
8	V	116	HIS
9	W	172	ASN
10	X	24	ASN
10	X	174	ASN
11	Y	163	GLN
12	Z	79	ASN
12	Z	157	ASN
13	a	89	HIS

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Mol	Chain	Res	Type
13	a	162	GLN
14	b	194	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

12 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	6V1	G	161	7	12,15,16	1.36	3 (25%)	9,20,22	2.63	6 (66%)
10	6V1	J	91	10	12,15,16	2.32	4 (33%)	9,20,22	4.56	6 (66%)
3	YCM	C	63	3	7,9,10	1.07	1 (14%)	4,10,12	1.27	1 (25%)
5	6V1	E	148	5	12,15,16	2.05	3 (25%)	9,20,22	3.56	4 (44%)
7	6V1	G	47	7	12,15,16	2.01	3 (25%)	9,20,22	1.15	1 (11%)
10	6V1	X	91	10	12,15,16	1.78	3 (25%)	9,20,22	4.89	6 (66%)
7	YCM	U	137	7	7,9,10	1.08	0	4,10,12	2.20	2 (50%)
3	YCM	Q	63	3	7,9,10	1.49	1 (14%)	4,10,12	2.99	3 (75%)
7	6V1	U	161	7	12,15,16	1.78	3 (25%)	9,20,22	3.41	5 (55%)
5	6V1	S	148	5	12,15,16	1.93	4 (33%)	9,20,22	2.93	4 (44%)
7	YCM	G	137	7	7,9,10	1.92	3 (42%)	4,10,12	2.45	2 (50%)
7	6V1	U	47	7	12,15,16	2.18	4 (33%)	9,20,22	2.10	2 (22%)

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

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	J	91	6V1	C1-SG	-6.50	1.76	1.83
5	E	148	6V1	CB-SG	-5.33	1.76	1.82
7	U	47	6V1	CB-SG	-5.19	1.76	1.82
5	S	148	6V1	CB-SG	-4.49	1.77	1.82
10	X	91	6V1	C1-SG	-4.28	1.78	1.83
7	G	47	6V1	CB-SG	-4.24	1.77	1.82
7	U	161	6V1	CB-SG	-4.09	1.77	1.82
7	G	47	6V1	C2-N3	-3.64	1.33	1.38
7	G	47	6V1	C4-N3	-3.27	1.33	1.38
7	U	47	6V1	C1-SG	-3.24	1.79	1.83
3	Q	63	YCM	CD-SG	-3.18	1.73	1.81
7	G	137	YCM	CD-SG	3.14	1.89	1.81
7	G	137	YCM	CE-NZ2	3.03	1.42	1.32
5	S	148	6V1	C5-C4	3.01	1.55	1.50
5	S	148	6V1	C2-N3	-2.89	1.34	1.38
7	U	47	6V1	C2-N3	-2.87	1.34	1.38
7	U	161	6V1	C4-N3	-2.68	1.34	1.38
10	X	91	6V1	C4-N3	-2.64	1.34	1.38
5	E	148	6V1	C4-N3	-2.63	1.34	1.38
7	U	161	6V1	C1-SG	-2.60	1.80	1.83
7	G	161	6V1	C4-N3	-2.53	1.34	1.38
7	U	47	6V1	C4-N3	-2.46	1.34	1.38
10	X	91	6V1	O7-C2	2.43	1.26	1.22
5	S	148	6V1	C4-N3	-2.39	1.34	1.38
10	J	91	6V1	CB-SG	2.28	1.84	1.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	J	91	6V1	C4-N3	-2.27	1.35	1.38
3	C	63	YCM	CD-SG	-2.16	1.76	1.81
7	G	161	6V1	C1-SG	-2.08	1.80	1.83
7	G	137	YCM	CB-SG	-2.07	1.72	1.80
7	G	161	6V1	C2-N3	-2.07	1.35	1.38
5	E	148	6V1	C5-C4	2.06	1.53	1.50
10	J	91	6V1	C2-N3	2.02	1.41	1.38

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	X	91	6V1	O7-C2-N3	7.71	133.57	124.14
10	X	91	6V1	C5-C4-N3	7.59	112.60	108.13
10	J	91	6V1	O7-C2-N3	7.55	133.38	124.14
10	J	91	6V1	C5-C4-N3	7.18	112.36	108.13
5	E	148	6V1	C2-N3-C4	-7.03	108.86	113.04
10	X	91	6V1	C2-N3-C4	-6.32	109.29	113.04
7	U	161	6V1	C2-N3-C4	-6.13	109.40	113.04
5	S	148	6V1	C2-N3-C4	-6.05	109.45	113.04
10	X	91	6V1	C6-N3-C2	5.92	130.86	123.36
10	J	91	6V1	C6-N3-C2	5.78	130.69	123.36
7	U	161	6V1	C5-C4-N3	5.57	111.41	108.13
5	E	148	6V1	C5-C4-N3	5.33	111.27	108.13
10	J	91	6V1	C2-N3-C4	-5.16	109.98	113.04
5	E	148	6V1	C6-N3-C2	4.92	129.60	123.36
5	S	148	6V1	C5-C4-N3	4.92	111.03	108.13
7	U	47	6V1	C5-C4-N3	4.62	110.85	108.13
7	G	137	YCM	CE-CD-SG	4.07	125.57	113.59
7	G	161	6V1	O8-C4-N3	3.94	128.28	123.92
7	U	161	6V1	O8-C4-C5	-3.81	121.68	127.24
7	G	161	6V1	O8-C4-C5	-3.80	121.70	127.24
7	U	137	YCM	CE-CD-SG	3.58	124.13	113.59
3	Q	63	YCM	CA-CB-SG	-3.55	100.72	113.74
3	Q	63	YCM	CE-CD-SG	-3.51	103.25	113.59
7	U	161	6V1	C6-N3-C2	3.47	127.76	123.36
10	X	91	6V1	O8-C4-C5	-3.37	122.33	127.24
7	U	47	6V1	C2-N3-C4	-3.30	111.08	113.04
10	J	91	6V1	C6-N3-C4	-3.14	118.50	122.59
7	G	161	6V1	O7-C2-N3	3.09	127.92	124.14
3	Q	63	YCM	CB-SG-CD	3.07	133.01	104.44
7	G	161	6V1	C5-C4-N3	3.01	109.91	108.13
10	X	91	6V1	C6-N3-C4	-3.01	118.67	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	47	6V1	C2-N3-C4	-2.93	111.30	113.04
7	U	161	6V1	O8-C4-N3	2.69	126.90	123.92
5	S	148	6V1	C6-N3-C4	2.65	126.05	122.59
7	G	161	6V1	C2-N3-C4	-2.62	111.49	113.04
10	J	91	6V1	O8-C4-C5	-2.31	123.88	127.24
5	E	148	6V1	C3-C6-N3	2.23	118.94	111.65
3	C	63	YCM	CE-CD-SG	-2.20	107.13	113.59
7	G	161	6V1	C6-N3-C2	2.14	126.07	123.36
7	G	137	YCM	CA-CB-SG	-2.10	106.05	113.74
7	U	137	YCM	CA-CB-SG	-2.10	106.05	113.74
5	S	148	6V1	O7-C2-N3	-2.01	121.68	124.14

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	U	47	6V1	C1

All (22) torsion outliers are listed below:

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



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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
18	1PE	H	305	-	15,15,15	0.46	0	14,14,14	0.58	0
18	1PE	L	301	-	15,15,15	0.55	0	14,14,14	0.70	0
19	6V7	Y	306	11	27,31,31	1.04	1 (3%)	36,42,42	1.47	5 (13%)
19	6V7	N	307	14	27,31,31	0.92	1 (3%)	36,42,42	1.54	8 (22%)
18	1PE	N	304	-	15,15,15	0.53	0	14,14,14	0.39	0
18	1PE	U	302	-	15,15,15	0.57	0	14,14,14	0.85	0
18	1PE	N	303	-	15,15,15	0.50	0	14,14,14	0.74	0
19	6V7	b	304	14	27,31,31	0.89	1 (3%)	36,42,42	1.54	4 (11%)
18	1PE	W	303	-	15,15,15	0.56	0	14,14,14	0.40	0
18	1PE	I	303	-	15,15,15	0.54	0	14,14,14	1.11	2 (14%)
19	6V7	K	305	11	27,31,31	1.43	4 (14%)	36,42,42	1.85	10 (27%)
18	1PE	Y	305	-	15,15,15	0.52	0	14,14,14	0.53	0
18	1PE	L	302	-	15,15,15	0.51	0	14,14,14	0.41	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	1PE	H	305	-	-	9/13/13/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	1PE	L	301	-	-	6/13/13/13	-
19	6V7	Y	306	11	1/1/7/9	5/26/32/32	0/2/2/2
19	6V7	N	307	14	1/1/7/9	4/26/32/32	0/2/2/2
18	1PE	N	304	-	-	7/13/13/13	-
18	1PE	U	302	-	-	7/13/13/13	-
18	1PE	N	303	-	-	4/13/13/13	-
19	6V7	b	304	14	-	8/26/32/32	0/2/2/2
18	1PE	W	303	-	-	6/13/13/13	-
18	1PE	I	303	-	-	8/13/13/13	-
19	6V7	K	305	11	-	8/26/32/32	0/2/2/2
18	1PE	Y	305	-	-	6/13/13/13	-
18	1PE	L	302	-	-	8/13/13/13	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	K	305	6V7	C2-N3	4.26	1.40	1.34
19	Y	306	6V7	O12-C9	-3.41	1.33	1.43
19	K	305	6V7	C11-C9	-2.72	1.43	1.51
19	b	304	6V7	C10-C18	-2.16	1.47	1.52
19	N	307	6V7	C2-N3	-2.11	1.31	1.34
19	K	305	6V7	C5-C4	2.04	1.43	1.38
19	K	305	6V7	C24-C15	2.01	1.43	1.39

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	b	304	6V7	C11-C9-C10	5.38	123.15	112.29
19	K	305	6V7	C6-C1-C2	-4.59	113.08	118.63
19	b	304	6V7	C2-C7-N9	4.20	123.00	115.20
19	K	305	6V7	C21-C22-C8	3.95	120.36	115.39
19	N	307	6V7	C2-C7-N9	3.92	122.48	115.20
19	N	307	6V7	O12-C9-C10	3.83	116.81	109.13
19	Y	306	6V7	C21-C22-C8	3.73	120.08	115.39
19	Y	306	6V7	O12-C9-C11	-3.65	98.94	109.74
19	K	305	6V7	O12-C9-C11	-3.47	99.45	109.74
19	K	305	6V7	C1-C2-N3	3.35	126.85	122.92
19	K	305	6V7	C7-C2-N3	-3.23	112.30	117.42
19	Y	306	6V7	C11-C9-C10	2.80	117.95	112.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	I	303	1PE	C25-OH5-C14	2.76	125.24	113.29
19	K	305	6V7	C6-C5-C4	2.72	122.60	118.90
19	K	305	6V7	C5-C4-N3	-2.66	118.53	121.97
19	K	305	6V7	O12-C9-C10	2.52	114.18	109.13
19	Y	306	6V7	C12-C8-C22	2.48	120.22	111.11
19	N	307	6V7	C9-C10-N9	-2.45	105.44	111.72
19	b	304	6V7	O8-C7-C2	-2.40	115.85	121.08
19	K	305	6V7	C2-C7-N9	2.40	119.65	115.20
18	I	303	1PE	OH5-C25-C15	2.33	120.89	110.39
19	b	304	6V7	C9-C10-C18	2.23	116.20	111.28
19	Y	306	6V7	C2-C7-N9	2.22	119.33	115.20
19	N	307	6V7	C11-C9-C10	2.18	116.68	112.29
19	N	307	6V7	C1-C2-C7	2.16	123.09	119.57
19	N	307	6V7	C20-C24-C15	-2.13	117.88	120.56
19	N	307	6V7	C7-C2-N3	-2.11	114.08	117.42
19	N	307	6V7	C4-N3-C2	2.08	121.66	118.11
19	K	305	6V7	C12-C8-C22	2.03	118.58	111.11

All (2) chirality outliers are listed below:

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

All (86) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	K	305	6V7	C21-C22-C8-C12
19	K	305	6V7	C18-C10-C9-O12
19	Y	306	6V7	C21-C22-C8-C12
19	b	304	6V7	C18-C10-C9-C11
19	b	304	6V7	C18-C10-C9-O12
19	b	304	6V7	N9-C10-C9-C11
19	b	304	6V7	N9-C10-C9-O12
19	N	307	6V7	N3-C2-C7-O8
19	b	304	6V7	N3-C2-C7-O8
19	N	307	6V7	C1-C2-C7-O8
19	b	304	6V7	C1-C2-C7-O8
19	K	305	6V7	N3-C2-C7-N9
19	N	307	6V7	N3-C2-C7-N9
19	Y	306	6V7	N3-C2-C7-N9
19	b	304	6V7	N3-C2-C7-N9

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Mol	Chain	Res	Type	Atoms
19	K	305	6V7	C1-C2-C7-N9
19	N	307	6V7	C1-C2-C7-N9
19	b	304	6V7	C1-C2-C7-N9
19	K	305	6V7	N3-C2-C7-O8
19	Y	306	6V7	N3-C2-C7-O8
19	K	305	6V7	C1-C2-C7-O8
19	Y	306	6V7	C1-C2-C7-O8
19	Y	306	6V7	C1-C2-C7-N9
18	I	303	1PE	C15-C25-OH5-C14
18	L	301	1PE	C16-C26-OH6-C15
18	U	302	1PE	C24-C14-OH5-C25
18	Y	305	1PE	OH6-C15-C25-OH5
18	L	302	1PE	OH4-C13-C23-OH3
18	N	304	1PE	OH4-C13-C23-OH3
18	U	302	1PE	OH4-C13-C23-OH3
18	H	305	1PE	OH4-C13-C23-OH3
18	N	304	1PE	OH5-C14-C24-OH4
18	L	302	1PE	OH5-C14-C24-OH4
18	W	303	1PE	OH6-C15-C25-OH5
18	N	303	1PE	OH2-C12-C22-OH3
18	I	303	1PE	OH2-C12-C22-OH3
18	N	303	1PE	OH4-C13-C23-OH3
18	U	302	1PE	OH6-C15-C25-OH5
18	N	304	1PE	OH7-C16-C26-OH6
18	H	305	1PE	C24-C14-OH5-C25
19	K	305	6V7	N9-C10-C9-O12
18	Y	305	1PE	C16-C26-OH6-C15
18	H	305	1PE	OH5-C14-C24-OH4
18	L	302	1PE	OH6-C15-C25-OH5
18	L	302	1PE	OH7-C16-C26-OH6
18	L	302	1PE	OH2-C12-C22-OH3
18	N	303	1PE	OH7-C16-C26-OH6
18	H	305	1PE	OH7-C16-C26-OH6
18	U	302	1PE	OH7-C16-C26-OH6
18	I	303	1PE	OH6-C15-C25-OH5
18	N	304	1PE	OH2-C12-C22-OH3
18	W	303	1PE	OH7-C16-C26-OH6
18	U	302	1PE	C25-C15-OH6-C26
18	H	305	1PE	OH2-C12-C22-OH3
18	L	301	1PE	C25-C15-OH6-C26
18	L	301	1PE	C13-C23-OH3-C22
18	L	301	1PE	C24-C14-OH5-C25

