



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 2, 2025 – 04:28 am BST

PDB ID : 2CFD / pdb_00002cfd
Title : AGAO in complex with wc4l3 (Ru-wire inhibitor, 4-carbon linker, lambda 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 : 2006-02-20
Resolution : 1.60 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

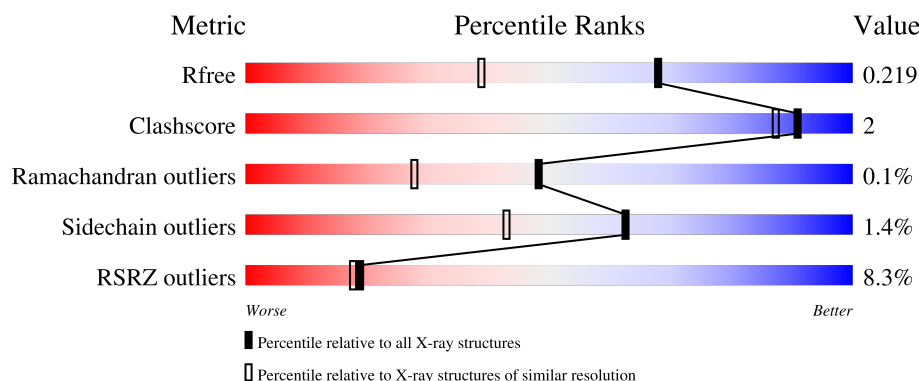
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

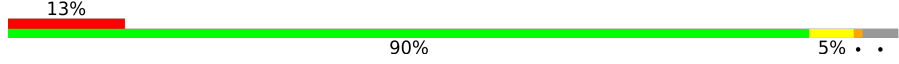
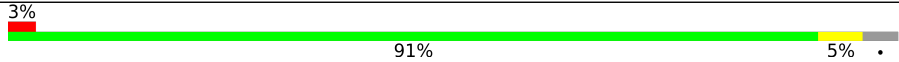
The reported resolution of this entry is 1.60 Å.

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}	164625	4274 (1.60-1.60)
Clashscore	180529	4682 (1.60-1.60)
Ramachandran outliers	177936	4583 (1.60-1.60)
Sidechain outliers	177891	4582 (1.60-1.60)
RSRZ outliers	164620	4272 (1.60-1.60)

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 $\leq 5\%$. 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:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	R4A	A	705	X	-	-	-
4	R4A	B	705	X	-	-	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 19634 atoms, of which 9073 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	3	0
			9344	3077	4473	853	931	10			
1	B	619	Total	C	H	N	O	S	0	5	0
			9359	3081	4483	853	931	11			

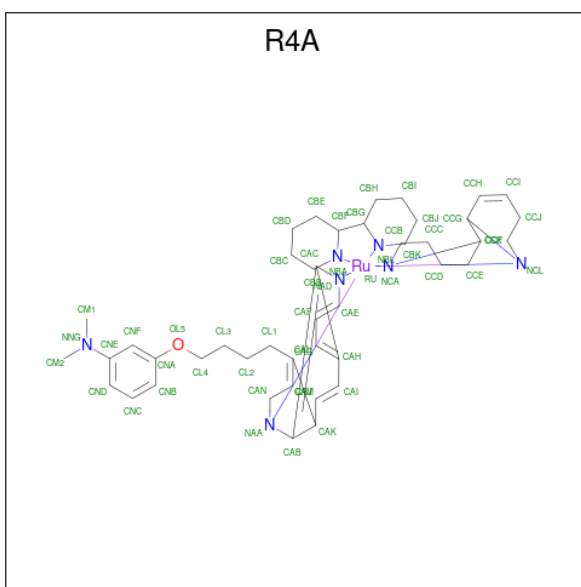
- Molecule 2 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

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).

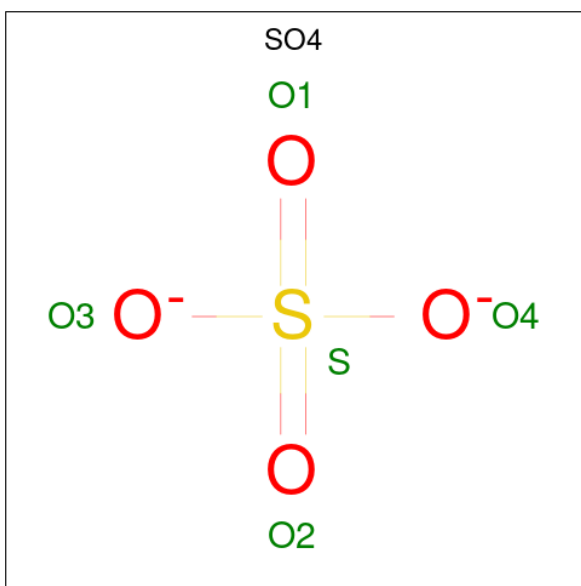
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		
3	B	1	Total	Na	0	0
			1	1		

- Molecule 4 is 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-DIMETHYLA
NILINATO(2-)}RUTHENIUM (CCD ID: R4A) (formula: C₄₄H₆₁N₇ORu).



