



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 04:04 am BST

PDB ID : 6DF6
Title : Crystal structure of estrogen receptor alpha in complex with receptor degrader 16ab
Authors : Kiefer, J.R.; Vinogradova, M.; Liang, J.; Zhang, B.; Ortwine, D.F.; Nettles, K.W.; Nwachukwu, J.C.
Deposited on : 2018-05-14
Resolution : 2.50 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 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 : 2.11
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) : 2.11

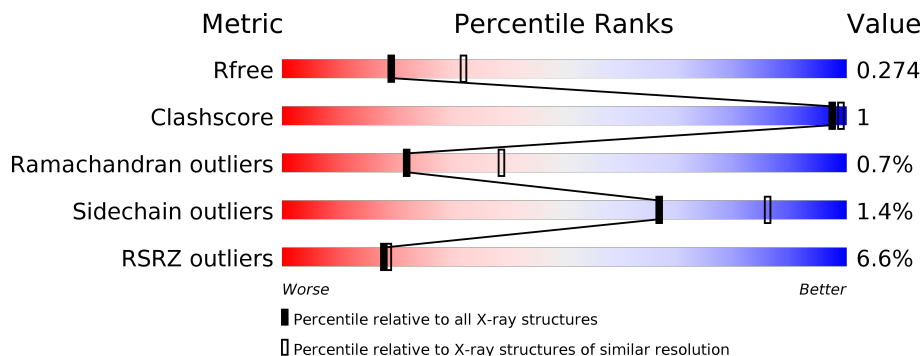
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	280	 5% 81% 16%
1	B	280	 6% 76% 21%
1	C	280	 5% 80% 17%
1	D	280	 6% 79% 18%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	D	602	-	-	-	X

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 7353 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 Estrogen receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	235	Total 1848	C 1184	N 311	O 335	S 18	0	1	0
1	B	220	Total 1710	C 1094	N 296	O 304	S 16	0	1	0
1	C	233	Total 1820	C 1168	N 306	O 328	S 18	0	0	0
1	D	231	Total 1799	C 1150	N 308	O 324	S 17	0	1	0

There are 104 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	274	MET	-	initiating methionine	UNP P03372
A	275	HIS	-	expression tag	UNP P03372
A	276	HIS	-	expression tag	UNP P03372
A	277	HIS	-	expression tag	UNP P03372
A	278	HIS	-	expression tag	UNP P03372
A	279	HIS	-	expression tag	UNP P03372
A	280	HIS	-	expression tag	UNP P03372
A	281	SER	-	expression tag	UNP P03372
A	282	SER	-	expression tag	UNP P03372
A	283	GLY	-	expression tag	UNP P03372
A	284	VAL	-	expression tag	UNP P03372
A	285	ASP	-	expression tag	UNP P03372
A	286	LEU	-	expression tag	UNP P03372
A	287	GLY	-	expression tag	UNP P03372
A	288	THR	-	expression tag	UNP P03372
A	289	GLU	-	expression tag	UNP P03372
A	290	ASN	-	expression tag	UNP P03372
A	291	LEU	-	expression tag	UNP P03372
A	292	TYR	-	expression tag	UNP P03372
A	293	PHE	-	expression tag	UNP P03372
A	294	GLN	-	expression tag	UNP P03372

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Chain	Residue	Modelled	Actual	Comment	Reference
A	295	SER	-	expression tag	UNP P03372
A	296	ASN	-	expression tag	UNP P03372
A	297	ALA	-	expression tag	UNP P03372
A	372	SER	LEU	conflict	UNP P03372
A	536	SER	LEU	conflict	UNP P03372
B	274	MET	-	initiating methionine	UNP P03372
B	275	HIS	-	expression tag	UNP P03372
B	276	HIS	-	expression tag	UNP P03372
B	277	HIS	-	expression tag	UNP P03372
B	278	HIS	-	expression tag	UNP P03372
B	279	HIS	-	expression tag	UNP P03372
B	280	HIS	-	expression tag	UNP P03372
B	281	SER	-	expression tag	UNP P03372
B	282	SER	-	expression tag	UNP P03372
B	283	GLY	-	expression tag	UNP P03372
B	284	VAL	-	expression tag	UNP P03372
B	285	ASP	-	expression tag	UNP P03372
B	286	LEU	-	expression tag	UNP P03372
B	287	GLY	-	expression tag	UNP P03372
B	288	THR	-	expression tag	UNP P03372
B	289	GLU	-	expression tag	UNP P03372
B	290	ASN	-	expression tag	UNP P03372
B	291	LEU	-	expression tag	UNP P03372
B	292	TYR	-	expression tag	UNP P03372
B	293	PHE	-	expression tag	UNP P03372
B	294	GLN	-	expression tag	UNP P03372
B	295	SER	-	expression tag	UNP P03372
B	296	ASN	-	expression tag	UNP P03372
B	297	ALA	-	expression tag	UNP P03372
B	372	SER	LEU	conflict	UNP P03372
B	536	SER	LEU	conflict	UNP P03372
C	274	MET	-	initiating methionine	UNP P03372
C	275	HIS	-	expression tag	UNP P03372
C	276	HIS	-	expression tag	UNP P03372
C	277	HIS	-	expression tag	UNP P03372
C	278	HIS	-	expression tag	UNP P03372
C	279	HIS	-	expression tag	UNP P03372
C	280	HIS	-	expression tag	UNP P03372
C	281	SER	-	expression tag	UNP P03372
C	282	SER	-	expression tag	UNP P03372
C	283	GLY	-	expression tag	UNP P03372
C	284	VAL	-	expression tag	UNP P03372

