



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:58 PM UTC

PDB ID : 1G9A / pdb_00001g9a
Title : CRYSTAL STRUCTURE OF CLOSTRIDIUM BOTULINUM NEUROTOXIN B COMPLEXED WITH AN INHIBITOR (EXPERIMENT 3)
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Deposited on : 2000-11-22
Resolution : 2.10 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

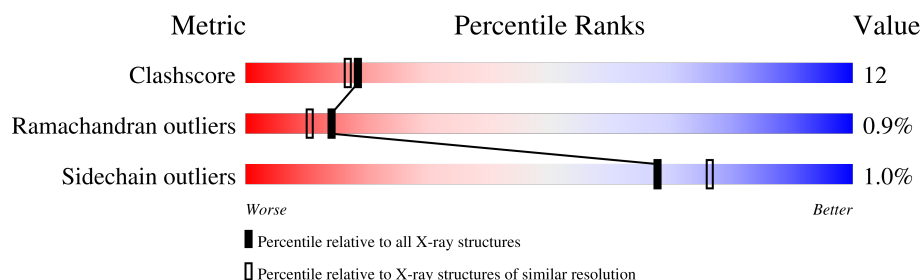
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)

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	1290	

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
3	BAB	A	1292	-	-	X	-
3	BAB	A	1293	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 11184 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.

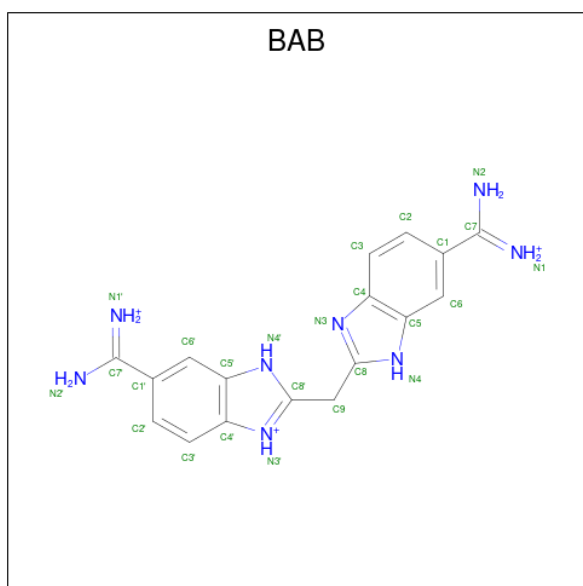
- Molecule 1 is a protein called BOTULINUM NEUROTOXIN TYPE B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1287	Total	C	N	O	S	0	0	0
			10586	6827	1704	2022	33			

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		

- Molecule 3 is BIS(5-AMIDINO-BENZIMIDAZOLYL)METHANE (CCD ID: BAB) (formula: C₁₇H₁₉N₈).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			25	17	8		
3	A	1	Total	C	N	0	0
			25	17	8		

- Molecule 4 is water.

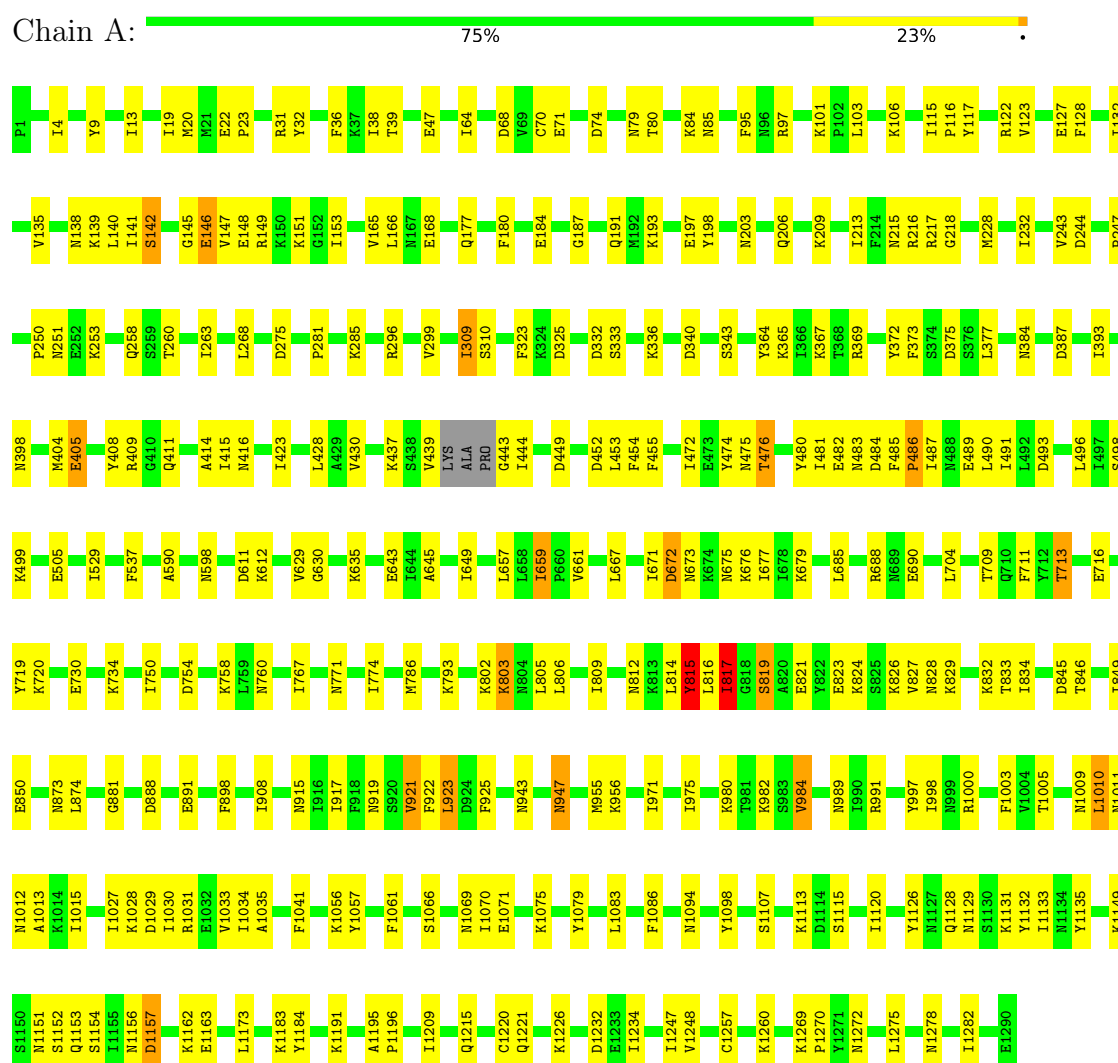
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	546	Total	O	0	0
			546	546		

