Full wwPDB X-ray Structure Validation Report (i)

Aug 22, 2026 – 03:14 am BST

PDB ID	:	2CFG / pdb_00002cfg
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 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:

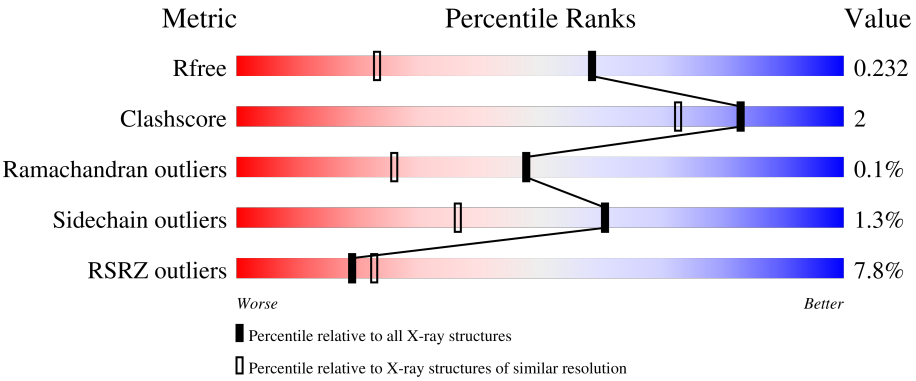
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 1.55 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}	180053	2145 (1.56-1.56)
Clashscore	190562	2189 (1.56-1.56)
Ramachandran outliers	187476	2153 (1.56-1.56)
Sidechain outliers	187428	2150 (1.56-1.56)
RSRZ outliers	180081	2146 (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 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	11% 91%
1	B	646	4% 91% 5%

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
1	A	619	Total	C	H	N	O	S	0	4	0
			9355	3080	4480	853	931	11			
1	B	619	Total	C	H	N	O	S	0	5	0
			9362	3082	4485	853	931	11			

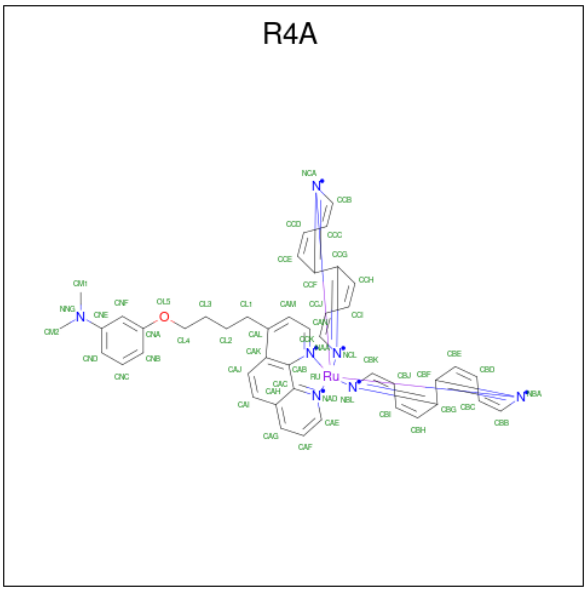
- Molecule 2 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

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

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

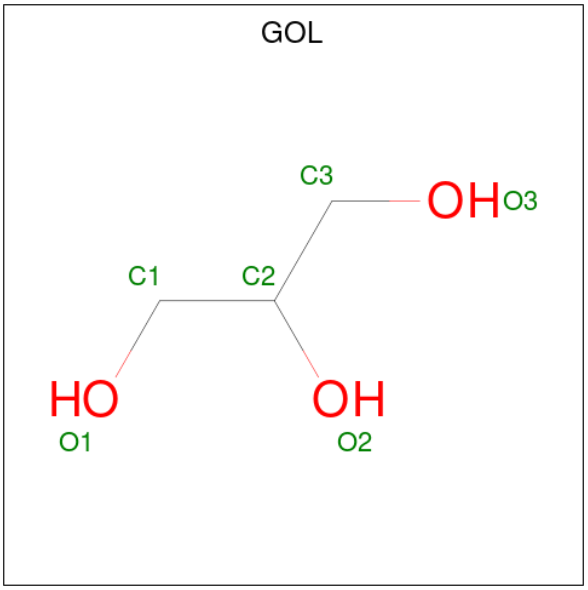
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		
3	B	1	Total	Na	0	0
			1	1		

- Molecule 4 is (OC-6-3'3-C)-bis(2,2'-bipyridine-kappa 2 N 1 ,N 1'){N,N-dimethyl-3-[4-(1,10-phenanthrolin-4-yl-kappa 2 N 1 ,N 10)butoxy]aniline}ruthenium (CCD ID: R4A) (formula: $C_{44}H_{41}N_7ORu$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	H	N	O	Ru	0	0
			94	44	41	7	1	1		
4	B	1	Total	C	H	N	O	Ru	0	0
			94	44	41	7	1	1		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



