Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:04 PM GMT

PDB ID	:	1S0F
Title	:	Crystal structure of botulinum neurotoxin type B at pH 7.0
Authors	:	Eswaramoorthy, S.; Kumaran, D.; Keller, J.; Swaminathan, S.
Deposited on	:	2003-12-30
Resolution	:	2.30 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

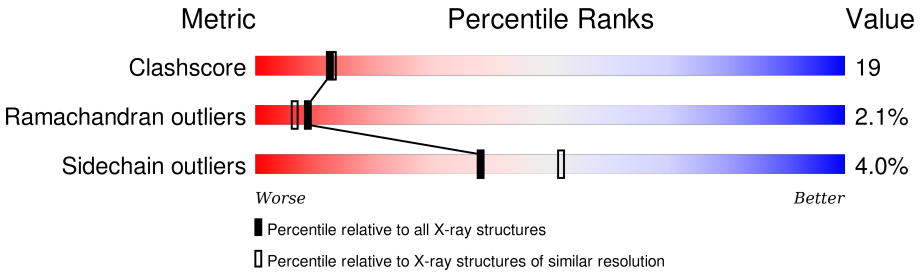
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 2.30 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	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)

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	62% 33%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 10851 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	1276	Total	C	N	O	S	0	0	0
			10429	6719	1676	2001	33			

- 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	419	Total	O	0	0
			419	419		

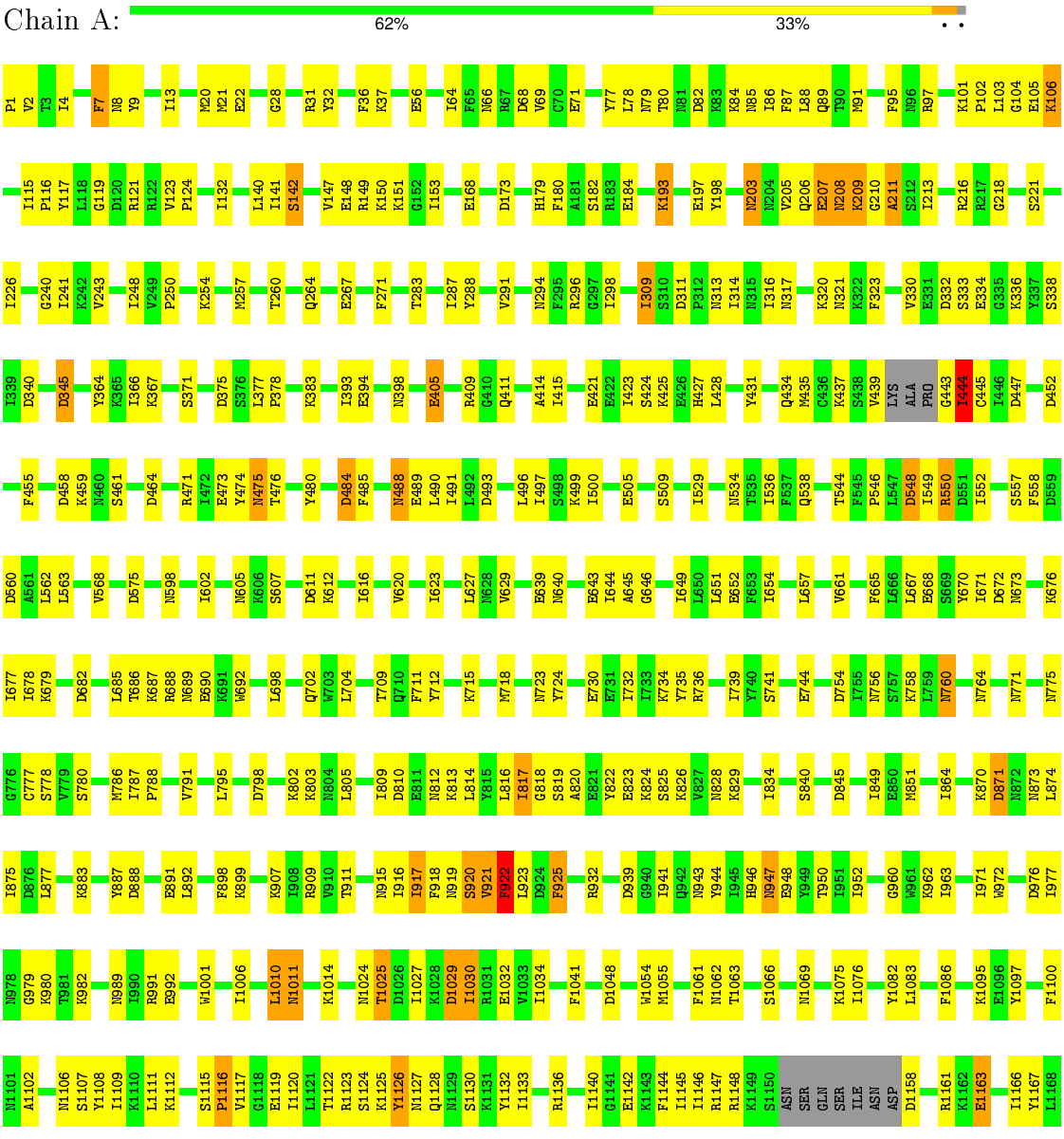
3 Residue-property plots (i)

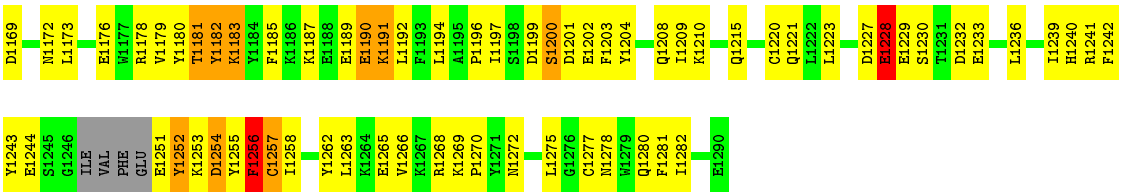
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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