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

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



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

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

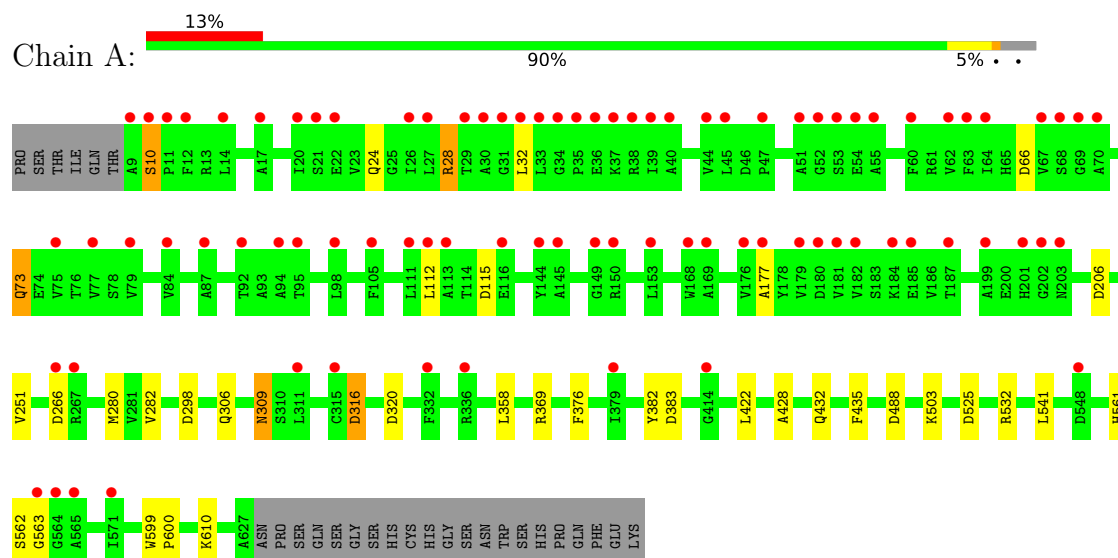
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	266	Total	O	0	0
			266	266		
7	B	386	Total	O	0	0
			386	386		

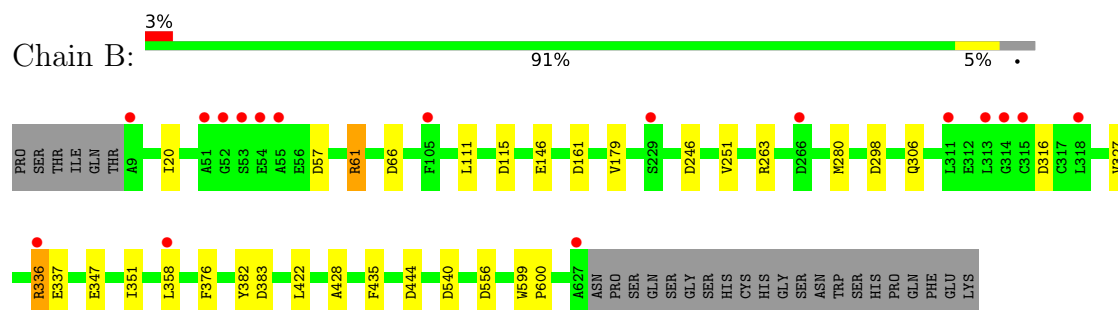
3 Residue-property plots

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



• Molecule 1: PHENYLETHYLAMINE OXIDASE



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	192.29Å 62.86Å 158.17Å 90.00° 117.47° 90.00°	Depositor
Resolution (Å)	29.99 – 1.60 29.99 – 1.60	Depositor EDS
% Data completeness (in resolution range)	93.9 (29.99-1.60) 93.9 (29.99-1.60)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.61 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.194 , 0.213 0.200 , 0.219	Depositor DCC
R_{free} test set	10382 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	21.7	Xtriage
Anisotropy	0.564	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 36.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	19634	wwPDB-VP
Average B, all atoms (Å ²)	21.0	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 77.91 % 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 7.7218e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CU, GOL, TPQ, R4A, NA, 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	0.51	0/4990	0.79	10/6793 (0.1%)
1	B	0.59	1/5006 (0.0%)	0.85	10/6815 (0.1%)
All	All	0.55	1/9996 (0.0%)	0.82	20/13608 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	347	GLU	CD-OE2	-5.40	1.19	1.25

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	61	ARG	NE-CZ-NH2	-8.72	115.94	120.30
1	B	298	ASP	CB-CG-OD2	7.33	124.89	118.30
1	A	383	ASP	CB-CG-OD2	6.42	124.08	118.30
1	A	66	ASP	CB-CG-OD2	6.20	123.88	118.30
1	B	540	ASP	CB-CG-OD2	6.11	123.80	118.30
1	B	316	ASP	CB-CG-OD2	5.74	123.46	118.30
1	A	298	ASP	CB-CG-OD2	5.62	123.36	118.30
1	B	115	ASP	CB-CG-OD2	5.60	123.34	118.30
1	A	488	ASP	CB-CG-OD2	5.60	123.34	118.30
1	A	206	ASP	CB-CG-OD2	5.52	123.27	118.30
1	A	525	ASP	CB-CG-OD2	5.51	123.26	118.30
1	A	320	ASP	CB-CG-OD2	5.46	123.21	118.30
1	B	161	ASP	CB-CG-OD2	5.42	123.17	118.30
1	B	57	ASP	CB-CG-OD2	5.39	123.15	118.30
1	B	383	ASP	CB-CG-OD2	5.36	123.12	118.30
1	A	266	ASP	CB-CG-OD2	5.34	123.11	118.30
1	A	115	ASP	CB-CG-OD2	5.13	122.91	118.30
1	B	246	ASP	CB-CG-OD2	5.05	122.85	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	66	ASP	CB-CG-OD2	5.05	122.84	118.30
1	A	316	ASP	CB-CG-OD2	5.00	122.80	118.30

