



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2026 – 06:25 PM UTC

PDB ID : 4LZ9 / pdb_00004lz9
Title : Structure of MATE multidrug transporter DinF-BH in complex with R6G
Authors : Lu, M.; Radchenko, M.; Symersky, J.; Nie, R.; Guo, Y.
Deposited on : 2013-07-31
Resolution : 3.70 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
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 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

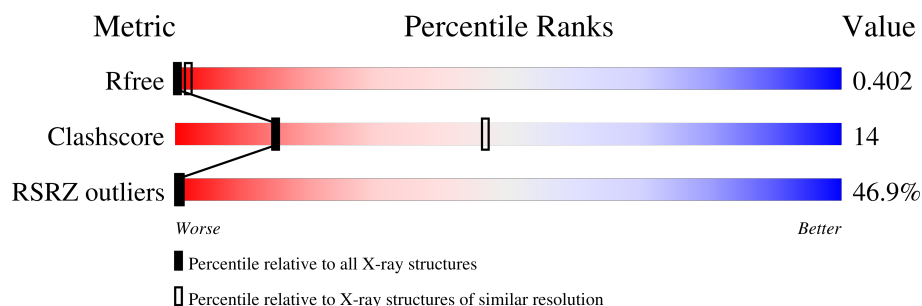
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.70 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	1131 (3.80-3.60)
Clashscore	190562	1171 (3.80-3.60)
RSRZ outliers	180081	1130 (3.80-3.60)

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	446	47% 100%

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
2	RHQ	A	501	-	-	-	X

2 Entry composition [i](#)

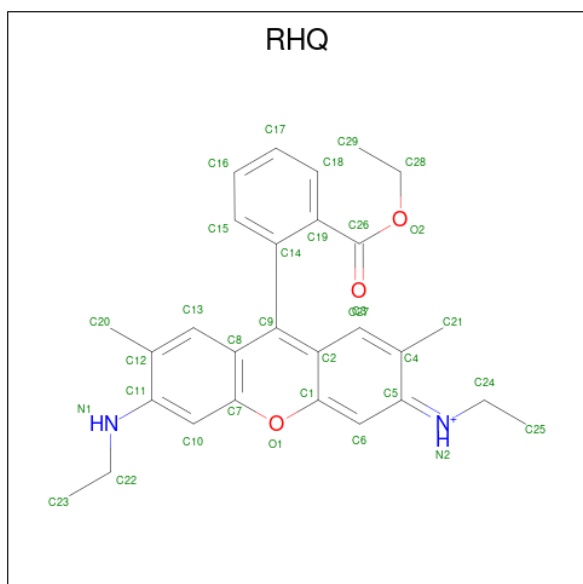
There are 2 unique types of molecules in this entry. The entry contains 479 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 BH2163 protein.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
1	A	446	Total	C		0	0	446
			446	446				

