



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 05:48 AM UTC

PDB ID : 6XQ3 / pdb_00006xq3
Title : Receptor for Advanced Glycation End Products VC1 domain in complex with 3-(3-(((3-(4-Carboxyphenoxy)benzyl)oxy)methyl)phenyl)-1H-indole-2-carboxylic acid
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Deposited on : 2020-07-09
Resolution : 1.71 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](#) ①) 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

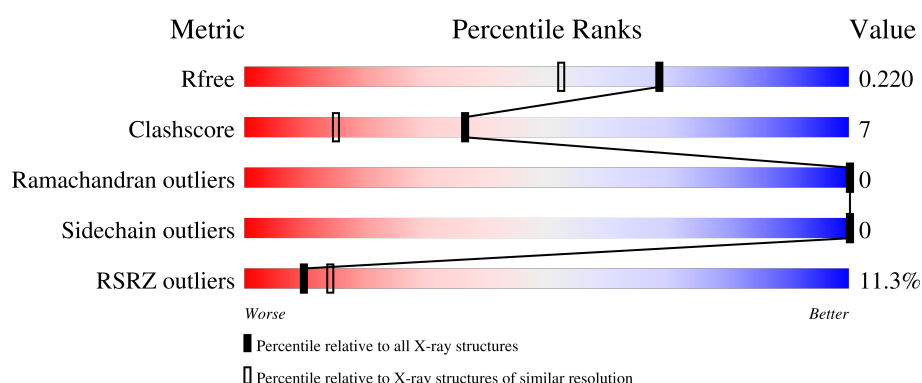
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.71 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	1039 (1.72-1.72)
Clashscore	190562	1049 (1.72-1.72)
Ramachandran outliers	187476	1041 (1.72-1.72)
Sidechain outliers	187428	1041 (1.72-1.72)
RSRZ outliers	180081	1039 (1.72-1.72)

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	11% 89% 10%
1	B	212	11% 87% 13%

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
4	V6Y	A	306	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 3678 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.

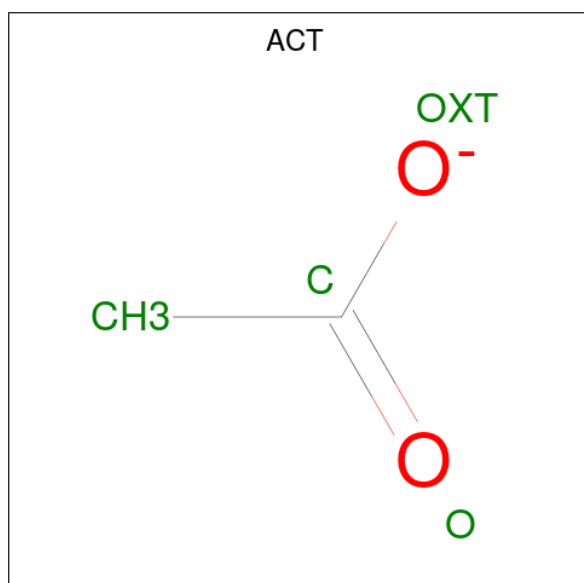
- Molecule 1 is a protein called Advanced glycosylation end product-specific receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	212	Total	C	N	O	S	0	10	0
			1619	1024	287	301	7			
1	B	212	Total	C	N	O	S	0	9	0
			1641	1037	298	299	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).

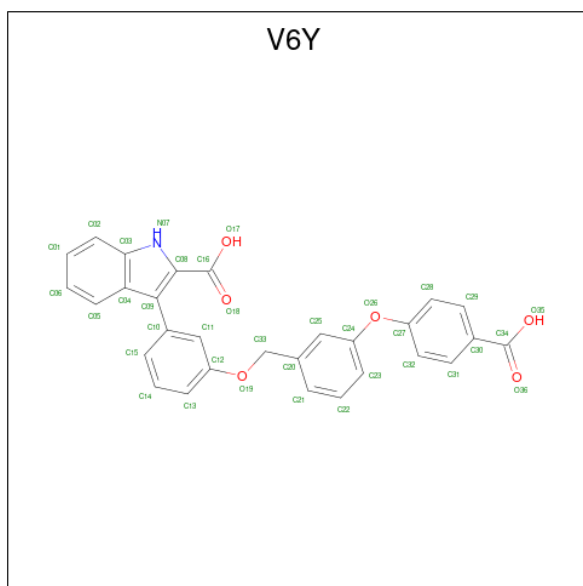


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Cl 1 1	0	0
3	B	1	Total Cl 1 1	0	0

- Molecule 4 is 3-(3-{[3-(4-carboxyphenoxy)phenyl]methoxy}phenyl)-1H-indole-2-carboxylic acid (CCD ID: V6Y) (formula: C₂₉H₂₁NO₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 36 29 1 6	0	0
4	A	1	Total C N O 36 29 1 6	0	0
4	B	1	Total C N O 36 29 1 6	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			36	29	1	6		

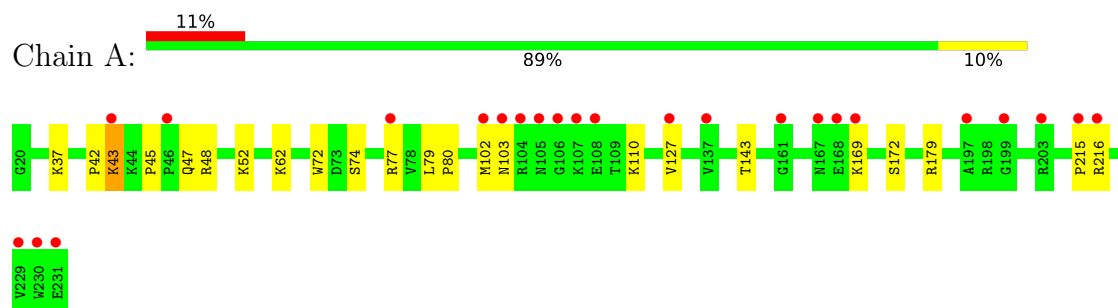
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	128	Total	O	0	0
			128	128		
5	B	128	Total	O	0	0
			128	128		

