Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 10:04 PM GMT

PDB ID	:	1S0D
Title	:	Crystal structure of botulinum neurotoxin type B at pH 5.5
Authors	:	Eswaramoorthy, S.; Kumaran, D.; Keller, J.; Swaminathan, S.
Deposited on	:	2003-12-30
Resolution	:	2.20 Å(reported)

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

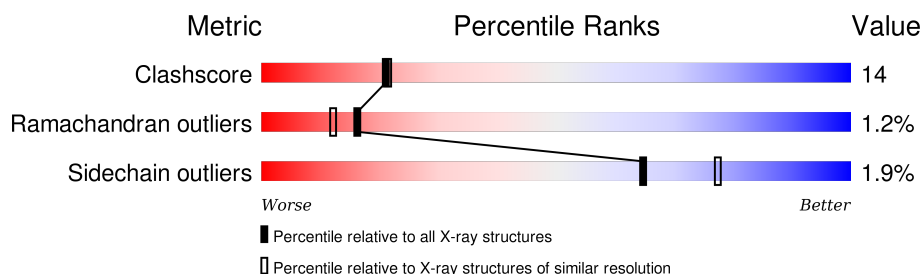|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance (i)

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	Percentile Ranks	Value
Clashscore		14
Ramachandran outliers		1.2%
Sidechain outliers		1.9%

Worse　　　　　*Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

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 >=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 <=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	72%　　　　　27%　　·

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 11145 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	3	0
			10595	6832	1704	2024	35			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Ca	0	0
			2	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	547	Total	O	0	0
			547	547		

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

• Molecule 1: Botulinum neurotoxin type B
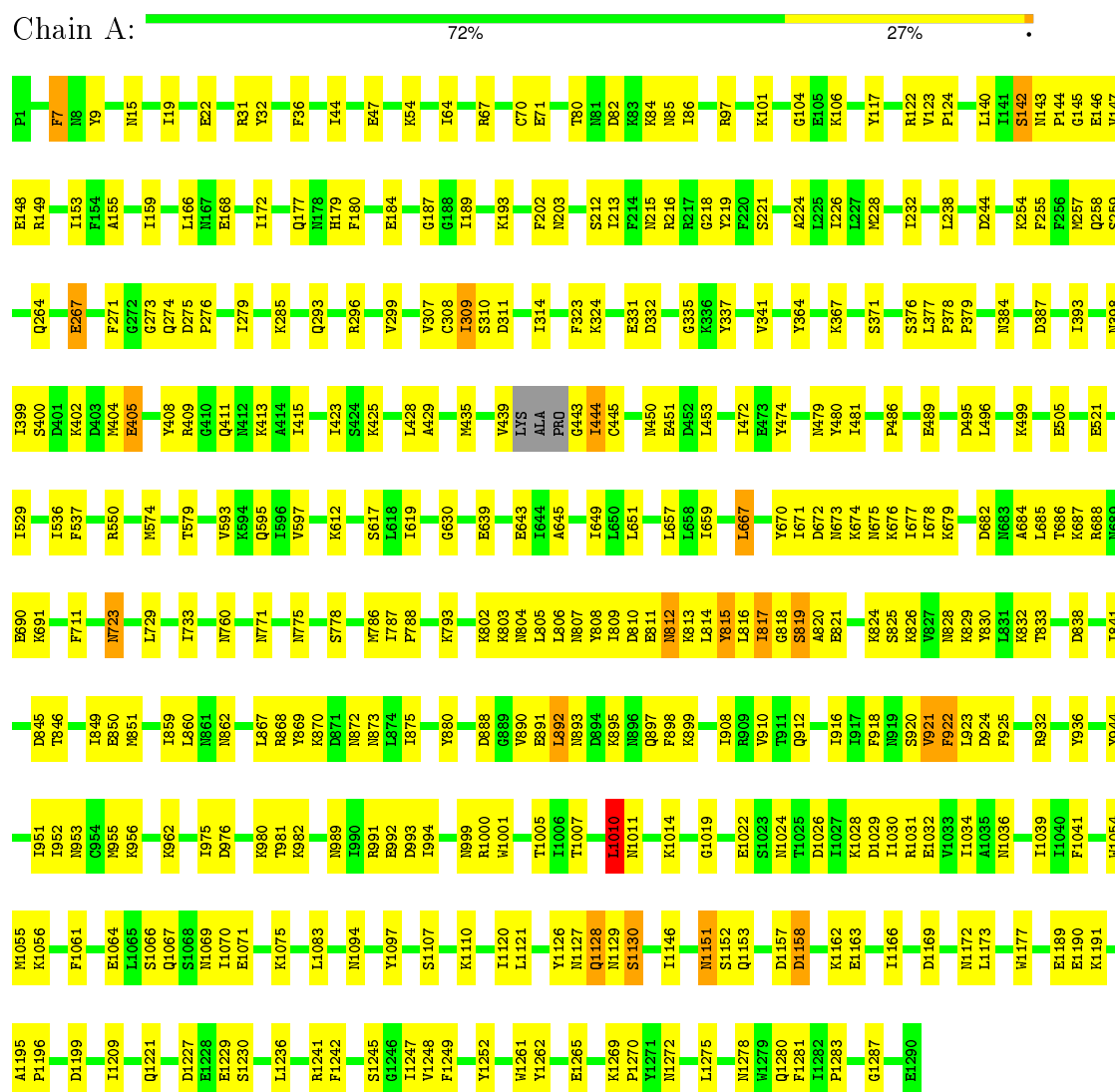
4 Data and refinement statistics (i)