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

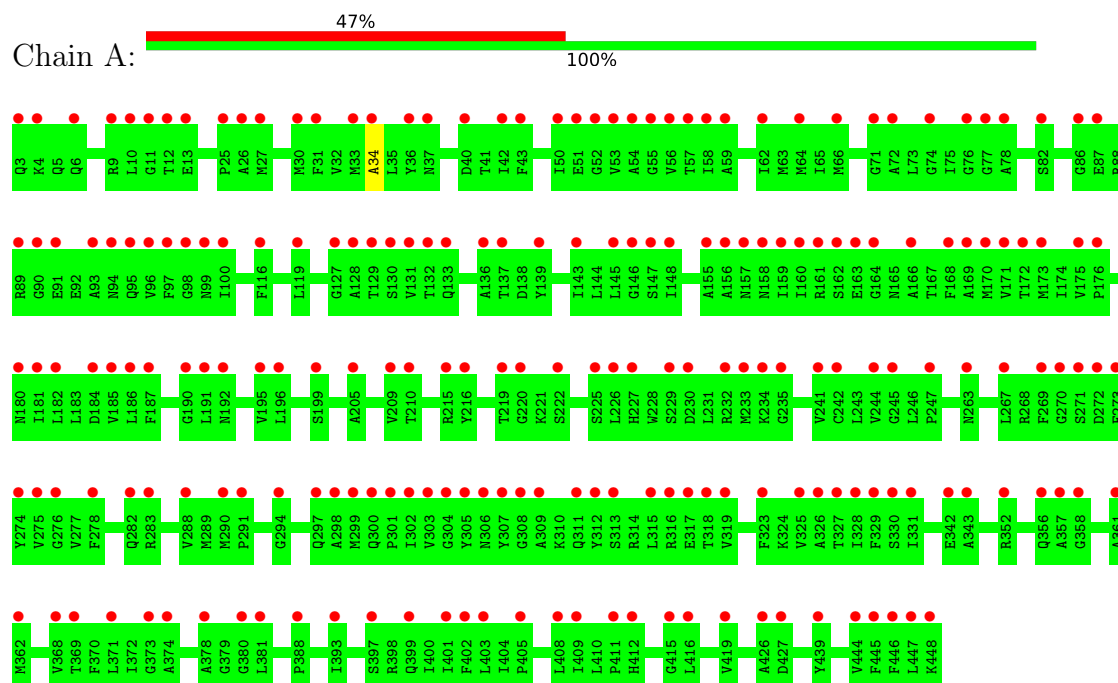


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			33	28	2	3		

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: BH2163 protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	90.18Å 93.89Å 102.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.70 20.00 – 3.70	Depositor EDS
% Data completeness (in resolution range)	95.0 (20.00-3.70) 94.4 (20.00-3.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 3.71Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.290 , 0.300 0.393 , 0.402	Depositor DCC
R_{free} test set	443 reflections (4.60%)	wwPDB-VP
Wilson B-factor (Å ²)	150.9	Xtriage
Anisotropy	0.422	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.73 , 0.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.34$, $\langle L^2 \rangle = 0.17$	Xtriage
Estimated twinning fraction	0.158 for k,h,-l	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	479	wwPDB-VP
Average B, all atoms (Å ²)	204.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.38% of the height of the origin peak. No significant pseudotranslation is detected.*

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 [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).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	446	0	0	1	0
2	A	33	0	31	7	0
All	All	479	0	31	7	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 14.

All (7) 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)
2:A:501:RHQ:H242	2:A:501:RHQ:H213	1.34	1.07
2:A:501:RHQ:H242	2:A:501:RHQ:C21	2.03	0.86
1:A:34:ALA:CA	2:A:501:RHQ:H292	2.32	0.59
2:A:501:RHQ:C20	2:A:501:RHQ:H222	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:501:RHQ:H213	2:A:501:RHQ:C24	2.24	0.49
2:A:501:RHQ:H222	2:A:501:RHQ:H201	1.99	0.43
2:A:501:RHQ:H201	2:A:501:RHQ:C22	2.51	0.41

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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 oligosaccharides 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	501	-	35,36,36	2.35	8 (22%)	49,51,51	2.11	15 (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	501	-	-	9/15/21/21	0/4/4/4

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	RHQ	C19-C14	6.63	1.51	1.40
2	A	501	RHQ	C11-C12	5.68	1.52	1.40
2	A	501	RHQ	C8-C7	5.64	1.51	1.40
2	A	501	RHQ	O2-C26	5.22	1.46	1.33
2	A	501	RHQ	C2-C1	4.09	1.51	1.43
2	A	501	RHQ	C2-C9	3.83	1.50	1.40
2	A	501	RHQ	C5-C4	2.53	1.51	1.45
2	A	501	RHQ	C14-C9	2.01	1.52	1.49

