Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 11:32 PM GMT

PDB ID	:	1XQB
Title	:	X-Ray Structure Of YaeB from Haemophilus influenzae. Northeast Structural Genomics Research Consortium (NESGC)target IR47.
Authors	:	Benach, J.; Lee, I.; Forouhar, F.; Kuzin, A.P.; Keller, J.P.; Itkin, A.; Xiao, R.; Acton, T.; Montelione, G.T.; Hunt, J.F.; Northeast Structural Genomics Consortium (NESG)
Deposited on	:	2004-10-11
Resolution	:	2.85 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:

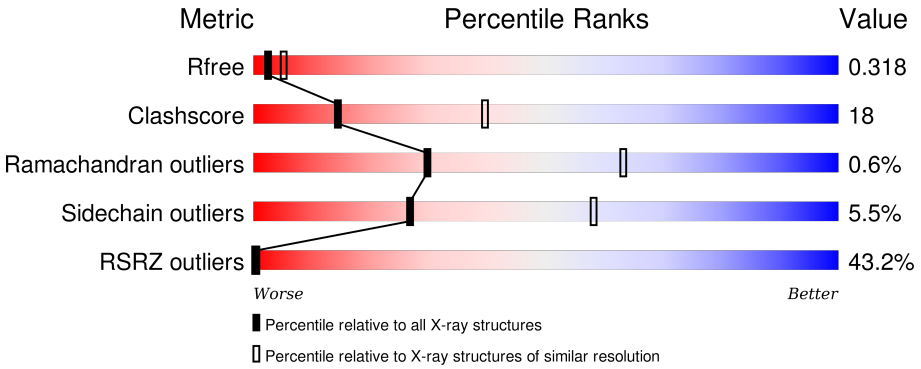
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.85 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	2228 (2.90-2.82)
Clashscore	102246	2499 (2.90-2.82)
Ramachandran outliers	100387	2439 (2.90-2.82)
Sidechain outliers	100360	2442 (2.90-2.82)
RSRZ outliers	91569	2236 (2.90-2.82)

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	247	33% 47% 27% · 25%
1	B	247	31% 48% 26% · 25%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3036 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 UPF0066 protein HI0510.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	186	Total	C	N	O	S	Se	0	0	0
			1484	952	254	271	4	3			
1	B	186	Total	C	N	O	S	Se	0	0	0
			1484	952	254	271	4	3			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	UNP P44740
A	63	MSE	PHE	ENGINEERED	UNP P44740
A	102	MSE	LEU	ENGINEERED	UNP P44740
A	161	MET	LEU	ENGINEERED	UNP P44740
A	240	LEU	-	CLONING ARTIFACT	UNP P44740
A	241	GLU	-	CLONING ARTIFACT	UNP P44740
A	242	HIS	-	EXPRESSION TAG	UNP P44740
A	243	HIS	-	EXPRESSION TAG	UNP P44740
A	244	HIS	-	EXPRESSION TAG	UNP P44740
A	245	HIS	-	EXPRESSION TAG	UNP P44740
A	246	HIS	-	EXPRESSION TAG	UNP P44740
A	247	HIS	-	EXPRESSION TAG	UNP P44740
B	1	MSE	MET	MODIFIED RESIDUE	UNP P44740
B	63	MSE	PHE	ENGINEERED	UNP P44740
B	102	MSE	LEU	ENGINEERED	UNP P44740
B	161	MET	LEU	ENGINEERED	UNP P44740
B	240	LEU	-	CLONING ARTIFACT	UNP P44740
B	241	GLU	-	CLONING ARTIFACT	UNP P44740
B	242	HIS	-	EXPRESSION TAG	UNP P44740
B	243	HIS	-	EXPRESSION TAG	UNP P44740
B	244	HIS	-	EXPRESSION TAG	UNP P44740
B	245	HIS	-	EXPRESSION TAG	UNP P44740
B	246	HIS	-	EXPRESSION TAG	UNP P44740
B	247	HIS	-	EXPRESSION TAG	UNP P44740

- Molecule 2 is water.

