



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 05:15 AM GMT

PDB ID : 1C4P
Title : BETA DOMAIN OF STREPTOKINASE
Authors : Wang, X.; Zhang, X.C.
Deposited on : 1999-09-15
Resolution : 2.40 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

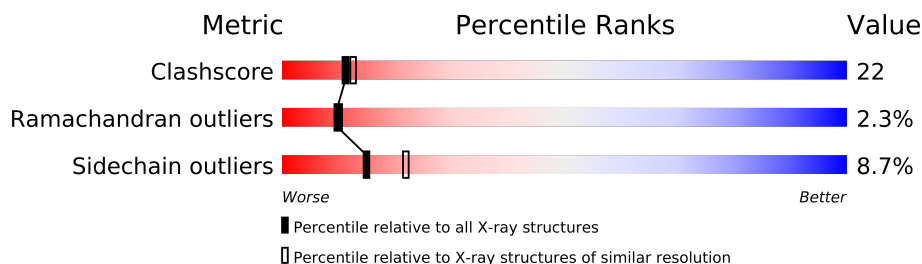
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.40 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	79885	2789 (2.40-2.40)
Ramachandran outliers	78287	2736 (2.40-2.40)
Sidechain outliers	78261	2737 (2.40-2.40)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	137	
1	B	137	
1	C	137	
1	D	137	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4471 atoms, of which 0 are hydrogen and 0 are deuterium.

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 PROTEIN (STREPTOKINASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	137	Total	C	N	O	S	0	0	0
			1105	697	185	222	1			
1	B	137	Total	C	N	O	S	0	0	0
			1105	697	185	222	1			
1	C	132	Total	C	N	O	S	0	0	0
			1070	675	179	215	1			
1	D	132	Total	C	N	O	S	0	0	0
			1070	675	179	215	1			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	42	Total	O	0	0
			42	42		
2	B	37	Total	O	0	0
			37	37		
2	C	13	Total	O	0	0
			13	13		
2	D	29	Total	O	0	0
			29	29		

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	73.97Å 83.99Å 97.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.40	Depositor
% Data completeness (in resolution range)	95.7 (20.00-2.40)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 0.5	Depositor
R, R_{free}	0.237 , 0.304	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4471	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	0.51	0/1125	0.70	0/1524
1	B	0.49	0/1125	0.72	0/1524
1	C	0.44	0/1089	0.67	0/1475
1	D	0.50	0/1089	0.73	0/1475
All	All	0.49	0/4428	0.71	0/5998

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1105	0	1090	49	0
1	B	1105	0	1090	60	0
1	C	1070	0	1060	59	0
1	D	1070	0	1060	42	0
2	A	42	0	0	0	0
2	B	37	0	0	1	0
2	C	13	0	0	1	0
2	D	29	0	0	0	0
All	All	4471	0	4300	194	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 22.