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: BOTULINUM NEUROTOXIN TYPE B



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	75.92Å 123.24Å 95.90Å 90.00° 113.72° 90.00°	Depositor
Resolution (Å)	50.00 – 2.10	Depositor
% Data completeness (in resolution range)	88.8 (50.00-2.10)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.213 , 0.248	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11184	wwPDB-VP
Average B, all atoms (Å ²)	35.0	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: ZN, BAB

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	0.40	0/10816	0.89	36/14611 (0.2%)

There are no bond length outliers.

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	672	ASP	N-CA-CB	-7.32	106.78	114.10
1	A	1183	LYS	N-CA-C	7.25	119.19	111.28
1	A	1012	ASN	N-CA-C	7.23	120.77	110.14
1	A	1133	ILE	N-CA-C	7.18	120.56	108.86
1	A	659	ILE	CA-C-N	7.14	127.13	119.78
1	A	659	ILE	C-N-CA	7.14	127.13	119.78
1	A	1184	TYR	N-CA-C	7.09	121.27	111.55
1	A	888	ASP	N-CA-C	6.92	120.60	111.75
1	A	187	GLY	N-CA-C	-6.90	103.99	112.68
1	A	971	ILE	N-CA-C	6.57	117.94	108.48
1	A	138	ASN	N-CA-C	6.28	120.28	110.17
1	A	947	ASN	N-CA-C	6.15	118.20	108.67
1	A	984	VAL	N-CA-C	-5.93	100.52	108.35
1	A	197	GLU	N-CA-C	5.81	118.84	111.69
1	A	881	GLY	N-CA-C	5.71	122.72	114.10
1	A	251	ASN	N-CA-C	-5.70	101.20	110.20
1	A	1098	TYR	N-CA-C	-5.69	101.27	110.32
1	A	1113	LYS	N-CA-C	5.62	117.86	111.11
1	A	661	VAL	N-CA-C	-5.55	100.32	108.54
1	A	915	ASN	N-CA-C	5.53	118.82	112.57
1	A	243	VAL	N-CA-C	5.51	116.44	110.21
1	A	193	LYS	N-CA-C	-5.51	99.43	108.41
1	A	128	PHE	N-CA-C	-5.46	100.00	108.90
1	A	123	VAL	N-CA-C	5.39	114.04	109.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1079	TYR	N-CA-C	5.22	117.80	110.23
1	A	71	GLU	N-CA-C	5.21	117.25	109.59
1	A	997	TYR	N-CA-C	5.18	120.08	113.55
1	A	1035	ALA	N-CA-C	5.13	119.63	113.17
1	A	1129	ASN	N-CA-C	5.12	118.55	112.72
1	A	1003	PHE	N-CA-C	5.10	117.05	108.73
1	A	127	GLU	N-CA-C	5.09	117.15	109.41
1	A	1173	LEU	CB-CA-C	-5.08	110.31	117.23
1	A	19	ILE	N-CA-C	5.05	114.98	108.82
1	A	23	PRO	CA-C-N	5.04	125.07	119.32
1	A	23	PRO	C-N-CA	5.04	125.07	119.32
1	A	824	LYS	N-CA-C	-5.01	105.72	111.14

