



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 05:17 AM UTC

PDB ID : 1T9V / pdb_00001t9v
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 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

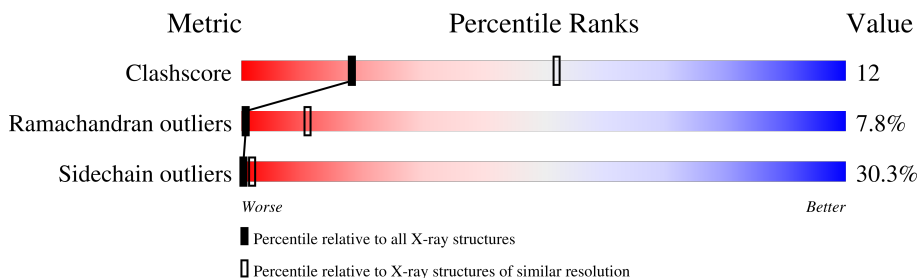
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 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	190562	1012 (3.94-3.66)
Ramachandran outliers	187476	1048 (3.96-3.64)
Sidechain outliers	187428	1043 (3.96-3.64)

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.

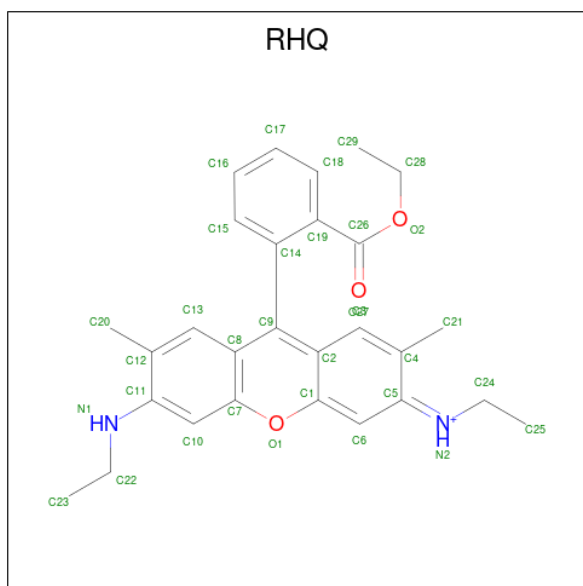
- Molecule 1 is a protein called Acriflavine resistance protein B.

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

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 (CCD ID: RHQ) (formula: $C_{28}H_{31}N_2O_3$).

