Full wwPDB X-ray Structure Validation Report (i)

Jun 13, 2024 – 09:38 AM EDT

PDB ID	:	1MIV
Title	:	Crystal structure of Bacillus stearothermophilus CCA-adding enzyme
Authors	:	Li, F.; Xiong, Y.; Wang, J.; Cho, H.D.; Weiner, A.M.; Steitz, T.A.
Deposited on	:	2002-08-23
Resolution	:	3.50 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 (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:

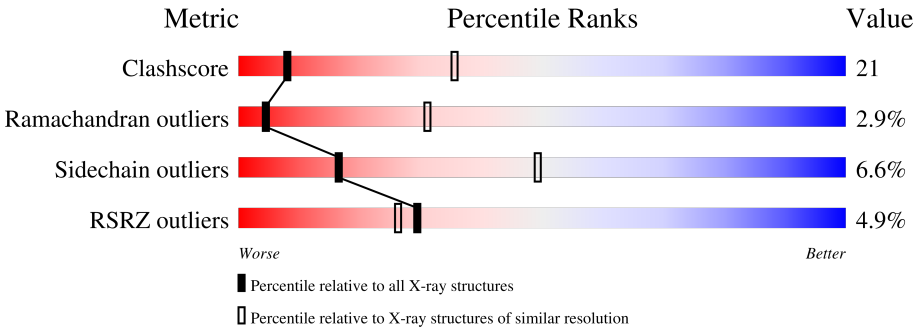
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 3.50 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	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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	404	4% 54% 38% 5% •
1	B	404	5% 56% 35% 6% •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6264 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 tRNA CCA-adding enzyme.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	395	Total	C	N	O	S	Se	0	0	0
			3113	1986	560	555	2	10			
1	B	395	Total	C	N	O	S	Se	0	0	0
			3113	1986	560	555	2	10			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		

- Molecule 3 is water.

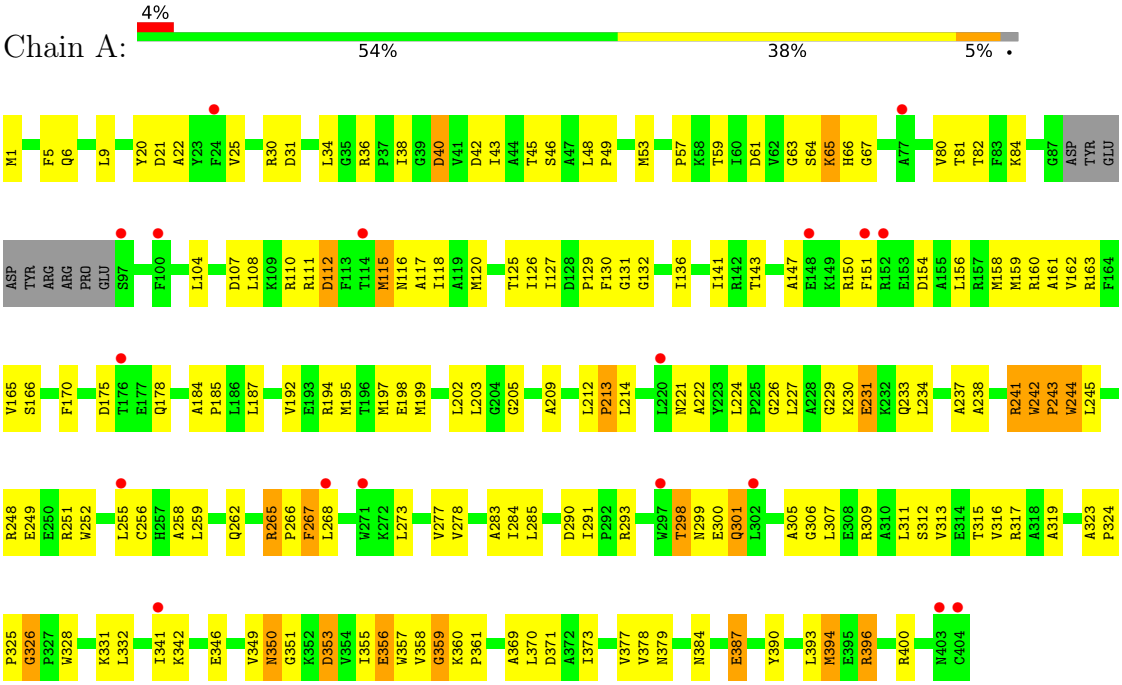
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	18	Total	O	0	0
			18	18		
3	B	18	Total	O	0	0
			18	18		

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.