All (194) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:197:GLN:HE21	1:C:197:GLN:N	1.59	0.99
1:C:197:GLN:H	1:C:197:GLN:NE2	1.67	0.91
1:A:197:GLN:NE2	1:A:197:GLN:H	1.71	0.88
1:A:197:GLN:H	1:A:197:GLN:HE21	0.92	0.87
1:D:185:LEU:HD11	1:D:202:GLN:HG3	1.54	0.87
1:B:251:ALA:H	1:B:266:ASN:HD21	1.25	0.85
1:B:177:PRO:HG2	1:D:249:GLU:HG2	1.57	0.85
1:D:255:ASN:C	1:D:255:ASN:HD22	1.80	0.85
1:A:195:THR:OG1	1:A:198:GLU:HG3	1.77	0.84
1:D:183:LYS:NZ	1:D:202:GLN:HE22	1.75	0.84
1:A:255:ASN:HB3	1:A:259:GLY:H	1.41	0.84
1:A:197:GLN:N	1:A:197:GLN:HE21	1.73	0.83
1:B:253:GLU:HG3	1:B:264:ILE:HD13	1.63	0.81
1:B:185:LEU:HD11	1:B:202:GLN:HG3	1.64	0.80
1:C:186:LYS:HE2	1:C:188:LEU:HD21	1.66	0.77
1:C:176:ARG:HH11	1:C:176:ARG:HG2	1.50	0.76
1:A:158:VAL:HG22	1:A:266:ASN:HB2	1.69	0.74
1:C:197:GLN:HE21	1:C:197:GLN:H	0.83	0.73
1:A:190:ILE:HD13	1:A:247:ASN:HD22	1.54	0.72
1:C:279:LYS:HA	1:C:279:LYS:HE3	1.69	0.72
1:A:226:HIS:HD2	1:A:268:ASP:OD1	1.73	0.72
1:A:223:ILE:HG12	1:A:234:ILE:HG23	1.70	0.72
1:B:255:ASN:ND2	1:B:258:SER:H	1.86	0.72
1:B:158:VAL:HG22	1:B:266:ASN:HB2	1.71	0.71
1:B:180:LYS:HD3	1:D:264:ILE:HD11	1.72	0.70
1:A:226:HIS:HE1	1:A:233:THR:CG2	2.05	0.70
1:A:172:ASP:OD1	1:A:174:ASP:HB2	1.93	0.68
1:A:160:VAL:HG22	1:A:186:LYS:O	1.93	0.68
1:D:175:PHE:O	1:D:177:PRO:HD3	1.94	0.67
1:C:175:PHE:HA	1:C:211:HIS:CE1	2.31	0.65
1:C:277:LEU:H	1:C:277:LEU:HD23	1.61	0.65
1:D:185:LEU:O	1:D:186:LYS:HG3	1.98	0.64
1:A:154:GLN:HG3	1:A:247:ASN:HD21	1.61	0.64
1:C:204:GLN:HE21	1:C:208:ASN:ND2	1.95	0.64
1:C:168:PRO:HD3	1:C:175:PHE:CE2	2.33	0.63
1:C:253:GLU:HG2	1:C:264:ILE:HG21	1.80	0.63
1:A:207:LEU:HD12	1:A:211:HIS:HB2	1.80	0.63
1:A:157:SER:HB3	1:A:265:ASN:HD21	1.64	0.63
1:B:179:LEU:HB2	1:D:252:TYR:CZ	2.34	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:177:PRO:CG	1:D:249:GLU:HG2	2.29	0.63
1:A:155:ALA:HB1	1:A:266:ASN:ND2	2.14	0.62
1:D:255:ASN:ND2	1:D:255:ASN:C	2.51	0.62
1:D:183:LYS:HZ2	1:D:202:GLN:HE22	1.43	0.62
1:C:220:ASP:O	1:C:237:MET:HG3	2.00	0.62
1:A:158:VAL:HG22	1:A:266:ASN:CB	2.29	0.62
1:B:247:ASN:HD22	1:B:248:ARG:N	1.99	0.61
1:D:224:VAL:HB	1:D:233:THR:HB	1.83	0.61
1:B:254:ILE:O	1:B:254:ILE:HG22	1.99	0.60
1:C:168:PRO:HD3	1:C:175:PHE:CD2	2.37	0.59
1:D:222:SER:HB2	1:D:235:LEU:HB2	1.85	0.59
1:C:159:ASP:HB3	1:C:184:LEU:HD11	1.84	0.59
1:C:186:LYS:CE	1:C:188:LEU:HD21	2.32	0.59
1:B:179:LEU:HD13	1:D:252:TYR:CE2	2.38	0.58
1:B:151:ILE:HD12	1:B:154:GLN:HB2	1.85	0.58
1:A:254:ILE:HG13	1:A:255:ASN:H	1.68	0.58
1:A:190:ILE:HD13	1:A:247:ASN:HA	1.84	0.58
1:A:237:MET:HB2	1:B:234:ILE:HG12	1.85	0.58
1:A:154:GLN:HG2	1:A:190:ILE:HD12	1.86	0.58
1:B:247:ASN:HD22	1:B:248:ARG:H	1.52	0.58
1:B:215:THR:HG23	1:B:279:LYS:HE2	1.85	0.58
1:C:222:SER:HB2	1:C:235:LEU:HB2	1.86	0.57
1:D:183:LYS:HZ3	1:D:202:GLN:HE22	1.51	0.57
1:A:160:VAL:HG23	1:A:185:LEU:HB3	1.87	0.57
1:C:175:PHE:HA	1:C:211:HIS:HE1	1.67	0.57
1:B:185:LEU:HD11	1:B:202:GLN:CG	2.35	0.56
1:A:164:VAL:HG22	1:A:165:GLN:H	1.71	0.56