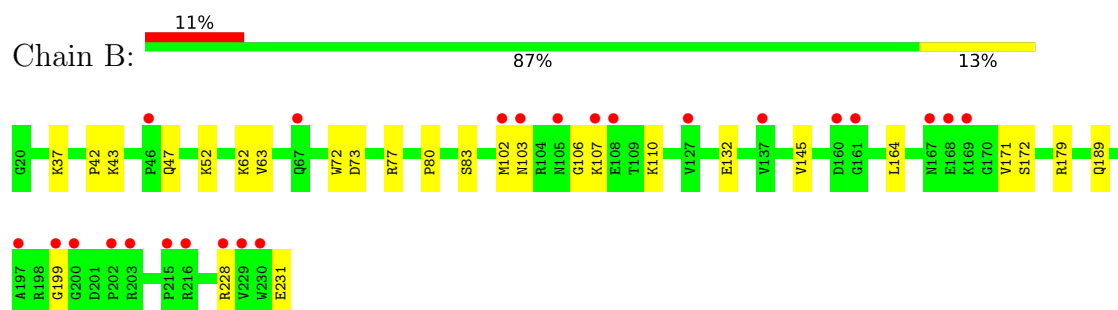
3 Residue-property plots [i](#)

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, α , β , γ	102.47Å 102.47Å 101.81Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.68 – 1.71 40.68 – 1.71	Depositor EDS
% Data completeness (in resolution range)	98.7 (40.68-1.71) 98.9 (40.68-1.71)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.02 (at 1.71Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.192 , 0.220 0.193 , 0.220	Depositor DCC
R_{free} test set	3191 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	20.5	Xtriage
Anisotropy	0.459	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 41.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.488 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3678	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% 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: ACT, CL, V6Y

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	0.81	0/1693	0.92	1/2313 (0.0%)
1	B	0.81	0/1712	0.90	0/2333
All	All	0.81	0/3405	0.91	1/4646 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	43	LYS	CD-CE-NZ	-9.02	83.03	111.90

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	1619	0	1585	21	1
1	B	1641	0	1632	22	1
2	A	12	0	9	1	0
2	B	4	0	3	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	72	0	0	14	0
4	B	72	0	0	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	128	0	0	5	1
5	B	128	0	0	3	1
All	All	3678	0	3229	48	2

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 (48) 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:110:LYS:NZ	4:B:303:V6Y:O17	2.03	0.91
2:A:303:ACT:OXT	5:A:401:HOH:O	1.98	0.82
4:A:306:V6Y:C33	4:B:304:V6Y:C31	2.62	0.78
1:B:43:LYS:NZ	5:B:401:HOH:O	2.25	0.69
1:B:172:SER:HB3	5:B:462:HOH:O	1.98	0.63
1:A:79:LEU:HD23	4:A:306:V6Y:C21	2.30	0.60
1:A:43:LYS:NZ	5:A:402:HOH:O	2.31	0.59
1:A:45:PRO:CG	4:A:306:V6Y:N07	2.69	0.56
1:A:62:LYS:HE2	1:A:72:TRP:CD1	2.40	0.56
1:B:52:LYS:HD3	4:B:303:V6Y:C01	2.36	0.55
1:B:73:ASP:O	4:B:304:V6Y:C23	2.54	0.55
1:A:110:LYS:HE3	4:A:305:V6Y:O18	2.08	0.54
4:A:306:V6Y:O26	4:B:304:V6Y:C33	2.56	0.54
1:A:79:LEU:HD23	4:A:306:V6Y:C22	2.39	0.53
1:B:132[A]:GLU:OE2	1:B:228:ARG:NH2	2.41	0.53
1:A:48:ARG:NH2	1:A:103:ASN:O	2.42	0.53
1:A:45:PRO:HG3	4:A:306:V6Y:N07	2.23	0.52
1:A:80:PRO:HA	4:A:306:V6Y:O18	2.10	0.52
1:B:62:LYS:HE2	1:B:72:TRP:CD1	2.45	0.52
1:A:42:PRO:HD2	1:A:47:GLN:HG2	1.92	0.51
4:B:304:V6Y:C20	4:B:304:V6Y:C13	2.86	0.50
1:A:77:ARG:HB3	4:A:306:V6Y:C23	2.42	0.50
1:A:48:ARG:NH1	1:A:102:MET:SD	2.85	0.49
1:A:52:LYS:HD3	4:A:305:V6Y:C01	2.43	0.49
1:A:37:LYS:HD2	5:A:435:HOH:O	2.13	0.48
1:B:52:LYS:HG2	1:B:63:VAL:HG22	1.97	0.47
4:A:306:V6Y:C33	4:B:304:V6Y:C32	2.93	0.47
1:A:77:ARG:HB3	4:A:306:V6Y:C22	2.44	0.46
1:A:74:SER:HA	4:A:306:V6Y:O35	2.16	0.46
1:B:42:PRO:HD2	1:B:47:GLN:HG2	1.98	0.46
1:B:37:LYS:HD3	1:B:37:LYS:HA	1.60	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:199:GLY:N	1:B:231:GLU:OE1	2.48	0.45
1:B:37:LYS:HD2	5:B:490:HOH:O	2.16	0.44
1:B:164:LEU:HD22	1:B:171:VAL:HG21	1.99	0.44
1:B:37:LYS:HD3	1:B:83:SER:OG	2.18	0.43
1:B:145:VAL:HG22	1:B:189:GLN:HG2	2.00	0.43
1:A:169:LYS:N	5:A:408:HOH:O	2.52	0.42
1:B:77:ARG:HD3	4:B:304:V6Y:C13	2.48	0.42
1:A:215:PRO:O	1:A:216:ARG:HB2	2.18	0.42
1:B:103:ASN:ND2	1:B:107:LYS:HB3	2.35	0.42
1:B:102:MET:SD	1:B:106:GLY:HA2	2.59	0.42
1:A:80:PRO:HG3	4:A:306:V6Y:O18	2.20	0.41
1:B:199:GLY:H	1:B:231:GLU:CD	2.27	0.41
1:A:127:VAL:HG23	1:A:143:THR:HB	2.01	0.41
1:B:52:LYS:HD3	4:B:303:V6Y:C02	2.51	0.41
1:B:102:MET:HE2	1:B:102:MET:HB2	1.89	0.41
1:B:80:PRO:HG3	4:B:304:V6Y:C02	2.49	0.40
1:A:172[B]:SER:HB3	5:A:412:HOH:O	2.22	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:ARG:NH1	5:B:508:HOH:O[2_454]	2.11	0.09
1:B:179[B]:ARG:NH2	5:A:511:HOH:O[3_445]	2.13	0.07

