Full wwPDB X-ray Structure Validation Report (i)

Jun 18, 2024 – 07:10 AM EDT

PDB ID	:	5RB5
Title	:	PanDDA analysis group deposition – Crystal Structure of JMJD1B in complex with FM010010a
Authors	:	Snee, M.; Nowak, R.; Johansson, C.; Burgess-Brown, N.A.; Arrowsmith, C.H.; Bountra, C.; Edwards, A.M.; Oppermann, U.
Deposited on	:	2020-03-16
Resolution	:	1.51 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:

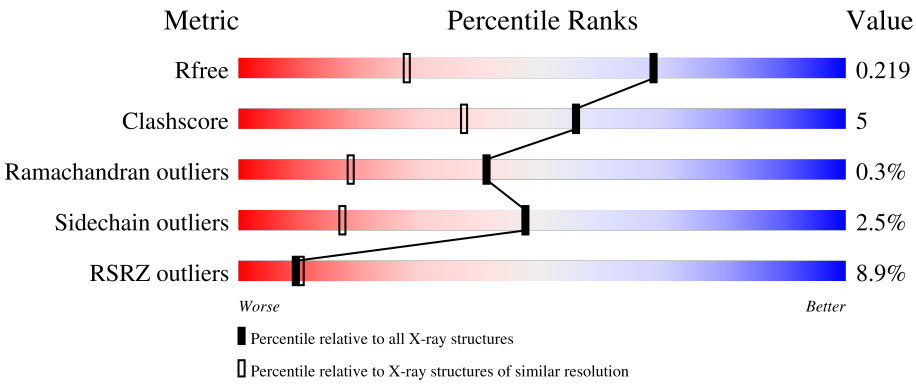
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 1.51 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	4009 (1.54-1.50)
Clashscore	141614	4249 (1.54-1.50)
Ramachandran outliers	138981	4148 (1.54-1.50)
Sidechain outliers	138945	4146 (1.54-1.50)
RSRZ outliers	127900	3943 (1.54-1.50)

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	372	9%, 81%, 9%, •, 9%
1	B	372	8%, 85%, 7%, •, 8%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 6324 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 Lysine-specific demethylase 3B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	340	2779	1758	487	518	16	0	5	0
1	B	344	2798	1774	492	517	15	0	2	0

There are 50 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1357	MET	-	initiating methionine	UNP Q7LBC6
A	1358	HIS	-	expression tag	UNP Q7LBC6
A	1359	HIS	-	expression tag	UNP Q7LBC6
A	1360	HIS	-	expression tag	UNP Q7LBC6
A	1361	HIS	-	expression tag	UNP Q7LBC6
A	1362	HIS	-	expression tag	UNP Q7LBC6
A	1363	HIS	-	expression tag	UNP Q7LBC6
A	1364	SER	-	expression tag	UNP Q7LBC6
A	1365	SER	-	expression tag	UNP Q7LBC6
A	1366	GLY	-	expression tag	UNP Q7LBC6
A	1367	VAL	-	expression tag	UNP Q7LBC6
A	1368	ASP	-	expression tag	UNP Q7LBC6
A	1369	LEU	-	expression tag	UNP Q7LBC6
A	1370	GLY	-	expression tag	UNP Q7LBC6
A	1371	THR	-	expression tag	UNP Q7LBC6
A	1372	GLU	-	expression tag	UNP Q7LBC6
A	1373	ASN	-	expression tag	UNP Q7LBC6
A	1374	LEU	-	expression tag	UNP Q7LBC6
A	1375	TYR	-	expression tag	UNP Q7LBC6
A	1376	PHE	-	expression tag	UNP Q7LBC6
A	1377	GLN	-	expression tag	UNP Q7LBC6
A	1378	SER	-	expression tag	UNP Q7LBC6
A	1379	MET	-	expression tag	UNP Q7LBC6
A	1601	GLU	GLN	conflict	UNP Q7LBC6
A	1606	HIS	GLY	conflict	UNP Q7LBC6

