



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:34 AM UTC

PDB ID : 1C4P / pdb_00001c4p
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

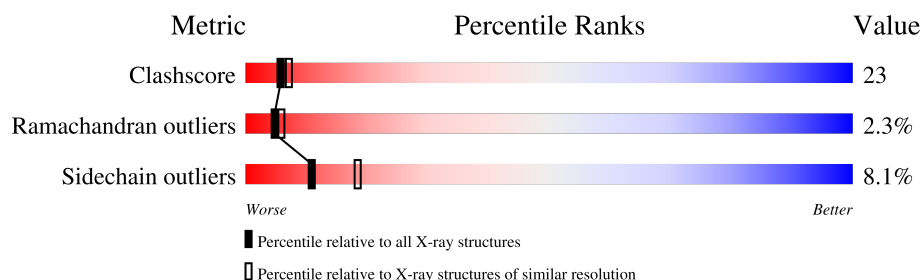
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	137	59% 36% 5%
1	B	137	56% 37% . .
1	C	137	50% 42% . . .
1	D	137	58% 34% . . .

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		

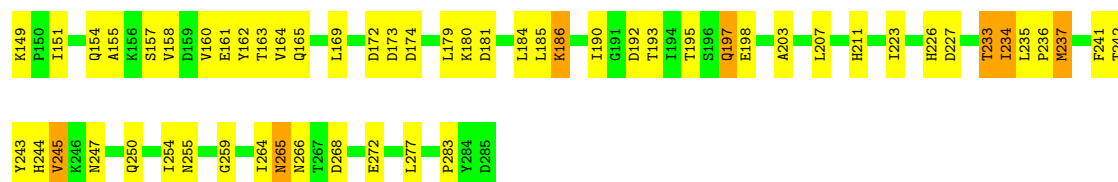
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

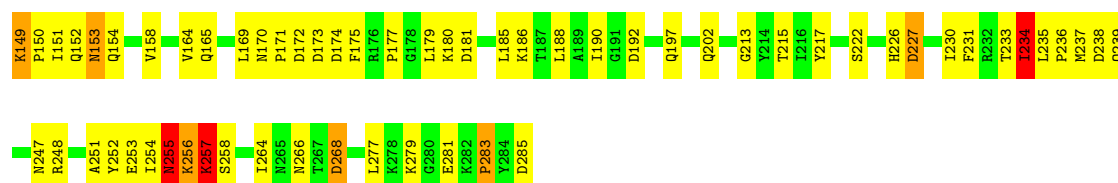
• Molecule 1: PROTEIN (STREPTOKINASE)

Chain A: 



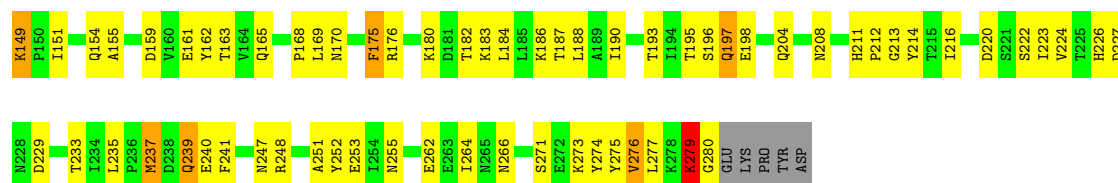
• Molecule 1: PROTEIN (STREPTOKINASE)

Chain B: 



• Molecule 1: PROTEIN (STREPTOKINASE)

Chain C: 



• Molecule 1: PROTEIN (STREPTOKINASE)

Chain D: 



L235	P236	D237	D238	Q239	T242	Y243	N247	R248	E249	Y252	E253	I254	N255	K256	K257	I264	N265	N266	L277	G280	GLU	LYS	PRO	TYR	ASP
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4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore 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	0.58	0/1125	1.01	3/1524 (0.2%)
1	B	0.57	0/1125	1.02	5/1524 (0.3%)
1	C	0.52	0/1089	0.93	2/1475 (0.1%)
1	D	0.59	0/1089	1.02	5/1475 (0.3%)
All	All	0.57	0/4428	1.00	15/5998 (0.3%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	237	MET	N-CA-C	7.29	122.53	112.04
1	D	256	LYS	N-CA-C	6.94	119.73	111.33
1	D	228	ASN	N-CA-C	6.92	121.47	113.38
1	A	237	MET	N-CA-C	6.84	121.89	112.04
1	C	255	ASN	N-CA-C	-6.24	99.71	109.25
1	B	213	GLY	N-CA-C	-5.62	107.51	115.43
1	C	229	ASP	N-CA-C	-5.48	103.16	110.55
1	D	227	ASP	CA-C-N	-5.41	114.93	123.91
1	D	227	ASP	C-N-CA	-5.41	114.93	123.91
1	A	235	LEU	CA-C-N	5.29	126.45	119.84
1	A	235	LEU	C-N-CA	5.29	126.45	119.84
1	B	234	ILE	CB-CA-C	-5.27	104.37	110.91
1	B	268	ASP	N-CA-C	-5.26	100.83	109.40
1	B	257	LYS	N-CA-C	5.17	116.60	111.07
1	D	188	LEU	N-CA-C	5.09	116.40	109.18

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	51	0
1	B	1105	0	1090	63	0
1	C	1070	0	1060	60	0
1	D	1070	0	1060	43	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	201	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 23.

