Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 12:21 AM EDT

PDB ID	:	1M1Z
Title	:	BETA-LACTAM SYNTHETASE APO ENZYME
Authors	:	Miller, M.T.; Bachmann, B.O.; Townsend, C.A.; Rosenzweig, A.C.
Deposited on	:	2002-06-20
Resolution	:	1.95 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 (i) 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 (1)) were used in the production of this report:

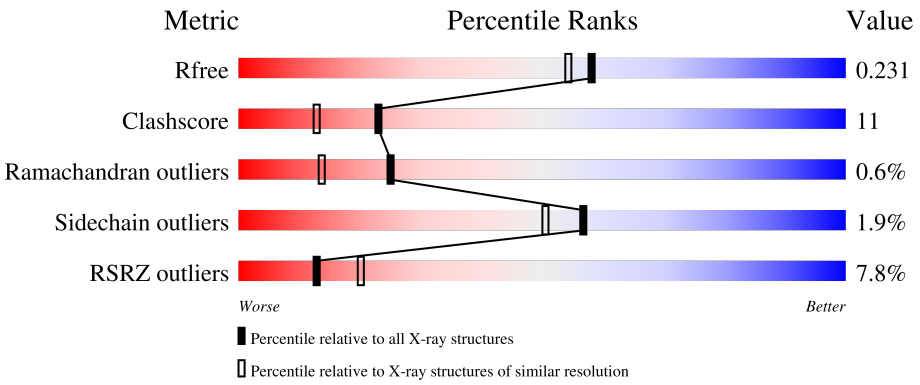
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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 <=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	513	10% 72% 20% • 6%
1	B	513	5% 74% 20% • •

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 7883 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-LACTAM SYNTHETASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	480	3604	2254	659	683	8	0	0	0
1	B	490	3676	2296	674	698	8	0	0	0

- Molecule 2 is water.

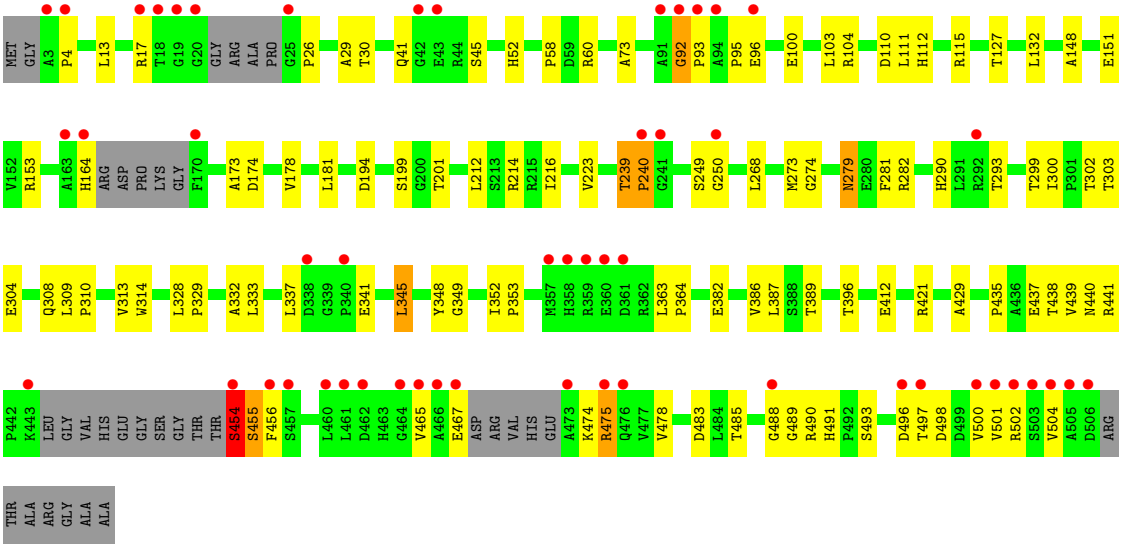
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	268	268	268	0	0
2	B	335	335	335	0	0

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.

