Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 10:34 PM GMT

PDB ID	:	1TZZ
Title	:	Crystal structure of the protein L1841, unknown member of enolase superfamily from Bradyrhizobium japonicum
Authors	:	Fedorov, A.A.; Fedorov, E.V.; Yew, W.S.; Gerlt, J.A.; Almo, S.C.; Burley, S.K.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on	:	2004-07-12
Resolution	:	1.86 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:

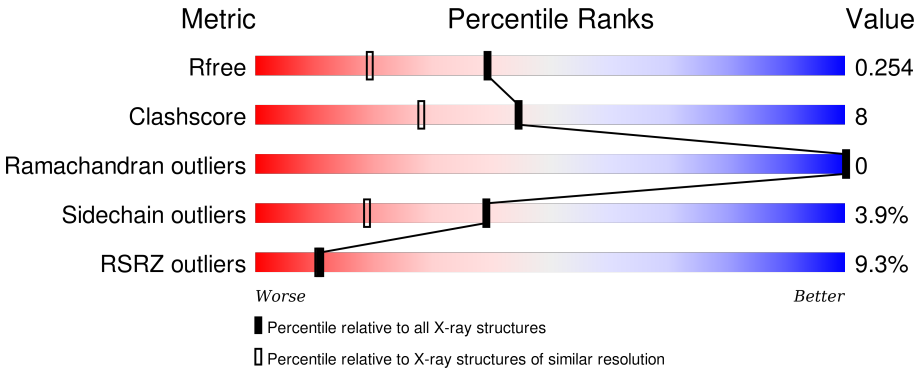
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 1.86 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	1745 (1.86-1.86)
Clashscore	102246	1898 (1.86-1.86)
Ramachandran outliers	100387	1875 (1.86-1.86)
Sidechain outliers	100360	1875 (1.86-1.86)
RSRZ outliers	91569	1747 (1.86-1.86)

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	392	14% 77% 17% • 5%
1	B	392	4% 78% 18% • •

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6155 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 Hypothetical protein L1841.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	374	Total	C	N	O	S	0	0	0
			2906	1840	511	538	17			
1	B	379	Total	C	N	O	S	0	0	0
			2944	1865	517	545	17			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1001	GLY	-	CLONING ARTIFACT	UNP Q89FH0
A	1002	SER	-	CLONING ARTIFACT	UNP Q89FH0
A	1003	HIS	-	CLONING ARTIFACT	UNP Q89FH0
B	2001	GLY	-	CLONING ARTIFACT	UNP Q89FH0
B	2002	SER	-	CLONING ARTIFACT	UNP Q89FH0
B	2003	HIS	-	CLONING ARTIFACT	UNP Q89FH0

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

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

- Molecule 3 is water.

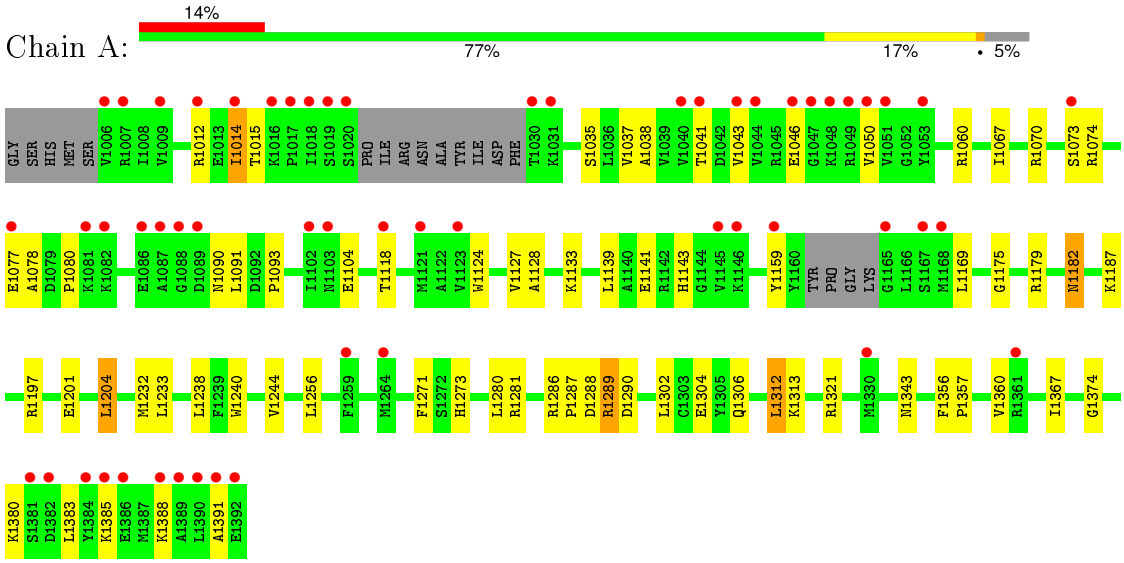
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	122	Total	O	0	0
			122	122		
3	B	181	Total	O	0	0
			181	181		

