Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 11:18 PM GMT

PDB ID	:	1X2G
Title	:	Crystal Structure of Lipate-Protein Ligase A from Escherichia coli
Authors	:	Fujiwara, K.; Toma, S.; Okamura-Ikeda, K.; Motokawa, Y.; Nakagawa, A.; Taniguchi, H.
Deposited on	:	2005-04-23
Resolution	:	2.40 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

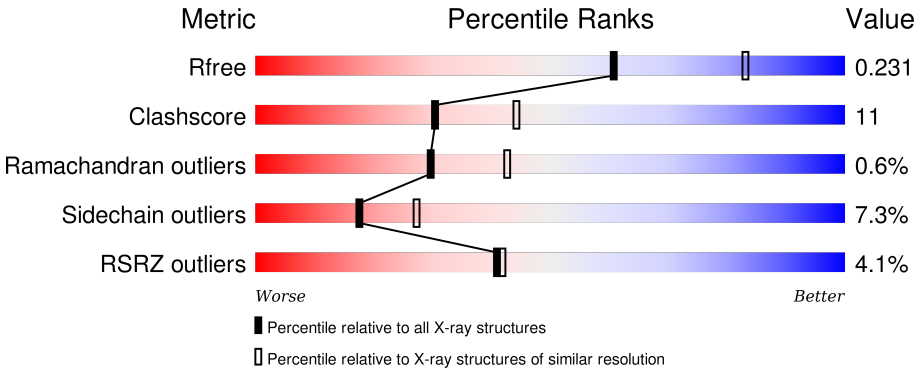
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.40 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}	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	337	3% 76% 19%
1	B	337	5% 78% 17%
1	C	337	4% 75% 20%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 8425 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 Lipoate-protein ligase A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	331	Total	C	N	O	S	Se	0	0	0
			2618	1646	467	494	6	5			
1	B	330	Total	C	N	O	S	Se	0	0	0
			2614	1644	466	493	6	5			
1	C	337	Total	C	N	O	S	Se	0	0	0
			2663	1673	476	503	6	5			

- Molecule 2 is water.

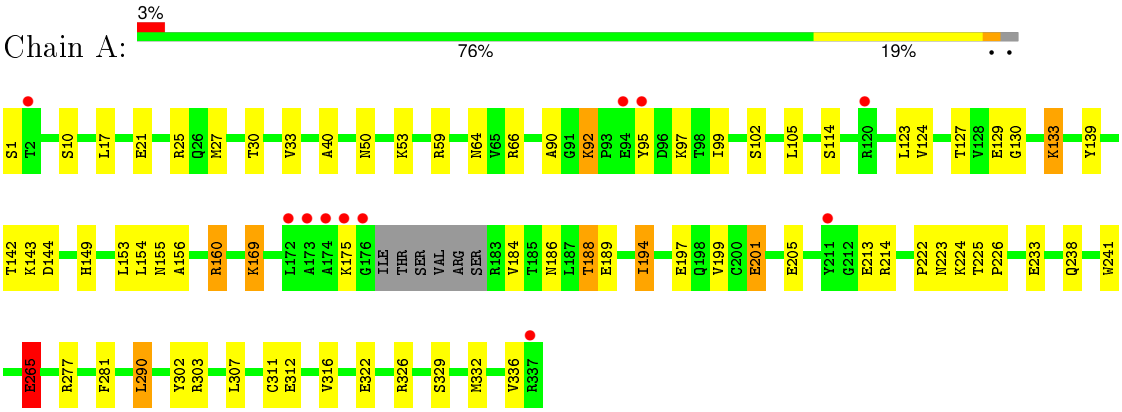
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	177	Total	O	0	0
			177	177		
2	B	175	Total	O	0	0
			175	175		
2	C	178	Total	O	0	0
			178	178		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

