WORLDWIDE PDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Feb 2, 2016 – 12:00 AM GMT

PDB ID : 7AHL
Title : ALPHA-HEMOLYSIN FROM STAPHYLOCOCCUS AUREUS
Authors : Song, L.; Hobaugh, M.; Shustak, C.; Cheley, S.; Bayley, H.; Gouaux, J.E.
Deposited on : 1996-12-02
Resolution : 1.89 Å(reported)

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

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 1.89 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		10
Ramachandran outliers		0.1%
Sidechain outliers		6.9%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
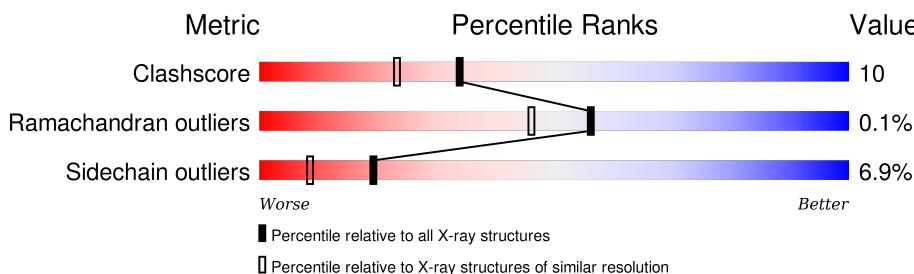
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)

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	293	74% 22% •
1	B	293	71% 26% •
1	C	293	80% 18% •
1	D	293	70% 27% •
1	E	293	77% 19% •
1	F	293	72% 27% •
1	G	293	76% 21% •
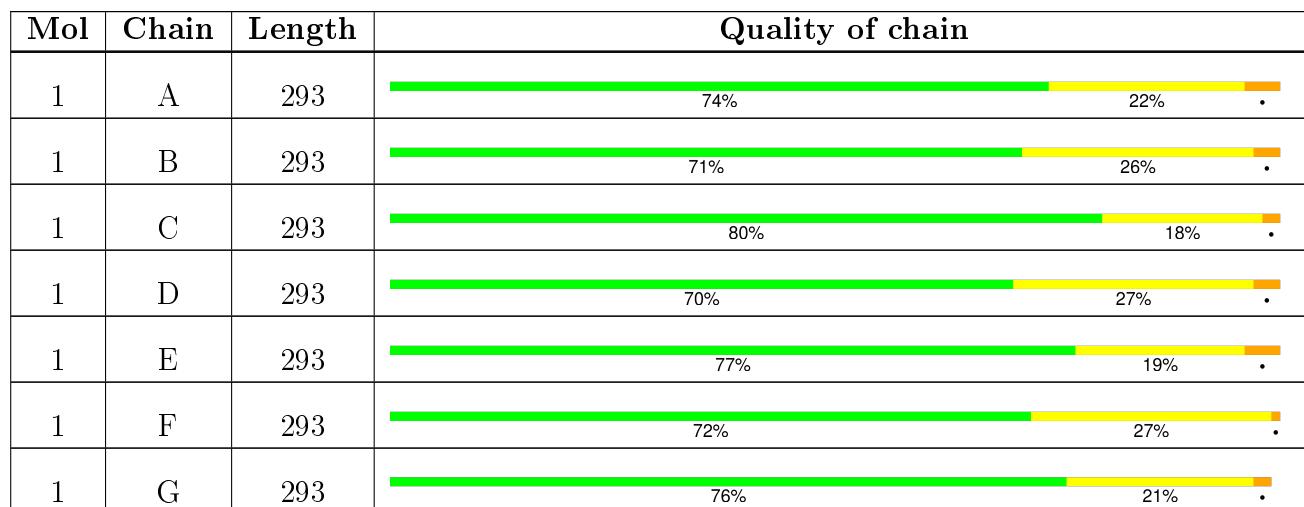
2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 22778 atoms, of which 5571 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 ALPHA-HEMOLYSIN.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	293	Total 2891	C 1466	H 556	N 397	O 465	S 7	0	0	0
1	B	293	Total 2909	C 1472	H 564	N 401	O 465	S 7	0	0	0
1	C	293	Total 2909	C 1472	H 564	N 401	O 465	S 7	0	0	0
1	D	293	Total 2896	C 1466	H 559	N 399	O 465	S 7	0	0	0
1	E	293	Total 2911	C 1472	H 566	N 401	O 465	S 7	0	0	0
1	F	293	Total 2904	C 1469	H 563	N 400	O 465	S 7	0	0	0
1	G	293	Total 2904	C 1469	H 563	N 400	O 465	S 7	0	0	0

- Molecule 2 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	118	Total 354	H 236	O 118	0	0
2	B	128	Total 384	H 256	O 128	0	0
2	C	119	Total 357	H 238	O 119	0	0
2	D	122	Total 366	H 244	O 122	0	0
2	E	126	Total 378	H 252	O 126	0	0
2	F	92	Total 276	H 184	O 92	0	0
2	G	113	Total 339	H 226	O 113	0	0