Chain A:




D1169
N1172
L1173
E1176
W1177
R1178
V1179
Y1180
T1181
Y1182
K1183
Y1184
F1185
K1186
K1187
E1188
E1189
E1190
K1191
L1192
F1193
L1194
A1195
P1196
I1197
S1198
D1199
S1200
D1201
E1202
F1203
Y1204
Q1208
I1209
K1210
Q1215
C1220
Q1221
L1222
L1223
D1227
E1228
E1229
S1230
T1231
D1232
E1233
L1236
I1239
H1240
R1241
F1242
Y1243
E1244
S1245
G1246
ILE
VAL
PHE
GLU
E1251
Y1252
K1253
D1254
Y1255
F1256
C1257
I1258
Y1262
L1263
K1264
E1265
V1266
K1267
R1268
K1269
P1270
Y1271
N1272
L1275
G1276
C1277
N1278
W1279
Q1280
F1281
I1282
E1290

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	77.60Å 122.85Å 93.41Å 90.00° 112.48° 90.00°	Depositor
Resolution (Å)	50.00 – 2.30	Depositor
% Data completeness (in resolution range)	80.8 (50.00-2.30)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.227 , 0.288	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10851	wwPDB-VP
Average B, all atoms (Å^2)	38.0	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, 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	0.41	0/10653	0.62	2/14403 (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	661	VAL	N-CA-C	-5.06	97.33	111.00
1	A	193	LYS	N-CA-C	-5.05	97.37	111.00

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	10429	0	10182	399	0
2	A	1	0	0	0	0
3	A	2	0	0	0	0
4	A	419	0	0	19	0
All	All	10851	0	10182	399	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 19.

