



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:52 PM UTC

PDB ID : 1CUD / pdb_00001cud
Title : CUTINASE, N172K, R196D MUTANT, MONOCLINIC CRYSTAL FORM
WITH THREE MOLECULES PER ASYMMETRIC UNIT
Authors : Longhi, S.; Cambillau, C.
Deposited on : 1995-11-16
Resolution : 2.70 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

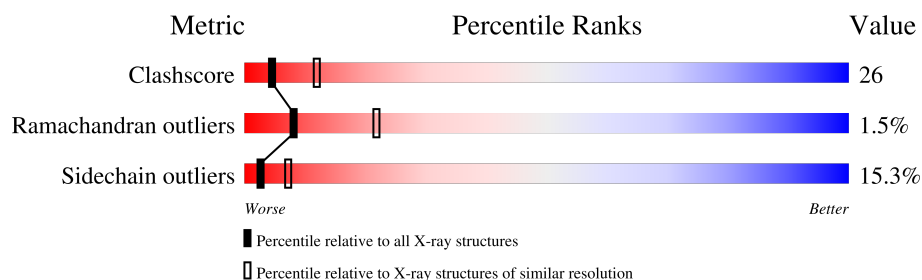
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)

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	214	
1	B	214	
1	C	214	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6762 atoms, of which 1964 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 CUTINASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	197	Total	C	H	N	O	S	0	0	0
			1770	894	332	257	282	5			
1	B	197	Total	C	H	N	O	S	0	0	0
			1770	894	332	257	282	5			
1	C	197	Total	C	H	N	O	S	0	0	0
			1770	894	332	257	282	5			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	32	ALA	ARG	conflict	UNP P00590
A	172	LYS	ASN	engineered mutation	UNP P00590
A	196	GLU	ARG	engineered mutation	UNP P00590
B	32	ALA	ARG	conflict	UNP P00590
B	172	LYS	ASN	engineered mutation	UNP P00590
B	196	GLU	ARG	engineered mutation	UNP P00590
C	32	ALA	ARG	conflict	UNP P00590
C	172	LYS	ASN	engineered mutation	UNP P00590
C	196	GLU	ARG	engineered mutation	UNP P00590

- Molecule 2 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	132	Total	H	O	0	0
			396	264	132		
2	B	193	Total	H	O	0	0
			579	386	193		
2	C	159	Total	H	O	0	0
			477	318	159		

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.

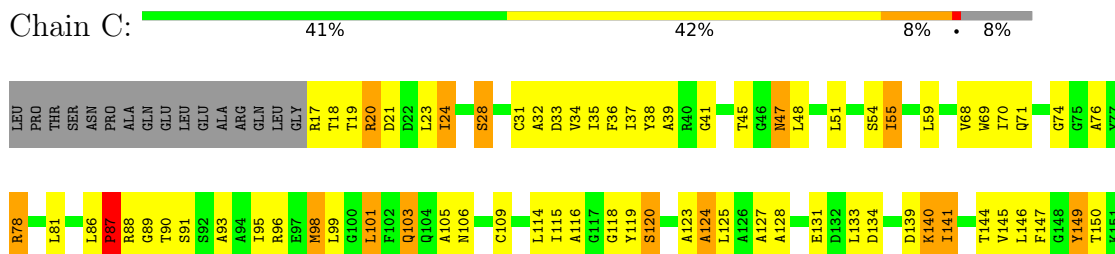
• Molecule 1: CUTINASE



• Molecule 1: CUTINASE



• Molecule 1: CUTINASE



M152	L153	Q154	N155	R156	G157	R158	I159		Y162	P163	A164		K168	V169	F170	C171	K172	T173	G174	D175	L176	V177	C178	T179		I183	V184	A185	A186	P187	H188	L189	A190	Y191	G192	P193	D194	A195	E196	G197	P198	A199	P200		L203	I204	E205	K206		V210	R211	G212	S213	ALA
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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 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	65.90Å 73.30Å 71.20Å 90.00° 112.70° 90.00°	Depositor
Resolution (Å)	6.00 – 2.70	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.70)	Depositor
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.141 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6762	wwPDB-VP
Average B, all atoms (Å ²)	12.0	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	0.88	1/1461 (0.1%)	1.36	12/1982 (0.6%)
1	B	0.81	1/1461 (0.1%)	1.27	16/1982 (0.8%)
1	C	0.69	0/1461	1.32	19/1982 (1.0%)
All	All	0.79	2/4383 (0.0%)	1.32	47/5946 (0.8%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	210	VAL	CA-CB	6.13	1.62	1.54
1	A	141	ILE	CA-CB	5.39	1.59	1.53