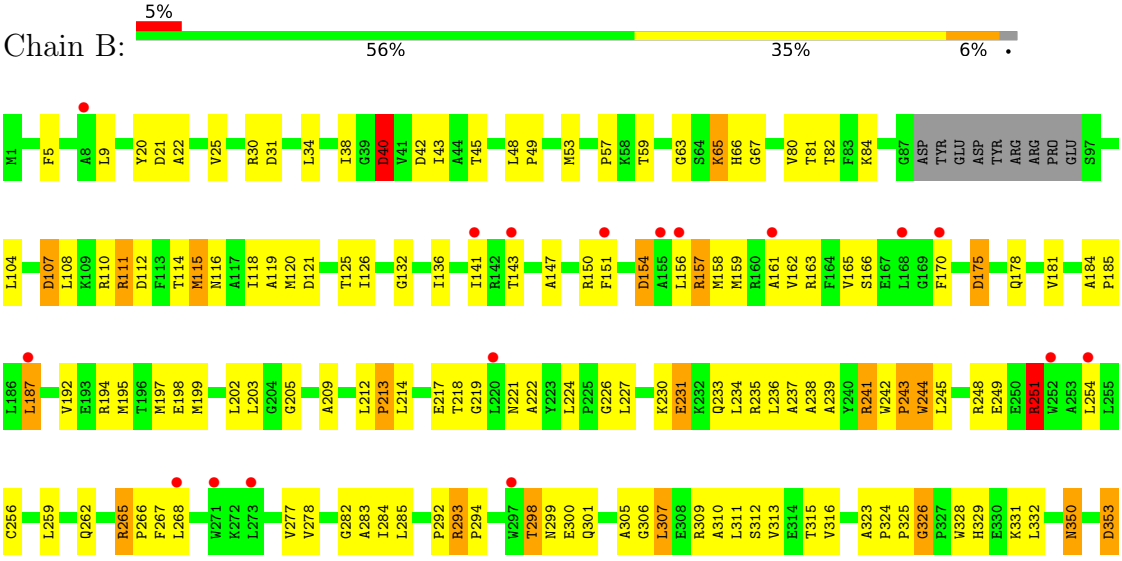
• Molecule 1: tRNA CCA-adding enzyme

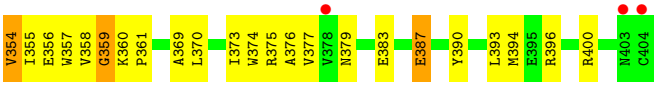
Chain A:



• Molecule 1: tRNA CCA-adding enzyme

Chain B:




V354
I355
E356
W357
V358
G359
K360
P361
A369
L370
I373
W374
R375
A376
V377
V378
N379
E383
E387
Y390
L393
M394
E395
R396
R400
N403
C404

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	105.86Å 105.86Å 183.66Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.50 82.03 – 3.41	Depositor EDS
% Data completeness (in resolution range)	99.5 (20.00-3.50) 88.5 (82.03-3.41)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	1.24 (at 3.41Å)	Xtriage
Refinement program	REFMAC 5.1.17	Depositor
R, R_{free}	0.289 , 0.328 0.266 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	131.8	Xtriage
Anisotropy	0.148	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 104.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.032 for -h,-k,l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6264	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 32.83 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.8258e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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	0.67	1/3172 (0.0%)	0.86	11/4278 (0.3%)
1	B	0.65	2/3172 (0.1%)	0.83	11/4278 (0.3%)
All	All	0.66	3/6344 (0.0%)	0.84	22/8556 (0.3%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	244	TRP	CB-CG	6.71	1.62	1.50
1	A	244	TRP	CB-CG	6.05	1.61	1.50
1	B	241	ARG	CG-CD	5.16	1.64	1.51

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	31	ASP	CB-CG-OD2	6.12	123.80	118.30
1	A	154	ASP	CB-CG-OD2	6.04	123.73	118.30
1	B	353	ASP	CB-CG-OD2	5.92	123.63	118.30
1	B	251	ARG	NE-CZ-NH2	-5.73	117.44	120.30
1	A	42	ASP	CB-CG-OD2	5.71	123.44	118.30
1	A	241	ARG	NE-CZ-NH2	-5.71	117.45	120.30
1	B	40	ASP	CB-CG-OD2	5.66	123.40	118.30
1	B	42	ASP	CB-CG-OD2	5.66	123.40	118.30
1	A	107	ASP	CB-CG-OD2	5.65	123.39	118.30
1	B	154	ASP	CB-CG-OD2	5.57	123.32	118.30
1	A	353	ASP	CB-CG-OD2	5.45	123.21	118.30
1	B	292	PRO	N-CD-CG	-5.39	95.12	103.20
1	A	290	ASP	CB-CG-OD2	5.29	123.06	118.30
1	B	121	ASP	CB-CG-OD2	5.24	123.02	118.30
1	B	112	ASP	CB-CG-OD2	5.17	122.95	118.30
1	B	175	ASP	CB-CG-OD2	5.14	122.92	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	393	LEU	CB-CG-CD2	-5.09	102.35	111.00
1	B	107	ASP	CB-CG-OD2	5.09	122.88	118.30
1	A	371	ASP	CB-CG-OD2	5.05	122.84	118.30
1	A	317	ARG	NE-CZ-NH2	-5.05	117.78	120.30
1	A	112	ASP	CB-CG-OD2	5.00	122.80	118.30
1	A	40	ASP	CB-CG-OD2	5.00	122.80	118.30

There are no chirality outliers.

