



Full wwPDB X-ray Structure Validation Report ⓘ

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 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

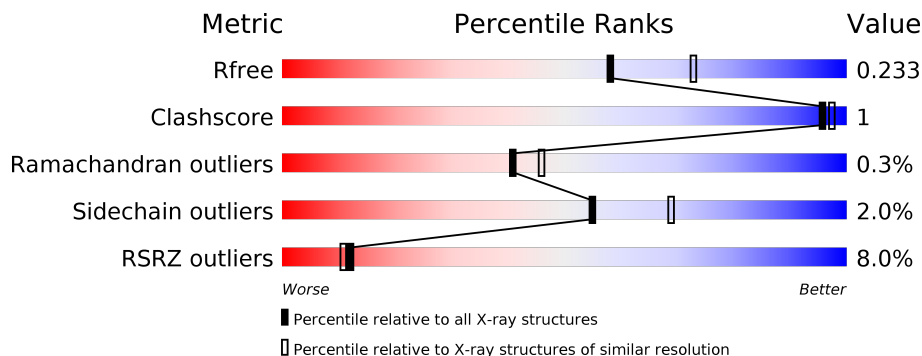
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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 $\leq 5\%$. 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	 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 [i](#)

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
			Total	C	H	N	O	S			
1	D	238	3811	1206	1925	321	340	19	0	3	0
1	A	220	3524	1111	1789	295	312	17	0	2	0
1	C	239	3811	1206	1925	321	340	19	0	2	0
1	B	225	3636	1149	1843	304	322	18	0	3	0

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

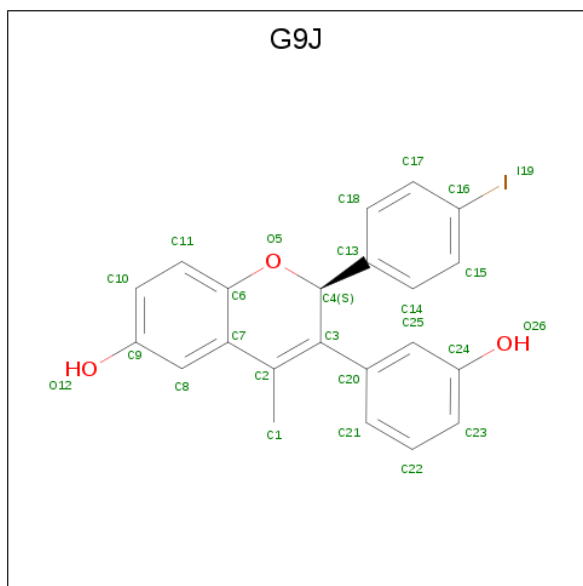
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Chain	Residue	Modelled	Actual	Comment	Reference
C	285	ASP	-	expression tag	UNP P03372
C	286	LEU	-	expression tag	UNP P03372
C	287	GLY	-	expression tag	UNP P03372
C	288	THR	-	expression tag	UNP P03372
C	289	GLU	-	expression tag	UNP P03372
C	290	ASN	-	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

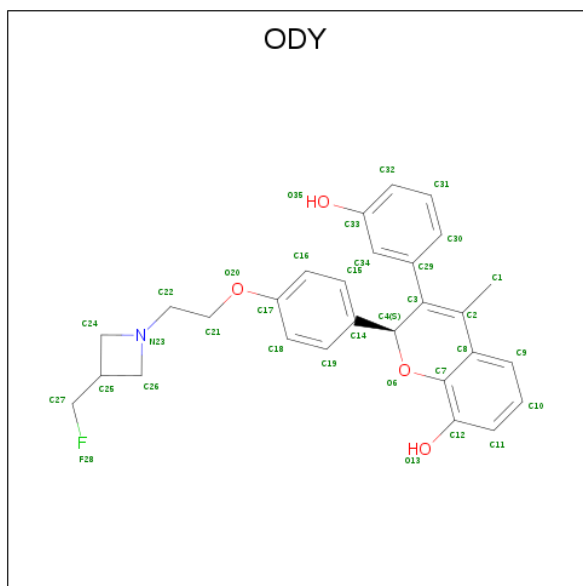
- Molecule 2 is (2S)-3-(3-hydroxyphenyl)-2-(4-iodophenyl)-4-methyl-2H-1-benzopyran-6-ol

(three-letter code: G9J) (formula: C₂₂H₁₇IO₃).



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

- 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: C₂₈H₂₈FNO₄) (labeled as "Ligand of Interest" by author).

