



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:14 PM UTC

PDB ID : 2OQC / pdb_00002oqc
Title : Crystal Structure of Penicillin V acylase from *Bacillus subtilis*
Authors : Suresh, C.G.; Rathinaswamy, P.; Pundle, A.V.; Prabhune, A.A.; Sivaraman, H.; Brannigan, J.A.; Dodson, G.G.
Deposited on : 2007-01-31
Resolution : 2.50 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)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

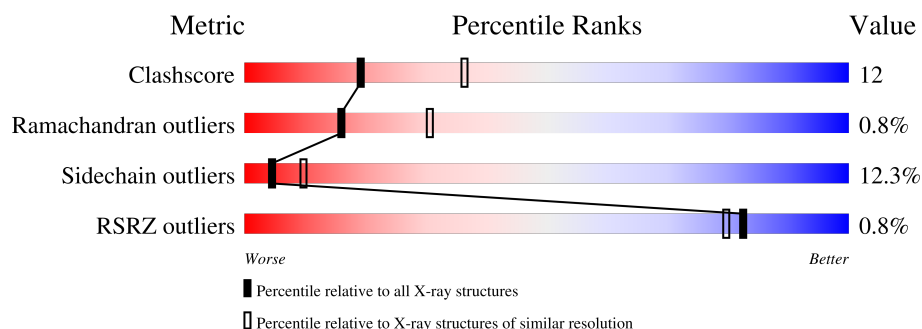
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	327	64% 24% 9% . .
1	B	327	65% 26% 5% . .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5502 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 V acylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	317	Total	C	N	O	S	0	0	0
			2541	1616	431	484	10			
1	B	317	Total	C	N	O	S	0	0	0
			2541	1616	431	484	10			

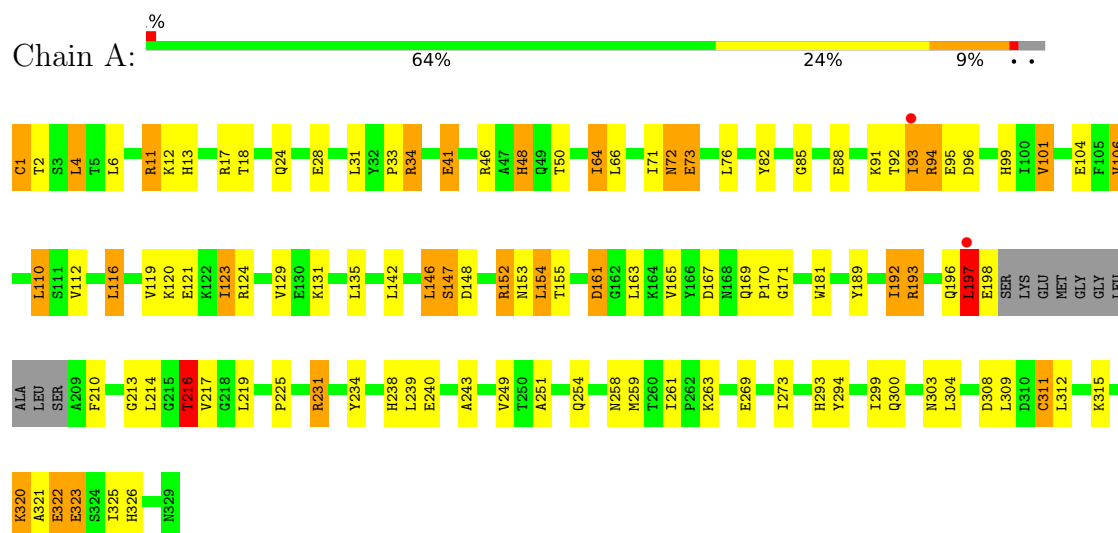
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	212	Total	O	0	0
			212	212		
2	B	208	Total	O	0	0
			208	208		