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	RHQ	C4-C5-N2	4.97	124.31	117.22
2	A	501	RHQ	O2-C26-C19	4.46	120.99	112.24
2	A	501	RHQ	C12-C11-N1	4.33	125.05	119.41
2	A	501	RHQ	C20-C12-C11	4.09	125.86	121.23
2	A	501	RHQ	C15-C14-C19	-3.76	115.05	119.26
2	A	501	RHQ	C14-C9-C2	3.70	124.86	120.33
2	A	501	RHQ	C10-C11-N1	-3.69	115.27	121.49
2	A	501	RHQ	O1-C7-C10	3.23	120.41	115.83
2	A	501	RHQ	C21-C4-C5	3.01	123.75	119.24
2	A	501	RHQ	C6-C1-C2	-2.69	119.14	122.86
2	A	501	RHQ	O2-C26-O27	-2.62	118.42	123.67
2	A	501	RHQ	C20-C12-C13	-2.41	115.33	119.57
2	A	501	RHQ	C17-C16-C15	2.39	123.19	120.24
2	A	501	RHQ	C21-C4-C3	-2.35	116.61	121.96
2	A	501	RHQ	C3-C2-C1	2.11	119.53	116.63

There are no chirality outliers.

All (9) torsion outliers are listed below:

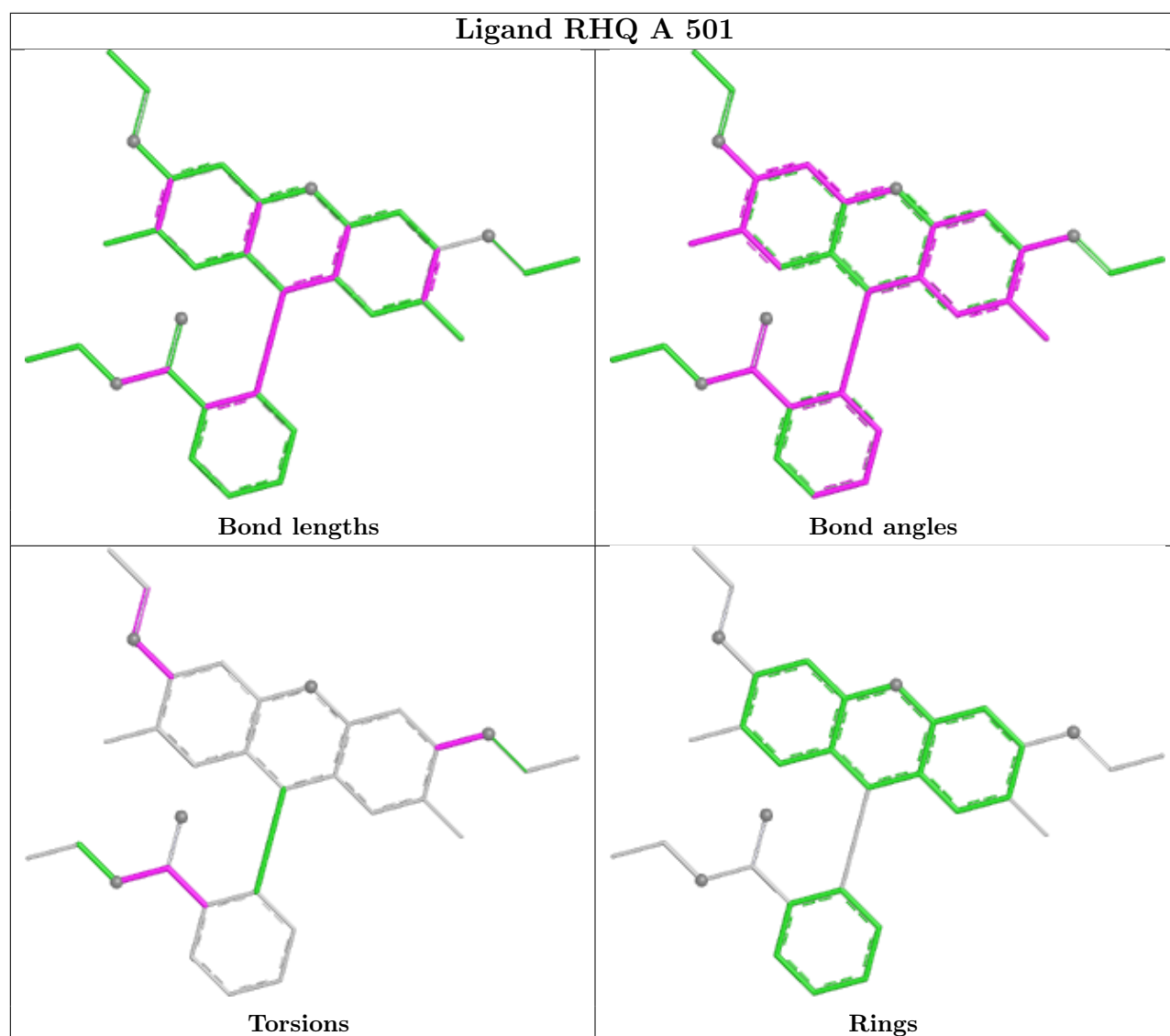
Mol	Chain	Res	Type	Atoms
2	A	501	RHQ	C6-C5-N2-C24
2	A	501	RHQ	C12-C11-N1-C22
2	A	501	RHQ	C19-C26-O2-C28
2	A	501	RHQ	O27-C26-O2-C28
2	A	501	RHQ	C10-C11-N1-C22
2	A	501	RHQ	C23-C22-N1-C11
2	A	501	RHQ	C18-C19-C26-O2
2	A	501	RHQ	C14-C19-C26-O2
2	A	501	RHQ	C18-C19-C26-O27

