



# wwPDB X-ray Structure Validation Summary Report

Feb 26, 2014 – 02:40 PM GMT

PDB ID : 2HN2  
Title : Crystal structure of the CorA Mg<sup>2+</sup> transporter homologue from *T. maritima*  
in complex with divalent cations  
Authors : Payandeh, J.; Pai, E.F.  
Deposited on : 2006-07-11  
Resolution : 3.70 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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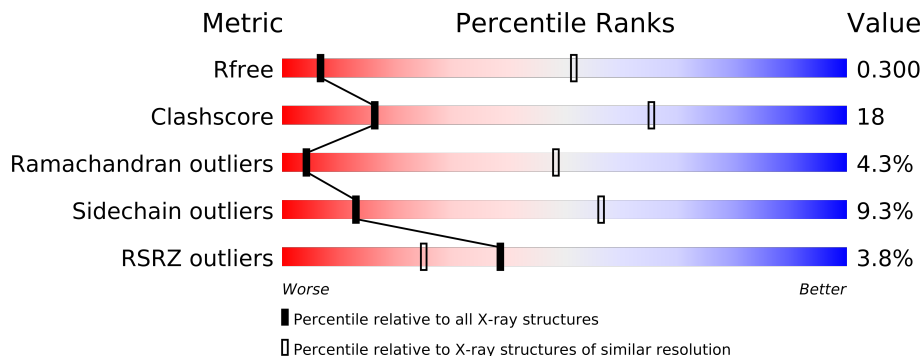
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	<b>FAILED</b>
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 3.70 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	1098 (4.00-3.40)
Clashscore	79885	1009 (3.94-3.46)
Ramachandran outliers	78287	1016 (3.98-3.42)
Sidechain outliers	78261	1014 (3.98-3.42)
RSRZ outliers	66119	1099 (4.00-3.40)

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  $\geq 3$ , 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	A	354	
1	B	354	
1	C	354	
1	D	354	
1	E	354	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	CA	A	6211	-	X
2	CA	B	6102	-	X
2	CA	B	6201	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
2	CA	B	6212	-	X
2	CA	D	6214	-	X
2	CA	E	6215	-	X

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13698 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 Magnesium transport protein corA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	331	Total	C	N	O	S	0	0	0
			2737	1782	445	501	9			
1	B	331	Total	C	N	O	S	0	0	0
			2737	1782	445	501	9			
1	C	331	Total	C	N	O	S	0	0	0
			2737	1782	445	501	9			
1	D	331	Total	C	N	O	S	0	0	0
			2737	1782	445	501	9			
1	E	331	Total	C	N	O	S	0	0	0
			2737	1782	445	501	9			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	998	GLY	-	CLONING ARTIFACT	UNP Q9WZ31
A	999	SER	-	CLONING ARTIFACT	UNP Q9WZ31
A	1000	HIS	-	CLONING ARTIFACT	UNP Q9WZ31
B	1998	GLY	-	CLONING ARTIFACT	UNP Q9WZ31
B	1999	SER	-	CLONING ARTIFACT	UNP Q9WZ31
B	2000	HIS	-	CLONING ARTIFACT	UNP Q9WZ31
C	2998	GLY	-	CLONING ARTIFACT	UNP Q9WZ31
C	2999	SER	-	CLONING ARTIFACT	UNP Q9WZ31
C	3000	HIS	-	CLONING ARTIFACT	UNP Q9WZ31
D	3998	GLY	-	CLONING ARTIFACT	UNP Q9WZ31
D	3999	SER	-	CLONING ARTIFACT	UNP Q9WZ31
D	4000	HIS	-	CLONING ARTIFACT	UNP Q9WZ31
E	4998	GLY	-	CLONING ARTIFACT	UNP Q9WZ31
E	4999	SER	-	CLONING ARTIFACT	UNP Q9WZ31
E	5000	HIS	-	CLONING ARTIFACT	UNP Q9WZ31

