Full wwPDB X-ray Structure Validation Report ⓘ

Apr 6, 2023 – 01:19 pm BST

PDB ID	:	6ZK0
Title	:	1.47A human IMPase with ebselen
Authors	:	Bax, B.D.; Fenn, G.D.
Deposited on	:	2020-06-29
Resolution	:	1.47 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

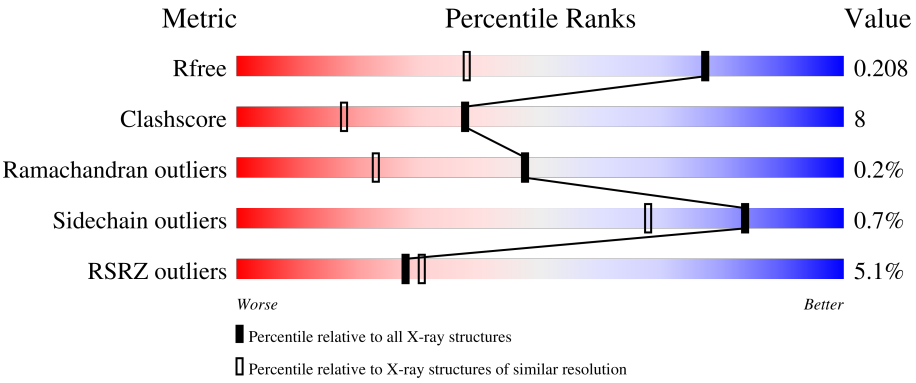
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.32.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.2

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 1.47 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	4690 (1.50-1.46)
Clashscore	141614	4955 (1.50-1.46)
Ramachandran outliers	138981	4846 (1.50-1.46)
Sidechain outliers	138945	4844 (1.50-1.46)
RSRZ outliers	127900	4614 (1.50-1.46)

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	AAA	279	5% 84% 13%
1	BBB	279	5% 86% 12%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SO4	AAA	305[B]	-	-	X	-
5	GOL	AAA	308	-	-	X	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 5165 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 Inositol monophosphatase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	274	Total 2250	C 1418	N 380	O 428	S 24	0	26	0
1	BBB	275	Total 2319	C 1450	N 406	O 439	S 24	0	24	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	-1	GLY	-	expression tag	UNP P29218
AAA	0	PRO	-	expression tag	UNP P29218
BBB	-1	GLY	-	expression tag	UNP P29218
BBB	0	PRO	-	expression tag	UNP P29218

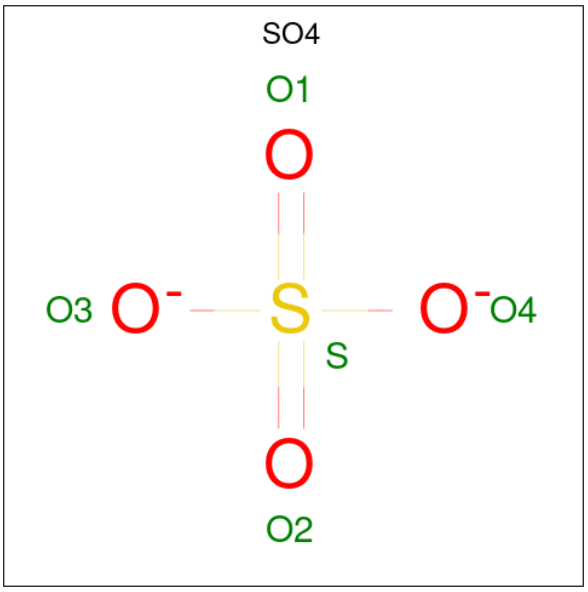
- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	AAA	6	Total 6	Na 6	0	1
2	BBB	2	Total 2	Na 2	0	1

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

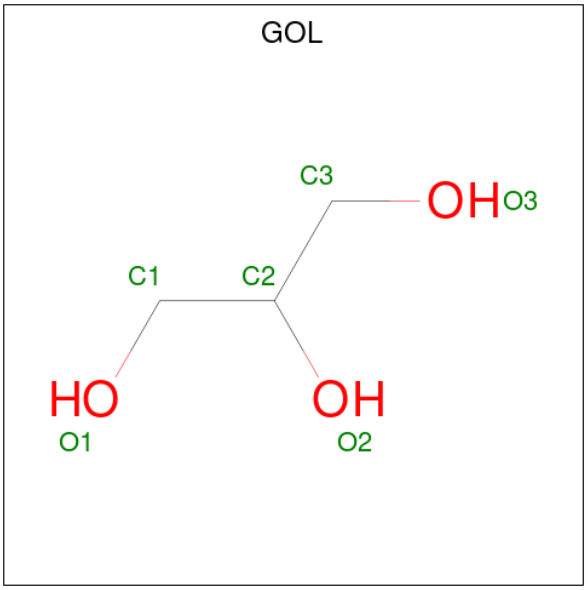
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	AAA	2	Total 3	Mn 3	0	2
3	BBB	4	Total 4	Mn 4	0	3

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	AAA	1	Total O S 10 8 2	0	1
4	BBB	1	Total O S 5 4 1	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	AAA	1	Total C O 6 3 3	0	0
5	AAA	1	Total C O 12 6 6	0	1