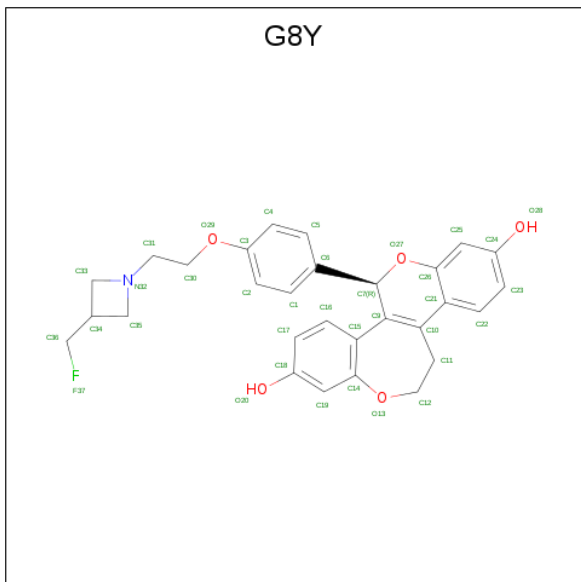
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Chain	Residue	Modelled	Actual	Comment	Reference
C	285	ASP	-	expression tag	UNP P03372
C	286	LEU	-	expression tag	UNP P03372
C	287	GLY	-	expression tag	UNP P03372
C	288	THR	-	expression tag	UNP P03372
C	289	GLU	-	expression tag	UNP P03372
C	290	ASN	-	expression tag	UNP P03372
C	291	LEU	-	expression tag	UNP P03372
C	292	TYR	-	expression tag	UNP P03372
C	293	PHE	-	expression tag	UNP P03372
C	294	GLN	-	expression tag	UNP P03372
C	295	SER	-	expression tag	UNP P03372
C	296	ASN	-	expression tag	UNP P03372
C	297	ALA	-	expression tag	UNP P03372
C	372	SER	LEU	conflict	UNP P03372
C	536	SER	LEU	conflict	UNP P03372
D	274	MET	-	initiating methionine	UNP P03372
D	275	HIS	-	expression tag	UNP P03372
D	276	HIS	-	expression tag	UNP P03372
D	277	HIS	-	expression tag	UNP P03372
D	278	HIS	-	expression tag	UNP P03372
D	279	HIS	-	expression tag	UNP P03372
D	280	HIS	-	expression tag	UNP P03372
D	281	SER	-	expression tag	UNP P03372
D	282	SER	-	expression tag	UNP P03372
D	283	GLY	-	expression tag	UNP P03372
D	284	VAL	-	expression tag	UNP P03372
D	285	ASP	-	expression tag	UNP P03372
D	286	LEU	-	expression tag	UNP P03372
D	287	GLY	-	expression tag	UNP P03372
D	288	THR	-	expression tag	UNP P03372
D	289	GLU	-	expression tag	UNP P03372
D	290	ASN	-	expression tag	UNP P03372
D	291	LEU	-	expression tag	UNP P03372
D	292	TYR	-	expression tag	UNP P03372
D	293	PHE	-	expression tag	UNP P03372
D	294	GLN	-	expression tag	UNP P03372
D	295	SER	-	expression tag	UNP P03372
D	296	ASN	-	expression tag	UNP P03372
D	297	ALA	-	expression tag	UNP P03372
D	372	SER	LEU	conflict	UNP P03372
D	536	SER	LEU	conflict	UNP P03372

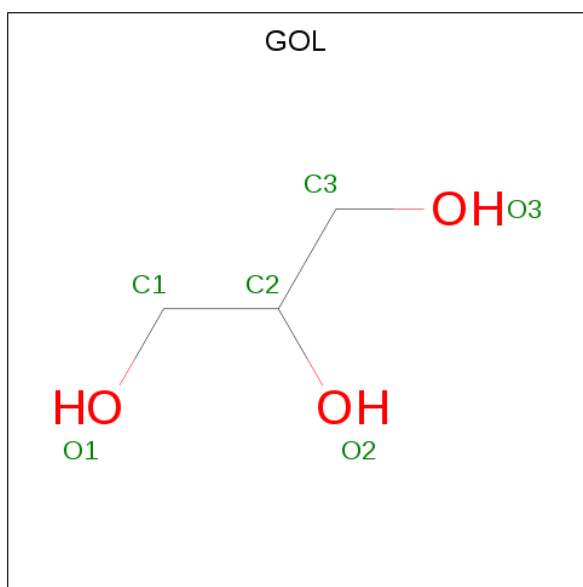
- Molecule 2 is (8R)-8-(4-{2-[3-(fluoromethyl)azetid-1-yl]ethoxy}phenyl)-1,8-dihydr

o-2H-[1]benzopyrano[4,3-d][1]benzoxepine-5,11-diol (three-letter code: G8Y) (formula: $C_{29}H_{28}FNO_5$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	F	N	O		
2	A	1	Total 36	C 29	F 1	N 1	O 5	0	0
2	B	1	Total 36	C 29	F 1	N 1	O 5	0	0
2	C	1	Total 36	C 29	F 1	N 1	O 5	0	0
2	D	1	Total 36	C 29	F 1	N 1	O 5	0	0

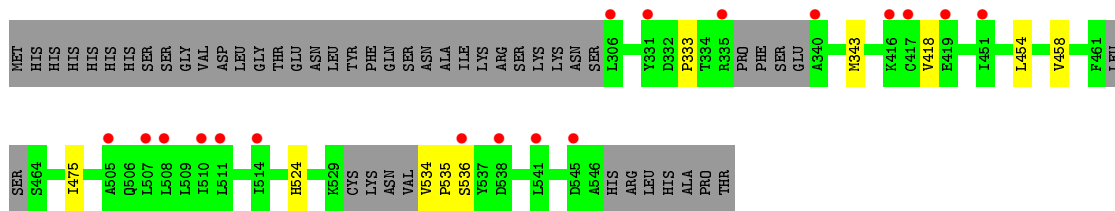
- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C O 6 3 3	0	0
3	D	1	Total C O 6 3 3	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	6	Total O 6 6	0	0
4	B	6	Total O 6 6	0	0
4	C	3	Total O 3 3	0	0
4	D	5	Total O 5 5	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	53.39Å 58.86Å 94.05Å 79.75° 75.42° 63.10°	Depositor
Resolution (Å)	35.00 – 2.50 30.26 – 2.50	Depositor EDS
% Data completeness (in resolution range)	79.7 (35.00-2.50) 79.8 (30.26-2.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.23 (at 2.51Å)	Xtrriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.218 , 0.273 0.221 , 0.274	Depositor DCC
R_{free} test set	1385 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	48.5	Xtrriage
Anisotropy	0.034	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 40.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.095 for h,h-k,h-l	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7353	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.47% 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: GOL, G8Y