All (399) 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:1223:LEU:HB2	1:A:1236:LEU:HD23	1.28	1.10
1:A:834:ILE:HD11	1:A:917:ILE:HG13	1.44	0.99
1:A:946:HIS:O	1:A:947:ASN:HB2	1.65	0.96
1:A:1075:LYS:HE2	1:A:1215:GLN:HE22	1.31	0.95
1:A:142:SER:OG	1:A:148:GLU:HG2	1.68	0.93
1:A:309:ILE:HD13	1:A:309:ILE:H	1.36	0.91
1:A:367:LYS:H	1:A:411:GLN:HE22	0.91	0.90
1:A:1241:ARG:HH21	1:A:1252:TYR:H	1.15	0.90
1:A:367:LYS:H	1:A:411:GLN:NE2	1.71	0.89
1:A:142:SER:HB2	1:A:149:ARG:H	1.38	0.88
1:A:1192:LEU:HD21	1:A:1258:ILE:HB	1.55	0.88
1:A:1223:LEU:HB2	1:A:1236:LEU:CD2	2.03	0.88
1:A:826:LYS:HA	1:A:829:LYS:HE2	1.58	0.85
1:A:425:LYS:HD3	1:A:428:LEU:HD12	1.58	0.85
1:A:1115:SER:HB2	1:A:1116:PRO:HD2	1.60	0.84
1:A:1241:ARG:HH21	1:A:1252:TYR:N	1.76	0.83
1:A:1272:ASN:HD22	1:A:1275:LEU:HG	1.42	0.82
1:A:802:LYS:HE2	1:A:828:ASN:ND2	1.93	0.82
1:A:367:LYS:N	1:A:411:GLN:HE22	1.75	0.81
1:A:612:LYS:HB3	1:A:1076:ILE:HD13	1.62	0.81
1:A:640:ASN:HB2	4:A:1500:HOH:O	1.82	0.80
1:A:211:ALA:HB1	1:A:764:ASN:HD21	1.45	0.80
1:A:309:ILE:CD1	1:A:309:ILE:H	1.96	0.79
1:A:493:ASP:OD2	1:A:496:LEU:HB2	1.81	0.79
1:A:1106:ASN:ND2	1:A:1136:ARG:HE	1.82	0.78
1:A:140:LEU:HD11	1:A:147:VAL:HA	1.66	0.77
1:A:563:LEU:HG	4:A:1695:HOH:O	1.85	0.76
1:A:213:ILE:H	1:A:760:ASN:HD21	1.34	0.76
1:A:1241:ARG:HA	1:A:1254:ASP:HA	1.69	0.75
1:A:203:ASN:HB3	1:A:218:GLY:HA2	1.68	0.75
1:A:211:ALA:HB1	1:A:764:ASN:ND2	2.02	0.74
1:A:657:LEU:HD11	1:A:786:MET:HG2	1.68	0.74
1:A:1125:LYS:HD3	1:A:1136:ARG:NH1	2.03	0.74
1:A:977:ILE:HG21	1:A:1032:GLU:OE1	1.87	0.74
1:A:550:ARG:HH11	1:A:550:ARG:HB2	1.52	0.74
1:A:435:MET:HG2	1:A:529:ILE:HD11	1.71	0.73
1:A:1192:LEU:HG	1:A:1256:PHE:O	1.90	0.72
1:A:976:ASP:OD2	1:A:980:LYS:HB3	1.90	0.71
1:A:670:TYR:CD2	1:A:676:LYS:HB3	2.25	0.71
1:A:1181:THR:O	1:A:1203:PHE:HB3	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1243:TYR:O	1:A:1244:GLU:HG3	1.90	0.70
1:A:193:LYS:HD3	4:A:1404:HOH:O	1.89	0.70
1:A:1014:LYS:HE2	1:A:1024:ASN:ND2	2.07	0.70
1:A:802:LYS:HE3	1:A:828:ASN:HA	1.74	0.69
1:A:870:LYS:HG3	1:A:875:ILE:HD11	1.74	0.68
1:A:309:ILE:HD13	1:A:309:ILE:N	2.07	0.68
1:A:919:ASN:C	1:A:921:VAL:H	1.95	0.68
1:A:1236:LEU:HD12	1:A:1262:TYR:CB	2.24	0.67
1:A:209:LYS:CB	1:A:218:GLY:H	2.07	0.67
1:A:205:VAL:HA	4:A:1608:HOH:O	1.94	0.67
1:A:812:ASN:O	1:A:816:LEU:HG	1.95	0.67
1:A:4:ILE:HD12	1:A:95:PHE:HB3	1.76	0.67
1:A:32:TYR:OH	1:A:150:LYS:HE2	1.94	0.67
1:A:439:VAL:HB	1:A:443:GLY:HA2	1.77	0.67
1:A:330:VAL:HG23	1:A:338:SER:HB3	1.75	0.67
1:A:548:ASP:HA	4:A:1466:HOH:O	1.96	0.66
1:A:213:ILE:N	1:A:760:ASN:HD21	1.93	0.65
1:A:1115:SER:HB2	1:A:1116:PRO:CD	2.25	0.65
1:A:1197:ILE:HA	4:A:1354:HOH:O	1.94	0.65
1:A:812:ASN:HB3	1:A:816:LEU:HG	1.79	0.65
1:A:394:GLU:HB3	4:A:1666:HOH:O	1.97	0.64
1:A:1126:TYR:CE1	1:A:1128:GLN:HB2	2.33	0.64
1:A:1107:SER:HB3	1:A:1120:ILE:CG2	2.28	0.64
1:A:670:TYR:CD2	1:A:676:LYS:HD3	2.33	0.63
1:A:920:SER:HG	1:A:922:PHE:HE1	1.46	0.63
1:A:437:LYS:HD2	1:A:444:ILE:HG23	1.80	0.63
1:A:85:ASN:ND2	1:A:89:GLN:HE21	1.97	0.63
1:A:471:ARG:HH11	1:A:471:ARG:HG3	1.64	0.62
1:A:825:SER:O	1:A:829:LYS:HG2	1.98	0.62
1:A:1142:GLU:HB2	1:A:1144:PHE:CE1	2.33	0.62
1:A:13:ILE:HD13	1:A:20:MET:HG2	1.82	0.62
1:A:550:ARG:HH11	1:A:550:ARG:CB	2.12	0.61
1:A:1126:TYR:CZ	1:A:1128:GLN:HB2	2.36	0.61
1:A:7:PHE:HZ	1:A:37:LYS:O	1.83	0.61
1:A:982:LYS:HG2	1:A:1030:ILE:HD11	1.83	0.61
1:A:685:LEU:O	1:A:688:ARG:HB3	2.01	0.61
1:A:1111:LEU:HD23	1:A:1172:ASN:ND2	2.14	0.61
1:A:845:ASP:O	1:A:849:ILE:HG12	2.01	0.61
1:A:946:HIS:O	1:A:947:ASN:CB	2.43	0.61
1:A:1086:PHE:HB2	1:A:1282:ILE:HG12	1.81	0.60
