



# Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 08:45 pm BST

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)

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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

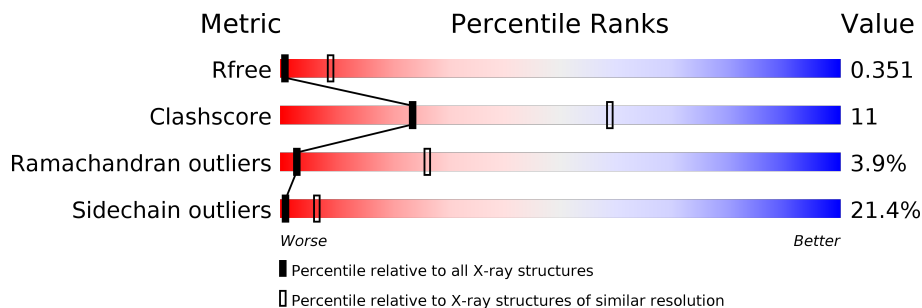
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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	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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

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

## 2 Entry composition [i](#)

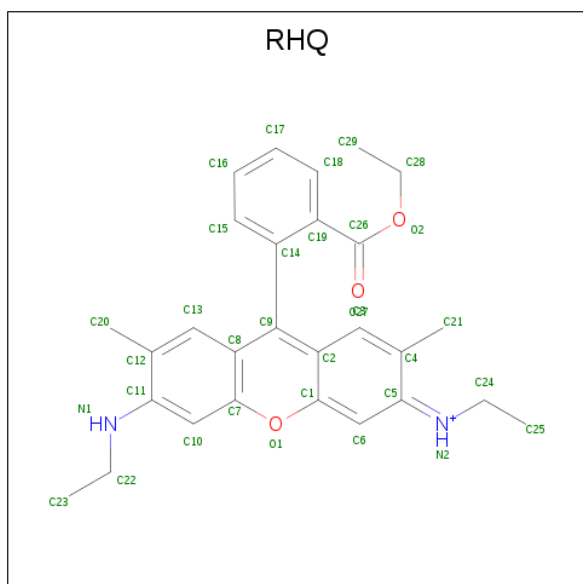
There are 2 unique types of molecules in this entry. The entry contains 7672 atoms, of which 0 are hydrogens and 0 are deuteriums.

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:  $C_{28}H_{31}N_2O_3$ ).

