



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 12:52 PM GMT

PDB ID : 4DNT
Title : Crystal structure of the CusBA heavy-metal efflux complex from Escherichia coli, mutant
Authors : Su, C.-C.; Long, F.; Yu, E.
Deposited on : 2012-02-09
Resolution : 3.10 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

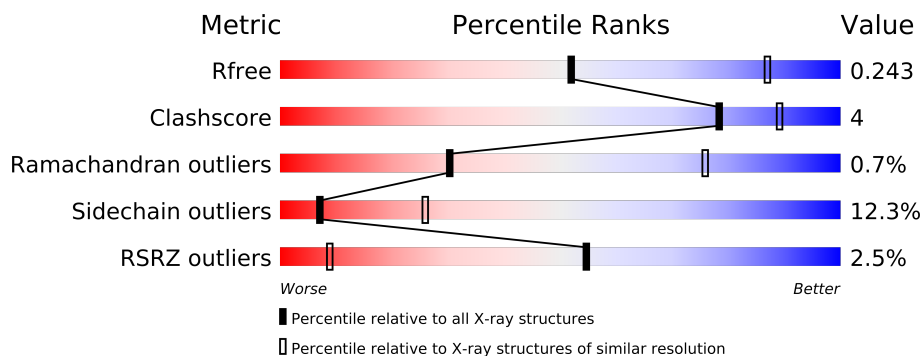
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.10 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}	66092	1007 (3.18-3.02)
Clashscore	79885	1078 (3.16-3.04)
Ramachandran outliers	78287	1044 (3.16-3.04)
Sidechain outliers	78261	1044 (3.16-3.04)
RSRZ outliers	66119	1008 (3.18-3.02)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	B	413	<div><div></div><div><div></div><div></div><div></div><div></div></div><div></div></div>
1	C	413	<div><div></div><div><div></div><div></div><div></div><div></div></div><div></div></div>
2	A	1054	<div><div></div><div><div></div><div></div><div></div><div></div></div><div></div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12895 atoms, of which 0 are hydrogen and 0 are deuterium.

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 CusB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	322	Total	C	N	O	S	0	0	0
			2458	1555	428	469	6			
1	C	324	Total	C	N	O	S	0	0	0
			2473	1563	430	474	6			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	408	HIS	-	EXPRESSION TAG	UNP P77239
B	409	HIS	-	EXPRESSION TAG	UNP P77239
B	410	HIS	-	EXPRESSION TAG	UNP P77239
B	411	HIS	-	EXPRESSION TAG	UNP P77239
B	412	HIS	-	EXPRESSION TAG	UNP P77239
B	413	HIS	-	EXPRESSION TAG	UNP P77239
C	408	HIS	-	EXPRESSION TAG	UNP P77239
C	409	HIS	-	EXPRESSION TAG	UNP P77239
C	410	HIS	-	EXPRESSION TAG	UNP P77239
C	411	HIS	-	EXPRESSION TAG	UNP P77239
C	412	HIS	-	EXPRESSION TAG	UNP P77239
C	413	HIS	-	EXPRESSION TAG	UNP P77239

- Molecule 2 is a protein called Cation efflux system protein CusA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	1031	Total	C	N	O	S	0	0	0
			7945	5139	1333	1436	37			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	EXPRESSION TAG	UNP P38054
A	-5	HIS	-	EXPRESSION TAG	UNP P38054

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	HIS	-	EXPRESSION TAG	UNP P38054
A	-3	HIS	-	EXPRESSION TAG	UNP P38054
A	-2	HIS	-	EXPRESSION TAG	UNP P38054
A	-1	HIS	-	EXPRESSION TAG	UNP P38054
A	0	HIS	-	EXPRESSION TAG	UNP P38054
A	405	ALA	ASP	ENGINEERED MUTATION	UNP P38054

- Molecule 3 is water.