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.

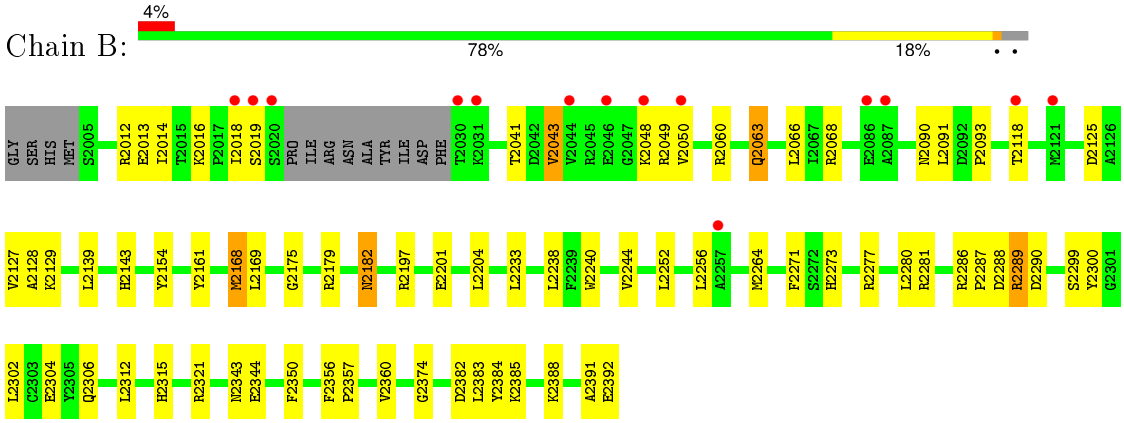
- Molecule 1: Hypothetical protein L1841

Chain A:



- Molecule 1: Hypothetical protein L1841

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	95.97Å 178.00Å 110.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.86 29.22 – 1.86	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-1.86) 99.3 (29.22-1.86)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.67 (at 1.87Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.234 , 0.254 0.235 , 0.254	Depositor DCC
R_{free} test set	3988 reflections (5.05%)	DCC
Wilson B-factor (Å^2)	23.5	Xtriage
Anisotropy	0.285	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 43.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Outliers	0 of 78948 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6155	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% 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

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	0.32	0/2969	0.59	0/4006
1	B	0.33	0/3010	0.61	0/4063
All	All	0.33	0/5979	0.60	0/8069

There are no bond length outliers.

There are no bond angle outliers.

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	2906	0	2861	43	0
1	B	2944	0	2899	50	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	122	0	0	2	0
3	B	181	0	0	1	0
All	All	6155	0	5760	92	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 8.