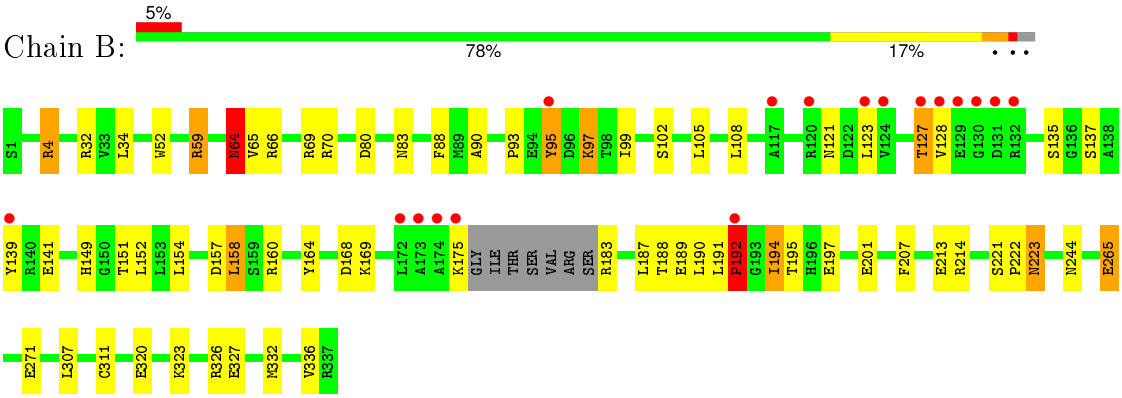
- Molecule 1: Lipoate-protein ligase A

Chain A:



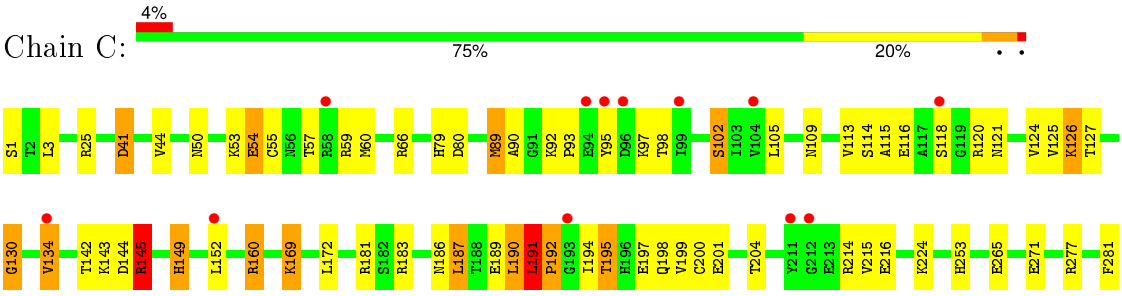
- Molecule 1: Lipoate-protein ligase A

Chain B:



- Molecule 1: Lipoate-protein ligase A

Chain C:




L290
L297
A304
L307
Q308
C311
L315
E322
K323
R326
M332
V336
R337

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	82.00Å 112.80Å 289.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.60 – 2.40 43.61 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.6 (43.60-2.40) 99.6 (43.61-2.40)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	6.71 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.171 , 0.233 0.169 , 0.231	Depositor DCC
R_{free} test set	2698 reflections (5.42%)	DCC
Wilson B-factor (Å^2)	43.0	Xtriage
Anisotropy	0.029	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 44.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 52725 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	8425	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.38% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	1.03	4/2669 (0.1%)	0.94	3/3606 (0.1%)
1	B	0.98	2/2665 (0.1%)	0.95	5/3601 (0.1%)
1	C	1.04	8/2715 (0.3%)	0.93	6/3670 (0.2%)
All	All	1.02	14/8049 (0.2%)	0.94	14/10877 (0.1%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	54	GLU	CB-CG	11.49	1.74	1.52
1	C	54	GLU	CD-OE2	9.15	1.35	1.25
1	B	265	GLU	CD-OE1	8.82	1.35	1.25
1	C	265	GLU	CD-OE1	8.79	1.35	1.25
1	A	265	GLU	CD-OE1	8.69	1.35	1.25
1	C	54	GLU	CG-CD	8.33	1.64	1.51
1	A	233	GLU	CG-CD	6.21	1.61	1.51
1	C	89	MSE	SE-CE	-5.99	1.60	1.95
1	C	201	GLU	CB-CG	5.98	1.63	1.52
1	C	201	GLU	CG-CD	5.53	1.60	1.51
1	A	302	TYR	CD2-CE2	5.33	1.47	1.39
1	B	64	ASN	CB-CG	5.22	1.63	1.51
1	C	55	CYS	CB-SG	-5.12	1.73	1.81
1	A	201	GLU	CG-CD	5.05	1.59	1.51

