wwPDB X-ray Structure Validation Summary Report (i)

May 15, 2020 – 10:56 am BST

PDB ID	:	6PET
Title	:	Crystal structure of 8-hydroxychromene compound 30 bound to estrogen receptor alpha
Authors	:	Kiefer, J.R.; Vinogradova, M.; Liang, J.; Wang, X.; Zbieg, J.; Labadie, S.S.; Zhang, B.; Li, J.; Liang, W.
Deposited on	:	2019-06-20
Resolution	:	2.20 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

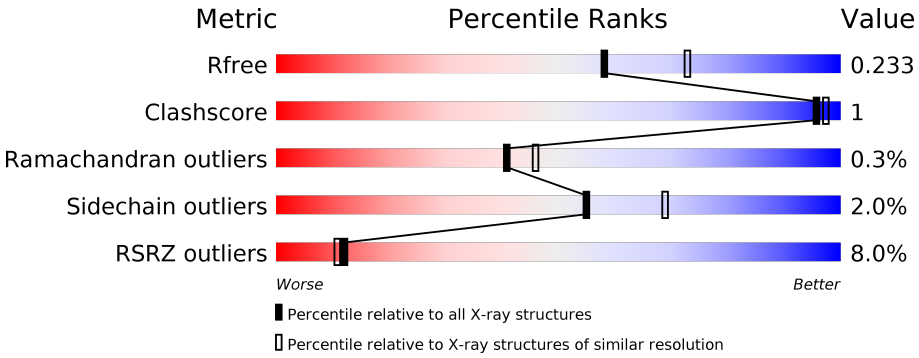
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 <=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	8% 76% 21%
1	B	280	5% 78% 20%
1	C	280	8% 81% 15%
1	D	280	5% 80% 5% 15%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 15062 atoms, of which 7544 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
1	D	238	Total	C	H	N	O	S	0	3	0
			3811	1206	1925	321	340	19			
1	A	220	Total	C	H	N	O	S	0	2	0
			3524	1111	1789	295	312	17			
1	C	239	Total	C	H	N	O	S	0	2	0
			3811	1206	1925	321	340	19			
1	B	225	Total	C	H	N	O	S	0	3	0
			3636	1149	1843	304	322	18			

There are 104 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	engineered mutation	UNP P03372
D	536	SER	LEU	engineered mutation	UNP P03372
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
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	engineered mutation	UNP P03372
A	536	SER	LEU	engineered mutation	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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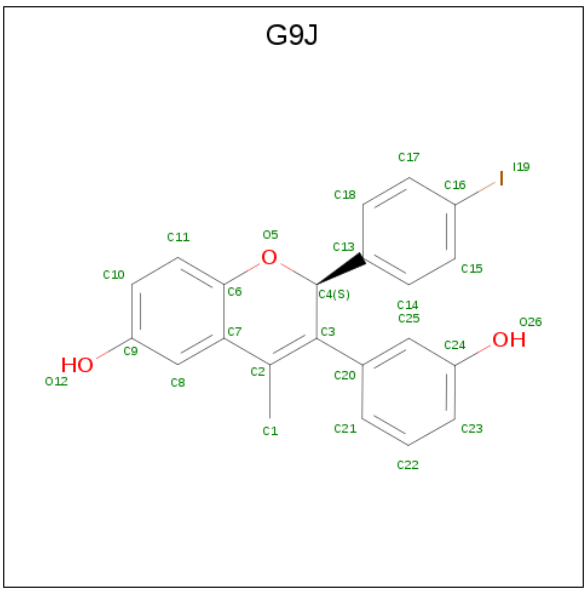
Chain	Residue	Modelled	Actual	Comment	Reference
C	285	ASP	-	expression tag	UNP P03372
C	286	LEU	-	expression tag	UNP P03372
C	287	GLY	-	expression tag	UNP P03372
C	288	THR	-	expression tag	UNP P03372
C	289	GLU	-	expression tag	UNP P03372
C	290	ASN	-	expression tag	UNP P03372
C	291	LEU	-	expression tag	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	engineered mutation	UNP P03372
C	536	SER	LEU	engineered mutation	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	engineered mutation	UNP P03372
B	536	SER	LEU	engineered mutation	UNP P03372

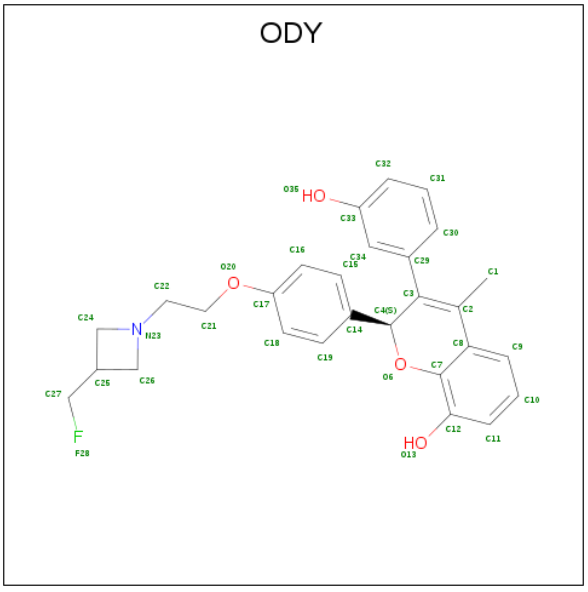
- Molecule 2 is (2S)-3-(3-hydroxyphenyl)-2-(4-iodophenyl)-4-methyl-2H-1-benzopyran-6-ol

(three-letter code: G9J) (formula: $C_{22}H_{17}IO_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total C I O 26 22 1 3	0	0
2	C	1	Total C I O 26 22 1 3	0	0

- Molecule 3 is (2S)-2-(4-{2-[3-(fluoromethyl)azetidin-1-yl]ethoxy}phenyl)-3-(3-hydroxyphenyl)-4-methyl-2H-1-benzopyran-8-ol (three-letter code: ODY) (formula: $C_{28}H_{28}FNO_4$) (labeled as "Ligand of Interest" by author).