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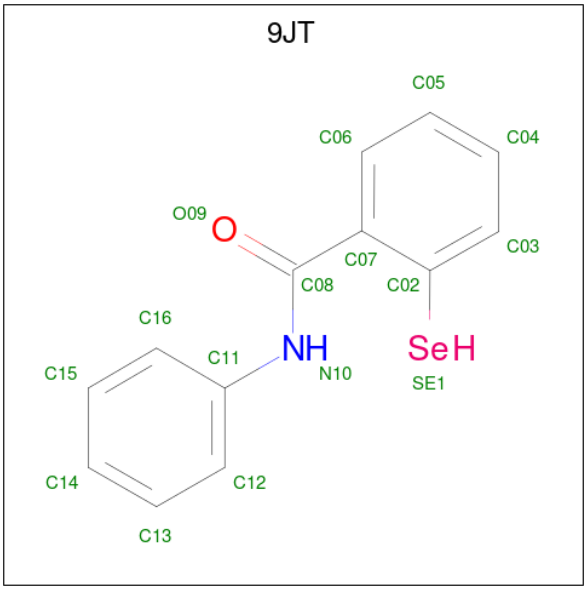
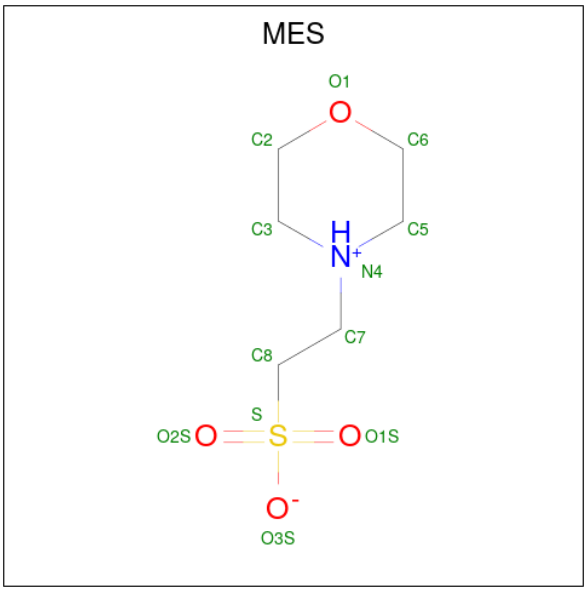
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	AAA	1	Total C O 6 3 3	0	0
5	AAA	1	Total C O 12 6 6	0	1
5	AAA	1	Total C O 6 3 3	0	0
5	AAA	1	Total C O 6 3 3	0	0
5	BBB	1	Total C O 6 3 3	0	0
5	BBB	1	Total C O 6 3 3	0	0
5	BBB	1	Total C O 6 3 3	0	0

- Molecule 6 is N-phenyl-2-selanylbenzamide (three-letter code: 9JT) (formula: $C_{13}H_{11}NOSe$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	AAA	1	Total C N O Se 17 13 1 1 2	0	1
6	BBB	1	Total C N O Se 32 26 2 2 2	0	1

- Molecule 7 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	BBB	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 8 is water.

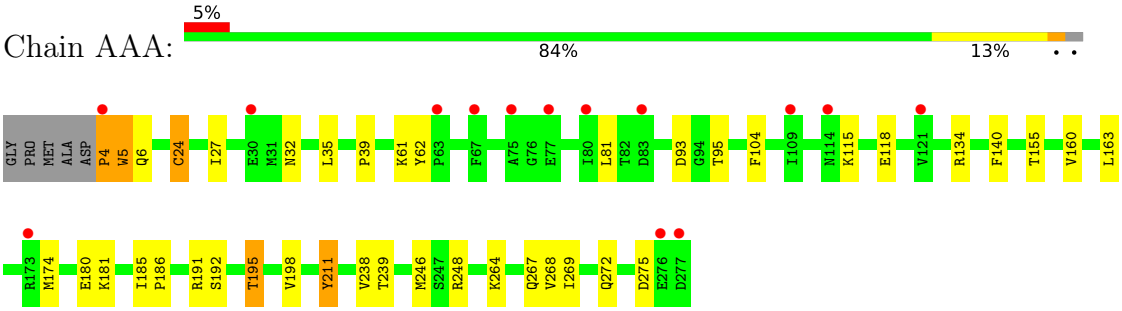
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	AAA	217	Total	O	0	14
			226	226		
8	BBB	209	Total	O	0	6
			213	213		

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.

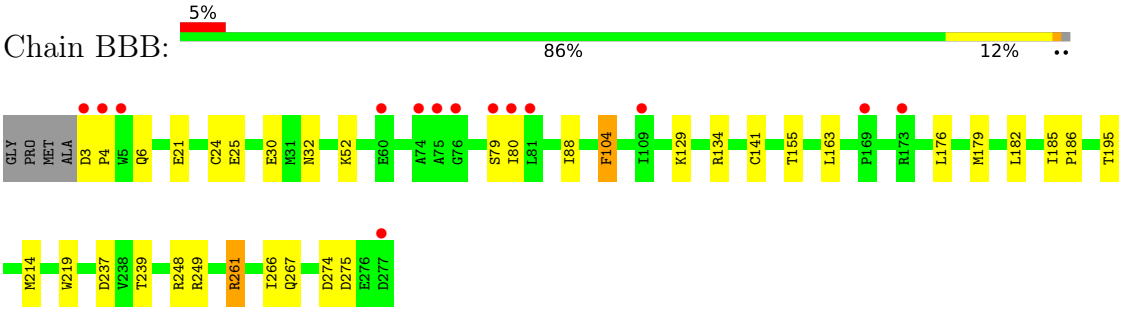
• Molecule 1: Inositol monophosphatase 1

Chain AAA:



• Molecule 1: Inositol monophosphatase 1

Chain BBB:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	84.02Å 84.02Å 150.22Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	24.44 – 1.47 24.44 – 1.47	Depositor EDS
% Data completeness (in resolution range)	100.0 (24.44-1.47) 100.0 (24.44-1.47)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.46 (at 1.47Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.179 , 0.208 0.179 , 0.208	Depositor DCC
R_{free} test set	5081 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å^2)	23.5	Xtriage
Anisotropy	0.005	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 49.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.018 for -h,-k,l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	5165	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.96% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MES, SO4, 9JT, GOL, MN, NA

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	AAA	0.53	0/2290	0.94	4/3104 (0.1%)
1	BBB	0.54	0/2353	0.96	3/3177 (0.1%)
All	All	0.54	0/4643	0.95	7/6281 (0.1%)

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	AAA	0	1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AAA	195	THR	CA-CB-OG1	7.61	124.98	109.00
1	AAA	211	TYR	CB-CG-CD2	-6.45	117.13	121.00
1	BBB	261[A]	ARG	NE-CZ-NH2	-5.39	117.60	120.30
1	BBB	261[B]	ARG	NE-CZ-NH2	-5.39	117.60	120.30
1	AAA	24[A]	CYS	CB-CA-C	5.08	120.55	110.40
1	AAA	24[B]	CYS	CB-CA-C	5.08	120.55	110.40
1	BBB	104	PHE	CB-CG-CD2	-5.04	117.27	120.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AAA	4[B]	PRO	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	AAA	2250	0	2189	36	0
1	BBB	2319	0	2285	29	0
2	AAA	6	0	0	1	0
2	BBB	2	0	0	0	0
3	AAA	3	0	0	0	0
3	BBB	4	0	0	0	0
4	AAA	10	0	0	3	0
4	BBB	5	0	0	0	0
5	AAA	48	0	62	12	0
5	BBB	18	0	23	2	0
6	AAA	17	0	0	1	0
6	BBB	32	0	0	6	0
7	BBB	12	0	13	1	0
8	AAA	226	0	0	10	0
8	BBB	213	0	0	1	0
All	All	5165	0	4572	72	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 8.