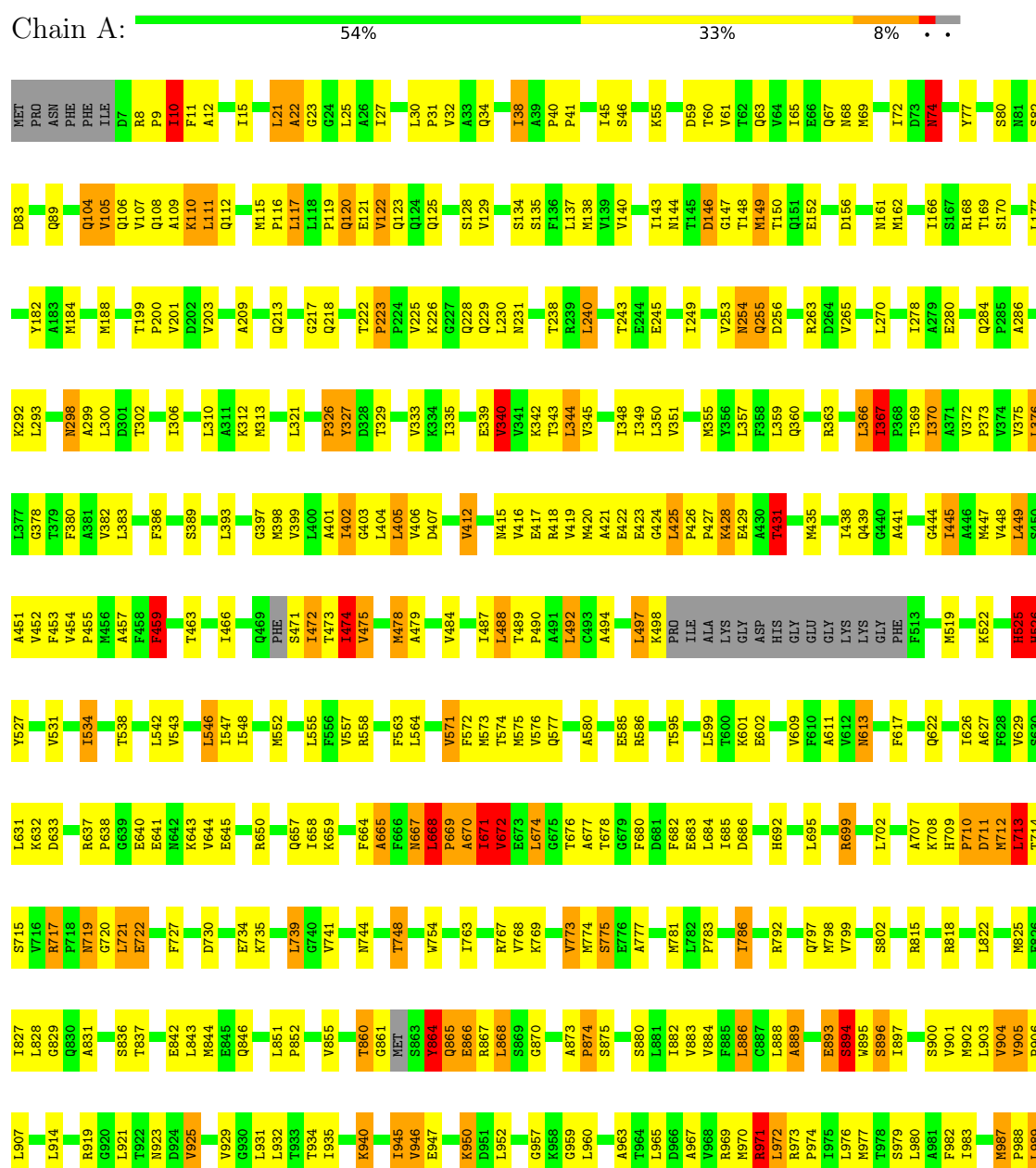


3 Residue-property plots

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. 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.

Note EDS was not executed.

• Molecule 1: Acriflavine resistance protein B



Y990	Y991	S992	T993	G994	A995	Q1000	V1007	M1008	T1013	A1014	T1015	V1016	L1017	A1018	T1019	F1020	F1021	V1022	P1023	V1024	F1025	F1026	V1027	V1028	V1029	R1030	R1031	R1032	R1035	R1036	ASN	GLU	ASP	ILE	GLU	HIS	SER	HIS	THR	VAL	ASP	HIS	HIS
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4 Data and refinement statistics

Xtriage (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.	Xtriage
Total number of atoms	7765	wwPDB-VP
Average B, all atoms (Å ²)	95.0	wwPDB-VP

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	0.55	4/7839 (0.1%)	0.91	11/10644 (0.1%)

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	367	ILE	CA-CB	6.47	1.57	1.54
1	A	668	LEU	C-O	5.83	1.31	1.24
1	A	667	ASN	CG-OD1	5.15	1.33	1.23
1	A	577	GLN	CD-OE1	5.10	1.33	1.23

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	474	ILE	N-CA-C	9.10	121.00	110.62
1	A	719	ASN	N-CA-C	8.90	124.86	112.04
1	A	426	PRO	N-CA-C	8.49	121.06	110.70
1	A	668	LEU	CA-C-N	6.94	128.51	119.84
1	A	668	LEU	C-N-CA	6.94	128.51	119.84
1	A	474	ILE	CB-CA-C	6.80	120.94	112.04
1	A	722	GLU	N-CA-C	6.52	124.69	110.80
1	A	711	ASP	N-CA-C	5.95	127.66	111.00
1	A	474	ILE	N-CA-CB	5.75	117.66	110.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	526	HIS	N-CA-C	-5.43	99.23	110.80
1	A	10	ILE	N-CA-C	5.27	120.31	109.34

