



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 15, 2020 – 03:12 am BST

PDB ID : 2CFG  
Title : AGAO in complex with wc4d3 (Ru-wire inhibitor, 4-carbon linker, delta enantiomer, data set 3)  
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 : 1.55 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) 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

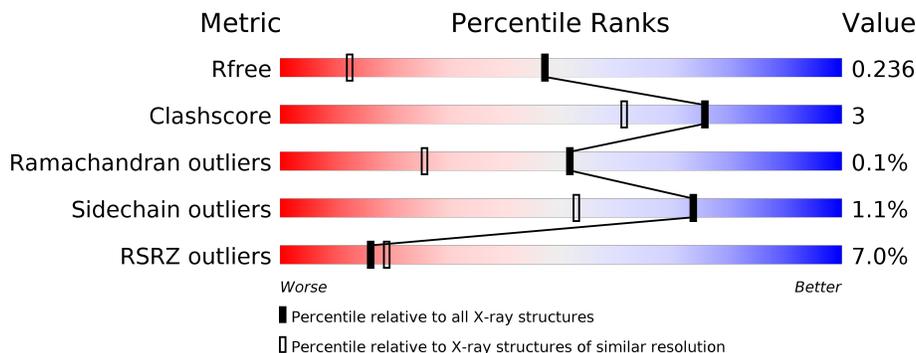
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.55 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	1483 (1.56-1.56)
Clashscore	141614	1529 (1.56-1.56)
Ramachandran outliers	138981	1498 (1.56-1.56)
Sidechain outliers	138945	1495 (1.56-1.56)
RSRZ outliers	127900	1465 (1.56-1.56)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	
1	B	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:

<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
4	R4A	A	1630	X	-	-	-
4	R4A	B	1632	X	-	X	-

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 19843 atoms, of which 9102 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	619	9355	3080	4480	853	931	11	0	4	0
1	B	619	9362	3082	4485	853	931	11	0	5	0

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

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

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

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

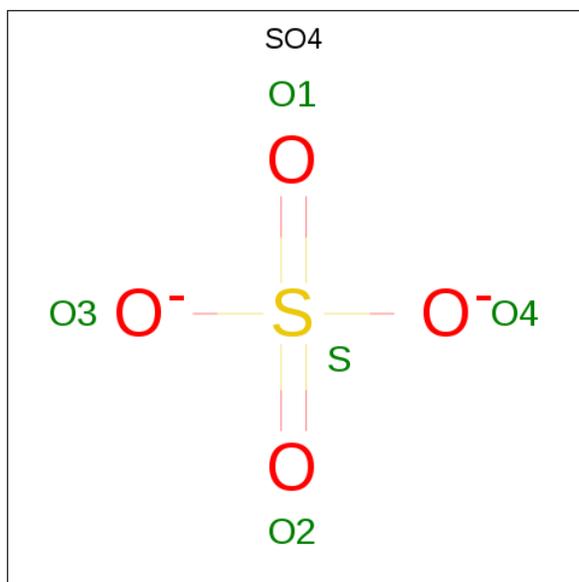
- Molecule 4 is BIS[1H,1'H-2,2'-BIPYRIDINATO(2-)-KAPPA 2 N 1 ,N 1' ]{3-[4-(1,10-DIHYDRO-1,10-PHENANTHROLIN-4-YL-KAPPA 2 N 1 ,N 10 )BUTOXY]-N,N-DIMETHYLANILINATO(2-)}RUTHENIUM (three-letter code: R4A) (formula: C<sub>44</sub>H<sub>61</sub>N<sub>7</sub>ORu).