All (72) 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:BBB:141[A]:CYS:SG	6:BBB:311[A]:9JT:SE1	2.47	1.22
1:AAA:4[A]:PRO:HG2	8:AAA:435[A]:HOH:O	1.50	1.11
5:AAA:309[A]:GOL:H12	8:AAA:453[A]:HOH:O	1.54	1.03
1:AAA:248:ARG:HH12	5:AAA:307[A]:GOL:H12	1.30	0.96
1:AAA:272[B]:GLN:HB3	5:AAA:307[B]:GOL:H11	1.59	0.85
1:AAA:192:SER:OG	5:AAA:308:GOL:H32	1.79	0.83
1:AAA:93:ASP:OD2	1:AAA:195:THR:HG23	1.82	0.80
1:AAA:195:THR:HG22	1:AAA:198:VAL:H	1.48	0.78
1:AAA:95:THR:OG1	4:AAA:305[B]:SO4:O2	2.07	0.73
2:AAA:316:NA:NA	8:AAA:530:HOH:O	1.62	0.72
1:AAA:6[A]:GLN:HB2	8:AAA:435[A]:HOH:O	1.93	0.67
1:AAA:272[B]:GLN:HB3	5:AAA:307[B]:GOL:C1	2.23	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:AAA:312[A]:9JT:SE1	6:AAA:312[A]:9JT:O09	2.64	0.66
1:AAA:181:LYS:NZ	8:AAA:404:HOH:O	2.29	0.66
1:BBB:267[B]:GLN:OE1	7:BBB:309:MES:O3S	2.14	0.65
5:AAA:308:GOL:H11	8:AAA:408:HOH:O	1.97	0.64
1:BBB:3[A]:ASP:HB3	1:BBB:6:GLN:HB2	1.79	0.63
5:AAA:308:GOL:C1	8:AAA:408:HOH:O	2.46	0.63
1:BBB:185:ILE:N	1:BBB:186:PRO:HA	2.15	0.61
1:BBB:141[B]:CYS:SG	6:BBB:311[B]:9JT:SE1	3.09	0.60
1:AAA:248:ARG:NH1	5:AAA:307[A]:GOL:H12	2.12	0.59
1:BBB:248:ARG:HH12	5:BBB:308:GOL:H32	1.68	0.57
1:AAA:24[B]:CYS:O	1:AAA:27:ILE:HG22	2.05	0.56
1:AAA:185:ILE:N	1:AAA:186:PRO:HA	2.21	0.54
1:AAA:4[B]:PRO:N	1:AAA:134[B]:ARG:HH22	2.06	0.54
1:AAA:246[B]:MET:SD	1:AAA:275:ASP:HB3	2.47	0.54
1:BBB:129:LYS:HE3	6:BBB:311[B]:9JT:SE1	2.59	0.53
1:AAA:155:THR:HA	1:AAA:186:PRO:O	2.09	0.52
1:AAA:195:THR:CG2	1:AAA:198:VAL:H	2.21	0.51
1:AAA:118:GLU:OE1	1:AAA:134[A]:ARG:NH1	2.42	0.51
1:AAA:264:LYS:NZ	8:AAA:411:HOH:O	2.43	0.51
6:BBB:311[A]:9JT:SE1	6:BBB:311[A]:9JT:O09	2.80	0.50
1:AAA:81:LEU:O	1:AAA:115:LYS:HE3	2.11	0.50
1:BBB:163:LEU:CD2	1:BBB:179[A]:MET:HE1	2.42	0.50
1:BBB:79:SER:HB3	1:BBB:274:ASP:O	2.13	0.48
1:AAA:32[A]:ASN:OD1	8:AAA:401:HOH:O	2.18	0.48
1:BBB:214:MET:HG2	1:BBB:249[A]:ARG:HG2	1.96	0.48
1:BBB:214:MET:HG2	1:BBB:249[B]:ARG:HG2	1.96	0.48
1:AAA:174[A]:MET:SD	1:AAA:267[A]:GLN:HG2	2.54	0.48
1:BBB:21[B]:GLU:O	1:BBB:25[B]:GLU:HG3	2.14	0.48
1:BBB:155:THR:HA	1:BBB:186:PRO:O	2.14	0.47
1:AAA:163:LEU:HG	5:AAA:308:GOL:O3	2.14	0.47
4:AAA:305[B]:SO4:O3	5:AAA:309[B]:GOL:O1	2.33	0.47
1:BBB:248:ARG:HH22	5:BBB:308:GOL:C3	2.28	0.47
1:AAA:61:LYS:HG2	1:AAA:62:TYR:CE2	2.49	0.46
1:AAA:239:THR:HG22	1:AAA:268:VAL:HG21	1.97	0.46
1:BBB:182:LEU:HD11	1:BBB:266[B]:ILE:HD11	1.97	0.46
1:BBB:141[A]:CYS:CB	6:BBB:311[A]:9JT:SE1	3.14	0.45
1:AAA:35:LEU:HD13	1:AAA:39:PRO:HA	1.98	0.45
1:BBB:80:ILE:HD12	1:BBB:275:ASP:HB2	1.99	0.45
1:AAA:238:VAL:HG23	1:AAA:268:VAL:HG22	1.98	0.45
1:BBB:261[B]:ARG:HA	1:BBB:261[B]:ARG:HD2	1.80	0.44
1:BBB:32:ASN:HB2	8:BBB:411:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:239:THR:HG23	1:BBB:249[C]:ARG:NH1	2.32	0.44
6:BBB:311[B]:9JT:O09	6:BBB:311[B]:9JT:C12	2.65	0.44
1:AAA:248:ARG:HH12	5:AAA:307[B]:GOL:H12	1.81	0.44
1:AAA:195:THR:HG21	1:AAA:198:VAL:HG23	2.00	0.43
1:BBB:179[A]:MET:HE2	1:BBB:179[A]:MET:HB2	1.77	0.43
1:AAA:160:VAL:HG23	1:AAA:211:TYR:HB2	2.00	0.42
1:AAA:160:VAL:HG12	1:AAA:191:ARG:HB2	2.00	0.42
1:AAA:5[B]:TRP:CE3	1:AAA:5[B]:TRP:HA	2.54	0.42
1:BBB:52[C]:LYS:HE3	1:BBB:52[C]:LYS:HB3	1.70	0.42
4:AAA:305[B]:SO4:O3	8:AAA:402[B]:HOH:O	2.21	0.42
1:AAA:180:GLU:HB2	1:BBB:176:LEU:CD1	2.50	0.41
1:BBB:3[A]:ASP:OD1	1:BBB:134:ARG:NH2	2.41	0.41
1:BBB:237[B]:ASP:OD2	1:BBB:239:THR:HG23	2.20	0.41
1:AAA:104:PHE:CZ	1:BBB:104:PHE:HZ	2.39	0.41
1:AAA:140:PHE:CD1	5:AAA:310:GOL:H12	2.56	0.41
1:BBB:249[C]:ARG:HH21	1:BBB:249[C]:ARG:HD3	1.66	0.41
1:BBB:3[A]:ASP:OD1	1:BBB:4:PRO:HD2	2.21	0.40
1:AAA:174[B]:MET:CE	1:AAA:269:ILE:HG12	2.51	0.40
1:BBB:88:ILE:HG22	1:BBB:219:TRP:HA	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	AAA	298/279 (107%)	292 (98%)	4 (1%)	2 (1%)	22 5
1	BBB	300/279 (108%)	295 (98%)	5 (2%)	0	100 100
All	All	598/558 (107%)	587 (98%)	9 (2%)	2 (0%)	47 18

