



Full wwPDB X-ray Structure Validation Report ⓘ

May 7, 2026 – 11:36 AM EDT

PDB ID : 1OY8 / pdb_00001oy8
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

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

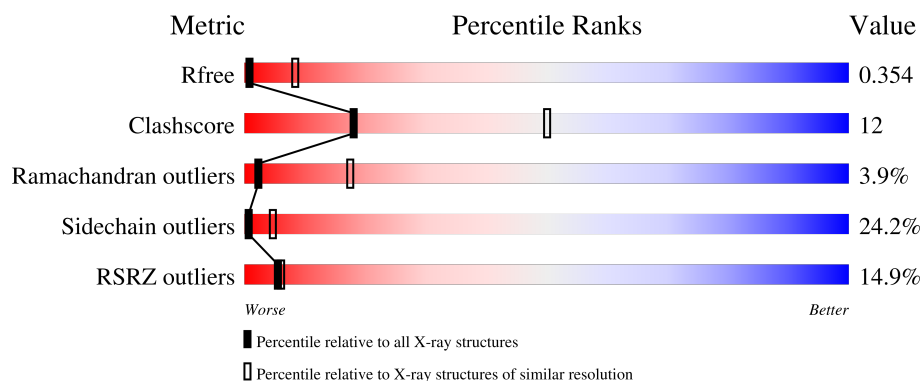
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.63 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}	180053	1132 (3.76-3.52)
Clashscore	190562	1014 (3.74-3.54)
Ramachandran outliers	187476	1123 (3.76-3.52)
Sidechain outliers	187428	1121 (3.76-3.52)
RSRZ outliers	180081	1130 (3.76-3.52)

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	1049	

2 Entry composition [i](#)

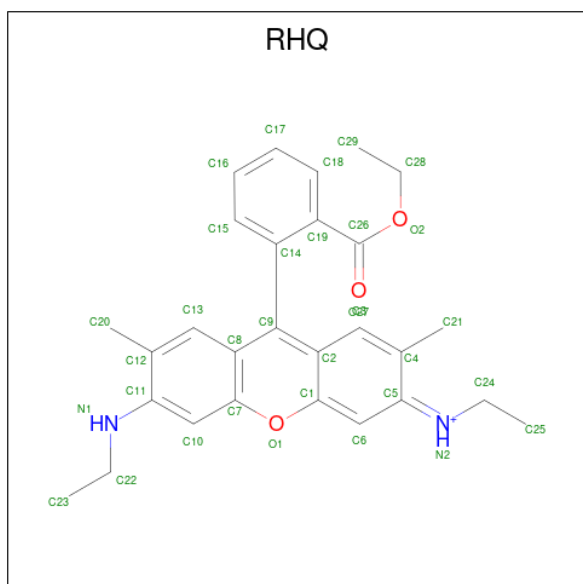
There are 2 unique types of molecules in this entry. The entry contains 7672 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
1	A	1006	Total	C	N	O	S	0	0	0
			7639	4916	1262	1419	42			

