



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:15 PM UTC

PDB ID : 6XQ7 / pdb_00006xq7
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

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>.

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

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

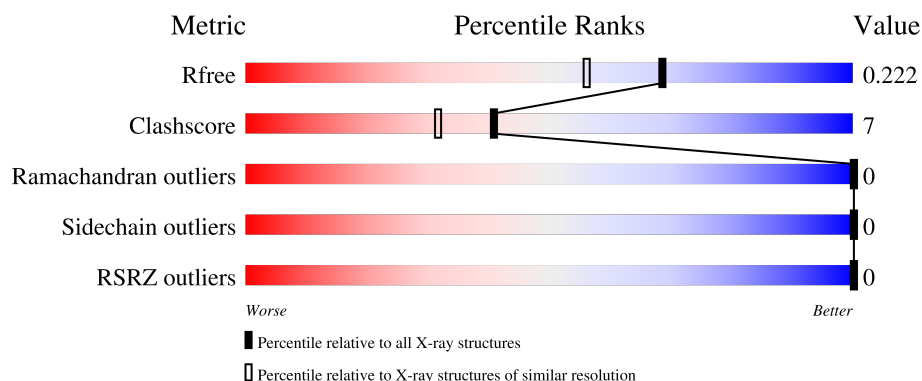
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (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 ≥ 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	 90% 10%
1	B	212	 88% 12%

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	A	307	-	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.

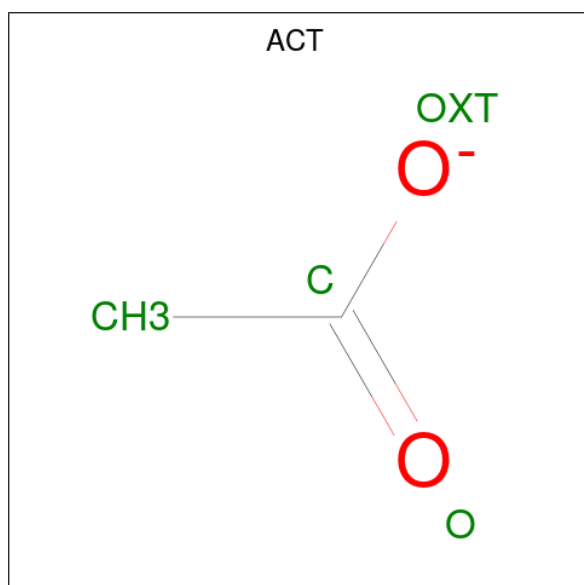
- Molecule 1 is a protein called Advanced glycosylation end product-specific receptor.

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

There are 6 discrepancies between the modelled and reference sequences:

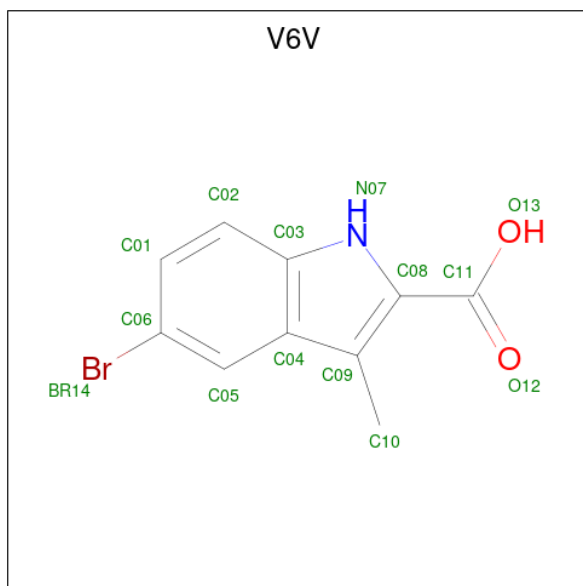
Chain	Residue	Modelled	Actual	Comment	Reference
A	20	GLY	-	expression tag	UNP Q15109
A	21	ALA	-	expression tag	UNP Q15109
A	22	MET	-	expression tag	UNP Q15109
B	20	GLY	-	expression tag	UNP Q15109
B	21	ALA	-	expression tag	UNP Q15109
B	22	MET	-	expression tag	UNP Q15109

- Molecule 2 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



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 (CCD ID: V6V) (formula: $C_{10}H_8BrNO_2$) (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

Continued on next page...

Continued from previous page...

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 (CCD ID: 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.

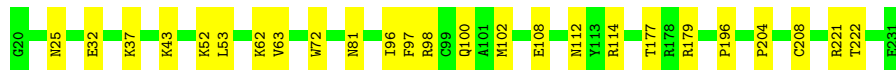
- Molecule 1: Advanced glycosylation end product-specific receptor

Chain A:  90% 10%



- Molecule 1: Advanced glycosylation end product-specific receptor

Chain B:  88% 12%



4 Data and refinement statistics

Property	Value	Source
Space group	P 62	Depositor
Cell constants a, b, c, α , β , γ	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) 99.8 (45.92-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.16 (at 1.79Å)	Xtriage
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 (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	23.2	Xtriage
Anisotropy	0.275	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 32.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.487 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	3458	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage'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.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, V6V, 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	0.77	0/1617	0.89	0/2217
1	B	0.75	0/1604	0.92	3/2196 (0.1%)
All	All	0.76	0/3221	0.91	3/4413 (0.1%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	177	THR	CA-C-N	-5.70	113.24	122.36
1	B	177	THR	C-N-CA	-5.70	113.24	122.36
1	B	25	ASN	N-CA-C	-5.67	100.43	109.96

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	24	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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	2	0	0	0	0
5	A	115	0	0	1	0
5	B	97	0	0	5	0
All	All	3458	0	3020	41	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 7.