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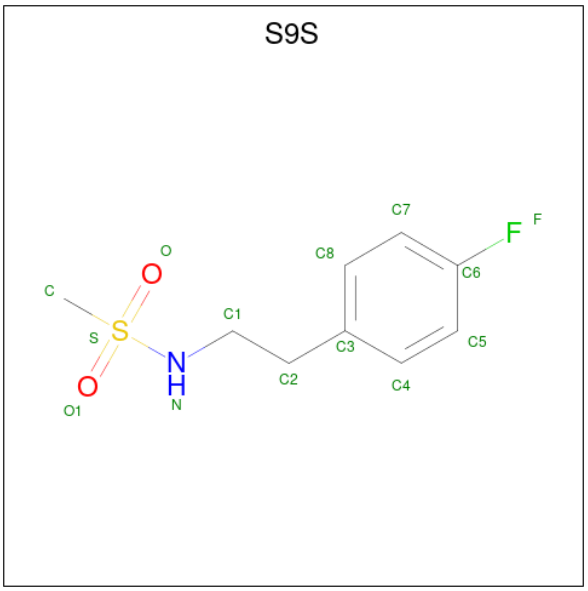
Chain	Residue	Modelled	Actual	Comment	Reference
B	1357	MET	-	initiating methionine	UNP Q7LBC6
B	1358	HIS	-	expression tag	UNP Q7LBC6
B	1359	HIS	-	expression tag	UNP Q7LBC6
B	1360	HIS	-	expression tag	UNP Q7LBC6
B	1361	HIS	-	expression tag	UNP Q7LBC6
B	1362	HIS	-	expression tag	UNP Q7LBC6
B	1363	HIS	-	expression tag	UNP Q7LBC6
B	1364	SER	-	expression tag	UNP Q7LBC6
B	1365	SER	-	expression tag	UNP Q7LBC6
B	1366	GLY	-	expression tag	UNP Q7LBC6
B	1367	VAL	-	expression tag	UNP Q7LBC6
B	1368	ASP	-	expression tag	UNP Q7LBC6
B	1369	LEU	-	expression tag	UNP Q7LBC6
B	1370	GLY	-	expression tag	UNP Q7LBC6
B	1371	THR	-	expression tag	UNP Q7LBC6
B	1372	GLU	-	expression tag	UNP Q7LBC6
B	1373	ASN	-	expression tag	UNP Q7LBC6
B	1374	LEU	-	expression tag	UNP Q7LBC6
B	1375	TYR	-	expression tag	UNP Q7LBC6
B	1376	PHE	-	expression tag	UNP Q7LBC6
B	1377	GLN	-	expression tag	UNP Q7LBC6
B	1378	SER	-	expression tag	UNP Q7LBC6
B	1379	MET	-	expression tag	UNP Q7LBC6
B	1601	GLU	GLN	conflict	UNP Q7LBC6
B	1606	HIS	GLY	conflict	UNP Q7LBC6

- Molecule 2 is {N}-[2-(4-fluorophenyl)ethyl]methanesulfonamide (three-letter code: S9S) (formula: $C_9H_{12}FNO_2S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	F	N	O	S		
2	A	1	14	9	1	1	2	1	0	0
			Total	C	F	N	O	S		
2	A	1	14	9	1	1	2	1	0	0
			Total	C	F	N	O	S		
2	B	1	14	9	1	1	2	1	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mn		
4	A	1	1	1	0	0
			Total	Mn		
4	B	1	1	1	0	0

- Molecule 5 is water.

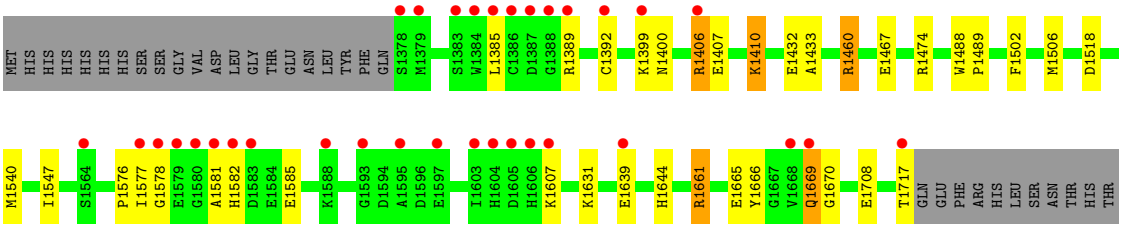
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	377	377	377	0	0
			Total	O		
5	B	321	321	321	0	0

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.

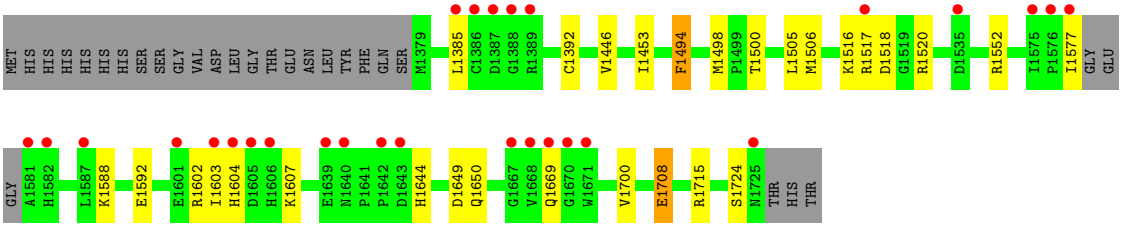
• Molecule 1: Lysine-specific demethylase 3B

Chain A:



• Molecule 1: Lysine-specific demethylase 3B

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	57.93Å 93.60Å 93.81Å 90.00° 107.80° 90.00°	Depositor
Resolution (Å)	55.11 – 1.51 55.05 – 1.51	Depositor EDS
% Data completeness (in resolution range)	98.9 (55.11-1.51) 99.0 (55.05-1.51)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.57 (at 1.51Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.185 , 0.208 0.198 , 0.219	Depositor DCC
R_{free} test set	7406 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	21.4	Xtriage
Anisotropy	0.068	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 46.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.022 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	6324	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 4.77% 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: MN, CL, S9S

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	0.93	4/2852 (0.1%)	0.97	6/3867 (0.2%)
1	B	0.88	2/2872 (0.1%)	0.89	1/3895 (0.0%)
All	All	0.91	6/5724 (0.1%)	0.93	7/7762 (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	A	0	1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1432	GLU	CD-OE1	7.10	1.33	1.25
1	B	1708	GLU	CD-OE1	6.44	1.32	1.25
1	A	1467	GLU	CD-OE1	-6.43	1.18	1.25
1	B	1708	GLU	CD-OE2	6.22	1.32	1.25
1	A	1708	GLU	CD-OE2	5.35	1.31	1.25
1	A	1577	ILE	C-O	5.23	1.33	1.23