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, α, β, γ	77.54Å 123.03Å 95.92Å 90.00° 113.45° 90.00°	Depositor
Resolution (Å)	50.00 – 2.20	Depositor
% Data completeness (in resolution range)	84.7 (50.00-2.20)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.223 , 0.273	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11145	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, CA

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	0/10837	0.62	2/14639 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	267[A]	GLU	N-CA-CB	-5.46	100.76	110.60
1	A	267[B]	GLU	N-CA-CB	-5.46	100.76	110.60

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	10595	0	10423	299	0
2	A	1	0	0	0	0
3	A	2	0	0	0	0
4	A	547	0	0	22	0
All	All	11145	0	10423	299	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 14.

All (299) 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	1.30	1.11
1:A:474:TYR:HB2	1:A:679:LYS:HD2	1.47	0.97
1:A:980:LYS:HE2	1:A:1029:ASP:HB3	1.46	0.96
1:A:1066:SER:H	1:A:1069:ASN:HD22	1.17	0.92
1:A:367:LYS:H	1:A:411:GLN:HE22	1.10	0.92
1:A:1110:LYS:HD3	1:A:1121:LEU:HD11	1.55	0.89
1:A:657:LEU:HD11	1:A:786:MET:HG2	1.58	0.84
1:A:341:VAL:HB	4:A:1721:HOH:O	1.78	0.84
1:A:425:LYS:HD3	1:A:428:LEU:HD12	1.60	0.83
1:A:1199:ASP:HB3	4:A:1597:HOH:O	1.78	0.82
1:A:846:THR:O	1:A:850:GLU:HG3	1.81	0.81
1:A:444:ILE:HD13	1:A:445:CYS:N	1.96	0.80
1:A:9:TYR:H	1:A:85:ASN:HD22	1.26	0.80
1:A:816:LEU:HB2	1:A:820:ALA:HB2	1.65	0.79
1:A:142:SER:OG	1:A:148:GLU:HG2	1.83	0.79
1:A:812:ASN:O	1:A:816:LEU:HG	1.84	0.77
1:A:989:ASN:HD22	1:A:992:GLU:HG3	1.50	0.77
1:A:976:ASP:OD2	1:A:980:LYS:HB3	1.85	0.75
1:A:1227:ASP:HA	4:A:1655:HOH:O	1.86	0.75
1:A:435:MET:HG2	1:A:529:ILE:HD11	1.69	0.74
1:A:989:ASN:ND2	1:A:991:ARG:H	1.85	0.74
1:A:9:TYR:H	1:A:85:ASN:ND2	1.85	0.73
1:A:639:GLU:O	1:A:643:GLU:HG3	1.89	0.73
1:A:956:LYS:HE2	1:A:1034:ILE:HG21	1.71	0.73
1:A:826:LYS:HA	1:A:829:LYS:CE	2.14	0.73
1:A:1026:ASP:OD2	1:A:1028:LYS:HE3	1.89	0.72
1:A:1010:LEU:HD13	1:A:1011:ASN:ND2	2.04	0.72
1:A:1014:LYS:HE2	1:A:1024:ASN:HD21	1.55	0.72
1:A:1157:ASP:O	1:A:1158:ASP:HB2	1.89	0.72
1:A:309:ILE:CD1	1:A:309:ILE:H	2.03	0.72
1:A:444:ILE:HD13	1:A:445:CYS:H	1.54	0.72
1:A:142:SER:HB2	1:A:149:ARG:H	1.55	0.71
1:A:47:GLU:HG2	1:A:84:LYS:HE3	1.71	0.71
1:A:255:PHE:HB2	1:A:529:ILE:HD12	1.73	0.71
