



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 12:07 am BST

PDB ID : 1FR1
Title : REFINED CRYSTAL STRUCTURE OF BETA-LACTAMASE FROM CITROBACTER FREUNDII INDICATES A MECHANISM FOR BETA-LACTAM HYDROLYSIS
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Deposited on : 2000-09-07
Resolution : 2.00 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

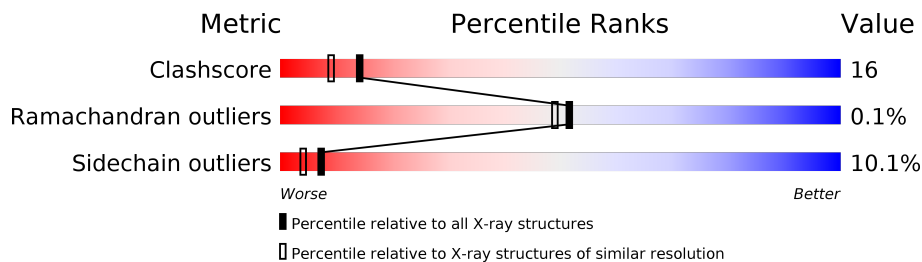
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)

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 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	361	
1	B	361	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6057 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
			Total	C	N	O	S			
1	A	361	2799	1796	477	517	9	0	0	0
1	B	361	2806	1801	479	517	9	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	175	SER	THR	SEE REMARK 999	UNP Q46041
A	176	LYS	THR	SEE REMARK 999	UNP Q46041
A	180	HIS	GLN	SEE REMARK 999	UNP Q46041
A	228	ILE	VAL	SEE REMARK 999	UNP Q46041
A	253	GLU	LYS	SEE REMARK 999	UNP Q46041
A	278	VAL	LEU	SEE REMARK 999	UNP Q46041
A	285	SER	ASN	SEE REMARK 999	UNP Q46041
A	348	VAL	ALA	SEE REMARK 999	UNP Q46041
B	175	SER	THR	SEE REMARK 999	UNP Q46041
B	176	LYS	THR	SEE REMARK 999	UNP Q46041
B	180	HIS	GLN	SEE REMARK 999	UNP Q46041
B	228	ILE	VAL	SEE REMARK 999	UNP Q46041
B	253	GLU	LYS	SEE REMARK 999	UNP Q46041
B	278	VAL	LEU	SEE REMARK 999	UNP Q46041
B	285	SER	ASN	SEE REMARK 999	UNP Q46041
B	348	VAL	ALA	SEE REMARK 999	UNP Q46041

- Molecule 2 is water.

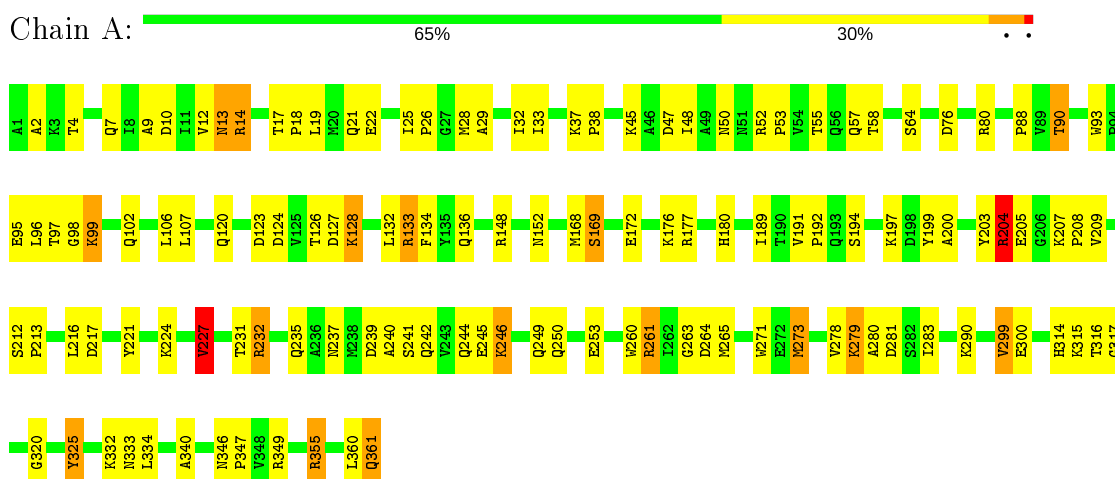
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	211	Total	O	0	0
			211	211		
2	B	241	Total	O	0	0
			241	241		

