



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 06:48 am GMT

PDB ID : 4KP2
Title : Crystal structure of homoaconitase large subunit from methanococcus jannaschii (MJ1003)
Authors : Hwang, K.Y.; Lee, E.H.
Deposited on : 2013-05-13
Resolution : 2.50 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

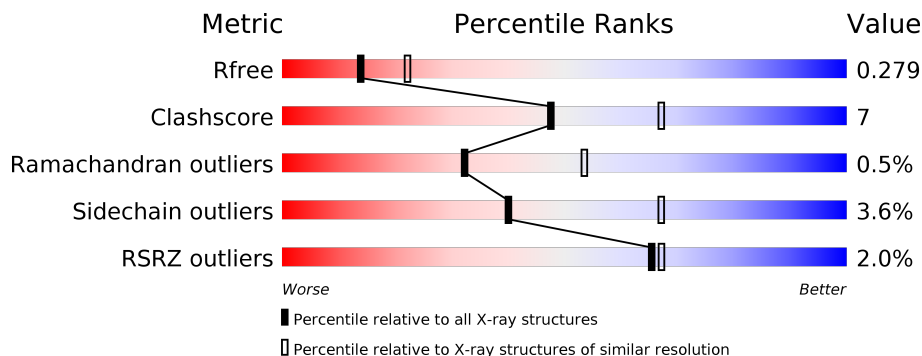
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	100719	3846 (2.50-2.50)
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (2.50-2.50)

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 $\leq 5\%$. 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	441	<div> <div>2%</div> <div> <div></div> <div>77%</div> <div>17%</div> <div>• 5%</div> </div> </div>
1	B	441	<div> <div>2%</div> <div> <div></div> <div>74%</div> <div>19%</div> <div>• 5%</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6470 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 Homoaconitase large subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	418	Total	C	N	O	S	0	0	0
			3209	2030	546	609	24			
1	B	418	Total	C	N	O	S	0	0	0
			3209	2030	546	609	24			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	EXPRESSION TAG	UNP Q58409
A	-19	GLY	-	EXPRESSION TAG	UNP Q58409
A	-18	SER	-	EXPRESSION TAG	UNP Q58409
A	-17	SER	-	EXPRESSION TAG	UNP Q58409
A	-16	HIS	-	EXPRESSION TAG	UNP Q58409
A	-15	HIS	-	EXPRESSION TAG	UNP Q58409
A	-14	HIS	-	EXPRESSION TAG	UNP Q58409
A	-13	HIS	-	EXPRESSION TAG	UNP Q58409
A	-12	HIS	-	EXPRESSION TAG	UNP Q58409
A	-11	HIS	-	EXPRESSION TAG	UNP Q58409
A	-10	SER	-	EXPRESSION TAG	UNP Q58409
A	-9	SER	-	EXPRESSION TAG	UNP Q58409
A	-8	GLY	-	EXPRESSION TAG	UNP Q58409
A	-7	LEU	-	EXPRESSION TAG	UNP Q58409
A	-6	VAL	-	EXPRESSION TAG	UNP Q58409
A	-5	PRO	-	EXPRESSION TAG	UNP Q58409
A	-4	ARG	-	EXPRESSION TAG	UNP Q58409
A	-3	GLY	-	EXPRESSION TAG	UNP Q58409
A	-2	SER	-	EXPRESSION TAG	UNP Q58409
A	-1	HIS	-	EXPRESSION TAG	UNP Q58409
A	0	MET	-	EXPRESSION TAG	UNP Q58409
B	-20	MET	-	EXPRESSION TAG	UNP Q58409
B	-19	GLY	-	EXPRESSION TAG	UNP Q58409
B	-18	SER	-	EXPRESSION TAG	UNP Q58409
B	-17	SER	-	EXPRESSION TAG	UNP Q58409

