



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 03:41 PM BST

PDB ID : 5X3X
Title : 2.8Å resolution structure of a cobalt energy-coupling factor transporter-CbiMQO
Authors : Bao, Z.; Qi, X.; Wang, J.; Zhang, P.
Deposited on : 2017-02-09
Resolution : 2.79 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

<https://www.wwpdb.org/validation/2017/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) : 1.13
EDS : 2.13
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13

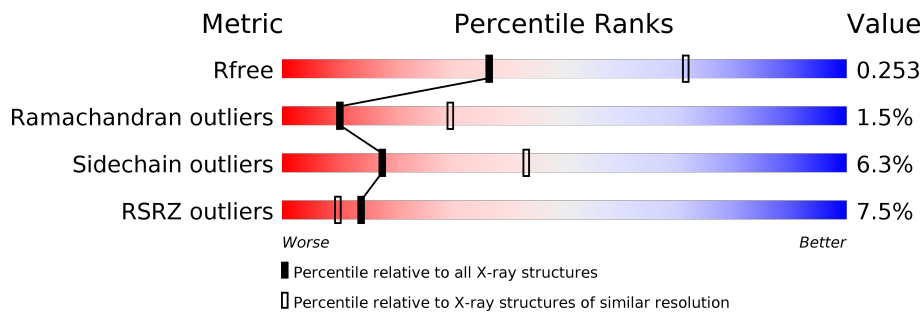
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.79 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}	130704	4107 (2.80-2.76)
Ramachandran outliers	138981	4487 (2.80-2.76)
Sidechain outliers	138945	4489 (2.80-2.76)
RSRZ outliers	127900	4027 (2.80-2.76)

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 respectively. 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	280	5% (poor fit), 94% (0-1 outliers), 6% (2-3 outliers)
1	B	280	4% (poor fit), 97% (0-1 outliers), 2% (2-3 outliers)
1	a	280	18% (poor fit), 91% (0-1 outliers), 8% (2-3 outliers)
1	b	280	10% (poor fit), 94% (0-1 outliers), 6% (2-3 outliers)
2	M	222	4% (poor fit), 86% (0-1 outliers), 7% (2 outliers), 7% (3 outliers)
2	m	222	3% (poor fit), 84% (0-1 outliers), 8% (2 outliers), 8% (3 outliers)
3	Q	244	7% (poor fit), 92% (0-1 outliers), 7% (2 outliers)

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Mol	Chain	Length	Quality of chain
3	q	244	 6% 90% 7% ..

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 14966 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 Cobalt ABC transporter ATP-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	280	Total 2067	C 1300	N 380	O 382	S 5	0	0	0
1	B	280	Total 2069	C 1301	N 380	O 383	S 5	0	0	0
1	a	279	Total 2058	C 1295	N 376	O 382	S 5	0	0	0
1	b	280	Total 2069	C 1301	N 380	O 383	S 5	0	0	0

- Molecule 2 is a protein called Cobalt transport protein CbiM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	M	207	Total 1474	C 978	N 237	O 252	S 7	0	0	0
2	m	205	Total 1461	C 970	N 234	O 250	S 7	0	0	0

- Molecule 3 is a protein called Uncharacterized protein CbiQ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	Q	243	Total 1815	C 1175	N 333	O 301	S 6	0	0	0
3	q	242	Total 1807	C 1169	N 332	O 300	S 6	0	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	24	Total O 24 24	0	0
4	B	19	Total O 19 19	0	0

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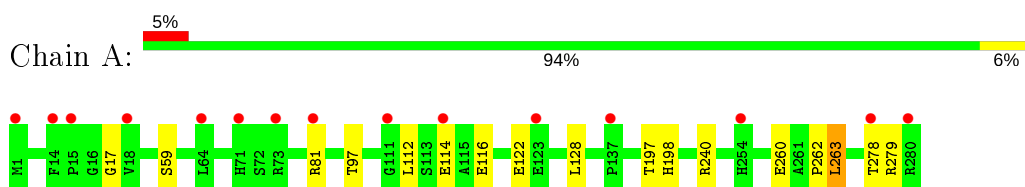
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	M	9	Total O 9 9	0	0
4	Q	28	Total O 28 28	0	0
4	a	19	Total O 19 19	0	0
4	b	16	Total O 16 16	0	0
4	m	13	Total O 13 13	0	0
4	q	18	Total O 18 18	0	0

