Full wwPDB X-ray Structure Validation Report (i)

Nov 14, 2023 – 02:25 PM JST

PDB ID	:	5ZG3
Title	:	Crystal structure of the GluA2o LBD in complex with glutamate and TAK-137
Authors	:	Sogabe, S.; Igaki, S.; Hirokawa, A.; Zama, Y.; Lane, W.; Snell, G.
Deposited on	:	2018-03-07
Resolution	:	1.65 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 (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:

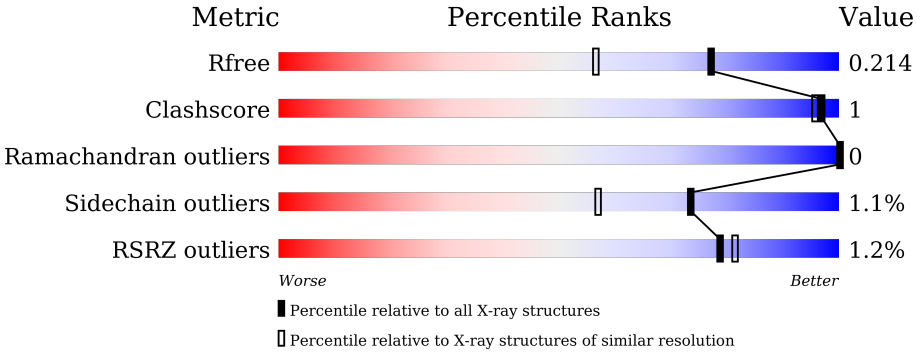
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 1.65 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	1827 (1.66-1.66)
Clashscore	141614	1931 (1.66-1.66)
Ramachandran outliers	138981	1891 (1.66-1.66)
Sidechain outliers	138945	1891 (1.66-1.66)
RSRZ outliers	127900	1791 (1.66-1.66)

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	263	% 95%
1	B	263	97%
1	C	263	% 95%
1	D	263	96%
1	E	263	3% 97%
1	F	263	3% 96%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 13577 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 Glutamate receptor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	260	2047	1305	342	385	15	0	2	0
1	B	260	2050	1307	342	385	16	0	3	0
1	C	260	2047	1303	343	386	15	0	2	0
1	D	262	2057	1308	345	389	15	0	2	0
1	E	260	2047	1305	342	385	15	0	2	0
1	F	260	2051	1307	342	386	16	0	3	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	411	GLY	-	expression tag	UNP P42262
A	412	SER	-	expression tag	UNP P42262
A	641	GLY	-	linker	UNP P42262
A	642	THR	-	linker	UNP P42262
B	411	GLY	-	expression tag	UNP P42262
B	412	SER	-	expression tag	UNP P42262
B	641	GLY	-	linker	UNP P42262
B	642	THR	-	linker	UNP P42262
C	411	GLY	-	expression tag	UNP P42262
C	412	SER	-	expression tag	UNP P42262
C	641	GLY	-	linker	UNP P42262
C	642	THR	-	linker	UNP P42262
D	411	GLY	-	expression tag	UNP P42262
D	412	SER	-	expression tag	UNP P42262
D	641	GLY	-	linker	UNP P42262
D	642	THR	-	linker	UNP P42262
E	411	GLY	-	expression tag	UNP P42262

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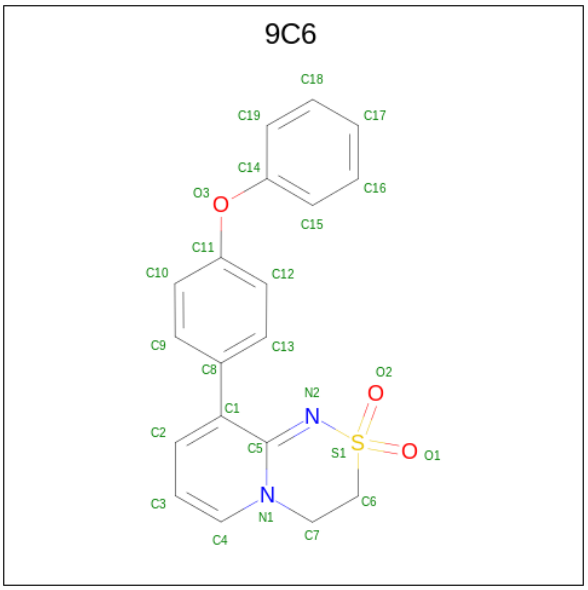
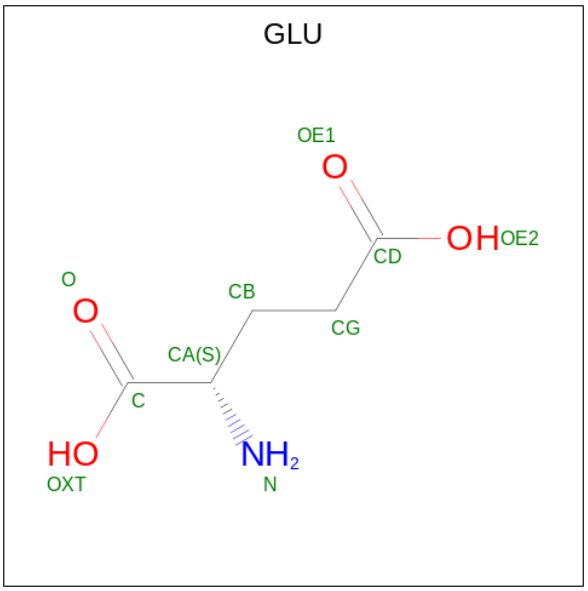
Chain	Residue	Modelled	Actual	Comment	Reference
E	412	SER	-	expression tag	UNP P42262
E	641	GLY	-	linker	UNP P42262
E	642	THR	-	linker	UNP P42262
F	411	GLY	-	expression tag	UNP P42262
F	412	SER	-	expression tag	UNP P42262
F	641	GLY	-	linker	UNP P42262
F	642	THR	-	linker	UNP P42262

- Molecule 2 is 9-(4-phenoxyphenyl)-3,4-dihydro-2H-2lambda 6 -pyrido[2,1-c][1,2,4]thiadiazine-2,2-dione (three-letter code: 9C6) (formula: $C_{19}H_{16}N_2O_3S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			25	19	2	3	1		
2	D	1	Total	C	N	O	S	0	1
			50	38	4	6	2		
2	E	1	Total	C	N	O	S	0	0
			25	19	2	3	1		

- Molecule 3 is GLUTAMIC ACID (three-letter code: GLU) (formula: $C_5H_9NO_4$).