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	0.36	0/1883	0.54	0/2549
1	B	0.36	0/1738	0.54	0/2349
1	C	0.38	0/1854	0.54	0/2510
1	D	0.36	0/1829	0.54	0/2474
All	All	0.36	0/7304	0.54	0/9882

There are no bond length outliers.

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	1848	0	1846	2	0
1	B	1710	0	1713	2	0
1	C	1820	0	1828	3	0
1	D	1799	0	1805	5	0
2	A	36	0	0	0	0
2	B	36	0	0	1	0
2	C	36	0	0	0	0
2	D	36	0	0	1	0
3	B	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	6	0	8	0	0
4	A	6	0	0	0	0
4	B	6	0	0	0	0
4	C	3	0	0	0	0
4	D	5	0	0	0	0
All	All	7353	0	7208	12	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 1.

All (12) 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:A:487:ILE:HD11	1:A:504:LEU:HD22	1.68	0.74
1:D:458:VAL:CG2	1:D:475:ILE:HG21	2.38	0.54
1:D:454:LEU:O	1:D:458:VAL:HG23	2.13	0.48
1:C:490:MET:HB3	1:C:495:LEU:HD12	1.98	0.44
1:A:403:LEU:HD13	1:A:409:LEU:HD13	2.03	0.41
1:B:524:HIS:ND1	2:B:601:G8Y:O28	2.50	0.41
1:D:343:MET:CE	1:D:418:VAL:HG21	2.51	0.41
1:D:458:VAL:HG21	1:D:475:ILE:HG21	2.01	0.41
1:C:310:LEU:HD22	1:C:314:GLN:HB3	2.02	0.41
1:C:388:MET:O	1:C:392:VAL:HG23	2.21	0.41
1:D:524:HIS:ND1	2:D:601:G8Y:O28	2.46	0.40
1:B:391:LEU:HD13	1:B:404:PHE:HA	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	230/280 (82%)	224 (97%)	6 (3%)	0	100	100
1	B	213/280 (76%)	209 (98%)	2 (1%)	2 (1%)	17	31
1	C	227/280 (81%)	223 (98%)	3 (1%)	1 (0%)	34	54
1	D	224/280 (80%)	218 (97%)	3 (1%)	3 (1%)	12	21
All	All	894/1120 (80%)	874 (98%)	14 (2%)	6 (1%)	22	39

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	341	SER
1	D	535	PRO
1	D	536	SER
1	B	340	ALA
1	C	419	GLU
1	D	333	PRO

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	203/252 (81%)	200 (98%)	3 (2%)	65	85
1	B	183/252 (73%)	180 (98%)	3 (2%)	62	84
1	C	200/252 (79%)	196 (98%)	4 (2%)	55	79
1	D	196/252 (78%)	195 (100%)	1 (0%)	88	96
All	All	782/1008 (78%)	771 (99%)	11 (1%)	67	86

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	416	LYS
1	A	419	GLU
1	A	441	GLN
1	B	372	SER
1	B	425	PHE

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Mol	Chain	Res	Type
1	B	544	LEU
1	C	416	LYS
1	C	417	CYS
1	C	419	GLU
1	C	538	ASP
1	D	534	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	441	GLN
1	A	519	ASN
1	B	375	GLN
1	B	519	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	G8Y	D	601	-	39,41,41	0.87	1 (2%)	43,59,59	1.25	3 (6%)
2	G8Y	B	601	-	39,41,41	0.86	2 (5%)	43,59,59	1.35	4 (9%)
3	GOL	B	602	-	5,5,5	0.33	0	5,5,5	0.28	0
3	GOL	D	602	-	5,5,5	0.34	0	5,5,5	0.24	0
2	G8Y	A	601	-	39,41,41	0.95	2 (5%)	43,59,59	1.28	4 (9%)
2	G8Y	C	601	-	39,41,41	0.89	1 (2%)	43,59,59	1.28	3 (6%)

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
2	G8Y	D	601	-	-	3/8/46/46	0/6/6/6
2	G8Y	B	601	-	-	2/8/46/46	0/6/6/6
3	GOL	B	602	-	-	2/4/4/4	-
3	GOL	D	602	-	-	2/4/4/4	-
2	G8Y	A	601	-	-	2/8/46/46	0/6/6/6
2	G8Y	C	601	-	-	3/8/46/46	0/6/6/6

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	G8Y	C15-C9	2.54	1.51	1.47
2	D	601	G8Y	C15-C9	2.49	1.51	1.47
2	B	601	G8Y	C15-C9	2.37	1.50	1.47
2	B	601	G8Y	C15-C14	2.21	1.44	1.40
2	C	601	G8Y	C15-C9	2.17	1.50	1.47
2	A	601	G8Y	C15-C14	2.05	1.44	1.40