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	5[A]	TRP
1	AAA	5[B]	TRP

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	AAA	239/232 (103%)	239 (100%)	0	100 100
1	BBB	248/232 (107%)	243 (98%)	5 (2%)	55 24
All	All	487/464 (105%)	482 (99%)	5 (1%)	84 54

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	BBB	24[A]	CYS
1	BBB	24[B]	CYS
1	BBB	30[A]	GLU
1	BBB	30[B]	GLU
1	BBB	195	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 34 ligands modelled in this entry, 15 are monoatomic and 1 is modelled with single atom - leaving 18 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	GOL	AAA	309[A]	2	5,5,5	0.17	0	5,5,5	0.60	0
6	9JT	BBB	311[A]	-	17,17,17	0.91	1 (5%)	21,22,22	1.01	1 (4%)
4	SO4	AAA	305[A]	2	4,4,4	0.65	0	6,6,6	0.74	0
6	9JT	AAA	312[A]	1	17,17,17	1.05	1 (5%)	21,22,22	1.71	1 (4%)
5	GOL	AAA	308	-	5,5,5	0.19	0	5,5,5	0.19	0
4	SO4	BBB	307	3	4,4,4	0.57	0	6,6,6	1.19	0
5	GOL	BBB	306	3,2	5,5,5	0.33	0	5,5,5	0.79	0
5	GOL	BBB	308	-	5,5,5	0.12	0	5,5,5	0.19	0
5	GOL	AAA	307[B]	-	5,5,5	0.09	0	5,5,5	0.31	0
5	GOL	BBB	310	-	5,5,5	0.14	0	5,5,5	0.48	0
5	GOL	AAA	311	-	5,5,5	0.10	0	5,5,5	0.35	0
5	GOL	AAA	306	-	5,5,5	0.12	0	5,5,5	0.36	0
6	9JT	BBB	311[B]	-	17,17,17	0.54	1 (5%)	21,22,22	0.50	0
7	MES	BBB	309	-	12,12,12	0.61	0	14,16,16	0.98	1 (7%)
4	SO4	AAA	305[B]	3,2	4,4,4	0.39	0	6,6,6	0.24	0
5	GOL	AAA	310	-	5,5,5	0.14	0	5,5,5	0.27	0
5	GOL	AAA	307[A]	-	5,5,5	0.10	0	5,5,5	0.27	0
5	GOL	AAA	309[B]	2	5,5,5	0.20	0	5,5,5	0.53	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
5	GOL	AAA	309[A]	2	-	1/4/4/4	-
6	9JT	BBB	311[A]	-	-	2/8/8/8	0/2/2/2
6	9JT	AAA	312[A]	1	-	2/8/8/8	0/2/2/2
5	GOL	AAA	308	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	BBB	306	3,2	-	0/4/4/4	-
5	GOL	BBB	308	-	-	0/4/4/4	-
5	GOL	AAA	307[B]	-	-	2/4/4/4	-
5	GOL	BBB	310	-	-	0/4/4/4	-
5	GOL	AAA	311	-	-	0/4/4/4	-
5	GOL	AAA	306	-	-	0/4/4/4	-
7	MES	BBB	309	-	-	5/6/14/14	0/1/1/1
6	9JT	BBB	311[B]	-	-	2/8/8/8	0/2/2/2
5	GOL	AAA	310	-	-	2/4/4/4	-
5	GOL	AAA	307[A]	-	-	2/4/4/4	-
5	GOL	AAA	309[B]	2	-	2/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	AAA	312[A]	9JT	SE1-C02	4.10	1.94	1.89
6	BBB	311[A]	9JT	SE1-C02	3.45	1.93	1.89
6	BBB	311[B]	9JT	SE1-C02	2.07	1.92	1.89

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	AAA	312[A]	9JT	SE1-C02-C03	6.74	126.28	119.47
6	BBB	311[A]	9JT	SE1-C02-C03	2.85	122.34	119.47
7	BBB	309	MES	C2-C3-N4	-2.05	107.00	110.10

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	AAA	309[B]	GOL	C1-C2-C3-O3
5	AAA	310	GOL	C1-C2-C3-O3
6	BBB	311[B]	9JT	C02-C07-C08-O09
6	BBB	311[B]	9JT	C02-C07-C08-N10
7	BBB	309	MES	C8-C7-N4-C3
7	BBB	309	MES	C7-C8-S-O2S
7	BBB	309	MES	C7-C8-S-O3S
5	AAA	309[A]	GOL	C1-C2-C3-O3
5	AAA	309[B]	GOL	O2-C2-C3-O3
5	AAA	310	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
6	BBB	311[A]	9JT	C16-C11-N10-C08
6	BBB	311[A]	9JT	C12-C11-N10-C08
6	AAA	312[A]	9JT	C12-C11-N10-C08
5	AAA	307[B]	GOL	O2-C2-C3-O3
6	AAA	312[A]	9JT	C16-C11-N10-C08
5	AAA	307[A]	GOL	O1-C1-C2-O2
7	BBB	309	MES	C7-C8-S-O1S
7	BBB	309	MES	C8-C7-N4-C5
5	AAA	307[A]	GOL	O1-C1-C2-C3
5	AAA	307[B]	GOL	C1-C2-C3-O3

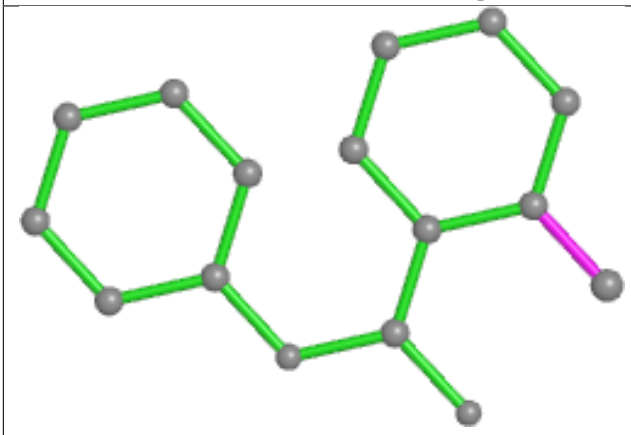
There are no ring outliers.