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

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

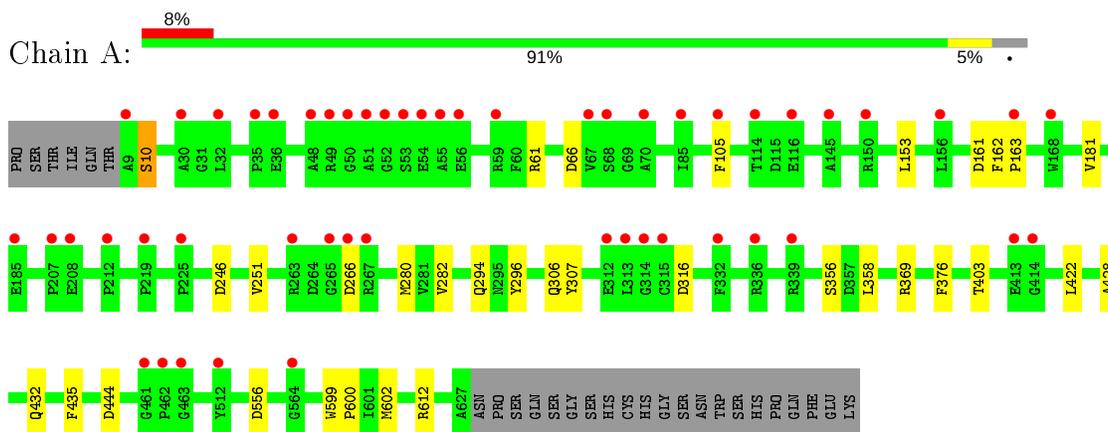
- Molecule 7 is water.

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
7	A	365	Total 365	O 365	0	0
7	B	438	Total 438	O 438	0	0

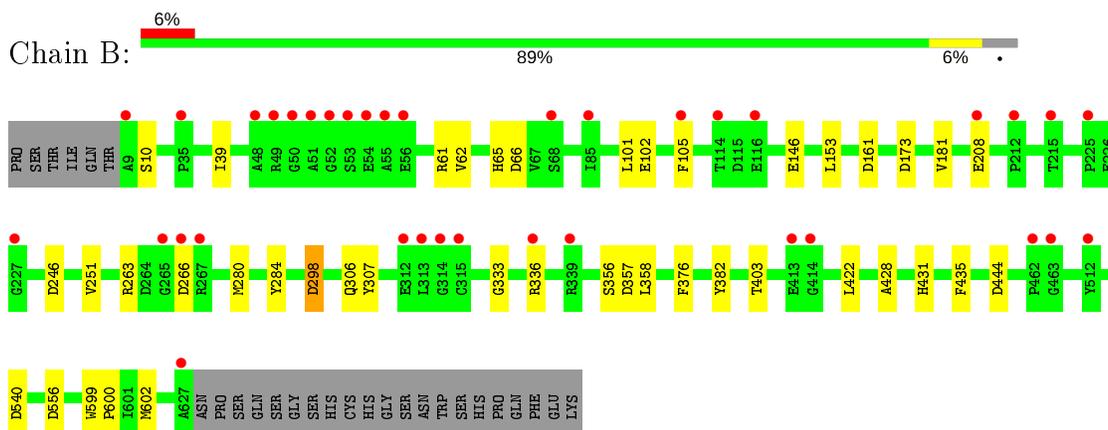
### 3 Residue-property plots [i](#)

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



- Molecule 1: PHENYLETHYLAMINE OXIDASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	192.37Å 62.95Å 158.13Å 90.00° 117.46° 90.00°	Depositor
Resolution (Å)	30.01 – 1.55 30.01 – 1.55	Depositor EDS
% Data completeness (in resolution range)	92.6 (30.01-1.55) 92.5 (30.01-1.55)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.48 (at 1.55Å)	Xtrriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.203 , 0.224 0.220 , 0.236	Depositor DCC
$R_{free}$ test set	11299 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.8	Xtrriage
Anisotropy	0.385	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.46 , 52.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	19843	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 93.62 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.8182e-09. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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, R4A, NA, SO4, TPQ, 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	0.50	0/4998	0.79	6/6804 (0.1%)
1	B	0.57	0/5006	0.83	8/6815 (0.1%)
All	All	0.54	0/10004	0.81	14/13619 (0.1%)

There are no bond length outliers.

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	246	ASP	CB-CG-OD2	6.62	124.26	118.30
1	B	540	ASP	CB-CG-OD2	6.58	124.23	118.30
1	A	246	ASP	CB-CG-OD2	6.38	124.04	118.30
1	B	298	ASP	CB-CG-OD2	6.26	123.93	118.30
1	A	66	ASP	CB-CG-OD2	5.51	123.26	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	4875	4480	4692	19	0
1	B	4877	4485	4693	37	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	53	41	53	8	0
4	B	53	41	56	21	0
5	A	24	20	32	1	0
5	B	42	35	56	1	0
6	B	10	0	0	1	0
7	A	365	0	0	1	0
7	B	438	0	0	2	0
All	All	10741	9102	9582	61	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.

