Full wwPDB X-ray Structure Validation Report (i)

May 16, 2020 – 01:32 pm BST

PDB ID	:	2CG1
Title	:	AGAO in complex with wc11b (Ru-wire inhibitor, 11-carbon linker, data set b)
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Deposited on	:	2006-02-27
Resolution	:	1.67 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 following versions of software and data (see references (i)) were used in the production of this report:

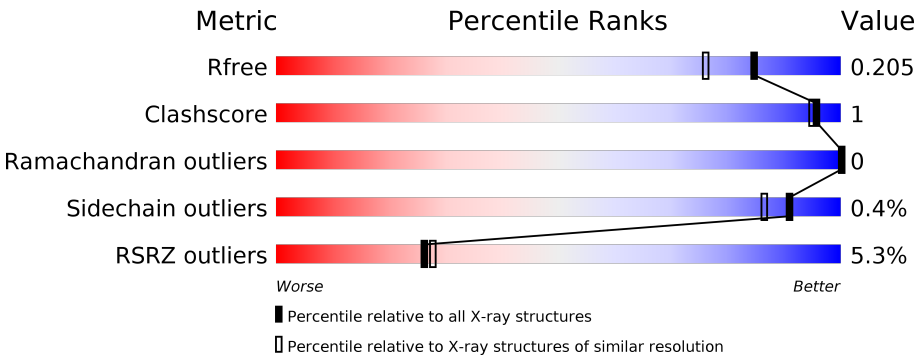
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

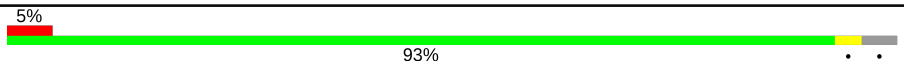
The reported resolution of this entry is 1.67 Å.

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	6780 (1.70-1.66)
Clashscore	141614	7310 (1.70-1.66)
Ramachandran outliers	138981	7173 (1.70-1.66)
Sidechain outliers	138945	7172 (1.70-1.66)
RSRZ outliers	127900	6661 (1.70-1.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on 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	

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	11R	A	1631	X	-	-	X

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 10015 atoms, of which 4573 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	9390	3091	4498	856	934	11	0	8	0

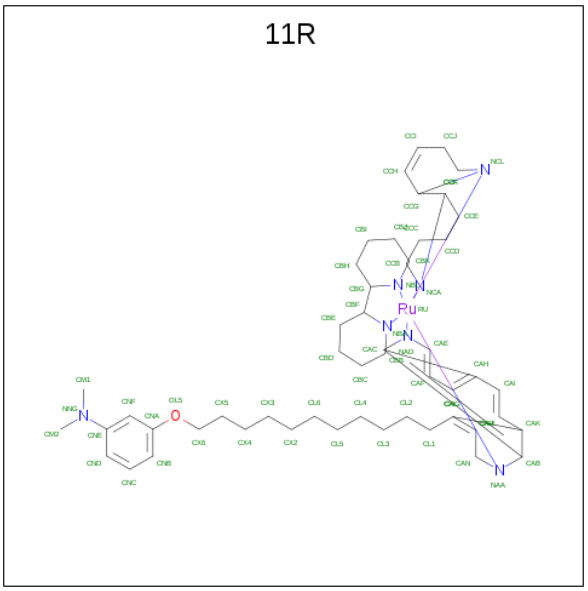
- Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

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).

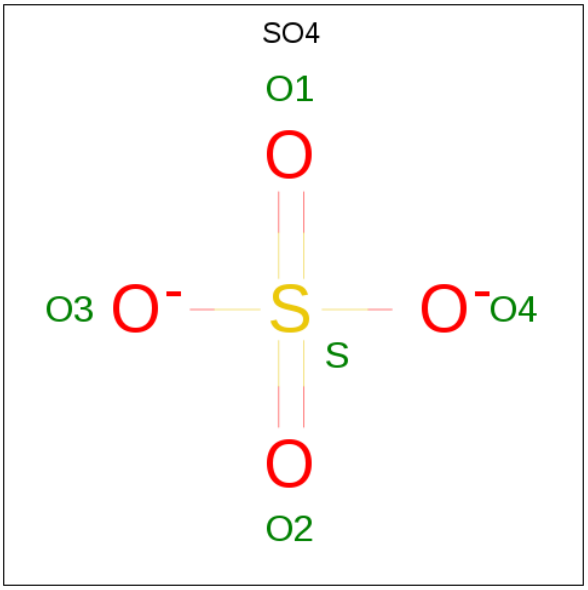
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
3	A	1	1	1	0	0

- Molecule 4 is RUTHENIUM WIRE, 11 CARBON LINKER (three-letter code: 11R) (formula: $C_{51}H_{75}N_7ORu$).