1:A:1117:VAL:HG22	4:A:1668:HOH:O	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:ARG:HH11	1:A:296:ARG:HG2	1.65	0.60
1:A:816:LEU:HB2	1:A:820:ALA:HB2	1.83	0.60
1:A:1241:ARG:NH2	1:A:1252:TYR:H	1.95	0.60
1:A:802:LYS:HE2	1:A:828:ASN:CG	2.21	0.60
1:A:1236:LEU:HD12	1:A:1262:TYR:HB3	1.84	0.60
1:A:1:PRO:HB2	1:A:105:GLU:OE2	2.01	0.60
1:A:330:VAL:CG2	1:A:338:SER:HB3	2.32	0.60
1:A:646:GLY:O	1:A:649:ILE:HG12	2.01	0.60
1:A:667:LEU:HD11	1:A:805:LEU:HD23	1.84	0.60
1:A:206:GLN:HA	1:A:771:ASN:ND2	2.17	0.60
1:A:1189:GLU:OE1	1:A:1189:GLU:N	2.35	0.59
1:A:921:VAL:O	1:A:922:PHE:HB3	2.02	0.59
1:A:1268:ARG:HH11	1:A:1268:ARG:HG3	1.67	0.59
1:A:1111:LEU:HD13	1:A:1194:LEU:HD12	1.83	0.59
1:A:1183:LYS:HD2	1:A:1202:GLU:O	2.03	0.59
1:A:1148:ARG:NH2	1:A:1158:ASP:HB3	2.17	0.59
1:A:409:ARG:NH1	1:A:415:ILE:HD13	2.18	0.59
1:A:1236:LEU:HD12	1:A:1262:TYR:HB2	1.84	0.59
1:A:977:ILE:HD13	1:A:1032:GLU:HB3	1.84	0.59
1:A:817:ILE:HG22	1:A:818:GLY:H	1.68	0.58
1:A:1145:ILE:HD13	1:A:1147:ARG:NH2	2.18	0.58
1:A:1241:ARG:HB2	1:A:1254:ASP:OD2	2.04	0.58
1:A:1223:LEU:CB	1:A:1236:LEU:HD23	2.20	0.58
1:A:1241:ARG:NH2	1:A:1251:GLU:HA	2.19	0.58
1:A:330:VAL:HG22	1:A:338:SER:O	2.04	0.58
1:A:976:ASP:HB3	1:A:1030:ILE:HG23	1.86	0.57
1:A:826:LYS:HA	1:A:829:LYS:CE	2.33	0.57
1:A:243:VAL:CG2	1:A:287:ILE:HG23	2.34	0.57
1:A:645:ALA:HB3	1:A:649:ILE:HG23	1.87	0.57
1:A:213:ILE:H	1:A:760:ASN:ND2	2.00	0.57
1:A:670:TYR:HB2	1:A:677:ILE:HG13	1.87	0.57
1:A:899:LYS:HD2	1:A:1054:TRP:CZ2	2.40	0.57
1:A:1106:ASN:HD22	1:A:1136:ARG:HE	1.53	0.56
1:A:645:ALA:HB3	1:A:649:ILE:CG2	2.35	0.56
1:A:639:GLU:O	1:A:643:GLU:HG3	2.04	0.56
1:A:1228:GLU:OE1	1:A:1228:GLU:N	2.38	0.56
1:A:546:PRO:HB2	1:A:549:ILE:HG12	1.87	0.56
1:A:819:SER:O	1:A:822:TYR:HB3	2.05	0.56
1:A:670:TYR:CG	1:A:676:LYS:HB3	2.41	0.56
1:A:101:LYS:HB2	1:A:364:TYR:CZ	2.40	0.56
1:A:332:ASP:OD2	1:A:336:LYS:HB3	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:ILE:CD1	1:A:431:TYR:HB2	2.36	0.56
1:A:1147:ARG:O	1:A:1166:ILE:HB	2.06	0.56
1:A:730:GLU:OE1	1:A:756:ASN:OD1	2.23	0.56
1:A:80:THR:O	1:A:84:LYS:HG3	2.07	0.55
1:A:840:SER:HB3	1:A:849:ILE:HD12	1.88	0.55
1:A:1185:PHE:C	1:A:1187:LYS:H	2.10	0.55
1:A:311:ASP:HB3	1:A:314:ILE:HG12	1.88	0.55
1:A:1181:THR:HG21	1:A:1258:ILE:HD13	1.88	0.55
1:A:909:ARG:HD2	4:A:1561:HOH:O	2.06	0.55
1:A:499:LYS:O	1:A:500:ILE:HD13	2.07	0.55
1:A:892:LEU:HD23	1:A:898:PHE:HB3	1.89	0.55
1:A:1255:TYR:C	1:A:1257:CYS:H	2.10	0.54
1:A:1265:GLU:HA	1:A:1268:ARG:HH11	1.73	0.54
1:A:1263:LEU:O	1:A:1266:VAL:HG22	2.06	0.54
1:A:260:THR:HG21	1:A:455:PHE:HE1	1.72	0.54
1:A:787:ILE:HB	1:A:788:PRO:HD3	1.90	0.54
1:A:1182:TYR:C	1:A:1182:TYR:CD2	2.81	0.54
1:A:332:ASP:OD1	1:A:334:GLU:HB2	2.08	0.54
1:A:485:PHE:HE2	1:A:490:LEU:HB2	1.73	0.54
1:A:377:LEU:HB3	1:A:378:PRO:CD	2.38	0.54
1:A:698:LEU:O	1:A:702:GLN:HG3	2.08	0.54
1:A:1083:LEU:HD13	1:A:1209:ILE:CD1	2.38	0.54
1:A:692:TRP:CH2	1:A:834:ILE:HB	2.43	0.53
1:A:1208:GLN:OE1	1:A:1210:LYS:HD3	2.07	0.53
1:A:1199:ASP:O	1:A:1201:ASP:N	2.42	0.53
1:A:823:GLU:HA	1:A:826:LYS:HB2	1.89	0.53
1:A:1272:ASN:ND2	1:A:1275:LEU:HG	2.16	0.53
1:A:670:TYR:HD2	1:A:676:LYS:HD3	1.74	0.53
1:A:813:LYS:HG3	1:A:814:LEU:N	2.23	0.53
1:A:1268:ARG:NH1	1:A:1268:ARG:HG3	2.23	0.53
1:A:887:TYR:HD1	1:A:907:LYS:HG3	1.73	0.53
1:A:1265:GLU:HA	1:A:1268:ARG:NH1	2.23	0.53
1:A:1180:TYR:HB3	1:A:1204:TYR:O	2.08	0.53
1:A:31:ARG:HG3	1:A:32:TYR:N	2.24	0.53
1:A:1086:PHE:CB	1:A:1282:ILE:HG12	2.40	0.53
1:A:817:ILE:HG22	1:A:818:GLY:N	2.24	0.53
1:A:296:ARG:HG2	1:A:296:ARG:NH1	2.23	0.52