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1540	MET	CG-SD-CE	-7.51	88.18	100.20
1	A	1474	ARG	NE-CZ-NH1	7.45	124.02	120.30
1	A	1474	ARG	NE-CZ-NH2	-7.04	116.78	120.30
1	B	1708	GLU	CB-CG-CD	5.75	129.72	114.20
1	A	1576	PRO	O-C-N	5.72	131.86	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1460	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	A	1576	PRO	C-N-CA	5.02	134.26	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1578	GLY	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	2779	0	2669	30	0
1	B	2798	0	2685	26	0
2	A	28	0	0	0	0
2	B	14	0	0	0	0
3	A	4	0	0	0	0
3	B	1	0	0	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	377	0	0	10	2
5	B	321	0	0	9	0
All	All	6324	0	5354	56	2

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 5.

All (56) 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:A:1400:ASN:ND2	5:A:1901:HOH:O	1.59	1.03
1:A:1406[A]:ARG:NH1	5:A:1904:HOH:O	2.06	0.88
1:B:1715:ARG:HG3	5:B:2136:HOH:O	1.77	0.82
1:B:1644:HIS:NE2	1:B:1649:ASP:OD2	2.12	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1639:GLU:O	5:A:1903:HOH:O	2.00	0.80
1:B:1517[B]:ARG:CG	1:B:1517[B]:ARG:HH11	1.95	0.80
1:A:1389[A]:ARG:NH1	5:A:1902:HOH:O	1.69	0.79
1:B:1518:ASP:HB3	5:B:2147:HOH:O	1.85	0.76
1:B:1516:LYS:HE3	5:B:1933:HOH:O	1.88	0.74
1:B:1517[B]:ARG:HH11	1:B:1517[B]:ARG:HG3	1.55	0.70
1:A:1582:HIS:CE1	5:A:1934:HOH:O	2.47	0.68
1:B:1517[B]:ARG:HH11	1:B:1517[B]:ARG:CB	2.07	0.67
1:B:1715:ARG:HD3	5:B:2177:HOH:O	1.97	0.64
1:B:1517[B]:ARG:HG3	1:B:1517[B]:ARG:NH1	2.12	0.64
1:B:1517[B]:ARG:HH11	1:B:1517[B]:ARG:HB2	1.62	0.63
1:B:1517[A]:ARG:NH1	5:B:1904:HOH:O	2.33	0.60
1:A:1407:GLU:HG3	1:A:1410:LYS:HE2	1.82	0.60
1:A:1518:ASP:OD1	5:A:1905:HOH:O	2.17	0.60
1:B:1494:PHE:CZ	1:B:1498:MET:HE3	2.37	0.60
1:A:1407:GLU:HG3	1:A:1410:LYS:NZ	2.18	0.59
1:A:1502:PHE:CE2	1:A:1506:MET:HE2	2.38	0.59
1:A:1547:ILE:HG23	1:A:1582:HIS:CD2	2.39	0.57
1:A:1406[A]:ARG:NH2	5:A:1911:HOH:O	2.38	0.56
1:A:1407:GLU:HG3	1:A:1410:LYS:CE	2.36	0.56
1:A:1407:GLU:CG	1:A:1410:LYS:HZ3	2.18	0.55
1:B:1552:ARG:NH1	1:B:1592:GLU:OE1	2.35	0.55
1:B:1517[B]:ARG:CG	1:B:1517[B]:ARG:NH1	2.63	0.54
1:A:1582:HIS:O	1:A:1582:HIS:CG	2.61	0.54
1:A:1407:GLU:O	1:A:1410:LYS:HG2	2.09	0.52
1:A:1407:GLU:HG3	1:A:1410:LYS:HZ3	1.72	0.52
1:B:1644:HIS:CE1	1:B:1649:ASP:OD2	2.63	0.52
1:B:1506:MET:O	1:B:1516:LYS:HE2	2.12	0.50
1:A:1407:GLU:CB	1:A:1410:LYS:HZ3	2.25	0.49
1:B:1505:LEU:HD22	1:B:1700:VAL:HG11	1.93	0.49
1:A:1631:LYS:HE2	1:A:1666:TYR:OH	2.13	0.49
1:B:1650:GLN:OE1	5:B:1901:HOH:O	2.20	0.48
1:B:1520:ARG:NE	5:B:1913:HOH:O	2.46	0.48
1:A:1407:GLU:CG	1:A:1410:LYS:NZ	2.77	0.47
1:A:1669:GLN:HE21	1:A:1670:GLY:H	1.63	0.47
1:B:1708:GLU:HG3	5:B:2203:HOH:O	2.15	0.47
1:A:1385:LEU:HD12	1:A:1392[B]:CYS:SG	2.55	0.46
1:B:1708:GLU:CG	5:B:2203:HOH:O	2.64	0.45
1:B:1385:LEU:HD12	1:B:1392:CYS:SG	2.56	0.44
1:A:1399:LYS:NZ	5:A:1919:HOH:O	2.50	0.44
1:B:1602:ARG:HG2	1:B:1602:ARG:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1433:ALA:HB3	5:A:1944:HOH:O	2.18	0.43
1:A:1661:ARG:HG2	1:A:1665:GLU:CD	2.38	0.43
1:A:1607:LYS:C	5:A:1920:HOH:O	2.58	0.42
1:B:1494:PHE:CE1	1:B:1498:MET:HE3	2.53	0.42
1:A:1547:ILE:HA	1:A:1582:HIS:NE2	2.35	0.42
1:A:1661:ARG:HG2	1:A:1665:GLU:OE2	2.20	0.41
1:B:1446:VAL:HG22	1:B:1453:ILE:CD1	2.50	0.41
1:A:1661:ARG:CG	1:A:1665:GLU:OE2	2.69	0.41
1:B:1500:THR:OG1	3:B:1802:CL:CL	2.68	0.41
1:A:1488:TRP:HA	1:A:1489:PRO:C	2.41	0.40
1:A:1385:LEU:HG	1:A:1392[B]:CYS:SG	2.62	0.40

