



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:49 PM UTC

PDB ID : 2CFK / pdb\_00002cfk  
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](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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

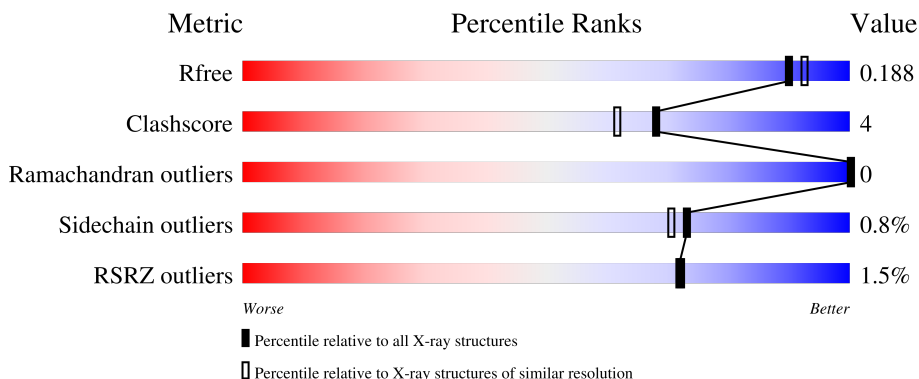
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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))
$R_{free}$	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (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  $\geq 3$ , 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	 91%

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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<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	R5A	A	1632[B]	X	-	-	-

## 2 Entry composition

There are 7 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

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	639	SER	-	expression tag	UNP P46881
A	640	ASN	-	expression tag	UNP P46881
A	641	TRP	-	expression tag	UNP P46881
A	642	SER	-	expression tag	UNP P46881
A	643	HIS	-	expression tag	UNP P46881
A	644	PRO	-	expression tag	UNP P46881
A	645	GLN	-	expression tag	UNP P46881
A	646	PHE	-	expression tag	UNP P46881
A	647	GLU	-	expression tag	UNP P46881
A	648	LYS	-	expression tag	UNP P46881

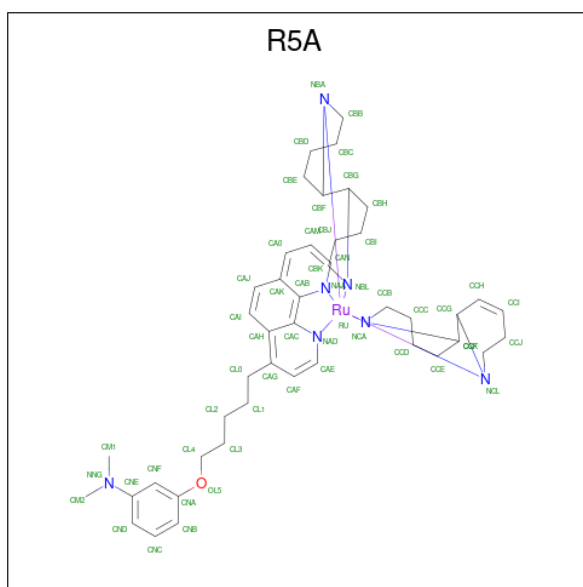
- Molecule 2 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

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

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

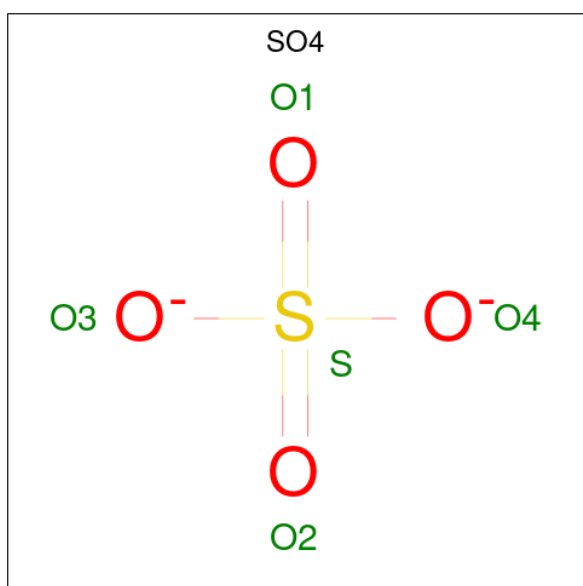
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		

- Molecule 4 is RUTHENIUM WIRE, 5 CARBON LINKER (CCD ID: R5A) (formula: C<sub>45</sub>H<sub>61</sub>N<sub>7</sub>ORu).