1:A:309:ILE:HD13	1:A:309:ILE:H	1.57	0.70
1:A:1028:LYS:HB2	1:A:1028:LYS:NZ	2.07	0.69
1:A:989:ASN:ND2	1:A:992:GLU:HG3	2.07	0.69
1:A:172:ILE:HD11	1:A:193:LYS:NZ	2.06	0.69
1:A:117:TYR:HA	1:A:323:PHE:CZ	2.26	0.69
1:A:324:LYS:NZ	1:A:331:GLU:HB3	2.08	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:826:LYS:CA	1:A:829:LYS:HE2	2.17	0.68
1:A:1221:GLN:HE21	1:A:1278:ASN:HD22	1.40	0.68
1:A:202:PHE:CE2	4:A:1639:HOH:O	2.46	0.68
1:A:771:ASN:HB3	4:A:1538:HOH:O	1.93	0.68
1:A:212:SER:HA	1:A:760:ASN:ND2	2.10	0.67
1:A:140:LEU:HD11	1:A:147:VAL:HA	1.77	0.67
1:A:956:LYS:HE2	1:A:1034:ILE:CG2	2.25	0.67
1:A:667:LEU:H	1:A:667:LEU:HD12	1.59	0.66
1:A:309:ILE:HD13	1:A:310:SER:H	1.60	0.66
1:A:1221:GLN:HE21	1:A:1278:ASN:ND2	1.95	0.65
1:A:486:PRO:HG2	1:A:489:GLU:HG2	1.79	0.65
1:A:1094:ASN:HD22	1:A:1157:ASP:HA	1.60	0.65
1:A:97:ARG:HA	1:A:393:ILE:HG23	1.78	0.65
1:A:309:ILE:N	1:A:309:ILE:HD13	2.13	0.63
1:A:812:ASN:C	1:A:816:LEU:HG	2.18	0.63
1:A:377:LEU:HB3	1:A:378:PRO:HD2	1.79	0.63
1:A:307:VAL:HG22	1:A:308:CYS:N	2.12	0.63
1:A:1022:GLU:HB3	4:A:1646:HOH:O	1.97	0.63
1:A:486:PRO:HA	4:A:1611:HOH:O	1.99	0.63
1:A:64:ILE:O	1:A:64:ILE:HD12	1.99	0.62
1:A:982:LYS:HG3	1:A:1030:ILE:HG12	1.81	0.62
1:A:439:VAL:HB	1:A:443:GLY:CA	2.29	0.62
1:A:472:ILE:HG21	1:A:684:ALA:HB2	1.81	0.62
1:A:645:ALA:HB3	1:A:649:ILE:CG2	2.29	0.61
1:A:816:LEU:CB	1:A:820:ALA:HB2	2.29	0.61
1:A:31:ARG:CD	1:A:32:TYR:H	2.13	0.61
1:A:812:ASN:HD22	1:A:812:ASN:N	1.99	0.60
1:A:480:TYR:OH	1:A:690:GLU:HA	2.01	0.60
1:A:106:LYS:HD3	1:A:496:LEU:HD23	1.84	0.60
1:A:659:ILE:CG2	1:A:793:LYS:HG3	2.31	0.60
1:A:817:ILE:HG22	1:A:818:GLY:N	2.17	0.60
1:A:67:ARG:NH1	1:A:259:SER:HB3	2.17	0.59
1:A:202:PHE:HE2	4:A:1639:HOH:O	1.81	0.59
1:A:213:ILE:H	1:A:760:ASN:HD22	1.50	0.59
1:A:521:GLU:HG2	4:A:1536:HOH:O	2.02	0.59
1:A:1071:GLU:OE2	1:A:1075:LYS:NZ	2.33	0.59
1:A:845:ASP:O	1:A:849:ILE:HG12	2.03	0.59
1:A:15:ASN:HA	1:A:19:ILE:HG22	1.85	0.59
1:A:817:ILE:HD12	1:A:817:ILE:N	2.18	0.59
1:A:817:ILE:HG22	1:A:818:GLY:H	1.67	0.59
1:A:44:ILE:HD13	1:A:159:ILE:HB	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1083:LEU:HD13	1:A:1209:ILE:CD1	2.34	0.58
1:A:1066:SER:H	1:A:1069:ASN:ND2	1.94	0.58
1:A:1014:LYS:HE2	1:A:1024:ASN:ND2	2.17	0.58
1:A:1236:LEU:HD12	1:A:1262:TYR:HB3	1.84	0.58
1:A:400:SER:HA	1:A:405:GLU:HB2	1.86	0.57
1:A:439:VAL:HB	1:A:443:GLY:N	2.19	0.57