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: ALPHA-HEMOLYSIN
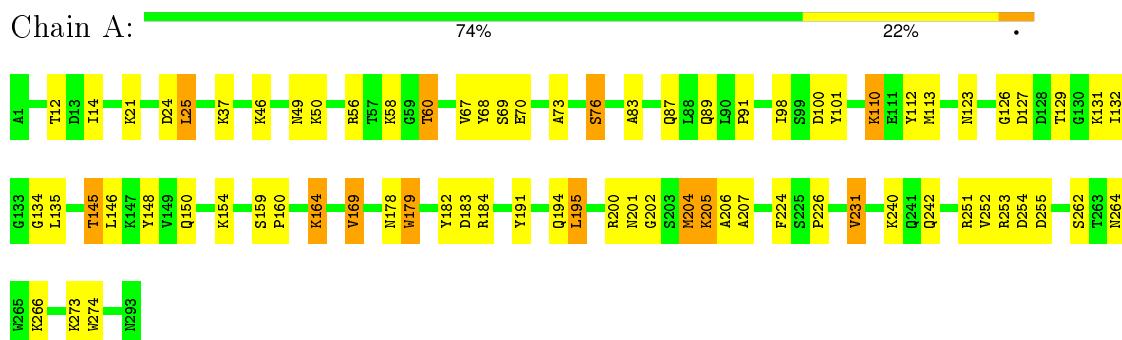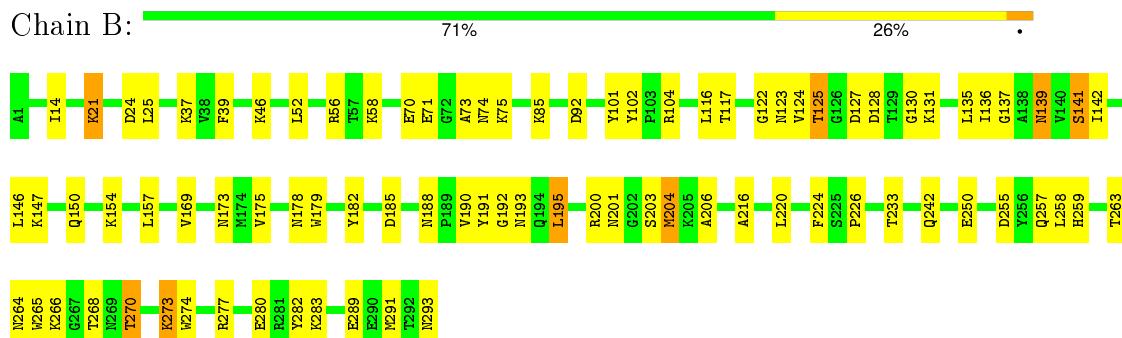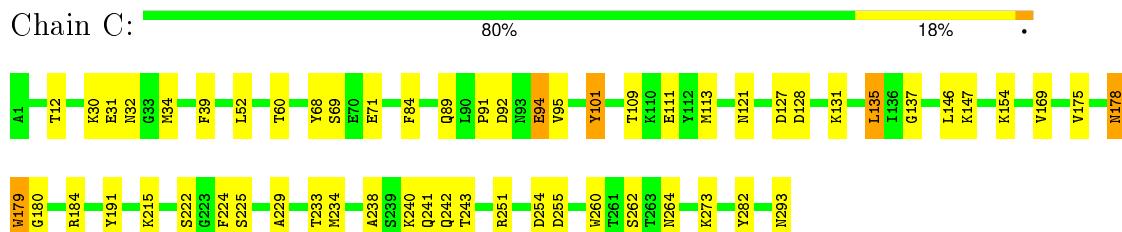
Chain A:

- Molecule 1: ALPHA-HEMOLYSIN

Chain B:

- Molecule 1: ALPHA-HEMOLYSIN

Chain C:

- Molecule 1: ALPHA-HEMOLYSIN

Chain D:

• Molecule 1: ALPHA-HEMOLYSIN

Chain E:

• Molecule 1: ALPHA-HEMOLYSIN

Chain F:

• Molecule 1: ALPHA-HEMOLYSIN

Chain G:
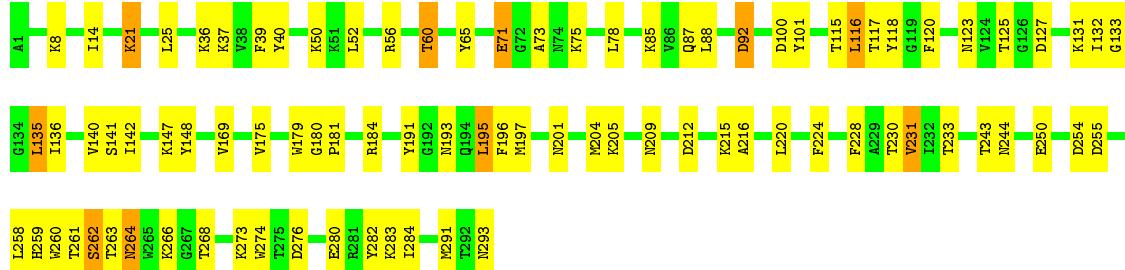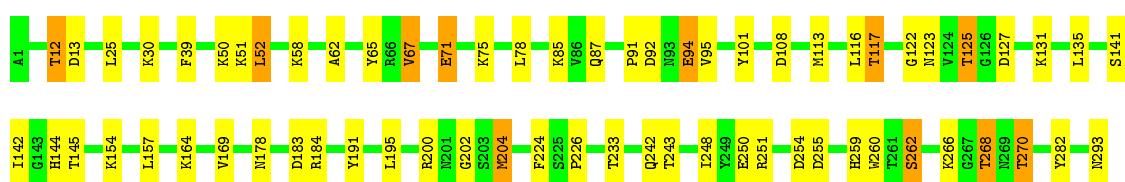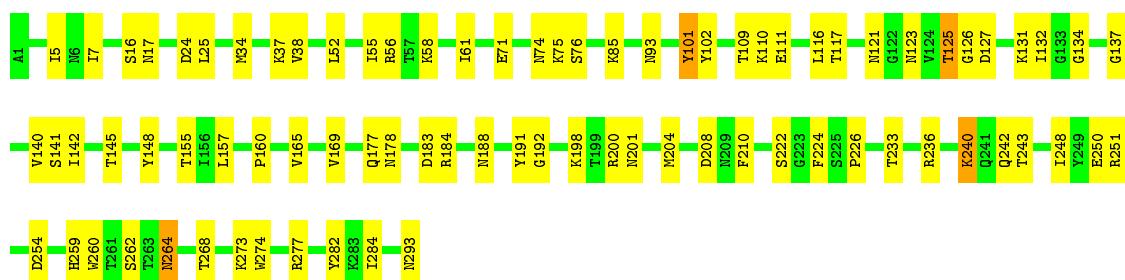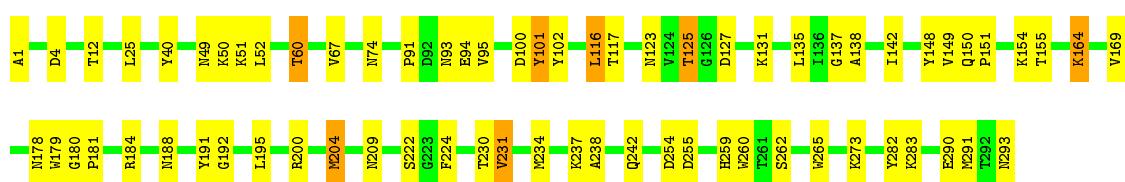
4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	151.92Å　　136.76Å　　135.12Å 90.00°　　91.40°　　90.00°	Depositor
Resolution (Å)	8.00　–　1.89	Depositor
% Data completeness (in resolution range)	93.3 (8.00-1.89)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.199　,　0.257	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	22778	wwPDB-VP
Average B, all atoms (Å²)	30.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

