



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:09 AM UTC

PDB ID : 1HD8 / pdb_00001hd8
Title : Crystal structure of a deacylation-defective mutant of penicillin-binding protein 5 at 2.3 Å resolution
Authors : Davies, C.; White, S.W.; Nicholas, R.A.
Deposited on : 2000-11-11
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

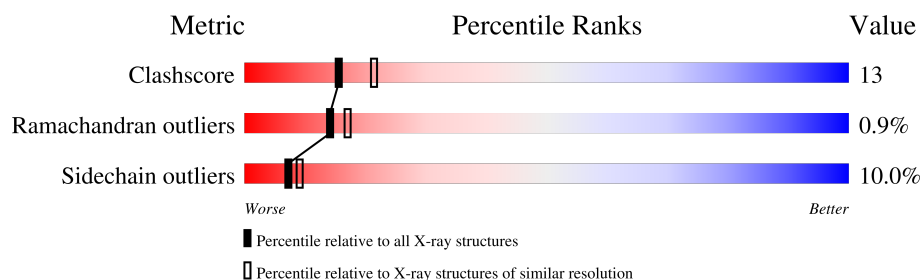
1 Overall quality at a glance

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	363	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2751 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 PENICILLIN-BINDING PROTEIN 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	337	2606	1641	453	500	12	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	105	ASP	GLY	engineered mutation	UNP P04287

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	145	Total	O	0	0
			145	145		

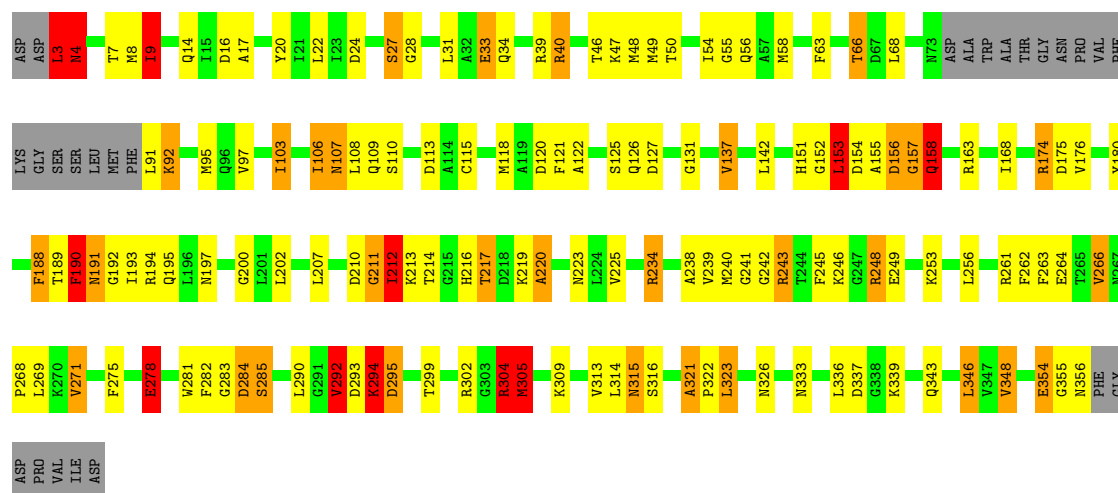
3 Residue-property plots

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: PENICILLIN-BINDING PROTEIN 5

Chain A: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	50.83Å 50.83Å 140.29Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	15.00 – 2.30	Depositor
% Data completeness (in resolution range)	95.4 (15.00-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.199 , 0.283	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2751	wwPDB-VP
Average B, all atoms (Å ²)	35.0	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	1.03	6/2649 (0.2%)	2.61	147/3575 (4.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	7

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	212	ILE	N-CA	-9.67	1.34	1.46
1	A	157	GLY	N-CA	-6.82	1.35	1.45
1	A	234	ARG	NE-CZ	-6.32	1.26	1.33
1	A	211	GLY	N-CA	-5.10	1.40	1.45
1	A	211	GLY	C-O	-5.06	1.18	1.23
1	A	211	GLY	C-N	-5.01	1.26	1.33

