



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:00 AM UTC

PDB ID : 1BLP / pdb_00001blp
Title : STRUCTURAL BASIS FOR THE INACTIVATION OF THE P54 MUTANT
OF BETA-LACTAMASE FROM STAPHYLOCOCCUS AUREUS PC1
Authors : Herzberg, O.
Deposited on : 1993-09-23
Resolution : 2.30 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

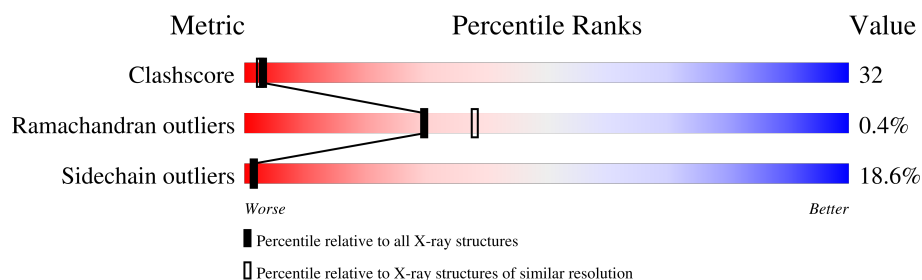
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)

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	257	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2108 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 BETA-LACTAMASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	253	Total	C	N	O	S	0	0	0
			1982	1264	334	381	3			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	179	ASN	ASP	engineered mutation	UNP P00807

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	126	Total	O	0	0
			126	126		

4 Data and refinement statistics

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

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	54.90Å 96.00Å 137.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.181 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2108	wwPDB-VP
Average B, all atoms (Å ²)	27.0	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	1.59	15/2010 (0.7%)	2.38	121/2697 (4.5%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	194	ILE	CA-CB	6.79	1.61	1.55
1	A	126	SER	CA-CB	6.68	1.63	1.53
1	A	79	ILE	C-O	6.64	1.31	1.24
1	A	133	THR	CA-CB	6.52	1.63	1.53
1	A	123	ILE	N-CA	6.44	1.54	1.46
1	A	177	LYS	CA-CB	-6.37	1.43	1.53
1	A	53	SER	C-O	6.23	1.32	1.24
1	A	220	LEU	CA-C	-5.93	1.50	1.53
1	A	125	ALA	C-O	5.86	1.30	1.24
1	A	259	ILE	C-O	5.76	1.30	1.24
1	A	132	ASN	C-O	5.71	1.30	1.24
1	A	49	LEU	N-CA	-5.37	1.40	1.46
1	A	119	LEU	N-CA	5.26	1.52	1.46
1	A	136	ASN	C-O	5.25	1.30	1.24
1	A	46	VAL	C-O	5.07	1.29	1.24