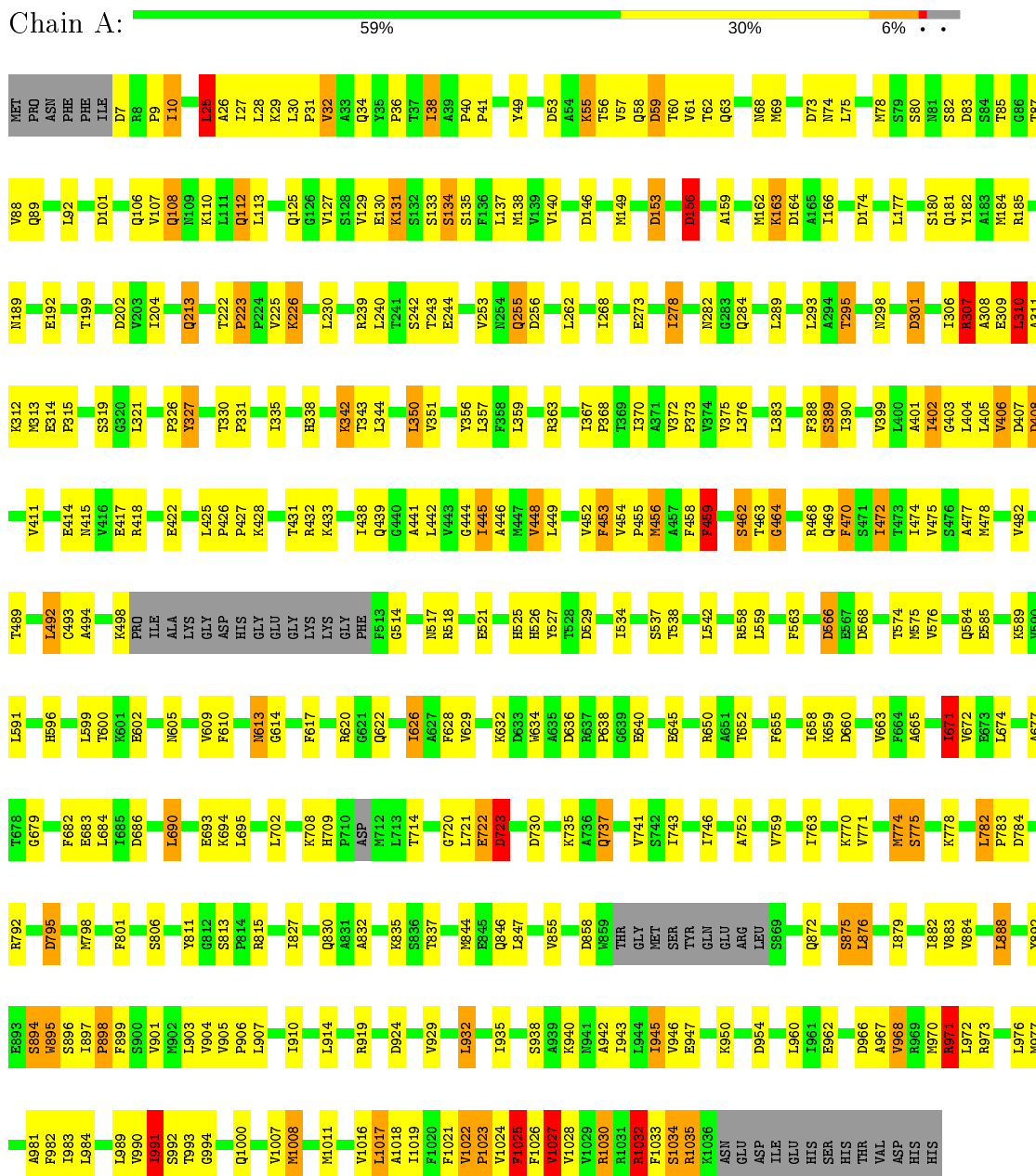


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	33	28	2	3	0	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.29 (at 3.57Å)	Xtrriage
Refinement program	REFMAC 5.0	Depositor
R, $R_{free}$	0.245 , 0.322 0.350 , 0.351	Depositor DCC
$R_{free}$ test set	1257 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	130.1	Xtrriage
Anisotropy	0.274	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 41.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.82	EDS
Total number of atoms	7672	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	101.0	wwPDB-VP

Xtrriage'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.*

<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: 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

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
1	A	568	ASP	CB-CG-OD2	5.94	123.65	118.30
1	A	795	ASP	CB-CG-OD2	5.87	123.59	118.30
1	A	310	LEU	CA-CB-CG	5.87	128.79	115.30
1	A	146	ASP	CB-CG-OD2	5.69	123.42	118.30
1	A	966	ASP	CB-CG-OD2	5.47	123.22	118.30
1	A	59	ASP	CB-CG-OD2	5.38	123.15	118.30
1	A	174	ASP	CB-CG-OD2	5.36	123.12	118.30
1	A	7	ASP	CB-CG-OD2	5.35	123.12	118.30
1	A	153	ASP	CB-CG-OD2	5.31	123.08	118.30
1	A	156	ASP	CB-CG-OD2	5.30	123.07	118.30
1	A	202	ASP	CB-CG-OD2	5.27	123.04	118.30
1	A	53	ASP	CB-CG-OD2	5.26	123.03	118.30
1	A	636	ASP	CB-CG-OD2	5.25	123.03	118.30
1	A	83	ASP	CB-CG-OD2	5.24	123.01	118.30
1	A	730	ASP	CB-CG-OD2	5.22	123.00	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	660	ASP	CB-CG-OD2	5.21	122.99	118.30
1	A	924	ASP	CB-CG-OD2	5.17	122.95	118.30
1	A	566	ASP	CB-CG-OD2	5.16	122.94	118.30
1	A	784	ASP	CB-CG-OD2	5.09	122.88	118.30
1	A	256	ASP	CB-CG-OD2	5.09	122.88	118.30
1	A	101	ASP	CB-CG-OD2	5.08	122.87	118.30
1	A	408	ASP	CB-CG-OD2	5.05	122.85	118.30
1	A	954	ASP	CB-CG-OD2	5.02	122.82	118.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7639	0	7800	168	0
2	A	33	0	31	6	0
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.