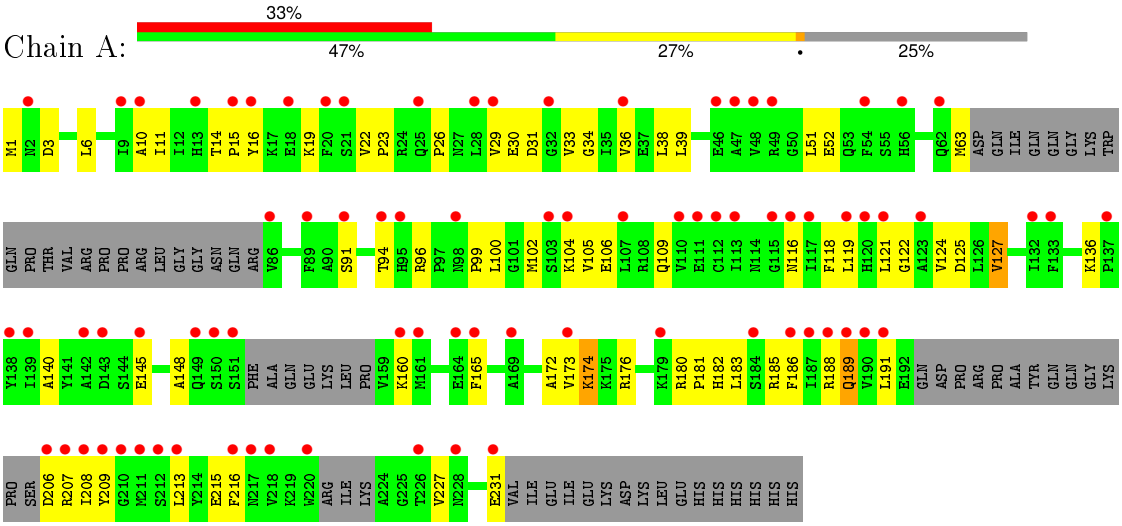
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	33	Total O 33 33	0	0
2	B	35	Total O 35 35	0	0

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.

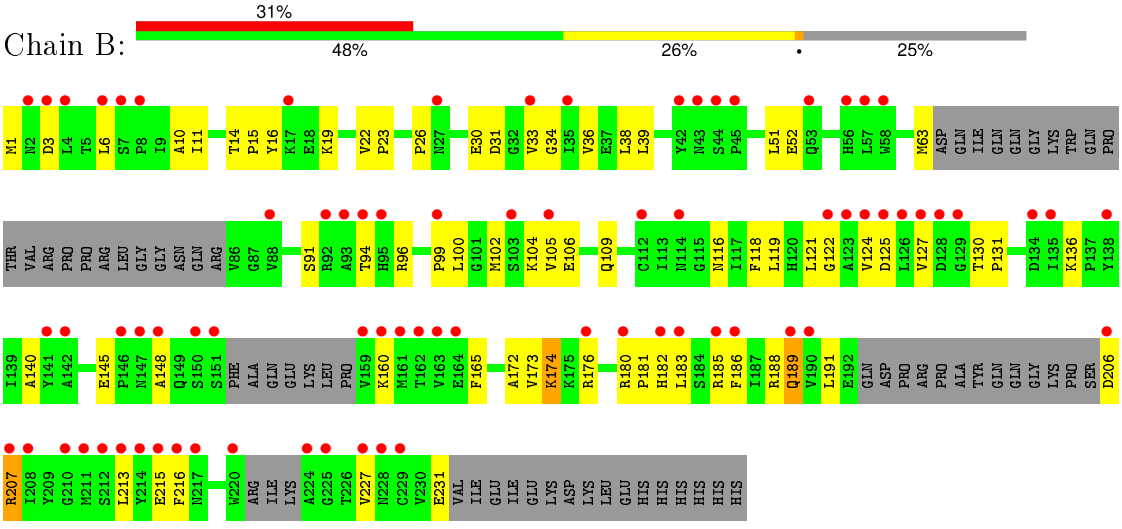
- Molecule 1: Hypothetical UPF0066 protein HI0510

Chain A:



- Molecule 1: Hypothetical UPF0066 protein HI0510

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	69.65Å 69.91Å 119.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.74 – 2.85 27.70 – 2.81	Depositor EDS
% Data completeness (in resolution range)	93.2 (19.74-2.85) 92.4 (27.70-2.81)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	40.10 (at 2.80Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.279 , 0.324 0.280 , 0.318	Depositor DCC
R_{free} test set	1334 reflections (10.08%)	DCC
Wilson B-factor (Å^2)	56.9	Xtriage
Anisotropy	0.580	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 25.8	EDS
Estimated twinning fraction	0.458 for k,h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Outliers	0 of 13694 reflections	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	3036	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.08% 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	0.43	0/1514	0.68	0/2045
1	B	0.44	0/1514	0.67	0/2045
All	All	0.43	0/3028	0.67	0/4090

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	1484	0	1486	61	0
1	B	1484	0	1486	57	0
2	A	33	0	0	1	0
2	B	35	0	0	2	0
All	All	3036	0	2972	107	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 18.

All (107) 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:102:MSE:HE2	1:B:136:LYS:HD2	1.52	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:11:ILE:HG13	1:B:39:LEU:HD21	1.55	0.88
1:A:11:ILE:HG13	1:A:39:LEU:HD21	1.56	0.88
1:A:63:MSE:HE1	1:A:96:ARG:HD2	1.59	0.84
1:A:136:LYS:HD2	1:B:102:MSE:HE2	1.58	0.82
1:B:63:MSE:HE1	1:B:96:ARG:HD2	1.61	0.80
1:A:207:ARG:HG3	1:A:209:TYR:CE1	2.20	0.77
1:A:172:ALA:O	1:A:176:ARG:HD3	1.95	0.66
1:A:36:VAL:HG23	1:A:121:LEU:HD11	1.78	0.65
1:B:172:ALA:O	1:B:176:ARG:HD3	1.98	0.64
1:A:215:GLU:CD	1:A:215:GLU:H	1.99	0.64
1:B:36:VAL:HG23	1:B:121:LEU:HD11	1.80	0.63
1:B:191:LEU:O	1:B:191:LEU:HD23	1.99	0.62
1:B:16:TYR:HE2	1:B:189:GLN:HE22	1.47	0.62
1:B:116:ASN:HB3	1:B:118:PHE:CE1	2.35	0.61
1:A:16:TYR:HE2	1:A:189:GLN:HE22	1.47	0.61
1:B:215:GLU:H	1:B:215:GLU:CD	2.04	0.60
1:A:191:LEU:HD23	1:A:191:LEU:O	2.02	0.59
1:A:104:LYS:NZ	1:B:145:GLU:HB2	2.19	0.58
1:B:160:LYS:HE2	1:B:191:LEU:HD11	1.85	0.57
1:A:160:LYS:HE2	1:A:191:LEU:HD11	1.86	0.57
1:A:116:ASN:HB3	1:A:118:PHE:CE1	2.39	0.57
1:A:6:LEU:HD11	1:B:6:LEU:HD11	1.88	0.56
1:B:207:ARG:HD3	2:B:3004:HOH:O	2.05	0.55
1:B:91:SER:O	1:B:96:ARG:NH2	2.39	0.55
1:A:207:ARG:CG	1:A:209:TYR:CE1	2.90	0.54
1:A:91:SER:O	1:A:96:ARG:NH2	2.41	0.53
1:A:207:ARG:CZ	1:A:209:TYR:HE1	2.21	0.53
1:B:19:LYS:HB3	1:B:19:LYS:NZ	2.24	0.53
1:A:207:ARG:NE	1:A:209:TYR:HE1	2.07	0.52
1:B:14:THR:HG23	1:B:15:PRO:HD2	1.92	0.52
1:B:174:LYS:NZ	1:B:174:LYS:HB2	2.25	0.52
1:B:30:GLU:H	1:B:188:ARG:NH1	2.08	0.51
1:A:39:LEU:HD11	1:B:1:MSE:HE1	1.92	0.51
1:A:145:GLU:HB2	1:B:104:LYS:NZ	2.26	0.51
1:A:1:MSE:HE1	1:B:39:LEU:HD11	1.92	0.51
1:A:19:LYS:HB3	1:A:19:LYS:NZ	2.26	0.51
1:A:14:THR:HG23	1:A:15:PRO:HD2	1.94	0.50
1:A:173:VAL:HG13	1:A:183:LEU:CD1	2.42	0.49
1:A:63:MSE:CE	1:A:96:ARG:HD2	2.38	0.49