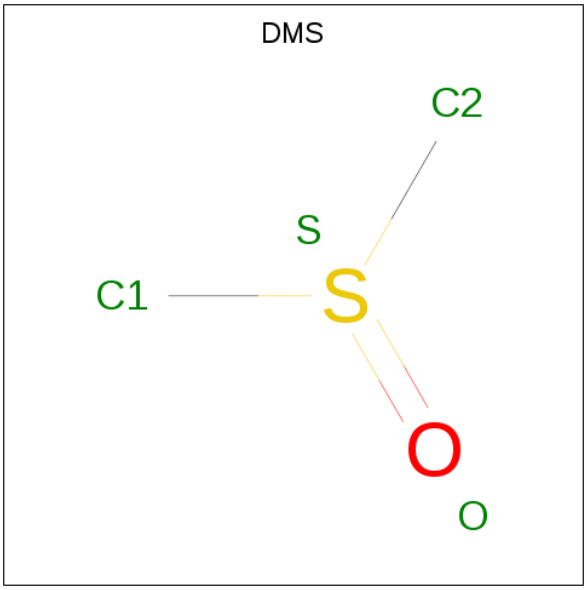


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	F	H	N	O	0	0
			62	28	1	28	1	4		
3	B	1	Total	C	F	H	N	O	0	0
			62	28	1	28	1	4		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		

- Molecule 5 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	H	O	S	0	0
			10	2	6	1	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	23	Total	O	0	0
			23	23		
6	A	23	Total	O	0	0
			23	23		
6	C	23	Total	O	0	0
			23	23		

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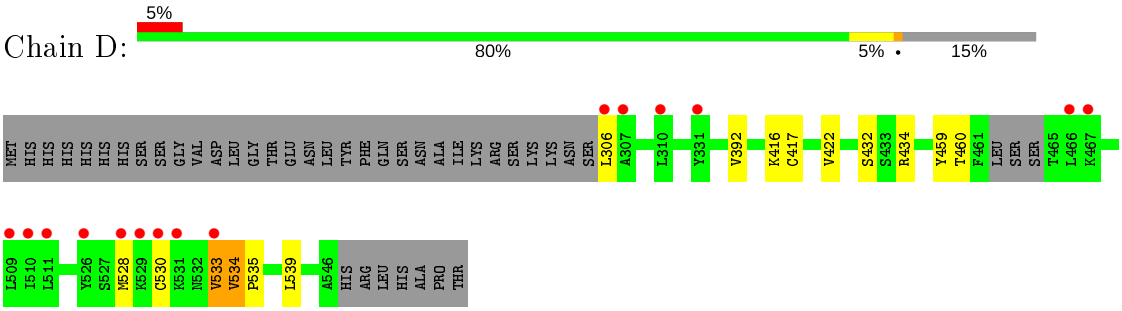
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	24	Total	O	0	0
			24	24		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

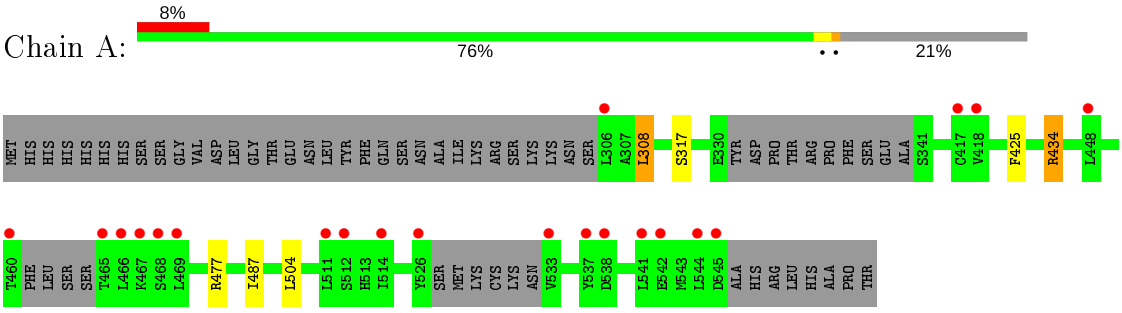
- Molecule 1: Estrogen receptor

Chain D:



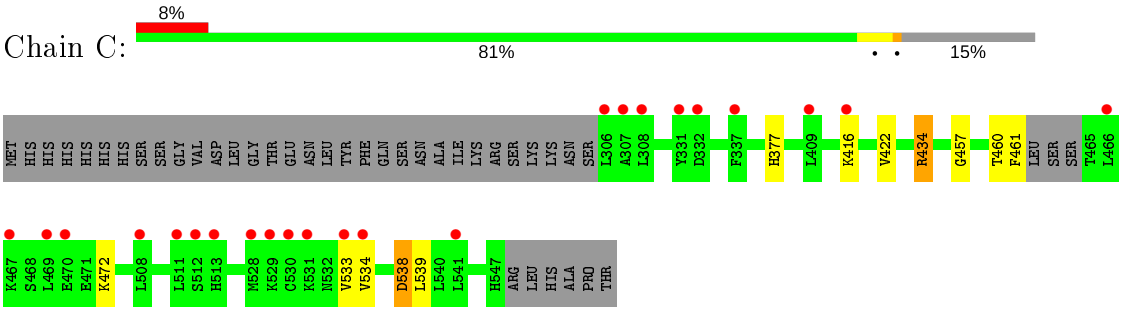
- Molecule 1: Estrogen receptor

Chain A:



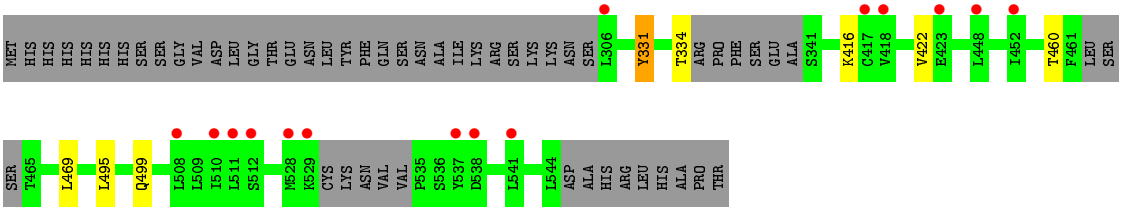
- Molecule 1: Estrogen receptor

Chain C:



- Molecule 1: Estrogen receptor

Chain B:


MET HIS HIS HIS HIS HIS SER SER GLY VAL ASP LEU GLY THR GLU ASN LEU TYR PHE GLN SER ASN ALA ILE LYS ARG SER LYS LYS ASN SER L306 Y331 T334 ARG PRO PHE SER GLU ALA S341 K416 C417 V418 V422 E423 L448 I452 T460 F461 LEU SER

SER T465 L469 L495 Q499 L508 L509 I510 L511 S512 M528 K529 CYS LYS ASN VAL VAL P535 S536 Y537 D538 L541 L544 ASP ALA HIS ARG LEU HIS ALA PRO THR

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	53.17Å 58.75Å 92.93Å 77.57° 74.40° 63.09°	Depositor
Resolution (Å)	32.14 – 2.20 32.14 – 2.20	Depositor EDS
% Data completeness (in resolution range)	67.5 (32.14-2.20) 67.5 (32.14-2.20)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.70 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.173 , 0.232 0.175 , 0.233	Depositor DCC
R_{free} test set	1634 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	40.6	Xtriage
Anisotropy	0.560	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 48.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.129 for h,h-k,h-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	15062	wwPDB-VP
Average B, all atoms (Å^2)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.90% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ODY, DMS, G9J, CL

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	0.32	0/1762	0.49	0/2378
1	B	0.35	0/1824	0.52	0/2460
1	C	0.32	0/1921	0.49	0/2597
1	D	0.34	0/1921	0.51	0/2597
All	All	0.33	0/7428	0.50	0/10032

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

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	1735	1789	1771	3	0
1	B	1793	1843	1821	2	0
1	C	1886	1925	1906	7	0
1	D	1886	1925	1905	6	0
2	C	26	0	0	0	0
2	D	26	0	0	0	0
3	A	34	28	0	0	0
3	B	34	28	0	0	0
4	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	4	6	6	0	0
6	A	23	0	0	0	0
6	B	24	0	0	0	0
6	C	23	0	0	1	0
6	D	23	0	0	1	0
All	All	7518	7544	7409	17	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.

The worst 5 of 17 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:C:377:HIS:HE2	1:C:460:THR:HG1	1.41	0.63
1:C:457:GLY:O	1:C:460:THR:OG1	2.29	0.50
1:A:308:LEU:HD21	1:A:477:ARG:HB3	1.95	0.48
1:D:528:MET:SD	6:D:717:HOH:O	2.60	0.48
1:C:461:PHE:HB2	1:C:472:LYS:HE3	1.97	0.47

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	212/280 (76%)	210 (99%)	2 (1%)	0	100 100
1	B	218/280 (78%)	215 (99%)	2 (1%)	1 (0%)	29 31
1	C	235/280 (84%)	227 (97%)	8 (3%)	0	100 100
1	D	235/280 (84%)	229 (97%)	4 (2%)	2 (1%)	17 16
All	All	900/1120 (80%)	881 (98%)	16 (2%)	3 (0%)	41 46

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	533	VAL
1	D	534	VAL
1	B	331	TYR

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	194/252 (77%)	190 (98%)	4 (2%)	53	67
1	B	200/252 (79%)	196 (98%)	4 (2%)	55	69
1	C	210/252 (83%)	207 (99%)	3 (1%)	67	80
1	D	210/252 (83%)	205 (98%)	5 (2%)	49	62
All	All	814/1008 (81%)	798 (98%)	16 (2%)	55	69

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	425	PHE
1	A	434	ARG
1	B	331	TYR
1	A	317	SER
1	B	334	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	439	ASN
1	A	441	GLN
1	C	547	HIS
1	B	373	HIS
1	B	488	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 1 is monoatomic - leaving 5 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	$\#\|Z\| > 2$
5	DMS	B	602	-	3,3,3	0.58	0	3,3,3	1.82	2 (66%)
2	G9J	D	601	-	29,29,29	0.58	0	38,42,42	1.16	4 (10%)
3	ODY	B	601	-	37,38,38	0.33	0	41,54,54	0.64	1 (2%)
2	G9J	C	601	-	29,29,29	0.63	1 (3%)	38,42,42	1.25	6 (15%)
3	ODY	A	601	-	37,38,38	0.34	0	41,54,54	0.65	1 (2%)

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	G9J	D	601	-	-	0/8/24/24	0/4/4/4
3	ODY	B	601	-	-	3/12/40/40	0/5/5/5
2	G9J	C	601	-	-	0/8/24/24	0/4/4/4
3	ODY	A	601	-	-	3/12/40/40	0/5/5/5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	G9J	C7-C2	2.27	1.49	1.45

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	601	G9J	O5-C6-C7	-3.52	118.05	122.09
2	D	601	G9J	O5-C4-C13	-3.39	104.45	109.53
2	D	601	G9J	O5-C6-C7	-2.70	119.00	122.09
2	C	601	G9J	O5-C6-C11	2.47	120.69	116.29
2	C	601	G9J	C14-C13-C4	-2.44	116.62	120.50

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

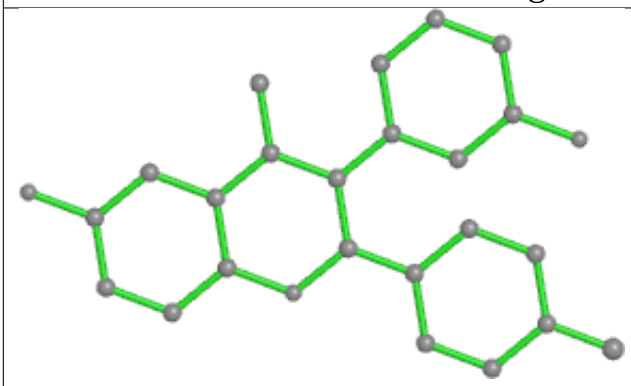
Mol	Chain	Res	Type	Atoms
3	A	601	ODY	O20-C21-C22-N23
3	B	601	ODY	O20-C21-C22-N23
3	A	601	ODY	C30-C29-C3-C2
3	A	601	ODY	C34-C29-C3-C2
3	B	601	ODY	C34-C29-C3-C2

There are no ring outliers.