There are no planarity outliers.

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	3113	0	3161	138	0
1	B	3113	0	3161	131	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	18	0	0	0	0
3	B	18	0	0	0	0
All	All	6264	0	6322	269	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 21.

All (269) 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:360:LYS:HG3	1:B:361:PRO:HD2	1.27	1.14
1:B:199:MSE:HE1	1:B:202:LEU:HD22	1.42	1.01
1:A:199:MSE:HE1	1:A:202:LEU:HD22	1.44	0.99
1:B:370:LEU:HA	1:B:373:ILE:HD12	1.48	0.92
1:A:360:LYS:HG3	1:A:361:PRO:HD2	1.54	0.90
1:A:34:LEU:HD13	1:A:136:ILE:HG23	1.56	0.88
1:B:373:ILE:O	1:B:377:VAL:HG23	1.73	0.88
1:A:30:ARG:HD3	1:A:115:MSE:HE3	1.56	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:ILE:O	1:A:377:VAL:HG23	1.75	0.86
1:A:199:MSE:CE	1:A:202:LEU:HD22	2.06	0.85
1:A:118:ILE:HD12	1:A:118:ILE:H	1.40	0.83
1:A:370:LEU:HA	1:A:373:ILE:HD12	1.60	0.83
1:B:312:SER:O	1:B:316:VAL:HG23	1.79	0.83
1:B:199:MSE:CE	1:B:202:LEU:HD22	2.08	0.83
1:A:312:SER:O	1:A:316:VAL:HG23	1.77	0.82
1:A:192:VAL:HA	1:A:195:MSE:HE3	1.62	0.82
1:A:249:GLU:CD	1:A:249:GLU:H	1.82	0.81
1:A:199:MSE:HE2	1:A:203:LEU:HG	1.62	0.79
1:B:249:GLU:H	1:B:249:GLU:CD	1.86	0.78
1:B:199:MSE:HE2	1:B:203:LEU:HG	1.65	0.78
1:A:115:MSE:HE2	1:A:116:ASN:OD1	1.84	0.77
1:A:159:MSE:HE3	1:A:198:GLU:HB2	1.65	0.77
1:B:30:ARG:HD3	1:B:115:MSE:HE3	1.65	0.77
1:B:159:MSE:HE3	1:B:198:GLU:HB2	1.70	0.73
1:A:30:ARG:HD3	1:A:115:MSE:CE	2.20	0.72
1:B:356:GLU:HG3	1:B:356:GLU:O	1.88	0.71
1:B:120:MSE:HE3	1:B:126:ILE:HD11	1.72	0.71
1:A:118:ILE:HD12	1:A:118:ILE:N	2.04	0.71
1:B:30:ARG:HD3	1:B:115:MSE:CE	2.21	0.70
1:A:242:TRP:HB2	1:A:243:PRO:CD	2.21	0.69
1:B:115:MSE:HE2	1:B:116:ASN:OD1	1.91	0.69
1:A:284:ILE:HG23	1:A:313:VAL:HG22	1.75	0.69
1:B:283:ALA:HB1	1:B:309:ARG:NE	2.09	0.68
1:B:192:VAL:HA	1:B:195:MSE:HE3	1.76	0.68
1:B:242:TRP:HB2	1:B:243:PRO:CD	2.24	0.68
1:A:203:LEU:HB3	1:A:251:ARG:HG2	1.75	0.67
1:A:358:VAL:HG12	1:A:358:VAL:O	1.93	0.67
1:B:268:LEU:HB2	1:B:278:VAL:HG13	1.77	0.67
1:B:49:PRO:HD3	1:B:82:THR:OG1	1.95	0.66
1:A:53:MSE:HG2	1:A:59:THR:HG21	1.78	0.66
1:B:203:LEU:HB3	1:B:251:ARG:HG2	1.77	0.66
1:B:360:LYS:HG3	1:B:361:PRO:CD	2.17	0.65
1:B:358:VAL:HG12	1:B:358:VAL:O	1.97	0.65
1:A:30:ARG:CD	1:A:115:MSE:HE3	2.27	0.64
1:A:161:ALA:O	1:A:165:VAL:HG23	1.98	0.64
1:B:161:ALA:O	1:B:165:VAL:HG23	1.98	0.64
1:B:48:LEU:HD23	1:B:82:THR:HG21	1.79	0.63
1:A:120:MSE:HE3	1:A:126:ILE:HD11	1.80	0.63