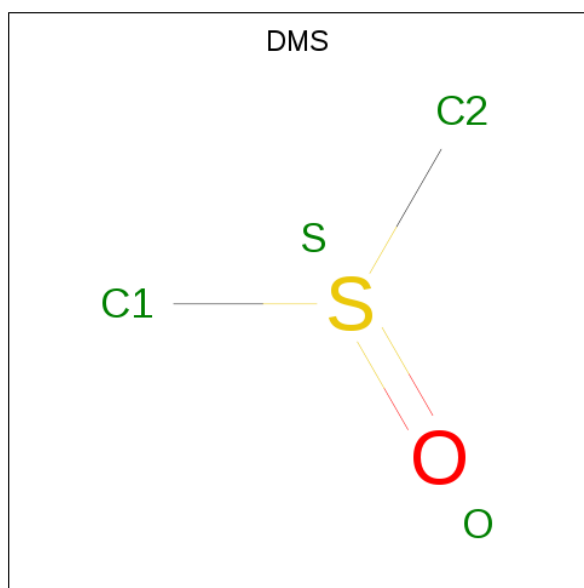


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	F	H	N			O
3	A	1	Total 62	C 28	F 1	H 28	N 1	O 4	0	0
3	B	1	Total 62	C 28	F 1	H 28	N 1	O 4	0	0

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

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

- Molecule 5 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C₂H₆OS).



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

- Molecule 6 is water.

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

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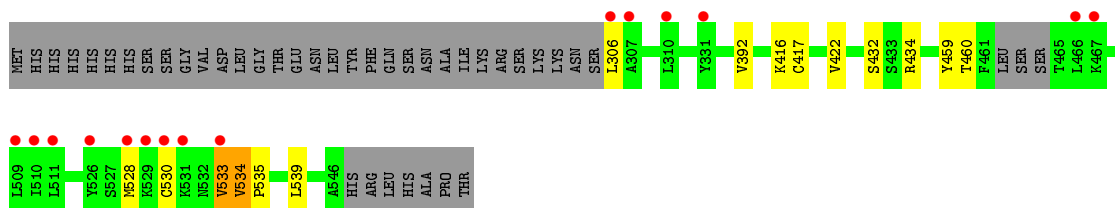
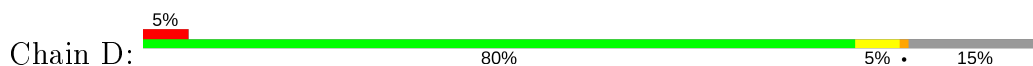
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	24	Total	O	0	0
			24	24		

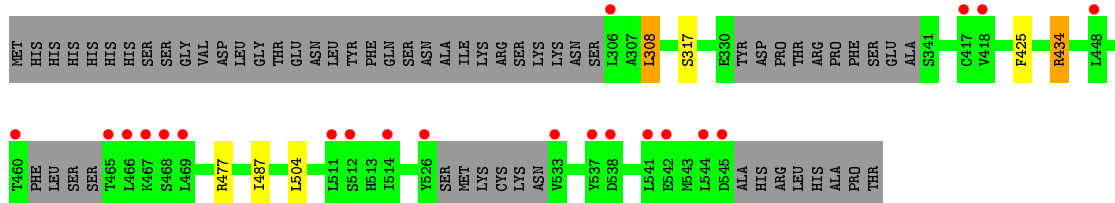
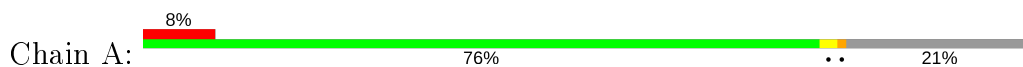
3 Residue-property plots [i](#)

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.

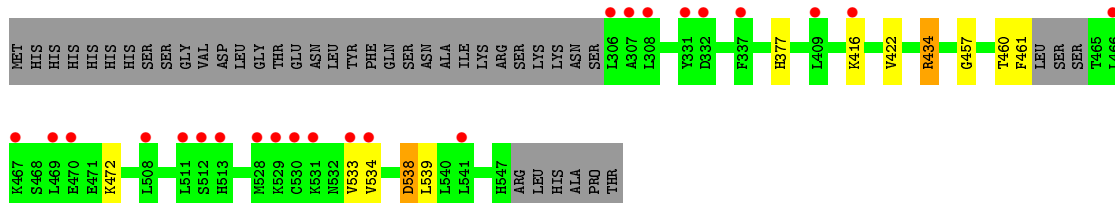
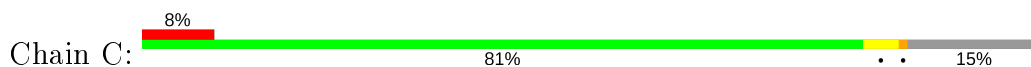
- Molecule 1: Estrogen receptor



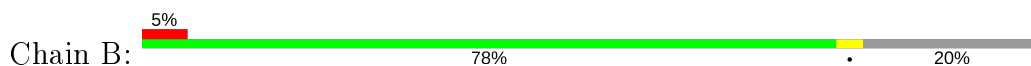
- Molecule 1: Estrogen receptor

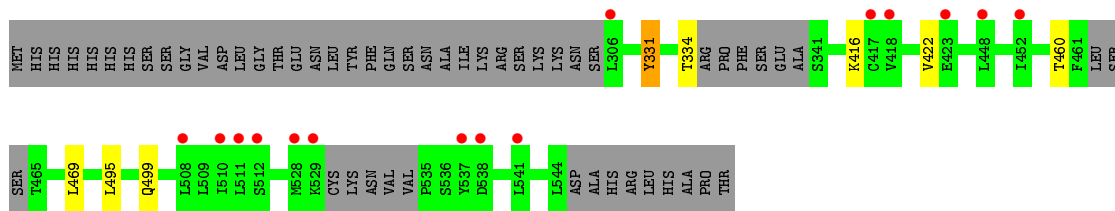


- Molecule 1: Estrogen receptor



- Molecule 1: Estrogen receptor





4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 2.20Å)	Xtrriage
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	Xtrriage
Anisotropy	0.560	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 48.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.129 for h,h-k,h-l	Xtrriage
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

Xtrriage'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.*

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: 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 [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	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.

