



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 11:06 AM UTC

PDB ID : 1KN9 / pdb_00001kn9
Title : CRYSTAL STRUCTURE OF A BACTERIAL SIGNAL PEPTIDASE APO-
ENZYME, IMPLICATIONS FOR SIGNAL PEPTIDE BINDING AND THE
SER-LYS DYAD MECHANISM.
Authors : Paetzel, M.; Dalbey, R.E.; Strynadka, N.C.J.
Deposited on : 2001-12-18
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

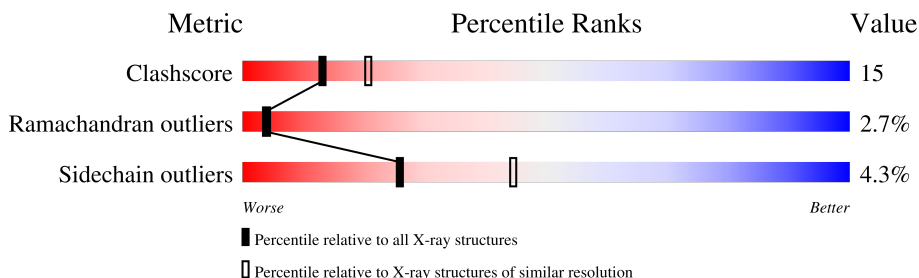
1 Overall quality at a glance

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	249	 68% 24% • 6%
1	B	249	 61% 26% • 11%
1	C	249	 59% 29% 5% 6%
1	D	249	 57% 26% • 14%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7154 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 Signal peptidase I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	234	Total	C	N	O	S	0	0	0
			1782	1132	306	337	7			
1	B	222	Total	C	N	O	S	0	0	0
			1688	1076	284	320	8			
1	C	234	Total	C	N	O	S	0	0	0
			1805	1156	303	339	7			
1	D	214	Total	C	N	O	S	0	0	0
			1623	1033	276	307	7			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	75	MET	-	initiating methionine	UNP P00803
B	75	MET	-	initiating methionine	UNP P00803
C	75	MET	-	initiating methionine	UNP P00803
D	75	MET	-	initiating methionine	UNP P00803

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	94	Total	O	0	0
			94	94		
2	B	64	Total	O	0	0
			64	64		
2	C	49	Total	O	0	0
			49	49		
2	D	49	Total	O	0	0
			49	49		

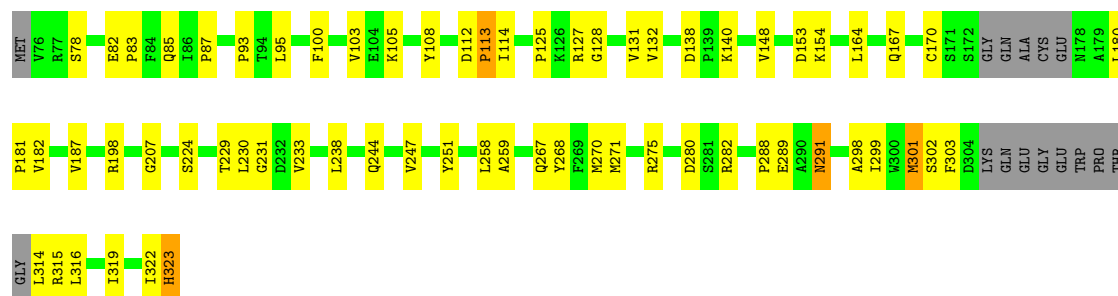
3 Residue-property plots [i](#)

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.

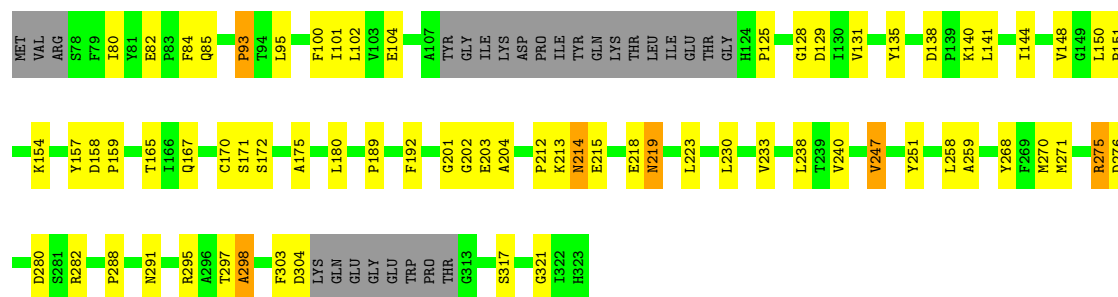
• Molecule 1: Signal peptidase I

Chain A: 