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	HIS	-	EXPRESSION TAG	UNP Q58409
B	-15	HIS	-	EXPRESSION TAG	UNP Q58409
B	-14	HIS	-	EXPRESSION TAG	UNP Q58409
B	-13	HIS	-	EXPRESSION TAG	UNP Q58409
B	-12	HIS	-	EXPRESSION TAG	UNP Q58409
B	-11	HIS	-	EXPRESSION TAG	UNP Q58409
B	-10	SER	-	EXPRESSION TAG	UNP Q58409
B	-9	SER	-	EXPRESSION TAG	UNP Q58409
B	-8	GLY	-	EXPRESSION TAG	UNP Q58409
B	-7	LEU	-	EXPRESSION TAG	UNP Q58409
B	-6	VAL	-	EXPRESSION TAG	UNP Q58409
B	-5	PRO	-	EXPRESSION TAG	UNP Q58409
B	-4	ARG	-	EXPRESSION TAG	UNP Q58409
B	-3	GLY	-	EXPRESSION TAG	UNP Q58409
B	-2	SER	-	EXPRESSION TAG	UNP Q58409
B	-1	HIS	-	EXPRESSION TAG	UNP Q58409
B	0	MET	-	EXPRESSION TAG	UNP Q58409

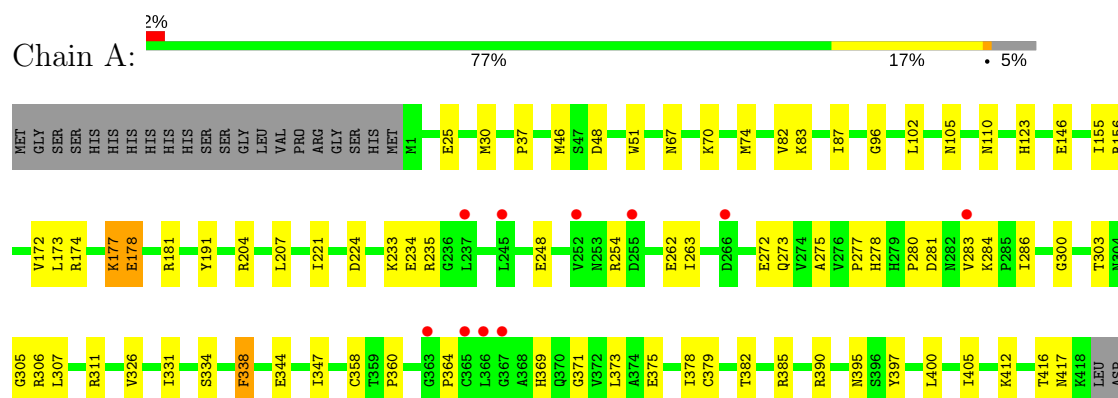
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	27	Total O 27 27	0	0
2	B	25	Total O 25 25	0	0

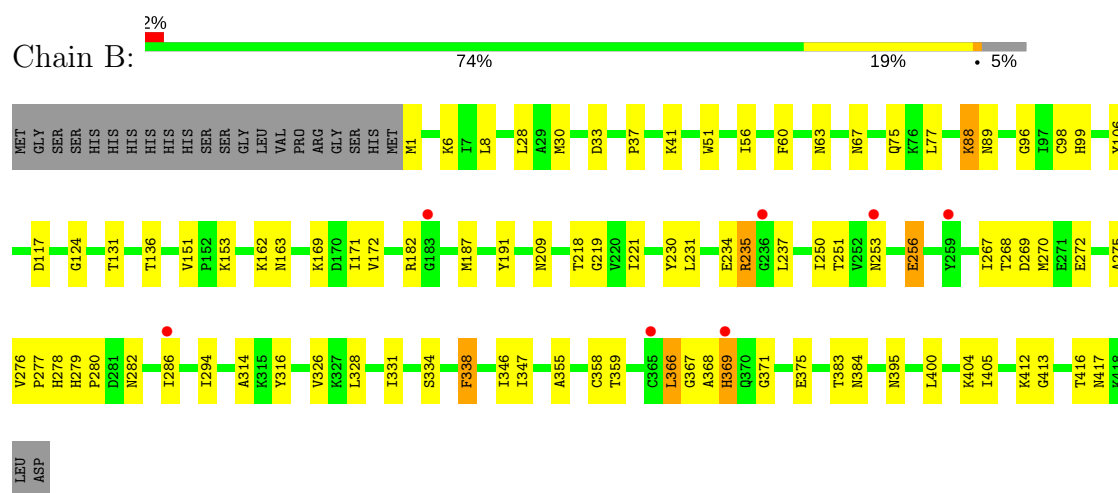
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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: Homoaconitase large subunit