All (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
1:C:538:ASP:OD1	1:C:538:ASP:N	2.50	0.44
1:D:530:CYS:HB2	1:D:533:VAL:CG1	2.48	0.44
1:C:416:LYS:HA	1:C:422:VAL:HG22	2.00	0.44
1:A:487:ILE:HD11	1:A:504:LEU:HD22	2.00	0.43
1:D:459:TYR:HE1	1:A:434:ARG:HD3	1.82	0.43
1:D:534:VAL:HA	1:D:535:PRO:HD2	1.95	0.43
1:C:533:VAL:HG23	1:C:534:VAL:N	2.35	0.42
1:D:392:VAL:HG13	1:D:432:SER:HA	2.01	0.42
1:D:416:LYS:HA	1:D:422:VAL:HG22	2.02	0.41
1:C:434:ARG:NH1	6:C:706:HOH:O	2.53	0.41
1:B:495:LEU:HD22	1:B:499:GLN:HB3	2.01	0.41
1:B:416:LYS:HA	1:B:422:VAL:HG22	2.02	0.41

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 [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	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

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	306	LEU
1	D	417	CYS
1	D	434	ARG
1	D	460	THR
1	D	539	LEU

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Mol	Chain	Res	Type
1	A	308	LEU
1	A	317	SER
1	A	425	PHE
1	A	434	ARG
1	C	434	ARG
1	C	538	ASP
1	C	539	LEU
1	B	331	TYR
1	B	334	THR
1	B	460	THR
1	B	469	LEU

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 [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](#)

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

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
2	C	601	G9J	C17-C18-C13	-2.35	118.83	121.20
5	B	602	DMS	O-S-C1	2.26	118.06	106.54
2	D	601	G9J	O5-C6-C11	2.20	120.22	116.29
2	D	601	G9J	C18-C13-C14	2.19	121.02	118.29
5	B	602	DMS	O-S-C2	-2.14	95.62	106.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	ODY	C1-C2-C3	-2.13	121.68	124.49
2	C	601	G9J	C18-C13-C14	2.12	120.94	118.29
3	B	601	ODY	O20-C17-C18	2.03	129.90	119.94
2	C	601	G9J	C1-C2-C3	-2.03	121.81	124.49

There are no chirality outliers.