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

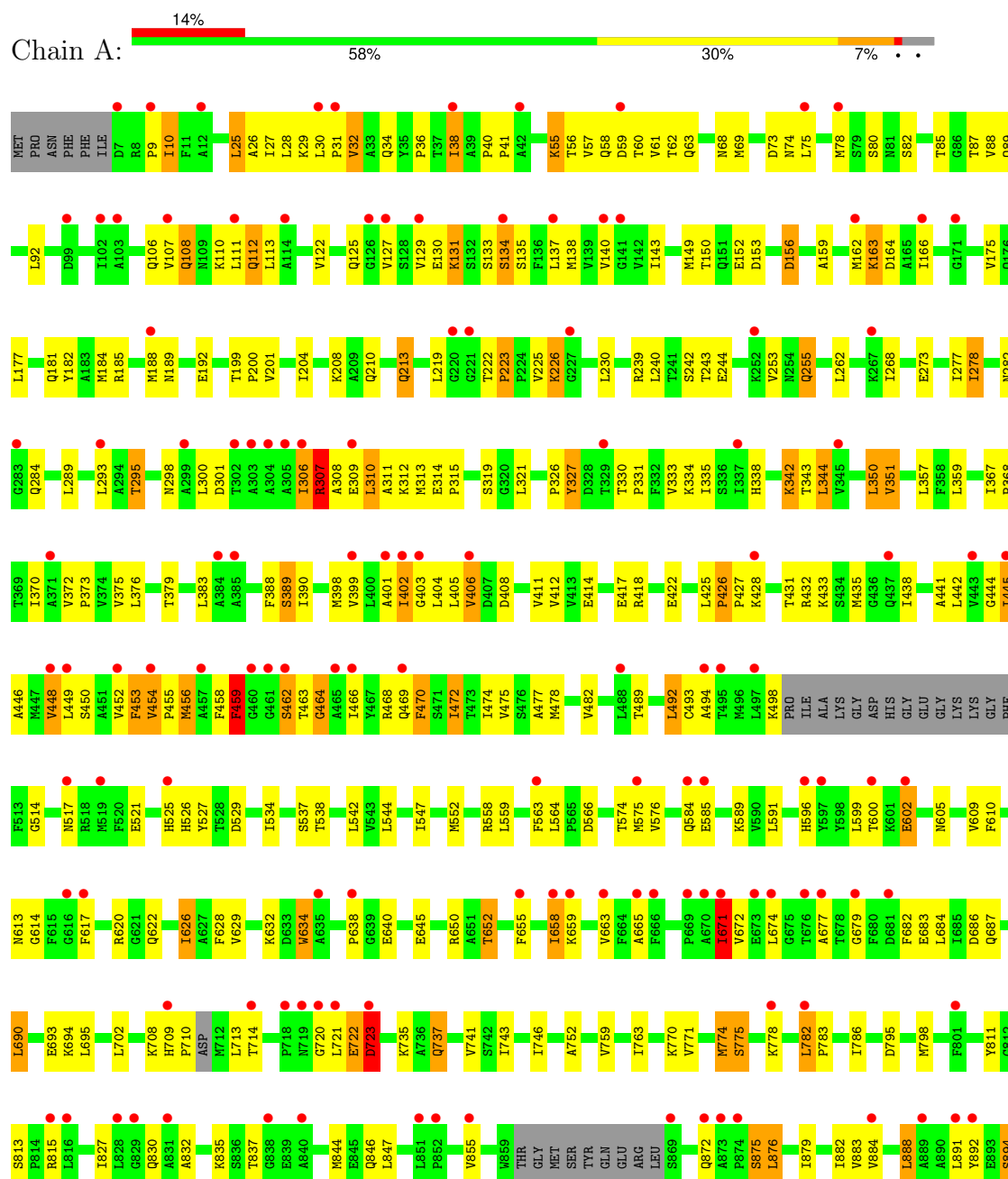


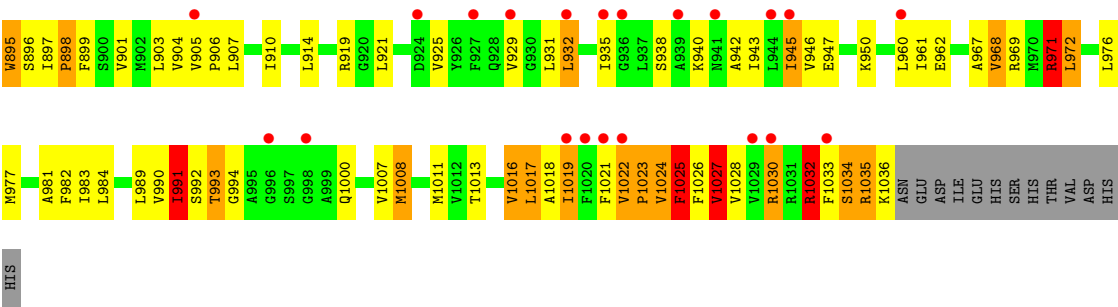
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			33	28	2	3		

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: 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 46.60 – 3.63	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.60-3.63) 99.0 (46.60-3.63)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.29 (at 3.57Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.245 , 0.322 0.353 , 0.354	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)	0.28 , 46.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.83	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.*

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: 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	0.46	1/7779 (0.0%)	0.89	1/10563 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1032	ARG	CZ-NH1	6.01	1.41	1.32

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	426	PRO	N-CA-C	7.37	119.69	110.70

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	180	0
2	A	33	0	31	9	0
All	All	7672	0	7831	189	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 12.