12 monomers are involved in 24 short contacts:

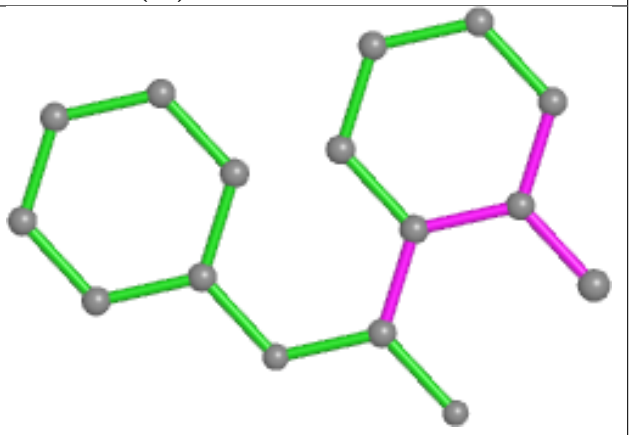
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	AAA	309[A]	GOL	1	0
6	BBB	311[A]	9JT	3	0
6	AAA	312[A]	9JT	1	0
5	AAA	308	GOL	4	0
5	BBB	308	GOL	2	0
5	AAA	307[B]	GOL	3	0
6	BBB	311[B]	9JT	3	0
7	BBB	309	MES	1	0
4	AAA	305[B]	SO4	3	0
5	AAA	310	GOL	1	0
5	AAA	307[A]	GOL	2	0
5	AAA	309[B]	GOL	1	0

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.

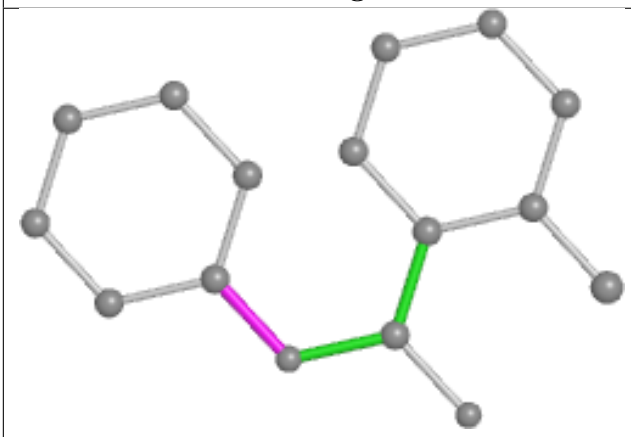
Ligand 9JT BBB 311 (A)



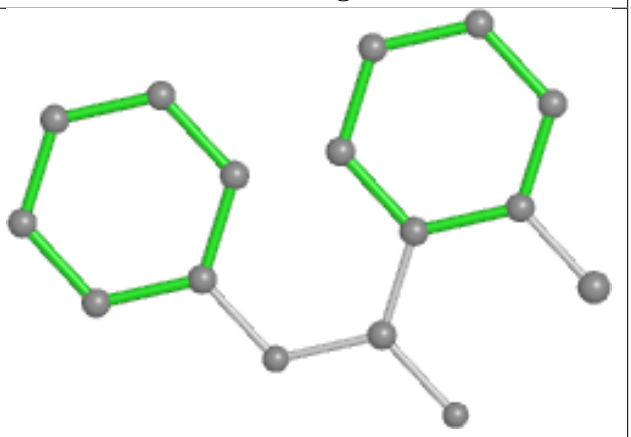
Bond lengths



Bond angles

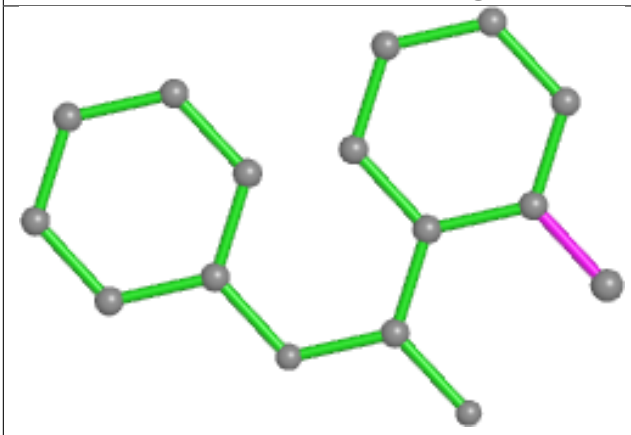


Torsions

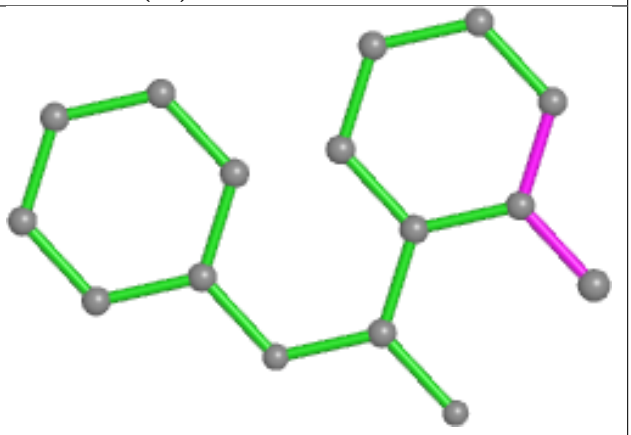


Rings

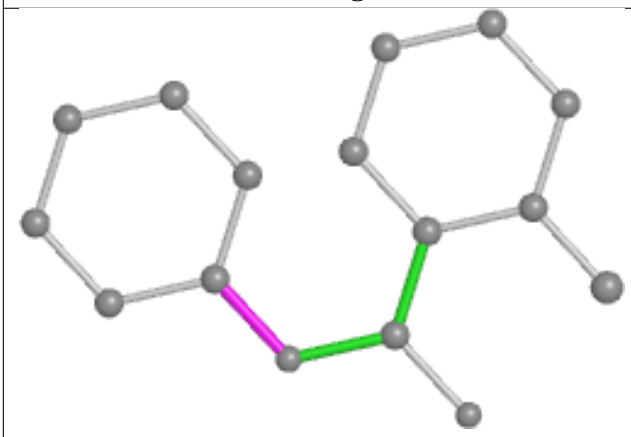
Ligand 9JT AAA 312 (A)