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 ⓘ

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	187	0
2	A	66	0	62	15	0
All	All	7765	0	7918	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:613:ASN:HD22	1:A:613:ASN:C	1.96	0.73
1:A:475:VAL:HG13	1:A:478:MET:HE2	1.71	0.73
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:717:ARG:CZ	2:A:2002:RHQ:H222	2.24	0.68
1:A:386:PHE:CE2	2:A:2001:RHQ:H61	2.30	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:721:LEU:HD22	1:A:825:MET:HE2	1.82	0.60
1:A:894:SER:HB2	1:A:895:TRP:C	2.27	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:380:PHE:CE2	1:A:398:MET:HE2	2.37	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
1:A:867:ARG:C	1:A:868:LEU:HD23	2.29	0.58
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:425:LEU:C	1:A:427:PRO:HD2	2.32	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:184:MET:HE3	1:A:184:MET:HA	1.91	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:326:PRO:O	1:A:327:TYR:C	2.52	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:188:MET:HE2	1:A:773:VAL:HG13	1.91	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: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:987:MET:HE2	1:A:1008:MET:HE3	1.93	0.50
1:A:61:VAL:HG21	1:A:122:VAL:HG21	1.95	0.49
1:A:1027:VAL:O	1:A:1028:VAL:C	2.56	0.49
2:A:2001:RHQ:H211	2:A:2001:RHQ:H242	1.94	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:21:LEU:O	1:A:22:ALA:C	2.56	0.49
1:A:931:LEU:O	1:A:935:ILE:HD12	2.13	0.49
2:A:2002:RHQ:H242	2:A:2002:RHQ:H211	1.94	0.49
1:A:886:LEU:O	1:A:889:ALA:HB3	2.13	0.48
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:188:MET:HE1	1:A:200:PRO:HB3	1.97	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:987:MET:CE	1:A:1008:MET:HE3	2.45	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:420:MET:HE1	1:A:497:LEU:HG	1.98	0.46
1:A:972:LEU:C	1:A:972:LEU:HD13	2.40	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:923:ASN:C	1:A:923:ASN:HD22	2.22	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:692:HIS:HD1	1:A:692:HIS:C	2.25	0.44
1:A:339:GLU:O	1:A:340:VAL:HG23	2.18	0.44
1:A:531:VAL:HA	1:A:534:ILE:HG12	1.98	0.44
1:A:376:LEU:HD23	1:A:398:MET:HE3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:GLN:C	1:A:122:VAL:N	2.75	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:959:GLY:O	1:A:960:LEU:C	2.61	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:950:LYS:N	1:A:950:LYS:HE3	2.34	0.43
1:A:678:THR:C	1:A:831:ALA:HB3	2.44	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:401:ALA:O	1:A:402:ILE:C	2.62	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:670:ALA:O	1:A:671:ILE:C	2.62	0.41
1:A:946:VAL:HG22	1:A:950:LYS:HZ2	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: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:111:LEU:C	1:A:111:LEU:HD23	2.46	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
1:A:228:GLN:HE21	1:A:229:GLN:H	1.70	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: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 11

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
1	A	893	GLU
1	A	995	ALA
1	A	74	ASN
1	A	170	SER
1	A	209	ALA

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Mol	Chain	Res	Type
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 ⓘ

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%)	574 (70%)	250 (30%)	0 2

All (250) 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	25	LEU
1	A	27	ILE
1	A	30	LEU
1	A	32	VAL
1	A	38	ILE
1	A	45	ILE
1	A	46	SER
1	A	55	LYS
1	A	59	ASP
1	A	63	GLN
1	A	65	ILE
1	A	67	GLN
1	A	68	ASN
1	A	69	MET
1	A	72	ILE
1	A	74	ASN
1	A	80	SER
1	A	82	SER
1	A	83	ASP
1	A	89	GLN
1	A	105	VAL
1	A	107	VAL
1	A	110	LYS
1	A	111	LEU
1	A	112	GLN
1	A	117	LEU
1	A	120	GLN
1	A	122	VAL
1	A	125	GLN
1	A	128	SER
1	A	137	LEU
1	A	138	MET
1	A	149	MET

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Mol	Chain	Res	Type
1	A	150	THR
1	A	162	MET
1	A	166	ILE
1	A	168	ARG
1	A	169	THR
1	A	177	LEU
1	A	182	TYR
1	A	199	THR
1	A	203	VAL
1	A	213	GLN
1	A	225	VAL
1	A	226	LYS
1	A	230	LEU
1	A	238	THR
1	A	240	LEU
1	A	243	THR
1	A	249	ILE
1	A	253	VAL
1	A	254	ASN
1	A	255	GLN
1	A	263	ARG
1	A	265	VAL
1	A	270	LEU
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	302	THR
1	A	306	ILE
1	A	312	LYS
1	A	313	MET
1	A	321	LEU
1	A	329	THR
1	A	333	VAL
1	A	335	ILE
1	A	340	VAL
1	A	342	LYS
1	A	343	THR
1	A	344	LEU

