



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:35 PM GMT

PDB ID : 1G9D  
Title : CRYSTAL STRUCTURE OF CLOSTRIDIUM BOTULINUM NEURO-  
TOXIN B COMPLEXED WITH AN INHIBITOR (EXPERIMENT 2)  
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Deposited on : 2000-11-22  
Resolution : 2.20 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

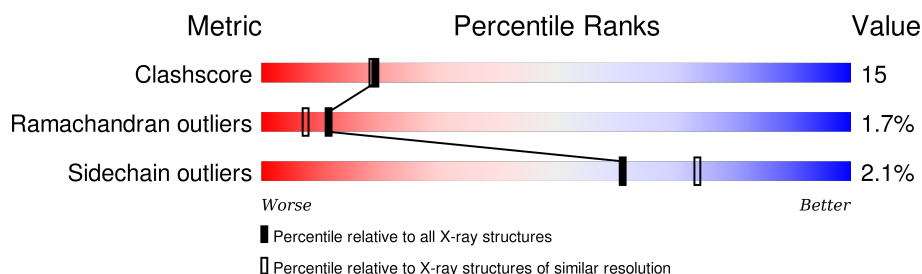
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	1290	<div> <div></div> <div>70%</div> <div>28%</div> <div>.</div> </div>

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 11021 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.

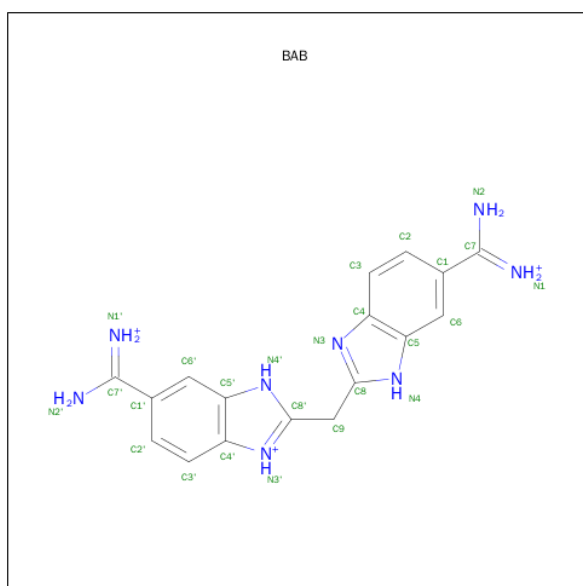
- Molecule 1 is a protein called BOTULINUM NEUROTOXIN TYPE B.

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 (three-letter code: 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 (three-letter code: BAB) (formula: C<sub>17</sub>H<sub>19</sub>N<sub>8</sub>).



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	383	Total	O	0	0
			383	383		



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	76.65Å 123.28Å 95.69Å 90.00° 112.92° 90.00°	Depositor
Resolution (Å)	50.00 – 2.20	Depositor
% Data completeness (in resolution range)	90.7 (50.00-2.20)	Depositor
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.263 , 0.283	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11021	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	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: 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	0.39	0/10816	0.61	0/14611

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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	10419	318	0
2	A	2	0	0	0	0
3	A	50	0	38	24	0
4	A	383	0	0	18	0
All	All	11021	0	10457	318	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 15.