1:A:255:LEU:HD12	1:A:255:LEU:O	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:284:ILE:HG23	1:B:313:VAL:HG22	1.80	0.63
1:B:118:ILE:HD12	1:B:118:ILE:H	1.62	0.63
1:B:5:PHE:HE1	1:B:38:ILE:HD13	1.64	0.62
1:A:369:ALA:O	1:A:373:ILE:HG13	1.99	0.62
1:A:104:LEU:HD11	1:A:108:LEU:HD21	1.82	0.61
1:A:298:THR:OG1	1:A:301:GLN:NE2	2.33	0.61
1:A:355:ILE:C	1:A:357:TRP:H	2.04	0.61
1:A:192:VAL:HA	1:A:195:MSE:CE	2.29	0.60
1:A:328:TRP:HA	1:A:328:TRP:CE3	2.35	0.60
1:B:156:LEU:O	1:B:159:MSE:HB2	2.02	0.60
1:B:63:GLY:HA2	1:B:65:LYS:HE2	1.84	0.60
1:B:53:MSE:HG2	1:B:59:THR:HG21	1.84	0.60
1:B:354:VAL:HG22	1:B:393:LEU:CD2	2.31	0.60
1:B:25:VAL:HG21	1:B:111:ARG:HH22	1.67	0.60
1:A:156:LEU:O	1:A:159:MSE:HB2	2.01	0.59
1:B:234:LEU:O	1:B:237:ALA:HB3	2.03	0.59
1:B:298:THR:O	1:B:299:ASN:C	2.40	0.59
1:B:353:ASP:O	1:B:357:TRP:CG	2.56	0.59
1:B:256:CYS:HB2	1:B:285:LEU:HD11	1.84	0.58
1:A:63:GLY:HA2	1:A:65:LYS:HE2	1.85	0.58
1:B:67:GLY:O	1:B:81:THR:HA	2.03	0.58
1:A:256:CYS:O	1:A:259:LEU:N	2.29	0.58
1:B:84:LYS:O	1:B:110:ARG:HD3	2.04	0.58
1:A:300:GLU:HG2	1:A:379:ASN:HD21	1.69	0.58
1:B:166:SER:OG	1:B:205:GLY:HA3	2.03	0.58
1:A:25:VAL:HG21	1:A:111:ARG:HH22	1.69	0.57
1:B:194:ARG:HA	1:B:197:MSE:HE2	1.85	0.57
1:B:248:ARG:HD3	1:B:277:VAL:HG21	1.86	0.57
1:B:242:TRP:HB2	1:B:243:PRO:HD3	1.86	0.57
1:A:48:LEU:HD23	1:A:82:THR:HG21	1.87	0.56
1:B:30:ARG:CD	1:B:115:MSE:HE3	2.34	0.56
1:B:265:ARG:HB3	1:B:266:PRO:HD3	1.86	0.56
1:B:298:THR:O	1:B:301:GLN:N	2.38	0.56
1:A:199:MSE:HE3	1:A:202:LEU:HB3	1.86	0.56
1:A:49:PRO:HD3	1:A:82:THR:OG1	2.06	0.55
1:B:370:LEU:HA	1:B:373:ILE:CD1	2.29	0.55
1:A:84:LYS:O	1:A:110:ARG:HD3	2.07	0.55
1:B:163:ARG:O	1:B:166:SER:N	2.39	0.55
1:B:298:THR:N	1:B:301:GLN:HE21	2.05	0.54
1:A:143:THR:HG21	1:A:147:ALA:HA	1.88	0.54
1:B:118:ILE:HD12	1:B:118:ILE:N	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:ALA:HB1	1:A:309:ARG:NE	2.22	0.54
1:A:325:PRO:O	1:A:326:GLY:C	2.46	0.54
1:A:268:LEU:HB2	1:A:278:VAL:HG13	1.89	0.54
1:B:300:GLU:HG2	1:B:379:ASN:HD21	1.72	0.54
1:B:245:LEU:N	1:B:245:LEU:HD23	2.23	0.54
1:A:1:MSE:HE3	1:A:9:LEU:CD2	2.38	0.54
1:B:224:LEU:HB2	1:B:227:LEU:HD12	1.90	0.53
1:B:199:MSE:HE3	1:B:202:LEU:HB3	1.90	0.53
1:B:104:LEU:HD11	1:B:108:LEU:HD21	1.89	0.53
1:A:298:THR:O	1:A:299:ASN:C	2.47	0.53
1:A:67:GLY:O	1:A:81:THR:HA	2.09	0.53
1:A:49:PRO:O	1:A:53:MSE:HG3	2.09	0.53
1:A:242:TRP:HB2	1:A:243:PRO:HD2	1.90	0.53
1:B:212:LEU:HB2	1:B:213:PRO:HD3	1.90	0.53