The worst 5 of 61 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:B:105:PHE:CZ	4:B:1632:R4A:HL12	1.38	1.58
1:B:105:PHE:CE2	4:B:1632:R4A:CAL	2.20	1.24
1:B:105:PHE:CZ	4:B:1632:R4A:CL1	2.21	1.22
1:B:105:PHE:CE2	4:B:1632:R4A:CL1	2.33	1.09
1:B:105:PHE:CE2	4:B:1632:R4A:HL12	1.87	1.06

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	620/646 (96%)	598 (96%)	21 (3%)	1 (0%)	47 23
1	B	621/646 (96%)	597 (96%)	24 (4%)	0	100 100
All	All	1241/1292 (96%)	1195 (96%)	45 (4%)	1 (0%)	51 26

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	10	SER

### 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	516/537 (96%)	512 (99%)	4 (1%)	81	66
1	B	517/537 (96%)	510 (99%)	7 (1%)	67	41
All	All	1033/1074 (96%)	1022 (99%)	11 (1%)	73	53

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	10	SER
1	B	146	GLU
1	B	336	ARG
1	A	444	ASP
1	B	263	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	421	GLN
1	B	306	GLN
1	B	421	GLN
1	B	507	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains

2 non-standard protein/DNA/RNA residues are 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	1.39	2 (15%)	15,19,21	1.73	1 (6%)
1	TPQ	B	382	1	13,14,15	1.33	2 (15%)	15,19,21	1.74	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	-	1/5/22/24	0/1/1/1
1	TPQ	B	382	1	-	1/5/22/24	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	382	TPQ	C3-C4	3.04	1.40	1.35
1	A	382	TPQ	O4-C4	-2.76	1.26	1.34
1	B	382	TPQ	O4-C4	-2.70	1.27	1.34
1	B	382	TPQ	C3-C4	2.67	1.39	1.35

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	382	TPQ	CB-CA-C	-5.75	100.69	111.47
1	A	382	TPQ	CB-CA-C	-5.45	101.26	111.47
1	B	382	TPQ	C6-C1-C2	2.42	120.49	118.64

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	382	TPQ	N-CA-CB-C1
1	B	382	TPQ	N-CA-CB-C1

There are no ring outliers.

1 monomer is involved in 1 short contact:

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 4 are monoatomic - leaving 15 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	A	1633	-	5,5,5	0.37	0	5,5,5	0.26	0
6	SO4	B	1633	-	4,4,4	0.12	0	6,6,6	0.49	0
5	GOL	B	1635	-	5,5,5	0.36	0	5,5,5	0.22	0
5	GOL	B	1636	-	5,5,5	0.29	0	5,5,5	0.50	0
5	GOL	A	1632	-	5,5,5	0.32	0	5,5,5	0.34	0
5	GOL	A	1631	-	5,5,5	0.39	0	5,5,5	0.25	0
6	SO4	B	1628	-	4,4,4	0.10	0	6,6,6	0.58	0
5	GOL	B	1638	-	5,5,5	0.35	0	5,5,5	0.17	0
4	R4A	B	1632	-	52,63,63	3.87	25 (48%)	44,101,101	2.91	22 (50%)
4	R4A	A	1630	-	52,63,63	3.86	25 (48%)	44,101,101	2.92	21 (47%)
5	GOL	B	1637	-	5,5,5	0.33	0	5,5,5	0.31	0
5	GOL	B	1639	-	5,5,5	0.25	0	5,5,5	0.68	0
5	GOL	B	1634	-	5,5,5	0.24	0	5,5,5	0.40	0
5	GOL	A	1634	-	5,5,5	0.30	0	5,5,5	0.82	0
5	GOL	B	1629	-	5,5,5	0.32	0	5,5,5	0.17	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	A	1633	-	-	2/4/4/4	-
5	GOL	B	1635	-	-	0/4/4/4	-
5	GOL	B	1636	-	-	0/4/4/4	-
5	GOL	A	1632	-	-	0/4/4/4	-
5	GOL	A	1631	-	-	0/4/4/4	-
5	GOL	B	1638	-	-	2/4/4/4	-
4	R4A	B	1632	-	5/5/19/19	6/12/150/150	0/10/11/11
4	R4A	A	1630	-	5/5/19/19	5/12/150/150	0/10/11/11
5	GOL	B	1637	-	-	2/4/4/4	-
5	GOL	B	1639	-	-	2/4/4/4	-
5	GOL	B	1634	-	-	0/4/4/4	-
5	GOL	A	1634	-	-	2/4/4/4	-
5	GOL	B	1629	-	-	2/4/4/4	-