All (2) 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)
5:A:1921:HOH:O	5:A:1962:HOH:O[2_658]	1.64	0.56
5:A:1943:HOH:O	5:A:2196:HOH:O[2_648]	1.71	0.49

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	343/372 (92%)	337 (98%)	5 (2%)	1 (0%)	41	18
1	B	342/372 (92%)	331 (97%)	10 (3%)	1 (0%)	41	18
All	All	685/744 (92%)	668 (98%)	15 (2%)	2 (0%)	41	18

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1581	ALA

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Mol	Chain	Res	Type
1	B	1669	GLN

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	301/331 (91%)	292 (97%)	9 (3%)	41	12
1	B	302/331 (91%)	295 (98%)	7 (2%)	50	20
All	All	603/662 (91%)	587 (97%)	16 (3%)	47	15

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

Mol	Chain	Res	Type
1	A	1406[A]	ARG
1	A	1406[B]	ARG
1	A	1410	LYS
1	A	1460	ARG
1	A	1585	GLU
1	A	1644	HIS
1	A	1661	ARG
1	A	1669	GLN
1	A	1717	THR
1	B	1494	PHE
1	B	1577	ILE
1	B	1588	LYS
1	B	1603	ILE
1	B	1604	HIS
1	B	1607	LYS
1	B	1724	SER

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	1650	GLN

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Mol	Chain	Res	Type
1	A	1669	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 10 ligands modelled in this entry, 7 are monoatomic - leaving 3 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	$\#\|Z\| > 2$
2	S9S	B	1801	-	14,14,14	1.75	6 (42%)	18,19,19	2.01	4 (22%)
2	S9S	A	1802	-	14,14,14	1.90	4 (28%)	18,19,19	3.28	4 (22%)
2	S9S	A	1801	-	14,14,14	1.37	2 (14%)	18,19,19	1.27	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	S9S	B	1801	-	-	0/7/7/7	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	S9S	A	1802	-	-	3/7/7/7	0/1/1/1
2	S9S	A	1801	-	-	0/7/7/7	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1801	S9S	C7-C6	3.82	1.44	1.37
2	A	1802	S9S	C5-C4	3.33	1.44	1.38
2	A	1802	S9S	C5-C6	3.16	1.43	1.37
2	A	1802	S9S	C-S	-3.01	1.68	1.75
2	B	1801	S9S	C7-C6	3.01	1.43	1.37
2	A	1802	S9S	C8-C7	2.89	1.44	1.38
2	B	1801	S9S	S-N	2.59	1.65	1.60
2	B	1801	S9S	O1-S	-2.56	1.39	1.43
2	B	1801	S9S	O-S	2.28	1.47	1.43
2	B	1801	S9S	C-S	-2.14	1.70	1.75
2	A	1801	S9S	C-S	-2.04	1.70	1.75
2	B	1801	S9S	C5-C6	2.03	1.41	1.37

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1802	S9S	C-S-N	-12.87	99.87	107.76
2	B	1801	S9S	O1-S-O	-5.10	111.52	118.85
2	B	1801	S9S	C-S-N	-5.09	104.64	107.76
2	B	1801	S9S	O-S-C	2.87	112.89	108.28
2	B	1801	S9S	O1-S-C	2.69	112.59	108.28
2	A	1801	S9S	F-C6-C7	2.68	123.10	118.54
2	A	1801	S9S	C7-C6-C5	-2.36	119.70	122.83
2	A	1802	S9S	F-C6-C7	2.19	122.26	118.54
2	A	1802	S9S	C2-C3-C4	-2.19	115.70	121.23
2	A	1802	S9S	C2-C3-C8	2.07	126.47	121.23

There are no chirality outliers.