All (189) 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
1:A:112:GLN:HG2	1:A:112:GLN:O	1.84	0.76
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:450:SER:HB3	1:A:478:MET:HE1	1.73	0.71
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
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:552:MET:HE2	1:A:906:PRO:HB3	1.77	0.66
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
2:A:2001:RHQ:C24	2:A:2001:RHQ:H211	2.29	0.62
1:A:306:ILE:HG23	1:A:307:ARG:N	2.16	0.60
1:A:456:MET:HA	1:A:876:LEU:HB3	1.81	0.60
1:A:610:PHE:HB3	1:A:628:PHE:HB2	1.82	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:634:TRP:H	1:A:634:TRP:CD1	2.22	0.57
1:A:383:LEU:HB3	1:A:388:PHE:HB2	1.85	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:613:ASN:HD22	1:A:613:ASN:C	2.13	0.56
1:A:110:LYS:HD3	1:A:113:LEU:HD12	1.85	0.56
1:A:188:MET:HE1	1:A:200:PRO:HB3	1.88	0.55
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:425:LEU:C	1:A:427:PRO:HD2	2.31	0.54
1:A:470:PHE:HD1	1:A:929:VAL:HG21	1.71	0.54
1:A:709:HIS:CG	1:A:709:HIS:O	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:307:ARG:H	1:A:308:ALA:C	2.17	0.53
1:A:306:ILE:C	1:A:308:ALA:HB3	2.35	0.52
1:A:10:ILE:HD13	1:A:10:ILE:N	2.25	0.52
1:A:475:VAL:HA	1:A:478:MET:HE2	1.91	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
2:A:2001:RHQ:C22	2:A:2001:RHQ:H203	2.41	0.50
1:A:204:ILE:HG23	1:A:759:VAL:HG13	1.93	0.50
1:A:390:ILE:HG22	1:A:390:ILE:O	2.10	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
2:A:2001:RHQ:H211	2:A:2001:RHQ:H242	1.92	0.49
1:A:453:PHE:CE2	1:A:474:ILE:HB	2.47	0.49
1:A:897:ILE:C	1:A:899:PHE:H	2.20	0.49
1:A:904:VAL:HG11	1:A:942:ALA:HB2	1.93	0.49
1:A:75:LEU:HD21	1:A:92:LEU:HD23	1.94	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: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
2:A:2001:RHQ:H222	2:A:2001:RHQ:H203	1.94	0.49
1:A:307:ARG:N	1:A:308:ALA:C	2.71	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:GLN:HB2	1:A:129:VAL:HG21	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:401:ALA:HB2	1:A:474:ILE:HG12	1.95	0.48
1:A:671:ILE:H	1:A:671:ILE:HG13	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:62:THR:OG1	1:A:88:VAL:HG21	2.14	0.47
1:A:428:LYS:HG2	1:A:494:ALA:HB1	1.96	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