All (318) 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:826:LYS:HA	1:A:829:LYS:HE2	1.39	1.00
1:A:375:ASP:HA	3:A:1292:BAB:H92	1.41	1.00
1:A:537:PHE:HD2	3:A:1293:BAB:H3'	1.28	0.98
1:A:439:VAL:HB	1:A:443:GLY:HA2	1.46	0.98
1:A:474:TYR:HB2	1:A:679:LYS:HD2	1.46	0.97
1:A:989:ASN:HD22	1:A:992:GLU:HG2	1.31	0.96
1:A:1066:SER:H	1:A:1069:ASN:HD22	0.95	0.94
1:A:436:CYS:HG	1:A:445:CYS:HG	0.95	0.90
1:A:203:ASN:HD21	3:A:1293:BAB:HN22	1.21	0.86
1:A:367:LYS:H	1:A:411:GLN:HE22	1.26	0.83
1:A:817:ILE:HB	4:A:1542:HOH:O	1.80	0.82
1:A:216:ARG:O	1:A:414:ALA:HB2	1.80	0.81
1:A:537:PHE:CD2	3:A:1293:BAB:H3'	2.15	0.81
1:A:805:LEU:O	1:A:809:ILE:HG13	1.81	0.80
1:A:716:GLU:HB3	3:A:1293:BAB:HN4	1.45	0.79
1:A:709:THR:HB	3:A:1292:BAB:N2'	1.98	0.78
1:A:1221:GLN:HE21	1:A:1278:ASN:HD22	1.32	0.78
1:A:255:PHE:HB2	1:A:529:ILE:CD1	2.15	0.77
1:A:1071:GLU:OE2	1:A:1075:LYS:HE3	1.85	0.77
1:A:455:PHE:H	3:A:1292:BAB:C7'	2.00	0.75
1:A:142:SER:HB3	1:A:149:ARG:HB2	1.69	0.74
1:A:31:ARG:HB3	4:A:1526:HOH:O	1.87	0.74
1:A:482:GLU:OE2	1:A:484:ASP:HB3	1.87	0.73
1:A:146:GLU:HG3	1:A:148:GLU:HG2	1.69	0.73
1:A:140:LEU:HD11	1:A:147:VAL:HA	1.71	0.73
1:A:255:PHE:HB2	1:A:529:ILE:HD12	1.70	0.72
1:A:278:ILE:HD13	1:A:705:SER:HB3	1.73	0.71
1:A:1026:ASP:OD1	1:A:1028:LYS:HG2	1.91	0.71
1:A:826:LYS:HA	1:A:829:LYS:CE	2.19	0.70
1:A:1126:TYR:CZ	1:A:1128:GLN:HB2	2.25	0.70
1:A:170:GLU:HB3	1:A:193:LYS:HD2	1.71	0.70
1:A:296:ARG:O	1:A:299:VAL:HG12	1.91	0.70
1:A:309:ILE:HD13	1:A:309:ILE:H	1.55	0.70
1:A:486:PRO:HG2	1:A:489:GLU:HG2	1.74	0.70
1:A:667:LEU:HD11	1:A:805:LEU:HD23	1.73	0.70
1:A:1154:SER:HB2	4:A:1649:HOH:O	1.92	0.69
1:A:1066:SER:H	1:A:1069:ASN:ND2	1.80	0.69
1:A:9:TYR:H	1:A:85:ASN:ND2	1.91	0.69
1:A:203:ASN:ND2	3:A:1293:BAB:HN22	1.90	0.68
1:A:922:PHE:HD2	1:A:1010:LEU:HB3	1.59	0.68
1:A:823:GLU:HA	1:A:826:LYS:HB3	1.75	0.68
1:A:13:ILE:HD13	1:A:20:MET:HG2	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:639:GLU:O	1:A:643:GLU:HG3	1.94	0.67
1:A:989:ASN:ND2	1:A:992:GLU:HG2	2.09	0.67
1:A:384:ASN:HD22	1:A:387:ASP:HB2	1.58	0.67
1:A:275:ASP:OD2	1:A:372:TYR:HB2	1.95	0.67
1:A:980:LYS:HE2	1:A:1029:ASP:HB3	1.76	0.66
1:A:809:ILE:HD11	1:A:827:VAL:HG21	1.78	0.66
1:A:212:SER:CB	1:A:215:ASN:HB3	2.26	0.66
1:A:709:THR:HB	3:A:1292:BAB:H2'1	1.60	0.65
1:A:763:ILE:O	1:A:767:ILE:HG12	1.97	0.65
1:A:635:LYS:HG3	4:A:1503:HOH:O	1.96	0.65
1:A:31:ARG:HD2	1:A:32:TYR:H	1.62	0.65
1:A:698:LEU:O	1:A:702:GLN:HG3	1.97	0.65
1:A:31:ARG:CD	1:A:32:TYR:H	2.11	0.64
1:A:646:GLY:O	1:A:649:ILE:HG12	1.97	0.64
1:A:435:MET:HG2	1:A:529:ILE:HD11	1.79	0.64
1:A:826:LYS:CA	1:A:829:LYS:HE2	2.24	0.64
1:A:142:SER:CB	1:A:148:GLU:HG3	2.27	0.64
1:A:656:GLU:HG3	4:A:1514:HOH:O	1.96	0.64
1:A:1247:ILE:HG13	1:A:1248:VAL:HG23	1.79	0.63
1:A:206:GLN:HA	1:A:771:ASN:ND2	2.13	0.63
1:A:716:GLU:HB3	3:A:1293:BAB:N4	2.12	0.62