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	220/212 (104%)	219 (100%)	1 (0%)	0	100 100
1	B	219/212 (103%)	218 (100%)	1 (0%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	439/424 (104%)	437 (100%)	2 (0%)	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	173/176 (98%)	173 (100%)	0	100	100
1	B	176/176 (100%)	176 (100%)	0	100	100
All	All	349/352 (99%)	349 (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 (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	GLN
1	A	226	GLN
1	B	100	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

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 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
4	V6Y	B	303	-	40,40,40	1.63	6 (15%)	55,56,56	1.53	10 (18%)
2	ACT	A	303	-	3,3,3	2.45	2 (66%)	3,3,3	1.22	0
4	V6Y	A	305	-	40,40,40	1.74	7 (17%)	55,56,56	1.30	7 (12%)
2	ACT	A	302	-	3,3,3	1.11	0	3,3,3	1.43	0
4	V6Y	B	304	-	40,40,40	1.62	5 (12%)	55,56,56	2.86	25 (45%)
2	ACT	A	301	-	3,3,3	1.85	1 (33%)	3,3,3	1.17	0
2	ACT	B	301	-	3,3,3	1.50	1 (33%)	3,3,3	1.01	0
4	V6Y	A	306	-	40,40,40	1.48	6 (15%)	55,56,56	2.83	22 (40%)

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
4	V6Y	B	303	-	-	8/21/21/21	0/5/5/5
4	V6Y	A	305	-	-	8/21/21/21	0/5/5/5
4	V6Y	B	304	-	-	7/21/21/21	0/5/5/5
4	V6Y	A	306	-	-	10/21/21/21	0/5/5/5

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	304	V6Y	C04-C09	-6.57	1.32	1.47
4	A	305	V6Y	C04-C09	-5.36	1.35	1.47
4	B	303	V6Y	C04-C09	-5.33	1.35	1.47
4	A	306	V6Y	C04-C09	-4.46	1.37	1.47
4	B	303	V6Y	C08-C16	4.16	1.54	1.48
4	A	305	V6Y	C08-C16	3.82	1.54	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	305	V6Y	C10-C09	3.71	1.55	1.49
4	A	305	V6Y	O35-C34	-3.66	1.19	1.30
4	B	303	V6Y	C10-C09	3.61	1.55	1.49
4	B	304	V6Y	C04-C03	-3.37	1.37	1.41
4	A	306	V6Y	C03-N07	-3.23	1.32	1.38
4	A	305	V6Y	C15-C10	3.07	1.44	1.39
2	A	303	ACT	CH3-C	3.06	1.61	1.49
4	A	306	V6Y	C08-C16	2.94	1.52	1.48
2	A	303	ACT	O-C	2.87	1.34	1.22
4	B	304	V6Y	C08-C16	2.75	1.52	1.48
4	B	304	V6Y	C30-C34	2.73	1.55	1.49
4	A	306	V6Y	C09-C08	-2.70	1.35	1.38
4	A	306	V6Y	C08-N07	-2.64	1.34	1.38
2	A	301	ACT	CH3-C	2.64	1.59	1.49
4	A	306	V6Y	C30-C34	2.46	1.54	1.49
4	B	303	V6Y	C15-C10	2.37	1.43	1.39
2	B	301	ACT	CH3-C	2.35	1.58	1.49
4	A	305	V6Y	C03-N07	-2.33	1.34	1.38
4	B	303	V6Y	C31-C30	2.25	1.42	1.39
4	B	303	V6Y	C03-N07	-2.24	1.34	1.38
4	B	304	V6Y	O36-C34	2.17	1.29	1.22
4	A	305	V6Y	C29-C30	2.07	1.42	1.39

