wwPDB X-ray Structure Validation Summary Report (i)

Oct 25, 2023 – 01:33 PM EDT

PDB ID	:	6WOK
Title	:	Crystal structure of estrogen receptor alpha in complex with receptor degrader 6
Authors	:	Kiefer, J.R.; Vinogradova, M.; Liang, J.; Zhang, B.; Wang, X.; Labadie, S.
Deposited on	:	2020-04-24
Resolution	:	2.31 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

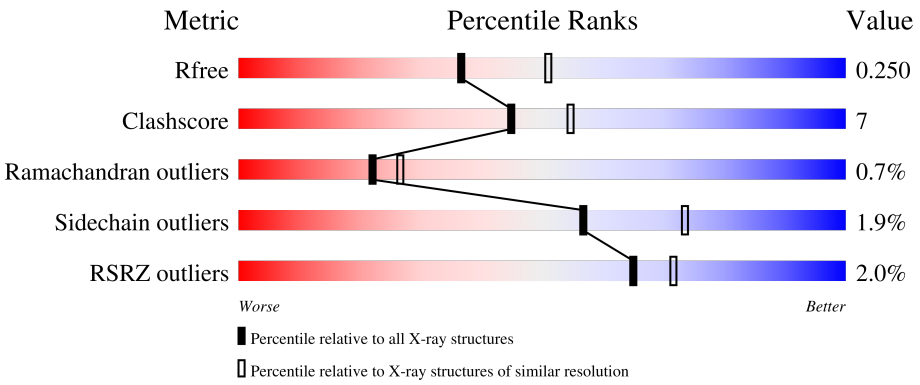
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.31 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 <=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	3% 66% 14% 20%
1	B	280	2% 69% 12% • 18%
1	C	280	% 69% 15% 17%
1	D	280	% 69% 13% • 18%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 7499 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	D	231	1818	1165	304	331	18	0	2	0
1	A	225	1764	1129	299	317	19	0	2	0
1	C	233	1799	1152	304	326	17	0	2	0
1	B	230	1797	1155	303	322	17	0	2	0

There are 104 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	274	MET	-	expression tag	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	-	expression tag	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	-	expression tag	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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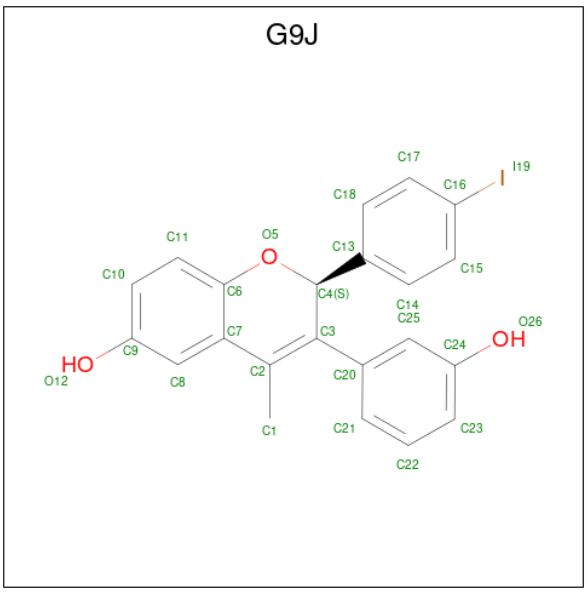
Chain	Residue	Modelled	Actual	Comment	Reference
C	285	ASP	-	expression tag	UNP P03372
C	286	LEU	-	expression tag	UNP P03372
C	287	GLY	-	expression tag	UNP P03372
C	288	THR	-	expression tag	UNP P03372
C	289	GLU	-	expression tag	UNP P03372
C	290	ASN	-	expression tag	UNP P03372
C	291	LEU	-	expression tag	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	-	expression tag	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

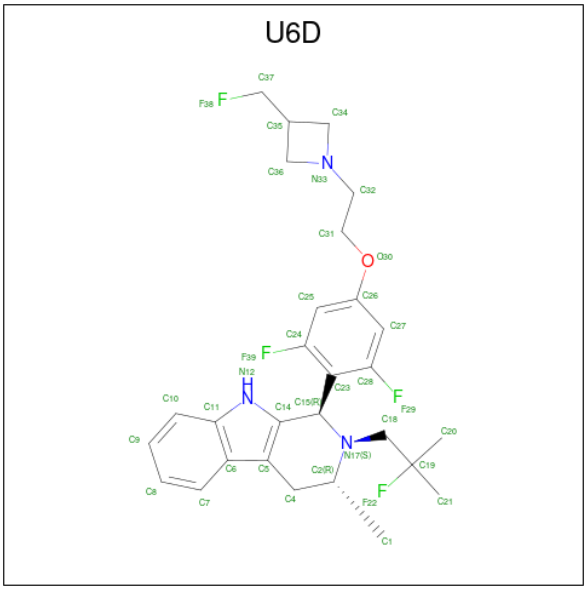
- Molecule 2 is (2S)-3-(3-hydroxyphenyl)-2-(4-iodophenyl)-4-methyl-2H-1-benzopyran-6-ol

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



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

- Molecule 3 is (1R,3R)-1-(2,6-difluoro-4-{2-[3-(fluoromethyl)azetidin-1-yl]ethoxy}phenyl)-2-(2-fluoro-2-methylpropyl)-3-methyl-2,3,4,9-tetrahydro-1H-beta-carboline (three-letter code: U6D) (formula: $C_{28}H_{33}F_4N_3O$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	F	N	O		
3	A	1	36	28	4	3	1	0	1
3	C	1	36	28	4	3	1	0	1
3	B	1	36	28	4	3	1	0	0

- Molecule 4 is water.

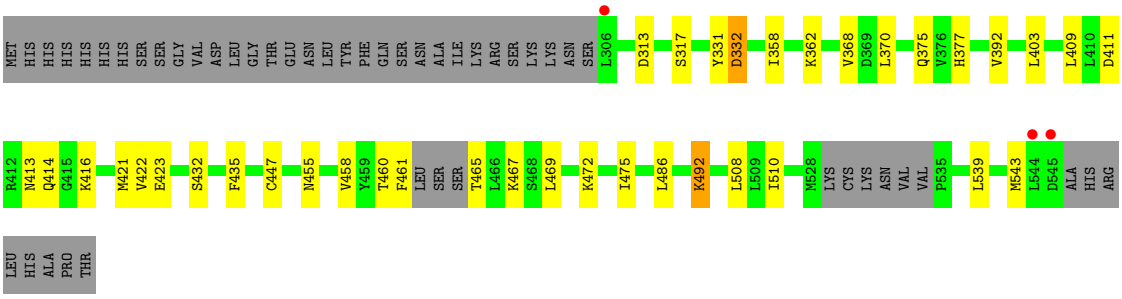
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	D	39	39	39	0	0
4	A	30	30	30	0	0
4	C	27	27	27	0	0
4	B	38	39	39	0	1

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.