All (41) 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:102:MET:HE2	1:B:108:GLU:CB	2.37	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:A:81:ASN:HD22	1:B:32[B]:GLU:CD	2.21	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:LYS:HE3	1:A:39:LYS:HB2	1.59	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
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 ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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 ⓘ

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
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 oligosaccharides 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$
2	ACT	A	302	-	3,3,3	1.66	1 (33%)	3,3,3	1.02	0
2	ACT	B	301	-	3,3,3	2.18	1 (33%)	3,3,3	1.20	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ACT	A	305	-	3,3,3	1.79	1 (33%)	3,3,3	1.55	1 (33%)
2	ACT	B	303	-	3,3,3	1.86	1 (33%)	3,3,3	1.51	0
3	V6V	A	306	-	14,15,15	4.90	7 (50%)	19,22,22	1.31	3 (15%)
3	V6V	B	310	-	14,15,15	5.46	9 (64%)	19,22,22	1.04	0
3	V6V	B	311	-	14,15,15	5.84	8 (57%)	19,22,22	4.70	11 (57%)
2	ACT	A	304	-	3,3,3	3.80	1 (33%)	3,3,3	2.26	2 (66%)
2	ACT	A	303	-	3,3,3	1.57	1 (33%)	3,3,3	1.57	0
3	V6V	B	308	-	14,15,15	4.92	8 (57%)	19,22,22	1.16	3 (15%)
3	V6V	B	309	-	14,15,15	5.15	8 (57%)	19,22,22	1.74	5 (26%)
3	V6V	A	307	-	14,15,15	6.13	8 (57%)	19,22,22	2.89	10 (52%)
2	ACT	B	304	-	3,3,3	3.35	2 (66%)	3,3,3	1.68	1 (33%)
3	V6V	B	307	-	14,15,15	5.24	9 (64%)	19,22,22	2.21	6 (31%)
2	ACT	B	302	-	3,3,3	1.68	0	3,3,3	1.39	1 (33%)
2	ACT	A	301	-	3,3,3	2.25	1 (33%)	3,3,3	1.18	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
3	V6V	B	310	-	-	0/4/4/4	0/2/2/2
3	V6V	B	311	-	-	4/4/4/4	0/2/2/2
3	V6V	A	306	-	-	4/4/4/4	0/2/2/2
3	V6V	B	308	-	-	4/4/4/4	0/2/2/2
3	V6V	B	309	-	-	3/4/4/4	0/2/2/2
3	V6V	A	307	-	-	4/4/4/4	0/2/2/2
3	V6V	B	307	-	-	0/4/4/4	0/2/2/2

All (66) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	311	V6V	C02-C03	13.37	1.61	1.39
3	A	307	V6V	C02-C03	13.15	1.61	1.39
3	B	310	V6V	C05-C04	12.08	1.58	1.39
3	B	309	V6V	C02-C03	11.37	1.58	1.39
3	A	307	V6V	C05-C04	11.35	1.57	1.39
3	B	307	V6V	C02-C03	11.21	1.57	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	307	V6V	C05-C04	10.59	1.56	1.39
3	B	310	V6V	C02-C03	10.44	1.56	1.39
3	B	309	V6V	C05-C04	10.25	1.55	1.39
3	B	308	V6V	C02-C03	10.11	1.56	1.39
3	B	308	V6V	C05-C04	10.04	1.55	1.39
3	A	306	V6V	C02-C03	9.95	1.55	1.39
3	A	306	V6V	C05-C04	9.90	1.55	1.39
3	A	307	V6V	C02-C01	9.69	1.54	1.38
3	B	311	V6V	C02-C01	9.65	1.54	1.38
3	B	311	V6V	C05-C04	9.35	1.54	1.39
3	B	307	V6V	C02-C01	7.92	1.51	1.38
3	B	310	V6V	C05-C06	7.24	1.52	1.38
3	A	307	V6V	C05-C06	7.10	1.52	1.38
3	A	306	V6V	C05-C06	6.87	1.51	1.38
3	B	309	V6V	C02-C01	6.81	1.49	1.38
3	B	308	V6V	C05-C06	6.50	1.50	1.38
2	A	304	ACT	CH3-C	-6.35	1.24	1.49
3	B	311	V6V	C01-C06	6.13	1.50	1.38
3	A	307	V6V	C01-C06	6.10	1.50	1.38
3	B	310	V6V	C02-C01	5.82	1.48	1.38
3	B	309	V6V	C01-C06	5.81	1.49	1.38
3	A	306	V6V	C02-C01	5.78	1.48	1.38
3	B	311	V6V	C05-C06	5.62	1.49	1.38
3	B	308	V6V	C02-C01	5.57	1.47	1.38
3	B	307	V6V	C01-C06	5.23	1.48	1.38
2	B	304	ACT	CH3-C	-5.13	1.29	1.49
3	B	310	V6V	C01-C06	4.95	1.48	1.38
3	B	309	V6V	C05-C06	4.90	1.47	1.38
3	B	307	V6V	C05-C06	4.86	1.47	1.38
3	B	311	V6V	C04-C09	-4.49	1.35	1.44
3	B	308	V6V	C04-C09	-4.32	1.36	1.44
3	A	306	V6V	C01-C06	4.29	1.46	1.38
3	B	308	V6V	C01-C06	4.16	1.46	1.38
3	A	306	V6V	C04-C09	-4.11	1.36	1.44
3	A	307	V6V	C08-C11	4.02	1.54	1.48
3	B	309	V6V	C04-C09	-4.00	1.36	1.44
2	B	301	ACT	CH3-C	3.71	1.63	1.49
3	B	310	V6V	C08-C11	3.68	1.53	1.48
3	B	307	V6V	C04-C09	-3.61	1.37	1.44
2	A	301	ACT	CH3-C	3.54	1.63	1.49
3	B	311	V6V	C08-C11	3.52	1.53	1.48
3	A	307	V6V	C04-C09	-3.36	1.38	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	310	V6V	C04-C03	-3.22	1.37	1.41
3	B	310	V6V	C04-C09	-3.06	1.38	1.44
2	A	305	ACT	CH3-C	2.63	1.59	1.49
2	A	303	ACT	CH3-C	2.50	1.58	1.49
2	B	303	ACT	CH3-C	2.46	1.58	1.49
3	B	308	V6V	C03-N07	-2.38	1.34	1.38
3	B	310	V6V	C08-N07	-2.27	1.35	1.38
3	B	308	V6V	C08-N07	-2.22	1.35	1.38
3	B	307	V6V	C08-C11	2.22	1.51	1.48
3	A	307	V6V	C10-C09	2.18	1.54	1.50
3	A	306	V6V	C03-N07	-2.16	1.34	1.38
3	B	307	V6V	C04-C03	-2.14	1.38	1.41
3	B	311	V6V	C10-C09	2.11	1.53	1.50
2	B	304	ACT	OXT-C	-2.10	1.21	1.30
2	A	302	ACT	CH3-C	2.04	1.57	1.49
3	B	309	V6V	C08-C11	2.03	1.51	1.48
3	B	307	V6V	O12-C11	2.01	1.27	1.22
3	B	309	V6V	C10-C09	2.00	1.53	1.50