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	159	ILE	N-CA-C	-9.93	97.72	107.55
1	C	109	CYS	CA-C-N	8.86	128.46	119.24
1	C	109	CYS	C-N-CA	8.86	128.46	119.24
1	A	138	ARG	N-CA-C	-8.03	102.61	111.36
1	C	134	ASP	N-CA-C	-7.69	98.29	109.59
1	A	210	VAL	CB-CA-C	-7.41	104.54	111.06
1	B	25	ASN	N-CA-C	-7.28	104.77	112.93
1	B	18	THR	N-CA-C	6.80	120.67	112.38
1	A	18	THR	N-CA-C	6.59	120.93	113.02
1	C	191	TYR	N-CA-C	6.50	121.38	113.38
1	C	141	ILE	N-CA-C	-6.27	98.16	107.51
1	C	140	LYS	N-CA-C	6.17	119.75	112.72
1	A	208	ARG	N-CA-C	6.16	118.80	111.71
1	B	195	ALA	N-CA-C	-6.16	105.92	113.50
1	B	175	ASP	N-CA-C	-6.10	95.74	107.57
1	A	169	VAL	N-CA-C	6.10	117.19	107.98
1	C	81	LEU	N-CA-C	6.08	118.40	111.11
1	C	124	ALA	N-CA-C	-6.07	104.66	111.28
1	B	172	LYS	N-CA-C	6.04	117.84	110.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	28	SER	N-CA-C	6.03	119.74	112.38
1	C	32	ALA	N-CA-C	-5.93	102.55	110.55
1	B	136	ALA	N-CA-C	5.87	119.54	112.38
1	B	31	CYS	N-CA-C	5.86	118.75	109.96
1	C	124	ALA	CA-C-N	5.79	127.96	120.44
1	C	124	ALA	C-N-CA	5.79	127.96	120.44
1	A	159	ILE	N-CA-C	-5.78	95.66	107.92
1	B	99	LEU	N-CA-C	-5.78	105.06	111.71
1	A	33	ASP	N-CA-C	-5.65	105.49	112.90
1	A	113	THR	N-CA-C	-5.63	100.01	109.07
1	A	207	VAL	N-CA-C	-5.59	105.05	110.42
1	C	120	SER	CB-CA-C	-5.58	108.52	116.34
1	B	45	THR	N-CA-C	5.54	117.88	110.35
1	B	35	ILE	CB-CA-C	5.49	117.27	110.73
1	A	190	ALA	N-CA-C	5.48	119.59	111.87
1	A	61	SER	N-CA-C	-5.43	104.78	111.40
1	A	56	ALA	N-CA-C	5.34	116.90	111.14
1	B	180	GLY	N-CA-C	5.32	125.78	113.18
1	C	174	GLY	N-CA-C	-5.23	108.46	114.69
1	B	121	GLN	N-CA-C	-5.23	105.66	111.36
1	C	176	LEU	N-CA-C	5.20	119.34	112.89
1	C	87	PRO	N-CA-C	5.14	123.07	112.47
1	B	206	LYS	N-CA-C	5.11	117.75	111.82
1	C	86	LEU	CA-C-N	5.11	126.22	119.84
1	C	86	LEU	C-N-CA	5.11	126.22	119.84
1	B	169	VAL	CB-CA-C	-5.10	103.53	110.77
1	B	192	GLY	CA-C-N	5.08	126.19	119.84
1	B	192	GLY	C-N-CA	5.08	126.19	119.84

There are no chirality outliers.

There are no planarity outliers.

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	1438	332	1424	81	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1438	332	1424	76	0
1	C	1438	332	1424	70	0
2	A	132	264	0	7	0
2	B	193	386	0	10	0
2	C	159	318	0	5	0
All	All	4798	1964	4272	224	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 26.