All (121) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	237	GLN	OE1-CD-NE2	11.86	134.46	122.60
1	A	177	LYS	N-CA-CB	11.54	128.61	110.73
1	A	264	PHE	CA-CB-CG	10.13	123.93	113.80
1	A	41	ASN	CA-CB-CG	-9.92	102.68	112.60
1	A	194	ILE	N-CA-C	9.01	119.95	111.48
1	A	245	ASN	CB-CG-ND2	8.93	129.79	116.40
1	A	233	ASP	CA-CB-CG	-8.61	103.99	112.60
1	A	82	GLU	CB-CG-CD	8.42	126.91	112.60
1	A	248	ALA	CA-C-O	8.13	130.15	121.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	234	LYS	N-CA-CB	8.13	123.58	110.90
1	A	261	LEU	CB-CA-C	8.10	124.36	109.70
1	A	132	ASN	CA-CB-CG	-8.04	104.56	112.60
1	A	262	VAL	O-C-N	7.88	131.38	123.18
1	A	35	ASP	O-C-N	7.77	131.31	122.22
1	A	137	LYS	N-CA-CB	7.69	121.54	110.16
1	A	84	VAL	O-C-N	7.60	129.76	121.10
1	A	279	ILE	O-C-N	7.52	129.72	121.90
1	A	262	VAL	CA-C-N	-7.49	112.58	122.99
1	A	262	VAL	C-N-CA	-7.49	112.58	122.99
1	A	220	LEU	N-CA-C	7.32	114.78	108.78
1	A	158	LYS	CA-CB-CG	7.19	128.49	114.10
1	A	104	ALA	CA-C-O	-7.14	113.73	121.44
1	A	268	ASP	CA-CB-CG	-7.07	105.53	112.60
1	A	98	ASN	N-CA-CB	7.02	121.58	111.05
1	A	141	GLU	O-C-N	6.89	130.28	122.22
1	A	214	ASN	CB-CA-C	6.87	121.69	110.22
1	A	177	LYS	O-C-N	6.83	130.38	122.25
1	A	124	GLU	CB-CG-CD	6.82	124.20	112.60
1	A	67	ALA	CA-C-O	-6.74	113.78	121.19
1	A	254	GLY	CA-C-N	6.73	132.49	121.58
1	A	254	GLY	C-N-CA	6.73	132.49	121.58
1	A	139	ILE	O-C-N	6.72	128.66	121.94
1	A	228	ASP	CA-CB-CG	-6.70	105.90	112.60
1	A	50	ASP	CA-CB-CG	-6.70	105.91	112.60
1	A	290	PHE	CB-CA-C	6.57	122.58	110.10
1	A	136	ASN	CA-C-O	-6.50	113.66	120.55
1	A	245	ASN	OD1-CG-ND2	-6.46	116.14	122.60
1	A	210	LEU	CD1-CG-CD2	-6.43	96.65	110.80
1	A	92	ASN	CA-C-O	-6.40	110.91	119.11
1	A	61	ASN	CA-CB-CG	-6.39	106.21	112.60
1	A	177	LYS	CA-CB-CG	6.36	126.83	114.10
1	A	122	LEU	CA-C-N	-6.27	112.66	120.56
1	A	122	LEU	C-N-CA	-6.27	112.66	120.56
1	A	237	GLN	CB-CA-C	-6.27	99.90	110.43
1	A	105	TYR	N-CA-CB	6.20	122.24	111.40
1	A	218	ASP	CA-CB-CG	-6.19	106.41	112.60
1	A	51	THR	OG1-CB-CG2	6.18	121.67	109.30
1	A	89	ASN	OD1-CG-ND2	-6.18	116.42	122.60
1	A	118	THR	CA-CB-OG1	-6.18	100.34	109.60
1	A	37	GLU	CG-CD-OE2	6.17	132.59	118.40
1	A	182	THR	O-C-N	6.13	126.56	121.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	116	ASP	N-CA-CB	6.11	120.53	110.69
1	A	151	ARG	NE-CZ-NH2	5.96	124.56	119.20
1	A	134	ALA	CA-C-O	-5.95	114.24	120.55
1	A	248	ALA	N-CA-C	5.94	117.81	108.96
1	A	136	ASN	CB-CG-ND2	5.93	125.30	116.40
1	A	46	VAL	N-CA-C	5.91	116.99	108.48
1	A	270	LYS	O-C-N	5.91	128.23	122.09