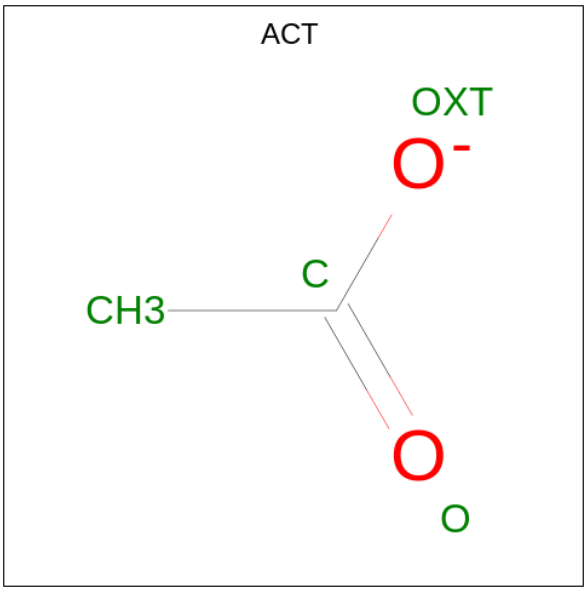


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	10	5	1	4	0	0
3	B	1	10	5	1	4	0	0
3	C	1	10	5	1	4	0	0
3	D	1	10	5	1	4	0	0
3	E	1	10	5	1	4	0	0
3	F	1	10	5	1	4	0	0

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
4	B	2	2	2	0	0
4	C	2	2	2	0	0
4	D	4	4	4	0	0
4	E	1	1	1	0	0
4	F	3	3	3	0	0

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	B	1	4	2	2	0	0
			Total	C	O		
5	B	1	4	2	2	0	0
			Total	C	O		
5	C	1	4	2	2	0	0
			Total	C	O		
5	C	1	4	2	2	0	0
			Total	C	O		
5	C	1	4	2	2	0	0
			Total	C	O		
5	D	1	4	2	2	0	0
			Total	C	O		
5	D	1	4	2	2	0	0
			Total	C	O		
5	E	1	4	2	2	0	0
			Total	C	O		
5	F	1	4	2	2	0	0
			Total	C	O		
5	F	1	4	2	2	0	0
			Total	C	O		
5	F	1	4	2	2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	153	153	153	0	0

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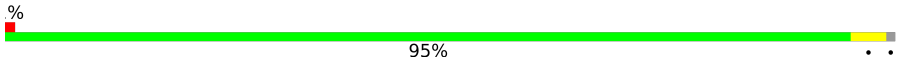
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	B	161	161	161	0	0
			Total	O		
6	C	229	229	229	0	0
			Total	O		
6	D	225	225	225	0	0
			Total	O		
6	E	137	137	137	0	0
			Total	O		
6	F	157	157	157	0	0

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.

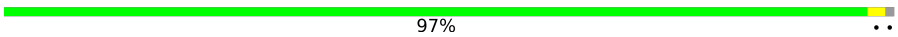
• Molecule 1: Glutamate receptor 2

Chain A:



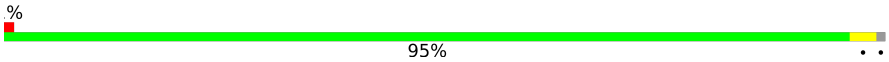
• Molecule 1: Glutamate receptor 2

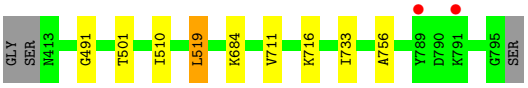
Chain B:



• Molecule 1: Glutamate receptor 2

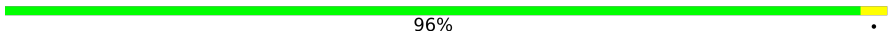
Chain C:





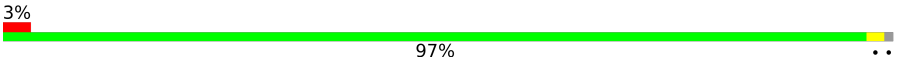
• Molecule 1: Glutamate receptor 2

Chain D:



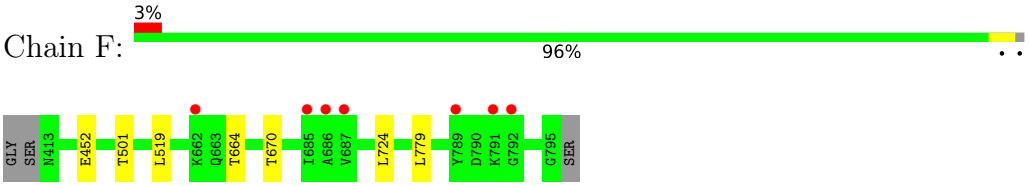
• Molecule 1: Glutamate receptor 2

Chain E:



• Molecule 1: Glutamate receptor 2

Chain F:


3%
96%
GLY
SER
N413
E452
T501
L519
K662
Q663
T664
T670
I685
A686
V687
L724
L779
Y789
D790
K791
G792
G795
SER

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	114.06Å 162.33Å 47.38Å 90.00° 90.02° 90.00°	Depositor
Resolution (Å)	40.00 – 1.65 42.26 – 1.65	Depositor EDS
% Data completeness (in resolution range)	99.2 (40.00-1.65) 99.2 (42.26-1.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	1.90 (at 1.65Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.184 , 0.215 0.184 , 0.214	Depositor DCC
R_{free} test set	10304 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	23.1	Xtriage
Anisotropy	0.130	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 29.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.468 for -h,-k,l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	13577	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.27% 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: ZN, ACT, 9C6