1:A:921:VAL:O	1:A:922:PHE:HB3	1.98	0.62
1:A:802:LYS:O	1:A:806:LEU:HG	1.99	0.62
1:A:101:LYS:HE3	1:A:364:TYR:HA	1.82	0.62
1:A:133:ALA:HB3	1:A:176:ILE:HD11	1.81	0.62
1:A:1010:LEU:HD13	1:A:1011:ASN:ND2	2.14	0.61
1:A:493:ASP:OD2	1:A:496:LEU:HB2	2.01	0.60
1:A:452:ASP:OD1	3:A:1293:BAB:N3	2.34	0.60
1:A:899:LYS:HD2	1:A:1054:TRP:CZ2	2.36	0.60
1:A:1126:TYR:OH	1:A:1128:GLN:HB2	2.02	0.59
1:A:285:LYS:HA	1:A:481:ILE:HD11	1.84	0.59
1:A:140:LEU:CD1	1:A:147:VAL:HA	2.32	0.59
1:A:1031:ARG:HG2	4:A:1474:HOH:O	2.02	0.59
1:A:309:ILE:HD13	1:A:309:ILE:N	2.17	0.59
1:A:1075:LYS:HE2	1:A:1215:GLN:NE2	2.18	0.59
1:A:454:PHE:HA	3:A:1292:BAB:N1'	2.18	0.58
1:A:455:PHE:O	3:A:1292:BAB:N2'	2.37	0.58
1:A:812:ASN:HD22	1:A:812:ASN:N	2.02	0.58
1:A:64:ILE:O	1:A:64:ILE:HD12	2.04	0.58
1:A:709:THR:CB	3:A:1292:BAB:N2'	2.67	0.57
1:A:22:GLU:HB2	1:A:32:TYR:CE2	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:475:ASN:HB2	4:A:1433:HOH:O	2.03	0.57
1:A:730:GLU:HG3	1:A:734:LYS:HE3	1.87	0.57
1:A:139:LYS:HG3	1:A:141:ILE:HD11	1.85	0.57
1:A:720:LYS:NZ	3:A:1293:BAB:HN4'	2.03	0.56
1:A:472:ILE:HB	1:A:667:LEU:HD23	1.85	0.56
1:A:482:GLU:C	1:A:484:ASP:H	2.08	0.56
1:A:203:ASN:HB3	1:A:218:GLY:HA2	1.88	0.56
1:A:489:GLU:HG3	1:A:490:LEU:N	2.20	0.56
1:A:912:GLN:NE2	1:A:1036:ASN:HA	2.21	0.56
1:A:892:LEU:HD23	1:A:898:PHE:HB3	1.88	0.56
1:A:1007:THR:HB	1:A:1064:GLU:HG3	1.87	0.55
1:A:228:MET:O	1:A:232:ILE:HG13	2.07	0.55
1:A:153:ILE:HA	1:A:505:GLU:O	2.06	0.55
1:A:384:ASN:ND2	1:A:387:ASP:HB2	2.21	0.55
1:A:332:ASP:OD2	1:A:336:LYS:HB3	2.06	0.55
1:A:285:LYS:HA	1:A:481:ILE:CD1	2.36	0.55
1:A:101:LYS:HB2	1:A:364:TYR:CZ	2.42	0.55
1:A:620:VAL:CG1	1:A:623:ILE:HG13	2.37	0.55
1:A:932:ARG:HD3	1:A:1001:TRP:CD1	2.41	0.55
1:A:97:ARG:HG3	1:A:97:ARG:HH11	1.71	0.55
1:A:677:ILE:HG21	1:A:816:LEU:HD21	1.88	0.55
1:A:268:LEU:HD22	1:A:275:ASP:HB3	1.88	0.54
1:A:249:VAL:HG23	1:A:458:ASP:HB3	1.89	0.54
1:A:141:ILE:HD11	1:A:151:LYS:HB3	1.89	0.54
1:A:404:MET:HE1	1:A:416:ASN:OD1	2.07	0.54
1:A:120:ASP:HB2	4:A:1563:HOH:O	2.07	0.54
1:A:209:LYS:CB	1:A:218:GLY:H	2.21	0.54
1:A:1221:GLN:HE21	1:A:1278:ASN:ND2	2.04	0.54
1:A:1066:SER:N	1:A:1069:ASN:HD22	1.81	0.54
1:A:127:GLU:OE2	1:A:309:ILE:HD12	2.07	0.54
1:A:250:PRO:HG3	1:A:260:THR:CG2	2.37	0.54
1:A:472:ILE:HG21	1:A:684:ALA:HB2	1.89	0.54
1:A:1146:ILE:HG23	1:A:1166:ILE:HD12	1.89	0.54
1:A:720:LYS:HZ3	3:A:1293:BAB:HN4'	1.54	0.53
1:A:439:VAL:CB	1:A:443:GLY:HA2	2.31	0.53
1:A:367:LYS:HB2	1:A:408:TYR:CD1	2.43	0.53
1:A:146:GLU:CG	1:A:148:GLU:HG2	2.36	0.53
1:A:675:ASN:HB3	1:A:679:LYS:HE2	1.90	0.53
1:A:670:TYR:CE2	1:A:676:LYS:HD3	2.44	0.53
1:A:670:TYR:CD2	1:A:676:LYS:HD3	2.44	0.53
1:A:142:SER:HB2	1:A:148:GLU:HG3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:989:ASN:ND2	1:A:991:ARG:H	2.06	0.53
1:A:9:TYR:H	1:A:85:ASN:HD22	1.56	0.53