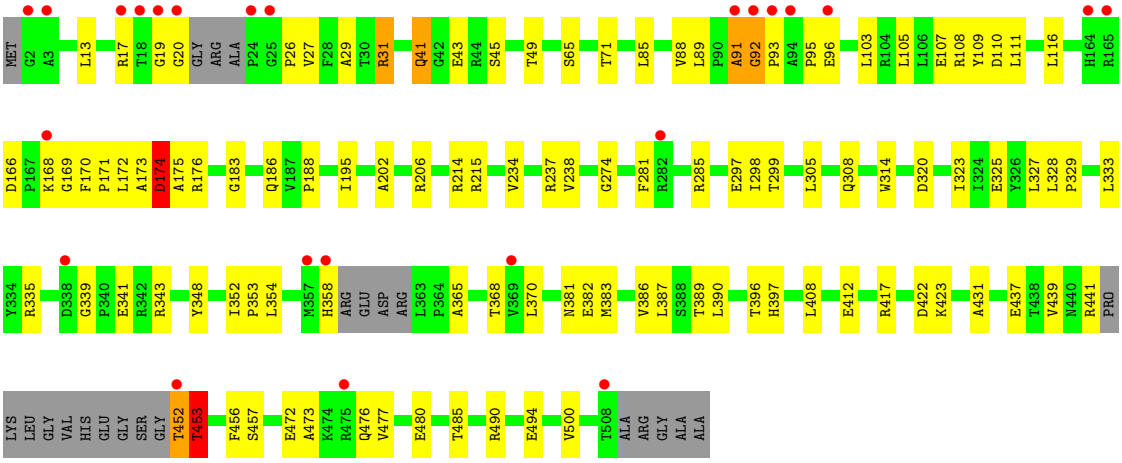
• Molecule 1: BETA-LACTAM SYNTHETASE

Chain A:



• Molecule 1: BETA-LACTAM SYNTHETASE

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	61.18Å 97.47Å 80.97Å 90.00° 90.42° 90.00°	Depositor
Resolution (Å)	23.88 – 1.95 29.19 – 1.90	Depositor EDS
% Data completeness (in resolution range)	91.2 (23.88-1.95) 91.4 (29.19-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	0.00 (at 1.91Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.197 , 0.231 0.197 , 0.231	Depositor DCC
R_{free} test set	6156 reflections (8.23%)	wwPDB-VP
Wilson B-factor (Å^2)	22.2	Xtriage
Anisotropy	0.341	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 55.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.036 for h,-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7883	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.82% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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	0.32	0/3674	0.62	3/5012 (0.1%)
1	B	0.45	2/3749 (0.1%)	0.80	13/5116 (0.3%)
All	All	0.39	2/7423 (0.0%)	0.72	16/10128 (0.2%)

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	4
All	All	0	5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	93	PRO	N-CD	13.49	1.66	1.47
1	B	92	GLY	C-N	6.54	1.46	1.34

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	91	ALA	C-N-CA	17.01	158.01	122.30
1	B	92	GLY	O-C-N	-15.30	92.03	121.10
1	B	93	PRO	CA-N-CD	-13.68	92.34	111.50
1	B	92	GLY	CA-C-N	10.34	146.04	117.10
1	B	174	ASP	CB-CG-OD1	7.94	125.45	118.30
1	B	91	ALA	CA-C-N	7.80	131.81	116.20
1	A	454	SER	O-C-N	-7.54	110.64	122.70
1	B	93	PRO	N-CA-CB	7.47	112.26	103.30
1	B	174	ASP	OD1-CG-OD2	-7.15	109.72	123.30
1	A	455	SER	CB-CA-C	6.99	123.38	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	91	ALA	CA-C-O	-6.29	106.90	120.10
1	B	92	GLY	N-CA-C	5.82	127.64	113.10
1	B	173	ALA	C-N-CA	5.66	135.85	121.70
1	A	454	SER	C-N-CA	-5.65	107.57	121.70
1	B	453	THR	CB-CA-C	-5.45	96.90	111.60
1	B	93	PRO	CB-CA-C	5.32	125.30	112.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	454	SER	Mainchain
1	B	174	ASP	Sidechain
1	B	452	THR	Mainchain
1	B	453	THR	Mainchain
1	B	91	ALA	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	3604	0	3595	79	0
1	B	3676	0	3663	91	0
2	A	268	0	0	4	0
2	B	335	0	0	4	0
All	All	7883	0	7258	165	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 11.

