Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:18 AM GMT

PDB ID	:	2Q74
Title	:	Mycobacterium tuberculosis SuhB
Authors	:	Brown, A.K.; Meng, G.; Ghadbane, H.; Besra, G.S.; Futterer, K.
Deposited on	:	2007-06-06
Resolution	:	2.60 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:

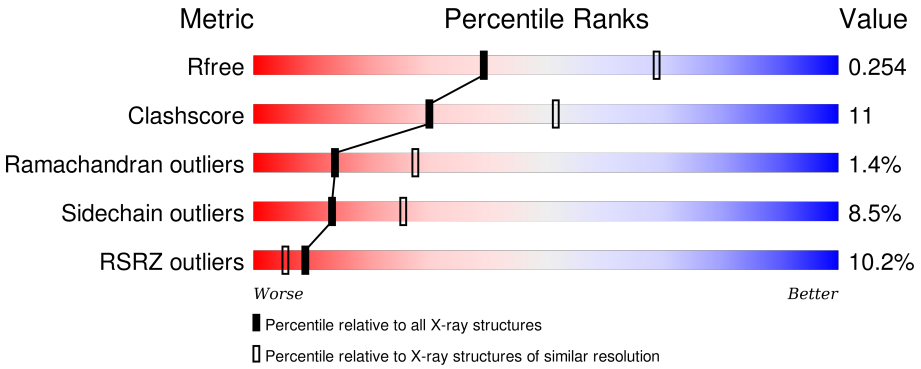
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.60 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	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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	299	7% 65% 15% • 18%
1	B	299	9% 66% 12% • 18%
1	C	299	9% 61% 17% • 19%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 5466 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 Inositol-1-monophosphatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	245	Total	C	N	O	S	0	0	0
			1784	1115	325	339	5			
1	B	245	Total	C	N	O	S	0	0	0
			1784	1115	325	338	6			
1	C	243	Total	C	N	O	S	0	0	0
			1774	1109	323	336	6			

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	291	ALA	-	expression tag	UNP P65165
A	292	LEU	-	expression tag	UNP P65165
A	293	GLU	-	expression tag	UNP P65165
A	294	HIS	-	expression tag	UNP P65165
A	295	HIS	-	expression tag	UNP P65165
A	296	HIS	-	expression tag	UNP P65165
A	297	HIS	-	expression tag	UNP P65165
A	298	HIS	-	expression tag	UNP P65165
A	299	HIS	-	expression tag	UNP P65165
B	291	ALA	-	expression tag	UNP P65165
B	292	LEU	-	expression tag	UNP P65165
B	293	GLU	-	expression tag	UNP P65165
B	294	HIS	-	expression tag	UNP P65165
B	295	HIS	-	expression tag	UNP P65165
B	296	HIS	-	expression tag	UNP P65165
B	297	HIS	-	expression tag	UNP P65165
B	298	HIS	-	expression tag	UNP P65165
B	299	HIS	-	expression tag	UNP P65165
C	291	ALA	-	expression tag	UNP P65165
C	292	LEU	-	expression tag	UNP P65165
C	293	GLU	-	expression tag	UNP P65165
C	294	HIS	-	expression tag	UNP P65165
C	295	HIS	-	expression tag	UNP P65165

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Chain	Residue	Modelled	Actual	Comment	Reference
C	296	HIS	-	expression tag	UNP P65165
C	297	HIS	-	expression tag	UNP P65165
C	298	HIS	-	expression tag	UNP P65165
C	299	HIS	-	expression tag	UNP P65165

- Molecule 2 is water.