1:A:97:ARG:HA	1:A:393:ILE:HG23	1.91	0.53
1:A:309:ILE:CD1	1:A:309:ILE:H	2.20	0.53
1:A:956:LYS:HE2	1:A:1034:ILE:CG2	2.39	0.52
1:A:409:ARG:NH1	1:A:415:ILE:HD13	2.24	0.52
1:A:60:LYS:HD3	1:A:61:SER:N	2.24	0.52
1:A:377:LEU:HB3	1:A:378:PRO:CD	2.39	0.52
1:A:483:ASN:HB3	4:A:1366:HOH:O	2.09	0.52
1:A:453:LEU:O	3:A:1292:BAB:HB6'	2.09	0.52
1:A:325:ASP:OD2	1:A:500:ILE:HG12	2.10	0.52
1:A:813:LYS:HG3	1:A:814:LEU:N	2.25	0.51
1:A:916:ILE:O	1:A:918:PHE:N	2.41	0.51
1:A:1066:SER:OG	1:A:1069:ASN:ND2	2.44	0.51
1:A:918:PHE:HD1	1:A:1036:ASN:HB3	1.74	0.51
1:A:667:LEU:HD22	1:A:680:THR:HG22	1.92	0.51
1:A:367:LYS:HB2	1:A:408:TYR:CG	2.46	0.51
1:A:139:LYS:HG3	1:A:141:ILE:CD1	2.41	0.51
1:A:823:GLU:O	1:A:827:VAL:HG23	2.11	0.50
1:A:846:THR:O	1:A:850:GLU:HG3	2.11	0.50
1:A:720:LYS:CE	3:A:1293:BAB:HN4'	2.24	0.50
1:A:674:LYS:O	1:A:678:ILE:HG13	2.10	0.50
1:A:486:PRO:O	1:A:489:GLU:HG2	2.12	0.50
1:A:922:PHE:HD2	1:A:1010:LEU:CB	2.25	0.50
1:A:1168:LEU:O	1:A:1179:VAL:HG23	2.11	0.50
1:A:1280:GLN:HA	4:A:1305:HOH:O	2.10	0.50
1:A:132:ILE:HD11	1:A:135:VAL:HG23	1.92	0.50
1:A:686:THR:HA	1:A:689:ASN:HD22	1.78	0.49
1:A:817:ILE:HG22	1:A:818:GLY:N	2.27	0.49
1:A:309:ILE:HG12	1:A:310:SER:N	2.28	0.49
1:A:1261:TRP:CH2	1:A:1265:GLU:HG3	2.48	0.49
1:A:1011:ASN:OD1	1:A:1028:LYS:HE2	2.13	0.49
1:A:791:VAL:O	1:A:795:LEU:HG	2.12	0.49
1:A:666:LEU:HD13	4:A:1412:HOH:O	2.12	0.49
1:A:422:GLU:HB2	4:A:1556:HOH:O	2.13	0.49
1:A:935:LYS:HD2	1:A:1288:TRP:CD2	2.48	0.49
1:A:845:ASP:O	1:A:849:ILE:HG12	2.13	0.48
1:A:250:PRO:HG3	1:A:260:THR:HG23	1.95	0.48
1:A:467:SER:HB3	1:A:660:PRO:HB2	1.95	0.48
1:A:946:HIS:HE1	4:A:1596:HOH:O	1.95	0.48
1:A:474:TYR:CE1	1:A:676:LYS:HE2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:486:PRO:HG2	1:A:489:GLU:CG	2.42	0.48
1:A:64:ILE:C	1:A:64:ILE:HD12	2.33	0.48
1:A:755:ILE:O	1:A:759:LEU:HG	2.13	0.48
1:A:480:TYR:OH	1:A:690:GLU:HA	2.14	0.48
1:A:814:LEU:O	1:A:817:ILE:HG13	2.13	0.48
1:A:82:ASP:O	1:A:86:ILE:HG13	2.13	0.48
1:A:485:PHE:HE2	1:A:490:LEU:HB2	1.78	0.48
1:A:490:LEU:HD13	4:A:1550:HOH:O	2.12	0.48
1:A:1195:ALA:HB1	1:A:1196:PRO:HD2	1.96	0.48
1:A:36:PHE:N	1:A:36:PHE:CD1	2.82	0.48
1:A:1097:TYR:CD2	1:A:1283:PRO:HB3	2.48	0.48
1:A:85:ASN:O	1:A:89:GLN:HG2	2.12	0.48
1:A:812:ASN:O	1:A:816:LEU:HG	2.14	0.48
1:A:817:ILE:HD12	1:A:817:ILE:N	2.28	0.48
1:A:454:PHE:CE2	1:A:713:THR:HG21	2.48	0.48
1:A:377:LEU:HD21	3:A:1293:BAB:C7	2.43	0.48
1:A:104:GLY:HA3	1:A:364:TYR:OH	2.13	0.47
1:A:783:MET:O	1:A:788:PRO:HD3	2.14	0.47
1:A:1110:LYS:HD3	1:A:1121:LEU:HD11	1.96	0.47
1:A:216:ARG:HD3	1:A:420:TYR:OH	2.15	0.47
1:A:27:ARG:HG2	1:A:27:ARG:HH11	1.79	0.47
1:A:908:ILE:HB	1:A:1041:PHE:HB2	1.96	0.47
1:A:811:GLU:C	1:A:812:ASN:HD22	2.17	0.47
1:A:907:LYS:HA	1:A:1041:PHE:O	2.14	0.47
1:A:405:GLU:HG2	4:A:1547:HOH:O	2.15	0.47
1:A:803:LYS:HB3	1:A:803:LYS:NZ	2.29	0.47