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	0.52	0/2089	0.64	1/2808 (0.0%)
1	B	0.49	0/2095	0.63	0/2816
1	C	0.54	0/2089	0.67	1/2808 (0.0%)
1	D	0.53	0/2099	0.68	1/2821 (0.0%)
1	E	0.50	0/2089	0.64	1/2808 (0.0%)
1	F	0.48	0/2096	0.62	0/2817
All	All	0.51	0/12557	0.65	4/16878 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	519	LEU	CA-CB-CG	5.88	128.82	115.30
1	A	519	LEU	CA-CB-CG	5.20	127.26	115.30
1	D	519	LEU	CA-CB-CG	5.15	127.15	115.30
1	E	519	LEU	CA-CB-CG	5.06	126.95	115.30

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	2047	0	2089	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2050	0	2094	1	0
1	C	2047	0	2084	5	0
1	D	2057	0	2092	6	0
1	E	2047	0	2089	2	0
1	F	2051	0	2094	3	0
2	A	25	0	0	0	0
2	D	50	0	0	0	0
2	E	25	0	0	0	0
3	A	10	0	5	1	0
3	B	10	0	5	1	0
3	C	10	0	5	1	0
3	D	10	0	5	1	0
3	E	10	0	5	1	0
3	F	10	0	5	1	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	4	0	0	0	0
4	E	1	0	0	0	0
4	F	3	0	0	0	1
5	B	8	0	6	0	0
5	C	12	0	9	0	0
5	D	8	0	6	0	0
5	E	4	0	3	0	0
5	F	12	0	9	0	0
6	A	153	0	0	1	1
6	B	161	0	0	0	0
6	C	229	0	0	2	0
6	D	225	0	0	1	0
6	E	137	0	0	0	0
6	F	157	0	0	0	0
All	All	13577	0	12605	23	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 1.

All (23) 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:D:474:ARG:HH11	1:D:479:LYS:HD2	1.65	0.61
1:A:501:THR:HG1	3:A:1002:GLU:N	2.05	0.54
1:E:452:GLU:HG3	1:E:779:LEU:HD21	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:501:THR:HG1	3:E:1002:GLU:N	2.08	0.51
1:C:711:VAL:HG21	1:C:733:ILE:HD13	1.94	0.49
1:B:501:THR:HG1	3:B:901:GLU:N	2.10	0.49
1:F:501:THR:HG1	3:F:802:GLU:N	2.11	0.48
1:A:452:GLU:HG3	1:A:779:LEU:HD21	1.95	0.47
1:C:716:LYS:HG3	6:C:1034:HOH:O	2.15	0.46
1:A:510:ILE:HD12	1:A:756:ALA:HB1	1.98	0.45
1:D:474:ARG:NH1	1:D:479:LYS:HD2	2.30	0.45
1:D:491:GLY:HA2	6:D:910:HOH:O	2.18	0.44
1:D:713:ARG:O	1:D:717:SER:HB3	2.17	0.43
1:C:491:GLY:HA2	6:C:926:HOH:O	2.18	0.43
1:A:491:GLY:HA2	6:A:1117:HOH:O	2.19	0.43
1:D:510:ILE:HD12	1:D:756:ALA:HB1	2.01	0.43
1:C:501:THR:HG1	3:C:802:GLU:N	2.18	0.42
1:F:452:GLU:HG3	1:F:779:LEU:HD11	2.02	0.41
1:A:434:GLU:H	1:A:434:GLU:HG2	1.68	0.41
1:C:510:ILE:HD12	1:C:756:ALA:HB1	2.03	0.41
1:A:497:ILE:HG12	1:A:755[B]:ILE:HD12	2.03	0.40
1:F:670:THR:HG22	1:F:724:LEU:HB2	2.03	0.40
1:D:501:THR:HG1	3:D:803:GLU:N	2.20	0.40

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)
4:F:804:ZN:ZN	6:A:1102:HOH:O[2_656]	1.50	0.70

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	260/263 (99%)	256 (98%)	4 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	261/263 (99%)	259 (99%)	2 (1%)	0	100	100
1	C	260/263 (99%)	257 (99%)	3 (1%)	0	100	100
1	D	262/263 (100%)	259 (99%)	3 (1%)	0	100	100
1	E	260/263 (99%)	257 (99%)	3 (1%)	0	100	100
1	F	261/263 (99%)	258 (99%)	3 (1%)	0	100	100
All	All	1564/1578 (99%)	1546 (99%)	18 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	221/221 (100%)	219 (99%)	2 (1%)	78	66
1	B	222/221 (100%)	217 (98%)	5 (2%)	50	25
1	C	221/221 (100%)	219 (99%)	2 (1%)	78	66
1	D	222/221 (100%)	221 (100%)	1 (0%)	88	81
1	E	221/221 (100%)	219 (99%)	2 (1%)	78	66
1	F	222/221 (100%)	220 (99%)	2 (1%)	78	66
All	All	1329/1326 (100%)	1315 (99%)	14 (1%)	73	57

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	519	LEU
1	A	791	LYS
1	B	519	LEU
1	B	664	THR
1	B	697	SER
1	B	779	LEU
1	B	784	LYS
1	C	519	LEU

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Mol	Chain	Res	Type
1	C	684	LYS
1	D	519	LEU
1	E	492	LYS
1	E	519	LEU
1	F	519	LEU
1	F	664	THR

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

Mol	Chain	Res	Type
1	F	765	ASN
1	F	777	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)

