



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2023 – 02:43 AM EDT

PDB ID : 6XQ7  
Title : Receptor for Advanced Glycation End Products VC1 domain in complex with Fragment 5  
Authors : Salay, L.E.; Kozlyuk, N.; Gilston, B.A.; Gogliotti, R.D.; Christov, P.P.; Kim, K.; Ovee, M.; Waterson, A.G.; Chazin, W.J.  
Deposited on : 2020-07-09  
Resolution : 1.80 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.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35.1  
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) : 2.35.1

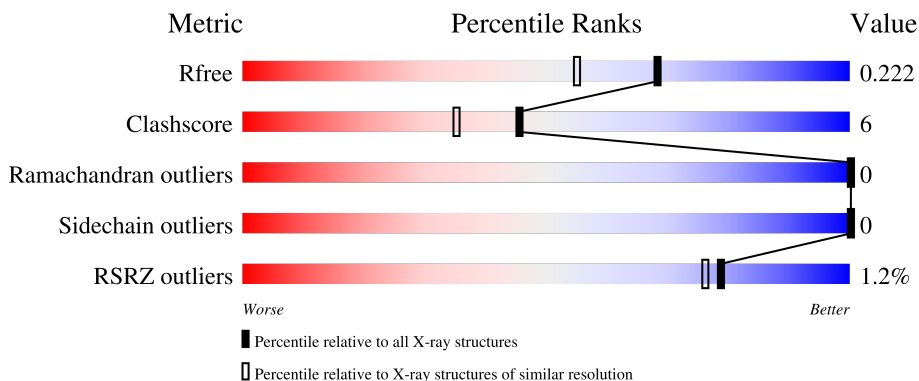
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	212	
1	B	212	

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
2	ACT	A	304	-	X	-	-
2	ACT	B	302	-	-	X	-
2	ACT	B	304	-	X	X	-
3	V6V	B	311	-	X	-	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 3458 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.

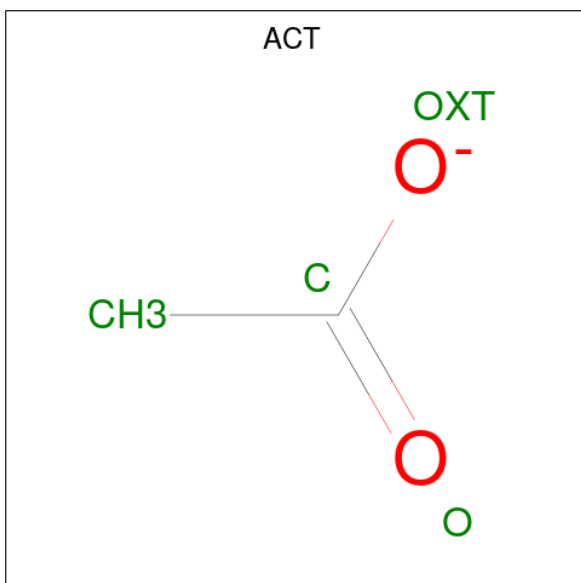
- Molecule 1 is a protein called Advanced glycosylation end product-specific receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	212	1557	987	273	291	6	0	6	0
1	B	212	1553	986	279	281	7	0	3	0

There are 6 discrepancies between the modelled and reference sequences:

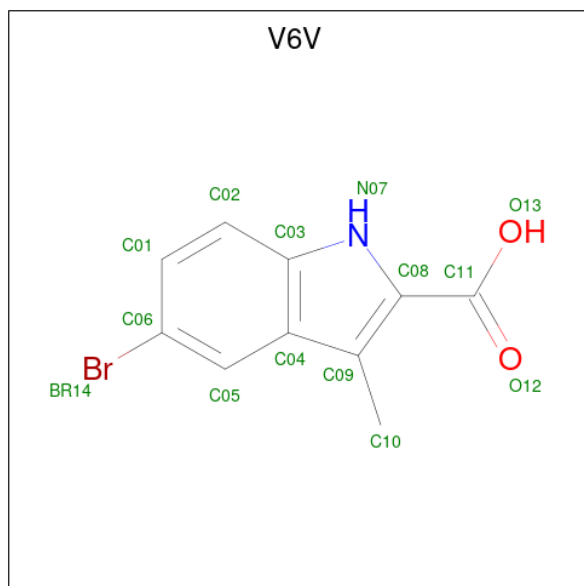
Chain	Residue	Modelled	Actual	Comment	Reference
A	20	GLY	-	expression tag	UNP Q15109
A	21	ALA	-	expression tag	UNP Q15109
A	22	MET	-	expression tag	UNP Q15109
B	20	GLY	-	expression tag	UNP Q15109
B	21	ALA	-	expression tag	UNP Q15109
B	22	MET	-	expression tag	UNP Q15109

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0

- Molecule 3 is 5-bromo-3-methyl-1H-indole-2-carboxylic acid (three-letter code: V6V) (formula: C<sub>10</sub>H<sub>8</sub>BrNO<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Br C N O 14 1 10 1 2	0	0
3	A	1	Total Br C N O 14 1 10 1 2	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	Br	C	N	O	0	0
			14	1	10	1	2		
3	B	1	Total	Br	C	N	O	0	0
			14	1	10	1	2		
3	B	1	Total	Br	C	N	O	0	0
			14	1	10	1	2		
3	B	1	Total	Br	C	N	O	0	0
			14	1	10	1	2		
3	B	1	Total	Br	C	N	O	0	0
			14	1	10	1	2		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total	Cl	0	0
			2	2		

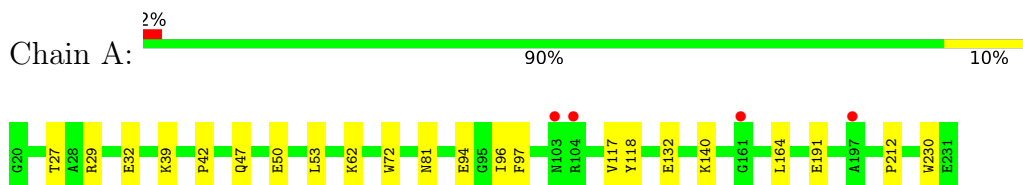
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	115	Total	O	0	0
			115	115		
5	B	97	Total	O	0	0
			97	97		

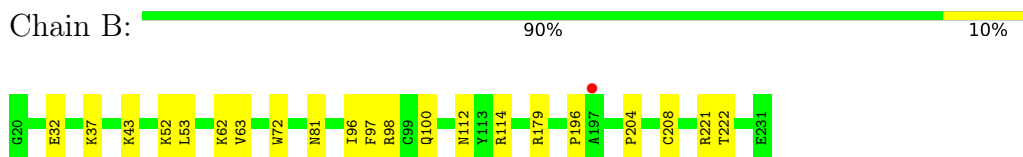
### 3 Residue-property plots [i](#)

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: Advanced glycosylation end product-specific receptor



- Molecule 1: Advanced glycosylation end product-specific receptor



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 62	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	102.91Å 102.91Å 101.77Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.92 – 1.80 45.92 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.6 (45.92-1.80) 99.6 (45.92-1.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.16 (at 1.79Å)	Xtrriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, $R_{free}$	0.199 , 0.222 0.199 , 0.222	Depositor DCC
$R_{free}$ test set	2802 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.2	Xtrriage
Anisotropy	0.275	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 37.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	0.487 for h,-h-k,-l	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	3458	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.07% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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



## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: V6V, CL, ACT

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	0.75	1/1617 (0.1%)	0.85	0/2217
1	B	0.71	0/1604	0.87	0/2196
All	All	0.73	1/3221 (0.0%)	0.86	0/4413

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	50	GLU	CB-CG	-5.16	1.42	1.52

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1557	0	1489	18	0
1	B	1553	0	1507	23	0
2	A	20	0	12	2	0
2	B	16	0	12	6	0
3	A	28	0	0	0	0
3	B	70	0	0	6	0
4	B	2	0	0	0	0
5	A	115	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	97	0	0	5	0
All	All	3458	0	3020	40	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (40) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:112[A]:ASN:H	2:B:302:ACT:H3	1.20	0.99
1:B:112[B]:ASN:H	2:B:302:ACT:H3	1.20	0.99
1:B:196:PRO:HB3	2:B:304:ACT:H2	1.50	0.93
1:B:37:LYS:NZ	5:B:401:HOH:O	2.16	0.77
1:A:140:LYS:HE2	1:A:191:GLU:HG3	1.67	0.77
1:B:100:GLN:HG2	3:B:311:V6V:BR14	2.44	0.73
1:A:96:ILE:HD12	2:A:301:ACT:H3	1.74	0.70
1:A:94[A]:GLU:HG2	1:A:117:VAL:HG13	1.73	0.69
1:A:212:PRO:HB3	2:A:305:ACT:H3	1.76	0.68
1:B:196:PRO:CB	2:B:304:ACT:H2	2.25	0.65
1:B:100:GLN:CG	3:B:311:V6V:BR14	3.00	0.64
1:A:132:GLU:CG	1:A:230:TRP:HE1	2.10	0.64
1:B:98:ARG:HB3	3:B:310:V6V:C01	2.30	0.61
1:B:179:ARG:HD3	3:B:309:V6V:BR14	2.57	0.59
1:A:27[B]:THR:HG22	1:A:118:TYR:CE1	2.40	0.57
1:A:29:ARG:HB3	1:A:32[B]:GLU:HG3	1.87	0.56
1:B:96:ILE:HD13	1:B:114:ARG:HD3	1.90	0.54
1:B:204:PRO:HG3	2:B:304:ACT:OXT	2.09	0.53
1:A:62:LYS:HE3	1:A:72:TRP:CD1	2.45	0.51
1:B:221:ARG:HG2	1:B:222:THR:N	2.27	0.49
1:A:47:GLN:HB2	5:A:441:HOH:O	2.13	0.48
1:B:81:ASN:ND2	5:B:401:HOH:O	2.47	0.48
1:B:37:LYS:HD3	5:B:443:HOH:O	2.14	0.47
1:B:53:LEU:HG	1:B:97:PHE:CD2	2.49	0.47
1:A:32[B]:GLU:OE2	5:B:401:HOH:O	2.20	0.45
1:A:132:GLU:HG2	1:A:230:TRP:HE1	1.82	0.45
1:B:43:LYS:NZ	5:B:405:HOH:O	2.47	0.44
1:B:62:LYS:HE3	1:B:72:TRP:CD1	2.52	0.43
1:A:39:LYS:HE3	1:A:39:LYS:HB2	1.59	0.43
1:A:81:ASN:HD22	1:B:32[B]:GLU:CD	2.21	0.43
1:A:53:LEU:HG	1:A:97:PHE:CD2	2.54	0.43
1:A:42:PRO:HD2	1:A:47:GLN:HG2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:ASN:ND2	1:B:32[B]:GLU:OE1	2.53	0.42
1:A:27[B]:THR:HG22	1:A:118:TYR:CD1	2.54	0.41
1:A:164:LEU:HD23	1:A:164:LEU:HA	1.93	0.41
1:B:208:CYS:O	1:B:221:ARG:HG3	2.21	0.41
1:B:112[A]:ASN:HB2	3:B:310:V6V:N07	2.36	0.40
1:B:112[B]:ASN:HB2	3:B:310:V6V:N07	2.36	0.40
1:B:52:LYS:HG2	1:B:63:VAL:HG22	2.02	0.40

There are no symmetry-related clashes.

### 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	216/212 (102%)	214 (99%)	2 (1%)	0	100	100
1	B	213/212 (100%)	212 (100%)	1 (0%)	0	100	100
All	All	429/424 (101%)	426 (99%)	3 (1%)	0	100	100

There are no Ramachandran outliers to report.

#### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	159/176 (90%)	159 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	158/176 (90%)	158 (100%)	0	100	100
All	All	317/352 (90%)	317 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	189	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 2 are monoatomic - leaving 16 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
3	V6V	B	310	-	14,15,15	4.72	6 (42%)	15,22,22	1.05	1 (6%)
3	V6V	B	309	-	14,15,15	4.43	6 (42%)	15,22,22	1.81	4 (26%)
2	ACT	B	301	-	3,3,3	2.04	1 (33%)	3,3,3	1.21	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	ACT	A	301	-	3,3,3	2.11	1 (33%)	3,3,3	1.19	0
3	V6V	A	306	-	14,15,15	4.39	6 (42%)	15,22,22	1.22	1 (6%)
2	ACT	B	303	-	3,3,3	1.75	1 (33%)	3,3,3	1.53	0
3	V6V	A	307	-	14,15,15	5.35	6 (42%)	15,22,22	2.07	6 (40%)
2	ACT	A	305	-	3,3,3	1.68	1 (33%)	3,3,3	1.57	1 (33%)
3	V6V	B	311	-	14,15,15	5.11	6 (42%)	15,22,22	3.73	8 (53%)
2	ACT	B	304	-	3,3,3	3.13	2 (66%)	3,3,3	1.70	1 (33%)
3	V6V	B	308	-	14,15,15	4.36	6 (42%)	15,22,22	1.08	1 (6%)
2	ACT	B	302	-	3,3,3	1.58	0	3,3,3	1.41	1 (33%)
2	ACT	A	303	-	3,3,3	1.47	1 (33%)	3,3,3	1.59	0
2	ACT	A	304	-	3,3,3	3.54	1 (33%)	3,3,3	2.31	2 (66%)
2	ACT	A	302	-	3,3,3	1.56	0	3,3,3	1.03	0
3	V6V	B	307	-	14,15,15	4.45	6 (42%)	15,22,22	2.28	5 (33%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	V6V	B	310	-	-	3/4/4/4	0/2/2/2
3	V6V	B	309	-	-	3/4/4/4	0/2/2/2
3	V6V	A	306	-	-	3/4/4/4	0/2/2/2
3	V6V	A	307	-	-	4/4/4/4	0/2/2/2
3	V6V	B	311	-	-	4/4/4/4	0/2/2/2
3	V6V	B	308	-	-	2/4/4/4	0/2/2/2
3	V6V	B	307	-	-	0/4/4/4	0/2/2/2