1:A:94:LEU:O	1:A:98:ILE:HG13	2.15	0.47
1:A:1107:SER:HB3	1:A:1120:ILE:CG2	2.45	0.47
1:A:994:ILE:HG13	1:A:1105:LYS:HB3	1.96	0.47
1:A:1056:LYS:HE2	1:A:1057:TYR:CE1	2.50	0.47
1:A:258:GLN:OE1	3:A:1292:BAB:N4'	2.47	0.46
1:A:922:PHE:CD2	1:A:1010:LEU:HB3	2.44	0.46
1:A:951:ILE:HG13	1:A:952:ILE:HG13	1.96	0.46
1:A:140:LEU:HD12	1:A:149:ARG:O	2.16	0.46
1:A:141:ILE:CD1	1:A:141:ILE:N	2.78	0.46
1:A:1195:ALA:HB1	1:A:1196:PRO:CD	2.45	0.46
1:A:1094:ASN:C	1:A:1145:ILE:HD11	2.36	0.46
1:A:27:ARG:HG2	1:A:27:ARG:NH1	2.30	0.46
1:A:387:ASP:C	1:A:389:GLU:H	2.19	0.46
1:A:276:PRO:HB3	4:A:1366:HOH:O	2.14	0.46
1:A:434:GLN:OE1	1:A:528:LYS:HD3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:475:ASN:O	1:A:476:THR:C	2.54	0.46
1:A:893:ASN:HD21	1:A:897:GLN:HB2	1.81	0.46
1:A:593:VAL:O	1:A:597:VAL:HG23	2.16	0.46
1:A:142:SER:HB3	1:A:149:ARG:CB	2.43	0.46
1:A:919:ASN:C	1:A:921:VAL:H	2.19	0.46
1:A:688:ARG:HG2	1:A:797:PHE:HE2	1.80	0.46
1:A:713:THR:CB	3:A:1292:BAB:HN1	2.28	0.46
1:A:716:GLU:OE1	3:A:1293:BAB:H6	2.16	0.46
1:A:402:LYS:HE3	1:A:404:MET:HE2	1.98	0.46
1:A:23:PRO:HA	1:A:24:PRO:HD3	1.87	0.46
1:A:1097:TYR:CG	1:A:1281:PHE:HB3	2.50	0.45
1:A:248:ILE:HD13	1:A:461:SER:HB3	1.99	0.45
1:A:106:LYS:O	1:A:110:MET:HG2	2.16	0.45
1:A:943:ASN:HB3	1:A:947:ASN:ND2	2.31	0.45
1:A:31:ARG:CG	1:A:32:TYR:N	2.80	0.45
1:A:1029:ASP:O	1:A:1030:ILE:C	2.54	0.45
1:A:982:LYS:HG3	1:A:1030:ILE:HG12	1.97	0.45
1:A:1100:PHE:HB2	1:A:1282:ILE:HD11	1.99	0.45
1:A:326:LYS:HD3	1:A:327:TYR:CE1	2.52	0.45
1:A:107:LEU:O	1:A:111:ILE:HG13	2.16	0.45
1:A:162:PRO:HG3	1:A:166:LEU:HD22	1.97	0.45
1:A:354:GLY:HA3	4:A:1550:HOH:O	2.16	0.45
1:A:821:GLU:HA	1:A:824:LYS:HB2	1.98	0.45
1:A:384:ASN:HD22	1:A:387:ASP:CB	2.29	0.45
1:A:984:VAL:HG13	1:A:1015:ILE:HD11	1.97	0.45
1:A:464:ASP:OD1	1:A:660:PRO:HB3	2.17	0.44
1:A:162:PRO:CG	1:A:166:LEU:HD22	2.48	0.44
1:A:331:GLU:HG3	1:A:335:GLY:HA2	1.99	0.44
1:A:1086:PHE:CG	1:A:1282:ILE:HG12	2.53	0.44
1:A:1086:PHE:CB	1:A:1282:ILE:HG12	2.47	0.44
1:A:925:PHE:HB2	1:A:1061:PHE:O	2.16	0.44
1:A:400:SER:C	1:A:402:LYS:H	2.20	0.44
1:A:698:LEU:HG	1:A:702:GLN:HE21	1.81	0.44
1:A:936:TYR:HB3	1:A:944:TYR:CD1	2.52	0.44
1:A:106:LYS:HD3	1:A:496:LEU:HD23	1.99	0.44
1:A:11:ASP:HA	1:A:12:PRO:HD3	1.85	0.44
1:A:487:ILE:O	1:A:491:ILE:HG13	2.18	0.44
1:A:917:ILE:O	1:A:917:ILE:HG22	2.17	0.44
1:A:1082:TYR:HA	1:A:1161:ARG:HA	2.00	0.44
1:A:296:ARG:HH11	1:A:296:ARG:HG2	1.83	0.44
1:A:832:LYS:HA	1:A:832:LYS:HD2	1.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:892:LEU:HD23	1:A:898:PHE:CB	2.47	0.44
1:A:1093:TYR:O	1:A:1157:ASP:OD1	2.35	0.44
1:A:910:VAL:HB	1:A:1039:ILE:HB	1.99	0.44
1:A:816:LEU:C	1:A:817:ILE:HD12	2.38	0.43
1:A:102:PRO:HB2	1:A:491:ILE:HG23	2.00	0.43
1:A:822:TYR:CD2	1:A:823:GLU:HG3	2.53	0.43
1:A:377:LEU:HD21	3:A:1293:BAB:H2	2.00	0.43
1:A:885:GLU:HB2	1:A:909:ARG:HB3	2.00	0.43