All (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
1:A:686:ASP:HB2	1:A:695:LEU:HD12	1.62	0.80
1:A:968:VAL:HB	1:A:1025:PHE:HZ	1.46	0.79
2:A:2001:RHQ:C24	2:A:2001:RHQ:H211	2.13	0.79
1:A:112:GLN:HG2	1:A:112:GLN:O	1.84	0.76
2:A:2001:RHQ:H241	2:A:2001:RHQ:H211	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:LYS:HB3	1:A:295:THR:H	1.52	0.74
1:A:1022:VAL:HG22	1:A:1023:PRO:HD2	1.71	0.72
1:A:403:GLY:HA3	1:A:982:PHE:HD1	1.55	0.71
1:A:403:GLY:HA3	1:A:982:PHE:CD1	2.26	0.71
1:A:306:ILE:HG23	1:A:307:ARG:H	1.56	0.70
2:A:2001:RHQ:H222	2:A:2001:RHQ:H202	1.73	0.70
1:A:1023:PRO:HA	1:A:1026:PHE:HB2	1.74	0.70
1:A:372:VAL:N	1:A:373:PRO:HD2	2.07	0.70
1:A:894:SER:O	1:A:895:TRP:HB2	1.92	0.70
1:A:901:VAL:O	1:A:904:VAL:HG22	1.92	0.68
1:A:31:PRO:HG2	1:A:389:SER:HB3	1.78	0.66
1:A:373:PRO:HA	1:A:376:LEU:HD12	1.78	0.65
1:A:159:ALA:HA	1:A:163:LYS:HB3	1.78	0.64
1:A:449:LEU:HB2	1:A:478:MET:SD	2.39	0.63
1:A:929:VAL:HA	1:A:932:LEU:HD12	1.80	0.62
1:A:306:ILE:HG23	1:A:307:ARG:N	2.16	0.60
1:A:610:PHE:HB3	1:A:628:PHE:HB2	1.82	0.60
1:A:456:MET:HA	1:A:876:LEU:HB3	1.81	0.60
1:A:306:ILE:CG2	1:A:307:ARG:N	2.64	0.60
1:A:446:ALA:HB2	1:A:482:VAL:HG21	1.82	0.60
1:A:330:THR:HB	1:A:331:PRO:HD3	1.83	0.60
1:A:454:VAL:N	1:A:455:PRO:HD2	2.17	0.60
1:A:1030:ARG:HA	1:A:1034:SER:HB3	1.84	0.60
1:A:298:ASN:HB2	1:A:301:ASP:HB2	1.84	0.59
1:A:463:THR:HG23	1:A:563:PHE:HE1	1.67	0.59
2:A:2001:RHQ:H222	2:A:2001:RHQ:C20	2.32	0.59
1:A:453:PHE:HE2	1:A:474:ILE:HB	1.68	0.57
1:A:472:ILE:HA	1:A:475:VAL:HB	1.86	0.57
1:A:383:LEU:HB3	1:A:388:PHE:HB2	1.85	0.57
1:A:110:LYS:HD3	1:A:113:LEU:HD12	1.85	0.56
1:A:189:ASN:HB3	1:A:192:GLU:HB2	1.88	0.55
1:A:945:ILE:HA	1:A:971:ARG:NH1	2.21	0.55
1:A:30:LEU:HD23	1:A:390:ILE:HG13	1.89	0.55
1:A:897:ILE:HG23	1:A:946:VAL:HG11	1.89	0.55
1:A:470:PHE:HD1	1:A:929:VAL:HG21	1.71	0.54
1:A:709:HIS:O	1:A:709:HIS:CG	2.60	0.54
1:A:888:LEU:HD12	1:A:898:PRO:HA	1.89	0.54
1:A:575:MET:HB3	1:A:626:ILE:HD12	1.91	0.53
1:A:458:PHE:O	1:A:459:PHE:O	2.26	0.53
1:A:10:ILE:HD13	1:A:10:ILE:N	2.25	0.52
1:A:613:ASN:HD22	1:A:613:ASN:C	2.13	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:390:ILE:HG22	1:A:390:ILE:O	2.10	0.51
1:A:993:THR:HB	1:A:994:GLY:CA	2.40	0.51
1:A:372:VAL:HG11	1:A:406:VAL:HG22	1.93	0.51
1:A:344:LEU:HD23	1:A:402:ILE:HD11	1.93	0.51
1:A:156:ASP:HA	1:A:181:GLN:HA	1.92	0.51
1:A:262:LEU:HG	1:A:268:ILE:HD11	1.92	0.51
1:A:445:ILE:O	1:A:449:LEU:HG	2.10	0.51
1:A:584:GLN:H	1:A:622:GLN:HE21	1.59	0.51
1:A:983:ILE:HG23	1:A:1008:MET:HG2	1.93	0.51