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	0.49	0/2387	0.75	1/3232 (0.0%)
1	B	0.50	0/2397	0.74	0/3243
1	C	0.50	0/2397	0.75	0/3243
1	D	0.48	0/2389	0.74	0/3235
1	E	0.51	0/2397	0.75	1/3243 (0.0%)
1	F	0.47	0/2393	0.73	1/3239 (0.0%)
1	G	0.49	0/2393	0.77	1/3239 (0.0%)
All	All	0.49	0/16753	0.75	4/22674 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	F	0	1
1	G	0	1
All	All	0	3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	52	LEU	CA-CB-CG	5.64	128.28	115.30
1	A	251	ARG	NE-CZ-NH2	-5.53	117.53	120.30
1	G	52	LEU	CA-CB-CG	5.13	127.10	115.30
1	F	251	ARG	NE-CZ-NH2	-5.01	117.80	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	102	TYR	Sidechain
1	F	102	TYR	Sidechain
1	G	102	TYR	Sidechain

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	2335	556	2248	60	0
1	B	2345	564	2270	62	0
1	C	2345	564	2270	45	0
1	D	2337	559	2248	66	0
1	E	2345	566	2270	55	0
1	F	2341	563	2259	59	0
1	G	2341	563	2259	50	0
2	A	118	236	0	5	1
2	B	128	256	0	4	0
2	C	119	238	0	5	0
2	D	122	244	0	4	0
2	E	126	252	0	6	0
2	F	92	184	0	2	0
2	G	113	226	0	7	0
All	All	17207	5571	15824	325	1

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 10.