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10586	0	10420	253	0
2	A	2	0	0	0	0
3	A	50	0	38	34	0
4	A	546	0	0	11	0
All	All	11184	0	10458	253	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 (253) 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:716:GLU:HB3	3:A:1293:BAB:HN4	1.18	1.08
1:A:537:PHE:HD2	3:A:1293:BAB:H3'	1.21	1.05
1:A:720:LYS:HE3	3:A:1293:BAB:HN4'	1.31	0.96
1:A:537:PHE:CD2	3:A:1293:BAB:H3'	2.01	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:989:ASN:ND2	1:A:991:ARG:H	1.65	0.94
1:A:709:THR:HB	3:A:1292:BAB:H2'1	1.33	0.92
1:A:709:THR:HB	3:A:1292:BAB:N2'	1.84	0.91
1:A:375:ASP:HA	3:A:1292:BAB:H92	1.55	0.87
1:A:826:LYS:HA	1:A:829:LYS:HE2	1.57	0.86
1:A:367:LYS:H	1:A:411:GLN:HE22	1.25	0.84
1:A:206:GLN:HA	1:A:771:ASN:ND2	1.94	0.83
1:A:1075:LYS:HE2	1:A:1215:GLN:HE22	1.44	0.83
1:A:1066:SER:H	1:A:1069:ASN:HD22	1.25	0.82
1:A:671:ILE:O	1:A:672:ASP:HB2	1.82	0.80
1:A:1247:ILE:HG13	1:A:1248:VAL:HG23	1.63	0.80
1:A:213:ILE:H	1:A:760:ASN:ND2	1.79	0.80
1:A:834:ILE:HD11	1:A:917:ILE:HG12	1.62	0.79
1:A:980:LYS:HE2	1:A:1029:ASP:HB3	1.64	0.78
1:A:439:VAL:HB	1:A:443:GLY:HA2	1.66	0.77
1:A:720:LYS:CE	3:A:1293:BAB:HN4'	1.97	0.77
1:A:369:ARG:HH22	3:A:1292:BAB:H6	1.50	0.75
1:A:165:VAL:CG1	1:A:168:GLU:HG3	2.16	0.75
1:A:454:PHE:HA	3:A:1292:BAB:N1'	2.02	0.74
1:A:659:ILE:HG22	1:A:793:LYS:HG3	1.72	0.72
1:A:716:GLU:HB3	3:A:1293:BAB:N4	2.00	0.71
1:A:989:ASN:HD22	1:A:991:ARG:H	1.37	0.71
1:A:486:PRO:HG2	1:A:489:GLU:HG2	1.73	0.71
1:A:165:VAL:HG11	1:A:168:GLU:HG3	1.74	0.69
1:A:332:ASP:OD2	1:A:336:LYS:HB3	1.92	0.69
1:A:437:LYS:HD2	1:A:444:ILE:CG2	2.23	0.69
1:A:449:ASP:HB2	1:A:452:ASP:OD2	1.91	0.69
1:A:398:ASN:HD21	1:A:411:GLN:HE21	1.40	0.68
1:A:377:LEU:HD11	3:A:1293:BAB:HN22	1.60	0.67
1:A:216:ARG:O	1:A:414:ALA:HB2	1.94	0.66
1:A:209:LYS:CB	1:A:218:GLY:H	2.08	0.66
1:A:1075:LYS:HE2	1:A:1215:GLN:NE2	2.09	0.66
1:A:142:SER:CB	1:A:148:GLU:HG3	2.25	0.66
1:A:455:PHE:H	3:A:1292:BAB:C7'	2.09	0.65
1:A:482:GLU:C	1:A:484:ASP:H	2.04	0.65
1:A:9:TYR:H	1:A:85:ASN:HD22	1.43	0.65
1:A:667:LEU:HD11	1:A:805:LEU:HD23	1.79	0.65
1:A:309:ILE:HD13	1:A:309:ILE:H	1.62	0.64
1:A:590:ALA:HA	1:A:750:ILE:HD11	1.77	0.64
1:A:805:LEU:O	1:A:809:ILE:HG13	1.97	0.64
1:A:635:LYS:HG3	4:A:1830:HOH:O	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:ARG:HH22	3:A:1292:BAB:C6	2.12	0.63
1:A:1010:LEU:HD13	1:A:1011:ASN:ND2	2.14	0.62
1:A:1083:LEU:HD13	1:A:1209:ILE:CD1	2.28	0.62
1:A:9:TYR:H	1:A:85:ASN:ND2	1.98	0.62
1:A:13:ILE:HD13	1:A:20:MET:HG2	1.82	0.61
1:A:453:LEU:O	3:A:1292:BAB:H6'	1.98	0.61
1:A:209:LYS:CB	1:A:217:ARG:HB2	2.31	0.61
1:A:908:ILE:HB	1:A:1041:PHE:HB2	1.82	0.61
1:A:819:SER:C	1:A:821:GLU:H	2.08	0.60
1:A:537:PHE:HA	3:A:1293:BAB:H2'	1.82	0.60
1:A:709:THR:CB	3:A:1292:BAB:N2'	2.63	0.60
1:A:1066:SER:H	1:A:1069:ASN:ND2	1.99	0.60
1:A:309:ILE:HD13	1:A:309:ILE:N	2.16	0.60
1:A:720:LYS:HE3	3:A:1293:BAB:N4'	2.12	0.60