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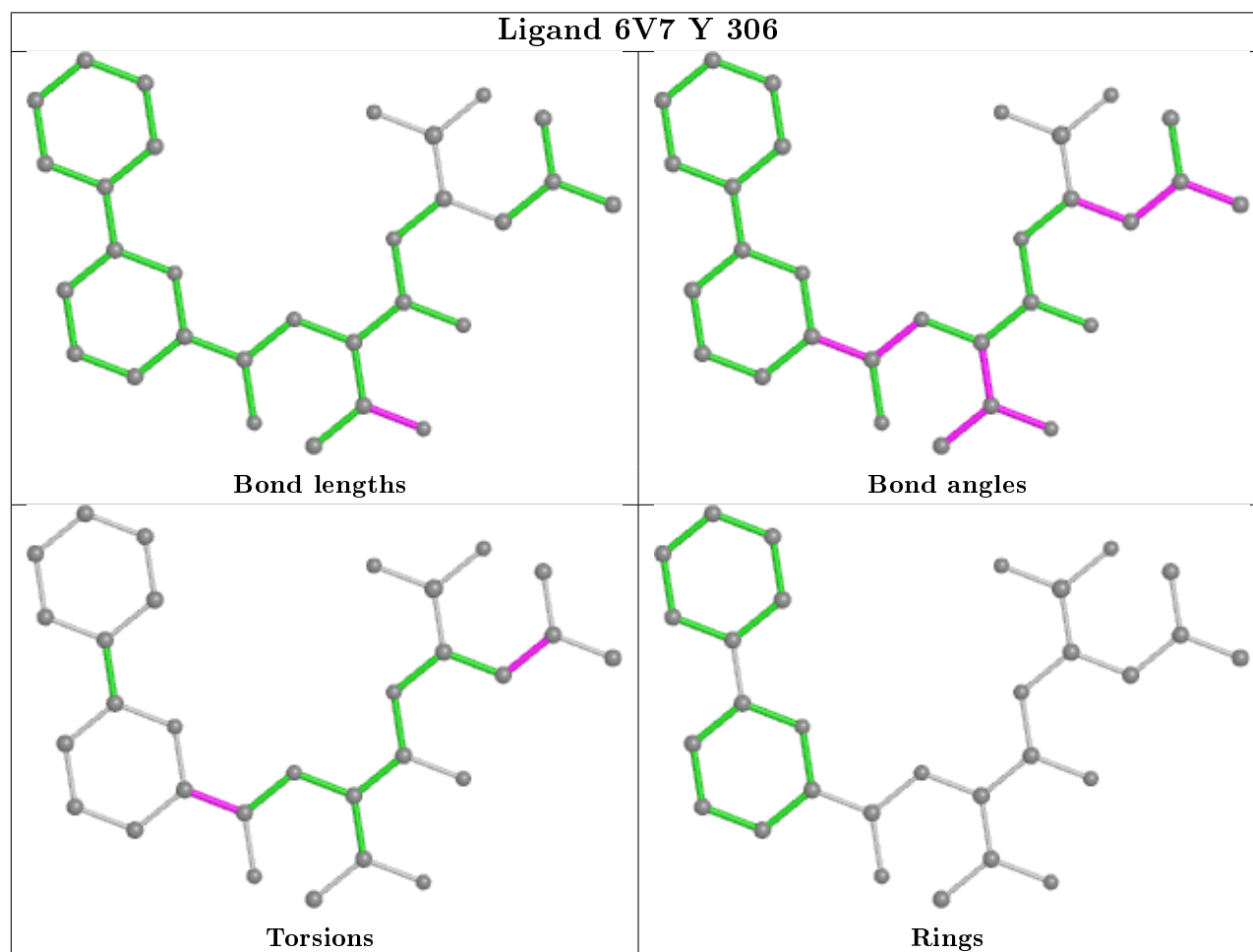
Mol	Chain	Res	Type	Atoms
18	L	302	1PE	C14-C24-OH4-C13
18	N	304	1PE	C25-C15-OH6-C26
18	I	303	1PE	C25-C15-OH6-C26
18	I	303	1PE	C24-C14-OH5-C25
18	H	305	1PE	C23-C13-OH4-C24
18	Y	305	1PE	C12-C22-OH3-C23
18	H	305	1PE	C15-C25-OH5-C14
18	H	305	1PE	C16-C26-OH6-C15
18	W	303	1PE	C24-C14-OH5-C25
18	I	303	1PE	C14-C24-OH4-C13
18	L	301	1PE	C23-C13-OH4-C24
18	W	303	1PE	C12-C22-OH3-C23
18	W	303	1PE	C23-C13-OH4-C24
18	L	302	1PE	C23-C13-OH4-C24
18	N	304	1PE	C23-C13-OH4-C24
18	H	305	1PE	OH6-C15-C25-OH5
18	N	304	1PE	C14-C24-OH4-C13
18	I	303	1PE	C13-C23-OH3-C22
19	K	305	6V7	C18-C10-C9-C11
18	Y	305	1PE	OH4-C13-C23-OH3
18	I	303	1PE	OH5-C14-C24-OH4
18	N	303	1PE	C12-C22-OH3-C23
18	L	302	1PE	C15-C25-OH5-C14
18	Y	305	1PE	C15-C25-OH5-C14
18	L	301	1PE	OH2-C12-C22-OH3
18	U	302	1PE	OH5-C14-C24-OH4
18	W	303	1PE	OH2-C12-C22-OH3
18	U	302	1PE	C14-C24-OH4-C13
18	Y	305	1PE	OH7-C16-C26-OH6

There are no ring outliers.

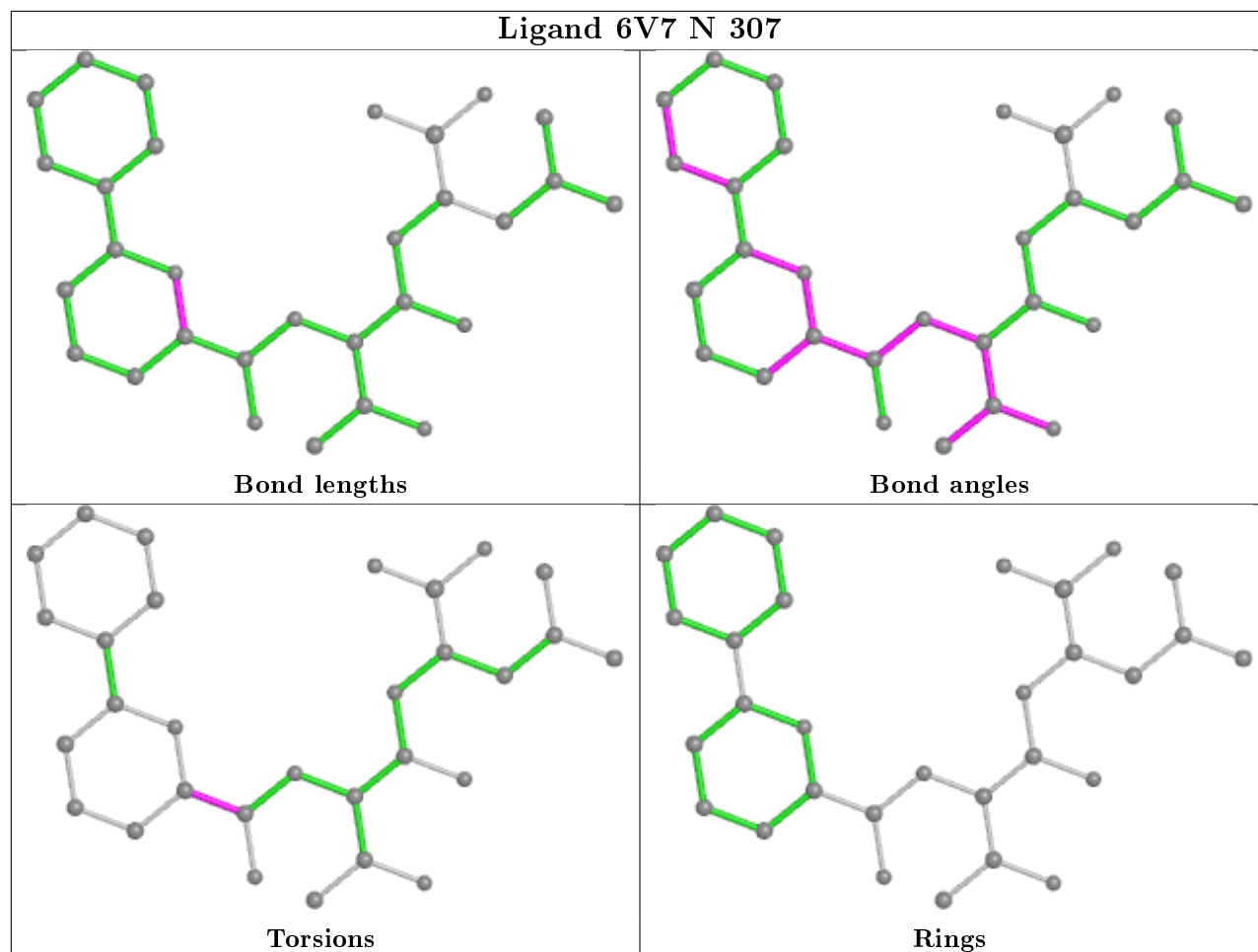
No monomer is involved in short contacts.

