Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2024 – 03:31 PM EST

PDB ID	:	4K7K
Title	:	Crystal structures of CusC review conformational changes accompanying folding and transmembrane channel formation
Authors	:	Su, C.-C.; Lei, H.-T.
Deposited on	:	2013-04-17
Resolution	:	2.53 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

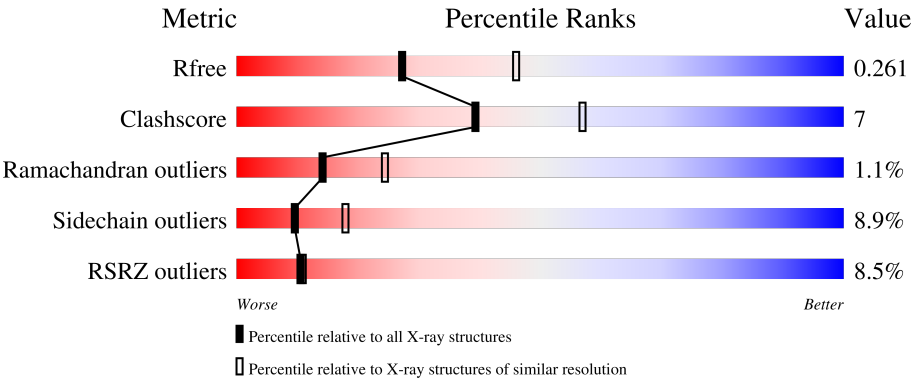
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.53 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	5743 (2.54-2.50)
Clashscore	141614	6463 (2.54-2.50)
Ramachandran outliers	138981	6335 (2.54-2.50)
Sidechain outliers	138945	6337 (2.54-2.50)
RSRZ outliers	127900	5630 (2.54-2.50)

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 of 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 <=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	446	6% 67% 16% · 15%
1	B	446	9% 63% 18% · 17%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 5970 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 Cation efflux system protein CusC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	380	Total	C	N	O	S	0	0	0
			2979	1860	537	577	5			
1	B	371	Total	C	N	O	S	0	0	0
			2903	1815	521	562	5			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	441	HIS	-	expression tag	UNP P77211
A	442	HIS	-	expression tag	UNP P77211
A	443	HIS	-	expression tag	UNP P77211
A	444	HIS	-	expression tag	UNP P77211
A	445	HIS	-	expression tag	UNP P77211
A	446	HIS	-	expression tag	UNP P77211
B	441	HIS	-	expression tag	UNP P77211
B	442	HIS	-	expression tag	UNP P77211
B	443	HIS	-	expression tag	UNP P77211
B	444	HIS	-	expression tag	UNP P77211
B	445	HIS	-	expression tag	UNP P77211
B	446	HIS	-	expression tag	UNP P77211

- Molecule 2 is water.

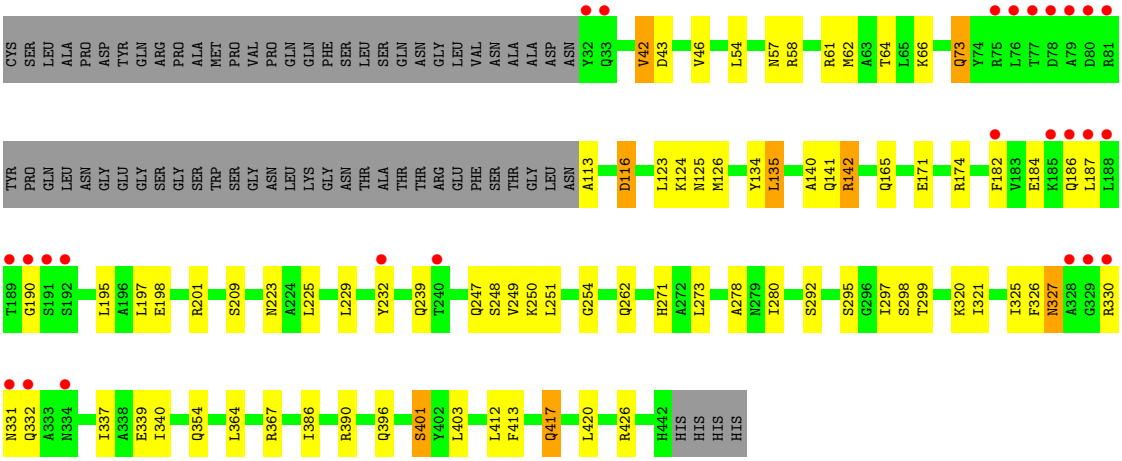
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	59	Total	O	0	0
			59	59		
2	B	29	Total	O	0	0
			29	29		