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	4	ARG	NE-CZ-NH2	-10.57	115.01	120.30
1	B	4	ARG	NE-CZ-NH1	7.81	124.20	120.30
1	C	160	ARG	NE-CZ-NH1	7.77	124.19	120.30
1	C	160	ARG	NE-CZ-NH2	-7.68	116.46	120.30
1	A	160	ARG	NE-CZ-NH2	-7.32	116.64	120.30
1	B	70	ARG	NE-CZ-NH2	-6.68	116.96	120.30
1	A	290	LEU	CA-CB-CG	-6.54	100.26	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	187	LEU	CA-CB-CG	6.49	130.22	115.30
1	B	80	ASP	CB-CG-OD1	6.35	124.02	118.30
1	B	168	ASP	CB-CG-OD1	5.61	123.35	118.30
1	C	145	ARG	NE-CZ-NH2	-5.27	117.66	120.30
1	C	80	ASP	CB-CG-OD1	5.20	122.98	118.30
1	C	290	LEU	CA-CB-CG	-5.10	103.57	115.30
1	A	303	ARG	NE-CZ-NH1	5.08	122.84	120.30

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	2618	0	2554	56	0
1	B	2614	0	2551	43	0
1	C	2663	0	2605	78	0
2	A	177	0	0	7	0
2	B	175	0	0	8	0
2	C	178	0	0	16	0
All	All	8425	0	7710	171	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 (171) 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:C:89:MSE:HE2	1:C:145:ARG:HB2	1.31	1.11
1:C:169:LYS:HD3	1:C:169:LYS:H	1.01	1.08
1:C:337:ARG:HG2	2:C:515:HOH:O	1.56	1.05
1:C:126:LYS:HG3	1:C:130:GLY:O	1.58	1.04
1:C:142:THR:HG22	1:C:144:ASP:H	1.26	1.00
1:C:1:SER:HB3	2:C:493:HOH:O	1.63	0.99
1:B:69:ARG:H	1:B:244:ASN:HD22	1.12	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:50:ASN:O	1:C:54:GLU:HG3	1.67	0.94
1:A:197:GLU:O	1:A:201:GLU:HG3	1.69	0.92
1:C:169:LYS:CD	1:C:169:LYS:H	1.84	0.89
1:C:169:LYS:HD3	1:C:169:LYS:N	1.87	0.88
1:C:215:VAL:HG11	2:C:376:HOH:O	1.74	0.87
1:A:169:LYS:H	1:A:169:LYS:HD2	1.41	0.86
1:C:127:THR:H	1:C:130:GLY:HA3	1.39	0.85
1:C:89:MSE:HE2	1:C:145:ARG:CB	2.09	0.83
1:A:1:SER:HB3	1:A:213:GLU:OE2	1.77	0.83
1:A:155:ASN:ND2	1:A:188:THR:HG21	1.94	0.82
1:C:191:LEU:H	1:C:192:PRO:HD3	1.46	0.81
1:C:54:GLU:HB3	2:C:505:HOH:O	1.81	0.80
1:C:134:VAL:HG21	1:C:187:LEU:HD13	1.67	0.75
1:A:265:GLU:HG3	2:A:493:HOH:O	1.87	0.75
1:A:155:ASN:HD22	1:A:188:THR:HG21	1.50	0.74
1:C:323:LYS:HA	1:C:326:ARG:HG2	1.70	0.73
1:C:89:MSE:CE	1:C:145:ARG:HB2	2.16	0.72
1:B:271:GLU:HG2	2:B:497:HOH:O	1.90	0.71
1:A:17:LEU:HG	2:A:471:HOH:O	1.89	0.71
1:A:194:ILE:HD11	1:A:199:VAL:CG2	2.21	0.71