Of 33 ligands modelled in this entry, 12 are monoatomic - leaving 21 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	ACT	E	1004	4	3,3,3	0.69	0	3,3,3	0.77	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	ACT	F	807	-	3,3,3	0.77	0	3,3,3	0.69	0
3	GLU	F	802	-	8,9,9	1.12	1 (12%)	10,11,11	1.14	1 (10%)
5	ACT	C	806	-	3,3,3	0.74	0	3,3,3	0.74	0
2	9C6	E	1001	-	28,28,28	2.47	6 (21%)	33,40,40	1.92	7 (21%)
2	9C6	D	802[B]	-	28,28,28	2.33	5 (17%)	33,40,40	2.24	10 (30%)
3	GLU	C	802	-	8,9,9	1.03	0	10,11,11	1.22	1 (10%)
5	ACT	C	805	-	3,3,3	0.75	0	3,3,3	0.75	0
5	ACT	D	807	4	3,3,3	0.78	0	3,3,3	0.77	0
5	ACT	B	904	-	3,3,3	0.77	0	3,3,3	0.71	0
5	ACT	B	903	-	3,3,3	0.73	0	3,3,3	0.85	0
3	GLU	A	1002	-	8,9,9	1.02	0	10,11,11	1.24	1 (10%)
3	GLU	B	901	-	8,9,9	1.10	1 (12%)	10,11,11	1.23	1 (10%)
5	ACT	C	804	-	3,3,3	0.77	0	3,3,3	0.68	0
5	ACT	F	806	4	3,3,3	0.81	0	3,3,3	0.72	0
3	GLU	D	803	-	8,9,9	1.10	1 (12%)	10,11,11	1.19	2 (20%)
2	9C6	A	1001	-	28,28,28	2.38	8 (28%)	33,40,40	1.96	8 (24%)
5	ACT	D	806	-	3,3,3	0.76	0	3,3,3	0.75	0
5	ACT	F	805	4	3,3,3	0.81	0	3,3,3	0.66	0
2	9C6	D	802[A]	-	28,28,28	2.40	6 (21%)	33,40,40	2.18	10 (30%)
3	GLU	E	1002	-	8,9,9	1.08	0	10,11,11	1.21	0

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	GLU	D	803	-	-	1/9/9/9	-
2	9C6	E	1001	-	-	0/8/19/19	0/3/4/4
2	9C6	D	802[B]	-	-	0/8/19/19	0/3/4/4
2	9C6	A	1001	-	-	0/8/19/19	0/3/4/4
3	GLU	A	1002	-	-	2/9/9/9	-
3	GLU	B	901	-	-	2/9/9/9	-
3	GLU	C	802	-	-	1/9/9/9	-
2	9C6	D	802[A]	-	-	0/8/19/19	0/3/4/4
3	GLU	F	802	-	-	1/9/9/9	-
3	GLU	E	1002	-	-	2/9/9/9	-

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1001	9C6	C6-S1	-7.20	1.67	1.76
2	D	802[A]	9C6	C6-S1	-7.18	1.67	1.76
2	D	802[B]	9C6	C6-S1	-7.02	1.67	1.76
2	A	1001	9C6	C6-S1	-6.87	1.68	1.76
2	D	802[A]	9C6	S1-N2	-6.57	1.52	1.62
2	D	802[B]	9C6	S1-N2	-6.26	1.52	1.62
2	E	1001	9C6	S1-N2	-5.83	1.53	1.62
2	A	1001	9C6	S1-N2	-5.52	1.53	1.62
2	E	1001	9C6	C5-N1	4.91	1.44	1.37
2	A	1001	9C6	C5-N1	4.66	1.43	1.37
2	D	802[A]	9C6	C5-N1	4.45	1.43	1.37
2	D	802[B]	9C6	C5-N1	4.43	1.43	1.37
2	E	1001	9C6	C1-C5	4.43	1.48	1.43
2	A	1001	9C6	C1-C5	4.27	1.48	1.43
2	A	1001	9C6	C4-N1	3.96	1.42	1.37
2	D	802[B]	9C6	C1-C5	3.94	1.48	1.43
2	E	1001	9C6	C4-N1	3.91	1.42	1.37
2	D	802[A]	9C6	C1-C5	3.73	1.48	1.43
2	D	802[A]	9C6	C4-N1	3.37	1.42	1.37
2	D	802[B]	9C6	C4-N1	3.29	1.41	1.37
3	D	803	GLU	OXT-C	-2.29	1.23	1.30
3	F	802	GLU	OXT-C	-2.17	1.23	1.30
2	A	1001	9C6	O1-S1	2.14	1.46	1.43
2	D	802[A]	9C6	O3-C14	-2.14	1.35	1.39
2	E	1001	9C6	C4-C3	2.12	1.40	1.35
3	B	901	GLU	OXT-C	-2.06	1.23	1.30
2	A	1001	9C6	C7-N1	2.05	1.49	1.47
2	A	1001	9C6	C4-C3	2.03	1.40	1.35

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	802[A]	9C6	O1-S1-O2	-6.70	108.94	118.28
2	D	802[B]	9C6	O1-S1-O2	-6.64	109.02	118.28
2	A	1001	9C6	C9-C8-C1	-5.30	113.52	120.98
2	E	1001	9C6	C9-C8-C1	-5.10	113.80	120.98
2	D	802[B]	9C6	O2-S1-C6	-5.08	102.84	109.50
2	A	1001	9C6	O1-S1-O2	-4.84	111.54	118.28
2	E	1001	9C6	O1-S1-O2	-4.39	112.16	118.28
2	D	802[A]	9C6	C9-C8-C1	-4.36	114.83	120.98
2	D	802[B]	9C6	C9-C8-C1	-4.13	115.17	120.98
2	D	802[A]	9C6	O2-S1-C6	-4.06	104.18	109.50
2	D	802[B]	9C6	C14-O3-C11	3.99	128.14	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	802[A]	9C6	C14-O3-C11	3.86	127.82	118.80
2	D	802[B]	9C6	O2-S1-N2	3.82	114.48	108.93
2	E	1001	9C6	O2-S1-C6	-3.80	104.52	109.50
2	A	1001	9C6	O2-S1-C6	-3.65	104.72	109.50
2	E	1001	9C6	C14-O3-C11	3.40	126.75	118.80
2	D	802[A]	9C6	O2-S1-N2	3.39	113.86	108.93
2	A	1001	9C6	C13-C8-C1	3.11	125.35	120.98
2	A	1001	9C6	C14-O3-C11	3.02	125.88	118.80
2	E	1001	9C6	C13-C8-C1	3.01	125.22	120.98
2	A	1001	9C6	C12-C13-C8	-2.79	117.53	120.78
2	D	802[B]	9C6	C8-C1-C5	-2.67	118.26	121.74
2	E	1001	9C6	C12-C13-C8	-2.67	117.68	120.78
2	A	1001	9C6	C6-C7-N1	2.55	117.96	113.54
2	A	1001	9C6	C8-C1-C5	-2.49	118.49	121.74
2	D	802[B]	9C6	C3-C4-N1	2.39	124.53	121.20
2	D	802[A]	9C6	C3-C4-N1	2.39	124.53	121.20
2	D	802[A]	9C6	C2-C1-C5	2.33	120.66	116.59
2	D	802[A]	9C6	C8-C1-C5	-2.29	118.75	121.74
3	C	802	GLU	OE2-CD-CG	2.28	121.36	114.03
2	D	802[B]	9C6	C1-C5-N1	2.25	120.34	116.84
2	D	802[B]	9C6	C2-C1-C5	2.24	120.52	116.59
2	E	1001	9C6	C8-C1-C5	-2.23	118.83	121.74
2	D	802[B]	9C6	C13-C8-C1	2.13	123.97	120.98
3	D	803	GLU	OE1-CD-CG	-2.10	116.34	123.08
3	B	901	GLU	OE2-CD-CG	2.10	120.77	114.03
3	A	1002	GLU	OE2-CD-CG	2.06	120.64	114.03
2	D	802[A]	9C6	C1-C5-N1	2.05	120.04	116.84
3	D	803	GLU	OE2-CD-CG	2.05	120.62	114.03
3	F	802	GLU	OE2-CD-CG	2.04	120.57	114.03
2	D	802[A]	9C6	C9-C8-C13	2.00	121.44	118.59

