



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 17, 2021 – 01:17 AM EDT

PDB ID : 1T9V
Title : Structural Basis of Multidrug Transport by the AcrB Multidrug Efflux Pump
Authors : Yu, E.W.; McDermott, G.; Nikaido, H.
Deposited on : 2004-05-18
Resolution : 3.80 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 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)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

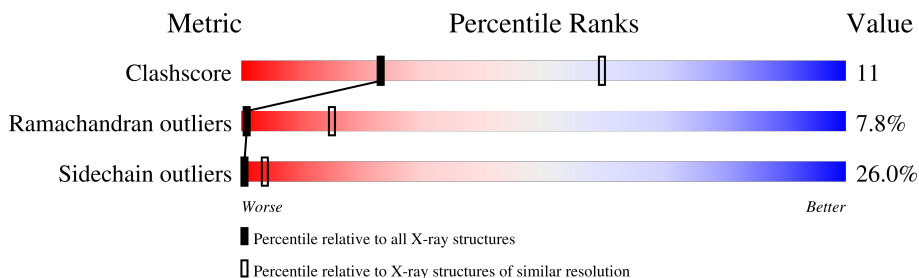
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 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))
Clashscore	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)

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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	1049	

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	2001	-	X	-	-
2	RHQ	A	2002	-	X	-	-

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 7765 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.

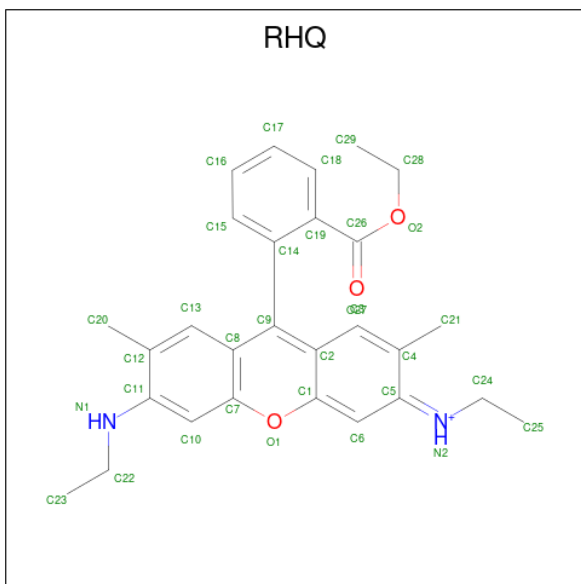
- Molecule 1 is a protein called Acriflavine resistance protein B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1014	7699	4950	1273	1434	42	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	109	ALA	ASN	engineered mutation	UNP P31224

- 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
2	A	1	33	28	2	3	0	0

V1007	M1008	T1013	A1014	T1015	V1016	L1017	A1018	I1019	F1020	F1021	V1022	P1023	V1024	F1025	F1026	V1027	V1028	V1029	R1030	R1031	R1032	R1035	K1036	ASN	GLU	ASP	ASP	ILE	GLU	GLU	HIS	SER	HIS	THR	VAL	ASP	HIS	HIS
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4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	144.37Å 144.37Å 518.44Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	182.57 – 3.80	Depositor
% Data completeness (in resolution range)	(Not available) (182.57-3.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.1	Depositor
R, R_{free}	0.277 , 0.331	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	7765	wwPDB-VP
Average B, all atoms (Å ²)	95.0	wwPDB-VP

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	0.37	0/7839	0.74	36/10644 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	4	4

There are no bond length outliers.

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1032	ARG	NE-CZ-NH1	7.17	123.89	120.30
1	A	711	ASP	N-CA-C	6.17	127.66	111.00
1	A	568	ASP	CB-CG-OD2	6.03	123.73	118.30
1	A	795	ASP	CB-CG-OD2	5.93	123.64	118.30
1	A	407	ASP	CB-CG-OD2	5.67	123.41	118.30
1	A	7	ASP	CB-CG-OD2	5.58	123.32	118.30
1	A	966	ASP	CB-CG-OD2	5.50	123.25	118.30
1	A	924	ASP	CB-CG-OD2	5.47	123.23	118.30
1	A	174	ASP	CB-CG-OD2	5.43	123.19	118.30
1	A	660	ASP	CB-CG-OD2	5.39	123.15	118.30
1	A	745	ASP	CB-CG-OD2	5.34	123.11	118.30
1	A	764	ASP	CB-CG-OD2	5.34	123.11	118.30
1	A	53	ASP	CB-CG-OD2	5.32	123.09	118.30
1	A	276	ASP	CB-CG-OD2	5.29	123.06	118.30
1	A	146	ASP	CB-CG-OD2	5.27	123.04	118.30
1	A	101	ASP	CB-CG-OD2	5.26	123.04	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	408	ASP	CB-CG-OD2	5.25	123.03	118.30
1	A	153	ASP	CB-CG-OD2	5.23	123.01	118.30
1	A	59	ASP	CB-CG-OD2	5.21	122.99	118.30
1	A	83	ASP	CB-CG-OD2	5.21	122.99	118.30
1	A	785	ASP	CB-CG-OD2	5.20	122.98	118.30
1	A	711	ASP	CB-CG-OD2	5.19	122.97	118.30
1	A	858	ASP	CB-CG-OD2	5.19	122.97	118.30
1	A	723	ASP	CB-CG-OD2	5.18	122.96	118.30
1	A	566	ASP	CB-CG-OD2	5.17	122.95	118.30
1	A	784	ASP	CB-CG-OD2	5.16	122.94	118.30
1	A	954	ASP	CB-CG-OD2	5.16	122.94	118.30
1	A	719	ASN	N-CA-C	5.13	124.86	111.00
1	A	256	ASP	CB-CG-OD2	5.12	122.91	118.30
1	A	730	ASP	CB-CG-OD2	5.12	122.91	118.30
1	A	636	ASP	CB-CG-OD2	5.09	122.88	118.30
1	A	633	ASP	CB-CG-OD2	5.08	122.87	118.30
1	A	722	GLU	N-CA-C	5.07	124.69	111.00
1	A	301	ASP	CB-CG-OD2	5.07	122.86	118.30
1	A	713	LEU	CA-CB-CG	5.06	126.94	115.30
1	A	202	ASP	CB-CG-OD2	5.02	122.82	118.30