1:C:155:ALA:HB3	1:C:190:ILE:HD11	1.88	0.55
1:A:169:LEU:HD12	1:A:277:LEU:HD13	1.88	0.55
1:A:164:VAL:HG22	1:A:165:GLN:N	2.21	0.55
1:C:195:THR:OG1	1:C:198:GLU:HG3	2.06	0.55
1:C:162:TYR:O	1:C:182:THR:HA	2.06	0.55
1:D:183:LYS:NZ	1:D:202:GLN:NE2	2.52	0.55
1:C:197:GLN:N	1:C:197:GLN:NE2	2.40	0.54
1:B:253:GLU:HG3	1:B:264:ILE:CD1	2.35	0.54
1:D:154:GLN:HG3	1:D:247:ASN:OD1	2.07	0.54
1:B:153:ASN:ND2	1:D:176:ARG:HH11	2.05	0.54
1:D:183:LYS:HD3	1:D:202:GLN:HE21	1.72	0.54
1:B:152:GLN:NE2	1:D:177:PRO:HD2	2.23	0.54
1:B:186:LYS:CD	1:B:188:LEU:HD21	2.38	0.54
1:B:251:ALA:N	1:B:266:ASN:HD21	2.01	0.53
1:D:183:LYS:HD2	1:D:206:ILE:HD11	1.91	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:226:HIS:CE1	1:A:233:THR:CG2	2.89	0.53
1:A:192:ASP:O	1:A:245:VAL:HG23	2.08	0.53
1:C:204:GLN:HE21	1:C:208:ASN:HD21	1.56	0.53
1:C:279:LYS:HE3	1:C:279:LYS:CA	2.36	0.53
1:B:256:LYS:HB3	1:B:256:LYS:NZ	2.24	0.53
1:C:154:GLN:NE2	1:C:247:ASN:OD1	2.42	0.52
1:B:230:ILE:HG22	1:B:231:PHE:CD1	2.45	0.52
1:A:226:HIS:CD2	1:A:268:ASP:OD1	2.60	0.51
1:B:255:ASN:HD22	1:B:255:ASN:C	2.13	0.51
1:C:165:GLN:HB3	1:C:273:LYS:HG2	1.92	0.51
1:D:169:LEU:HD11	1:D:217:TYR:CD2	2.46	0.51
1:B:149:LYS:HG2	1:B:149:LYS:O	2.11	0.51
1:A:195:THR:HG1	1:A:198:GLU:HG3	1.75	0.50
1:C:251:ALA:H	1:C:266:ASN:HD21	1.59	0.50
1:D:153:ASN:N	1:D:249:GLU:OE2	2.44	0.50
1:A:190:ILE:HD13	1:A:247:ASN:ND2	2.22	0.50
1:C:213:GLY:O	1:C:279:LYS:HB2	2.12	0.50
1:B:217:TYR:CE1	1:B:283:PRO:HG2	2.45	0.50
1:A:185:LEU:O	1:A:186:LYS:HB2	2.11	0.50
1:A:179:LEU:HB2	1:C:252:TYR:CZ	2.47	0.50
1:C:252:TYR:HB2	1:C:262:GLU:O	2.12	0.50
1:B:256:LYS:HB3	1:B:256:LYS:HZ2	1.77	0.49
1:C:222:SER:HB3	1:C:235:LEU:HD12	1.93	0.49
1:A:157:SER:HB3	1:A:265:ASN:ND2	2.26	0.49
1:D:172:ASP:OD1	1:D:174:ASP:N	2.46	0.48
1:C:176:ARG:NH1	1:C:176:ARG:HG2	2.23	0.48
1:C:253:GLU:HG2	1:C:264:ILE:CG2	2.42	0.48
1:D:193:THR:HA	1:D:243:TYR:O	2.14	0.48
1:B:251:ALA:H	1:B:266:ASN:ND2	2.03	0.48
1:C:204:GLN:NE2	1:C:208:ASN:HD21	2.10	0.48
1:A:161:GLU:OE1	1:A:184:LEU:HA	2.14	0.48
1:B:149:LYS:HB2	1:B:149:LYS:NZ	2.29	0.48
1:B:149:LYS:N	1:B:150:PRO:HD3	2.29	0.48
1:C:227:ASP:OD2	1:C:248:ARG:HD3	2.13	0.47
1:B:151:ILE:O	1:B:151:ILE:HG13	2.14	0.47
1:D:169:LEU:HD12	1:D:277:LEU:HG	1.96	0.47
1:C:224:VAL:HB	1:C:233:THR:HB	1.95	0.47
1:B:172:ASP:OD1	1:B:175:PHE:HD1	1.97	0.47
1:A:160:VAL:O	1:A:160:VAL:HG23	2.14	0.47
1:D:183:LYS:HD3	1:D:202:GLN:NE2	2.30	0.47
1:C:204:GLN:NE2	1:C:208:ASN:ND2	2.63	0.47
1:D:185:LEU:HD11	1:D:202:GLN:CG	2.34	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:179:LEU:HB2	1:D:252:TYR:OH	2.15	0.47
1:C:169:LEU:HG	1:C:275:TYR:CD1	2.50	0.47
1:A:162:TYR:OH	1:A:203:ALA:HB2	2.15	0.46
1:C:149:LYS:O	1:C:151:ILE:N	2.46	0.46
1:C:187:THR:O	1:C:188:LEU:HD23	2.16	0.46
1:C:226:HIS:CE1	1:C:233:THR:OG1	2.69	0.46
1:A:237:MET:HB2	1:B:234:ILE:CG1	2.45	0.46
1:B:230:ILE:HG22	1:B:231:PHE:HD1	1.78	0.46
1:A:164:VAL:HA	1:A:272:GLU:O	2.16	0.46
1:C:216:ILE:HG23	1:C:274:TYR:HB3	1.98	0.45