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	311	V6V	C02-C03	11.23	1.61	1.41
3	A	307	V6V	C02-C03	11.02	1.61	1.41
3	B	310	V6V	C05-C06	9.91	1.52	1.36
3	A	307	V6V	C05-C06	9.74	1.52	1.36
3	A	306	V6V	C05-C06	9.45	1.51	1.36
3	B	309	V6V	C02-C03	9.36	1.58	1.41
3	B	307	V6V	C02-C03	9.21	1.57	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	308	V6V	C05-C06	9.01	1.50	1.36
3	B	310	V6V	C02-C03	8.50	1.56	1.41
3	A	307	V6V	C02-C01	8.47	1.54	1.36
3	B	311	V6V	C02-C01	8.44	1.54	1.36
3	B	310	V6V	C05-C04	8.32	1.58	1.42
3	B	308	V6V	C02-C03	8.19	1.56	1.41
3	A	306	V6V	C02-C03	8.04	1.55	1.41
3	B	311	V6V	C05-C06	7.93	1.49	1.36
3	A	307	V6V	C05-C04	7.75	1.57	1.42
3	B	307	V6V	C05-C04	7.14	1.56	1.42
3	B	307	V6V	C02-C01	7.11	1.51	1.36
3	B	309	V6V	C05-C06	7.04	1.47	1.36
3	B	307	V6V	C05-C06	6.99	1.47	1.36
3	B	309	V6V	C05-C04	6.88	1.55	1.42
3	B	308	V6V	C05-C04	6.71	1.55	1.42
3	A	306	V6V	C05-C04	6.61	1.55	1.42
3	B	309	V6V	C02-C01	6.26	1.49	1.36
3	B	311	V6V	C05-C04	6.17	1.54	1.42
2	A	304	ACT	CH3-C	-5.91	1.24	1.49
3	B	311	V6V	C01-C06	5.80	1.50	1.38
3	A	307	V6V	C01-C06	5.77	1.50	1.38
3	B	310	V6V	C02-C01	5.51	1.48	1.36
3	B	309	V6V	C01-C06	5.50	1.49	1.38
3	A	306	V6V	C02-C01	5.48	1.48	1.36
3	B	308	V6V	C02-C01	5.31	1.47	1.36
3	B	307	V6V	C01-C06	4.95	1.48	1.38
2	B	304	ACT	CH3-C	-4.78	1.29	1.49
3	B	310	V6V	C01-C06	4.69	1.48	1.38
3	B	311	V6V	C09-C04	-4.69	1.35	1.40
3	B	308	V6V	C09-C04	-4.40	1.36	1.40
3	A	306	V6V	C01-C06	4.07	1.46	1.38
3	A	306	V6V	C09-C04	-4.03	1.36	1.40
3	B	308	V6V	C01-C06	3.94	1.46	1.38
3	B	309	V6V	C09-C04	-3.83	1.36	1.40
2	B	301	ACT	CH3-C	3.47	1.63	1.49
2	A	301	ACT	CH3-C	3.31	1.63	1.49
3	B	307	V6V	C09-C04	-3.14	1.37	1.40
3	A	307	V6V	C09-C04	-2.70	1.38	1.40
2	A	305	ACT	CH3-C	2.47	1.59	1.49
2	A	303	ACT	CH3-C	2.34	1.58	1.49
2	B	303	ACT	CH3-C	2.30	1.58	1.49
3	B	310	V6V	C09-C04	-2.17	1.38	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	304	ACT	OXT-C	-2.01	1.21	1.30

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	311	V6V	BR14-C06-C05	-9.07	106.39	119.72
3	B	311	V6V	BR14-C06-C01	8.35	131.44	119.30
3	B	307	V6V	BR14-C06-C05	-4.60	112.96	119.72
3	B	307	V6V	C01-C06-C05	4.14	127.77	121.99
3	B	311	V6V	C02-C01-C06	-3.98	113.95	119.17
3	A	307	V6V	C02-C01-C06	-3.74	114.27	119.17
3	B	307	V6V	C02-C01-C06	-3.72	114.30	119.17
3	A	307	V6V	BR14-C06-C05	-3.35	114.79	119.72
3	B	309	V6V	BR14-C06-C05	-3.28	114.89	119.72
2	A	304	ACT	O-C-CH3	-3.12	110.20	122.33
3	B	311	V6V	C09-C08-C11	-3.00	121.51	130.34
3	B	309	V6V	C06-C05-C04	-2.99	116.09	119.79
3	B	307	V6V	C06-C05-C04	-2.87	116.23	119.79
3	B	309	V6V	C01-C06-C05	2.84	125.96	121.99
3	A	307	V6V	C08-N07-C03	2.77	109.59	103.90
3	A	306	V6V	BR14-C06-C01	-2.76	115.29	119.30
3	A	307	V6V	BR14-C06-C01	2.60	123.08	119.30
3	B	310	V6V	C08-N07-C03	2.53	109.09	103.90
3	B	311	V6V	C08-N07-C03	2.50	109.04	103.90
3	B	311	V6V	C06-C05-C04	2.45	122.83	119.79
3	A	307	V6V	C09-C08-C11	-2.44	123.15	130.34
2	B	304	ACT	OXT-C-O	2.44	131.05	122.05
2	A	304	ACT	OXT-C-O	2.30	130.52	122.05
3	B	311	V6V	O13-C11-C08	2.29	121.89	114.46
3	A	307	V6V	O13-C11-O12	-2.23	118.39	123.35
3	B	309	V6V	C02-C01-C06	-2.18	116.31	119.17
3	B	307	V6V	O12-C11-C08	-2.16	116.28	120.73
3	B	308	V6V	BR14-C06-C01	-2.10	116.24	119.30
2	B	302	ACT	OXT-C-O	2.05	129.62	122.05
3	B	311	V6V	C02-C03-N07	2.03	136.64	130.78
2	A	305	ACT	OXT-C-O	2.02	129.51	122.05

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	306	V6V	C09-C08-C11-O12

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Mol	Chain	Res	Type	Atoms
3	A	306	V6V	C09-C08-C11-O13
3	A	306	V6V	N07-C08-C11-O13
3	A	307	V6V	C09-C08-C11-O12
3	A	307	V6V	C09-C08-C11-O13
3	A	307	V6V	N07-C08-C11-O13
3	B	308	V6V	N07-C08-C11-O13
3	B	309	V6V	C09-C08-C11-O12
3	B	309	V6V	C09-C08-C11-O13
3	B	309	V6V	N07-C08-C11-O13
3	B	310	V6V	C09-C08-C11-O12
3	B	310	V6V	C09-C08-C11-O13
3	B	310	V6V	N07-C08-C11-O13
3	B	311	V6V	C09-C08-C11-O12
3	B	311	V6V	C09-C08-C11-O13
3	B	311	V6V	N07-C08-C11-O13
3	B	311	V6V	N07-C08-C11-O12
3	B	308	V6V	C09-C08-C11-O13
3	A	307	V6V	N07-C08-C11-O12

There are no ring outliers.