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	4871	4473	4687	16	0
1	B	4876	4483	4693	14	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	56	2	0
4	B	53	41	56	3	0
5	A	5	0	0	0	0
5	B	5	0	0	0	0
6	A	12	10	16	0	0
6	B	30	25	40	1	0
7	A	266	0	0	1	0
7	B	386	0	0	2	0
All	All	10561	9073	9548	32	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (32) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:336:ARG:NH2	4:B:705:R4A:HCD1	2.11	0.66
1:B:599:TRP:CD2	1:B:600:PRO:HA	2.36	0.60
1:A:358:LEU:HA	4:B:705:R4A:HBD1	1.84	0.59
1:A:532:ARG:HB3	1:A:563:GLY:HA3	1.84	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:599:TRP:CD2	1:A:600:PRO:HA	2.38	0.58
1:B:422:LEU:HD11	1:B:428:ALA:HB2	1.85	0.58
1:B:61:ARG:HH22	1:B:556:ASP:CG	2.09	0.55
1:A:422:LEU:HD11	1:A:428:ALA:HB2	1.89	0.54
4:A:705:R4A:HBD1	1:B:358:LEU:HA	1.91	0.53
1:B:251:VAL:HG22	1:B:306:GLN:HB3	1.90	0.53
1:B:280[B]:MET:HG3	1:B:435:PHE:CE2	2.44	0.52
1:B:20:ILE:HD12	1:B:327:VAL:HG12	1.93	0.51
1:A:32:LEU:HD22	1:A:73:GLN:NE2	2.26	0.51
1:A:251:VAL:HG22	1:A:306:GLN:HB3	1.92	0.51
1:A:561:HIS:ND1	1:A:562:SER:O	2.39	0.50
1:B:61:ARG:NH2	1:B:556:ASP:OD2	2.41	0.50
1:B:556:ASP:OD1	7:B:2329:HOH:O	2.19	0.49
6:B:726:GOL:H32	7:B:2224:HOH:O	2.13	0.48
1:B:251:VAL:CG2	1:B:306:GLN:HB3	2.43	0.48
1:A:24:GLN:O	1:A:28:ARG:HG2	2.14	0.48
1:A:112:LEU:HD21	1:A:177:ALA:HB1	1.96	0.47
1:A:251:VAL:CG2	1:A:306:GLN:HB3	2.45	0.47
1:A:610:LYS:NZ	7:A:2251:HOH:O	2.48	0.46
1:A:309:ASN:HD22	1:A:309:ASN:N	2.16	0.43
1:B:280[B]:MET:HG3	1:B:435:PHE:CD2	2.53	0.43
4:A:705:R4A:HNF	4:A:705:R4A:HM23	1.86	0.43
4:B:705:R4A:HM23	4:B:705:R4A:HNF	1.77	0.42
1:A:280[B]:MET:HG3	1:A:435:PHE:CE2	2.54	0.42
1:A:316:ASP:HA	1:B:351:ILE:HD11	2.01	0.41
1:B:111:LEU:HD12	1:B:179:VAL:HG11	2.02	0.41
1:A:280[B]:MET:HG3	1:A:435:PHE:CD2	2.56	0.40
1:A:282:VAL:HA	1:A:432:GLN:O	2.21	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	619/646 (96%)	598 (97%)	20 (3%)	1 (0%)	44	25
1	B	621/646 (96%)	596 (96%)	25 (4%)	0	100	100
All	All	1240/1292 (96%)	1194 (96%)	45 (4%)	1 (0%)	48	28

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	10	SER

5.3.2 Protein sidechains ⓘ

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	515/537 (96%)	507 (98%)	8 (2%)	58	37
1	B	517/537 (96%)	511 (99%)	6 (1%)	67	50
All	All	1032/1074 (96%)	1018 (99%)	14 (1%)	62	43

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	SER
1	A	28	ARG
1	A	73	GLN
1	A	309	ASN
1	A	369	ARG
1	A	376	PHE
1	A	503	LYS
1	A	541	LEU
1	B	146	GLU
1	B	263	ARG
1	B	336	ARG
1	B	337	GLU
1	B	376	PHE
1	B	444	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	73	GLN
1	A	309	ASN
1	B	421	GLN

5.3.3 RNA ⓘ

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	1.46	3 (23%)	15,19,21	1.37	1 (6%)
1	TPQ	B	382	1	13,14,15	1.52	3 (23%)	15,19,21	1.72	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 (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	382	TPQ	C3-C4	3.47	1.41	1.35
1	A	382	TPQ	O4-C4	-2.75	1.26	1.34
1	A	382	TPQ	C3-C4	2.56	1.39	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	382	TPQ	O4-C4	-2.36	1.27	1.34
1	A	382	TPQ	C6-C1	2.14	1.40	1.34
1	B	382	TPQ	C6-C1	2.02	1.40	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	382	TPQ	CB-CA-C	-4.59	102.86	111.47
1	B	382	TPQ	C6-C1-C2	3.74	121.51	118.64
1	A	382	TPQ	CB-CA-C	-3.71	104.51	111.47