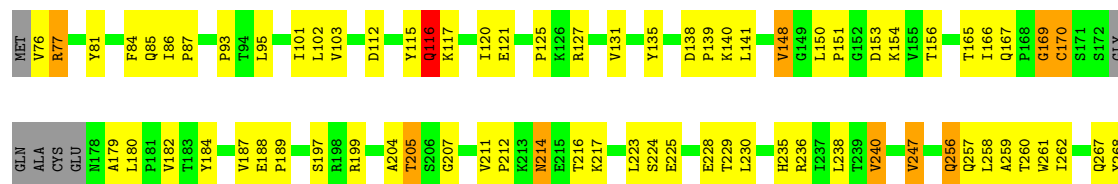
• Molecule 1: Signal peptidase I

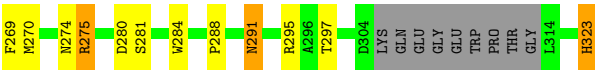
Chain B: 



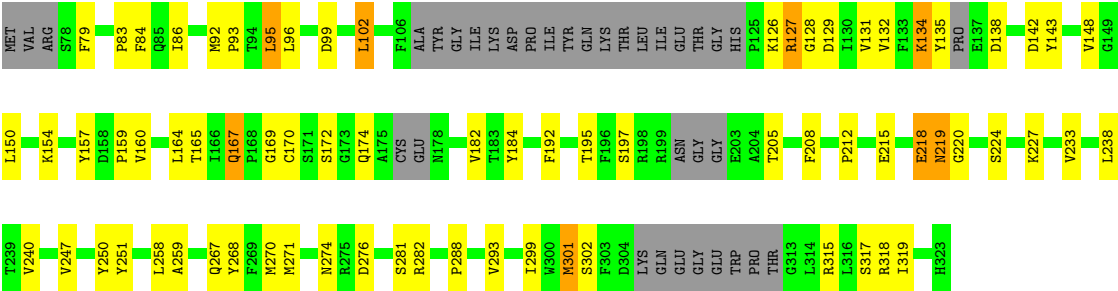
• Molecule 1: Signal peptidase I

Chain C: 





● Molecule 1: Signal peptidase I



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	112.44Å 112.44Å 198.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.05 – 2.40	Depositor
% Data completeness (in resolution range)	98.7 (40.05-2.40)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.239 , 0.278	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7154	wwPDB-VP
Average B, all atoms (Å ²)	45.0	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	0.43	0/1827	0.98	6/2472 (0.2%)
1	B	0.44	0/1730	1.04	14/2344 (0.6%)
1	C	0.40	0/1852	0.92	8/2509 (0.3%)
1	D	0.38	0/1660	0.96	6/2243 (0.3%)
All	All	0.41	0/7069	0.98	34/9568 (0.4%)

There are no bond length outliers.