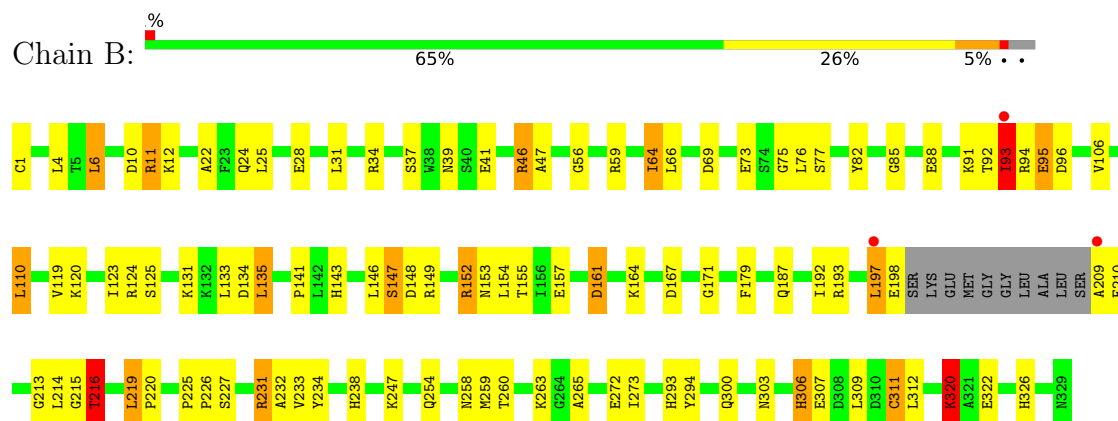
3 Residue-property plots

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

• Molecule 1: Penicillin V acylase



• Molecule 1: Penicillin V acylase



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	110.96Å 307.96Å 56.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50 20.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.7 (20.00-2.50) 93.3 (20.00-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	138.74 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.155 , 0.218 0.155 , (Not available)	Depositor DCC
R_{free} test set	1705 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	37.5	Xtriage
Anisotropy	0.104	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 39.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5502	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.18% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	1.75	29/2601 (1.1%)	1.50	27/3532 (0.8%)
1	B	1.66	13/2601 (0.5%)	1.39	13/3532 (0.4%)
All	All	1.71	42/5202 (0.8%)	1.45	40/7064 (0.6%)

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	3
1	B	0	1
All	All	0	4

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	41	GLU	C-N	18.10	1.56	1.33
1	A	41	GLU	C-N	16.85	1.55	1.33
1	A	64	ILE	C-N	15.34	1.54	1.33
1	B	64	ILE	C-N	11.47	1.50	1.33
1	A	210	PHE	C-O	7.67	1.33	1.24
1	B	119	VAL	CA-CB	7.65	1.64	1.54
1	A	243	ALA	CA-CB	6.88	1.64	1.53
1	A	46	ARG	CD-NE	6.45	1.55	1.46
1	B	187	GLN	CB-CG	6.44	1.71	1.52
1	A	142	LEU	CA-C	-6.38	1.44	1.52
1	A	46	ARG	NE-CZ	6.21	1.39	1.33
1	B	141	PRO	CA-C	6.20	1.58	1.52
1	A	311	CYS	CA-C	6.17	1.61	1.52
1	B	179	PHE	CA-C	6.15	1.60	1.52
1	A	273	ILE	N-CA	-6.10	1.38	1.46
1	A	119	VAL	CA-CB	6.09	1.61	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	106	VAL	CA-CB	6.07	1.61	1.54
1	A	13	HIS	C-O	5.83	1.31	1.23
1	B	232	ALA	N-CA	5.79	1.53	1.46
1	B	320	LYS	CG-CD	5.70	1.69	1.52
1	A	116	LEU	C-O	-5.67	1.17	1.24
1	B	210	PHE	C-O	5.53	1.31	1.24
1	A	28	GLU	CD-OE2	5.52	1.35	1.25
1	A	249	VAL	C-O	5.50	1.30	1.24
1	A	165	VAL	C-O	-5.44	1.18	1.24
1	A	147	SER	CB-OG	-5.44	1.31	1.42
1	A	323	GLU	N-CA	-5.41	1.39	1.46
1	A	217	VAL	CA-CB	5.37	1.59	1.54
1	A	193	ARG	C-O	-5.37	1.17	1.24
1	A	148	ASP	C-O	-5.33	1.18	1.23
1	A	33	PRO	CA-C	5.32	1.58	1.52
1	A	50	THR	CA-C	5.26	1.59	1.52
1	A	48	HIS	CA-C	-5.24	1.46	1.52
1	B	187	GLN	CG-CD	5.20	1.65	1.52
1	A	299	ILE	CB-CG2	5.19	1.69	1.52
1	A	192	ILE	CA-C	5.11	1.58	1.52
1	A	101	VAL	CA-C	5.09	1.58	1.52
1	B	215	GLY	C-O	-5.08	1.18	1.24
1	B	265	ALA	CA-CB	5.06	1.61	1.53
1	B	260	THR	CA-CB	5.03	1.60	1.53
1	A	72	ASN	N-CA	5.03	1.51	1.45
1	A	269	GLU	CG-CD	5.03	1.64	1.52