All (224) 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:B:62:ALA:HA	1:C:179:THR:HG21	1.47	0.95
1:C:96:ARG:HG3	1:C:96:ARG:HH11	1.39	0.87
1:B:35:ILE:HG22	1:B:114:LEU:HB3	1.61	0.83
1:A:158:ARG:HG3	2:A:221:HOH:O	1.77	0.83
1:A:19:THR:HA	1:A:47:ASN:ND2	1.94	0.81
1:A:20:ARG:H	1:A:47:ASN:HD21	1.27	0.79
1:C:150:THR:HA	1:C:177:VAL:HB	1.65	0.78
2:A:264:HOH:O	1:B:182:LEU:HD12	1.84	0.77
1:A:151:LYS:O	1:A:155:ASN:HB2	1.86	0.76
1:A:88:ARG:HG2	1:A:88:ARG:HH11	1.50	0.75
1:A:48:LEU:HB3	1:A:53:PRO:HD3	1.68	0.74
1:C:99:LEU:O	1:C:103:GLN:HG2	1.88	0.73
1:B:47:ASN:HD22	1:B:72:GLY:HA3	1.53	0.73
1:C:23:LEU:HD11	1:C:105:ALA:HA	1.69	0.73
1:A:34:VAL:HG13	1:A:68:VAL:HG23	1.71	0.72
1:C:78:ARG:HA	1:C:78:ARG:HH11	1.53	0.72
1:B:19:THR:HG23	1:B:47:ASN:OD1	1.90	0.71
1:C:17:ARG:O	1:C:48:LEU:HD12	1.90	0.71
1:C:96:ARG:HG3	1:C:96:ARG:NH1	2.04	0.71
1:A:185:ALA:HA	1:B:81:LEU:HD23	1.71	0.71
1:B:114:LEU:O	1:B:141:ILE:HA	1.91	0.70
1:A:103:GLN:HG3	2:A:285:HOH:O	1.89	0.70
1:C:156:ARG:HE	1:C:158:ARG:NE	1.90	0.70
1:C:200:PRO:O	1:C:204:ILE:HG13	1.91	0.70
1:B:62:ALA:HA	1:C:179:THR:CG2	2.22	0.69
1:B:88:ARG:HH11	1:B:95:ILE:HD13	1.59	0.68
1:C:152:ASN:HB3	1:C:178:CYS:HA	1.76	0.67
1:C:156:ARG:HE	1:C:158:ARG:HE	1.42	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:ASN:O	1:A:61:SER:HB2	1.94	0.67
1:C:116:ALA:O	1:C:144:THR:HG23	1.94	0.67
1:C:172:LYS:HG3	2:C:354:HOH:O	1.93	0.67
1:C:20:ARG:H	1:C:47:ASN:HD21	1.43	0.67
1:B:42:SER:HB3	1:B:81:LEU:HD12	1.76	0.67
1:B:200:PRO:O	1:B:204:ILE:HG13	1.94	0.67
1:B:99:LEU:HD12	1:B:99:LEU:N	2.10	0.67
1:A:17:ARG:NE	1:A:17:ARG:HA	2.09	0.66
1:C:183:ILE:HA	2:C:266:HOH:O	1.95	0.66
1:B:176:LEU:HA	1:B:179:THR:HG22	1.80	0.64
1:A:39:ALA:O	1:A:122:GLY:HA3	1.98	0.64
1:C:36:PHE:CE2	1:C:38:TYR:HB2	2.33	0.64
1:B:186:ALA:N	1:B:187:PRO:HD2	2.13	0.64
1:A:197:GLY:O	1:A:200:PRO:HD2	1.99	0.62
1:C:21:ASP:HA	1:C:71:GLN:OE1	1.99	0.62
1:A:82:GLY:HA3	2:A:341:HOH:O	1.98	0.62
1:B:145:VAL:HG21	1:B:199:ALA:HB1	1.80	0.62
1:B:208:ARG:HG2	2:B:308:HOH:O	1.99	0.62
1:C:88:ARG:HH12	1:C:128:ALA:HB1	1.66	0.60
1:B:40:ARG:HD2	1:B:44:GLU:HB3	1.83	0.60
1:C:156:ARG:NE	1:C:158:ARG:HE	2.00	0.60
1:A:175:ASP:OD2	1:A:188:HIS:HA	2.02	0.60
1:B:37:ILE:HG22	1:B:98:MET:HE3	1.84	0.60
1:B:197:GLY:O	1:B:201:GLU:HB2	2.01	0.60
1:C:74:GLY:HA3	2:C:231:HOH:O	2.02	0.60
1:C:20:ARG:HE	1:C:70:ILE:HB	1.67	0.60
1:A:20:ARG:H	1:A:47:ASN:ND2	2.00	0.59
1:C:123:ALA:HB1	1:C:146:LEU:HD22	1.84	0.58
1:B:44:GLU:HG2	1:B:49:GLY:HA2	1.85	0.57