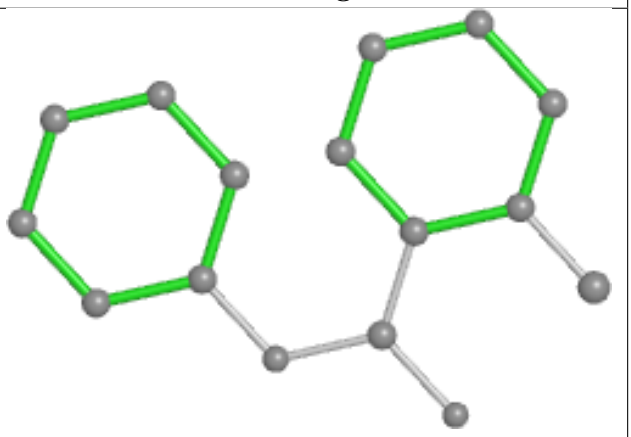
Bond lengths



Bond angles

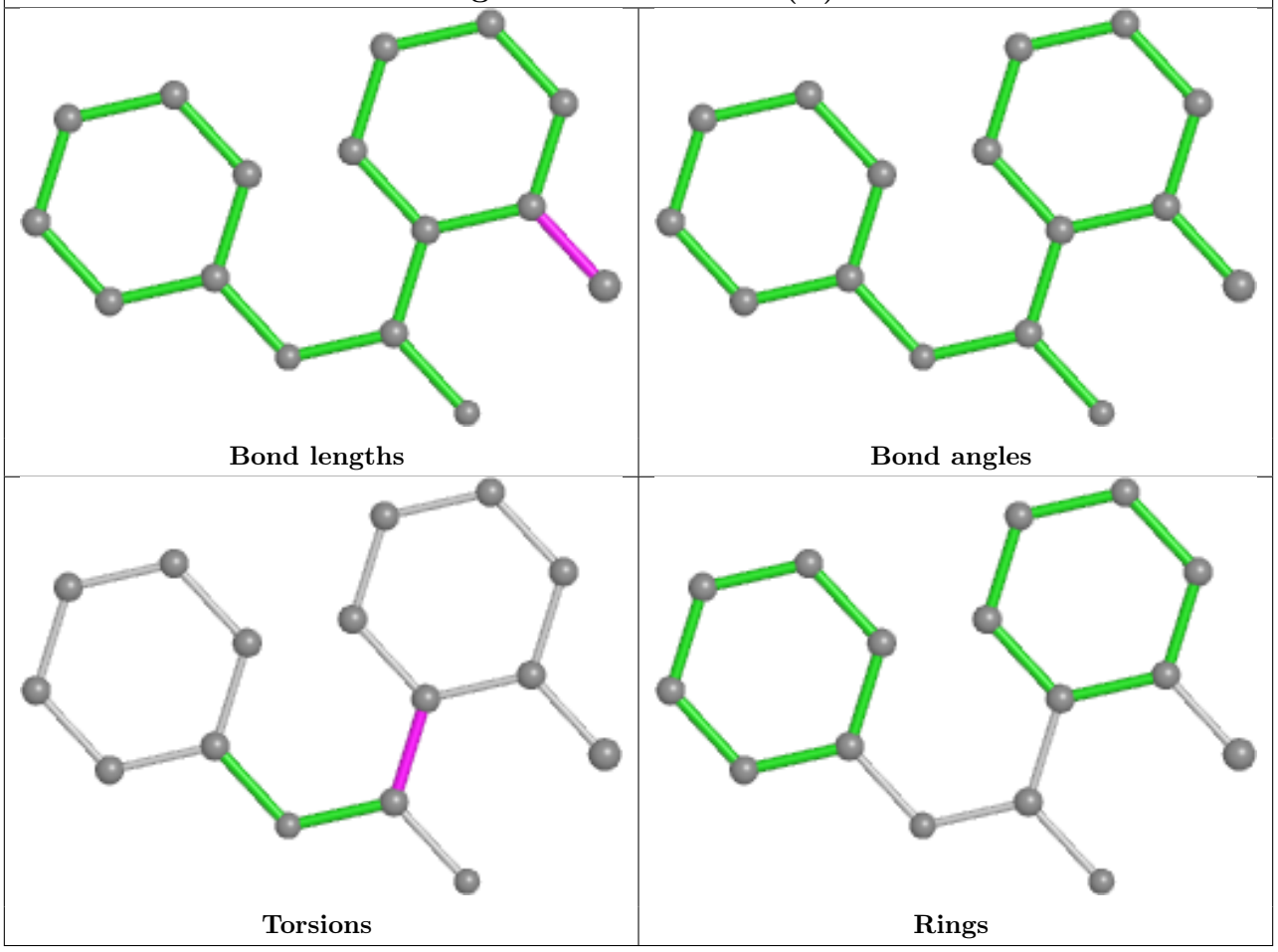


Torsions



Rings

Ligand 9JT BBB 311 (B)