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	474	ILE	CA
1	A	711	ASP	CA
1	A	719	ASN	CA
1	A	722	GLU	CA

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1022	VAL	Peptide
1	A	525	HIS	Peptide
1	A	712	MET	Peptide
1	A	864	TYR	Peptide

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	7699	0	7856	174	0
2	A	66	0	62	18	0
All	All	7765	0	7918	178	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 (178) 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:717:ARG:HD3	2:A:2002:RHQ:C22	1.86	1.05
1:A:717:ARG:HD3	2:A:2002:RHQ:H221	1.44	0.99
1:A:717:ARG:CD	2:A:2002:RHQ:H222	2.04	0.88
1:A:717:ARG:HD3	2:A:2002:RHQ:H222	1.56	0.88
1:A:1023:PRO:HB3	1:A:1027:VAL:HG13	1.56	0.88
1:A:525:HIS:HB2	1:A:526:HIS:HB2	1.56	0.87
1:A:717:ARG:NE	2:A:2002:RHQ:H222	1.93	0.84
1:A:710:PRO:HB2	1:A:713:LEU:HA	1.64	0.80
1:A:717:ARG:CD	2:A:2002:RHQ:C22	2.60	0.80
1:A:709:HIS:CD2	1:A:709:HIS:O	2.39	0.76
1:A:471:SER:O	1:A:473:THR:N	2.19	0.75
1:A:860:THR:HG22	1:A:861:GLY:HA3	1.68	0.74
1:A:525:HIS:CB	1:A:526:HIS:HB2	2.19	0.73
1:A:298:ASN:HD22	1:A:298:ASN:N	1.90	0.70
1:A:613:ASN:HD22	1:A:613:ASN:C	1.96	0.69
1:A:717:ARG:CZ	2:A:2002:RHQ:H222	2.24	0.68
2:A:2002:RHQ:H242	2:A:2002:RHQ:H211	1.76	0.67
1:A:386:PHE:CE2	2:A:2001:RHQ:H61	2.30	0.66
2:A:2001:RHQ:H211	2:A:2001:RHQ:H242	1.76	0.66
1:A:399:VAL:HA	1:A:402:ILE:HD12	1.79	0.64
1:A:1015:THR:O	1:A:1019:ILE:HG22	1.99	0.63
1:A:344:LEU:HD23	1:A:402:ILE:HD11	1.81	0.61
1:A:463:THR:OG1	1:A:868:LEU:HD22	1.99	0.61
1:A:1024:VAL:O	1:A:1025:PHE:CG	2.53	0.61
1:A:218:GLN:HE21	1:A:231:ASN:HD21	1.49	0.60
1:A:595:THR:HG22	1:A:599:LEU:HD12	1.84	0.59
1:A:383:LEU:HD21	1:A:473:THR:HA	1.83	0.59
1:A:668:LEU:O	1:A:668:LEU:HD13	2.02	0.58
1:A:1023:PRO:HA	1:A:1026:PHE:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:897:ILE:O	1:A:900:SER:OG	2.22	0.57
1:A:527:TYR:O	1:A:531:VAL:HG23	2.05	0.56
1:A:684:LEU:HD11	1:A:855:VAL:CG1	2.35	0.56
1:A:563:PHE:CD1	1:A:868:LEU:HD13	2.41	0.56
1:A:1032:ARG:CG	1:A:1032:ARG:HH11	2.19	0.55
1:A:108:GLN:HB3	1:A:129:VAL:HG21	1.88	0.55
1:A:676:THR:HB	2:A:2002:RHQ:C28	2.37	0.55
1:A:441:ALA:HB2	1:A:947:GLU:HG2	1.88	0.55
1:A:929:VAL:HA	1:A:932:LEU:HD12	1.89	0.55
1:A:894:SER:HB2	1:A:895:TRP:C	2.27	0.55
1:A:710:PRO:HB2	1:A:713:LEU:CA	2.36	0.54
1:A:60:THR:HG23	1:A:61:VAL:HG23	1.89	0.54
1:A:873:ALA:HB3	1:A:874:PRO:CD	2.38	0.54
1:A:684:LEU:HD23	1:A:699:ARG:HB2	1.88	0.54
1:A:989:LEU:HD22	1:A:1000:GLN:HE21	1.73	0.54
1:A:867:ARG:HB3	1:A:868:LEU:HG	1.90	0.53
1:A:868:LEU:O	1:A:873:ALA:HB2	2.08	0.53
1:A:1027:VAL:HG23	1:A:1028:VAL:H	1.73	0.53
1:A:867:ARG:C	1:A:868:LEU:HD23	2.29	0.53
1:A:905:VAL:HG23	1:A:906:PRO:HD3	1.90	0.52
1:A:709:HIS:O	1:A:709:HIS:CG	2.63	0.52
1:A:344:LEU:CD2	1:A:402:ILE:HD11	2.40	0.52
1:A:709:HIS:N	1:A:710:PRO:HD3	2.25	0.52