3 Residue-property plots

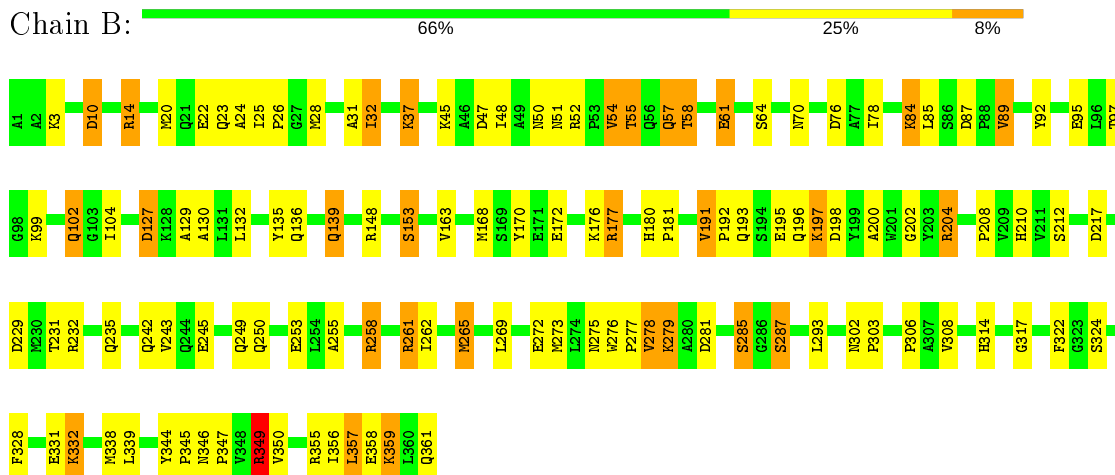
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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: BETA-LACTAMASE



- Molecule 1: BETA-LACTAMASE



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	98.07Å 84.63Å 89.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.00	Depositor
% Data completeness (in resolution range)	87.0 (6.00-2.00)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.182 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6057	wwPDB-VP
Average B, all atoms (Å ²)	17.0	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	1.04	2/2874 (0.1%)	1.51	25/3918 (0.6%)
1	B	1.10	4/2881 (0.1%)	1.63	32/3925 (0.8%)
All	All	1.07	6/5755 (0.1%)	1.57	57/7843 (0.7%)

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	1
1	B	0	2
All	All	0	3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	61	GLU	CD-OE1	-6.77	1.18	1.25
1	B	355	ARG	CD-NE	-6.17	1.35	1.46
1	B	278	VAL	N-CA	-5.60	1.35	1.46
1	A	278	VAL	N-CA	-5.53	1.35	1.46
1	A	227	VAL	CB-CG2	5.37	1.64	1.52
1	B	349	ARG	NE-CZ	-5.29	1.26	1.33