1:A:224:LEU:HB2	1:A:227:LEU:HD12	1.89	0.52
1:A:84:LYS:HG3	1:A:110:ARG:NE	2.24	0.52
1:A:1:MSE:HE3	1:A:9:LEU:HD21	1.91	0.52
1:A:131:GLY:O	1:A:132:GLY:C	2.46	0.52
1:A:163:ARG:HD3	1:A:198:GLU:OE2	2.10	0.52
1:B:194:ARG:HG2	1:B:197:MSE:CE	2.40	0.52
1:B:298:THR:H	1:B:301:GLN:HE21	1.58	0.52
1:A:353:ASP:O	1:A:357:TRP:CG	2.62	0.52
1:A:120:MSE:HG3	1:A:126:ILE:HD13	1.91	0.51
1:B:237:ALA:O	1:B:238:ALA:C	2.48	0.51
1:A:234:LEU:O	1:A:237:ALA:HB3	2.10	0.51
1:A:242:TRP:CB	1:A:243:PRO:CD	2.88	0.51
1:B:143:THR:HG21	1:B:147:ALA:HA	1.91	0.51
1:A:165:VAL:HG13	1:A:170:PHE:O	2.10	0.51
1:B:298:THR:O	1:B:300:GLU:N	2.43	0.51
1:A:342:LYS:N	1:A:346:GLU:OE2	2.34	0.51
1:B:300:GLU:CG	1:B:379:ASN:HD21	2.24	0.51
1:B:298:THR:CB	1:B:301:GLN:HG3	2.41	0.51
1:B:328:TRP:HA	1:B:328:TRP:CE3	2.45	0.51
1:A:194:ARG:HA	1:A:197:MSE:HE2	1.92	0.50
1:B:350:ASN:O	1:B:353:ASP:HB2	2.11	0.50
1:A:244:TRP:HD1	1:A:315:THR:HG23	1.75	0.50
1:A:248:ARG:HD3	1:A:277:VAL:HG21	1.93	0.50
1:A:298:THR:CB	1:A:301:GLN:HG3	2.42	0.50
1:A:300:GLU:CG	1:A:379:ASN:HD21	2.23	0.50
1:B:244:TRP:HD1	1:B:315:THR:HG23	1.76	0.50
1:A:237:ALA:O	1:A:238:ALA:C	2.50	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:34:LEU:HD13	1:B:136:ILE:HG23	1.93	0.50
1:B:355:ILE:C	1:B:357:TRP:H	2.14	0.50
1:A:212:LEU:HB2	1:A:213:PRO:HD3	1.93	0.50
1:A:298:THR:N	1:A:301:GLN:HE21	2.10	0.50
1:A:118:ILE:H	1:A:118:ILE:CD1	2.19	0.49
1:A:30:ARG:HB2	1:A:115:MSE:O	2.12	0.49
1:A:221:ASN:O	1:A:222:ALA:HB3	2.13	0.49
1:A:53:MSE:CG	1:A:59:THR:HG21	2.42	0.49
1:B:242:TRP:CB	1:B:243:PRO:CD	2.91	0.49
1:B:354:VAL:HG22	1:B:393:LEU:HD21	1.95	0.49
1:B:233:GLN:HB2	1:B:259:LEU:HD23	1.95	0.49
1:B:242:TRP:CZ3	1:B:254:LEU:HD23	2.48	0.49
1:B:369:ALA:O	1:B:373:ILE:HG13	2.12	0.49
1:A:163:ARG:O	1:A:166:SER:N	2.45	0.49
1:A:252:TRP:CE2	1:A:273:LEU:HD11	2.47	0.49
1:A:358:VAL:O	1:A:359:GLY:C	2.50	0.49
1:B:298:THR:HB	1:B:301:GLN:HG3	1.94	0.49
1:A:350:ASN:O	1:A:353:ASP:HB2	2.12	0.48
1:B:154:ASP:O	1:B:157:ARG:HG3	2.13	0.48
1:B:192:VAL:HA	1:B:195:MSE:CE	2.43	0.48
1:B:184:ALA:HB3	1:B:185:PRO:HD3	1.95	0.48
1:B:226:GLY:HA3	1:B:267:PHE:CE1	2.49	0.48
1:B:358:VAL:O	1:B:359:GLY:C	2.51	0.48
1:A:127:ILE:O	1:A:127:ILE:HG22	2.12	0.48
1:A:349:VAL:O	1:A:349:VAL:HG12	2.12	0.48
1:A:355:ILE:C	1:A:357:TRP:N	2.67	0.48
1:A:184:ALA:HB3	1:A:185:PRO:HD3	1.95	0.48
1:B:22:ALA:HB2	1:B:45:THR:HB	1.96	0.48
1:A:357:TRP:O	1:A:394:MSE:HE1	2.14	0.48