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	64	ILE	O-C-N	-18.62	100.84	122.62
1	A	64	ILE	CA-C-N	12.72	138.76	120.95
1	A	64	ILE	C-N-CA	12.72	138.76	120.95
1	B	41	GLU	N-CA-C	-7.62	103.95	113.18
1	A	225	PRO	N-CA-C	7.26	119.56	110.70
1	A	231	ARG	N-CA-C	-6.89	103.21	111.69
1	A	34	ARG	NE-CZ-NH2	-6.68	113.19	119.20
1	B	41	GLU	O-C-N	-6.59	112.80	122.43
1	A	41	GLU	N-CA-C	-6.49	104.62	112.54
1	A	46	ARG	NE-CZ-NH1	6.27	127.77	121.50
1	A	161	ASP	N-CA-C	6.25	120.40	113.21
1	A	322	GLU	CB-CA-C	-6.25	99.48	109.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	261	ILE	N-CA-C	6.04	113.06	107.56
1	A	64	ILE	CB-CA-C	-5.82	104.37	111.88
1	A	321	ALA	N-CA-C	5.80	119.54	112.23
1	A	85	GLY	N-CA-C	-5.77	108.21	115.08
1	A	325	ILE	N-CA-C	5.76	116.40	107.99
1	B	12	LYS	CD-CE-NZ	-5.76	93.47	111.90
1	B	147	SER	N-CA-CB	-5.74	101.35	111.39
1	A	181	TRP	CA-C-N	5.69	127.84	120.44
1	A	181	TRP	C-N-CA	5.69	127.84	120.44
1	A	146	LEU	CA-CB-CG	5.67	136.13	116.30
1	B	231	ARG	N-CA-C	-5.51	105.35	111.36
1	B	233	VAL	N-CA-C	-5.45	105.40	110.53
1	B	133	LEU	N-CA-C	-5.45	98.35	107.99
1	A	193	ARG	CA-C-N	5.38	125.19	119.28
1	A	193	ARG	C-N-CA	5.38	125.19	119.28
1	A	251	ALA	N-CA-C	-5.35	105.36	111.14
1	A	34	ARG	CD-NE-CZ	5.33	131.86	124.40
1	B	216	THR	N-CA-CB	-5.32	102.11	110.46
1	B	120	LYS	N-CA-C	-5.30	106.08	112.54
1	B	306	HIS	N-CA-C	-5.28	106.82	113.20
1	A	216	THR	N-CA-CB	-5.22	102.26	110.46
1	B	93	ILE	CB-CA-C	5.20	117.02	111.35
1	A	34	ARG	CG-CD-NE	-5.13	100.72	112.00
1	A	119	VAL	N-CA-C	5.09	115.23	110.30
1	A	73	GLU	CA-C-N	-5.05	114.56	122.49
1	A	73	GLU	C-N-CA	-5.05	114.56	122.49
1	B	73	GLU	CA-C-N	-5.04	114.58	122.49
1	B	73	GLU	C-N-CA	-5.04	114.58	122.49