All (325) 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:113:MET:HG3	1:A:145:THR:HG23	1.50	0.92
1:F:260:TRP:NE1	1:F:262:SER:HA	1.92	0.84
1:E:282:TYR:CD2	1:E:293:ASN:HB3	2.14	0.82
1:B:125:THR:HG23	1:C:135:LEU:HD22	1.61	0.82
1:E:260:TRP:NE1	1:E:262:SER:HA	1.96	0.81
1:D:123:ASN:HB2	1:D:135:LEU:HB3	1.62	0.81
1:E:255:ASP:HB3	1:E:270:THR:HG23	1.63	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:ALA:HA	1:A:205:LYS:HE3	1.66	0.78
1:B:127:ASP:HB2	1:C:131:LYS:HZ2	1.47	0.78
1:E:144:HIS:HE1	1:G:179:TRP:CZ2	2.02	0.77
1:B:179:TRP:HD1	1:B:182:TYR:HH	1.32	0.75
1:A:135:LEU:HD13	1:G:125:THR:HG23	1.68	0.75
1:G:282:TYR:CD1	1:G:293:ASN:HB3	2.22	0.74
1:E:202:GLY:HA3	1:E:204:MET:HE3	1.69	0.73
1:E:144:HIS:HE1	1:G:179:TRP:HZ2	1.38	0.72
1:A:12:THR:HG21	1:B:56:ARG:NH1	2.05	0.71
1:F:201:ASN:HB3	1:F:264:ASN:HA	1.73	0.70
1:D:123:ASN:HD22	1:E:135:LEU:HD11	1.57	0.70
1:A:127:ASP:HB2	1:B:131:LYS:NZ	2.07	0.69
1:B:255:ASP:HB3	1:B:270:THR:HG23	1.74	0.69
1:B:179:TRP:HD1	1:B:182:TYR:OH	1.77	0.68
1:E:12:THR:HG21	1:F:56:ARG:NH1	2.09	0.68
1:F:282:TYR:CD1	1:F:293:ASN:HB3	2.30	0.67
1:D:255:ASP:HB2	1:D:273:LYS:HD2	1.75	0.67
1:B:52:LEU:HD22	1:B:233:THR:HG22	1.75	0.67
1:D:273:LYS:HD3	1:D:274:TRP:CZ2	2.29	0.67
1:F:52:LEU:CD2	1:F:233:THR:HG22	2.25	0.66
1:A:60:THR:HG22	1:G:101:TYR:OH	1.95	0.66
1:F:109:THR:HG22	1:G:151:PRO:HA	1.77	0.66
1:E:259:HIS:CE1	1:E:266:LYS:HD3	2.31	0.66
1:E:12:THR:HG21	1:F:56:ARG:HH12	1.61	0.66
1:G:91:PRO:HD2	1:G:94:GLU:HG3	1.77	0.65
1:C:282:TYR:CD1	1:C:293:ASN:HB3	2.32	0.64
1:D:116:LEU:HD23	1:D:142:ILE:CD1	2.27	0.64
1:B:127:ASP:HB2	1:C:131:LYS:NZ	2.12	0.64
1:D:50:LYS:HD3	1:D:233:THR:HB	1.79	0.64
1:F:169:VAL:HG21	1:F:224:PHE:CZ	2.32	0.63
1:C:178:ASN:HD22	1:C:178:ASN:N	1.97	0.63
1:A:205:LYS:HE2	1:A:206:ALA:N	2.14	0.63
2:A:368:HOH:O	1:B:21:LYS:HD3	1.99	0.63
1:F:71:GLU:O	1:F:75:LYS:HB3	1.97	0.63
1:A:14:ILE:HD11	1:B:39:PHE:HE1	1.63	0.63
1:C:127:ASP:HB2	1:D:131:LYS:NZ	2.14	0.62
1:E:270:THR:HG22	2:E:373:HOH:O	1.98	0.62
1:D:273:LYS:HD3	1:D:274:TRP:CE2	2.35	0.62
1:D:8:LYS:HD2	1:E:13:ASP:HB2	1.81	0.62
1:B:282:TYR:CD2	1:B:293:ASN:HB3	2.35	0.62
1:F:85:LYS:HB2	1:F:250:GLU:HB2	1.81	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:116:LEU:HD23	1:E:142:ILE:CD1	2.30	0.62
1:B:123:ASN:HB2	1:B:135:LEU:HB3	1.80	0.62
1:A:183:ASP:HB2	2:A:294:HOH:O	1.99	0.62
1:A:202:GLY:HA3	1:A:204:MET:HE3	1.80	0.62
1:C:52:LEU:CD2	1:C:233:THR:HG22	2.30	0.61
1:A:134:GLY:O	1:G:125:THR:HG22	2.01	0.61
1:B:273:LYS:HD2	1:B:274:TRP:CZ2	2.35	0.61
1:E:85:LYS:HB2	1:E:250:GLU:HB3	1.82	0.61
1:F:148:TYR:OH	1:G:178:ASN:HA	2.00	0.61
1:A:205:LYS:HE2	1:A:207:ALA:H	1.66	0.60
1:B:74:ASN:O	1:B:259:HIS:HA	2.01	0.60
1:F:111:GLU:HG2	1:G:149:VAL:HG22	1.82	0.60
1:B:52:LEU:CD2	1:B:233:THR:HG22	2.31	0.60
1:E:94:GLU:HG2	1:E:243:THR:HG23	1.84	0.59
1:E:51:LYS:HG2	2:E:330:HOH:O	2.03	0.59
1:C:169:VAL:HG21	1:C:224:PHE:CZ	2.38	0.58
1:F:183:ASP:HB2	2:F:327:HOH:O	2.02	0.58
1:C:238:ALA:HB3	1:C:241:GLN:NE2	2.19	0.58
1:D:195:LEU:HD13	1:D:196:PHE:CE2	2.39	0.58
1:C:260:TRP:NE1	1:C:262:SER:HA	2.18	0.58
1:A:154:LYS:O	1:A:169:VAL:HA	2.04	0.58
1:D:85:LYS:HB2	1:D:250:GLU:HG2	1.85	0.57
1:G:51:LYS:HB3	2:G:332:HOH:O	2.05	0.57
1:E:71:GLU:HG2	1:E:75:LYS:HE3	1.86	0.57
1:G:116:LEU:HD23	1:G:142:ILE:HG12	1.87	0.57
1:D:127:ASP:HB2	1:E:131:LYS:NZ	2.20	0.56
1:A:184:ARG:HD2	1:A:254:ASP:OD2	2.05	0.56
1:E:117:THR:HG23	1:E:141:SER:HB3	1.86	0.56
1:A:87:GLN:HB3	2:A:400:HOH:O	2.05	0.56
1:D:260:TRP:NE1	1:D:262:SER:HA	2.20	0.56
1:E:50:LYS:HG2	1:E:233:THR:HB	1.87	0.55
1:F:127:ASP:OD2	1:F:131:LYS:HB3	2.07	0.55