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	306	V6Y	C10-C09-C08	-7.81	111.35	127.68
4	A	306	V6Y	C16-C08-N07	7.66	130.76	121.22
4	B	304	V6Y	C15-C10-C09	-7.56	107.88	120.91
4	A	306	V6Y	C04-C09-C10	7.17	140.82	123.61
4	B	304	V6Y	C04-C09-C08	6.73	109.61	106.06
4	A	306	V6Y	O17-C16-C08	6.43	126.93	116.73
4	B	304	V6Y	C33-O19-C12	-5.92	103.52	117.62
4	B	304	V6Y	C10-C11-C12	-5.85	113.51	119.56
4	B	303	V6Y	O35-C34-C30	5.24	128.28	114.84
4	B	304	V6Y	C27-O26-C24	-5.17	106.97	118.78
4	A	306	V6Y	C33-C20-C21	-4.96	109.22	120.64
4	B	304	V6Y	C11-C10-C09	4.66	128.14	120.62
4	B	304	V6Y	O19-C33-C20	4.58	122.61	109.16
4	B	304	V6Y	C16-C08-N07	4.51	126.83	121.22
4	A	306	V6Y	O18-C16-C08	-4.28	112.75	120.20
4	B	304	V6Y	C15-C10-C11	4.08	123.97	119.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	303	V6Y	C28-C29-C30	-3.98	116.54	120.80
4	B	304	V6Y	C09-C08-N07	-3.97	106.88	109.80
4	B	304	V6Y	C15-C14-C13	-3.93	115.19	120.24
4	A	306	V6Y	C31-C32-C27	3.76	124.03	119.73
4	A	306	V6Y	C33-C20-C25	3.69	128.98	120.30
4	A	305	V6Y	C03-C04-C09	3.68	109.23	106.92
4	A	306	V6Y	C24-C25-C20	-3.67	115.74	119.76
4	B	303	V6Y	C03-C04-C09	3.61	109.19	106.92
4	A	305	V6Y	C32-C31-C30	-3.61	116.95	120.80
4	B	304	V6Y	C32-C31-C30	3.47	124.51	120.80
4	B	304	V6Y	C23-C24-C25	-3.41	115.91	120.50
4	A	306	V6Y	C04-C09-C08	3.36	107.83	106.06
4	B	304	V6Y	C22-C23-C24	3.23	123.87	118.98
4	B	303	V6Y	O17-C16-C08	3.19	121.79	116.73
4	B	304	V6Y	C05-C04-C03	3.18	122.13	118.84
4	A	306	V6Y	C02-C03-C04	3.17	125.25	122.19
4	B	304	V6Y	C32-C27-C28	-3.13	115.59	120.16
4	B	304	V6Y	C29-C28-C27	3.13	123.30	119.73
4	B	303	V6Y	O35-C34-O36	-3.12	116.64	123.35
4	A	305	V6Y	O35-C34-O36	-3.12	116.64	123.35
4	B	304	V6Y	C02-C03-C04	-3.02	119.27	122.19
4	A	306	V6Y	C29-C30-C34	2.94	126.19	120.37
4	B	304	V6Y	C14-C13-C12	2.94	123.42	118.98
4	A	306	V6Y	O35-C34-C30	2.91	122.30	114.84
4	A	306	V6Y	C09-C08-N07	-2.90	107.66	109.80
4	B	304	V6Y	C21-C20-C25	2.89	122.54	118.55
4	A	306	V6Y	O35-C34-O36	-2.86	117.21	123.35
4	A	306	V6Y	C27-O26-C24	2.77	125.12	118.78
4	A	306	V6Y	C01-C06-C05	2.68	123.55	120.24
4	B	303	V6Y	C31-C30-C29	2.63	121.91	118.57
4	B	304	V6Y	C31-C30-C29	-2.57	115.30	118.57
4	A	306	V6Y	C31-C30-C34	-2.55	115.32	120.37
4	A	305	V6Y	C31-C30-C29	2.47	121.70	118.57
4	B	303	V6Y	O36-C34-C30	-2.44	115.06	121.46
4	A	306	V6Y	C21-C20-C25	2.35	121.79	118.55
4	B	304	V6Y	C29-C30-C34	2.32	124.96	120.37
4	B	304	V6Y	C22-C21-C20	-2.31	117.36	120.61
4	A	305	V6Y	C10-C11-C12	2.29	121.93	119.56
4	A	305	V6Y	O17-C16-O18	-2.25	118.53	123.90
4	B	304	V6Y	O26-C24-C25	2.20	126.07	119.16
4	B	303	V6Y	C10-C11-C12	2.19	121.82	119.56
4	A	306	V6Y	O26-C24-C25	2.18	125.99	119.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	305	V6Y	O36-C34-C30	2.17	127.14	121.46
4	A	306	V6Y	C05-C04-C03	-2.15	116.62	118.84
4	B	303	V6Y	C27-O26-C24	-2.14	113.89	118.78
4	B	303	V6Y	O17-C16-O18	-2.07	118.98	123.90
4	B	304	V6Y	O35-C34-C30	2.04	120.08	114.84
4	A	306	V6Y	C32-C31-C30	-2.03	118.63	120.80

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	305	V6Y	C09-C08-C16-O17
4	A	305	V6Y	N07-C08-C16-O17
4	A	305	V6Y	N07-C08-C16-O18
4	A	306	V6Y	C09-C08-C16-O17
4	A	306	V6Y	C09-C08-C16-O18
4	A	306	V6Y	N07-C08-C16-O17
4	A	306	V6Y	N07-C08-C16-O18
4	B	303	V6Y	C09-C08-C16-O17
4	B	303	V6Y	N07-C08-C16-O17
4	B	303	V6Y	N07-C08-C16-O18
4	B	304	V6Y	C29-C30-C34-O35
4	B	304	V6Y	C29-C30-C34-O36
4	B	304	V6Y	C31-C30-C34-O36
4	B	304	V6Y	C31-C30-C34-O35
4	A	306	V6Y	C31-C30-C34-O35
4	A	306	V6Y	C29-C30-C34-O36
4	A	306	V6Y	C31-C30-C34-O36
4	A	306	V6Y	C29-C30-C34-O35
4	A	305	V6Y	C31-C30-C34-O36
4	B	303	V6Y	C31-C30-C34-O35
4	A	305	V6Y	C29-C30-C34-O36
4	A	305	V6Y	C31-C30-C34-O35
4	B	303	V6Y	C29-C30-C34-O35
4	A	305	V6Y	C29-C30-C34-O35
4	B	303	V6Y	C29-C30-C34-O36
4	B	303	V6Y	C31-C30-C34-O36
4	A	305	V6Y	C09-C08-C16-O18
4	B	303	V6Y	C09-C08-C16-O18
4	A	306	V6Y	C11-C12-O19-C33
4	A	306	V6Y	C13-C12-O19-C33
4	B	304	V6Y	C11-C12-O19-C33