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

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



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

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

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula:  $C_3H_8O_3$ ).



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

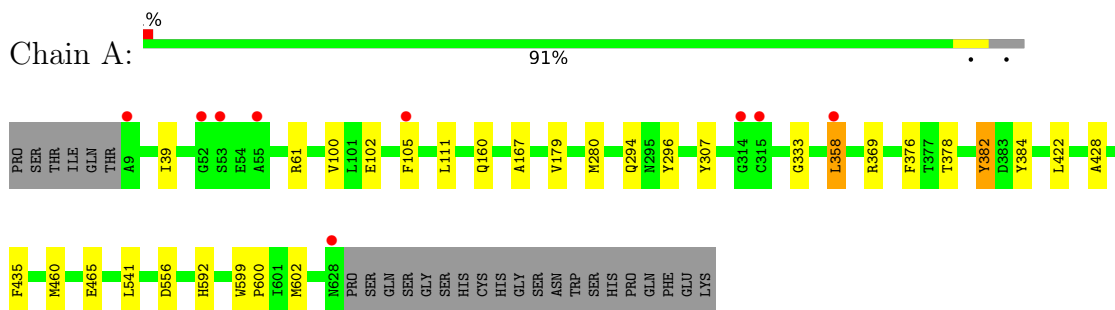
- Molecule 7 is water.

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

### 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



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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) 98.8 (15.02-1.80)	Depositor EDS
$R_{merge}$	0.03	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.70 (at 1.79Å)	Xtrriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.145 , 0.165 0.172 , 0.188	Depositor DCC
$R_{free}$ test set	3847 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	21.9	Xtrriage
Anisotropy	0.602	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.45 , 43.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	10117	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtrriage'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.*

<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: R5A, NA, CU, GOL, SO4, 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	0.60	0/5045	0.78	0/6869

There are no bond length outliers.

There are no bond angle outliers.

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	30	0
2	A	1	0	0	0	0
3	A	1	0	0	0	0
4	A	108	86	114	15	0
5	A	15	0	0	0	0
6	A	42	35	56	2	0
7	A	425	0	0	3	0
All	All	5489	4628	4882	36	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 4.

All (36) 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
6:A:1639:GOL:O3	7: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:1632[B]:R5A:HM12	2.08	0.54
1:A:382:TPQ:O5	4:A:1631[A]:R5A:HM12	2.08	0.54
6:A:1641:GOL:H32	7: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:280[B]:MET:HE1	1:A:384:TYR:CE2	2.45	0.50
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:61:ARG:HH22	1:A:556:ASP:CG	2.24	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
4:A:1632[B]:R5A:HNF	4:A:1632[B]:R5A: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
4:A:1632[B]:R5A:HM13	4:A:1632[B]:R5A:HND	1.78	0.43
1:A:358:LEU:HD23	7:A:2231:HOH:O	2.18	0.43
1:A:160:GLN:HG3	1:A:167:ALA:HB2	2.01	0.42
1:A:460:MET:HE3	1:A:465:GLU:O	2.19	0.42
1:A:111:LEU:HD12	1:A:179:VAL:HG11	2.02	0.42
1:A:602[A]:MET:HE2	1:A:602[A]:MET:HB2	1.83	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:280[A]:MET:HE1	1:A:384:TYR:CZ	2.54	0.41
1:A:296:TYR:CE2	4:A:1632[B]:R5A: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
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:105:PHE:HE2	1:A:307:TYR:HH	1.66	0.40
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%)	73 70

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
1	A	541	LEU

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	418	ASN
1	A	458	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](#)

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	1.35	2 (15%)	13,19,21	1.50	2 (15%)

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	O4-C4	-3.05	1.26	1.33
1	A	382	TPQ	C3-C4	2.47	1.40	1.36

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	382	TPQ	C6-C1-C2	3.68	121.28	118.66
1	A	382	TPQ	O5-C5-C4	2.47	123.33	119.43