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	RHQ	7	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	446/446 (100%)	2.74	209 (46%) 0 1	116, 193, 286, 374	0

All (209) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	131	VAL	22.3
1	A	129	THR	21.7
1	A	270	GLY	19.0
1	A	271	SER	16.7
1	A	132	THR	14.3
1	A	269	PHE	14.2
1	A	447	LEU	12.7
1	A	4	LYS	12.7
1	A	127	GLY	12.4
1	A	128	ALA	12.2
1	A	162	SER	12.1
1	A	155	ALA	11.9
1	A	87	GLU	11.4
1	A	12	THR	11.0
1	A	74	GLY	10.6
1	A	163	GLU	10.4
1	A	358	GLY	10.4
1	A	164	GLY	9.9
1	A	205	ALA	9.8
1	A	352	ARG	9.8
1	A	230	ASP	9.7
1	A	308	GLY	9.6
1	A	90	GLY	9.1
1	A	226	LEU	9.0
1	A	59	ALA	9.0
1	A	130	SER	8.8
1	A	343	ALA	8.5

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Mol	Chain	Res	Type	RSRZ
1	A	302	ILE	8.3
1	A	219	THR	8.1
1	A	374	ALA	7.6
1	A	3	GLN	7.6
1	A	373	GLY	7.5
1	A	299	MET	7.1
1	A	55	GLY	7.1
1	A	294	GLY	7.1
1	A	82	SER	7.0
1	A	40	ASP	6.7
1	A	362	MET	6.7
1	A	225	SER	6.6
1	A	53	VAL	6.5
1	A	133	GLN	6.5
1	A	301	PRO	6.4
1	A	100	ILE	6.4
1	A	357	ALA	6.4
1	A	96	VAL	6.3
1	A	166	ALA	6.3
1	A	37	ASN	6.3
1	A	190	GLY	6.3
1	A	402	PHE	6.2
1	A	172	THR	6.0
1	A	272	ASP	6.0
1	A	156	ALA	5.8
1	A	416	LEU	5.8
1	A	184	ASP	5.7
1	A	222	SER	5.7
1	A	11	GLY	5.6
1	A	327	THR	5.5
1	A	300	GLN	5.5
1	A	94	ASN	5.5
1	A	309	ALA	5.4
1	A	275	VAL	5.4
1	A	210	THR	5.4
1	A	380	GLY	5.4
1	A	136	ALA	5.3
1	A	312	TYR	5.2
1	A	216	TYR	5.2
1	A	361	ALA	5.1
1	A	369	THR	5.1
1	A	186	LEU	5.1