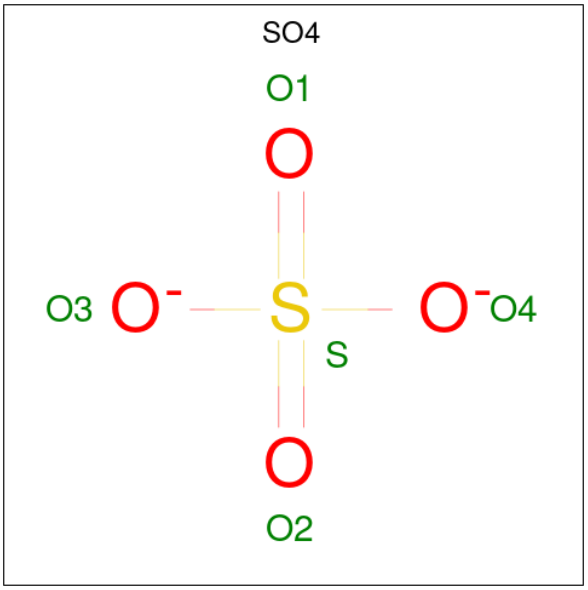
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			11	3	5	3		
5	A	1	Total	C	H	O	0	0
			11	3	5	3		

Continued on next page...

Continued from previous page...

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		
5	B	1	Total	C	H	O	0	0
			11	3	5	3		

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



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.

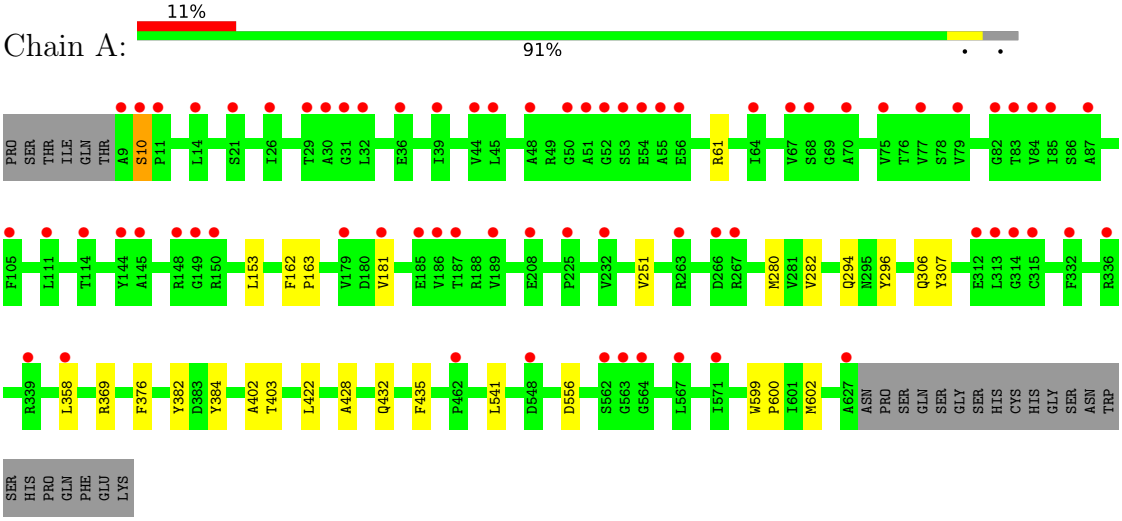
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	365	Total O 365 365	0	0
7	B	438	Total O 438 438	0	0

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.

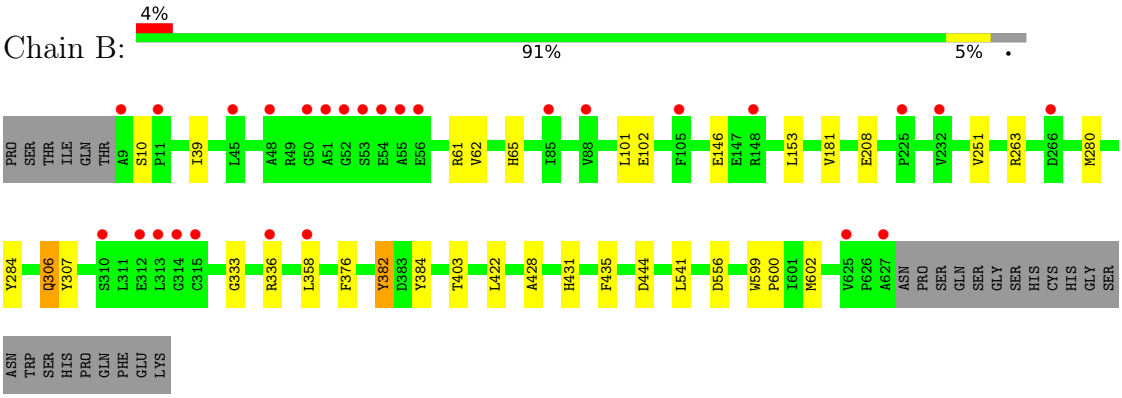
• Molecule 1: PHENYLETHYLAMINE OXIDASE

Chain A:



• Molecule 1: PHENYLETHYLAMINE OXIDASE

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	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) 92.6 (30.01-1.55)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.48 (at 1.55Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.203 , 0.224 0.215 , 0.232	Depositor DCC
R_{free} test set	11299 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	25.8	Xtriage
Anisotropy	0.385	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.43 , 37.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	19843	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage'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.*

[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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: R4A, NA, CU, TPQ, GOL, SO4

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	0.61	0/4998	0.80	0/6804
1	B	0.68	0/5006	0.83	0/6815
All	All	0.65	0/10004	0.81	0/13619

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

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	23	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	53	41	53	6	0
4	B	53	41	56	7	0
5	A	24	20	32	1	0
5	B	42	35	56	1	0
6	B	10	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	365	0	0	1	0
7	B	438	0	0	2	0
All	All	10741	9102	9582	47	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 2.

All (47) 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:307:TYR:CE1	4:A:1630:R4A:HAM	2.12	0.85
1:B:307:TYR:CE1	4:B:1632:R4A:HAM	2.27	0.70
1:B:599:TRP:CD2	1:B:600:PRO:HA	2.34	0.63
1:A:251:VAL:HG22	1:A:306:GLN:HB3	1.83	0.61
1:B:102:GLU:HB3	4:B:1632:R4A:HBI1	1.82	0.61
1:A:599:TRP:CD2	1:A:600:PRO:HA	2.37	0.59
1:B:61:ARG:NH2	1:B:556:ASP:OD2	2.38	0.56
1:A:307:TYR:CE1	4:A:1630:R4A:CAM	2.87	0.55
1:A:280[B]:MET:HE1	1:A:384:TYR:CE2	2.42	0.55
1:B:251:VAL:HG22	1:B:306:GLN:HB3	1.90	0.54
1:B:280[B]:MET:HG3	1:B:435:PHE:CE2	2.43	0.54
5:A:1634:GOL:H11	7:A:2205:HOH:O	2.08	0.52
1:A:422:LEU:HD11	1:A:428:ALA:HB2	1.93	0.51
1:A:307:TYR:CZ	4:A:1630:R4A:HAM	2.45	0.50
1:A:358:LEU:HD12	4:B:1632:R4A:CAI	2.41	0.50
1:B:307:TYR:CE1	4:B:1632:R4A:CAM	2.95	0.50
1:B:422:LEU:HD11	1:B:428:ALA:HB2	1.94	0.49
1:A:61:ARG:HH22	1:A:556:ASP:CG	2.22	0.48
1:B:307:TYR:CZ	4:B:1632:R4A:HAM	2.48	0.47
1:B:382:TPQ:O5	4:B:1632:R4A:HM21	2.14	0.47
4:A:1630:R4A:HNF	4:A:1630:R4A:HM23	1.62	0.47
4:B:1632:R4A:HM23	4:B:1632:R4A:HNF	1.61	0.47
1:B:280[B]:MET:HE1	1:B:384:TYR:CE2	2.50	0.46
1:B:251:VAL:CG2	1:B:306:GLN:HB3	2.46	0.46
1:B:39[B]:ILE:HD12	1:B:333:GLY:HA2	1.98	0.46
1:B:61:ARG:HH22	1:B:556:ASP:CG	2.24	0.45
1:B:39[B]:ILE:HD12	1:B:333:GLY:CA	2.46	0.45
1:B:280[B]:MET:HG3	1:B:435:PHE:CD2	2.52	0.45
1:A:403:THR:HA	1:A:602[A]:MET:HG3	1.99	0.45
1:B:403:THR:HA	1:B:602[A]:MET:HG3	1.99	0.45
1:B:403:THR:HA	1:B:602[A]:MET:CG	2.47	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:PHE:HB2	1:A:163:PRO:CD	2.47	0.44
5:B:1639:GOL:H32	7:B:2260:HOH:O	2.16	0.44
1:A:307:TYR:CD1	4:A:1630:R4A:HAM	2.52	0.44
1:B:39[A]:ILE:HD12	1:B:62:VAL:CG1	2.49	0.43
1:A:153:LEU:HD12	1:A:181:VAL:HG11	2.00	0.43
6:B:1633:SO4:O2	7:B:2428:HOH:O	2.19	0.43
1:A:280[B]:MET:HG3	1:A:435:PHE:CD2	2.54	0.42
4:A:1630:R4A:CAI	1:B:358:LEU:HD12	2.49	0.42
1:B:284:TYR:CD2	1:B:431:HIS:HB3	2.54	0.42
1:A:280[B]:MET:HG3	1:A:435:PHE:CE2	2.54	0.42
1:A:282:VAL:HA	1:A:432:GLN:O	2.20	0.42
1:A:402:ALA:O	1:A:602[A]:MET:HE2	2.19	0.41
1:A:403:THR:HA	1:A:602[A]:MET:CG	2.49	0.41
1:A:294:GLN:HB2	1:A:296:TYR:CZ	2.55	0.41
1:B:153:LEU:HD12	1:B:181:VAL:HG11	2.02	0.40
1:B:65:HIS:CD2	1:B:101:LEU:HD11	2.56	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	620/646 (96%)	598 (96%)	21 (3%)	1 (0%)	43 24
1	B	621/646 (96%)	597 (96%)	24 (4%)	0	100 100
All	All	1241/1292 (96%)	1195 (96%)	45 (4%)	1 (0%)	48 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%)	73 56
1	B	517/537 (96%)	508 (98%)	9 (2%)	53 25
All	All	1033/1074 (96%)	1020 (99%)	13 (1%)	61 36