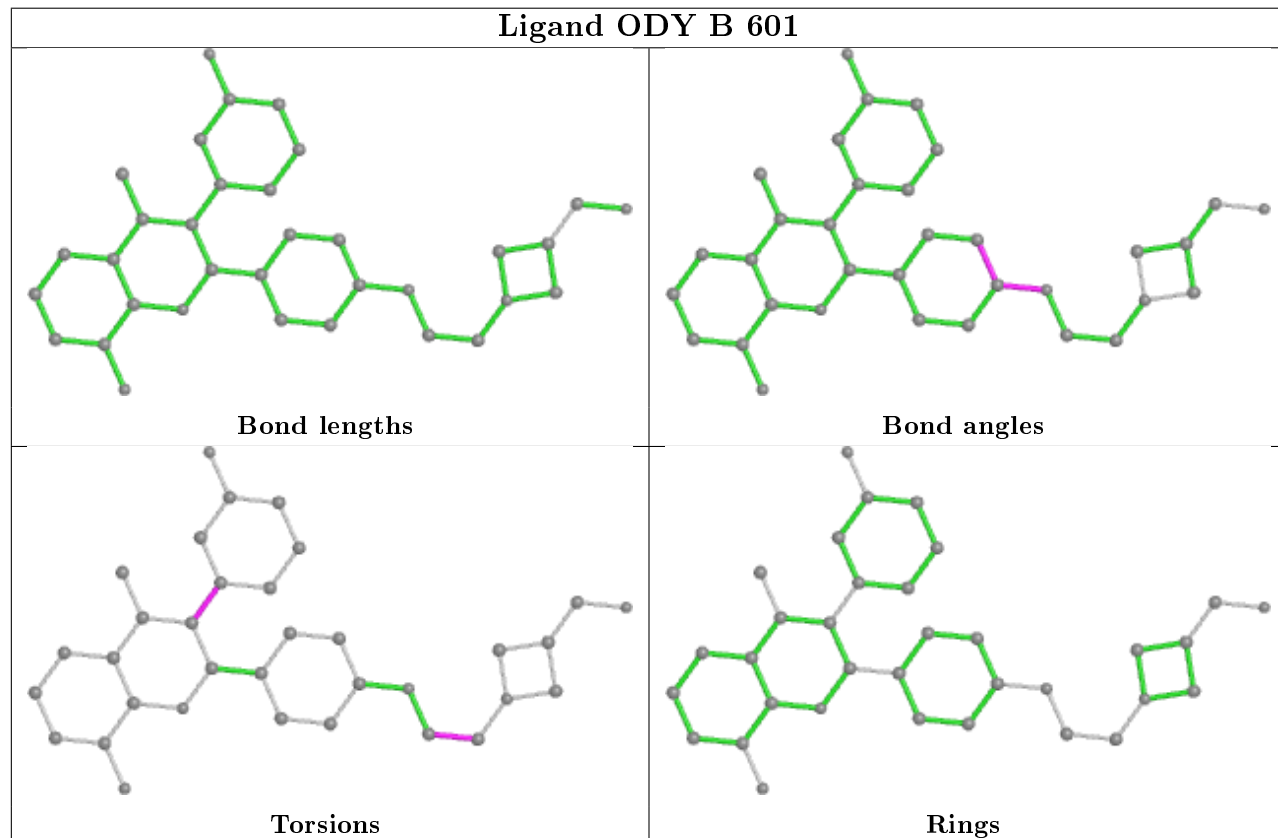
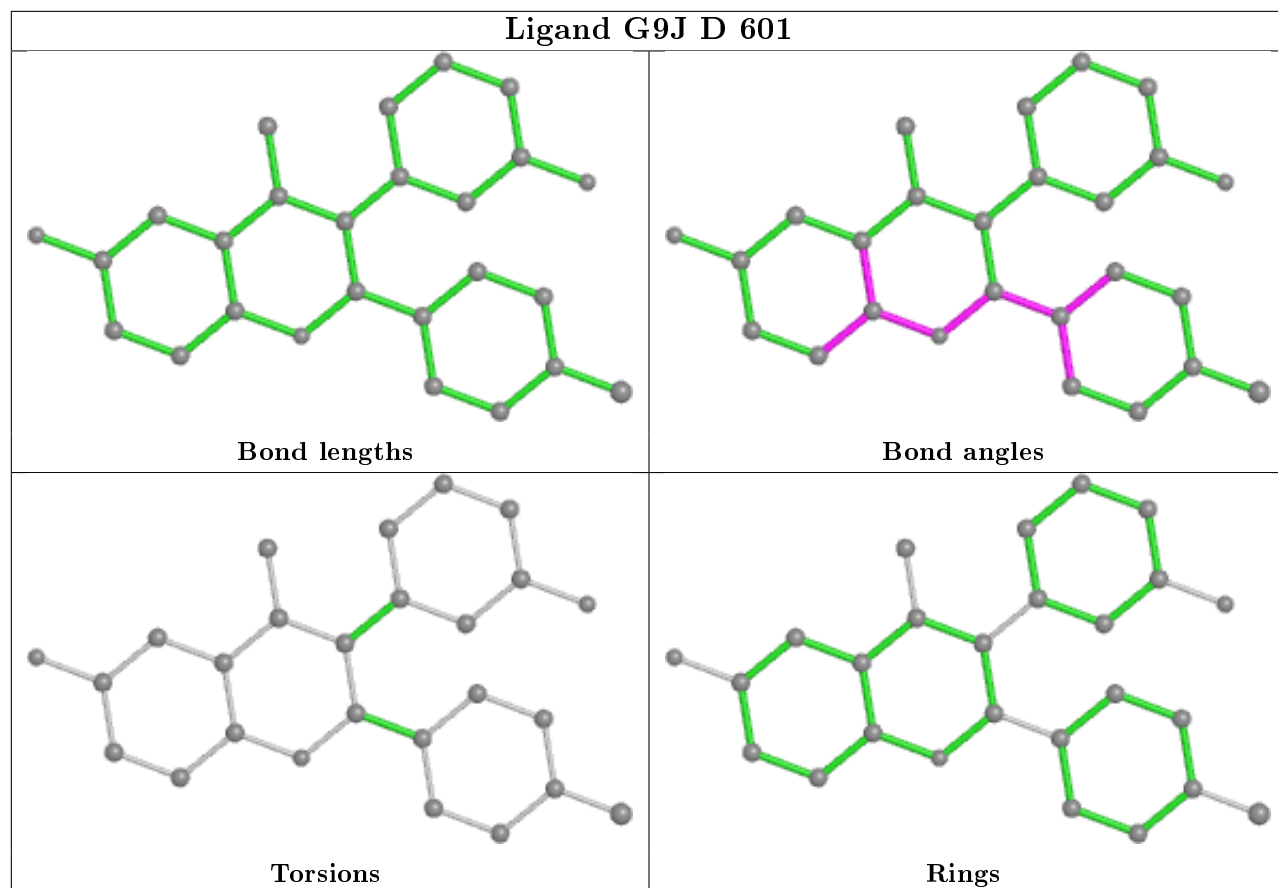
All (6) torsion outliers are listed below:

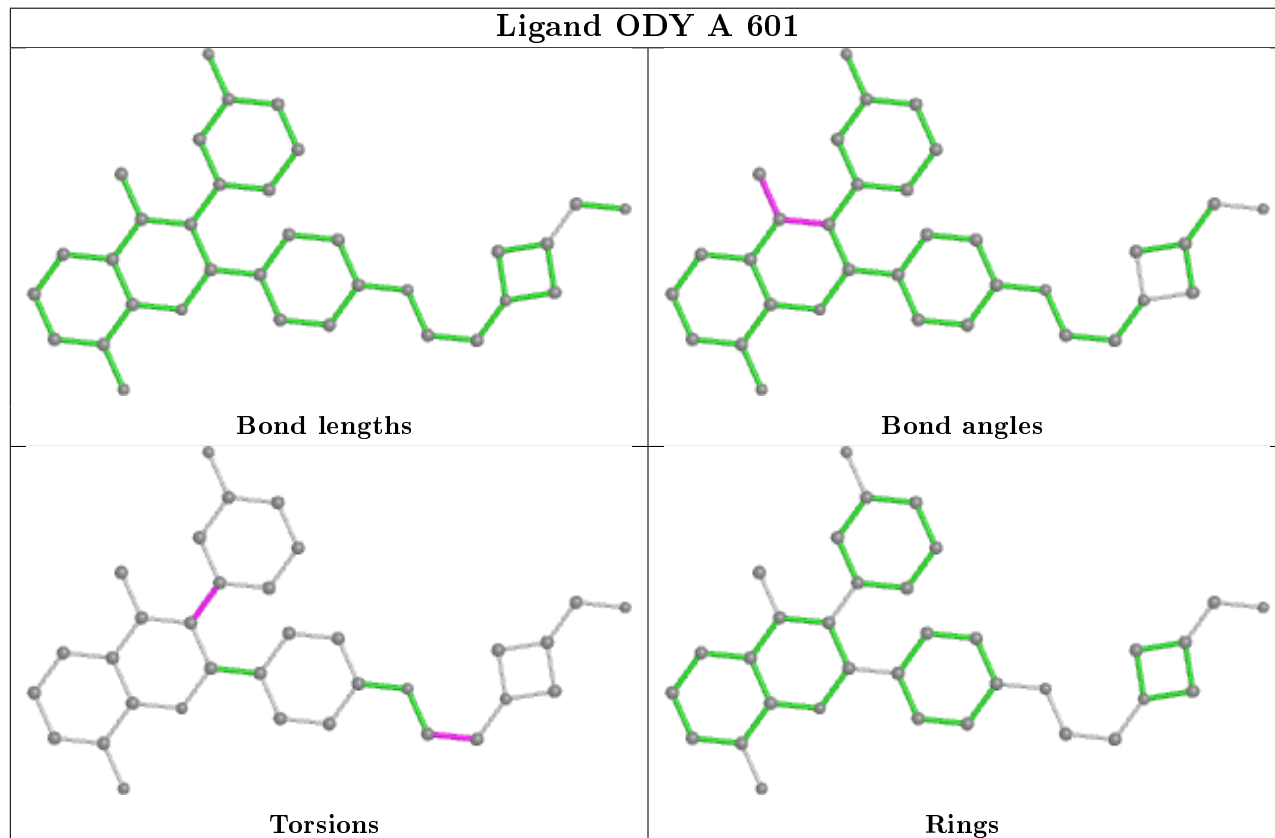
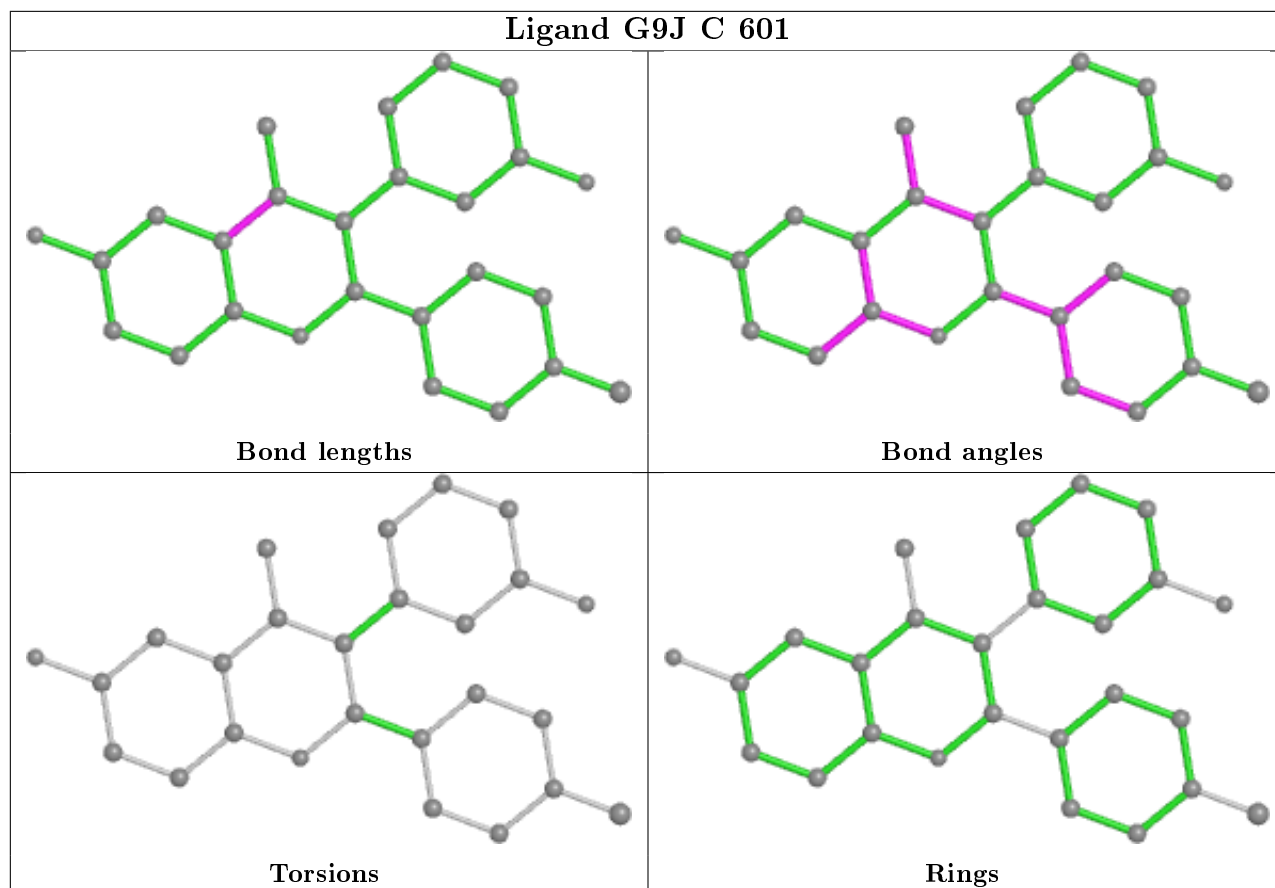
Mol	Chain	Res	Type	Atoms
3	A	601	ODY	O20-C21-C22-N23
3	B	601	ODY	O20-C21-C22-N23
3	A	601	ODY	C30-C29-C3-C2
3	A	601	ODY	C34-C29-C3-C2
3	B	601	ODY	C34-C29-C3-C2
3	B	601	ODY	C30-C29-C3-C2