All (165) 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:41:GLN:HE21	1:B:45:SER:HB3	1.28	0.93
1:A:92:GLY:H	1:A:93:PRO:HD2	1.34	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:308:GLN:NE2	1:B:335:ARG:HH11	1.73	0.86
1:A:112:HIS:HD2	1:A:115:ARG:HE	1.23	0.85
1:B:174:ASP:O	1:B:188:PRO:HG3	1.79	0.82
1:B:31:ARG:HH11	1:B:31:ARG:HB2	1.45	0.81
1:A:41:GLN:HG2	1:A:45:SER:OG	1.86	0.75
1:A:216:ILE:HD11	1:B:116:LEU:HD22	1.70	0.74
1:A:148:ALA:HB3	1:A:151:GLU:HG3	1.70	0.73
1:A:216:ILE:HD12	1:B:88:VAL:HG11	1.72	0.72
1:B:186:GLN:HE22	1:B:381:ASN:HD21	1.37	0.72
1:B:174:ASP:O	1:B:188:PRO:CG	2.38	0.71
1:B:383:MET:HG2	1:B:397:HIS:CD2	2.25	0.71
1:B:41:GLN:NE2	1:B:45:SER:HB3	2.06	0.69
1:B:348:TYR:CE2	1:B:383:MET:HG3	2.28	0.69
1:B:308:GLN:HE21	1:B:335:ARG:HD3	1.60	0.66
1:B:328:LEU:HB2	1:B:329:PRO:HD3	1.79	0.64
1:A:95:PRO:HB3	1:A:100:GLU:HB3	1.79	0.64
1:A:314:TRP:CD1	1:A:485:THR:HB	2.34	0.62
1:B:214:ARG:NH2	1:B:370:LEU:HD12	2.14	0.62
1:B:27:VAL:O	1:B:27:VAL:HG23	1.99	0.61
1:A:13:LEU:HD23	1:A:26:PRO:HG3	1.83	0.60
1:B:169:GLY:HA3	1:B:183:GLY:O	2.02	0.59
1:B:103:LEU:O	1:B:107:GLU:HG3	2.03	0.59
1:A:456:PHE:CE2	1:A:474:LYS:HD3	2.38	0.59
1:B:308:GLN:NE2	1:B:335:ARG:NH1	2.49	0.59
1:A:239:THR:HG22	1:A:240:PRO:HD2	1.84	0.59
1:A:273:MET:HB2	1:A:333:LEU:HD13	1.83	0.59
1:B:176:ARG:HD2	2:B:657:HOH:O	2.01	0.58
1:B:41:GLN:HE21	1:B:45:SER:CB	2.08	0.58
1:B:437:GLU:HG2	1:B:441:ARG:NH2	2.19	0.58
1:A:437:GLU:O	1:A:441:ARG:HB2	2.04	0.57
1:B:314:TRP:CD1	1:B:485:THR:HB	2.39	0.57
1:A:456:PHE:CD2	1:A:474:LYS:HD3	2.40	0.57
1:B:26:PRO:HG3	1:B:49:THR:HG21	1.87	0.57
1:A:52:HIS:NE2	1:A:58:PRO:HG3	2.19	0.56
1:B:352:ILE:O	1:B:370:LEU:HD23	2.05	0.56
1:A:279:ASN:HD22	1:A:281:PHE:H	1.53	0.56
1:A:250:GLY:O	1:A:441:ARG:HD2	2.06	0.56
1:B:325:GLU:HG2	1:B:456:PHE:HD2	1.72	0.55
1:B:298:ILE:N	1:B:298:ILE:HD12	2.22	0.55
1:A:309:LEU:HD11	1:A:456:PHE:CE1	2.41	0.55
1:B:437:GLU:HG2	1:B:441:ARG:HH22	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:308:GLN:NE2	1:B:335:ARG:HD3	2.22	0.55
1:B:354:LEU:HD21	1:B:408:LEU:HD22	1.88	0.54
1:B:490:ARG:HG2	1:B:494:GLU:HG3	1.90	0.54
1:B:327:LEU:HD13	1:B:387:LEU:HD21	1.87	0.54
1:B:386:VAL:HA	1:B:389:THR:OG1	2.07	0.54
1:A:92:GLY:N	1:A:93:PRO:HD2	2.14	0.53
1:A:112:HIS:CD2	1:A:115:ARG:HE	2.14	0.53
1:B:348:TYR:OH	1:B:382:GLU:HG3	2.08	0.53
1:B:65:SER:HB3	1:B:71:THR:HB	1.90	0.53
1:B:453:THR:CG2	1:B:457:SER:HB2	2.39	0.53
1:B:472:GLU:HG3	1:B:476:GLN:HE21	1.73	0.53
1:B:215:ARG:HH11	1:B:215:ARG:HG3	1.74	0.52