1:A:950:THR:HA	1:A:964:SER:HB3	2.00	0.43
1:A:455:PHE:N	3:A:1292:BAB:N2'	2.66	0.43
1:A:128:PHE:CZ	1:A:305:VAL:HG21	2.54	0.43
1:A:170:GLU:CB	1:A:193:LYS:HD2	2.45	0.43
1:A:657:LEU:HD11	1:A:786:MET:HG2	2.01	0.43
1:A:807:ASN:O	1:A:811:GLU:HG3	2.18	0.43
1:A:1017:ILE:CG1	1:A:1022:GLU:HG3	2.49	0.43
1:A:1269:LYS:HA	1:A:1270:PRO:C	2.38	0.43
1:A:1083:LEU:CD2	1:A:1220:CYS:HB2	2.49	0.43
1:A:398:ASN:HA	1:A:404:MET:O	2.19	0.42
1:A:558:PHE:CZ	1:A:562:LEU:HD11	2.53	0.42
1:A:382:ILE:HG21	1:A:385:LEU:CD2	2.50	0.42
1:A:775:ASN:O	1:A:779:VAL:HG23	2.19	0.42
1:A:406:LYS:O	1:A:409:ARG:HG3	2.19	0.42
1:A:304:LYS:O	1:A:306:LEU:HG	2.19	0.42
1:A:919:ASN:O	1:A:921:VAL:N	2.53	0.42
1:A:683:ASN:HD22	1:A:683:ASN:N	2.17	0.42
1:A:474:TYR:CZ	1:A:676:LYS:HE2	2.55	0.42
1:A:490:LEU:HD12	1:A:496:LEU:HD22	2.00	0.42
1:A:8:ASN:HA	1:A:85:ASN:HD21	1.83	0.42
1:A:206:GLN:HA	1:A:771:ASN:HD21	1.83	0.42
1:A:98:ILE:O	1:A:364:TYR:OH	2.33	0.42
1:A:117:TYR:HA	1:A:323:PHE:CZ	2.54	0.42
1:A:480:TYR:CE1	1:A:690:GLU:HG3	2.54	0.42
1:A:692:TRP:CH2	1:A:834:ILE:HB	2.55	0.42
1:A:254:LYS:HB2	1:A:257:MET:HG3	2.00	0.42
1:A:620:VAL:HG12	1:A:623:ILE:HG13	2.00	0.42
1:A:474:TYR:CD1	1:A:676:LYS:HG2	2.54	0.42
1:A:84:LYS:O	1:A:87:PHE:HB3	2.20	0.42
1:A:122:ARG:NH2	1:A:176:ILE:HG21	2.35	0.42
1:A:685:LEU:O	1:A:688:ARG:HB3	2.19	0.42
1:A:382:ILE:HG21	1:A:385:LEU:HD21	2.01	0.42
1:A:489:GLU:O	1:A:493:ASP:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:LYS:H	1:A:411:GLN:NE2	2.06	0.41
1:A:482:GLU:C	1:A:484:ASP:N	2.72	0.41
1:A:250:PRO:HG3	1:A:260:THR:HG22	2.01	0.41
1:A:1149:LYS:HD2	1:A:1167:TYR:CZ	2.55	0.41
1:A:9:TYR:CZ	1:A:84:LYS:HD3	2.55	0.41
1:A:477:GLN:HG3	4:A:1636:HOH:O	2.19	0.41
1:A:1240:HIS:O	1:A:1254:ASP:HA	2.20	0.41
1:A:31:ARG:HD2	1:A:32:TYR:N	2.34	0.41
1:A:696:TYR:HB2	1:A:842:TYR:OH	2.21	0.41
1:A:612:LYS:HB3	1:A:1076:ILE:HD13	2.02	0.41
1:A:203:ASN:ND2	1:A:377:LEU:HD11	2.35	0.41
1:A:692:TRP:CE3	1:A:794:LEU:HD13	2.56	0.41
1:A:1107:SER:HB3	1:A:1120:ILE:HG23	2.02	0.41
1:A:867:LEU:O	1:A:868:ARG:HD3	2.20	0.41
1:A:72:TYR:CD1	1:A:423:ILE:HG21	2.56	0.41
1:A:919:ASN:OD1	1:A:919:ASN:N	2.50	0.41
1:A:398:ASN:HB3	1:A:405:GLU:HA	2.02	0.41
1:A:291:VAL:O	1:A:294:ASN:HB2	2.21	0.41
1:A:923:LEU:HD13	1:A:1033:VAL:HB	2.03	0.41
1:A:1163:GLU:OE1	1:A:1163:GLU:HA	2.21	0.41
1:A:256:PHE:O	1:A:453:LEU:HB3	2.21	0.40
1:A:1083:LEU:HD13	1:A:1209:ILE:HD13	2.03	0.40
1:A:79:ASN:OD1	1:A:80:THR:HG23	2.21	0.40
1:A:141:ILE:HD12	1:A:141:ILE:N	2.35	0.40
1:A:139:LYS:HG2	1:A:151:LYS:O	2.22	0.40
1:A:4:ILE:HD12	1:A:95:PHE:HB3	2.03	0.40
1:A:436:CYS:CB	1:A:445:CYS:HG	2.35	0.40
1:A:828:ASN:O	1:A:832:LYS:HB2	2.21	0.40
1:A:738:ASN:HA	1:A:745:LYS:CE	2.51	0.40
1:A:14:ASP:O	1:A:15:ASN:HB2	2.22	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	1283/1290 (100%)	1181 (92%)	80 (6%)	22 (2%)	11 7

