Full wwPDB X-ray Structure Validation Report (i)

Dec 10, 2023 – 01:23 am GMT

PDB ID	:	2CFK
Title	:	AGAO in complex with wc5 (Ru-wire inhibitor, 5-carbon linker)
Authors	:	Langley, D.B.; Duff, A.P.; Freeman, H.C.; Guss, J.M.; Juda, G.A.; Dooley, D.M.; Contakes, S.M.; Halpern-Manners, N.W.; Dunn, A.R.; Gray, H.B.
Deposited on	:	2006-02-21
Resolution	:	1.80 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:

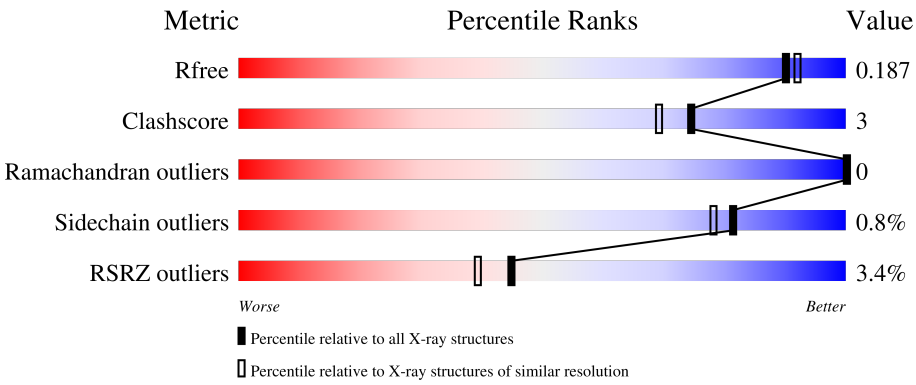
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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	646	3% 91% 5% •

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	R5A	A	1631[A]	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	R5B	A	1632[B]	X	-	-	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 10117 atoms, of which 4628 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 PHENYLETHYLAMINE OXIDASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	620	9404	3095	4507	856	935	11	0	9	0

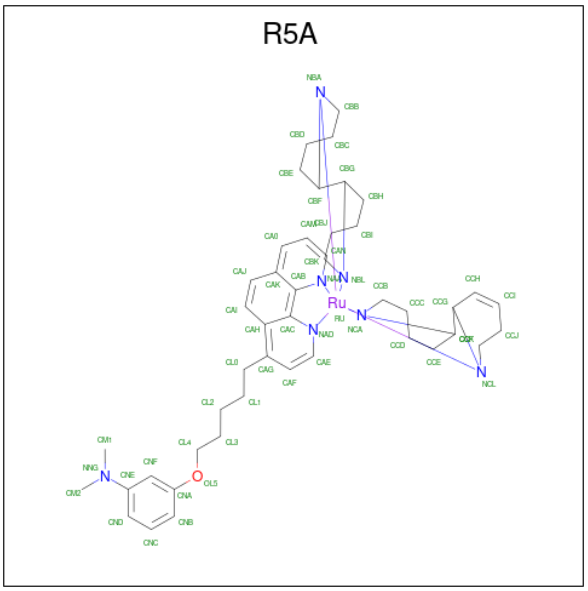
- Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cu		
2	A	1	1	1	0	0

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

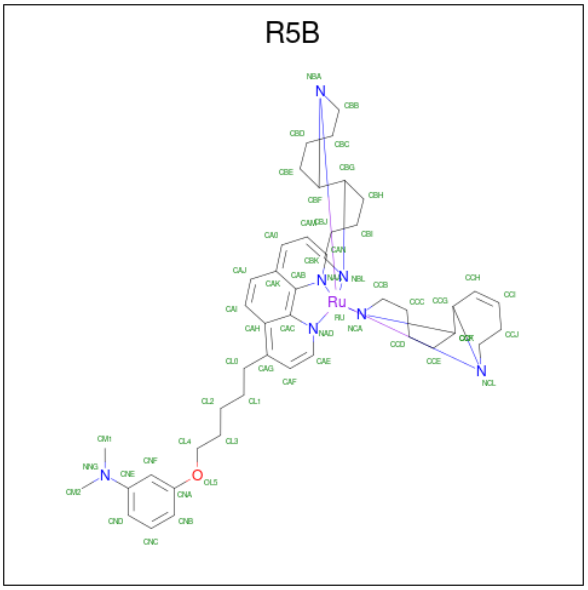
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
3	A	1	1	1	0	0

- Molecule 4 is RUTHENIUM WIRE, 5 CARBON LINKER (three-letter code: R5A) (formula: $C_{45}H_{61}N_7ORu$).