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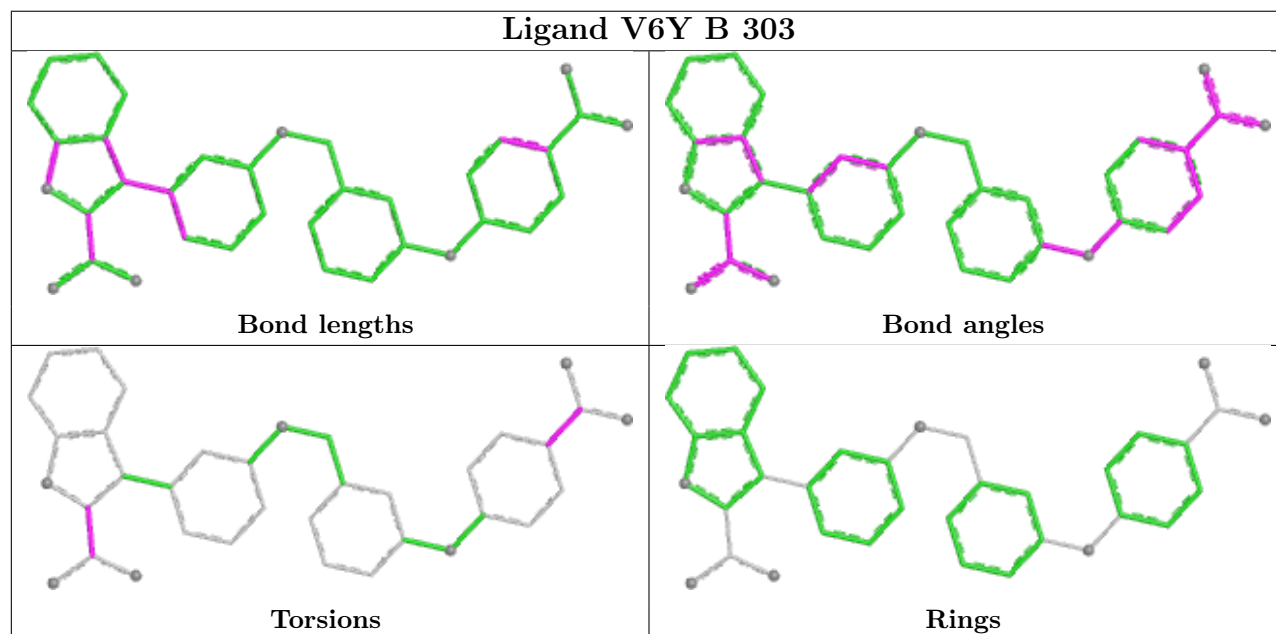
Mol	Chain	Res	Type	Atoms
4	B	304	V6Y	C13-C12-O19-C33
4	B	304	V6Y	C20-C33-O19-C12

There are no ring outliers.

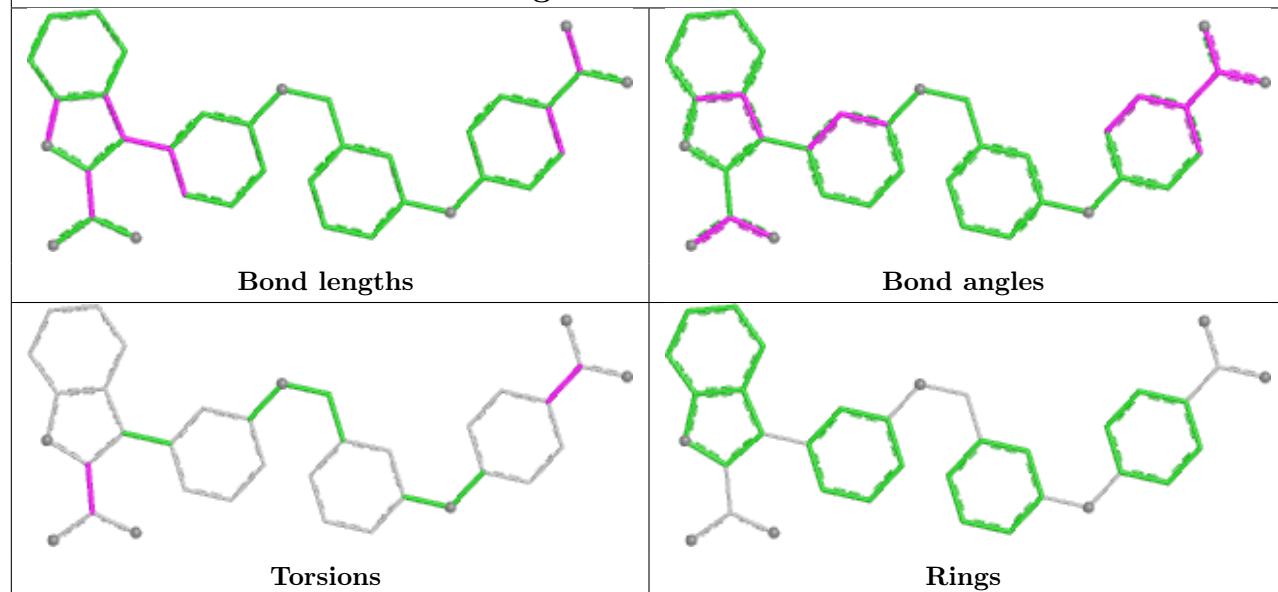
5 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	303	V6Y	3	0
2	A	303	ACT	1	0
4	A	305	V6Y	2	0
4	B	304	V6Y	7	0
4	A	306	V6Y	12	0