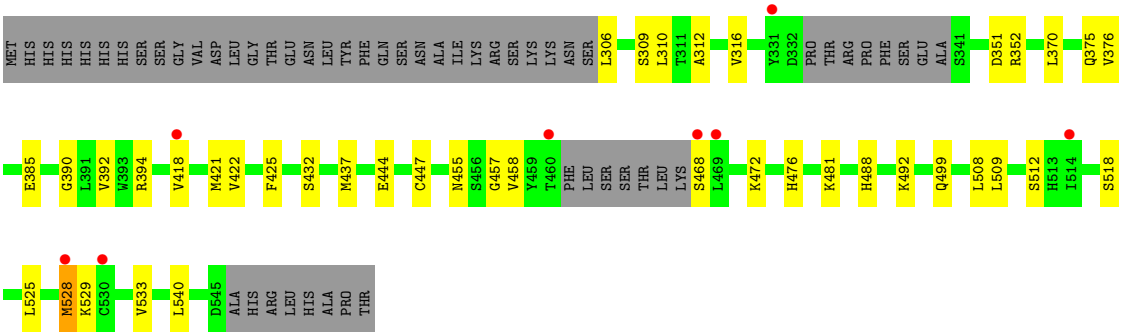
• Molecule 1: Estrogen receptor

Chain D:



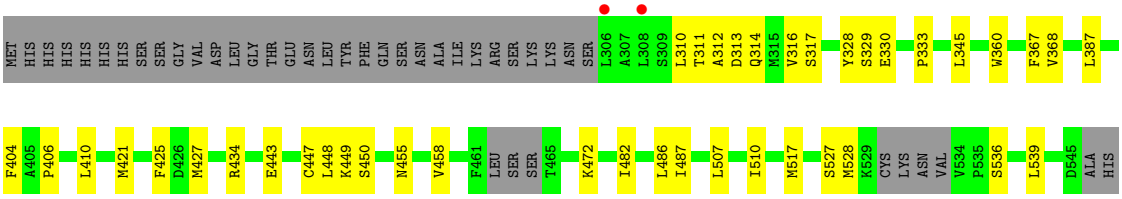
• Molecule 1: Estrogen receptor

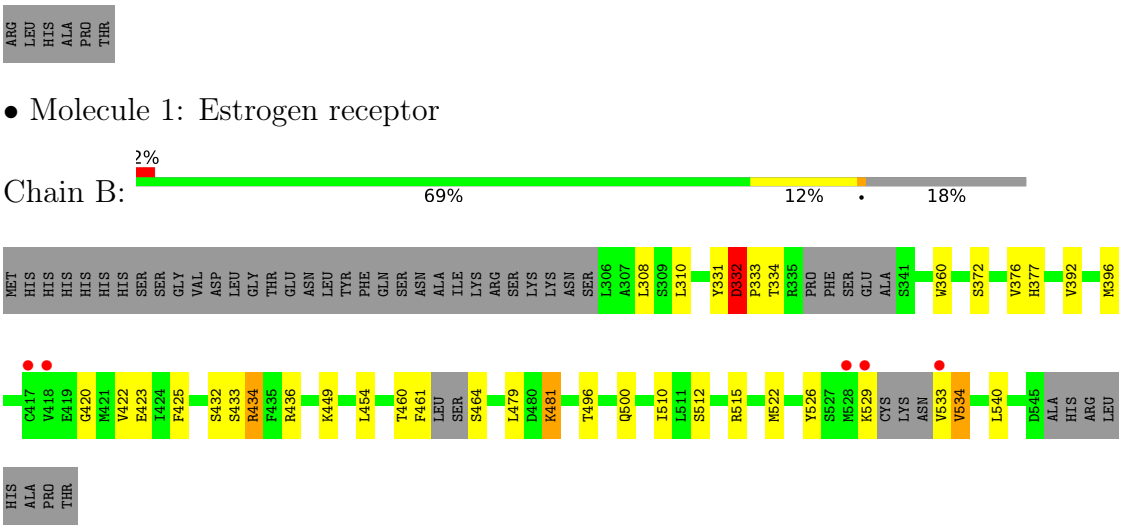
Chain A:



• Molecule 1: Estrogen receptor

Chain C:




ARG LEU HIS ALA PRO THR
• Molecule 1: Estrogen receptor
Chain B:
2%
69%
12%
18%
MET HIS 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 A307 L308 S309 L310 Y331 D332 P333 T334 R335 PRO PHE SER GLU ALA S341 W360 S372 V376 H377 V392 M396
C417 V418 E419 G420 M421 V422 E423 I424 F425 S432 S433 R434 F435 R436 K449 L454 T460 F461 LEU SER S464 L479 D480 K481 T496 Q500 I510 L511 S512 R515 M522 Y526 S527 M528 K529 CYS LYS ASN V533 V534 L540 D545 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	53.61Å 59.10Å 94.72Å 86.61° 74.78° 63.29°	Depositor
Resolution (Å)	38.45 – 2.31 38.45 – 2.31	Depositor EDS
% Data completeness (in resolution range)	73.5 (38.45-2.31) 73.5 (38.45-2.31)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.61 (at 2.31Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.172 , 0.250 0.172 , 0.250	Depositor DCC
R_{free} test set	1214 reflections (3.76%)	wwPDB-VP
Wilson B-factor (Å^2)	40.3	Xtriage
Anisotropy	0.197	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 38.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.159 for h,h-k,h-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7499	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.55% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: G9J, U6D

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	0.43	0/1796	0.60	0/2427
1	B	0.43	0/1831	0.60	0/2478
1	C	0.42	0/1835	0.56	0/2488
1	D	0.42	0/1855	0.58	0/2509
All	All	0.43	0/7317	0.59	0/9902

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	332	ASP	Peptide

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	1764	0	1791	23	1
1	B	1797	0	1814	21	0
1	C	1799	0	1779	25	0
1	D	1818	0	1822	27	1
2	A	26	0	0	1	0
2	C	26	0	0	1	0
2	D	26	0	0	1	0
3	A	36	0	0	1	0
3	B	36	0	0	0	0
3	C	36	0	0	0	0
4	A	30	0	0	2	0
4	B	39	0	0	0	0
4	C	27	0	0	2	0
4	D	39	0	0	3	0
All	All	7499	0	7206	95	1

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.