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	275	ARG	N-CA-C	8.24	122.29	111.75
1	A	275	ARG	N-CA-C	8.18	122.22	111.75
1	B	158	ASP	CA-C-N	8.11	128.05	119.05
1	B	158	ASP	C-N-CA	8.11	128.05	119.05
1	A	131	VAL	N-CA-C	7.90	119.85	108.48
1	A	251	TYR	N-CA-C	-7.11	98.46	109.76
1	C	207	GLY	N-CA-C	6.96	119.64	111.63
1	D	131	VAL	N-CA-C	6.83	118.43	108.53
1	C	131	VAL	N-CA-C	6.48	117.81	108.48
1	B	251	TYR	N-CA-C	-6.46	99.37	109.25
1	A	303	PHE	N-CA-C	6.35	118.96	108.49
1	B	170	CYS	CA-CB-SG	-6.20	100.14	114.40
1	B	298	ALA	N-CA-C	6.03	116.38	107.88
1	C	274	ASN	N-CA-C	-5.95	100.69	109.62
1	B	131	VAL	N-CA-C	5.93	117.13	108.53
1	A	207	GLY	N-CA-C	5.75	117.95	111.85
1	B	192	PHE	N-CA-C	5.74	118.75	109.40
1	D	274	ASN	N-CA-C	-5.70	101.06	109.62
1	B	167	GLN	CA-C-N	5.68	126.00	119.92
1	B	167	GLN	C-N-CA	5.68	126.00	119.92
1	D	192	PHE	N-CA-C	5.62	118.72	109.72
1	C	275	ARG	N-CA-C	5.57	122.67	110.80
1	B	202	GLY	N-CA-C	-5.56	108.47	115.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	101	ILE	N-CA-C	5.56	117.41	108.85
1	C	240	VAL	CA-C-N	5.46	125.54	119.32
1	C	240	VAL	C-N-CA	5.46	125.54	119.32
1	B	154	LYS	N-CA-C	-5.43	98.91	108.20
1	D	251	TYR	N-CA-C	-5.27	100.58	108.96
1	B	180	LEU	N-CA-C	-5.14	99.44	108.69
1	D	160	VAL	N-CA-C	5.13	115.80	110.82
1	D	268	TYR	N-CA-C	5.13	116.99	109.24
1	C	284	TRP	N-CA-C	5.09	119.03	112.41
1	A	298	ALA	N-CA-C	5.06	115.84	108.14
1	C	240	VAL	N-CA-C	-5.02	102.58	107.55

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	1782	0	1696	45	0
1	B	1688	0	1602	42	0
1	C	1805	0	1722	65	0
1	D	1623	0	1537	52	0
2	A	94	0	0	0	0
2	B	64	0	0	1	0
2	C	49	0	0	1	0
2	D	49	0	0	1	0
All	All	7154	0	6557	200	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 15.

