



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 9, 2014 – 11:40 AM EDT

PDB ID : 2OQC
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 validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

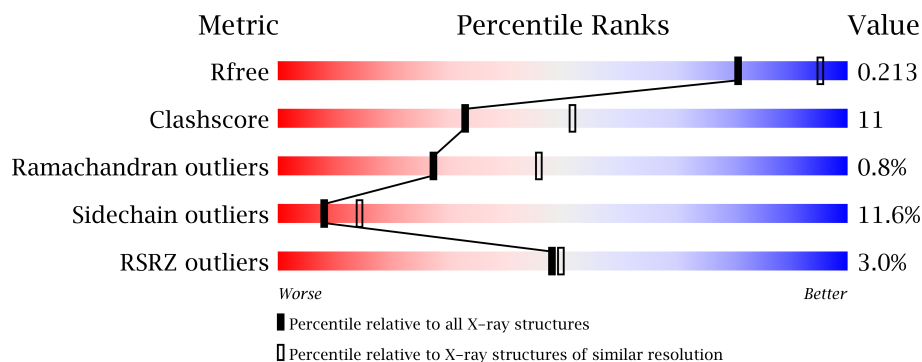
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1439
EDS	:	stable22978
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22978

1 Overall quality at a glance

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))
R_{free}	66092	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	327	
1	B	327	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5502 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

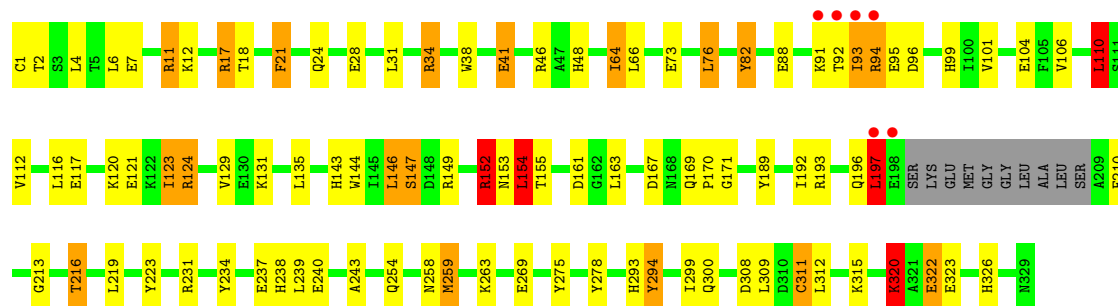
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	212	Total	O	0	0
			212	212		
2	B	208	Total	O	0	0
			208	208		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

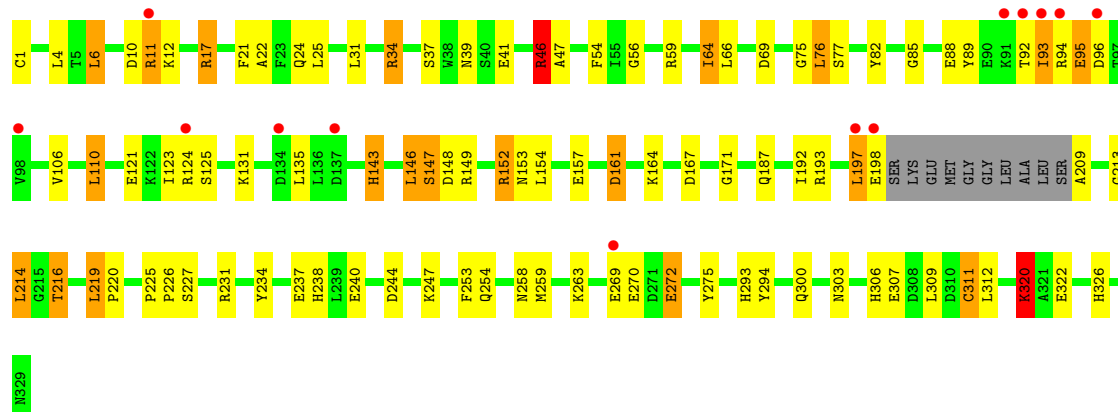
- Molecule 1: Penicillin V acylase

Chain A: 