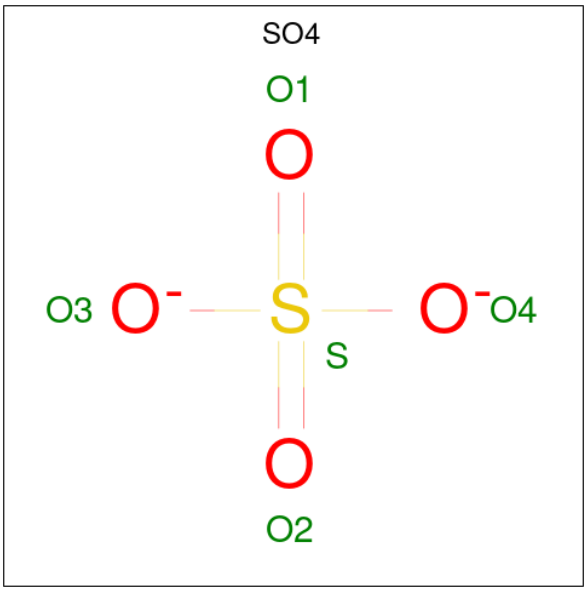
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	N	O	Ru		
4	A	1	97	45	43	7	1	1	0	1

- Molecule 5 is RUTHENIUM WIRE WC5 (three-letter code: R5B) (formula: $C_{45}H_{61}N_7ORu$).



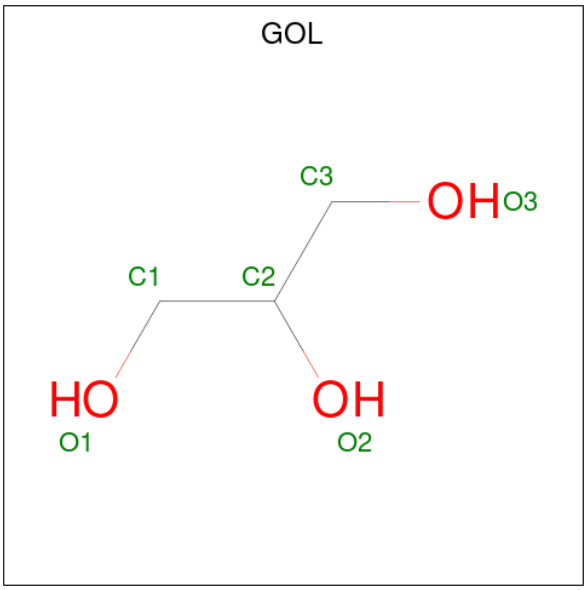
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	N	O	Ru		
5	A	1	97	45	43	7	1	1	0	1

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	O	S			
6	A	1	5	4	1		0	0
			Total	O	S			
6	A	1	5	4	1		0	0
			Total	O	S			
6	A	1	5	4	1		0	0

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
7	A	1	11	3	5	3	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
7	A	1	11	3	5	3	0	0
			Total	C	H	O		
7	A	1	11	3	5	3	0	0
			Total	C	H	O		
7	A	1	11	3	5	3	0	0
			Total	C	H	O		
7	A	1	11	3	5	3	0	0
			Total	C	H	O		
7	A	1	11	3	5	3	0	0
			Total	C	H	O		
7	A	1	11	3	5	3	0	0

- Molecule 8 is water.

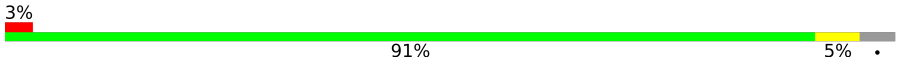
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	A	425	425	425	0	0

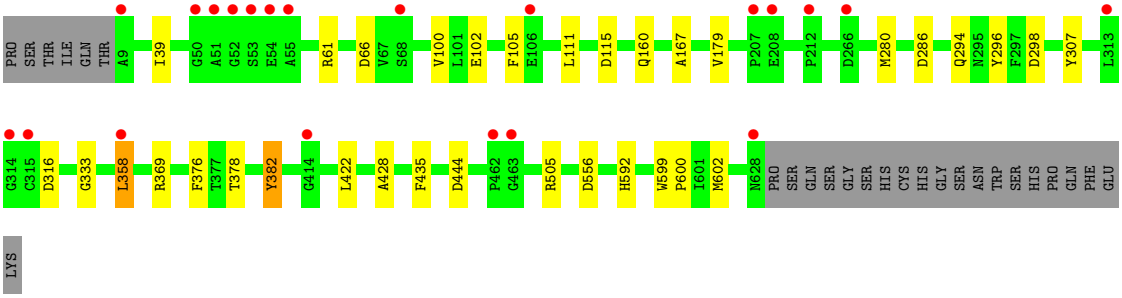
3 Residue-property plots (i)

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: PHENYLETHYLAMINE OXIDASE

Chain A:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	157.88Å 62.94Å 92.01Å 90.00° 112.20° 90.00°	Depositor
Resolution (Å)	15.02 – 1.80 15.02 – 1.80	Depositor EDS
% Data completeness (in resolution range)	98.9 (15.02-1.80) 98.9 (15.02-1.80)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.70 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.145 , 0.165 0.171 , 0.187	Depositor DCC
R_{free} test set	3847 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	21.9	Xtriage
Anisotropy	0.602	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.48 , 53.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	10117	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.19% 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: R5B, NA, CU, SO4, GOL, R5A, TPQ

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	0.50	0/5045	0.79	7/6869 (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	A	505	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	A	505	ARG	NE-CZ-NH1	5.87	123.23	120.30
1	A	298	ASP	CB-CG-OD2	5.71	123.44	118.30
1	A	286	ASP	CB-CG-OD1	5.45	123.21	118.30
1	A	316	ASP	CB-CG-OD2	5.45	123.20	118.30
1	A	66	ASP	CB-CG-OD2	5.22	123.00	118.30
1	A	115	ASP	CB-CG-OD2	5.05	122.84	118.30

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	4897	4507	4712	26	0
2	A	1	0	0	0	0
3	A	1	0	0	0	0
4	A	54	43	57	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	54	43	57	4	0
6	A	15	0	0	0	0
7	A	42	35	56	2	0
8	A	425	0	0	3	0
All	All	5489	4628	4882	32	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 3.