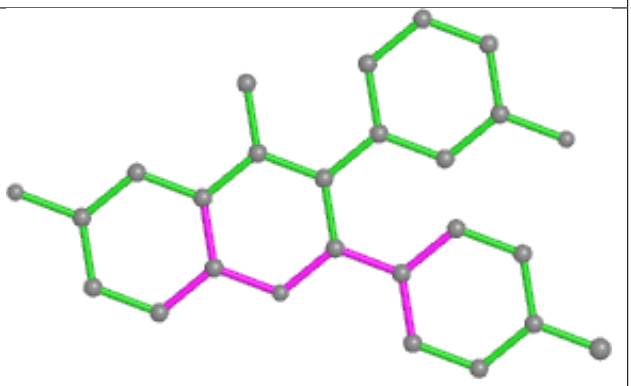
No monomer is involved in short contacts.

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

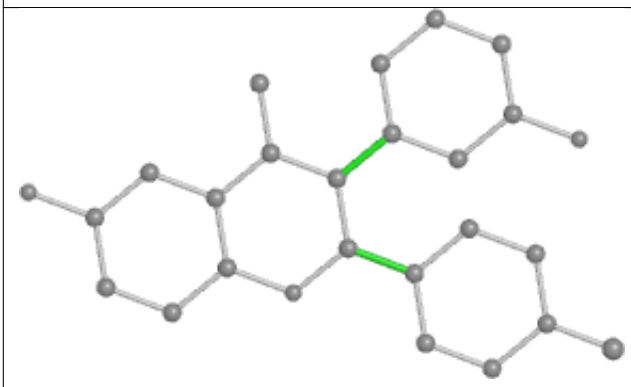
Ligand G9J D 601



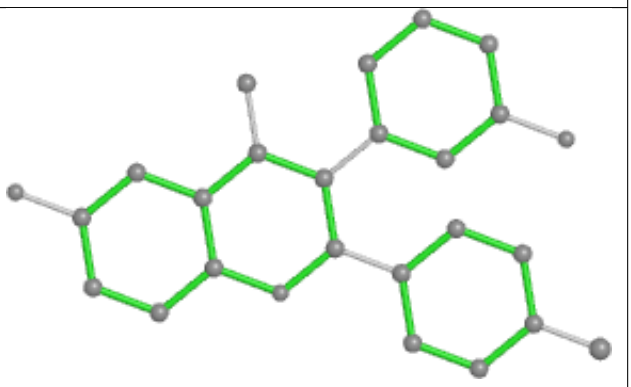
Bond lengths



Bond angles

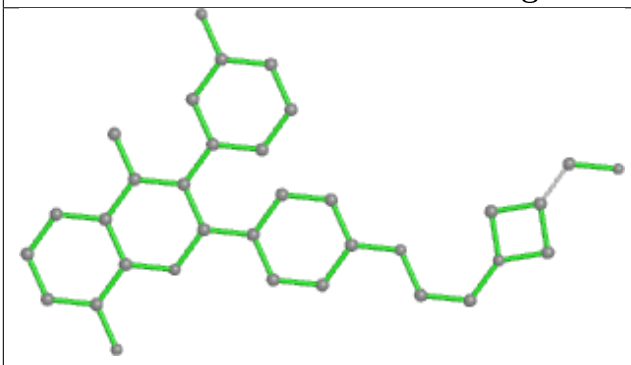


Torsions

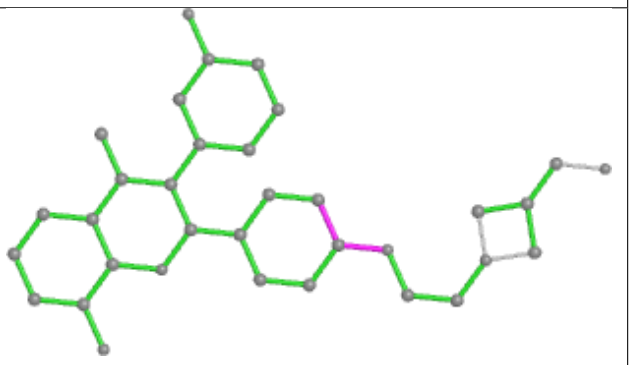


Rings

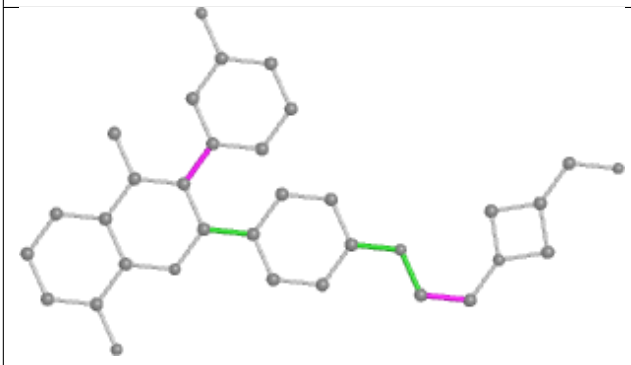
Ligand ODY B 601



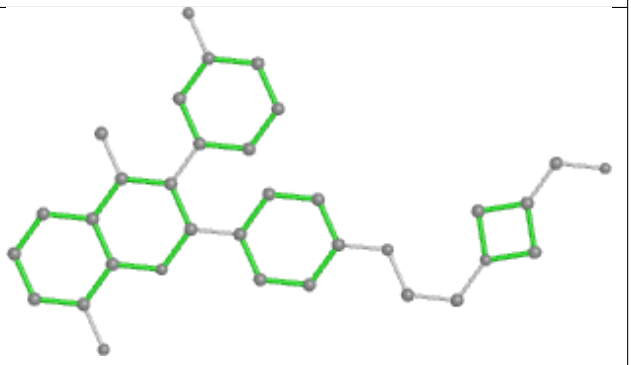
Bond lengths



Bond angles

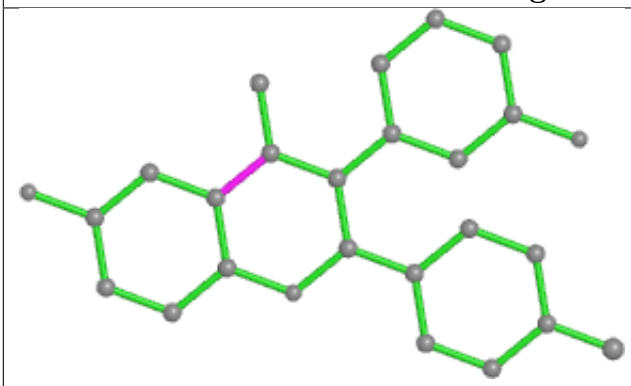


Torsions

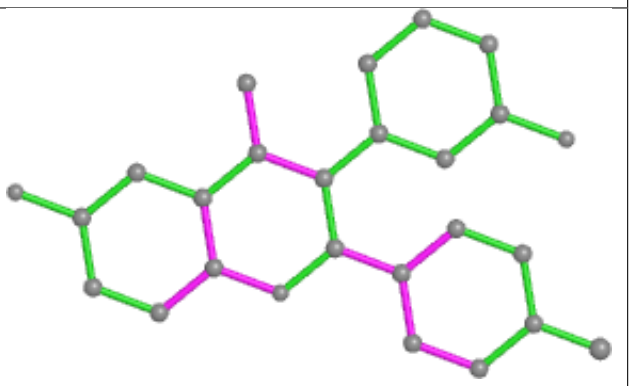


Rings

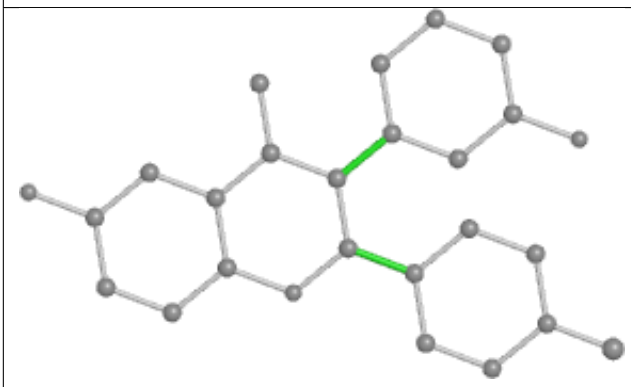