- Molecule 1: Penicillin V acylase

Chain B: 



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 39.41 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.7 (20.00-2.50) 98.7 (39.41-2.50)	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 0.156 , 0.213	Depositor DCC
R_{free} test set	1705 reflections (5.35%)	DCC
Wilson B-factor (Å ²)	37.5	Xtriage
Anisotropy	0.104	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 31.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 33564 reflections	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.

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	1.54	28/2601 (1.1%)	1.26	21/3532 (0.6%)
1	B	1.46	17/2601 (0.7%)	1.19	14/3532 (0.4%)
All	All	1.50	45/5202 (0.9%)	1.23	35/7064 (0.5%)

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 (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	41	GLU	C-N	9.93	1.56	1.34
1	A	28	GLU	CD-OE2	9.26	1.35	1.25
1	A	41	GLU	C-N	9.23	1.55	1.34
1	A	64	ILE	C-N	8.90	1.54	1.34
1	A	269	GLU	CG-CD	8.45	1.64	1.51
1	A	147	SER	CB-OG	-8.44	1.31	1.42
1	A	237	GLU	CG-CD	8.12	1.64	1.51
1	A	237	GLU	CD-OE2	7.41	1.33	1.25
1	A	82	TYR	CD1-CE1	7.26	1.50	1.39
1	B	187	GLN	CB-CG	7.12	1.71	1.52
1	B	237	GLU	CG-CD	7.08	1.62	1.51
1	B	64	ILE	C-N	6.97	1.50	1.34
1	B	89	TYR	CD1-CE1	6.69	1.49	1.39
1	A	7	GLU	CG-CD	6.63	1.61	1.51
1	A	82	TYR	CD2-CE2	6.62	1.49	1.39
1	A	28	GLU	CD-OE1	6.57	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	269	GLU	CG-CD	6.37	1.61	1.51
1	B	237	GLU	CD-OE2	6.28	1.32	1.25
1	B	187	GLN	CG-CD	6.09	1.65	1.51
1	A	144	TRP	CZ3-CH2	6.04	1.49	1.40
1	B	152	ARG	CG-CD	5.87	1.66	1.51
1	A	223	TYR	CE1-CZ	5.68	1.46	1.38
1	B	272	GLU	CG-CD	5.66	1.60	1.51
1	A	237	GLU	CD-OE1	5.58	1.31	1.25
1	A	320	LYS	CD-CE	5.53	1.65	1.51
1	A	243	ALA	CA-CB	5.51	1.64	1.52
1	B	121	GLU	CG-CD	5.48	1.60	1.51
1	A	210	PHE	C-O	5.47	1.33	1.23
1	A	299	ILE	CB-CG2	5.42	1.69	1.52
1	B	270	GLU	CG-CD	5.42	1.60	1.51
1	A	278	TYR	CG-CD1	5.29	1.46	1.39
1	A	21	PHE	CE1-CZ	5.28	1.47	1.37
1	B	275	TYR	CD2-CE2	5.27	1.47	1.39
1	A	46	ARG	NE-CZ	5.25	1.39	1.33
1	A	294	TYR	CG-CD2	5.25	1.46	1.39
1	A	149	ARG	CZ-NH2	5.24	1.39	1.33
1	B	240	GLU	CD-OE1	5.21	1.31	1.25
1	A	46	ARG	CD-NE	5.19	1.55	1.46
1	B	253	PHE	CE2-CZ	5.17	1.47	1.37
1	A	311	CYS	CB-SG	-5.15	1.73	1.81
1	A	117	GLU	CG-CD	5.13	1.59	1.51
1	A	38	TRP	CG-CD1	5.11	1.44	1.36
1	B	320	LYS	CG-CD	5.03	1.69	1.52
1	A	294	TYR	CE2-CZ	5.01	1.45	1.38
1	B	54	PHE	CE2-CZ	5.01	1.46	1.37