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.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 4 are monoatomic - leaving 11 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	SO4	B	710	-	4,4,4	0.12	0	6,6,6	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	SO4	A	710	-	4,4,4	0.15	0	6,6,6	0.50	0
6	GOL	B	725	-	5,5,5	0.38	0	5,5,5	0.20	0
6	GOL	A	725	-	5,5,5	0.37	0	5,5,5	0.24	0
6	GOL	B	726	-	5,5,5	0.29	0	5,5,5	0.73	0
6	GOL	A	723	-	5,5,5	0.40	0	5,5,5	0.28	0
4	R4A	A	705	-	51,63,63	3.77	25 (49%)	43,101,101	2.82	20 (46%)
4	R4A	B	705	-	51,63,63	3.75	23 (45%)	43,101,101	2.84	20 (46%)
6	GOL	B	720	-	5,5,5	0.29	0	5,5,5	0.52	0
6	GOL	B	723	-	5,5,5	0.36	0	5,5,5	0.29	0
6	GOL	B	721	-	5,5,5	0.42	0	5,5,5	0.37	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	B	725	-	-	2/4/4/4	-
6	GOL	A	725	-	-	1/4/4/4	-
6	GOL	B	726	-	-	2/4/4/4	-
6	GOL	A	723	-	-	4/4/4/4	-
4	R4A	A	705	-	5/5/19/19	7/12/150/150	0/10/11/11
4	R4A	B	705	-	5/5/19/19	4/12/150/150	0/10/11/11
6	GOL	B	720	-	-	0/4/4/4	-
6	GOL	B	723	-	-	2/4/4/4	-
6	GOL	B	721	-	-	0/4/4/4	-

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	705	R4A	CCB-NCA	-11.18	1.27	1.49
4	A	705	R4A	CCB-NCA	-10.92	1.27	1.49
4	B	705	R4A	CBB-NBA	-10.58	1.28	1.49
4	A	705	R4A	CBB-NBA	-10.51	1.28	1.49
4	B	705	R4A	CBD-CBE	-7.82	1.32	1.53
4	A	705	R4A	CCD-CCE	-7.76	1.32	1.53
4	B	705	R4A	CCD-CCE	-7.64	1.33	1.53
4	A	705	R4A	CBD-CBE	-7.46	1.33	1.53
4	A	705	R4A	CBK-NBL	-7.41	1.34	1.49
4	A	705	R4A	CCK-NCL	-7.19	1.35	1.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	705	R4A	CCK-NCL	-7.09	1.35	1.49
4	B	705	R4A	CBK-NBL	-6.86	1.35	1.49
4	A	705	R4A	CBH-CBG	-6.38	1.39	1.53
4	B	705	R4A	CBH-CBG	-5.87	1.40	1.53
4	B	705	R4A	CBI-CBH	-5.10	1.39	1.53
4	A	705	R4A	CBI-CBH	-5.10	1.39	1.53
4	B	705	R4A	CCB-CCC	-4.82	1.34	1.51
4	A	705	R4A	CCB-CCC	-4.72	1.34	1.51
4	A	705	R4A	CBB-CBC	-4.69	1.34	1.51
4	B	705	R4A	CBB-CBC	-4.56	1.35	1.51
4	A	705	R4A	CAK-CAL	-4.31	1.48	1.54
4	B	705	R4A	CAK-CAL	-4.26	1.48	1.54
4	A	705	R4A	CCK-CCJ	-4.08	1.40	1.51
4	A	705	R4A	CAI-CAJ	4.06	1.41	1.33
4	B	705	R4A	CCK-CCJ	-4.02	1.40	1.51
4	A	705	R4A	CAM-CAL	3.96	1.41	1.33
4	B	705	R4A	CAI-CAJ	3.96	1.41	1.33
4	B	705	R4A	CAM-CAL	3.59	1.40	1.33
4	B	705	R4A	CBK-CBJ	-3.03	1.40	1.51
4	A	705	R4A	CBK-CBJ	-3.02	1.40	1.51
4	A	705	R4A	CBI-CBJ	-3.01	1.39	1.51
4	B	705	R4A	CCH-CCI	2.88	1.39	1.32
4	B	705	R4A	CBI-CBJ	-2.84	1.40	1.51
4	A	705	R4A	CCH-CCI	2.75	1.39	1.32
4	B	705	R4A	CAK-CAJ	-2.67	1.40	1.51
4	A	705	R4A	CAE-CAF	2.61	1.41	1.35
4	B	705	R4A	CAH-CAC	2.60	1.46	1.41
4	A	705	R4A	CAH-CAC	2.56	1.46	1.41
4	A	705	R4A	CCE-CCF	-2.56	1.47	1.53
4	A	705	R4A	CAK-CAJ	-2.48	1.41	1.51
4	A	705	R4A	CAK-CAB	-2.46	1.46	1.52
4	B	705	R4A	CAE-CAF	2.44	1.40	1.35
4	B	705	R4A	CCE-CCF	-2.42	1.47	1.53
4	B	705	R4A	CCJ-CCI	-2.37	1.40	1.48
4	A	705	R4A	CCJ-CCI	-2.32	1.40	1.48
4	A	705	R4A	CAN-CAM	-2.19	1.40	1.48
4	B	705	R4A	CAK-CAB	-2.16	1.46	1.52
4	A	705	R4A	CNE-NNG	2.05	1.42	1.37