1:A:537:PHE:HD2	3:A:1293:BAB:C3'	2.07	0.59
1:A:296:ARG:O	1:A:299:VAL:HG12	2.02	0.59
1:A:1083:LEU:HD13	1:A:1209:ILE:HD13	1.83	0.59
1:A:101:LYS:HE3	1:A:364:TYR:HA	1.83	0.58
1:A:921:VAL:HG12	1:A:921:VAL:O	2.02	0.58
1:A:31:ARG:CD	1:A:32:TYR:H	2.16	0.57
1:A:333:SER:HA	4:A:1796:HOH:O	2.03	0.57
1:A:1149:LYS:HE3	4:A:1699:HOH:O	2.04	0.56
1:A:97:ARG:HA	1:A:393:ILE:HG23	1.87	0.56
1:A:817:ILE:N	1:A:817:ILE:HD12	2.21	0.56
1:A:1126:TYR:CZ	1:A:1128:GLN:HB2	2.41	0.56
1:A:713:THR:OG1	3:A:1292:BAB:N1'	2.34	0.55
1:A:275:ASP:OD2	1:A:372:TYR:HB2	2.07	0.55
1:A:309:ILE:H	1:A:309:ILE:CD1	2.19	0.55
1:A:64:ILE:HD12	1:A:64:ILE:O	2.06	0.55
1:A:140:LEU:HD11	1:A:147:VAL:HA	1.89	0.55
1:A:482:GLU:HG3	1:A:484:ASP:HB3	1.88	0.54
1:A:828:ASN:O	1:A:832:LYS:HB2	2.06	0.54
1:A:834:ILE:CD1	1:A:917:ILE:HG12	2.36	0.54
1:A:1107:SER:HB3	1:A:1120:ILE:CG2	2.37	0.54
1:A:1226:LYS:HB2	1:A:1232:ASP:HB3	1.90	0.54
1:A:31:ARG:HD2	1:A:32:TYR:H	1.73	0.54
1:A:455:PHE:O	3:A:1292:BAB:N2'	2.40	0.54
1:A:645:ALA:HB3	1:A:649:ILE:CG2	2.38	0.54
1:A:982:LYS:HG3	1:A:1030:ILE:HG12	1.89	0.54
1:A:20:MET:HE2	1:A:31:ARG:HH21	1.73	0.54
1:A:213:ILE:N	1:A:760:ASN:HD21	2.05	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:ILE:HD12	1:A:141:ILE:N	2.22	0.53
1:A:203:ASN:ND2	3:A:1293:BAB:HN22	2.06	0.53
1:A:819:SER:C	1:A:821:GLU:N	2.67	0.52
1:A:74:ASP:HB3	1:A:166:LEU:HD11	1.91	0.52
1:A:384:ASN:ND2	1:A:387:ASP:HB2	2.25	0.52
1:A:228:MET:O	1:A:232:ILE:HG13	2.10	0.52
1:A:980:LYS:HE2	1:A:1029:ASP:CB	2.37	0.52
1:A:730:GLU:HG3	1:A:734:LYS:HE3	1.92	0.52
1:A:1094:ASN:HD22	1:A:1157:ASP:HA	1.74	0.52
1:A:213:ILE:H	1:A:760:ASN:HD21	1.51	0.51
1:A:203:ASN:ND2	1:A:217:ARG:NH1	2.59	0.51
1:A:1221:GLN:HE21	1:A:1278:ASN:HD22	1.58	0.51
1:A:142:SER:HB3	1:A:148:GLU:HG3	1.91	0.51
1:A:258:GLN:OE1	3:A:1292:BAB:N4'	2.44	0.51
1:A:802:LYS:O	1:A:806:LEU:HG	2.11	0.51
1:A:1126:TYR:CE1	1:A:1128:GLN:HB2	2.46	0.51
1:A:1272:ASN:HB3	1:A:1275:LEU:HG	1.91	0.51
1:A:499:LYS:HG2	4:A:1691:HOH:O	2.11	0.51
1:A:250:PRO:HG3	1:A:260:THR:HG22	1.93	0.51
1:A:367:LYS:H	1:A:411:GLN:NE2	2.03	0.51
1:A:846:THR:O	1:A:850:GLU:HG3	2.11	0.51
1:A:203:ASN:ND2	3:A:1293:BAB:N2	2.59	0.50
1:A:956:LYS:HE2	1:A:1034:ILE:CG2	2.41	0.50
1:A:140:LEU:CD1	1:A:147:VAL:HA	2.40	0.50
1:A:833:THR:HG22	1:A:921:VAL:HG21	1.92	0.50
1:A:472:ILE:HB	1:A:667:LEU:HD23	1.93	0.50
1:A:489:GLU:HG3	1:A:490:LEU:N	2.26	0.50
1:A:22:GLU:HB2	1:A:32:TYR:CE2	2.46	0.50
1:A:268:LEU:HD22	1:A:275:ASP:HB3	1.93	0.50
1:A:79:ASN:OD1	1:A:80:THR:HG23	2.12	0.50
1:A:217:ARG:NH2	3:A:1293:BAB:N1	2.60	0.50
1:A:404:MET:HE1	1:A:416:ASN:HB2	1.93	0.50
1:A:487:ILE:O	1:A:491:ILE:HG13	2.11	0.50
1:A:122:ARG:HH11	1:A:177:GLN:NE2	2.10	0.49
1:A:823:GLU:O	1:A:827:VAL:HG23	2.12	0.49
1:A:47:GLU:HG2	1:A:84:LYS:HE3	1.93	0.49
1:A:141:ILE:HD11	1:A:151:LYS:HB3	1.93	0.49
1:A:1075:LYS:CE	1:A:1215:GLN:HE22	2.22	0.49