All (32) 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:294[A]:GLN:HG3	1:A:296:TYR:CZ	2.29	0.68
7:A:1639:GOL:O3	8:A:2418:HOH:O	2.15	0.62
1:A:599:TRP:CD2	1:A:600:PRO:HA	2.36	0.61
1:A:102:GLU:HB3	4:A:1631[A]:R5A:HAG	1.82	0.61
1:A:382:TPQ:O5	4:A:1631[A]:R5A:HM12	2.08	0.54
1:A:382:TPQ:O5	5:A:1632[B]:R5B:HM12	2.08	0.54
7:A:1641:GOL:H32	8:A:2249:HOH:O	2.08	0.54
1:A:378:THR:O	4:A:1631[A]:R5A:HL22	2.08	0.53
1:A:422:LEU:HD11	1:A:428:ALA:HB2	1.92	0.51
1:A:592:HIS:HE1	1:A:602[A]:MET:SD	2.33	0.50
1:A:39[B]:ILE:HD12	1:A:333:GLY:HA2	1.93	0.49
1:A:280[B]:MET:HG3	1:A:435:PHE:CD2	2.48	0.49
1:A:105:PHE:HE2	1:A:307:TYR:HH	1.60	0.46
1:A:280[B]:MET:HG3	1:A:435:PHE:CE2	2.52	0.45
4:A:1631[A]:R5A:HNF	4:A:1631[A]:R5A:HM23	1.76	0.45
5:A:1632[B]:R5B:HNF	5:A:1632[B]:R5B:HM23	1.76	0.45
1:A:105:PHE:HD2	4:A:1631[A]:R5A:CAJ	2.31	0.44
1:A:105:PHE:CZ	4:A:1631[A]:R5A:HL51	2.53	0.43
4:A:1631[A]:R5A:HND	4:A:1631[A]:R5A:HM13	1.78	0.43
5:A:1632[B]:R5B:HM13	5:A:1632[B]:R5B:HND	1.78	0.43
1:A:358:LEU:HD23	8:A:2231:HOH:O	2.18	0.43
1:A:160:GLN:HG3	1:A:167:ALA:HB2	2.01	0.42
1:A:111:LEU:HD12	1:A:179:VAL:HG11	2.02	0.42
1:A:105:PHE:CD2	4:A:1631[A]:R5A:CAJ	3.02	0.42
1:A:105:PHE:CD2	4:A:1631[A]:R5A:HAI	2.55	0.42
1:A:61:ARG:HH22	1:A:556:ASP:CG	2.24	0.41
1:A:296:TYR:CE2	5:A:1632[B]:R5B:HM11	2.56	0.41
1:A:100:VAL:HG11	1:A:105:PHE:HE1	1.85	0.41
1:A:61:ARG:NH2	1:A:556:ASP:OD2	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:GLU:HG2	4:A:1631[A]:R5A:HAI	2.03	0.41
1:A:296:TYR:CE2	4:A:1631[A]:R5A:HM11	2.56	0.41
1:A:592:HIS:CE1	1:A:602[A]:MET:SD	3.13	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	A	626/646 (97%)	608 (97%)	18 (3%)	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	522/537 (97%)	518 (99%)	4 (1%)	81	78

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	358	LEU
1	A	369	ARG
1	A	376	PHE

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Mol	Chain	Res	Type
1	A	444	ASP

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)

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	TPQ	A	382	1	13,14,15	1.44	2 (15%)	15,19,21	2.05	3 (20%)

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
1	TPQ	A	382	1	-	0/5/22/24	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	382	TPQ	C3-C4	3.14	1.40	1.35
1	A	382	TPQ	O4-C4	-3.06	1.26	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	382	TPQ	CB-CA-C	-6.01	100.20	111.47
1	A	382	TPQ	C6-C1-C2	3.43	121.28	118.64
1	A	382	TPQ	O5-C5-C4	2.41	123.33	119.38