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.

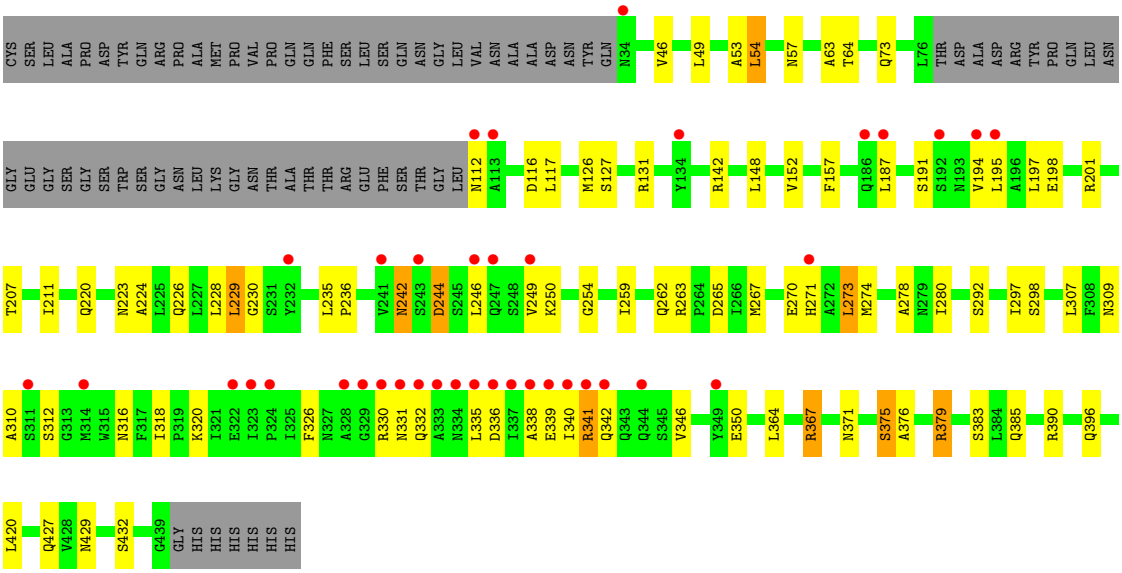
• Molecule 1: Cation efflux system protein CusC

Chain A:



• Molecule 1: Cation efflux system protein CusC

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	62.01Å 104.49Å 72.06Å 90.00° 101.06° 90.00°	Depositor
Resolution (Å)	46.01 – 2.53 46.01 – 2.53	Depositor EDS
% Data completeness (in resolution range)	99.6 (46.01-2.53) 99.6 (46.01-2.53)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.03 (at 2.54Å)	Xtriage
Refinement program	PHENIX 1.7.3_928	Depositor
R, R_{free}	0.208 , 0.267 0.201 , 0.261	Depositor DCC
R_{free} test set	1507 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	39.8	Xtriage
Anisotropy	0.363	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 56.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5970	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.59% 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, 0.333 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	0.44	0/3020	0.57	1/4086 (0.0%)
1	B	0.41	0/2941	0.56	0/3979
All	All	0.42	0/5961	0.57	1/8065 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	135	LEU	CA-CB-CG	5.50	127.94	115.30