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 oligosaccharides 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	GOL	A	1639	-	5,5,5	0.36	0	5,5,5	0.07	0
5	SO4	A	1633	-	4,4,4	0.22	0	6,6,6	0.21	0
5	SO4	A	1634	-	4,4,4	0.26	0	6,6,6	0.20	0
5	SO4	A	1642	-	4,4,4	0.22	0	6,6,6	0.30	0
6	GOL	A	1640	-	5,5,5	0.42	0	5,5,5	0.19	0
6	GOL	A	1641	-	5,5,5	0.24	0	5,5,5	0.50	0
4	R5A	A	1632[B]	-	46,64,64	2.80	16 (34%)	44,102,102	2.55	16 (36%)
6	GOL	A	1636	-	5,5,5	0.32	0	5,5,5	0.33	0
6	GOL	A	1637	-	5,5,5	0.36	0	5,5,5	0.17	0
6	GOL	A	1638	-	5,5,5	0.36	0	5,5,5	0.22	0
6	GOL	A	1635	-	5,5,5	0.38	0	5,5,5	0.31	0
4	R5A	A	1631[A]	-	46,64,64	2.80	16 (34%)	44,102,102	2.65	18 (40%)

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	1639	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	A	1640	-	-	2/4/4/4	-
6	GOL	A	1641	-	-	0/4/4/4	-
4	R5A	A	1632[B]	-	4/4/12/12	6/13/125/125	0/11/11/11
6	GOL	A	1636	-	-	0/4/4/4	-
6	GOL	A	1637	-	-	4/4/4/4	-
6	GOL	A	1638	-	-	2/4/4/4	-
6	GOL	A	1635	-	-	0/4/4/4	-
4	R5A	A	1631[A]	-	4/4/12/12	7/13/125/125	0/11/11/11

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1631[A]	R5A	CCD-CCE	-8.13	1.32	1.53
4	A	1631[A]	R5A	CBD-CBE	-8.09	1.32	1.53
4	A	1632[B]	R5A	CCD-CCE	-8.04	1.33	1.53
4	A	1632[B]	R5A	CBD-CBE	-7.99	1.33	1.53
4	A	1632[B]	R5A	CBH-CBG	-6.31	1.39	1.53
4	A	1631[A]	R5A	CBH-CBG	-6.28	1.39	1.53
4	A	1632[B]	R5A	CBI-CBH	-5.32	1.39	1.53
4	A	1631[A]	R5A	CBI-CBH	-5.30	1.39	1.53
4	A	1632[B]	R5A	CBB-CBC	-4.96	1.34	1.51
4	A	1631[A]	R5A	CBB-CBC	-4.94	1.34	1.51
4	A	1631[A]	R5A	CCB-CCC	-4.92	1.34	1.51
4	A	1632[B]	R5A	CCB-CCC	-4.92	1.34	1.51
4	A	1631[A]	R5A	CCK-CCJ	-4.29	1.40	1.51
4	A	1632[B]	R5A	CCK-CCJ	-4.26	1.40	1.51
4	A	1631[A]	R5A	CAB-CAC	3.90	1.46	1.39
4	A	1632[B]	R5A	CAB-CAC	3.74	1.45	1.39
4	A	1631[A]	R5A	CBK-CBJ	-3.30	1.39	1.51
4	A	1632[B]	R5A	CBK-CBJ	-3.26	1.40	1.51
4	A	1631[A]	R5A	CBI-CBJ	-3.20	1.40	1.51
4	A	1632[B]	R5A	CBI-CBJ	-3.18	1.40	1.51
4	A	1632[B]	R5A	CCH-CCI	3.07	1.39	1.32
4	A	1631[A]	R5A	CCH-CCI	3.06	1.39	1.32
4	A	1632[B]	R5A	CAN-CAM	2.87	1.41	1.35
4	A	1632[B]	R5A	CAE-CAF	2.55	1.41	1.35
4	A	1631[A]	R5A	CAN-CAM	2.46	1.40	1.35
4	A	1631[A]	R5A	CCJ-CCI	-2.44	1.39	1.48
4	A	1632[B]	R5A	CCJ-CCI	-2.38	1.40	1.48
4	A	1631[A]	R5A	CAE-CAF	2.35	1.40	1.35
4	A	1631[A]	R5A	CCE-CCF	-2.19	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1632[B]	R5A	CBE-CBF	-2.18	1.48	1.53
4	A	1632[B]	R5A	CCE-CCF	-2.17	1.48	1.53
4	A	1631[A]	R5A	CBE-CBF	-2.13	1.48	1.53