The worst 5 of 95 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:536:SER:HB2	1:C:539:LEU:H	1.42	0.83
1:B:377:HIS:NE2	1:B:460:THR:OG1	2.11	0.82
1:B:377:HIS:HE2	1:B:460:THR:HG1	1.29	0.79
1:A:529:LYS:HA	1:A:533:VAL:HG21	1.69	0.74
1:D:539:LEU:HD23	1:D:543:MET:SD	2.30	0.71

All (1) 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:D:332:ASP:OD1	1:A:499:GLN:NE2[1_465]	2.08	0.12

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	220/280 (79%)	216 (98%)	4 (2%)	0	100	100
1	B	223/280 (80%)	213 (96%)	6 (3%)	4 (2%)	8	7
1	C	228/280 (81%)	222 (97%)	5 (2%)	1 (0%)	34	42
1	D	226/280 (81%)	222 (98%)	3 (1%)	1 (0%)	34	42
All	All	897/1120 (80%)	873 (97%)	18 (2%)	6 (1%)	22	26

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	332	ASP
1	B	333	PRO
1	B	534	VAL
1	C	528	MET
1	D	332	ASP

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	196/252 (78%)	193 (98%)	3 (2%)	65	79
1	B	198/252 (79%)	190 (96%)	8 (4%)	31	44
1	C	194/252 (77%)	191 (98%)	3 (2%)	65	79
1	D	201/252 (80%)	200 (100%)	1 (0%)	88	95
All	All	789/1008 (78%)	774 (98%)	15 (2%)	57	73

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	425	PHE
1	B	515	ARG

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Mol	Chain	Res	Type
1	B	433	SER
1	B	522	MET
1	B	481	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	501	HIS
1	C	506	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 monosaccharides 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	$\#\|Z\| > 2$
3	U6D	C	601[A]	-	34,40,40	0.91	2 (5%)	37,60,60	1.75	11 (29%)
2	G9J	D	601	-	29,29,29	0.72	2 (6%)	38,42,42	1.08	2 (5%)
2	G9J	C	602[B]	-	29,29,29	0.48	0	38,42,42	1.00	3 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	U6D	A	601[A]	-	34,40,40	0.82	1 (2%)	37,60,60	1.65	9 (24%)
2	G9J	A	602[B]	-	29,29,29	0.43	0	38,42,42	1.03	2 (5%)
3	U6D	B	601	-	34,40,40	0.99	2 (5%)	37,60,60	1.54	8 (21%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	U6D	C	601[A]	-	-	6/13/41/41	0/5/5/5
2	G9J	D	601	-	-	2/8/24/24	0/4/4/4
2	G9J	C	602[B]	-	-	2/8/24/24	0/4/4/4
3	U6D	A	601[A]	-	-	5/13/41/41	0/5/5/5
2	G9J	A	602[B]	-	-	2/8/24/24	0/4/4/4
3	U6D	B	601	-	-	3/13/41/41	0/5/5/5

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	601	U6D	C15-N17	3.38	1.50	1.48
3	B	601	U6D	C5-C14	-2.37	1.35	1.39
3	A	601[A]	U6D	C5-C14	-2.33	1.35	1.39
3	C	601[A]	U6D	C15-N17	2.32	1.49	1.48
3	C	601[A]	U6D	C5-C14	-2.29	1.35	1.39

The worst 5 of 35 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	601[A]	U6D	C28-C23-C24	4.04	118.04	114.16
3	C	601[A]	U6D	C28-C23-C24	3.98	117.99	114.16
3	B	601	U6D	F39-C24-C23	3.31	121.37	118.13
3	A	601[A]	U6D	C25-C24-C23	-3.21	120.60	124.63
3	C	601[A]	U6D	C25-C24-C23	-3.11	120.72	124.63

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	601[A]	U6D	N17-C18-C19-C20
3	A	601[A]	U6D	N17-C18-C19-C21
3	A	601[A]	U6D	N17-C18-C19-F22
3	C	601[A]	U6D	N17-C18-C19-C20
3	C	601[A]	U6D	N17-C18-C19-C21

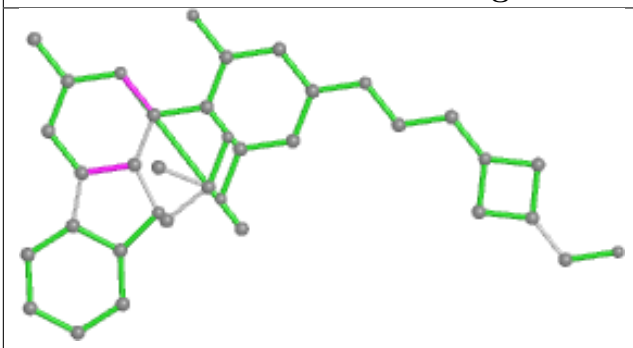
There are no ring outliers.

4 monomers are involved in 4 short contacts:

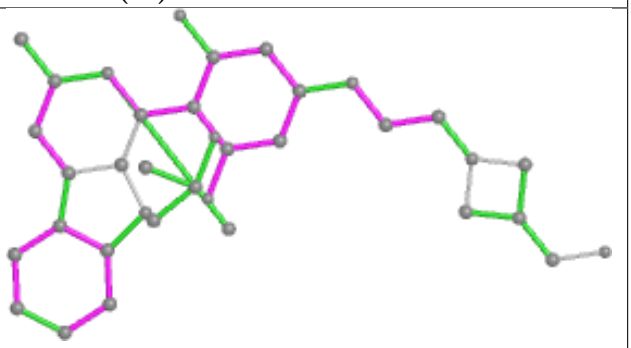
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	601	G9J	1	0
2	C	602[B]	G9J	1	0
3	A	601[A]	U6D	1	0
2	A	602[B]	G9J	1	0

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 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.