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	311	V6V	C03-C04-C09	9.90	112.33	107.52
3	B	311	V6V	BR14-C06-C05	-9.08	106.39	119.23
3	B	311	V6V	BR14-C06-C01	8.91	131.44	119.30
3	B	311	V6V	C11-C08-N07	7.49	130.55	121.22
3	A	307	V6V	C11-C08-N07	6.80	129.69	121.22
3	B	311	V6V	C11-C08-C09	-5.21	121.51	133.02
3	A	307	V6V	C03-C04-C09	4.59	109.75	107.52
3	A	307	V6V	C11-C08-C09	-4.47	123.15	133.02
3	B	307	V6V	BR14-C06-C05	-4.44	112.96	119.23
3	B	311	V6V	C02-C01-C06	-4.37	113.95	119.18
3	B	307	V6V	C01-C06-C05	4.33	127.77	121.53
3	A	307	V6V	C02-C01-C06	-4.10	114.27	119.18
3	B	307	V6V	C02-C01-C06	-4.08	114.30	119.18
3	B	307	V6V	C03-C04-C09	4.03	109.48	107.52
3	B	311	V6V	C04-C03-N07	-3.52	104.27	108.23
3	B	311	V6V	O13-C11-C08	3.25	121.89	116.73
3	B	311	V6V	C02-C03-C04	-3.21	119.09	122.19
3	A	307	V6V	BR14-C06-C05	-3.14	114.79	119.23
3	B	309	V6V	C01-C06-C05	3.07	125.96	121.53
3	B	309	V6V	BR14-C06-C05	-3.07	114.89	119.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	304	ACT	O-C-CH3	-3.01	110.20	122.53
3	A	306	V6V	BR14-C06-C01	-2.94	115.29	119.30
3	B	309	V6V	C03-C04-C09	2.93	108.94	107.52
3	B	311	V6V	C02-C03-N07	2.88	136.64	130.83
3	A	307	V6V	BR14-C06-C01	2.78	123.08	119.30
3	B	309	V6V	C11-C08-C09	-2.71	127.03	133.02
2	B	304	ACT	OXT-C-O	2.43	131.05	122.03
3	B	309	V6V	C02-C01-C06	-2.40	116.31	119.18
3	A	307	V6V	C04-C03-N07	-2.36	105.57	108.23
3	A	307	V6V	C02-C03-C04	-2.36	119.91	122.19
3	A	307	V6V	O13-C11-O12	-2.31	118.39	123.90
3	A	306	V6V	BR14-C06-C05	2.31	122.50	119.23
2	A	304	ACT	OXT-C-O	2.29	130.52	122.03
3	A	306	V6V	C11-C08-C09	-2.28	127.97	133.02
3	B	308	V6V	C11-C08-C09	-2.25	128.04	133.02
3	A	307	V6V	O13-C11-C08	2.25	120.31	116.73
3	B	307	V6V	O12-C11-C08	-2.25	116.28	120.20
3	B	308	V6V	BR14-C06-C01	-2.24	116.24	119.30
3	B	311	V6V	C04-C05-C06	2.23	122.83	118.99
3	B	307	V6V	C11-C08-C09	-2.18	128.20	133.02
3	B	308	V6V	BR14-C06-C05	2.05	122.14	119.23
2	B	302	ACT	OXT-C-O	2.05	129.62	122.03
2	A	305	ACT	OXT-C-O	2.02	129.51	122.03

There are no chirality outliers.

All (19) torsion outliers are listed below:

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

Continued on next page...

Continued from previous page...