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	AAA	274/279 (98%)	0.09	14 (5%)	28	30	17, 27, 47, 111	0
1	BBB	275/279 (98%)	0.04	14 (5%)	28	30	17, 25, 44, 73	0
All	All	549/558 (98%)	0.06	28 (5%)	28	30	17, 26, 46, 111	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	80[A]	ILE	8.2
1	AAA	277	ASP	7.7
1	AAA	4[A]	PRO	5.3
1	AAA	109	ILE	4.8
1	BBB	80	ILE	4.6
1	BBB	277	ASP	4.2
1	BBB	76	GLY	4.1
1	BBB	75	ALA	4.1
1	BBB	3[A]	ASP	3.5
1	BBB	81	LEU	3.3
1	BBB	4	PRO	3.0
1	AAA	30[A]	GLU	2.8
1	BBB	173[A]	ARG	2.7
1	BBB	169	PRO	2.5
1	AAA	63	PRO	2.4
1	BBB	79	SER	2.3
1	BBB	5	TRP	2.3
1	AAA	77	GLU	2.3
1	AAA	67	PHE	2.2
1	BBB	109	ILE	2.2
1	BBB	74	ALA	2.2
1	AAA	173[A]	ARG	2.2
1	AAA	276	GLU	2.1
1	BBB	60	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	AAA	121	VAL	2.1
1	AAA	83	ASP	2.0
1	AAA	114	ASN	2.0
1	AAA	75	ALA	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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	MES	BBB	309	12/12	0.70	0.18	34,41,58,60	12
5	GOL	AAA	307[B]	6/6	0.71	0.17	56,59,63,74	6
5	GOL	AAA	307[A]	6/6	0.71	0.17	45,53,55,65	6
2	NA	AAA	314	1/1	0.72	0.29	61,61,61,61	0
5	GOL	AAA	309[B]	6/6	0.75	0.21	25,34,37,38	6
5	GOL	AAA	309[A]	6/6	0.75	0.21	33,38,42,43	6
5	GOL	BBB	310	6/6	0.76	0.31	49,72,81,84	0
5	GOL	AAA	308	6/6	0.80	0.15	39,43,46,46	0
5	GOL	AAA	310	6/6	0.81	0.17	35,40,42,47	6
2	NA	AAA	315	1/1	0.83	0.23	61,61,61,61	0
5	GOL	BBB	308	6/6	0.83	0.16	43,47,55,58	0
5	GOL	BBB	306	6/6	0.88	0.10	27,27,30,34	0
5	GOL	AAA	306	6/6	0.90	0.16	56,63,66,85	0
5	GOL	AAA	311	6/6	0.90	0.17	70,73,73,76	0
2	NA	AAA	316	1/1	0.93	0.40	51,51,51,51	0
6	9JT	AAA	312[B]	1/16	0.94	0.12	42,42,42,42	1
6	9JT	AAA	312[A]	16/16	0.94	0.12	25,29,34,34	16
6	9JT	BBB	311[A]	16/16	0.95	0.13	24,26,28,31	16
6	9JT	BBB	311[B]	16/16	0.95	0.13	34,36,38,40	16

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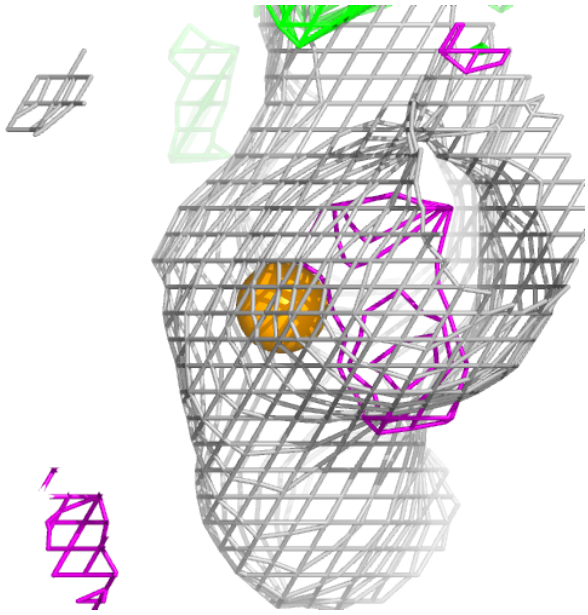
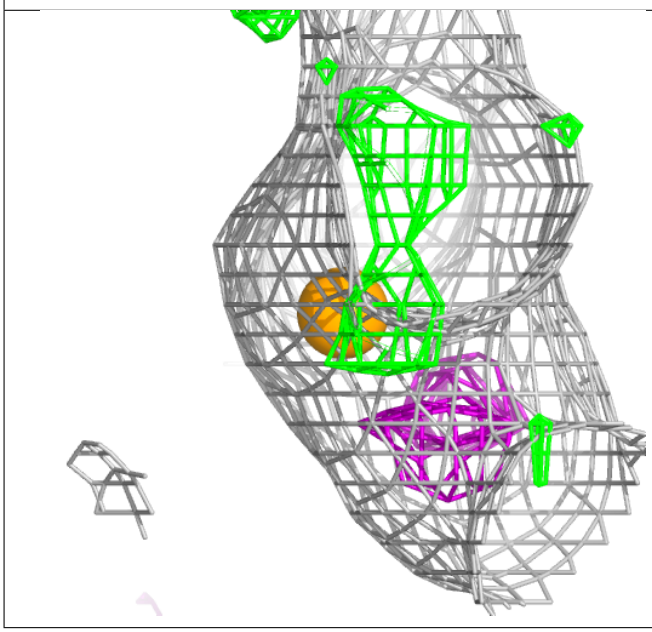
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NA	BBB	312	1/1	0.95	0.08	36,36,36,36	0
2	NA	AAA	304	1/1	0.98	0.05	19,19,19,19	0
2	NA	AAA	313	1/1	0.98	0.43	41,41,41,41	0
4	SO4	AAA	305[A]	5/5	0.98	0.11	17,19,30,34	5
4	SO4	AAA	305[B]	5/5	0.98	0.11	12,22,26,28	5
3	MN	AAA	302[B]	1/1	0.99	0.06	20,20,20,20	1
4	SO4	BBB	307	5/5	0.99	0.04	19,22,31,34	0
3	MN	AAA	303[B]	1/1	1.00	0.04	16,16,16,16	1
3	MN	BBB	302[B]	1/1	1.00	0.10	14,14,14,14	1
3	MN	BBB	303	1/1	1.00	0.05	17,17,17,17	0
3	MN	BBB	304[A]	1/1	1.00	0.06	13,13,13,13	1
3	MN	BBB	305[B]	1/1	1.00	0.03	28,28,28,28	1
2	NA	AAA	301[A]	1/1	1.00	0.05	18,18,18,18	1
2	NA	BBB	301[A]	1/1	1.00	0.10	14,14,14,14	1
3	MN	AAA	303[A]	1/1	1.00	0.04	16,16,16,16	1