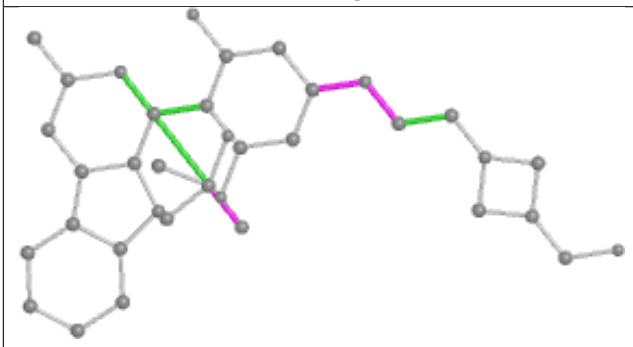
Ligand U6D C 601 (A)



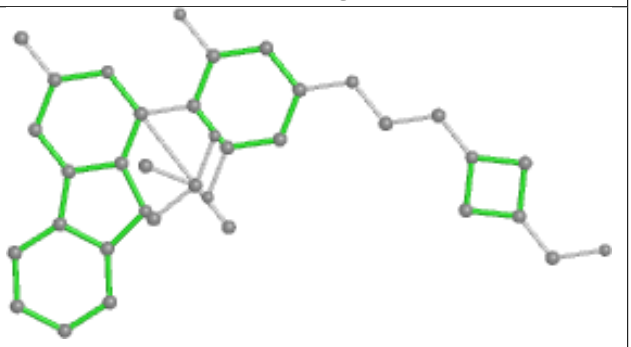
Bond lengths



Bond angles

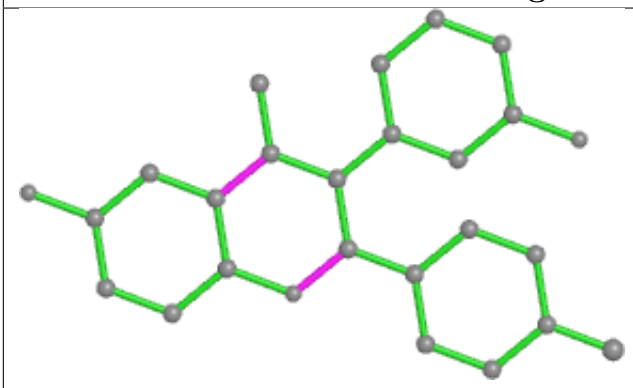


Torsions

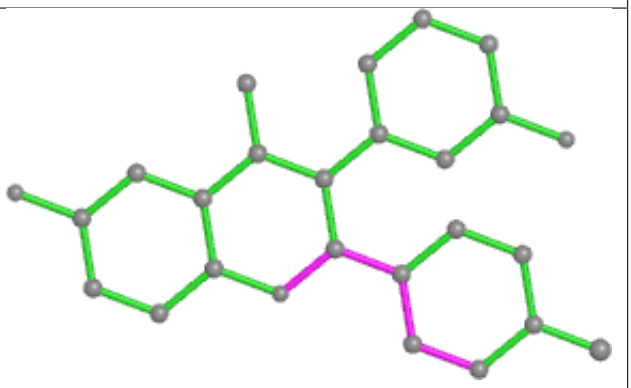


Rings

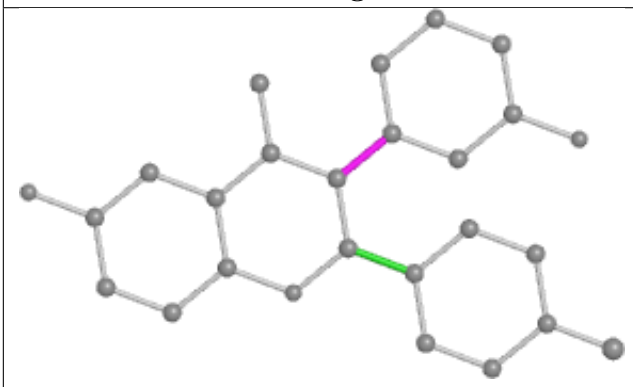
Ligand G9J D 601