1:A:20:ARG:N	1:A:47:ASN:HD21	1.99	0.57
1:A:69:TRP:CZ3	1:A:109:CYS:SG	2.97	0.57
1:A:153:LEU:HD23	1:A:153:LEU:C	2.30	0.56
1:B:115:ILE:HG22	1:B:143:GLY:H	1.70	0.56
1:A:80:THR:HB	1:A:83:ASP:OD2	2.05	0.56
1:C:55:ILE:O	1:C:59:LEU:HG	2.05	0.56
1:A:31:CYS:HA	1:A:69:TRP:CZ2	2.41	0.56
1:A:199:ALA:HB3	1:A:200:PRO:HD3	1.88	0.56
1:A:74:GLY:O	1:A:97:GLU:HG2	2.06	0.55
1:A:106:ASN:C	1:A:106:ASN:HD22	2.14	0.55
1:B:38:TYR:HE2	1:B:48:LEU:O	1.89	0.55
1:B:43:THR:O	1:B:43:THR:HG22	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:99:LEU:HD12	1:B:99:LEU:H	1.71	0.55
1:C:88:ARG:NH1	1:C:95:ILE:HD13	2.21	0.55
1:A:59:LEU:HD21	1:A:115:ILE:CD1	2.36	0.55
1:B:34:VAL:HB	1:B:68:VAL:HG23	1.87	0.55
1:C:38:TYR:OH	1:C:119:TYR:HB3	2.07	0.55
1:B:176:LEU:HA	1:B:179:THR:CG2	2.37	0.55
1:C:89:GLY:HA3	1:C:124:ALA:HB1	1.88	0.55
1:A:24:ILE:HG22	1:A:25:ASN:OD1	2.07	0.54
1:A:106:ASN:C	1:A:106:ASN:ND2	2.65	0.54
1:C:33:ASP:HB3	1:C:211:ARG:HH21	1.72	0.54
1:A:168:LYS:HG3	1:A:170:PHE:CE1	2.43	0.54
1:B:21:ASP:HA	1:B:71:GLN:OE1	2.08	0.54
1:C:37:ILE:HG22	1:C:98:MET:HE3	1.90	0.54
1:C:76:ALA:HB1	1:C:93:ALA:HB1	1.89	0.54
1:C:78:ARG:HA	1:C:78:ARG:NH1	2.21	0.54
1:B:44:GLU:HG2	1:B:49:GLY:CA	2.38	0.54
1:C:88:ARG:HH11	1:C:95:ILE:HD13	1.74	0.53
1:C:106:ASN:ND2	1:C:140:LYS:HE3	2.24	0.53
1:A:158:ARG:HD2	1:A:164:ALA:HB2	1.90	0.53
1:B:28:SER:HB3	2:B:240:HOH:O	2.09	0.53
1:C:186:ALA:HB3	1:C:187:PRO:HD3	1.91	0.52
1:B:202:PHE:CE2	1:B:206:LYS:HE3	2.44	0.52
1:B:24:ILE:HD12	1:B:71:GLN:HE22	1.75	0.52
1:C:45:THR:HG23	2:C:280:HOH:O	2.08	0.52
1:C:149:TYR:HB3	1:C:152:ASN:HB2	1.90	0.52
1:A:158:ARG:NE	1:A:164:ALA:HB2	2.25	0.52
1:C:206:LYS:O	1:C:210:VAL:HG22	2.09	0.52
1:A:207:VAL:O	1:A:210:VAL:HG22	2.11	0.51
1:B:119:TYR:O	1:B:122:GLY:N	2.43	0.51
1:C:158:ARG:HH11	1:C:164:ALA:HB2	1.74	0.51
1:B:77:TYR:CE1	1:B:125:LEU:HD22	2.44	0.51
1:B:155:ASN:HB3	1:B:158:ARG:O	2.11	0.51
1:A:200:PRO:O	1:A:204:ILE:HG13	2.09	0.51
1:C:170:PHE:HZ	1:C:198:PRO:HB2	1.75	0.51
1:A:39:ALA:HB1	1:A:125:LEU:HD23	1.93	0.51
1:B:17:ARG:NH2	1:B:53:PRO:HB3	2.26	0.51
1:C:54:SER:HB3	1:C:196:GLU:HG2	1.92	0.51
1:A:37:ILE:HG22	1:A:98:MET:HE3	1.93	0.50
1:A:62:ALA:HB2	1:A:204:ILE:HD13	1.93	0.50
1:A:36:PHE:HA	1:A:115:ILE:O	2.11	0.50
1:A:40:ARG:HG2	2:A:223:HOH:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:152:ASN:ND2	1:B:157:GLY:HA2	2.26	0.50
1:A:38:TYR:HA	1:A:117:GLY:O	2.12	0.50
1:A:55:ILE:HD11	1:A:147:PHE:CZ	2.46	0.50
1:C:88:ARG:HH11	1:C:95:ILE:CD1	2.25	0.50