1:A:1162:LYS:O	1:A:1163:GLU:HB2	2.13	0.49
1:A:70:CYS:SG	1:A:428:LEU:HD13	2.51	0.49
1:A:719:TYR:HA	1:A:767:ILE:HD11	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:823:GLU:HA	1:A:826:LYS:HB3	1.94	0.49
1:A:1234:ILE:O	1:A:1260:LYS:HG2	2.12	0.49
1:A:373:PHE:O	3:A:1292:BAB:H3'	2.13	0.49
1:A:409:ARG:NH1	1:A:415:ILE:HD13	2.27	0.49
1:A:145:GLY:O	1:A:146:GLU:HB3	2.12	0.49
1:A:645:ALA:HB3	1:A:649:ILE:HG23	1.93	0.49
1:A:823:GLU:HA	1:A:826:LYS:CB	2.43	0.48
1:A:1010:LEU:HD12	1:A:1011:ASN:H	1.78	0.48
1:A:489:GLU:O	1:A:493:ASP:N	2.46	0.48
1:A:675:ASN:O	1:A:679:LYS:HG3	2.13	0.48
1:A:1195:ALA:HB1	1:A:1196:PRO:CD	2.43	0.48
1:A:1163:GLU:HA	1:A:1163:GLU:OE1	2.14	0.48
1:A:485:PHE:HE2	1:A:490:LEU:HB2	1.78	0.48
1:A:989:ASN:ND2	1:A:991:ARG:N	2.47	0.48
1:A:1011:ASN:OD1	1:A:1028:LYS:HE2	2.14	0.48
1:A:367:LYS:HB2	1:A:408:TYR:CG	2.49	0.48
1:A:475:ASN:O	1:A:476:THR:C	2.56	0.48
1:A:1071:GLU:OE2	1:A:1075:LYS:HE3	2.14	0.48
1:A:657:LEU:HD11	1:A:786:MET:HG2	1.95	0.47
1:A:711:PHE:HB3	1:A:774:ILE:CG2	2.44	0.47
1:A:989:ASN:HD21	1:A:991:ARG:HB2	1.79	0.47
1:A:141:ILE:HD11	1:A:151:LYS:CB	2.44	0.47
1:A:191:GLN:HG3	4:A:1697:HOH:O	2.14	0.47
1:A:984:VAL:HG13	1:A:1015:ILE:HD11	1.96	0.47
1:A:1195:ALA:HB1	1:A:1196:PRO:HD2	1.96	0.47
1:A:537:PHE:HA	3:A:1293:BAB:C2'	2.43	0.47
1:A:1221:GLN:HE21	1:A:1278:ASN:ND2	2.12	0.47
1:A:309:ILE:HG12	1:A:310:SER:N	2.30	0.47
1:A:64:ILE:HD12	1:A:64:ILE:C	2.40	0.47
1:A:919:ASN:C	1:A:921:VAL:H	2.22	0.47
1:A:375:ASP:HA	3:A:1292:BAB:C9	2.38	0.46
1:A:480:TYR:OH	1:A:690:GLU:HA	2.15	0.46
1:A:437:LYS:HD2	1:A:444:ILE:HG23	1.96	0.46
1:A:263:ILE:HD11	4:A:1722:HOH:O	2.15	0.46
1:A:1131:LYS:HE3	1:A:1132:TYR:CZ	2.50	0.46
1:A:31:ARG:CG	1:A:32:TYR:N	2.78	0.46
1:A:296:ARG:HH11	1:A:296:ARG:HG2	1.81	0.46
1:A:493:ASP:OD2	1:A:496:LEU:HB2	2.15	0.46
1:A:529:ILE:HD12	1:A:529:ILE:C	2.39	0.46
1:A:70:CYS:HA	1:A:430:VAL:HG22	1.97	0.46
1:A:103:LEU:CD1	1:A:487:ILE:HD11	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:730:GLU:CG	1:A:734:LYS:HE3	2.45	0.46
1:A:730:GLU:CD	1:A:734:LYS:HE3	2.41	0.46
1:A:814:LEU:C	1:A:816:LEU:H	2.22	0.46
1:A:1010:LEU:HD12	1:A:1010:LEU:N	2.30	0.46
1:A:1086:PHE:HB2	1:A:1282:ILE:HG12	1.98	0.46
1:A:198:TYR:HD2	1:A:423:ILE:HD11	1.81	0.46
1:A:31:ARG:HG3	1:A:32:TYR:N	2.31	0.45
1:A:365:LYS:NZ	1:A:405:GLU:OE2	2.49	0.45
1:A:891:GLU:O	1:A:898:PHE:HA	2.16	0.45
1:A:1013:ALA:HB2	1:A:1027:ILE:HD13	1.98	0.45
1:A:106:LYS:HD3	1:A:496:LEU:HD23	1.99	0.45
1:A:802:LYS:NZ	1:A:806:LEU:HD11	2.31	0.45
1:A:215:ASN:OD1	1:A:216:ARG:N	2.45	0.45
1:A:812:ASN:O	1:A:816:LEU:HG	2.17	0.45
1:A:4:ILE:HD12	1:A:95:PHE:HB3	1.98	0.45
1:A:203:ASN:OD1	1:A:203:ASN:O	2.34	0.45
1:A:482:GLU:O	1:A:484:ASP:N	2.47	0.45
1:A:165:VAL:HG12	1:A:168:GLU:HG3	1.98	0.45
1:A:955:MET:HE1	1:A:975:ILE:HD12	1.98	0.45
1:A:1094:ASN:HD22	1:A:1157:ASP:N	2.15	0.45
1:A:1156:ASN:O	1:A:1157:ASP:HB2	2.17	0.45
1:A:1009:ASN:OD1	1:A:1009:ASN:C	2.60	0.45