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	922	PHE
1	A	1151	ASN
1	A	476	THR
1	A	819	SER
1	A	923	LEU
1	A	1030	ILE
1	A	388	ASN
1	A	872	ASN
1	A	920	SER
1	A	1230	SER
1	A	438	SER
1	A	817	ILE
1	A	871	ASP
1	A	919	ASN
1	A	1029	ASP
1	A	1128	GLN
1	A	342	GLU
1	A	917	ILE
1	A	573	SER
1	A	1157	ASP
1	A	1228	GLU
1	A	921	VAL

### 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	1176/1189 (99%)	1151 (98%)	25 (2%)	61 74



All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	PHE
1	A	60	LYS
1	A	68	ASP
1	A	128	PHE
1	A	193	LYS
1	A	309	ILE
1	A	340	ASP
1	A	345	ASP
1	A	405	GLU
1	A	484	ASP
1	A	501	GLU
1	A	713	THR
1	A	760	ASN
1	A	803	LYS
1	A	812	ASN
1	A	815	TYR
1	A	873	ASN
1	A	888	ASP
1	A	918	PHE
1	A	919	ASN
1	A	925	PHE
1	A	1010	LEU
1	A	1055	MET
1	A	1157	ASP
1	A	1189	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	ASN
1	A	177	GLN
1	A	178	ASN
1	A	203	ASN
1	A	313	ASN
1	A	384	ASN
1	A	411	GLN
1	A	475	ASN
1	A	523	GLN
1	A	605	ASN
1	A	683	ASN
1	A	689	ASN