1:A:1014:LYS:HE2	1:A:1024:ASN:HD21	1.74	0.52
1:A:221:SER:HB2	1:A:226:ILE:HD11	1.90	0.52
1:A:1125:LYS:HB3	1:A:1136:ARG:HH11	1.74	0.52
1:A:907:LYS:HA	1:A:1041:PHE:O	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:ASP:O	1:A:86:ILE:HG13	2.10	0.52
1:A:887:TYR:CD1	1:A:907:LYS:HG3	2.44	0.52
1:A:1066:SER:H	1:A:1069:ASN:HD22	1.57	0.52
1:A:1191:LYS:HG3	1:A:1242:PHE:HE1	1.74	0.52
1:A:972:TRP:CD2	1:A:1006:ILE:HG21	2.44	0.52
1:A:1163:GLU:OE1	1:A:1210:LYS:HD2	2.10	0.52
1:A:1179:VAL:HG22	1:A:1194:LEU:HD22	1.92	0.51
1:A:1182:TYR:O	1:A:1183:LYS:CB	2.58	0.51
1:A:1230:SER:C	1:A:1232:ASP:N	2.62	0.51
1:A:64:ILE:HD11	1:A:431:TYR:CD1	2.45	0.51
1:A:864:ILE:HG21	1:A:916:ILE:HG21	1.91	0.51
1:A:241:ILE:HG22	1:A:291:VAL:HG13	1.91	0.51
1:A:932:ARG:HD3	1:A:1001:TRP:CD1	2.45	0.51
1:A:1010:LEU:HD13	1:A:1011:ASN:OD1	2.10	0.51
1:A:102:PRO:O	1:A:106:LYS:HD2	2.10	0.51
1:A:665:PHE:CZ	1:A:687:LYS:HG3	2.46	0.51
1:A:338:SER:HB2	4:A:1557:HOH:O	2.10	0.51
1:A:32:TYR:N	1:A:32:TYR:CD1	2.78	0.51
1:A:925:PHE:HB2	1:A:1061:PHE:O	2.11	0.51
1:A:1275:LEU:HD13	1:A:1277:CYS:SG	2.50	0.50
1:A:1169:ASP:OD2	1:A:1176:GLU:OE2	2.29	0.50
1:A:1262:TYR:O	1:A:1265:GLU:N	2.44	0.50
1:A:826:LYS:CA	1:A:829:LYS:HE2	2.34	0.50
1:A:425:LYS:HB3	4:A:1468:HOH:O	2.11	0.50
1:A:1272:ASN:HD22	1:A:1275:LEU:CG	2.20	0.50
1:A:444:ILE:O	1:A:444:ILE:HG13	2.11	0.50
1:A:819:SER:O	1:A:822:TYR:N	2.43	0.50
1:A:960:GLY:HA2	1:A:1034:ILE:O	2.11	0.50
1:A:22:GLU:CD	1:A:28:GLY:HA2	2.32	0.50
1:A:627:LEU:HD11	1:A:718:MET:HG2	1.94	0.50
1:A:66:ASN:OD1	1:A:69:VAL:HG23	2.12	0.50
1:A:775:ASN:HB3	1:A:851:MET:HG2	1.93	0.50
1:A:1215:GLN:HA	1:A:1215:GLN:HE21	1.76	0.49
1:A:1112:LYS:HA	1:A:1119:GLU:OE2	2.11	0.49
1:A:1253:LYS:CB	1:A:1255:TYR:HE1	2.24	0.49
1:A:1227:ASP:C	1:A:1229:GLU:H	2.16	0.49
1:A:439:VAL:O	1:A:439:VAL:HG12	2.12	0.49
1:A:976:ASP:HA	1:A:1032:GLU:O	2.12	0.49
1:A:817:ILE:CG2	1:A:818:GLY:H	2.25	0.49
1:A:142:SER:CB	1:A:148:GLU:HG2	2.42	0.49
1:A:1123:ARG:HG2	1:A:1140:ILE:HD11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:989:ASN:HD22	1:A:992:GLU:HG3	1.77	0.49
1:A:686:THR:HA	1:A:689:ASN:HD22	1.78	0.49
1:A:1025:THR:HG22	1:A:1027:ILE:HG23	1.95	0.49
1:A:103:LEU:HB2	1:A:491:ILE:HD11	1.95	0.49
1:A:791:VAL:HB	1:A:915:ASN:HB3	1.94	0.48
1:A:1265:GLU:O	1:A:1268:ARG:HB2	2.13	0.48
1:A:71:GLU:HG2	1:A:168:GLU:OE2	2.12	0.48
1:A:952:ILE:HD12	1:A:963:ILE:HD12	1.95	0.48
1:A:809:ILE:HG23	1:A:816:LEU:HD12	1.96	0.48
1:A:605:ASN:C	1:A:607:SER:H	2.15	0.48
1:A:260:THR:CG2	1:A:455:PHE:HE1	2.27	0.48
1:A:1272:ASN:HB3	1:A:1275:LEU:HG	1.96	0.48
1:A:1257:CYS:SG	1:A:1257:CYS:O	2.72	0.48
1:A:1191:LYS:CG	1:A:1242:PHE:HE1	2.27	0.48
1:A:182:SER:O	1:A:240:GLY:HA2	2.14	0.48
1:A:678:ILE:HG12	1:A:823:GLU:OE1	2.14	0.48
1:A:919:ASN:C	1:A:921:VAL:N	2.63	0.48
1:A:1111:LEU:HD23	1:A:1172:ASN:HD22	1.76	0.48
1:A:1111:LEU:CD2	1:A:1172:ASN:HD22	2.26	0.48
1:A:730:GLU:O	1:A:734:LYS:HG3	2.14	0.48
1:A:950:THR:OG1	1:A:962:LYS:HD2	2.14	0.48
1:A:678:ILE:HG22	1:A:682:ASP:OD2	2.14	0.48
1:A:1182:TYR:O	1:A:1183:LYS:HB2	2.14	0.48
1:A:1132:TYR:CD1	1:A:1132:TYR:N	2.82	0.47
1:A:802:LYS:CE	1:A:828:ASN:HA	2.44	0.47
1:A:612:LYS:HE3	4:A:1463:HOH:O	2.14	0.47
1:A:670:TYR:O	1:A:677:ILE:HD11	2.14	0.47
1:A:497:ILE:HD13	4:A:1710:HOH:O	2.13	0.47
1:A:1120:ILE:HD12	1:A:1239:ILE:HD13	1.96	0.47
1:A:919:ASN:O	1:A:921:VAL:N	2.48	0.47
1:A:645:ALA:CB	1:A:649:ILE:HG23	2.44	0.47
1:A:474:TYR:HB2	1:A:679:LYS:HB2	1.97	0.47
1:A:203:ASN:HD22	1:A:203:ASN:N	2.12	0.47
1:A:1147:ARG:HB2	1:A:1167:TYR:HB2	1.96	0.47
1:A:704:LEU:O	1:A:709:THR:HG23	2.13	0.47