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	SER
1	A	369	ARG
1	A	376	PHE
1	A	541	LEU
1	B	10	SER
1	B	146	GLU
1	B	208	GLU
1	B	263	ARG
1	B	306	GLN
1	B	336	ARG
1	B	376	PHE
1	B	444	ASP
1	B	541	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	418	ASN
1	A	458	GLN
1	A	561	HIS
1	B	418	ASN
1	B	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)

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(^{o})	Ideal(^{o})
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 oligosaccharides 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	1632	-	5,5,5	0.32	0	5,5,5	0.34	0
5	GOL	B	1634	-	5,5,5	0.24	0	5,5,5	0.40	0
5	GOL	B	1636	-	5,5,5	0.29	0	5,5,5	0.50	0
5	GOL	B	1637	-	5,5,5	0.33	0	5,5,5	0.31	0
5	GOL	B	1635	-	5,5,5	0.36	0	5,5,5	0.22	0
4	R4A	A	1630	1	54,63,63	1.74	13 (24%)	47,101,101	1.79	9 (19%)
4	R4A	B	1632	-	54,63,63	1.76	14 (25%)	47,101,101	1.79	9 (19%)
5	GOL	B	1629	-	5,5,5	0.32	0	5,5,5	0.17	0
5	GOL	B	1639	-	5,5,5	0.25	0	5,5,5	0.68	0
6	SO4	B	1628	-	4,4,4	0.10	0	6,6,6	0.58	0
5	GOL	A	1634	-	5,5,5	0.30	0	5,5,5	0.82	0
6	SO4	B	1633	-	4,4,4	0.12	0	6,6,6	0.49	0
5	GOL	A	1633	-	5,5,5	0.37	0	5,5,5	0.26	0
5	GOL	B	1638	-	5,5,5	0.35	0	5,5,5	0.17	0
5	GOL	A	1631	-	5,5,5	0.39	0	5,5,5	0.25	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	1632	-	-	0/4/4/4	-
5	GOL	B	1634	-	-	0/4/4/4	-
5	GOL	B	1636	-	-	0/4/4/4	-
5	GOL	B	1637	-	-	2/4/4/4	-
5	GOL	B	1635	-	-	0/4/4/4	-
4	R4A	A	1630	1	-	5/12/124/124	0/11/11/11
4	R4A	B	1632	-	-	5/12/124/124	0/11/11/11
5	GOL	B	1629	-	-	2/4/4/4	-
5	GOL	B	1639	-	-	2/4/4/4	-
5	GOL	A	1634	-	-	2/4/4/4	-
5	GOL	A	1633	-	-	2/4/4/4	-
5	GOL	B	1638	-	-	2/4/4/4	-
5	GOL	A	1631	-	-	0/4/4/4	-