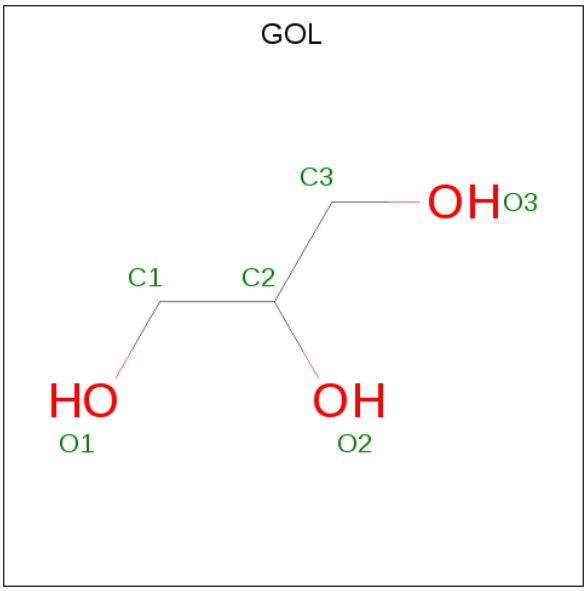
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	N	O	Ru		
4	A	1	115	51	55	7	1	1	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 7 is water.

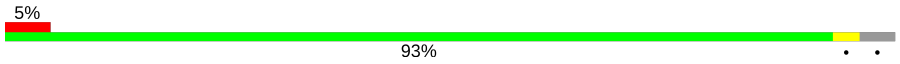
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	459	459	459	0	0

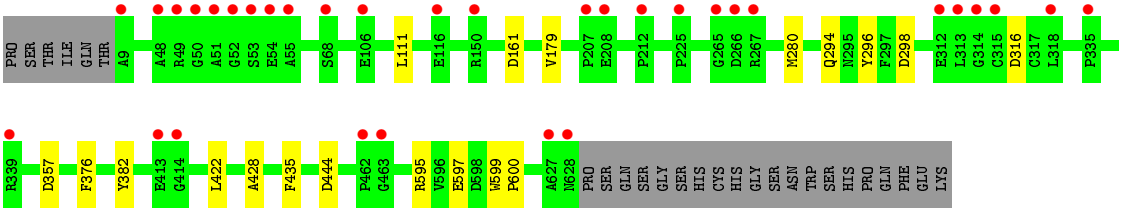
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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	157.92Å 63.04Å 92.07Å 90.00° 112.19° 90.00°	Depositor
Resolution (Å)	14.99 – 1.67 14.98 – 1.67	Depositor EDS
% Data completeness (in resolution range)	97.3 (14.99-1.67) 97.3 (14.98-1.67)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.21 (at 1.67Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.160 , 0.179 0.191 , 0.205	Depositor DCC
R_{free} test set	4738 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	20.4	Xtriage
Anisotropy	0.653	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.48 , 60.9	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	0.95	EDS
Total number of atoms	10015	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 5.13% 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: GOL, NA, SO4, TPQ, 11R, CU

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.43	0/5030	0.76	4/6848 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	316	ASP	CB-CG-OD2	5.74	123.46	118.30
1	A	357	ASP	CB-CG-OD2	5.39	123.15	118.30
1	A	298	ASP	CB-CG-OD2	5.28	123.06	118.30
1	A	161	ASP	CB-CG-OD2	5.11	122.90	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	4892	4498	4706	9	0
2	A	1	0	0	0	0
3	A	1	0	0	0	0
4	A	60	55	70	3	0
5	A	5	0	0	0	0
6	A	24	20	32	0	0
7	A	459	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	5442	4573	4808	11	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 1.