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Mol	Chain	Res	Type
1	A	345	VAL
1	A	348	ILE
1	A	349	ILE
1	A	350	LEU
1	A	351	VAL
1	A	355	MET
1	A	357	LEU
1	A	359	LEU
1	A	360	GLN
1	A	363	ARG
1	A	366	LEU
1	A	367	ILE
1	A	369	THR
1	A	370	ILE
1	A	376	LEU
1	A	393	LEU
1	A	402	ILE
1	A	406	VAL
1	A	407	ASP
1	A	412	VAL
1	A	417	GLU
1	A	418	ARG
1	A	419	VAL
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	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	475	VAL
1	A	478	MET
1	A	484	VAL
1	A	492	LEU

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Mol	Chain	Res	Type
1	A	497	LEU
1	A	498	LYS
1	A	519	MET
1	A	522	LYS
1	A	526	HIS
1	A	534	ILE
1	A	542	LEU
1	A	546	LEU
1	A	547	ILE
1	A	548	ILE
1	A	552	MET
1	A	555	LEU
1	A	557	VAL
1	A	558	ARG
1	A	564	LEU
1	A	573	MET
1	A	574	THR
1	A	575	MET
1	A	576	VAL
1	A	585	GLU
1	A	586	ARG
1	A	601	LYS
1	A	602	GLU
1	A	609	VAL
1	A	613	ASN
1	A	617	PHE
1	A	622	GLN
1	A	632	LYS
1	A	633	ASP
1	A	640	GLU
1	A	641	GLU
1	A	643	LYS
1	A	645	GLU
1	A	650	ARG
1	A	657	GLN
1	A	658	ILE
1	A	659	LYS
1	A	667	ASN
1	A	668	LEU
1	A	671	ILE
1	A	672	VAL
1	A	674	LEU

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Mol	Chain	Res	Type
1	A	683	GLU
1	A	685	ILE
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	735	LYS
1	A	739	LEU
1	A	741	VAL
1	A	748	THR
1	A	763	ILE
1	A	767	ARG
1	A	768	VAL
1	A	773	VAL
1	A	774	MET
1	A	786	ILE
1	A	792	ARG
1	A	797	GLN
1	A	798	MET
1	A	802	SER
1	A	815	ARG
1	A	818	ARG
1	A	822	LEU
1	A	828	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	866	GLU

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Mol	Chain	Res	Type
1	A	868	LEU
1	A	880	SER
1	A	882	ILE
1	A	884	VAL
1	A	886	LEU
1	A	893	GLU
1	A	894	SER
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	921	LEU
1	A	925	VAL
1	A	934	THR
1	A	940	LYS
1	A	945	ILE
1	A	946	VAL
1	A	950	LYS
1	A	965	LEU
1	A	969	ARG
1	A	971	ARG
1	A	972	LEU
1	A	976	LEU
1	A	977	MET
1	A	980	LEU
1	A	983	ILE
1	A	987	MET
1	A	989	LEU
1	A	990	VAL
1	A	991	ILE
1	A	992	SER
1	A	993	THR
1	A	1007	VAL
1	A	1008	MET
1	A	1017	LEU
1	A	1020	PHE
1	A	1022	VAL
1	A	1024	VAL
1	A	1027	VAL
1	A	1028	VAL

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Mol	Chain	Res	Type
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 (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	GLN
1	A	58	GLN
1	A	68	ASN
1	A	74	ASN
1	A	89	GLN
1	A	112	GLN
1	A	189	ASN
1	A	194	ASN
1	A	213	GLN
1	A	228	GLN
1	A	231	ASN
1	A	284	GLN
1	A	298	ASN
1	A	439	GLN
1	A	525	HIS
1	A	569	GLN
1	A	604	ASN
1	A	605	ASN
1	A	613	ASN
1	A	622	GLN
1	A	657	GLN
1	A	687	GLN
1	A	700	ASN
1	A	709	HIS
1	A	760	ASN
1	A	872	GLN
1	A	923	ASN
1	A	1000	GLN

5.3.3 RNA ⓘ

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](#)