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

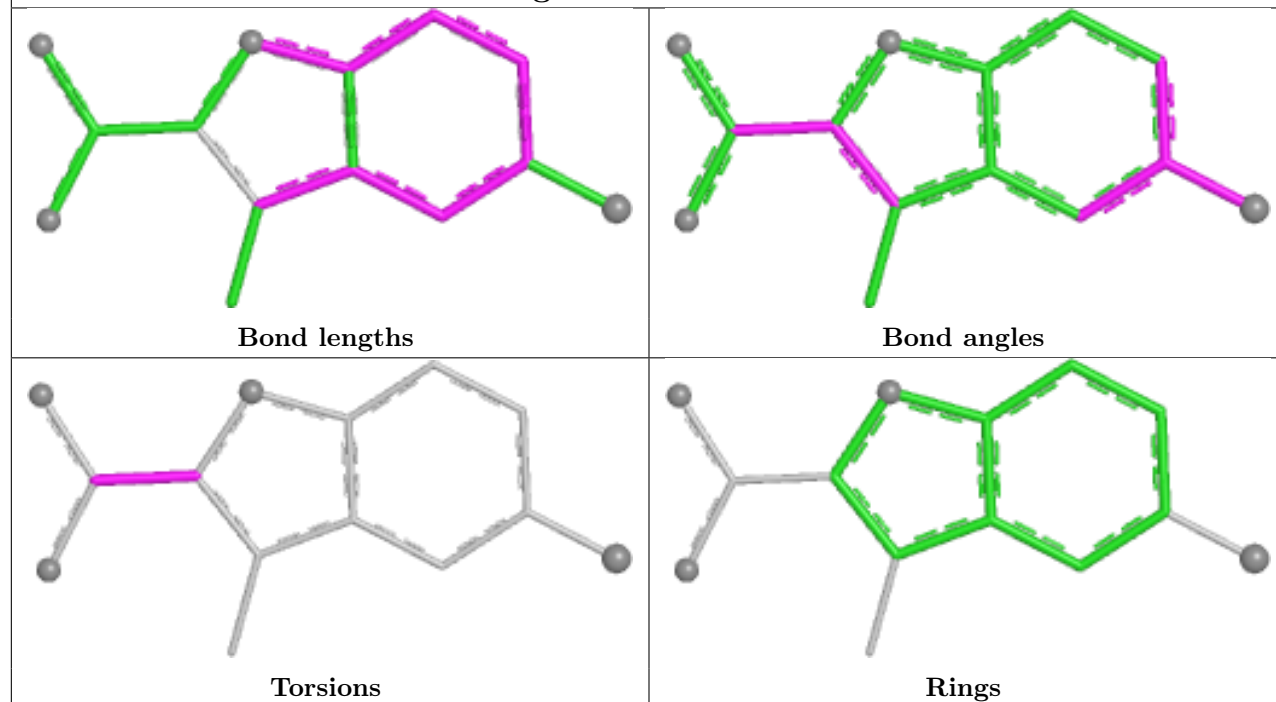
There are no ring outliers.

7 monomers are involved in 14 short contacts:

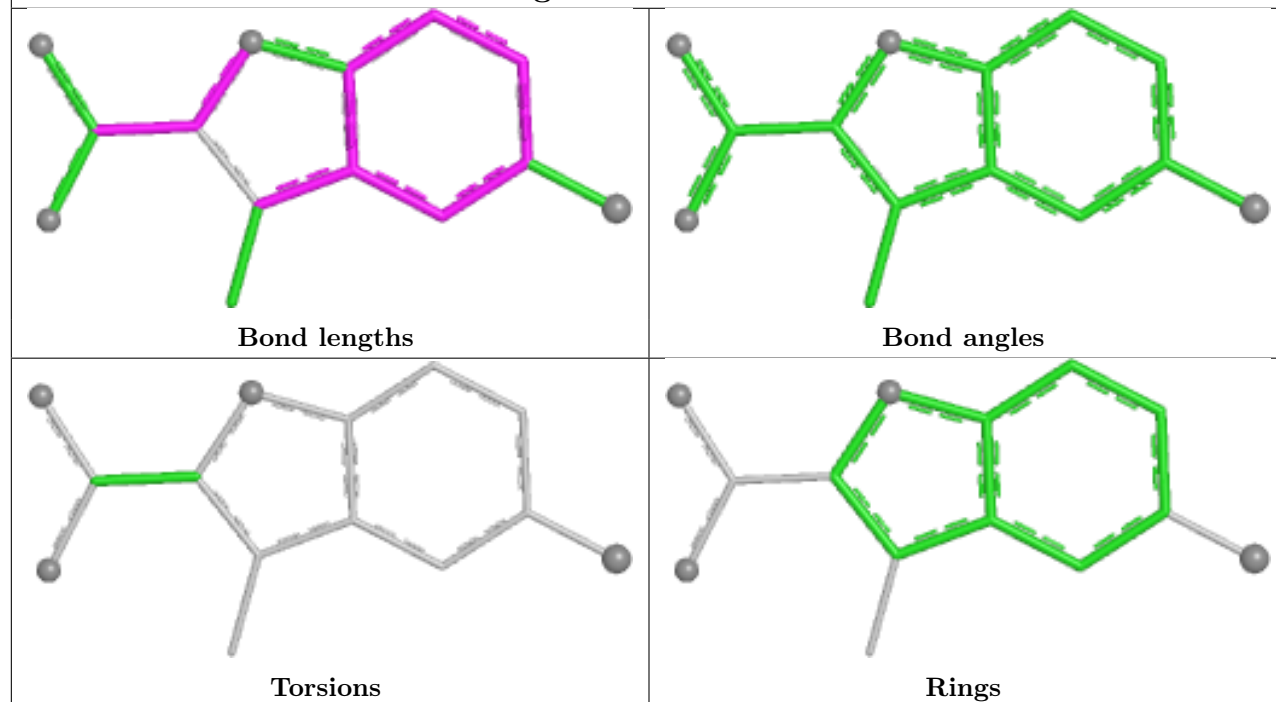
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	305	ACT	1	0
3	B	310	V6V	3	0
3	B	311	V6V	2	0
3	B	309	V6V	1	0
2	B	304	ACT	3	0
2	B	302	ACT	3	0
2	A	301	ACT	1	0

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.