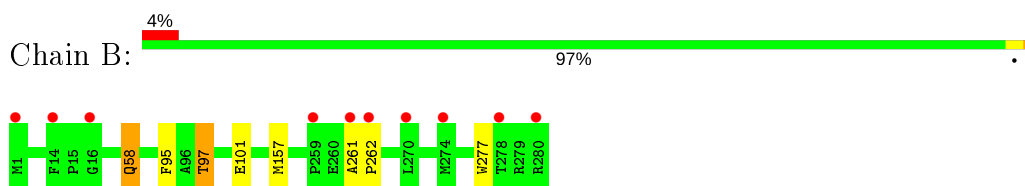
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

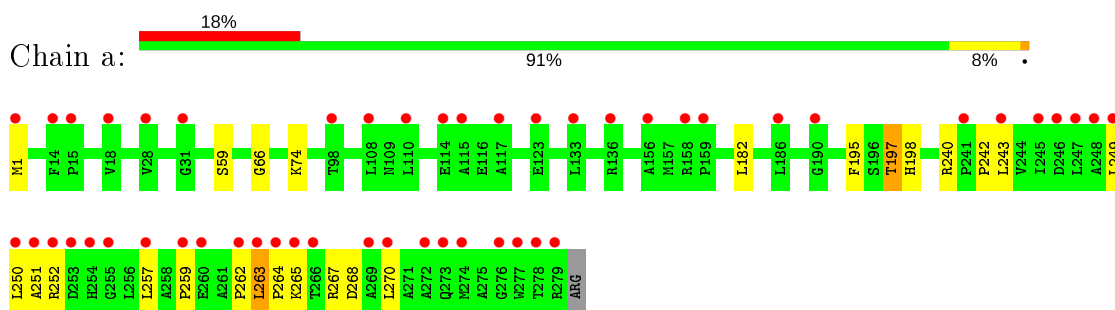
- Molecule 1: Cobalt ABC transporter ATP-binding protein



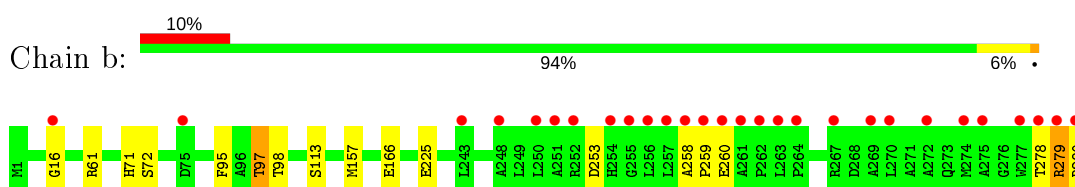
- Molecule 1: Cobalt ABC transporter ATP-binding protein



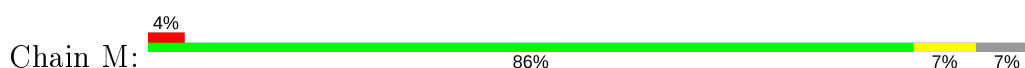
- Molecule 1: Cobalt ABC transporter ATP-binding protein

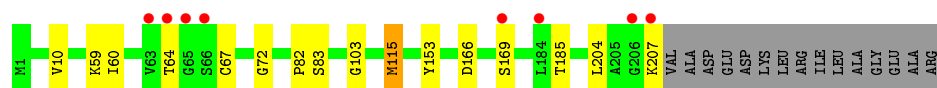


- Molecule 1: Cobalt ABC transporter ATP-binding protein

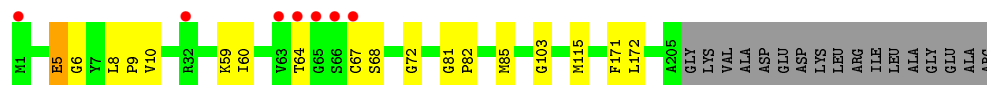
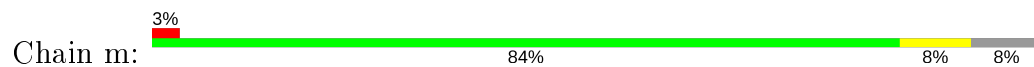