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 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

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	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

All (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
1	A	465	THR	7.6
1	C	529	LYS	7.3
1	D	528	MET	6.0
1	B	528	MET	5.8
1	C	306	LEU	5.2
1	C	332	ASP	4.9
1	D	306	LEU	4.9
1	C	466	LEU	4.7
1	A	467	LYS	4.5
1	C	531	LYS	4.5
1	C	331	TYR	4.2
1	D	331	TYR	4.2
1	C	533	VAL	4.1
1	B	511	LEU	4.1
1	C	467	LYS	4.0
1	B	538	ASP	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	511	LEU	3.9
1	C	528	MET	3.8
1	A	417	CYS	3.8
1	B	418	VAL	3.7
1	C	469	LEU	3.7
1	A	538	ASP	3.6
1	C	511	LEU	3.5
1	A	533	VAL	3.4
1	B	537	TYR	3.4
1	A	537	TYR	3.2
1	D	466	LEU	3.2
1	D	509	LEU	3.1
1	A	512	SER	3.1
1	D	511	LEU	3.1
1	A	544	LEU	3.1
1	A	545	ASP	3.0
1	C	508	LEU	3.0
1	B	417	CYS	2.9
1	A	460	THR	2.9
1	B	541	LEU	2.9
1	B	512	SER	2.8
1	C	337	PHE	2.8
1	C	307	ALA	2.8
1	D	307	ALA	2.7
1	D	531	LYS	2.6
1	C	541	LEU	2.6
1	C	308	LEU	2.5
1	A	526	TYR	2.5
1	C	512	SER	2.5
1	B	452	ILE	2.5
1	B	508	LEU	2.5
1	B	510	ILE	2.5
1	A	469	LEU	2.5
1	B	529	LYS	2.4
1	A	468	SER	2.4
1	D	310	LEU	2.3
1	A	542	GLU	2.3
1	C	416	LYS	2.3
1	A	306	LEU	2.3
1	A	541	LEU	2.3
1	A	418	VAL	2.2
1	D	526	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	470	GLU	2.2
1	C	409	LEU	2.2
1	D	510	ILE	2.1
1	A	448	LEU	2.1
1	B	306	LEU	2.1
1	B	423	GLU	2.0
1	C	534	VAL	2.0
1	C	513	HIS	2.0
1	A	514	ILE	2.0
1	B	448	LEU	2.0
1	D	467	LYS	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](#)