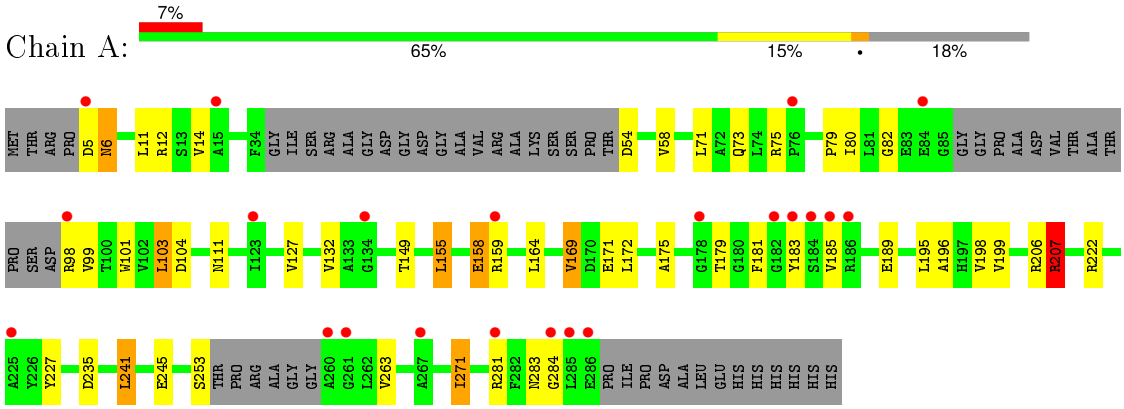
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	41	Total O 41 41	0	0
2	B	31	Total O 31 31	0	0
2	C	52	Total O 52 52	0	0

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.

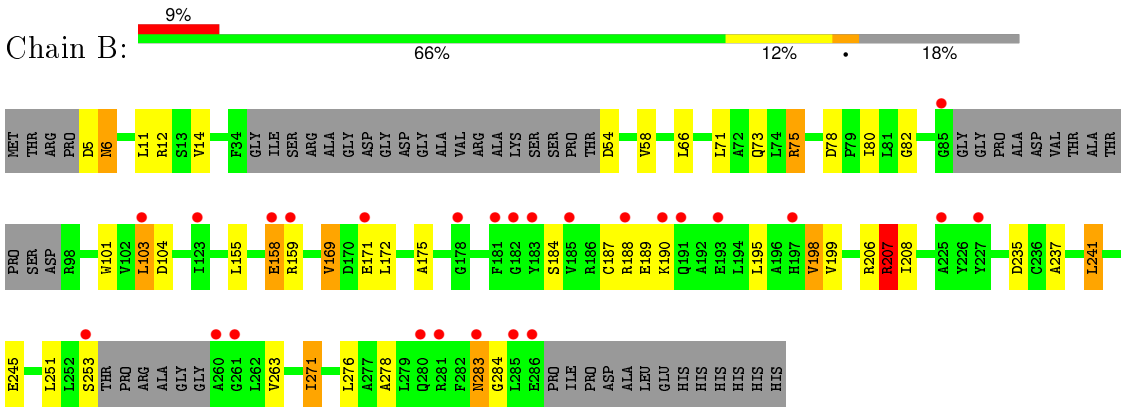
- Molecule 1: Inositol-1-monophosphatase

Chain A:



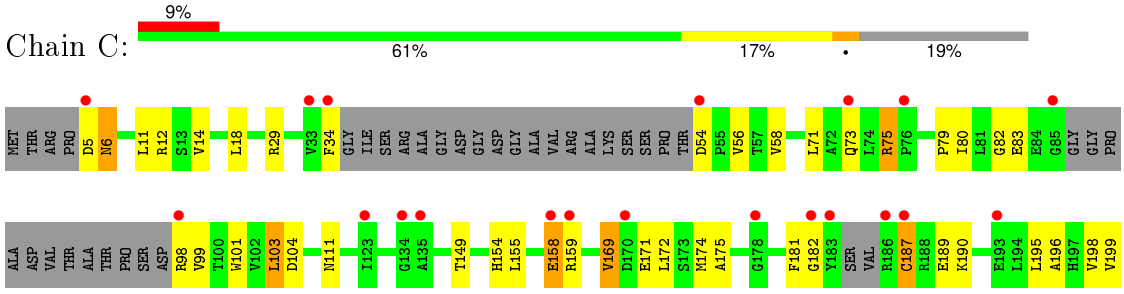
- Molecule 1: Inositol-1-monophosphatase

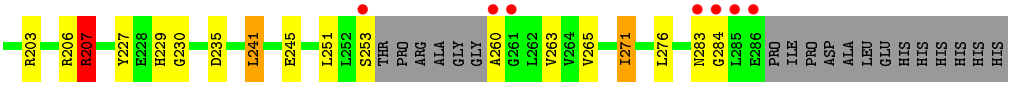
Chain B:



- Molecule 1: Inositol-1-monophosphatase

Chain C:




R203
R206
R207
Y227
E228
H229
G230
D235
L241
E245
L251
L252
S253
THR
PRO
ARG
ALA
GLY
GLY
A260
G261
L262
V263
V264
V265
I271
L276
N283
G284
L285
E286
PRO
ILE
PRO
ASP
ALA
LEU
GLU
HIS
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	101.40Å 185.60Å 107.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.88 – 2.60 19.90 – 2.60	Depositor EDS
% Data completeness (in resolution range)	93.2 (19.88-2.60) 92.6 (19.90-2.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	3.28 (at 2.59Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.223 , 0.245 0.217 , 0.254	Depositor DCC
R_{free} test set	1469 reflections (5.33%)	DCC
Wilson B-factor (Å^2)	68.9	Xtriage
Anisotropy	0.069	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 71.4	EDS
Estimated twinning fraction	0.015 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.021 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	1 of 29034 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5466	wwPDB-VP
Average B, all atoms (Å^2)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.62% 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	0.56	0/1806	0.72	1/2457 (0.0%)
1	B	0.44	0/1806	0.66	1/2457 (0.0%)
1	C	0.58	0/1795	0.72	1/2440 (0.0%)
All	All	0.53	0/5407	0.70	3/7354 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	207	ARG	NE-CZ-NH1	7.12	123.86	120.30
1	B	207	ARG	NE-CZ-NH1	7.04	123.82	120.30
1	A	207	ARG	NE-CZ-NH1	6.91	123.75	120.30

There are no chirality outliers.

There are no planarity outliers.

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	1784	0	1769	38	0
1	B	1784	0	1769	38	1
1	C	1774	0	1764	50	0
2	A	41	0	0	5	0
2	B	31	0	0	9	1
2	C	52	0	0	16	0
All	All	5466	0	5302	118	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 11.