- Molecule 2: Cobalt transport protein CbiM





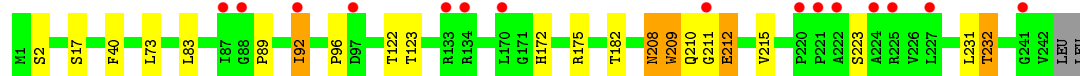
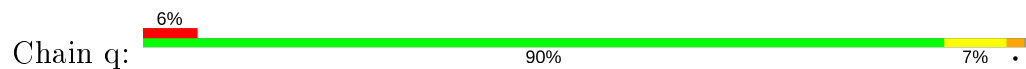
- Molecule 2: Cobalt transport protein CbiM



- Molecule 3: Uncharacterized protein CbiQ



- Molecule 3: Uncharacterized protein CbiQ



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	63.68Å 220.56Å 301.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.33 – 2.79 48.33 – 2.79	Depositor EDS
% Data completeness (in resolution range)	87.0 (48.33-2.79) 87.0 (48.33-2.79)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.47 (at 2.77Å)	Xtrriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.214 , 0.249 0.225 , 0.253	Depositor DCC
R_{free} test set	2376 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	48.3	Xtrriage
Anisotropy	0.071	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 65.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	14966	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 41.63 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.2942e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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	0.71	1/2096 (0.0%)	0.81	2/2847 (0.1%)
1	B	0.66	1/2098 (0.0%)	0.79	3/2850 (0.1%)
1	a	0.60	0/2087	0.83	5/2836 (0.2%)
1	b	0.65	1/2098 (0.0%)	0.81	2/2850 (0.1%)
2	M	0.82	0/1508	0.84	2/2059 (0.1%)
2	m	0.87	1/1495 (0.1%)	0.84	4/2043 (0.2%)
3	Q	0.69	0/1850	0.81	1/2525 (0.0%)
3	q	0.71	0/1842	0.86	5/2514 (0.2%)
All	All	0.71	4/15074 (0.0%)	0.82	24/20524 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2
1	b	0	1
3	Q	0	1
3	q	0	1
All	All	0	5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	198	HIS	C-O	-5.86	1.12	1.23
1	B	101	GLU	CD-OE1	-5.53	1.19	1.25
1	b	259	PRO	N-CD	5.47	1.55	1.47
2	m	5	GLU	CD-OE2	-5.12	1.20	1.25

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	198	HIS	N-CA-C	-8.66	87.61	111.00
1	a	197	THR	N-CA-C	-6.87	92.45	111.00
3	Q	70	VAL	N-CA-C	6.79	129.34	111.00
3	q	211	GLY	N-CA-C	6.53	129.41	113.10
1	a	242	PRO	N-CA-C	-6.21	95.95	112.10
2	m	82	PRO	N-CA-C	6.09	127.94	112.10
2	m	6	GLY	N-CA-C	-6.01	98.08	113.10
1	A	278	THR	N-CA-C	5.99	127.17	111.00
3	q	210	GLN	N-CA-CB	-5.85	100.07	110.60
1	a	198	HIS	C-N-CA	5.84	136.29	121.70
2	m	8	LEU	C-N-CD	-5.78	107.90	120.60
1	A	128	LEU	CA-CB-CG	-5.63	102.35	115.30
2	M	82	PRO	N-CA-C	5.57	126.58	112.10
1	b	258	ALA	C-N-CD	5.46	139.87	128.40
1	b	157	MET	N-CA-C	-5.41	96.40	111.00
1	B	277	TRP	N-CA-C	5.38	125.53	111.00
3	q	40	PHE	C-N-CD	5.38	139.70	128.40
3	q	212	GLU	N-CA-C	-5.34	96.58	111.00
1	B	261	ALA	C-N-CD	-5.30	108.95	120.60
2	m	81	GLY	C-N-CD	-5.25	109.04	120.60
1	B	157	MET	N-CA-C	-5.10	97.24	111.00
1	a	66	GLY	N-CA-C	-5.07	100.42	113.10
3	q	209	TRP	N-CA-CB	5.05	119.68	110.60
2	M	115	MET	C-N-CA	-5.02	109.16	121.70