1:A:1110:LYS:HD3	1:A:1121:LEU:CD1	2.33	0.57
1:A:685:LEU:O	1:A:688:ARG:HB3	2.05	0.57
1:A:908:ILE:HB	1:A:1041:PHE:HB2	1.87	0.56
1:A:70[A]:CYS:SG	1:A:428:LEU:HD13	2.45	0.56
1:A:838:ASP:HB3	1:A:841:ILE:HG12	1.87	0.56
1:A:1028:LYS:HB2	1:A:1028:LYS:HZ2	1.69	0.56
1:A:324:LYS:HD2	1:A:337:TYR:HE2	1.70	0.56
1:A:806:LEU:HD22	1:A:824:LYS:HE3	1.89	0.56
1:A:1083:LEU:HD13	1:A:1209:ILE:HD13	1.88	0.55
1:A:148:GLU:HG3	1:A:149:ARG:N	2.22	0.55
1:A:31:ARG:HG3	1:A:32:TYR:N	2.22	0.55
1:A:667:LEU:N	1:A:667:LEU:HD12	2.21	0.55
1:A:22:GLU:HB2	1:A:32:TYR:CE2	2.41	0.55
1:A:332:ASP:OD1	1:A:335:GLY:N	2.40	0.55
1:A:479:ASN:N	1:A:690:GLU:OE1	2.39	0.55
1:A:833:THR:HG22	1:A:921:VAL:HG21	1.89	0.54
1:A:293:GLN:HB3	4:A:1656:HOH:O	2.07	0.54
1:A:1146:ILE:HG23	1:A:1166:ILE:HD12	1.88	0.54
1:A:659:ILE:HG22	1:A:793:LYS:HG3	1.89	0.54
1:A:1011:ASN:OD1	1:A:1028:LYS:HG2	2.08	0.54
1:A:143:ASN:HA	4:A:1304:HOH:O	2.07	0.54
1:A:31:ARG:CG	1:A:32:TYR:N	2.71	0.54
1:A:499:LYS:HG2	4:A:1666:HOH:O	2.07	0.54
1:A:1107:SER:HB3	1:A:1120:ILE:CG2	2.38	0.53
1:A:1031:ARG:NE	4:A:1664:HOH:O	2.41	0.53
1:A:486:PRO:HG2	1:A:489:GLU:CG	2.38	0.53
1:A:213:ILE:H	1:A:760:ASN:ND2	2.06	0.53
1:A:398:ASN:HD21	1:A:411:GLN:HE21	1.57	0.53
1:A:274:GLN:HG3	1:A:275:ASP:N	2.23	0.53
1:A:921:VAL:O	1:A:921:VAL:HG12	2.07	0.53
1:A:101:LYS:HB2	1:A:364:TYR:CZ	2.44	0.53
1:A:146:GLU:HG2	1:A:148:GLU:HG2	1.90	0.53
1:A:122:ARG:HH11	1:A:177:GLN:NE2	2.07	0.53
1:A:215:ASN:OD1	1:A:216:ARG:N	2.41	0.53
1:A:1005:THR:HG21	1:A:1070:ILE:HG12	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1248:VAL:HG23	1:A:1249:PHE:H	1.74	0.52
1:A:1162:LYS:O	1:A:1163:GLU:HB2	2.08	0.52
1:A:932:ARG:HD3	1:A:1001:TRP:CD1	2.45	0.52
1:A:324:LYS:HZ2	1:A:331:GLU:HB3	1.73	0.52
1:A:486:PRO:HG2	1:A:489:GLU:CD	2.30	0.52
1:A:453:LEU:HD22	1:A:537:PHE:CZ	2.45	0.52
1:A:830:TYR:C	1:A:832:LYS:H	2.11	0.51
1:A:153:ILE:HA	1:A:505:GLU:O	2.09	0.51
1:A:976:ASP:HB3	1:A:1030:ILE:HG23	1.92	0.51
1:A:31:ARG:CG	1:A:32:TYR:H	2.23	0.51
1:A:612:LYS:HZ2	1:A:617:SER:CB	2.23	0.51
1:A:981:THR:HG22	1:A:982:LYS:N	2.25	0.51
1:A:922:PHE:HB2	1:A:1010:LEU:HB3	1.93	0.51
1:A:413:LYS:HE2	4:A:1678:HOH:O	2.09	0.51
1:A:674:LYS:HZ1	1:A:816:LEU:C	2.14	0.51
1:A:172:ILE:HD11	1:A:193:LYS:HZ1	1.73	0.51
1:A:384:ASN:ND2	1:A:387:ASP:HB2	2.26	0.50
1:A:409:ARG:NH1	1:A:415:ILE:HD13	2.26	0.50
1:A:332:ASP:HB2	4:A:1706:HOH:O	2.11	0.50