1:D:264:ASN:HD22	1:D:264:ASN:C	2.10	0.55
1:A:150:GLN:HG2	2:A:392:HOH:O	2.06	0.55
1:F:273:LYS:HB3	1:F:274:TRP:CE3	2.41	0.55
1:B:191:TYR:CE1	1:B:200:ARG:HB3	2.42	0.55
1:G:100:ASP:HB3	1:G:231:VAL:HG13	1.89	0.55
1:F:101:TYR:OH	1:G:60:THR:HG22	2.07	0.54
1:G:95:VAL:HG12	2:G:335:HOH:O	2.08	0.54
1:D:212:ASP:HB3	1:D:215:LYS:HD2	1.88	0.54
1:E:58:LYS:HA	1:E:226:PRO:O	2.08	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:169:VAL:HG21	1:E:224:PHE:CZ	2.42	0.54
1:A:131:LYS:HD2	1:A:132:ILE:H	1.73	0.54
1:D:71:GLU:HG3	1:D:75:LYS:HB3	1.89	0.54
1:C:146:LEU:HD21	1:D:175:VAL:HG22	1.89	0.54
1:A:201:ASN:ND2	1:A:264:ASN:HB3	2.23	0.54
1:F:125:THR:HG23	1:G:135:LEU:HD13	1.90	0.54
1:D:50:LYS:HE2	2:D:335:HOH:O	2.07	0.53
1:D:37:LYS:HE3	1:D:39:PHE:HB2	1.91	0.53
1:G:154:LYS:O	1:G:169:VAL:HA	2.07	0.53
1:A:76:SER:HB2	1:A:206:ALA:HB3	1.89	0.53
1:C:191:TYR:HE1	1:C:264:ASN:HB2	1.73	0.53
1:F:264:ASN:HD22	1:F:264:ASN:C	2.11	0.53
1:E:191:TYR:CE1	1:E:200:ARG:HB3	2.44	0.53
1:D:52:LEU:HD23	1:D:233:THR:HG22	1.90	0.53
1:A:113:MET:HB3	1:B:147:LYS:HG3	1.90	0.53
1:D:73:ALA:HB1	1:D:205:LYS:HA	1.91	0.52
1:C:238:ALA:HB3	1:C:241:GLN:HE22	1.71	0.52
1:B:71:GLU:HB2	1:B:75:LYS:HB3	1.91	0.52
1:D:100:ASP:HB3	1:D:231:VAL:HG13	1.91	0.52
1:A:179:TRP:HZ2	1:F:116:LEU:HB2	1.74	0.52
1:E:184:ARG:HD2	1:E:254:ASP:OD2	2.10	0.52
1:E:113:MET:HG2	1:E:145:THR:HB	1.90	0.52
1:E:154:LYS:O	1:E:169:VAL:HA	2.09	0.52
1:C:127:ASP:HB2	1:D:131:LYS:HZ2	1.74	0.52
1:F:250:GLU:HG2	1:F:277:ARG:HG2	1.92	0.52
1:B:185:ASP:OD2	1:C:215:LYS:HE3	2.10	0.52
1:G:150:GLN:HG2	2:G:388:HOH:O	2.09	0.52
1:D:87:GLN:HB3	2:D:376:HOH:O	2.10	0.52
1:B:154:LYS:O	1:B:169:VAL:HA	2.10	0.52
1:F:188:ASN:O	1:F:192:GLY:N	2.42	0.52
1:D:141:SER:O	1:D:142:ILE:HD13	2.09	0.52
1:D:52:LEU:CD2	1:D:233:THR:HG22	2.40	0.52
1:E:116:LEU:HD23	1:E:142:ILE:HD13	1.91	0.52
1:B:85:LYS:HB2	1:B:250:GLU:HB2	1.92	0.52
1:A:131:LYS:HZ1	1:G:127:ASP:CG	2.14	0.51
1:F:126:GLY:HA2	1:F:131:LYS:O	2.10	0.51
1:A:14:ILE:HD11	1:B:39:PHE:CE1	2.44	0.51
1:D:132:ILE:HG22	1:D:133:GLY:N	2.25	0.51
1:B:125:THR:CG2	1:C:135:LEU:HD22	2.35	0.51
1:F:52:LEU:HD23	1:F:233:THR:HG22	1.91	0.51
1:E:52:LEU:CD2	1:E:233:THR:HG22	2.41	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:197:MET:HB3	1:D:258:LEU:HD21	1.93	0.51
1:E:123:ASN:ND2	1:F:137:GLY:HA3	2.25	0.51
1:A:112:TYR:HB2	1:B:150:GLN:NE2	2.26	0.51
1:B:257:GLN:HB2	1:B:268:THR:HG22	1.92	0.51
1:F:191:TYR:CZ	1:F:200:ARG:HD3	2.46	0.51
1:A:148:TYR:OH	1:B:178:ASN:HA	2.12	0.50
1:B:75:LYS:HA	1:B:258:LEU:O	2.12	0.50
1:B:24:ASP:OD1	1:B:37:LYS:HE3	2.12	0.50
1:D:282:TYR:CD1	1:D:293:ASN:HB3	2.47	0.50
1:C:94:GLU:CG	1:C:243:THR:HG23	2.41	0.50
1:F:260:TRP:CE2	1:F:262:SER:HA	2.45	0.50
1:E:125:THR:HG22	1:F:134:GLY:O	2.12	0.50
1:D:131:LYS:HG3	1:D:132:ILE:N	2.26	0.50
1:G:290:GLU:HG3	2:G:350:HOH:O	2.12	0.50
1:A:178:ASN:HA	1:G:148:TYR:OH	2.11	0.50
1:E:116:LEU:HD23	1:E:142:ILE:HD11	1.92	0.49
1:G:1:ALA:HB3	1:G:4:ASP:OD2	2.12	0.49
1:B:169:VAL:HG21	1:B:224:PHE:CZ	2.47	0.49
1:A:146:LEU:HD21	1:B:175:VAL:HG22	1.93	0.49
1:E:183:ASP:HB2	2:E:352:HOH:O	2.12	0.49
1:E:30:LYS:HE2	2:E:417:HOH:O	2.12	0.49
1:C:12:THR:HG23	2:C:309:HOH:O	2.12	0.49
1:G:282:TYR:CE1	1:G:293:ASN:HB3	2.47	0.49
1:F:71:GLU:OE1	1:F:76:SER:HA	2.12	0.49
1:D:216:ALA:HB1	1:D:220:LEU:HD12	1.93	0.49
1:F:127:ASP:HB2	1:G:131:LYS:NZ	2.27	0.49
1:D:14:ILE:HD11	1:E:39:PHE:HE1	1.76	0.49
1:D:184:ARG:HD2	1:D:254:ASP:OD2	2.12	0.49
1:D:169:VAL:HG21	1:D:224:PHE:CZ	2.48	0.49
1:E:127:ASP:HB2	1:F:131:LYS:NZ	2.28	0.49
1:C:128:ASP:CG	1:D:131:LYS:HZ3	2.16	0.49
1:A:154:LYS:HD2	2:B:407:HOH:O	2.13	0.48
