W O R L D W I D E
wwPDB
PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Jun 12, 2024 – 08:45 AM EDT

PDB ID	:	1OY8
Title	:	Structural Basis of Multiple Drug Binding Capacity of the AcrB Multidrug Efflux Pump
Authors	:	Yu, E.W.; McDermott, G.; Zgurskaya, H.I.; Nikaido, H.; Koshland Jr., D.E.
Deposited on	:	2003-04-03
Resolution	:	3.63 Å(reported)

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

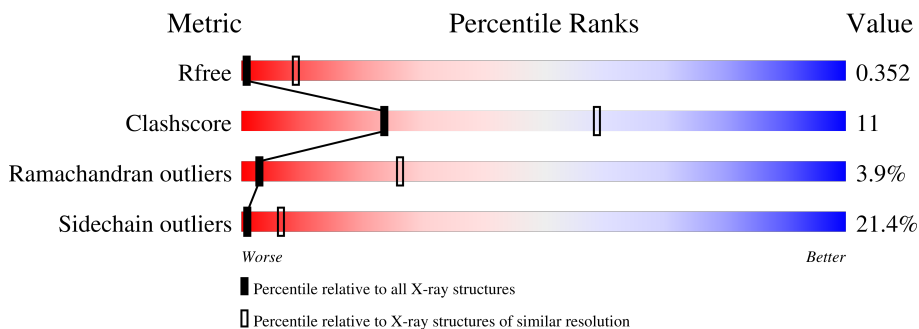|		
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 3.63 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	Percentile Ranks	Value
Rfree		0.352
Clashscore		11
Ramachandran outliers		3.9%
Sidechain outliers		21.4%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1341 (3.78-3.50)
Clashscore	141614	1439 (3.78-3.50)
Ramachandran outliers	138981	1391 (3.78-3.50)
Sidechain outliers	138945	1391 (3.78-3.50)

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%

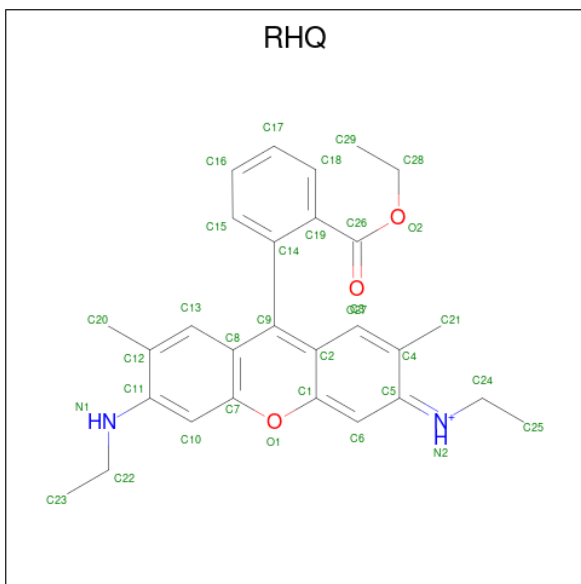| Mol	Chain	Length	Quality of chain
1	A	1049	59% 30% 6% · ·

2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 7672 atoms, of which 0 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 Acriflavine resistance protein B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1006	7639	4916	1262	1419	42	0	0	0

- Molecule 2 is RHODAMINE 6G (three-letter code: RHQ) (formula: $C_{28}H_{31}N_2O_3$).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	33	28	2	3	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. 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. 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: Acriflavine resistance protein B

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	144.80Å 144.80Å 518.61Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.60 – 3.63 46.62 – 3.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.60-3.63) 99.1 (46.62-3.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.29 (at 3.57Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.245 , 0.322 0.353 , 0.352	Depositor DCC
R_{free} test set	1257 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å^2)	130.1	Xtriage
Anisotropy	0.274	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 41.4	EDS
L-test for twinning[2]	$< \lvert L \rvert > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.82	EDS
Total number of atoms	7672	wwPDB-VP
Average B, all atoms (Å^2)	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.50% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< \lvert L \rvert >$, $< L^2 >$ 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: RHQ

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	0.36	1/7779 (0.0%)	0.67	28/10563 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1032	ARG	CZ-NH1	6.24	1.41	1.33

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1032	ARG	NE-CZ-NH2	-7.26	116.67	120.30
1	A	723	ASP	CB-CG-OD2	6.43	124.08	118.30
1	A	407	ASP	CB-CG-OD2	6.41	124.06	118.30
1	A	858	ASP	CB-CG-OD2	6.16	123.84	118.30
1	A	25	LEU	CA-CB-CG	6.01	129.12	115.30

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	7639	0	7800	168	0
2	A	33	0	31	6	0

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	7672	0	7831	174	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 11.