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Mol	Chain	Res	Type	RSRZ
1	A	58	ILE	5.0
1	A	215	ARG	5.0
1	A	444	VAL	4.9
1	A	77	GLY	4.9
1	A	137	THR	4.8
1	A	297	GLN	4.8
1	A	244	VAL	4.7
1	A	26	ALA	4.7
1	A	185	VAL	4.7
1	A	415	GLY	4.7
1	A	303	VAL	4.6
1	A	445	PHE	4.6
1	A	448	LYS	4.6
1	A	181	ILE	4.6
1	A	419	VAL	4.5
1	A	147	SER	4.4
1	A	91	GLU	4.3
1	A	307	TYR	4.3
1	A	446	PHE	4.3
1	A	245	GLY	4.3
1	A	234	LYS	4.2
1	A	10	LEU	4.2
1	A	235	GLY	4.2
1	A	148	ILE	4.2
1	A	56	VAL	4.1
1	A	401	ILE	4.1
1	A	99	ASN	4.1
1	A	305	TYR	4.1
1	A	169	ALA	4.0
1	A	439	TYR	4.0
1	A	97	PHE	3.9
1	A	143	ILE	3.9
1	A	9	ARG	3.8
1	A	98	GLY	3.8
1	A	161	ARG	3.8
1	A	315	LEU	3.8
1	A	330	SER	3.7
1	A	368	VAL	3.7
1	A	412	HIS	3.7
1	A	72	ALA	3.7
1	A	171	VAL	3.7
1	A	54	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	36	TYR	3.6
1	A	51	GLU	3.6
1	A	247	PRO	3.6
1	A	393	ILE	3.5
1	A	173	MET	3.5
1	A	273	PHE	3.5
1	A	405	PRO	3.5
1	A	191	LEU	3.4
1	A	146	GLY	3.4
1	A	13	GLU	3.4
1	A	116	PHE	3.4
1	A	93	ALA	3.4
1	A	170	MET	3.3
1	A	408	LEU	3.3
1	A	57	THR	3.3
1	A	50	ILE	3.3
1	A	329	PHE	3.3
1	A	176	PRO	3.2
1	A	427	ASP	3.2
1	A	326	ALA	3.2
1	A	34	ALA	3.1
1	A	33	MET	3.1
1	A	263	ASN	3.1
1	A	319	VAL	3.1
1	A	52	GLY	3.1
1	A	304	GLY	3.1
1	A	95	GLN	3.1
1	A	316	ARG	3.0
1	A	356	GLN	3.0
1	A	139	TYR	2.9
1	A	187	PHE	2.9
1	A	6	GLN	2.9
1	A	323	PHE	2.9
1	A	291	PRO	2.9
1	A	119	LEU	2.8
1	A	160	ILE	2.8
1	A	209	VAL	2.8
1	A	180	ASN	2.8
1	A	306	ASN	2.8
1	A	276	GLY	2.7
1	A	158	ASN	2.7
1	A	313	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	43	PHE	2.7
1	A	229	SER	2.7
1	A	175	VAL	2.6
1	A	66	MET	2.6
1	A	328	ILE	2.6
1	A	282	GLN	2.6
1	A	71	GLY	2.6
1	A	381	LEU	2.6
1	A	342	GLU	2.6
1	A	242	CYS	2.5
1	A	89	ARG	2.5
1	A	388	PRO	2.5
1	A	411	PRO	2.5
1	A	195	VAL	2.5
1	A	317	GLU	2.5
1	A	42	ILE	2.5
1	A	62	ILE	2.5
1	A	182	LEU	2.4
1	A	157	ASN	2.4
1	A	199	SER	2.4
1	A	278	PHE	2.4
1	A	311	GLN	2.4
1	A	399	GLN	2.4
1	A	159	ILE	2.4
1	A	274	TYR	2.4
1	A	227	HIS	2.4
1	A	78	ALA	2.4
1	A	318	THR	2.4
1	A	288	VAL	2.4
1	A	220	GLY	2.3
1	A	267	LEU	2.3
1	A	241	VAL	2.3
1	A	378	ALA	2.3
1	A	409	ILE	2.3
1	A	325	VAL	2.3
1	A	233	MET	2.3
1	A	168	PHE	2.3
1	A	25	PRO	2.3
1	A	86	GLY	2.3
1	A	31	PHE	2.3
1	A	290	MET	2.3
1	A	192	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	27	MET	2.2
1	A	331	ILE	2.2
1	A	145	LEU	2.2
1	A	426	ALA	2.2
1	A	196	LEU	2.1
1	A	371	LEU	2.1
1	A	283	ARG	2.1
1	A	232	ARG	2.1
1	A	76	GLY	2.1
1	A	397	SER	2.1
1	A	30	MET	2.1
1	A	403	LEU	2.0
1	A	64	MET	2.0
1	A	298	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