All (147) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	174	ARG	CD-NE-CZ	32.89	170.45	124.40
1	A	211	GLY	CA-C-N	31.54	178.74	121.97
1	A	211	GLY	C-N-CA	31.54	178.74	121.97
1	A	156	ASP	CA-C-N	19.41	159.44	121.41
1	A	156	ASP	C-N-CA	19.41	159.44	121.41
1	A	156	ASP	CA-C-O	18.24	142.64	122.03
1	A	284	ASP	CA-CB-CG	17.98	130.58	112.60
1	A	3	LEU	CA-C-N	17.18	154.36	121.54
1	A	3	LEU	C-N-CA	17.18	154.36	121.54
1	A	321	ALA	CA-C-O	-17.00	100.95	121.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	40	ARG	NE-CZ-NH2	16.73	134.26	119.20
1	A	4	ASN	CA-CB-CG	16.59	129.19	112.60
1	A	3	LEU	CA-C-O	16.31	148.53	120.80
1	A	156	ASP	CA-CB-CG	-14.28	98.32	112.60
1	A	234	ARG	NE-CZ-NH1	-12.94	108.56	121.50
1	A	155	ALA	N-CA-C	-12.68	97.50	111.07
1	A	154	ASP	CA-CB-CG	12.06	124.66	112.60
1	A	63	PHE	CA-CB-CG	11.56	125.36	113.80
1	A	40	ARG	NE-CZ-NH1	-11.53	109.97	121.50
1	A	321	ALA	O-C-N	11.43	134.68	121.31
1	A	4	ASN	OD1-CG-ND2	-11.21	111.39	122.60
1	A	156	ASP	O-C-N	-11.02	109.67	122.68
1	A	154	ASP	CA-C-O	10.83	133.50	120.62
1	A	157	GLY	CA-C-N	10.81	136.22	120.87
1	A	157	GLY	C-N-CA	10.81	136.22	120.87
1	A	234	ARG	NE-CZ-NH2	10.49	128.64	119.20
1	A	211	GLY	CA-C-O	10.44	131.73	121.60
1	A	293	ASP	CA-CB-CG	10.05	122.65	112.60
1	A	155	ALA	CA-C-O	-10.00	110.32	120.82
1	A	211	GLY	N-CA-C	9.47	126.08	110.55
1	A	261	ARG	NE-CZ-NH2	9.12	127.40	119.20
1	A	50	THR	CA-C-O	8.84	130.10	120.82
1	A	156	ASP	N-CA-C	8.82	121.72	110.33
1	A	158	GLN	OE1-CD-NE2	-8.74	113.86	122.60
1	A	3	LEU	CB-CA-C	8.63	126.49	110.10
1	A	337	ASP	CA-CB-CG	8.47	121.07	112.60
1	A	118	MET	CA-C-O	-8.24	111.10	120.24
1	A	121	PHE	CA-CB-CG	8.24	122.04	113.80
1	A	120	ASP	CA-C-O	-8.20	111.86	120.55
1	A	153	LEU	CA-C-O	8.14	129.17	120.55
1	A	322	PRO	N-CD-CG	7.91	113.30	103.80
1	A	225	VAL	N-CA-CB	7.62	121.50	111.90
1	A	292	VAL	N-CA-CB	-7.58	97.91	111.93
1	A	157	GLY	CA-C-O	7.50	133.62	120.57
1	A	248	ARG	CD-NE-CZ	7.47	134.86	124.40
1	A	248	ARG	CG-CD-NE	7.44	128.38	112.00
1	A	3	LEU	O-C-N	-7.44	111.10	123.00
1	A	243	ARG	NE-CZ-NH1	-7.43	114.07	121.50
1	A	49	MET	CA-C-O	7.35	128.43	119.97
1	A	127	ASP	CA-CB-CG	-7.35	105.25	112.60
1	A	9	ILE	CA-C-O	7.32	127.87	119.89
1	A	158	GLN	CG-CD-NE2	7.27	127.30	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	157	GLY	N-CA-C	7.17	130.18	113.18
1	A	262	PHE	N-CA-C	7.16	122.19	113.38
1	A	192	GLY	N-CA-C	-7.08	105.95	115.36
1	A	304	ARG	N-CA-C	7.05	121.60	112.92
1	A	241	GLY	CA-C-N	7.02	126.66	119.92
1	A	241	GLY	C-N-CA	7.02	126.66	119.92
1	A	154	ASP	N-CA-CB	7.00	121.08	109.60
1	A	305	MET	N-CA-CB	-6.98	99.89	110.01
1	A	322	PRO	N-CA-CB	6.87	110.16	102.60
1	A	248	ARG	NE-CZ-NH2	6.86	125.37	119.20
1	A	210	ASP	CA-C-O	6.84	126.13	119.08
1	A	256	LEU	CA-C-O	6.83	127.99	120.82
1	A	256	LEU	CA-C-N	6.82	129.30	120.44
1	A	256	LEU	C-N-CA	6.82	129.30	120.44
1	A	304	ARG	CA-C-N	6.81	129.29	120.44
1	A	304	ARG	C-N-CA	6.81	129.29	120.44
1	A	322	PRO	CA-N-CD	-6.81	101.97	111.50
1	A	304	ARG	CG-CD-NE	6.77	126.89	112.00
1	A	56	GLN	OE1-CD-NE2	-6.73	115.87	122.60
1	A	285	SER	N-CA-CB	6.71	122.86	111.66