All (3) torsion outliers are listed below:

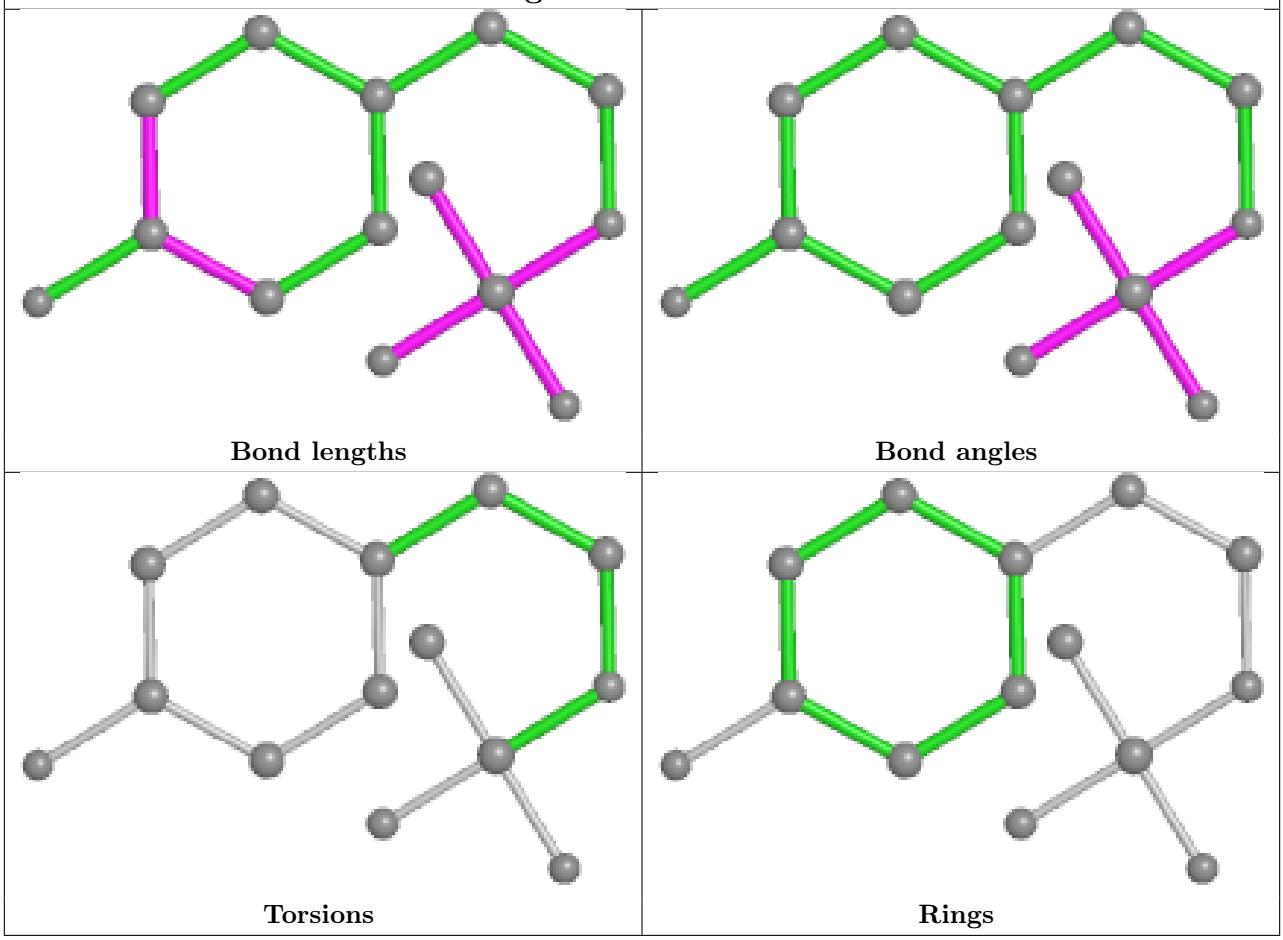
Mol	Chain	Res	Type	Atoms
2	A	1802	S9S	N-C1-C2-C3
2	A	1802	S9S	C1-C2-C3-C8
2	A	1802	S9S	C1-C2-C3-C4

There are no ring outliers.

