Full wwPDB X-ray Structure Validation Report (i)

Jun 18, 2024 – 11:11 PM EDT

PDB ID	:	4DK0
Title	:	Crystal structure of MacA from Actinobacillus actinomycetemcomitans
Authors	:	Xu, Y.; Piao, S.; Ha, N.C.
Deposited on	:	2012-02-03
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:

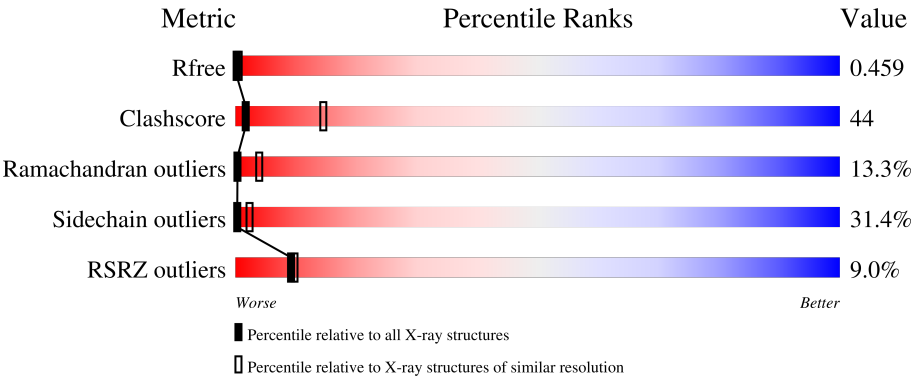
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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))
R_{free}	130704	1659 (3.60-3.40)
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	369	8% 21% 43% 21% • 12%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2486 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 Putative MacA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	Se			
1	A	324	2486	1550	419	514	3	4	0	0

There are 8 discrepancies between the modelled and reference sequences:

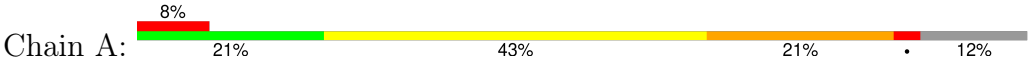
Chain	Residue	Modelled	Actual	Comment	Reference
A	26	GLY	-	EXPRESSION TAG	UNP Q2EHL9
A	27	ALA	-	EXPRESSION TAG	UNP Q2EHL9
A	28	MSE	-	EXPRESSION TAG	UNP Q2EHL9
A	29	ASP	-	EXPRESSION TAG	UNP Q2EHL9
A	68	ILE	VAL	SEE REMARK 999	UNP Q2EHL9
A	85	LEU	ILE	SEE REMARK 999	UNP Q2EHL9
A	126	GLN	ASN	SEE REMARK 999	UNP Q2EHL9
A	177	LEU	VAL	SEE REMARK 999	UNP Q2EHL9

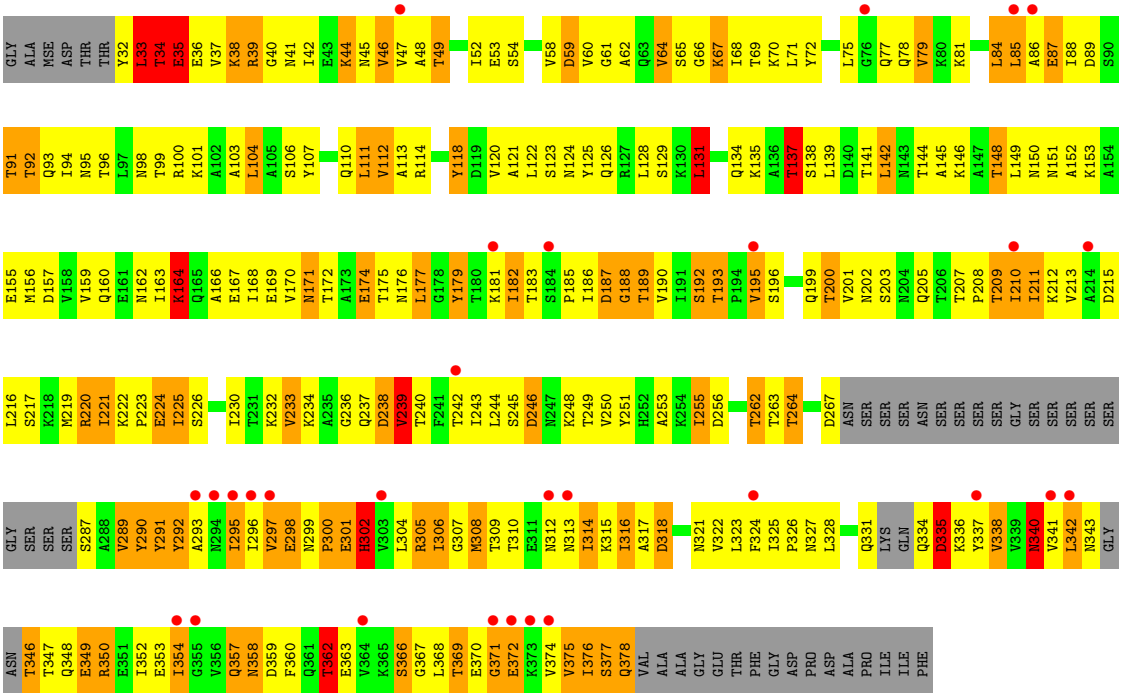
3 Residue-property plots (i)