1:B:207:ARG:HG2	2:B:3002:HOH:O	2.11	0.49
1:A:30:GLU:H	1:A:188:ARG:NH1	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:VAL:HG11	1:B:124:VAL:HG12	1.95	0.49
1:A:140:ALA:HB2	1:B:148:ALA:HB3	1.94	0.49
1:B:176:ARG:HG2	1:B:216:PHE:CE2	2.48	0.49
1:B:63:MSE:HE3	1:B:99:PRO:HA	1.94	0.48
1:A:63:MSE:HE3	1:A:99:PRO:HA	1.95	0.48
1:A:104:LYS:HG3	1:A:104:LYS:O	2.14	0.48
1:B:173:VAL:HG13	1:B:183:LEU:CD1	2.43	0.48
1:B:33:VAL:HG12	1:B:34:GLY:N	2.29	0.48
1:A:105:VAL:HG11	1:A:124:VAL:HG12	1.96	0.48
1:A:165:PHE:HD2	1:A:227:VAL:HG11	1.80	0.47
1:A:174:LYS:NZ	1:A:174:LYS:HB2	2.30	0.47
1:B:10:ALA:HA	1:B:39:LEU:HG	1.96	0.47
1:A:176:ARG:HG2	1:A:216:PHE:CE2	2.50	0.47
1:B:63:MSE:SE	1:B:94:THR:HA	2.65	0.47
1:A:33:VAL:HG12	1:A:34:GLY:N	2.30	0.47
1:A:208:ILE:O	1:A:208:ILE:HG23	2.15	0.47
1:B:105:VAL:CG1	1:B:124:VAL:HG12	2.45	0.46
1:A:104:LYS:HZ3	1:B:145:GLU:HB2	1.78	0.46
1:A:206:ASP:CG	1:A:207:ARG:H	2.19	0.46
1:B:104:LYS:HG3	1:B:104:LYS:O	2.15	0.46
1:A:10:ALA:HA	1:A:39:LEU:HG	1.97	0.46
1:A:207:ARG:HG3	1:A:209:TYR:CZ	2.50	0.46
1:B:33:VAL:HA	1:B:122:GLY:O	2.16	0.46
1:A:26:PRO:HG2	1:A:125:ASP:HB3	1.98	0.46
1:B:63:MSE:CE	1:B:96:ARG:HD2	2.40	0.45
1:B:26:PRO:HG2	1:B:125:ASP:HB3	1.97	0.45
1:B:185:ARG:O	1:B:188:ARG:HG3	2.17	0.45
1:B:165:PHE:HD2	1:B:227:VAL:HG11	1.81	0.45
1:A:63:MSE:SE	1:A:94:THR:HA	2.67	0.45
1:A:63:MSE:HE2	1:A:100:LEU:C	2.37	0.45
1:A:33:VAL:HA	1:A:122:GLY:O	2.17	0.45
1:A:148:ALA:HB3	1:B:140:ALA:HB2	1.97	0.45
1:B:181:PRO:O	1:B:182:HIS:HB2	2.16	0.45
1:A:105:VAL:CG1	1:A:124:VAL:HG12	2.46	0.45
1:B:105:VAL:HG21	1:B:121:LEU:HD13	1.99	0.45
1:B:63:MSE:HE2	1:B:100:LEU:C	2.37	0.45
1:A:29:VAL:HG11	1:A:189:GLN:OE1	2.17	0.44
1:B:183:LEU:O	1:B:183:LEU:HD22	2.18	0.43
1:A:181:PRO:O	1:A:182:HIS:HB2	2.17	0.43
1:B:31:ASP:HB2	1:B:186:PHE:CD1	2.54	0.43
1:B:19:LYS:HZ2	1:B:19:LYS:HB3	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:THR:HA	1:B:131:PRO:HD3	1.86	0.43
1:B:206:ASP:HB2	1:B:207:ARG:CZ	2.48	0.42
1:A:165:PHE:HD2	1:A:227:VAL:CG1	2.31	0.42
1:A:127:VAL:HG13	2:A:3035:HOH:O	2.19	0.42
1:A:189:GLN:HE21	1:A:213:LEU:HD21	1.83	0.42
1:B:207:ARG:HG2	1:B:207:ARG:O	2.19	0.42
1:A:165:PHE:CD2	1:A:227:VAL:HG11	2.55	0.42
1:A:185:ARG:O	1:A:188:ARG:HG3	2.19	0.42
1:B:189:GLN:HE21	1:B:213:LEU:HD21	1.85	0.41
1:A:31:ASP:HB2	1:A:186:PHE:CD1	2.54	0.41
1:A:109:GLN:HE21	1:A:109:GLN:HB3	1.70	0.41
1:A:173:VAL:HG13	1:A:183:LEU:HD12	2.01	0.41
1:A:36:VAL:HB	1:A:119:LEU:HB2	2.03	0.41
1:B:36:VAL:HB	1:B:119:LEU:HB2	2.03	0.41
1:A:22:VAL:HA	1:A:23:PRO:HD3	1.90	0.41
1:B:165:PHE:HD2	1:B:227:VAL:CG1	2.32	0.41
1:B:106:GLU:O	1:B:122:GLY:N	2.54	0.41
1:A:105:VAL:CG2	1:A:121:LEU:HD22	2.51	0.41
1:B:176:ARG:HG2	1:B:216:PHE:CZ	2.56	0.41
1:B:165:PHE:CD2	1:B:227:VAL:HG11	2.56	0.41
1:A:106:GLU:O	1:A:122:GLY:N	2.54	0.41
1:A:145:GLU:HB2	1:B:104:LYS:HZ3	1.85	0.40
1:A:23:PRO:HG2	1:A:29:VAL:HG21	2.03	0.40
1:B:22:VAL:HA	1:B:23:PRO:HD3	1.87	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	176/247 (71%)	153 (87%)	22 (12%)	1 (1%)	30 63