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	2001	-	35,36,36	6.35	28 (80%)	49,51,51	3.80	27 (55%)
2	RHQ	A	2002	-	35,36,36	6.34	27 (77%)	49,51,51	3.82	27 (55%)

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

All (55) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2002	RHQ	C13-C8	12.94	1.60	1.39
2	A	2001	RHQ	C13-C8	12.93	1.60	1.39
2	A	2001	RHQ	C14-C9	12.47	1.66	1.49
2	A	2002	RHQ	C14-C9	12.38	1.66	1.49
2	A	2001	RHQ	C16-C15	11.63	1.58	1.38
2	A	2002	RHQ	C16-C15	11.62	1.58	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2002	RHQ	C19-C14	11.00	1.58	1.40
2	A	2001	RHQ	C19-C14	10.99	1.58	1.40
2	A	2002	RHQ	C8-C7	9.22	1.57	1.40
2	A	2001	RHQ	C8-C7	9.19	1.57	1.40
2	A	2002	RHQ	C2-C9	9.04	1.65	1.40
2	A	2001	RHQ	C2-C9	8.99	1.65	1.40
2	A	2001	RHQ	O1-C7	8.87	1.51	1.38
2	A	2002	RHQ	O1-C7	8.84	1.51	1.38
2	A	2002	RHQ	C3-C4	8.66	1.52	1.35
2	A	2001	RHQ	C3-C4	8.64	1.52	1.35
2	A	2002	RHQ	C10-C11	8.32	1.52	1.39
2	A	2001	RHQ	C10-C11	8.28	1.52	1.39
2	A	2001	RHQ	C11-C12	7.87	1.56	1.40
2	A	2002	RHQ	C11-C12	7.81	1.56	1.40
2	A	2002	RHQ	O2-C26	6.83	1.50	1.33
2	A	2001	RHQ	O2-C26	6.82	1.50	1.33
2	A	2001	RHQ	C17-C16	6.65	1.52	1.38
2	A	2002	RHQ	C17-C16	6.62	1.52	1.38
2	A	2002	RHQ	C6-C1	5.87	1.53	1.37
2	A	2001	RHQ	C6-C1	5.85	1.53	1.37
2	A	2002	RHQ	O1-C1	5.81	1.47	1.37
2	A	2001	RHQ	O1-C1	5.80	1.47	1.37
2	A	2001	RHQ	C15-C14	5.76	1.48	1.39
2	A	2002	RHQ	C15-C14	5.74	1.48	1.39
2	A	2002	RHQ	C21-C4	4.76	1.62	1.50
2	A	2001	RHQ	C21-C4	4.74	1.62	1.50
2	A	2001	RHQ	C18-C19	4.57	1.46	1.39
2	A	2002	RHQ	C18-C19	4.52	1.46	1.39
2	A	2002	RHQ	C2-C1	4.44	1.52	1.43
2	A	2001	RHQ	C2-C1	4.44	1.52	1.43
2	A	2002	RHQ	C13-C12	4.15	1.45	1.39
2	A	2001	RHQ	C13-C12	4.09	1.45	1.39
2	A	2002	RHQ	C17-C18	4.09	1.45	1.38
2	A	2001	RHQ	C17-C18	4.03	1.45	1.38
2	A	2002	RHQ	O27-C26	3.92	1.33	1.22
2	A	2001	RHQ	O27-C26	3.89	1.33	1.22
2	A	2002	RHQ	C20-C12	3.68	1.57	1.51
2	A	2001	RHQ	C20-C12	3.63	1.57	1.51
2	A	2002	RHQ	C19-C26	-3.63	1.42	1.50
2	A	2001	RHQ	C19-C26	-3.62	1.42	1.50
2	A	2001	RHQ	C3-C2	3.42	1.51	1.41
2	A	2002	RHQ	C3-C2	3.38	1.51	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2001	RHQ	C22-N1	3.24	1.56	1.46
2	A	2002	RHQ	C22-N1	3.19	1.56	1.46
2	A	2001	RHQ	C8-C9	2.78	1.54	1.47
2	A	2002	RHQ	C8-C9	2.77	1.54	1.47
2	A	2001	RHQ	C6-C5	2.73	1.48	1.42
2	A	2002	RHQ	C6-C5	2.71	1.48	1.42
2	A	2001	RHQ	C10-C7	2.02	1.42	1.38