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	355	ARG	CD-NE-CZ	21.10	153.14	123.60
1	B	349	ARG	NE-CZ-NH1	19.52	130.06	120.30
1	A	273	MET	CA-CB-CG	16.61	141.53	113.30
1	B	355	ARG	NE-CZ-NH1	16.36	128.48	120.30
1	B	349	ARG	CD-NE-CZ	12.24	140.74	123.60
1	B	349	ARG	NE-CZ-NH2	-11.52	114.54	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	232	ARG	NE-CZ-NH1	11.21	125.91	120.30
1	A	133	ARG	NE-CZ-NH1	11.13	125.86	120.30
1	B	355	ARG	NE-CZ-NH2	-10.98	114.81	120.30
1	A	204	ARG	NE-CZ-NH2	-8.99	115.81	120.30
1	B	14	ARG	NE-CZ-NH1	8.70	124.65	120.30
1	A	133	ARG	NE-CZ-NH2	-8.50	116.05	120.30
1	B	177	ARG	NE-CZ-NH2	-8.16	116.22	120.30
1	B	261	ARG	NE-CZ-NH2	-7.76	116.42	120.30
1	B	232	ARG	CD-NE-CZ	-7.36	113.30	123.60
1	B	76	ASP	CB-CG-OD2	-7.06	111.94	118.30
1	B	204	ARG	NE-CZ-NH2	-7.06	116.77	120.30
1	A	148	ARG	NE-CZ-NH1	6.78	123.69	120.30
1	A	133	ARG	CD-NE-CZ	6.56	132.79	123.60
1	A	124	ASP	CB-CG-OD1	6.55	124.19	118.30
1	A	14	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	B	217	ASP	CB-CG-OD1	6.45	124.11	118.30
1	A	80	ARG	NE-CZ-NH2	-6.43	117.09	120.30
1	B	258	ARG	CD-NE-CZ	-6.27	114.83	123.60
1	A	204	ARG	NE-CZ-NH1	6.27	123.43	120.30
1	B	232	ARG	NE-CZ-NH2	-6.03	117.29	120.30
1	A	199	TYR	CB-CG-CD2	-5.91	117.45	121.00
1	B	14	ARG	CD-NE-CZ	5.91	131.88	123.60
1	B	61	GLU	OE1-CD-OE2	5.89	130.37	123.30
1	A	199	TYR	CB-CG-CD1	5.88	124.53	121.00
1	B	130	ALA	CB-CA-C	5.85	118.88	110.10
1	A	177	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	B	127	ASP	CB-CG-OD1	5.74	123.46	118.30
1	A	227	VAL	CA-CB-CG2	-5.72	102.33	110.90
1	B	52	ARG	NE-CZ-NH2	-5.65	117.47	120.30
1	A	261	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	A	148	ARG	CD-NE-CZ	5.46	131.24	123.60
1	B	229	ASP	N-CA-CB	5.39	120.31	110.60
1	A	205	GLU	CA-CB-CG	5.34	125.16	113.40
1	B	10	ASP	CB-CG-OD2	-5.32	113.51	118.30
1	A	80	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	B	55	THR	N-CA-CB	-5.32	100.20	110.30
1	A	169	SER	CB-CA-C	-5.31	100.01	110.10
1	B	55	THR	CA-CB-CG2	5.30	119.82	112.40
1	B	217	ASP	CB-CA-C	5.25	120.91	110.40
1	A	76	ASP	CB-CG-OD2	-5.23	113.59	118.30
1	A	180	HIS	CB-CA-C	5.22	120.83	110.40
1	B	31	ALA	N-CA-CB	5.18	117.35	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	153	SER	N-CA-CB	-5.17	102.75	110.50
1	A	355	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	A	325	TYR	O-C-N	5.16	130.95	122.70
1	B	328	PHE	O-C-N	5.15	130.94	122.70
1	B	261	ARG	O-C-N	5.12	130.89	122.70
1	B	61	GLU	CG-CD-OE2	-5.11	108.08	118.30
1	B	54	VAL	O-C-N	5.05	130.78	122.70
1	A	148	ARG	NH1-CZ-NH2	-5.01	113.89	119.40
1	B	135	TYR	CB-CG-CD2	-5.01	117.99	121.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	204	ARG	Sidechain
1	B	177	ARG	Sidechain
1	B	349	ARG	Sidechain

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	2799	0	2776	89	7
1	B	2806	0	2796	90	12
2	A	211	0	0	18	18
2	B	241	0	0	9	26
All	All	6057	0	5572	174	34

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 16.