All (40) bond angle outliers are listed below:

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	705	R4A	CCC-CCB-NCA	6.08	122.91	113.00
4	B	705	R4A	CBC-CBB-NBA	5.68	122.26	113.00
4	B	705	R4A	CCC-CCB-NCA	5.63	122.18	113.00
4	A	705	R4A	CBC-CBB-NBA	5.57	122.08	113.00
4	B	705	R4A	CBK-CBJ-CBI	5.37	120.53	111.44
4	B	705	R4A	CCF-CCG-NCL	5.05	113.77	107.55
4	A	705	R4A	CBK-CBJ-CBI	5.03	119.96	111.44
4	B	705	R4A	CBB-CBC-CBD	5.00	119.92	111.44
4	A	705	R4A	CBB-CBC-CBD	4.88	119.71	111.44
4	B	705	R4A	CAJ-CAK-CAB	4.86	118.62	108.39
4	A	705	R4A	CCB-CCC-CCD	4.81	119.58	111.44
4	A	705	R4A	CAJ-CAK-CAB	4.79	118.47	108.39
4	A	705	R4A	CCF-CCG-NCL	4.65	113.27	107.55
4	B	705	R4A	CCB-CCC-CCD	4.65	119.31	111.44
4	A	705	R4A	CCD-CCE-CCF	4.44	119.22	111.22
4	A	705	R4A	CBI-CBH-CBG	4.40	119.15	111.22
4	B	705	R4A	CBI-CBH-CBG	4.34	119.04	111.22
4	B	705	R4A	CBJ-CBK-NBL	4.31	120.02	113.00
4	A	705	R4A	CBJ-CBK-NBL	4.20	119.86	113.00
4	A	705	R4A	CBJ-CBI-CBH	4.20	119.99	111.42
4	B	705	R4A	CBJ-CBI-CBH	3.94	119.45	111.42
4	B	705	R4A	CBD-CBE-CBF	3.68	117.86	111.22
4	A	705	R4A	CBD-CBE-CBF	3.62	117.74	111.22
4	B	705	R4A	CCD-CCE-CCF	3.56	117.64	111.22
4	B	705	R4A	CAC-CAB-NAA	3.33	117.14	106.05
4	A	705	R4A	CAC-CAB-NAA	3.19	116.67	106.05
4	B	705	R4A	CCC-CCD-CCE	3.03	117.60	111.42
4	B	705	R4A	CAB-CAC-NAD	3.03	116.43	108.46
4	B	705	R4A	CL4-OL5-CNA	2.96	125.66	117.93
4	A	705	R4A	CBC-CBD-CBE	2.94	117.41	111.42
4	A	705	R4A	CAB-CAC-NAD	2.84	115.94	108.46
4	B	705	R4A	CBC-CBD-CBE	2.81	117.15	111.42
4	A	705	R4A	CAK-CAL-CAM	2.73	118.02	112.14
4	B	705	R4A	CAK-CAL-CAM	2.39	117.27	112.14
4	A	705	R4A	CCC-CCD-CCE	2.38	116.26	111.42
4	A	705	R4A	CCJ-CCK-NCL	2.22	119.59	111.94
4	B	705	R4A	CCJ-CCK-NCL	2.18	119.48	111.94
4	A	705	R4A	CL4-OL5-CNA	2.07	123.33	117.93
4	B	705	R4A	CAG-CAH-CAC	-2.06	116.00	118.51
4	A	705	R4A	CCJ-CCI-CCH	-2.01	120.04	123.61

All (10) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	705	R4A	CCG
4	A	705	R4A	CBF
4	A	705	R4A	CCF
4	A	705	R4A	CBG
4	A	705	R4A	CAK
4	B	705	R4A	CCG
4	B	705	R4A	CBF
4	B	705	R4A	CCF
4	B	705	R4A	CBG
4	B	705	R4A	CAK

All (22) torsion outliers are listed below:

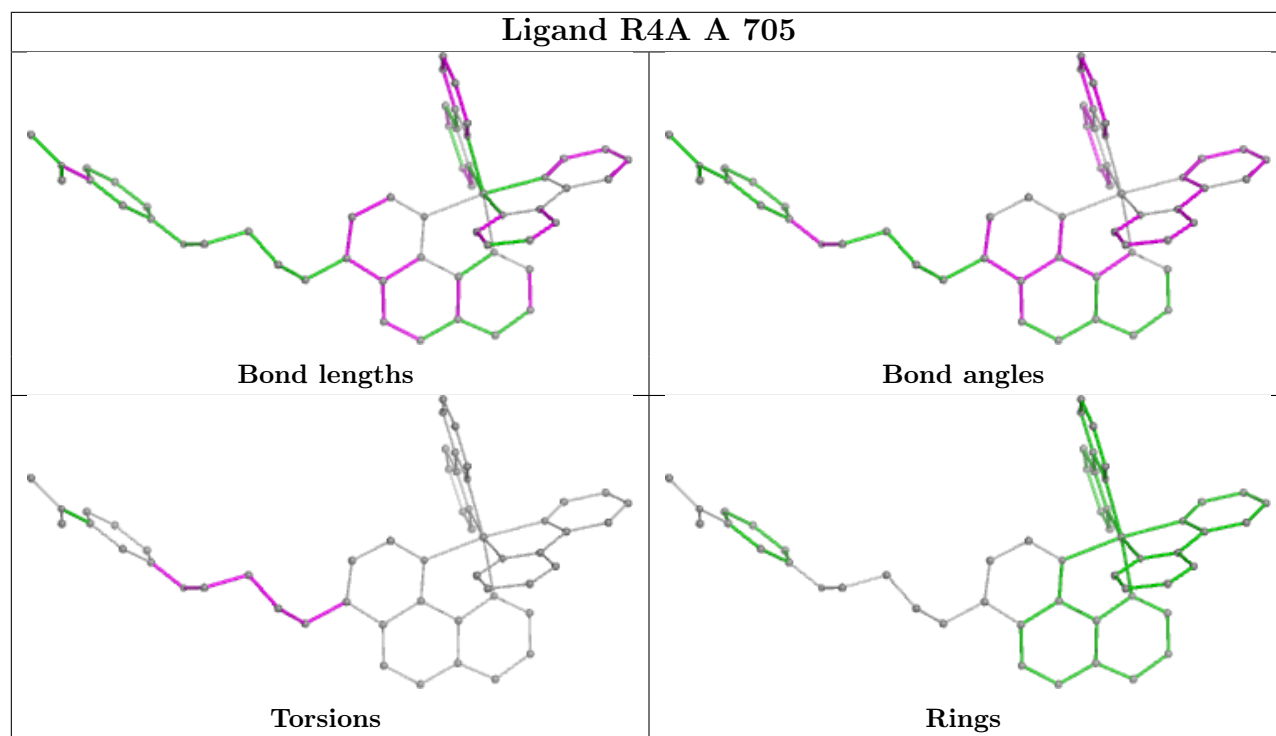
Mol	Chain	Res	Type	Atoms
6	A	723	GOL	C1-C2-C3-O3
6	B	723	GOL	C1-C2-C3-O3
6	B	725	GOL	O1-C1-C2-C3
6	B	726	GOL	O1-C1-C2-C3
4	A	705	R4A	CL2-CL3-CL4-OL5
4	B	705	R4A	CL2-CL3-CL4-OL5
6	A	723	GOL	O1-C1-C2-C3
4	B	705	R4A	CAL-CL1-CL2-CL3
4	A	705	R4A	CL1-CL2-CL3-CL4
4	B	705	R4A	CL1-CL2-CL3-CL4
6	A	723	GOL	O2-C2-C3-O3
6	B	723	GOL	O2-C2-C3-O3
6	B	725	GOL	O1-C1-C2-O2
6	B	726	GOL	O1-C1-C2-O2
4	A	705	R4A	CAL-CL1-CL2-CL3
4	A	705	R4A	CL3-CL4-OL5-CNA
4	B	705	R4A	CL3-CL4-OL5-CNA
6	A	723	GOL	O1-C1-C2-O2
4	A	705	R4A	CNB-CNA-OL5-CL4
4	A	705	R4A	CNF-CNA-OL5-CL4
4	A	705	R4A	CAK-CAL-CL1-CL2
6	A	725	GOL	C1-C2-C3-O3

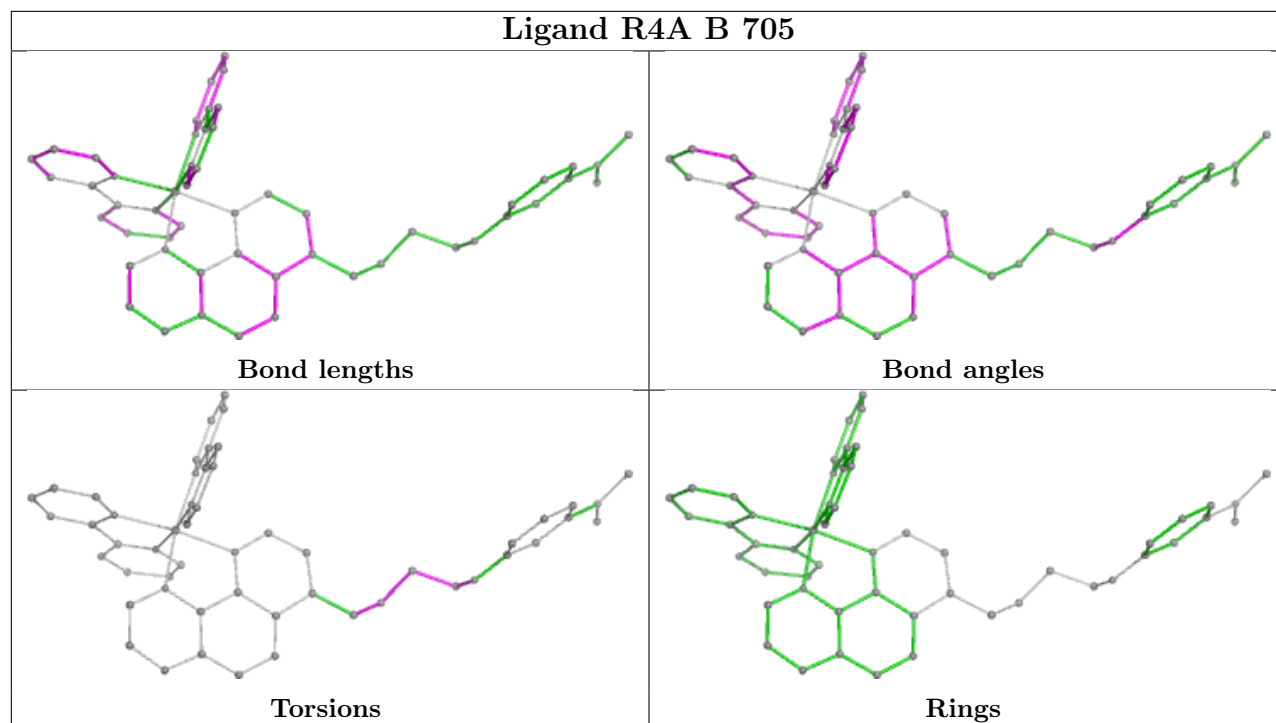
There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	726	GOL	1	0
4	A	705	R4A	2	0
4	B	705	R4A	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 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