All (92) 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:2244:VAL:HG11	1:B:2256:LEU:HD21	1.60	0.84
1:B:2041:THR:OG1	1:B:2050:VAL:HG13	1.83	0.79
1:B:2357:PRO:O	1:B:2360:VAL:HG22	1.81	0.79
1:B:2161:TYR:CD2	1:B:2168:MET:HG2	2.20	0.77
1:B:2357:PRO:HD2	1:B:2360:VAL:HG21	1.71	0.73
1:A:1093:PRO:HG3	1:A:1127:VAL:HG21	1.68	0.73
1:B:2244:VAL:HG21	1:B:2264:MET:HE3	1.71	0.72
1:A:1012:ARG:HD2	1:A:1391:ALA:HB2	1.70	0.72
1:A:1014:ILE:HD13	1:A:1015:THR:N	2.06	0.71
1:B:2288:ASP:OD1	1:B:2289:ARG:HD3	1.90	0.70
1:A:1357:PRO:O	1:A:1360:VAL:HG22	1.92	0.69
1:A:1385:LYS:HA	1:A:1388:LYS:HE2	1.75	0.69
1:A:1357:PRO:HD2	1:A:1360:VAL:HG21	1.74	0.68
1:A:1288:ASP:OD1	1:A:1289:ARG:HD3	1.94	0.66
1:B:2244:VAL:HG21	1:B:2256:LEU:HD23	1.78	0.66
1:A:1244:VAL:HG11	1:A:1256:LEU:HD21	1.77	0.65
1:B:2384:TYR:CE2	1:B:2388:LYS:HD2	2.32	0.63
1:A:1041:THR:OG1	1:A:1050:VAL:HG13	1.98	0.63
1:B:2290:ASP:O	1:B:2321:ARG:HD3	1.98	0.62
1:B:2175:GLY:O	1:B:2179:ARG:HG2	1.99	0.62
1:B:2273:HIS:HD2	1:B:2304:GLU:OE2	1.85	0.60
1:A:1043:VAL:O	1:A:1050:VAL:HG12	2.03	0.59
1:A:1290:ASP:O	1:A:1321:ARG:HD3	2.03	0.59
1:B:2281:ARG:HG2	1:B:2315:HIS:CE1	2.37	0.58
1:B:2244:VAL:CG2	1:B:2264:MET:HE3	2.33	0.58
1:B:2043:VAL:O	1:B:2050:VAL:HG12	2.04	0.57
1:A:1175:GLY:O	1:A:1179:ARG:HG2	2.04	0.57
1:A:1273:HIS:HD2	1:A:1304:GLU:OE2	1.87	0.56
1:A:1244:VAL:HG21	1:A:1256:LEU:HD23	1.87	0.56
1:B:2280:LEU:HD11	1:B:2312:LEU:HD22	1.88	0.56
1:A:1280:LEU:HD11	1:A:1312:LEU:HD22	1.89	0.55
1:A:1128:ALA:HB3	1:A:1374:GLY:HA2	1.90	0.54
1:B:2277:ARG:O	1:B:2281:ARG:HG3	2.08	0.54
1:B:2118:THR:HG21	3:B:3025:HOH:O	2.07	0.54
1:B:2049:ARG:HH21	1:B:2392:GLU:C	2.11	0.54
1:A:1139:LEU:HD21	1:A:1302:LEU:HD21	1.91	0.53
1:B:2252:LEU:O	1:B:2256:LEU:HD13	2.09	0.53
1:B:2244:VAL:HG21	1:B:2256:LEU:CD2	2.38	0.52
1:B:2043:VAL:HG13	1:B:2050:VAL:CG1	2.39	0.52
1:B:2154:TYR:CE2	1:B:2344:GLU:HB3	2.45	0.52
1:A:1197:ARG:O	1:A:1201:GLU:HG3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2128:ALA:HB3	1:B:2374:GLY:HA2	1.91	0.51
1:A:1133:LYS:HE2	1:A:1141:GLU:OE2	2.11	0.51
1:A:1143:HIS:HE1	1:A:1306:GLN:NE2	2.08	0.51
1:A:1090:ASN:OD1	1:A:1091:LEU:N	2.43	0.51
1:B:2382:ASP:O	1:B:2385:LYS:HG2	2.11	0.51
1:B:2018:ILE:HG13	1:B:2019:SER:N	2.26	0.50
1:B:2197:ARG:O	1:B:2201:GLU:HG3	2.12	0.49
1:A:1313:LYS:HB2	1:A:1313:LYS:NZ	2.27	0.49