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1631[A]	R5A	CBC-CBB-NBA	6.07	122.48	112.97
4	A	1632[B]	R5A	CBC-CBB-NBA	5.93	122.27	112.97
4	A	1632[B]	R5A	CCC-CCB-NCA	5.81	122.08	112.97
4	A	1631[A]	R5A	CCC-CCB-NCA	5.59	121.73	112.97
4	A	1631[A]	R5A	CCF-CCG-NCL	5.18	113.92	107.55
4	A	1632[B]	R5A	CBK-CBJ-CBI	5.10	120.32	111.46
4	A	1631[A]	R5A	CBK-CBJ-CBI	5.07	120.26	111.46
4	A	1631[A]	R5A	CCB-CCC-CCD	4.96	120.07	111.46
4	A	1632[B]	R5A	CCB-CCC-CCD	4.81	119.81	111.46
4	A	1632[B]	R5A	CCF-CCG-NCL	4.65	113.27	107.55
4	A	1632[B]	R5A	CBB-CBC-CBD	4.59	119.42	111.46
4	A	1631[A]	R5A	CBB-CBC-CBD	4.52	119.30	111.46
4	A	1631[A]	R5A	CBJ-CBK-NBL	4.29	119.69	112.97
4	A	1631[A]	R5A	CBJ-CBI-CBH	4.22	120.10	111.42
4	A	1632[B]	R5A	CBJ-CBK-NBL	4.21	119.57	112.97
4	A	1632[B]	R5A	CBJ-CBI-CBH	4.19	120.03	111.42
4	A	1631[A]	R5A	CBI-CBH-CBG	3.95	118.62	111.25
4	A	1632[B]	R5A	CBI-CBH-CBG	3.87	118.46	111.25
4	A	1631[A]	R5A	CBD-CBE-CBF	3.81	118.36	111.25
4	A	1632[B]	R5A	CBD-CBE-CBF	3.56	117.90	111.25
4	A	1631[A]	R5A	CCD-CCE-CCF	3.56	117.89	111.25
4	A	1632[B]	R5A	CCD-CCE-CCF	3.48	117.75	111.25
4	A	1631[A]	R5A	CAC-CAH-CAI	-2.99	115.40	120.24
4	A	1632[B]	R5A	CBC-CBD-CBE	2.87	117.32	111.42
4	A	1631[A]	R5A	CBC-CBD-CBE	2.84	117.25	111.42
4	A	1632[B]	R5A	CCC-CCD-CCE	2.81	117.20	111.42
4	A	1631[A]	R5A	CCC-CCD-CCE	2.79	117.15	111.42
4	A	1631[A]	R5A	CCJ-CCK-NCL	2.30	119.87	111.94
4	A	1631[A]	R5A	CAH-CAC-NAD	-2.25	123.24	128.06
4	A	1632[B]	R5A	CCJ-CCK-NCL	2.23	119.64	111.94
4	A	1631[A]	R5A	CL4-OL5-CNA	2.18	123.59	117.93
4	A	1632[B]	R5A	CAH-CAC-NAD	-2.05	123.67	128.06
4	A	1632[B]	R5A	CCJ-CCI-CCH	-2.04	119.98	123.57
4	A	1631[A]	R5A	CCJ-CCI-CCH	-2.01	120.03	123.57

All (8) chirality outliers are listed below:

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

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1631[A]	R5A	CAH-CAG-CL0-CL1
4	A	1632[B]	R5A	CAH-CAG-CL0-CL1
6	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
6	A	1637	GOL	C1-C2-C3-O3
6	A	1638	GOL	O2-C2-C3-O3
4	A	1632[B]	R5A	CL2-CL3-CL4-OL5
4	A	1631[A]	R5A	CNB-CNA-OL5-CL4
4	A	1632[B]	R5A	CNB-CNA-OL5-CL4
4	A	1631[A]	R5A	CNF-CNA-OL5-CL4
4	A	1632[B]	R5A	CNF-CNA-OL5-CL4
4	A	1632[B]	R5A	CL3-CL4-OL5-CNA
6	A	1637	GOL	O2-C2-C3-O3
4	A	1631[A]	R5A	CAF-CAG-CL0-CL1
4	A	1632[B]	R5A	CAF-CAG-CL0-CL1
6	A	1637	GOL	O1-C1-C2-C3
6	A	1640	GOL	C1-C2-C3-O3
6	A	1640	GOL	O2-C2-C3-O3
4	A	1631[A]	R5A	CL3-CL4-OL5-CNA
6	A	1637	GOL	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 17 short contacts:

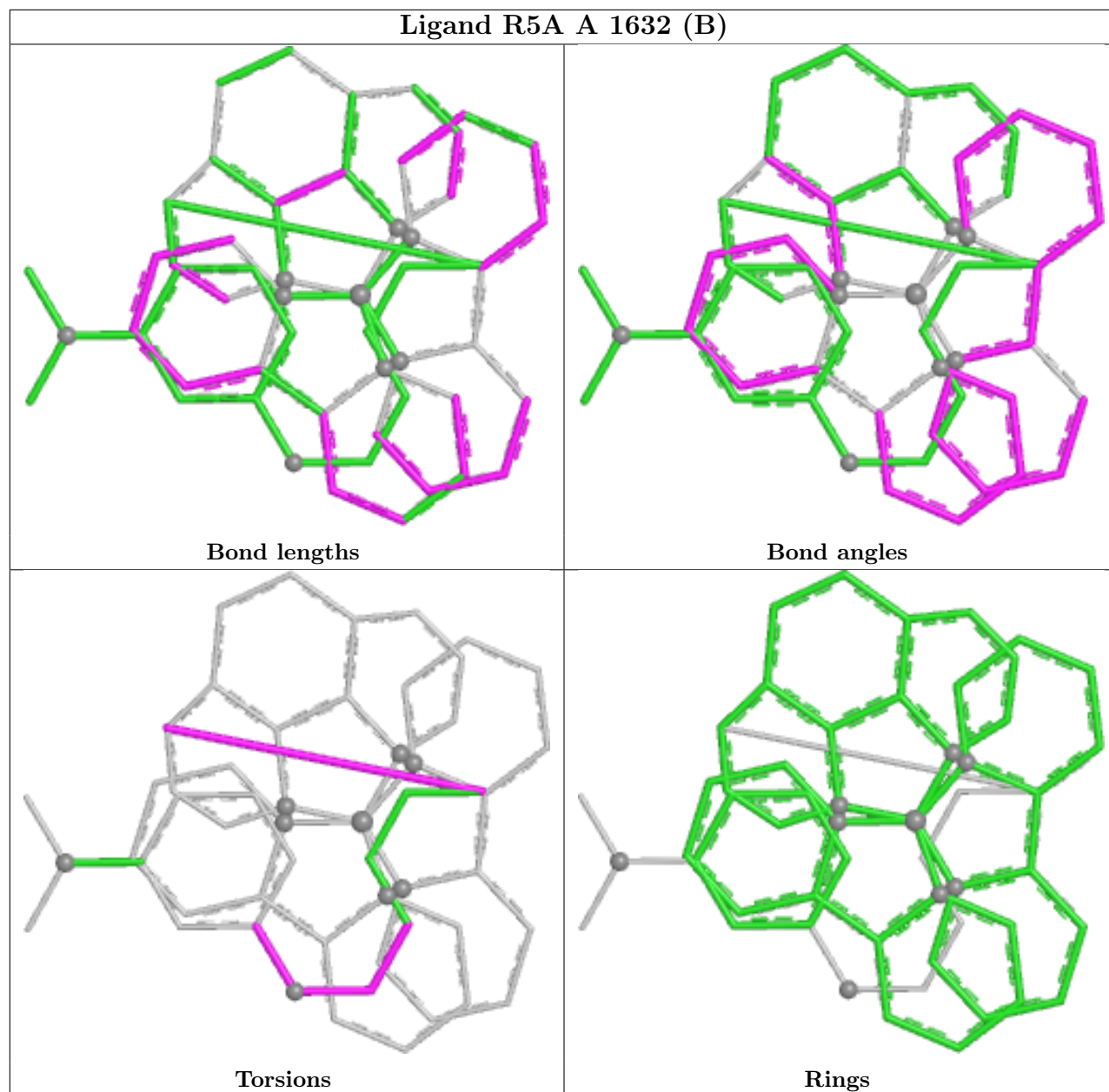
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1639	GOL	1	0
6	A	1641	GOL	1	0
4	A	1632[B]	R5A	4	0