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	G8Y	C12-O13-C14	5.57	123.78	116.03
2	A	601	G8Y	C12-O13-C14	5.01	122.99	116.03
2	C	601	G8Y	C12-O13-C14	4.43	122.18	116.03
2	D	601	G8Y	C12-O13-C14	4.23	121.91	116.03
2	C	601	G8Y	O27-C26-C21	-4.12	117.36	122.09
2	B	601	G8Y	O27-C26-C21	-3.73	117.81	122.09
2	D	601	G8Y	O27-C26-C21	-3.69	117.85	122.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	601	G8Y	O27-C26-C25	3.31	121.60	116.38
2	B	601	G8Y	O27-C26-C25	3.22	121.44	116.38
2	A	601	G8Y	O27-C26-C21	-3.17	118.46	122.09
2	C	601	G8Y	O27-C26-C25	3.05	121.19	116.38
2	A	601	G8Y	O27-C26-C25	2.37	120.11	116.38
2	B	601	G8Y	O13-C14-C19	-2.25	113.68	116.95
2	A	601	G8Y	O13-C14-C19	-2.02	114.03	116.95

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	602	GOL	O1-C1-C2-C3
2	B	601	G8Y	C2-C3-O29-C30
2	B	601	G8Y	C4-C3-O29-C30
2	D	601	G8Y	O29-C30-C31-N32
2	D	601	G8Y	C2-C3-O29-C30
2	D	601	G8Y	C4-C3-O29-C30
2	C	601	G8Y	C2-C3-O29-C30
2	C	601	G8Y	C4-C3-O29-C30
3	D	602	GOL	O1-C1-C2-C3
2	C	601	G8Y	O29-C30-C31-N32
3	B	602	GOL	O1-C1-C2-O2
3	D	602	GOL	O1-C1-C2-O2
2	A	601	G8Y	C4-C3-O29-C30
2	A	601	G8Y	C2-C3-O29-C30

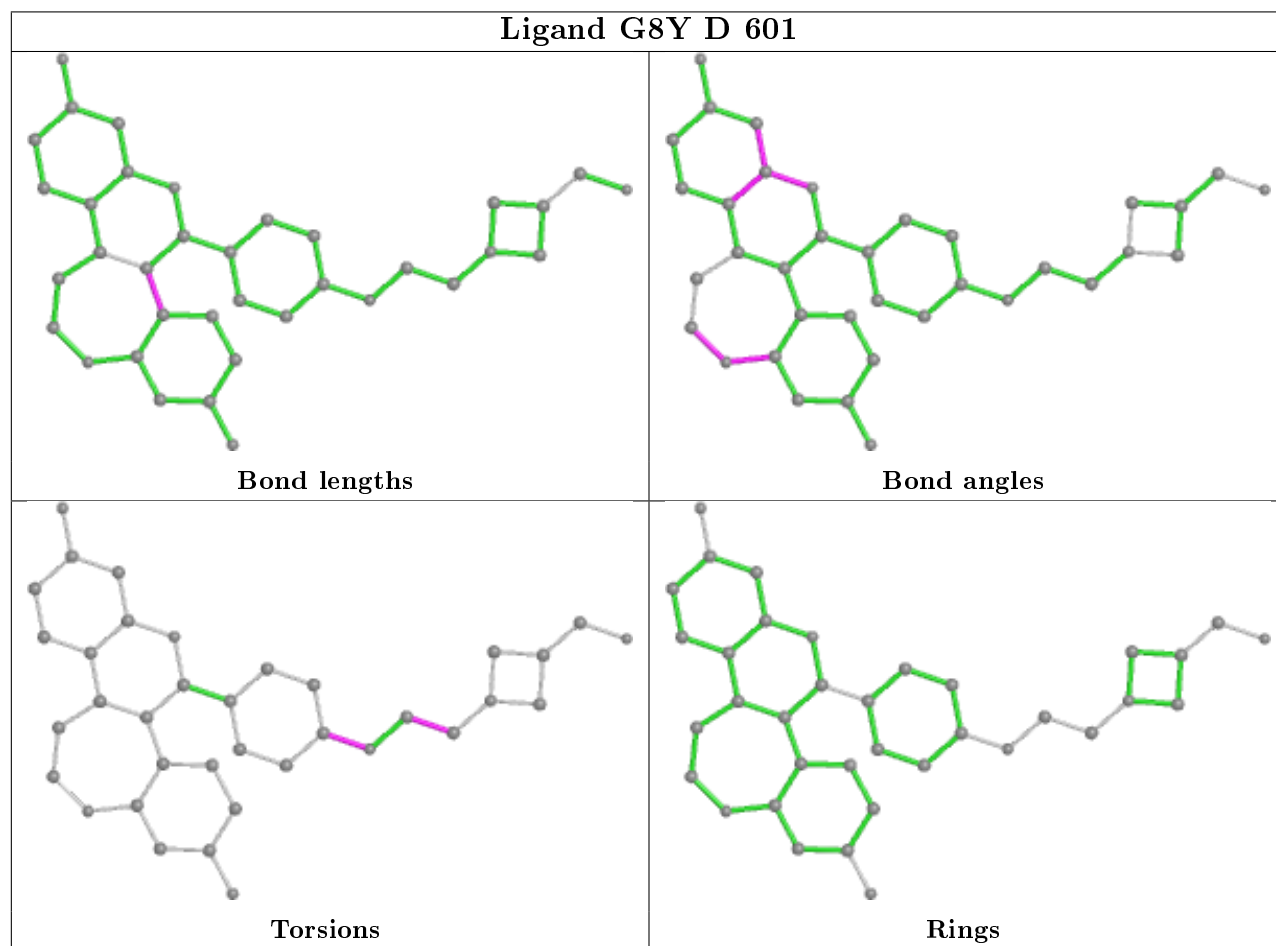
There are no ring outliers.