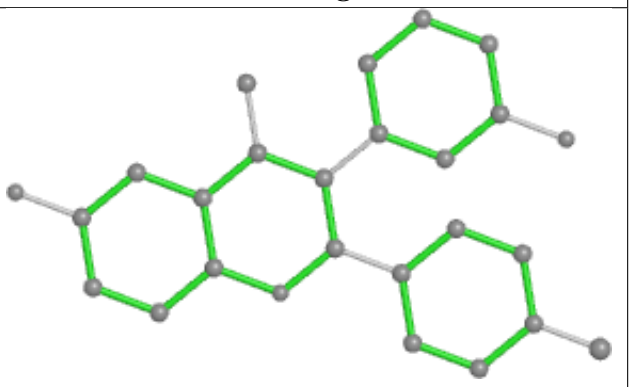
Bond lengths



Bond angles

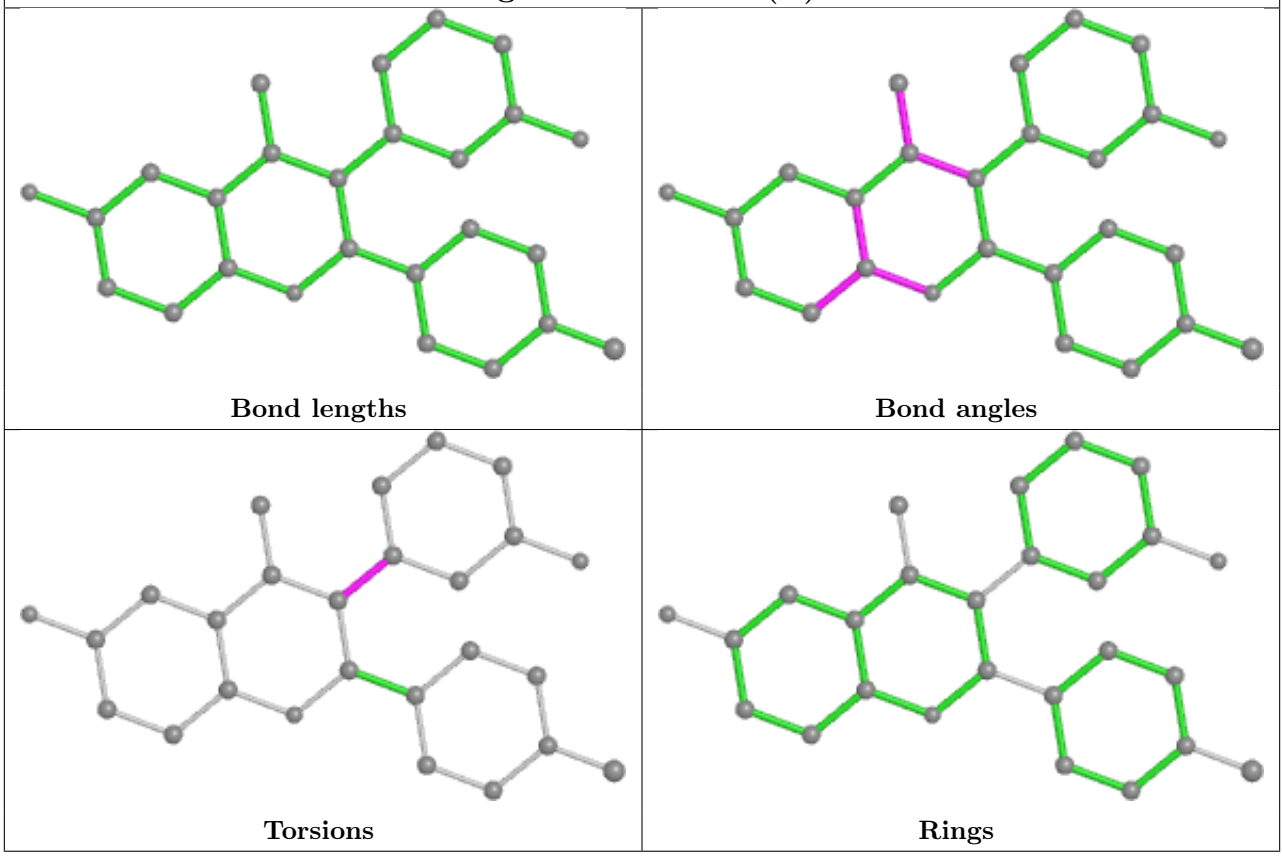


Torsions

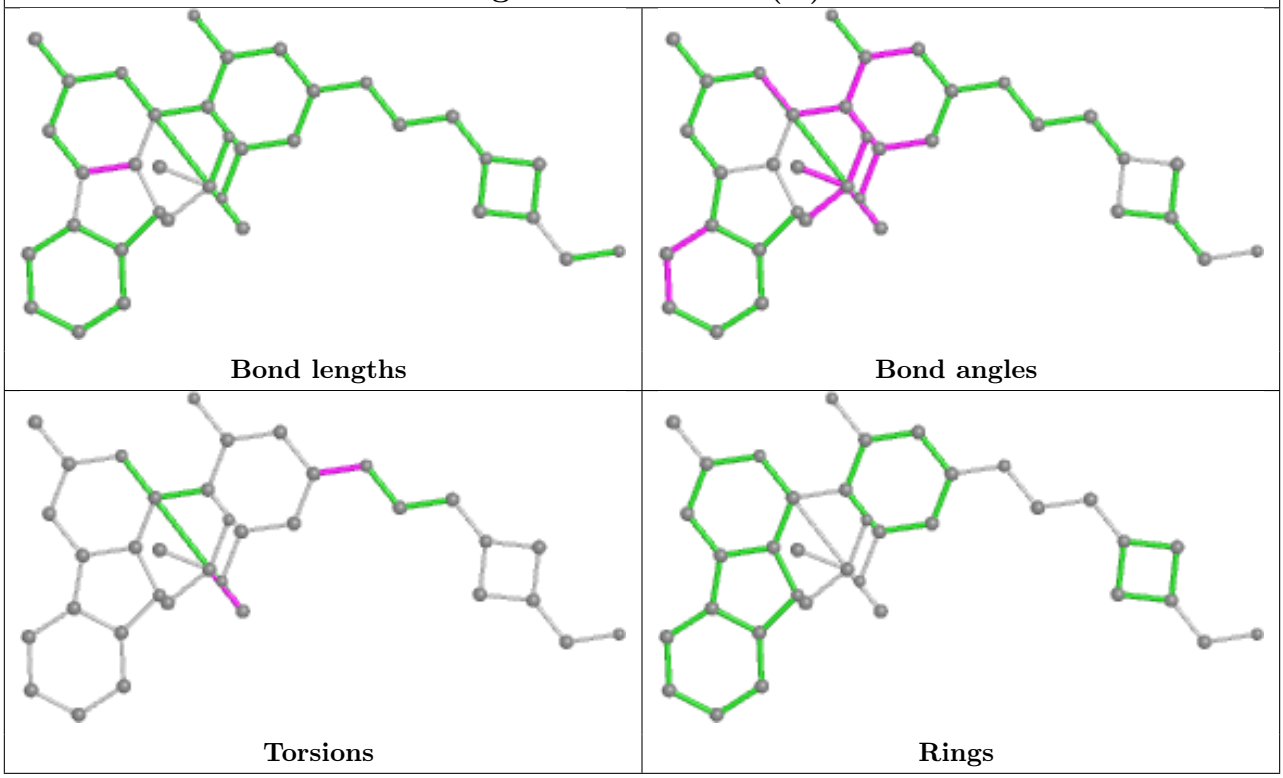


Rings

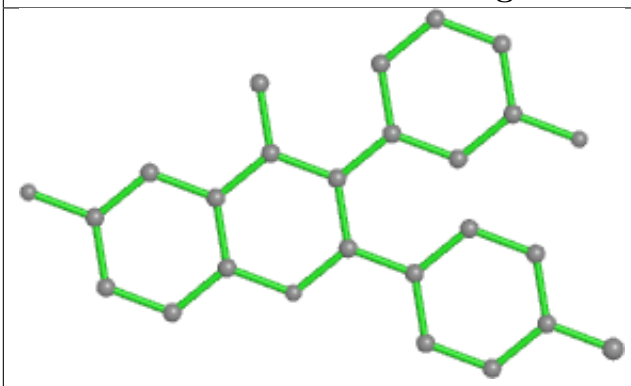
Ligand G9J C 602 (B)



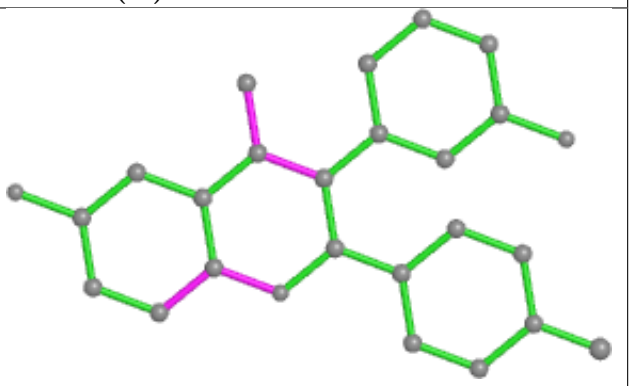
Ligand U6D A 601 (A)