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	382	TPQ	2	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 14 ligands modelled in this entry, 2 are monoatomic - leaving 12 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	$\#\|Z\| > 2$
6	SO4	A	1634	-	4,4,4	0.15	0	6,6,6	0.25	0
6	SO4	A	1642	-	4,4,4	0.11	0	6,6,6	0.29	0
7	GOL	A	1635	-	5,5,5	0.37	0	5,5,5	0.27	0
7	GOL	A	1637	-	5,5,5	0.35	0	5,5,5	0.18	0
7	GOL	A	1640	-	5,5,5	0.41	0	5,5,5	0.19	0
4	R5A	A	1631[A]	-	52,64,64	3.58	20 (38%)	44,102,102	2.67	18 (40%)
7	GOL	A	1639	-	5,5,5	0.36	0	5,5,5	0.08	0
6	SO4	A	1633	-	4,4,4	0.11	0	6,6,6	0.17	0
7	GOL	A	1636	-	5,5,5	0.31	0	5,5,5	0.31	0
7	GOL	A	1641	-	5,5,5	0.23	0	5,5,5	0.47	0
7	GOL	A	1638	-	5,5,5	0.35	0	5,5,5	0.19	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	R5B	A	1632[B]	-	52,64,64	3.60	20 (38%)	44,102,102	2.59	16 (36%)

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
7	GOL	A	1637	-	-	3/4/4/4	-
7	GOL	A	1635	-	-	0/4/4/4	-
7	GOL	A	1640	-	-	2/4/4/4	-
4	R5A	A	1631[A]	-	4/4/12/12	7/13/125/125	0/11/11/11
7	GOL	A	1639	-	-	0/4/4/4	-
7	GOL	A	1636	-	-	0/4/4/4	-
7	GOL	A	1641	-	-	0/4/4/4	-
7	GOL	A	1638	-	-	2/4/4/4	-
5	R5B	A	1632[B]	-	4/4/12/12	6/13/125/125	0/11/11/11

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1632[B]	R5B	CCB-NCA	-10.81	1.28	1.49
4	A	1631[A]	R5A	CCB-NCA	-10.79	1.28	1.49
5	A	1632[B]	R5B	CBB-NBA	-10.73	1.28	1.49
4	A	1631[A]	R5A	CBB-NBA	-10.67	1.28	1.49
4	A	1631[A]	R5A	CCD-CCE	-7.75	1.32	1.53
4	A	1631[A]	R5A	CBD-CBE	-7.71	1.32	1.53
5	A	1632[B]	R5B	CCD-CCE	-7.67	1.33	1.53
5	A	1632[B]	R5B	CBD-CBE	-7.62	1.33	1.53
5	A	1632[B]	R5B	CCK-NCL	-7.50	1.34	1.49
5	A	1632[B]	R5B	CBK-NBL	-7.42	1.34	1.49
4	A	1631[A]	R5A	CBK-NBL	-7.40	1.34	1.49
4	A	1631[A]	R5A	CCK-NCL	-7.30	1.34	1.49
5	A	1632[B]	R5B	CBH-CBG	-6.24	1.39	1.53
4	A	1631[A]	R5A	CBH-CBG	-6.21	1.39	1.53
5	A	1632[B]	R5B	CBI-CBH	-5.07	1.39	1.53
4	A	1631[A]	R5A	CBI-CBH	-5.05	1.39	1.53
5	A	1632[B]	R5B	CBB-CBC	-4.79	1.34	1.51
4	A	1631[A]	R5A	CBB-CBC	-4.77	1.34	1.51
4	A	1631[A]	R5A	CCB-CCC	-4.76	1.34	1.51
5	A	1632[B]	R5B	CCB-CCC	-4.76	1.34	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1631[A]	R5A	CCK-CCJ	-4.20	1.40	1.51
5	A	1632[B]	R5B	CCK-CCJ	-4.17	1.40	1.51
4	A	1631[A]	R5A	CBK-CBJ	-3.19	1.39	1.51
5	A	1632[B]	R5B	CBK-CBJ	-3.15	1.40	1.51
5	A	1632[B]	R5B	CCH-CCI	2.93	1.39	1.32
4	A	1631[A]	R5A	CCH-CCI	2.93	1.39	1.32
4	A	1631[A]	R5A	CBI-CBJ	-2.92	1.40	1.51
5	A	1632[B]	R5B	CBI-CBJ	-2.90	1.40	1.51
5	A	1632[B]	R5B	CAN-CAM	2.62	1.41	1.35
5	A	1632[B]	R5B	CAE-CAF	2.57	1.41	1.35
4	A	1631[A]	R5A	CCJ-CCI	-2.46	1.39	1.48
4	A	1631[A]	R5A	CAB-CAC	2.43	1.46	1.40
5	A	1632[B]	R5B	CCJ-CCI	-2.39	1.40	1.48
4	A	1631[A]	R5A	CAE-CAF	2.37	1.40	1.35
5	A	1632[B]	R5B	CAB-CAC	2.32	1.45	1.40
4	A	1631[A]	R5A	CAN-CAM	2.25	1.40	1.35
4	A	1631[A]	R5A	CCE-CCF	-2.15	1.48	1.53
5	A	1632[B]	R5B	CBE-CBF	-2.15	1.48	1.53
5	A	1632[B]	R5B	CCE-CCF	-2.13	1.48	1.53
4	A	1631[A]	R5A	CBE-CBF	-2.10	1.48	1.53