1:A:325:ASP:OD1	1:A:498:SER:HB2	2.17	0.44
1:A:439:VAL:HB	1:A:443:GLY:CA	2.41	0.44
1:A:101:LYS:HB2	1:A:364:TYR:CZ	2.52	0.44
1:A:332:ASP:HB2	4:A:1625:HOH:O	2.18	0.44
1:A:629:VAL:HG22	1:A:630:GLY:N	2.33	0.44
1:A:36:PHE:CD1	1:A:36:PHE:N	2.85	0.44
1:A:213:ILE:N	1:A:760:ASN:ND2	2.54	0.44
1:A:285:LYS:HA	1:A:481:ILE:HD11	1.99	0.44
1:A:1094:ASN:HD22	1:A:1157:ASP:CA	2.31	0.44
1:A:38:ILE:HG23	1:A:39:THR:HG23	1.98	0.44
1:A:922:PHE:HD2	1:A:1010:LEU:HB3	1.82	0.44
1:A:873:ASN:ND2	1:A:874:LEU:H	2.16	0.43
1:A:474:TYR:CZ	1:A:676:LYS:HE2	2.53	0.43
1:A:672:ASP:N	1:A:815:TYR:CD2	2.85	0.43
1:A:1191:LYS:HA	1:A:1257:CYS:SG	2.58	0.43
1:A:452:ASP:HA	3:A:1293:BAB:N3	2.32	0.43
1:A:452:ASP:OD1	3:A:1293:BAB:N3	2.52	0.43
1:A:803:LYS:NZ	1:A:803:LYS:HB3	2.34	0.43
1:A:845:ASP:O	1:A:849:ILE:HG12	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1152:SER:C	1:A:1154:SER:H	2.27	0.43
1:A:141:ILE:N	1:A:141:ILE:CD1	2.82	0.43
1:A:142:SER:HB3	1:A:149:ARG:HB2	2.00	0.43
1:A:611:ASP:OD2	1:A:643:GLU:OE2	2.37	0.43
1:A:377:LEU:HD21	3:A:1293:BAB:C7	2.49	0.43
1:A:923:LEU:HD13	1:A:1033:VAL:HB	1.99	0.43
1:A:704:LEU:O	1:A:709:THR:HG23	2.19	0.43
1:A:816:LEU:C	1:A:817:ILE:HD12	2.43	0.43
1:A:253:LYS:HD2	4:A:1542:HOH:O	2.18	0.42
1:A:598:ASN:HB2	4:A:1694:HOH:O	2.19	0.42
1:A:9:TYR:CZ	1:A:84:LYS:HD3	2.54	0.42
1:A:922:PHE:HA	4:A:1808:HOH:O	2.19	0.42
1:A:117:TYR:HA	1:A:323:PHE:CZ	2.55	0.42
1:A:802:LYS:HZ2	1:A:806:LEU:HD11	1.85	0.42
1:A:1247:ILE:HG13	1:A:1248:VAL:N	2.35	0.42
1:A:673:ASN:O	1:A:677:ILE:HG13	2.19	0.42
1:A:943:ASN:HB3	1:A:947:ASN:ND2	2.35	0.42
1:A:1056:LYS:HE2	1:A:1057:TYR:CE1	2.55	0.42
1:A:1153:GLN:O	1:A:1154:SER:HB2	2.20	0.42
1:A:612:LYS:HD2	4:A:1741:HOH:O	2.19	0.42
1:A:998:ILE:O	1:A:1000:ARG:HG3	2.20	0.42
1:A:139:LYS:HG2	1:A:151:LYS:O	2.19	0.41
1:A:805:LEU:HD12	1:A:827:VAL:HG13	2.01	0.41
1:A:180:PHE:O	1:A:184:GLU:HG3	2.21	0.41
1:A:1135:TYR:CD1	1:A:1135:TYR:C	2.99	0.41
1:A:1269:LYS:HA	1:A:1270:PRO:C	2.45	0.41
1:A:1031:ARG:HA	1:A:1031:ARG:HD3	1.79	0.41
1:A:153:ILE:HA	1:A:505:GLU:O	2.21	0.41
1:A:372:TYR:CZ	3:A:1292:BAB:H2	2.55	0.41
1:A:482:GLU:C	1:A:484:ASP:N	2.70	0.41
1:A:720:LYS:HE3	3:A:1293:BAB:N4	2.36	0.41
1:A:206:GLN:HA	1:A:771:ASN:HD21	1.81	0.41
1:A:709:THR:CB	3:A:1292:BAB:H2'1	2.16	0.41
1:A:1083:LEU:HD22	1:A:1220:CYS:CB	2.51	0.41
1:A:1086:PHE:CB	1:A:1282:ILE:HG12	2.51	0.41
1:A:115:ILE:HA	1:A:116:PRO:HD3	1.98	0.41
1:A:754:ASP:OD1	1:A:758:LYS:HE3	2.21	0.40
1:A:1005:THR:HG21	1:A:1070:ILE:HG12	2.03	0.40
1:A:685:LEU:O	1:A:688:ARG:HB3	2.20	0.40
1:A:925:PHE:HB2	1:A:1061:PHE:O	2.21	0.40
1:A:340:ASP:HB3	1:A:343:SER:OG	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1009:ASN:OD1	1:A:1011:ASN:N	2.54	0.40
1:A:31:ARG:CG	1:A:32:TYR:H	2.35	0.40
1:A:132:ILE:HD11	1:A:135:VAL:HG23	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	1283/1290 (100%)	1213 (94%)	58 (4%)	12 (1%)	14 10