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1002	GLU	O-C-CA-N
3	B	901	GLU	O-C-CA-N
3	C	802	GLU	O-C-CA-N
3	D	803	GLU	O-C-CA-N
3	E	1002	GLU	O-C-CA-N
3	F	802	GLU	O-C-CA-N
3	B	901	GLU	OXT-C-CA-CB

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Mol	Chain	Res	Type	Atoms
3	A	1002	GLU	OE2-CD-CG-CB
3	E	1002	GLU	OE2-CD-CG-CB

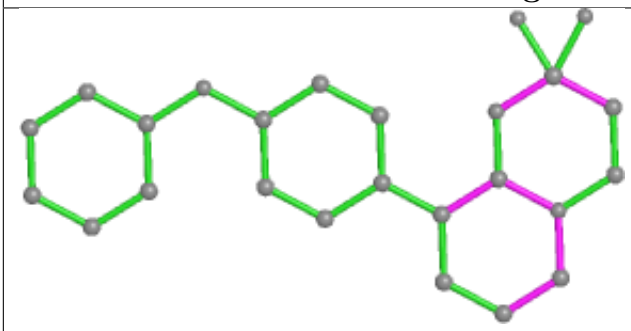
There are no ring outliers.

6 monomers are involved in 6 short contacts:

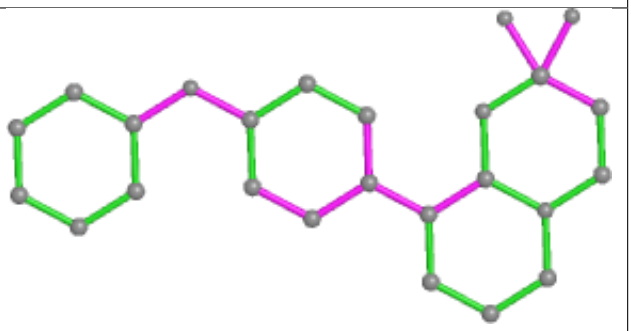
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	802	GLU	1	0
3	C	802	GLU	1	0
3	A	1002	GLU	1	0
3	B	901	GLU	1	0
3	D	803	GLU	1	0
3	E	1002	GLU	1	0

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.

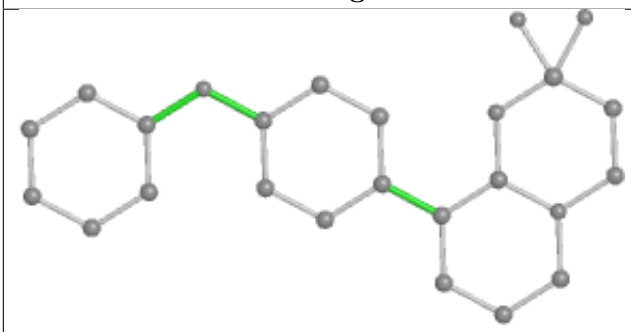
Ligand 9C6 E 1001



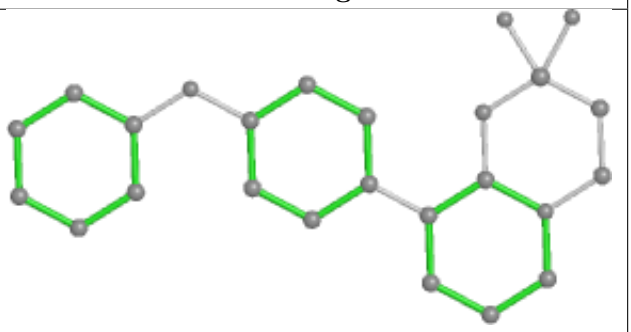
Bond lengths



Bond angles

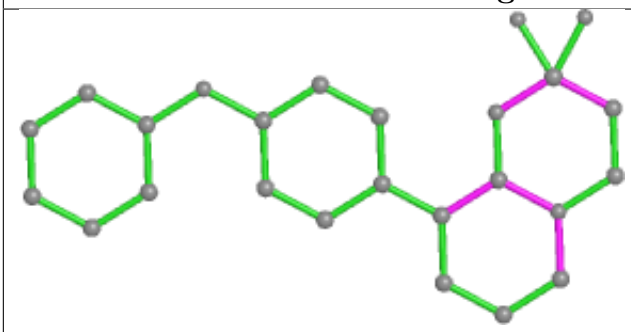


Torsions

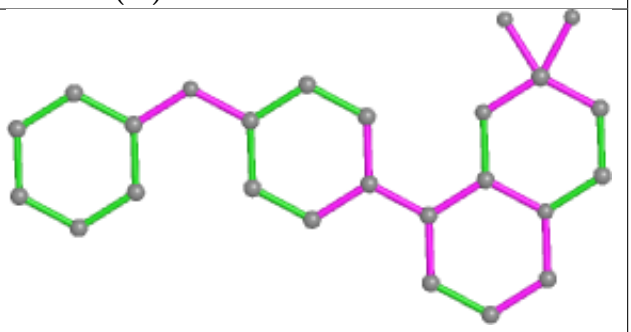


Rings

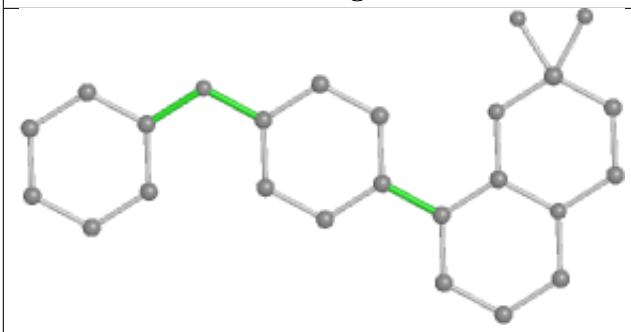
Ligand 9C6 D 802 (B)