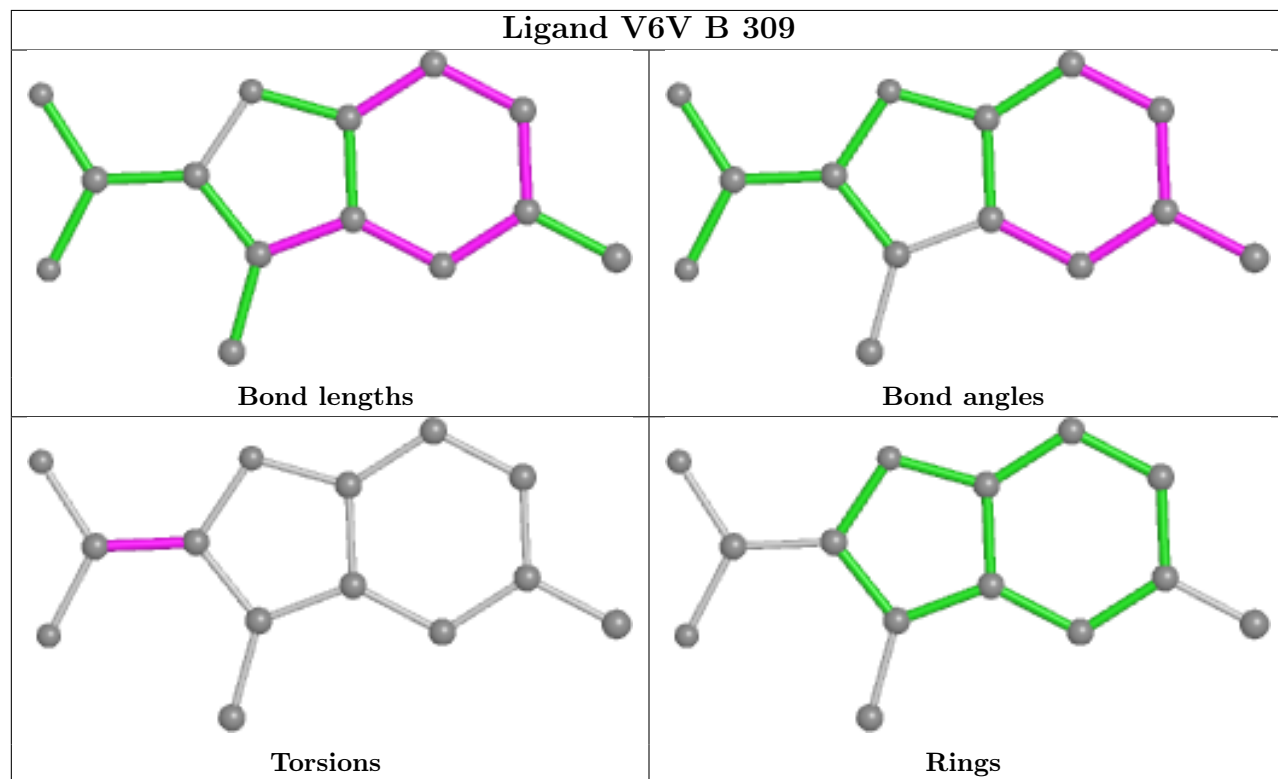
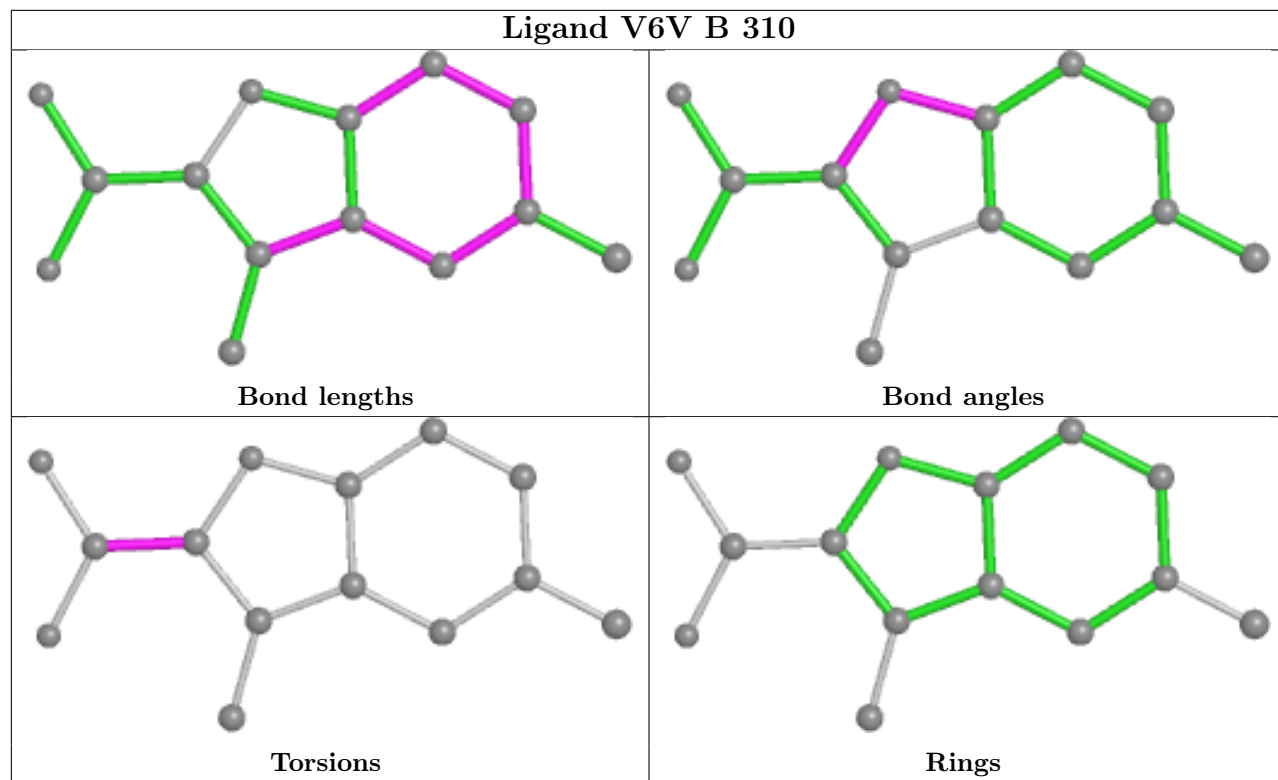
7 monomers are involved in 14 short contacts:

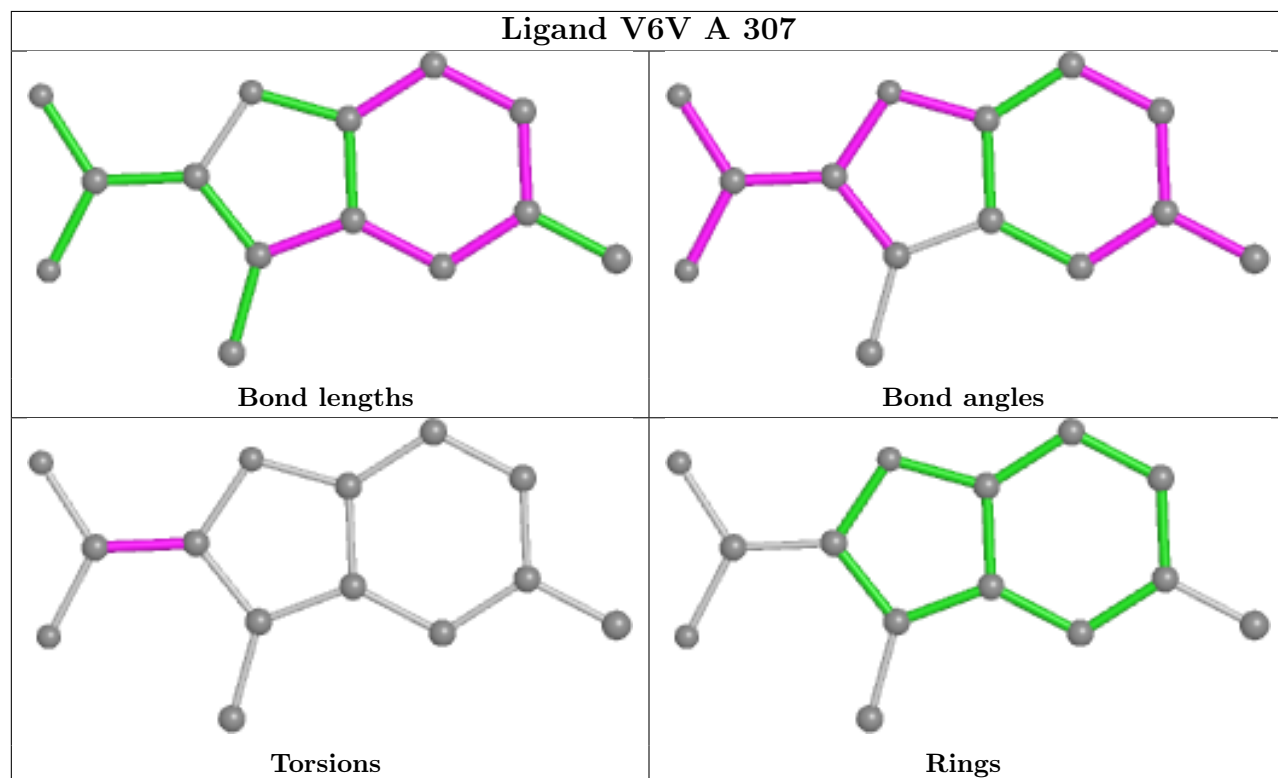
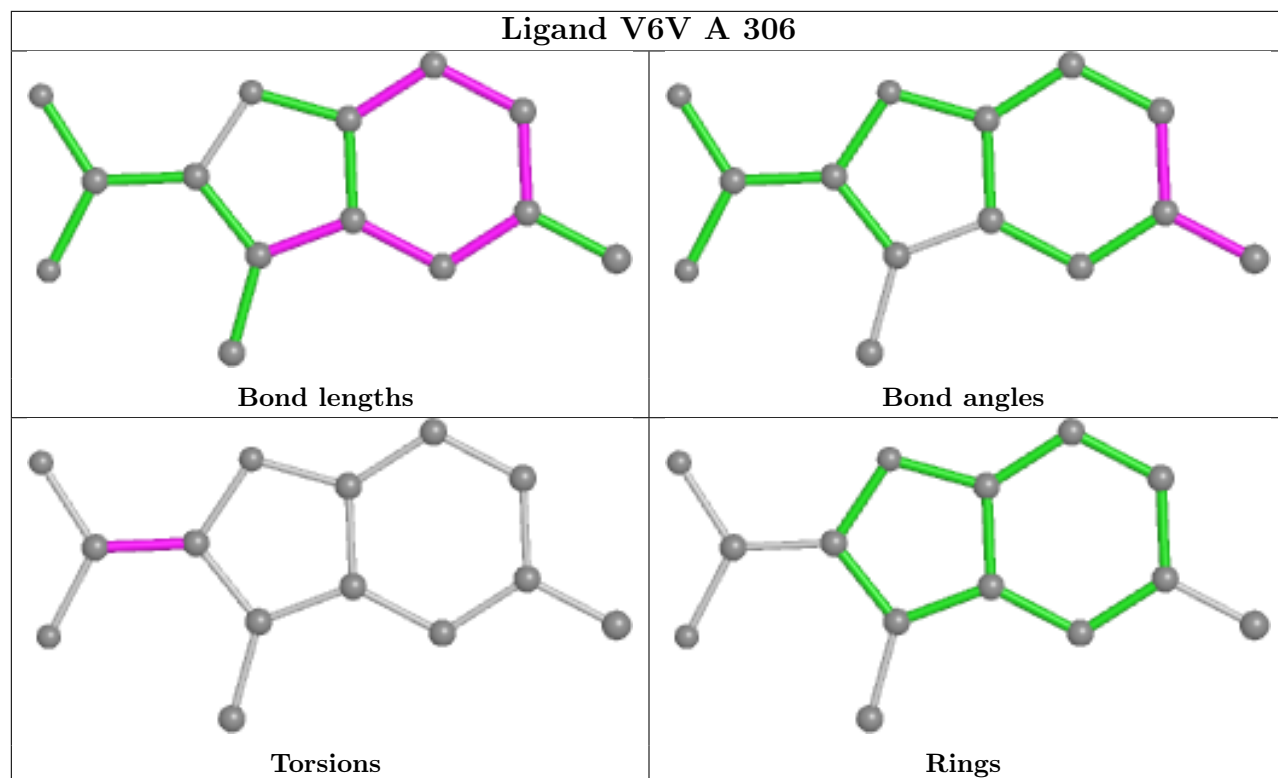
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	310	V6V	3	0
3	B	309	V6V	1	0
2	A	301	ACT	1	0
2	A	305	ACT	1	0
3	B	311	V6V	2	0
2	B	304	ACT	3	0
2	B	302	ACT	3	0