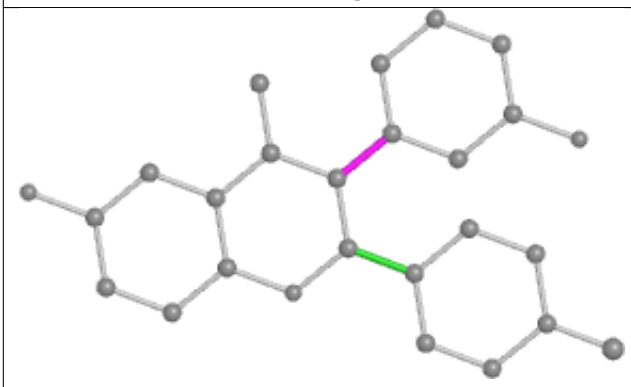
Ligand G9J A 602 (B)



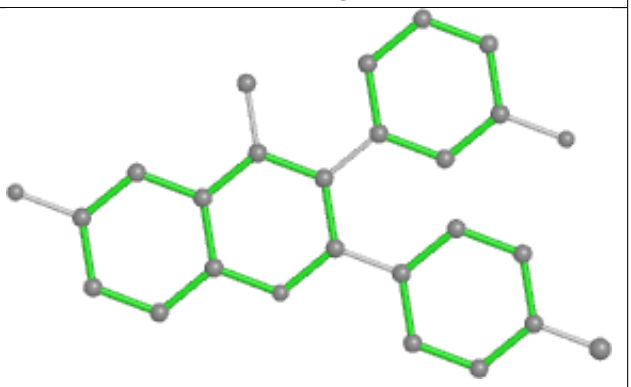
Bond lengths



Bond angles

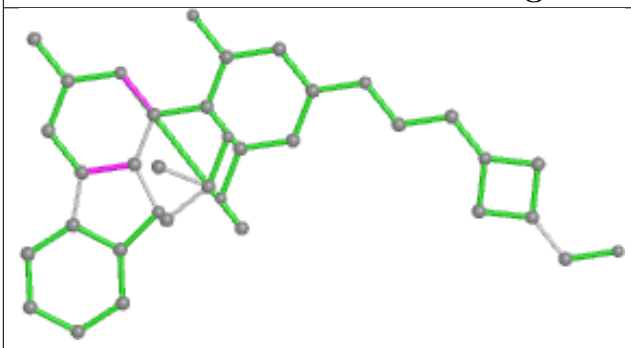


Torsions

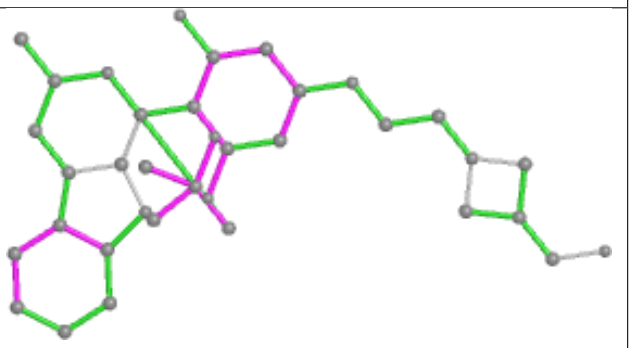


Rings

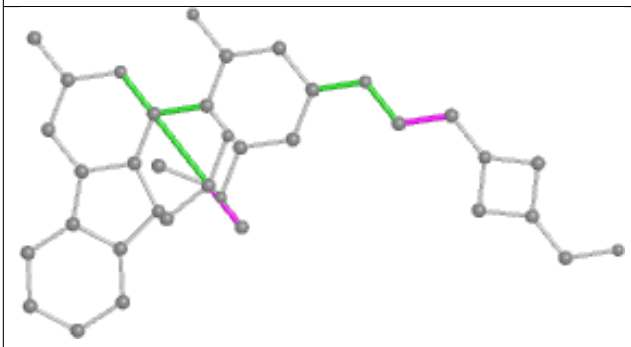
Ligand U6D B 601



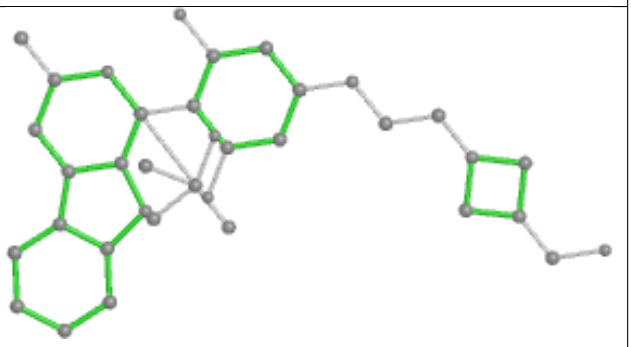
Bond lengths



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 (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	225/280 (80%)	-0.27	8 (3%)	42	49	29, 48, 82, 140	0
1	B	230/280 (82%)	-0.35	5 (2%)	62	69	29, 46, 81, 119	0
1	C	233/280 (83%)	-0.37	2 (0%)	84	88	31, 51, 79, 102	0
1	D	231/280 (82%)	-0.45	3 (1%)	77	81	28, 47, 80, 99	0
All	All	919/1120 (82%)	-0.36	18 (1%)	65	71	28, 48, 81, 140	0

The worst 5 of 18 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	306	LEU	3.5
1	A	530	CYS	3.5
1	A	460	THR	3.4
1	D	306	LEU	3.2
1	B	528	MET	3.1

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 monosaccharides in this entry.

6.4 Ligands (i)

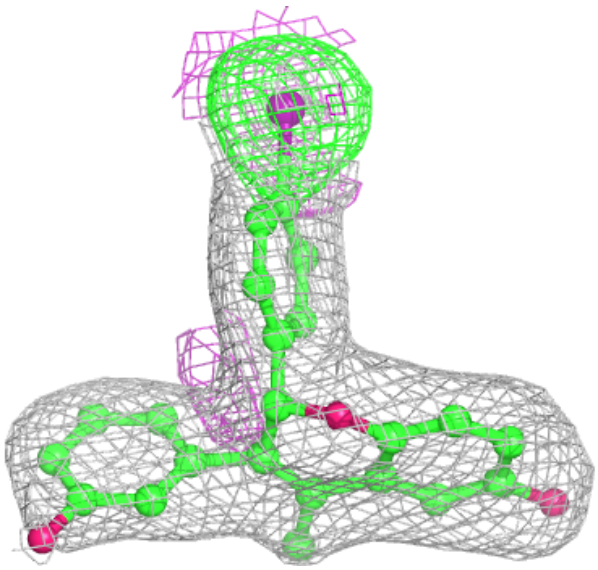
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