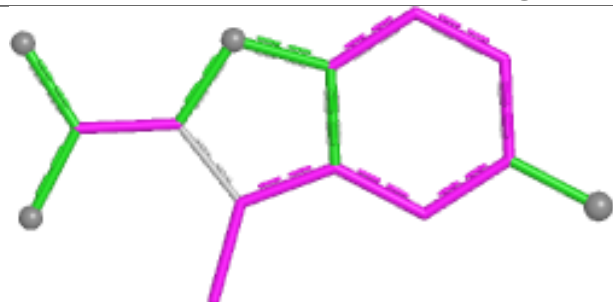
Ligand V6V A 306



Ligand V6V B 310



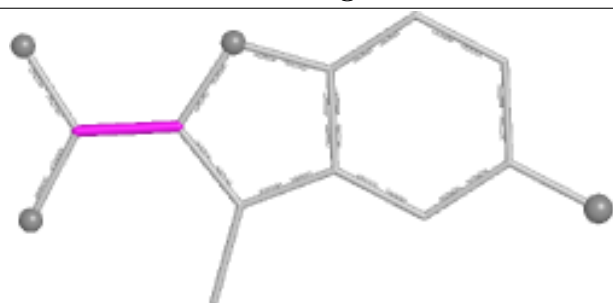
Ligand V6V B 311



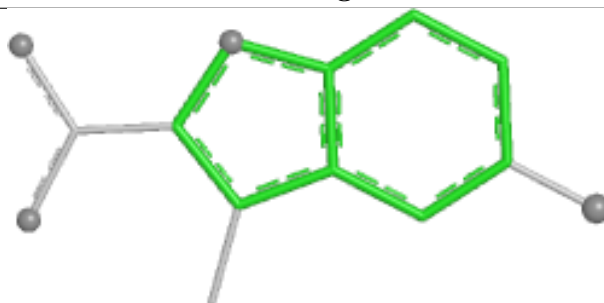
Bond lengths



Bond angles

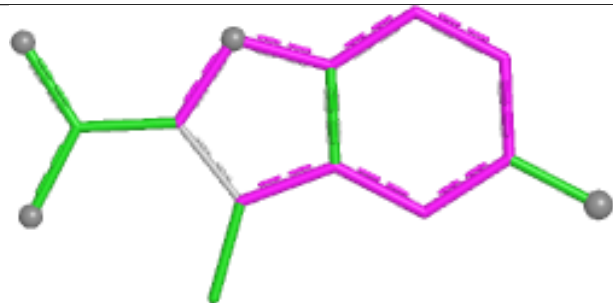


Torsions

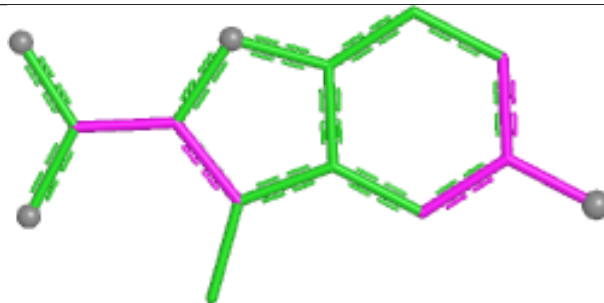


Rings

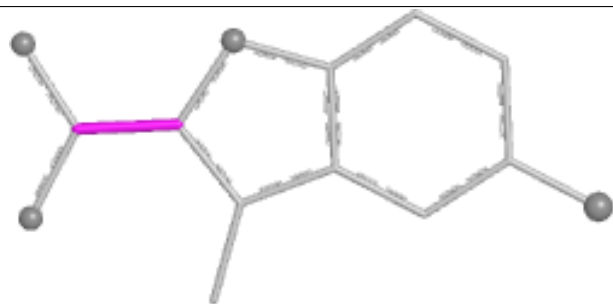
Ligand V6V B 308



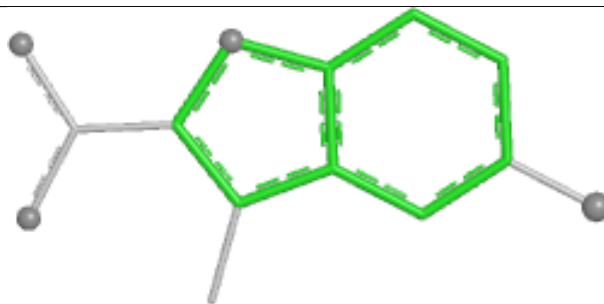
Bond lengths



Bond angles

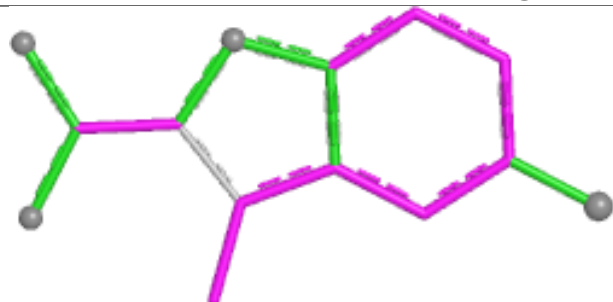


Torsions

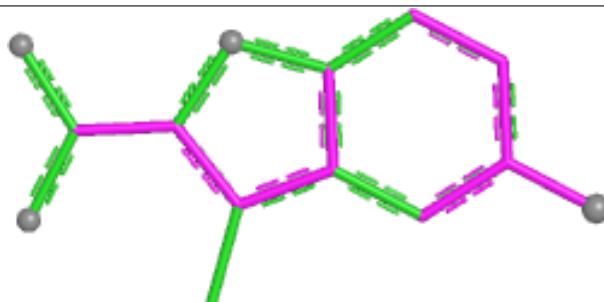


Rings

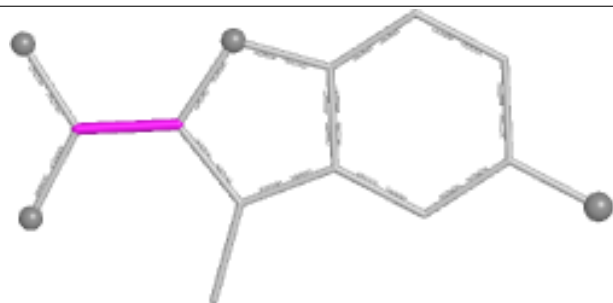
Ligand V6V B 309



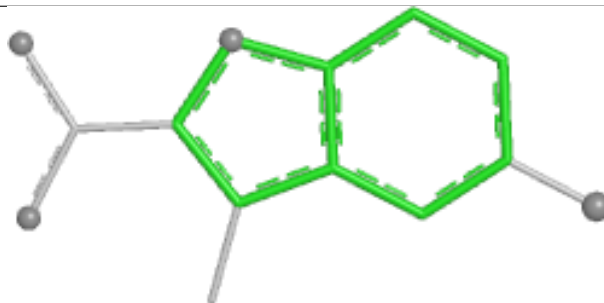
Bond lengths