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1631[A]	R5A	CBC-CBB-NBA	5.81	122.48	113.00
5	A	1632[B]	R5B	CBC-CBB-NBA	5.69	122.27	113.00
5	A	1632[B]	R5B	CCC-CCB-NCA	5.57	122.08	113.00
4	A	1631[A]	R5A	CCC-CCB-NCA	5.35	121.73	113.00
5	A	1632[B]	R5B	CBK-CBJ-CBI	5.24	120.32	111.44
4	A	1631[A]	R5A	CBK-CBJ-CBI	5.21	120.26	111.44
4	A	1631[A]	R5A	CCF-CCG-NCL	5.18	113.92	107.55
4	A	1631[A]	R5A	CCB-CCC-CCD	5.10	120.07	111.44
5	A	1632[B]	R5B	CCB-CCC-CCD	4.94	119.81	111.44
5	A	1632[B]	R5B	CBB-CBC-CBD	4.71	119.42	111.44
5	A	1632[B]	R5B	CCF-CCG-NCL	4.65	113.27	107.55
4	A	1631[A]	R5A	CBB-CBC-CBD	4.64	119.30	111.44
4	A	1631[A]	R5A	CBJ-CBI-CBH	4.26	120.10	111.42
5	A	1632[B]	R5B	CBJ-CBI-CBH	4.23	120.03	111.42
4	A	1631[A]	R5A	CBJ-CBK-NBL	4.11	119.69	113.00
4	A	1631[A]	R5A	CBI-CBH-CBG	4.11	118.62	111.22
5	A	1632[B]	R5B	CBJ-CBK-NBL	4.03	119.57	113.00
5	A	1632[B]	R5B	CBI-CBH-CBG	4.02	118.46	111.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1631[A]	R5A	CBD-CBE-CBF	3.96	118.36	111.22
4	A	1631[A]	R5A	CAF-CAE-NAD	-3.81	120.44	124.23
5	A	1632[B]	R5B	CBD-CBE-CBF	3.71	117.90	111.22
4	A	1631[A]	R5A	CCD-CCE-CCF	3.70	117.89	111.22
5	A	1632[B]	R5B	CCD-CCE-CCF	3.62	117.75	111.22
5	A	1632[B]	R5B	CAF-CAE-NAD	-3.22	121.03	124.23
5	A	1632[B]	R5B	CBC-CBD-CBE	2.89	117.32	111.42
4	A	1631[A]	R5A	CBC-CBD-CBE	2.86	117.25	111.42
5	A	1632[B]	R5B	CCC-CCD-CCE	2.84	117.20	111.42
4	A	1631[A]	R5A	CCC-CCD-CCE	2.81	117.15	111.42
4	A	1631[A]	R5A	CAB-CAK-CAJ	-2.48	116.77	119.74
4	A	1631[A]	R5A	CCJ-CCK-NCL	2.30	119.87	111.94
5	A	1632[B]	R5B	CCJ-CCK-NCL	2.23	119.64	111.94
4	A	1631[A]	R5A	CL4-OL5-CNA	2.17	123.59	117.93
5	A	1632[B]	R5B	CCJ-CCI-CCH	-2.03	119.98	123.61
4	A	1631[A]	R5A	CCJ-CCI-CCH	-2.01	120.03	123.61

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	1631[A]	R5A	CBF
4	A	1631[A]	R5A	CBG
4	A	1631[A]	R5A	CCG
4	A	1631[A]	R5A	CCF
5	A	1632[B]	R5B	CBF
5	A	1632[B]	R5B	CBG
5	A	1632[B]	R5B	CCG
5	A	1632[B]	R5B	CCF

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1631[A]	R5A	CAH-CAG-CL0-CL1
5	A	1632[B]	R5B	CAH-CAG-CL0-CL1
7	A	1637	GOL	C1-C2-C3-O3
7	A	1638	GOL	C1-C2-C3-O3
4	A	1631[A]	R5A	CAG-CL0-CL1-CL2
4	A	1631[A]	R5A	CL0-CL1-CL2-CL3
7	A	1638	GOL	O2-C2-C3-O3
5	A	1632[B]	R5B	CL2-CL3-CL4-OL5
5	A	1632[B]	R5B	CNB-CNA-OL5-CL4
4	A	1631[A]	R5A	CNB-CNA-OL5-CL4

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Mol	Chain	Res	Type	Atoms
4	A	1631[A]	R5A	CNF-CNA-OL5-CL4
5	A	1632[B]	R5B	CNF-CNA-OL5-CL4
5	A	1632[B]	R5B	CL3-CL4-OL5-CNA
7	A	1637	GOL	O2-C2-C3-O3
7	A	1640	GOL	C1-C2-C3-O3
4	A	1631[A]	R5A	CAF-CAG-CL0-CL1
5	A	1632[B]	R5B	CAF-CAG-CL0-CL1
7	A	1637	GOL	O1-C1-C2-C3
7	A	1640	GOL	O2-C2-C3-O3
4	A	1631[A]	R5A	CL3-CL4-OL5-CNA