1:B:20:ARG:CG	1:B:48:LEU:HD11	2.40	0.50
1:B:171:CYS:HA	1:B:191:TYR:OH	2.12	0.50
1:A:88:ARG:HG2	1:A:88:ARG:NH1	2.19	0.50
1:C:88:ARG:NH1	1:C:128:ALA:HB1	2.26	0.50
1:B:210:VAL:HG13	2:B:270:HOH:O	2.12	0.49
1:C:162:TYR:CD1	1:C:163:PRO:HD2	2.47	0.49
1:A:19:THR:HA	1:A:47:ASN:HD22	1.75	0.49
1:A:77:TYR:HD1	1:A:94:ALA:HB1	1.77	0.49
1:C:192:GLY:N	1:C:193:PRO:CD	2.75	0.49
1:C:35:ILE:HB	1:C:114:LEU:HD22	1.93	0.49
1:B:47:ASN:ND2	1:B:72:GLY:HA3	2.25	0.49
1:B:106:ASN:C	1:B:106:ASN:HD22	2.19	0.49
1:A:59:LEU:HD21	1:A:115:ILE:HD12	1.94	0.49
1:C:59:LEU:HD21	1:C:203:LEU:HD12	1.95	0.49
1:A:168:LYS:HB2	1:A:202:PHE:CE2	2.48	0.48
1:B:113:THR:OG1	1:B:211:ARG:HD2	2.12	0.48
1:C:127:ALA:HA	1:C:159:ILE:HG23	1.93	0.48
1:A:28:SER:C	1:A:30:SER:H	2.21	0.48
1:A:31:CYS:HA	1:A:69:TRP:CH2	2.48	0.48
1:B:101:LEU:HD12	1:B:101:LEU:HA	1.70	0.48
1:B:202:PHE:O	1:B:206:LYS:HG2	2.13	0.48
1:A:175:ASP:OD1	1:A:177:VAL:HG22	2.13	0.48
1:B:145:VAL:HG12	1:B:168:LYS:HB3	1.95	0.48
1:B:65:LYS:HE3	2:B:235:HOH:O	2.13	0.48
1:B:174:GLY:O	1:B:187:PRO:HG3	2.13	0.48
1:C:199:ALA:HB3	1:C:200:PRO:CD	2.43	0.48
1:A:126:ALA:O	1:A:130:ILE:HG13	2.14	0.48
1:A:34:VAL:HG13	1:A:68:VAL:CG2	2.41	0.47
1:A:86:LEU:HB3	1:A:87:PRO:HD2	1.96	0.47
1:C:145:VAL:HG12	1:C:168:LYS:HB3	1.96	0.47
1:A:98:MET:HB3	1:A:129:SER:OG	2.15	0.47
1:A:194:ASP:HA	1:A:198:PRO:HG2	1.95	0.47
1:A:17:ARG:HA	1:A:17:ARG:HE	1.79	0.47
1:A:210:VAL:HG23	1:A:211:ARG:HG3	1.97	0.47
1:C:34:VAL:O	1:C:68:VAL:HA	2.15	0.47
1:C:39:ALA:HB1	1:C:125:LEU:HD23	1.97	0.47
1:B:39:ALA:O	1:B:122:GLY:HA3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:TYR:O	1:B:72:GLY:HA2	2.15	0.46
1:C:152:ASN:OD1	1:C:169:VAL:HG11	2.15	0.46
1:B:150:THR:HA	1:B:177:VAL:HG23	1.98	0.46
1:C:55:ILE:HD13	1:C:200:PRO:HD3	1.97	0.46
1:A:190:ALA:HA	2:A:269:HOH:O	2.16	0.46
1:A:23:LEU:HD11	1:A:105:ALA:HA	1.98	0.46
1:A:102:PHE:O	1:A:105:ALA:HB3	2.16	0.46
1:B:134:ASP:OD1	1:B:137:ILE:HG13	2.15	0.46
1:C:35:ILE:HG12	1:C:69:TRP:HB2	1.98	0.46
1:B:88:ARG:NH1	1:B:95:ILE:HD13	2.26	0.45
1:A:158:ARG:CD	1:A:164:ALA:HB2	2.45	0.45
1:B:202:PHE:CE1	1:B:206:LYS:HG3	2.51	0.45
1:A:36:PHE:CE2	1:A:38:TYR:HB2	2.52	0.45
1:B:62:ALA:HB2	1:B:204:ILE:HD13	1.98	0.45
1:B:99:LEU:O	1:B:103:GLN:HG3	2.17	0.45
1:A:99:LEU:HD21	1:A:132:ASP:CB	2.47	0.45
1:B:20:ARG:HG3	1:B:48:LEU:HD11	1.99	0.45
1:C:41:GLY:HA3	1:C:120:SER:HB2	1.99	0.45
1:C:174:GLY:HA3	1:C:187:PRO:HG2	1.99	0.45
1:B:24:ILE:C	1:B:26:GLY:H	2.25	0.45
1:C:103:GLN:HG2	1:C:103:GLN:H	1.65	0.44