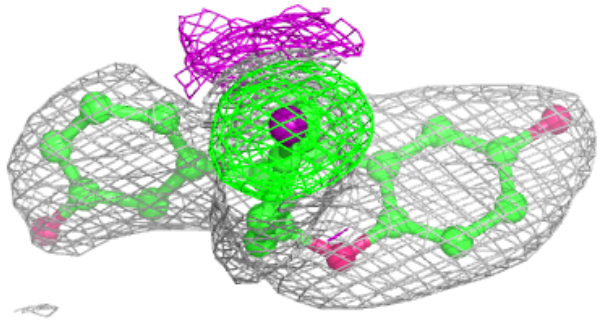
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	G9J	D	601	26/26	0.79	0.15	27,48,80,244	0
3	U6D	B	601	36/36	0.95	0.14	25,51,75,81	0
3	U6D	A	601[A]	36/36	0.96	0.12	36,46,63,69	36
2	G9J	A	602[B]	26/26	0.96	0.10	39,43,51,74	26
3	U6D	C	601[A]	36/36	0.97	0.15	35,46,59,62	36
2	G9J	C	602[B]	26/26	0.97	0.13	36,44,54,57	26

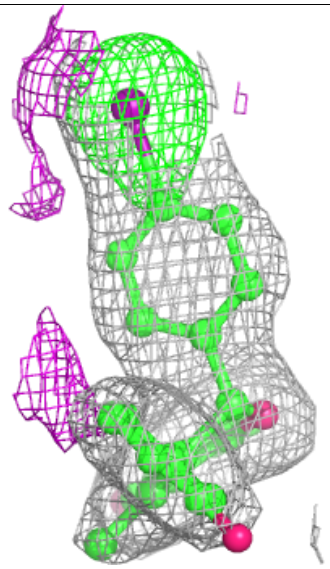
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 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)

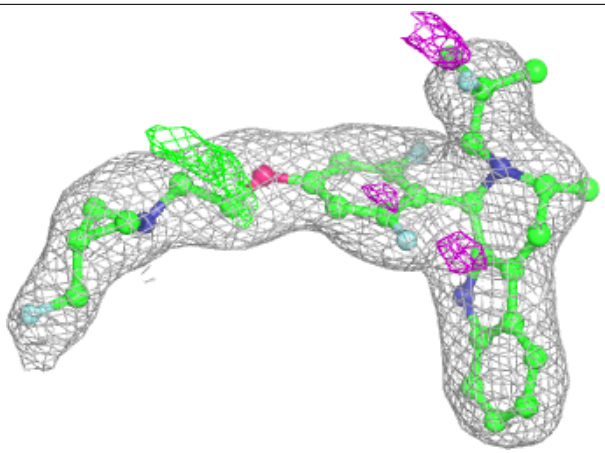


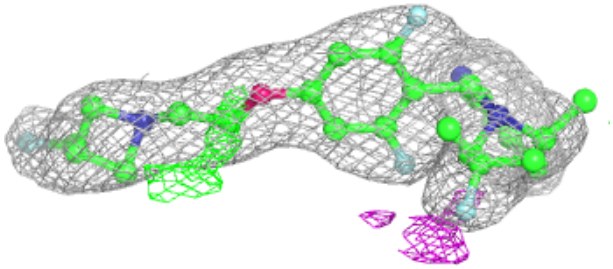


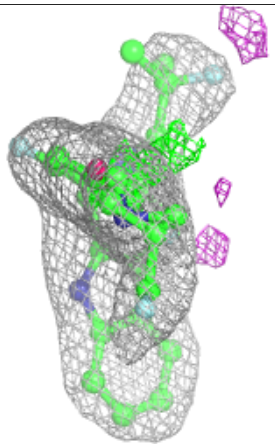


Electron density around U6D B 601:

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

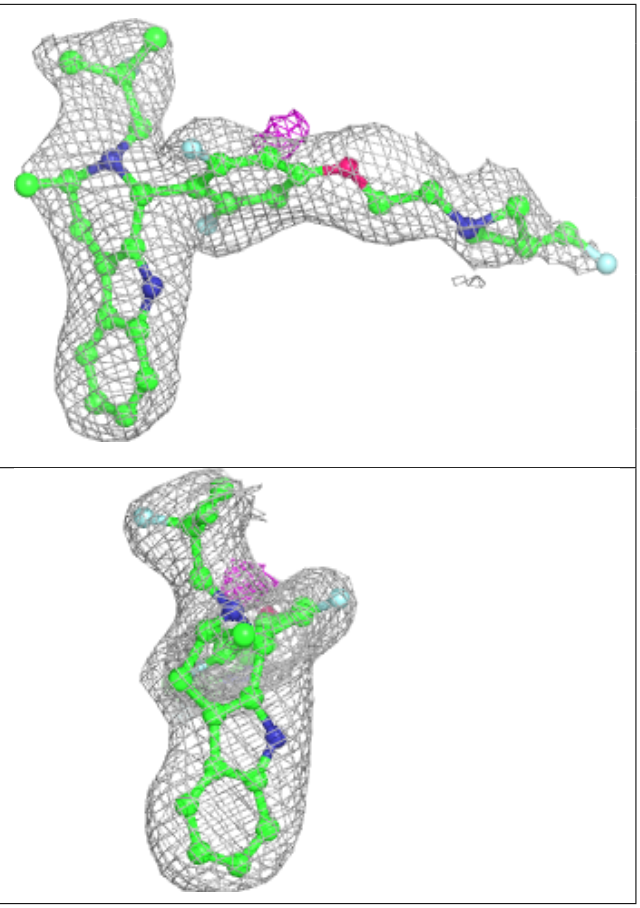


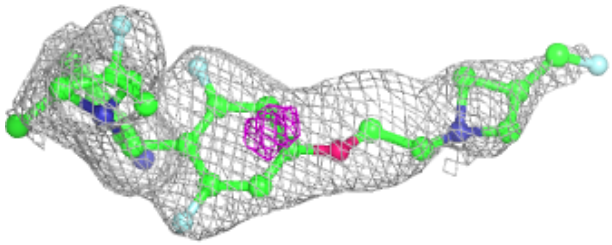




Electron density around U6D A 601 (A):

$2mF_o$-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 A 602 (B):