1:A:313:VAL:HG11	1:A:478:VAL:HG13	1.91	0.52
1:B:353:PRO:HA	1:B:370:LEU:HD21	1.92	0.51
1:B:422:ASP:OD2	1:B:423:LYS:HE2	2.09	0.51
1:A:454:SER:O	1:A:455:SER:C	2.48	0.51
1:B:297:GLU:C	1:B:298:ILE:HD12	2.30	0.51
1:B:348:TYR:HH	1:B:382:GLU:CD	2.13	0.51
1:B:85:LEU:O	1:B:89:LEU:HD13	2.11	0.51
1:A:302:THR:CG2	1:A:455:SER:HB2	2.41	0.51
1:B:480:GLU:OE1	1:B:500:VAL:HG13	2.11	0.50
1:B:341:GLU:HG2	2:B:542:HOH:O	2.10	0.50
1:B:382:GLU:HG2	2:B:827:HOH:O	2.10	0.50
1:B:453:THR:HG22	1:B:457:SER:HB2	1.93	0.50
1:A:349:GLY:O	1:A:353:PRO:HD2	2.11	0.50
1:A:212:LEU:HD13	1:B:206:ARG:HB2	1.93	0.49
1:A:52:HIS:CD2	1:A:58:PRO:HG3	2.48	0.49
1:B:327:LEU:HD22	1:B:387:LEU:HD13	1.95	0.49
1:A:386:VAL:HA	1:A:389:THR:OG1	2.12	0.48
1:B:85:LEU:O	1:B:88:VAL:HG22	2.13	0.48
1:A:30:THR:HG23	1:A:389:THR:HB	1.96	0.48
1:A:112:HIS:HE1	1:B:368:THR:OG1	1.97	0.48
1:A:345:LEU:HD22	1:A:396:THR:CG2	2.43	0.48
1:B:358:HIS:HB3	1:B:417:ARG:NH2	2.28	0.48
1:A:17:ARG:NH1	1:A:151:GLU:HB3	2.29	0.48
1:B:370:LEU:C	1:B:370:LEU:HD13	2.35	0.48
1:A:148:ALA:HB3	1:A:151:GLU:CG	2.41	0.47
1:B:353:PRO:HA	1:B:370:LEU:CD2	2.44	0.47
1:A:29:ALA:HA	1:A:314:TRP:CH2	2.50	0.47
1:B:166:ASP:O	1:B:168:LYS:HD2	2.14	0.47
1:B:325:GLU:OE2	1:B:456:PHE:HB3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:ALA:HA	1:B:314:TRP:CH2	2.49	0.47
1:A:4:PRO:HB3	2:A:717:HOH:O	2.15	0.47
1:B:170:PHE:HB3	1:B:171:PRO:HD2	1.95	0.47
1:B:195:ILE:HG12	1:B:202:ALA:HB2	1.97	0.47
1:A:110:ASP:CG	1:A:111:LEU:H	2.18	0.47
1:B:41:GLN:HB2	1:B:45:SER:HB3	1.97	0.47
1:A:73:ALA:HB2	1:A:103:LEU:HD13	1.97	0.46
1:B:308:GLN:HE22	1:B:335:ARG:NH1	2.12	0.46
1:B:473:ALA:O	1:B:477:VAL:HG23	2.15	0.46
1:A:435:PRO:HG2	1:A:438:THR:OG1	2.16	0.46
1:A:249:SER:HB3	2:A:519:HOH:O	2.16	0.46
1:B:305:LEU:C	1:B:305:LEU:HD23	2.36	0.46
1:B:431:ALA:HA	1:B:439:VAL:HG11	1.98	0.46
1:A:303:THR:HG23	1:A:304:GLU:N	2.30	0.46
1:B:308:GLN:HE21	1:B:335:ARG:HH11	1.57	0.46
1:B:308:GLN:HE22	1:B:335:ARG:HH11	1.60	0.46
1:A:127:THR:HG23	1:A:127:THR:O	2.15	0.46
1:A:496:ASP:O	1:A:500:VAL:HG23	2.16	0.46
1:A:223:VAL:HG13	1:A:429:ALA:HA	1.97	0.46
1:A:308:GLN:HB2	1:A:328:LEU:HD22	1.97	0.45
1:B:358:HIS:HE2	1:B:365:ALA:HB3	1.82	0.45
1:A:214:ARG:HB2	1:B:116:LEU:HD23	1.97	0.45
1:A:132:LEU:HD23	1:A:194:ASP:HA	1.99	0.45
1:A:268:LEU:O	1:A:293:THR:HB	2.17	0.45
1:A:497:THR:O	1:A:501:VAL:HG23	2.17	0.45
1:B:17:ARG:NH2	1:B:20:GLY:HA2	2.32	0.45
1:A:313:VAL:CG1	1:A:478:VAL:HG13	2.47	0.45
1:B:333:LEU:C	1:B:333:LEU:HD23	2.37	0.44