1:A:204:ILE:HG23	1:A:759:VAL:HG13	1.93	0.50
1:A:55:LYS:HE3	1:A:813:SER:H	1.76	0.50
1:A:1018:ALA:HB1	1:A:1024:VAL:HG21	1.94	0.49
1:A:425:LEU:C	1:A:427:PRO:HD2	2.31	0.49
1:A:453:PHE:CE2	1:A:474:ILE:HB	2.47	0.49
1:A:904:VAL:HG11	1:A:942:ALA:HB2	1.93	0.49
1:A:426:PRO:N	1:A:427:PRO:HD2	2.28	0.49
1:A:468:ARG:O	1:A:472:ILE:HG22	2.13	0.49
1:A:75:LEU:HD21	1:A:92:LEU:HD23	1.94	0.49
1:A:576:VAL:HG13	1:A:663:VAL:HG22	1.93	0.49
1:A:682:PHE:HB3	1:A:827:ILE:HB	1.94	0.49
1:A:108:GLN:HB2	1:A:129:VAL:HG21	1.95	0.48
2:A:2001:RHQ:H242	2:A:2001:RHQ:H211	1.95	0.48
1:A:282:ASN:HD22	1:A:599:LEU:HD21	1.79	0.48
1:A:879:ILE:HA	1:A:882:ILE:HD12	1.96	0.48
1:A:307:ARG:H	1:A:308:ALA:C	2.17	0.48
1:A:401:ALA:HB2	1:A:474:ILE:HG12	1.95	0.48
1:A:671:ILE:HG13	1:A:671:ILE:H	1.40	0.48
1:A:60:THR:HG23	1:A:61:VAL:HG23	1.96	0.48
1:A:456:MET:O	1:A:876:LEU:HD13	2.14	0.47
1:A:306:ILE:C	1:A:308:ALA:HB3	2.35	0.47
1:A:428:LYS:HG2	1:A:494:ALA:HB1	1.96	0.47
1:A:62:THR:OG1	1:A:88:VAL:HG21	2.14	0.47
1:A:375:VAL:HG11	1:A:405:LEU:HD22	1.97	0.47
1:A:401:ALA:O	1:A:405:LEU:HG	2.15	0.47
1:A:613:ASN:HD22	1:A:614:GLY:N	2.13	0.47
1:A:832:ALA:HB3	1:A:835:LYS:HB2	1.97	0.47
1:A:993:THR:HB	1:A:994:GLY:HA2	1.97	0.47
1:A:367:ILE:HB	1:A:368:PRO:HD3	1.96	0.46
1:A:993:THR:CB	1:A:994:GLY:HA2	2.44	0.46
1:A:721:LEU:O	1:A:723:ASP:N	2.48	0.46
1:A:59:ASP:HA	1:A:63:GLN:HB2	1.95	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:VAL:N	1:A:373:PRO:CD	2.77	0.46
1:A:655:PHE:HB3	1:A:663:VAL:HB	1.96	0.46
1:A:991:ILE:O	1:A:993:THR:N	2.49	0.46
1:A:73:ASP:H	1:A:106:GLN:HE22	1.64	0.46
1:A:879:ILE:O	1:A:883:VAL:HG23	2.16	0.46
1:A:350:LEU:HD12	1:A:984:LEU:HB3	1.98	0.46
1:A:905:VAL:HB	1:A:906:PRO:CD	2.38	0.46
1:A:892:TYR:HB3	1:A:897:ILE:HD13	1.98	0.46
1:A:25:LEU:HA	1:A:28:LEU:HD12	1.99	0.45
1:A:166:ILE:HG13	1:A:289:LEU:HD13	1.98	0.45
1:A:414:GLU:O	1:A:417:GLU:HB2	2.16	0.45
1:A:596:HIS:O	1:A:600:THR:HG22	2.16	0.45
1:A:896:SER:HB2	1:A:1032:ARG:HA	1.98	0.45
1:A:489:THR:O	1:A:493:CYS:HB2	2.17	0.45
1:A:897:ILE:C	1:A:899:PHE:H	2.20	0.45
1:A:527:TYR:OH	1:A:1019:ILE:HG13	2.17	0.44
1:A:441:ALA:HB2	1:A:947:GLU:HG2	1.99	0.44
1:A:343:THR:HG21	1:A:989:LEU:HD21	1.98	0.44
1:A:213:GLN:HG2	1:A:239:ARG:H	1.82	0.44
1:A:278:ILE:HG13	1:A:613:ASN:HB3	1.99	0.44
1:A:351:VAL:HG22	1:A:981:ALA:HB1	1.99	0.44
1:A:972:LEU:HD23	1:A:1019:ILE:HG12	1.99	0.44
1:A:438:ILE:HG22	1:A:442:LEU:HG	1.99	0.44
2:A:2001:RHQ:C22	2:A:2001:RHQ:C20	2.96	0.44
1:A:370:ILE:O	1:A:370:ILE:HG22	2.18	0.44
1:A:307:ARG:N	1:A:308:ALA:C	2.71	0.43