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2001	RHQ	C4-C5-N2	10.59	132.33	117.22
2	A	2002	RHQ	C4-C5-N2	10.57	132.31	117.22
2	A	2002	RHQ	C15-C14-C19	-7.85	110.45	119.26
2	A	2001	RHQ	C15-C14-C19	-7.82	110.48	119.26
2	A	2002	RHQ	C12-C11-N1	7.69	129.41	119.41
2	A	2001	RHQ	C12-C11-N1	7.65	129.36	119.41
2	A	2002	RHQ	C18-C19-C14	7.43	127.60	119.26
2	A	2001	RHQ	C18-C19-C14	7.40	127.57	119.26
2	A	2002	RHQ	C14-C9-C8	7.29	129.33	119.91
2	A	2001	RHQ	C14-C9-C8	7.23	129.25	119.91
2	A	2002	RHQ	C8-C9-C2	-6.38	106.34	120.00
2	A	2001	RHQ	C8-C9-C2	-6.36	106.38	120.00
2	A	2001	RHQ	C19-C14-C9	5.99	131.81	123.42
2	A	2002	RHQ	C19-C14-C9	5.99	131.80	123.42
2	A	2002	RHQ	C7-C8-C9	5.81	126.37	118.65
2	A	2001	RHQ	C7-C8-C9	5.74	126.28	118.65
2	A	2002	RHQ	C10-C11-N1	-5.48	112.25	121.49
2	A	2001	RHQ	C10-C11-N1	-5.48	112.25	121.49
2	A	2002	RHQ	C28-O2-C26	4.93	127.50	116.45
2	A	2001	RHQ	C28-O2-C26	4.91	127.44	116.45
2	A	2002	RHQ	C18-C19-C26	-4.64	109.26	118.66
2	A	2001	RHQ	C18-C19-C26	-4.58	109.38	118.66
2	A	2002	RHQ	O1-C1-C2	4.56	125.82	120.36
2	A	2001	RHQ	O1-C1-C2	4.48	125.72	120.36
2	A	2001	RHQ	C9-C2-C1	4.36	124.75	119.37
2	A	2002	RHQ	C9-C2-C1	4.29	124.67	119.37
2	A	2002	RHQ	C3-C2-C9	-4.13	116.94	123.82
2	A	2001	RHQ	C3-C2-C9	-4.11	116.97	123.82
2	A	2002	RHQ	C7-O1-C1	-3.72	113.12	119.73
2	A	2002	RHQ	O1-C1-C6	-3.70	111.21	116.73
2	A	2001	RHQ	C7-O1-C1	-3.70	113.14	119.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2001	RHQ	O1-C1-C6	-3.68	111.24	116.73
2	A	2002	RHQ	C6-C5-C4	3.26	124.67	119.14
2	A	2001	RHQ	C6-C5-C4	3.25	124.66	119.14
2	A	2002	RHQ	C22-N1-C11	3.17	129.88	123.22
2	A	2001	RHQ	C22-N1-C11	3.17	129.87	123.22
2	A	2002	RHQ	C13-C8-C9	-2.64	118.50	123.00
2	A	2002	RHQ	C1-C6-C5	-2.62	115.00	119.11
2	A	2001	RHQ	C1-C6-C5	-2.62	115.01	119.11
2	A	2001	RHQ	C13-C8-C9	-2.60	118.56	123.00
2	A	2002	RHQ	C16-C17-C18	-2.57	117.07	120.24
2	A	2001	RHQ	C16-C17-C18	-2.55	117.09	120.24
2	A	2001	RHQ	C20-C12-C11	2.42	123.97	121.23
2	A	2002	RHQ	C20-C12-C11	2.41	123.95	121.23
2	A	2001	RHQ	O1-C7-C8	2.36	123.71	121.57
2	A	2002	RHQ	C13-C8-C7	-2.34	115.12	118.28
2	A	2002	RHQ	O1-C7-C8	2.31	123.67	121.57
2	A	2001	RHQ	C13-C8-C7	-2.31	115.16	118.28
2	A	2002	RHQ	C2-C3-C4	-2.28	118.54	123.09
2	A	2001	RHQ	C2-C3-C4	-2.25	118.59	123.09
2	A	2002	RHQ	O2-C26-C19	2.25	116.66	112.24
2	A	2001	RHQ	O2-C26-C19	2.19	116.54	112.24
2	A	2002	RHQ	C20-C12-C13	-2.06	115.94	119.57
2	A	2001	RHQ	C20-C12-C13	-2.05	115.96	119.57

There are no chirality outliers.