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: Putative MacA

Chain A:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 6 2 2	Depositor
Cell constants a, b, c, α, β, γ	109.19Å 109.19Å 255.44Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	9.99 – 3.50 47.28 – 3.00	Depositor EDS
% Data completeness (in resolution range)	97.9 (9.99-3.50) 97.1 (47.28-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.83 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, R_{free}	0.338 , 0.390 0.404 , 0.459	Depositor DCC
R_{free} test set	1833 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å^2)	69.4	Xtriage
Anisotropy	0.403	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 124.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.38$, $< L^2 > = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	2486	wwPDB-VP
Average B, all atoms (Å^2)	121.0	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 40.91 % 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 2.5499e-04.*

[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

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	0.66	0/2503	0.97	2/3391 (0.1%)

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

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	85	LEU	CA-CB-CG	5.09	127.01	115.30
1	A	131	LEU	CA-CB-CG	5.05	126.92	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	248	LYS	Peptide
1	A	33	LEU	Peptide
1	A	34	THR	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of 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	2486	0	2535	222	1
All	All	2486	0	2535	222	1

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 44.

All (222) 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:220:ARG:HH21	1:A:222:LYS:HE3	1.32	0.92
1:A:239:VAL:HA	1:A:314:ILE:HA	1.58	0.86
1:A:305:ARG:O	1:A:307:GLY:N	2.08	0.85
1:A:239:VAL:HG23	1:A:314:ILE:HG22	1.57	0.84
1:A:70:LYS:HB2	1:A:87:GLU:HB2	1.60	0.83
1:A:195:VAL:HG11	1:A:210:ILE:HD13	1.62	0.80
1:A:67:LYS:HG3	1:A:200:THR:HG23	1.62	0.80
1:A:239:VAL:HG11	1:A:295:ILE:HD11	1.64	0.79
1:A:142:LEU:HD12	1:A:146:LYS:HE3	1.64	0.79
1:A:129:SER:HA	1:A:142:LEU:HD21	1.66	0.78
1:A:221:ILE:H	1:A:295:ILE:HG22	1.49	0.77
1:A:186:ILE:HG13	1:A:187:ASP:H	1.52	0.75