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

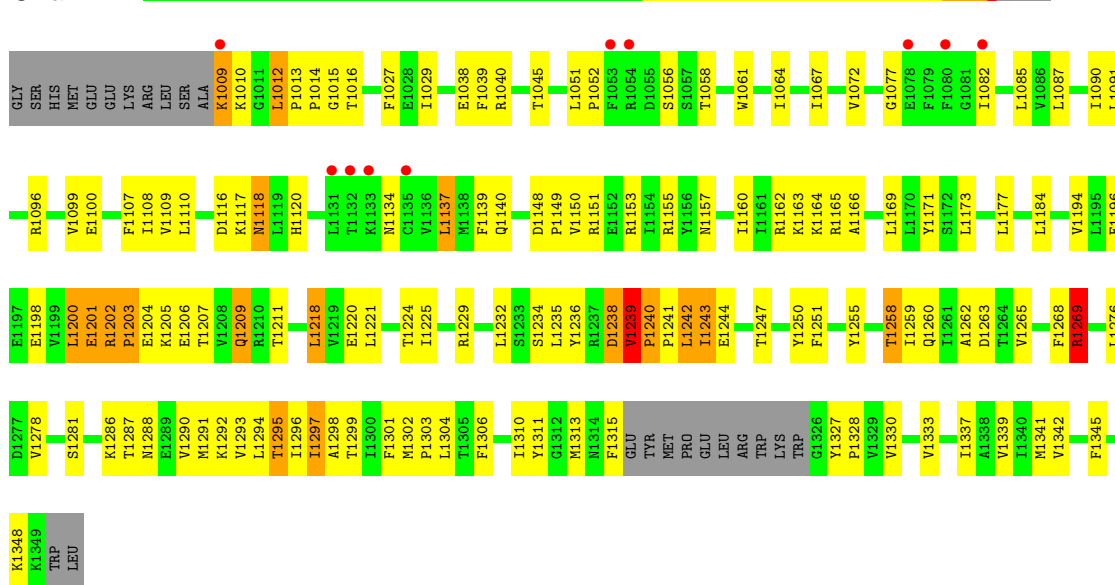
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	3	Total 3	Ca 3	0	0
2	A	4	Total 4	Ca 4	0	0
2	D	3	Total 3	Ca 3	0	0
2	C	2	Total 2	Ca 2	0	0
2	E	1	Total 1	Ca 1	0	0

### 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.

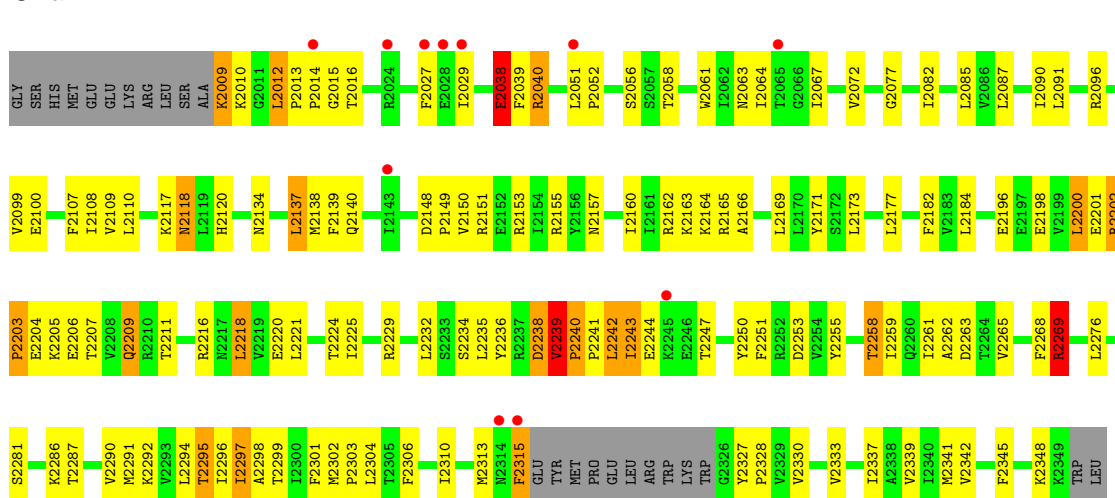
- Molecule 1: Magnesium transport protein corA