1:A:1070:ARG:HD3	1:A:1104:GLU:OE2	2.12	0.49
1:B:2093:PRO:HG3	1:B:2127:VAL:HG21	1.95	0.49
1:B:2143:HIS:HE1	1:B:2306:GLN:NE2	2.11	0.49
1:B:2018:ILE:HG13	1:B:2019:SER:H	1.78	0.48
1:B:2182:ASN:HD22	1:B:2182:ASN:C	2.17	0.48
1:A:1232:MET:SD	1:A:1233:LEU:HD12	2.54	0.47
1:B:2384:TYR:CD2	1:B:2388:LYS:HD2	2.50	0.46
1:A:1014:ILE:HD13	1:A:1014:ILE:C	2.36	0.46
1:A:1367:ILE:HD12	1:A:1367:ILE:C	2.36	0.46
1:B:2012:ARG:HD2	1:B:2391:ALA:HB2	1.97	0.46
1:B:2125:ASP:OD1	1:B:2129:LYS:HE3	2.16	0.46
1:A:1118:THR:HG21	3:A:3263:HOH:O	2.15	0.46
1:A:1060:ARG:HD2	1:A:1271:PHE:CZ	2.52	0.45
1:A:1078:ALA:O	1:A:1080:PRO:HD3	2.17	0.45
1:A:1380:LYS:HD3	1:A:1383:LEU:HD12	1.98	0.45
1:B:2013:GLU:OE1	1:B:2068:ARG:NE	2.51	0.44
1:A:1356:PHE:HB2	1:A:1360:VAL:HG23	2.00	0.44
1:A:1073:SER:O	1:A:1077:GLU:HG3	2.17	0.44
1:A:1037:VAL:HG21	1:A:1067:ILE:HD13	2.00	0.44
1:A:1037:VAL:HG12	1:A:1038:ALA:N	2.33	0.43
1:A:1046:GLU:O	1:A:1046:GLU:HG3	2.19	0.43
1:B:2060:ARG:HD2	1:B:2271:PHE:CZ	2.54	0.43
1:B:2356:PHE:HB2	1:B:2360:VAL:HG23	2.00	0.43
1:A:1070:ARG:HG2	1:A:1074:ARG:CZ	2.49	0.43
1:A:1287:PRO:HG2	1:B:2287:PRO:HG2	2.01	0.43
1:A:1182:ASN:C	1:A:1182:ASN:HD22	2.21	0.43
1:B:2356:PHE:HB3	1:B:2360:VAL:CG2	2.49	0.43
1:B:2018:ILE:HG12	1:B:2350:PHE:HD2	1.85	0.42
1:B:2014:ILE:HD13	1:B:2016:LYS:HE2	2.02	0.42
1:B:2360:VAL:O	1:B:2360:VAL:HG23	2.20	0.42
1:B:2090:ASN:OD1	1:B:2091:LEU:N	2.49	0.42
1:A:1124:TRP:CD2	1:A:1302:LEU:HD23	2.55	0.41
1:B:2356:PHE:CB	1:B:2360:VAL:HG23	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2139:LEU:HD21	1:B:2302:LEU:HD21	2.01	0.41
1:A:1204:LEU:HA	1:A:1204:LEU:HD12	1.92	0.41
1:B:2281:ARG:HG2	1:B:2315:HIS:HE1	1.85	0.41
1:A:1035:SER:HB2	3:A:3263:HOH:O	2.21	0.41
1:A:1281:ARG:HH11	1:A:1281:ARG:HG3	1.86	0.41
1:A:1159:TYR:CD1	1:A:1187:LYS:HE3	2.56	0.40
1:B:2356:PHE:CB	1:B:2360:VAL:CG2	2.99	0.40
1:B:2299:SER:O	1:B:2300:TYR:HB2	2.20	0.40
1:B:2063:GLN:HG3	1:B:2066:LEU:HD12	2.03	0.40
1:B:2048:LYS:HB3	1:B:2048:LYS:HE3	1.95	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	368/392 (94%)	355 (96%)	13 (4%)	0	100	100
1	B	375/392 (96%)	367 (98%)	8 (2%)	0	100	100
All	All	743/784 (95%)	722 (97%)	21 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	296/311 (95%)	286 (97%)	10 (3%)	44 24
1	B	300/311 (96%)	287 (96%)	13 (4%)	35 16
All	All	596/622 (96%)	573 (96%)	23 (4%)	39 19