1:A:107:TYR:CD1	1:A:162:ASN:HB3	2.23	0.73
1:A:263:THR:O	1:A:263:THR:OG1	2.05	0.73
1:A:220:ARG:NH2	1:A:222:LYS:HE3	2.03	0.73
1:A:334:GLN:HA	1:A:335:ASP:HB2	1.69	0.72
1:A:219:MSE:HE2	1:A:299:ASN:ND2	2.05	0.71
1:A:237:GLN:O	1:A:239:VAL:N	2.24	0.70
1:A:159:VAL:O	1:A:163:ILE:HG12	1.91	0.70
1:A:79:VAL:O	1:A:187:ASP:HA	1.93	0.69
1:A:68:ILE:HG22	1:A:199:GLN:O	1.92	0.69
1:A:374:VAL:HG12	1:A:375:VAL:H	1.58	0.69
1:A:144:THR:OG1	1:A:145:ALA:N	2.22	0.68
1:A:328:LEU:HB3	1:A:377:SER:HB2	1.74	0.68
1:A:210:ILE:HG22	1:A:211:ILE:HG22	1.75	0.68
1:A:315:LYS:O	1:A:316:ILE:HB	1.92	0.68
1:A:107:TYR:HD1	1:A:162:ASN:HB3	1.58	0.68
1:A:325:ILE:HD11	1:A:368:LEU:HD21	1.76	0.67
1:A:221:ILE:HG23	1:A:295:ILE:HG21	1.74	0.67
1:A:216:LEU:HD21	1:A:306:ILE:HD13	1.77	0.66
1:A:326:PRO:HB2	1:A:376:ILE:HG21	1.77	0.66
1:A:346:THR:O	1:A:346:THR:OG1	2.13	0.66
1:A:338:VAL:HB	1:A:375:VAL:HG11	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:GLY:HA3	1:A:215:ASP:HA	1.76	0.65
1:A:331:GLN:HB2	1:A:336:LYS:O	1.95	0.65
1:A:340:ASN:ND2	1:A:342:LEU:O	2.29	0.65
1:A:230:ILE:HA	1:A:233:VAL:HG23	1.80	0.64
1:A:88:ILE:HG22	1:A:89:ASP:H	1.63	0.64
1:A:179:TYR:CD1	1:A:179:TYR:N	2.64	0.64
1:A:61:GLY:HA2	1:A:209:THR:HA	1.79	0.63
1:A:221:ILE:HG13	1:A:310:THR:OG1	1.98	0.63
1:A:37:VAL:HG13	1:A:324:PHE:H	1.64	0.63
1:A:151:ASN:O	1:A:155:GLU:HG2	1.99	0.63
1:A:298:GLU:HB3	1:A:300:PRO:HD3	1.82	0.62
1:A:195:VAL:HG21	1:A:210:ILE:HG23	1.82	0.61
1:A:230:ILE:HG21	1:A:291:TYR:HD2	1.65	0.61
1:A:187:ASP:OD1	1:A:187:ASP:N	2.33	0.61
1:A:93:GLN:HB3	1:A:177:LEU:HD22	1.82	0.60
1:A:353:GLU:HA	1:A:354:ILE:HB	1.84	0.60
1:A:54:SER:OG	1:A:306:ILE:HG21	2.02	0.60
1:A:137:THR:O	1:A:137:THR:OG1	2.14	0.60
1:A:328:LEU:HB3	1:A:377:SER:CB	2.31	0.60
1:A:69:THR:N	1:A:87:GLU:O	2.27	0.59
1:A:52:ILE:HD12	1:A:308:MSE:HB2	1.84	0.59
1:A:211:ILE:HD11	1:A:213:VAL:HG23	1.85	0.59
1:A:377:SER:HA	1:A:378:GLN:C	2.23	0.59
1:A:243:ILE:C	1:A:245:SER:H	2.08	0.57
1:A:98:ASN:HA	1:A:101:LYS:HD3	1.86	0.57
1:A:66:GLY:C	1:A:67:LYS:HE2	2.25	0.57
1:A:62:ALA:O	1:A:208:PRO:HD2	2.04	0.57
1:A:251:TYR:OH	1:A:301:GLU:OE1	2.23	0.57
1:A:357:GLN:O	1:A:358:ASN:HB2	2.05	0.57
1:A:223:PRO:HB2	1:A:293:ALA:HB3	1.87	0.56
1:A:38:LYS:HE3	1:A:38:LYS:H	1.69	0.56