1:A:375:VAL:HG11	1:A:405:LEU:HD22	1.92	0.51
1:A:10:ILE:CD1	1:A:10:ILE:N	2.73	0.51
1:A:1022:VAL:HG22	1:A:1023:PRO:HD2	1.92	0.51
1:A:459:PHE:CD1	1:A:459:PHE:N	2.78	0.51
1:A:222:THR:HB	1:A:223:PRO:HD3	1.93	0.51
1:A:1032:ARG:HH11	1:A:1032:ARG:HG3	1.76	0.51
1:A:156:ASP:OD2	1:A:769:LYS:NZ	2.44	0.50
1:A:74:ASN:HD22	1:A:74:ASN:N	2.09	0.50
1:A:383:LEU:HD11	1:A:473:THR:HG23	1.94	0.50
1:A:425:LEU:C	1:A:427:PRO:HD2	2.32	0.50
1:A:531:VAL:O	1:A:534:ILE:HG13	2.10	0.50
1:A:386:PHE:HE2	2:A:2001:RHQ:H61	1.74	0.50
1:A:372:VAL:H	1:A:373:PRO:HD2	1.77	0.50
1:A:61:VAL:HG21	1:A:122:VAL:HG21	1.95	0.49
1:A:777:ALA:O	1:A:781:MET:HG2	2.11	0.49
1:A:240:LEU:HD12	1:A:245:GLU:HB3	1.93	0.49
1:A:931:LEU:O	1:A:935:ILE:HD12	2.13	0.49
1:A:886:LEU:O	1:A:889:ALA:HB3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:452:VAL:O	1:A:932:LEU:HD22	2.13	0.48
1:A:894:SER:HB2	1:A:895:TRP:CA	2.44	0.48
1:A:739:LEU:HD12	1:A:799:VAL:HG11	1.94	0.48
1:A:475:VAL:HG13	1:A:478:MET:HE2	1.96	0.48
1:A:77:TYR:OH	1:A:861:GLY:O	2.20	0.48
1:A:298:ASN:N	1:A:298:ASN:ND2	2.61	0.48
1:A:146:ASP:O	1:A:148:THR:N	2.47	0.47
1:A:386:PHE:CZ	2:A:2001:RHQ:H61	2.49	0.47
1:A:864:TYR:CD2	1:A:864:TYR:N	2.82	0.47
1:A:38:ILE:HG21	1:A:466:ILE:HD11	1.95	0.47
1:A:428:LYS:HE3	1:A:494:ALA:HB1	1.96	0.47
1:A:543:VAL:HA	1:A:546:LEU:HD12	1.97	0.47
1:A:326:PRO:O	1:A:327:TYR:C	2.52	0.47
1:A:416:VAL:O	1:A:420:MET:HG3	2.15	0.47
1:A:669:PRO:HB3	1:A:671:ILE:HD12	1.96	0.47
1:A:611:ALA:HA	1:A:627:ALA:HA	1.97	0.47
1:A:672:VAL:HG23	1:A:674:LEU:HD23	1.97	0.47
1:A:115:MET:N	1:A:116:PRO:CD	2.77	0.47
1:A:366:LEU:O	1:A:370:ILE:HG13	2.15	0.47
1:A:727:PHE:CZ	1:A:783:PRO:HB3	2.50	0.47
1:A:664:PHE:O	1:A:665:ALA:CB	2.63	0.46
1:A:1024:VAL:H	1:A:1027:VAL:HG22	1.80	0.46
1:A:378:GLY:O	1:A:382:VAL:HG23	2.14	0.46
1:A:143:ILE:HG22	1:A:286:ALA:HB2	1.96	0.46
1:A:669:PRO:O	1:A:670:ALA:CB	2.64	0.46
1:A:873:ALA:HB3	1:A:874:PRO:HD3	1.98	0.46
1:A:117:LEU:HD23	1:A:117:LEU:N	2.31	0.46
1:A:894:SER:CB	1:A:895:TRP:HA	2.45	0.46
1:A:970:MET:HG3	1:A:970:MET:O	2.15	0.46
1:A:973:ARG:HB3	1:A:974:PRO:CD	2.45	0.46
1:A:21:LEU:O	1:A:23:GLY:N	2.48	0.45
1:A:487:ILE:HG22	1:A:488:LEU:N	2.31	0.45
1:A:631:LEU:HD13	1:A:637:ARG:NH1	2.31	0.45
1:A:412:VAL:O	1:A:416:VAL:HG23	2.16	0.45
1:A:987:MET:N	1:A:988:PRO:HD2	2.32	0.45
1:A:466:ILE:CG2	1:A:925:VAL:HG21	2.47	0.45
1:A:894:SER:CB	1:A:895:TRP:CA	2.94	0.45
1:A:466:ILE:HG21	1:A:925:VAL:HG21	1.98	0.45
1:A:572:PHE:CE2	1:A:629:VAL:HG11	2.51	0.45
1:A:367:ILE:HG23	1:A:492:LEU:HD22	1.99	0.44
1:A:1027:VAL:O	1:A:1028:VAL:C	2.56	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339:GLU:O	1:A:340:VAL:HG23	2.18	0.44
1:A:21:LEU:O	1:A:22:ALA:C	2.56	0.44
1:A:531:VAL:HA	1:A:534:ILE:HG12	1.98	0.44
1:A:463:THR:CB	1:A:868:LEU:HD22	2.48	0.43
1:A:415:ASN:HB3	1:A:438:ILE:HD11	2.00	0.43