1:A:458:ASP:OD2	1:A:459:LYS:N	2.47	0.47
1:A:398:ASN:HD21	1:A:411:GLN:HE21	1.62	0.47
1:A:21:MET:HG2	1:A:22:GLU:N	2.30	0.47
1:A:1082:TYR:HA	1:A:1161:ARG:HA	1.96	0.47
1:A:64:ILE:HD12	1:A:431:TYR:HB2	1.97	0.47
1:A:1199:ASP:O	1:A:1199:ASP:OD1	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:989:ASN:HD22	1:A:992:GLU:CG	2.28	0.47
1:A:558:PHE:CZ	1:A:562:LEU:HD11	2.50	0.47
1:A:97:ARG:HG3	1:A:97:ARG:HH11	1.79	0.47
1:A:216:ARG:O	1:A:414:ALA:HB2	2.14	0.47
1:A:405:GLU:C	1:A:405:GLU:OE1	2.54	0.46
1:A:1230:SER:C	1:A:1232:ASP:H	2.17	0.46
1:A:1100:PHE:HD2	1:A:1280:GLN:HB2	1.80	0.46
1:A:1190:GLU:O	1:A:1258:ILE:HG22	2.16	0.46
1:A:283:THR:HA	4:A:1638:HOH:O	2.15	0.46
1:A:1220:CYS:SG	1:A:1281:PHE:HE1	2.39	0.46
1:A:1241:ARG:HB2	1:A:1254:ASP:CG	2.35	0.46
1:A:434:GLN:HG2	1:A:445:CYS:HB3	1.97	0.46
1:A:85:ASN:HD21	1:A:89:GLN:HE21	1.64	0.46
1:A:892:LEU:HD23	1:A:898:PHE:CB	2.46	0.46
1:A:552:ILE:HD12	1:A:568:VAL:HG21	1.98	0.46
1:A:921:VAL:O	1:A:922:PHE:CB	2.63	0.46
1:A:377:LEU:N	1:A:377:LEU:HD23	2.29	0.46
1:A:1227:ASP:O	1:A:1229:GLU:N	2.49	0.46
1:A:184:GLU:HA	1:A:294:ASN:ND2	2.31	0.46
1:A:629:VAL:HG23	1:A:652:GLU:OE1	2.15	0.45
1:A:437:LYS:HD2	1:A:444:ILE:CG2	2.45	0.45
1:A:873:ASN:ND2	1:A:874:LEU:H	2.14	0.45
1:A:1233:GLU:HB2	4:A:1706:HOH:O	2.16	0.45
1:A:1240:HIS:N	1:A:1257:CYS:SG	2.89	0.45
1:A:557:SER:HB3	1:A:560:ASP:HB2	1.98	0.45
1:A:671:ILE:O	1:A:672:ASP:HB2	2.17	0.45
1:A:434:GLN:HG3	1:A:447:ASP:OD1	2.16	0.45
1:A:97:ARG:HA	1:A:393:ILE:HG23	1.99	0.45
1:A:316:ILE:O	1:A:320:LYS:HG3	2.16	0.45
1:A:711:PHE:CE1	1:A:778:SER:HA	2.51	0.45
1:A:31:ARG:HG3	1:A:32:TYR:H	1.80	0.45
1:A:1107:SER:HB3	1:A:1120:ILE:HG23	1.99	0.45
1:A:529:ILE:HD12	1:A:529:ILE:C	2.37	0.45
1:A:117:TYR:HA	1:A:323:PHE:CE2	2.52	0.45
1:A:141:ILE:CD1	1:A:151:LYS:HB2	2.47	0.45
1:A:1146:ILE:HG23	1:A:1166:ILE:HD12	1.99	0.44
1:A:651:LEU:HD12	1:A:654:ILE:HD13	1.99	0.44
1:A:317:ASN:O	1:A:321:ASN:ND2	2.47	0.44
1:A:1185:PHE:CD2	1:A:1190:GLU:HG2	2.53	0.44
1:A:85:ASN:HD21	1:A:89:GLN:NE2	2.14	0.44
1:A:22:GLU:OE2	1:A:28:GLY:HA2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:GLY:HA2	1:A:132:ILE:HD13	1.98	0.44
1:A:153:ILE:HA	1:A:505:GLU:O	2.16	0.44
1:A:1269:LYS:HA	1:A:1270:PRO:C	2.37	0.44
1:A:489:GLU:O	1:A:493:ASP:HB2	2.17	0.44
1:A:473:GLU:HB3	1:A:670:TYR:OH	2.17	0.44
1:A:1083:LEU:HD13	1:A:1209:ILE:HD13	1.99	0.44
1:A:216:ARG:HG2	4:A:1590:HOH:O	2.16	0.44
1:A:1:PRO:HB2	1:A:2:VAL:H	1.66	0.44
1:A:754:ASP:OD2	1:A:758:LYS:HE3	2.17	0.44
1:A:1215:GLN:HA	1:A:1215:GLN:NE2	2.33	0.44
1:A:1220:CYS:C	1:A:1221:GLN:NE2	2.71	0.44
1:A:208:ASN:O	1:A:210:GLY:N	2.51	0.44
1:A:870:LYS:O	1:A:871:ASP:C	2.56	0.44
1:A:9:TYR:H	1:A:85:ASN:HD22	1.64	0.44
1:A:1169:ASP:HB3	1:A:1176:GLU:HG2	2.00	0.44
1:A:670:TYR:HB2	1:A:677:ILE:CG1	2.47	0.44
1:A:948:GLU:O	1:A:948:GLU:HG3	2.17	0.44
1:A:425:LYS:C	1:A:427:HIS:N	2.71	0.43
1:A:925:PHE:HA	1:A:1063:THR:N	2.33	0.43
1:A:1145:ILE:HG23	1:A:1145:ILE:O	2.16	0.43
1:A:605:ASN:C	1:A:607:SER:N	2.72	0.43
1:A:198:TYR:HD2	1:A:423:ILE:HD11	1.83	0.43
1:A:544:THR:HG22	1:A:724:TYR:CE2	2.52	0.43
1:A:550:ARG:NH1	1:A:550:ARG:CB	2.79	0.43
1:A:471:ARG:HH11	1:A:471:ARG:CG	2.30	0.43
1:A:787:ILE:O	1:A:791:VAL:HG23	2.18	0.43
1:A:963:ILE:HA	1:A:971:ILE:O	2.18	0.43
1:A:823:GLU:O	1:A:824:LYS:C	2.56	0.43
1:A:741:SER:OG	1:A:744:GLU:HG3	2.19	0.43
1:A:980:LYS:HE2	1:A:1029:ASP:CG	2.38	0.43
1:A:1200:SER:C	1:A:1202:GLU:H	2.21	0.43
1:A:864:ILE:CG2	1:A:1062:ASN:HD22	2.32	0.43
1:A:147:VAL:O	1:A:147:VAL:HG23	2.18	0.43
1:A:813:LYS:HG3	1:A:814:LEU:H	1.82	0.43
1:A:1102:ALA:HB3	1:A:1278:ASN:HB2	2.01	0.43