Ligand G9J C 601



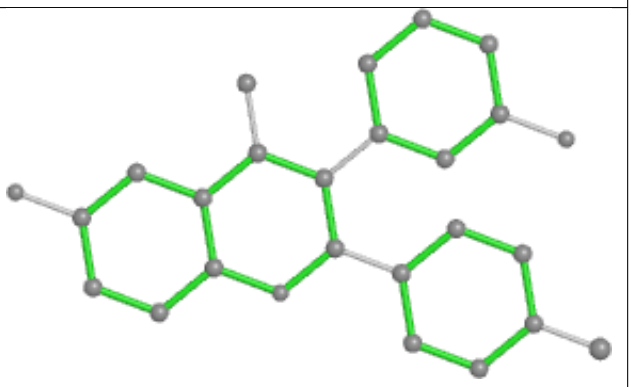
Bond lengths



Bond angles

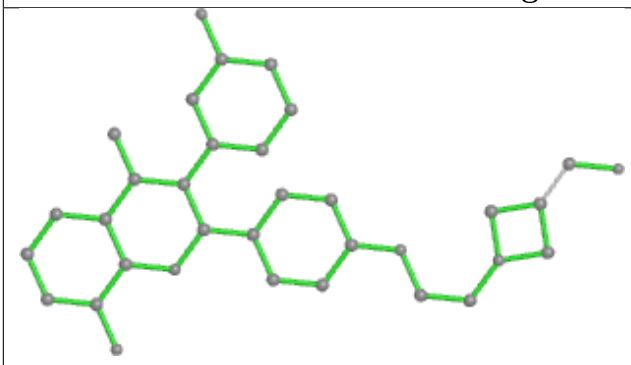


Torsions

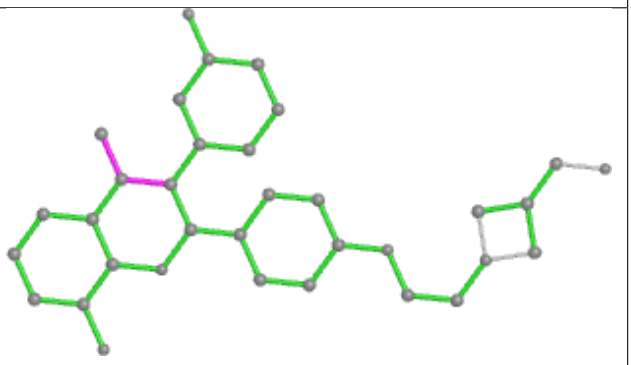


Rings

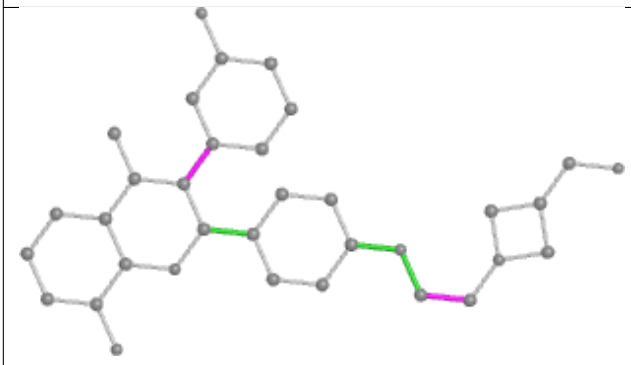
Ligand ODY A 601



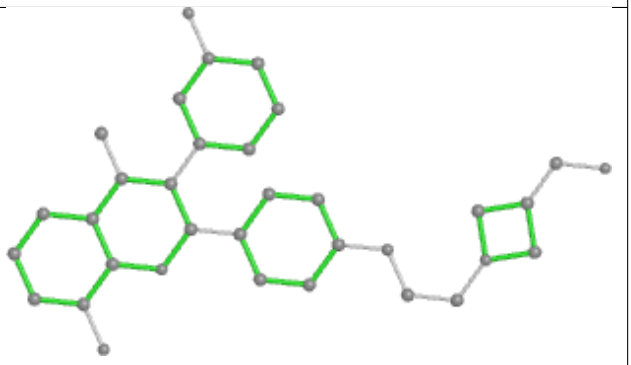
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	220/280 (78%)	0.37	21 (9%)	8 7	39, 64, 122, 178	0
1	B	225/280 (80%)	0.20	15 (6%)	17 16	37, 60, 108, 140	0
1	C	239/280 (85%)	0.31	23 (9%)	8 6	37, 65, 119, 158	0
1	D	238/280 (85%)	0.16	15 (6%)	20 19	40, 61, 117, 169	0
All	All	922/1120 (82%)	0.26	74 (8%)	12 11	37, 62, 117, 178	0