1	A	126	GLN	CG-CD-OE1	6.61	134.01	120.80
1	A	174	ARG	CG-CD-NE	6.51	126.32	112.00
1	A	153	LEU	N-CA-C	6.48	118.34	111.28
1	A	191	ASN	N-CA-C	6.39	124.42	110.80
1	A	155	ALA	CA-C-N	-6.32	109.71	120.95
1	A	155	ALA	C-N-CA	-6.32	109.71	120.95
1	A	3	LEU	N-CA-CB	-6.31	99.78	110.50
1	A	126	GLN	OE1-CD-NE2	-6.29	116.31	122.60
1	A	326	ASN	OD1-CG-ND2	-6.27	116.33	122.60
1	A	315	ASN	CA-CB-CG	6.27	118.87	112.60
1	A	295	ASP	N-CA-C	6.22	119.02	110.24
1	A	220	ALA	N-CA-C	-6.22	105.52	113.23
1	A	294	LYS	CA-C-O	6.11	128.06	120.54
1	A	216	HIS	CA-C-N	6.08	132.82	122.37
1	A	216	HIS	C-N-CA	6.08	132.82	122.37
1	A	281	TRP	CA-C-N	6.04	131.16	122.40
1	A	281	TRP	C-N-CA	6.04	131.16	122.40
1	A	107	ASN	N-CA-C	6.03	117.66	111.14
1	A	175	ASP	N-CA-C	5.91	117.80	111.36
1	A	190	PHE	CB-CA-C	5.90	119.45	109.84
1	A	40	ARG	CD-NE-CZ	-5.89	116.15	124.40
1	A	234	ARG	CD-NE-CZ	5.86	132.60	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	190	PHE	O-C-N	-5.83	116.21	123.04
1	A	4	ASN	CB-CG-OD1	5.83	132.46	120.80
1	A	282	PHE	N-CA-C	5.83	119.70	112.24
1	A	155	ALA	N-CA-CB	5.80	118.42	110.01
1	A	7	THR	CA-C-N	5.79	128.93	120.71
1	A	7	THR	C-N-CA	5.79	128.93	120.71
1	A	151	HIS	CA-C-O	-5.78	112.78	118.97
1	A	33	GLU	CB-CG-CD	5.75	122.38	112.60
1	A	46	THR	CA-C-O	-5.75	113.76	120.20
1	A	242	GLY	N-CA-C	-5.75	104.64	111.36
1	A	92	LYS	CA-C-O	5.71	125.50	120.19
1	A	125	SER	CA-C-N	5.68	127.83	120.44
1	A	125	SER	C-N-CA	5.68	127.83	120.44
1	A	248	ARG	CB-CA-C	-5.65	101.94	110.92
1	A	122	ALA	CA-C-O	-5.64	113.12	120.00
1	A	191	ASN	CB-CA-C	-5.61	99.25	110.42
1	A	212	ILE	CA-CB-CG2	-5.59	101.00	110.50
1	A	239	VAL	CA-C-O	5.57	126.18	120.39
1	A	137	VAL	CA-C-O	-5.57	115.16	120.95
1	A	106	ILE	CA-C-N	5.56	128.01	120.44
1	A	106	ILE	C-N-CA	5.56	128.01	120.44
1	A	262	PHE	N-CA-CB	-5.55	102.26	110.53
1	A	243	ARG	CA-C-O	-5.51	112.83	119.27
1	A	188	PHE	CA-C-N	-5.50	115.30	123.11
1	A	188	PHE	C-N-CA	-5.50	115.30	123.11
1	A	256	LEU	O-C-N	-5.49	116.42	122.07
1	A	17	ALA	CA-C-O	-5.48	115.57	121.38
1	A	211	GLY	O-C-N	-5.43	117.09	123.55
1	A	174	ARG	NE-CZ-NH2	5.42	124.08	119.20
1	A	55	GLY	O-C-N	-5.36	117.04	122.18
1	A	39	ARG	NE-CZ-NH1	-5.26	116.24	121.50
1	A	157	GLY	O-C-N	-5.26	115.86	122.70
1	A	348	VAL	CB-CA-C	5.26	117.23	111.08
1	A	281	TRP	CA-C-O	5.24	127.46	121.28
1	A	49	MET	O-C-N	-5.22	115.84	122.27
1	A	176	VAL	CA-C-N	5.21	125.01	119.28
1	A	176	VAL	C-N-CA	5.21	125.01	119.28
1	A	248	ARG	CA-CB-CG	5.21	124.52	114.10
1	A	66	THR	CB-CA-C	5.13	120.17	109.95
1	A	202	LEU	CA-C-O	-5.13	115.11	120.55
1	A	304	ARG	O-C-N	-5.13	116.19	122.34
1	A	354	GLU	CB-CA-C	5.13	118.42	109.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	278	GLU	CA-CB-CG	5.12	124.34	114.10
1	A	131	GLY	CA-C-N	5.12	127.56	120.29
1	A	131	GLY	C-N-CA	5.12	127.56	120.29
1	A	292	VAL	CA-CB-CG1	5.10	119.07	110.40
1	A	197	ASN	OD1-CG-ND2	-5.07	117.53	122.60
1	A	282	PHE	CA-C-O	-5.07	114.52	120.81
1	A	243	ARG	NH1-CZ-NH2	5.06	125.88	119.30
1	A	28	GLY	N-CA-C	-5.04	108.30	115.30
1	A	153	LEU	CB-CA-C	-5.03	102.43	110.79
1	A	103	ILE	CA-C-O	-5.02	114.83	120.25
1	A	197	ASN	CA-C-O	-5.00	115.56	121.16