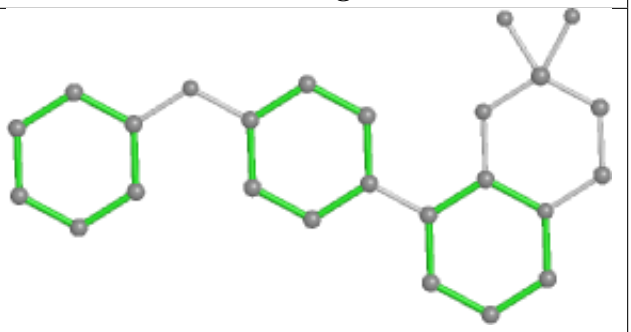
Bond lengths



Bond angles

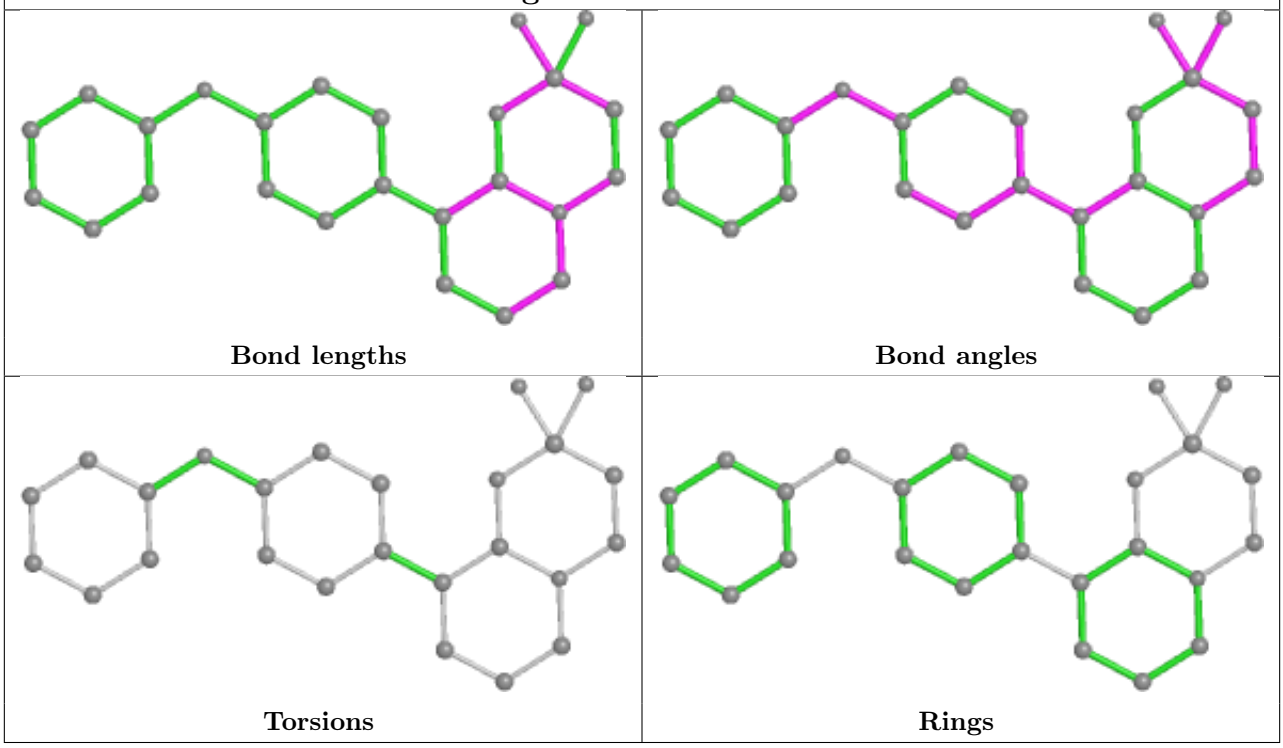


Torsions

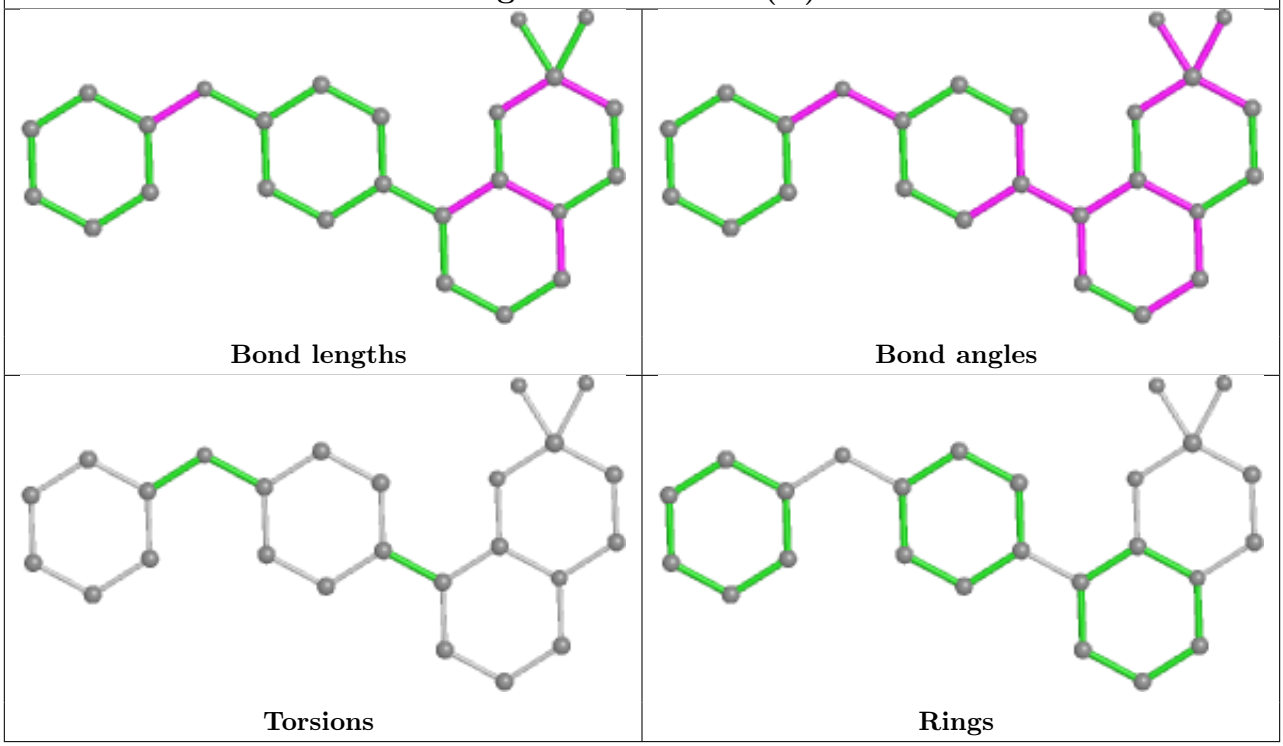


Rings

Ligand 9C6 A 1001



Ligand 9C6 D 802 (A)



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	260/263 (98%)	-0.04	2 (0%)	86	88	19, 28, 52, 75	0
1	B	260/263 (98%)	-0.07	0	100	100	18, 29, 55, 79	0
1	C	260/263 (98%)	-0.27	2 (0%)	86	88	16, 24, 43, 69	0
1	D	262/263 (99%)	-0.33	1 (0%)	92	93	16, 24, 44, 68	0
1	E	260/263 (98%)	-0.12	7 (2%)	54	55	20, 29, 53, 77	0
1	F	260/263 (98%)	-0.09	7 (2%)	54	55	19, 30, 56, 75	0
All	All	1562/1578 (98%)	-0.15	19 (1%)	79	81	16, 28, 51, 79	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	686	ALA	4.7
1	F	789	TYR	3.2
1	F	685	ILE	3.0
1	E	476	ALA	2.9
1	D	789	TYR	2.8
1	C	789	TYR	2.8
1	F	687	VAL	2.8
1	E	686	ALA	2.7
1	F	792	GLY	2.6
1	E	477	ASP	2.5
1	F	686	ALA	2.4
1	E	664	THR	2.3
1	E	795	GLY	2.3
1	E	792	GLY	2.2
1	E	687	VAL	2.2
1	F	791	LYS	2.1
1	A	477	ASP	2.1
1	F	662	LYS	2.0
1	C	791	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 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
5	ACT	B	903	4/4	0.62	0.18	47,51,53,56	0
5	ACT	C	806	4/4	0.62	0.16	44,51,58,60	0
5	ACT	D	806	4/4	0.69	0.24	38,41,42,47	0
5	ACT	C	804	4/4	0.79	0.17	33,33,40,40	0
4	ZN	D	801	1/1	0.81	0.05	93,93,93,93	0