The worst 5 of 50 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1630	R4A	CBB-NBA	-10.91	1.27	1.49
4	B	1632	R4A	CBB-NBA	-10.85	1.28	1.49
4	A	1630	R4A	CCB-NCA	-10.76	1.28	1.49
4	B	1632	R4A	CCB-NCA	-10.62	1.28	1.49
4	B	1632	R4A	CBD-CBE	-7.83	1.32	1.53

The worst 5 of 43 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1632	R4A	CBC-CBB-NBA	5.91	122.64	113.00
4	A	1630	R4A	CBC-CBB-NBA	5.87	122.56	113.00
4	B	1632	R4A	CBK-CBJ-CBI	5.36	120.52	111.44
4	A	1630	R4A	CCC-CCB-NCA	5.35	121.73	113.00
4	B	1632	R4A	CCC-CCB-NCA	5.26	121.57	113.00

5 of 10 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	B	1632	R4A	CAK

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Mol	Chain	Res	Type	Atom
4	B	1632	R4A	CBG
4	B	1632	R4A	CCF
4	B	1632	R4A	CBF
4	B	1632	R4A	CCG

5 of 23 torsion outliers are listed below:

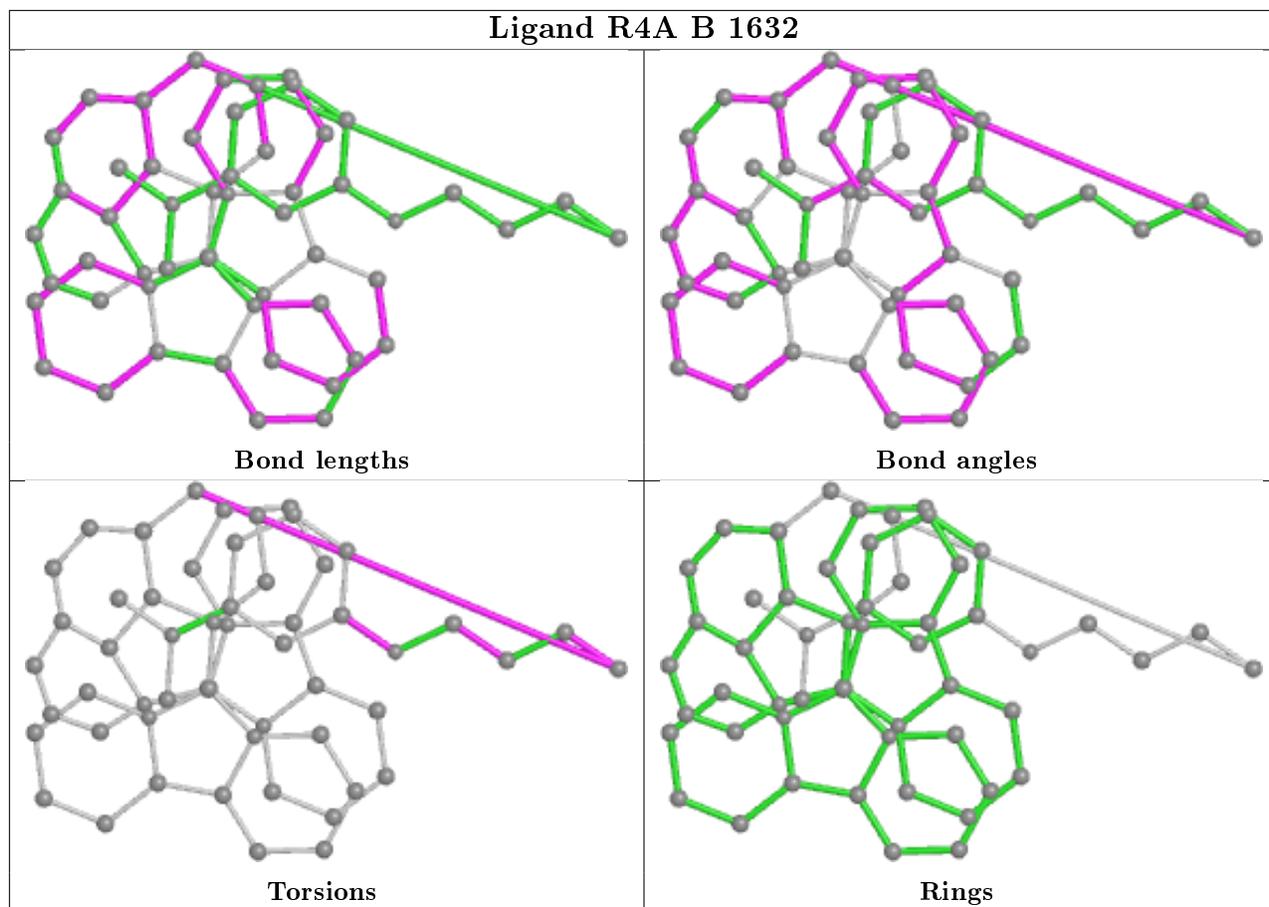
Mol	Chain	Res	Type	Atoms
5	A	1633	GOL	C1-C2-C3-O3
5	A	1633	GOL	O2-C2-C3-O3
5	B	1638	GOL	O1-C1-C2-C3
5	B	1637	GOL	C1-C2-C3-O3
5	B	1637	GOL	O2-C2-C3-O3