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	2979	0	2957	42	0
1	B	2903	0	2896	45	0
2	A	59	0	0	1	0
2	B	29	0	0	2	0
All	All	5970	0	5853	87	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 (87) 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:336:ASP:HB2	1:B:339:GLU:HB2	1.52	0.92
1:A:248:SER:HB3	1:A:426:ARG:HD2	1.70	0.74
1:B:309:ASN:HB3	1:B:312:SER:HB2	1.70	0.72
1:A:171:GLU:HG2	1:A:174:ARG:HH21	1.56	0.71
1:A:73:GLN:HG3	1:A:223:ASN:HD22	1.58	0.67
1:B:73:GLN:HE22	1:B:220:GLN:HA	1.59	0.67
1:A:142:ARG:HH11	1:A:262:GLN:HB2	1.61	0.65
1:A:73:GLN:HG3	1:A:223:ASN:ND2	2.13	0.64
1:B:126:MET:HE2	1:B:131:ARG:HG2	1.80	0.64
1:B:376:ALA:HA	1:B:379:ARG:HD2	1.79	0.64
1:A:165:GLN:HG2	1:A:417:GLN:OE1	2.00	0.62
1:A:134:TYR:O	1:A:135:LEU:HB3	2.00	0.62
1:B:198:GLU:OE2	1:B:201:ARG:NH1	2.34	0.61
1:B:390:ARG:NH1	2:B:517:HOH:O	2.35	0.60
1:B:270:GLU:HA	1:B:273:LEU:HD22	1.84	0.59
1:A:251:LEU:H	1:A:298:SER:HG	1.48	0.59
1:B:338:ALA:O	1:B:342:GLN:HG3	2.03	0.58
1:A:57:ASN:OD1	1:A:66:LYS:HD2	2.04	0.57
1:A:251:LEU:N	1:A:298:SER:OG	2.25	0.57
1:A:297:ILE:HG12	1:A:298:SER:N	2.19	0.57
1:B:326:PHE:CE2	1:B:342:GLN:HG2	2.44	0.52
1:B:339:GLU:HA	1:B:342:GLN:HB2	1.92	0.52
1:B:278:ALA:HB2	1:B:326:PHE:CE2	2.45	0.51
1:B:307:LEU:O	1:B:316:ASN:N	2.40	0.51
1:A:187:LEU:HD22	1:A:197:LEU:HD22	1.91	0.51
1:A:327:ASN:OD1	1:A:327:ASN:N	2.41	0.51
1:B:242:ASN:OD1	1:B:244:ASP:HB2	2.11	0.51
1:B:148:LEU:O	1:B:152:VAL:HG23	2.10	0.51
1:B:339:GLU:HG3	1:B:342:GLN:OE1	2.12	0.50
1:A:225:LEU:O	1:A:229:LEU:HB2	2.12	0.49
1:B:73:GLN:NE2	1:B:223:ASN:HD22	2.11	0.49
1:A:198:GLU:OE2	1:A:201:ARG:NH1	2.46	0.48
1:A:182:PHE:O	1:A:186:GLN:HG2	2.14	0.47
1:B:254:GLY:HA2	1:B:292:SER:OG	2.14	0.47
1:A:171:GLU:HB3	1:A:413:PHE:CZ	2.49	0.47
1:A:42:VAL:HG21	1:A:249:VAL:HG21	1.96	0.47
1:A:386:ILE:O	1:A:390:ARG:HG3	2.14	0.47
1:B:57:ASN:HB3	1:B:63:ALA:HB2	1.97	0.47
1:B:126:MET:CE	1:B:131:ARG:HA	2.44	0.47
1:B:224:ALA:O	1:B:228:LEU:HG	2.14	0.47
1:A:116:ASP:OD2	1:A:116:ASP:N	2.47	0.47
1:A:43:ASP:O	1:A:46:VAL:HG12	2.14	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:197:LEU:HD23	1:B:201:ARG:HH21	1.80	0.46