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.

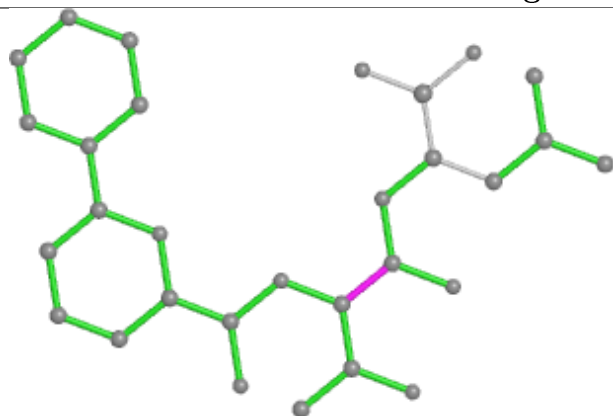
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



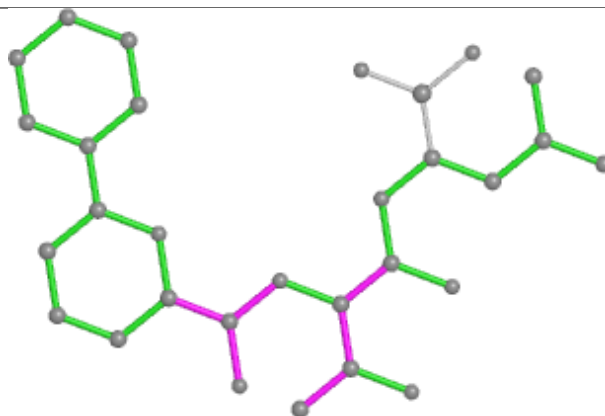
## Ligand 6V7 N 307



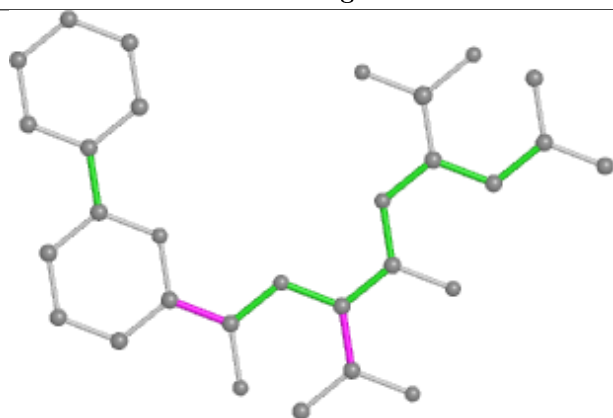
## Ligand 6V7 b 304



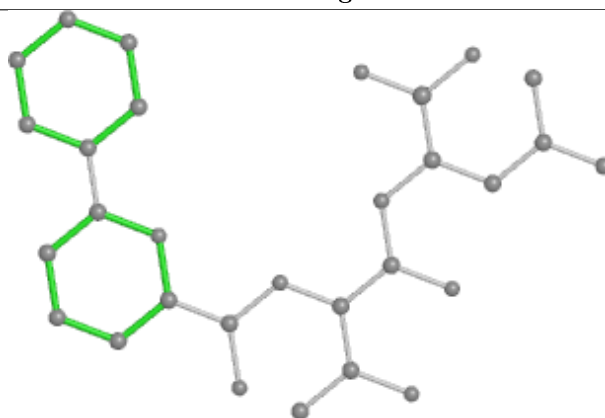
Bond lengths



Bond angles

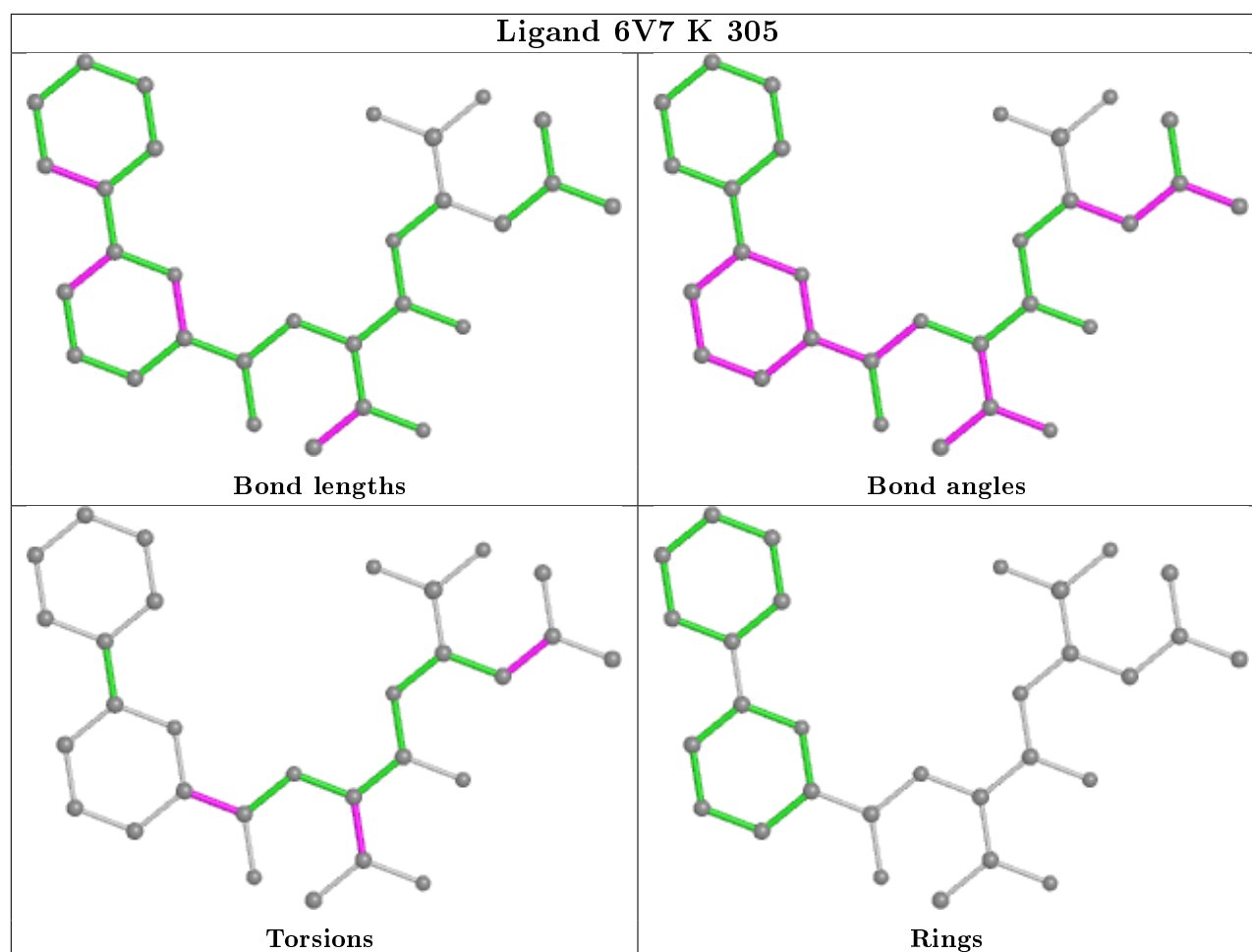


Torsions



Rings





## 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%)	0.13	7 (3%) 50 49	27, 46, 86, 102	0
1	O	230/234 (98%)	0.81	40 (17%) 1 1	40, 68, 117, 148	0
2	B	248/261 (95%)	0.49	18 (7%) 15 14	32, 53, 98, 144	0
2	P	248/261 (95%)	1.02	50 (20%) 1 0	40, 64, 127, 174	0
3	C	236/248 (95%)	0.78	30 (12%) 3 3	36, 65, 112, 146	0
3	Q	238/248 (95%)	1.10	51 (21%) 0 0	33, 66, 138, 175	0
4	D	233/241 (96%)	0.38	20 (8%) 10 9	37, 62, 95, 139	0
4	R	233/241 (96%)	0.17	10 (4%) 35 34	30, 44, 75, 106	0
5	E	233/263 (88%)	0.27	14 (6%) 21 20	25, 41, 92, 116	0
5	S	237/263 (90%)	0.24	12 (5%) 28 27	32, 48, 86, 118	0
6	F	239/255 (93%)	-0.07	2 (0%) 86 85	22, 34, 59, 77	0
6	T	240/255 (94%)	0.47	24 (10%) 7 6	34, 57, 97, 137	0
7	G	241/246 (97%)	0.17	6 (2%) 57 56	23, 39, 73, 110	0
7	U	235/246 (95%)	0.85	39 (16%) 1 1	44, 67, 107, 136	0
8	H	220/234 (94%)	-0.01	7 (3%) 47 46	23, 35, 77, 133	0
8	V	220/234 (94%)	0.31	7 (3%) 47 46	34, 50, 91, 130	0
9	I	204/205 (99%)	0.11	2 (0%) 82 81	26, 36, 62, 81	0
9	W	204/205 (99%)	0.28	2 (0%) 82 81	34, 51, 80, 92	0
10	J	195/201 (97%)	0.05	4 (2%) 63 62	28, 43, 61, 84	0
10	X	195/201 (97%)	0.06	1 (0%) 91 90	32, 44, 60, 84	0
11	K	200/204 (98%)	0.26	4 (2%) 65 63	33, 47, 76, 97	0
11	Y	201/204 (98%)	0.13	3 (1%) 73 72	25, 35, 60, 81	0
12	L	213/213 (100%)	0.03	0 100 100	29, 49, 75, 95	0