1:A:156:ARG:O	1:A:156:ARG:HD3	2.17	0.44
1:B:208:ARG:HD2	2:B:250:HOH:O	2.16	0.44
1:C:170:PHE:CZ	1:C:198:PRO:HB2	2.52	0.44
1:A:23:LEU:HD21	1:A:101:LEU:O	2.17	0.44
1:A:37:ILE:HG22	1:A:98:MET:CE	2.47	0.44
1:C:96:ARG:NH1	1:C:96:ARG:CG	2.77	0.44
1:A:96:ARG:HD3	2:A:252:HOH:O	2.17	0.44
1:C:18:THR:O	1:C:48:LEU:HB2	2.18	0.44
1:C:28:SER:HA	1:C:31:CYS:SG	2.58	0.44
1:B:184:VAL:HG12	1:B:184:VAL:O	2.17	0.43
1:B:96:ARG:NE	2:B:262:HOH:O	2.49	0.43
1:C:20:ARG:H	1:C:47:ASN:ND2	2.14	0.43
1:B:93:ALA:HB2	2:B:304:HOH:O	2.17	0.43
1:A:102:PHE:CG	1:A:133:LEU:HD11	2.54	0.43
1:C:55:ILE:HD11	1:C:147:PHE:HZ	1.84	0.43
1:A:43:THR:HG22	1:A:43:THR:O	2.18	0.43
1:A:184:VAL:HG12	1:A:184:VAL:O	2.18	0.43
1:A:211:ARG:HG2	1:A:211:ARG:HH11	1.84	0.43
1:A:37:ILE:HA	1:A:71:GLN:O	2.18	0.43
1:C:172:LYS:HE3	1:C:190:ALA:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:THR:N	1:B:79:ALA:O	2.49	0.42
1:A:27:ASN:OD1	1:A:30:SER:HB2	2.19	0.42
1:A:211:ARG:HG2	1:A:211:ARG:NH1	2.34	0.42
1:B:36:PHE:HD2	1:B:70:ILE:HG23	1.84	0.42
1:B:99:LEU:N	1:B:99:LEU:CD1	2.81	0.42
1:B:173:THR:HG23	2:B:348:HOH:O	2.19	0.42
1:B:174:GLY:HA2	2:B:219:HOH:O	2.19	0.42
1:C:90:THR:OG1	1:C:91:SER:N	2.52	0.42
1:B:86:LEU:HB3	1:B:87:PRO:HD2	2.00	0.42
1:B:175:ASP:OD2	1:B:188:HIS:HA	2.20	0.42
1:B:187:PRO:O	1:B:190:ALA:HB3	2.20	0.42
1:B:146:LEU:HD13	1:B:149:TYR:CD1	2.54	0.42
1:C:24:ILE:CD1	1:C:101:LEU:HD11	2.48	0.42
1:C:186:ALA:HB2	2:C:258:HOH:O	2.19	0.42
1:A:194:ASP:HA	1:A:198:PRO:CG	2.50	0.41
1:B:100:GLY:O	1:B:104:GLN:HB2	2.19	0.41
1:C:118:GLY:O	1:C:123:ALA:HB2	2.20	0.41
1:A:99:LEU:HD11	1:A:129:SER:HA	2.02	0.41
1:A:146:LEU:HD11	1:A:159:ILE:HD11	2.03	0.41
1:B:43:THR:OG1	1:B:81:LEU:HD13	2.20	0.41
1:A:98:MET:C	1:A:100:GLY:N	2.74	0.41
1:A:77:TYR:CD1	1:A:94:ALA:HB1	2.56	0.41
1:A:77:TYR:CE1	1:A:125:LEU:HD22	2.56	0.41
1:A:95:ILE:O	1:A:99:LEU:HD12	2.21	0.41
1:B:151:LYS:HG3	2:B:248:HOH:O	2.21	0.41
1:B:152:ASN:HB3	1:B:178:CYS:O	2.21	0.41
1:A:44:GLU:HB3	1:A:49:GLY:HA2	2.02	0.40
1:B:165:ASP:OD1	1:B:166:ARG:HG3	2.21	0.40
1:A:36:PHE:HD2	1:A:70:ILE:HG23	1.87	0.40
1:A:192:GLY:N	1:A:193:PRO:HD3	2.37	0.40
1:B:62:ALA:CB	1:B:204:ILE:HD13	2.52	0.40
1:C:155:ASN:O	1:C:156:ARG:HG3	2.22	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	195/214 (91%)	170 (87%)	23 (12%)	2 (1%)	12	32
1	B	195/214 (91%)	169 (87%)	22 (11%)	4 (2%)	5	15
1	C	195/214 (91%)	173 (89%)	19 (10%)	3 (2%)	8	22
All	All	585/642 (91%)	512 (88%)	64 (11%)	9 (2%)	8	22