1:A:574:MET:HG2	4:A:1493:HOH:O	2.10	0.50
1:A:104:GLY:HA3	1:A:364:TYR:OH	2.11	0.50
1:A:71:GLU:HG2	1:A:168:GLU:OE2	2.11	0.50
1:A:687:LYS:O	1:A:691:LYS:HG2	2.12	0.50
1:A:809:ILE:HG23	1:A:816:LEU:CD1	2.41	0.50
1:A:258:GLN:HG3	1:A:450:ASN:O	2.11	0.50
1:A:296:ARG:O	1:A:299:VAL:HG12	2.12	0.49
1:A:279:ILE:HA	4:A:1560:HOH:O	2.10	0.49
1:A:1007:THR:HB	1:A:1064:GLU:HG3	1.95	0.49
1:A:893:ASN:OD1	1:A:895:LYS:HB2	2.13	0.49
1:A:1066:SER:N	1:A:1069:ASN:HD22	1.99	0.49
1:A:1195:ALA:HB1	1:A:1196:PRO:HD2	1.95	0.49
1:A:671:ILE:O	1:A:672:ASP:HB2	2.12	0.49
1:A:550:ARG:HG2	1:A:550:ARG:HH11	1.77	0.49
1:A:1195:ALA:HB1	1:A:1196:PRO:CD	2.43	0.49
1:A:221:SER:HB2	1:A:226:ILE:HD11	1.94	0.49
1:A:31:ARG:HD2	1:A:32:TYR:H	1.76	0.49
1:A:1097:TYR:CD2	1:A:1283:PRO:HB3	2.48	0.49
1:A:807:ASN:O	1:A:811:GLU:HG3	2.13	0.48
1:A:869:TYR:CE1	1:A:872:ASN:HA	2.48	0.48
1:A:367:LYS:H	1:A:411:GLN:NE2	1.93	0.48
1:A:82:ASP:O	1:A:86:ILE:HG13	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:898:PHE:CZ	1:A:1055:MET:HB3	2.49	0.48
1:A:859:ILE:HA	1:A:862:ASN:HD22	1.78	0.48
1:A:825:SER:O	1:A:829:LYS:HG2	2.14	0.48
1:A:213:ILE:CB	1:A:723:ASN:HD21	2.26	0.48
1:A:870:LYS:HG3	1:A:875:ILE:HD11	1.96	0.48
1:A:912:GLN:NE2	1:A:1036:ASN:HA	2.29	0.48
1:A:1241:ARG:NH1	1:A:1252:TYR:CD1	2.82	0.48
1:A:803:LYS:HG3	1:A:804:ASN:N	2.29	0.48
1:A:376:SER:O	1:A:451:GLU:OE1	2.31	0.48
1:A:670:TYR:CE2	1:A:676:LYS:HD3	2.50	0.47
1:A:1248:VAL:HG23	1:A:1249:PHE:CD1	2.49	0.47
1:A:893:ASN:HD21	1:A:897:GLN:HB2	1.78	0.47
1:A:955:MET:CE	1:A:975:ILE:HD12	2.43	0.47
1:A:999:ASN:ND2	1:A:1287:GLY:HA3	2.30	0.47
1:A:155:ALA:O	1:A:189:ILE:HG12	2.13	0.47
1:A:285:LYS:HA	1:A:481:ILE:CD1	2.44	0.47
1:A:659:ILE:HG21	1:A:793:LYS:HG3	1.95	0.47
1:A:254:LYS:HB2	1:A:257:MET:HG3	1.97	0.47
1:A:1169:ASP:HB3	1:A:1177:TRP:O	2.15	0.47
1:A:273:GLY:O	1:A:276:PRO:HD2	2.14	0.47
1:A:830:TYR:C	1:A:832:LYS:N	2.68	0.46
1:A:54:LYS:HE3	4:A:1755:HOH:O	2.13	0.46
1:A:891:GLU:C	1:A:892:LEU:HD23	2.35	0.46
1:A:867:LEU:O	1:A:868:ARG:HD3	2.15	0.46
1:A:271:PHE:CE2	1:A:371:SER:HA	2.50	0.46
1:A:1094:ASN:HD22	1:A:1157:ASP:CA	2.28	0.46
1:A:1126:TYR:CE1	1:A:1128:GLN:HB2	2.51	0.46
1:A:711:PHE:CE1	1:A:778:SER:HA	2.51	0.46
1:A:678:ILE:HG22	1:A:682:ASP:OD2	2.16	0.46
1:A:307:VAL:CG2	1:A:308:CYS:N	2.77	0.46
1:A:367:LYS:HB2	1:A:408:TYR:CG	2.51	0.46