1:A:37:VAL:HB	1:A:370:GLU:HA	1.88	0.56
1:A:367:GLY:HA2	1:A:368:LEU:HB3	1.87	0.56
1:A:338:VAL:HA	1:A:349:GLU:HA	1.87	0.56
1:A:357:GLN:OE1	1:A:358:ASN:N	2.40	0.55
1:A:46:VAL:HB	1:A:314:ILE:HD11	1.88	0.55
1:A:91:THR:OG1	1:A:92:THR:N	2.39	0.55
1:A:219:MSE:SE	1:A:306:ILE:HG23	2.57	0.55
1:A:60:VAL:HB	1:A:211:ILE:O	2.07	0.54
1:A:171:ASN:O	1:A:174:GLU:HG3	2.07	0.54
1:A:221:ILE:HD13	1:A:295:ILE:HB	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:TYR:HB2	1:A:145:ALA:HB1	1.89	0.54
1:A:211:ILE:HD11	1:A:213:VAL:CG2	2.38	0.54
1:A:48:ALA:HB1	1:A:224:GLU:O	2.07	0.54
1:A:181:LYS:HD2	1:A:183:THR:HG22	1.90	0.54
1:A:58:VAL:HG11	1:A:213:VAL:O	2.07	0.54
1:A:327:ASN:HD22	1:A:360:PHE:HA	1.71	0.54
1:A:36:GLU:HG2	1:A:371:GLY:H	1.73	0.54
1:A:85:LEU:CD1	1:A:211:ILE:HD12	2.38	0.53
1:A:221:ILE:HG21	1:A:310:THR:HG21	1.90	0.53
1:A:222:LYS:HD2	1:A:292:TYR:CD2	2.43	0.53
1:A:327:ASN:HD22	1:A:360:PHE:HD1	1.55	0.53
1:A:350:ARG:NH1	1:A:372:GLU:OE1	2.42	0.53
1:A:230:ILE:HG21	1:A:291:TYR:CD2	2.44	0.52
1:A:62:ALA:HB3	1:A:208:PRO:HG2	1.89	0.52
1:A:222:LYS:HB3	1:A:292:TYR:CE2	2.44	0.52
1:A:34:THR:O	1:A:35:GLU:HB2	2.09	0.52
1:A:219:MSE:HG2	1:A:299:ASN:HB2	1.92	0.52
1:A:40:GLY:O	1:A:322:VAL:N	2.22	0.52
1:A:325:ILE:HG13	1:A:368:LEU:HD11	1.90	0.52
1:A:67:LYS:HA	1:A:200:THR:HA	1.92	0.52
1:A:85:LEU:HD11	1:A:211:ILE:HD12	1.92	0.52
1:A:290:TYR:O	1:A:291:TYR:CD1	2.62	0.52
1:A:70:LYS:O	1:A:86:ALA:HA	2.11	0.51
1:A:85:LEU:HD12	1:A:182:ILE:O	2.10	0.51
1:A:221:ILE:HD11	1:A:312:ASN:ND2	2.25	0.51
1:A:256:ASP:HB2	1:A:296:ILE:HG12	1.92	0.51
1:A:58:VAL:HG11	1:A:213:VAL:C	2.30	0.51
1:A:338:VAL:HG13	1:A:347:THR:HB	1.93	0.51
1:A:89:ASP:HB2	1:A:91:THR:HG23	1.92	0.51
1:A:376:ILE:HA	1:A:377:SER:HB2	1.93	0.51
1:A:239:VAL:HG12	1:A:253:ALA:C	2.32	0.51
1:A:36:GLU:HG2	1:A:371:GLY:HA2	1.92	0.50
1:A:219:MSE:O	1:A:297:VAL:HG23	2.10	0.50
1:A:236:GLY:H	1:A:255:ILE:HG22	1.77	0.50
1:A:32:TYR:N	1:A:378:GLN:HB2	2.26	0.50
1:A:322:VAL:HB	1:A:363:GLU:HG3	1.93	0.50
1:A:211:ILE:HG12	1:A:212:LYS:N	2.26	0.50
1:A:120:VAL:O	1:A:124:ASN:HB2	2.12	0.49
1:A:44:LYS:HG3	1:A:358:ASN:CG	2.32	0.49
1:A:221:ILE:O	1:A:223:PRO:HD3	2.11	0.49
1:A:44:LYS:HG3	1:A:358:ASN:ND2	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:ALA:N	1:A:181:LYS:O	2.35	0.49