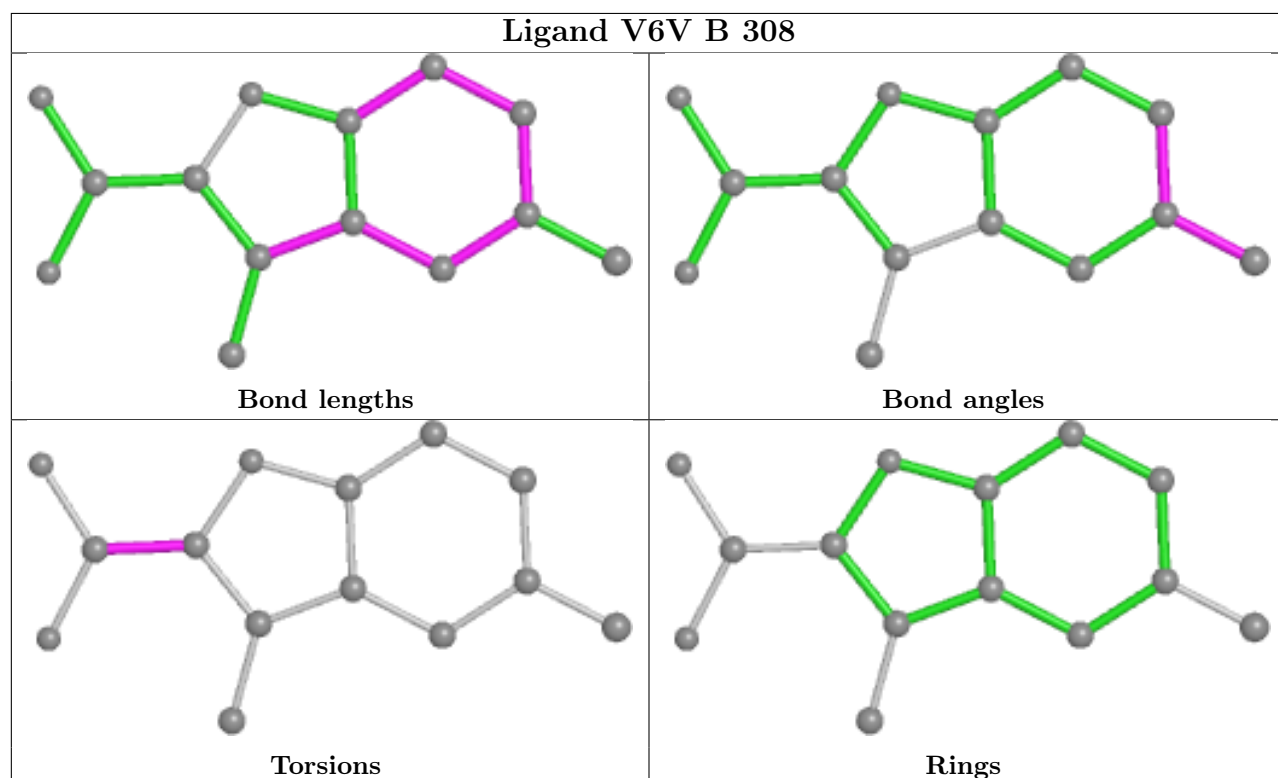
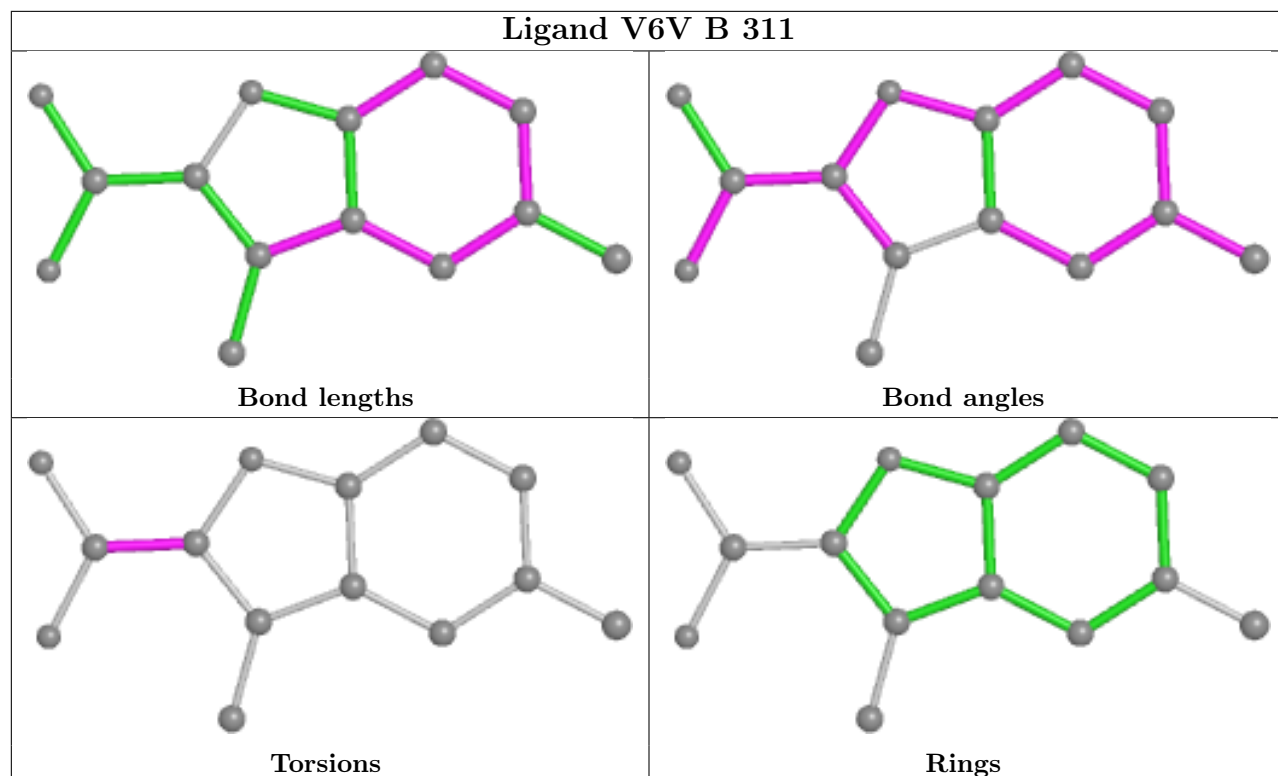
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

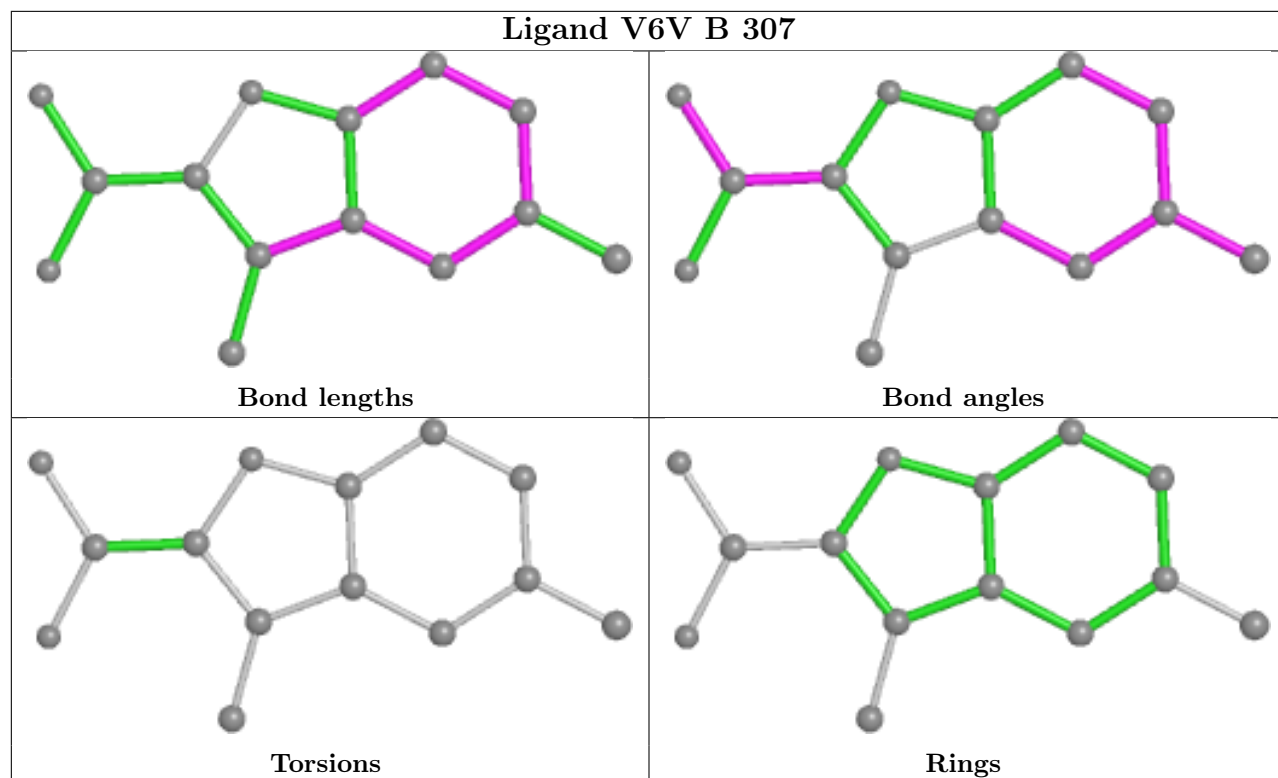


equivalents in the CSD to analyse the geometry.









## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	212/212 (100%)	-0.29	4 (1%) 66 63	17, 29, 62, 79	0
1	B	212/212 (100%)	-0.30	1 (0%) 91 89	17, 29, 60, 80	0
All	All	424/424 (100%)	-0.30	5 (1%) 79 76	17, 29, 61, 80	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	197	ALA	3.2
1	B	197	ALA	2.9
1	A	103	ASN	2.1
1	A	104	ARG	2.1
1	A	161	GLY	2.1

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

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

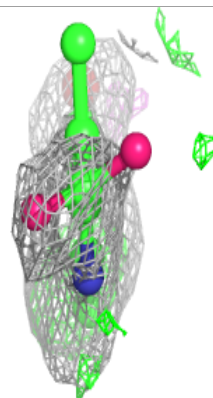
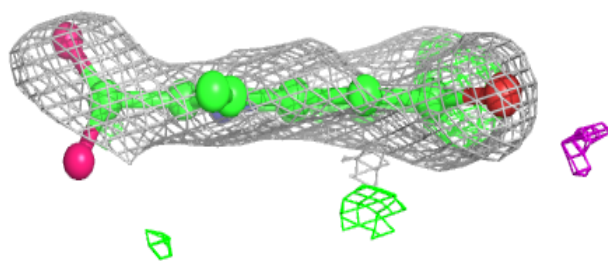
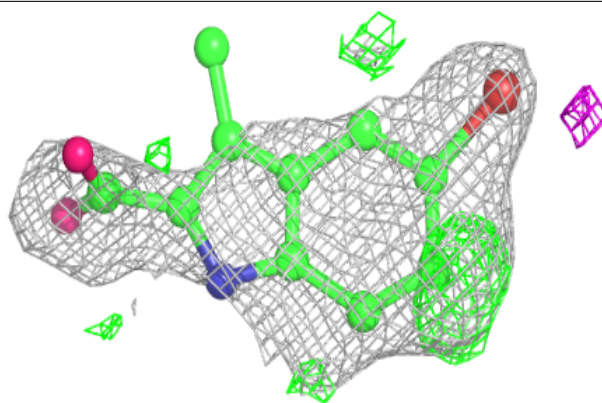
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	V6V	B	311	14/14	0.67	0.30	30,59,72,144	14
3	V6V	A	307	14/14	0.72	0.27	27,63,68,127	14
3	V6V	B	310	14/14	0.84	0.19	27,43,53,88	14
2	ACT	B	304	4/4	0.92	0.21	25,39,49,57	0
2	ACT	A	305	4/4	0.93	0.15	37,38,46,49	0
3	V6V	B	307	14/14	0.95	0.12	17,21,29,32	14
3	V6V	B	309	14/14	0.95	0.11	17,24,32,34	14
3	V6V	A	306	14/14	0.95	0.13	29,37,50,50	14
2	ACT	A	302	4/4	0.95	0.12	28,29,34,48	0
3	V6V	B	308	14/14	0.96	0.12	28,36,50,50	14
2	ACT	A	303	4/4	0.96	0.19	33,34,37,38	0
2	ACT	B	303	4/4	0.96	0.18	34,34,37,38	0
2	ACT	A	304	4/4	0.96	0.24	15,21,32,45	0
2	ACT	A	301	4/4	0.97	0.16	30,33,36,37	0
2	ACT	B	301	4/4	0.97	0.11	30,32,34,36	0
2	ACT	B	302	4/4	0.97	0.13	20,40,41,69	0
4	CL	B	305	1/1	0.97	0.05	33,33,33,33	0
4	CL	B	306	1/1	0.97	0.06	35,35,35,35	0

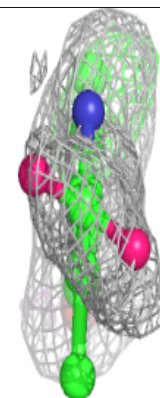
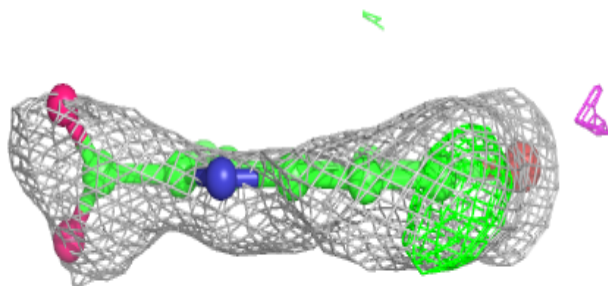
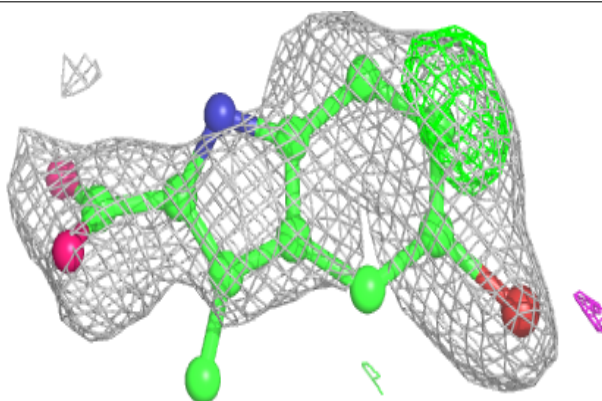
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around V6V B 311:**

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

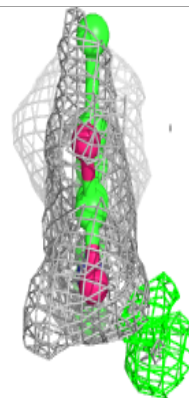
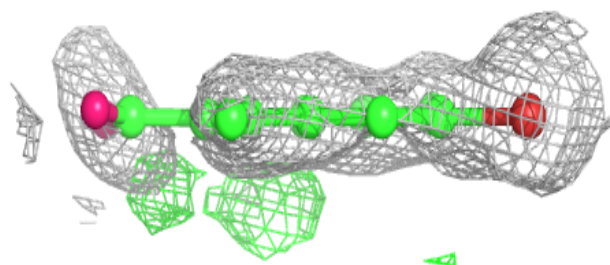
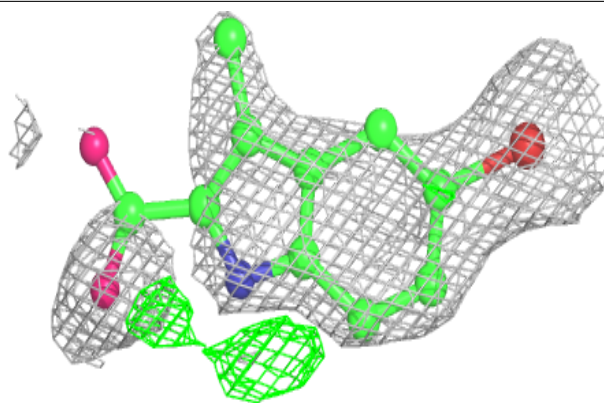
**Electron density around V6V A 307:**

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

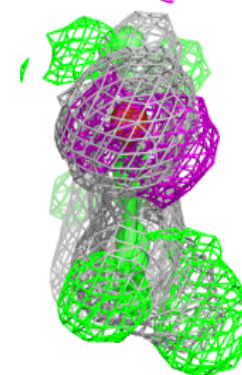
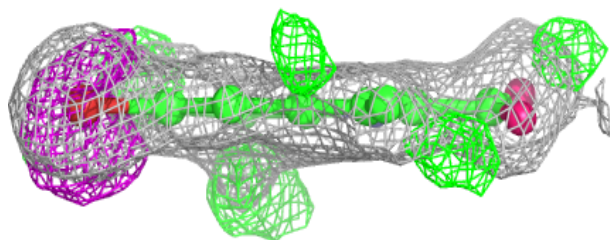
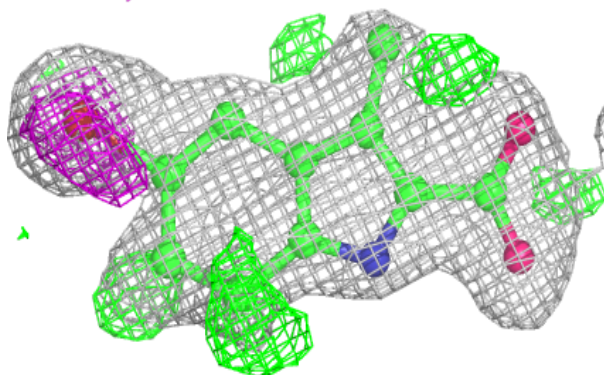