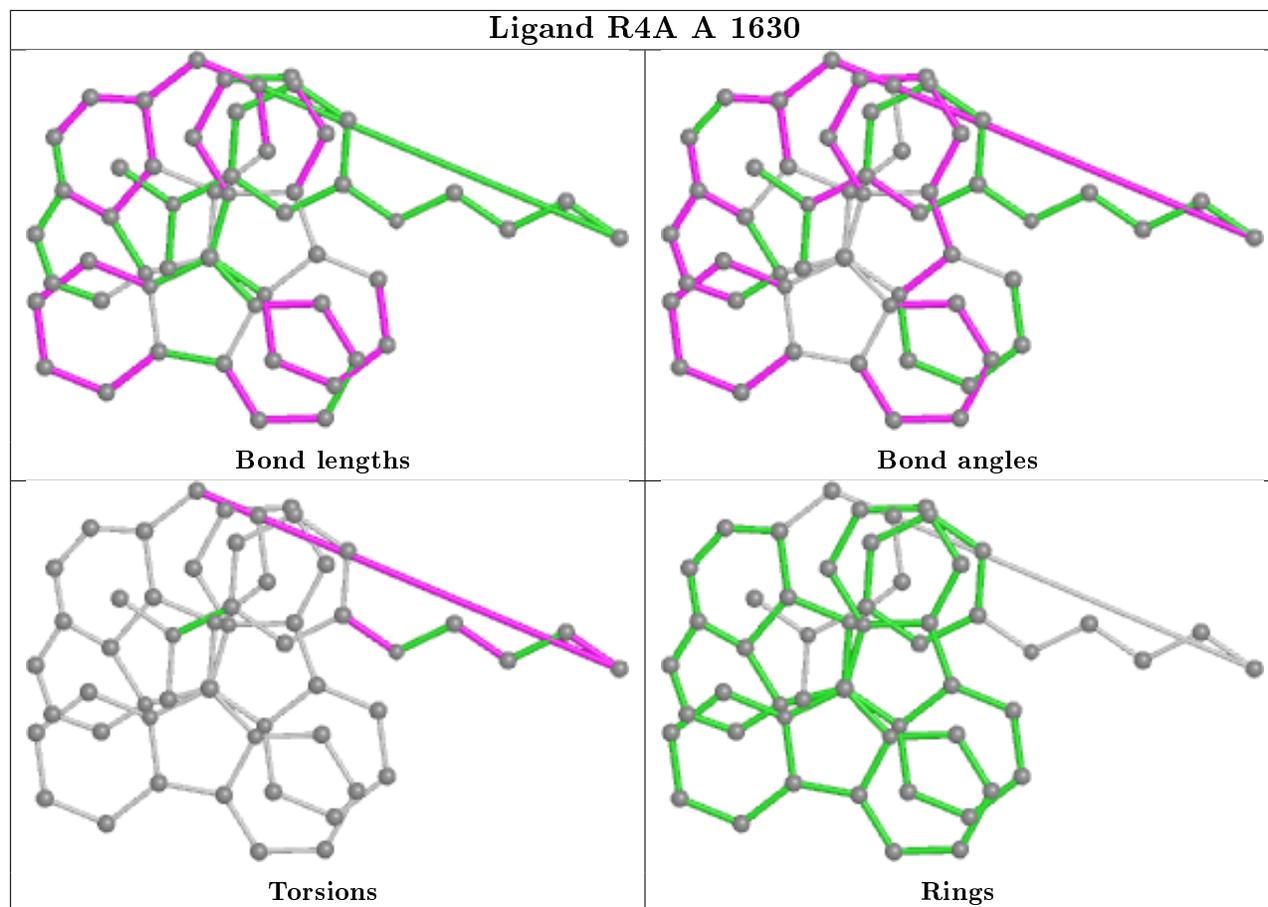
There are no ring outliers.