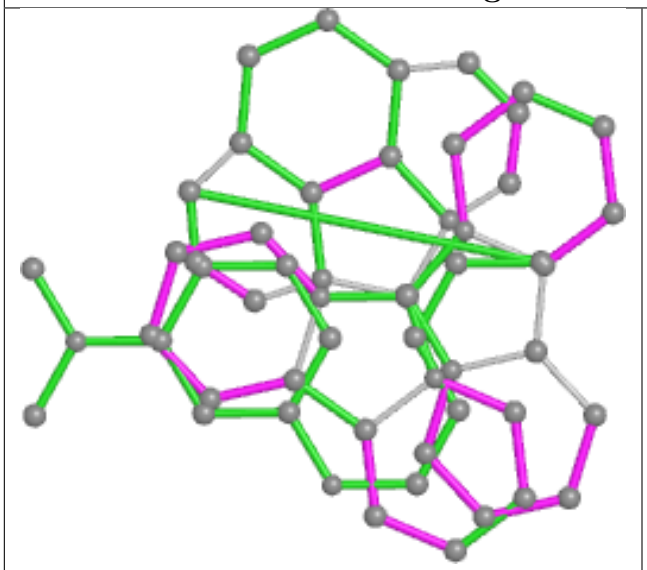
There are no ring outliers.

4 monomers are involved in 17 short contacts:

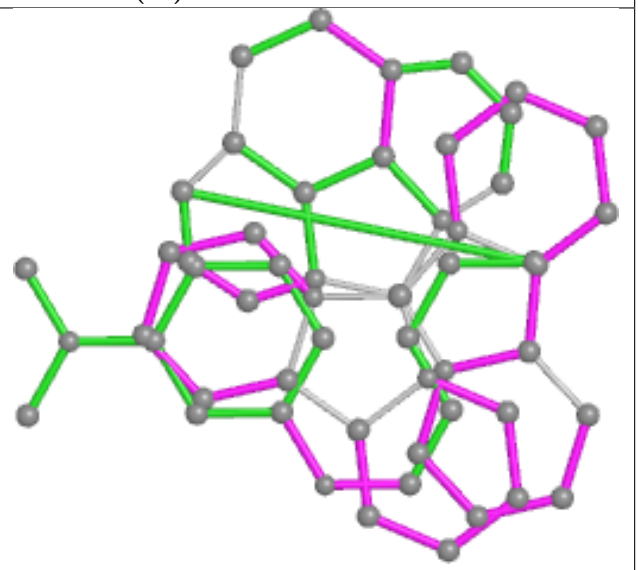
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1631[A]	R5A	11	0
7	A	1639	GOL	1	0
7	A	1641	GOL	1	0
5	A	1632[B]	R5B	4	0

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.

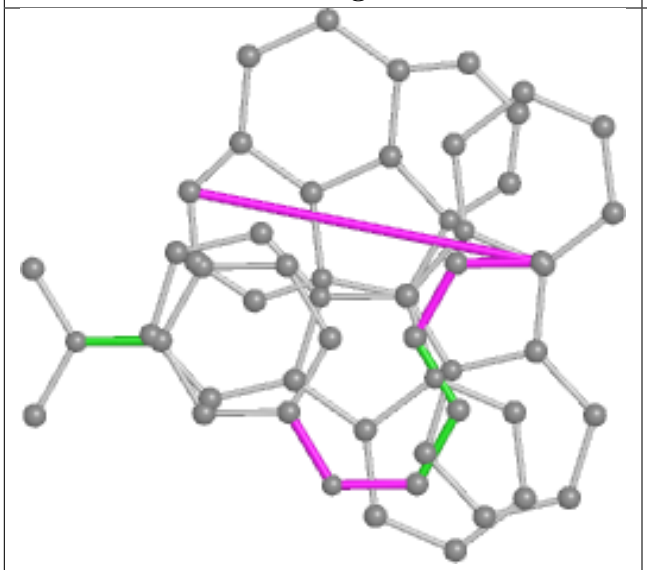
Ligand R5A A 1631 (A)