All (174) 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:361:GLN:CA	2:A:503:HOH:O	1.86	1.24

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:361:GLN:C	2:A:503:HOH:O	1.84	1.13
1:A:227:VAL:HG23	2:A:417:HOH:O	1.51	1.10
1:B:55:THR:H	1:B:58:THR:CG2	1.78	0.96
1:A:55:THR:HG22	1:A:57:GLN:H	1.35	0.88
1:B:172:GLU:HG2	1:B:176:LYS:HZ2	1.39	0.86
1:B:265:MET:HE1	1:B:272:GLU:HG2	1.58	0.84
1:A:232:ARG:HD3	2:A:382:HOH:O	1.78	0.84
1:B:281:ASP:O	1:B:285:SER:HB2	1.80	0.81
1:A:246:LYS:HE3	1:A:250:GLN:HG3	1.63	0.78
1:B:132:LEU:HD11	1:B:136:GLN:NE2	1.99	0.78
1:B:48:ILE:O	2:B:516:HOH:O	2.02	0.78
1:A:120:GLN:HE22	1:A:152:ASN:ND2	1.82	0.76
1:B:55:THR:HG22	1:B:57:GLN:H	1.51	0.75
1:B:258:ARG:HH12	1:B:275:ASN:HD21	1.36	0.74
1:B:258:ARG:HH22	1:B:275:ASN:HD22	1.36	0.74
1:B:258:ARG:HH22	1:B:275:ASN:ND2	1.85	0.73
1:B:55:THR:H	1:B:58:THR:HG23	1.54	0.72
1:B:346:ASN:HA	1:B:349:ARG:HD3	1.73	0.71
1:B:3:LYS:O	2:B:493:HOH:O	2.08	0.71
1:B:32:ILE:HD11	1:B:356:ILE:HG21	1.74	0.70
1:A:361:GLN:HA	2:A:503:HOH:O	1.67	0.68
1:A:133:ARG:HH12	1:B:347:PRO:HB2	1.59	0.67
1:B:132:LEU:HD11	1:B:136:GLN:HE21	1.59	0.67
1:B:54:VAL:HA	1:B:58:THR:HG21	1.76	0.67
1:B:25:ILE:HG21	1:B:28:MET:HE2	1.77	0.66
1:A:207:LYS:HE3	1:A:208:PRO:HD2	1.78	0.66
1:A:17:THR:HB	1:A:18:PRO:HD3	1.76	0.65
1:B:99:LYS:HD3	1:B:102:GLN:HG3	1.80	0.64
1:B:243:VAL:HG22	1:B:249:GLN:HB2	1.79	0.64
1:A:227:VAL:CG2	2:A:417:HOH:O	2.21	0.64
1:B:265:MET:CE	1:B:272:GLU:HG2	2.28	0.63
1:B:127:ASP:OD2	1:B:129:ALA:HB3	1.99	0.63
1:A:28:MET:HE2	1:A:340:ALA:HB2	1.81	0.62
1:A:120:GLN:NE2	1:A:152:ASN:ND2	2.47	0.62
1:A:235:GLN:NE2	2:A:415:HOH:O	2.31	0.62
1:A:28:MET:CE	1:A:340:ALA:HB2	2.30	0.62
1:B:204:ARG:HH11	1:B:204:ARG:HG3	1.63	0.62
1:A:128:LYS:HD2	1:A:128:LYS:H	1.63	0.62
1:A:361:GLN:OXT	2:A:503:HOH:O	2.08	0.61
1:A:244:GLN:HG3	2:A:480:HOH:O	2.00	0.61
1:A:93:TRP:O	1:A:96:LEU:HB3	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:GLU:HG2	1:A:132:LEU:HD21	1.83	0.59
1:B:25:ILE:HG21	1:B:28:MET:CE	2.32	0.59
1:A:12:VAL:HG21	1:A:32:ILE:HD13	1.86	0.58
1:B:78:ILE:HD11	1:B:85:LEU:HG	1.87	0.57
1:B:346:ASN:O	1:B:349:ARG:HB2	2.05	0.57
1:A:47:ASP:OD1	1:A:50:ASN:HB2	2.05	0.57
1:B:168:MET:CE	1:B:176:LYS:HD2	2.34	0.57
1:B:55:THR:CG2	1:B:57:GLN:HG3	2.35	0.57
1:A:126:THR:HG22	1:B:204:ARG:NH1	2.20	0.56
1:A:126:THR:HG22	1:B:204:ARG:HH12	1.69	0.56
1:B:84:LYS:NZ	1:B:84:LYS:HB2	2.20	0.56
1:A:88:PRO:HB2	1:A:90:THR:HG23	1.87	0.56
1:B:14:ARG:HG3	1:B:14:ARG:HH11	1.70	0.56
1:A:29:ALA:HB1	1:A:227:VAL:HG21	1.88	0.56