The worst 5 of 174 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:306:ILE:O	1:A:307:ARG:HB2	1.74	0.87
1:A:905:VAL:HB	1:A:906:PRO:HD3	1.57	0.85
1:A:308:ALA:HB1	1:A:309:GLU:HA	1.59	0.82
1:A:399:VAL:HA	1:A:402:ILE:HD12	1.62	0.81
1:A:222:THR:HB	1:A:223:PRO:HD3	1.64	0.80

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	998/1049 (95%)	858 (86%)	101 (10%)	39 (4%)	3 26

5 of 39 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	34	GLN
1	A	255	GLN
1	A	459	PHE
1	A	526	HIS
1	A	671	ILE

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	818/855 (96%)	643 (79%)	175 (21%)	1 6

5 of 175 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	690	LEU
1	A	895	TRP
1	A	714	THR
1	A	792	ARG
1	A	938	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	622	GLN
1	A	747	ASN
1	A	231	ASN
1	A	282	ASN
1	A	391	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

1 ligand 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	$\#|Z| > 2$
2	RHQ	A	2001	-	34,36,36	2.53	8 (23%)	39,51,51	2.04	12 (30%)

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
2	RHQ	A	2001	-	-	6/11/21/21	0/4/4/4

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2001	RHQ	C8-C7	6.75	1.49	1.41
2	A	2001	RHQ	C2-C1	6.69	1.49	1.41
2	A	2001	RHQ	C4-C5	5.21	1.51	1.43
2	A	2001	RHQ	C11-C12	5.19	1.51	1.40
2	A	2001	RHQ	O2-C26	5.11	1.46	1.33

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	2001	RHQ	O2-C26-C19	5.63	120.03	111.65
2	A	2001	RHQ	C12-C11-N1	4.31	125.02	119.41
2	A	2001	RHQ	C7-O1-C1	3.83	123.32	120.37
2	A	2001	RHQ	C6-C1-C2	-3.35	119.51	123.11
2	A	2001	RHQ	C10-C7-C8	-3.33	119.54	123.11

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2001	RHQ	C12-C11-N1-C22
2	A	2001	RHQ	C19-C26-O2-C28
2	A	2001	RHQ	O27-C26-O2-C28
2	A	2001	RHQ	C10-C11-N1-C22
2	A	2001	RHQ	C23-C22-N1-C11

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2001	RHQ	6	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 RHQ A 2001

Bond lengths

Bond angles

Torsions

Rings
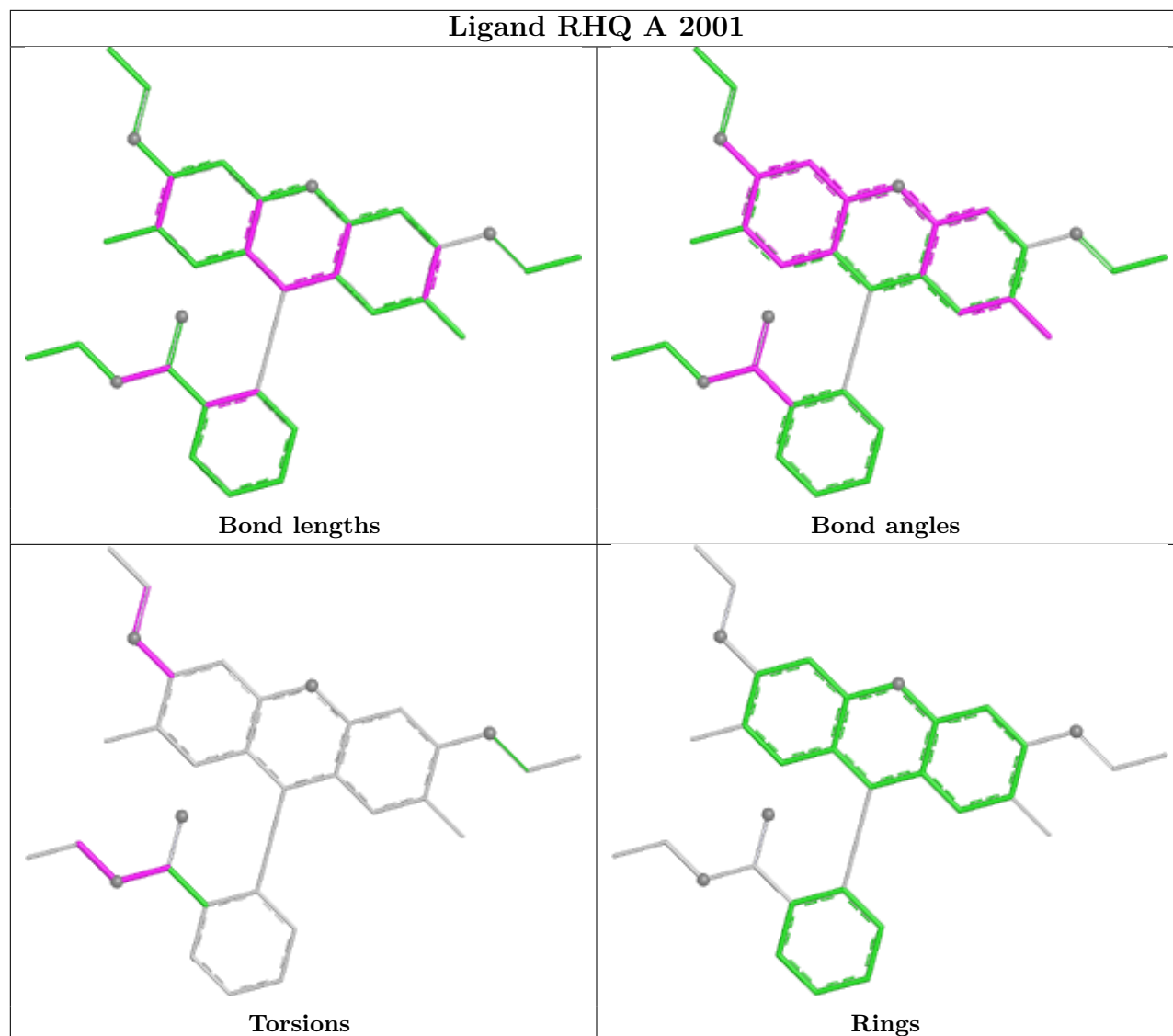
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