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	46	ARG	NE-CZ-NH1	14.94	127.77	120.30
1	A	34	ARG	NE-CZ-NH2	-14.22	113.19	120.30
1	A	64	ILE	O-C-N	-13.66	100.84	122.70
1	B	34	ARG	NE-CZ-NH1	12.14	126.37	120.30
1	B	34	ARG	NE-CZ-NH2	-10.32	115.14	120.30
1	A	34	ARG	NE-CZ-NH1	9.45	125.03	120.30
1	A	146	LEU	CA-CB-CG	9.06	136.13	115.30
1	B	12	LYS	CD-CE-NZ	-7.92	93.47	111.70
1	B	11	ARG	NE-CZ-NH1	7.42	124.01	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	214	LEU	CB-CG-CD2	-7.41	98.40	111.00
1	B	146	LEU	CA-CB-CG	7.19	131.85	115.30
1	B	46	ARG	NE-CZ-NH1	7.19	123.89	120.30
1	A	152	ARG	NE-CZ-NH1	6.95	123.77	120.30
1	B	17	ARG	NE-CZ-NH1	-6.87	116.86	120.30
1	A	64	ILE	C-N-CA	6.83	138.76	121.70
1	A	124	ARG	NE-CZ-NH2	-6.64	116.98	120.30
1	A	154	LEU	CA-CB-CG	6.55	130.37	115.30
1	A	124	ARG	NE-CZ-NH1	6.51	123.55	120.30
1	B	244	ASP	CB-CG-OD1	6.47	124.13	118.30
1	A	146	LEU	CB-CG-CD2	6.47	121.99	111.00
1	B	64	ILE	CA-C-N	-6.23	103.49	117.20
1	B	41	GLU	O-C-N	-6.19	112.80	122.70
1	B	11	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	B	147	SER	N-CA-CB	-6.10	101.35	110.50
1	B	76	LEU	CB-CG-CD2	6.06	121.30	111.00
1	A	146	LEU	CB-CG-CD1	5.91	121.05	111.00
1	A	110	LEU	CB-CG-CD1	5.90	121.04	111.00
1	A	34	ARG	CD-NE-CZ	5.90	131.86	123.60
1	A	76	LEU	CA-CB-CG	5.63	128.25	115.30
1	A	76	LEU	CB-CG-CD2	5.46	120.29	111.00
1	A	322	GLU	CB-CA-C	-5.46	99.48	110.40
1	A	147	SER	CB-CA-C	-5.36	99.92	110.10
1	A	46	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	A	46	ARG	CD-NE-CZ	5.30	131.03	123.60
1	A	34	ARG	CG-CD-NE	-5.28	100.72	111.80

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit,

and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2541	0	2477	55	0
1	B	2541	0	2477	57	4
2	A	212	0	0	18	3
2	B	208	0	0	16	12
All	All	5502	0	4954	112	13

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 11.