1:A:168:MET:HE2	1:A:172:GLU:HG2	1.88	0.55
1:B:202:GLY:O	1:B:208:PRO:HA	2.05	0.55
1:B:55:THR:HB	1:B:58:THR:HG22	1.89	0.55
1:A:107:LEU:HD21	2:A:431:HOH:O	2.05	0.55
1:A:10:ASP:O	1:A:14:ARG:HG2	2.07	0.55
1:B:20:MET:HG2	1:B:28:MET:CE	2.37	0.55
1:A:25:ILE:HG21	1:A:28:MET:CE	2.37	0.54
1:A:25:ILE:HG21	1:A:28:MET:HE3	1.90	0.54
1:A:9:ALA:O	1:A:13:ASN:HB2	2.07	0.54
1:A:45:LYS:HA	1:A:53:PRO:HA	1.88	0.54
1:B:287:SER:OG	1:B:350:VAL:HG21	2.08	0.53
1:B:231:THR:O	1:B:235:GLN:HG3	2.07	0.53
1:A:176:LYS:HE2	2:A:477:HOH:O	2.09	0.53
1:B:332:LYS:CE	2:B:574:HOH:O	2.57	0.53
1:B:20:MET:HG2	1:B:28:MET:HE3	1.91	0.53
1:B:95:GLU:O	1:B:136:GLN:NE2	2.42	0.53
1:A:58:THR:CG2	1:A:200:ALA:HB2	2.38	0.52
1:A:168:MET:CE	1:A:172:GLU:HG2	2.38	0.52
1:A:127:ASP:HA	1:A:128:LYS:HZ2	1.74	0.52
1:A:360:LEU:C	2:A:503:HOH:O	2.48	0.52
1:B:302:ASN:HD22	1:B:303:PRO:HA	1.74	0.52
1:B:200:ALA:O	1:B:210:HIS:HE1	1.93	0.51
1:B:148:ARG:HD2	1:B:262:ILE:CD1	2.40	0.51
1:B:70:ASN:HB2	1:B:170:TYR:OH	2.10	0.51
1:A:189:ILE:O	1:A:224:LYS:NZ	2.42	0.51
1:B:255:ALA:HA	1:B:269:LEU:HB2	1.91	0.51
1:A:361:GLN:N	2:A:503:HOH:O	2.23	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:LYS:HD2	2:A:421:HOH:O	2.11	0.51
1:A:232:ARG:HG2	1:A:232:ARG:HH11	1.76	0.51
1:B:22:GLU:HG2	2:B:380:HOH:O	2.09	0.51
1:A:95:GLU:HG2	1:A:132:LEU:CD2	2.42	0.50
1:A:17:THR:CB	1:A:18:PRO:HD3	2.40	0.50
1:B:55:THR:CG2	1:B:57:GLN:H	2.22	0.50
1:B:132:LEU:O	1:B:136:GLN:HG3	2.12	0.50
1:A:128:LYS:CD	1:A:128:LYS:H	2.24	0.50
1:A:120:GLN:HE22	1:A:152:ASN:HD21	1.54	0.50
1:A:33:ILE:O	1:A:334:LEU:HA	2.11	0.50
1:A:93:TRP:CE3	1:A:96:LEU:HD22	2.46	0.50
1:A:64:SER:HB2	1:A:317:GLY:HA2	1.93	0.50
1:B:84:LYS:HB2	1:B:84:LYS:HZ3	1.75	0.50
1:B:197:LYS:HE3	1:B:198:ASP:OD2	2.12	0.49
1:B:99:LYS:CD	1:B:102:GLN:HG3	2.42	0.49
1:A:26:PRO:HB3	1:A:48:ILE:HD11	1.93	0.49
1:B:168:MET:HE3	1:B:176:LYS:HD2	1.93	0.49
1:A:240:ALA:O	1:A:249:GLN:HG3	2.12	0.49
1:B:148:ARG:HD2	1:B:262:ILE:HD13	1.94	0.48
1:B:331:GLU:HG3	1:B:332:LYS:HE3	1.95	0.48
1:A:207:LYS:CE	1:A:208:PRO:HD2	2.42	0.48
1:A:25:ILE:HD13	1:A:28:MET:CE	2.43	0.48
1:A:48:ILE:HG13	1:A:203:TYR:CZ	2.49	0.48
1:A:204:ARG:HH11	1:A:204:ARG:CG	2.27	0.47
1:A:221:TYR:HE1	2:A:542:HOH:O	1.97	0.47
1:A:120:GLN:NE2	1:A:152:ASN:HD22	2.12	0.47
1:B:172:GLU:CG	1:B:176:LYS:HZ2	2.20	0.47
1:A:290:LYS:CE	1:B:139:GLN:NE2	2.78	0.47
1:B:276:TRP:CG	1:B:277:PRO:HA	2.50	0.47
1:A:29:ALA:HB1	1:A:227:VAL:CG2	2.45	0.46
1:A:88:PRO:HB2	1:A:90:THR:CG2	2.46	0.46
1:B:64:SER:HB2	1:B:317:GLY:HA2	1.95	0.46
1:B:127:ASP:OD2	1:B:129:ALA:N	2.48	0.46