All (118) 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:195:LEU:CD2	2:A:312:HOH:O	1.93	1.17
1:C:29:ARG:HD3	2:C:287:HOH:O	1.50	1.08
1:B:199:VAL:HG11	2:B:316:HOH:O	1.68	0.92
1:A:195:LEU:HD23	2:A:312:HOH:O	1.56	0.92
1:B:278:ALA:HB1	2:B:310:HOH:O	1.72	0.90
1:C:56:VAL:HG12	2:C:310:HOH:O	1.81	0.80
1:C:251:LEU:HD23	2:C:323:HOH:O	1.86	0.75
1:B:237:ALA:HB1	2:B:306:HOH:O	1.86	0.74
1:C:171:GLU:C	1:C:271:ILE:HD11	2.10	0.72
1:C:227:TYR:HB2	2:C:322:HOH:O	1.89	0.72
1:A:111:ASN:OD1	1:C:206:ARG:NH1	2.22	0.72
1:A:171:GLU:C	1:A:271:ILE:HD11	2.09	0.71
1:C:182:GLY:HA3	1:C:230:GLY:O	1.91	0.70
1:C:79:PRO:HD2	1:C:99:VAL:O	1.92	0.70
1:B:171:GLU:C	1:B:271:ILE:HD11	2.13	0.69
1:A:132:VAL:HG22	2:A:318:HOH:O	1.91	0.69
1:C:265:VAL:HG13	2:C:322:HOH:O	1.94	0.67
1:C:265:VAL:HG22	2:C:322:HOH:O	1.98	0.64
1:A:206:ARG:NH1	1:C:111:ASN:OD1	2.33	0.62
1:C:18:LEU:HD23	2:C:338:HOH:O	1.99	0.61
2:B:303:HOH:O	1:C:187:CYS:HB2	2.00	0.61
1:C:34:PHE:CD1	2:C:330:HOH:O	2.51	0.60
1:A:281:ARG:HH22	1:B:283:ASN:ND2	2.00	0.60
1:C:54:ASP:O	1:C:58:VAL:HG23	2.03	0.59
1:A:281:ARG:HH22	1:B:283:ASN:CG	2.06	0.59
1:A:196:ALA:O	1:C:189:GLU:HG3	2.01	0.59
1:B:54:ASP:O	1:B:58:VAL:HG23	2.01	0.59
1:C:187:CYS:SG	1:C:187:CYS:O	2.61	0.58
1:A:54:ASP:O	1:A:58:VAL:HG23	2.03	0.58
1:A:71:LEU:HD13	1:A:80:ILE:HD12	1.86	0.58
1:C:169:VAL:HB	1:C:271:ILE:HD12	1.87	0.57
1:B:14:VAL:HB	2:B:297:HOH:O	2.05	0.57
1:C:83:GLU:HB3	2:C:299:HOH:O	2.04	0.57
1:A:189:GLU:HG3	1:C:196:ALA:O	2.04	0.57
1:C:71:LEU:HD13	1:C:80:ILE:HD12	1.87	0.56
1:B:206:ARG:CD	2:B:311:HOH:O	2.53	0.56
1:B:206:ARG:NE	2:B:311:HOH:O	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:VAL:HB	1:B:271:ILE:HD12	1.87	0.56
1:A:169:VAL:HB	1:A:271:ILE:HD12	1.87	0.55
1:B:187:CYS:O	1:B:189:GLU:N	2.40	0.55
1:A:195:LEU:HD21	2:A:312:HOH:O	1.82	0.55
1:C:171:GLU:O	1:C:271:ILE:HD11	2.07	0.54
1:A:207:ARG:HB3	1:C:207:ARG:HB3	1.90	0.54
1:C:6:ASN:HB2	2:C:306:HOH:O	2.08	0.53
1:B:171:GLU:O	1:B:271:ILE:HD11	2.08	0.53
1:B:5:ASP:C	2:B:302:HOH:O	2.47	0.53
1:A:14:VAL:CG2	1:A:101:TRP:CH2	2.92	0.52
1:B:71:LEU:HD13	1:B:80:ILE:HD12	1.91	0.52
1:C:260:ALA:HB2	2:C:325:HOH:O	2.09	0.52
1:C:195:LEU:O	1:C:199:VAL:HG23	2.09	0.52
1:A:171:GLU:O	1:A:271:ILE:HD11	2.09	0.51
1:A:79:PRO:HD2	1:A:99:VAL:O	2.11	0.51
1:C:34:PHE:CG	2:C:330:HOH:O	2.62	0.51
1:A:207:ARG:HD2	2:C:291:HOH:O	2.10	0.51
1:C:14:VAL:CG2	1:C:101:TRP:CH2	2.94	0.50
1:A:99:VAL:HG22	1:A:127:VAL:HG22	1.93	0.49
1:B:206:ARG:HD3	2:B:311:HOH:O	2.11	0.49
1:B:14:VAL:CG2	1:B:101:TRP:CH2	2.96	0.48
1:C:5:ASP:O	1:C:6:ASN:HB2	2.14	0.48
1:B:104:ASP:OD2	1:B:235:ASP:OD1	2.32	0.48