1:A:680:PHE:CZ	1:A:829:GLY:HA3	2.54	0.43
1:A:10:ILE:HG12	1:A:11:PHE:CD2	2.53	0.43
1:A:445:ILE:O	1:A:449:LEU:HB2	2.19	0.43
1:A:744:ASN:O	1:A:748:THR:HG22	2.18	0.43
1:A:1027:VAL:HG12	1:A:1031:ARG:HE	1.82	0.43
1:A:448:VAL:HG11	1:A:888:LEU:HG	2.00	0.43
1:A:686:ASP:HB2	1:A:695:LEU:HD12	2.01	0.43
1:A:104:GLN:O	1:A:106:GLN:N	2.52	0.43
1:A:240:LEU:HD12	1:A:245:GLU:CB	2.49	0.43
1:A:420:MET:HE1	1:A:497:LEU:HG	1.99	0.43
1:A:950:LYS:N	1:A:950:LYS:HE3	2.34	0.43
1:A:12:ALA:HB1	1:A:487:ILE:HG22	1.99	0.43
1:A:201:VAL:HG22	1:A:748:THR:HG23	2.01	0.42
1:A:478:MET:HG2	1:A:479:ALA:N	2.33	0.42
1:A:254:ASN:O	1:A:256:ASP:N	2.52	0.42
1:A:457:ALA:HB2	1:A:471:SER:HB3	1.99	0.42
1:A:1018:ALA:O	1:A:1024:VAL:HB	2.19	0.42
1:A:404:LEU:HD11	1:A:449:LEU:HD21	2.00	0.42
1:A:945:ILE:HA	1:A:971:ARG:CZ	2.49	0.42
1:A:970:MET:O	1:A:971:ARG:HB3	2.19	0.42
1:A:451:ALA:HB1	1:A:883:VAL:HB	2.01	0.42
1:A:463:THR:HG23	1:A:466:ILE:HG21	2.01	0.42
1:A:1016:VAL:O	1:A:1017:LEU:HB2	2.20	0.42
1:A:40:PRO:HA	1:A:41:PRO:HD3	1.91	0.42
1:A:534:ILE:HB	1:A:1026:PHE:CZ	2.55	0.42
1:A:1024:VAL:N	1:A:1027:VAL:HG22	2.35	0.42
1:A:397:GLY:HA2	1:A:474:ILE:HD11	2.02	0.42
1:A:682:PHE:HB3	1:A:827:ILE:HB	2.01	0.41
1:A:851:LEU:HB3	1:A:852:PRO:CD	2.49	0.41
1:A:967:ALA:O	1:A:971:ARG:HG3	2.20	0.41
1:A:31:PRO:HG2	1:A:389:SER:HB3	2.02	0.41
1:A:120:GLN:HA	1:A:123:GLN:HB2	2.01	0.41
1:A:972:LEU:C	1:A:972:LEU:HD13	2.40	0.41
1:A:946:VAL:HG22	1:A:950:LYS:HZ1	1.84	0.41
1:A:188:MET:N	1:A:775:SER:HA	2.36	0.41
1:A:489:THR:HB	1:A:490:PRO:CD	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:613:ASN:C	1:A:613:ASN:ND2	2.68	0.41
1:A:676:THR:HB	2:A:2002:RHQ:H281	2.03	0.41
1:A:959:GLY:HA3	1:A:963:ALA:HB2	2.03	0.41
1:A:1013:THR:HG22	1:A:1017:LEU:HD22	2.02	0.41
1:A:144:ASN:ND2	1:A:149:MET:SD	2.94	0.41
1:A:403:GLY:HA3	1:A:982:PHE:CD1	2.56	0.41
1:A:717:ARG:NH2	2:A:2002:RHQ:H203	2.36	0.41
1:A:372:VAL:N	1:A:373:PRO:HD2	2.36	0.41
1:A:386:PHE:HE2	2:A:2001:RHQ:C6	2.33	0.41
1:A:431:THR:O	1:A:435:MET:HG2	2.21	0.41
1:A:451:ALA:O	1:A:455:PRO:HG2	2.21	0.41
1:A:754:TRP:CZ2	1:A:786:ILE:HG12	2.56	0.41
1:A:979:SER:CB	1:A:1015:THR:HG21	2.51	0.41
2:A:2001:RHQ:H232	2:A:2001:RHQ:H202	2.03	0.41
1:A:228:GLN:HE21	1:A:229:GLN:H	1.70	0.40
2:A:2002:RHQ:H202	2:A:2002:RHQ:H232	2.03	0.40
1:A:140:VAL:HG11	1:A:310:LEU:HD11	2.03	0.40
1:A:901:VAL:O	1:A:904:VAL:HG23	2.21	0.40
1:A:952:LEU:O	1:A:957:GLY:O	2.39	0.40
1:A:420:MET:HG2	1:A:425:LEU:O	2.21	0.40
1:A:571:VAL:O	1:A:668:LEU:HG	2.22	0.40
1:A:707:ALA:HA	1:A:710:PRO:HG3	2.04	0.40
1:A:923:ASN:C	1:A:923:ASN:HD22	2.22	0.40
1:A:894:SER:HB2	1:A:896:SER:N	2.36	0.40
1:A:907:LEU:HG	1:A:1022:VAL:CG1	2.51	0.40
1:A:973:ARG:HB3	1:A:974:PRO:HD3	2.03	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	1006/1049 (96%)	797 (79%)	131 (13%)	78 (8%)	1 15