1:A:498:ASP:HB3	1:A:502:ARG:NH2	2.32	0.44
1:A:96:GLU:HG2	1:A:100:GLU:OE1	2.17	0.44
1:B:89:LEU:HD11	1:B:105:LEU:HD23	1.99	0.44
1:B:390:LEU:C	1:B:390:LEU:HD12	2.38	0.44
1:B:281:PHE:O	1:B:285:ARG:HG3	2.18	0.44
1:A:500:VAL:O	1:A:504:VAL:HG23	2.17	0.44
1:A:348:TYR:HH	1:A:382:GLU:CD	2.21	0.43
1:A:95:PRO:HG3	1:A:104:ARG:HG3	2.00	0.43
1:A:178:VAL:HG11	1:A:181:LEU:HD12	2.00	0.43
1:B:108:ARG:NH1	1:B:109:TYR:OH	2.52	0.43
1:A:290:HIS:CG	1:A:435:PRO:HD3	2.54	0.43
1:A:421:ARG:HH21	1:A:440:ASN:HA	1.84	0.43
1:B:110:ASP:CG	1:B:111:LEU:H	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:465:VAL:HG12	1:A:467:GLU:H	1.84	0.43
1:B:348:TYR:OH	1:B:382:GLU:CD	2.56	0.43
1:A:60:ARG:HG3	2:A:668:HOH:O	2.18	0.43
1:A:173:ALA:O	1:A:174:ASP:HB2	2.18	0.43
1:A:475:ARG:HG2	1:A:475:ARG:HH11	1.83	0.43
1:B:89:LEU:HD11	1:B:105:LEU:CD2	2.49	0.43
1:B:237:ARG:O	1:B:343:ARG:HD3	2.18	0.43
1:B:422:ASP:C	1:B:423:LYS:HG2	2.39	0.43
1:A:92:GLY:H	1:A:93:PRO:CD	2.17	0.42
1:A:491:HIS:HD2	1:A:493:SER:H	1.68	0.42
1:A:153:ARG:HE	1:A:164:HIS:CD2	2.38	0.42
1:B:352:ILE:HB	1:B:353:PRO:CD	2.49	0.42
1:B:43:GLU:H	1:B:43:GLU:HG2	1.70	0.42
1:B:341:GLU:OE1	1:B:341:GLU:N	2.53	0.42
1:A:300:ILE:HD13	1:A:332:ALA:HB1	2.02	0.42
1:A:352:ILE:HB	1:A:353:PRO:CD	2.50	0.42
1:B:320:ASP:HB3	1:B:323:ILE:HD13	2.02	0.41
1:A:348:TYR:CG	1:A:349:GLY:N	2.89	0.41
1:A:199:SER:OG	1:A:201:THR:HG22	2.20	0.41
1:A:341:GLU:H	1:A:341:GLU:HG3	1.64	0.41
1:B:172:LEU:HB2	1:B:175:ALA:HB3	2.01	0.41
1:B:234:VAL:O	1:B:238:VAL:HG23	2.20	0.41
1:A:26:PRO:HD3	2:A:657:HOH:O	2.21	0.41
1:A:308:GLN:HG3	1:A:332:ALA:HB2	2.02	0.41
1:B:237:ARG:HB3	1:B:396:THR:HG21	2.02	0.41
1:A:216:ILE:HD13	1:A:412:GLU:HG2	2.01	0.41
1:B:174:ASP:O	1:B:188:PRO:HG2	2.17	0.41
1:A:483:ASP:O	1:A:488:GLY:N	2.54	0.41
1:A:274:GLY:O	1:A:299:THR:HA	2.20	0.41
1:A:421:ARG:HH22	1:A:439:VAL:HG12	1.86	0.41
1:A:352:ILE:HB	1:A:353:PRO:HD3	2.02	0.41
1:B:274:GLY:O	1:B:299:THR:HA	2.20	0.41
1:A:309:LEU:N	1:A:310:PRO:HD2	2.36	0.40
1:A:328:LEU:N	1:A:329:PRO:HD2	2.36	0.40
1:A:490:ARG:HH11	1:A:490:ARG:HG2	1.85	0.40
1:B:13:LEU:HD23	1:B:26:PRO:HB3	2.03	0.40
1:B:215:ARG:HG3	1:B:215:ARG:NH1	2.36	0.40
1:B:490:ARG:CG	1:B:494:GLU:HG3	2.49	0.40
1:A:363:LEU:N	1:A:364:PRO:CD	2.85	0.40
1:B:95:PRO:HB3	2:B:810:HOH:O	2.21	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	470/513 (92%)	452 (96%)	15 (3%)	3 (1%)	25	14
1	B	482/513 (94%)	463 (96%)	16 (3%)	3 (1%)	25	14
All	All	952/1026 (93%)	915 (96%)	31 (3%)	6 (1%)	25	14