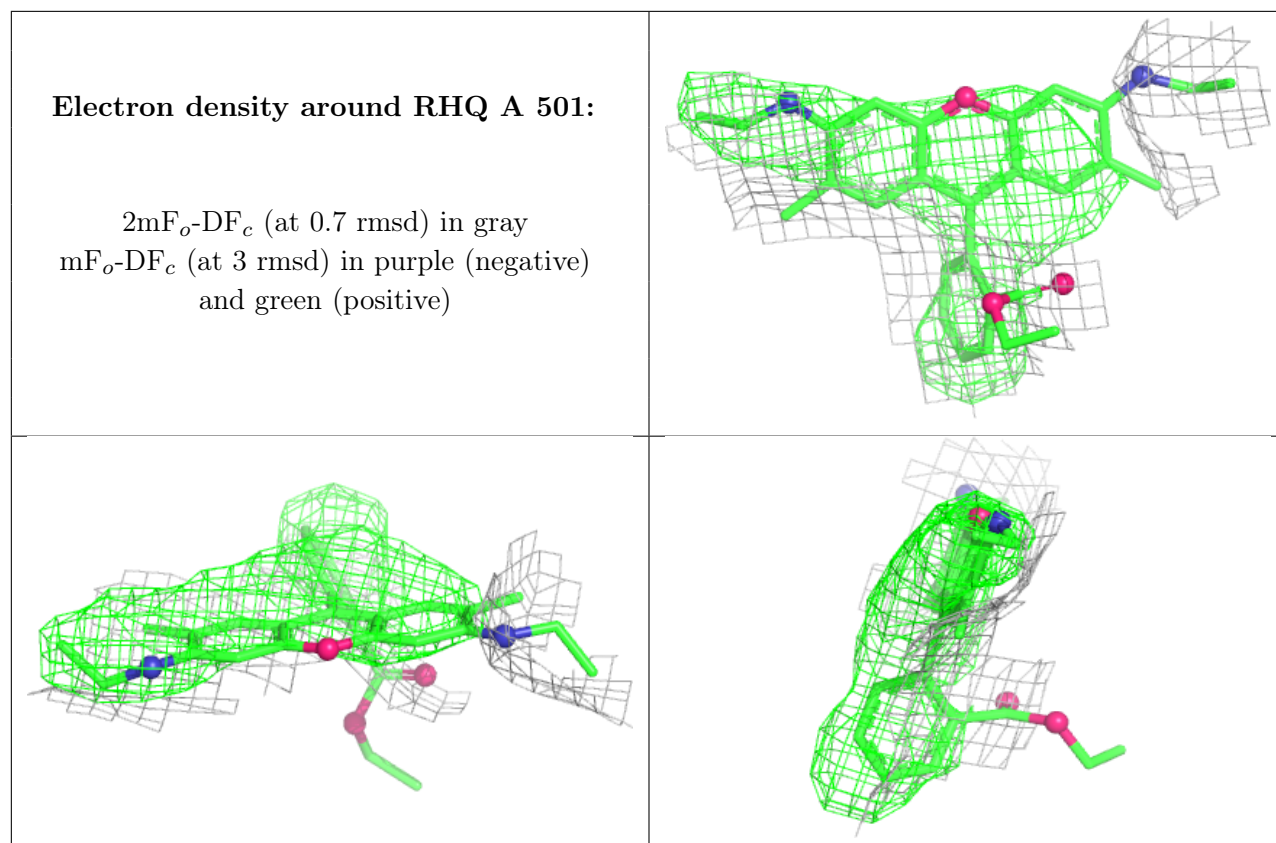
There are no oligosaccharides in this entry.

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, 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
2	RHQ	A	501	33/33	0.40	0.60	180,300,300,300	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.