All (8) torsion outliers are listed below:

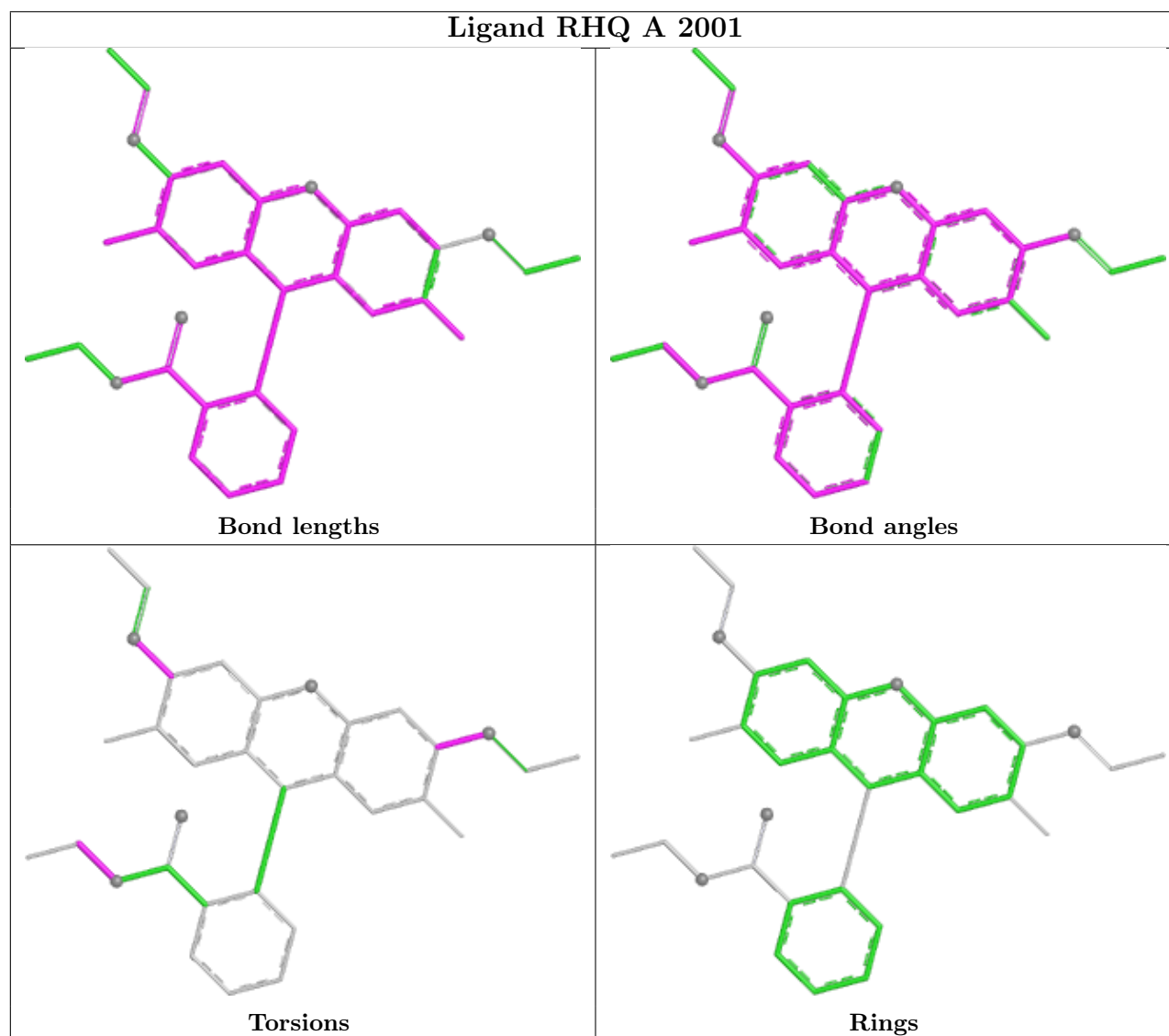
Mol	Chain	Res	Type	Atoms
2	A	2001	RHQ	C6-C5-N2-C24
2	A	2001	RHQ	C12-C11-N1-C22
2	A	2002	RHQ	C6-C5-N2-C24
2	A	2002	RHQ	C12-C11-N1-C22
2	A	2001	RHQ	C29-C28-O2-C26
2	A	2002	RHQ	C29-C28-O2-C26
2	A	2001	RHQ	C10-C11-N1-C22
2	A	2002	RHQ	C10-C11-N1-C22