1:A:36:PRO:O	1:A:38:ILE:HG13	2.18	0.43
1:A:782:LEU:HB3	1:A:783:PRO:HD2	2.00	0.43
1:A:884:VAL:O	1:A:888:LEU:HB2	2.18	0.43
1:A:945:ILE:HG21	1:A:1024:VAL:O	2.18	0.43
1:A:56:THR:O	1:A:60:THR:HG22	2.18	0.43
1:A:967:ALA:HB1	1:A:971:ARG:NH1	2.33	0.43
1:A:306:ILE:HG12	1:A:309:GLU:H	1.83	0.43
1:A:32:VAL:HA	1:A:390:ILE:HB	1.99	0.43
1:A:743:ILE:HA	1:A:746:ILE:HD12	1.99	0.43
1:A:1033:PHE:O	1:A:1035:ARG:N	2.51	0.43
1:A:737:GLN:HG2	1:A:737:GLN:H	1.64	0.43
1:A:184:MET:HB3	1:A:771:VAL:HG13	2.00	0.43
1:A:945:ILE:HD11	1:A:1019:ILE:HD12	2.01	0.43
1:A:10:ILE:N	1:A:10:ILE:CD1	2.81	0.43
1:A:112:GLN:O	1:A:112:GLN:CG	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:454:VAL:HG22	1:A:475:VAL:HG21	2.01	0.43
1:A:388:PHE:CE1	1:A:469:GLN:HG2	2.55	0.42
1:A:367:ILE:HG12	1:A:492:LEU:HD22	2.00	0.42
1:A:57:VAL:HG23	1:A:82:SER:HB3	2.01	0.42
1:A:444:GLY:O	1:A:448:VAL:HG23	2.19	0.42
1:A:514:GLY:HA2	1:A:517:ASN:HD22	1.84	0.42
1:A:534:ILE:HD12	1:A:1026:PHE:HE1	1.85	0.42
1:A:402:ILE:O	1:A:406:VAL:HG23	2.20	0.42
1:A:690:LEU:HB3	1:A:694:LYS:HD2	2.01	0.42
1:A:905:VAL:HG13	1:A:935:ILE:HG12	2.02	0.42
1:A:967:ALA:O	1:A:971:ARG:HG3	2.18	0.42
1:A:40:PRO:HA	1:A:41:PRO:HD3	1.91	0.42
1:A:426:PRO:N	1:A:427:PRO:CD	2.83	0.42
1:A:982:PHE:CD2	1:A:1011:MET:HG3	2.55	0.42
1:A:314:GLU:N	1:A:315:PRO:CD	2.83	0.42
1:A:517:ASN:O	1:A:521:GLU:HB2	2.20	0.42
1:A:26:ALA:O	1:A:30:LEU:HB2	2.20	0.42
1:A:832:ALA:HB3	1:A:835:LYS:H	1.84	0.42
1:A:162:MET:O	1:A:166:ILE:HG12	2.20	0.41
1:A:405:LEU:HD21	1:A:477:ALA:HB1	2.03	0.41
1:A:1023:PRO:HB3	1:A:1027:VAL:HG13	2.02	0.41
1:A:326:PRO:O	1:A:327:TYR:C	2.58	0.41
1:A:752:ALA:O	1:A:774:MET:HA	2.19	0.41
1:A:774:MET:HB3	1:A:775:SER:H	1.62	0.41
1:A:1026:PHE:O	1:A:1030:ARG:HG3	2.21	0.41
1:A:709:HIS:HE1	1:A:847:LEU:HD21	1.85	0.41
1:A:311:ALA:O	1:A:315:PRO:HD3	2.20	0.41
1:A:470:PHE:HA	1:A:470:PHE:HD2	1.68	0.41
1:A:312:LYS:HD2	1:A:312:LYS:HA	1.77	0.41
1:A:652:THR:HG23	1:A:665:ALA:HB3	2.03	0.41
1:A:671:ILE:HB	1:A:672:VAL:H	1.48	0.41
1:A:459:PHE:HB2	1:A:464:GLY:HA2	2.03	0.41
1:A:30:LEU:HA	1:A:31:PRO:HD2	1.94	0.40
1:A:441:ALA:O	1:A:445:ILE:HG13	2.21	0.40
1:A:897:ILE:N	1:A:898:PRO:CD	2.84	0.40
1:A:133:SER:O	1:A:135:SER:N	2.50	0.40
1:A:338:HIS:O	1:A:342:LYS:HB2	2.21	0.40
1:A:462:SER:C	1:A:464:GLY:H	2.25	0.40
1:A:602:GLU:HG3	1:A:605:ASN:HB2	2.02	0.40
1:A:989:LEU:HB3	1:A:1000:GLN:O	2.21	0.40
1:A:679:GLY:HA2	1:A:830:GLN:HA	2.04	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	998/1049 (95%)	858 (86%)	101 (10%)	39 (4%)	<b>3</b> <b>26</b>