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	153	LEU	Mainchain
1	A	180	TYR	Mainchain
1	A	211	GLY	Peptide
1	A	27	SER	Mainchain
1	A	315	ASN	Mainchain
1	A	321	ALA	Peptide,Mainchain

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	2606	0	2605	70	0
2	A	145	0	0	6	0
All	All	2751	0	2605	70	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 13.

All (70) 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:294:LYS:HA	1:A:294:LYS:HE2	1.60	0.80
1:A:207:LEU:HD11	1:A:253:LYS:HG3	1.65	0.77
1:A:217:THR:HG22	1:A:220:ALA:H	1.48	0.77
1:A:58:MET:HE3	2:A:2080:HOH:O	1.87	0.74
1:A:58:MET:HE1	1:A:103:ILE:HD13	1.72	0.72
1:A:245:PHE:O	1:A:248:ARG:HG3	1.90	0.71
1:A:278:GLU:HG2	1:A:314:LEU:HD11	1.75	0.68
1:A:234:ARG:NH1	2:A:2101:HOH:O	2.28	0.65
1:A:200:GLY:HA3	1:A:249:GLU:OE2	1.98	0.64
1:A:354:GLU:HG3	1:A:356:ASN:O	1.99	0.62
1:A:14:GLN:NE2	1:A:14:GLN:HA	2.14	0.62
1:A:189:THR:HG22	1:A:194:ARG:HG3	1.84	0.59
1:A:266:VAL:HG11	1:A:305:MET:HG2	1.86	0.58
1:A:109:GLN:NE2	1:A:195:GLN:HB3	2.19	0.57
1:A:217:THR:HG22	1:A:220:ALA:N	2.18	0.57
1:A:3:LEU:N	1:A:4:ASN:OD1	2.37	0.56
1:A:213:LYS:HE2	2:A:2082:HOH:O	2.04	0.56
1:A:47:LYS:HE2	1:A:110:SER:O	2.05	0.56
1:A:40:ARG:NH1	1:A:40:ARG:HB3	2.21	0.56
1:A:109:GLN:HE22	1:A:195:GLN:HB3	1.70	0.56
1:A:223:ASN:HD22	1:A:240:MET:HG2	1.72	0.56
1:A:40:ARG:NH1	2:A:2029:HOH:O	2.28	0.55
1:A:31:LEU:HD21	1:A:299:THR:HG21	1.89	0.54
1:A:92:LYS:O	1:A:95:MET:HG2	2.07	0.54
1:A:292:VAL:HG13	1:A:294:LYS:O	2.11	0.50
1:A:290:LEU:HD13	1:A:346:LEU:HD13	1.93	0.50
1:A:20:TYR:HA	1:A:238:ALA:O	2.12	0.50
1:A:20:TYR:CE2	1:A:34:GLN:HB3	2.48	0.49
1:A:58:MET:HE1	1:A:103:ILE:CD1	2.42	0.48
1:A:264:GLU:HG2	1:A:302:ARG:HA	1.94	0.48
1:A:219:LYS:O	1:A:219:LYS:HG2	2.14	0.48
1:A:54:ILE:HG22	1:A:58:MET:HE2	1.95	0.47
1:A:108:LEU:HD22	1:A:188:PHE:CD1	2.49	0.47
1:A:158:GLN:O	1:A:158:GLN:HG2	2.12	0.47
1:A:14:GLN:HA	1:A:14:GLN:HE21	1.78	0.47
1:A:304:ARG:HH11	1:A:304:ARG:HG2	1.79	0.47
1:A:8:MET:HG2	1:A:9:ILE:N	2.28	0.46
1:A:33:GLU:HG2	2:A:2020:HOH:O	2.14	0.46
1:A:304:ARG:HH11	1:A:304:ARG:CG	2.28	0.46
1:A:16:ASP:OD1	1:A:243:ARG:NH1	2.44	0.46
1:A:290:LEU:HD13	1:A:346:LEU:CD1	2.46	0.46