All (78) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	9	PRO
1	A	22	ALA
1	A	34	GLN
1	A	110	LYS
1	A	121	GLU
1	A	134	SER
1	A	255	GLN
1	A	299	ALA
1	A	340	VAL
1	A	459	PHE
1	A	472	ILE
1	A	526	HIS
1	A	669	PRO
1	A	670	ALA
1	A	713	LEU
1	A	865	GLN
1	A	874	PRO
1	A	889	ALA
1	A	896	SER
1	A	971	ARG
1	A	1017	LEU
1	A	1021	PHE
1	A	1023	PRO
1	A	1025	PHE
1	A	1027	VAL
1	A	10	ILE
1	A	104	GLN
1	A	135	SER
1	A	147	GLY
1	A	152	GLU
1	A	161	ASN
1	A	327	TYR
1	A	421	ALA
1	A	722	GLU
1	A	775	SER
1	A	864	TYR
1	A	870	GLY
1	A	875	SER

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Mol	Chain	Res	Type
1	A	893	GLU
1	A	995	ALA
1	A	74	ASN
1	A	170	SER
1	A	209	ALA
1	A	431	THR
1	A	488	LEU
1	A	665	ALA
1	A	671	ILE
1	A	866	GLU
1	A	894	SER
1	A	991	ILE
1	A	105	VAL
1	A	119	PRO
1	A	146	ASP
1	A	405	LEU
1	A	525	HIS
1	A	538	THR
1	A	580	ALA
1	A	638	PRO
1	A	677	ALA
1	A	837	THR
1	A	21	LEU
1	A	109	ALA
1	A	223	PRO
1	A	424	GLY
1	A	672	VAL
1	A	992	SER
1	A	1028	VAL
1	A	1035	ARG
1	A	326	PRO
1	A	644	VAL
1	A	940	LYS
1	A	217	GLY
1	A	571	VAL
1	A	720	GLY
1	A	710	PRO
1	A	1029	VAL
1	A	444	GLY
1	A	626	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	824/854 (96%)	610 (74%)	214 (26%)	0 4

All (214) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ARG
1	A	10	ILE
1	A	15	ILE
1	A	27	ILE
1	A	30	LEU
1	A	32	VAL
1	A	38	ILE
1	A	46	SER
1	A	49	TYR
1	A	55	LYS
1	A	58	GLN
1	A	59	ASP
1	A	67	GLN
1	A	68	ASN
1	A	74	ASN
1	A	80	SER
1	A	82	SER
1	A	83	ASP
1	A	89	GLN
1	A	110	LYS
1	A	112	GLN
1	A	117	LEU
1	A	120	GLN
1	A	122	VAL
1	A	128	SER
1	A	137	LEU
1	A	138	MET
1	A	149	MET
1	A	150	THR
1	A	153	ASP

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Mol	Chain	Res	Type
1	A	162	MET
1	A	164	ASP
1	A	166	ILE
1	A	168	ARG
1	A	169	THR
1	A	177	LEU
1	A	182	TYR
1	A	185	ARG
1	A	213	GLN
1	A	225	VAL
1	A	226	LYS
1	A	230	LEU
1	A	238	THR
1	A	243	THR
1	A	249	ILE
1	A	253	VAL
1	A	255	GLN
1	A	263	ARG
1	A	265	VAL
1	A	278	ILE
1	A	280	GLU
1	A	284	GLN
1	A	292	LYS
1	A	293	LEU
1	A	298	ASN
1	A	300	LEU
1	A	312	LYS
1	A	313	MET
1	A	321	LEU
1	A	333	VAL
1	A	335	ILE
1	A	340	VAL
1	A	342	LYS
1	A	343	THR
1	A	349	ILE
1	A	350	LEU
1	A	351	VAL
1	A	355	MET
1	A	359	LEU
1	A	360	GLN
1	A	363	ARG
1	A	366	LEU

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Mol	Chain	Res	Type
1	A	376	LEU
1	A	386	PHE
1	A	393	LEU
1	A	406	VAL
1	A	407	ASP
1	A	408	ASP
1	A	412	VAL
1	A	415	ASN
1	A	417	GLU
1	A	418	ARG
1	A	422	GLU
1	A	423	GLU
1	A	425	LEU
1	A	428	LYS
1	A	429	GLU
1	A	431	THR
1	A	433	LYS
1	A	439	GLN
1	A	445	ILE
1	A	447	MET
1	A	449	LEU
1	A	453	PHE
1	A	454	VAL
1	A	459	PHE
1	A	472	ILE
1	A	474	ILE
1	A	478	MET
1	A	484	VAL
1	A	492	LEU
1	A	497	LEU
1	A	498	LYS
1	A	519	MET
1	A	522	LYS
1	A	526	HIS
1	A	536	ARG
1	A	542	LEU
1	A	546	LEU
1	A	547	ILE
1	A	552	MET
1	A	555	LEU
1	A	557	VAL
1	A	558	ARG

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Mol	Chain	Res	Type
1	A	574	THR
1	A	575	MET
1	A	585	GLU
1	A	586	ARG
1	A	596	HIS
1	A	602	GLU
1	A	613	ASN
1	A	617	PHE
1	A	622	GLN
1	A	632	LYS
1	A	633	ASP
1	A	636	ASP
1	A	640	GLU
1	A	641	GLU
1	A	643	LYS
1	A	645	GLU
1	A	650	ARG
1	A	658	ILE
1	A	659	LYS
1	A	667	ASN
1	A	668	LEU
1	A	672	VAL
1	A	674	LEU
1	A	685	ILE
1	A	692	HIS
1	A	699	ARG
1	A	702	LEU
1	A	708	LYS
1	A	711	ASP
1	A	712	MET
1	A	713	LEU
1	A	714	THR
1	A	715	SER
1	A	717	ARG
1	A	719	ASN
1	A	721	LEU
1	A	730	ASP
1	A	734	GLU
1	A	739	LEU
1	A	741	VAL
1	A	742	SER
1	A	748	THR

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Mol	Chain	Res	Type
1	A	765	ARG
1	A	767	ARG
1	A	768	VAL
1	A	773	VAL
1	A	774	MET
1	A	792	ARG
1	A	797	GLN
1	A	798	MET
1	A	801	PHE
1	A	802	SER
1	A	804	PHE
1	A	815	ARG
1	A	818	ARG
1	A	822	LEU
1	A	836	SER
1	A	842	GLU
1	A	843	LEU
1	A	844	MET
1	A	846	GLN
1	A	860	THR
1	A	864	TYR
1	A	865	GLN
1	A	868	LEU
1	A	871	ASN
1	A	880	SER
1	A	882	ILE
1	A	884	VAL
1	A	886	LEU
1	A	902	MET
1	A	903	LEU
1	A	904	VAL
1	A	905	VAL
1	A	914	LEU
1	A	919	ARG
1	A	923	ASN
1	A	934	THR
1	A	940	LYS
1	A	950	LYS
1	A	969	ARG
1	A	971	ARG
1	A	972	LEU
1	A	976	LEU