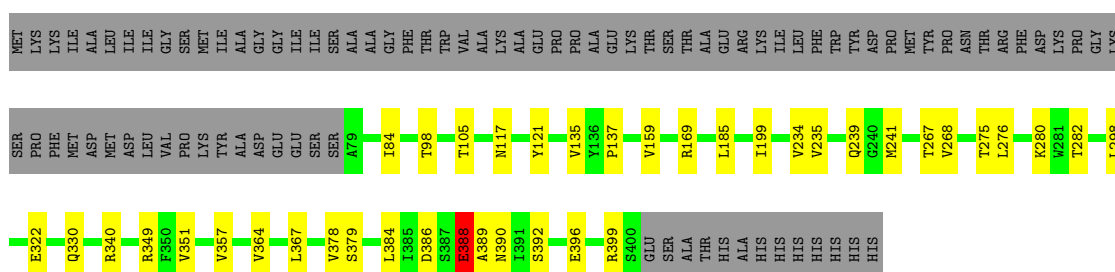
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	4	Total O 4 4	0	0
3	C	10	Total O 10 10	0	0
3	A	5	Total O 5 5	0	0

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 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.

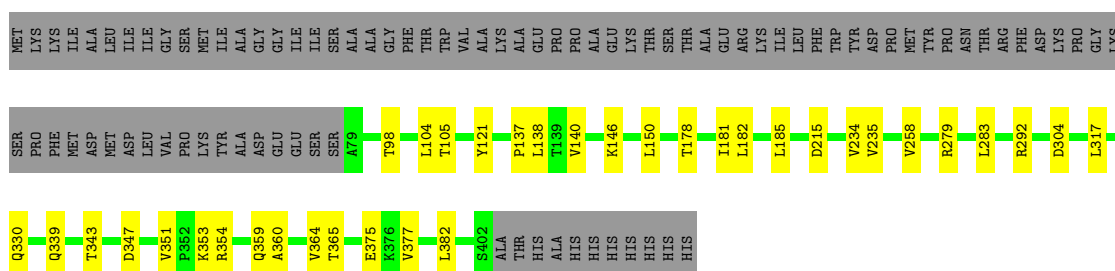
- Molecule 1: Cation efflux system protein CusB

Chain B:



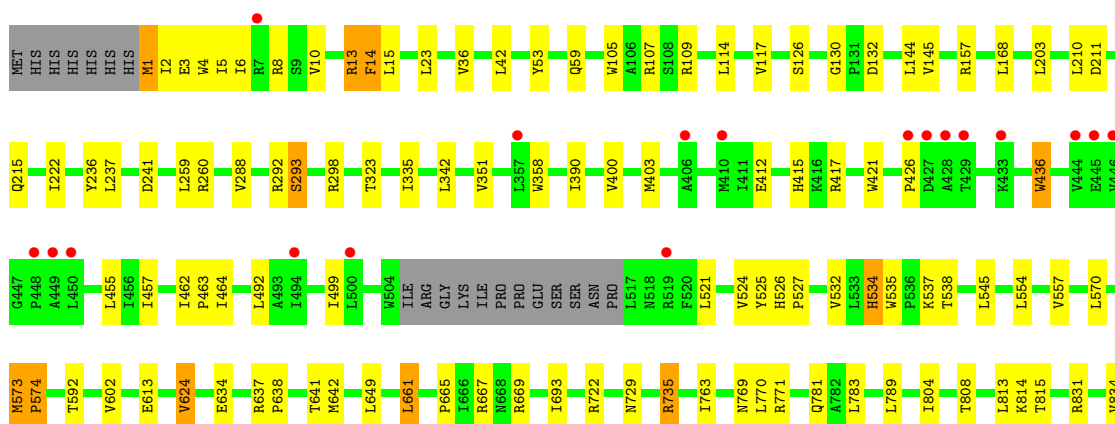
- Molecule 1: Cation efflux system protein CusB

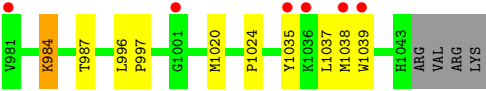
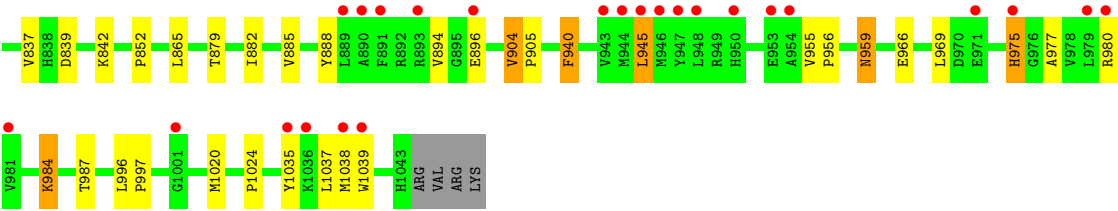
Chain C:



- Molecule 2: Cation efflux system protein CusA

Chain A:





4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	159.64Å 159.64Å 681.10Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	107.33 – 3.10 107.33 – 3.10	Depositor EDS
% Data completeness (in resolution range)	92.0 (107.33-3.10) 99.9 (107.33-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 3.13Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.219 , 0.244 0.217 , 0.243	Depositor DCC
R_{free} test set	3095 reflections (5.06%)	DCC
Wilson B-factor (Å ²)	70.5	Xtriage
Anisotropy	0.385	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 44.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 61235 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	12895	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.25% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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	B	0.23	0/2498	0.45	1/3401 (0.0%)
1	C	0.22	0/2513	0.43	0/3421
2	A	0.21	0/8111	0.42	0/11044
All	All	0.22	0/13122	0.43	1/17866 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	388	GLU	N-CA-C	5.12	124.83	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2458	0	21	3	0
1	C	2473	0	9	2	0
2	A	7945	0	111	42	0
3	A	5	0	0	0	0
3	B	4	0	0	0	0
3	C	10	0	0	0	0
All	All	12895	0	141	47	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 4.

All (47) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:896:GLU:OE1	2:A:945:LEU:CD1	2.20	0.90
2:A:896:GLU:OE1	2:A:945:LEU:CG	2.20	0.90
2:A:14:PHE:CD2	2:A:14:PHE:O	2.30	0.84
2:A:13:ARG:NH1	2:A:436:TRP:CZ3	2.53	0.77
2:A:13:ARG:O	2:A:13:ARG:CD	2.32	0.77
2:A:13:ARG:CB	2:A:499:ILE:CD1	2.65	0.75
2:A:888:TYR:OH	2:A:894:VAL:CG2	2.36	0.72
2:A:2:ILE:H	2:A:2:ILE:HD12	1.55	0.69
1:B:386:ASP:O	1:B:388:GLU:N	2.25	0.69
1:B:388:GLU:CA	1:B:388:GLU:OE1	2.41	0.68
2:A:888:TYR:CZ	2:A:894:VAL:CG2	2.80	0.65
2:A:4:TRP:O	2:A:8:ARG:HG3	1.98	0.64
2:A:735:ARG:CG	2:A:735:ARG:NH2	2.60	0.62
2:A:888:TYR:CE2	2:A:894:VAL:CG2	2.83	0.62
2:A:940:PHE:C	2:A:940:PHE:CD2	2.73	0.61
2:A:13:ARG:C	2:A:13:ARG:CD	2.70	0.60
2:A:6:ILE:O	2:A:10:VAL:HG23	2.02	0.60
2:A:535:TRP:O	2:A:537:LYS:N	2.37	0.58
2:A:13:ARG:O	2:A:14:PHE:CB	2.52	0.56
2:A:436:TRP:C	2:A:436:TRP:CD1	2.82	0.52
2:A:574:PRO:CG	2:A:624:VAL:CG1	2.89	0.51
2:A:534:HIS:CD2	2:A:534:HIS:C	2.84	0.50
2:A:3:GLU:H	2:A:3:GLU:CD	2.15	0.50
2:A:955:VAL:N	2:A:956:PRO:CD	2.75	0.49
2:A:940:PHE:CE1	2:A:984:LYS:CE	2.95	0.49
1:B:388:GLU:O	1:B:389:ALA:C	2.52	0.48
2:A:959:ASN:N	2:A:959:ASN:OD1	2.46	0.48
2:A:535:TRP:O	2:A:538:THR:N	2.47	0.47
1:C:359:GLN:CG	1:C:360:ALA:N	2.77	0.47
2:A:904:VAL:N	2:A:905:PRO:CD	2.77	0.47
2:A:1:MET:O	2:A:5:ILE:HG13	2.15	0.47
2:A:573:MET:O	2:A:661:LEU:CB	2.63	0.46
2:A:526:HIS:N	2:A:527:PRO:CD	2.79	0.46
2:A:831:ARG:NH2	2:A:839:ASP:OD1	2.49	0.46
2:A:132:ASP:O	2:A:293:SER:OG	2.35	0.45
2:A:2:ILE:N	2:A:2:ILE:HD12	2.28	0.45
2:A:421:TRP:O	2:A:421:TRP:CD1	2.72	0.43
2:A:996:LEU:N	2:A:997:PRO:CD	2.82	0.42
2:A:975:HIS:C	2:A:977:ALA:N	2.73	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:525:TYR:OH	2:A:980:ARG:NH2	2.53	0.41
2:A:804:ILE:CG1	2:A:804:ILE:O	2.68	0.41
1:C:146:LYS:N	1:C:215:ASP:OD2	2.53	0.41
2:A:2:ILE:CD1	2:A:2:ILE:H	2.29	0.41
2:A:292:ARG:O	2:A:293:SER:C	2.58	0.41
2:A:2:ILE:O	2:A:6:ILE:HG13	2.21	0.41
2:A:462:ILE:N	2:A:463:PRO:CD	2.84	0.40
2:A:107:ARG:NH1	2:A:130:GLY:O	2.53	0.40