5	ACT	C	805	4/4	0.82	0.11	41,49,56,58	0
4	ZN	F	803	1/1	0.91	0.07	59,59,59,59	0
4	ZN	B	902	1/1	0.91	0.05	56,56,56,56	0
2	9C6	E	1001	25/25	0.92	0.10	25,29,34,37	0
2	9C6	A	1001	25/25	0.93	0.10	23,28,33,36	0
5	ACT	D	807	4/4	0.93	0.15	40,45,49,60	0
5	ACT	F	805	4/4	0.93	0.10	39,46,49,53	0
2	9C6	D	802[B]	25/25	0.94	0.14	18,20,24,24	25
2	9C6	D	802[A]	25/25	0.94	0.14	18,20,23,23	25
4	ZN	F	804	1/1	0.95	0.06	31,31,31,31	0
3	GLU	F	802	10/10	0.95	0.08	19,20,25,26	0
5	ACT	F	806	4/4	0.95	0.15	34,37,50,54	0
5	ACT	F	807	4/4	0.95	0.18	37,40,42,44	0
5	ACT	E	1004	4/4	0.96	0.10	35,43,46,46	0
5	ACT	B	904	4/4	0.96	0.18	36,38,40,50	0
3	GLU	B	901	10/10	0.96	0.08	18,19,24,24	0
4	ZN	B	905	1/1	0.96	0.06	80,80,80,80	0
3	GLU	E	1002	10/10	0.97	0.06	22,23,27,27	0
4	ZN	E	1003	1/1	0.97	0.04	31,31,31,31	0
3	GLU	A	1002	10/10	0.97	0.07	20,22,25,25	0
3	GLU	D	803	10/10	0.98	0.07	15,17,20,20	0
3	GLU	C	802	10/10	0.98	0.08	15,18,20,20	0

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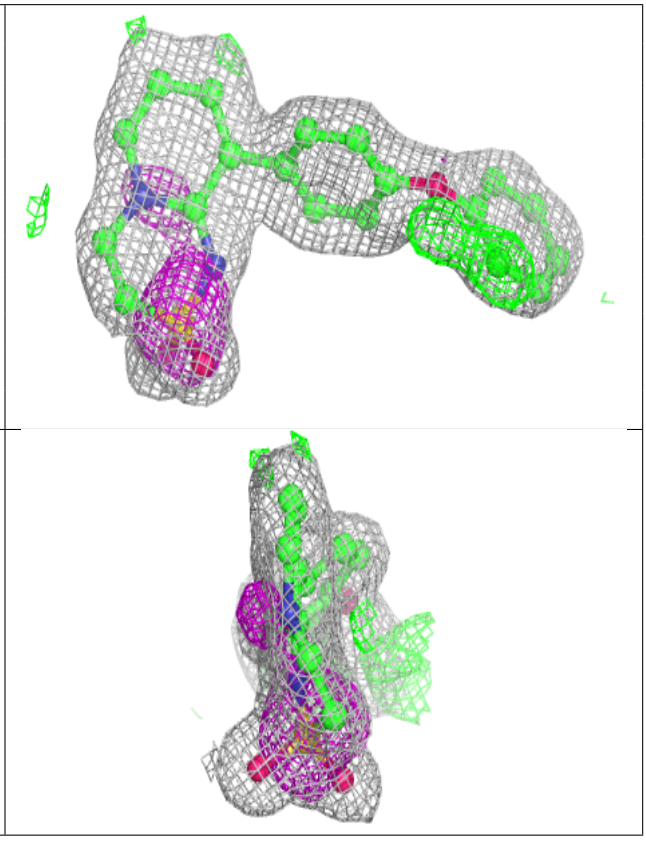
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	ZN	D	805	1/1	0.99	0.03	26,26,26,26	0
4	ZN	D	808	1/1	0.99	0.03	25,25,25,25	0
4	ZN	C	803	1/1	0.99	0.06	25,25,25,25	0
4	ZN	C	801	1/1	0.99	0.07	24,24,24,24	0
4	ZN	F	801	1/1	1.00	0.04	25,25,25,25	0
4	ZN	D	804	1/1	1.00	0.07	25,25,25,25	0

