Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:43 PM 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 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:

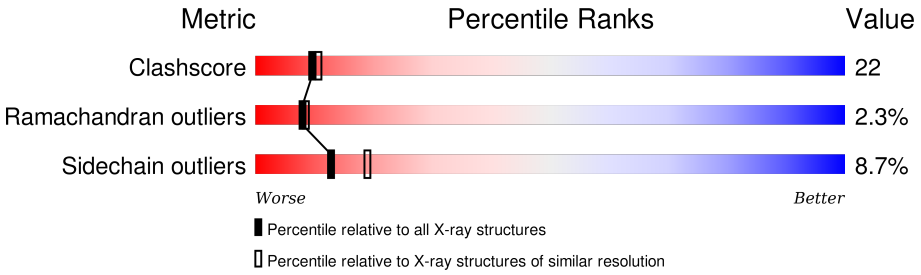
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

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	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (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. 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	137	61% 31% 7%
1	B	137	58% 36%
1	C	137	51% 40%
1	D	137	62% 31%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4471 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 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		

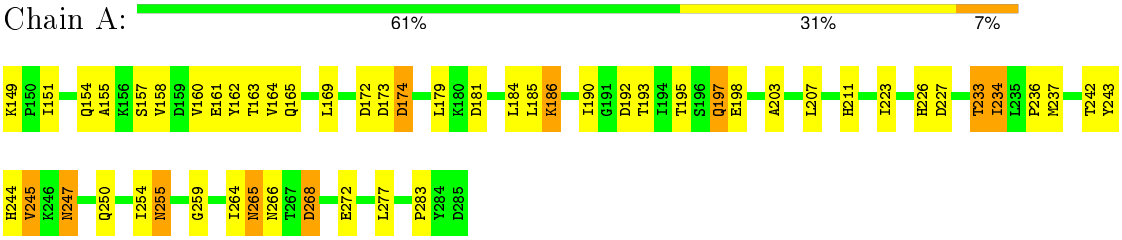
3 Residue-property plots (i)

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.

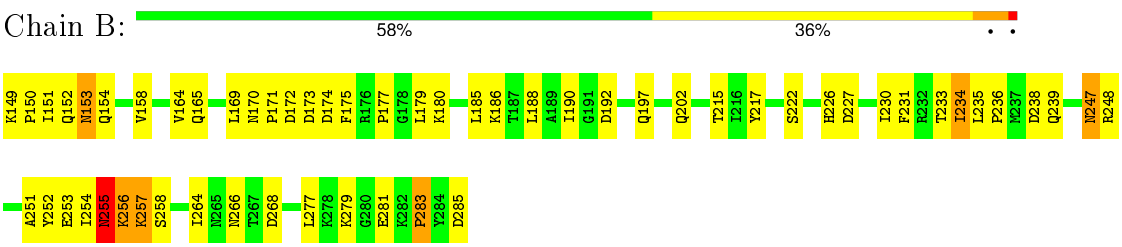
- Molecule 1: PROTEIN (STREPTOKINASE)

Chain A:



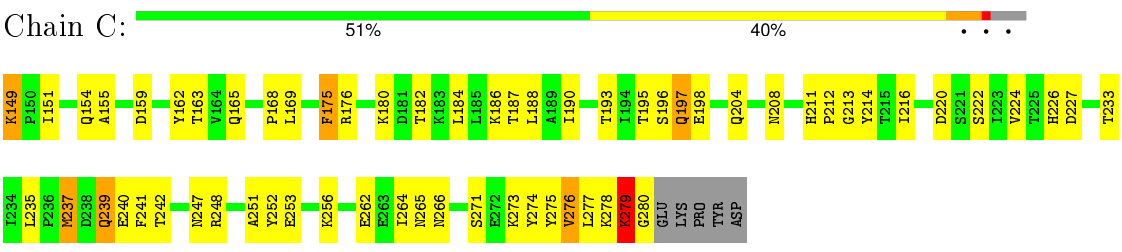
- Molecule 1: PROTEIN (STREPTOKINASE)

Chain B:



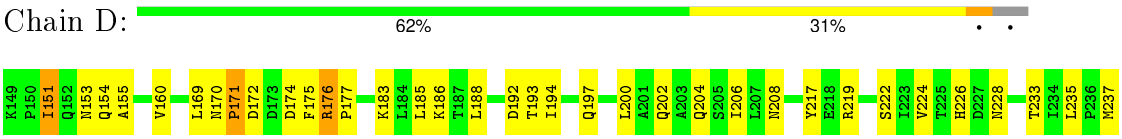
- Molecule 1: PROTEIN (STREPTOKINASE)

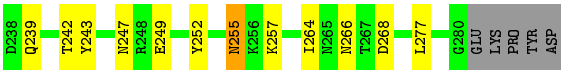
Chain C:



- Molecule 1: PROTEIN (STREPTOKINASE)

Chain D:




D238
Q239
T242
Y243
N247
R248
E249
Y252
N255
K256
K257
I264
N265
N266
T267
D268
L277
G280
GLU
LYS
PRO
TYR
ASP

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 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 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	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

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 22.

All (194) 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: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
1:B:177:PRO:CG	1:D:249:GLU:HG2	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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	Interatomic distance (Å)	Clash overlap (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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:185:LEU:HD11	1:D:202:GLN:CG	2.34	0.47
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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 (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	135/137 (98%)	120 (89%)	11 (8%)	4 (3%)	5 4
1	B	135/137 (98%)	121 (90%)	11 (8%)	3 (2%)	8 9
1	C	130/137 (95%)	111 (85%)	16 (12%)	3 (2%)	8 8
1	D	130/137 (95%)	119 (92%)	9 (7%)	2 (2%)	13 17
All	All	530/548 (97%)	471 (89%)	47 (9%)	12 (2%)	8 8

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 (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	125/127 (98%)	113 (90%)	12 (10%)	10 15
1	B	125/127 (98%)	114 (91%)	11 (9%)	12 18
1	C	122/127 (96%)	111 (91%)	11 (9%)	12 17
1	D	122/127 (96%)	113 (93%)	9 (7%)	17 26
All	All	494/508 (97%)	451 (91%)	43 (9%)	13 19

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

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Mol	Chain	Res	Type
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

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Mol	Chain	Res	Type
1	D	265	ASN
1	D	266	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

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.