All (11) 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	2.32	0.64
1:A:599:TRP:CD2	1:A:600:PRO:HA	2.35	0.62
1:A:422:LEU:HD11	1:A:428:ALA:HB2	1.88	0.54
1:A:294[A]:GLN:HG3	1:A:296:TYR:CE2	2.47	0.50
1:A:280[B]:MET:HG3	1:A:435:PHE:CD2	2.50	0.47
1:A:111:LEU:HD12	1:A:179:VAL:HG11	1.96	0.47
4:A:1631:11R:HND	4:A:1631:11R:HM13	1.79	0.45
1:A:280[B]:MET:HG3	1:A:435:PHE:CE2	2.52	0.45
4:A:1631:11R:HNF	4:A:1631:11R:HM23	1.73	0.43
1:A:595:ARG:HG3	1:A:597:GLU:HB2	2.00	0.42
1:A:382:TPQ:O5	4:A:1631:11R:HM12	2.21	0.41

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	624/646 (97%)	604 (97%)	20 (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	520/537 (97%)	518 (100%)	2 (0%)	91 86

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	376	PHE
1	A	444	ASP

Some 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	1.38	2 (15%)	15,19,21	1.97	2 (13%)

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	2.99	1.40	1.35
1	A	382	TPQ	O4-C4	-2.83	1.26	1.34

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	382	TPQ	CB-CA-C	-6.16	99.91	111.47
1	A	382	TPQ	C6-C1-C2	2.48	120.54	118.64

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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	GOL	A	1636	-	5,5,5	0.37	0	5,5,5	0.27	0
6	GOL	A	1633	-	5,5,5	0.22	0	5,5,5	0.24	0
6	GOL	A	1634	-	5,5,5	0.30	0	5,5,5	0.25	0
5	SO4	A	1632	-	4,4,4	0.13	0	6,6,6	0.25	0
4	11R	A	1631	-	59,70,70	3.61	24 (40%)	51,108,108	2.63	22 (43%)
6	GOL	A	1635	-	5,5,5	0.31	0	5,5,5	0.44	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
6	GOL	A	1634	-	-	0/4/4/4	-
4	11R	A	1631	-	5/5/19/19	8/19/157/157	0/10/11/11
6	GOL	A	1636	-	-	2/4/4/4	-
6	GOL	A	1633	-	-	0/4/4/4	-
6	GOL	A	1635	-	-	2/4/4/4	-

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1631	11R	CCB-NCA	-10.84	1.28	1.49
4	A	1631	11R	CBB-NBA	-10.81	1.28	1.49
4	A	1631	11R	CBD-CBE	-7.70	1.33	1.53
4	A	1631	11R	CCD-CCE	-7.66	1.33	1.53
4	A	1631	11R	CBK-NBL	-7.50	1.34	1.49
4	A	1631	11R	CCK-NCL	-7.48	1.34	1.49
4	A	1631	11R	CBH-CBG	-6.21	1.39	1.53
4	A	1631	11R	CAI-CAJ	5.57	1.41	1.33
4	A	1631	11R	CBI-CBH	-5.08	1.39	1.53
4	A	1631	11R	CAC-CAB	4.82	1.45	1.38
4	A	1631	11R	CCB-CCC	-4.75	1.34	1.51
4	A	1631	11R	CBB-CBC	-4.72	1.34	1.51
4	A	1631	11R	CCK-CCJ	-4.17	1.40	1.51
4	A	1631	11R	CAK-CAL	-3.89	1.49	1.54
4	A	1631	11R	CAC-CAH	3.80	1.46	1.42
4	A	1631	11R	CAM-CAL	3.77	1.41	1.33
4	A	1631	11R	CBK-CBJ	-3.16	1.40	1.51
4	A	1631	11R	CBI-CBJ	-2.90	1.40	1.51
4	A	1631	11R	CCH-CCI	2.88	1.39	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1631	11R	CAK-CAJ	-2.60	1.40	1.51
4	A	1631	11R	CCJ-CCI	-2.40	1.40	1.48
4	A	1631	11R	CCE-CCF	-2.20	1.48	1.53
4	A	1631	11R	CBE-CBF	-2.19	1.48	1.53
4	A	1631	11R	CAK-CAB	-2.14	1.46	1.52