1:B:307:LEU:CD1	1:B:336:VAL:HG21	2.21	0.69
1:B:83:ASN:HD22	1:B:151:THR:HG21	1.57	0.69
1:B:69:ARG:H	1:B:244:ASN:ND2	1.88	0.68
1:B:59:ARG:HH11	1:B:59:ARG:HG3	1.59	0.68
1:A:142:THR:HG22	1:A:144:ASP:H	1.59	0.68
1:C:304:ALA:O	1:C:308:GLN:HG3	1.94	0.67
1:A:66:ARG:HH21	1:B:64:ASN:HD22	1.42	0.67
1:A:27:MSE:HE1	1:A:33:VAL:CG2	2.24	0.67
1:A:27:MSE:HE1	1:A:33:VAL:HG21	1.77	0.67
1:C:59:ARG:HG3	1:C:59:ARG:HH11	1.59	0.66
1:A:1:SER:CB	1:A:213:GLU:OE2	2.43	0.66
1:C:90:ALA:HB3	1:C:95:TYR:CD1	2.31	0.66
1:C:89:MSE:CE	1:C:145:ARG:CB	2.73	0.65
1:B:265:GLU:HG3	2:B:373:HOH:O	1.96	0.65
1:C:127:THR:H	1:C:130:GLY:CA	2.09	0.64
1:A:127:THR:HB	1:A:130:GLY:O	1.97	0.64
1:C:89:MSE:HE3	1:C:145:ARG:NE	2.13	0.64
1:B:64:ASN:HB3	2:B:446:HOH:O	1.97	0.64
1:C:57:THR:HA	1:C:60:MSE:HE2	1.80	0.63
1:A:238:GLN:HG3	2:A:452:HOH:O	1.99	0.63
1:B:323:LYS:O	1:B:327:GLU:HG3	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:SER:HA	2:A:437:HOH:O	1.99	0.62
1:C:125:VAL:HG21	1:C:190:LEU:HD12	1.82	0.62
1:C:1:SER:H2	1:C:215:VAL:HG22	1.65	0.61
1:A:307:LEU:CD1	1:A:336:VAL:HG21	2.31	0.61
1:C:224:LYS:HD2	2:C:472:HOH:O	2.00	0.60
1:C:191:LEU:N	1:C:192:PRO:HD3	2.13	0.60
1:A:133:LYS:HB3	1:A:184:VAL:HG22	1.83	0.60
1:B:59:ARG:CG	1:B:59:ARG:HH11	2.13	0.60
1:C:41:ASP:OD2	1:C:160:ARG:NH2	2.35	0.59
1:B:83:ASN:HD22	1:B:151:THR:CG2	2.15	0.59
1:C:66:ARG:HG3	2:C:503:HOH:O	2.03	0.58
1:A:316:VAL:HB	2:C:486:HOH:O	2.03	0.58
1:C:190:LEU:O	1:C:191:LEU:HB2	2.03	0.58
1:C:253:HIS:CE1	2:C:498:HOH:O	2.56	0.58
1:A:154:LEU:O	1:A:188:THR:HB	2.04	0.57
1:C:307:LEU:HD13	1:C:336:VAL:HG21	1.85	0.57
1:C:152:LEU:HD13	1:C:199:VAL:HG11	1.85	0.57
1:C:271:GLU:HG2	2:C:496:HOH:O	2.05	0.57
1:C:253:HIS:HE1	2:C:498:HOH:O	1.88	0.56
1:C:44:VAL:HG23	1:C:79:HIS:HD2	1.70	0.56
1:C:297:LEU:HD22	1:C:307:LEU:HD23	1.87	0.56
1:C:50:ASN:O	1:C:54:GLU:CG	2.48	0.56
1:C:118:SER:OG	1:C:124:VAL:HG23	2.07	0.55
1:B:139:TYR:CE2	1:B:141:GLU:HG3	2.42	0.55
1:C:200:CYS:O	1:C:204:THR:HG23	2.06	0.55
1:C:191:LEU:H	1:C:192:PRO:CD	2.16	0.55
1:B:195:THR:HG22	1:B:197:GLU:OE1	2.07	0.55
1:B:69:ARG:N	1:B:244:ASN:HD22	1.94	0.55
1:C:115:ALA:O	1:C:116:GLU:HG3	2.07	0.55