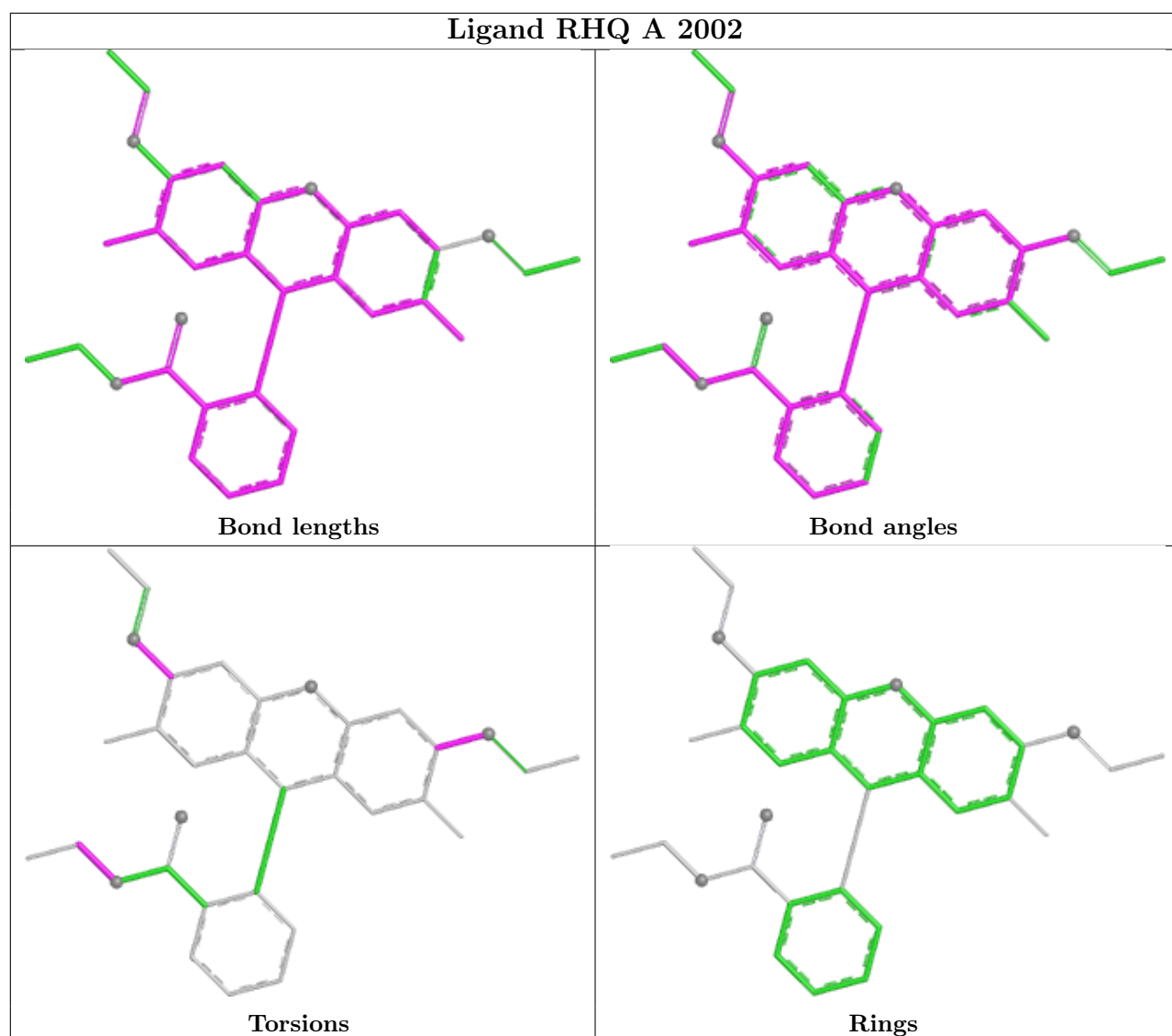
There are no ring outliers.

2 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2001	RHQ	5	0
2	A	2002	RHQ	10	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](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.