Bond angles

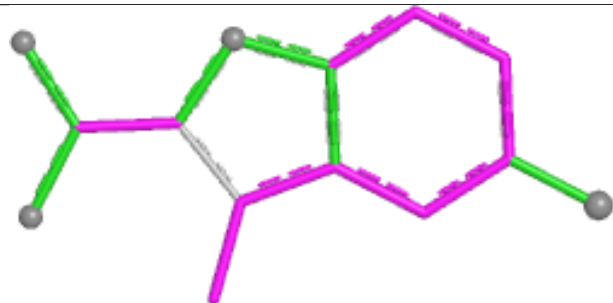


Torsions

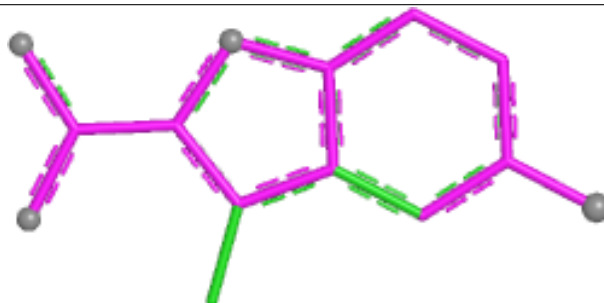


Rings

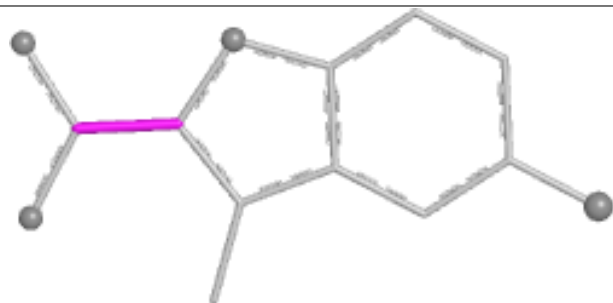
Ligand V6V A 307



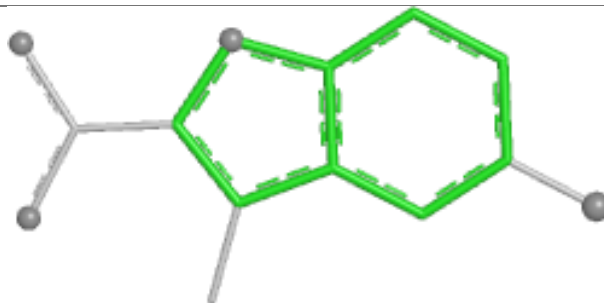
Bond lengths



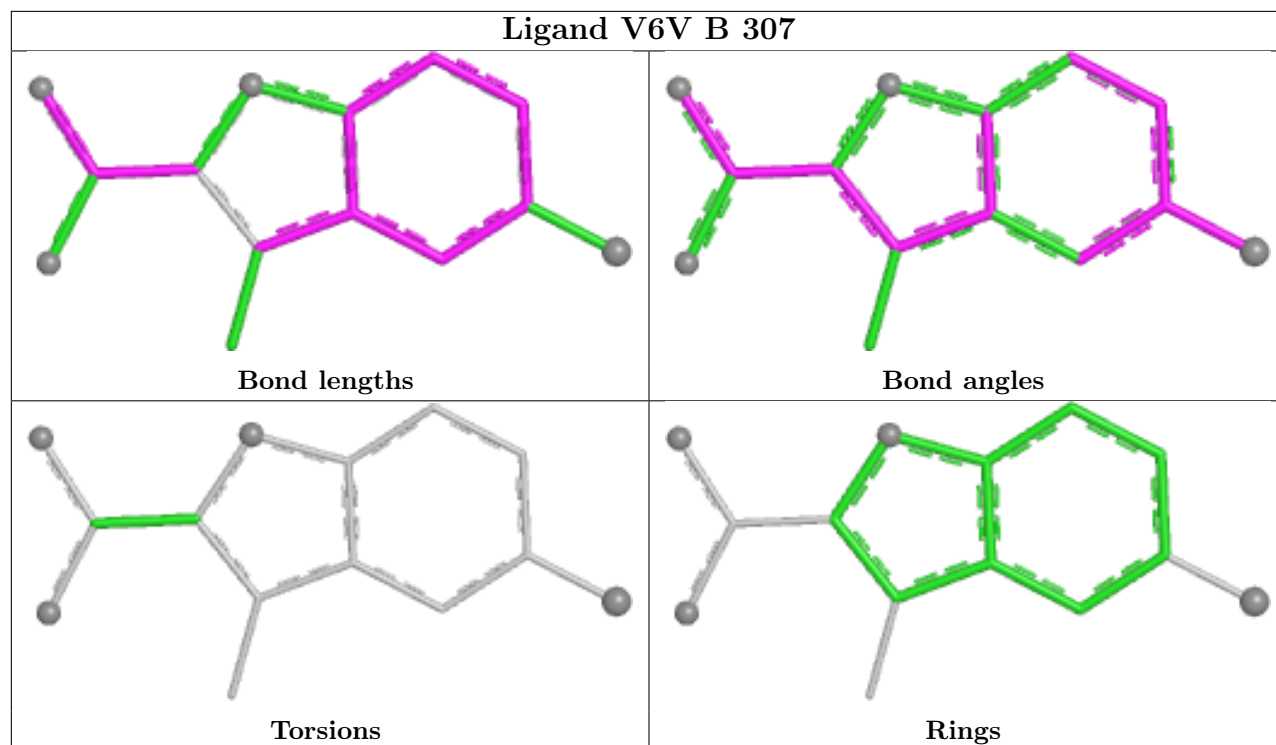
Bond angles



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 [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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	212/212 (100%)	-1.14	0 100 100	12, 29, 62, 79	6 (2%)
1	B	212/212 (100%)	-1.13	0 100 100	13, 29, 60, 80	3 (1%)
All	All	424/424 (100%)	-1.13	0 100 100	12, 29, 61, 80	9 (2%)

There are no RSRZ outliers to report.