1:C:169:LYS:HD2	2:C:480:HOH:O	2.07	0.54
1:A:307:LEU:HD13	1:A:336:VAL:HG21	1.89	0.54
1:A:194:ILE:HD11	1:A:199:VAL:HG22	1.90	0.54
1:A:225:THR:HG22	1:A:226:PRO:O	2.08	0.53
1:B:4:ARG:NH2	2:B:410:HOH:O	2.41	0.53
1:C:144:ASP:OD1	1:C:145:ARG:HD2	2.08	0.53
1:B:307:LEU:HD12	1:B:336:VAL:HG21	1.88	0.53
1:C:1:SER:N	1:C:215:VAL:HG22	2.23	0.53
1:A:10:SER:HB2	1:A:222:PRO:HD3	1.90	0.52
1:A:142:THR:CG2	1:A:143:LYS:N	2.72	0.52
1:B:97:LYS:HG3	1:B:139:TYR:CD1	2.44	0.52
1:C:125:VAL:HG21	1:C:190:LEU:CD1	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:ARG:HD3	2:A:348:HOH:O	2.09	0.52
1:B:121:ASN:HB3	1:B:137:SER:O	2.10	0.51
1:C:311:CYS:HB2	1:C:332:MSE:HE1	1.94	0.50
1:C:98:THR:O	1:C:102:SER:HB3	2.11	0.50
1:A:205:GLU:OE1	1:A:214:ARG:NH2	2.44	0.50
1:A:27:MSE:CE	1:A:33:VAL:HG21	2.41	0.49
1:C:215:VAL:HG12	1:C:216:GLU:N	2.27	0.49
1:C:326:ARG:HD3	2:C:514:HOH:O	2.13	0.49
1:A:127:THR:HG22	1:A:129:GLU:N	2.28	0.49
1:A:194:ILE:HD11	1:A:199:VAL:HG23	1.95	0.48
1:C:59:ARG:HD3	2:C:388:HOH:O	2.13	0.48
1:C:194:ILE:HG23	1:C:198:GLN:HE21	1.78	0.48
1:A:156:ALA:H	1:A:186:ASN:ND2	2.12	0.48
1:B:97:LYS:HG3	1:B:139:TYR:CG	2.49	0.47
1:B:195:THR:HG21	2:B:392:HOH:O	2.14	0.47
1:B:93:PRO:HD2	2:B:466:HOH:O	2.14	0.47
1:A:156:ALA:H	1:A:186:ASN:HD21	1.62	0.47
1:A:142:THR:HG22	1:A:144:ASP:N	2.26	0.47
1:B:187:LEU:C	1:B:194:ILE:HD11	2.35	0.47
1:B:123:LEU:HB2	1:B:135:SER:HB3	1.97	0.47
1:B:188:THR:N	1:B:194:ILE:HD11	2.30	0.46
1:A:97:LYS:HD2	1:A:139:TYR:HB2	1.97	0.46
1:C:127:THR:N	1:C:130:GLY:HA3	2.20	0.46
1:A:194:ILE:CD1	1:A:199:VAL:CG2	2.92	0.46
1:C:142:THR:CG2	1:C:143:LYS:N	2.79	0.46
1:A:127:THR:HG23	1:A:129:GLU:OE1	2.16	0.46
1:C:118:SER:OG	1:C:124:VAL:CG2	2.63	0.46
1:B:83:ASN:HB3	1:B:151:THR:HG23	1.99	0.45
1:A:92:LYS:NZ	1:A:143:LYS:O	2.49	0.45
1:B:105:LEU:HD23	1:B:105:LEU:HA	1.80	0.45
1:C:25:ARG:NH1	2:C:500:HOH:O	2.49	0.45
1:C:326:ARG:CD	2:C:514:HOH:O	2.64	0.45
1:A:90:ALA:HB3	1:A:95:TYR:CG	2.52	0.45
1:B:34:LEU:HD13	1:B:88:PHE:CE1	2.51	0.45
1:B:90:ALA:HB3	1:B:95:TYR:CG	2.52	0.45
1:C:50:ASN:HB2	1:C:281:PHE:CG	2.53	0.44
1:C:66:ARG:HD3	1:C:66:ARG:HA	1.73	0.44
1:B:213:GLU:HG2	1:B:214:ARG:N	2.32	0.44