• Molecule 1: Homoaconitase large subunit



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	68.33Å 103.10Å 112.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.89 – 2.50 46.89 – 2.50	Depositor EDS
% Data completeness (in resolution range)	96.1 (46.89-2.50) 96.1 (46.89-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.44 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.226 , 0.277 0.223 , 0.279	Depositor DCC
R_{free} test set	1998 reflections (7.39%)	DCC
Wilson B-factor (Å ²)	32.2	Xtriage
Anisotropy	0.249	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 28.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	6470	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.71% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	0.21	0/3263	0.39	0/4401
1	B	0.21	0/3263	0.39	0/4401
All	All	0.21	0/6526	0.39	0/8802

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	3209	0	3245	43	0
1	B	3209	0	3245	48	0
2	A	27	0	0	0	0
2	B	25	0	0	1	0
All	All	6470	0	6490	90	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 7.

All (90) 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:163:ASN:ND2	1:B:269:ASP:O	2.22	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:231:LEU:HB3	1:B:237:LEU:HD22	1.75	0.68
1:A:412:LYS:HD3	1:A:416:THR:HG21	1.75	0.67
1:B:37:PRO:HB3	1:B:77:LEU:HD23	1.77	0.67
1:B:153:LYS:HB2	1:B:187:MET:HG2	1.78	0.66
1:A:67:ASN:HD22	1:A:369:HIS:HB2	1.62	0.65
1:B:1:MET:N	1:B:256:GLU:O	2.30	0.65
1:A:273:GLN:HB3	1:A:283:VAL:HG21	1.80	0.63
1:B:275:ALA:HB3	1:B:400:LEU:HB2	1.81	0.62
1:A:191:TYR:HB2	1:A:221:ILE:HG12	1.80	0.62
1:B:1:MET:HG2	1:B:6:LYS:HG2	1.82	0.61
1:B:191:TYR:HB2	1:B:221:ILE:HG12	1.84	0.59
1:B:282:ASN:ND2	2:B:521:HOH:O	2.34	0.59
1:B:209:ASN:OD1	1:B:384:ASN:ND2	2.33	0.59
1:B:96:GLY:HA3	1:B:334:SER:HA	1.85	0.58
1:A:181:ARG:NH2	1:A:281:ASP:OD1	2.35	0.57
1:A:110:ASN:ND2	1:A:248:GLU:O	2.36	0.57
1:B:412:LYS:HG3	1:B:416:THR:HG21	1.88	0.56
1:A:275:ALA:HB3	1:A:400:LEU:HB2	1.88	0.55
1:A:378:ILE:HG12	1:A:397:TYR:HB2	1.87	0.55
1:A:303:THR:O	1:A:306:ARG:NH2	2.40	0.55
1:A:233:LYS:NZ	1:A:234:GLU:OE2	2.41	0.54
1:A:303:THR:OG1	1:A:382:THR:O	2.26	0.53
1:A:204:ARG:NH1	1:A:224:ASP:OD1	2.35	0.53
1:A:173:LEU:O	1:A:177:LYS:HE3	2.10	0.52
1:B:99:HIS:NE2	1:B:117:ASP:OD2	2.33	0.52
1:B:366:LEU:HG	1:B:368:ALA:HB2	1.91	0.51
1:B:286:ILE:HG21	1:B:417:ASN:HB2	1.92	0.51
1:A:338:PHE:HE1	1:A:347:ILE:HG12	1.76	0.51
1:B:6:LYS:NZ	1:B:251:THR:O	2.43	0.51
1:A:311:ARG:NH1	1:A:344:GLU:OE2	2.43	0.51
1:A:331:ILE:HG12	1:A:358:CYS:HB2	1.93	0.51
1:A:375:GLU:HG3	1:A:395:ASN:HB2	1.92	0.50
1:A:156:ARG:HG2	1:A:254:ARG:HH22	1.77	0.50