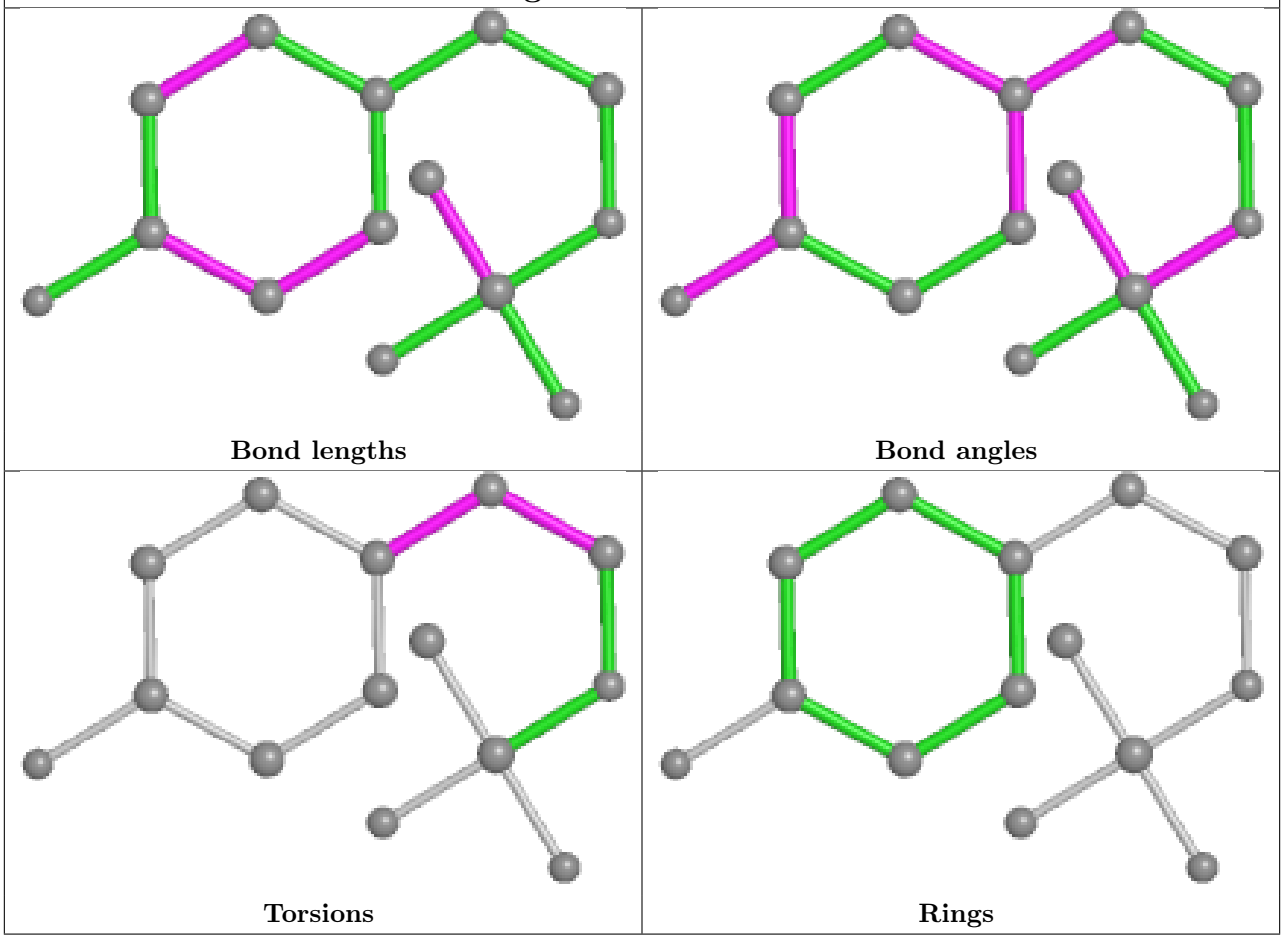
No monomer is involved in short contacts.

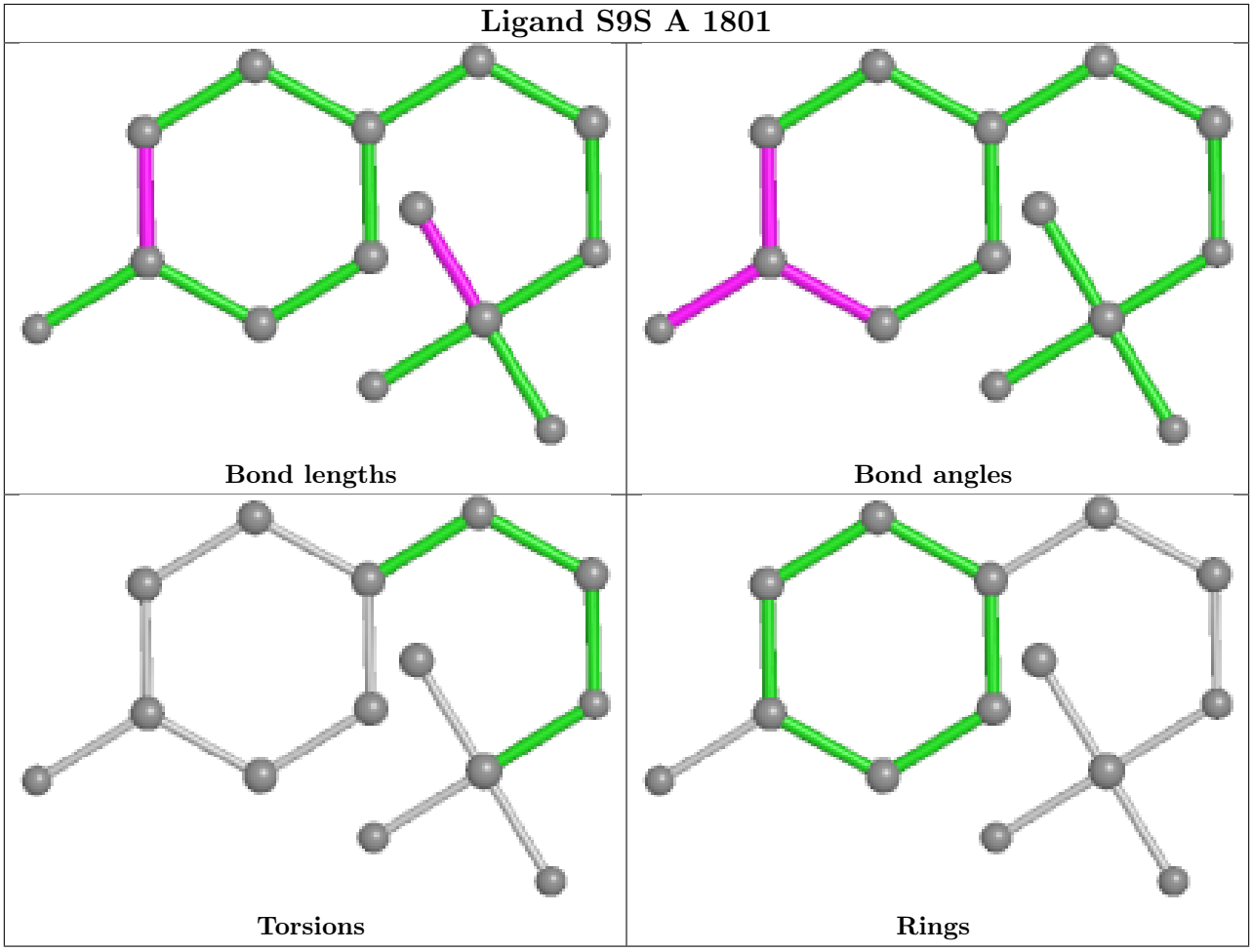
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand S9S B 1801