All (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
1	A	837	THR
1	A	1021	PHE
1	A	1023	PRO
1	A	1034	SER
1	A	307	ARG
1	A	327	TYR
1	A	722	GLU
1	A	876	LEU
1	A	894	SER
1	A	971	ARG
1	A	1017	LEU
1	A	1025	PHE
1	A	9	PRO
1	A	74	ASN
1	A	310	LEU
1	A	295	THR
1	A	525	HIS
1	A	677	ALA
1	A	723	ASP
1	A	875	SER

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Mol	Chain	Res	Type
1	A	134	SER
1	A	226	LYS
1	A	720	GLY
1	A	775	SER
1	A	992	SER
1	A	223	PRO
1	A	898	PRO
1	A	991	ILE
1	A	1027	VAL
1	A	464	GLY
1	A	638	PRO
1	A	1016	VAL
1	A	402	ILE
1	A	658	ILE

### 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	818/855 (96%)	643 (79%)	175 (21%)	<b>1</b> <b>6</b>

All (175) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ILE
1	A	25	LEU
1	A	27	ILE
1	A	29	LYS
1	A	32	VAL
1	A	38	ILE
1	A	49	TYR
1	A	55	LYS
1	A	58	GLN
1	A	68	ASN
1	A	69	MET
1	A	78	MET

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	80	SER
1	A	85	THR
1	A	87	THR
1	A	89	GLN
1	A	107	VAL
1	A	108	GLN
1	A	112	GLN
1	A	125	GLN
1	A	127	VAL
1	A	130	GLU
1	A	131	LYS
1	A	134	SER
1	A	137	LEU
1	A	138	MET
1	A	140	VAL
1	A	149	MET
1	A	153	ASP
1	A	156	ASP
1	A	163	LYS
1	A	164	ASP
1	A	177	LEU
1	A	180	SER
1	A	182	TYR
1	A	185	ARG
1	A	199	THR
1	A	213	GLN
1	A	225	VAL
1	A	226	LYS
1	A	230	LEU
1	A	240	LEU
1	A	242	SER
1	A	243	THR
1	A	244	GLU
1	A	253	VAL
1	A	255	GLN
1	A	273	GLU
1	A	278	ILE
1	A	284	GLN
1	A	293	LEU
1	A	301	ASP
1	A	307	ARG
1	A	310	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	313	MET
1	A	319	SER
1	A	321	LEU
1	A	335	ILE
1	A	342	LYS
1	A	350	LEU
1	A	356	TYR
1	A	357	LEU
1	A	359	LEU
1	A	363	ARG
1	A	389	SER
1	A	404	LEU
1	A	406	VAL
1	A	408	ASP
1	A	411	VAL
1	A	415	ASN
1	A	418	ARG
1	A	422	GLU
1	A	431	THR
1	A	432	ARG
1	A	433	LYS
1	A	439	GLN
1	A	445	ILE
1	A	448	VAL
1	A	452	VAL
1	A	453	PHE
1	A	456	MET
1	A	459	PHE
1	A	462	SER
1	A	470	PHE
1	A	472	ILE
1	A	492	LEU
1	A	498	LYS
1	A	518	ARG
1	A	529	ASP
1	A	537	SER
1	A	538	THR
1	A	542	LEU
1	A	558	ARG
1	A	559	LEU
1	A	566	ASP
1	A	574	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	585	GLU
1	A	589	LYS
1	A	591	LEU
1	A	609	VAL
1	A	613	ASN
1	A	617	PHE
1	A	620	ARG
1	A	626	ILE
1	A	629	VAL
1	A	632	LYS
1	A	634	TRP
1	A	640	GLU
1	A	645	GLU
1	A	650	ARG
1	A	659	LYS
1	A	671	ILE
1	A	674	LEU
1	A	683	GLU
1	A	684	LEU
1	A	690	LEU
1	A	693	GLU
1	A	702	LEU
1	A	708	LYS
1	A	714	THR
1	A	722	GLU
1	A	723	ASP
1	A	735	LYS
1	A	737	GLN
1	A	741	VAL
1	A	763	ILE
1	A	770	LYS
1	A	774	MET
1	A	778	LYS
1	A	782	LEU
1	A	792	ARG
1	A	795	ASP
1	A	798	MET
1	A	801	PHE
1	A	806	SER
1	A	811	TYR
1	A	815	ARG
1	A	844	MET

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	846	GLN
1	A	855	VAL
1	A	872	GLN
1	A	875	SER
1	A	888	LEU
1	A	895	TRP
1	A	903	LEU
1	A	907	LEU
1	A	910	ILE
1	A	914	LEU
1	A	919	ARG
1	A	932	LEU
1	A	938	SER
1	A	940	LYS
1	A	943	ILE
1	A	945	ILE
1	A	950	LYS
1	A	960	LEU
1	A	962	GLU
1	A	968	VAL
1	A	970	MET
1	A	971	ARG
1	A	973	ARG
1	A	976	LEU
1	A	977	MET
1	A	990	VAL
1	A	991	ILE
1	A	1007	VAL
1	A	1008	MET
1	A	1017	LEU
1	A	1022	VAL
1	A	1025	PHE
1	A	1027	VAL
1	A	1028	VAL
1	A	1030	ARG
1	A	1032	ARG
1	A	1035	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	67	GLN

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Mol	Chain	Res	Type
1	A	68	ASN
1	A	106	GLN
1	A	181	GLN
1	A	194	ASN
1	A	213	GLN
1	A	228	GLN
1	A	231	ASN
1	A	282	ASN
1	A	391	ASN
1	A	517	ASN
1	A	526	HIS
1	A	605	ASN
1	A	613	ASN
1	A	622	GLN
1	A	657	GLN
1	A	747	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