1:A:131:LEU:HA	1:A:134:GLN:HG2	1.94	0.49
1:A:62:ALA:O	1:A:203:SER:HB2	2.13	0.49
1:A:151:ASN:OD1	1:A:152:ALA:N	2.46	0.49
1:A:262:THR:OG1	1:A:263:THR:N	2.46	0.49
1:A:44:LYS:HA	1:A:358:ASN:HD22	1.77	0.48
1:A:42:ILE:HD11	1:A:363:GLU:H	1.78	0.48
1:A:186:ILE:HG13	1:A:187:ASP:N	2.24	0.48
1:A:334:GLN:HA	1:A:335:ASP:CB	2.41	0.48
1:A:150:ASN:HA	1:A:153:LYS:HE2	1.94	0.48
1:A:236:GLY:N	1:A:255:ILE:HG22	2.29	0.48
1:A:369:THR:HB	1:A:370:GLU:H	1.43	0.48
1:A:128:LEU:HD12	1:A:128:LEU:O	2.14	0.48
1:A:222:LYS:HB3	1:A:292:TYR:HE2	1.79	0.47
1:A:221:ILE:HG23	1:A:295:ILE:CG2	2.43	0.47
1:A:72:TYR:CD1	1:A:84:LEU:HB2	2.50	0.47
1:A:100:ARG:NH1	1:A:169:GLU:OE1	2.47	0.47
1:A:38:LYS:HB3	1:A:40:GLY:N	2.30	0.47
1:A:81:LYS:HG3	1:A:185:PRO:O	2.15	0.47
1:A:112:VAL:HG12	1:A:113:ALA:N	2.29	0.47
1:A:262:THR:HA	1:A:291:TYR:HD1	1.78	0.47
1:A:327:ASN:HB2	1:A:360:PHE:C	2.34	0.47
1:A:327:ASN:HB2	1:A:360:PHE:O	2.15	0.47
1:A:337:TYR:CE2	1:A:352:ILE:HG12	2.49	0.47
1:A:295:ILE:HG23	1:A:297:VAL:HG22	1.97	0.47
1:A:78:GLN:HA	1:A:189:THR:HA	1.97	0.46
1:A:94:ILE:HG13	1:A:95:ASN:N	2.31	0.46
1:A:195:VAL:HG11	1:A:210:ILE:CD1	2.39	0.46
1:A:99:THR:HG22	1:A:100:ARG:N	2.31	0.46
1:A:142:LEU:HA	1:A:142:LEU:HD22	1.65	0.46
1:A:35:GLU:OE1	1:A:36:GLU:N	2.44	0.46
1:A:104:LEU:HB2	1:A:166:ALA:HB1	1.98	0.46
1:A:219:MSE:HE3	1:A:304:LEU:C	2.35	0.46
1:A:157:ASP:HA	1:A:160:GLN:HG2	1.98	0.46
1:A:230:ILE:HG21	1:A:291:TYR:HB2	1.97	0.46
1:A:88:ILE:HG22	1:A:89:ASP:N	2.30	0.46
1:A:201:VAL:CG1	1:A:208:PRO:HG3	2.46	0.46
1:A:327:ASN:ND2	1:A:360:PHE:HD1	2.14	0.46
1:A:38:LYS:O	1:A:323:LEU:HA	2.15	0.46
1:A:70:LYS:HB2	1:A:87:GLU:CB	2.40	0.46
1:A:336:LYS:O	1:A:337:TYR:HD1	1.99	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:SER:OG	1:A:193:THR:N	2.49	0.45
1:A:33:LEU:HG	1:A:376:ILE:O	2.16	0.45
1:A:66:GLY:O	1:A:67:LYS:HE2	2.15	0.45
1:A:236:GLY:HA2	1:A:255:ILE:O	2.16	0.45
1:A:220:ARG:HH21	1:A:222:LYS:CE	2.16	0.45
1:A:358:ASN:HA	1:A:359:ASP:HA	1.53	0.45
1:A:156:MSE:HE2	1:A:156:MSE:HB3	1.93	0.45
1:A:314:ILE:HD12	1:A:315:LYS:O	2.15	0.45
1:A:42:ILE:HG22	1:A:44:LYS:H	1.82	0.45
1:A:226:SER:HA	1:A:290:TYR:HA	1.98	0.45
1:A:58:VAL:HG22	1:A:59:ASP:N	2.32	0.45
1:A:64:VAL:CG2	1:A:179:TYR:HD2	2.30	0.45
1:A:246:ASP:OD1	1:A:249:THR:HB	2.17	0.45