5 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	1633	SO4	1	0
4	B	1632	R4A	21	0
4	A	1630	R4A	8	0
5	B	1639	GOL	1	0
5	A	1634	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 than 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.





## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	618/646 (95%)	0.41	51 (8%) 11 12	18, 27, 40, 60	1 (0%)
1	B	618/646 (95%)	0.23	36 (5%) 23 26	16, 24, 35, 58	1 (0%)
All	All	1236/1292 (95%)	0.32	87 (7%) 16 19	16, 25, 38, 60	2 (0%)

The worst 5 of 87 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	52	GLY	11.9
1	A	53	SER	10.9
1	B	53	SER	10.5
1	A	51	ALA	9.3
1	A	9	ALA	8.8

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	TPQ	A	382	14/15	0.94	0.11	22,28,35,39	0
1	TPQ	B	382	14/15	0.94	0.12	19,26,33,38	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands

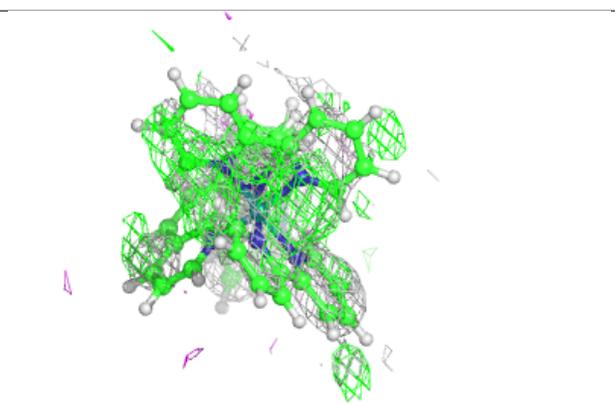
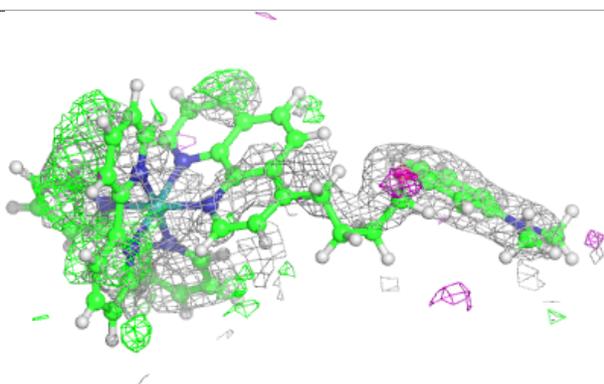
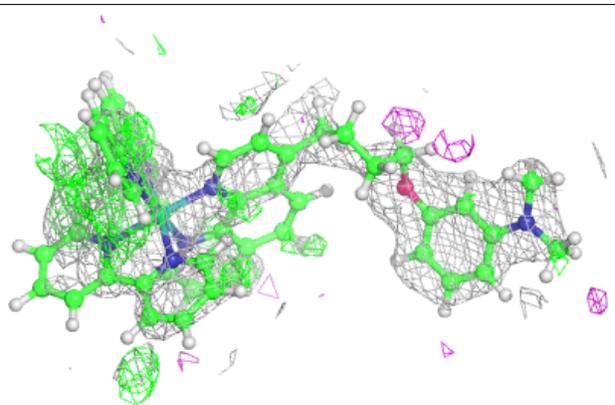
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	GOL	B	1638	6/6	0.65	0.21	53,54,55,56	0
5	GOL	B	1637	6/6	0.67	0.23	56,59,59,60	0
5	GOL	A	1631	6/6	0.71	0.13	43,49,51,52	0
5	GOL	B	1629	6/6	0.72	0.20	54,55,55,57	0
5	GOL	B	1635	6/6	0.73	0.14	42,46,47,49	0
5	GOL	A	1632	6/6	0.73	0.23	66,66,67,67	0
5	GOL	A	1633	6/6	0.73	0.20	59,60,61,61	0
5	GOL	B	1636	6/6	0.74	0.21	62,63,63,64	0
5	GOL	B	1634	6/6	0.78	0.16	33,33,34,35	0
5	GOL	A	1634	6/6	0.79	0.18	43,51,52,54	0
5	GOL	B	1639	6/6	0.79	0.20	46,51,52,54	0
4	R4A	A	1630	53/53	0.87	0.25	46,52,53,53	71
4	R4A	B	1632	53/53	0.90	0.21	37,41,43,43	71
6	SO4	B	1633	5/5	0.93	0.13	56,56,57,58	0
6	SO4	B	1628	5/5	0.96	0.09	50,50,53,54	0
3	NA	A	1629	1/1	0.98	0.25	34,34,34,34	0
3	NA	B	1631	1/1	0.99	0.17	30,30,30,30	0
2	CU	B	1630	1/1	0.99	0.14	30,30,30,30	0
2	CU	A	1628	1/1	1.00	0.16	32,32,32,32	0