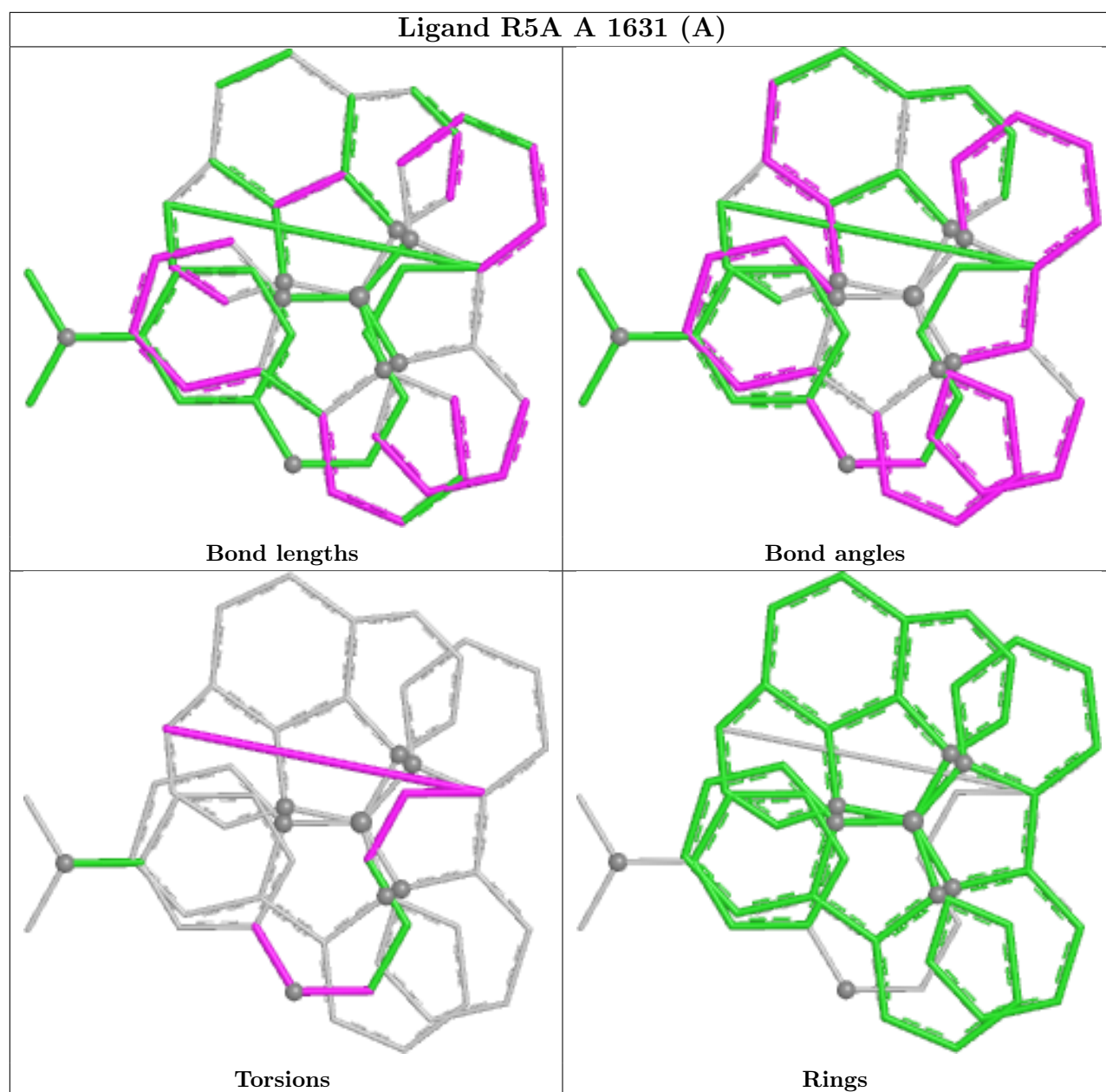
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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Clashes</b>	<b>Symm-Clashes</b>
4	A	1631[A]	R5A	11	0

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	619/646 (95%)	-0.48	9 (1%) 72 72	9, 18, 34, 70	9 (1%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	105	PHE	3.9
1	A	358	LEU	3.9
1	A	628	ASN	3.5
1	A	52	GLY	3.4
1	A	53	SER	3.1
1	A	314	GLY	2.9
1	A	315	CYS	2.8
1	A	9	ALA	2.7
1	A	55	ALA	2.1