All (112) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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:HH11	1:A:11:ARG:HG2	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:231:ARG:HB3	1:A:259:MET:HE2	1.68	0.75
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: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:HH11	1:B:46:ARG:HG2	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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:A:275:TYR:OH	2:A:512:HOH:O	2.16	0.60
1:B:231:ARG:NH1	1:B:258:ASN:CB	2.61	0.60
1:B:46:ARG:CG	1:B:46:ARG:HH11	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:220:PRO:HB2	1:B:227:SER:HB3	1.87	0.56
1:B:39:ASN:ND2	1:B:47:ALA:HA	2.20	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:131:LYS:CD	2:A:458:HOH:O	2.55	0.55
1:B:152:ARG:NH1	1:B:152:ARG:HG3	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:234:TYR:O	1:A:238:HIS:HD2	1.92	0.51
1:A:95:GLU:O	1:A:96:ASP:HB2	2.10	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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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: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:NH1	1:B:46:ARG:HG2	2.29	0.45
1:B:93:ILE:HG13	1:B:93:ILE:O	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:231:ARG:HD3	1:A:259:MET:HE3	1.99	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:B:231:ARG:HD3	1:B:259:MET:HE3	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:B:24:GLN:CG	2:B:513:HOH:O	2.59	0.41
1:B:4:LEU:CD1	1:B:6:LEU:HD13	2.50	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
1:B:56:GLY:HA3	1:B:69:ASP:O	2.20	0.41
1:B:11:ARG:HG2	1:B:11:ARG:NH1	2.36	0.41
1:B:225:PRO:HB2	1:B:226:PRO:HD3	2.03	0.41
1:B:39:ASN:ND2	1:B:47:ALA:CA	2.84	0.41
1:A:308:ASP:O	1:A:311:CYS:HB2	2.21	0.41
1:B:219:LEU:HA	1:B:219:LEU:HD23	1.90	0.41
1:A:101:VAL:HG22	1:A:104:GLU:HG3	2.02	0.40
1:A:4:LEU:HA	1:A:171:GLY:O	2.21	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	Distance(Å)	Clash(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
1:B:306:HIS:O	2:B:366:HOH:O[4_556]	2.16	0.04
2:A:487:HOH:O	2:A:497:HOH:O[3_756]	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%)	33	55
1	B	313/327 (96%)	300 (96%)	10 (3%)	3 (1%)	22	38
All	All	626/654 (96%)	598 (96%)	23 (4%)	5 (1%)	27	46

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%)	244 (88%)	32 (12%)	8	14
1	B	276/283 (98%)	244 (88%)	32 (12%)	8	14
All	All	552/566 (98%)	488 (88%)	64 (12%)	8	14

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	11	ARG
1	A	17	ARG
1	A	21	PHE
1	A	31	LEU
1	A	66	LEU
1	A	76	LEU
1	A	82	TYR
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	143	HIS
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	216	THR
1	A	219	LEU
1	A	259	MET
1	A	312	LEU

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Mol	Chain	Res	Type
1	A	320	LYS
1	A	322	GLU
1	A	323	GLU
1	B	1	CYS
1	B	6	LEU
1	B	17	ARG
1	B	21	PHE
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	93	ILE
1	B	95	GLU
1	B	110	LEU
1	B	123	ILE
1	B	125	SER
1	B	131	LYS
1	B	135	LEU
1	B	143	HIS
1	B	146	LEU
1	B	154	LEU
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	311	CYS
1	B	312	LEU
1	B	320	LYS
1	B	322	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	HIS
1	A	99	HIS
1	A	114	GLN

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Mol	Chain	Res	Type
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	188	GLN
1	B	238	HIS
1	B	274	HIS
1	B	284	ASN
1	B	292	HIS
1	B	293	HIS
1	B	300	GLN
1	B	306	HIS

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates 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 ⓘ

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%)	-0.45	6 (1%) 64 66	25, 34, 58, 93	0
1	B	317/327 (96%)	-0.25	13 (4%) 35 36	27, 38, 62, 94	0
All	All	634/654 (96%)	-0.35	19 (2%) 48 50	25, 36, 60, 94	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	197	LEU	5.6
1	A	197	LEU	4.6
1	A	92	THR	4.1
1	B	92	THR	3.7
1	B	94	ARG	3.4
1	B	93	ILE	3.1
1	A	94	ARG	2.8
1	A	198	GLU	2.8
1	B	198	GLU	2.6
1	B	91	LYS	2.4
1	A	91	LYS	2.4
1	A	93	ILE	2.3
1	B	96	ASP	2.2
1	B	124	ARG	2.2
1	B	134	ASP	2.1
1	B	98	VAL	2.1
1	B	269	GLU	2.1
1	B	11	ARG	2.0
1	B	137	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.