



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 19, 2023 – 02:31 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 X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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 : 4.02b-467  
Xtrriage (Phenix) : 1.13  
EDS : 2.36  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

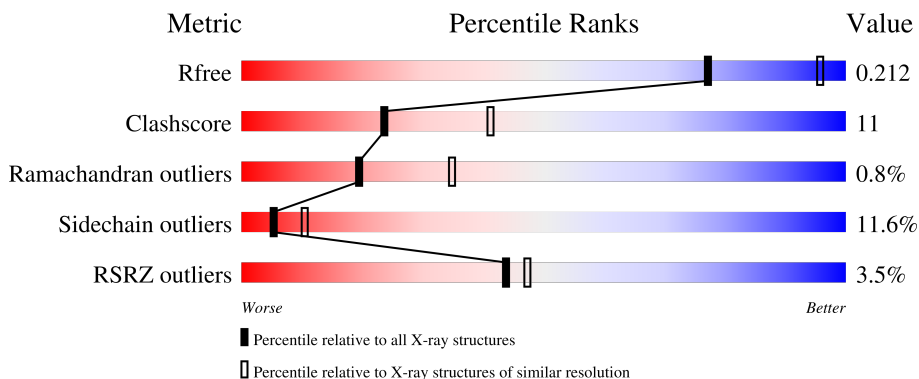
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

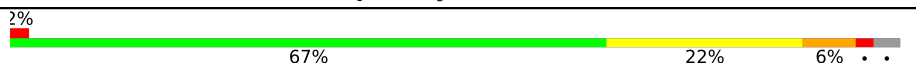

The reported resolution of this entry is 2.50 Å.

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))
$R_{free}$	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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  $\geq 3$ , 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	 2% 67% 22% 6% . .
1	B	327	 5% 67% 24% 6% . .

## 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
			Total	C	N	O	S			
1	A	317	2541	1616	431	484	10	0	0	0
1	B	317	2541	1616	431	484	10	0	0	0

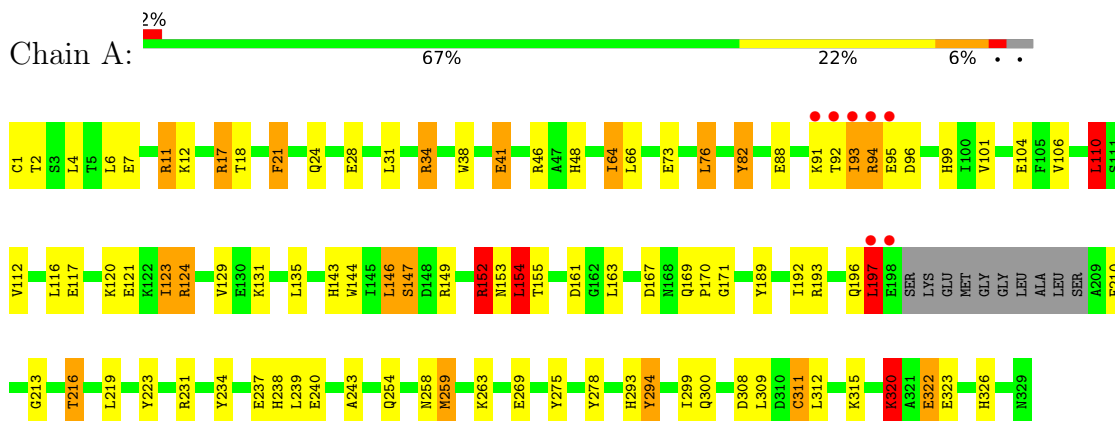
- Molecule 2 is water.