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1151	ASN
1	A	146	GLU
1	A	817	ILE
1	A	476	THR
1	A	483	ASN
1	A	819	SER
1	A	921	VAL
1	A	923	LEU
1	A	142	SER
1	A	1157	ASP
1	A	815	TYR
1	A	486	PRO

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	1176/1189 (99%)	1164 (99%)	12 (1%)	68 76

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	ASP
1	A	244	ASP
1	A	247	PRO
1	A	281	PRO
1	A	309	ILE
1	A	405	GLU
1	A	713	THR
1	A	803	LYS
1	A	815	TYR
1	A	817	ILE
1	A	1010	LEU
1	A	1115	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	ASN
1	A	17	ASN
1	A	85	ASN
1	A	177	GLN
1	A	178	ASN
1	A	203	ASN
1	A	293	GLN
1	A	313	ASN
1	A	411	GLN
1	A	475	ASN
1	A	605	ASN
1	A	683	ASN
1	A	760	ASN
1	A	764	ASN
1	A	765	GLN
1	A	771	ASN
1	A	799	ASN

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Mol	Chain	Res	Type
1	A	828	ASN
1	A	844	ASN
1	A	862	ASN
1	A	866	ASN
1	A	873	ASN
1	A	947	ASN
1	A	953	ASN
1	A	989	ASN
1	A	999	ASN
1	A	1069	ASN
1	A	1094	ASN
1	A	1128	GLN
1	A	1134	ASN
1	A	1215	GLN
1	A	1278	ASN

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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
3	BAB	A	1293	-	28,28,28	4.23	16 (57%)	35,41,41	2.19	9 (25%)
3	BAB	A	1292	2	28,28,28	4.56	18 (64%)	35,41,41	2.26	8 (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
3	BAB	A	1293	-	-	7/12/12/12	0/4/4/4
3	BAB	A	1292	2	-	2/12/12/12	0/4/4/4

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1292	BAB	C8'-N3'	10.80	1.49	1.32
3	A	1292	BAB	C8-N3	10.57	1.49	1.32
3	A	1293	BAB	C8'-N3'	9.01	1.46	1.32
3	A	1293	BAB	C8-N3	8.72	1.46	1.32
3	A	1293	BAB	C8'-N4'	6.78	1.48	1.35
3	A	1292	BAB	C8-N4	6.65	1.48	1.35
3	A	1292	BAB	C7-N2	6.56	1.50	1.33
3	A	1293	BAB	C7-N2	6.44	1.50	1.33
3	A	1293	BAB	C7'-N2'	6.32	1.50	1.33
3	A	1293	BAB	C8-N4	5.98	1.47	1.35
3	A	1292	BAB	C8'-N4'	5.83	1.46	1.35
3	A	1292	BAB	C5-N4	5.75	1.49	1.38
3	A	1293	BAB	C7'-N1'	5.72	1.51	1.27
3	A	1292	BAB	C7-N1	5.65	1.51	1.27
3	A	1292	BAB	C7'-N2'	5.61	1.48	1.33
3	A	1293	BAB	C7-N1	5.51	1.50	1.27
3	A	1292	BAB	C7'-N1'	4.86	1.47	1.27
3	A	1292	BAB	C5'-N4'	4.81	1.47	1.38
3	A	1293	BAB	C5'-N4'	4.72	1.47	1.38
3	A	1293	BAB	C5-N4	4.62	1.47	1.38
3	A	1292	BAB	C4-N3	4.43	1.48	1.39
3	A	1292	BAB	C4'-N3'	4.15	1.48	1.39
3	A	1293	BAB	C4'-N3'	4.03	1.48	1.39
3	A	1293	BAB	C4-N3	3.53	1.47	1.39
3	A	1293	BAB	C5'-C4'	-3.01	1.35	1.40
3	A	1293	BAB	C5-C4	-2.89	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1292	BAB	C5'-C4'	-2.87	1.36	1.40
3	A	1292	BAB	C5-C4	-2.85	1.36	1.40
3	A	1293	BAB	C3'-C4'	-2.65	1.35	1.40
3	A	1292	BAB	C2'-C1'	2.46	1.43	1.39
3	A	1292	BAB	C1-C7	2.43	1.51	1.47
3	A	1292	BAB	C6'-C5'	-2.42	1.35	1.39
3	A	1293	BAB	C1'-C7'	2.23	1.51	1.47
3	A	1292	BAB	C9-C8'	2.15	1.53	1.49

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1293	BAB	C8'-C9-C8	-7.45	103.09	113.55
3	A	1292	BAB	C8'-C9-C8	-5.84	105.35	113.55
3	A	1292	BAB	N4'-C8'-N3'	-4.58	107.13	112.72
3	A	1292	BAB	N4-C8-N3	-4.45	107.29	112.72
3	A	1292	BAB	C4'-C5'-N4'	4.34	110.92	105.71
3	A	1292	BAB	C4-C5-N4	4.08	110.62	105.71
3	A	1293	BAB	N4'-C8'-N3'	-4.06	107.77	112.72
3	A	1292	BAB	C9-C8-N4	3.83	126.67	122.77
3	A	1293	BAB	C4-C5-N4	3.80	110.27	105.71
3	A	1293	BAB	C9-C8-N4	3.72	126.56	122.77
3	A	1293	BAB	N4-C8-N3	-3.59	108.34	112.72
3	A	1292	BAB	C9-C8'-N4'	3.36	126.19	122.77
3	A	1293	BAB	C4'-C5'-N4'	3.06	109.38	105.71
3	A	1293	BAB	C9-C8'-N4'	3.02	125.85	122.77
3	A	1292	BAB	C9-C8'-N3'	2.60	126.67	124.33
3	A	1293	BAB	C3-C4-C5	2.31	122.80	120.26
3	A	1293	BAB	C9-C8'-N3'	2.27	126.38	124.33

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1293	BAB	C2-C1-C7-N2
3	A	1293	BAB	C6-C1-C7-N2
3	A	1293	BAB	N3'-C8'-C9-C8
3	A	1292	BAB	N3'-C8'-C9-C8
3	A	1293	BAB	N3-C8-C9-C8'
3	A	1292	BAB	C6'-C1'-C7'-N2'
3	A	1293	BAB	C6'-C1'-C7'-N2'
3	A	1293	BAB	N4'-C8'-C9-C8