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1632	R4A	CAK-CAB	6.75	1.46	1.39
4	A	1630	R4A	CAK-CAB	6.40	1.46	1.39
4	A	1630	R4A	CBG-NBL	4.09	1.40	1.33
4	B	1632	R4A	CBG-NBL	4.05	1.40	1.33
4	A	1630	R4A	CCG-NCL	3.80	1.40	1.33
4	B	1632	R4A	CCG-NCL	3.80	1.40	1.33
4	A	1630	R4A	CBF-NBA	-3.11	1.28	1.33
4	B	1632	R4A	CCF-NCA	-3.07	1.28	1.33
4	A	1630	R4A	CCF-NCA	-2.96	1.28	1.33
4	B	1632	R4A	CBF-NBA	-2.91	1.28	1.33
4	A	1630	R4A	CBE-CBF	2.67	1.48	1.42
4	B	1632	R4A	CBE-CBF	2.61	1.48	1.42
4	A	1630	R4A	CBF-CBG	2.51	1.50	1.45
4	A	1630	R4A	CCE-CCF	2.49	1.48	1.42
4	B	1632	R4A	CAN-NAA	2.47	1.33	1.29
4	B	1632	R4A	CCF-CCG	2.39	1.50	1.45
4	A	1630	R4A	CAN-NAA	2.36	1.33	1.29
4	B	1632	R4A	CCE-CCF	2.34	1.47	1.42
4	A	1630	R4A	CCF-CCG	2.33	1.50	1.45
4	B	1632	R4A	CCC-CCD	2.31	1.46	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1632	R4A	CBF-CBG	2.30	1.50	1.45
4	A	1630	R4A	CCC-CCD	2.25	1.46	1.40
4	A	1630	R4A	CAE-CAF	2.16	1.41	1.36
4	B	1632	R4A	CAE-CAF	2.13	1.41	1.36
4	B	1632	R4A	CBC-CBD	2.11	1.46	1.40
4	A	1630	R4A	CBC-CBD	2.10	1.46	1.40
4	B	1632	R4A	CBD-CBE	-2.04	1.32	1.37

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	1632	R4A	CCE-CCF-NCA	-4.85	119.53	124.86
4	A	1630	R4A	CCH-CCG-NCL	-4.56	119.84	124.86
4	B	1632	R4A	CCH-CCG-NCL	-4.54	119.87	124.86
4	A	1630	R4A	CCE-CCF-NCA	-4.51	119.89	124.86
4	A	1630	R4A	CBH-CBG-NBL	-4.30	120.13	124.86
4	B	1632	R4A	CBH-CBG-NBL	-4.28	120.15	124.86
4	A	1630	R4A	CL1-CAL-CAK	4.25	123.55	118.62
4	A	1630	R4A	CBE-CBF-NBA	-4.17	120.28	124.86
4	B	1632	R4A	CL1-CAL-CAK	4.10	123.39	118.62
4	B	1632	R4A	CBE-CBF-NBA	-3.77	120.71	124.86
4	B	1632	R4A	CNF-CNE-NNG	-3.72	117.03	121.33
4	A	1630	R4A	CNF-CNE-NNG	-3.34	117.47	121.33
4	A	1630	R4A	CBC-CBD-CBE	-3.02	117.01	121.23
4	B	1632	R4A	CBC-CBD-CBE	-2.92	117.15	121.23
4	A	1630	R4A	CAJ-CAK-CAL	2.58	128.63	123.78
4	A	1630	R4A	CCC-CCD-CCE	-2.50	117.74	121.23
4	B	1632	R4A	CAJ-CAK-CAL	2.47	128.41	123.78
4	B	1632	R4A	CCC-CCD-CCE	-2.40	117.87	121.23

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1630	R4A	CAK-CAL-CL1-CL2
4	B	1632	R4A	CAK-CAL-CL1-CL2
5	A	1633	GOL	C1-C2-C3-O3
5	A	1633	GOL	O2-C2-C3-O3
5	A	1634	GOL	C1-C2-C3-O3
5	B	1629	GOL	O1-C1-C2-C3
5	B	1637	GOL	C1-C2-C3-O3
5	B	1637	GOL	O2-C2-C3-O3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	B	1638	GOL	O1-C1-C2-C3
5	B	1639	GOL	O1-C1-C2-C3
5	B	1629	GOL	O1-C1-C2-O2
5	B	1639	GOL	O1-C1-C2-O2
4	A	1630	R4A	CL2-CL3-CL4-OL5
4	B	1632	R4A	CL2-CL3-CL4-OL5
4	A	1630	R4A	CAL-CL1-CL2-CL3
4	B	1632	R4A	CAL-CL1-CL2-CL3
5	A	1634	GOL	O2-C2-C3-O3
5	B	1638	GOL	O1-C1-C2-O2
4	B	1632	R4A	CNB-CNA-OL5-CL4
4	B	1632	R4A	CNF-CNA-OL5-CL4
4	A	1630	R4A	CNB-CNA-OL5-CL4
4	A	1630	R4A	CNF-CNA-OL5-CL4

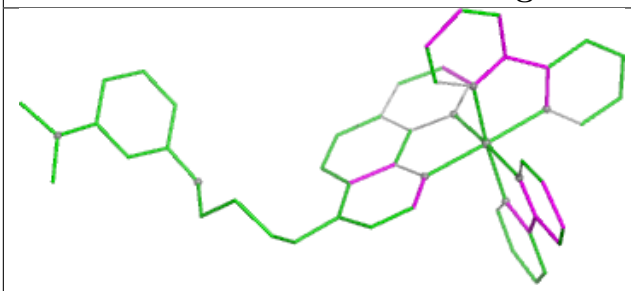
There are no ring outliers.