1:A:475:ASN:HA	1:A:475:ASN:HD22	1.53	0.43
1:A:243:VAL:HG21	1:A:287:ILE:HG23	1.99	0.43
1:A:97:ARG:NH2	1:A:366:ILE:HD11	2.34	0.43
1:A:1095:LYS:HD3	1:A:1097:TYR:OH	2.18	0.43
1:A:1108:TYR:HE2	1:A:1122:THR:O	2.01	0.43
1:A:271:PHE:CE2	1:A:371:SER:HA	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:977:ILE:CD1	1:A:1032:GLU:HB3	2.49	0.43
1:A:667:LEU:HD11	1:A:805:LEU:CD2	2.48	0.43
1:A:891:GLU:O	1:A:898:PHE:HA	2.19	0.43
1:A:711:PHE:O	1:A:715:LYS:HG3	2.18	0.43
1:A:735:TYR:O	1:A:739:ILE:HG12	2.19	0.43
1:A:777:CYS:O	1:A:780:SER:HB3	2.19	0.43
1:A:87:PHE:O	1:A:91:MET:HG2	2.19	0.43
1:A:330:VAL:HG11	1:A:340:ASP:HB2	2.01	0.42
1:A:1083:LEU:HD22	1:A:1220:CYS:CB	2.48	0.42
1:A:488:ASN:HA	1:A:488:ASN:HD22	1.58	0.42
1:A:943:ASN:O	1:A:946:HIS:O	2.37	0.42
1:A:104:GLY:HA3	1:A:364:TYR:OH	2.20	0.42
1:A:123:VAL:HA	1:A:124:PRO:HD3	1.90	0.42
1:A:1192:LEU:CD2	1:A:1258:ILE:HB	2.37	0.42
1:A:267:GLU:HB2	4:A:1529:HOH:O	2.19	0.42
1:A:1014:LYS:HG2	1:A:1024:ASN:ND2	2.35	0.42
1:A:809:ILE:HG23	1:A:816:LEU:CD1	2.49	0.42
1:A:536:ILE:HA	1:A:627:LEU:O	2.19	0.42
1:A:9:TYR:H	1:A:85:ASN:ND2	2.17	0.42
1:A:333:SER:O	1:A:334:GLU:HG2	2.20	0.42
1:A:1083:LEU:HD22	1:A:1220:CYS:HB2	2.00	0.42
1:A:732:ILE:O	1:A:736:ARG:HG2	2.19	0.42
1:A:36:PHE:N	1:A:36:PHE:CD1	2.88	0.42
1:A:920:SER:OG	1:A:922:PHE:HE1	2.02	0.42
1:A:56:GLU:HG3	4:A:1609:HOH:O	2.19	0.42
1:A:115:ILE:HA	1:A:116:PRO:HD3	1.90	0.42
1:A:1236:LEU:HB2	1:A:1262:TYR:CD2	2.55	0.42
1:A:101:LYS:HB2	1:A:364:TYR:OH	2.20	0.42
1:A:1178:ARG:HB3	1:A:1180:TYR:CE2	2.55	0.42
1:A:1242:PHE:N	1:A:1242:PHE:CD2	2.86	0.42
1:A:117:TYR:HA	1:A:323:PHE:CZ	2.55	0.42
1:A:1130:SER:HB3	1:A:1133:ILE:HG12	2.02	0.42
1:A:254:LYS:HB2	1:A:257:MET:HG3	2.02	0.42
1:A:620:VAL:CG1	1:A:623:ILE:HG13	2.49	0.42
1:A:250:PRO:HB3	1:A:455:PHE:CE1	2.55	0.41
1:A:207:GLU:O	1:A:208:ASN:CB	2.67	0.41
1:A:79:ASN:OD1	1:A:80:THR:HG23	2.20	0.41
1:A:1201:ASP:CG	1:A:1201:ASP:O	2.58	0.41
1:A:941:ILE:HD12	1:A:944:TYR:HB3	2.02	0.41
1:A:480:TYR:OH	1:A:690:GLU:HA	2.20	0.41
1:A:288:TYR:OH	1:A:345:ASP:OD1	2.32	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:644:ILE:HA	1:A:877:LEU:HD22	2.01	0.41
1:A:611:ASP:HB3	1:A:616:ILE:HB	2.01	0.41
1:A:1185:PHE:C	1:A:1187:LYS:N	2.73	0.41
1:A:13:ILE:CD1	1:A:20:MET:HG2	2.50	0.41
1:A:484:ASP:OD1	1:A:485:PHE:N	2.53	0.41
1:A:248:ILE:HD13	1:A:461:SER:HB3	2.03	0.41
1:A:1189:GLU:HG3	1:A:1240:HIS:CD2	2.55	0.41
1:A:1182:TYR:O	1:A:1183:LYS:HG3	2.20	0.41
1:A:671:ILE:C	1:A:673:ASN:H	2.24	0.41
1:A:375:ASP:OD1	1:A:712:TYR:HE2	2.03	0.41
1:A:898:PHE:CZ	1:A:1055:MET:HB3	2.56	0.41
1:A:264:GLN:O	1:A:267:GLU:HB3	2.20	0.41
1:A:383:LYS:NZ	1:A:421:GLU:HG2	2.36	0.41
1:A:77:TYR:OH	1:A:197:GLU:OE1	2.24	0.41
1:A:424:SER:HB3	4:A:1423:HOH:O	2.21	0.41
1:A:598:ASN:O	1:A:602:ILE:HG13	2.21	0.41
1:A:260:THR:HG21	1:A:455:PHE:CE1	2.55	0.40
1:A:173:ASP:HB2	1:A:182:SER:OG	2.22	0.40
1:A:534:ASN:HA	1:A:538:GLN:HG2	2.03	0.40
1:A:668:GLU:HB3	1:A:670:TYR:CE1	2.57	0.40
1:A:294:ASN:O	1:A:298:ILE:HG12	2.22	0.40
1:A:883:LYS:HB2	1:A:911:THR:HB	2.04	0.40
1:A:1109:ILE:HD13	1:A:1256:PHE:CE2	2.56	0.40
1:A:141:ILE:HD11	1:A:151:LYS:HB2	2.03	0.40
1:A:795:LEU:HD21	1:A:834:ILE:HG21	2.04	0.40
1:A:834:ILE:CD1	1:A:917:ILE:HG13	2.32	0.40
1:A:1111:LEU:CD2	1:A:1172:ASN:ND2	2.84	0.40
1:A:180:PHE:O	1:A:184:GLU:HG3	2.22	0.40
1:A:475:ASN:O	1:A:476:THR:C	2.60	0.40
1:A:77:TYR:CD2	1:A:78:LEU:HG	2.55	0.40
1:A:121:ARG:HD3	1:A:179:HIS:CG	2.57	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	1268/1290 (98%)	1127 (89%)	115 (9%)	26 (2%)	9 7