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	196	GLN	Peptide
1	A	41	GLU	Mainchain
1	A	64	ILE	Mainchain
1	B	64	ILE	Mainchain

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	2541	0	2477	57	0
1	B	2541	0	2477	60	4
2	A	212	0	0	17	3
2	B	208	0	0	16	12
All	All	5502	0	4954	117	13

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 12.

All (117) 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:231:ARG:HH11	1:B:258:ASN:HB3	1.15	1.06
1:B:167:ASP:HB3	2:B:496:HOH:O	1.59	1.02
1:A:231:ARG:HH11	1:A:258:ASN:HB3	1.28	0.97
1:A:11:ARG:HG2	1:A:11:ARG:HH11	1.31	0.95
1:B:231:ARG:NH1	1:B:258:ASN:HB3	1.88	0.89
1:A:124:ARG:HD2	2:A:345:HOH:O	1.80	0.81
1:A:300:GLN:HE22	1:A:320:LYS:H	1.35	0.74
1:B:197:LEU:HD22	2:B:531:HOH:O	1.87	0.74
1:A:315:LYS:HE3	2:A:425:HOH:O	1.86	0.73
1:B:303:ASN:HB3	2:B:345:HOH:O	1.88	0.73
1:A:231:ARG:HD3	1:A:259:MET:HE3	1.70	0.72
1:B:24:GLN:HG2	2:B:513:HOH:O	1.88	0.72
1:B:92:THR:HG23	2:B:404:HOH:O	1.88	0.72
1:B:300:GLN:HE22	1:B:320:LYS:H	1.38	0.71
1:B:152:ARG:HH11	1:B:152:ARG:HG3	1.55	0.70
1:A:11:ARG:HG2	1:A:11:ARG:NH1	2.03	0.70
1:A:116:LEU:HD22	1:A:154:LEU:HD22	1.74	0.69
1:A:231:ARG:NH1	1:A:258:ASN:OD1	2.25	0.69
1:B:326:HIS:HD2	2:B:435:HOH:O	1.76	0.69
1:B:46:ARG:HG2	1:B:46:ARG:HH11	1.56	0.68
1:A:231:ARG:NH1	1:A:258:ASN:HB3	2.05	0.68
1:B:213:GLY:O	1:B:216:THR:HB	1.96	0.65
1:A:167:ASP:HB3	2:A:403:HOH:O	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:231:ARG:HH11	1:B:258:ASN:CB	2.02	0.65
1:A:152:ARG:HD3	2:A:485:HOH:O	1.96	0.65
1:A:193:ARG:HH21	1:A:197:LEU:H	1.44	0.64
1:A:326:HIS:HD2	2:A:434:HOH:O	1.81	0.63
1:A:93:ILE:HD12	1:A:94:ARG:O	1.99	0.62
1:B:231:ARG:NH1	1:B:258:ASN:OD1	2.31	0.62
1:B:193:ARG:NH2	2:B:531:HOH:O	2.32	0.61
1:A:34:ARG:HD3	1:A:73:GLU:OE2	2.01	0.60
1:A:24:GLN:HG2	2:A:512:HOH:O	2.01	0.60