5 monomers are involved in 16 short contacts:

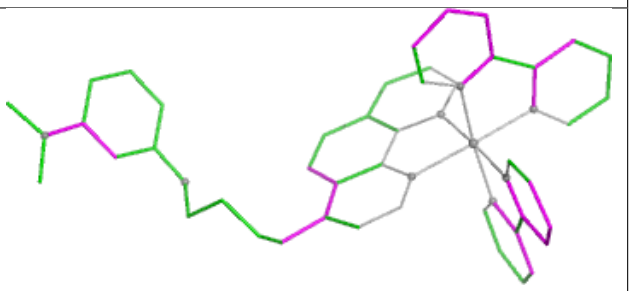
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1630	R4A	6	0
4	B	1632	R4A	7	0
5	B	1639	GOL	1	0
5	A	1634	GOL	1	0
6	B	1633	SO4	1	0

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 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.

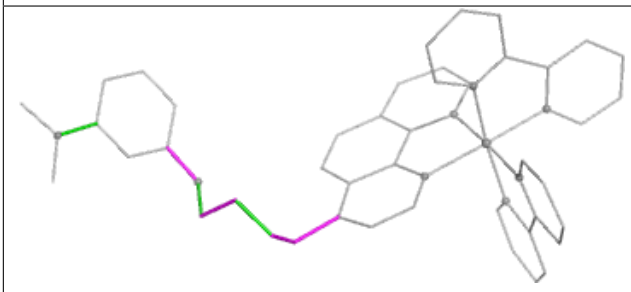
Ligand R4A A 1630



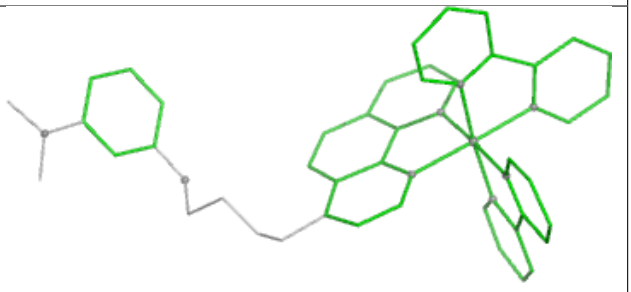
Bond lengths



Bond angles

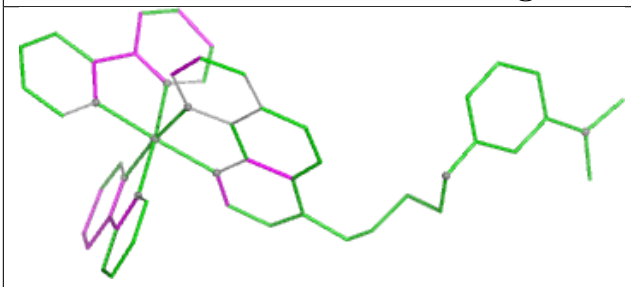


Torsions

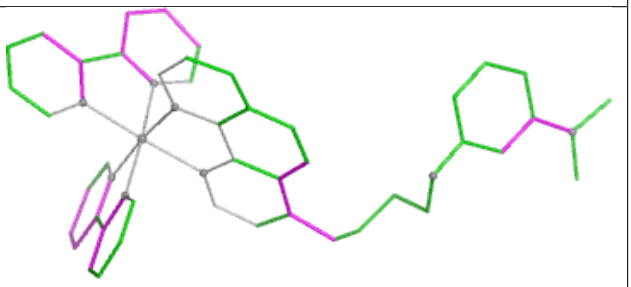


Rings

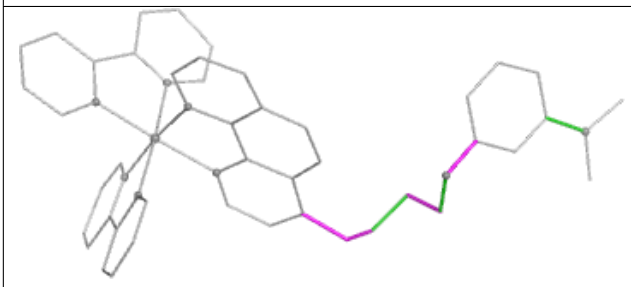
Ligand R4A B 1632



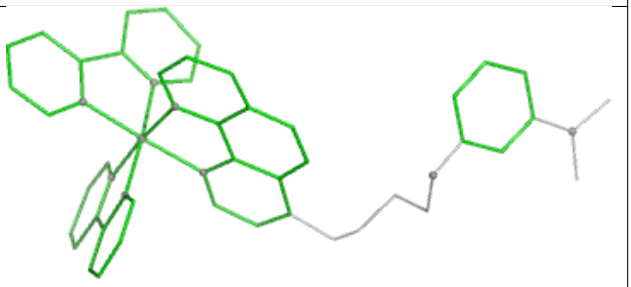
Bond lengths



Bond angles



Torsions



Rings

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

6.1 Protein, DNA and RNA chains

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^{th} 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	618/646 (95%)	0.77	70 (11%)	10	12	15, 27, 39, 59	5 (0%)
1	B	618/646 (95%)	0.43	27 (4%)	39	47	14, 24, 34, 58	6 (0%)
All	All	1236/1292 (95%)	0.60	97 (7%)	19	23	14, 25, 38, 59	11 (0%)

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	9	ALA	8.3
1	B	9	ALA	7.8
1	B	105	PHE	6.7
1	A	105	PHE	5.9
1	B	52	GLY	5.3
1	B	51	ALA	4.8
1	A	266	ASP	4.7
1	B	55	ALA	4.6
1	A	67	VAL	4.2
1	A	55	ALA	4.2
1	A	53	SER	4.1
1	B	53	SER	4.1
1	A	564	GLY	4.0
1	A	51	ALA	3.9
1	B	315	CYS	3.6
1	A	52	GLY	3.6
1	A	179	VAL	3.5
1	B	314	GLY	3.3
1	A	48	ALA	3.3
1	B	266	ASP	3.2
1	A	314	GLY	3.2
1	A	563	GLY	3.2
1	A	313	LEU	3.2