12	Z	213/213 (100%)	0.12	6 (2%) 53 51	22, 36, 63, 86	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	M	216/219 (98%)	0.19	5 (2%) 60 59	23, 37, 65, 98	0
13	a	216/219 (98%)	0.07	3 (1%) 75 74	24, 38, 60, 86	0
14	N	202/205 (98%)	-0.07	0 100 100	22, 32, 55, 81	0
14	b	203/205 (99%)	0.27	6 (2%) 50 49	29, 41, 69, 97	0
All	All	6223/6458 (96%)	0.32	373 (5%) 21 20	22, 47, 93, 175	0

All (373) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	232	ILE	14.7
2	P	204	SER	13.4
2	P	203	VAL	10.8
4	D	241	ILE	10.8
3	Q	232	ILE	9.9
3	Q	234	LYS	8.2
3	Q	202	GLY	8.1
3	Q	229	VAL	7.8
3	Q	203	GLY	7.8
3	Q	238	GLU	7.6
7	G	187	PHE	7.5
3	C	232	ILE	7.4
2	B	203	VAL	6.8
8	H	204	CYS	6.7
2	P	247	ALA	6.5
7	U	206	LEU	6.2
3	C	229	VAL	6.2
3	Q	233	GLU	6.1
2	P	202	ASP	6.0
3	C	225	ILE	6.0
2	P	61	PHE	6.0
7	U	242	LEU	5.9
3	C	202	GLY	5.9
3	Q	236	LYS	5.9
8	V	203	ARG	5.8
2	B	61	PHE	5.8
7	U	208	ILE	5.8
2	P	233	VAL	5.7
6	T	208	ALA	5.7
3	Q	239	ASN	5.7
3	Q	201	SER	5.6
2	P	205	LYS	5.6

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Mol	Chain	Res	Type	RSRZ
11	K	41	TYR	5.6
1	O	192	LEU	5.5
7	U	199	ILE	5.5
3	Q	192	ILE	5.5
3	Q	230	ALA	5.5
3	C	49	SER	5.4
4	R	241	ILE	5.3
7	U	2	SER	5.3
2	B	248	GLU	5.3
2	P	234	GLU	5.3
3	C	201	SER	5.3
3	C	234	LYS	5.3
1	O	181	LEU	5.2
4	R	128	ALA	5.2
3	C	203	GLY	5.2
1	O	229	LEU	5.1
3	C	236	LYS	5.0
5	E	54	SER	5.0
4	D	237	VAL	5.0
1	O	201	GLN	5.0
7	U	243	ALA	5.0
4	D	240	ASP	4.9
13	a	216	SER	4.9
3	Q	223	GLU	4.9
1	O	177	TYR	4.9
11	Y	41	TYR	4.9
3	Q	48	LYS	4.9
3	Q	240	GLU	4.9
2	B	247	ALA	4.8
12	Z	161	VAL	4.8
7	G	189	TRP	4.8
2	P	206	LEU	4.8
1	A	232	ILE	4.7
5	E	237	GLU	4.7
3	C	48	LYS	4.7
1	A	230	ALA	4.7
10	J	1[A]	MET	4.6
4	R	130	PRO	4.6
8	H	203	ARG	4.6
2	B	202	ASP	4.4
2	P	52	ILE	4.4
4	D	239	LYS	4.4