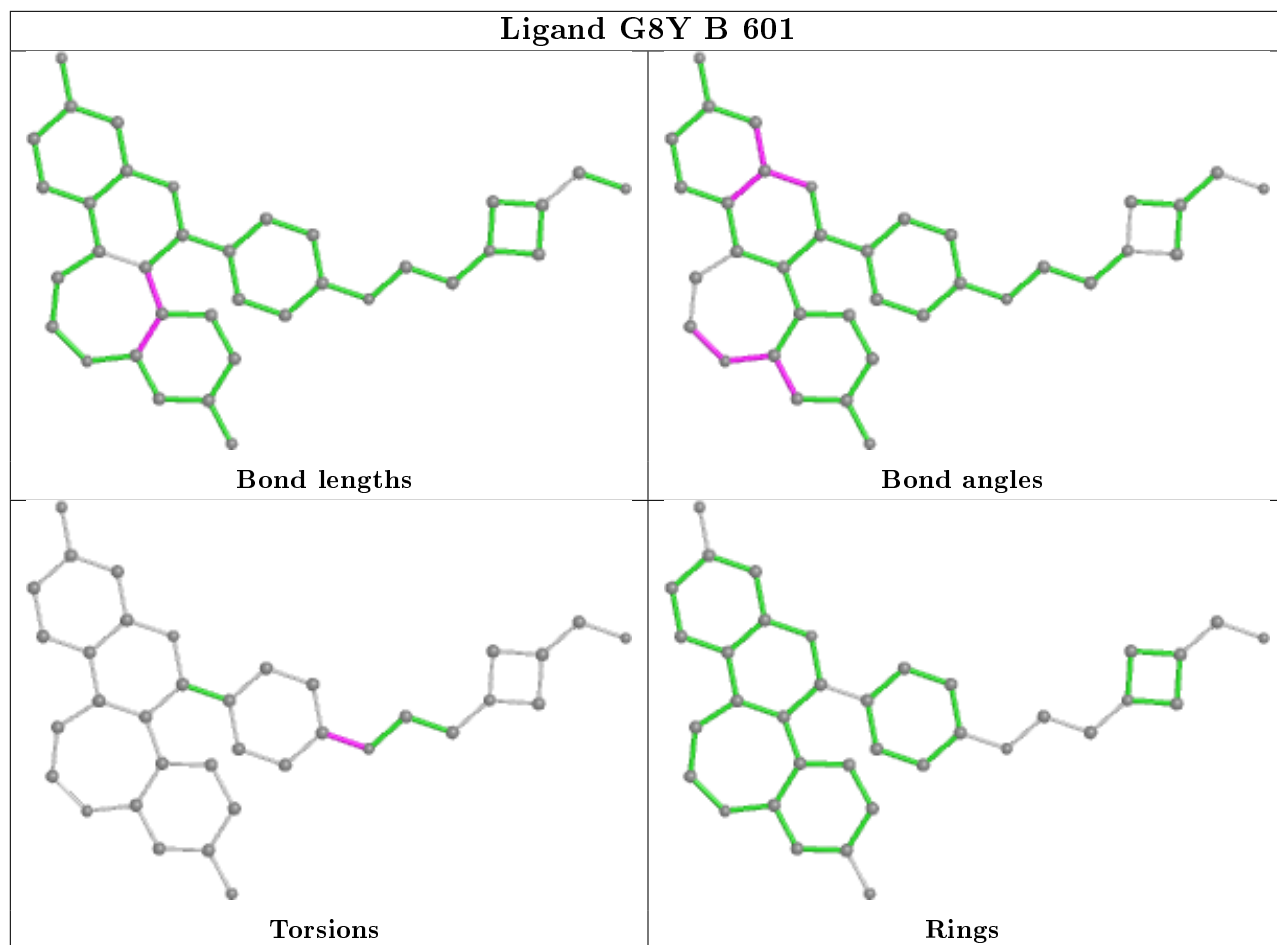
2 monomers are involved in 2 short contacts:

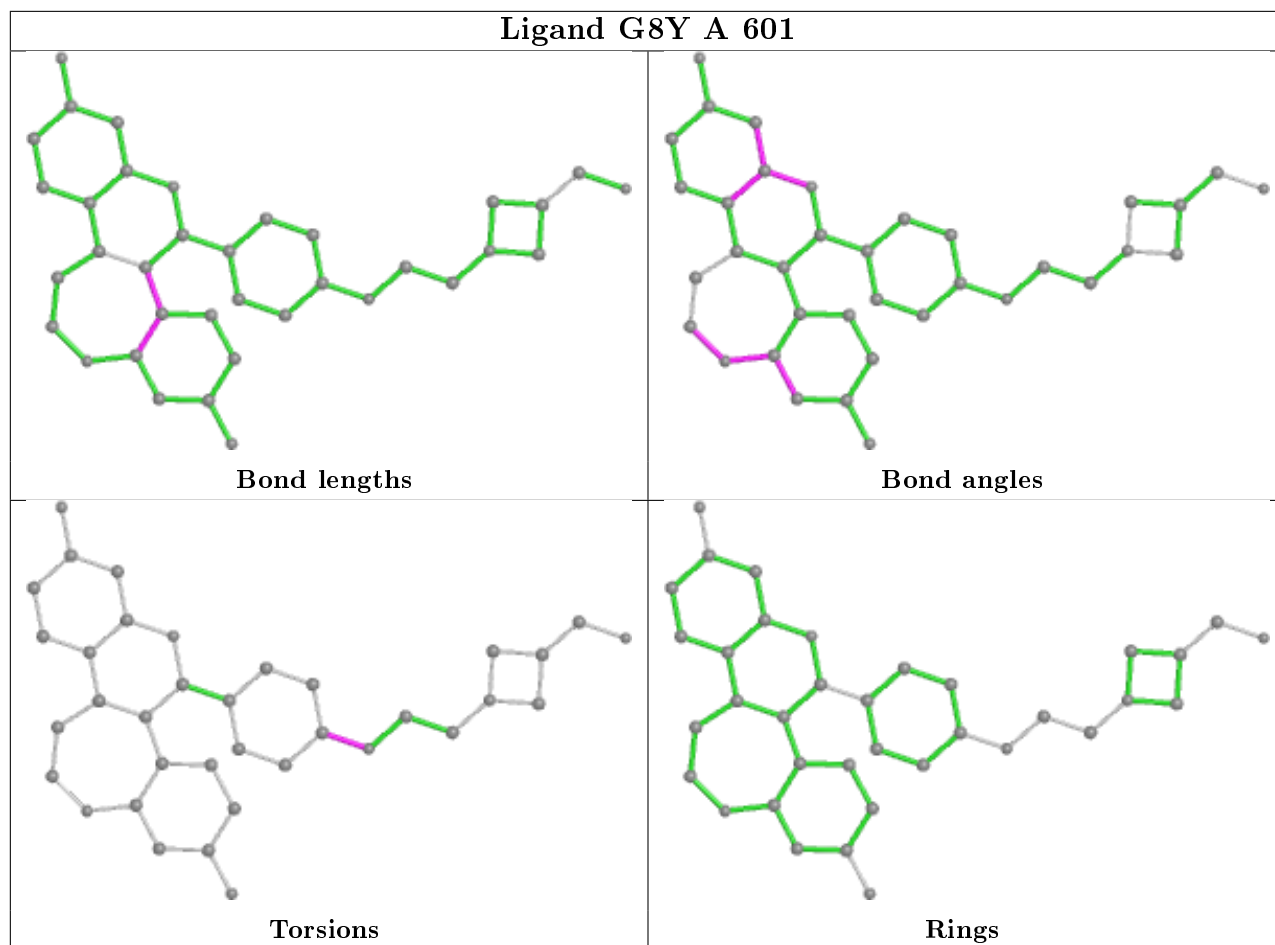
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	601	G8Y	1	0
2	B	601	G8Y	1	0