1:D:140:VAL:HG12	1:D:141:SER:N	2.28	0.48
1:F:198:LYS:HE3	1:F:210:PHE:O	2.12	0.48
1:A:60:THR:CG2	1:G:101:TYR:OH	2.60	0.48
1:C:255:ASP:HB2	1:C:273:LYS:HG3	1.94	0.48
1:D:250:GLU:HB2	1:D:276:ASP:O	2.13	0.48
1:F:236:ARG:HH11	1:F:236:ARG:HG3	1.79	0.48
1:A:127:ASP:HB2	1:B:131:LYS:HZ1	1.77	0.48
1:A:49:ASN:O	1:A:50:LYS:HG3	2.13	0.48
1:F:123:ASN:ND2	1:G:137:GLY:HA3	2.29	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:LEU:CD2	1:B:142:ILE:HG12	2.44	0.48
1:A:135:LEU:HD11	1:G:123:ASN:HB3	1.96	0.47
1:A:37:LYS:C	1:A:37:LYS:HD2	2.35	0.47
1:A:100:ASP:HB3	1:A:231:VAL:HG13	1.95	0.47
1:F:184:ARG:HD2	1:F:254:ASP:OD2	2.13	0.47
1:F:243:THR:HB	1:F:284:ILE:HB	1.96	0.47
1:G:188:ASN:O	1:G:192:GLY:N	2.44	0.47
1:B:58:LYS:HA	1:B:226:PRO:O	2.14	0.47
1:B:127:ASP:CB	1:C:131:LYS:HZ2	2.23	0.47
1:E:62:ALA:O	1:E:251:ARG:NH1	2.47	0.47
1:A:12:THR:HG22	2:G:307:HOH:O	2.14	0.47
1:A:127:ASP:HB2	1:B:131:LYS:HZ3	1.78	0.47
1:E:127:ASP:HB2	1:F:131:LYS:HZ3	1.77	0.47
1:G:74:ASN:O	1:G:259:HIS:HA	2.14	0.47
1:D:135:LEU:HD12	1:D:136:ILE:N	2.29	0.47
1:E:91:PRO:O	1:E:94:GLU:HB2	2.15	0.47
1:G:169:VAL:HG11	1:G:224:PHE:CZ	2.49	0.47
1:A:129:THR:HG23	1:B:131:LYS:HE2	1.96	0.47
1:C:113:MET:HG3	1:D:147:LYS:HG3	1.97	0.47
1:B:14:ILE:HD11	1:C:39:PHE:CE1	2.50	0.47
1:E:127:ASP:HB2	1:F:132:ILE:O	2.16	0.46
1:F:160:PRO:HB3	1:F:165:VAL:HG23	1.97	0.46
1:G:260:TRP:NE1	1:G:262:SER:HA	2.29	0.46
1:G:40:TYR:CE2	1:G:291:MET:HB3	2.51	0.46
1:F:268:THR:HG22	2:F:373:HOH:O	2.15	0.46
1:C:101:TYR:HA	1:C:229:ALA:O	2.15	0.46
1:D:212:ASP:HB2	2:D:413:HOH:O	2.14	0.46
1:E:113:MET:CG	1:E:145:THR:HB	2.45	0.46
1:A:70:GLU:HG3	1:A:205:LYS:HZ3	1.81	0.46
1:D:36:LYS:HZ1	1:D:280:GLU:HG3	1.81	0.46
1:B:203:SER:C	1:B:204:MET:HG3	2.35	0.46
1:B:259:HIS:CD2	1:B:266:LYS:HB3	2.51	0.46
1:D:56:ARG:HA	1:D:228:PHE:O	2.16	0.46
1:B:139:ASN:N	1:B:139:ASN:ND2	2.64	0.46
1:B:188:ASN:HB3	1:B:192:GLY:N	2.30	0.46
1:F:240:LYS:HA	1:F:240:LYS:HD2	1.51	0.45
1:D:88:LEU:HD12	1:D:88:LEU:N	2.30	0.45
1:D:127:ASP:HB2	1:E:131:LYS:HZ2	1.81	0.45
1:F:282:TYR:CE1	1:F:293:ASN:HB3	2.51	0.45
1:A:24:ASP:O	1:A:25:LEU:HD13	2.16	0.45
1:G:204:MET:HE3	1:G:209:ASN:HB2	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:243:THR:HB	1:D:284:ILE:HB	1.98	0.45
1:C:32:ASN:O	1:C:34:MET:HG3	2.16	0.45
1:A:159:SER:HA	1:A:160:PRO:HD3	1.75	0.45
1:E:259:HIS:HE1	1:E:266:LYS:HD3	1.76	0.45
1:G:91:PRO:HB2	1:G:94:GLU:HG2	1.98	0.45
1:C:180:GLY:HA3	2:C:405:HOH:O	2.15	0.45
1:C:101:TYR:OH	1:D:60:THR:HG22	2.16	0.45
1:C:32:ASN:O	1:C:251:ARG:NH2	2.48	0.45
1:B:206:ALA:HA	1:B:265:TRP:CH2	2.51	0.45
1:F:121:ASN:HB2	1:G:138:ALA:O	2.17	0.45
1:A:201:ASN:HD22	1:A:264:ASN:HB3	1.80	0.45
1:E:65:TYR:CE2	1:E:78:LEU:HD21	2.52	0.45
1:E:260:TRP:CE2	1:E:262:SER:HA	2.52	0.45
1:A:179:TRP:CH2	1:F:116:LEU:HD22	2.52	0.45
1:B:122:GLY:O	1:C:137:GLY:HA2	2.16	0.45
1:G:204:MET:H	1:G:204:MET:HE2	1.83	0.44
1:C:111:GLU:HB3	1:C:147:LYS:HB3	1.99	0.44
1:E:144:HIS:CE1	1:G:179:TRP:HZ2	2.27	0.44
1:B:21:LYS:HE3	1:B:289:GLU:HB2	2.00	0.44
1:D:73:ALA:CB	1:D:205:LYS:HA	2.47	0.44
1:E:157:LEU:O	1:F:222:SER:HB3	2.18	0.44
1:F:248:ILE:N	1:F:248:ILE:HD12	2.32	0.44
2:C:304:HOH:O	1:D:21:LYS:HD3	2.16	0.44
1:D:209:ASN:HD22	1:D:258:LEU:HD13	1.82	0.44
1:D:259:HIS:NE2	1:D:266:LYS:HD3	2.33	0.44
1:A:21:LYS:HE2	2:G:398:HOH:O	2.17	0.44
1:A:194:GLN:HE22	1:A:200:ARG:CZ	2.31	0.44
1:B:141:SER:C	1:B:142:ILE:HG13	2.38	0.44
1:C:184:ARG:HD2	1:C:254:ASP:OD2	2.17	0.44
1:F:250:GLU:CG	1:F:277:ARG:HG2	2.47	0.44
1:D:193:ASN:OD1	1:D:195:LEU:HB2	2.18	0.44
1:G:191:TYR:CE1	1:G:200:ARG:HB3	2.53	0.44