1:A:61:ARG:O	1:A:64:THR:HB	2.16	0.46
1:B:53:ALA:HB2	1:B:229:LEU:HD23	1.97	0.46
1:A:123:LEU:HA	1:A:126:MET:HE3	1.98	0.45
1:A:135:LEU:HA	1:A:140:ALA:CB	2.47	0.45
1:B:318:ILE:HD13	1:B:318:ILE:HA	1.90	0.45
1:B:429:ASN:O	1:B:432:SER:HB2	2.17	0.45
1:B:73:GLN:NE2	1:B:220:GLN:HA	2.29	0.45
1:A:248:SER:HB3	1:A:426:ARG:HH21	1.81	0.44
1:A:401:SER:HB3	2:B:510:HOH:O	2.16	0.44
1:A:295:SER:OG	1:A:299:THR:OG1	2.24	0.44
1:B:49:LEU:HD11	1:B:236:PRO:HG2	1.99	0.44
1:B:338:ALA:HA	1:B:341:ARG:HD2	2.00	0.44
1:B:259:ILE:O	1:B:262:GLN:HG2	2.17	0.44
1:B:339:GLU:HA	1:B:342:GLN:CG	2.47	0.44
1:B:249:VAL:HG13	1:B:367:ARG:HH12	1.82	0.44
1:A:73:GLN:O	1:A:73:GLN:HG2	2.18	0.43
1:A:320:LYS:HD2	1:A:321:ILE:H	1.83	0.43
1:B:54:LEU:HD12	1:B:148:LEU:HD23	1.99	0.43
1:B:267:MET:O	1:B:271:HIS:ND1	2.48	0.43
1:B:274:MET:HG3	1:B:280:ILE:HD11	2.00	0.43
1:A:321:ILE:HD13	1:A:325:ILE:HD12	2.00	0.43
1:B:246:LEU:HA	1:B:246:LEU:HD23	1.76	0.43
1:A:142:ARG:HH21	1:A:142:ARG:HB2	1.83	0.42
1:A:250:LYS:NZ	1:A:297:ILE:HG13	2.33	0.42
1:B:320:LYS:HA	1:B:320:LYS:HD2	1.82	0.42
1:B:339:GLU:HG3	1:B:342:GLN:CD	2.39	0.42
1:B:371:ASN:O	1:B:375:SER:HB2	2.19	0.42
1:B:250:LYS:HG3	1:B:298:SER:OG	2.19	0.42
1:A:254:GLY:HA2	1:A:292:SER:OG	2.20	0.42
1:A:278:ALA:HB2	1:A:326:PHE:CE2	2.54	0.42
1:A:113:ALA:N	2:A:544:HOH:O	2.53	0.42
1:A:62:MET:O	1:A:66:LYS:HG3	2.20	0.42
1:A:412:LEU:HD12	1:A:412:LEU:HA	1.83	0.42
1:B:226:GLN:HG2	1:B:235:LEU:HD21	2.01	0.42
1:B:207:THR:O	1:B:211:ILE:HG13	2.20	0.41
1:B:73:GLN:HG3	1:B:223:ASN:ND2	2.36	0.41
1:B:346:VAL:O	1:B:350:GLU:HG3	2.19	0.41
1:A:195:LEU:HA	1:A:198:GLU:HB2	2.02	0.41
1:A:403:LEU:HD23	1:A:403:LEU:HA	1.90	0.40
1:B:157:PHE:CD2	1:B:427:GLN:HB3	2.56	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:263:ARG:HB3	1:B:265:ASP:OD1	2.21	0.40
1:A:124:LYS:C	1:A:126:MET:H	2.24	0.40
1:A:280:ILE:HD13	1:A:280:ILE:HA	1.85	0.40
1:A:171:GLU:HG2	1:A:174:ARG:NH2	2.31	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	376/446 (84%)	355 (94%)	17 (4%)	4 (1%)	14	24
1	B	367/446 (82%)	347 (95%)	16 (4%)	4 (1%)	14	24
All	All	743/892 (83%)	702 (94%)	33 (4%)	8 (1%)	14	24