### 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	0.09	14,24,44,54	0

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands

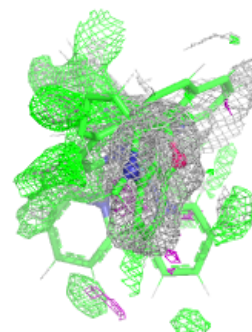
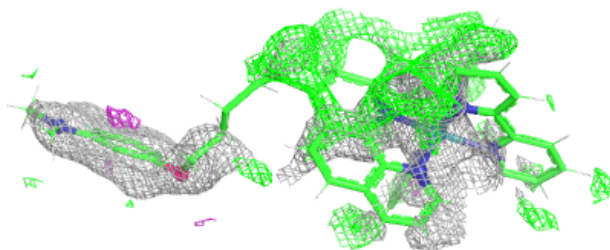
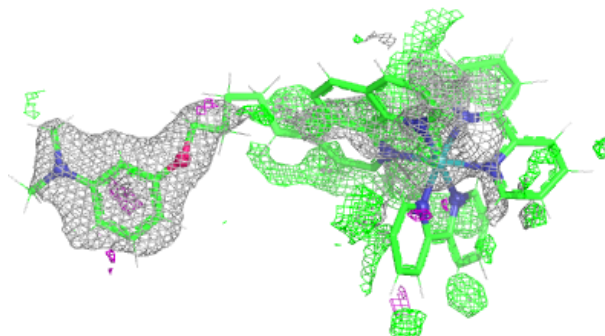
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<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
4	R5A	A	1631[A]	54/54	0.67	0.37	36,47,54,54	97
5	SO4	A	1633	5/5	0.68	0.17	89,95,96,99	0
5	SO4	A	1634	5/5	0.68	0.17	67,75,81,83	0
6	GOL	A	1640	6/6	0.70	0.22	54,58,61,65	0
6	GOL	A	1637	6/6	0.73	0.21	68,73,76,77	0
4	R5A	A	1632[B]	54/54	0.75	0.29	36,46,50,54	97
6	GOL	A	1636	6/6	0.79	0.16	38,45,48,54	0
6	GOL	A	1641	6/6	0.81	0.16	34,49,53,59	0
6	GOL	A	1638	6/6	0.85	0.13	40,55,58,59	0
6	GOL	A	1639	6/6	0.86	0.14	37,59,67,67	0
5	SO4	A	1642	5/5	0.88	0.12	56,58,60,64	0
6	GOL	A	1635	6/6	0.89	0.11	27,31,34,36	0
3	NA	A	1630	1/1	0.99	0.14	26,26,26,26	0
2	CU	A	1629	1/1	1.00	0.10	28,28,28,28	0

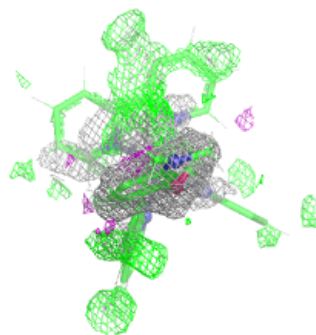
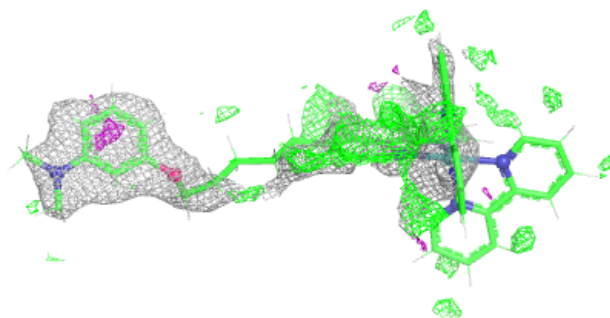
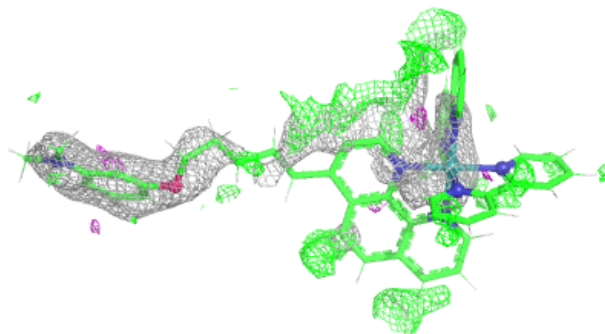
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation 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 R5A 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.