1:A:195:LEU:O	1:A:199:VAL:HG23	2.14	0.47
1:B:175:ALA:HB2	1:B:271:ILE:HD13	1.95	0.47
1:C:174:MET:O	1:C:203:ARG:HD2	2.14	0.47
1:B:207:ARG:HH11	1:B:207:ARG:HB2	1.80	0.47
1:B:195:LEU:O	1:B:199:VAL:HG23	2.15	0.46
1:A:99:VAL:HG22	1:A:127:VAL:CG2	2.45	0.46
1:C:241:LEU:HD22	1:C:245:GLU:HG2	1.98	0.46
1:B:207:ARG:CB	1:B:207:ARG:HH11	2.28	0.46
1:C:82:GLY:HA2	1:C:103:LEU:HD23	1.97	0.45
1:A:104:ASP:OD2	1:A:235:ASP:OD1	2.33	0.45
1:A:181:PHE:CZ	1:A:207:ARG:NH2	2.85	0.45
1:B:251:LEU:HD21	1:B:276:LEU:HD11	1.99	0.45
1:C:182:GLY:CA	1:C:230:GLY:O	2.64	0.45
1:B:207:ARG:HH11	1:B:207:ARG:CG	2.30	0.45
1:A:82:GLY:HA2	1:A:103:LEU:HD23	1.98	0.45
1:B:253:SER:HB3	1:B:263:VAL:HB	1.99	0.44
1:A:179:THR:HG22	1:A:227:TYR:O	2.17	0.44
1:A:207:ARG:HH11	1:A:207:ARG:CG	2.30	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:LEU:C	1:B:66:LEU:HD23	2.38	0.44
1:C:75:ARG:HA	1:C:75:ARG:HD2	1.92	0.44
1:C:207:ARG:HH11	1:C:207:ARG:CB	2.31	0.44
1:C:207:ARG:HH11	1:C:207:ARG:CG	2.30	0.44
1:A:172:LEU:N	1:A:271:ILE:HD11	2.32	0.44
1:A:14:VAL:CG2	1:A:101:TRP:HH2	2.30	0.44
1:A:207:ARG:CB	1:A:207:ARG:HH11	2.31	0.43
1:B:241:LEU:HD22	1:B:245:GLU:HG2	2.01	0.43
1:B:14:VAL:HG23	1:B:101:TRP:CH2	2.54	0.43
1:C:253:SER:HB3	1:C:263:VAL:HB	2.00	0.43
1:B:172:LEU:N	1:B:271:ILE:HD11	2.34	0.43
1:A:158:GLU:HG2	1:A:159:ARG:N	2.33	0.43
1:C:158:GLU:HG2	1:C:159:ARG:N	2.34	0.43
1:C:175:ALA:HB2	1:C:271:ILE:HD13	2.01	0.43
1:C:14:VAL:HG23	1:C:101:TRP:CH2	2.53	0.42
1:A:14:VAL:HG23	1:A:101:TRP:CH2	2.54	0.42
1:B:158:GLU:HG2	1:B:159:ARG:N	2.34	0.42
1:B:195:LEU:HA	1:B:198:VAL:HG13	2.00	0.42
1:B:82:GLY:HA2	1:B:103:LEU:HD23	2.02	0.42
1:C:181:PHE:CZ	1:C:207:ARG:NH2	2.88	0.42
1:B:75:ARG:NH1	1:B:78:ASP:OD2	2.53	0.42
1:A:5:ASP:O	1:A:6:ASN:HB2	2.18	0.42
1:C:172:LEU:N	1:C:271:ILE:HD11	2.35	0.41
1:A:241:LEU:HD22	1:A:245:GLU:HG2	2.03	0.41
1:C:207:ARG:HB2	1:C:207:ARG:HH11	1.86	0.41
1:C:14:VAL:CG2	1:C:101:TRP:HH2	2.33	0.41
1:A:222:ARG:NE	2:A:308:HOH:O	2.54	0.41
1:C:229:HIS:ND1	1:C:263:VAL:HG22	2.35	0.41
1:C:104:ASP:OD2	1:C:235:ASP:OD1	2.38	0.41
1:C:251:LEU:HD21	1:C:276:LEU:HD11	2.03	0.41
1:C:187:CYS:HA	2:C:300:HOH:O	2.20	0.41
1:A:155:LEU:HB2	1:A:164:LEU:HD21	2.03	0.41
1:B:190:LYS:HE3	2:C:300:HOH:O	2.20	0.41
1:B:189:GLU:CB	1:C:190:LYS:HE2	2.50	0.41
1:B:75:ARG:HA	1:B:75:ARG:HD2	1.90	0.40
1:A:253:SER:HB3	1:A:263:VAL:HB	2.03	0.40
1:C:154:HIS:HD2	2:C:298:HOH:O	2.04	0.40
1:B:14:VAL:CG2	1:B:101:TRP:HH2	2.34	0.40
1:B:5:ASP:O	1:B:6:ASN:HB2	2.21	0.40
1:A:175:ALA:HB2	1:A:271:ILE:HD13	2.02	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:208:ILE:C	2:B:311:HOH:O[3_655]	2.17	0.03