1:A:667:LEU:HD21	1:A:805:LEU:HD23	1.96	0.46
1:A:951:ILE:HG13	1:A:952:ILE:HG13	1.97	0.46
1:A:775:ASN:HB3	1:A:851:MET:HG2	1.98	0.46
1:A:311:ASP:HB3	1:A:314:ILE:HG12	1.99	0.45
1:A:439:VAL:HB	1:A:443:GLY:HA2	1.97	0.45
1:A:673:ASN:O	1:A:677:ILE:HG13	2.16	0.45
1:A:953:ASN:HD22	1:A:962:LYS:HB3	1.82	0.45
1:A:379:PRO:HG2	1:A:423:ILE:HD12	1.99	0.45
1:A:729:LEU:O	1:A:733:ILE:HG13	2.17	0.45
1:A:880:TYR:CG	1:A:916:ILE:HD11	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:SER:CB	1:A:148:GLU:HG2	2.47	0.45
1:A:645:ALA:HB3	1:A:649:ILE:HG21	1.98	0.45
1:A:399:ILE:HD12	1:A:402:LYS:HE2	1.98	0.45
1:A:1172:ASN:OD1	1:A:1173:LEU:HG	2.17	0.45
1:A:682:ASP:O	1:A:685:LEU:HB2	2.16	0.45
1:A:659:ILE:N	1:A:659:ILE:HD12	2.32	0.45
1:A:910:VAL:HB	1:A:1039:ILE:HB	1.98	0.45
1:A:819:SER:C	1:A:821:GLU:N	2.70	0.45
1:A:499:LYS:HE2	4:A:1496:HOH:O	2.17	0.44
1:A:36:PHE:CD1	1:A:36:PHE:N	2.85	0.44
1:A:869:TYR:O	1:A:870:LYS:HG2	2.18	0.44
1:A:1127:ASN:O	1:A:1128:GLN:O	2.36	0.44
1:A:1248:VAL:HG23	1:A:1249:PHE:N	2.32	0.44
1:A:672:ASP:N	1:A:815:TYR:CD2	2.78	0.44
1:A:805:LEU:O	1:A:808:TYR:HB3	2.18	0.44
1:A:982:LYS:HG2	1:A:1030:ILE:HD11	1.98	0.44
1:A:1129:ASN:O	1:A:1130:SER:HB2	2.18	0.43
1:A:802:LYS:HZ1	1:A:828:ASN:HD21	1.64	0.43
1:A:1269:LYS:HA	1:A:1270:PRO:C	2.39	0.43
1:A:216:ARG:HG2	4:A:1455:HOH:O	2.18	0.43
1:A:1097:TYR:CG	1:A:1281:PHE:HB3	2.53	0.43
1:A:862:ASN:O	1:A:1061:PHE:HA	2.19	0.43
1:A:166:LEU:N	1:A:166:LEU:HD23	2.33	0.43
1:A:674:LYS:HE3	1:A:819:SER:OG	2.18	0.43
1:A:97:ARG:HG3	1:A:97:ARG:HH11	1.84	0.43
1:A:1236:LEU:HD12	1:A:1262:TYR:CB	2.49	0.43
1:A:1031:ARG:HD3	1:A:1031:ARG:HA	1.79	0.43
1:A:7:PHE:CZ	1:A:36:PHE:HB3	2.54	0.43
1:A:817:ILE:CG2	1:A:818:GLY:H	2.26	0.43
1:A:787:ILE:HB	1:A:788:PRO:HD3	2.01	0.43
1:A:1151:ASN:C	1:A:1153:GLN:H	2.22	0.43
1:A:228:MET:O	1:A:232:ILE:HG13	2.19	0.43
1:A:1261:TRP:CH2	1:A:1265:GLU:HG3	2.54	0.43
1:A:1028:LYS:CB	1:A:1028:LYS:NZ	2.81	0.43
1:A:97:ARG:CA	1:A:393:ILE:HG23	2.46	0.43
1:A:802:LYS:NZ	1:A:828:ASN:HD21	2.17	0.43
1:A:486:PRO:O	1:A:489:GLU:HG2	2.18	0.42
1:A:890:VAL:HG12	1:A:892:LEU:CD2	2.48	0.42
1:A:1190:GLU:HG3	1:A:1191:LYS:N	2.34	0.42
1:A:899:LYS:HD2	1:A:1054:TRP:CZ2	2.54	0.42
1:A:812:ASN:O	1:A:814:LEU:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:981:THR:CG2	1:A:982:LYS:N	2.81	0.42
1:A:811:GLU:C	1:A:812:ASN:HD22	2.21	0.42