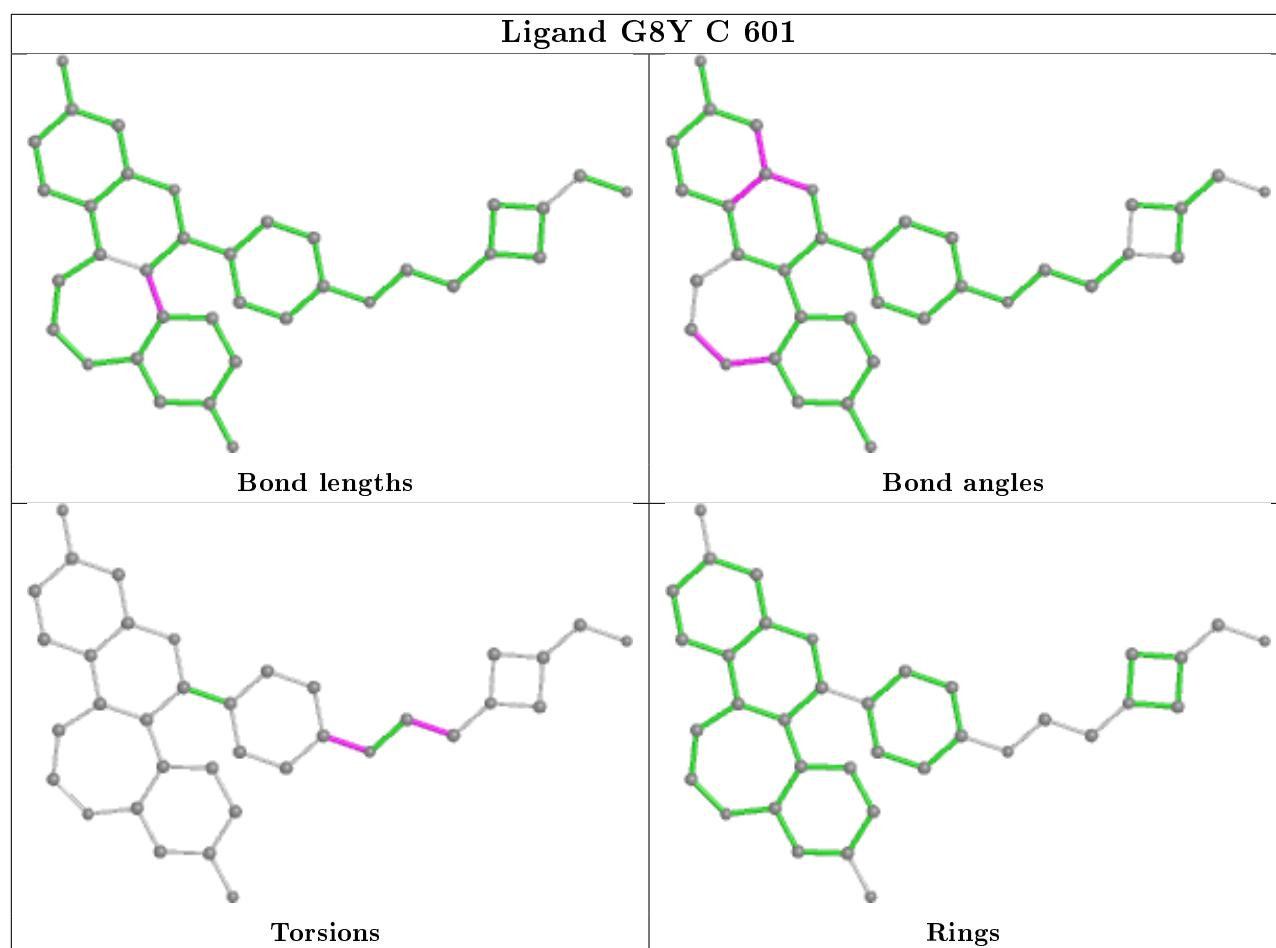
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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