Ligand S9S A 1802





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	340/372 (91%)	0.37	33 (9%)	7	8	14, 23, 56, 124	21 (6%)
1	B	344/372 (92%)	0.30	28 (8%)	12	13	16, 28, 58, 122	12 (3%)
All	All	684/744 (91%)	0.34	61 (8%)	9	10	14, 25, 57, 124	33 (4%)

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1581	ALA	18.0
1	A	1577	ILE	11.5
1	B	1605	ASP	10.5
1	B	1581	ALA	10.4
1	A	1668	VAL	10.4
1	B	1577	ILE	10.0
1	A	1392[A]	CYS	9.6
1	A	1384	TRP	9.0
1	A	1386	CYS	8.7
1	A	1564[A]	SER	8.4
1	B	1385	LEU	7.8
1	A	1606	HIS	7.4
1	A	1406[A]	ARG	7.4
1	B	1671	TRP	7.2
1	A	1385	LEU	7.2
1	A	1578	GLY	7.1
1	A	1580	GLY	7.0
1	B	1517[A]	ARG	6.9
1	B	1386	CYS	6.7
1	B	1668	VAL	6.6
1	A	1582	HIS	6.6
1	B	1606	HIS	6.3
1	A	1388	GLY	5.7
1	B	1669	GLN	5.3

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Mol	Chain	Res	Type	RSRZ
1	A	1389[A]	ARG	5.2
1	B	1388	GLY	5.1
1	A	1579	GLU	4.9
1	A	1603	ILE	4.7
1	A	1583	ASP	4.4
1	B	1587	LEU	4.3
1	A	1383	SER	4.3
1	A	1399	LYS	4.3
1	A	1595	ALA	4.2
1	B	1603	ILE	4.1
1	B	1582	HIS	3.9
1	A	1669	GLN	3.8
1	A	1379	MET	3.8
1	A	1378	SER	3.8
1	B	1575	ILE	3.7
1	A	1593	GLY	3.5
1	A	1605	ASP	3.5
1	B	1604	HIS	3.5
1	B	1642	PRO	3.4
1	B	1643	ASP	3.3
1	B	1639	GLU	3.2
1	B	1601	GLU	3.2
1	A	1607	LYS	3.1
1	B	1389	ARG	3.0
1	B	1640	ASN	2.8
1	A	1717	THR	2.8
1	B	1725	ASN	2.8
1	B	1670	GLY	2.8
1	B	1535	ASP	2.6
1	A	1588[A]	LYS	2.6
1	B	1667	GLY	2.5
1	A	1387	ASP	2.5
1	B	1576	PRO	2.4
1	A	1639	GLU	2.3
1	A	1604	HIS	2.2
1	A	1597	GLU	2.2
1	B	1387	ASP	2.1

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)

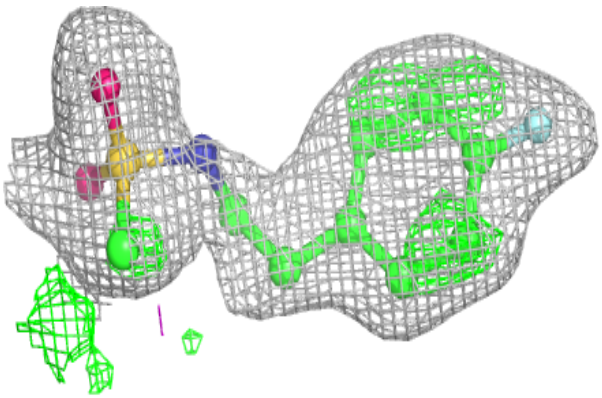
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