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1631	11R	CBC-CBB-NBA	5.63	122.17	113.00
4	A	1631	11R	CCC-CCB-NCA	5.60	122.13	113.00
4	A	1631	11R	CBK-CBJ-CBI	5.20	120.24	111.44
4	A	1631	11R	CBB-CBC-CBD	5.02	119.94	111.44
4	A	1631	11R	CCB-CCC-CCD	4.94	119.81	111.44
4	A	1631	11R	CCF-CCG-NCL	4.93	113.62	107.55
4	A	1631	11R	CAJ-CAK-CAB	4.77	118.42	108.39
4	A	1631	11R	CBJ-CBI-CBH	4.26	120.11	111.42
4	A	1631	11R	CAG-CAH-CAC	-4.14	115.69	118.54
4	A	1631	11R	CBI-CBH-CBG	4.04	118.51	111.22
4	A	1631	11R	CBJ-CBK-NBL	4.00	119.52	113.00
4	A	1631	11R	CAC-CAH-CAI	-3.56	118.05	124.02
4	A	1631	11R	CBD-CBE-CBF	3.22	117.02	111.22
4	A	1631	11R	CCD-CCE-CCF	3.21	117.00	111.22
4	A	1631	11R	CCC-CCD-CCE	2.89	117.31	111.42
4	A	1631	11R	CBC-CBD-CBE	2.86	117.25	111.42
4	A	1631	11R	CAK-CAL-CAM	2.82	118.20	112.14
4	A	1631	11R	CAG-CAH-CAI	2.68	126.27	121.54
4	A	1631	11R	CCJ-CCK-NCL	2.24	119.67	111.94
4	A	1631	11R	CAE-NAD-CAC	2.15	118.94	117.41
4	A	1631	11R	CAE-CAF-CAG	2.10	122.49	119.44
4	A	1631	11R	CCJ-CCI-CCH	-2.00	120.04	123.61

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	1631	11R	CAK
4	A	1631	11R	CBG
4	A	1631	11R	CCF
4	A	1631	11R	CBF
4	A	1631	11R	CCG

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1636	GOL	C1-C2-C3-O3
6	A	1635	GOL	C1-C2-C3-O3
4	A	1631	11R	CAL-CL1-CL2-CL3
6	A	1636	GOL	O2-C2-C3-O3
4	A	1631	11R	CNB-CNA-OL5-CX6
4	A	1631	11R	CNF-CNA-OL5-CX6
4	A	1631	11R	CL5-CL6-CX2-CX3
4	A	1631	11R	CX2-CX3-CX4-CX5
6	A	1635	GOL	O2-C2-C3-O3
4	A	1631	11R	CL1-CL2-CL3-CL4
4	A	1631	11R	CL6-CX2-CX3-CX4
4	A	1631	11R	CX5-CX6-OL5-CNA

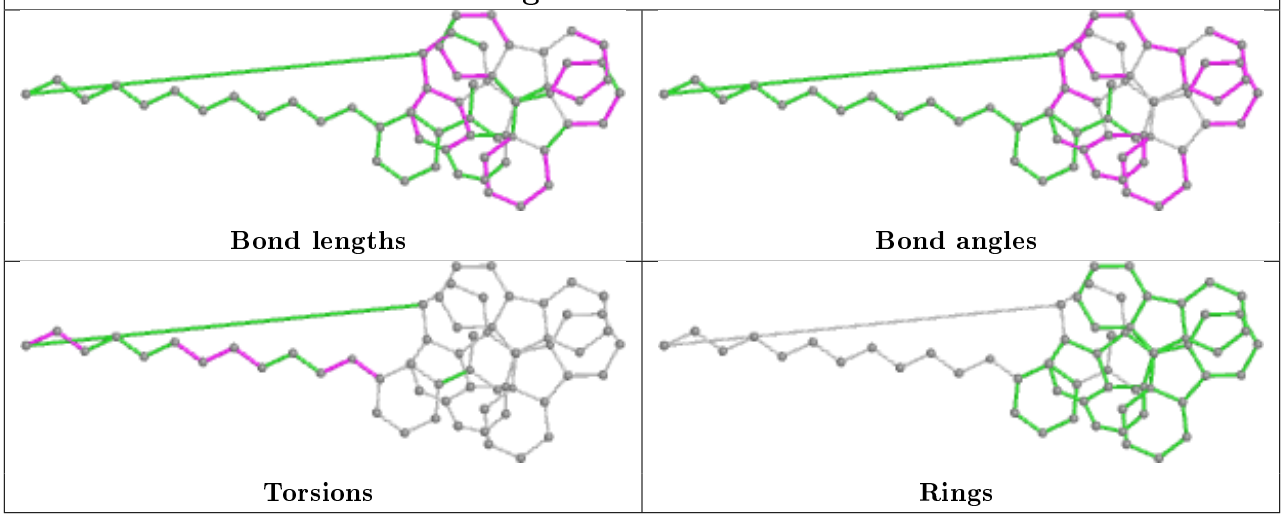
There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1631	11R	3	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 11R A 1631