1:B:324:SER:HA	1:B:338:MET:O	2.14	0.46
1:A:316:THR:HG22	1:A:325:TYR:CD2	2.51	0.46
1:B:191:VAL:HG22	1:B:196:GLN:NE2	2.31	0.45
1:A:123:ASP:HA	2:A:571:HOH:O	2.15	0.45
1:B:28:MET:HE3	1:B:28:MET:HB2	1.64	0.45
1:B:55:THR:O	1:B:58:THR:HG23	2.17	0.45
1:A:25:ILE:HD13	1:A:28:MET:HE1	1.99	0.45
1:A:355:ARG:HD2	2:A:530:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:THR:HG22	1:A:98:GLY:H	1.82	0.45
1:A:212:SER:HB2	1:A:213:PRO:HD2	1.98	0.44
1:A:260:TRP:CH2	1:A:300:GLU:HG3	2.53	0.44
1:A:261:ARG:HB3	1:A:299:VAL:HG13	1.98	0.44
1:A:280:ALA:O	1:A:283:ILE:HG12	2.18	0.44
1:A:134:PHE:HE1	2:B:430:HOH:O	2.00	0.44
1:A:204:ARG:HH11	1:A:204:ARG:HG2	1.82	0.44
1:A:191:VAL:HA	1:A:192:PRO:HD3	1.91	0.43
1:B:28:MET:HG3	1:B:339:LEU:O	2.18	0.43
1:B:332:LYS:HE2	2:B:574:HOH:O	2.17	0.43
1:B:358:GLU:HA	1:B:361:GLN:HE21	1.83	0.43
1:A:239:ASP:O	1:A:242:GLN:HG2	2.19	0.43
1:B:195:GLU:HA	1:B:197:LYS:HE2	2.01	0.43
1:B:32:ILE:HD11	1:B:356:ILE:CG2	2.47	0.43
1:B:37:LYS:HB2	1:B:37:LYS:HE3	1.58	0.43
1:B:23:GLN:O	1:B:24:ALA:HB3	2.18	0.42
1:A:37:LYS:HA	1:A:38:PRO:HD3	1.91	0.42
1:B:242:GLN:HG3	1:B:243:VAL:N	2.34	0.42
1:A:346:ASN:O	1:A:349:ARG:HB2	2.19	0.42
1:A:19:LEU:HD23	1:A:19:LEU:C	2.40	0.42
1:B:47:ASP:CG	1:B:50:ASN:HB2	2.39	0.42
1:A:231:THR:O	1:A:235:GLN:HG3	2.20	0.42
1:A:216:LEU:HD23	2:A:564:HOH:O	2.19	0.42
1:B:276:TRP:CD1	1:B:277:PRO:HA	2.54	0.42
1:A:237:ASN:ND2	1:A:271:TRP:HE1	2.17	0.41
1:A:320:GLY:HA3	2:B:528:HOH:O	2.19	0.41
1:B:61:GLU:HB2	1:B:322:PHE:CD2	2.55	0.41
1:B:89:VAL:CG1	1:B:104:ILE:HG22	2.50	0.41
1:A:315:LYS:HG3	1:A:316:THR:O	2.20	0.41
1:B:346:ASN:HD22	1:B:346:ASN:HA	1.67	0.41
1:B:204:ARG:HG3	1:B:204:ARG:NH1	2.32	0.41
1:B:197:LYS:HG3	1:B:197:LYS:H	1.66	0.41
1:B:25:ILE:HA	1:B:26:PRO:HD3	1.89	0.41
1:A:127:ASP:HA	1:A:128:LYS:NZ	2.36	0.41
1:A:209:VAL:HG21	2:B:528:HOH:O	2.21	0.41
1:B:191:VAL:HA	1:B:192:PRO:HD3	1.82	0.41
1:B:212:SER:HB2	2:B:501:HOH:O	2.21	0.41
1:B:258:ARG:HH12	1:B:275:ASN:ND2	2.12	0.41
1:B:87:ASP:OD1	1:B:92:TYR:OH	2.32	0.41
1:A:346:ASN:N	1:A:347:PRO:CD	2.84	0.41
1:B:25:ILE:HD13	1:B:28:MET:CE	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:357:LEU:HD12	1:B:357:LEU:HA	1.89	0.41
1:A:224:LYS:HD2	1:A:224:LYS:N	2.36	0.40
1:B:278:VAL:HG22	1:B:279:LYS:N	2.36	0.40
1:A:290:LYS:CE	1:B:139:GLN:HE21	2.34	0.40
1:B:168:MET:HE3	1:B:176:LYS:CD	2.52	0.40
1:B:180:HIS:N	1:B:181:PRO:HD2	2.37	0.40
1:A:19:LEU:HD23	1:A:25:ILE:HD12	2.04	0.40
1:A:260:TRP:CE3	1:A:300:GLU:HA	2.57	0.40
1:B:344:TYR:HA	1:B:345:PRO:HD3	1.93	0.40