The worst 5 of 74 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	533	VAL	10.1
1	D	530	CYS	9.5
1	C	530	CYS	8.5
1	A	466	LEU	8.4
1	D	529	LYS	8.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

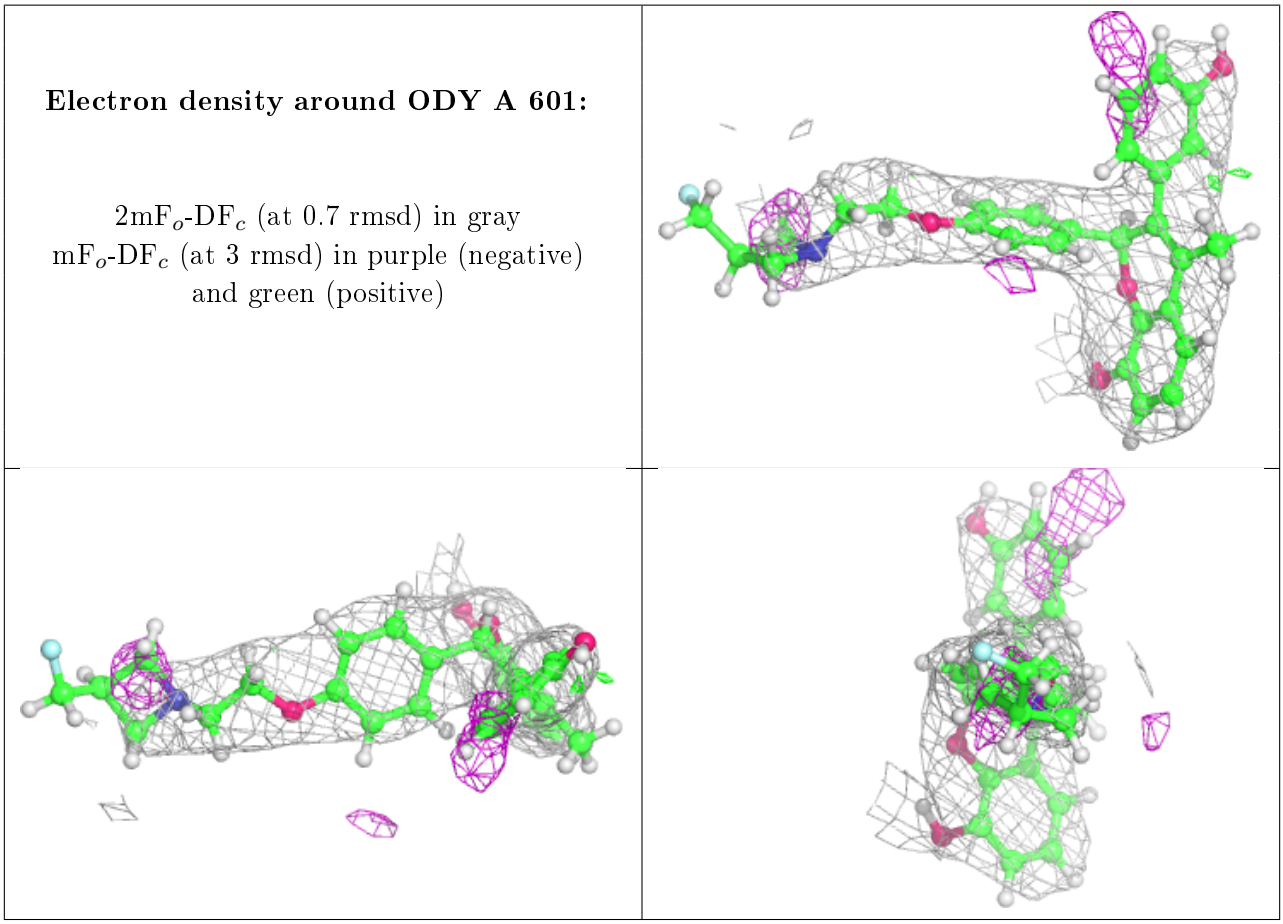
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	ODY	A	601	34/34	0.90	0.20	45,74,168,203	0
3	ODY	B	601	34/34	0.94	0.16	24,67,176,213	0
4	CL	A	602	1/1	0.95	0.17	79,79,79,79	0
2	G9J	C	601	26/26	0.96	0.12	48,55,74,91	0
5	DMS	B	602	4/4	0.97	0.10	75,90,117,117	0
2	G9J	D	601	26/26	0.97	0.11	42,52,63,73	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.