All (200) 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:SER:HB3	1:C:204:ALA:HB3	1.38	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:MET:HE3	1:A:319:ILE:HD11	1.44	0.99
1:A:323:HIS:H	1:A:323:HIS:CD2	1.88	0.90
1:D:127:ARG:HB2	1:D:127:ARG:HH21	1.38	0.89
1:C:257:GLN:HE21	1:C:258:LEU:H	1.13	0.89
1:D:301:MET:HE2	1:D:319:ILE:HD11	1.56	0.88
1:A:244:GLN:HE21	1:B:219:ASN:HD22	1.25	0.82
1:C:116:GLN:HE21	1:C:116:GLN:H	1.28	0.81
1:A:138:ASP:OD1	1:A:140:LYS:HE2	1.83	0.78
1:A:113:PRO:HG2	1:A:114:ILE:H	1.48	0.77
1:B:128:GLY:HA3	1:B:233:VAL:HG11	1.64	0.76
1:C:247:VAL:HG12	1:C:258:LEU:HD13	1.68	0.75
1:C:216:THR:HG22	1:C:217:LYS:H	1.52	0.74
1:C:216:THR:HG22	1:C:217:LYS:N	2.05	0.71
1:C:188:GLU:HG2	1:C:189:PRO:HD2	1.73	0.71
1:D:267:GLN:HE21	1:D:288:PRO:HG3	1.54	0.70
1:B:138:ASP:OD1	1:B:140:LYS:HE2	1.92	0.70
1:A:93:PRO:HD3	1:A:238:LEU:HG	1.73	0.70
1:C:291:ASN:HD22	1:C:291:ASN:N	1.89	0.69
1:C:257:GLN:NE2	1:C:258:LEU:H	1.89	0.69
1:D:79:PHE:HB3	1:D:102:LEU:HD21	1.75	0.68
1:B:247:VAL:CG1	1:B:258:LEU:HD13	2.24	0.68
1:C:154:LYS:HB3	1:C:167:GLN:HB2	1.74	0.68
1:D:134:LYS:O	1:D:135:TYR:HB2	1.94	0.67
1:C:116:GLN:H	1:C:116:GLN:NE2	1.93	0.67
1:C:267:GLN:NE2	1:C:288:PRO:HG3	2.09	0.67
1:A:301:MET:HE2	1:A:302:SER:H	1.60	0.66
1:C:295:ARG:NH1	1:C:297:THR:HG22	2.10	0.66
1:A:323:HIS:H	1:A:323:HIS:HD2	1.38	0.66
1:D:218:GLU:H	1:D:218:GLU:CD	2.04	0.65
1:B:247:VAL:HG12	1:B:258:LEU:HD13	1.79	0.65
1:D:164:LEU:O	1:D:182:VAL:HG21	1.97	0.65
1:D:92:MET:HG2	1:D:96:LEU:HD23	1.78	0.65
1:D:195:THR:HG22	1:D:220:GLY:HA3	1.78	0.64
1:C:93:PRO:HD3	1:C:238:LEU:HG	1.79	0.64
1:C:236:ARG:HH21	1:C:323:HIS:CB	2.10	0.64
1:D:271:MET:HE3	1:D:282:ARG:NE	2.13	0.63
1:A:244:GLN:NE2	1:B:219:ASN:HD22	1.95	0.63
1:B:247:VAL:HG13	1:B:258:LEU:HB3	1.80	0.62
1:C:214:ASN:H	1:C:214:ASN:HD22	1.47	0.62
1:C:76:VAL:O	1:C:77:ARG:HG3	2.00	0.61
1:B:125:PRO:HG2	1:B:268:TYR:CE2	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:LEU:HD23	1:A:181:PRO:N	2.16	0.60
1:C:116:GLN:NE2	1:C:116:GLN:N	2.49	0.60
1:B:214:ASN:HD22	1:B:215:GLU:N	2.00	0.60
1:D:157:TYR:O	1:D:159:PRO:HD3	2.03	0.59
1:A:182:VAL:HG23	1:A:182:VAL:O	2.01	0.58
1:C:223:LEU:HD22	1:C:240:VAL:HG22	1.85	0.58
1:A:180:LEU:HD21	1:A:231:GLY:CA	2.34	0.58
1:A:299:ILE:HG13	1:A:322:ILE:HD13	1.86	0.58
1:B:223:LEU:HD22	1:B:240:VAL:HG22	1.84	0.58
1:D:247:VAL:O	1:D:250:TYR:HB2	2.04	0.57
1:B:214:ASN:HD22	1:B:215:GLU:H	1.51	0.57
1:B:270:MET:O	1:B:280:ASP:HB2	2.05	0.57
1:C:148:VAL:HG22	1:C:230:LEU:HD11	1.87	0.57
1:A:314:LEU:HD13	1:A:316:LEU:HG	1.86	0.56
1:C:261:TRP:C	1:C:262:ILE:HD12	2.31	0.56
1:C:257:GLN:HG3	1:C:258:LEU:N	2.21	0.56
1:A:267:GLN:HG2	1:A:288:PRO:HA	1.88	0.55
1:A:247:VAL:HG13	1:A:258:LEU:HB3	1.87	0.55
1:C:256:GLN:HG3	1:C:260:THR:HG23	1.87	0.55
1:C:135:TYR:HD2	1:C:138:ASP:HB3	1.72	0.55
1:C:116:GLN:HE21	1:C:116:GLN:N	1.99	0.55
1:B:214:ASN:HD22	1:B:214:ASN:N	2.03	0.54
1:B:258:LEU:O	1:B:259:ALA:HB3	2.06	0.54
1:A:271:MET:HE3	1:A:282:ARG:NE	2.23	0.53
1:D:182:VAL:O	1:D:182:VAL:HG23	2.09	0.53