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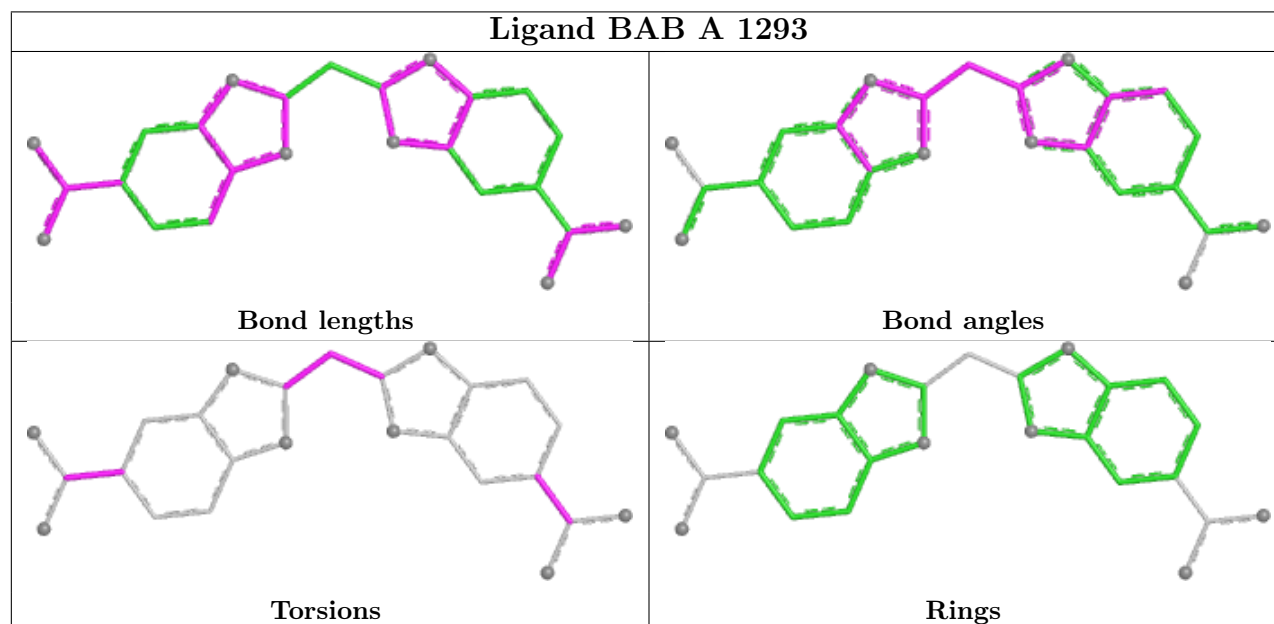
Mol	Chain	Res	Type	Atoms
3	A	1293	BAB	C6-C1-C7-N1

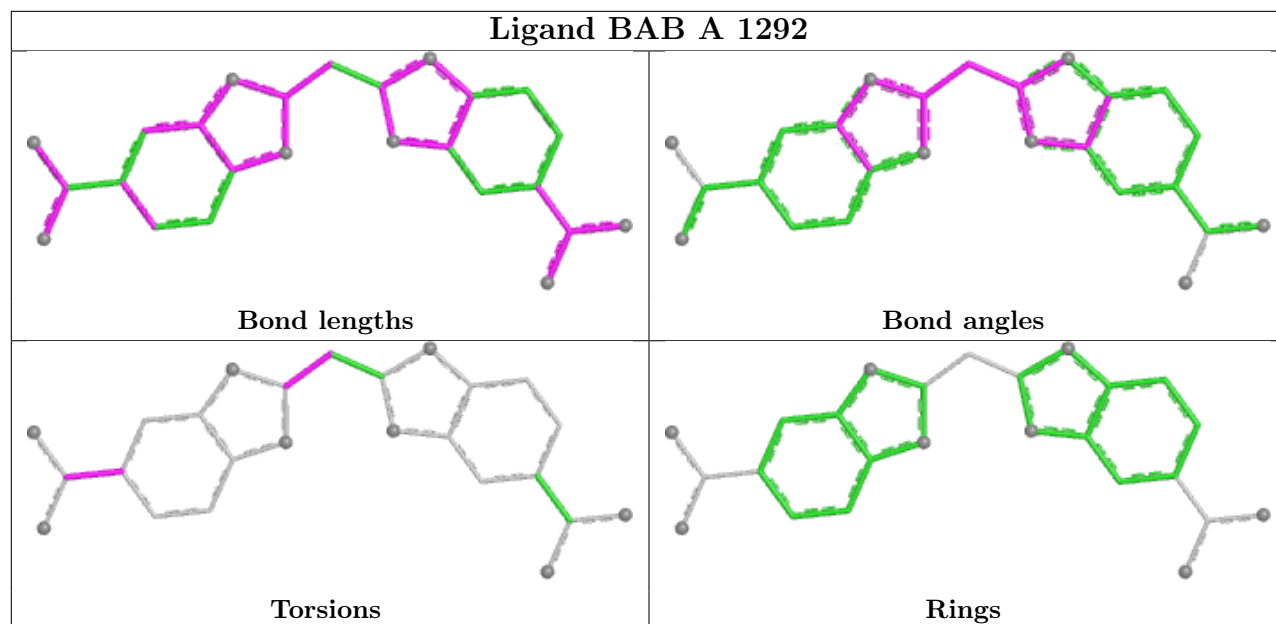
There are no ring outliers.

2 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1293	BAB	18	0
3	A	1292	BAB	16	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.