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Mol	Chain	Res	Type
1	A	771	ASN
1	A	772	ASN
1	A	799	ASN
1	A	862	ASN
1	A	873	ASN
1	A	912	GLN
1	A	947	ASN
1	A	953	ASN
1	A	989	ASN
1	A	999	ASN
1	A	1069	ASN
1	A	1215	GLN
1	A	1272	ASN
1	A	1278	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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	1292	2	22,28,28	3.28	16 (72%)	18,41,41	1.51	4 (22%)
3	BAB	A	1293	-	22,28,28	3.62	16 (72%)	18,41,41	1.60	4 (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	1292	2	-	0/12/12/12	0/4/4/4
3	BAB	A	1293	-	-	0/12/12/12	0/4/4/4

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1292	BAB	C6'-C5'	-3.03	1.37	1.41
3	A	1292	BAB	C6-C5	-2.80	1.37	1.41
3	A	1293	BAB	C3'-C4'	-2.79	1.36	1.41
3	A	1293	BAB	C6-C5	-2.60	1.37	1.41
3	A	1292	BAB	C3'-C4'	-2.17	1.37	1.41
3	A	1292	BAB	C3-C4	-2.09	1.38	1.41
3	A	1292	BAB	C6-C1	2.01	1.40	1.37
3	A	1292	BAB	C3-C2	2.06	1.40	1.36
3	A	1293	BAB	C6-C1	2.07	1.40	1.37
3	A	1293	BAB	C2-C1	2.10	1.42	1.39
3	A	1292	BAB	C1-C7	2.16	1.51	1.47
3	A	1292	BAB	C3'-C2'	2.24	1.41	1.36
3	A	1292	BAB	C5'-N4'	2.41	1.47	1.39
3	A	1293	BAB	C1-C7	2.51	1.51	1.47
3	A	1293	BAB	C3-C2	2.55	1.42	1.36
3	A	1292	BAB	C4-N3	2.63	1.47	1.39
3	A	1292	BAB	C4'-N3'	2.67	1.47	1.39
3	A	1292	BAB	C5-N4	2.77	1.48	1.39
3	A	1293	BAB	C4-N3	2.79	1.48	1.39
3	A	1293	BAB	C5-N4	2.80	1.48	1.39
3	A	1293	BAB	C1'-C7'	2.87	1.52	1.47
3	A	1293	BAB	C5'-N4'	3.02	1.49	1.39
3	A	1293	BAB	C4'-N3'	3.31	1.50	1.39
3	A	1293	BAB	C6'-C1'	3.49	1.43	1.37
3	A	1292	BAB	C7'-N1'	5.49	1.48	1.28
3	A	1292	BAB	C7-N1	5.91	1.49	1.28
3	A	1293	BAB	C7-N1	6.13	1.50	1.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1293	BAB	C7'-N1'	6.17	1.50	1.28
3	A	1292	BAB	C7'-N2'	6.20	1.48	1.33
3	A	1292	BAB	C7-N2	6.78	1.49	1.33
3	A	1293	BAB	C7-N2	7.16	1.50	1.33
3	A	1293	BAB	C7'-N2'	7.61	1.51	1.33

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1293	BAB	C1'-C6'-C5'	-3.57	117.10	120.80
3	A	1293	BAB	C2-C3-C4	-3.16	117.45	120.88
3	A	1292	BAB	C2'-C3'-C4'	-3.06	117.56	120.88
3	A	1292	BAB	C2-C3-C4	-2.98	117.64	120.88
3	A	1292	BAB	C1-C6-C5	-2.76	117.94	120.80
3	A	1293	BAB	C1-C6-C5	-2.65	118.06	120.80
3	A	1292	BAB	C1'-C6'-C5'	-2.58	118.13	120.80
3	A	1293	BAB	C2'-C1'-C7'	-2.09	118.02	120.67

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1292	BAB	11	0
3	A	1293	BAB	13	0

## 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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.