1:A:270:MET:O	1:A:280:ASP:HB2	2.08	0.53
1:A:302:SER:OG	1:A:315:ARG:HB2	2.08	0.53
1:B:271:MET:HE3	1:B:282:ARG:NE	2.23	0.53
1:C:216:THR:CG2	1:C:217:LYS:H	2.21	0.53
1:A:258:LEU:O	1:A:259:ALA:HB3	2.07	0.53
1:A:323:HIS:CD2	1:A:323:HIS:N	2.64	0.53
1:B:138:ASP:OD1	1:B:140:LYS:HB2	2.07	0.53
1:A:164:LEU:O	1:A:182:VAL:HG21	2.09	0.53
1:C:257:GLN:O	1:C:260:THR:HG22	2.09	0.53
1:C:267:GLN:HE21	1:C:288:PRO:HG3	1.73	0.53
1:C:85:GLN:O	1:C:87:PRO:HD3	2.09	0.52
1:D:93:PRO:HD3	1:D:238:LEU:HG	1.92	0.52
1:D:218:GLU:O	1:D:219:ASN:HB2	2.09	0.52
1:B:82:GLU:OE1	1:B:82:GLU:HA	2.10	0.52
1:D:212:PRO:HB2	1:D:215:GLU:HG2	1.90	0.52
1:A:138:ASP:OD1	1:A:140:LYS:HB2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:212:PRO:HB2	1:D:215:GLU:CG	2.40	0.52
1:D:299:ILE:HD13	1:D:318:ARG:NH1	2.25	0.51
1:A:301:MET:HE2	1:A:301:MET:HA	1.92	0.51
1:C:236:ARG:HH21	1:C:323:HIS:HB2	1.75	0.51
1:C:225:GLU:OE2	1:C:236:ARG:HD2	2.11	0.51
1:C:223:LEU:CD2	1:C:240:VAL:HG22	2.41	0.51
1:C:112:ASP:HB3	1:C:115:TYR:O	2.10	0.51
1:C:187:VAL:HG13	1:C:224:SER:HB3	1.92	0.50
1:C:115:TYR:O	1:C:117:LYS:N	2.39	0.50
1:A:198:ARG:NH2	1:B:276:ASP:O	2.44	0.50
1:A:180:LEU:HD23	1:A:180:LEU:C	2.37	0.50
1:B:275:ARG:HG3	2:B:328:HOH:O	2.12	0.50
1:D:315:ARG:HD3	1:D:318:ARG:HD3	1.92	0.50
1:B:102:LEU:HD12	1:B:297:THR:OG1	2.12	0.50
1:C:291:ASN:N	1:C:291:ASN:ND2	2.60	0.50
1:B:85:GLN:HG2	1:B:100:PHE:CZ	2.47	0.49
1:A:103:VAL:HG21	1:A:132:VAL:HG21	1.94	0.49
1:B:298:ALA:HB2	1:B:321:GLY:HA2	1.93	0.49
1:B:212:PRO:HG2	1:B:215:GLU:HB2	1.94	0.49
1:B:230:LEU:O	1:B:233:VAL:HG12	2.13	0.49
1:A:113:PRO:CG	1:A:114:ILE:H	2.23	0.49
1:D:218:GLU:OE1	1:D:218:GLU:N	2.39	0.49
1:B:157:TYR:O	1:B:159:PRO:HD3	2.13	0.49
1:A:148:VAL:HG22	1:A:230:LEU:HD11	1.94	0.48
1:D:258:LEU:O	1:D:259:ALA:HB3	2.13	0.48
1:B:140:LYS:N	1:B:140:LYS:HD3	2.29	0.48
1:B:288:PRO:HG2	1:B:291:ASN:OD1	2.14	0.47
1:C:169:GLY:O	1:C:170:CYS:HB2	2.14	0.47
1:A:85:GLN:O	1:A:87:PRO:HD3	2.14	0.47
1:C:262:ILE:HD12	1:C:262:ILE:N	2.29	0.47
1:C:216:THR:CG2	1:C:217:LYS:N	2.74	0.47
1:A:125:PRO:HG2	1:A:268:TYR:CE2	2.50	0.47
1:D:224:SER:O	1:D:238:LEU:HA	2.15	0.47
1:D:302:SER:OG	1:D:315:ARG:HD2	2.15	0.47
1:D:127:ARG:HD3	1:D:150:LEU:HG	1.97	0.47
1:D:195:THR:HG22	1:D:220:GLY:CA	2.44	0.47
1:B:129:ASP:CG	1:B:295:ARG:HD2	2.40	0.46
1:C:228:GLU:OE1	1:C:235:HIS:NE2	2.46	0.46
1:D:271:MET:HE3	1:D:282:ARG:CD	2.45	0.46
1:B:144:ILE:N	1:B:144:ILE:HD12	2.31	0.46
1:C:150:LEU:HB3	1:C:151:PRO:HD2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:VAL:HG12	1:A:258:LEU:HD13	1.97	0.46
1:C:247:VAL:CG1	1:C:258:LEU:HB3	2.45	0.46
1:D:127:ARG:HH21	1:D:127:ARG:CB	2.18	0.46
1:D:299:ILE:CD1	1:D:318:ARG:HH12	2.28	0.46
1:D:83:PRO:HG2	1:D:84:PHE:CD1	2.51	0.46
1:D:92:MET:HE1	1:D:208:PHE:HB3	1.97	0.46
1:D:197:SER:OG	1:D:205:THR:HG23	2.16	0.46
1:A:128:GLY:HA3	1:A:233:VAL:HG11	1.97	0.46
1:C:211:VAL:O	1:C:212:PRO:C	2.59	0.46
1:C:270:MET:O	1:C:280:ASP:HB2	2.16	0.46
1:B:303:PHE:O	1:B:304:ASP:HB2	2.16	0.45
1:D:154:LYS:HB3	1:D:167:GLN:HG3	1.98	0.45