1:B:231:ARG:NH1	1:B:258:ASN:CB	2.61	0.60
1:B:46:ARG:HH11	1:B:46:ARG:CG	2.13	0.59
1:B:34:ARG:HG2	1:B:309:LEU:O	2.03	0.59
1:A:152:ARG:HH11	1:A:152:ARG:HG3	1.68	0.58
1:B:10:ASP:O	1:B:11:ARG:HB2	2.03	0.58
1:B:293:HIS:HD2	2:B:400:HOH:O	1.86	0.58
1:B:209:ALA:N	2:B:418:HOH:O	2.37	0.57
1:B:106:VAL:HG13	1:B:110:LEU:HD22	1.87	0.56
1:B:124:ARG:HD2	2:B:349:HOH:O	2.05	0.56
1:A:293:HIS:HD2	2:A:398:HOH:O	1.87	0.56
1:B:39:ASN:ND2	1:B:47:ALA:HA	2.20	0.56
1:B:220:PRO:HB2	1:B:227:SER:HB3	1.87	0.56
1:A:239:LEU:HG	1:A:240:GLU:O	2.06	0.55
1:A:11:ARG:HD3	2:A:435:HOH:O	2.07	0.55
1:A:231:ARG:CD	1:A:259:MET:HE3	2.36	0.55
1:A:131:LYS:CD	2:A:458:HOH:O	2.55	0.55
1:B:152:ARG:HG3	1:B:152:ARG:NH1	2.21	0.54
1:A:34:ARG:HG2	1:A:309:LEU:O	2.08	0.54
1:A:293:HIS:CD2	2:A:398:HOH:O	2.61	0.54
1:A:123:ILE:CD1	1:A:163:LEU:HD13	2.37	0.53
1:A:231:ARG:HH11	1:A:258:ASN:CB	2.11	0.53
1:B:11:ARG:HD3	2:B:436:HOH:O	2.07	0.53
1:A:213:GLY:O	1:A:216:THR:HB	2.09	0.53
1:A:263:LYS:HG3	1:A:294:TYR:CZ	2.44	0.53
1:A:169:GLN:HB2	1:A:170:PRO:HD3	1.91	0.52
1:A:123:ILE:HD11	1:A:163:LEU:HD13	1.92	0.52
1:A:293:HIS:HE1	1:A:320:LYS:O	1.92	0.52
1:A:95:GLU:O	1:A:96:ASP:HB2	2.10	0.51
1:A:234:TYR:O	1:A:238:HIS:HD2	1.92	0.51
1:B:149:ARG:CZ	2:B:366:HOH:O	2.58	0.51
1:A:99:HIS:HD2	2:A:423:HOH:O	1.95	0.50
1:B:254:GLN:HA	1:B:254:GLN:OE1	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:293:HIS:HE1	1:B:320:LYS:O	1.95	0.49
1:B:11:ARG:HG2	1:B:11:ARG:HH11	1.76	0.49
1:A:48:HIS:HD2	2:A:373:HOH:O	1.95	0.49
1:B:25:LEU:O	1:B:59:ARG:HD2	2.12	0.49
1:B:234:TYR:O	1:B:238:HIS:HD2	1.96	0.48
1:A:153:ASN:HD22	1:A:171:GLY:HA2	1.78	0.48
1:A:231:ARG:HB3	1:A:259:MET:HE2	1.94	0.48
1:A:91:LYS:HG2	2:A:499:HOH:O	2.12	0.48
1:B:77:SER:HB3	1:B:147:SER:HB3	1.96	0.47
1:A:197:LEU:HD12	1:A:197:LEU:HA	1.57	0.47