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	-	33,36,36	2.59	7 (21%)	43,51,51	1.78	10 (23%)

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	-	-	6/15/21/21	0/4/4/4

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2001	RHQ	C2-C9	6.67	1.50	1.39
2	A	2001	RHQ	C19-C14	6.01	1.50	1.40
2	A	2001	RHQ	C8-C7	5.96	1.49	1.41
2	A	2001	RHQ	C11-C12	5.23	1.51	1.40
2	A	2001	RHQ	C5-C4	5.04	1.51	1.43
2	A	2001	RHQ	O2-C26	4.94	1.46	1.33
2	A	2001	RHQ	C9-C8	3.71	1.50	1.43

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2001	RHQ	C12-C11-N1	4.45	125.02	119.38
2	A	2001	RHQ	O2-C26-C19	3.96	120.03	112.21
2	A	2001	RHQ	C10-C11-N1	-3.45	116.15	121.58
2	A	2001	RHQ	C10-C7-C8	-3.17	119.54	123.05
2	A	2001	RHQ	C13-C8-C7	3.03	119.80	116.39
2	A	2001	RHQ	O1-C1-C6	2.95	119.52	116.03
2	A	2001	RHQ	O1-C7-C10	2.86	119.46	116.11
2	A	2001	RHQ	C2-C9-C8	-2.81	117.24	119.63
2	A	2001	RHQ	C21-C4-C3	-2.57	116.98	120.74
2	A	2001	RHQ	O2-C26-O27	-2.56	118.47	123.67

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2001	RHQ	C10-C11-N1-C22
2	A	2001	RHQ	C12-C11-N1-C22

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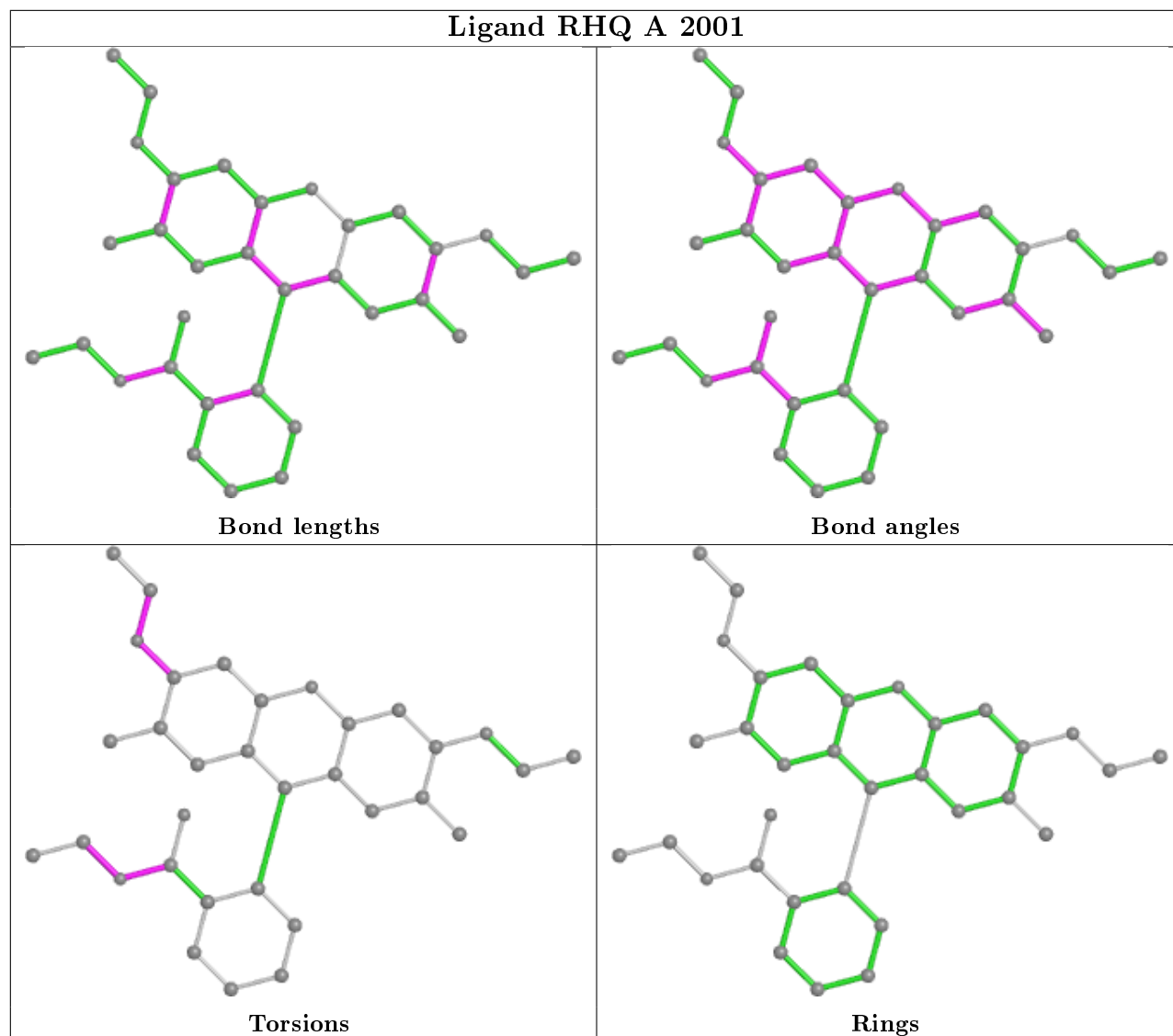
Mol	Chain	Res	Type	Atoms
2	A	2001	RHQ	C19-C26-O2-C28
2	A	2001	RHQ	O27-C26-O2-C28
2	A	2001	RHQ	C23-C22-N1-C11
2	A	2001	RHQ	C29-C28-O2-C26