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	58	GLN	Sidechain
1	B	95	PHE	Peptide
3	Q	208	ASN	Peptide
1	b	95	PHE	Peptide
3	q	208	ASN	Peptide

5.2 Too-close contacts

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	278/280 (99%)	260 (94%)	14 (5%)	4 (1%)	11	31
1	B	278/280 (99%)	267 (96%)	9 (3%)	2 (1%)	22	50
1	a	277/280 (99%)	259 (94%)	14 (5%)	4 (1%)	11	31
1	b	278/280 (99%)	264 (95%)	9 (3%)	5 (2%)	8	25
2	M	205/222 (92%)	191 (93%)	12 (6%)	2 (1%)	15	41
2	m	203/222 (91%)	188 (93%)	11 (5%)	4 (2%)	7	22
3	Q	241/244 (99%)	223 (92%)	14 (6%)	4 (2%)	9	27
3	q	240/244 (98%)	219 (91%)	16 (7%)	5 (2%)	7	21
All	All	2000/2052 (98%)	1871 (94%)	99 (5%)	30 (2%)	10	30

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	263	LEU
1	B	262	PRO
2	M	72	GLY
1	a	262	PRO
1	a	263	LEU
1	a	264	PRO
1	b	278	THR
2	m	9	PRO
2	m	72	GLY
2	m	103	GLY
3	q	73	LEU
3	q	89	PRO
1	A	17	GLY
1	A	114	GLU
1	A	262	PRO
1	B	97	THR
3	Q	210	GLN

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Mol	Chain	Res	Type
1	b	279	ARG
3	q	92	ILE
3	Q	212	GLU
1	a	251	ALA
1	b	260	GLU
2	m	64	THR
3	q	208	ASN
3	Q	96	PRO
1	b	97	THR
3	Q	89	PRO
1	b	16	GLY
2	M	103	GLY
3	q	96	PRO

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	208/209 (100%)	197 (95%)	11 (5%)	22	51
1	B	209/209 (100%)	207 (99%)	2 (1%)	76	91
1	a	208/209 (100%)	190 (91%)	18 (9%)	10	27
1	b	209/209 (100%)	198 (95%)	11 (5%)	22	51
2	M	144/155 (93%)	131 (91%)	13 (9%)	9	26
2	m	143/155 (92%)	133 (93%)	10 (7%)	15	37
3	Q	179/180 (99%)	166 (93%)	13 (7%)	14	35
3	q	178/180 (99%)	163 (92%)	15 (8%)	11	29
All	All	1478/1506 (98%)	1385 (94%)	93 (6%)	18	43

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	SER
1	A	81	ARG

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Mol	Chain	Res	Type
1	A	97	THR
1	A	112	LEU
1	A	116	GLU
1	A	122	GLU
1	A	197	THR
1	A	240	ARG
1	A	260	GLU
1	A	263	LEU
1	A	279	ARG
1	B	58	GLN
1	B	97	THR
2	M	10	VAL
2	M	59	LYS
2	M	60	ILE
2	M	64	THR
2	M	67	CYS
2	M	83	SER
2	M	115	MET
2	M	153	TYR
2	M	166	ASP
2	M	169	SER
2	M	185	THR
2	M	204	LEU
2	M	207	LYS
3	Q	5	SER
3	Q	8	ARG
3	Q	17	SER
3	Q	18	ARG
3	Q	71	LEU
3	Q	73	LEU
3	Q	75	PHE
3	Q	76	LEU
3	Q	210	GLN
3	Q	213	MET
3	Q	215	VAL
3	Q	217	SER
3	Q	225	ARG
1	a	1	MET
1	a	59	SER
1	a	74	LYS
1	a	182	LEU
1	a	195	PHE