1:B:161:ASP:HB3	1:B:164:LYS:HE2	1.96	0.47
1:B:143:HIS:HB2	1:B:157:GLU:HG2	1.98	0.46
1:A:153:ASN:ND2	2:A:466:HOH:O	2.49	0.46
1:B:231:ARG:HB3	1:B:259:MET:HE3	1.98	0.46
1:A:197:LEU:HD22	2:A:531:HOH:O	2.15	0.46
1:B:293:HIS:CD2	2:B:400:HOH:O	2.64	0.46
1:B:326:HIS:CD2	2:B:435:HOH:O	2.60	0.46
1:A:1:CYS:HB3	1:A:18:THR:O	2.16	0.45
1:A:120:LYS:HE2	1:A:154:LEU:HD11	1.98	0.45
1:B:46:ARG:HG2	1:B:46:ARG:NH1	2.29	0.45
1:B:93:ILE:O	1:B:93:ILE:HG13	2.16	0.45
1:A:231:ARG:NH1	1:A:258:ASN:CB	2.74	0.45
1:B:263:LYS:HG3	1:B:294:TYR:CZ	2.52	0.45
1:B:161:ASP:HB3	1:B:164:LYS:CE	2.47	0.44
1:A:189:TYR:HB3	1:A:192:ILE:HD12	2.00	0.44
1:A:254:GLN:HA	1:A:254:GLN:OE1	2.17	0.44
1:B:95:GLU:O	1:B:96:ASP:HB2	2.18	0.44
1:A:300:GLN:HE22	1:A:320:LYS:N	2.10	0.44
1:B:106:VAL:CG1	1:B:110:LEU:HD22	2.47	0.44
1:A:2:THR:O	1:A:17:ARG:HA	2.18	0.43
1:B:192:ILE:HG22	1:B:234:TYR:CE2	2.53	0.43
1:A:106:VAL:HG13	1:A:110:LEU:HD22	2.01	0.43
1:A:167:ASP:HB3	2:A:496:HOH:O	2.18	0.42
1:B:153:ASN:HD22	1:B:171:GLY:HA2	1.84	0.42
1:A:12:LYS:HE2	2:A:464:HOH:O	2.19	0.42
1:A:72:ASN:OD1	1:A:72:ASN:C	2.63	0.42
1:B:4:LEU:CD1	1:B:6:LEU:HD13	2.50	0.41
1:B:24:GLN:CG	2:B:513:HOH:O	2.59	0.41
1:A:303:ASN:O	1:A:304:LEU:C	2.63	0.41
1:B:22:ALA:HB1	1:B:272:GLU:HB3	2.02	0.41
1:B:209:ALA:HB1	2:B:476:HOH:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:GLY:HA3	1:B:69:ASP:O	2.20	0.41
1:A:308:ASP:O	1:A:311:CYS:HB2	2.21	0.41
1:B:11:ARG:HG2	1:B:11:ARG:NH1	2.36	0.41
1:B:39:ASN:ND2	1:B:47:ALA:CA	2.84	0.41
1:B:225:PRO:HB2	1:B:226:PRO:HD3	2.03	0.41
1:B:134:ASP:O	1:B:135:LEU:C	2.60	0.41
1:B:219:LEU:HD23	1:B:219:LEU:HA	1.90	0.41
1:A:101:VAL:HG22	1:A:104:GLU:HG3	2.02	0.40
1:B:231:ARG:NH1	1:B:258:ASN:CG	2.78	0.40
1:A:4:LEU:HA	1:A:171:GLY:O	2.21	0.40
1:B:231:ARG:CD	1:B:259:MET:HE3	2.51	0.40
1:B:75:GLY:O	1:B:148:ASP:HA	2.22	0.40