1	A	237	GLN	CA-C-O	-5.84	114.68	121.10
1	A	264	PHE	CA-C-O	-5.83	113.85	120.32
1	A	43	HIS	CA-CB-CG	-5.83	107.97	113.80
1	A	134	ALA	N-CA-CB	5.79	118.63	110.12
1	A	237	GLN	CA-CB-CG	-5.77	102.57	114.10
1	A	156	GLY	CA-C-O	5.72	124.67	118.95
1	A	35	ASP	CA-C-O	-5.71	113.64	120.10
1	A	102	ILE	N-CA-C	5.71	116.44	109.30
1	A	206	PHE	CA-C-O	5.71	127.35	121.07
1	A	134	ALA	O-C-N	5.70	128.16	122.12
1	A	71	THR	N-CA-C	-5.69	105.60	112.54
1	A	173	SER	O-C-N	5.67	127.85	121.32
1	A	145	ILE	CA-C-N	5.66	128.19	120.54
1	A	145	ILE	C-N-CA	5.66	128.19	120.54
1	A	76	ASN	CA-C-O	-5.62	114.59	120.55
1	A	161	ASN	CB-CA-C	5.61	117.63	110.34
1	A	96	HIS	CA-C-O	5.60	127.36	120.92
1	A	248	ALA	CA-C-N	5.60	131.06	123.11
1	A	248	ALA	C-N-CA	5.60	131.06	123.11
1	A	48	ALA	CA-C-N	5.59	130.55	122.44
1	A	48	ALA	C-N-CA	5.59	130.55	122.44
1	A	88	TYR	CA-C-N	5.59	131.38	120.99
1	A	88	TYR	C-N-CA	5.59	131.38	120.99
1	A	172	TYR	CA-C-O	5.59	127.41	120.54
1	A	230	LYS	O-C-N	5.55	129.84	123.29
1	A	278	LEU	O-C-N	5.55	128.00	122.12
1	A	226	PRO	CA-C-N	5.48	129.45	120.63
1	A	226	PRO	C-N-CA	5.48	129.45	120.63
1	A	245	ASN	CA-CB-CG	5.47	118.07	112.60
1	A	212	LEU	O-C-N	5.40	127.63	122.07
1	A	208	LEU	O-C-N	5.40	127.84	122.12
1	A	220	LEU	CA-C-O	5.39	121.07	117.94
1	A	122	LEU	CB-CA-C	-5.38	101.85	110.79
1	A	84	VAL	N-CA-CB	5.38	118.74	111.21
1	A	262	VAL	CA-C-O	-5.35	114.87	120.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	99	LYS	O-C-N	5.34	127.78	122.12
1	A	237	GLN	N-CA-CB	-5.30	103.50	111.56
1	A	276	ASP	N-CA-CB	5.29	119.32	110.32
1	A	177	LYS	N-CA-C	-5.27	106.08	112.88
1	A	49	LEU	O-C-N	5.27	129.99	123.14
1	A	150	GLN	CA-CB-CG	5.26	124.63	114.10
1	A	198	LYS	CG-CD-CE	5.25	123.38	111.30
1	A	65	ARG	NE-CZ-NH2	5.23	123.91	119.20
1	A	214	ASN	CA-CB-CG	5.22	117.82	112.60
1	A	163	VAL	CB-CA-C	5.21	118.73	110.81
1	A	42	ALA	O-C-N	5.20	129.51	122.96
1	A	181	SER	O-C-N	5.20	129.01	122.92
1	A	257	GLU	CG-CD-OE1	5.18	130.31	118.40
1	A	90	LYS	CA-CB-CG	-5.16	103.78	114.10
1	A	273	LYS	N-CA-CB	5.16	121.13	110.45
1	A	119	LEU	O-C-N	5.15	127.58	122.12
1	A	60	PHE	CB-CA-C	5.14	117.52	110.94
1	A	76	ASN	CA-CB-CG	5.13	117.73	112.60
1	A	76	ASN	CA-C-N	-5.11	113.44	120.28
1	A	76	ASN	C-N-CA	-5.11	113.44	120.28
1	A	135	ASN	O-C-N	5.07	127.29	122.07
1	A	187	GLY	O-C-N	5.05	127.03	122.18
1	A	198	LYS	CB-CG-CD	5.02	122.85	111.30
1	A	51	THR	CA-CB-OG1	-5.02	102.08	109.60
1	A	142	ILE	O-C-N	5.02	128.69	121.82
1	A	104	ALA	CA-C-N	5.02	130.40	122.78
1	A	104	ALA	C-N-CA	5.02	130.40	122.78
1	A	157	ASP	O-C-N	5.01	129.01	123.05