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	197	GLY
1	C	87	PRO
1	A	197	GLY
1	B	149	TYR
1	C	149	TYR
1	A	29	ALA
1	B	30	SER
1	B	40	ARG
1	C	211	ARG

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	146/159 (92%)	124 (85%)	22 (15%)	3	7
1	B	146/159 (92%)	125 (86%)	21 (14%)	3	8
1	C	146/159 (92%)	122 (84%)	24 (16%)	2	6
All	All	438/477 (92%)	371 (85%)	67 (15%)	3	7

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ARG
1	A	18	THR
1	A	34	VAL
1	A	47	ASN
1	A	59	LEU
1	A	61	SER
1	A	65	LYS
1	A	81	LEU
1	A	88	ARG
1	A	106	ASN
1	A	107	THR
1	A	114	LEU
1	A	120	SER
1	A	134	ASP
1	A	141	ILE
1	A	156	ARG
1	A	165	ASP
1	A	171	CYS
1	A	179	THR
1	A	181	SER
1	A	189	LEU
1	A	201	GLU
1	B	35	ILE
1	B	45	THR
1	B	70	ILE
1	B	87	PRO
1	B	101	LEU
1	B	104	GLN
1	B	114	LEU
1	B	115	ILE
1	B	131	GLU
1	B	135	SER
1	B	137	ILE
1	B	138	ARG
1	B	140	LYS
1	B	152	ASN
1	B	153	LEU
1	B	171	CYS
1	B	177	VAL
1	B	189	LEU
1	B	201	GLU
1	B	207	VAL
1	B	213	SER

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Mol	Chain	Res	Type
1	C	19	THR
1	C	20	ARG
1	C	24	ILE
1	C	47	ASN
1	C	51	LEU
1	C	55	ILE
1	C	78	ARG
1	C	87	PRO
1	C	98	MET
1	C	101	LEU
1	C	103	GLN
1	C	115	ILE
1	C	131	GLU
1	C	133	LEU
1	C	139	ASP
1	C	141	ILE
1	C	153	LEU
1	C	171	CYS
1	C	176	LEU
1	C	179	THR
1	C	184	VAL
1	C	189	LEU
1	C	194	ASP
1	C	211	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	ASN
1	A	84	ASN
1	A	103	GLN
1	A	121	GLN
1	B	121	GLN
1	B	152	ASN
1	C	47	ASN
1	C	106	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.