1:A:291:TYR:O	1:A:292:TYR:HB2	2.16	0.45
1:A:72:TYR:HB2	1:A:84:LEU:O	2.16	0.44
1:A:370:GLU:O	1:A:372:GLU:N	2.50	0.44
1:A:167:GLU:O	1:A:170:VAL:HG12	2.16	0.44
1:A:179:TYR:N	1:A:179:TYR:HD1	2.15	0.44
1:A:366:SER:HA	1:A:367:GLY:HA3	1.57	0.44
1:A:325:ILE:HG13	1:A:368:LEU:CD1	2.48	0.44
1:A:301:GLU:HB3	1:A:302:HIS:H	1.44	0.44
1:A:111:LEU:HD23	1:A:111:LEU:HA	1.79	0.44
1:A:128:LEU:HD21	1:A:141:THR:O	2.17	0.44
1:A:135:LYS:HA	1:A:135:LYS:HD3	1.84	0.43
1:A:375:VAL:O	1:A:375:VAL:HG13	2.18	0.43
1:A:141:THR:HA	1:A:144:THR:HG23	1.99	0.43
1:A:230:ILE:HG12	1:A:291:TYR:CD2	2.54	0.43
1:A:37:VAL:HG13	1:A:324:PHE:N	2.31	0.43
1:A:367:GLY:HA2	1:A:368:LEU:CB	2.47	0.43
1:A:87:GLU:HA	1:A:88:ILE:HD12	2.01	0.43
1:A:70:LYS:HB3	1:A:72:TYR:CE2	2.54	0.42
1:A:42:ILE:HG22	1:A:44:LYS:N	2.34	0.42
1:A:290:TYR:CD2	1:A:290:TYR:N	2.87	0.42
1:A:38:LYS:HB3	1:A:39:ARG:C	2.39	0.42
1:A:44:LYS:HG3	1:A:358:ASN:CB	2.50	0.42
1:A:88:ILE:HD12	1:A:88:ILE:N	2.34	0.42
1:A:246:ASP:CG	1:A:249:THR:HB	2.39	0.42
1:A:118:TYR:CD2	1:A:118:TYR:C	2.92	0.42
1:A:123:SER:HA	1:A:126:GLN:HG2	2.00	0.42
1:A:164:LYS:O	1:A:167:GLU:N	2.53	0.42
1:A:316:ILE:HG21	1:A:316:ILE:HD13	1.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:TYR:N	1:A:33:LEU:HD23	2.34	0.42
1:A:375:VAL:HG22	1:A:378:GLN:C	2.40	0.42
1:A:148:THR:HG23	1:A:151:ASN:HD21	1.85	0.41
1:A:196:SER:HB2	1:A:199:GLN:HB2	2.02	0.41
1:A:296:ILE:H	1:A:296:ILE:HG13	1.75	0.41
1:A:343:ASN:N	1:A:343:ASN:OD1	2.53	0.41
1:A:64:VAL:N	1:A:203:SER:OG	2.53	0.41
1:A:89:ASP:HB2	1:A:91:THR:CG2	2.49	0.41
1:A:223:PRO:CB	1:A:225:ILE:HD12	2.50	0.41
1:A:232:LYS:O	1:A:316:ILE:HD11	2.20	0.41
1:A:243:ILE:C	1:A:245:SER:N	2.73	0.41
1:A:49:THR:O	1:A:224:GLU:HB2	2.20	0.41
1:A:223:PRO:HB2	1:A:225:ILE:HD12	2.03	0.41
1:A:52:ILE:HG22	1:A:306:ILE:HA	2.02	0.41
1:A:121:ALA:O	1:A:149:LEU:HD23	2.19	0.41
1:A:357:GLN:HB2	1:A:362:THR:HG23	2.01	0.41
1:A:44:LYS:CG	1:A:45:ASN:H	2.34	0.41
1:A:92:THR:O	1:A:96:THR:HG23	2.21	0.41
1:A:125:TYR:HE1	1:A:146:LYS:HG3	1.86	0.41
1:A:287:SER:O	1:A:289:VAL:HG12	2.21	0.41
1:A:340:ASN:HA	1:A:347:THR:HG22	2.03	0.41
1:A:107:TYR:CE1	1:A:162:ASN:HB3	2.54	0.40
1:A:86:ALA:HB3	1:A:182:ILE:HB	2.04	0.40
1:A:177:LEU:HD13	1:A:177:LEU:HA	1.73	0.40
1:A:203:SER:HA	1:A:208:PRO:HD3	2.03	0.40