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:326:PRO:O	1:A:327:TYR:C	2.58	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:462:SER:C	1:A:464:GLY:H	2.25	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:613:ASN:C	1:A:613:ASN:ND2	2.75	0.45
1:A:489:THR:O	1:A:493:CYS:HB2	2.17	0.45
1:A:441:ALA:HB2	1:A:947:GLU:HG2	1.99	0.44
1:A:527:TYR:OH	1:A:1019:ILE:HG13	2.17	0.44
1:A:111:LEU:C	1:A:113:LEU:H	2.25	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C20	2:A:2001:RHQ:C22	2.96	0.44
1:A:370:ILE:HG22	1:A:370:ILE:O	2.18	0.44
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:32:VAL:HA	1:A:390:ILE:HB	1.99	0.43
1:A:306:ILE:HG12	1:A:309:GLU:H	1.83	0.43
1:A:412:VAL:HG13	1:A:435:MET:HE1	1.99	0.43
1:A:743:ILE:HA	1:A:746:ILE:HD12	1.99	0.43
1:A:737:GLN:H	1:A:737:GLN:HG2	1.64	0.43
1:A:1033:PHE:O	1:A:1035:ARG:N	2.51	0.43
2:A:2001:RHQ:C24	2:A:2001:RHQ:C21	2.93	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
1:A:454:VAL:HG22	1:A:475:VAL:HG21	2.01	0.43
1:A:57:VAL:HG23	1:A:82:SER:HB3	2.01	0.42
1:A:367:ILE:HG12	1:A:492:LEU:HD22	2.00	0.42
1:A:388:PHE:CE1	1:A:469:GLN:HG2	2.55	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:458:PHE:C	1:A:459:PHE:HD1	2.27	0.42
1:A:402:ILE:O	1:A:406:VAL:HG23	2.20	0.42
1:A:534:ILE:HD12	1:A:1026:PHE:HE1	1.85	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: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:982:PHE:CD2	1:A:1011:MET:HG3	2.55	0.42
1:A:26:ALA:O	1:A:30:LEU:HB2	2.20	0.42
1:A:150:THR:C	1:A:152:GLU:H	2.27	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:379:THR:HB	1:A:398:MET:HE1	2.01	0.41
1:A:405:LEU:HD21	1:A:477:ALA:HB1	2.03	0.41
1:A:710:PRO:C	1:A:713:LEU:HA	2.45	0.41
1:A:752:ALA:O	1:A:774:MET:HA	2.19	0.41
1:A:1023:PRO:HB3	1:A:1027:VAL:HG13	2.02	0.41
1:A:774:MET:HB3	1:A:775:SER:H	1.62	0.41
1:A:709:HIS:HE1	1:A:847:LEU:HD21	1.85	0.41
1:A:1026:PHE:O	1:A:1030:ARG:HG3	2.21	0.41
1:A:311:ALA:O	1:A:315:PRO:HD3	2.20	0.41
1:A:470:PHE:HD2	1:A:470:PHE:HA	1.68	0.41
1:A:312:LYS:HA	1:A:312:LYS:HD2	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
2:A:2001:RHQ:H211	2:A:2001:RHQ:H241	2.02	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:602:GLU:HG3	1:A:605:ASN:HB2	2.02	0.40
2:A:2001:RHQ:C21	2:A:2001:RHQ:H241	2.52	0.40
1:A:679:GLY:HA2	1:A:830:GLN:HA	2.04	0.40
1:A:989:LEU:HB3	1:A:1000:GLN:O	2.21	0.40