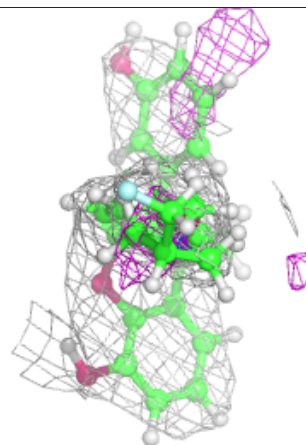
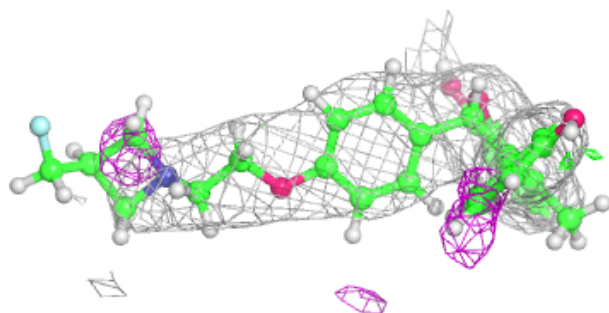
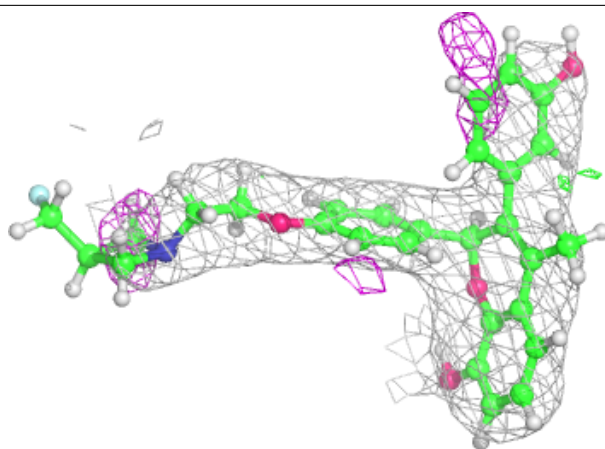
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(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.

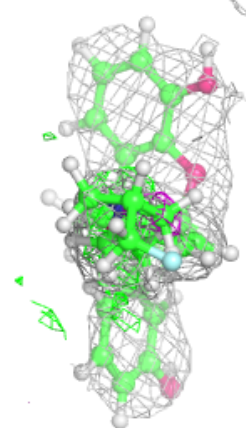
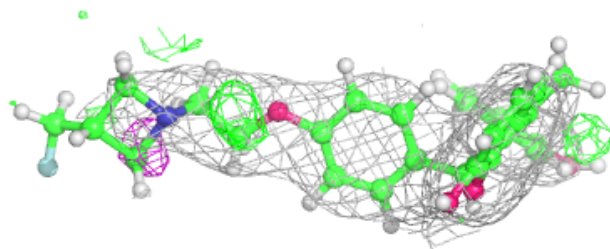
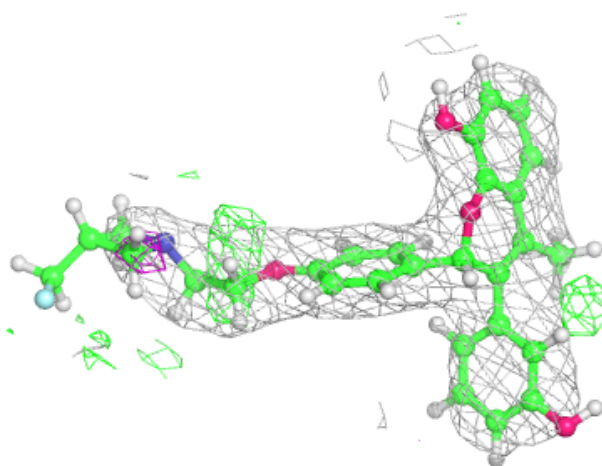
Electron density around ODY A 601:

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



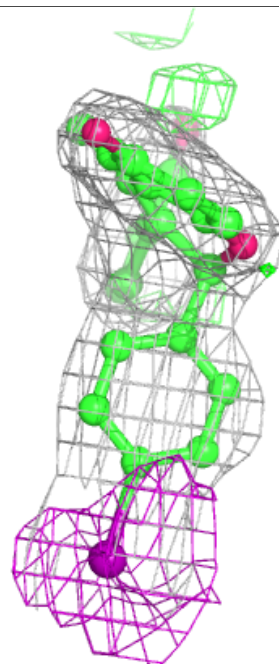
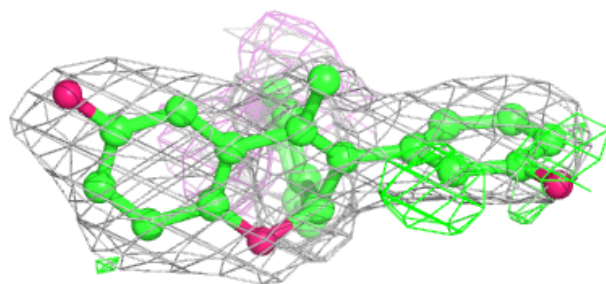
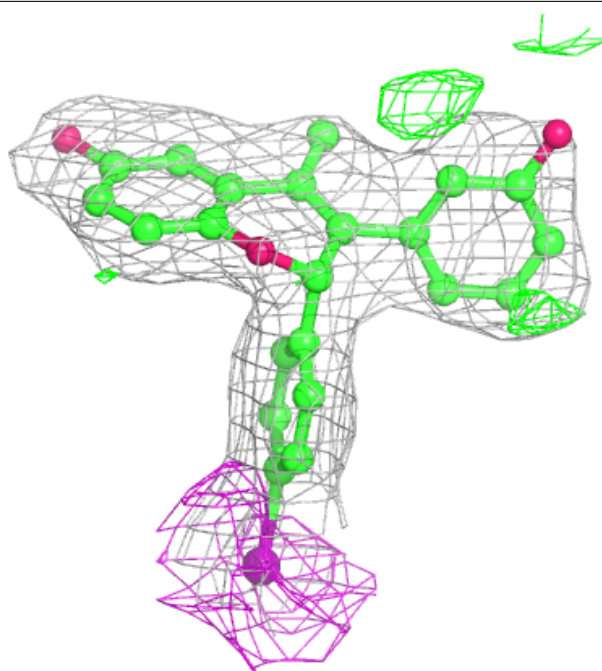
Electron density around ODY B 601:

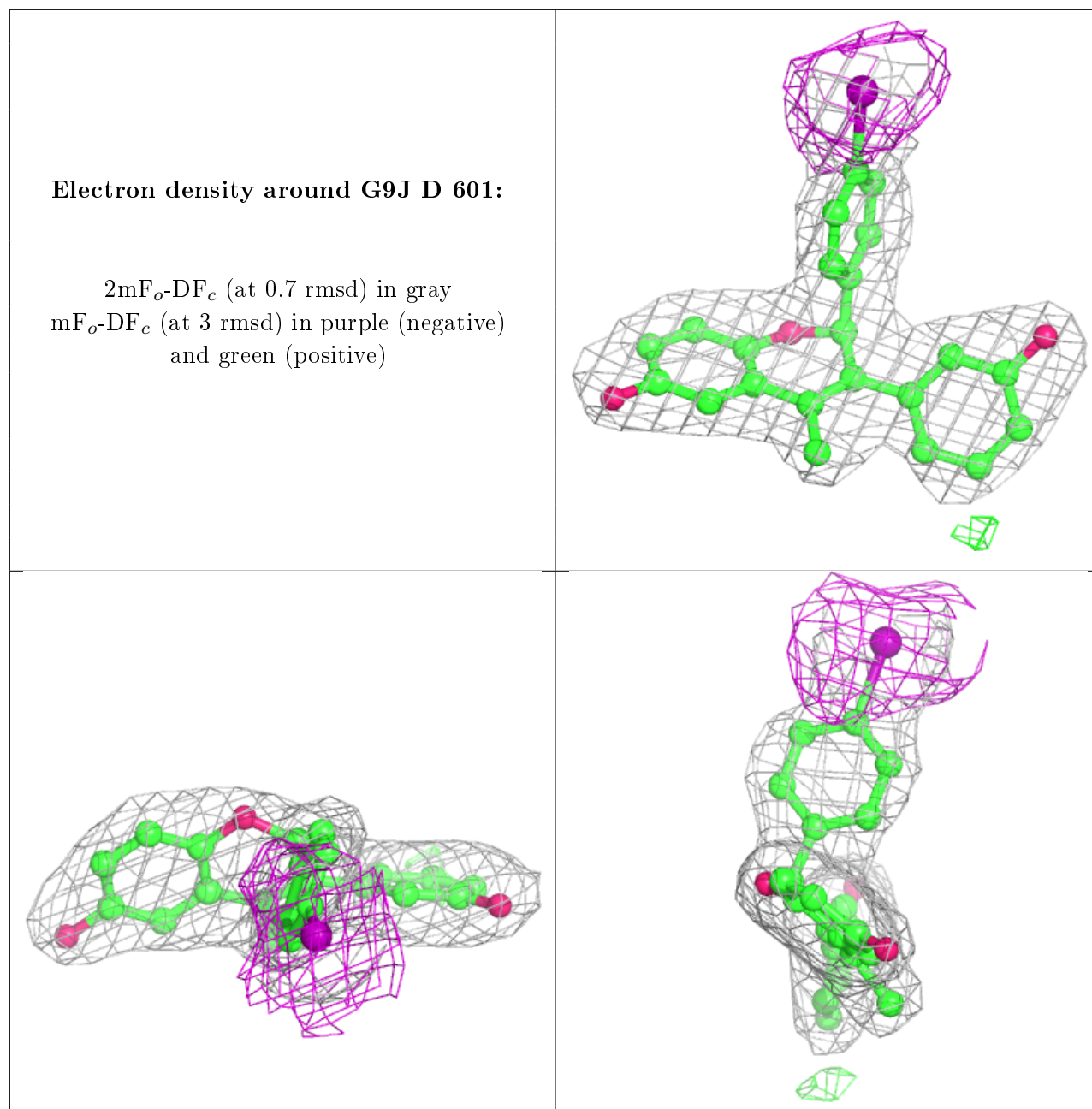
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





6.5 Other polymers [i](#)

There are no such residues in this entry.