All (201) 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:D:255:ASN:C	1:D:255:ASN:HD22	1.80	0.89
1:A:197:GLN:H	1:A:197:GLN:NE2	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: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:HE21	1:A:197:GLN:N	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:HG2	1:C:176:ARG:HH11	1.50	0.76
1:D:183:LYS:HZ3	1:D:202:GLN:HE22	1.32	0.74
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:255:ASN:C	1:D:255:ASN:ND2	2.51	0.67
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:HD23	1:C:277:LEU:H	1.61	0.65
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:D:185:LEU:O	1:D:186:LYS:HG3	1.98	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
1:A:155:ALA:HB1	1:A:266:ASN:ND2	2.14	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:HG22	1:B:254:ILE:O	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:151:ILE:HD12	1:B:154:GLN:HB2	1.85	0.58
1:B:179:LEU:HD13	1:D:252:TYR:CE2	2.38	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:215:THR:HG23	1:B:279:LYS:HE2	1.85	0.58
1:B:247:ASN:HD22	1:B:248:ARG:H	1.52	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:222:SER:HB2	1:C:235:LEU:HB2	1.86	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:B:255:ASN:HD22	1:B:255:ASN:C	2.13	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: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:D:183:LYS:HD3	1:D:202:GLN:HE21	1.72	0.54
1:B:251:ALA:N	1:B:266:ASN:HD21	2.01	0.53
1:B:256:LYS:HB3	1:B:256:LYS:HZ2	1.73	0.53
1:A:192:ASP:O	1:A:245:VAL:HG23	2.08	0.53
1:A:226:HIS:CE1	1:A:233:THR:CG2	2.89	0.53
1:D:183:LYS:HD2	1:D:206:ILE:HD11	1.91	0.53
1:C:204:GLN:HE21	1:C:208:ASN:HD21	1.56	0.53
1:B:256:LYS:HB3	1:B:256:LYS:NZ	2.24	0.53
1:C:279:LYS:HE3	1:C:279:LYS:CA	2.36	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: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:A:190:ILE:HD13	1:A:247:ASN:ND2	2.22	0.50
1:B:217:TYR:CE1	1:B:283:PRO:HG2	2.45	0.50
1:C:213:GLY:O	1:C:279:LYS:HB2	2.12	0.50
1:D:153:ASN:N	1:D:249:GLU:OE2	2.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:252:TYR:HB2	1:C:262:GLU:O	2.12	0.50
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:HG2	1:C:176:ARG:NH1	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:NZ	1:B:149:LYS:HB2	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:B:172:ASP:OD1	1:B:175:PHE:HD1	1.97	0.47
1:C:224:VAL:HB	1:C:233:THR:HB	1.95	0.47
1:D:169:LEU:HD12	1:D:277:LEU:HG	1.96	0.47
1:A:160:VAL:HG23	1:A:160:VAL:O	2.14	0.47
1:C:204:GLN:NE2	1:C:208:ASN:ND2	2.63	0.47
1:D:183:LYS:HD3	1:D:202:GLN:NE2	2.30	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:D:185:LEU:HD11	1:D:202:GLN:CG	2.34	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:B:255:ASN:ND2	1:B:255:ASN:C	2.73	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:A:193:THR:HA	1:A:243:TYR:O	2.16	0.45
1:C:216:ILE:HG23	1:C:274:TYR:HB3	1.98	0.45
1:A:207:LEU:CD1	1:A:211:HIS:HB2	2.44	0.45
1:B:254:ILE:O	1:B:255:ASN:C	2.59	0.45
1:D:183:LYS:HZ2	1:D:202:GLN:HE22	1.61	0.45
1:B:226:HIS:HD2	1:B:268:ASP:OD1	2.00	0.45
1:C:226:HIS:HE1	1:C:233:THR:OG1	2.00	0.45
1:A:226:HIS:O	1:A:227:ASP:C	2.60	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:LEU:HD12	1:B:277:LEU:HD13	1.98	0.45
1:D:255:ASN:ND2	1:D:257:LYS:H	2.15	0.45
1:D:226:HIS:O	1:D:227:ASP:C	2.60	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:A:181:ASP:O	1:A:181:ASP:OD1	2.35	0.44
1:B:277:LEU:HD22	1:B:283:PRO:HG3	1.99	0.44
1:C:165:GLN:NE2	1:C:273:LYS:HE2	2.33	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:164:VAL:HG22	1:B:165:GLN:N	2.33	0.43
1:B:277:LEU:HD21	1:B:281:GLU:O	2.18	0.43
1:A:234:ILE:H	1:A:234:ILE:HD12	1.83	0.43
1:B:238:ASP:HB3	2:B:48:HOH:O	2.18	0.43
1:C:151:ILE:HG12	1:C:247:ASN:HD21	1.83	0.43
1:C:222:SER:C	1:C:223:ILE:HD12	2.43	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:B:188:LEU:HB3	1:B:192:ASP:HB2	2.00	0.43
1:C:190:ILE:CG2	1:C:247:ASN:HA	2.49	0.43
1:C:196:SER:HB3	1:C:241:PHE:CE2	2.54	0.43
1:B:226:HIS:O	1:B:227:ASP:C	2.62	0.43
1:C:239:GLN:HE21	1:C:239:GLN:HB2	1.52	0.42
1:B:153:ASN:ND2	1:D:176:ARG:NH1	2.67	0.42
1:B:222:SER:HB2	1:B:235:LEU:HB2	2.01	0.42
1:B:253:GLU:CG	1:B:264:ILE:HD13	2.40	0.42
1:C:151:ILE:O	1:C:151:ILE:HG23	2.18	0.42
1:B:255:ASN:O	1:B:256:LYS:C	2.61	0.42
1:A:241:PHE:CD1	1:A:241:PHE:C	2.98	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:A:181:ASP:O	1:A:181:ASP:CG	2.62	0.41
1:B:257:LYS:HA	1:B:257:LYS:NZ	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:180:LYS:HD3	1:D:264:ILE:CD1	2.47	0.41
1:C:222:SER:CB	1:C:235:LEU:HB2	2.50	0.41
1:D:226:HIS:HE1	1:D:233:THR:OG1	2.03	0.41
1:C:279:LYS:HE3	1:C:280:GLY:N	2.36	0.41
1:D:189:ALA:O	1:D:190:ILE:C	2.62	0.41
1:B:181:ASP:O	1:B:181:ASP:CG	2.63	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: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:A:193:THR:HG22	1:A:244:HIS:ND1	2.36	0.40
1:B:185:LEU:HD12	1:B:185:LEU:HA	1.79	0.40
1:B:186:LYS:HD3	1:B:188:LEU:HD21	2.03	0.40
1:B:252:TYR:CE2	1:D:176:ARG:HD2	2.57	0.40
1:C:168:PRO:C	1:C:170:ASN:H	2.30	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%)	3	3
1	B	135/137 (98%)	121 (90%)	11 (8%)	3 (2%)	5	6
1	C	130/137 (95%)	111 (85%)	16 (12%)	3 (2%)	5	6
1	D	130/137 (95%)	119 (92%)	9 (7%)	2 (2%)	8	12
All	All	530/548 (97%)	471 (89%)	47 (9%)	12 (2%)	5	6