1:D:301:MET:HE2	1:D:301:MET:HA	1.97	0.45
1:D:270:MET:H	1:D:281:SER:HG	1.63	0.45
1:B:141:LEU:HD22	1:B:141:LEU:N	2.31	0.45
1:A:301:MET:HE3	1:A:319:ILE:CD1	2.32	0.45
1:D:318:ARG:HH11	1:D:318:ARG:HG3	1.81	0.45
1:B:104:GLU:O	1:B:104:GLU:HG3	2.17	0.45
1:C:120:ILE:HD12	1:C:120:ILE:N	2.31	0.45
1:C:236:ARG:NH2	1:C:323:HIS:CB	2.78	0.45
1:C:84:PHE:HB3	1:C:101:ILE:HG12	1.99	0.45
1:B:214:ASN:N	1:B:214:ASN:ND2	2.64	0.44
1:D:132:VAL:HA	1:D:143:TYR:O	2.17	0.44
1:C:258:LEU:O	1:C:259:ALA:HB3	2.18	0.44
1:D:240:VAL:HG23	1:D:276:ASP:HB2	2.00	0.44
1:D:276:ASP:HB2	2:D:328:HOH:O	2.18	0.44
1:C:138:ASP:C	1:C:140:LYS:H	2.25	0.44
1:D:142:ASP:OD2	1:D:293:VAL:HG21	2.18	0.44
1:C:166:ILE:HB	1:C:180:LEU:HB3	2.00	0.44
1:C:275:ARG:HG3	2:C:332:HOH:O	2.17	0.44
1:A:113:PRO:HG2	1:A:114:ILE:N	2.26	0.43
1:C:156:THR:HB	1:C:165:THR:HB	1.99	0.43
1:D:299:ILE:HD13	1:D:318:ARG:HH12	1.82	0.43
1:A:182:VAL:HA	1:A:229:THR:O	2.17	0.43
1:B:218:GLU:O	1:B:219:ASN:HB2	2.18	0.43
1:B:150:LEU:HB3	1:B:151:PRO:HD2	2.00	0.43
1:C:236:ARG:NH2	1:C:323:HIS:CG	2.86	0.43
1:D:267:GLN:NE2	1:D:288:PRO:HG3	2.27	0.43
1:D:99:ASP:OD1	1:D:318:ARG:NH1	2.51	0.43
1:C:84:PHE:HB3	1:C:101:ILE:CG1	2.48	0.43
1:D:184:TYR:HA	1:D:227:LYS:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:86:ILE:HD11	1:C:101:ILE:HD13	2.01	0.43
1:A:127:ARG:HH21	1:A:153:ASP:CG	2.27	0.43
1:A:187:VAL:HG13	1:A:224:SER:HB3	2.01	0.43
1:C:127:ARG:HH21	1:C:153:ASP:CG	2.27	0.43
1:C:148:VAL:HG22	1:C:230:LEU:CD1	2.48	0.43
1:D:86:ILE:CD1	1:D:95:LEU:HG	2.49	0.43
1:B:135:TYR:O	1:B:138:ASP:C	2.62	0.42
1:D:99:ASP:OD2	1:D:318:ARG:NH1	2.52	0.42
1:D:134:LYS:O	1:D:135:TYR:CB	2.66	0.42
1:A:154:LYS:HB3	1:A:167:GLN:HB2	2.01	0.42
1:A:314:LEU:HD13	1:A:314:LEU:O	2.19	0.42
1:C:184:TYR:CE2	1:C:228:GLU:HG3	2.55	0.42
1:B:214:ASN:ND2	1:B:215:GLU:N	2.65	0.42
1:A:85:GLN:NE2	1:A:100:PHE:CE1	2.88	0.42
1:B:138:ASP:CG	1:B:140:LYS:HE2	2.45	0.42
1:C:81:TYR:HA	1:C:103:VAL:O	2.20	0.42
1:A:82:GLU:HA	1:A:83:PRO:HD3	1.89	0.42
1:A:291:ASN:HD22	1:A:291:ASN:N	2.17	0.42
1:C:269:PHE:CE1	1:C:281:SER:HB3	2.54	0.42
1:D:128:GLY:HA3	1:D:233:VAL:HG11	2.00	0.42
1:A:301:MET:HE2	1:A:302:SER:N	2.32	0.42
1:B:317:SER:HA	1:D:317:SER:HA	2.01	0.42
1:D:154:LYS:HB2	1:D:170:CYS:HB3	2.02	0.42
1:A:78:SER:O	1:A:108:TYR:HB2	2.20	0.41
1:C:125:PRO:HG2	1:C:268:TYR:CE2	2.55	0.41
1:C:197:SER:H	1:C:205:THR:H	1.68	0.41
1:C:257:GLN:CG	1:C:258:LEU:N	2.83	0.41
1:C:214:ASN:HD22	1:C:214:ASN:N	2.09	0.41
1:D:218:GLU:O	1:D:219:ASN:CB	2.69	0.41
1:D:126:LYS:N	1:D:129:ASP:OD2	2.53	0.41
1:B:84:PHE:CD1	1:B:84:PHE:C	2.99	0.40
1:B:189:PRO:O	1:B:213:LYS:HE3	2.22	0.40
1:D:127:ARG:HD2	1:D:148:VAL:O	2.22	0.40
1:B:93:PRO:HD3	1:B:238:LEU:HG	2.02	0.40
1:C:182:VAL:HA	1:C:229:THR:O	2.21	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	228/249 (92%)	214 (94%)	12 (5%)	2 (1%)	14	22
1	B	216/249 (87%)	199 (92%)	10 (5%)	7 (3%)	3	3
1	C	228/249 (92%)	209 (92%)	10 (4%)	9 (4%)	2	2
1	D	202/249 (81%)	185 (92%)	11 (5%)	6 (3%)	3	3
All	All	874/996 (88%)	807 (92%)	43 (5%)	24 (3%)	4	4