1:A:193:THR:HA	1:A:243:TYR:O	2.16	0.45
1:A:207:LEU:CD1	1:A:211:HIS:HB2	2.44	0.45
1:C:226:HIS:HE1	1:C:233:THR:OG1	2.00	0.45
1:B:226:HIS:HD2	1:B:268:ASP:OD1	2.00	0.45
1:B:169:LEU:HD12	1:B:277:LEU:HD13	1.98	0.45
1:A:250:GLN:NE2	1:A:264:ILE:O	2.50	0.45
1:A:264:ILE:HD12	1:C:180:LYS:HD3	1.97	0.45
1:D:183:LYS:HZ2	1:D:202:GLN:NE2	2.13	0.45
1:D:255:ASN:ND2	1:D:257:LYS:H	2.15	0.45
1:B:179:LEU:HD12	1:B:180:LYS:H	1.82	0.45
1:B:285:ASP:CB	1:C:235:LEU:HD23	2.47	0.45
1:D:155:ALA:HB1	1:D:266:ASN:ND2	2.31	0.45
1:B:255:ASN:HD22	1:B:258:SER:H	1.65	0.44
1:C:216:ILE:HA	1:C:276:VAL:HG12	1.98	0.44
1:B:226:HIS:HE1	1:B:233:THR:OG1	2.00	0.44
1:D:200:LEU:O	1:D:204:GLN:HG3	2.17	0.44
1:C:165:GLN:NE2	1:C:273:LYS:HE2	2.33	0.44
1:B:277:LEU:HD22	1:B:283:PRO:HG3	1.99	0.44
1:A:181:ASP:OD1	1:A:181:ASP:O	2.35	0.44
1:D:151:ILE:HG12	1:D:247:ASN:ND2	2.32	0.44
1:A:161:GLU:OE1	1:A:161:GLU:HA	2.18	0.44
1:B:179:LEU:HD12	1:B:180:LYS:N	2.33	0.43
1:D:208:ASN:N	1:D:208:ASN:HD22	2.15	0.43
1:B:277:LEU:HD21	1:B:281:GLU:O	2.18	0.43
1:B:164:VAL:HG22	1:B:165:GLN:N	2.33	0.43
1:A:234:ILE:H	1:A:234:ILE:HD12	1.83	0.43
1:C:151:ILE:HG12	1:C:247:ASN:HD21	1.83	0.43
1:B:238:ASP:HB3	2:B:48:HOH:O	2.18	0.43
1:D:160:VAL:HG11	1:D:194:ILE:CD1	2.48	0.43
1:B:190:ILE:HG13	1:B:247:ASN:HA	2.01	0.43
1:A:226:HIS:CE1	1:A:233:THR:HG23	2.53	0.43
1:C:151:ILE:O	1:C:151:ILE:HG23	2.18	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:190:ILE:CG2	1:C:247:ASN:HA	2.49	0.43
1:B:188:LEU:HB3	1:B:192:ASP:HB2	2.00	0.43
1:C:196:SER:HB3	1:C:241:PHE:CE2	2.54	0.43
1:C:239:GLN:HB2	1:C:239:GLN:HE21	1.52	0.42
1:B:153:ASN:ND2	1:D:176:ARG:NH1	2.67	0.42
1:B:253:GLU:CG	1:B:264:ILE:HD13	2.40	0.42
1:B:222:SER:HB2	1:B:235:LEU:HB2	2.01	0.42
1:C:168:PRO:HA	1:C:276:VAL:O	2.20	0.42
1:C:193:THR:HG22	2:C:18:HOH:O	2.20	0.42
1:B:257:LYS:HA	1:B:257:LYS:NZ	2.35	0.41
1:B:180:LYS:HD3	1:D:264:ILE:CD1	2.47	0.41
1:D:226:HIS:HE1	1:D:233:THR:OG1	2.03	0.41
1:C:222:SER:CB	1:C:235:LEU:HB2	2.50	0.41
1:C:279:LYS:HE3	1:C:280:GLY:N	2.36	0.41
1:D:170:ASN:HA	1:D:171:PRO:HD2	1.91	0.41
1:D:188:LEU:HB3	1:D:192:ASP:HB2	2.03	0.41
1:C:220:ASP:HB3	1:C:273:LYS:O	2.21	0.41
1:B:254:ILE:O	1:B:255:ASN:C	2.59	0.41
1:B:255:ASN:ND2	1:B:255:ASN:C	2.73	0.41
1:C:154:GLN:HG3	1:C:247:ASN:OD1	2.20	0.41
1:A:163:THR:O	1:A:163:THR:HG23	2.20	0.40
1:B:185:LEU:HA	1:B:185:LEU:HD12	1.79	0.40
1:A:193:THR:HG22	1:A:244:HIS:ND1	2.36	0.40
1:C:242:THR:O	1:C:242:THR:HG23	2.21	0.40
1:A:226:HIS:O	1:A:227:ASP:C	2.60	0.40
1:B:252:TYR:CE2	1:D:176:ARG:HD2	2.57	0.40
1:B:186:LYS:HD3	1:B:188:LEU:HD21	2.03	0.40
1:B:170:ASN:HA	1:B:171:PRO:HD3	1.98	0.40
1:C:163:THR:CG2	1:C:271:SER:HA	2.51	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	135/137 (98%)	120 (89%)	11 (8%)	4 (3%)	7	5
1	B	135/137 (98%)	121 (90%)	11 (8%)	3 (2%)	10	11
1	C	130/137 (95%)	111 (85%)	16 (12%)	3 (2%)	10	10
1	D	130/137 (95%)	119 (92%)	9 (7%)	2 (2%)	15	20
All	All	530/548 (97%)	471 (89%)	47 (9%)	12 (2%)	10	10