1:A:256:CYS:HB2	1:A:285:LEU:HD11	1.95	0.48
1:B:163:ARG:HD3	1:B:198:GLU:OE2	2.14	0.48
1:A:162:VAL:HG13	1:A:214:LEU:HD23	1.96	0.47
1:A:221:ASN:ND2	1:A:227:LEU:HB3	2.29	0.47
1:A:226:GLY:HA3	1:A:267:PHE:CE1	2.48	0.47
1:A:166:SER:OG	1:A:205:GLY:HA3	2.14	0.47
1:B:181:VAL:HG22	1:B:218:THR:HA	1.97	0.47
1:B:374:TRP:C	1:B:376:ALA:H	2.17	0.47
1:A:356:GLU:O	1:A:356:GLU:HG3	2.13	0.47
1:A:22:ALA:HB2	1:A:45:THR:HB	1.96	0.47
1:A:265:ARG:HB3	1:A:266:PRO:HD3	1.96	0.47
1:B:151:PHE:CD2	1:B:158:MSE:HG2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:325:PRO:O	1:B:326:GLY:C	2.53	0.47
1:A:305:ALA:HA	1:A:309:ARG:NH1	2.30	0.46
1:A:233:GLN:HB2	1:A:259:LEU:HD23	1.96	0.46
1:B:219:GLY:O	1:B:221:ASN:O	2.33	0.46
1:B:374:TRP:O	1:B:376:ALA:N	2.47	0.46
1:A:284:ILE:HG21	1:A:316:VAL:HG21	1.97	0.46
1:A:151:PHE:CD2	1:A:158:MSE:HG2	2.51	0.46
1:A:285:LEU:HD23	1:A:285:LEU:HA	1.71	0.46
1:A:328:TRP:HA	1:A:328:TRP:HE3	1.79	0.46
1:B:45:THR:O	1:B:82:THR:HA	2.14	0.46
1:B:49:PRO:O	1:B:53:MSE:HG3	2.16	0.46
1:A:387:GLU:O	1:A:390:TYR:HB3	2.16	0.46
1:B:244:TRP:CD1	1:B:315:THR:HG23	2.50	0.45
1:B:298:THR:OG1	1:B:301:GLN:NE2	2.49	0.45
1:A:298:THR:O	1:A:300:GLU:N	2.50	0.45
1:B:221:ASN:ND2	1:B:227:LEU:HB3	2.32	0.45
1:B:256:CYS:CB	1:B:285:LEU:HD11	2.46	0.45
1:A:202:LEU:C	1:A:202:LEU:HD23	2.37	0.45
1:B:187:LEU:HD23	1:B:187:LEU:HA	1.78	0.45
1:B:9:LEU:HD12	1:B:9:LEU:HA	1.77	0.45
1:B:84:LYS:HG3	1:B:110:ARG:NE	2.32	0.45
1:B:43:ILE:O	1:B:80:VAL:HA	2.17	0.44
1:B:107:ASP:O	1:B:110:ARG:HG2	2.16	0.44
1:A:143:THR:CG2	1:A:150:ARG:HG3	2.47	0.44
1:A:309:ARG:O	1:A:313:VAL:HG23	2.17	0.44
1:A:245:LEU:HD21	1:A:319:ALA:HB2	1.98	0.44
1:A:394:MSE:O	1:A:396:ARG:N	2.50	0.44
1:B:40:ASP:OD1	1:B:40:ASP:N	2.49	0.44
1:B:387:GLU:O	1:B:390:TYR:HB3	2.16	0.44
1:B:311:LEU:HD23	1:B:332:LEU:HD12	2.00	0.44
1:A:298:THR:O	1:A:301:GLN:N	2.51	0.44
1:B:241:ARG:HH22	1:B:244:TRP:CB	2.31	0.44
1:A:20:TYR:O	1:A:21:ASP:CB	2.66	0.43
1:B:282:GLY:O	1:B:283:ALA:C	2.56	0.43
1:B:162:VAL:HG13	1:B:214:LEU:HD23	2.00	0.43
1:A:311:LEU:HD23	1:A:332:LEU:HD12	2.00	0.43
1:A:9:LEU:HD12	1:A:9:LEU:HA	1.79	0.43
1:B:315:THR:OG1	1:B:329:HIS:CE1	2.71	0.43
1:A:226:GLY:HA3	1:A:267:PHE:HE1	1.82	0.43
1:A:242:TRP:HB2	1:A:243:PRO:HD3	1.97	0.43
1:A:256:CYS:O	1:A:258:ALA:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:374:TRP:C	1:B:376:ALA:N	2.72	0.43
1:A:360:LYS:HG3	1:A:361:PRO:CD	2.37	0.43
1:A:31:ASP:OD1	1:A:36:ARG:HD3	2.19	0.43
1:A:298:THR:HB	1:A:301:GLN:HG3	2.01	0.43