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	176/247 (71%)	154 (88%)	21 (12%)	1 (1%)	30 63
All	All	352/494 (71%)	307 (87%)	43 (12%)	2 (1%)	30 63

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	3	ASP
1	A	3	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	165/217 (76%)	157 (95%)	8 (5%)	31 65
1	B	165/217 (76%)	155 (94%)	10 (6%)	23 52
All	All	330/434 (76%)	312 (94%)	18 (6%)	27 58

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	LEU
1	A	51	LEU
1	A	52	GLU
1	A	127	VAL
1	A	174	LYS
1	A	180	ARG
1	A	189	GLN
1	A	231	GLU
1	B	38	LEU
1	B	51	LEU
1	B	52	GLU
1	B	109	GLN
1	B	127	VAL
1	B	174	LYS

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Mol	Chain	Res	Type
1	B	180	ARG
1	B	189	GLN
1	B	207	ARG
1	B	231	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	ASN
1	A	56	HIS
1	A	109	GLN
1	B	27	ASN
1	B	56	HIS
1	B	109	GLN
1	B	168	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

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	183/247 (74%)	2.16	81 (44%) 0 0	25, 50, 74, 94	0
1	B	183/247 (74%)	2.11	77 (42%) 0 0	25, 50, 74, 94	0
All	All	366/494 (74%)	2.14	158 (43%) 0 0	25, 50, 74, 94	0

All (158) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	88	VAL	10.2
1	A	207	ARG	10.0
1	B	27	ASN	9.5
1	A	206	ASP	8.4
1	A	190	VAL	8.3
1	B	163	VAL	8.1
1	A	189	GLN	7.7
1	B	160	LYS	7.2
1	B	92	ARG	7.2
1	B	94	THR	7.2
1	A	86	VAL	7.1
1	A	32	GLY	6.9
1	A	29	VAL	6.8
1	B	214	TYR	6.3
1	B	183	LEU	6.2
1	B	162	THR	6.2
1	A	191	LEU	6.0
1	A	209	TYR	6.0
1	A	49	ARG	6.0
1	B	213	LEU	5.9
1	A	48	VAL	5.8
1	B	103	SER	5.7
1	B	122	GLY	5.6
1	A	145	GLU	5.5