1:A:674:LYS:HZ3	1:A:817:ILE:HD13	1.85	0.42
1:A:812:ASN:O	1:A:813:LYS:C	2.57	0.42
1:A:1067:GLN:NE2	1:A:1071:GLU:HB2	2.35	0.42
1:A:936:TYR:HB3	1:A:944:TYR:CD1	2.55	0.42
1:A:219:TYR:HA	1:A:411:GLN:O	2.20	0.42
1:A:64:ILE:HG22	1:A:429:ALA:HB1	2.02	0.42
1:A:1272:ASN:HB3	1:A:1275:LEU:HG	2.01	0.42
1:A:1019:GLY:HA2	1:A:1070:ILE:HG22	2.00	0.42
1:A:1247:ILE:HG13	1:A:1248:VAL:HG13	2.01	0.42
1:A:859:ILE:HG23	1:A:860:LEU:N	2.35	0.42
1:A:1242:PHE:O	1:A:1252:TYR:HA	2.20	0.42
1:A:819:SER:C	1:A:821:GLU:H	2.23	0.42
1:A:307:VAL:HG22	1:A:308:CYS:H	1.83	0.42
1:A:670:TYR:CD2	1:A:676:LYS:HD3	2.54	0.42
1:A:976:ASP:HA	1:A:1032:GLU:O	2.19	0.42
1:A:807:ASN:O	1:A:810:ASP:HB3	2.20	0.42
1:A:264:GLN:HB2	1:A:267[A]:GLU:HG3	2.02	0.42
1:A:674:LYS:NZ	1:A:816:LEU:C	2.74	0.41
1:A:307:VAL:HG23	4:A:1780:HOH:O	2.20	0.41
1:A:203:ASN:HB3	1:A:218:GLY:HA2	2.02	0.41
1:A:936:TYR:HB3	1:A:944:TYR:CE1	2.54	0.41
1:A:80:THR:O	1:A:84:LYS:HG3	2.20	0.41
1:A:536:ILE:HG23	1:A:537:PHE:N	2.36	0.41
1:A:920:SER:HB2	1:A:922:PHE:CE1	2.56	0.41
1:A:1000:ARG:NH2	1:A:1280:GLN:OE1	2.54	0.41
1:A:179:HIS:HB2	4:A:1502:HOH:O	2.19	0.41
1:A:324:LYS:HZ1	1:A:331:GLU:HB3	1.82	0.41
1:A:285:LYS:HA	1:A:481:ILE:HD11	2.03	0.41
1:A:1162:LYS:O	1:A:1163:GLU:CB	2.68	0.41
1:A:1127:ASN:C	1:A:1128:GLN:O	2.58	0.41
1:A:224:ALA:O	1:A:228:MET:HG3	2.19	0.41
1:A:1010:LEU:N	1:A:1010:LEU:HD12	2.35	0.41
1:A:999:ASN:HD21	1:A:1287:GLY:HA3	1.84	0.41
1:A:123:VAL:HA	1:A:124:PRO:HD3	1.93	0.41
1:A:212:SER:HA	1:A:760:ASN:HD21	1.82	0.41
1:A:922:PHE:CE2	1:A:924:ASP:HB2	2.55	0.41
1:A:1067:GLN:HE22	1:A:1071:GLU:HB2	1.86	0.41
1:A:895:LYS:O	1:A:1056:LYS:HE3	2.20	0.41
1:A:630:GLY:HA2	1:A:651:LEU:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:TYR:HA	1:A:323:PHE:CE2	2.56	0.40
1:A:993:ASP:O	1:A:994:ILE:HD13	2.21	0.40
1:A:982:LYS:HG3	1:A:1030:ILE:CG1	2.49	0.40
1:A:674:LYS:O	1:A:678:ILE:HG13	2.22	0.40
1:A:579:THR:HG21	1:A:595:GLN:HE21	1.86	0.40
1:A:187:GLY:HA3	1:A:238:LEU:O	2.21	0.40
1:A:920:SER:C	1:A:921:VAL:HG23	2.41	0.40
1:A:398:ASN:HA	1:A:404:MET:O	2.22	0.40
1:A:814:LEU:C	1:A:816:LEU:H	2.25	0.40
1:A:956:LYS:HB3	1:A:1034:ILE:HG21	2.04	0.40
1:A:824:LYS:HA	1:A:824:LYS:HD2	1.90	0.40
1:A:593:VAL:O	1:A:597:VAL:HG23	2.21	0.40
1:A:180:PHE:O	1:A:184:GLU:HG3	2.22	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	1286/1290 (100%)	1189 (92%)	82 (6%)	15 (1%)	16	12