There are no symmetry-related clashes.

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	B	320/413 (78%)	297 (93%)	20 (6%)	3 (1%)	25	71
1	C	322/413 (78%)	309 (96%)	12 (4%)	1 (0%)	50	87
2	A	1027/1054 (97%)	942 (92%)	77 (8%)	8 (1%)	27	74
All	All	1669/1880 (89%)	1548 (93%)	109 (6%)	12 (1%)	30	76

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	638	PRO
2	A	574	PRO
2	A	613	GLU
1	B	388	GLU
1	B	390	ASN
2	A	14	PHE
2	A	426	PRO
2	A	1024	PRO
2	A	665	PRO
1	B	137	PRO
1	C	137	PRO

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Mol	Chain	Res	Type
2	A	852	PRO

5.3.2 Protein sidechains ⓘ

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	B	263/338 (78%)	227 (86%)	36 (14%)	5	21
1	C	265/338 (78%)	234 (88%)	31 (12%)	8	29
2	A	849/871 (98%)	747 (88%)	102 (12%)	7	27
All	All	1377/1547 (89%)	1208 (88%)	169 (12%)	7	26

All (169) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	84	ILE
1	B	98	THR
1	B	105	THR
1	B	117	ASN
1	B	121	TYR
1	B	135	VAL
1	B	159	VAL
1	B	169	ARG
1	B	185	LEU
1	B	199	ILE
1	B	234	VAL
1	B	235	VAL
1	B	239	GLN
1	B	241	MET
1	B	267	THR
1	B	268	VAL
1	B	275	THR
1	B	276	LEU
1	B	280	LYS
1	B	282	THR
1	B	298	LEU
1	B	322	GLU

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Mol	Chain	Res	Type
1	B	330	GLN
1	B	340	ARG
1	B	349	ARG
1	B	351	VAL
1	B	357	VAL
1	B	364	VAL
1	B	367	LEU
1	B	378	VAL
1	B	379	SER
1	B	384	LEU
1	B	388	GLU
1	B	392	SER
1	B	396	GLU
1	B	399	ARG
1	C	98	THR
1	C	104	LEU
1	C	105	THR
1	C	121	TYR
1	C	138	LEU
1	C	140	VAL
1	C	150	LEU
1	C	178	THR
1	C	181	ILE
1	C	182	LEU
1	C	185	LEU
1	C	234	VAL
1	C	235	VAL
1	C	258	VAL
1	C	279	ARG
1	C	283	LEU
1	C	292	ARG
1	C	304	ASP
1	C	317	LEU
1	C	330	GLN
1	C	339	GLN
1	C	343	THR
1	C	347	ASP
1	C	351	VAL
1	C	353	LYS
1	C	354	ARG
1	C	364	VAL
1	C	365	THR