1:A:107:ASN:O	1:A:213:LYS:NZ	2.42	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:ARG:HD3	2:A:2069:HOH:O	2.16	0.46
1:A:152:GLY:HA2	1:A:158:GLN:OE1	2.16	0.45
1:A:40:ARG:CB	1:A:40:ARG:HH11	2.30	0.45
1:A:54:ILE:CG2	1:A:58:MET:HE2	2.46	0.45
1:A:48:MET:HE2	1:A:168:ILE:HG22	1.98	0.45
1:A:271:VAL:HG22	1:A:295:ASP:OD1	2.15	0.45
1:A:48:MET:HG3	1:A:213:LYS:HG3	1.98	0.45
1:A:283:GLY:HA2	1:A:355:GLY:H	1.81	0.45
1:A:266:VAL:HG23	1:A:268:PRO:HD3	1.99	0.44
1:A:189:THR:HG22	1:A:194:ARG:CG	2.46	0.44
1:A:24:ASP:HB3	1:A:27:SER:OG	2.18	0.44
1:A:106:ILE:HD11	1:A:115:CYS:HA	1.99	0.44
1:A:269:LEU:HD21	1:A:275:PHE:HB2	1.99	0.44
1:A:137:VAL:HG13	1:A:142:LEU:HB2	2.00	0.43
1:A:294:LYS:HD3	1:A:295:ASP:N	2.33	0.43
1:A:48:MET:HE3	1:A:212:ILE:HG21	2.01	0.42
1:A:40:ARG:HB3	1:A:40:ARG:HH11	1.82	0.42
1:A:153:LEU:HD23	1:A:153:LEU:HA	1.80	0.42
1:A:294:LYS:CE	1:A:295:ASP:H	2.33	0.42
1:A:91:LEU:HD23	1:A:113:ASP:HB3	2.02	0.42
1:A:190:PHE:O	1:A:193:ILE:N	2.45	0.42
1:A:323:LEU:HG	1:A:348:VAL:HG21	2.01	0.42
1:A:336:LEU:O	1:A:339:LYS:HB2	2.21	0.41
1:A:294:LYS:HD3	1:A:295:ASP:H	1.84	0.41
1:A:309:LYS:HE3	1:A:309:LYS:HB2	1.90	0.41
1:A:333:ASN:OD1	1:A:343:GLN:HG2	2.20	0.41
1:A:91:LEU:HD11	1:A:97:VAL:HG21	2.03	0.41
1:A:263:PHE:O	1:A:302:ARG:NH2	2.53	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	333/363 (92%)	321 (96%)	9 (3%)	3 (1%)	14 17

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	ASN
1	A	157	GLY
1	A	212	ILE

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	281/302 (93%)	253 (90%)	28 (10%)	7 9

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	A	4	ASN
1	A	9	ILE
1	A	22	LEU
1	A	66	THR
1	A	68	LEU
1	A	156	ASP
1	A	158	GLN
1	A	174	ARG
1	A	190	PHE
1	A	191	ASN
1	A	212	ILE
1	A	214	THR
1	A	217	THR
1	A	246	LYS
1	A	266	VAL
1	A	271	VAL
1	A	278	GLU

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Mol	Chain	Res	Type
1	A	284	ASP
1	A	285	SER
1	A	292	VAL
1	A	294	LYS
1	A	304	ARG
1	A	305	MET
1	A	313	VAL
1	A	316	SER
1	A	323	LEU
1	A	346	LEU

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	4	ASN
1	A	14	GLN
1	A	101	GLN
1	A	109	GLN
1	A	151	HIS
1	A	223	ASN
1	A	232	GLN
1	A	343	GLN

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 [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.