1	A	315	CYS	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	232	VAL	3.2
1	A	85	ILE	3.1
1	B	358	LEU	3.1
1	B	48	ALA	3.1
1	A	56	GLU	3.0
1	A	84	VAL	3.0
1	A	54	GLU	3.0
1	A	44	VAL	3.0
1	A	145	ALA	2.9
1	A	562	SER	2.8
1	A	571	ILE	2.8
1	B	85	ILE	2.8
1	A	79	VAL	2.8
1	A	70	ALA	2.8
1	A	627	ALA	2.8
1	B	225	PRO	2.8
1	A	144	TYR	2.7
1	A	225	PRO	2.7
1	A	336	ARG	2.7
1	A	185	GLU	2.7
1	B	313	LEU	2.6
1	A	187	THR	2.6
1	B	336	ARG	2.6
1	A	11	PRO	2.6
1	B	54	GLU	2.6
1	A	39	ILE	2.6
1	B	627	ALA	2.6
1	B	148	ARG	2.6
1	A	87	ALA	2.5
1	A	75	VAL	2.5
1	A	181	VAL	2.5
1	A	31	GLY	2.5
1	A	14	LEU	2.5
1	A	548	ASP	2.5
1	A	82	GLY	2.4
1	A	312	GLU	2.4
1	B	312	GLU	2.4
1	A	332	PHE	2.4
1	A	26	ILE	2.4
1	A	148	ARG	2.3
1	A	30	ALA	2.3
1	A	111	LEU	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	263	ARG	2.3
1	A	10	SER	2.3
1	A	462	PRO	2.3
1	B	88	VAL	2.3
1	A	29	THR	2.3
1	A	358	LEU	2.3
1	A	567	LEU	2.3
1	A	114	THR	2.2
1	A	149	GLY	2.2
1	A	267	ARG	2.2
1	A	186	VAL	2.2
1	A	32	LEU	2.2
1	A	45	LEU	2.2
1	A	64	ILE	2.2
1	B	56	GLU	2.2
1	B	50	GLY	2.2
1	A	232	VAL	2.2
1	A	50	GLY	2.1
1	A	68	SER	2.1
1	A	150	ARG	2.1
1	B	11	PRO	2.1
1	A	83	THR	2.1
1	B	45	LEU	2.1
1	A	36	GLU	2.1
1	A	208	GLU	2.1
1	A	77	VAL	2.0
1	A	189	VAL	2.0
1	A	339	ARG	2.0
1	B	625	VAL	2.0
1	A	21	SER	2.0
1	B	310	SER	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, 95^{th} 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	22,28,35,39	0
1	TPQ	B	382	14/15	0.94	0.09	19,26,33,38	0

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

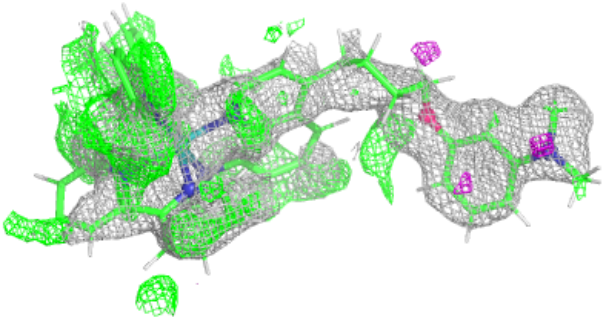
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