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Mol	Chain	Res	Type
1	A	977	MET
1	A	980	LEU
1	A	987	MET
1	A	991	ILE
1	A	992	SER
1	A	993	THR
1	A	1007	VAL
1	A	1008	MET
1	A	1020	PHE
1	A	1022	VAL
1	A	1024	VAL
1	A	1027	VAL
1	A	1030	ARG
1	A	1031	ARG
1	A	1032	ARG
1	A	1035	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	ASN
1	A	74	ASN
1	A	125	GLN
1	A	161	ASN
1	A	181	GLN
1	A	194	ASN
1	A	213	GLN
1	A	218	GLN
1	A	228	GLN
1	A	298	ASN
1	A	605	ASN
1	A	613	ASN
1	A	622	GLN
1	A	657	GLN
1	A	709	HIS
1	A	760	ASN
1	A	872	GLN
1	A	923	ASN
1	A	928	GLN
1	A	1000	GLN
1	A	1001	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands 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
2	RHQ	A	2002	-	33,36,36	6.95	27 (81%)	43,51,51	4.11	21 (48%)
2	RHQ	A	2001	-	33,36,36	6.95	27 (81%)	43,51,51	4.09	21 (48%)

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	2002	-	-	3/15/21/21	0/4/4/4
2	RHQ	A	2001	-	-	3/15/21/21	0/4/4/4

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2002	RHQ	C2-C9	15.76	1.65	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2001	RHQ	C2-C9	15.68	1.65	1.39
2	A	2001	RHQ	C14-C9	13.98	1.66	1.50
2	A	2002	RHQ	C14-C9	13.87	1.66	1.50
2	A	2002	RHQ	C8-C7	11.82	1.57	1.41
2	A	2001	RHQ	C8-C7	11.79	1.57	1.41
2	A	2002	RHQ	C19-C14	11.59	1.58	1.40
2	A	2001	RHQ	C19-C14	11.59	1.58	1.40
2	A	2001	RHQ	C16-C15	9.44	1.58	1.38
2	A	2002	RHQ	C16-C15	9.43	1.58	1.38
2	A	2002	RHQ	C13-C8	8.99	1.60	1.42
2	A	2001	RHQ	C13-C8	8.98	1.60	1.42
2	A	2002	RHQ	C3-C4	8.94	1.52	1.37
2	A	2001	RHQ	C3-C4	8.92	1.52	1.37
2	A	2001	RHQ	O1-C7	8.61	1.51	1.36
2	A	2002	RHQ	O1-C7	8.59	1.51	1.36
2	A	2001	RHQ	C11-C12	7.90	1.56	1.40
2	A	2002	RHQ	C11-C12	7.85	1.56	1.40
2	A	2002	RHQ	C6-C1	7.72	1.53	1.36
2	A	2001	RHQ	C6-C1	7.69	1.53	1.36
2	A	2002	RHQ	C10-C11	7.65	1.52	1.37
2	A	2001	RHQ	C10-C11	7.61	1.52	1.37
2	A	2001	RHQ	C3-C2	6.94	1.51	1.39
2	A	2001	RHQ	C6-C5	6.89	1.48	1.40
2	A	2002	RHQ	C3-C2	6.87	1.51	1.39
2	A	2002	RHQ	C6-C5	6.86	1.48	1.40
2	A	2002	RHQ	O2-C26	6.61	1.50	1.33
2	A	2001	RHQ	O2-C26	6.60	1.50	1.33
2	A	2002	RHQ	C21-C4	5.93	1.62	1.51
2	A	2001	RHQ	C21-C4	5.89	1.62	1.51
2	A	2001	RHQ	C9-C8	5.78	1.54	1.43
2	A	2002	RHQ	C9-C8	5.77	1.54	1.43
2	A	2001	RHQ	C17-C16	5.60	1.52	1.38
2	A	2002	RHQ	C17-C16	5.57	1.52	1.38
2	A	2001	RHQ	C15-C14	5.55	1.48	1.40
2	A	2002	RHQ	C15-C14	5.53	1.48	1.40
2	A	2001	RHQ	C18-C19	4.38	1.46	1.39
2	A	2002	RHQ	C18-C19	4.34	1.46	1.39
2	A	2002	RHQ	O27-C26	4.03	1.33	1.22
2	A	2001	RHQ	O27-C26	4.00	1.33	1.22
2	A	2002	RHQ	C19-C26	-3.58	1.42	1.50
2	A	2001	RHQ	C19-C26	-3.57	1.42	1.50
2	A	2002	RHQ	C20-C12	3.44	1.57	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2001	RHQ	C20-C12	3.39	1.57	1.51
2	A	2002	RHQ	C17-C18	3.31	1.45	1.38
2	A	2001	RHQ	C17-C18	3.26	1.45	1.38
2	A	2001	RHQ	C22-N1	2.97	1.56	1.46
2	A	2002	RHQ	C13-C12	2.97	1.45	1.37
2	A	2001	RHQ	C13-C12	2.93	1.45	1.37
2	A	2002	RHQ	C22-N1	2.92	1.56	1.46
2	A	2001	RHQ	C10-C7	2.30	1.42	1.37
2	A	2002	RHQ	C10-C7	2.26	1.42	1.37
2	A	2001	RHQ	C25-C24	2.01	1.60	1.47
2	A	2002	RHQ	C25-C24	2.00	1.60	1.47