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	1982	0	2069	128	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	126	0	0	13	0
All	All	2108	0	2069	128	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 32.

All (128) 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:A:146:LYS:HD2	1:A:147:LYS:HG2	1.26	1.10
1:A:177:LYS:HB2	1:A:177:LYS:NZ	1.74	1.01
1:A:64:LYS:HB2	2:A:307:HOH:O	1.60	1.00
1:A:198:LYS:N	1:A:198:LYS:HE3	1.79	0.97
1:A:146:LYS:HD2	1:A:147:LYS:CG	1.95	0.96
1:A:68:TYR:OH	1:A:162:PRO:HA	1.65	0.95
1:A:110:GLU:HG3	1:A:111:LYS:HD2	1.57	0.87
1:A:169:LEU:N	2:A:416:HOH:O	2.10	0.84
1:A:198:LYS:HE3	1:A:198:LYS:H	1.40	0.84
1:A:177:LYS:HB2	1:A:177:LYS:HZ3	1.39	0.81
1:A:146:LYS:CD	1:A:147:LYS:HG2	2.10	0.81
1:A:89:ASN:ND2	1:A:90:LYS:HD2	1.96	0.80
1:A:222:LYS:HE3	1:A:231:VAL:O	1.82	0.79
1:A:105:TYR:CZ	1:A:107:PRO:HG3	2.19	0.77
1:A:201:LYS:CE	1:A:205:LYS:HD2	2.16	0.75
1:A:44:ILE:HD11	1:A:278:LEU:HD11	1.70	0.74
1:A:201:LYS:HE3	1:A:201:LYS:HA	1.72	0.72
1:A:229:TYR:HE2	1:A:287:MET:HE2	1.56	0.70
1:A:259:ILE:CD1	1:A:287:MET:HE1	2.21	0.70
1:A:229:TYR:CE2	1:A:287:MET:HE2	2.27	0.69
1:A:33:LEU:HD12	1:A:36:LEU:HD12	1.73	0.69
1:A:146:LYS:HG3	1:A:147:LYS:H	1.57	0.69
1:A:215:LYS:HE2	1:A:215:LYS:HA	1.73	0.69
1:A:64:LYS:HD3	1:A:66:PHE:CZ	2.30	0.67
1:A:257:GLU:OE1	2:A:292:HOH:O	2.13	0.66
1:A:92:ASN:ND2	2:A:345:HOH:O	2.27	0.66
1:A:87:PRO:HB2	1:A:89:ASN:OD1	1.96	0.65
1:A:189:THR:O	1:A:193:LEU:HB2	1.96	0.65
1:A:150:GLN:O	1:A:154:GLU:HG3	1.97	0.65
1:A:175:LYS:NZ	1:A:175:LYS:HA	2.12	0.64
1:A:198:LYS:N	1:A:198:LYS:CE	2.56	0.64
1:A:175:LYS:N	1:A:175:LYS:HD2	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:LYS:CE	1:A:231:VAL:O	2.46	0.63
1:A:207:LEU:HA	1:A:210:LEU:HD12	1.79	0.63
1:A:151:ARG:HH21	1:A:198:LYS:HD2	1.64	0.62
1:A:229:TYR:HE2	1:A:287:MET:CE	2.12	0.62
1:A:89:ASN:CG	1:A:90:LYS:HD2	2.25	0.61
1:A:87:PRO:HG2	1:A:90:LYS:NZ	2.16	0.60
1:A:82:GLU:OE2	2:A:293:HOH:O	2.16	0.59
1:A:155:LEU:O	1:A:192:LYS:HE3	2.02	0.59
1:A:259:ILE:HD12	1:A:287:MET:HE1	1.85	0.58
1:A:103:VAL:O	1:A:106:SER:OG	2.20	0.58
1:A:87:PRO:HG2	1:A:90:LYS:HZ2	1.69	0.57
1:A:126:SER:O	1:A:130:SER:HA	2.04	0.57
1:A:105:TYR:HB3	1:A:132:ASN:HD22	1.68	0.57
1:A:198:LYS:HE3	2:A:293:HOH:O	2.04	0.57
1:A:273:LYS:HE2	2:A:315:HOH:O	2.06	0.56
1:A:146:LYS:HG2	2:A:402:HOH:O	2.05	0.56
1:A:64:LYS:HD3	1:A:66:PHE:HZ	1.70	0.56
1:A:48:ALA:HA	1:A:260:VAL:O	2.06	0.56
1:A:136:ASN:O	1:A:140:LYS:HG2	2.05	0.56
1:A:201:LYS:HE3	1:A:205:LYS:HD2	1.86	0.56
1:A:99:LYS:HE2	1:A:99:LYS:O	2.05	0.56
1:A:197:GLY:C	1:A:198:LYS:HE3	2.30	0.55
1:A:151:ARG:NH2	1:A:198:LYS:HD2	2.22	0.54
1:A:175:LYS:HA	1:A:175:LYS:HZ3	1.71	0.54
1:A:89:ASN:HD21	1:A:90:LYS:HD2	1.70	0.54
1:A:192:LYS:NZ	2:A:387:HOH:O	2.39	0.54
1:A:201:LYS:O	1:A:205:LYS:HD3	2.09	0.53
1:A:201:LYS:HG3	1:A:205:LYS:HE2	1.90	0.53
1:A:209:ASP:OD2	2:A:412:HOH:O	2.18	0.52
1:A:120:LYS:O	1:A:124:GLU:HG3	2.09	0.52