1:A:37:PRO:HG2	1:A:74:MET:HB3	1.93	0.50
1:A:67:ASN:N	1:A:67:ASN:OD1	2.38	0.50
1:A:272:GLU:HB3	1:A:405:ILE:HD11	1.94	0.49
1:B:169:LYS:HA	1:B:172:VAL:HG12	1.94	0.49
1:B:272:GLU:HG2	1:B:405:ILE:HD11	1.95	0.49
1:A:373:LEU:HD21	1:A:379:CYS:HB2	1.95	0.49
1:A:272:GLU:OE1	1:A:417:ASN:ND2	2.44	0.48
1:B:375:GLU:HG3	1:B:395:ASN:HB2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:326:VAL:HG21	1:B:413:GLY:HA2	1.95	0.48
1:B:6:LYS:HB3	1:B:250:ILE:HG21	1.95	0.48
1:B:63:ASN:O	1:B:75:GLN:NE2	2.47	0.48
1:A:82:VAL:HG13	1:A:87:ILE:HB	1.96	0.47
1:A:105:ASN:HA	1:A:235:ARG:HG2	1.96	0.47
1:A:177:LYS:NZ	1:A:280:PRO:O	2.36	0.47
1:A:48:ASP:N	1:A:48:ASP:OD1	2.48	0.47
1:A:96:GLY:HA3	1:A:334:SER:HA	1.98	0.46
1:B:171:ILE:HG12	1:B:267:ILE:HD11	1.98	0.46
1:A:177:LYS:NZ	1:A:283:VAL:HG12	2.30	0.46
1:A:254:ARG:NH1	1:A:262:GLU:OE1	2.48	0.46
1:B:230:TYR:CZ	1:B:234:GLU:HG3	2.50	0.45
1:B:235:ARG:HG3	1:B:237:LEU:HD13	1.98	0.45
1:B:314:ALA:HB2	1:B:346:ILE:HG23	1.99	0.45
1:B:331:ILE:HG12	1:B:358:CYS:HB2	1.98	0.45
1:B:253:ASN:HB3	1:B:256:GLU:HG2	1.99	0.45
1:B:416:THR:OG1	1:B:417:ASN:N	2.50	0.45
1:B:338:PHE:HE1	1:B:347:ILE:HG12	1.82	0.44
1:B:277:PRO:HA	1:B:278:HIS:HA	1.59	0.44
1:B:33:ASP:N	1:B:33:ASP:OD1	2.49	0.44
1:A:102:LEU:HB3	1:A:123:HIS:CE1	2.53	0.44
1:B:279:HIS:HA	1:B:280:PRO:HD3	1.88	0.44
1:A:416:THR:OG1	1:A:417:ASN:N	2.51	0.44
1:A:177:LYS:HE2	1:A:281:ASP:HA	2.00	0.43
1:B:383:THR:OG1	1:B:384:ASN:N	2.49	0.43
1:B:28:LEU:HD21	1:B:106:TYR:HB3	2.00	0.43
1:B:41:LYS:HE2	1:B:77:LEU:HD21	1.99	0.43
1:B:124:GLY:HA3	1:B:219:GLY:O	2.18	0.43
1:A:286:ILE:HG12	1:A:417:ASN:HB2	2.00	0.43
1:A:70:LYS:HE2	1:A:70:LYS:H	1.84	0.43
1:B:276:VAL:N	1:B:282:ASN:O	2.45	0.42
1:B:88:LYS:HE2	1:B:88:LYS:HB3	1.88	0.42
1:A:172:VAL:HB	1:A:207:LEU:HD12	2.00	0.42
1:A:277:PRO:HA	1:A:278:HIS:HA	1.62	0.42
1:A:174:ARG:NH1	1:A:178:GLU:OE1	2.53	0.42
1:A:300:GLY:HA2	1:A:305:GLY:HA2	2.02	0.42
1:A:364:PRO:HB3	1:A:371:GLY:H	1.84	0.42
1:A:181:ARG:HH11	1:B:182:ARG:NE	2.18	0.41
1:B:131:THR:HG22	1:B:218:THR:HB	2.02	0.41
1:B:33:ASP:HB3	1:B:60:PHE:CD1	2.55	0.41
1:B:316:TYR:CE2	1:B:404:LYS:HG3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:MET:HE3	1:A:46:MET:HB2	1.97	0.41
1:B:56:ILE:O	1:B:89:ASN:HB2	2.21	0.41
1:B:30:MET:SD	1:B:98:CYS:HB2	2.60	0.41
1:B:328:LEU:HD23	1:B:355:ALA:HB2	2.03	0.40
1:A:25:GLU:HG2	1:A:146:GLU:HG2	2.04	0.40
1:B:67:ASN:ND2	1:B:369:HIS:HB2	2.37	0.40
1:B:8:LEU:HD23	1:B:151:VAL:HG22	2.03	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	416/441 (94%)	390 (94%)	25 (6%)	1 (0%)	51	73
1	B	416/441 (94%)	390 (94%)	23 (6%)	3 (1%)	25	43
All	All	832/882 (94%)	780 (94%)	48 (6%)	4 (0%)	32	53