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Mol	Chain	Res	Type
1	a	197	THR
1	a	240	ARG
1	a	243	LEU
1	a	249	LEU
1	a	250	LEU
1	a	252	ARG
1	a	257	LEU
1	a	259	PRO
1	a	263	LEU
1	a	265	LYS
1	a	267	ARG
1	a	268	ASP
1	a	270	LEU
1	b	61	ARG
1	b	71	HIS
1	b	72	SER
1	b	97	THR
1	b	98	THR
1	b	113	SER
1	b	166	GLU
1	b	225	GLU
1	b	253	ASP
1	b	279	ARG
1	b	280	ARG
2	m	5	GLU
2	m	10	VAL
2	m	59	LYS
2	m	60	ILE
2	m	67	CYS
2	m	68	SER
2	m	85	MET
2	m	115	MET
2	m	171	PHE
2	m	172	LEU
3	q	2	SER
3	q	17	SER
3	q	83	LEU
3	q	92	ILE
3	q	122	THR
3	q	123	THR
3	q	172	HIS
3	q	175	ARG

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Mol	Chain	Res	Type
3	q	182	THR
3	q	209	TRP
3	q	212	GLU
3	q	215	VAL
3	q	223	SER
3	q	231	LEU
3	q	232	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	58	GLN
1	B	93	GLN
2	M	102	HIS
2	M	186	GLN
1	b	178	GLN
1	b	273	GLN
2	m	102	HIS
2	m	186	GLN
3	q	86	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 monosaccharides 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, 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	280/280 (100%)	0.23	15 (5%) 25 20	25, 43, 74, 112	0
1	B	280/280 (100%)	-0.00	10 (3%) 42 37	21, 38, 70, 106	0
1	a	279/280 (99%)	0.80	50 (17%) 1 1	29, 53, 100, 130	0
1	b	280/280 (100%)	0.46	28 (10%) 7 5	27, 48, 96, 170	0
2	M	207/222 (93%)	0.10	8 (3%) 39 34	23, 37, 66, 121	0
2	m	205/222 (92%)	0.08	7 (3%) 45 39	20, 39, 71, 131	0
3	Q	243/244 (99%)	0.28	18 (7%) 14 10	20, 44, 80, 115	0
3	q	242/244 (99%)	0.32	15 (6%) 20 15	23, 45, 80, 116	0
All	All	2016/2052 (98%)	0.30	151 (7%) 14 10	20, 44, 89, 170	0

All (151) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	b	261	ALA	11.3
1	b	259	PRO	8.5
1	b	262	PRO	8.4
2	m	65	GLY	8.3
2	m	66	SER	7.2
1	a	254	HIS	6.9
1	b	260	GLU	6.0
2	M	66	SER	5.7
1	A	280	ARG	5.6
1	a	115	ALA	5.3
1	a	250	LEU	5.1
1	a	274	MET	5.0
2	m	64	THR	4.8
1	a	277	TRP	4.8
3	q	88	GLY	4.7
1	b	251	ALA	4.7

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Mol	Chain	Res	Type	RSRZ
1	a	270	LEU	4.6
1	b	264	PRO	4.5
1	b	257	LEU	4.5
3	q	133	ARG	4.5
1	b	256	LEU	4.4
2	m	67	CYS	4.3
1	a	279	ARG	4.3
1	b	278	THR	4.2
1	a	266	THR	4.2
1	B	1	MET	4.2
3	Q	224	ALA	4.1
3	q	227	LEU	4.1
3	Q	90	GLU	4.1
3	Q	87	ILE	4.0
1	a	248	ALA	4.0
2	M	207	LYS	4.0
2	m	1	MET	4.0
3	Q	243	LEU	4.0
1	a	263	LEU	4.0
1	a	136	ARG	3.9
1	A	15	PRO	3.9
1	b	277	TRP	3.9
3	q	241	GLY	3.9
1	b	248	ALA	3.8
1	b	254	HIS	3.8
1	a	255	GLY	3.8
1	b	258	ALA	3.7
2	M	206	GLY	3.7
3	q	221	PRO	3.6
1	b	280	ARG	3.6
2	M	65	GLY	3.6
1	b	252	ARG	3.6
1	a	260	GLU	3.5
3	q	220	PRO	3.5
3	Q	241	GLY	3.4
3	Q	88	GLY	3.4
1	a	265	LYS	3.4
1	a	278	THR	3.4
1	a	264	PRO	3.4
1	B	261	ALA	3.3
3	q	211	GLY	3.3
2	M	64	THR	3.3