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	235/280 (83%)	0.20	13 (5%) 25 26	36, 52, 78, 89	0
1	B	220/280 (78%)	0.31	16 (7%) 15 15	35, 54, 89, 103	0
1	C	233/280 (83%)	0.25	14 (6%) 21 22	35, 55, 80, 87	0
1	D	231/280 (82%)	0.39	18 (7%) 13 13	34, 55, 92, 113	0
All	All	919/1120 (82%)	0.29	61 (6%) 18 19	34, 54, 86, 113	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	340	ALA	6.7
1	B	545	ASP	4.8
1	D	511	LEU	4.2
1	C	491	ALA	4.2
1	B	511	LEU	3.9
1	C	511	LEU	3.8
1	D	306	LEU	3.8
1	B	336	PRO	3.5
1	D	508	LEU	3.3
1	D	335	ARG	3.0
1	D	417	CYS	3.0
1	C	509	LEU	3.0
1	D	536	SER	3.0
1	D	451	ILE	3.0
1	A	511	LEU	3.0
1	B	541	LEU	3.0
1	A	526	TYR	2.9
1	C	308	LEU	2.8
1	B	537	TYR	2.8
1	D	505	ALA	2.8
1	C	331	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	509	LEU	2.6
1	C	419	GLU	2.6
1	C	512	SER	2.6
1	C	492	LYS	2.6
1	C	508	LEU	2.6
1	C	510	ILE	2.5
1	A	528	MET	2.5
1	D	545	ASP	2.5
1	A	466	LEU	2.5
1	B	368	VAL	2.5
1	B	417	CYS	2.5
1	A	512	SER	2.5
1	B	340	ALA	2.5
1	A	513[A]	HIS	2.4
1	A	510	ILE	2.4
1	C	416	LYS	2.4
1	B	508	LEU	2.4
1	B	306	LEU	2.3
1	D	510	ILE	2.3
1	D	416	LYS	2.3
1	C	337	PHE	2.3
1	A	508	LEU	2.3
1	C	418	VAL	2.2
1	D	331	TYR	2.2
1	B	536	SER	2.2
1	A	542	GLU	2.2
1	C	466	LEU	2.2
1	B	451	ILE	2.2
1	B	419	GLU	2.2
1	A	544	LEU	2.1
1	B	373	HIS	2.1
1	D	419	GLU	2.1
1	B	418	VAL	2.1
1	D	538	ASP	2.1
1	D	514	ILE	2.1
1	B	527	SER	2.1
1	A	307	ALA	2.0
1	D	541	LEU	2.0
1	A	464	SER	2.0
1	D	507	LEU	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 carbohydrates in this entry.

6.4 Ligands [i](#)

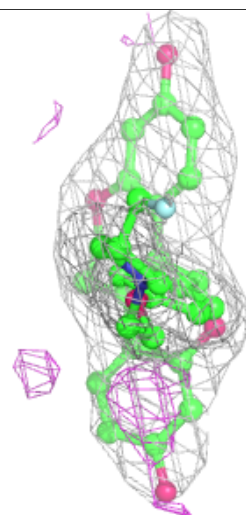
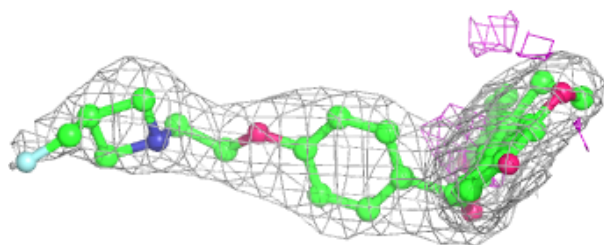
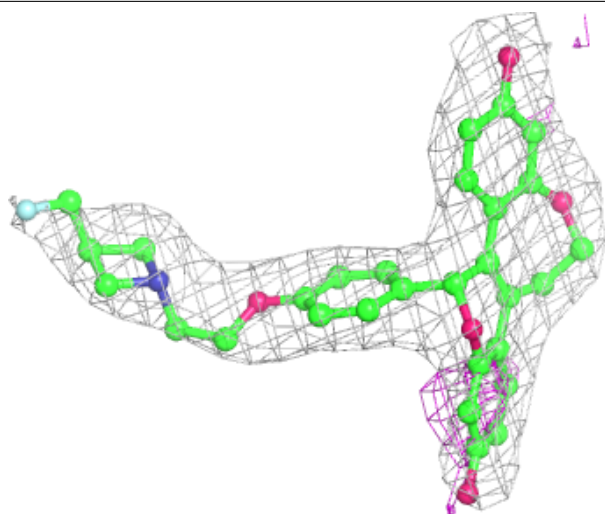
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	GOL	D	602	6/6	0.63	0.48	81,87,87,88	0
3	GOL	B	602	6/6	0.76	0.33	65,68,69,70	0
2	G8Y	A	601	36/36	0.86	0.19	44,48,66,72	0
2	G8Y	B	601	36/36	0.88	0.21	53,59,88,90	0
2	G8Y	D	601	36/36	0.88	0.20	50,54,74,82	0
2	G8Y	C	601	36/36	0.90	0.19	48,53,66,72	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.

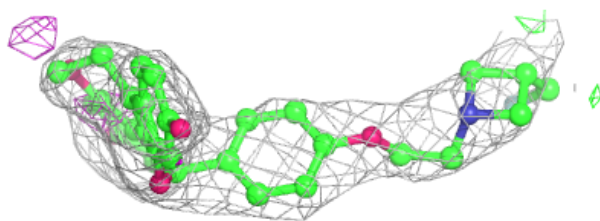
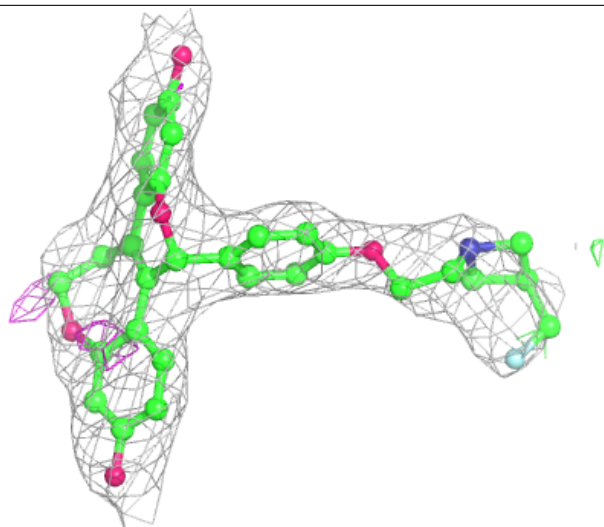
Electron density around G8Y A 601:

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



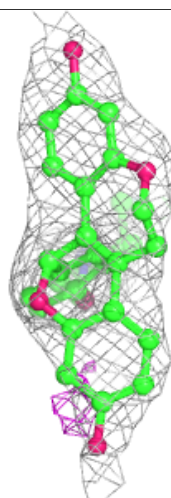
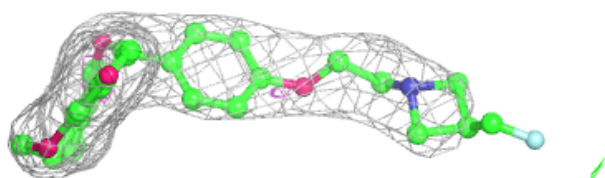
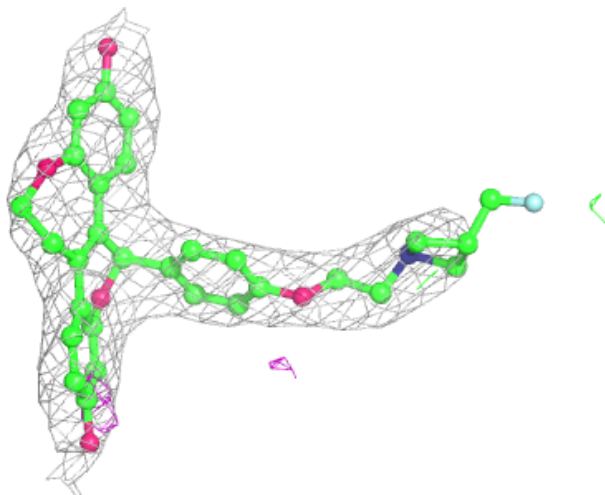
Electron density around G8Y B 601:

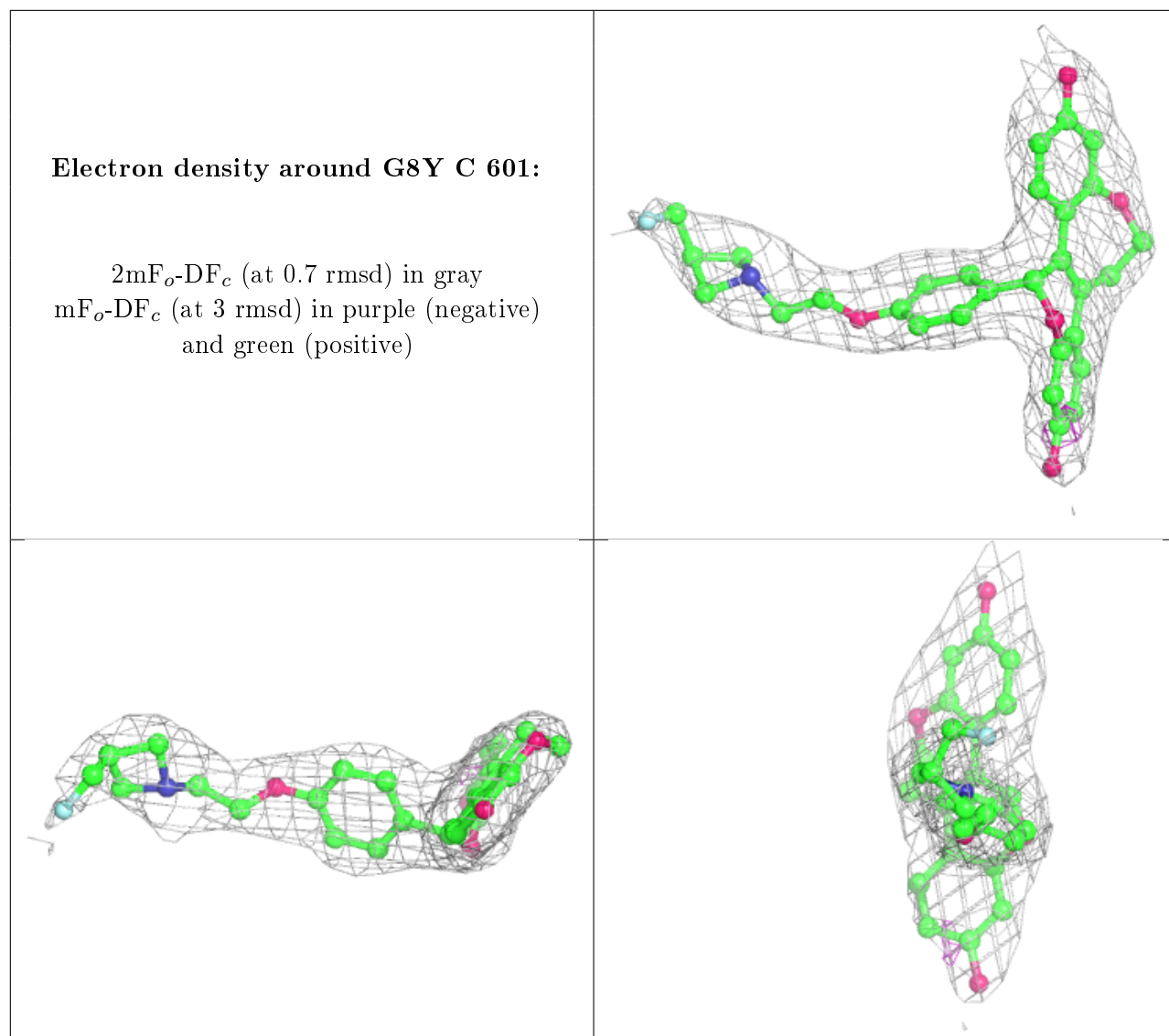
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around G8Y D 601:

$2mF_o-DF_c$ (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.