All (34) 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:A:507:HOH:O	2:B:529:HOH:O[2_664]	0.07	2.13
2:A:511:HOH:O	2:B:553:HOH:O[2_664]	0.17	2.03
2:B:436:HOH:O	2:B:477:HOH:O[2_665]	0.34	1.86
2:A:561:HOH:O	2:B:596:HOH:O[4_455]	0.36	1.84
2:A:508:HOH:O	2:B:549:HOH:O[3_645]	0.39	1.81
2:A:463:HOH:O	2:B:508:HOH:O[4_455]	0.45	1.75
2:A:396:HOH:O	2:B:414:HOH:O[4_455]	0.82	1.38
2:A:481:HOH:O	2:A:482:HOH:O[3_654]	1.09	1.11
2:A:498:HOH:O	2:B:534:HOH:O[2_564]	1.14	1.06
2:A:456:HOH:O	2:B:494:HOH:O[3_645]	1.23	0.97
2:B:577:HOH:O	2:B:578:HOH:O[2_664]	1.38	0.82
1:B:308:VAL:CG1	2:B:546:HOH:O[2_665]	1.65	0.55
1:B:261:ARG:CD	2:B:562:HOH:O[2_665]	1.75	0.45
1:B:306:PRO:O	2:B:581:HOH:O[2_665]	1.76	0.44
2:A:471:HOH:O	2:B:412:HOH:O[4_455]	1.79	0.41
2:A:403:HOH:O	2:B:422:HOH:O[2_564]	1.83	0.37
1:B:208:PRO:CG	2:B:589:HOH:O[2_664]	1.84	0.36
1:B:250:GLN:OE1	2:B:488:HOH:O[2_665]	1.85	0.35
1:B:97:THR:OG1	2:A:461:HOH:O[2_565]	1.87	0.33
1:A:332:LYS:NZ	2:A:470:HOH:O[4_455]	1.88	0.32
1:A:2:ALA:CB	2:B:514:HOH:O[2_564]	1.92	0.28
1:B:22:GLU:CB	2:A:535:HOH:O[4_555]	1.96	0.24
1:B:261:ARG:NH1	2:B:562:HOH:O[2_665]	2.00	0.20
1:B:261:ARG:NE	2:B:570:HOH:O[2_665]	2.01	0.19
1:A:299:VAL:CG2	2:B:586:HOH:O[4_455]	2.05	0.15
1:B:279:LYS:CE	2:A:459:HOH:O[4_555]	2.06	0.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:ARG:NH2	2:B:500:HOH:O[4_455]	2.11	0.09
1:B:250:GLN:NE2	2:B:481:HOH:O[2_665]	2.12	0.08
1:B:359:LYS:NZ	2:A:471:HOH:O[4_555]	2.12	0.08
1:A:279:LYS:N	2:A:537:HOH:O[4_455]	2.14	0.06
1:A:217:ASP:OD1	2:B:565:HOH:O[2_664]	2.15	0.05
1:A:99:LYS:CE	1:A:361:GLN:O[4_555]	2.15	0.05
2:B:477:HOH:O	2:B:578:HOH:O[2_664]	2.17	0.03
2:A:403:HOH:O	2:B:534:HOH:O[2_564]	2.17	0.03