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1014	ILE
1	A	1169	LEU
1	A	1182	ASN
1	A	1204	LEU
1	A	1238	LEU
1	A	1240	TRP
1	A	1286	ARG
1	A	1289	ARG
1	A	1312	LEU
1	A	1343	ASN
1	B	2043	VAL
1	B	2063	GLN
1	B	2168	MET
1	B	2169	LEU
1	B	2182	ASN
1	B	2204	LEU
1	B	2233	LEU
1	B	2238	LEU
1	B	2240	TRP
1	B	2286	ARG
1	B	2289	ARG
1	B	2343	ASN
1	B	2383	LEU

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

Mol	Chain	Res	Type
1	A	1063	GLN
1	A	1143	HIS
1	A	1182	ASN
1	A	1253	GLN
1	A	1273	HIS
1	A	1306	GLN
1	A	1329	GLN

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Mol	Chain	Res	Type
1	B	2063	GLN
1	B	2143	HIS
1	B	2182	ASN
1	B	2273	HIS
1	B	2315	HIS
1	B	2351	GLN

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 carbohydrates 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

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	374/392 (95%)	0.75	56 (14%) 3 3	15, 30, 50, 62	0
1	B	379/392 (96%)	0.26	14 (3%) 45 43	14, 25, 49, 61	0
All	All	753/784 (96%)	0.51	70 (9%) 11 11	14, 27, 49, 62	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1019	SER	7.7
1	A	1047	GLY	7.3
1	B	2030	THR	7.2
1	A	1046	GLU	6.7
1	A	1020	SER	6.3
1	B	2020	SER	5.9
1	A	1009	VAL	5.8
1	A	1018	ILE	5.7
1	A	1048	LYS	5.6
1	A	1081	LYS	5.3
1	A	1030	THR	5.1
1	A	1087	ALA	4.9
1	A	1044	VAL	4.6
1	A	1006	VAL	4.6
1	A	1031	LYS	4.6
1	A	1388	LYS	4.4
1	A	1043	VAL	4.1
1	B	2019	SER	4.0
1	B	2046	GLU	4.0
1	B	2018	ILE	3.9
1	A	1082	LYS	3.9
1	A	1392	GLU	3.8
1	A	1381	SER	3.6
1	A	1012	ARG	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	1385	LYS	3.5
1	A	1259	PHE	3.3
1	A	1086	GLU	3.3
1	A	1390	LEU	3.3
1	A	1389	ALA	3.3
1	A	1051	VAL	3.1
1	B	2031	LYS	3.0
1	A	1041	THR	2.9
1	A	1121	MET	2.9
1	A	1103	ASN	2.8
1	A	1102	ILE	2.8
1	A	1050	VAL	2.7
1	A	1167	SER	2.6
1	A	1053	TYR	2.6
1	A	1049	ARG	2.6
1	A	1165	GLY	2.6
1	B	2121	MET	2.6
1	A	1330	MET	2.5
1	A	1017	PRO	2.4
1	A	1040	VAL	2.4
1	A	1016	LYS	2.4
1	B	2044	VAL	2.4
1	A	1089	ASP	2.4
1	A	1145	VAL	2.4
1	A	1159	TYR	2.3
1	A	1361	ARG	2.3
1	A	1014	ILE	2.3
1	A	1123	VAL	2.3
1	A	1386	GLU	2.2
1	A	1264	MET	2.2
1	A	1391	ALA	2.2
1	A	1007	ARG	2.2
1	B	2257	ALA	2.1
1	A	1088	GLY	2.1
1	A	1382	ASP	2.1
1	A	1146	LYS	2.1
1	B	2118	THR	2.1
1	A	1168	MET	2.1
1	B	2048	LYS	2.1
1	A	1384	TYR	2.1
1	A	1118	THR	2.0
1	A	1077	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	2086	GLU	2.0
1	A	1073	SER	2.0
1	B	2087	ALA	2.0
1	B	2050	VAL	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)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
2	MG	A	3501	1/1	0.92	0.09	-0.95	25,25,25,25	0
2	MG	B	3502	1/1	0.94	0.07	-1.39	22,22,22,22	0

6.5 Other polymers (i)

There are no such residues in this entry.