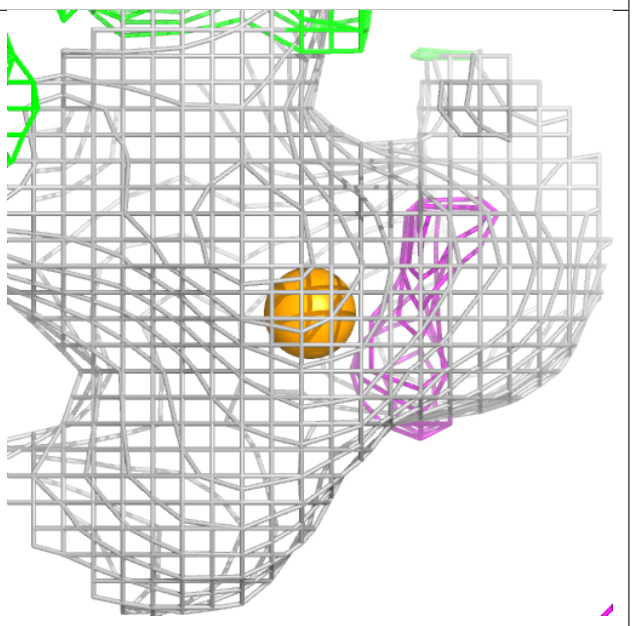
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 9JT AAA 312 (B):

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

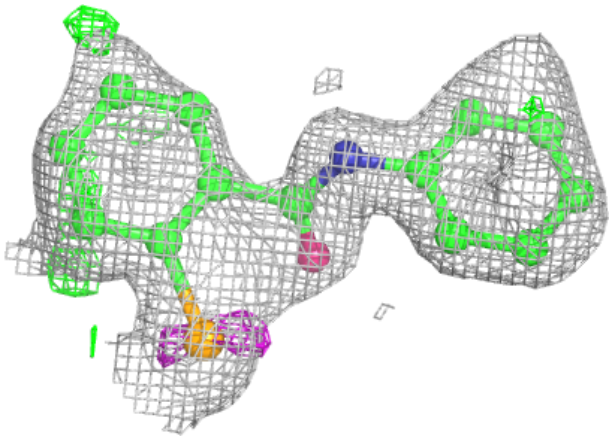


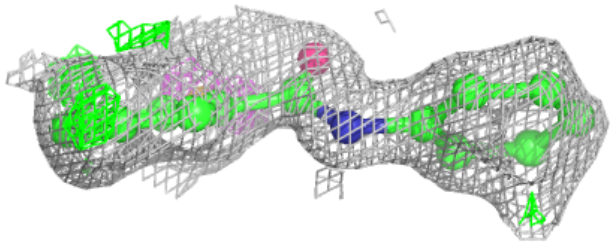


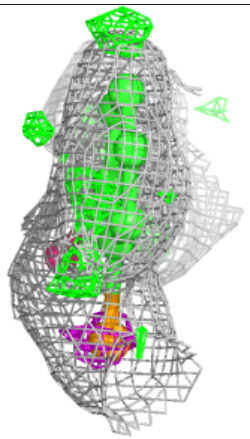


Electron density around 9JT AAA 312 (A):

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

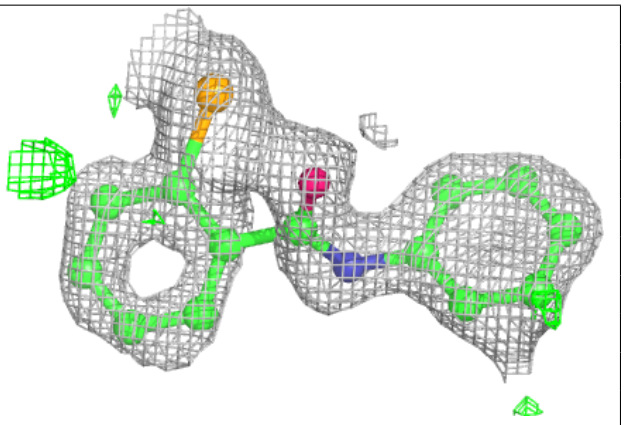


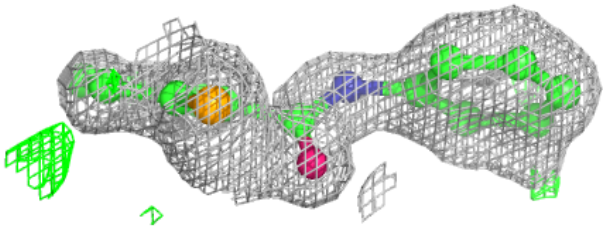


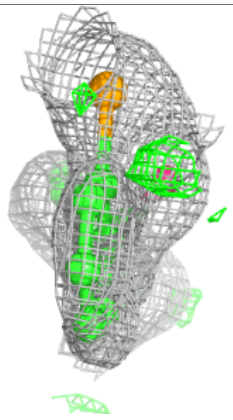


Electron density around 9JT BBB 311 (A):

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

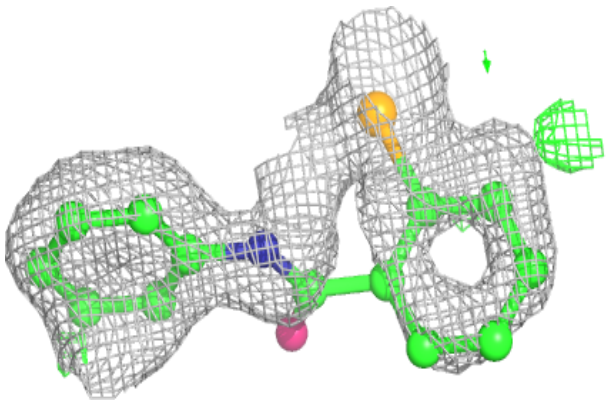


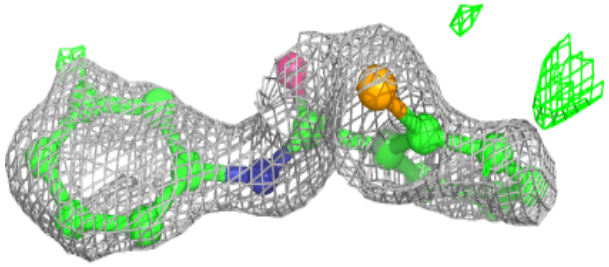


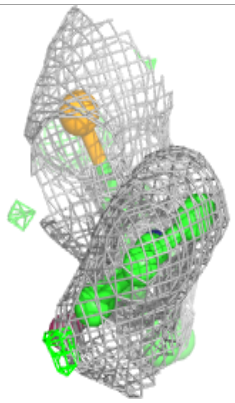


Electron density around 9JT BBB 311 (B):

$2mF_o$-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.