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%)	116 (93%)	9 (7%)	13	23
1	B	125/127 (98%)	114 (91%)	11 (9%)	9	15
1	C	122/127 (96%)	112 (92%)	10 (8%)	10	18
1	D	122/127 (96%)	112 (92%)	10 (8%)	10	18
All	All	494/508 (97%)	454 (92%)	40 (8%)	11	18

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	149	LYS
1	A	173	ASP
1	A	180	LYS
1	A	197	GLN
1	A	233	THR
1	A	234	ILE
1	A	236	PRO
1	A	242	THR
1	A	265	ASN
1	B	149	LYS

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Mol	Chain	Res	Type
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	255	ASN
1	B	256	LYS
1	B	257	LYS
1	C	149	LYS
1	C	161	GLU
1	C	175	PHE
1	C	183	LYS
1	C	197	GLN
1	C	237	MET
1	C	239	GLN
1	C	240	GLU
1	C	276	VAL
1	C	279	LYS
1	D	151	ILE
1	D	161	GLU
1	D	176	ARG
1	D	179	LEU
1	D	197	GLN
1	D	237	MET
1	D	239	GLN
1	D	242	THR
1	D	254	ILE
1	D	255	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	197	GLN
1	A	208	ASN
1	A	226	HIS
1	A	247	ASN
1	A	255	ASN
1	A	261	ASN
1	A	265	ASN
1	A	266	ASN

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Mol	Chain	Res	Type
1	B	152	GLN
1	B	153	ASN
1	B	154	GLN
1	B	170	ASN
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	204	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 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 [i](#)

There are no oligosaccharides 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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.