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%)	2	17

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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	658	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%)	620 (76%)	198 (24%)	1 5

All (198) 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	55	LYS
1	A	58	GLN
1	A	68	ASN
1	A	69	MET
1	A	78	MET
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	122	VAL
1	A	125	GLN
1	A	127	VAL
1	A	130	GLU
1	A	131	LYS
1	A	134	SER
1	A	137	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	138	MET
1	A	140	VAL
1	A	143	ILE
1	A	149	MET
1	A	153	ASP
1	A	156	ASP
1	A	163	LYS
1	A	164	ASP
1	A	175	VAL
1	A	177	LEU
1	A	182	TYR
1	A	185	ARG
1	A	199	THR
1	A	201	VAL
1	A	208	LYS
1	A	210	GLN
1	A	213	GLN
1	A	219	LEU
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	277	ILE
1	A	278	ILE
1	A	284	GLN
1	A	293	LEU
1	A	300	LEU
1	A	306	ILE
1	A	307	ARG
1	A	310	LEU
1	A	313	MET
1	A	319	SER
1	A	321	LEU
1	A	333	VAL
1	A	334	LYS
1	A	335	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	342	LYS
1	A	344	LEU
1	A	350	LEU
1	A	351	VAL
1	A	357	LEU
1	A	359	LEU
1	A	389	SER
1	A	404	LEU
1	A	406	VAL
1	A	408	ASP
1	A	411	VAL
1	A	418	ARG
1	A	422	GLU
1	A	431	THR
1	A	432	ARG
1	A	433	LYS
1	A	445	ILE
1	A	448	VAL
1	A	452	VAL
1	A	453	PHE
1	A	454	VAL
1	A	456	MET
1	A	459	PHE
1	A	462	SER
1	A	466	ILE
1	A	470	PHE
1	A	472	ILE
1	A	492	LEU
1	A	498	LYS
1	A	529	ASP
1	A	537	SER
1	A	538	THR
1	A	542	LEU
1	A	544	LEU
1	A	547	ILE
1	A	558	ARG
1	A	559	LEU
1	A	564	LEU
1	A	566	ASP
1	A	574	THR
1	A	585	GLU
1	A	589	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	591	LEU
1	A	602	GLU
1	A	609	VAL
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	652	THR
1	A	658	ILE
1	A	659	LYS
1	A	671	ILE
1	A	674	LEU
1	A	683	GLU
1	A	684	LEU
1	A	687	GLN
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	786	ILE
1	A	795	ASP
1	A	798	MET
1	A	811	TYR
1	A	815	ARG
1	A	844	MET
1	A	846	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	855	VAL
1	A	872	GLN
1	A	875	SER
1	A	888	LEU
1	A	891	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	921	LEU
1	A	925	VAL
1	A	931	LEU
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	961	ILE
1	A	962	GLU
1	A	968	VAL
1	A	969	ARG
1	A	971	ARG
1	A	972	LEU
1	A	976	LEU
1	A	977	MET
1	A	990	VAL
1	A	991	ILE
1	A	993	THR
1	A	1007	VAL
1	A	1008	MET
1	A	1013	THR
1	A	1016	VAL
1	A	1017	LEU
1	A	1019	ILE
1	A	1022	VAL
1	A	1024	VAL
1	A	1025	PHE
1	A	1027	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1028	VAL
1	A	1030	ARG
1	A	1032	ARG
1	A	1035	ARG
1	A	1036	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	GLN
1	A	68	ASN
1	A	106	GLN
1	A	151	GLN
1	A	189	ASN
1	A	194	ASN
1	A	218	GLN
1	A	228	GLN
1	A	237	GLN
1	A	254	ASN
1	A	282	ASN
1	A	391	ASN
1	A	439	GLN
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	701	GLN

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 [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	2001	-	35,36,36	2.10	8 (22%)	49,51,51	1.75	11 (22%)

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	-	-	7/15/21/21	0/4/4/4

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2001	RHQ	C19-C14	5.75	1.50	1.40
2	A	2001	RHQ	C11-C12	5.19	1.51	1.40
2	A	2001	RHQ	O2-C26	5.11	1.46	1.33
2	A	2001	RHQ	C8-C7	4.85	1.49	1.40
2	A	2001	RHQ	C2-C9	3.68	1.50	1.40
2	A	2001	RHQ	C2-C1	3.09	1.49	1.43
2	A	2001	RHQ	C5-C4	2.31	1.51	1.45
2	A	2001	RHQ	C3-C4	2.13	1.39	1.35

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2001	RHQ	C4-C5-N2	5.67	125.31	117.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2001	RHQ	C12-C11-N1	4.31	125.02	119.41
2	A	2001	RHQ	O2-C26-C19	3.97	120.03	112.24
2	A	2001	RHQ	C10-C11-N1	-3.17	116.15	121.49
2	A	2001	RHQ	C21-C4-C5	2.71	123.29	119.24
2	A	2001	RHQ	O2-C26-O27	-2.60	118.47	123.67
2	A	2001	RHQ	O1-C7-C10	2.56	119.46	115.83
2	A	2001	RHQ	C6-C1-C2	-2.42	119.51	122.86
2	A	2001	RHQ	C3-C2-C1	2.36	119.87	116.63
2	A	2001	RHQ	C21-C4-C3	-2.19	116.98	121.96
2	A	2001	RHQ	C7-O1-C1	2.02	123.32	119.73

There are no chirality outliers.