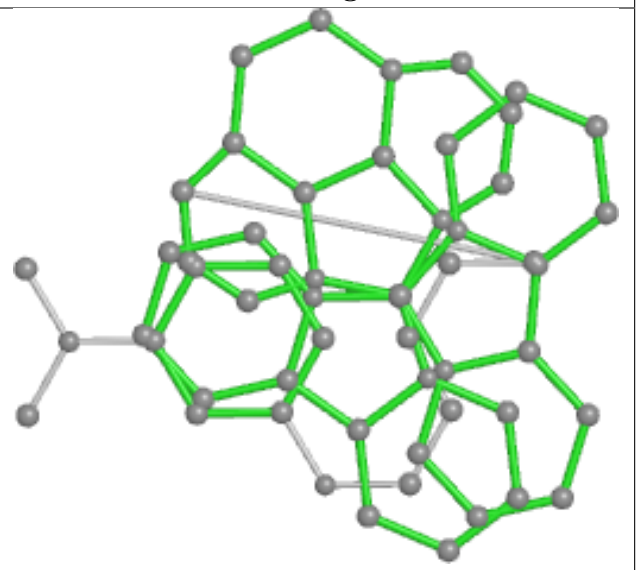
Bond lengths



Bond angles

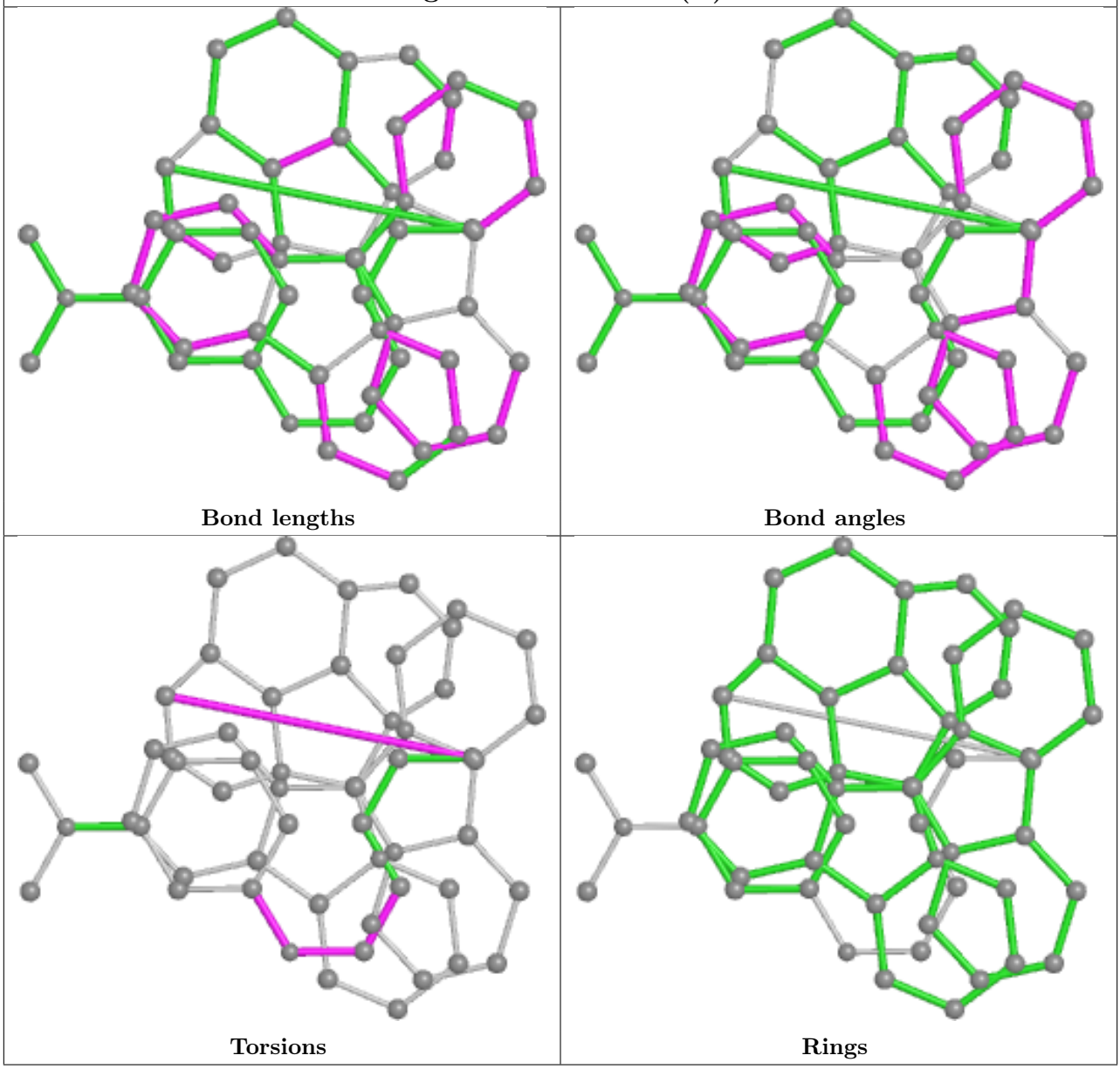


Torsions



Rings

Ligand R5B A 1632 (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 (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	619/646 (95%)	-0.45	21 (3%) 45 39	11, 18, 34, 71	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	53	SER	8.7
1	A	52	GLY	8.7
1	A	54	GLU	6.3
1	A	628	ASN	5.4
1	A	266	ASP	4.1
1	A	51	ALA	4.0
1	A	314	GLY	3.6
1	A	9	ALA	3.4
1	A	55	ALA	3.2
1	A	50	GLY	3.0
1	A	315	CYS	2.8
1	A	106	GLU	2.7
1	A	358	LEU	2.7
1	A	414	GLY	2.7
1	A	313	LEU	2.6
1	A	207	PRO	2.5
1	A	208	GLU	2.5
1	A	212	PRO	2.3
1	A	462	PRO	2.3
1	A	68	SER	2.1
1	A	463	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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
1	TPQ	A	382	14/15	0.94	0.10	14,24,44,54	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