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 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 [\(i\)](#)

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

### 6.2 Non-standard residues in protein, DNA, RNA chains [\(i\)](#)

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

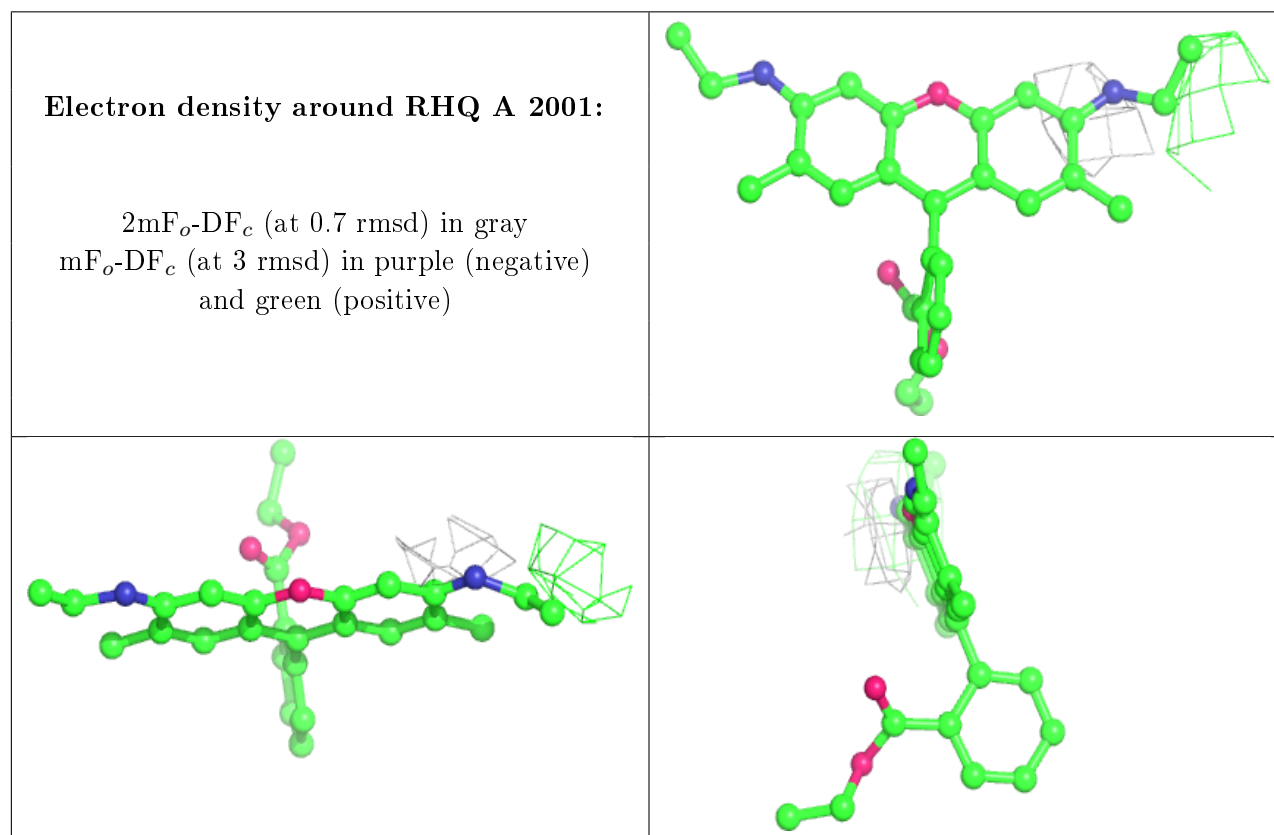
### 6.3 Carbohydrates [\(i\)](#)

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

### 6.4 Ligands [\(i\)](#)

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.



## 6.5 Other polymers

Unable to reproduce the depositor's R factor - this section is therefore empty.