1:A:219:THR:OG1	2:A:397:HOH:O	2.19	0.51
1:A:75:ILE:O	1:A:78:ALA:HB3	2.10	0.51
1:A:105:TYR:CE1	1:A:107:PRO:HG3	2.45	0.51
1:A:201:LYS:HG3	1:A:205:LYS:CD	2.40	0.50
1:A:285:SER:O	1:A:288:LYS:HB2	2.11	0.50
1:A:161:ASN:ND2	1:A:178:LYS:HA	2.27	0.50
1:A:81:LEU:HD21	1:A:123:ILE:HD13	1.93	0.50
1:A:237:GLN:HG3	1:A:244:ARG:HD2	1.93	0.49
1:A:201:LYS:HE2	1:A:205:LYS:HD2	1.91	0.48
1:A:169:LEU:CA	2:A:416:HOH:O	2.58	0.48
1:A:174:PRO:HD3	1:A:241:TYR:CE2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:LYS:CE	2:A:387:HOH:O	2.61	0.47
1:A:247:VAL:HG12	1:A:262:VAL:HG13	1.95	0.47
1:A:143:GLY:O	1:A:147:LYS:HG3	2.14	0.47
1:A:237:GLN:HG3	1:A:244:ARG:HH11	1.79	0.47
1:A:253:LYS:O	1:A:254:GLY:C	2.58	0.47
1:A:177:LYS:HB2	1:A:177:LYS:HZ2	1.71	0.46
1:A:172:TYR:O	1:A:240:THR:OG1	2.27	0.46
1:A:267:LYS:HD2	1:A:272:ASP:HB3	1.97	0.46
1:A:197:GLY:CA	1:A:198:LYS:HE3	2.45	0.46
1:A:173:SER:C	1:A:175:LYS:H	2.22	0.46
1:A:201:LYS:CG	1:A:205:LYS:HE2	2.46	0.46
1:A:209:ASP:OD1	1:A:213:ASN:ND2	2.50	0.45
1:A:153:LYS:O	1:A:158:LYS:NZ	2.43	0.45
1:A:215:LYS:HA	1:A:218:ASP:OD2	2.15	0.45
1:A:91:LEU:HB3	1:A:120:LYS:HB2	1.97	0.45
1:A:105:TYR:C	1:A:107:PRO:HD3	2.41	0.45
1:A:201:LYS:CE	1:A:201:LYS:HA	2.43	0.45
1:A:222:LYS:HG3	1:A:231:VAL:HG11	1.99	0.45
1:A:201:LYS:O	1:A:205:LYS:CD	2.65	0.45
1:A:64:LYS:HG2	1:A:66:PHE:CE1	2.52	0.45
1:A:215:LYS:HE2	1:A:215:LYS:CA	2.46	0.45
1:A:146:LYS:HD2	1:A:147:LYS:CD	2.47	0.44
1:A:84:VAL:O	1:A:203:ASN:ND2	2.49	0.44
1:A:222:LYS:HG3	1:A:231:VAL:CG1	2.48	0.44
1:A:68:TYR:HE1	1:A:72:SER:HB3	1.82	0.44
1:A:146:LYS:HG3	1:A:147:LYS:N	2.29	0.43
1:A:103:VAL:HG22	1:A:133:THR:CA	2.49	0.43
1:A:77:SER:O	1:A:81:LEU:HG	2.19	0.43
1:A:208:LEU:HA	1:A:208:LEU:HD23	1.73	0.43
1:A:60:PHE:CE1	1:A:61:ASN:ND2	2.87	0.43
1:A:251:TYR:HA	1:A:252:PRO:HD3	1.88	0.43
1:A:76:ASN:O	1:A:142:ILE:HD11	2.19	0.42
1:A:146:LYS:CG	1:A:147:LYS:H	2.30	0.42
1:A:99:LYS:HE2	1:A:99:LYS:CA	2.49	0.42
1:A:229:TYR:CD1	1:A:229:TYR:N	2.87	0.42
1:A:173:SER:C	1:A:175:LYS:N	2.76	0.42
1:A:192:LYS:O	1:A:197:GLY:HA2	2.20	0.42
1:A:103:VAL:HG22	1:A:133:THR:HA	2.01	0.42
1:A:259:ILE:HD13	1:A:287:MET:HE1	2.00	0.42
1:A:143:GLY:O	1:A:146:LYS:HE3	2.20	0.41
1:A:201:LYS:HE3	1:A:201:LYS:CA	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:ALA:O	1:A:56:GLU:HA	2.21	0.41
1:A:201:LYS:HG3	1:A:205:LYS:CE	2.50	0.41
1:A:223:ASP:OD2	1:A:277:LYS:NZ	2.52	0.41
1:A:44:ILE:HG22	1:A:46:VAL:HG23	2.02	0.41
1:A:61:ASN:O	1:A:64:LYS:HB3	2.20	0.41
1:A:67:ALA:HB2	1:A:172:TYR:CD1	2.56	0.41
1:A:181:SER:OG	1:A:182:THR:N	2.54	0.41
1:A:201:LYS:HD3	1:A:205:LYS:HE2	2.03	0.41
1:A:237:GLN:HG3	1:A:244:ARG:CD	2.51	0.41
1:A:92:ASN:HD22	1:A:92:ASN:N	2.19	0.40
1:A:225:VAL:HA	1:A:226:PRO:HD3	1.88	0.40
1:A:105:TYR:HB3	1:A:132:ASN:ND2	2.36	0.40
1:A:32:GLU:HG2	1:A:34:ASN:HD22	1.87	0.40
1:A:229:TYR:N	1:A:229:TYR:HD1	2.19	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	249/257 (97%)	241 (97%)	7 (3%)	1 (0%)	30	38