1:C:128:ASP:OD2	1:D:131:LYS:HA	2.18	0.43
1:A:178:ASN:ND2	1:G:148:TYR:OH	2.51	0.43
1:F:71:GLU:HB2	1:F:75:LYS:CG	2.48	0.43
1:A:83:ALA:HB3	1:A:252:VAL:HB	2.00	0.43
1:D:40:TYR:CG	1:D:291:MET:HE3	2.54	0.43
1:A:169:VAL:HG11	1:A:224:PHE:CZ	2.53	0.43
1:F:177:GLN:O	1:F:178:ASN:HB2	2.19	0.43
1:F:74:ASN:O	1:F:259:HIS:HA	2.18	0.43
1:F:157:LEU:O	1:G:222:SER:HB3	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:91:PRO:O	1:C:94:GLU:HB2	2.18	0.43
1:A:46:LYS:HD3	1:A:46:LYS:HA	1.90	0.43
1:B:128:ASP:C	1:B:130:GLY:H	2.22	0.43
1:D:191:TYR:O	1:D:266:LYS:HA	2.19	0.42
1:A:58:LYS:HA	1:A:226:PRO:O	2.19	0.42
1:G:184:ARG:HD2	1:G:254:ASP:OD2	2.18	0.42
1:G:49:ASN:O	1:G:50:LYS:HG3	2.19	0.42
1:E:282:TYR:HD2	1:E:293:ASN:HB3	1.79	0.42
1:F:109:THR:HG22	1:G:151:PRO:CA	2.48	0.42
1:G:180:GLY:HA3	1:G:181:PRO:HA	1.87	0.42
1:F:110:LYS:HE2	2:G:366:HOH:O	2.18	0.42
1:G:255:ASP:HB2	1:G:273:LYS:HD2	2.01	0.42
1:A:89:GLN:HG3	1:A:164:LYS:HB3	2.01	0.42
1:D:261:THR:OG1	1:D:264:ASN:ND2	2.53	0.42
1:D:260:TRP:HE1	1:D:262:SER:HA	1.85	0.42
1:A:126:GLY:HA2	1:A:131:LYS:O	2.20	0.42
1:D:184:ARG:HG3	2:D:398:HOH:O	2.18	0.42
1:B:116:LEU:HD23	1:B:142:ILE:HG12	2.01	0.42
1:E:122:GLY:HA2	1:E:135:LEU:O	2.20	0.42
1:E:268:THR:HG22	2:E:373:HOH:O	2.20	0.42
1:E:144:HIS:CE1	1:G:179:TRP:CZ2	2.94	0.42
1:B:283:LYS:NZ	2:B:414:HOH:O	2.52	0.42
1:A:255:ASP:HB2	1:A:273:LYS:HG2	2.02	0.42
1:A:110:LYS:NZ	1:B:173:ASN:OD1	2.45	0.41
1:F:34:MET:HG2	1:F:61:ILE:HG23	2.02	0.41
1:B:157:LEU:O	1:C:222:SER:HB3	2.20	0.41
1:C:127:ASP:HA	1:D:133:GLY:HA2	2.02	0.41
1:B:135:LEU:HD13	1:B:136:ILE:N	2.36	0.41
1:C:179:TRP:C	2:C:405:HOH:O	2.58	0.41
1:D:148:TYR:OH	1:E:178:ASN:ND2	2.53	0.41
1:D:127:ASP:OD2	1:D:131:LYS:HB3	2.20	0.41
1:C:95:VAL:HG22	2:C:371:HOH:O	2.19	0.41
1:F:140:VAL:HG12	1:F:141:SER:N	2.35	0.41
1:C:91:PRO:HB2	1:C:94:GLU:OE1	2.19	0.41
1:G:164:LYS:HB2	1:G:164:LYS:HE3	1.89	0.41
1:C:178:ASN:N	1:C:178:ASN:ND2	2.67	0.41
1:F:38:VAL:HG13	1:F:55:ILE:HG23	2.02	0.41
1:E:87:GLN:HB3	2:E:358:HOH:O	2.20	0.41
1:B:193:ASN:OD1	1:B:195:LEU:HB2	2.19	0.41
1:B:216:ALA:HB1	1:B:220:LEU:HD12	2.03	0.41
1:A:123:ASN:ND2	1:B:137:GLY:HA3	2.35	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:ARG:HB2	1:A:274:TRP:HB2	2.03	0.41
1:E:282:TYR:CE2	1:E:293:ASN:HB3	2.54	0.41
1:G:260:TRP:HB2	1:G:265:TRP:CZ3	2.55	0.41
1:C:68:TYR:CE2	1:C:69:SER:HB3	2.56	0.41
1:B:104:ARG:HD3	1:C:225:SER:CB	2.50	0.41
1:A:12:THR:HG21	1:B:56:ARG:HH12	1.83	0.41
1:F:5:ILE:O	1:F:7:ILE:HG13	2.21	0.41
1:B:277:ARG:NE	2:B:403:HOH:O	2.53	0.41
1:D:180:GLY:HA3	1:D:181:PRO:HA	1.93	0.41
1:A:191:TYR:C	1:A:266:LYS:HD2	2.42	0.41
1:D:280:GLU:OE1	1:D:293:ASN:ND2	2.54	0.41
1:A:56:ARG:NH1	2:A:366:HOH:O	2.53	0.41
1:G:237:LYS:HE2	1:G:237:LYS:HB3	1.88	0.41
1:D:244:ASN:ND2	1:D:283:LYS:HG2	2.35	0.41
1:G:95:VAL:HG11	1:G:238:ALA:HB1	2.03	0.40
1:A:68:TYR:CG	1:A:69:SER:N	2.89	0.40
1:F:24:ASP:OD1	1:F:37:LYS:HD3	2.21	0.40
1:C:154:LYS:O	1:C:169:VAL:HA	2.22	0.40
1:F:58:LYS:HA	1:F:226:PRO:O	2.20	0.40
1:E:248:ILE:N	1:E:248:ILE:HD12	2.37	0.40
1:C:84:PHE:HB2	1:C:169:VAL:HB	2.02	0.40
1:E:67:VAL:HA	1:E:78:LEU:HA	2.03	0.40
1:B:280:GLU:HG3	2:B:317:HOH:O	2.21	0.40
1:C:94:GLU:HG2	1:C:243:THR:HG23	2.03	0.40
1:B:142:ILE:HG23	1:D:179:TRP:HH2	1.86	0.40
1:B:146:LEU:HD21	1:C:175:VAL:HG22	2.02	0.40
1:D:117:THR:HG22	1:D:118:TYR:N	2.36	0.40
1:F:191:TYR:CE1	1:F:200:ARG:HB3	2.56	0.40
1:A:182:TYR:HB2	1:A:195:LEU:HD23	2.04	0.40
1:B:46:LYS:HA	1:B:46:LYS:HD3	1.82	0.40
1:D:65:TYR:CE1	1:D:78:LEU:HD21	2.57	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:338:HOH:H1	2:A:338:HOH:H1[2_656]	1.34	0.26