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

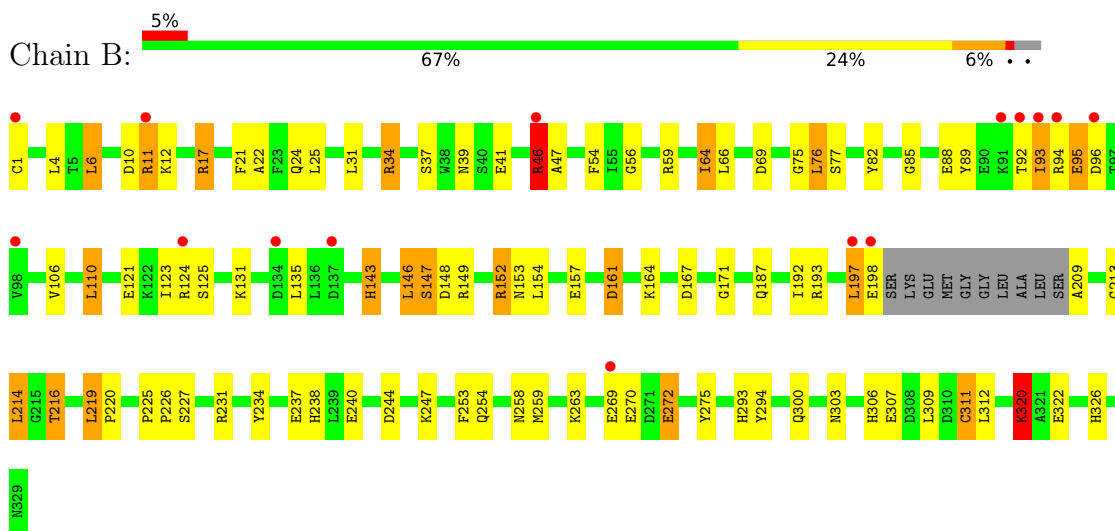
### 3 Residue-property plots [i](#)

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, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	138.74 (at 2.51Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.155 , 0.218 0.156 , 0.212	Depositor DCC
$R_{free}$ test set	1705 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	37.5	Xtrriage
Anisotropy	0.104	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 41.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	5502	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtrriage'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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 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	1.54	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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

Continued from previous page...

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 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	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

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 11.

All (112) 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: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: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
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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (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: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: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
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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:ASN:HD22	1:A:171:GLY:HA2	1.78	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: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: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: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: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: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: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

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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	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 [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	313/327 (96%)	298 (95%)	13 (4%)	2 (1%)	25	43
1	B	313/327 (96%)	300 (96%)	10 (3%)	3 (1%)	15	28
All	All	626/654 (96%)	598 (96%)	23 (4%)	5 (1%)	19	35

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 [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	276/283 (98%)	244 (88%)	32 (12%)	5	10
1	B	276/283 (98%)	244 (88%)	32 (12%)	5	10
All	All	552/566 (98%)	488 (88%)	64 (12%)	5	10

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

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
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
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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 (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	HIS
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	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 [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 monosaccharides 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	317/327 (96%)	-0.40	7 (2%) 62 65	25, 34, 58, 93	0
1	B	317/327 (96%)	-0.19	15 (4%) 31 33	27, 38, 62, 94	0
All	All	634/654 (96%)	-0.29	22 (3%) 44 47	25, 36, 60, 94	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	197	LEU	5.8
1	A	92	THR	4.4
1	B	92	THR	4.3
1	A	197	LEU	4.1
1	B	93	ILE	3.7
1	B	94	ARG	3.6
1	A	94	ARG	3.4
1	A	93	ILE	2.8
1	B	124	ARG	2.7
1	A	198	GLU	2.6
1	A	91	LYS	2.6
1	B	137	ASP	2.6
1	B	96	ASP	2.4
1	B	91	LYS	2.4
1	B	198	GLU	2.3
1	B	11	ARG	2.3
1	B	269	GLU	2.2
1	B	134	ASP	2.1
1	A	95	GLU	2.1
1	B	98	VAL	2.0
1	B	1	CYS	2.0
1	B	46	ARG	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 monosaccharides 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.