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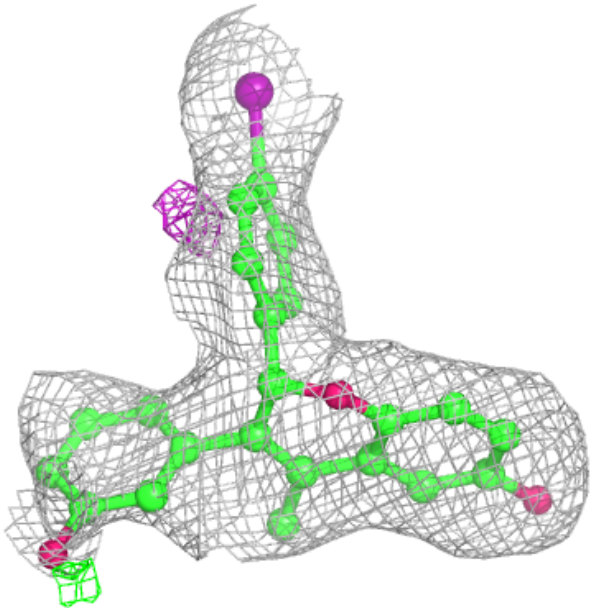
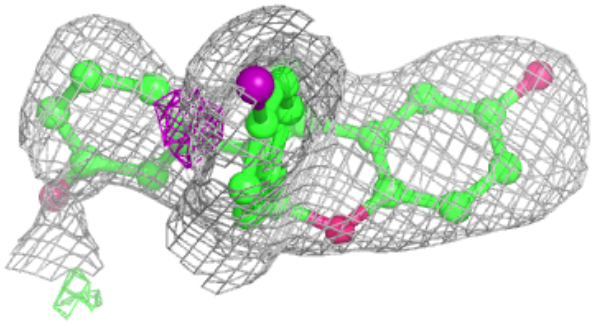
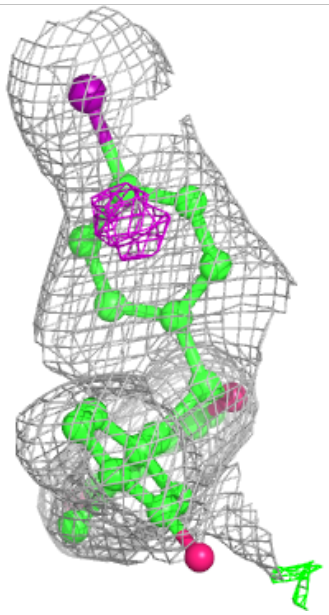
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

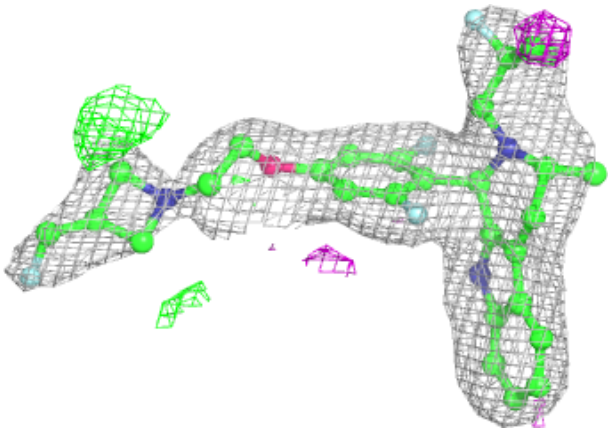


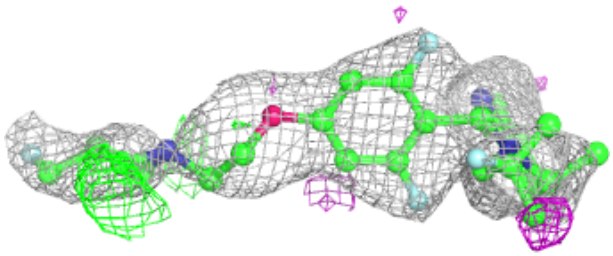


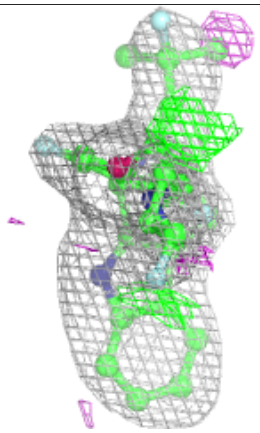


Electron density around U6D C 601 (A):

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

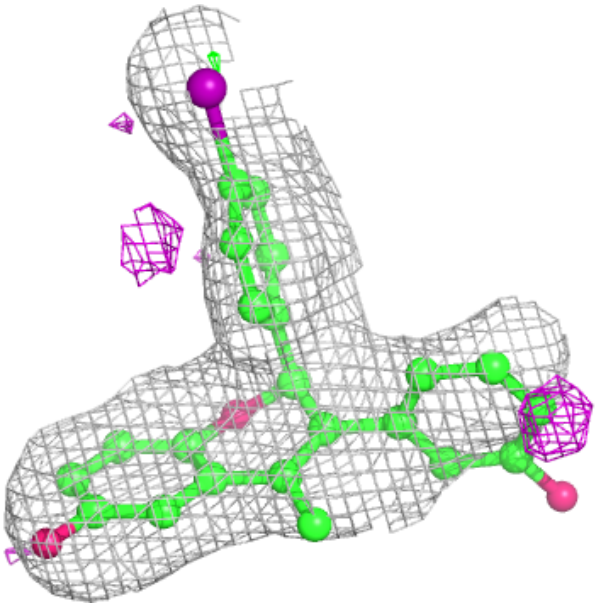


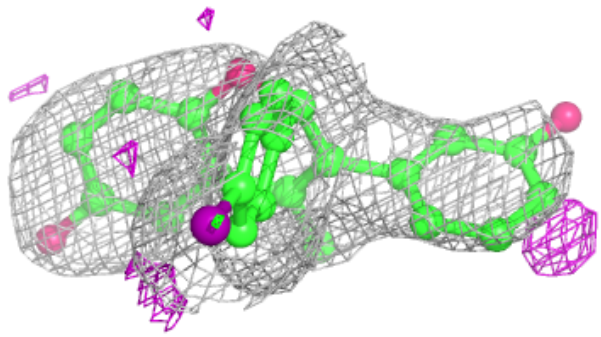


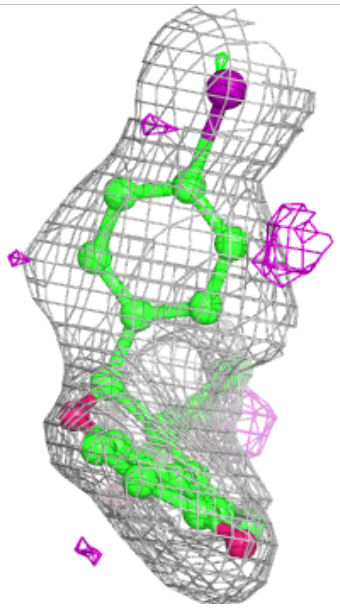


Electron density around G9J C 602 (B):

$2mF_o$-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.