1:A:160:ARG:HD2	2:A:353:HOH:O	2.18	0.44
1:A:21:GLU:O	1:A:25:ARG:HG2	2.18	0.43
1:C:191:LEU:N	1:C:192:PRO:CD	2.79	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:THR:HG22	1:A:143:LYS:N	2.34	0.43
1:C:60:MSE:HB2	1:C:60:MSE:HE2	1.92	0.43
1:A:153:LEU:HD13	1:A:184:VAL:HG13	2.00	0.43
1:C:194:ILE:HG22	1:C:195:THR:N	2.34	0.43
1:B:158:LEU:HD12	1:B:158:LEU:H	1.83	0.43
1:B:189:GLU:O	1:B:192:PRO:HD3	2.19	0.43
1:B:157:ASP:HB3	1:B:160:ARG:HG3	2.01	0.43
1:C:224:LYS:CD	2:C:472:HOH:O	2.63	0.43
1:C:92:LYS:HD3	1:C:143:LYS:O	2.19	0.42
1:C:194:ILE:HG23	1:C:198:GLN:NE2	2.34	0.42
1:C:41:ASP:CG	1:C:160:ARG:NH2	2.72	0.42
1:C:195:THR:HG22	1:C:197:GLU:OE1	2.19	0.42
1:B:65:VAL:HG21	1:B:164:TYR:CZ	2.54	0.42
1:A:40:ALA:HB1	2:B:512:HOH:O	2.19	0.42
1:A:105:LEU:HD21	1:A:123:LEU:HD22	2.02	0.42
1:C:190:LEU:O	1:C:191:LEU:CB	2.68	0.42
1:A:153:LEU:CD1	1:A:184:VAL:HG13	2.50	0.42
1:C:92:LYS:HB2	1:C:93:PRO:HA	2.02	0.42
1:A:64:ASN:ND2	1:B:66:ARG:HH12	2.18	0.41
1:A:50:ASN:HB2	1:A:281:PHE:CD1	2.55	0.41
1:A:223:ASN:HB3	1:B:52:TRP:CZ3	2.55	0.41
1:A:64:ASN:HB3	1:B:64:ASN:HB2	2.03	0.41
1:C:59:ARG:HG3	1:C:59:ARG:NH1	2.32	0.41
1:B:326:ARG:HD2	2:B:477:HOH:O	2.20	0.41
1:C:109:ASN:HA	1:C:113:VAL:O	2.20	0.41
1:B:127:THR:HB	1:B:128:VAL:H	1.69	0.41
1:B:108:LEU:HD21	1:B:152:LEU:HD22	2.03	0.41
1:A:27:MSE:HE1	1:A:33:VAL:HG22	2.03	0.41
1:A:241:TRP:CZ2	1:B:222:PRO:HB2	2.56	0.41
1:B:221:SER:OG	1:B:223:ASN:ND2	2.54	0.41
1:C:315:LEU:HD11	1:C:322:GLU:HG2	2.02	0.41
1:C:50:ASN:HB2	1:C:281:PHE:CD1	2.56	0.41
1:A:311:CYS:HB2	1:A:332:MSE:HE1	2.02	0.41
1:B:311:CYS:HB2	1:B:332:MSE:HE1	2.03	0.40
1:A:312:GLU:OE2	1:A:329:SER:OG	2.35	0.40
1:A:277:ARG:HB3	1:C:277:ARG:HB3	2.03	0.40
1:A:322:GLU:HG3	2:A:514:HOH:O	2.22	0.40
1:C:44:VAL:CG2	1:C:79:HIS:CD2	3.04	0.40
1:A:142:THR:HG21	1:A:144:ASP:OD1	2.20	0.40
1:C:149:HIS:N	1:C:149:HIS:CD2	2.89	0.40
1:C:149:HIS:H	1:C:149:HIS:CD2	2.39	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	327/337 (97%)	318 (97%)	9 (3%)	0	100	100
1	B	326/337 (97%)	313 (96%)	12 (4%)	1 (0%)	46	63
1	C	335/337 (99%)	314 (94%)	16 (5%)	5 (2%)	13	17
All	All	988/1011 (98%)	945 (96%)	37 (4%)	6 (1%)	30	43