5.3 Torsion angles

5.3.1 Protein backbone

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	237/299 (79%)	222 (94%)	11 (5%)	4 (2%)	11	22
1	B	237/299 (79%)	221 (93%)	12 (5%)	4 (2%)	11	22
1	C	233/299 (78%)	218 (94%)	13 (6%)	2 (1%)	21	42
All	All	707/897 (79%)	661 (94%)	36 (5%)	10 (1%)	14	28

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	6	ASN
1	B	6	ASN
1	C	6	ASN
1	A	185	VAL
1	B	188	ARG
1	A	183	TYR
1	B	184	SER
1	C	284	GLY
1	A	284	GLY
1	B	284	GLY

5.3.2 Protein sidechains

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	172/217 (79%)	157 (91%)	15 (9%)	13	24
1	B	172/217 (79%)	159 (92%)	13 (8%)	16	32
1	C	172/217 (79%)	156 (91%)	16 (9%)	11	21
All	All	516/651 (79%)	472 (92%)	44 (8%)	13	25

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LEU
1	A	12	ARG
1	A	73	GLN
1	A	75	ARG
1	A	98	ARG
1	A	103	LEU
1	A	149	THR
1	A	155	LEU
1	A	158	GLU
1	A	169	VAL
1	A	198	VAL
1	A	207	ARG
1	A	241	LEU
1	A	271	ILE
1	A	283	ASN
1	B	11	LEU
1	B	12	ARG
1	B	73	GLN
1	B	75	ARG
1	B	103	LEU
1	B	155	LEU
1	B	158	GLU
1	B	169	VAL
1	B	198	VAL
1	B	207	ARG
1	B	241	LEU
1	B	271	ILE
1	B	283	ASN
1	C	11	LEU
1	C	12	ARG
1	C	73	GLN

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Mol	Chain	Res	Type
1	C	75	ARG
1	C	98	ARG
1	C	103	LEU
1	C	149	THR
1	C	155	LEU
1	C	158	GLU
1	C	169	VAL
1	C	187	CYS
1	C	198	VAL
1	C	207	ARG
1	C	241	LEU
1	C	271	ILE
1	C	283	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	126	GLN
1	A	232	GLN
1	A	280	GLN
1	A	283	ASN
1	B	6	ASN
1	B	126	GLN
1	B	232	GLN
1	B	280	GLN
1	B	283	ASN
1	C	6	ASN
1	C	126	GLN
1	C	232	GLN
1	C	280	GLN
1	C	283	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	245/299 (81%)	0.35	22 (8%)	12	8	52, 69, 87, 94	0
1	B	245/299 (81%)	0.53	26 (10%)	8	5	52, 69, 87, 92	0
1	C	243/299 (81%)	0.32	27 (11%)	7	4	52, 69, 86, 93	0
All	All	733/897 (81%)	0.40	75 (10%)	9	5	52, 69, 87, 94	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	185	VAL	10.5
1	B	197	HIS	5.5
1	A	260	ALA	5.5
1	B	286	GLU	5.4
1	A	184	SER	5.4
1	A	183	TYR	5.2
1	B	253	SER	5.0
1	B	183	TYR	5.0
1	B	190	LYS	5.0
1	C	5	ASP	5.0
1	A	185	VAL	4.8
1	B	261	GLY	4.2
1	A	182	GLY	4.2
1	C	85	GLY	4.1
1	B	182	GLY	3.9
1	C	285	LEU	3.9
1	A	98	ARG	3.9
1	A	286	GLU	3.8
1	A	225	ALA	3.8
1	C	76	PRO	3.7
1	A	186	ARG	3.7
1	B	158	GLU	3.6
1	C	261	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	260	ALA	3.4
1	C	134	GLY	3.4
1	C	34	PHE	3.3
1	C	186	ARG	3.2
1	B	85	GLY	3.2
1	C	253	SER	3.2
1	C	33	VAL	3.1
1	A	15	ALA	3.1
1	C	178	GLY	3.1
1	A	159	ARG	3.0
1	B	188	ARG	3.0
1	B	159	ARG	3.0
1	B	178	GLY	3.0
1	C	158	GLU	3.0
1	C	135	ALA	3.0
1	B	191	GLN	3.0
1	A	84	GLU	2.9
1	C	286	GLU	2.9
1	B	260	ALA	2.9
1	C	54	ASP	2.9
1	A	123	ILE	2.8
1	C	98	ARG	2.8
1	A	285	LEU	2.7
1	B	285	LEU	2.7
1	B	193	GLU	2.7
1	B	225	ALA	2.7
1	B	181	PHE	2.7
1	C	182	GLY	2.6
1	B	283	ASN	2.5
1	B	227	TYR	2.5
1	C	159	ARG	2.5
1	B	280	GLN	2.4
1	A	261	GLY	2.4
1	C	283	ASN	2.3
1	B	103	LEU	2.3
1	A	178	GLY	2.3
1	A	267	ALA	2.3
1	B	171	GLU	2.3
1	A	76	PRO	2.3
1	B	281	ARG	2.3
1	B	123	ILE	2.2
1	C	284	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	123	ILE	2.2
1	A	5	ASP	2.2
1	C	73	GLN	2.1
1	C	170	ASP	2.1
1	C	193	GLU	2.1
1	A	284	GLY	2.1
1	C	183	TYR	2.0
1	A	281	ARG	2.0
1	C	187	CYS	2.0
1	A	134	GLY	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 carbohydrates 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.