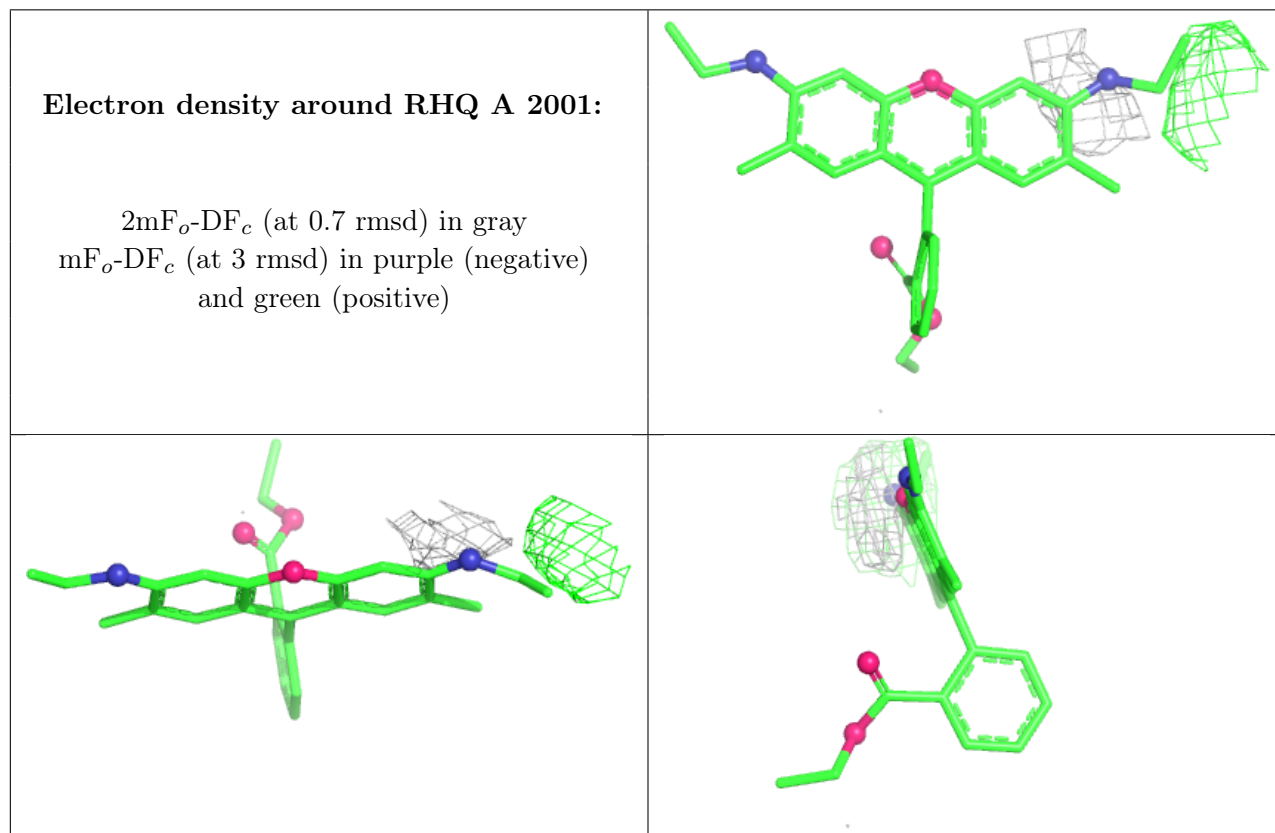Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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 RHQ A 2001:

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

6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.