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Mol	Chain	Res	Type	RSRZ
1	a	273	GLN	3.3
3	Q	56	LEU	3.2
1	a	159	PRO	3.2
1	b	243	LEU	3.2
1	b	250	LEU	3.2
1	a	276	GLY	3.2
1	A	278	THR	3.1
1	A	1	MET	3.1
1	a	110	LEU	3.1
3	Q	91	GLY	3.0
1	b	75	ASP	3.0
1	b	275	ALA	3.0
1	A	18	VAL	3.0
1	a	257	LEU	3.0
1	a	272	ALA	3.0
1	A	73	ARG	3.0
1	a	186	LEU	3.0
3	q	87	ILE	2.9
1	a	252	ARG	2.9
2	M	63	VAL	2.9
1	a	253	ASP	2.9
1	a	249	LEU	2.8
1	a	262	PRO	2.8
3	q	222	ALA	2.8
3	Q	94	LEU	2.8
3	Q	225	ARG	2.8
3	Q	134	ARG	2.8
1	a	1	MET	2.8
3	Q	89	PRO	2.8
1	B	16	GLY	2.8
2	m	32	ARG	2.8
1	a	243	LEU	2.8
1	b	279	ARG	2.7
1	a	14	PHE	2.7
3	Q	232	THR	2.7
1	b	255	GLY	2.7
1	a	251	ALA	2.6
1	a	246	ASP	2.6
1	A	111	GLY	2.6
1	a	245	ILE	2.6
1	a	28	VAL	2.6
3	q	92	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	a	190	GLY	2.5
1	A	14	PHE	2.5
1	A	114	GLU	2.5
1	a	247	LEU	2.5
1	B	274	MET	2.5
1	a	15	PRO	2.4
1	a	18	VAL	2.4
1	A	64	LEU	2.4
1	A	123	GLU	2.4
1	A	137	PRO	2.4
1	a	241	PRO	2.4
1	B	278	THR	2.4
1	a	133	LEU	2.4
1	a	31	GLY	2.4
1	B	280	ARG	2.4
3	q	224	ALA	2.4
1	b	263	LEU	2.3
1	b	270	LEU	2.3
1	a	114	GLU	2.3
1	B	262	PRO	2.3
3	Q	227	LEU	2.3
3	q	225	ARG	2.3
1	A	81	ARG	2.2
2	M	184	LEU	2.2
3	q	134	ARG	2.2
1	a	117	ALA	2.2
1	b	272	ALA	2.2
1	a	156	ALA	2.2
2	m	63	VAL	2.1
1	a	158	ARG	2.1
3	Q	173	ALA	2.1
1	B	270	LEU	2.1
3	q	170	LEU	2.1
1	b	269	ALA	2.1
1	a	98	THR	2.1
1	B	14	PHE	2.1
2	M	169	SER	2.1
1	a	269	ALA	2.1
3	Q	222	ALA	2.1
1	b	274	MET	2.1
1	a	108	LEU	2.1
1	a	123	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	a	259	PRO	2.1
3	q	97	ASP	2.1
1	b	267	ARG	2.1
3	Q	175	ARG	2.0
1	A	254	HIS	2.0
3	Q	231	LEU	2.0
1	b	16	GLY	2.0
1	A	71	HIS	2.0
1	B	259	PRO	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 monosaccharides 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.