1:A:351:GLY:HA2	1:A:370:LEU:HD11	2.01	0.43
1:B:114:THR:HB	1:B:132:GLY:HA2	2.01	0.43
1:A:341:ILE:HD11	1:A:378:VAL:HG23	2.00	0.42
1:B:315:THR:HG1	1:B:329:HIS:CE1	2.37	0.42
1:A:129:PRO:HD2	1:A:130:PHE:HD1	1.84	0.42
1:B:143:THR:CG2	1:B:150:ARG:HG3	2.49	0.42
1:B:194:ARG:HG2	1:B:197:MSE:HE2	2.01	0.42
1:B:221:ASN:O	1:B:222:ALA:HB3	2.18	0.42
1:B:323:ALA:HA	1:B:324:PRO:HD3	1.88	0.42
1:A:202:LEU:HD23	1:A:202:LEU:O	2.19	0.42
1:B:236:LEU:O	1:B:237:ALA:C	2.57	0.42
1:A:241:ARG:N	1:A:319:ALA:O	2.41	0.42
1:B:237:ALA:O	1:B:239:ALA:N	2.52	0.42
1:B:230:LYS:O	1:B:231:GLU:C	2.58	0.42
1:B:53:MSE:CG	1:B:59:THR:HG21	2.48	0.42
1:A:5:PHE:HE1	1:A:38:ILE:HD13	1.84	0.42
1:B:20:TYR:O	1:B:21:ASP:CB	2.68	0.42
1:B:118:ILE:HG22	1:B:119:ALA:H	1.84	0.42
1:B:245:LEU:O	1:B:251:ARG:NH2	2.48	0.42
1:B:293:ARG:HB3	1:B:293:ARG:NH1	2.35	0.42
1:A:45:THR:OG1	1:A:46:SER:N	2.53	0.41
1:A:355:ILE:O	1:A:357:TRP:N	2.52	0.41
1:B:217:GLU:HG3	1:B:235:ARG:NH2	2.35	0.41
1:A:6:GLN:O	1:A:9:LEU:HB2	2.20	0.41
1:B:108:LEU:HD23	1:B:108:LEU:N	2.35	0.41
1:A:377:VAL:CG1	1:A:384:ASN:HB2	2.51	0.41
1:B:48:LEU:O	1:B:49:PRO:C	2.58	0.41
1:A:229:GLY:HA2	1:A:231:GLU:OE2	2.20	0.41
1:A:230:LYS:O	1:A:231:GLU:C	2.59	0.41
1:B:305:ALA:HA	1:B:309:ARG:NH1	2.36	0.41
1:A:43:ILE:HB	1:A:80:VAL:HG22	2.02	0.41
1:A:45:THR:O	1:A:82:THR:HA	2.20	0.41
1:A:323:ALA:HA	1:A:324:PRO:HD3	1.87	0.41
1:A:104:LEU:CD1	1:A:108:LEU:HD21	2.50	0.41
1:A:141:ILE:HG13	1:A:170:PHE:HB3	2.03	0.41
1:A:324:PRO:HA	1:A:325:PRO:HD3	1.83	0.41
1:B:141:ILE:HG13	1:B:170:PHE:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:165:VAL:HG13	1:B:170:PHE:O	2.21	0.41
1:B:226:GLY:HA3	1:B:267:PHE:HE1	1.84	0.41
1:B:249:GLU:CD	1:B:249:GLU:N	2.64	0.41
1:B:307:LEU:O	1:B:310:ALA:HB3	2.21	0.41
1:A:112:ASP:OD2	1:A:160:ARG:NH2	2.54	0.40
1:A:244:TRP:O	1:A:244:TRP:CG	2.73	0.40
1:B:293:ARG:HA	1:B:294:PRO:HD3	1.95	0.40
1:A:61:ASP:OD2	1:A:64:SER:HB3	2.21	0.40
1:A:108:LEU:HD23	1:A:108:LEU:N	2.37	0.40
1:A:233:GLN:H	1:A:233:GLN:HG2	1.69	0.40
1:A:111:ARG:HB2	1:A:117:ALA:HB2	2.03	0.40
1:A:221:ASN:HD21	1:A:227:LEU:HB3	1.86	0.40
1:A:284:ILE:O	1:A:285:LEU:C	2.59	0.40
1:B:114:THR:C	1:B:116:ASN:H	2.24	0.40
1:B:285:LEU:HA	1:B:285:LEU:HD23	1.80	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	391/404 (97%)	312 (80%)	67 (17%)	12 (3%)	4 30
1	B	391/404 (97%)	314 (80%)	66 (17%)	11 (3%)	5 32
All	All	782/808 (97%)	626 (80%)	133 (17%)	23 (3%)	4 31