All (7) torsion outliers are listed below:

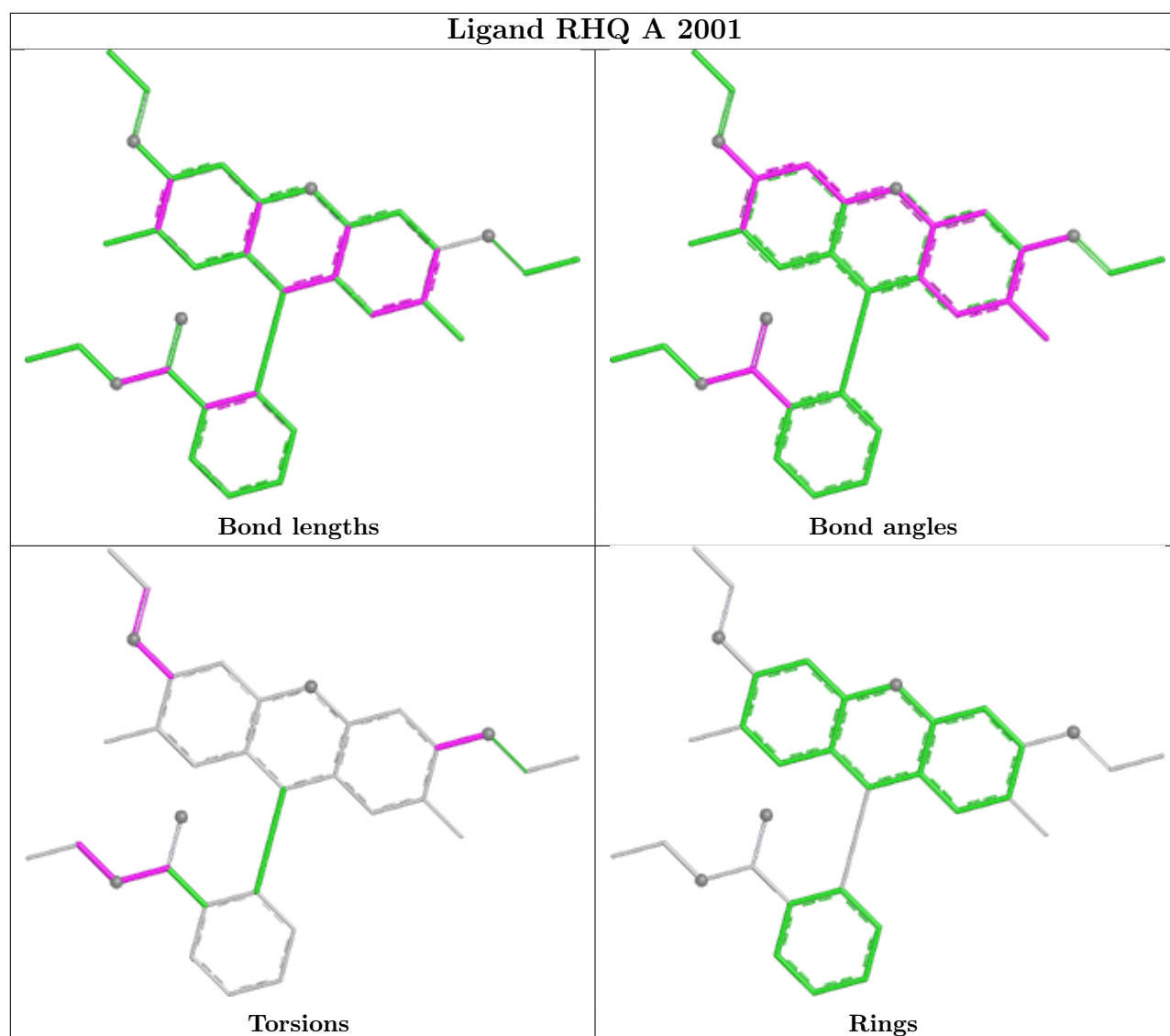
Mol	Chain	Res	Type	Atoms
2	A	2001	RHQ	C6-C5-N2-C24
2	A	2001	RHQ	C12-C11-N1-C22
2	A	2001	RHQ	C19-C26-O2-C28
2	A	2001	RHQ	O27-C26-O2-C28
2	A	2001	RHQ	C10-C11-N1-C22
2	A	2001	RHQ	C23-C22-N1-C11
2	A	2001	RHQ	C29-C28-O2-C26

There are no ring outliers.