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	113	PRO
1	B	171	SER
1	B	204	ALA
1	C	77	ARG
1	C	170	CYS
1	C	179	ALA
1	C	205	THR
1	D	134	LYS
1	D	138	ASP
1	D	172	SER
1	D	174	GLN
1	B	175	ALA
1	B	201	GLY
1	C	116	GLN
1	C	169	GLY
1	C	199	ARG
1	A	112	ASP
1	B	172	SER
1	D	169	GLY
1	B	219	ASN
1	B	203	GLU
1	D	219	ASN

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Mol	Chain	Res	Type
1	C	139	PRO
1	C	247	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	186/214 (87%)	179 (96%)	7 (4%)	29	49
1	B	177/214 (83%)	170 (96%)	7 (4%)	28	47
1	C	189/214 (88%)	179 (95%)	10 (5%)	20	36
1	D	169/214 (79%)	162 (96%)	7 (4%)	27	46
All	All	721/856 (84%)	690 (96%)	31 (4%)	26	44

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	95	LEU
1	A	105	LYS
1	A	170	CYS
1	A	289	GLU
1	A	291	ASN
1	A	301	MET
1	A	323	HIS
1	B	80	ILE
1	B	93	PRO
1	B	95	LEU
1	B	148	VAL
1	B	165	THR
1	B	214	ASN
1	B	247	VAL
1	C	95	LEU
1	C	102	LEU
1	C	116	GLN
1	C	121	GLU
1	C	141	LEU

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Mol	Chain	Res	Type
1	C	148	VAL
1	C	214	ASN
1	C	256	GLN
1	C	291	ASN
1	C	323	HIS
1	D	95	LEU
1	D	102	LEU
1	D	127	ARG
1	D	165	THR
1	D	167	GLN
1	D	218	GLU
1	D	301	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	194	GLN
1	A	244	GLN
1	A	252	GLN
1	A	256	GLN
1	A	277	ASN
1	A	291	ASN
1	A	323	HIS
1	B	194	GLN
1	B	214	ASN
1	B	256	GLN
1	B	277	ASN
1	C	116	GLN
1	C	194	GLN
1	C	214	ASN
1	C	246	GLN
1	C	256	GLN
1	C	257	GLN
1	C	277	ASN
1	C	291	ASN

5.3.3 RNA ⓘ

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 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.