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	326	GLY
1	B	326	GLY
1	A	243	PRO

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Mol	Chain	Res	Type
1	A	306	GLY
1	A	359	GLY
1	B	57	PRO
1	B	209	ALA
1	B	306	GLY
1	B	307	LEU
1	B	359	GLY
1	A	57	PRO
1	A	307	LEU
1	A	356	GLU
1	B	243	PRO
1	A	209	ALA
1	A	231	GLU
1	A	267	PHE
1	B	231	GLU
1	B	375	ARG
1	B	383	GLU
1	A	213	PRO
1	A	242	TRP
1	B	213	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	316/315 (100%)	296 (94%)	20 (6%)	18	51
1	B	316/315 (100%)	294 (93%)	22 (7%)	15	46
All	All	632/630 (100%)	590 (93%)	42 (7%)	16	49

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ASP
1	A	65	LYS
1	A	66	HIS

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Mol	Chain	Res	Type
1	A	115	MSE
1	A	125	THR
1	A	175	ASP
1	A	178	GLN
1	A	187	LEU
1	A	262	GLN
1	A	265	ARG
1	A	291	ILE
1	A	293	ARG
1	A	298	THR
1	A	301	GLN
1	A	331	LYS
1	A	350	ASN
1	A	387	GLU
1	A	394	MSE
1	A	396	ARG
1	A	400	ARG
1	B	40	ASP
1	B	65	LYS
1	B	66	HIS
1	B	111	ARG
1	B	115	MSE
1	B	125	THR
1	B	157	ARG
1	B	175	ASP
1	B	178	GLN
1	B	187	LEU
1	B	251	ARG
1	B	262	GLN
1	B	265	ARG
1	B	293	ARG
1	B	298	THR
1	B	331	LYS
1	B	350	ASN
1	B	354	VAL
1	B	387	GLU
1	B	394	MSE
1	B	396	ARG
1	B	400	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	HIS
1	A	182	GLN
1	A	221	ASN
1	A	257	HIS
1	A	301	GLN
1	A	329	HIS
1	A	379	ASN
1	B	66	HIS
1	B	182	GLN
1	B	221	ASN
1	B	301	GLN
1	B	329	HIS
1	B	379	ASN

5.3.3 RNA

There are no RNA molecules 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 monosaccharides in this entry.

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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

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^{th} 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	385/404 (95%)	0.15	18 (4%)	31	28	5, 31, 71, 83	0
1	B	385/404 (95%)	0.11	20 (5%)	27	24	5, 31, 71, 83	0
All	All	770/808 (95%)	0.13	38 (4%)	29	26	5, 31, 72, 83	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	404	CYS	6.7
1	A	403	ASN	5.2
1	A	100	PHE	5.0
1	B	141	ILE	3.8
1	B	151	PHE	3.7
1	A	152	ARG	3.4
1	B	155	ALA	3.2
1	B	156	LEU	3.2
1	A	271	TRP	3.1
1	B	271	TRP	3.1
1	B	404	CYS	3.0
1	B	168	LEU	3.0
1	A	297	TRP	3.0
1	B	254	LEU	2.9
1	A	220	LEU	2.8
1	A	268	LEU	2.8
1	B	143	THR	2.8
1	A	255	LEU	2.8
1	B	170	PHE	2.8
1	B	403	ASN	2.7
1	B	252	TRP	2.6
1	A	148	GLU	2.6
1	B	268	LEU	2.6
1	A	151	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	378	VAL	2.5
1	B	187	LEU	2.4
1	A	341	ILE	2.4
1	A	24	PHE	2.3
1	A	97	SER	2.3
1	B	297	TRP	2.2
1	A	77	ALA	2.2
1	B	8	ALA	2.2
1	A	114	THR	2.1
1	A	302	LEU	2.1
1	B	220	LEU	2.1
1	A	176	THR	2.0
1	B	161	ALA	2.0
1	B	273	LEU	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)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MG	B	6611	1/1	0.79	0.37	8,8,8,8	0
2	MG	A	5611	1/1	0.90	0.40	8,8,8,8	0

6.5 Other polymers (i)

There are no such residues in this entry.