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Mol	Chain	Res	Type	RSRZ
1	B	126	LEU	5.3
1	B	8	PRO	5.1
1	B	228	ASN	5.0
1	B	159	VAL	5.0
1	A	218	VAL	5.0
1	B	142	ALA	4.9
1	B	44	SER	4.9
1	A	217	ASN	4.9
1	A	110	VAL	4.8
1	A	121	LEU	4.4
1	B	147	ASN	4.4
1	B	135	ILE	4.2
1	B	225	GLY	4.2
1	B	105	VAL	4.1
1	A	89	PHE	4.1
1	A	115	GLY	4.0
1	B	208	ILE	4.0
1	A	226	THR	4.0
1	B	45	PRO	4.0
1	A	150	SER	4.0
1	A	47	ALA	4.0
1	B	227	VAL	4.0
1	B	17	LYS	3.9
1	A	95	HIS	3.9
1	A	2	ASN	3.9
1	B	217	ASN	3.9
1	A	20	PHE	3.9
1	B	125	ASP	3.9
1	A	56	HIS	3.8
1	B	43	ASN	3.8
1	B	224	ALA	3.7
1	A	91	SER	3.7
1	B	229	CYS	3.7
1	B	99	PRO	3.7
1	B	134	ASP	3.6
1	B	180	ARG	3.6
1	A	169	ALA	3.6
1	A	164	GLU	3.6
1	A	208	ILE	3.6
1	A	161	MET	3.5
1	A	137	PRO	3.5
1	B	141	TYR	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	54	PHE	3.5
1	A	151	SER	3.4
1	B	189	GLN	3.4
1	A	212	SER	3.3
1	A	25	GLN	3.3
1	A	231	GLU	3.3
1	A	165	PHE	3.3
1	B	215	GLU	3.3
1	B	35	ILE	3.3
1	B	4	LEU	3.3
1	A	123	ALA	3.3
1	B	127	VAL	3.2
1	B	206	ASP	3.2
1	A	184	SER	3.2
1	B	93	ALA	3.2
1	A	21	SER	3.2
1	A	28	LEU	3.1
1	B	185	ARG	3.1
1	B	212	SER	3.1
1	B	42	TYR	3.0
1	B	220	TRP	3.0
1	B	138	TYR	3.0
1	A	18	GLU	3.0
1	B	123	ALA	3.0
1	A	104	LYS	3.0
1	B	114	ASN	2.9
1	B	161	MET	2.9
1	A	94	THR	2.8
1	B	124	VAL	2.8
1	A	13	HIS	2.8
1	B	216	PHE	2.8
1	B	7	SER	2.8
1	A	116	ASN	2.8
1	B	210	GLY	2.7
1	B	33	VAL	2.7
1	B	95	HIS	2.7
1	A	211	MET	2.7
1	B	151	SER	2.7
1	B	58	TRP	2.6
1	A	139	ILE	2.6
1	A	119	LEU	2.6
1	A	187	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	98	ASN	2.6
1	A	210	GLY	2.6
1	A	138	TYR	2.6
1	A	16	TYR	2.6
1	A	10	ALA	2.5
1	B	176	ARG	2.5
1	A	112	CYS	2.5
1	A	46	GLU	2.5
1	B	128	ASP	2.5
1	B	164	GLU	2.5
1	B	148	ALA	2.5
1	B	2	ASN	2.5
1	B	3	ASP	2.4
1	A	179	LYS	2.4
1	A	142	ALA	2.4
1	B	182	HIS	2.4
1	B	53	GLN	2.4
1	A	213	LEU	2.3
1	A	117	ILE	2.3
1	B	186	PHE	2.3
1	A	103	SER	2.3
1	A	133	PHE	2.3
1	A	143	ASP	2.3
1	A	228	ASN	2.3
1	B	207	ARG	2.3
1	B	57	LEU	2.2
1	A	216	PHE	2.2
1	A	173	VAL	2.2
1	A	132	ILE	2.2
1	A	188	ARG	2.2
1	B	150	SER	2.2
1	B	146	PRO	2.2
1	A	111	GLU	2.2
1	B	211	MET	2.1
1	A	15	PRO	2.1
1	A	36	VAL	2.1
1	B	6	LEU	2.1
1	A	160	LYS	2.1
1	A	186	PHE	2.1
1	A	62	GLN	2.1
1	B	56	HIS	2.1
1	A	107	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	190	VAL	2.1
1	A	9	ILE	2.0
1	A	113	ILE	2.0
1	A	120	HIS	2.0
1	A	149	GLN	2.0
1	B	129	GLY	2.0
1	B	112	CYS	2.0
1	A	220	TRP	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.