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	331	ASN
1	B	230	GLY
1	A	332	GLN
1	B	310	ALA
1	B	297	ILE
1	A	125	ASN
1	B	332	GLN
1	A	190	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	313/367 (85%)	287 (92%)	26 (8%)	11 20
1	B	306/367 (83%)	277 (90%)	29 (10%)	8 15
All	All	619/734 (84%)	564 (91%)	55 (9%)	9 18

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	VAL
1	A	54	LEU
1	A	58	ARG
1	A	73	GLN
1	A	116	ASP
1	A	141	GLN
1	A	142	ARG
1	A	184	GLU
1	A	209	SER
1	A	232	TYR
1	A	239	GLN
1	A	247	GLN
1	A	271	HIS
1	A	273	LEU
1	A	327	ASN
1	A	330	ARG
1	A	337	ILE
1	A	339	GLU
1	A	340	ILE
1	A	354	GLN
1	A	364	LEU
1	A	367	ARG
1	A	396	GLN
1	A	401	SER
1	A	417	GLN
1	A	420	LEU
1	B	46	VAL
1	B	54	LEU
1	B	64	THR
1	B	112	ASN
1	B	116	ASP
1	B	117	LEU
1	B	127	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	142	ARG
1	B	187	LEU
1	B	191	SER
1	B	194	VAL
1	B	195	LEU
1	B	229	LEU
1	B	242	ASN
1	B	244	ASP
1	B	273	LEU
1	B	330	ARG
1	B	331	ASN
1	B	335	LEU
1	B	340	ILE
1	B	341	ARG
1	B	364	LEU
1	B	367	ARG
1	B	375	SER
1	B	379	ARG
1	B	383	SER
1	B	385	GLN
1	B	396	GLN
1	B	420	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	223	ASN
1	B	73	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, 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	380/446 (85%)	0.38	26 (6%) 17 18	22, 38, 84, 128	0
1	B	371/446 (83%)	0.68	38 (10%) 6 6	27, 46, 95, 123	0
All	All	751/892 (84%)	0.53	64 (8%) 10 11	22, 42, 94, 128	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	333	ALA	13.2
1	B	335	LEU	12.1
1	B	329	GLY	10.4
1	B	337	ILE	9.7
1	B	338	ALA	9.5
1	A	77	THR	8.5
1	B	339	GLU	8.4
1	B	331	ASN	8.1
1	B	334	ASN	8.0
1	B	330	ARG	7.8
1	B	341	ARG	7.7
1	A	191	SER	7.7
1	B	340	ILE	7.6
1	A	79	ALA	7.3
1	A	81	ARG	7.0
1	A	80	ASP	6.9
1	A	76	LEU	6.5
1	B	336	ASP	6.0
1	B	187	LEU	5.8
1	A	189	THR	5.6
1	A	329	GLY	5.6
1	A	328	ALA	5.4
1	B	332	GLN	5.2
1	B	342	GLN	5.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	232	TYR	4.7
1	B	249	VAL	4.2
1	A	332	GLN	4.1
1	A	78	ASP	4.0
1	A	331	ASN	4.0
1	B	112	ASN	3.9
1	A	190	GLY	3.9
1	A	188	LEU	3.7
1	A	75	ARG	3.6
1	A	330	ARG	3.5
1	B	328	ALA	3.4
1	B	241	VAL	3.3
1	A	33	GLN	3.0
1	A	32	TYR	3.0
1	A	186	GLN	2.9
1	A	182	PHE	2.8
1	B	34	ASN	2.7
1	B	247	GLN	2.7
1	B	311	SER	2.6
1	B	232	TYR	2.6
1	B	271	HIS	2.6
1	B	186	GLN	2.6
1	B	323	ILE	2.6
1	B	246	LEU	2.6
1	A	240	THR	2.5
1	A	185	LYS	2.4
1	B	324	PRO	2.3
1	A	192	SER	2.3
1	B	243	SER	2.3
1	A	334	ASN	2.2
1	B	322	GLU	2.2
1	B	192	SER	2.2
1	B	314	MET	2.2
1	B	344	GLN	2.1
1	B	194	VAL	2.1
1	B	113	ALA	2.1
1	B	195	LEU	2.1
1	A	187	LEU	2.1
1	B	134	TYR	2.1
1	B	349	TYR	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.