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, 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	618/646 (95%)	0.79	86 (13%) 7 6	11, 21, 38, 49	3 (0%)
1	B	618/646 (95%)	-0.01	17 (2%) 55 56	10, 17, 27, 47	5 (0%)
All	All	1236/1292 (95%)	0.39	103 (8%) 19 18	10, 19, 35, 49	8 (0%)

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	52	GLY	5.6
1	A	34	GLY	5.0
1	A	9	ALA	5.0
1	B	53	SER	5.0
1	A	563	GLY	4.9
1	B	55	ALA	4.3
1	A	67	VAL	4.1
1	A	315	CYS	4.1
1	A	53	SER	4.0
1	A	29	THR	4.0
1	A	182	VAL	3.9
1	A	33	LEU	3.7
1	B	315	CYS	3.7
1	B	9	ALA	3.7
1	A	14	LEU	3.7
1	A	52	GLY	3.5
1	A	26	ILE	3.4
1	A	55	ALA	3.4
1	A	332	PHE	3.3
1	B	51	ALA	3.3
1	A	44	VAL	3.2
1	A	179	VAL	3.2
1	A	32	LEU	3.2
1	A	30	ALA	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	266	ASP	3.2
1	A	202	GLY	3.2
1	A	20	ILE	3.1
1	A	94	ALA	3.1
1	A	54	GLU	3.1
1	A	70	ALA	3.1
1	B	54	GLU	3.1
1	A	95	THR	3.0
1	A	145	ALA	3.0
1	A	565	ALA	3.0
1	A	84	VAL	3.0
1	A	98	LEU	2.9
1	A	60	PHE	2.9
1	A	92	THR	2.9
1	B	358	LEU	2.9
1	B	105	PHE	2.9
1	A	111	LEU	2.8
1	A	64	ILE	2.8
1	A	571	ILE	2.8
1	A	564	GLY	2.8
1	A	201	HIS	2.8
1	A	22	GLU	2.7
1	A	144	TYR	2.7
1	A	37	LYS	2.7
1	A	68	SER	2.7
1	A	112	LEU	2.7
1	A	548	ASP	2.7
1	A	79	VAL	2.7
1	A	38	ARG	2.7
1	B	314	GLY	2.6
1	A	12	PHE	2.6
1	A	39	ILE	2.6
1	A	77	VAL	2.6
1	A	336	ARG	2.6
1	A	185	GLU	2.6
1	A	169	ALA	2.5
1	B	336	ARG	2.5
1	A	10	SER	2.5
1	A	35	PRO	2.5
1	A	27	LEU	2.5
1	A	63	PHE	2.5
1	A	153	LEU	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	11	PRO	2.4
1	A	40	ALA	2.4
1	A	113	ALA	2.4
1	A	105	PHE	2.4
1	A	203	ASN	2.4
1	A	267	ARG	2.4
1	A	180	ASP	2.4
1	B	313	LEU	2.3
1	A	177	ALA	2.3
1	A	31	GLY	2.3
1	A	150	ARG	2.3
1	A	187	THR	2.3
1	A	116	GLU	2.3
1	A	181	VAL	2.3
1	A	47	PRO	2.2
1	B	266	ASP	2.2
1	B	318	LEU	2.2
1	A	149	GLY	2.2
1	A	51	ALA	2.2
1	A	87	ALA	2.2
1	A	199	ALA	2.2
1	A	176	VAL	2.2
1	A	45	LEU	2.2
1	A	168	TRP	2.2
1	A	21	SER	2.2
1	A	69	GLY	2.2
1	B	627	ALA	2.1
1	A	62	VAL	2.1
1	A	414	GLY	2.1
1	B	229	SER	2.1
1	A	184	LYS	2.1
1	A	75	VAL	2.1
1	A	17	ALA	2.1
1	B	311	LEU	2.1
1	A	311	LEU	2.0
1	A	36	GLU	2.0
1	A	379	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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	0.08	18,19,23,27	0
1	TPQ	B	382	14/15	0.94	0.09	13,17,21,27	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