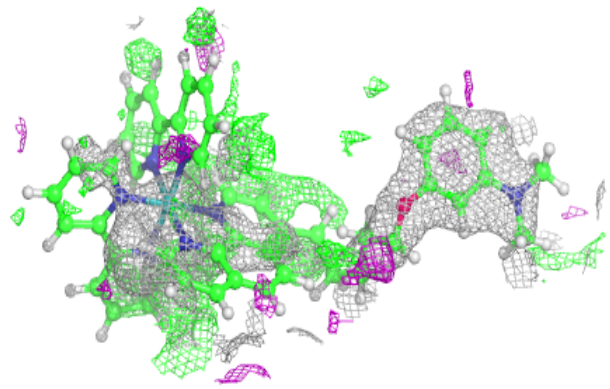
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

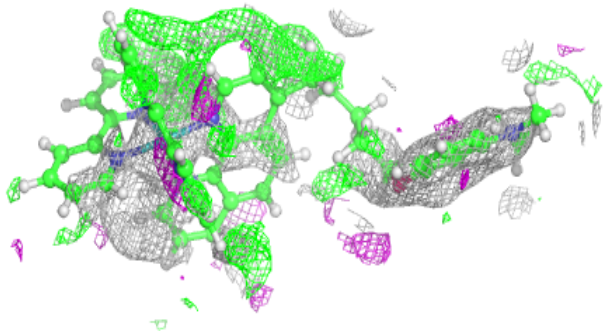
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	GOL	A	1637	6/6	0.65	0.24	68,73,76,77	0
6	SO4	A	1634	5/5	0.69	0.38	67,75,81,83	0
4	R5A	A	1631[A]	54/54	0.70	0.39	36,47,54,54	97
7	GOL	A	1640	6/6	0.71	0.27	54,58,61,65	0
5	R5B	A	1632[B]	54/54	0.72	0.38	36,46,50,54	97
7	GOL	A	1636	6/6	0.74	0.17	38,45,48,54	0
7	GOL	A	1638	6/6	0.75	0.23	40,55,58,59	0
6	SO4	A	1633	5/5	0.78	0.28	89,95,96,99	0
7	GOL	A	1635	6/6	0.84	0.11	27,31,34,36	0
7	GOL	A	1641	6/6	0.88	0.14	34,49,53,59	0
7	GOL	A	1639	6/6	0.92	0.12	37,59,67,67	0
6	SO4	A	1642	5/5	0.95	0.11	56,58,60,64	0
3	NA	A	1630	1/1	0.98	0.24	26,26,26,26	0
2	CU	A	1629	1/1	1.00	0.10	28,28,28,28	0

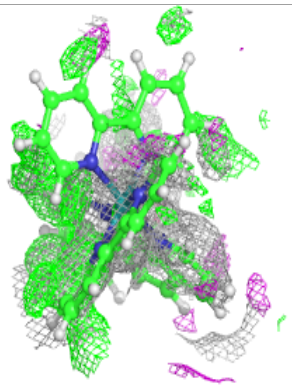
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around R5A A 1631 (A):

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

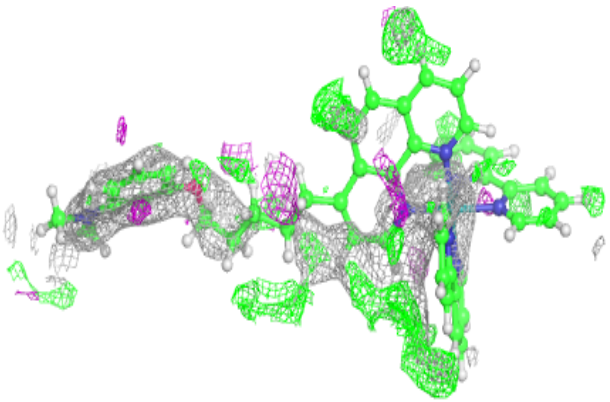


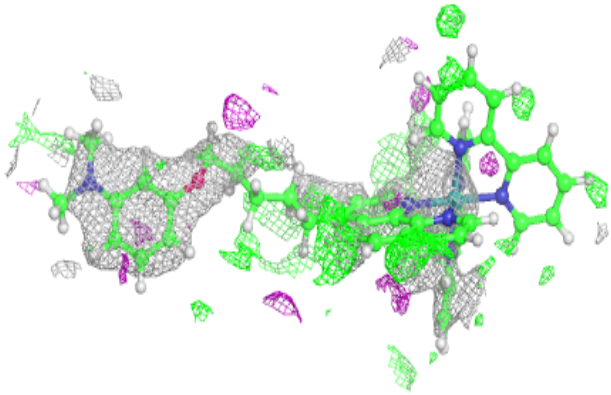


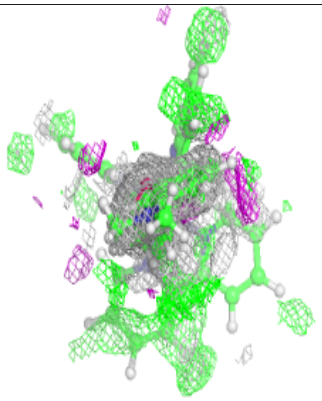


Electron density around R5B A 1632 (B):

$2mF_o$-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.