1 monomer is involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2001	RHQ	9	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	1006/1049 (95%)	1.01	150 (14%) 5 6	55, 101, 129, 149	0

All (150) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	494	ALA	6.2
1	A	935	ILE	5.9
1	A	306	ILE	5.2
1	A	585	GLU	5.1
1	A	309	GLU	5.0
1	A	461	GLY	5.0
1	A	401	ALA	4.9
1	A	303	ALA	4.6
1	A	960	LEU	4.5
1	A	1033	PHE	4.5
1	A	829	GLY	4.4
1	A	9	PRO	4.4
1	A	448	VAL	4.4
1	A	714	THR	4.3
1	A	460	GLY	4.3
1	A	402	ILE	4.1
1	A	658	ILE	4.0
1	A	709	HIS	4.0
1	A	111	LEU	4.0
1	A	828	LEU	4.0
1	A	892	TYR	4.0
1	A	1019	ILE	3.9
1	A	495	THR	3.9
1	A	252	LYS	3.8
1	A	488	LEU	3.7
1	A	852	PRO	3.6
1	A	220	GLY	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	998	GLY	3.6
1	A	723	ASP	3.6
1	A	1021	PHE	3.6
1	A	299	ALA	3.5
1	A	399	VAL	3.5
1	A	1020	PHE	3.5
1	A	517	ASN	3.5
1	A	406	VAL	3.4
1	A	676	THR	3.4
1	A	840	ALA	3.4
1	A	428	LYS	3.4
1	A	107	VAL	3.4
1	A	12	ALA	3.4
1	A	816	LEU	3.3
1	A	638	PRO	3.3
1	A	371	ALA	3.3
1	A	78	MET	3.3
1	A	437	GLN	3.2
1	A	137	LEU	3.2
1	A	457	ALA	3.2
1	A	134	SER	3.2
1	A	293	LEU	3.2
1	A	42	ALA	3.1
1	A	721	LEU	3.1
1	A	945	ILE	3.0
1	A	129	VAL	3.0
1	A	851	LEU	3.0
1	A	31	PRO	2.9
1	A	891	LEU	2.9
1	A	519	MET	2.9
1	A	403	GLY	2.8
1	A	466	ILE	2.8
1	A	944	LEU	2.8
1	A	563	PHE	2.8
1	A	227	GLY	2.8
1	A	941	ASN	2.8
1	A	905	VAL	2.7
1	A	59	ASP	2.7
1	A	936	GLY	2.7
1	A	596	HIS	2.7
1	A	1029	VAL	2.7
1	A	782	LEU	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	102	ILE	2.7
1	A	663	VAL	2.6
1	A	673	GLU	2.6
1	A	677	ALA	2.6
1	A	600	THR	2.6
1	A	345	VAL	2.6
1	A	932	LEU	2.6
1	A	996	GLY	2.6
1	A	838	GLY	2.6
1	A	449	LEU	2.5
1	A	305	ALA	2.5
1	A	384	ALA	2.5
1	A	681	ASP	2.5
1	A	873	ALA	2.5
1	A	126	GLY	2.5
1	A	815	ARG	2.5
1	A	445	ILE	2.5
1	A	141	GLY	2.5
1	A	778	LYS	2.4
1	A	385	ALA	2.4
1	A	1030	ARG	2.4
1	A	171	GLY	2.4
1	A	720	GLY	2.4
1	A	929	VAL	2.4
1	A	597	TYR	2.4
1	A	671	ILE	2.4
1	A	869	SER	2.4
1	A	304	ALA	2.4
1	A	872	GLN	2.4
1	A	602	GLU	2.4
1	A	465	ALA	2.4
1	A	831	ALA	2.4
1	A	525	HIS	2.3
1	A	452	VAL	2.3
1	A	7	ASP	2.3
1	A	462	SER	2.3
1	A	718	PRO	2.3
1	A	855	VAL	2.3
1	A	659	LYS	2.3
1	A	655	PHE	2.3
1	A	616	GLY	2.3
1	A	162	MET	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	924	ASP	2.2
1	A	927	PHE	2.2
1	A	939	ALA	2.2
1	A	497	LEU	2.2
1	A	679	GLY	2.2
1	A	666	PHE	2.2
1	A	719	ASN	2.2
1	A	454	VAL	2.2
1	A	665	ALA	2.2
1	A	166	ILE	2.2
1	A	103	ALA	2.1
1	A	635	ALA	2.1
1	A	127	VAL	2.1
1	A	801	PHE	2.1
1	A	584	GLN	2.1
1	A	874	PRO	2.1
1	A	75	LEU	2.1
1	A	114	ALA	2.1
1	A	267	LYS	2.1
1	A	674	LEU	2.1
1	A	38	ILE	2.1
1	A	337	ILE	2.1
1	A	140	VAL	2.1
1	A	329	THR	2.1
1	A	670	ALA	2.1
1	A	469	GLN	2.1
1	A	884	VAL	2.1
1	A	1022	VAL	2.1
1	A	221	GLY	2.1
1	A	443	VAL	2.1
1	A	575	MET	2.1
1	A	188	MET	2.0
1	A	283	GLY	2.0
1	A	99	ASP	2.0
1	A	617	PHE	2.0
1	A	30	LEU	2.0
1	A	889	ALA	2.0
1	A	669	PRO	2.0
1	A	302	THR	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](#)