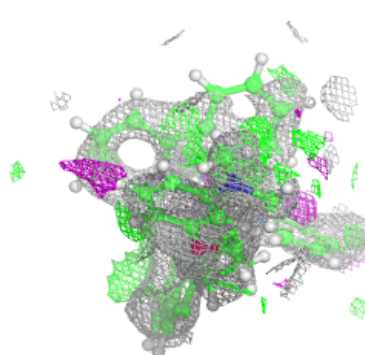
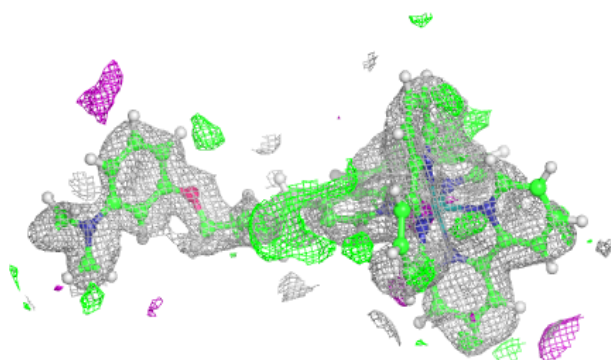
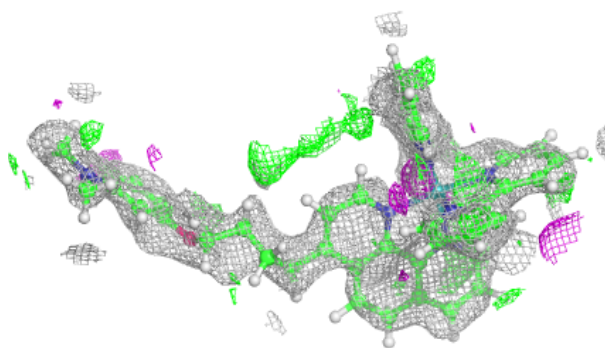
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	SO4	B	710	5/5	0.68	0.23	64,64,65,66	0
5	SO4	A	710	5/5	0.70	0.24	54,55,57,58	0
6	GOL	B	723	6/6	0.78	0.19	52,55,55,57	0
6	GOL	A	723	6/6	0.81	0.20	48,51,51,51	0
6	GOL	A	725	6/6	0.86	0.17	43,44,45,45	0
6	GOL	B	725	6/6	0.89	0.17	47,48,48,49	0
6	GOL	B	726	6/6	0.89	0.13	37,41,42,43	0
6	GOL	B	721	6/6	0.91	0.13	37,40,41,44	0
6	GOL	B	720	6/6	0.93	0.10	25,28,28,29	0
4	R4A	A	705	53/53	0.94	0.17	34,37,41,41	71
4	R4A	B	705	53/53	0.95	0.16	29,33,36,37	71
3	NA	A	703	1/1	0.98	0.08	28,28,28,28	0
2	CU	A	701	1/1	0.98	0.06	28,28,28,28	0
3	NA	B	703	1/1	0.99	0.05	22,22,22,22	0
2	CU	B	701	1/1	0.99	0.04	23,23,23,23	0

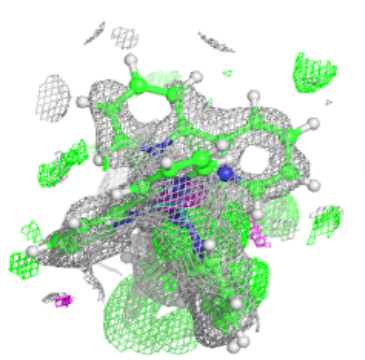
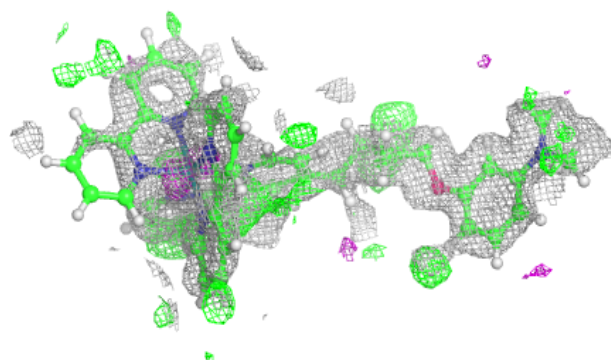
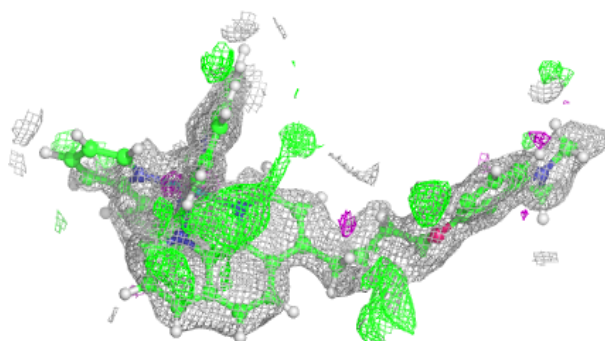
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around R4A A 705:

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

**Electron density around R4A B 705:**

$2mF_o-DF_c$ (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.