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	V6V	B	311	14/14	0.97	0.11	30,59,72,144	14
2	ACT	B	303	4/4	0.98	0.09	34,34,37,38	0
3	V6V	A	307	14/14	0.98	0.09	27,63,68,127	14
3	V6V	B	310	14/14	0.98	0.08	27,43,53,88	14
2	ACT	A	303	4/4	0.98	0.09	33,34,37,38	0
2	ACT	B	301	4/4	0.99	0.05	30,32,34,36	0
2	ACT	B	302	4/4	0.99	0.05	20,40,41,69	0

Continued on next page...

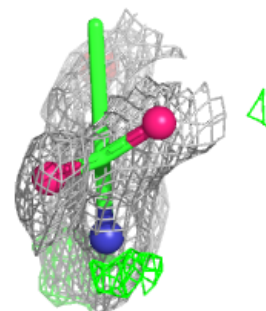
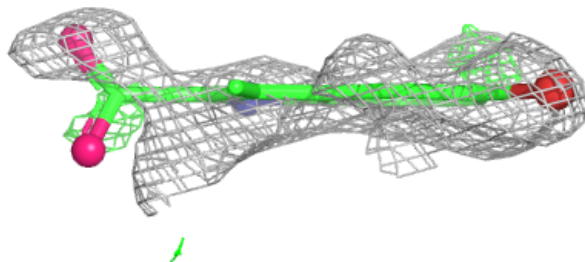
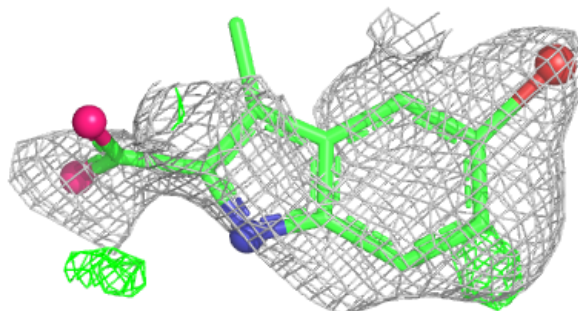
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ACT	A	302	4/4	0.99	0.04	28,29,34,48	0
2	ACT	B	304	4/4	0.99	0.06	25,39,49,57	0
3	V6V	A	306	14/14	0.99	0.04	29,37,50,50	14
2	ACT	A	301	4/4	0.99	0.07	30,33,36,37	0
3	V6V	B	307	14/14	0.99	0.06	17,21,29,32	14
3	V6V	B	308	14/14	0.99	0.04	28,36,50,50	14
3	V6V	B	309	14/14	0.99	0.06	17,24,32,34	14
2	ACT	A	304	4/4	0.99	0.07	15,21,32,45	0
2	ACT	A	305	4/4	0.99	0.04	37,38,46,49	0
4	CL	B	305	1/1	1.00	0.06	33,33,33,33	0
4	CL	B	306	1/1	1.00	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.

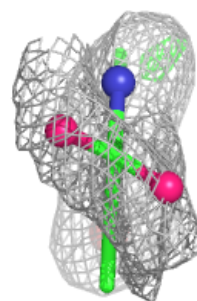
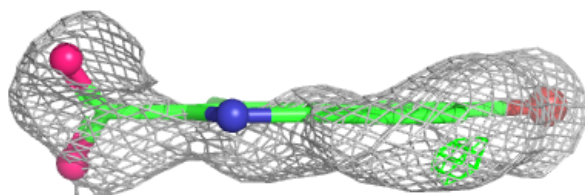
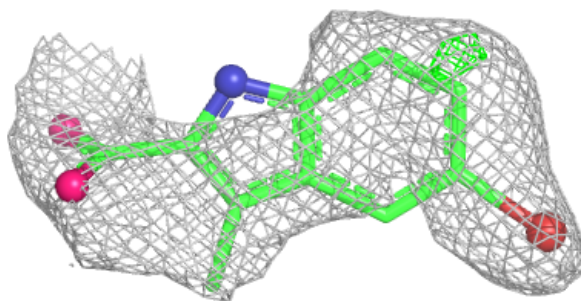
Electron density around V6V B 311:

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

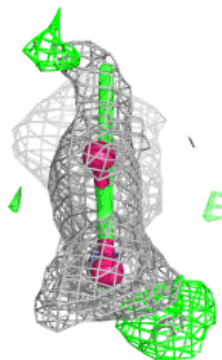
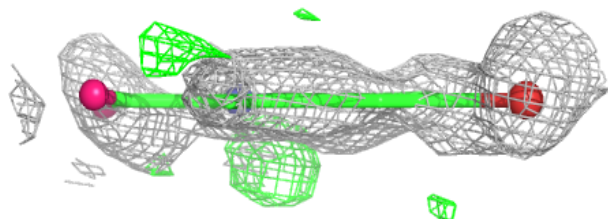
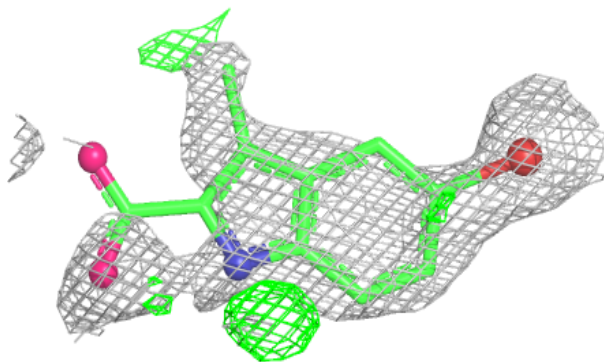


Electron density around V6V A 307:

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

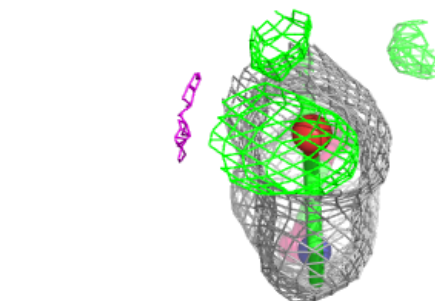
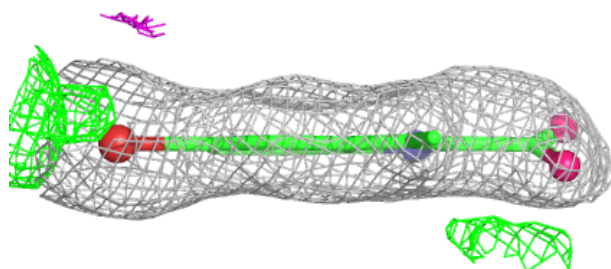
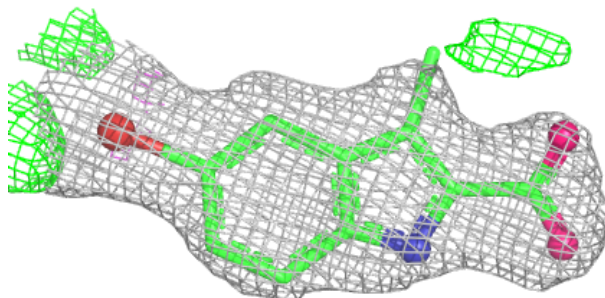
**Electron density around V6V B 310:**

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

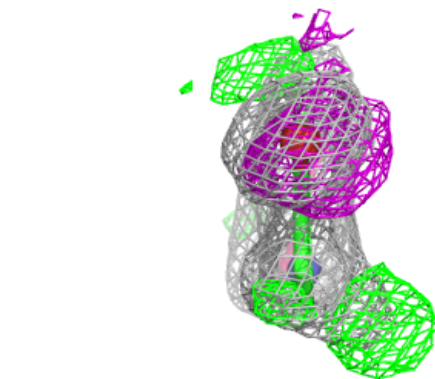
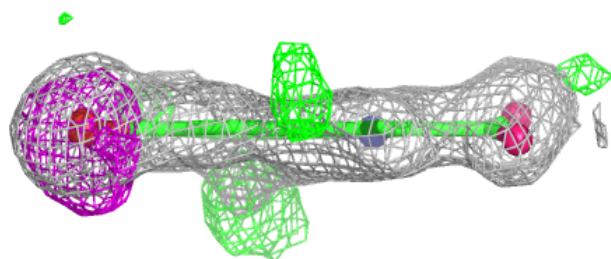
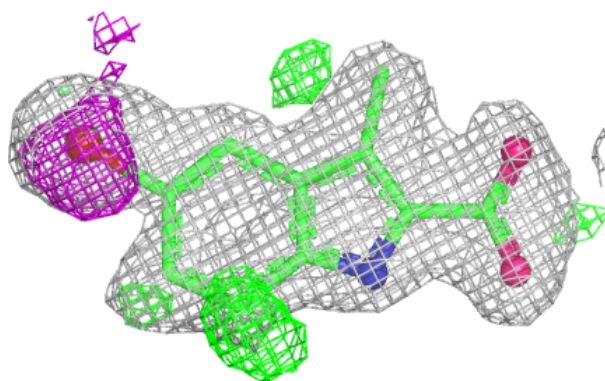


Electron density around V6V A 306:

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

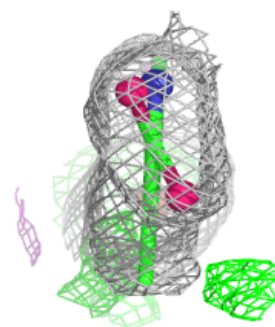
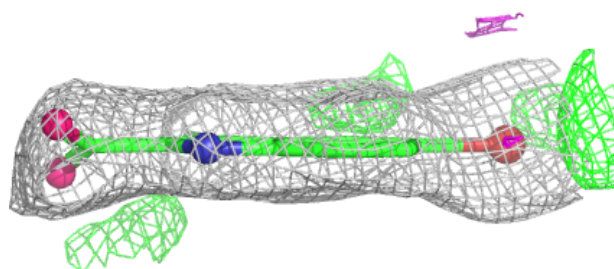
**Electron density around V6V B 307:**

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

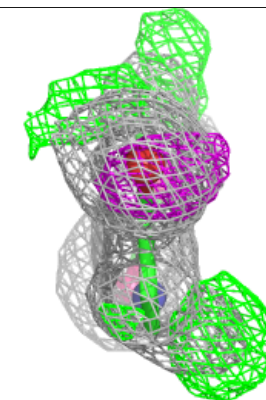
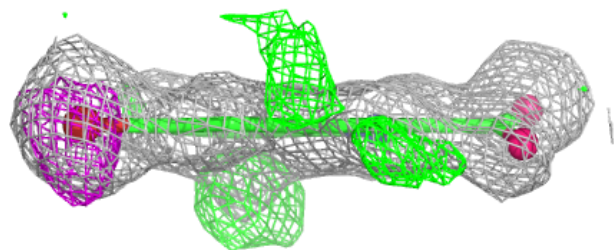
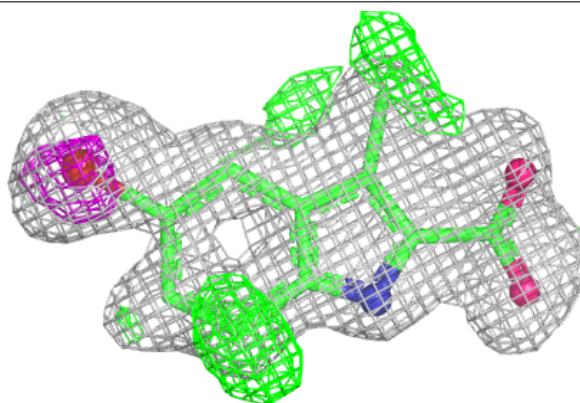


Electron density around V6V B 308:

$2mF_o-DF_c$ (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)



6.5 Other polymers [i](#)

There are no such residues in this entry.