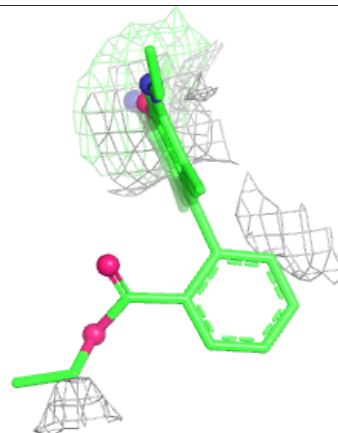
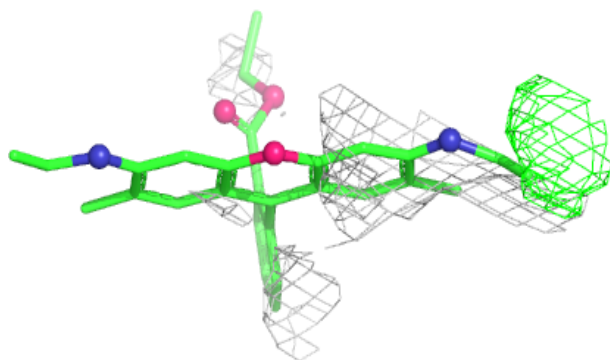
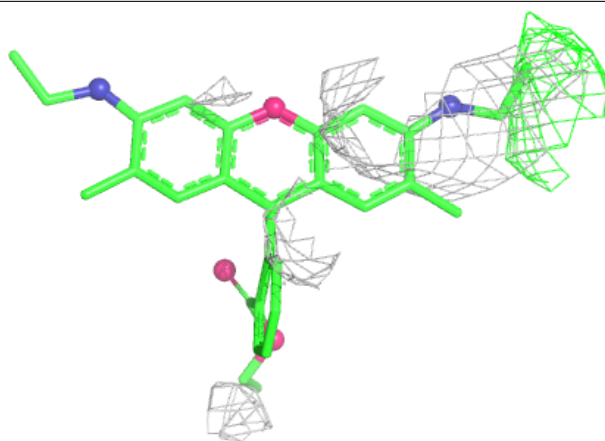
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	RHQ	A	2001	33/33	0.34	0.23	169,195,208,210	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 RHQ A 2001:

$2mF_o-DF_c$ (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.