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	359/361 (99%)	350 (98%)	8 (2%)	1 (0%)	41	37
1	B	359/361 (99%)	345 (96%)	14 (4%)	0	100	100
All	All	718/722 (99%)	695 (97%)	22 (3%)	1 (0%)	51	49

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	263	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	290/292 (99%)	260 (90%)	30 (10%)	7	4
1	B	292/292 (100%)	263 (90%)	29 (10%)	8	4
All	All	582/584 (100%)	523 (90%)	59 (10%)	7	4

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	THR
1	A	7	GLN
1	A	13	ASN
1	A	21	GLN
1	A	22	GLU
1	A	52	ARG
1	A	90	THR
1	A	99	LYS
1	A	102	GLN
1	A	106	LEU
1	A	128	LYS
1	A	136	GLN
1	A	169	SER
1	A	194	SER
1	A	197	LYS
1	A	204	ARG
1	A	227	VAL
1	A	241	SER
1	A	245	GLU
1	A	246	LYS
1	A	253	GLU
1	A	264	ASP
1	A	265	MET
1	A	273	MET
1	A	279	LYS
1	A	281	ASP
1	A	299	VAL
1	A	314	HIS
1	A	333	ASN
1	A	361	GLN
1	B	10	ASP
1	B	32	ILE
1	B	37	LYS
1	B	45	LYS
1	B	51	ASN

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Mol	Chain	Res	Type
1	B	57	GLN
1	B	58	THR
1	B	84	LYS
1	B	89	VAL
1	B	102	GLN
1	B	139	GLN
1	B	153	SER
1	B	163	VAL
1	B	191	VAL
1	B	193	GLN
1	B	197	LYS
1	B	245	GLU
1	B	253	GLU
1	B	265	MET
1	B	273	MET
1	B	279	LYS
1	B	285	SER
1	B	287	SER
1	B	293	LEU
1	B	314	HIS
1	B	332	LYS
1	B	349	ARG
1	B	357	LEU
1	B	359	LYS

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

Mol	Chain	Res	Type
1	A	21	GLN
1	A	35	GLN
1	A	91	GLN
1	A	102	GLN
1	A	152	ASN
1	A	237	ASN
1	A	256	GLN
1	A	361	GLN
1	B	6	GLN
1	B	35	GLN
1	B	50	ASN
1	B	56	GLN
1	B	91	GLN
1	B	102	GLN

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Mol	Chain	Res	Type
1	B	136	GLN
1	B	137	ASN
1	B	139	GLN
1	B	196	GLN
1	B	210	HIS
1	B	275	ASN
1	B	302	ASN
1	B	346	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 carbohydrates 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

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.