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	254	GLY

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	221/227 (97%)	180 (81%)	41 (19%)	1 1

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	LYS
1	A	32	GLU
1	A	33	LEU
1	A	38	LYS
1	A	59	LYS
1	A	64	LYS
1	A	73	LYS
1	A	83	GLN
1	A	84	VAL
1	A	90	LYS
1	A	92	ASN
1	A	93	LYS
1	A	95	VAL
1	A	99	LYS
1	A	111	LYS
1	A	115	LYS
1	A	137	LYS
1	A	140	LYS
1	A	142	ILE
1	A	146	LYS
1	A	147	LYS
1	A	149	LYS
1	A	158	LYS
1	A	169	LEU
1	A	175	LYS
1	A	177	LYS
1	A	193	LEU
1	A	198	LYS
1	A	201	LYS
1	A	204	LYS
1	A	205	LYS
1	A	210	LEU
1	A	214	ASN
1	A	215	LYS

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Mol	Chain	Res	Type
1	A	216	SER
1	A	227	LYS
1	A	239	ILE
1	A	253	LYS
1	A	273	LYS
1	A	277	LYS
1	A	284	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	ASN
1	A	76	ASN
1	A	92	ASN
1	A	132	ASN
1	A	150	GLN
1	A	161	ASN
1	A	245	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 oligosaccharides 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 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.