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2002	RHQ	C2-C9-C8	-15.61	106.34	119.63
2	A	2001	RHQ	C2-C9-C8	-15.56	106.38	119.63
2	A	2002	RHQ	C12-C11-N1	7.90	129.41	119.38
2	A	2001	RHQ	C12-C11-N1	7.86	129.36	119.38
2	A	2002	RHQ	C9-C8-C7	7.61	126.37	119.21
2	A	2001	RHQ	C9-C8-C7	7.51	126.28	119.21
2	A	2002	RHQ	C18-C19-C14	6.84	127.60	119.74
2	A	2001	RHQ	C18-C19-C14	6.81	127.57	119.74
2	A	2002	RHQ	C15-C14-C19	-6.68	110.45	118.03
2	A	2001	RHQ	C15-C14-C19	-6.66	110.48	118.03
2	A	2002	RHQ	C10-C11-N1	-5.93	112.25	121.58
2	A	2001	RHQ	C10-C11-N1	-5.92	112.25	121.58
2	A	2002	RHQ	C14-C9-C8	5.89	129.33	119.42
2	A	2001	RHQ	C14-C9-C8	5.84	129.25	119.42
2	A	2002	RHQ	C3-C2-C9	-5.13	116.94	123.97
2	A	2001	RHQ	C3-C2-C9	-5.11	116.97	123.97
2	A	2002	RHQ	C28-O2-C26	4.75	127.50	116.46
2	A	2001	RHQ	C28-O2-C26	4.72	127.44	116.46
2	A	2002	RHQ	C5-C6-C1	-4.68	115.00	119.46
2	A	2001	RHQ	C5-C6-C1	-4.68	115.01	119.46
2	A	2002	RHQ	C18-C19-C26	-4.58	109.26	118.66
2	A	2001	RHQ	C18-C19-C26	-4.52	109.38	118.66
2	A	2002	RHQ	O1-C1-C6	-4.06	111.21	116.03
2	A	2001	RHQ	O1-C1-C6	-4.03	111.24	116.03
2	A	2002	RHQ	C11-C10-C7	3.42	122.72	119.46
2	A	2001	RHQ	C11-C10-C7	3.38	122.67	119.46
2	A	2002	RHQ	C22-N1-C11	3.21	129.88	123.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2001	RHQ	C22-N1-C11	3.21	129.87	123.21
2	A	2001	RHQ	O1-C7-C8	2.61	123.71	121.03
2	A	2002	RHQ	O1-C7-C8	2.57	123.67	121.03
2	A	2001	RHQ	C20-C12-C11	2.40	123.97	121.25
2	A	2002	RHQ	C20-C12-C11	2.39	123.95	121.25
2	A	2001	RHQ	C6-C1-C2	2.39	123.03	118.69
2	A	2002	RHQ	C6-C1-C2	2.35	122.97	118.69
2	A	2002	RHQ	O2-C26-C19	2.25	116.66	112.21
2	A	2002	RHQ	C13-C8-C9	-2.21	118.50	122.24
2	A	2001	RHQ	O2-C26-C19	2.19	116.54	112.21
2	A	2001	RHQ	C13-C8-C9	-2.17	118.56	122.24
2	A	2002	RHQ	C2-C3-C4	-2.06	118.54	122.00
2	A	2002	RHQ	C16-C17-C18	-2.05	117.07	120.19
2	A	2001	RHQ	C16-C17-C18	-2.03	117.09	120.19
2	A	2001	RHQ	C2-C3-C4	-2.02	118.59	122.00

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
2	A	2002	RHQ	C10-C11-N1-C22
2	A	2002	RHQ	C12-C11-N1-C22
2	A	2001	RHQ	C29-C28-O2-C26
2	A	2002	RHQ	C29-C28-O2-C26

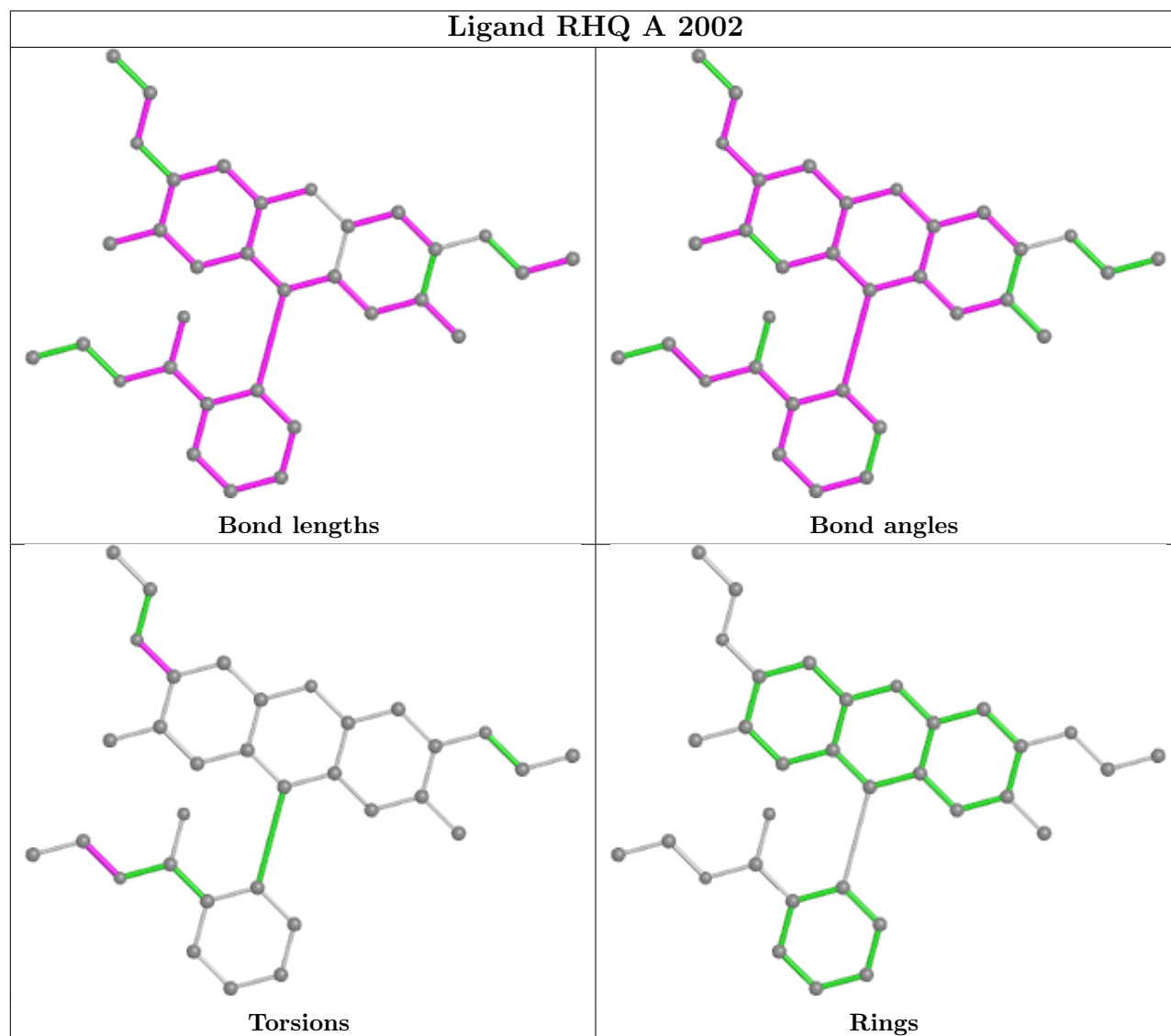
There are no ring outliers.