All (1) 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)
1:A:95:ASN:ND2	1:A:172:THR:OG1[5_565]	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	316/369 (86%)	206 (65%)	68 (22%)	42 (13%)	0 4

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	35	GLU
1	A	46	VAL
1	A	137	THR
1	A	238	ASP
1	A	264	THR
1	A	305	ARG
1	A	306	ILE
1	A	314	ILE
1	A	316	ILE
1	A	318	ASP
1	A	335	ASP
1	A	349	GLU
1	A	358	ASN
1	A	44	LYS
1	A	112	VAL
1	A	188	GLY
1	A	189	THR
1	A	250	VAL
1	A	301	GLU
1	A	302	HIS
1	A	321	ASN
1	A	340	ASN
1	A	362	THR
1	A	371	GLY
1	A	375	VAL
1	A	65	SER
1	A	103	ALA
1	A	300	PRO
1	A	317	ALA
1	A	342	LEU
1	A	366	SER
1	A	104	LEU
1	A	138	SER
1	A	239	VAL
1	A	372	GLU

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Mol	Chain	Res	Type
1	A	291	TYR
1	A	292	TYR
1	A	354	ILE
1	A	377	SER
1	A	164	LYS
1	A	182	ILE
1	A	168	ILE

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	283/314 (90%)	194 (69%)	89 (31%)	0 2

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	LEU
1	A	34	THR
1	A	35	GLU
1	A	38	LYS
1	A	39	ARG
1	A	41	ASN
1	A	47	VAL
1	A	49	THR
1	A	53	GLU
1	A	59	ASP
1	A	64	VAL
1	A	67	LYS
1	A	71	LEU
1	A	75	LEU
1	A	77	GLN
1	A	79	VAL
1	A	84	LEU
1	A	87	GLU
1	A	91	THR

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Mol	Chain	Res	Type
1	A	92	THR
1	A	106	SER
1	A	110	GLN
1	A	111	LEU
1	A	114	ARG
1	A	118	TYR
1	A	122	LEU
1	A	131	LEU
1	A	137	THR
1	A	139	LEU
1	A	142	LEU
1	A	148	THR
1	A	164	LYS
1	A	171	ASN
1	A	174	GLU
1	A	175	THR
1	A	176	ASN
1	A	177	LEU
1	A	179	TYR
1	A	187	ASP
1	A	190	VAL
1	A	192	SER
1	A	193	THR
1	A	195	VAL
1	A	200	THR
1	A	202	ASN
1	A	205	GLN
1	A	207	THR
1	A	209	THR
1	A	210	ILE
1	A	211	ILE
1	A	217	SER
1	A	220	ARG
1	A	221	ILE
1	A	224	GLU
1	A	225	ILE
1	A	233	VAL
1	A	234	LYS
1	A	238	ASP
1	A	239	VAL
1	A	240	THR
1	A	242	THR

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Mol	Chain	Res	Type
1	A	244	LEU
1	A	246	ASP
1	A	255	ILE
1	A	262	THR
1	A	264	THR
1	A	267	ASP
1	A	289	VAL
1	A	290	TYR
1	A	295	ILE
1	A	297	VAL
1	A	298	GLU
1	A	302	HIS
1	A	308	MSE
1	A	309	THR
1	A	313	ASN
1	A	318	ASP
1	A	335	ASP
1	A	338	VAL
1	A	340	ASN
1	A	341	VAL
1	A	346	THR
1	A	348	GLN
1	A	350	ARG
1	A	357	GLN
1	A	362	THR
1	A	369	THR
1	A	376	ILE
1	A	378	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	327	ASN
1	A	340	ASN
1	A	358	ASN

5.3.3 RNA

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

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	321/369 (86%)	0.39	29 (9%)	9	10	60, 112, 201, 266	1 (0%)

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	373	LYS	7.2
1	A	341	VAL	6.3
1	A	374	VAL	5.7
1	A	47	VAL	4.8
1	A	295	ILE	4.5
1	A	324	PHE	4.5
1	A	342	LEU	4.3
1	A	313	ASN	3.9
1	A	354	ILE	3.8
1	A	364	VAL	3.7
1	A	355	GLY	3.6
1	A	181	LYS	3.5
1	A	86	ALA	3.2
1	A	296	ILE	2.9
1	A	242	THR	2.9
1	A	303	VAL	2.9
1	A	85	LEU	2.8
1	A	293	ALA	2.7
1	A	371	GLY	2.7
1	A	312	ASN	2.5
1	A	372	GLU	2.5
1	A	214	ALA	2.3
1	A	195	VAL	2.3
1	A	184	SER	2.3
1	A	76	GLY	2.2
1	A	294	ASN	2.2
1	A	210	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	297	VAL	2.1
1	A	337	TYR	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.