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	142	SER
1	A	817	ILE
1	A	921	VAL
1	A	1128	GLN
1	A	1130	SER
1	A	1151	ASN
1	A	922	PHE
1	A	1152	SER

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Mol	Chain	Res	Type
1	A	1158	ASP
1	A	1230	SER
1	A	819	SER
1	A	923	LEU
1	A	1010	LEU
1	A	145	GLY
1	A	144	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	1179/1189 (99%)	1157 (98%)	22 (2%)	65	77

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	PHE
1	A	244	ASP
1	A	309	ILE
1	A	405	GLU
1	A	444	ILE
1	A	495	ASP
1	A	619	ILE
1	A	667	LEU
1	A	675	ASN
1	A	686	THR
1	A	723	ASN
1	A	812	ASN
1	A	815	TYR
1	A	873	ASN
1	A	888	ASP
1	A	892	LEU
1	A	918	PHE
1	A	925	PHE
1	A	1010	LEU

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Mol	Chain	Res	Type
1	A	1189	GLU
1	A	1229	GLU
1	A	1245	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	ASN
1	A	177	GLN
1	A	178	ASN
1	A	411	GLN
1	A	427	HIS
1	A	595	GLN
1	A	605	ASN
1	A	683	ASN
1	A	723	ASN
1	A	727	GLN
1	A	760	ASN
1	A	764	ASN
1	A	799	ASN
1	A	812	ASN
1	A	853	ASN
1	A	862	ASN
1	A	872	ASN
1	A	873	ASN
1	A	943	ASN
1	A	947	ASN
1	A	953	ASN
1	A	957	ASN
1	A	989	ASN
1	A	999	ASN
1	A	1067	GLN
1	A	1069	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 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.