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Mol	Chain	Res	Type	RSRZ
3	C	200	GLN	4.3
2	B	237	ILE	4.3
3	Q	186	LEU	4.3
7	U	240	VAL	4.3
8	V	199	LEU	4.2
3	Q	237	GLU	4.2
7	U	207	SER	4.2
7	U	204	THR	4.2
7	U	178	PHE	4.2
3	C	230	ALA	4.1
9	W	116	PHE	4.1
2	B	205	LYS	4.1
3	Q	225	ILE	4.1
3	Q	138	PHE	4.1
8	V	204	CYS	4.0
2	P	230	GLN	4.0
11	K	146	TYR	4.0
2	B	204	SER	4.0
7	U	3	ARG	4.0
1	O	199	GLU	4.0
1	O	225	VAL	3.9
2	P	220	ASN	3.9
1	O	186	ALA	3.9
3	Q	179	GLU	3.9
1	O	200	GLY	3.9
1	O	194	LEU	3.8
7	U	235	ILE	3.8
12	Z	164	VAL	3.8
3	Q	181	ILE	3.8
1	O	187	ILE	3.8
7	U	198	ALA	3.8
6	T	206	ASP	3.8
3	C	138	PHE	3.8
2	P	246	LYS	3.8
3	Q	180	ALA	3.7
3	C	233	GLU	3.7
5	E	56	LEU	3.7
7	G	188	ASP	3.7
2	P	248	GLU	3.7
3	C	228	TYR	3.7
6	T	209	PHE	3.7
1	A	231	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
3	C	237	GLU	3.6
2	P	237	ILE	3.6
4	D	230	THR	3.6
2	P	243	GLU	3.6
6	T	243	LEU	3.6
1	O	172	PHE	3.6
9	W	113	PRO	3.6
12	Z	165	PRO	3.6
1	O	191	ILE	3.6
7	U	205	VAL	3.6
1	O	198	PHE	3.6
1	O	223	THR	3.6
1	O	184	GLU	3.6
2	P	244	GLU	3.6
11	Y	201	SER	3.6
5	E	235	GLY	3.6
3	Q	228	TYR	3.5
3	Q	226	GLU	3.5
2	P	249	ARG	3.5
5	S	2	PHE	3.5
7	U	177	SER	3.5
7	U	58	ASP	3.5
1	O	176	ARG	3.5
5	E	53	GLN	3.5
3	Q	219	ILE	3.4
3	C	238	GLU	3.4
5	S	3	ARG	3.4
6	T	207	LYS	3.4
2	P	51	ASN	3.4
2	P	241	GLU	3.4
3	Q	213	ARG	3.4
2	B	245	ALA	3.4
4	D	238	ILE	3.4
2	P	200	THR	3.3
3	Q	190	LEU	3.3
2	P	201	MET	3.3
8	H	201	ARG	3.3
7	U	183	VAL	3.3
1	O	228	TYR	3.3
4	R	127	ASP	3.3
2	P	177	GLN	3.3
14	b	204	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
6	T	205	LYS	3.2
9	I	116	PHE	3.2
12	Z	163	HIS	3.2
4	D	131	GLY	3.2
4	D	232	GLU	3.2
5	E	52	ALA	3.2
5	S	174	ARG	3.2
1	O	157	TRP	3.2
13	M	215	ILE	3.2
8	H	202	TYR	3.1
6	T	204	VAL	3.1
4	D	234	LEU	3.1
2	P	58	GLU	3.1
3	Q	199	VAL	3.1
2	P	197	LEU	3.1
6	T	54	LEU	3.1
6	T	203	GLU	3.1
5	E	58	ALA	3.1
7	G	3	ARG	3.1
2	P	235	GLN	3.1
2	P	190	LEU	3.0
5	S	56	LEU	3.0
2	B	241	GLU	3.0
8	H	200	GLY	3.0
7	U	200	THR	3.0
4	R	131	GLY	3.0
1	O	182	GLU	3.0
7	U	223	GLU	3.0
3	Q	37	GLY	3.0
1	O	40	ALA	3.0
3	C	195	LEU	3.0
14	b	27	ILE	3.0
5	S	57	ALA	3.0
7	U	212	PRO	3.0
5	E	232	PHE	2.9
2	P	238	LYS	2.9
4	D	188	SER	2.9
5	E	182	CYS	2.9
7	U	239	LEU	2.9
2	P	194	ILE	2.9
3	Q	205	ASN	2.9
4	D	212	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
4	D	236	GLU	2.9
3	Q	204	LYS	2.9
5	E	201	ALA	2.9
3	Q	39	ASP	2.9
7	U	179	LEU	2.8
10	X	95	ARG	2.8
3	C	226	GLU	2.8
13	M	216	SER	2.8
1	O	227	ASP	2.8
3	Q	183	THR	2.8
6	T	240	LYS	2.8
7	U	196	GLU	2.8
3	Q	200	GLN	2.8
1	A	229	LEU	2.8
5	S	239	ARG	2.8
3	Q	191	VAL	2.8
4	D	130	PRO	2.8
1	O	211	ILE	2.8
3	Q	206	ILE	2.8
2	B	246	LYS	2.7
3	C	204	LYS	2.7
4	D	127	ASP	2.7
1	O	226	LYS	2.7
5	S	18[A]	ARG	2.7
3	C	220	LEU	2.7
5	S	236	LEU	2.7
1	A	201	GLN	2.7
8	H	220	GLU	2.7
6	T	5	THR	2.7
3	Q	171	PHE	2.7
3	Q	210	VAL	2.7
2	P	30	HIS	2.7
6	T	197	ILE	2.7
1	O	59	ARG	2.7
6	T	180	GLN	2.7
2	B	206	LEU	2.7
3	Q	178	ASP	2.6
1	O	3	ARG	2.6
1	O	41	ASN	2.6
2	P	55	LEU	2.6
8	V	132	LEU	2.6
6	T	239	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
11	Y	202	GLY	2.6
7	U	211	LYS	2.6
5	E	60	GLN	2.6
2	B	242	GLU	2.6
8	V	197	THR	2.6
3	C	235	GLU	2.6
1	O	171	THR	2.5
3	Q	177	THR	2.5
4	D	195	ILE	2.5
4	R	238	ILE	2.5
6	T	241	GLU	2.5
7	U	202	LEU	2.5
2	P	198	ASN	2.5
5	S	4	ASN	2.5
1	O	138	TRP	2.5
7	U	194	THR	2.5
4	D	183	GLU	2.5
2	P	178	ASP	2.5
2	P	179	TYR	2.5
5	E	218	ASP	2.5
7	U	7	ALA	2.5
2	P	219	GLU	2.5
4	R	186	HIS	2.5
13	M	33	LEU	2.5
3	C	227	LYS	2.5
7	G	57	PRO	2.5
3	Q	42	VAL	2.5
10	J	26	VAL	2.5
6	F	180	GLN	2.5
5	S	204	ASP	2.5
3	C	208	LEU	2.5
4	D	235	GLU	2.5
2	B	249	ARG	2.5
3	C	222	PRO	2.4
2	P	180	LYS	2.4
2	P	240	HIS	2.4
14	b	200	VAL	2.4
1	O	178	ASN	2.4
3	Q	175	ASN	2.4
7	U	173	THR	2.4
10	J	95	ARG	2.4
3	Q	185	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
2	P	217	THR	2.4
3	Q	235	GLU	2.4
3	Q	140	GLY	2.4
2	P	175	LEU	2.4
7	U	245	ARG	2.4
7	U	210	PHE	2.4
2	P	187	LYS	2.4
2	B	208	ALA	2.4
7	G	209	ASP	2.4
6	T	238	TYR	2.4
6	T	181	MET	2.4
7	U	213	SER	2.3
1	O	202	MET	2.3
12	Z	160	ASN	2.3
2	P	199	LYS	2.3
2	P	29	GLY	2.3
4	D	128	ALA	2.3
5	S	235	GLY	2.3
2	P	192	LEU	2.3
6	T	237	LYS	2.3
7	U	56	VAL	2.3
1	O	54	ILE	2.3
7	U	186	LYS	2.3
7	U	195	VAL	2.3
9	I	179	VAL	2.3
6	T	176	ILE	2.3
7	U	57	PRO	2.3
3	Q	220	LEU	2.3
8	V	202	TYR	2.3
3	C	231	GLU	2.3
2	P	245	ALA	2.3
6	T	231	ILE	2.3
4	R	58	LEU	2.3
4	D	224	GLN	2.2
3	C	196	LEU	2.2
3	Q	197	GLU	2.2
1	O	168	ASN	2.2
13	M	181	ALA	2.2
7	U	209	ASP	2.2
11	K	150	VAL	2.2
2	B	243	GLU	2.2
2	P	183	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
4	D	223	GLY	2.2
11	K	90	GLN	2.2
13	a	176	LEU	2.2
1	A	3	ARG	2.2
3	Q	184	ASP	2.2
1	O	50	LYS	2.2
1	O	175	LYS	2.2
2	P	157	GLY	2.2
3	Q	47	LYS	2.2
1	O	188	HIS	2.2
2	P	172	VAL	2.2
2	P	56	LEU	2.2
14	b	104	TRP	2.2
14	b	151	GLU	2.2
3	C	171	PHE	2.2
6	T	53	VAL	2.2
1	O	183	LEU	2.1
12	Z	1	ARG	2.1
5	E	59	HIS	2.1
6	T	233	GLU	2.1
2	P	236	LEU	2.1
1	O	230	ALA	2.1
3	Q	224	GLU	2.1
14	b	28	ALA	2.1
2	B	220	ASN	2.1
2	B	244	GLU	2.1
5	S	238	GLU	2.1
6	T	142	VAL	2.1
5	E	233	LEU	2.1
6	F	243	LEU	2.1
7	U	230	LEU	2.1
1	A	228	TYR	2.0
4	R	240	ASP	2.0
10	J	67	TYR	2.0
13	a	194	GLU	2.0
1	O	167	VAL	2.0
3	C	50	VAL	2.0
8	V	186	LEU	2.0
6	T	230	ASP	2.0
3	C	183	THR	2.0
7	U	221	THR	2.0
8	H	181	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
2	P	53	HIS	2.0
4	R	237	VAL	2.0
7	U	222	VAL	2.0
13	M	143	ALA	2.0
3	Q	49	SER	2.0