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	270	MET
1	B	367	GLY
1	A	360	PRO
1	B	371	GLY

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	344/364 (94%)	331 (96%)	13 (4%)	38	64
1	B	344/364 (94%)	332 (96%)	12 (4%)	41	68
All	All	688/728 (94%)	663 (96%)	25 (4%)	40	67

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	MET
1	A	51	TRP
1	A	83	LYS
1	A	155	ILE
1	A	177	LYS
1	A	178	GLU
1	A	263	ILE
1	A	284	LYS
1	A	307	LEU
1	A	326	VAL
1	A	338	PHE
1	A	385	ARG
1	A	390	ARG
1	B	51	TRP
1	B	88	LYS
1	B	136	THR
1	B	162	LYS
1	B	235	ARG
1	B	256	GLU
1	B	268	THR
1	B	294	ILE
1	B	338	PHE
1	B	359	THR
1	B	366	LEU
1	B	369	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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, 95th 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	418/441 (94%)	0.17	10 (2%) 59 61	39, 54, 74, 90	0
1	B	418/441 (94%)	0.11	7 (1%) 70 72	38, 53, 72, 89	0
All	All	836/882 (94%)	0.14	17 (2%) 65 67	38, 53, 72, 90	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	237	LEU	5.1
1	A	366	LEU	5.0
1	B	236	GLY	4.5
1	A	367	GLY	3.9
1	A	365	CYS	3.1
1	A	266	ASP	3.0
1	A	252	VAL	2.8
1	B	253	ASN	2.8
1	A	245	LEU	2.6
1	A	283	VAL	2.6
1	B	369	HIS	2.6
1	A	255	ASP	2.6
1	B	259	TYR	2.5
1	B	183	GLY	2.3
1	B	286	ILE	2.2
1	B	365	CYS	2.1
1	A	363	GLY	2.1

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.