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%)	-0.01	33 (5%) 26 28	13, 20, 33, 60	1 (0%)

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	52	GLY	10.6
1	A	53	SER	9.1
1	A	628	ASN	7.3
1	A	54	GLU	6.7
1	A	51	ALA	6.0
1	A	55	ALA	5.1
1	A	314	GLY	5.0
1	A	9	ALA	4.7
1	A	50	GLY	4.6
1	A	266	ASP	4.5
1	A	315	CYS	4.3
1	A	313	LEU	3.7
1	A	265	GLY	3.6
1	A	225	PRO	3.5
1	A	207	PRO	3.4
1	A	208	GLU	3.3
1	A	462	PRO	3.2
1	A	414	GLY	3.1
1	A	68	SER	3.0
1	A	463	GLY	2.9
1	A	212	PRO	2.7
1	A	318	LEU	2.7
1	A	116	GLU	2.6
1	A	267	ARG	2.4
1	A	106	GLU	2.4
1	A	627	ALA	2.4
1	A	49	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	339	ARG	2.3
1	A	150	ARG	2.3
1	A	413	GLU	2.2
1	A	48	ALA	2.2
1	A	312	GLU	2.1
1	A	335	PRO	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	0.11	16,23,38,51	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

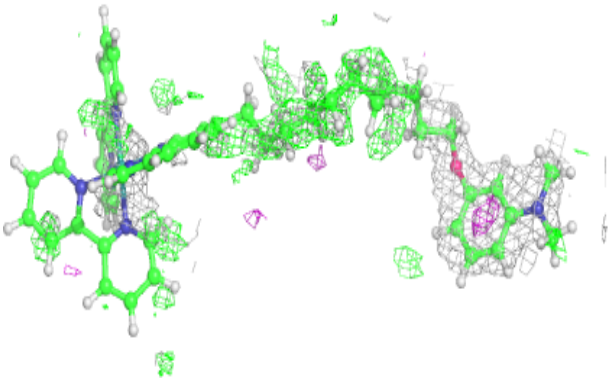
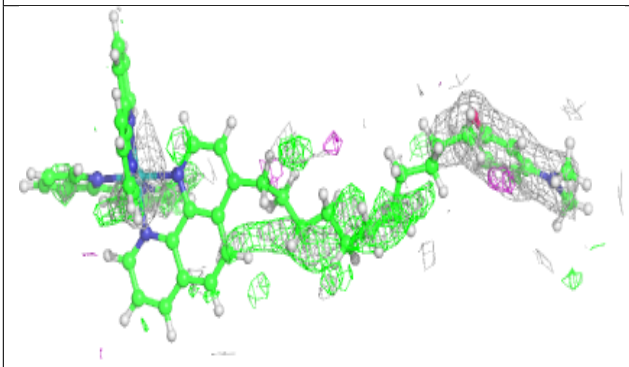
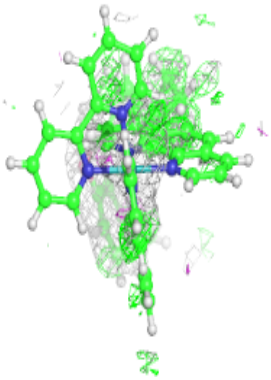
6.4 Ligands (i)

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
4	11R	A	1631	60/60	0.69	0.46	38,59,62,62	89
6	GOL	A	1634	6/6	0.76	0.16	36,42,47,49	0
6	GOL	A	1635	6/6	0.83	0.15	52,53,56,61	0
6	GOL	A	1636	6/6	0.84	0.22	39,50,53,55	0
6	GOL	A	1633	6/6	0.87	0.11	28,29,30,30	0
5	SO4	A	1632	5/5	0.94	0.11	49,50,54,64	0
2	CU	A	1629	1/1	0.99	0.10	26,26,26,26	0
3	NA	A	1630	1/1	0.99	0.23	26,26,26,26	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 11R A 1631: 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.