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Mol	Chain	Res	Type
1	C	375	GLU
1	C	377	VAL
1	C	382	LEU
2	A	1	MET
2	A	13	ARG
2	A	15	LEU
2	A	23	LEU
2	A	36	VAL
2	A	42	LEU
2	A	53	TYR
2	A	59	GLN
2	A	105	TRP
2	A	109	ARG
2	A	114	LEU
2	A	117	VAL
2	A	126	SER
2	A	144	LEU
2	A	145	VAL
2	A	157	ARG
2	A	168	LEU
2	A	203	LEU
2	A	210	LEU
2	A	211	ASP
2	A	215	GLN
2	A	222	ILE
2	A	236	TYR
2	A	237	LEU
2	A	241	ASP
2	A	259	LEU
2	A	260	ARG
2	A	288	VAL
2	A	293	SER
2	A	298	ARG
2	A	323	THR
2	A	335	ILE
2	A	342	LEU
2	A	351	VAL
2	A	358	TRP
2	A	390	ILE
2	A	400	VAL
2	A	403	MET
2	A	412	GLU

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Mol	Chain	Res	Type
2	A	415	HIS
2	A	417	ARG
2	A	436	TRP
2	A	455	LEU
2	A	457	ILE
2	A	464	ILE
2	A	492	LEU
2	A	521	LEU
2	A	524	VAL
2	A	532	VAL
2	A	534	HIS
2	A	545	LEU
2	A	554	LEU
2	A	557	VAL
2	A	570	LEU
2	A	573	MET
2	A	592	THR
2	A	602	VAL
2	A	624	VAL
2	A	634	GLU
2	A	637	ARG
2	A	641	THR
2	A	642	MET
2	A	649	LEU
2	A	661	LEU
2	A	667	ARG
2	A	669	ARG
2	A	693	ILE
2	A	722	ARG
2	A	729	ASN
2	A	735	ARG
2	A	763	ILE
2	A	769	ASN
2	A	770	LEU
2	A	771	ARG
2	A	781	GLN
2	A	783	LEU
2	A	789	LEU
2	A	808	THR
2	A	813	LEU
2	A	814	LYS
2	A	815	THR

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Mol	Chain	Res	Type
2	A	834	VAL
2	A	837	VAL
2	A	842	LYS
2	A	865	LEU
2	A	879	THR
2	A	882	ILE
2	A	885	VAL
2	A	904	VAL
2	A	940	PHE
2	A	945	LEU
2	A	959	ASN
2	A	966	GLU
2	A	969	LEU
2	A	975	HIS
2	A	984	LYS
2	A	987	THR
2	A	1020	MET
2	A	1035	TYR
2	A	1037	LEU
2	A	1038	MET
2	A	1039	TRP

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 chains 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, 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	B	322/413 (77%)	-0.09	0	100 100	26, 53, 97, 153	0
1	C	324/413 (78%)	-0.06	0	100 100	31, 54, 100, 142	0
2	A	1031/1054 (97%)	0.18	42 (4%)	35 5	26, 77, 184, 278	0
All	All	1677/1880 (89%)	0.08	42 (2%)	54 9	26, 65, 166, 278	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	946	MET	4.1
2	A	1035	TYR	4.1
2	A	948	LEU	4.1
2	A	980	ARG	3.8
2	A	410	MET	3.5
2	A	1036	LYS	3.3
2	A	947	TYR	3.1
2	A	429	THR	3.1
2	A	1001	GLY	3.1
2	A	1038	MET	3.0
2	A	950	HIS	2.9
2	A	953	GLU	2.9
2	A	954	ALA	2.9
2	A	428	ALA	2.8
2	A	427	ASP	2.7
2	A	449	ALA	2.6
2	A	893	ARG	2.6
2	A	519	ARG	2.5
2	A	445	GLU	2.5
2	A	494	ILE	2.5
2	A	433	LYS	2.5
2	A	446	VAL	2.4
2	A	406	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
2	A	1039	TRP	2.4
2	A	979	LEU	2.4
2	A	943	VAL	2.4
2	A	896	GLU	2.3
2	A	945	LEU	2.3
2	A	971	GLU	2.3
2	A	426	PRO	2.2
2	A	890	ALA	2.2
2	A	889	LEU	2.1
2	A	450	LEU	2.1
2	A	448	PRO	2.1
2	A	7	ARG	2.1
2	A	944	MET	2.1
2	A	444	VAL	2.1
2	A	975	HIS	2.1
2	A	357	LEU	2.1
2	A	981	VAL	2.1
2	A	500	LEU	2.0
2	A	891	PHE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.