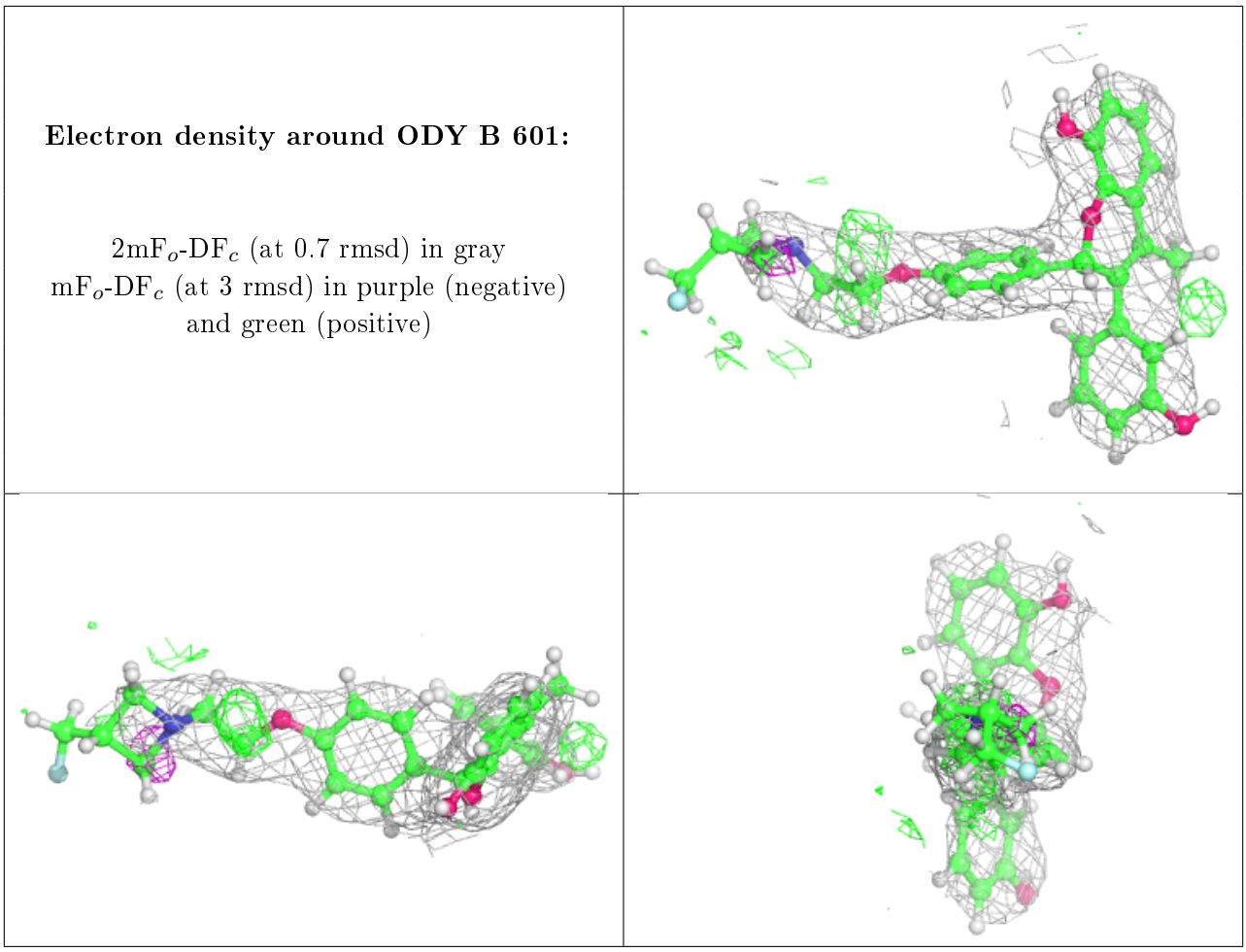
Electron density around ODY A 601:

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



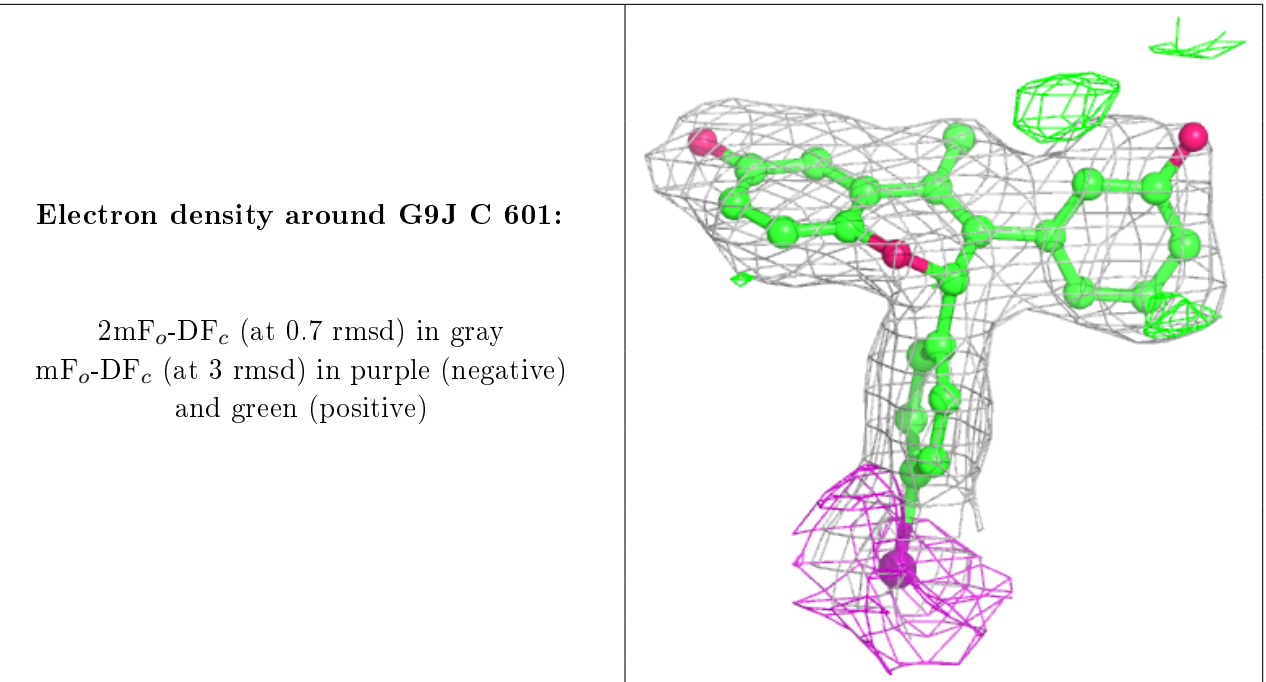
Electron density around ODY B 601:

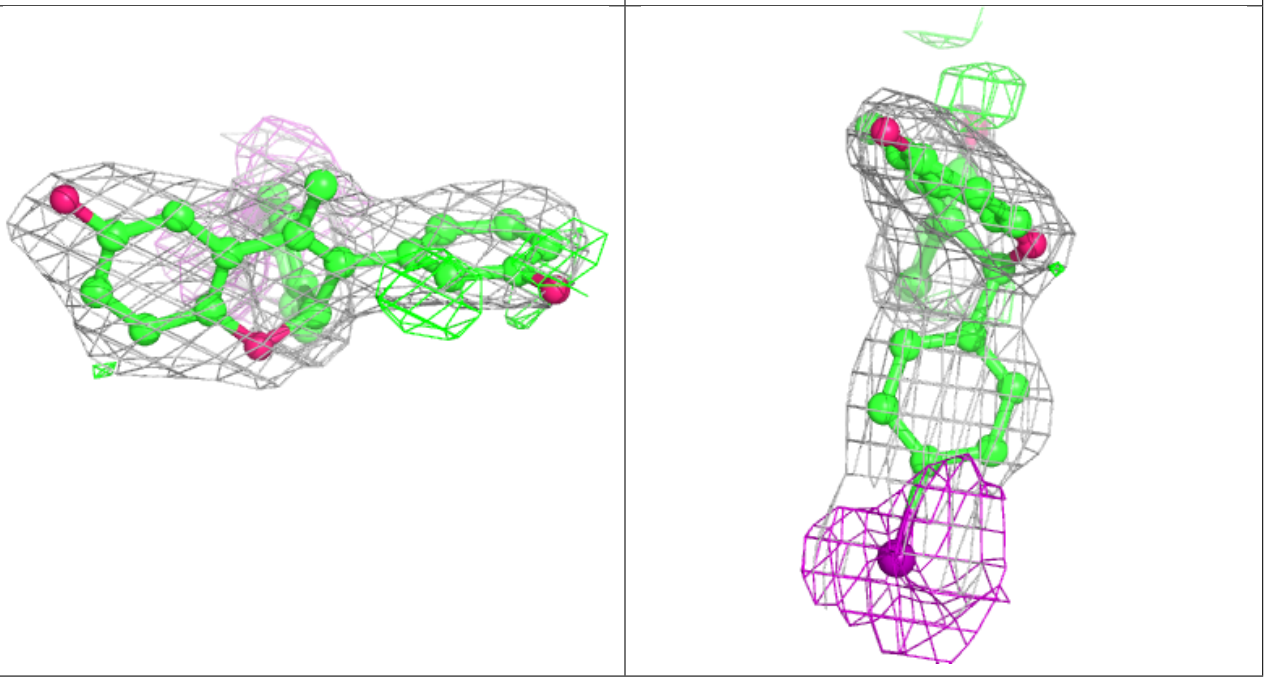
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around G9J C 601:

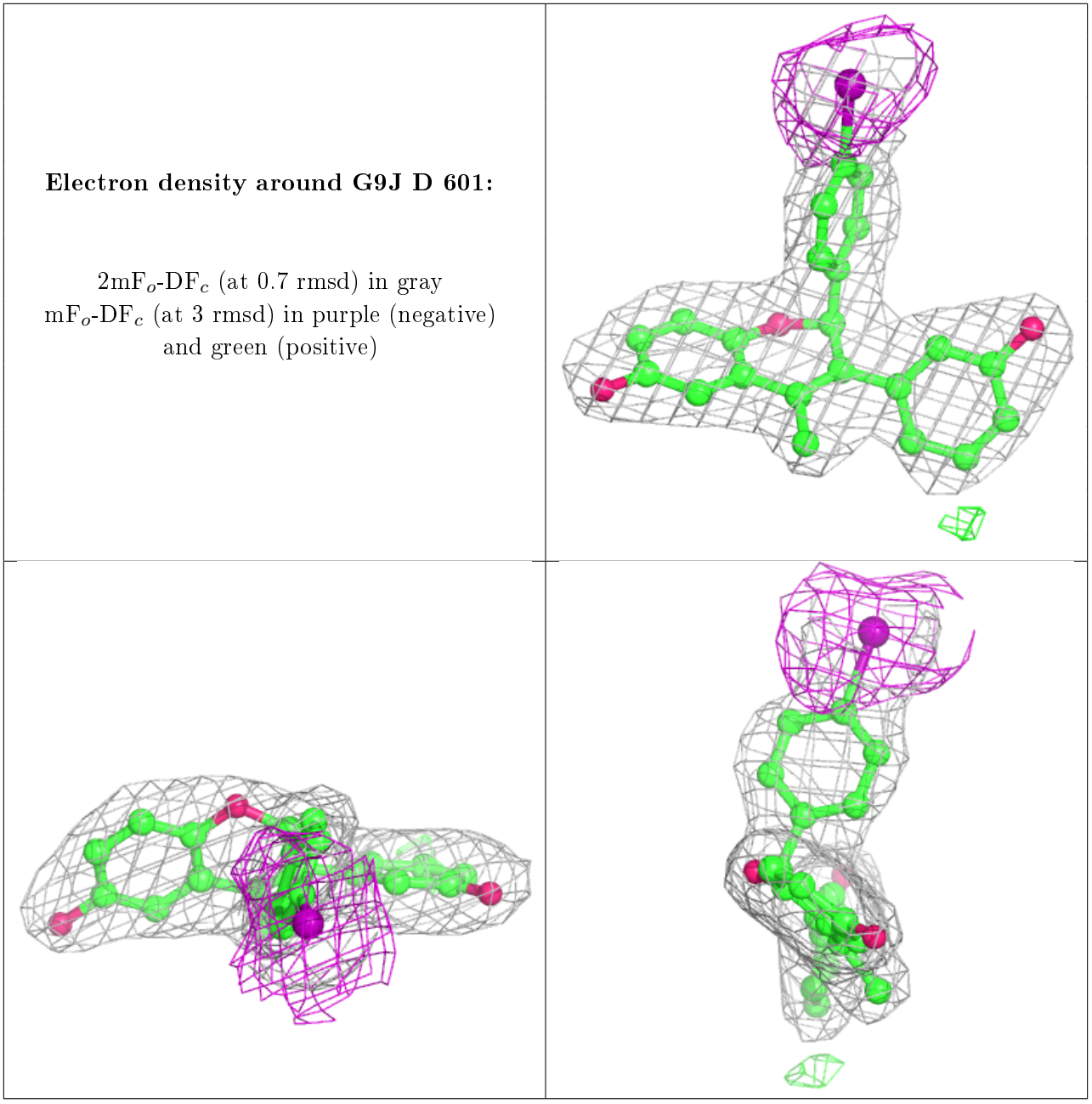
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





Electron density around G9J 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

There are no such residues in this entry.