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	255	ASN
1	A	151	ILE
1	B	227	ASP
1	C	279	LYS
1	D	151	ILE
1	B	283	PRO
1	C	212	PRO
1	A	186	LYS
1	A	283	PRO
1	C	214	TYR
1	D	171	PRO
1	A	245	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	125/127 (98%)	113 (90%)	12 (10%)	12	17
1	B	125/127 (98%)	114 (91%)	11 (9%)	14	21
1	C	122/127 (96%)	111 (91%)	11 (9%)	14	20
1	D	122/127 (96%)	113 (93%)	9 (7%)	20	30
All	All	494/508 (97%)	451 (91%)	43 (9%)	15	22

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	149	LYS
1	A	173	ASP
1	A	174	ASP
1	A	197	GLN
1	A	233	THR
1	A	234	ILE
1	A	236	PRO
1	A	242	THR
1	A	247	ASN
1	A	255	ASN
1	A	265	ASN
1	A	268	ASP
1	B	153	ASN
1	B	173	ASP
1	B	174	ASP
1	B	197	GLN
1	B	234	ILE
1	B	236	PRO
1	B	239	GLN
1	B	247	ASN
1	B	255	ASN
1	B	256	LYS
1	B	257	LYS
1	C	149	LYS
1	C	175	PHE
1	C	197	GLN
1	C	237	MET
1	C	239	GLN
1	C	240	GLU
1	C	256	LYS
1	C	265	ASN
1	C	276	VAL
1	C	278	LYS
1	C	279	LYS
1	D	176	ARG
1	D	197	GLN
1	D	219	ARG
1	D	228	ASN
1	D	237	MET
1	D	239	GLN
1	D	242	THR
1	D	255	ASN
1	D	268	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	197	GLN
1	A	204	GLN
1	A	208	ASN
1	A	226	HIS
1	A	247	ASN
1	A	261	ASN
1	A	266	ASN
1	B	152	GLN
1	B	153	ASN
1	B	154	GLN
1	B	197	GLN
1	B	202	GLN
1	B	226	HIS
1	B	239	GLN
1	B	244	HIS
1	B	247	ASN
1	B	255	ASN
1	B	265	ASN
1	B	266	ASN
1	C	165	GLN
1	C	197	GLN
1	C	202	GLN
1	C	208	ASN
1	C	211	HIS
1	C	226	HIS
1	C	239	GLN
1	C	265	ASN
1	C	266	ASN
1	D	165	GLN
1	D	197	GLN
1	D	202	GLN
1	D	208	ASN
1	D	226	HIS
1	D	228	ASN
1	D	239	GLN
1	D	255	ASN
1	D	261	ASN
1	D	265	ASN
1	D	266	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

There are no ligands in this entry.

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.