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	92	GLY
1	B	339	GLY
1	B	19	GLY
1	A	92	GLY
1	A	489	GLY
1	A	240	PRO

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	373/395 (94%)	365 (98%)	8 (2%)	53	46
1	B	381/395 (96%)	375 (98%)	6 (2%)	62	58
All	All	754/790 (95%)	740 (98%)	14 (2%)	57	50

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	239	THR
1	A	279	ASN
1	A	282	ARG
1	A	337	LEU
1	A	345	LEU
1	A	387	LEU
1	A	454	SER
1	A	475	ARG
1	B	31	ARG
1	B	41	GLN
1	B	96	GLU
1	B	174	ASP
1	B	412	GLU
1	B	452	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	112	HIS
1	A	118	ASN
1	A	164	HIS
1	A	236	GLN
1	A	279	ASN
1	A	491	HIS
1	B	41	GLN
1	B	236	GLN
1	B	308	GLN
1	B	381	ASN
1	B	440	ASN
1	B	476	GLN

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, 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	480/513 (93%)	0.64	52 (10%)	5	9	13, 26, 63, 76	0
1	B	490/513 (95%)	0.33	24 (4%)	29	39	14, 23, 45, 68	0
All	All	970/1026 (94%)	0.48	76 (7%)	13	20	13, 24, 55, 76	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	3	ALA	10.9
1	A	465	VAL	7.9
1	B	91	ALA	7.5
1	A	18	THR	7.0
1	A	4	PRO	6.5
1	A	163	ALA	6.4
1	B	20	GLY	5.9
1	B	93	PRO	5.9
1	A	170	PHE	5.6
1	A	460	LEU	5.5
1	A	20	GLY	5.4
1	A	359	ARG	5.3
1	A	461	LEU	5.3
1	A	506	ASP	5.2
1	B	2	GLY	5.2
1	A	94	ALA	5.1
1	A	500	VAL	5.0
1	B	92	GLY	5.0
1	A	502	ARG	5.0
1	B	358	HIS	4.8
1	B	165	ARG	4.8
1	A	466	ALA	4.6
1	A	164	HIS	4.6
1	B	164	HIS	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	93	PRO	4.4
1	A	443	LYS	4.2
1	A	240	PRO	4.2
1	B	24	PRO	4.2
1	B	452	THR	4.1
1	A	91	ALA	3.8
1	A	19	GLY	3.8
1	B	94	ALA	3.8
1	A	467	GLU	3.7
1	A	473	ALA	3.7
1	A	496	ASP	3.6
1	A	454	SER	3.6
1	A	25	GLY	3.6
1	A	241	GLY	3.4
1	B	18	THR	3.3
1	A	360	GLU	3.1
1	A	357	MET	3.1
1	A	358	HIS	3.0
1	B	168	LYS	3.0
1	B	3	ALA	3.0
1	A	96	GLU	2.9
1	A	505	ALA	2.9
1	A	456	PHE	2.8
1	B	282	ARG	2.8
1	A	43	GLU	2.8
1	B	338	ASP	2.8
1	A	42	GLY	2.8
1	B	475	ARG	2.8
1	A	92	GLY	2.7
1	B	17	ARG	2.7
1	B	19	GLY	2.5
1	B	357	MET	2.5
1	A	250	GLY	2.5
1	A	17	ARG	2.5
1	A	464	GLY	2.4
1	B	369	VAL	2.4
1	A	497	THR	2.4
1	A	503	SER	2.4
1	A	361	ASP	2.4
1	A	501	VAL	2.4
1	A	475	ARG	2.4
1	B	508	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	292	ARG	2.3
1	A	504	VAL	2.3
1	B	25	GLY	2.3
1	B	96	GLU	2.3
1	A	457	SER	2.1
1	A	338	ASP	2.1
1	A	462	ASP	2.1
1	A	488	GLY	2.1
1	A	476	GLN	2.1
1	A	340	PRO	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.