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	291/293 (99%)	272 (94%)	19 (6%)	0	100	100
1	B	291/293 (99%)	274 (94%)	16 (6%)	1 (0%)	46	35
1	C	291/293 (99%)	273 (94%)	18 (6%)	0	100	100
1	D	291/293 (99%)	272 (94%)	17 (6%)	2 (1%)	26	14
1	E	291/293 (99%)	273 (94%)	18 (6%)	0	100	100
1	F	291/293 (99%)	271 (93%)	20 (7%)	0	100	100
1	G	291/293 (99%)	274 (94%)	17 (6%)	0	100	100
All	All	2037/2051 (99%)	1909 (94%)	125 (6%)	3 (0%)	56	46

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	262	SER
1	B	73	ALA
1	D	92	ASP

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	257/259 (99%)	238 (93%)	19 (7%)	17	7
1	B	259/259 (100%)	239 (92%)	20 (8%)	16	6
1	C	259/259 (100%)	243 (94%)	16 (6%)	23	11

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	257/259 (99%)	238 (93%)	19 (7%)	17	7
1	E	259/259 (100%)	241 (93%)	18 (7%)	19	8
1	F	258/259 (100%)	243 (94%)	15 (6%)	25	13
1	G	258/259 (100%)	240 (93%)	18 (7%)	19	8
All	All	1807/1813 (100%)	1682 (93%)	125 (7%)	19	8

All (125) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	LEU
1	A	60	THR
1	A	67	VAL
1	A	76	SER
1	A	91	PRO
1	A	98	ILE
1	A	101	TYR
1	A	110	LYS
1	A	145	THR
1	A	164	LYS
1	A	169	VAL
1	A	179	TRP
1	A	195	LEU
1	A	204	MET
1	A	205	LYS
1	A	231	VAL
1	A	240	LYS
1	A	242	GLN
1	A	262	SER
1	B	21	LYS
1	B	25	LEU
1	B	70	GLU
1	B	92	ASP
1	B	101	TYR
1	B	117	THR
1	B	124	VAL
1	B	125	THR
1	B	139	ASN
1	B	141	SER
1	B	190	VAL
1	B	195	LEU
1	B	201	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	204	MET
1	B	242	GLN
1	B	263	THR
1	B	264	ASN
1	B	270	THR
1	B	273	LYS
1	B	291	MET
1	C	30	LYS
1	C	31	GLU
1	C	60	THR
1	C	71	GLU
1	C	89	GLN
1	C	92	ASP
1	C	94	GLU
1	C	101	TYR
1	C	109	THR
1	C	121	ASN
1	C	135	LEU
1	C	178	ASN
1	C	179	TRP
1	C	234	MET
1	C	240	LYS
1	C	242	GLN
1	D	21	LYS
1	D	25	LEU
1	D	60	THR
1	D	71	GLU
1	D	92	ASP
1	D	101	TYR
1	D	115	THR
1	D	116	LEU
1	D	120	PHE
1	D	125	THR
1	D	135	LEU
1	D	195	LEU
1	D	201	ASN
1	D	204	MET
1	D	230	THR
1	D	231	VAL
1	D	263	THR
1	D	264	ASN
1	D	268	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	12	THR
1	E	25	LEU
1	E	67	VAL
1	E	71	GLU
1	E	92	ASP
1	E	94	GLU
1	E	95	VAL
1	E	101	TYR
1	E	108	ASP
1	E	117	THR
1	E	125	THR
1	E	164	LYS
1	E	195	LEU
1	E	204	MET
1	E	242	GLN
1	E	262	SER
1	E	268	THR
1	E	270	THR
1	F	16	SER
1	F	17	ASN
1	F	25	LEU
1	F	93	ASN
1	F	101	TYR
1	F	117	THR
1	F	125	THR
1	F	142	ILE
1	F	145	THR
1	F	155	THR
1	F	204	MET
1	F	208	ASP
1	F	240	LYS
1	F	242	GLN
1	F	264	ASN
1	G	12	THR
1	G	25	LEU
1	G	60	THR
1	G	67	VAL
1	G	93	ASN
1	G	101	TYR
1	G	116	LEU
1	G	117	THR
1	G	125	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	155	THR
1	G	164	LYS
1	G	195	LEU
1	G	204	MET
1	G	230	THR
1	G	231	VAL
1	G	234	MET
1	G	242	GLN
1	G	283	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	ASN
1	A	89	GLN
1	A	177	GLN
1	A	178	ASN
1	A	194	GLN
1	A	201	ASN
1	A	257	GLN
1	A	259	HIS
1	B	64	GLN
1	B	74	ASN
1	B	139	ASN
1	B	150	GLN
1	B	178	ASN
1	B	194	GLN
1	B	242	GLN
1	B	264	ASN
1	C	64	GLN
1	C	139	ASN
1	C	150	GLN
1	C	178	ASN
1	C	241	GLN
1	C	264	ASN
1	D	74	ASN
1	D	89	GLN
1	D	121	ASN
1	D	123	ASN
1	D	178	ASN
1	D	244	ASN
1	D	257	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	264	ASN
1	E	64	GLN
1	E	74	ASN
1	E	123	ASN
1	E	144	HIS
1	E	150	GLN
1	E	178	ASN
1	E	259	HIS
1	F	93	ASN
1	F	178	ASN
1	F	264	ASN
1	G	17	ASN
1	G	89	GLN
1	G	93	ASN
1	G	144	HIS
1	G	177	GLN
1	G	257	GLN

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)

There are no ligands in this entry.

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.