## 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	0.85	0.33	81,117,124,127	0
3	YCM	Q	63	10/11	0.91	0.15	53,58,69,69	0
7	YCM	G	137	10/11	0.91	0.15	27,36,52,53	0
7	YCM	U	137	10/11	0.91	0.14	54,64,77,80	0
5	6V1	S	148	15/16	0.92	0.16	38,70,77,78	0
3	YCM	C	63	10/11	0.92	0.11	58,62,76,78	0
10	6V1	X	91	15/16	0.92	0.20	34,57,64,68	0
5	6V1	E	148	15/16	0.94	0.14	31,59,70,71	0
7	6V1	G	47	15/16	0.94	0.15	39,60,67,69	0
10	6V1	J	91	15/16	0.94	0.18	32,51,60,60	0
7	6V1	G	161	15/16	0.94	0.15	32,53,59,62	0
7	6V1	U	161	15/16	0.95	0.10	58,74,81,82	0

## 6.3 Carbohydrates [i](#)

There are no monosaccharides 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
17	MG	V	301	1/1	0.58	0.22	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
18	1PE	L	301	16/16	0.77	0.19	60,77,83,91	0
18	1PE	L	302	16/16	0.80	0.35	75,84,119,120	0
18	1PE	W	303	16/16	0.80	0.19	65,69,85,87	0
18	1PE	N	304	16/16	0.82	0.30	72,74,112,114	0
15	CL	O	303	1/1	0.82	0.10	99,99,99,99	0
18	1PE	Y	305	16/16	0.82	0.16	59,75,81,84	0
18	1PE	H	305	16/16	0.84	0.26	60,83,112,113	0
15	CL	D	301	1/1	0.85	0.14	81,81,81,81	0
15	CL	Q	302	1/1	0.87	0.14	72,72,72,72	0
15	CL	O	304	1/1	0.87	0.12	77,77,77,77	0
18	1PE	I	303	16/16	0.89	0.16	60,62,82,83	0
15	CL	a	302	1/1	0.89	0.17	69,69,69,69	0
18	1PE	U	302	16/16	0.90	0.14	50,57,92,92	0
15	CL	D	302	1/1	0.90	0.12	72,72,72,72	0
15	CL	C	301	1/1	0.91	0.12	76,76,76,76	0
15	CL	K	304	1/1	0.91	0.20	80,80,80,80	0
15	CL	Y	304	1/1	0.91	0.21	75,75,75,75	0
15	CL	V	302	1/1	0.91	0.11	68,68,68,68	0
15	CL	V	303	1/1	0.91	0.10	62,62,62,62	0
15	CL	A	304	1/1	0.92	0.10	63,63,63,63	0
18	1PE	N	303	16/16	0.92	0.12	39,48,65,68	0
15	CL	B	302	1/1	0.92	0.10	64,64,64,64	0
15	CL	K	303	1/1	0.92	0.12	74,74,74,74	0
15	CL	M	303	1/1	0.92	0.11	65,65,65,65	0
15	CL	R	301	1/1	0.92	0.14	67,67,67,67	0
15	CL	K	302	1/1	0.93	0.15	84,84,84,84	0
15	CL	a	304	1/1	0.93	0.14	67,67,67,67	0
15	CL	a	303	1/1	0.94	0.12	46,46,46,46	0
19	6V7	K	305	30/30	0.94	0.11	34,37,46,49	0
15	CL	A	302	1/1	0.94	0.16	72,72,72,72	0
17	MG	H	301	1/1	0.94	0.16	71,71,71,71	0
15	CL	I	302	1/1	0.94	0.08	51,51,51,51	0
15	CL	N	301	1/1	0.94	0.10	68,68,68,68	0
15	CL	M	301	1/1	0.94	0.18	62,62,62,62	0
15	CL	H	303	1/1	0.94	0.09	63,63,63,63	0
17	MG	K	301	1/1	0.94	0.10	37,37,37,37	0
15	CL	S	302	1/1	0.94	0.07	72,72,72,72	0
19	6V7	b	304	30/30	0.95	0.14	32,36,44,45	0
15	CL	O	301	1/1	0.95	0.11	61,61,61,61	0
15	CL	S	303	1/1	0.95	0.10	59,59,59,59	0
15	CL	a	301	1/1	0.95	0.12	74,74,74,74	0
15	CL	E	302	1/1	0.95	0.17	62,62,62,62	0

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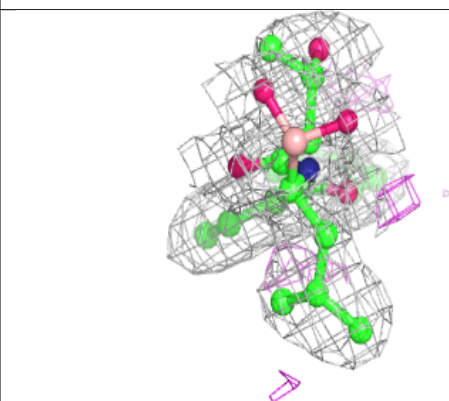
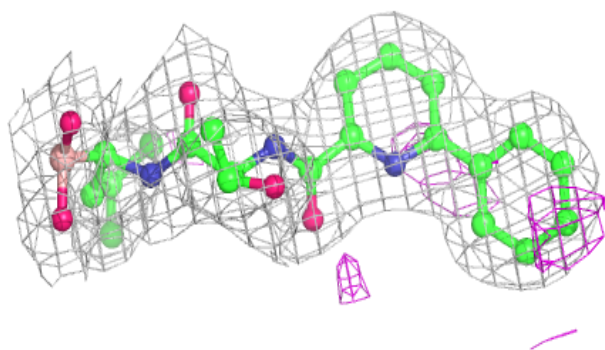
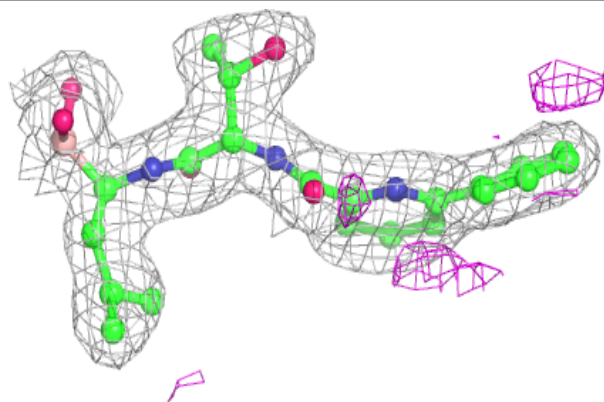
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
15	CL	S	301	1/1	0.95	0.14	81,81,81,81	0
17	MG	J	301	1/1	0.95	0.04	59,59,59,59	0
15	CL	R	302	1/1	0.95	0.11	61,61,61,61	0
15	CL	C	302	1/1	0.95	0.13	76,76,76,76	0
15	CL	E	303	1/1	0.96	0.13	74,74,74,74	0
15	CL	Y	302	1/1	0.96	0.18	68,68,68,68	0
15	CL	b	301	1/1	0.96	0.11	69,69,69,69	0
16	K	b	303	1/1	0.96	0.10	48,48,48,48	0
15	CL	O	302	1/1	0.96	0.09	72,72,72,72	0
15	CL	A	303	1/1	0.96	0.10	57,57,57,57	0
16	K	L	303	1/1	0.96	0.06	53,53,53,53	0
16	K	b	302	1/1	0.96	0.09	43,43,43,43	0
17	MG	H	302	1/1	0.96	0.08	32,32,32,32	0
16	K	U	303	1/1	0.96	0.08	46,46,46,46	0
15	CL	Y	303	1/1	0.96	0.08	68,68,68,68	0
15	CL	P	301	1/1	0.96	0.14	56,56,56,56	0
17	MG	I	301	1/1	0.96	0.11	33,33,33,33	0
19	6V7	Y	306	30/30	0.96	0.12	24,28,34,37	0
15	CL	G	301	1/1	0.96	0.13	53,53,53,53	0
15	CL	E	301	1/1	0.96	0.12	68,68,68,68	0
15	CL	M	302	1/1	0.97	0.10	42,42,42,42	0
15	CL	G	302	1/1	0.97	0.07	68,68,68,68	0
19	6V7	N	307	30/30	0.97	0.11	25,26,37,38	0
15	CL	H	304	1/1	0.97	0.07	50,50,50,50	0
17	MG	W	301	1/1	0.97	0.08	37,37,37,37	0
17	MG	I	304	1/1	0.97	0.12	29,29,29,29	0
16	K	N	305	1/1	0.97	0.10	41,41,41,41	0
15	CL	B	301	1/1	0.97	0.11	44,44,44,44	0
17	MG	L	304	1/1	0.97	0.05	39,39,39,39	0
16	K	Z	301	1/1	0.97	0.10	41,41,41,41	0
15	CL	U	301	1/1	0.97	0.15	67,67,67,67	0
15	CL	Q	301	1/1	0.97	0.14	84,84,84,84	0
15	CL	Y	301	1/1	0.97	0.14	69,69,69,69	0
15	CL	A	301	1/1	0.98	0.11	55,55,55,55	0
17	MG	X	301	1/1	0.98	0.08	58,58,58,58	0
15	CL	W	302	1/1	0.98	0.06	61,61,61,61	0
16	K	G	303	1/1	0.98	0.06	36,36,36,36	0
15	CL	F	301	1/1	0.98	0.07	61,61,61,61	0
16	K	N	306	1/1	0.98	0.12	40,40,40,40	0
15	CL	N	302	1/1	0.99	0.08	59,59,59,59	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