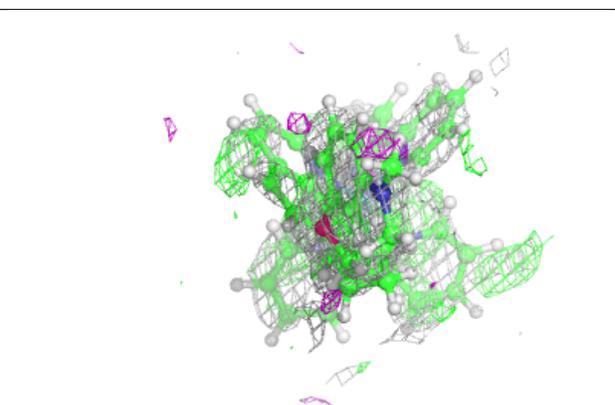
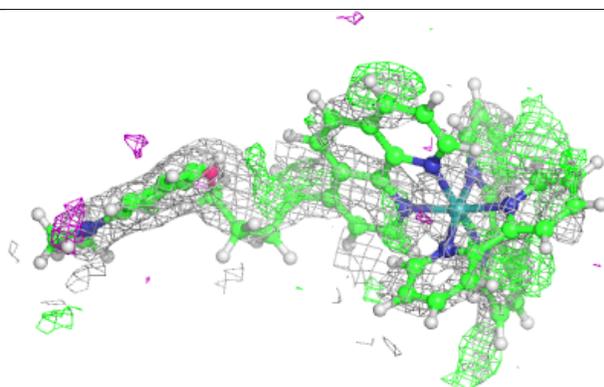
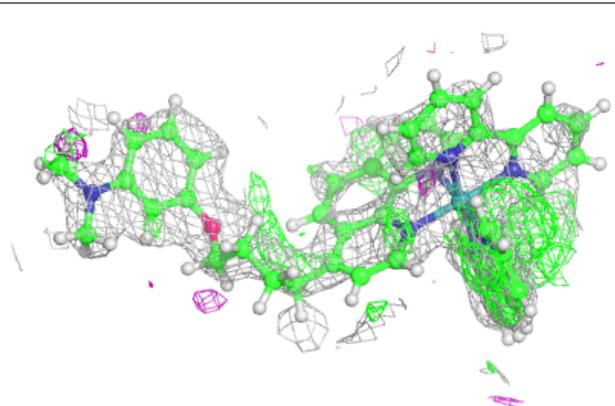
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around R4A A 1630:**

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

**Electron density around R4A B 1632:**

$2mF_o-DF_c$  (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.