All (13) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:441:HOH:O	2:B:475:HOH:O[4_556]	1.12	1.08
1:B:306:HIS:NE2	2:B:390:HOH:O[4_556]	1.65	0.55
2:B:509:HOH:O	2:B:536:HOH:O[4_556]	1.65	0.55
1:B:307:GLU:O	2:B:468:HOH:O[4_556]	1.86	0.34
1:B:307:GLU:N	2:B:468:HOH:O[4_556]	1.89	0.31
2:B:368:HOH:O	2:B:390:HOH:O[4_556]	1.89	0.31
2:B:395:HOH:O	2:B:464:HOH:O[2_755]	1.91	0.29
2:B:487:HOH:O	2:B:497:HOH:O[3_756]	1.94	0.26
2:B:388:HOH:O	2:B:446:HOH:O[4_556]	1.98	0.22
2:A:457:HOH:O	2:B:484:HOH:O[3_756]	2.06	0.14
2:A:484:HOH:O	2:B:457:HOH:O[3_756]	2.15	0.05
2:A:487:HOH:O	2:A:497:HOH:O[3_756]	2.16	0.04
1:B:306:HIS:O	2:B:366:HOH:O[4_556]	2.16	0.04

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	313/327 (96%)	298 (95%)	13 (4%)	2 (1%)	21	38
1	B	313/327 (96%)	300 (96%)	10 (3%)	3 (1%)	12	24
All	All	626/654 (96%)	598 (96%)	23 (4%)	5 (1%)	16	31

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	197	LEU
1	B	94	ARG
1	B	311	CYS
1	A	94	ARG
1	B	85	GLY

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	276/283 (98%)	243 (88%)	33 (12%)	5	10
1	B	276/283 (98%)	241 (87%)	35 (13%)	4	9
All	All	552/566 (98%)	484 (88%)	68 (12%)	4	10

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	CYS
1	A	4	LEU
1	A	6	LEU
1	A	11	ARG
1	A	31	LEU
1	A	66	LEU
1	A	71	ILE
1	A	76	LEU
1	A	82	TYR

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Mol	Chain	Res	Type
1	A	88	GLU
1	A	92	THR
1	A	93	ILE
1	A	110	LEU
1	A	112	VAL
1	A	121	GLU
1	A	123	ILE
1	A	129	VAL
1	A	135	LEU
1	A	146	LEU
1	A	147	SER
1	A	152	ARG
1	A	154	LEU
1	A	155	THR
1	A	161	ASP
1	A	197	LEU
1	A	198	GLU
1	A	214	LEU
1	A	216	THR
1	A	219	LEU
1	A	312	LEU
1	A	320	LYS
1	A	322	GLU
1	A	323	GLU
1	B	1	CYS
1	B	6	LEU
1	B	11	ARG
1	B	28	GLU
1	B	31	LEU
1	B	37	SER
1	B	46	ARG
1	B	66	LEU
1	B	76	LEU
1	B	82	TYR
1	B	88	GLU
1	B	91	LYS
1	B	93	ILE
1	B	95	GLU
1	B	110	LEU
1	B	123	ILE
1	B	125	SER
1	B	131	LYS

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Mol	Chain	Res	Type
1	B	135	LEU
1	B	146	LEU
1	B	152	ARG
1	B	154	LEU
1	B	155	THR
1	B	161	ASP
1	B	197	LEU
1	B	198	GLU
1	B	214	LEU
1	B	216	THR
1	B	219	LEU
1	B	247	LYS
1	B	273	ILE
1	B	311	CYS
1	B	312	LEU
1	B	320	LYS
1	B	322	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	HIS
1	A	51	GLN
1	A	99	HIS
1	A	114	GLN
1	A	153	ASN
1	A	188	GLN
1	A	238	HIS
1	A	274	HIS
1	A	292	HIS
1	A	293	HIS
1	A	300	GLN
1	B	39	ASN
1	B	114	GLN
1	B	153	ASN
1	B	182	HIS
1	B	238	HIS
1	B	274	HIS
1	B	284	ASN
1	B	292	HIS
1	B	293	HIS
1	B	300	GLN

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Mol	Chain	Res	Type
1	B	303	ASN

5.3.3 RNA [i](#)

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	317/327 (96%)	-0.72	2 (0%) 85 83	25, 34, 58, 93	0
1	B	317/327 (96%)	-0.65	3 (0%) 81 78	27, 38, 62, 94	0
All	All	634/654 (96%)	-0.69	5 (0%) 82 80	25, 36, 60, 94	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	197	LEU	3.6
1	B	209	ALA	2.9
1	A	93	ILE	2.3
1	B	197	LEU	2.2
1	B	93	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.