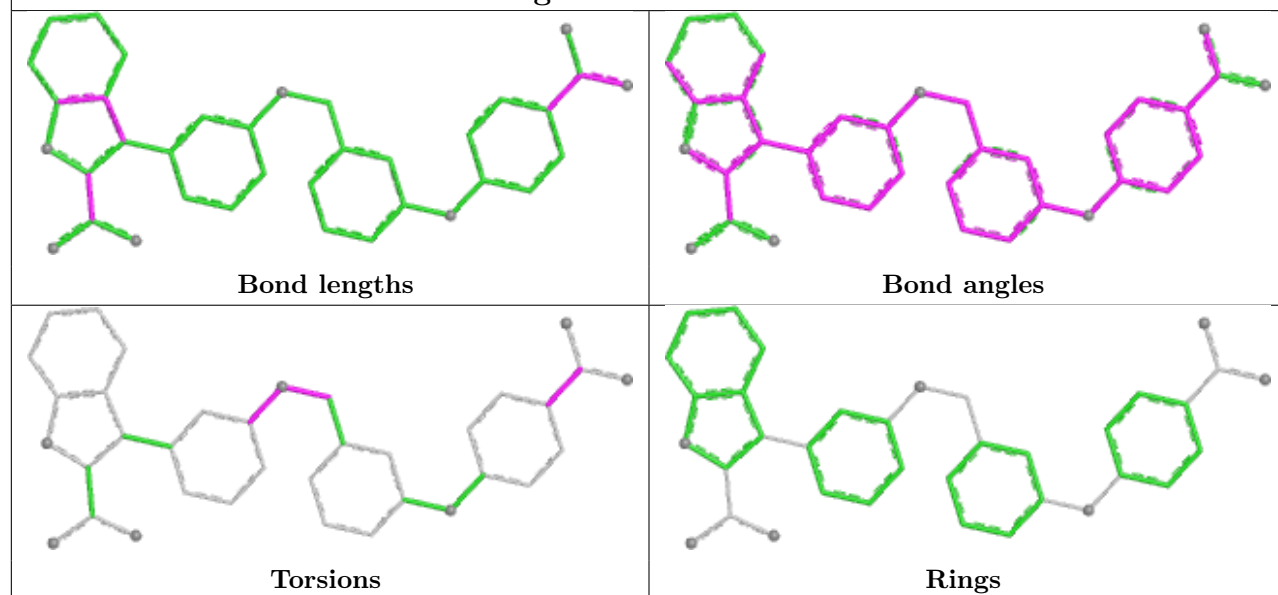
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

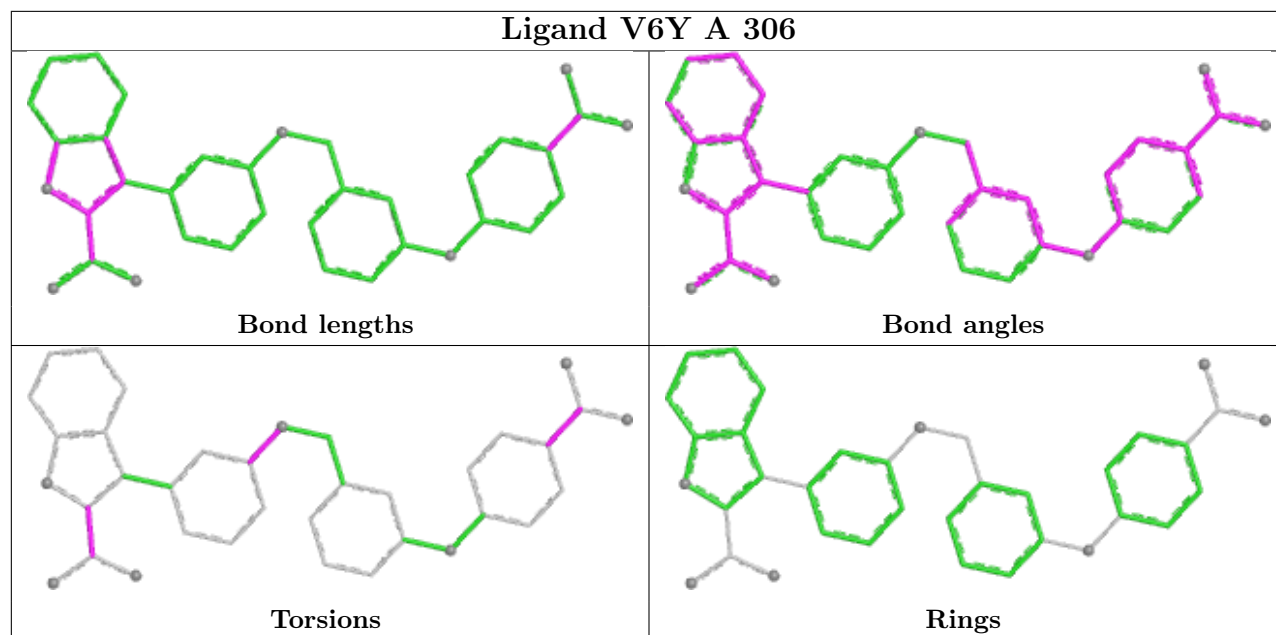


Ligand V6Y A 305



Ligand V6Y B 304





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, 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%)	0.61	24 (11%)	10 14	11, 27, 58, 69	10 (4%)
1	B	212/212 (100%)	0.59	24 (11%)	10 14	11, 27, 58, 72	9 (4%)
All	All	424/424 (100%)	0.60	48 (11%)	10 14	11, 27, 58, 72	19 (4%)