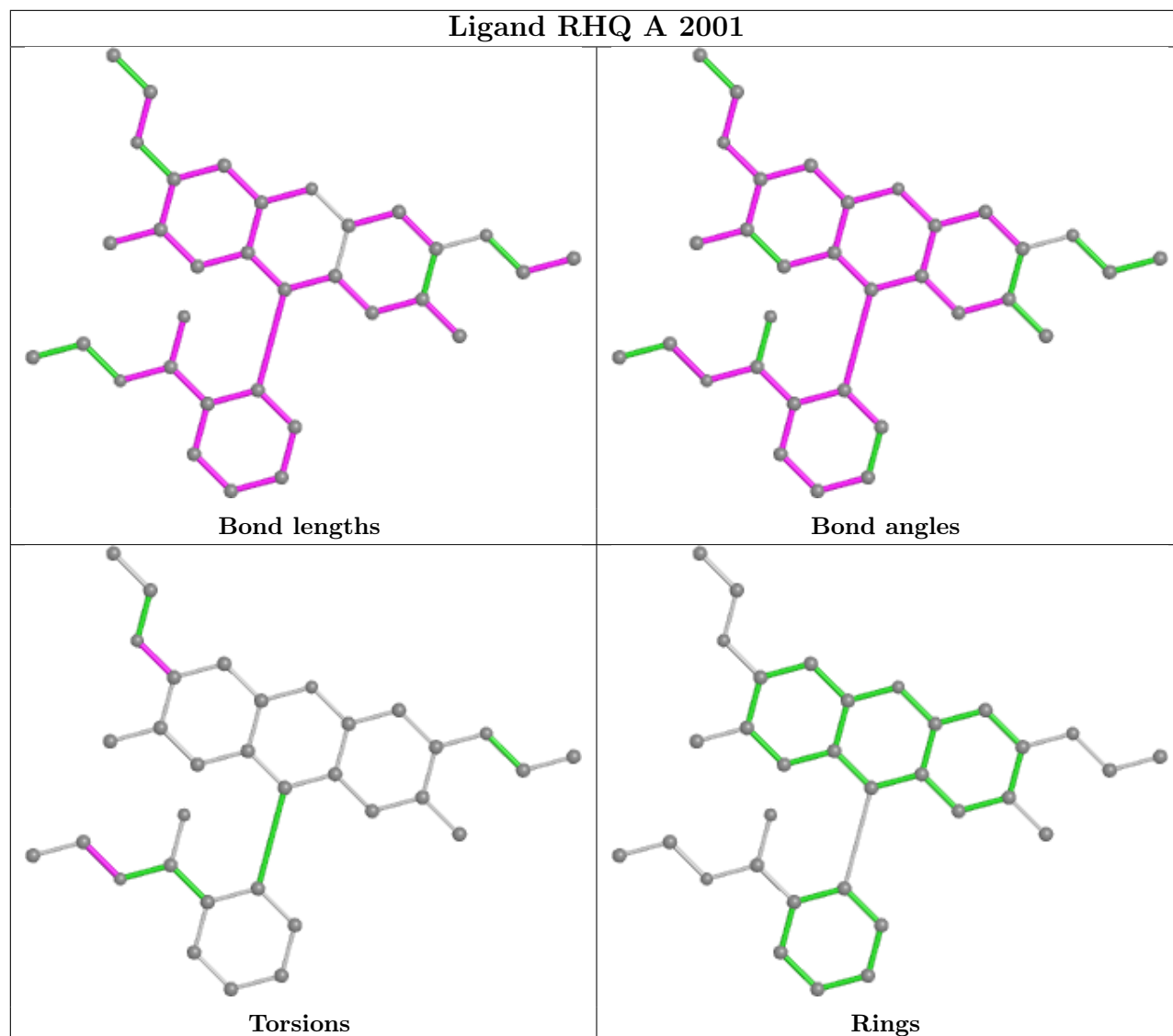
2 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2002	RHQ	12	0
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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.