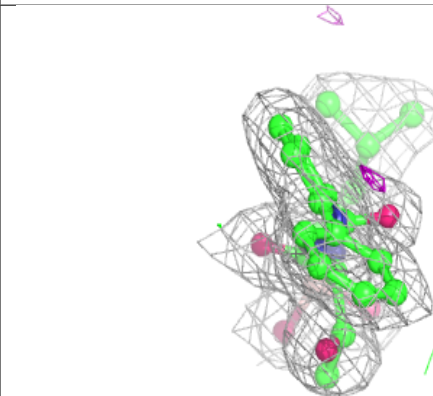
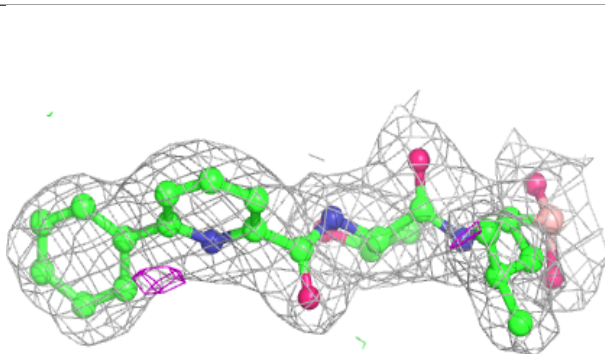
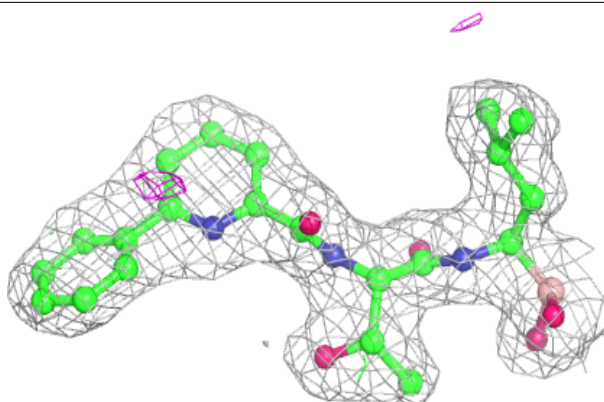
**Electron density around 6V7 K 305:**

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



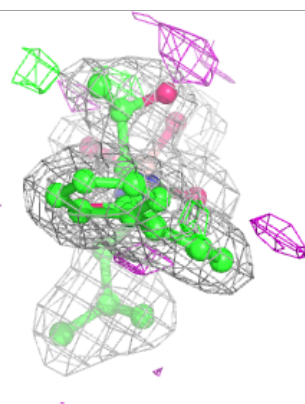
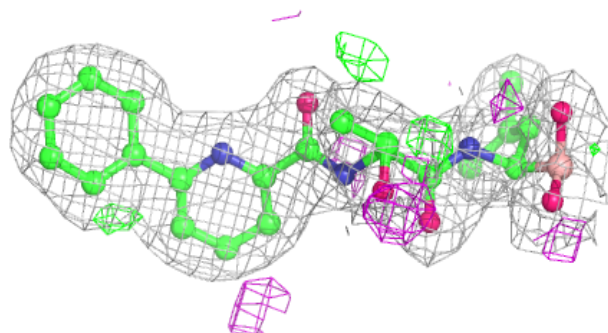
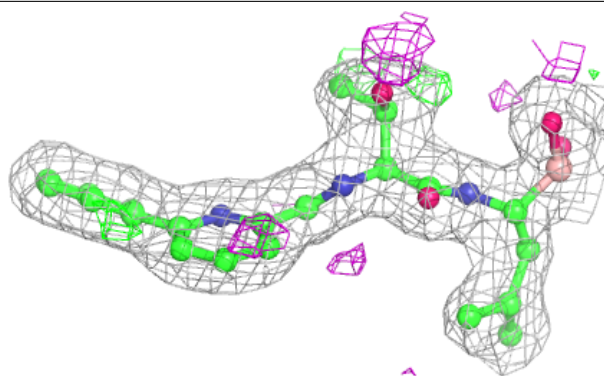
**Electron density around 6V7 b 304:**

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

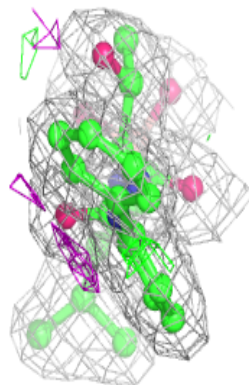
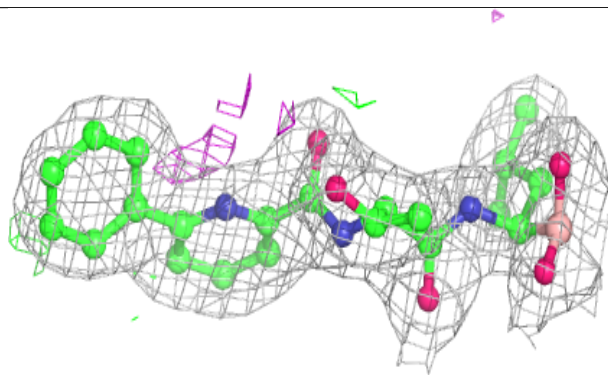
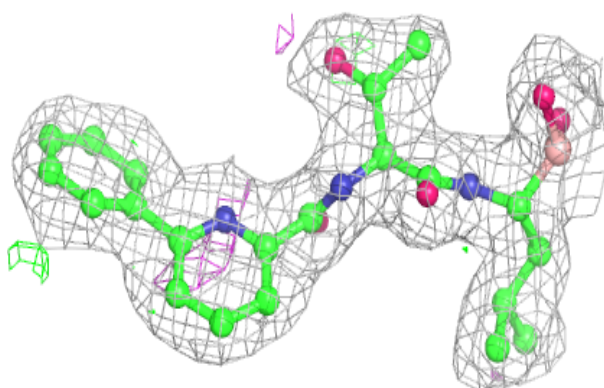


**Electron density around 6V7 Y 306:**

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

**Electron density around 6V7 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.