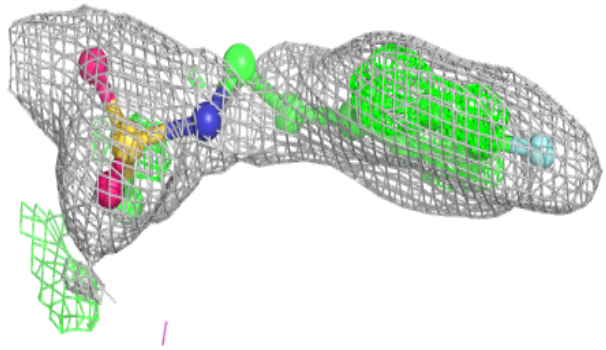
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	S9S	A	1802	14/14	0.77	0.19	25,29,52,55	14
3	CL	A	1806	1/1	0.88	0.08	48,48,48,48	0
2	S9S	A	1801	14/14	0.93	0.26	15,19,21,25	14
2	S9S	B	1801	14/14	0.94	0.20	23,29,32,34	14
4	MN	A	1807	1/1	0.96	0.06	46,46,46,46	0
3	CL	A	1805	1/1	0.97	0.07	36,36,36,36	0
3	CL	B	1802	1/1	0.98	0.05	41,41,41,41	0
4	MN	B	1803	1/1	0.98	0.04	30,30,30,30	0
3	CL	A	1804	1/1	0.99	0.06	34,34,34,34	0
3	CL	A	1803	1/1	0.99	0.11	21,21,21,21	0

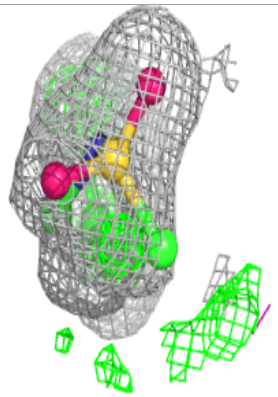
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around S9S A 1802:

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

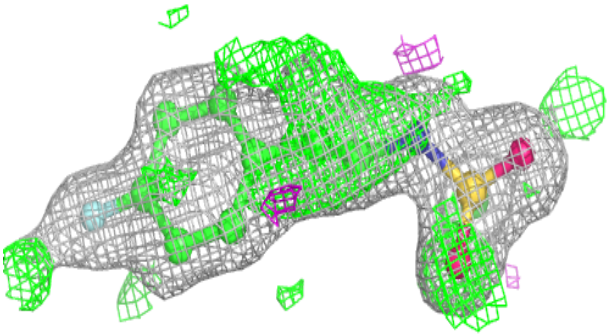


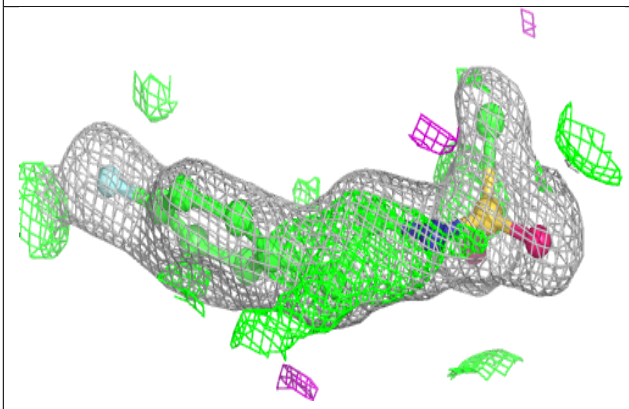


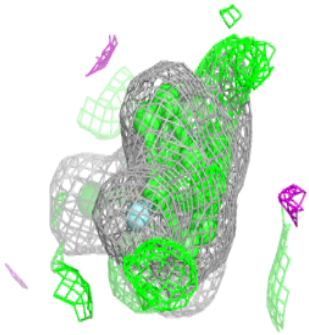


Electron density around S9S A 1801:

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

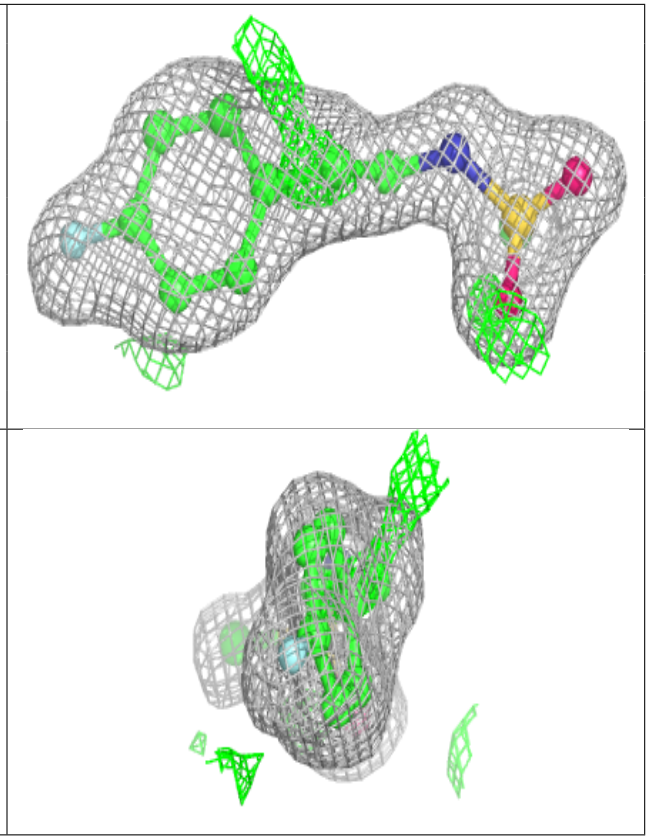






Electron density around S9S B 1801:

$2mF_o$-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.