**Electron density around V6V B 310:**

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

**Electron density around V6V B 307:**

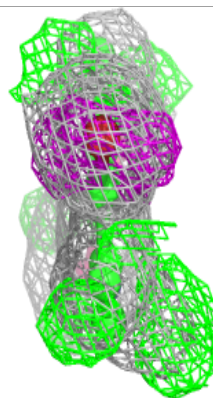
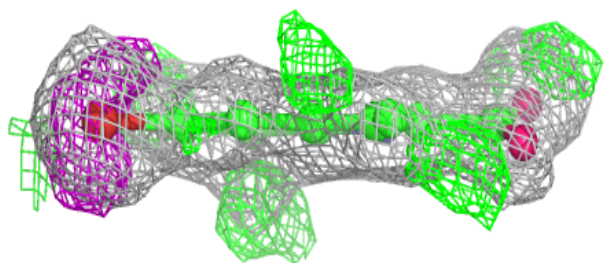
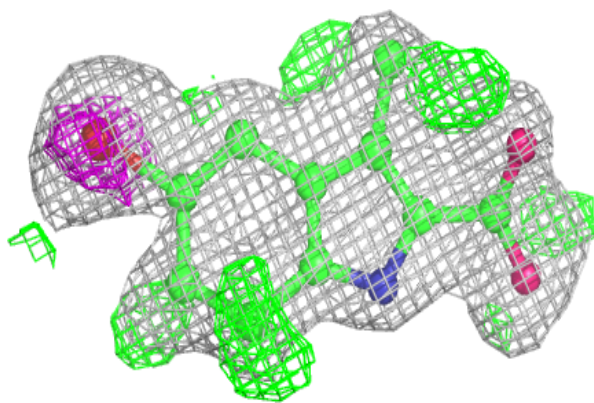
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



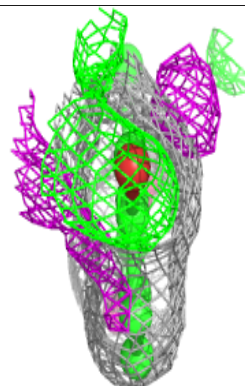
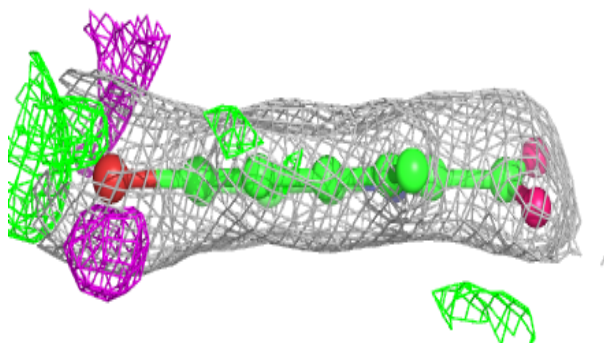
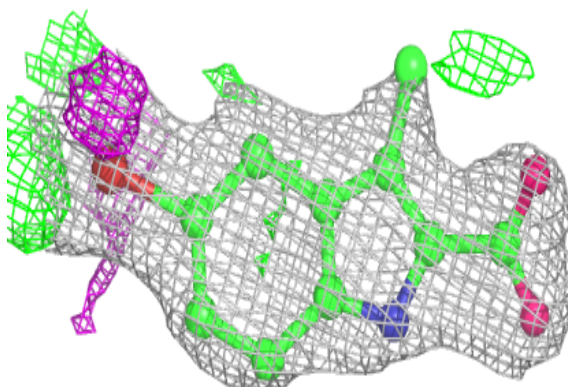


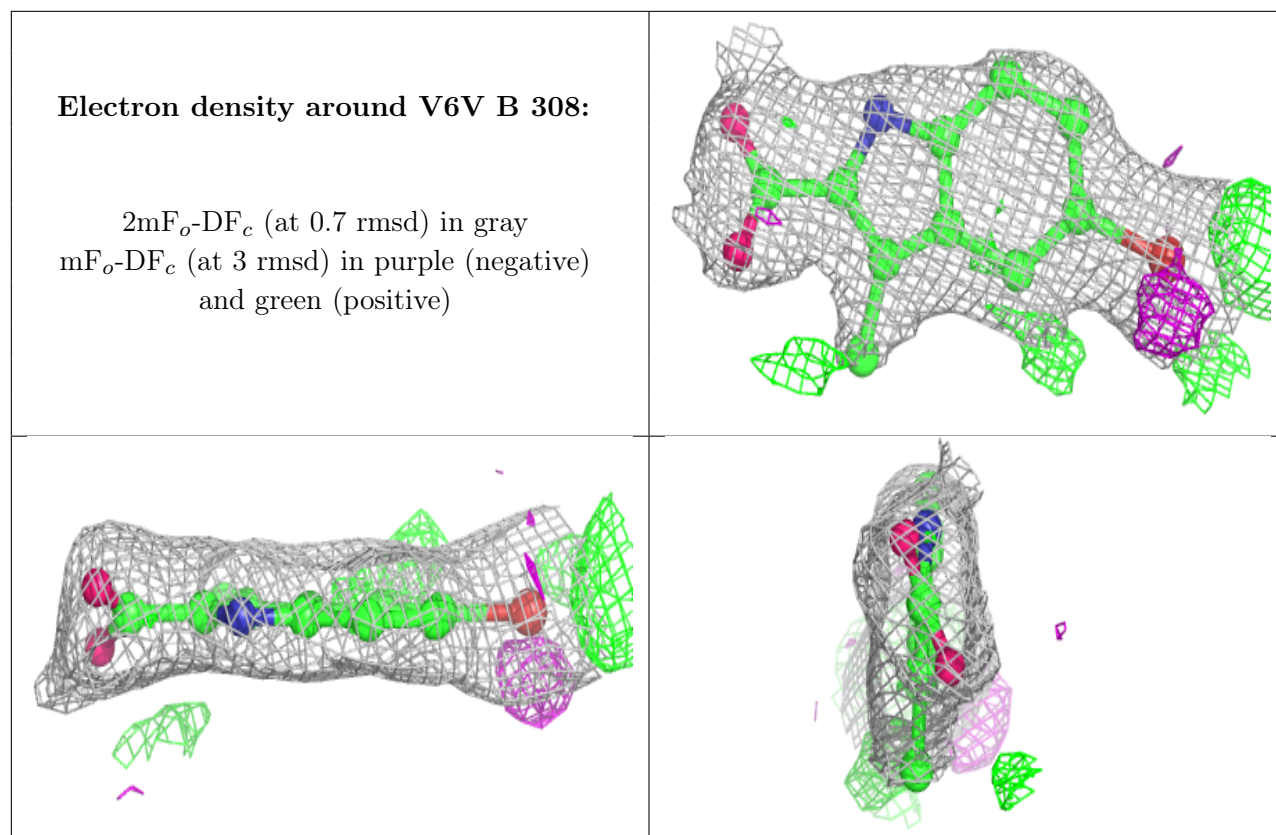
**Electron density around V6V B 309:**

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

**Electron density around V6V A 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.