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	191	LEU
1	B	192	PRO
1	C	130	GLY
1	C	186	ASN
1	C	192	PRO
1	C	41	ASP

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	276/277 (100%)	259 (94%)	17 (6%)	23	35
1	B	276/277 (100%)	254 (92%)	22 (8%)	15	23
1	C	282/277 (102%)	260 (92%)	22 (8%)	16	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	834/831 (100%)	773 (93%)	61 (7%)	17 27

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	THR
1	A	53	LYS
1	A	92	LYS
1	A	99	ILE
1	A	102	SER
1	A	124	VAL
1	A	133	LYS
1	A	149	HIS
1	A	169	LYS
1	A	175	LYS
1	A	188	THR
1	A	189	GLU
1	A	194	ILE
1	A	224	LYS
1	A	265	GLU
1	A	290	LEU
1	A	326	ARG
1	B	32	ARG
1	B	59	ARG
1	B	64	ASN
1	B	95	TYR
1	B	97	LYS
1	B	99	ILE
1	B	102	SER
1	B	127	THR
1	B	149	HIS
1	B	154	LEU
1	B	158	LEU
1	B	169	LYS
1	B	175	LYS
1	B	183	ARG
1	B	190	LEU
1	B	191	LEU
1	B	192	PRO
1	B	194	ILE
1	B	201	GLU
1	B	207	PHE

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Mol	Chain	Res	Type
1	B	223	ASN
1	B	320	GLU
1	C	3	LEU
1	C	53	LYS
1	C	97	LYS
1	C	102	SER
1	C	105	LEU
1	C	114	SER
1	C	120	ARG
1	C	121	ASN
1	C	126	LYS
1	C	134	VAL
1	C	145	ARG
1	C	149	HIS
1	C	169	LYS
1	C	172	LEU
1	C	181	ARG
1	C	183	ARG
1	C	189	GLU
1	C	190	LEU
1	C	191	LEU
1	C	195	THR
1	C	214	ARG
1	C	332	MSE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	ASN
1	A	155	ASN
1	A	186	ASN
1	A	230	ASN
1	A	238	GLN
1	A	279	GLN
1	B	26	GLN
1	B	64	ASN
1	B	83	ASN
1	B	166	ASN
1	B	223	ASN
1	B	230	ASN
1	B	244	ASN
1	B	279	GLN

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Mol	Chain	Res	Type
1	B	298	GLN
1	C	50	ASN
1	C	79	HIS
1	C	121	ASN
1	C	149	HIS
1	C	166	ASN
1	C	198	GLN
1	C	253	HIS
1	C	279	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 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

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	326/337 (96%)	-0.17	11 (3%)	49	49	26, 41, 66, 97	0
1	B	325/337 (96%)	-0.12	17 (5%)	31	31	27, 42, 87, 99	0
1	C	332/337 (98%)	0.08	12 (3%)	46	47	29, 48, 88, 98	0
All	All	983/1011 (97%)	-0.06	40 (4%)	41	42	26, 43, 86, 99	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	176	GLY	5.3
1	B	130	GLY	4.4
1	A	174	ALA	4.1
1	A	95	TYR	3.9
1	A	120	ARG	3.9
1	A	173	ALA	3.8
1	B	132	ARG	3.8
1	A	175	LYS	3.6
1	A	172	LEU	3.5
1	B	131	ASP	3.5
1	B	174	ALA	3.3
1	C	95	TYR	3.2
1	B	123	LEU	3.2
1	B	127	THR	3.2
1	B	128	VAL	3.1
1	B	124	VAL	3.0
1	C	118	SER	2.9
1	C	104	VAL	2.9
1	B	120	ARG	2.7
1	C	58	ARG	2.7
1	B	173	ALA	2.7
1	C	94	GLU	2.7
1	B	192	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	2	THR	2.4
1	C	99	ILE	2.4
1	B	175	LYS	2.4
1	A	211	TYR	2.4
1	A	337	ARG	2.3
1	C	193	GLY	2.2
1	C	211	TYR	2.2
1	B	172	LEU	2.1
1	B	117	ALA	2.1
1	C	212	GLY	2.1
1	C	152	LEU	2.1
1	B	95	TYR	2.1
1	B	139	TYR	2.1
1	C	96	ASP	2.1
1	B	129	GLU	2.1
1	A	94	GLU	2.0
1	C	134	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.