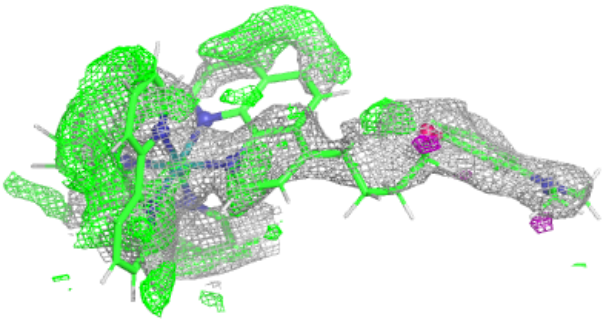
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	R4A	A	1630	53/53	0.80	0.36	46,52,53,53	71
5	GOL	B	1637	6/6	0.81	0.20	56,59,59,60	0
5	GOL	B	1636	6/6	0.82	0.23	62,63,63,64	0
5	GOL	A	1632	6/6	0.83	0.23	66,66,67,67	0
5	GOL	A	1633	6/6	0.84	0.21	59,60,61,61	0
5	GOL	A	1634	6/6	0.84	0.18	43,51,52,54	0
4	R4A	B	1632	53/53	0.85	0.31	37,41,43,43	71
6	SO4	B	1633	5/5	0.85	0.19	56,56,57,58	0
5	GOL	B	1638	6/6	0.86	0.22	53,54,55,56	0
5	GOL	B	1639	6/6	0.86	0.18	46,51,52,54	0
6	SO4	B	1628	5/5	0.86	0.17	50,50,53,54	0
5	GOL	B	1629	6/6	0.86	0.22	54,55,55,57	0
5	GOL	B	1635	6/6	0.90	0.15	42,46,47,49	0
5	GOL	A	1631	6/6	0.91	0.14	43,49,51,52	0
5	GOL	B	1634	6/6	0.93	0.11	33,33,34,35	0
3	NA	B	1631	1/1	0.98	0.11	30,30,30,30	0
2	CU	B	1630	1/1	0.99	0.11	30,30,30,30	0
3	NA	A	1629	1/1	0.99	0.14	34,34,34,34	0
2	CU	A	1628	1/1	0.99	0.14	32,32,32,32	0

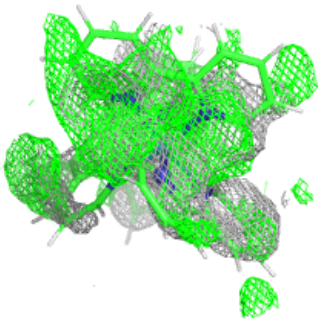
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

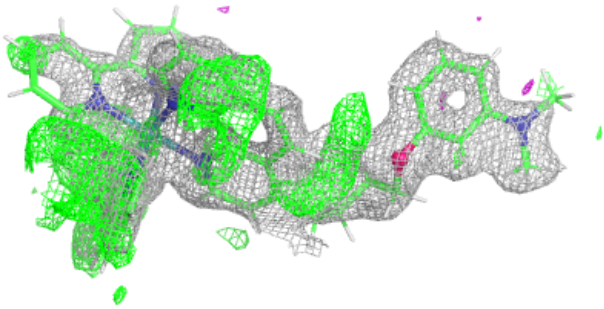


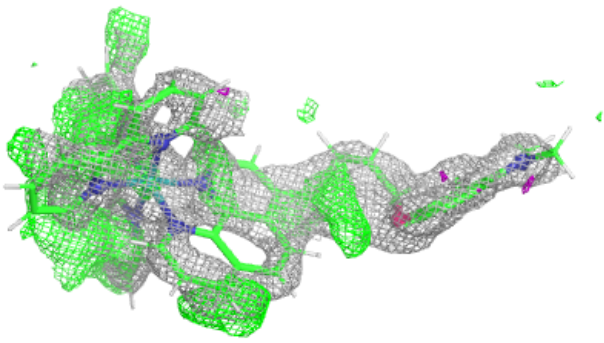


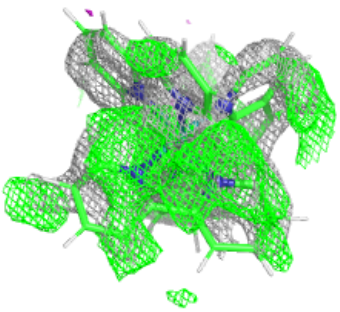


Electron density around R4A B 1632:

$2mF_o$-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.