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	230	TRP	10.9
1	B	230	TRP	10.0
1	B	105	ASN	5.1
1	A	105	ASN	5.0
1	B	102	MET	4.6
1	A	46	PRO	4.5
1	B	46	PRO	4.5
1	A	102	MET	4.4
1	B	167	ASN	4.3
1	A	197	ALA	4.0
1	A	216	ARG	3.6
1	A	167	ASN	3.5
1	B	161	GLY	3.5
1	A	169	LYS	3.1
1	B	199	GLY	3.1
1	B	197	ALA	3.1
1	A	161	GLY	3.0
1	B	127	VAL	2.9
1	A	104	ARG	2.7
1	B	216	ARG	2.7
1	A	103	ASN	2.7
1	B	228	ARG	2.6
1	B	103	ASN	2.6
1	B	160	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	137	VAL	2.6
1	B	202	PRO	2.6
1	B	169	LYS	2.5
1	B	137	VAL	2.5
1	B	107	LYS	2.5
1	A	77	ARG	2.5
1	A	107	LYS	2.4
1	B	168	GLU	2.4
1	A	127	VAL	2.4
1	B	229	VAL	2.4
1	A	108	GLU	2.4
1	A	106	GLY	2.3
1	A	231	GLU	2.3
1	A	203	ARG	2.3
1	A	43	LYS	2.3
1	A	168	GLU	2.2
1	B	203	ARG	2.2
1	A	215	PRO	2.1
1	A	229	VAL	2.1
1	B	215	PRO	2.1
1	A	199	GLY	2.1
1	B	200	GLY	2.1
1	B	67	GLN	2.1
1	B	108	GLU	2.0

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](#)

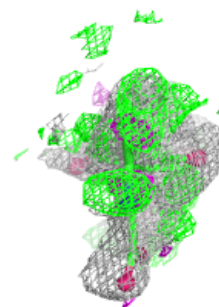
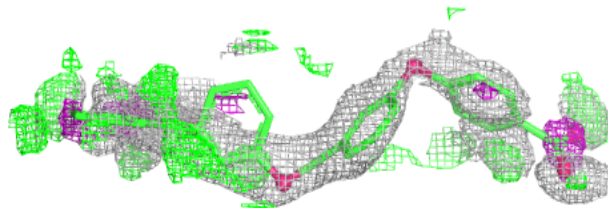
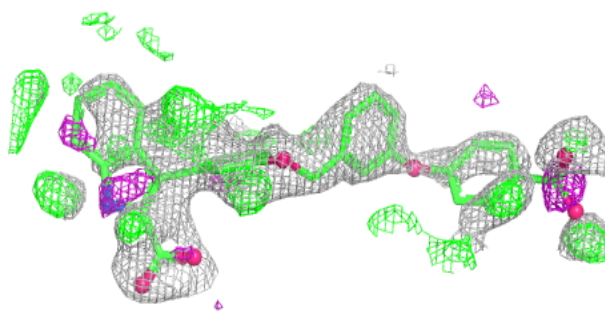
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	V6Y	B	304	36/36	0.66	0.33	44,54,68,70	36
4	V6Y	A	306	36/36	0.67	0.31	37,53,64,66	36
4	V6Y	B	303	36/36	0.85	0.15	21,36,52,54	36
4	V6Y	A	305	36/36	0.85	0.16	21,35,57,58	36
2	ACT	A	303	4/4	0.91	0.19	23,36,42,47	0
2	ACT	A	302	4/4	0.94	0.13	27,29,31,37	0
2	ACT	A	301	4/4	0.97	0.06	24,26,26,27	0
2	ACT	B	301	4/4	0.97	0.06	26,27,28,28	0
3	CL	A	304	1/1	0.99	0.05	25,25,25,25	0
3	CL	B	302	1/1	0.99	0.04	24,24,24,24	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.

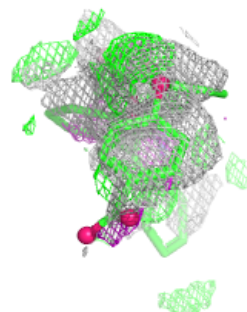
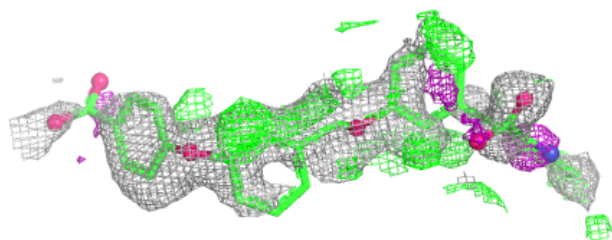
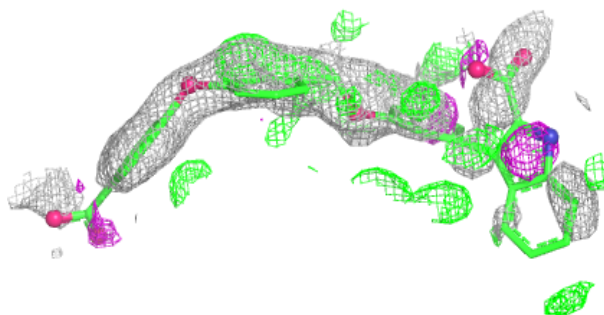
Electron density around V6Y B 304:

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

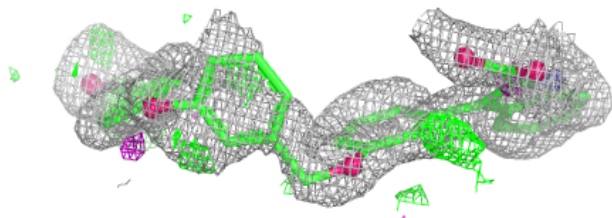
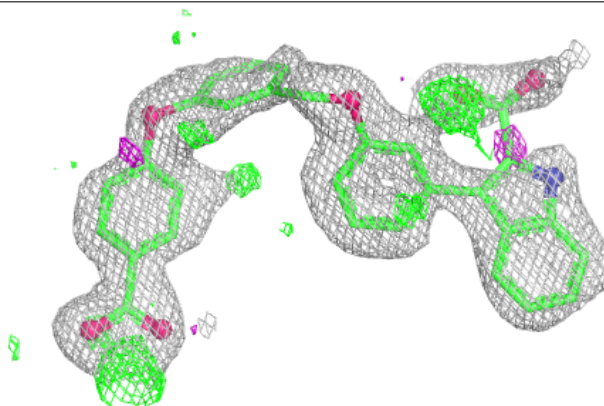


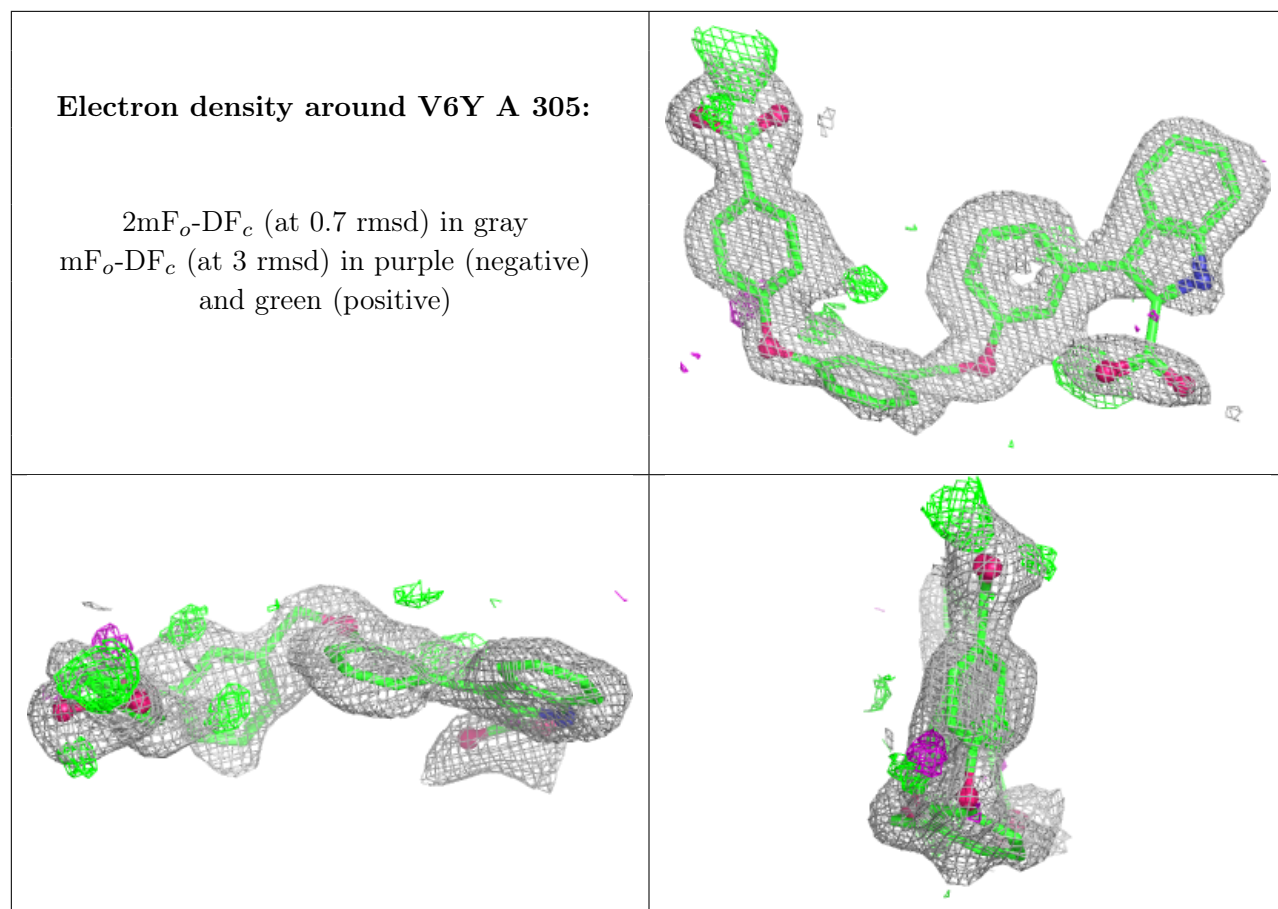
Electron density around V6Y A 306:

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

**Electron density around V6Y B 303:**

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





6.5 Other polymers ⓘ

There are no such residues in this entry.