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	207	GLU
1	A	208	ASN
1	A	444	ILE
1	A	922	PHE
1	A	1030	ILE
1	A	1183	LYS
1	A	142	SER
1	A	209	LYS
1	A	211	ALA
1	A	947	ASN
1	A	1029	ASP
1	A	1126	TYR
1	A	1200	SER
1	A	1228	GLU
1	A	1252	TYR
1	A	817	ILE
1	A	920	SER
1	A	1191	LYS
1	A	871	ASP
1	A	923	LEU
1	A	979	GLY
1	A	1173	LEU
1	A	1256	PHE
1	A	921	VAL
1	A	1116	PRO
1	A	1196	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	1150/1189 (97%)	1104 (96%)	46 (4%)	38 52

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	PHE
1	A	8	ASN
1	A	68	ASP
1	A	88	LEU
1	A	106	LYS
1	A	203	ASN
1	A	309	ILE
1	A	313	ASN
1	A	345	ASP
1	A	405	GLU
1	A	444	ILE
1	A	452	ASP
1	A	464	ASP
1	A	475	ASN
1	A	484	ASP
1	A	488	ASN
1	A	509	SER
1	A	548	ASP
1	A	550	ARG
1	A	575	ASP
1	A	723	ASN
1	A	760	ASN
1	A	798	ASP
1	A	803	LYS
1	A	810	ASP
1	A	888	ASP
1	A	917	ILE
1	A	918	PHE
1	A	922	PHE
1	A	925	PHE
1	A	939	ASP
1	A	991	ARG
1	A	1010	LEU
1	A	1011	ASN
1	A	1025	THR
1	A	1048	ASP
1	A	1124	SER
1	A	1127	ASN

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Mol	Chain	Res	Type
1	A	1163	GLU
1	A	1181	THR
1	A	1182	TYR
1	A	1190	GLU
1	A	1228	GLU
1	A	1254	ASP
1	A	1256	PHE
1	A	1257	CYS

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	16	ASN
1	A	85	ASN
1	A	411	GLN
1	A	475	ASN
1	A	488	ASN
1	A	523	GLN
1	A	605	ASN
1	A	683	ASN
1	A	689	ASN
1	A	723	ASN
1	A	727	GLN
1	A	753	ASN
1	A	760	ASN
1	A	764	ASN
1	A	873	ASN
1	A	946	HIS
1	A	989	ASN
1	A	999	ASN
1	A	1008	ASN
1	A	1024	ASN
1	A	1062	ASN
1	A	1069	ASN
1	A	1106	ASN
1	A	1215	GLN
1	A	1240	HIS
1	A	1272	ASN
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 carbohydrates in this entry.

5.6 Ligand geometry

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

There are no such residues in this entry.

5.8 Polymer linkage issues

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 will therefore be empty.

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

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

6.3 Carbohydrates

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

6.4 Ligands

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

6.5 Other polymers

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