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.

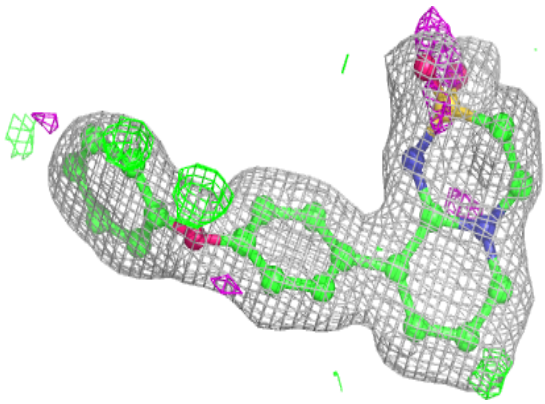
Electron density around 9C6 E 1001:

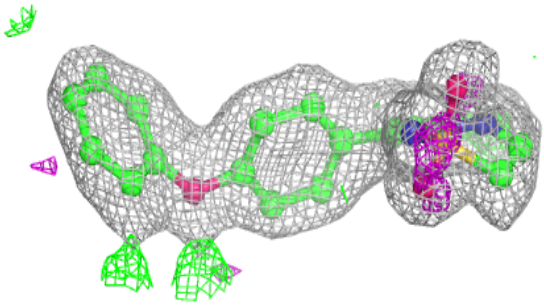
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)



Electron density around 9C6 A 1001:

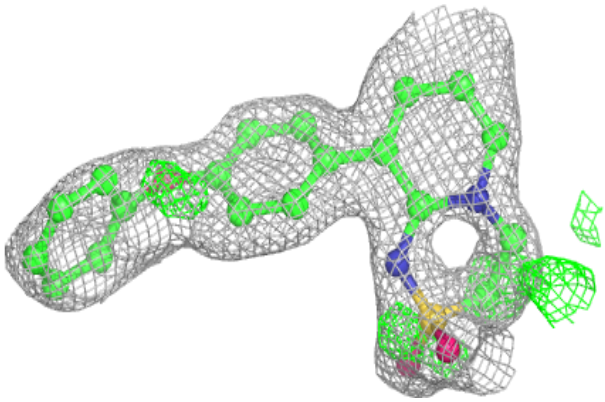
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

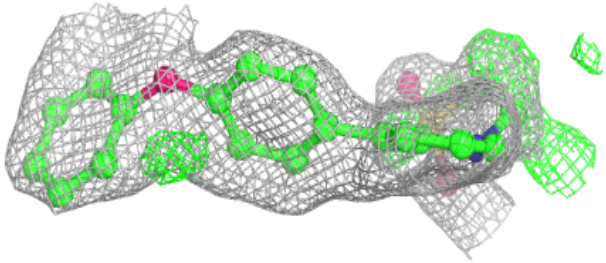


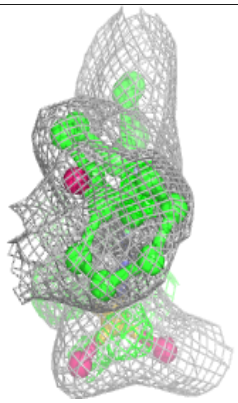


Electron density around 9C6 D 802 (B):

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

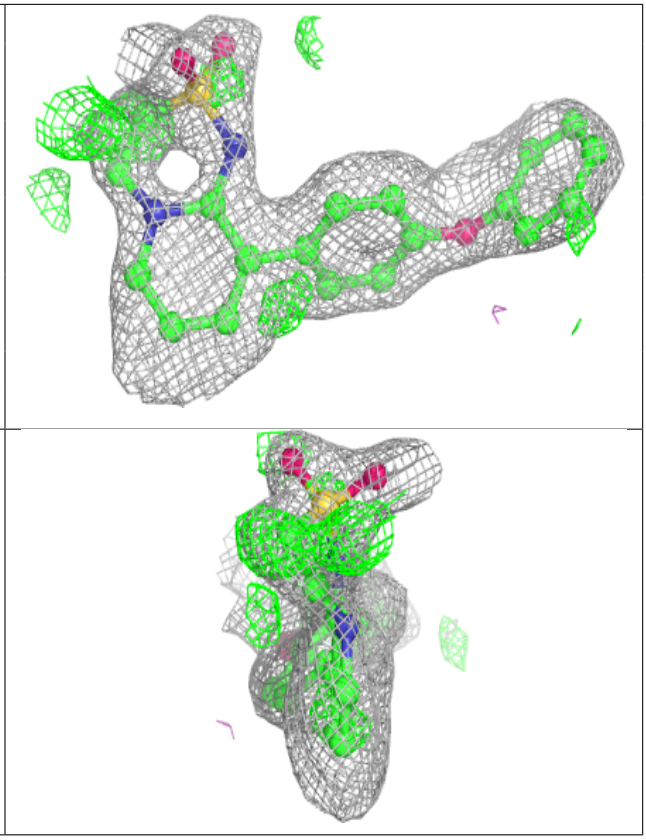






Electron density around 9C6 D 802 (A):

$2mF_o$-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.