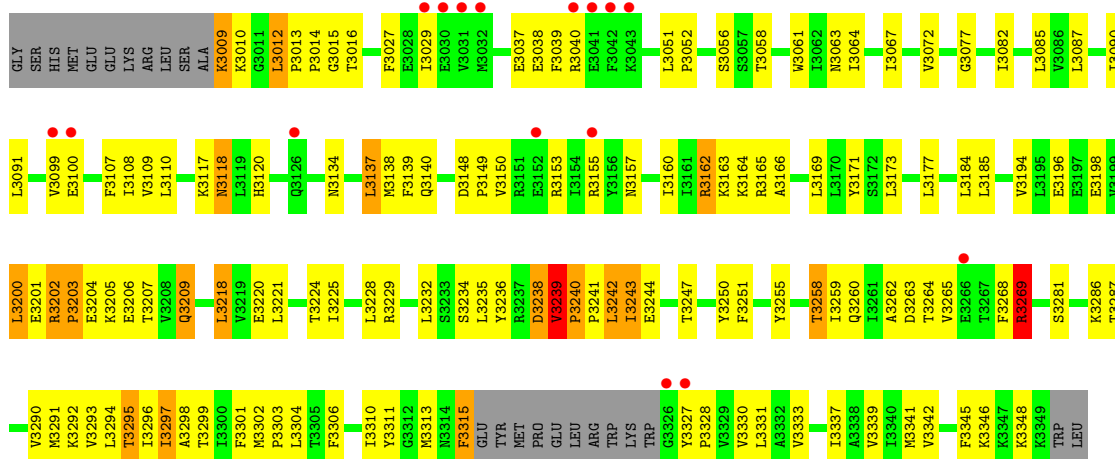
Chain A:



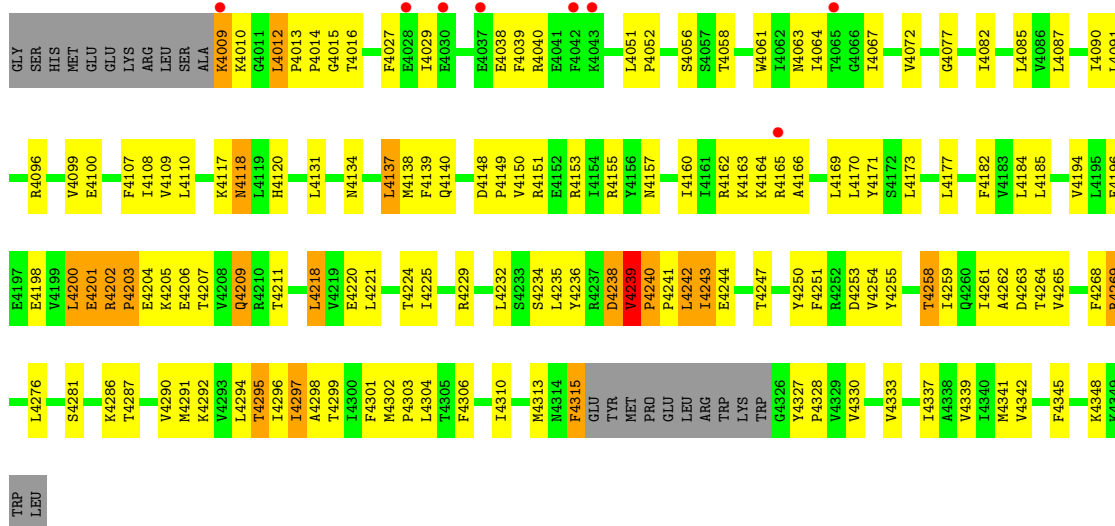
- Molecule 1: Magnesium transport protein corA

Chain B:

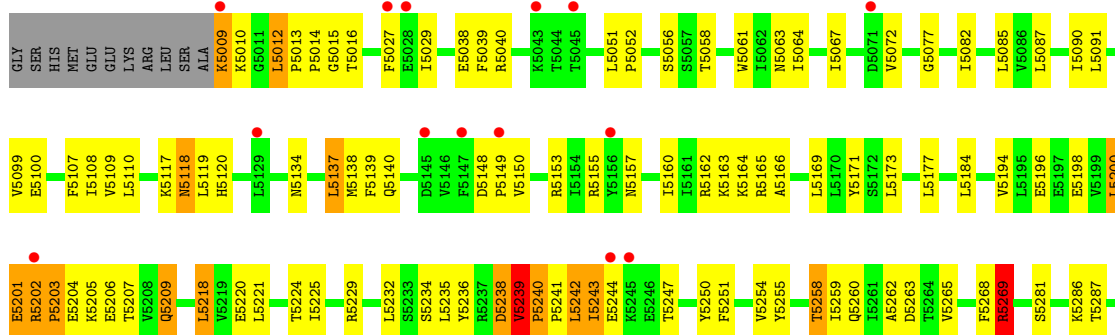




- Molecule 1: Magnesium transport protein corA



- Molecule 1: Magnesium transport protein corA



V5290	M5291	K5292	V5293	L5294	T5295	I5296	A5297	A5298	T5299	I5300	F5301	M5302	F5303	L5304	T5305	F5306	I5310	Y5311	G5312	M5313	M5314	F5315	GLI	TYR	NET	PRO	GLU	LEU	ARG	TRP	LYS	TRP	G5326	Y5327	P5328	V5329	V5330	V5333	I5337	A5338	V5339	I5340	M5341	V5342	V5343	Y5344	F5345	K5348	F5349	TRP	LEU
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## 4 Data and refinement statistics

Xtriage (Phenix) failed to run properly - this section will therefore be incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	214.25Å 86.30Å 181.53Å 90.00° 112.23° 90.00°	Depositor
Resolution (Å)	20.00 – 3.70 49.58 – 3.66	Depositor EDS
% Data completeness (in resolution range)	92.0 (20.00-3.70) 90.5 (49.58-3.66)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS	Depositor
R, $R_{free}$	0.295 , 0.316 0.294 , 0.300	Depositor DCC
$R_{free}$ test set	1521 reflections (5.02%)	DCC
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.24 , 74.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.85	EDS
Total number of atoms	13698	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	137.0	wwPDB-VP

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CA

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	0.34	0/2794	0.55	1/3785 (0.0%)
1	B	0.34	0/2794	0.55	3/3785 (0.1%)
1	C	0.35	0/2794	0.55	1/3785 (0.0%)
1	D	0.35	0/2794	0.68	3/3785 (0.1%)
1	E	0.34	0/2794	0.55	1/3785 (0.0%)
All	All	0.34	0/13970	0.58	9/18925 (0.0%)

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	4269	ARG	NE-CZ-NH2	-17.72	111.44	120.30
1	D	4269	ARG	NE-CZ-NH1	17.20	128.90	120.30
1	D	4269	ARG	CD-NE-CZ	8.40	135.36	123.60
1	B	2269	ARG	NE-CZ-NH1	-5.24	117.68	120.30
1	C	3269	ARG	NE-CZ-NH1	-5.17	117.72	120.30

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	A	2737	0	2790	113	1
1	B	2737	0	2790	116	1
1	C	2737	0	2790	114	1
1	D	2737	0	2790	116	0
1	E	2737	0	2790	115	1
2	A	4	0	0	0	0
2	B	3	0	0	0	0
2	C	2	0	0	0	0
2	D	3	0	0	0	0
2	E	1	0	0	0	0
All	All	13698	0	13950	499	3

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 18.

The worst 5 of 499 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:5240:PRO:HB2	1:E:5241:PRO:HD3	1.33	1.10
1:A:1240:PRO:HB2	1:A:1241:PRO:HD3	1.33	1.09
1:D:4240:PRO:HB2	1:D:4241:PRO:HD3	1.33	1.08
1:B:2240:PRO:HB2	1:B:2241:PRO:HD3	1.33	1.07
1:C:3240:PRO:HB2	1:C:3241:PRO:HD3	1.33	1.07

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:2038:GLU:OE2	1:E:5119:LEU:CD1[1_545]	2.07	0.13
1:C:3037:GLU:OE2	1:C:3162:ARG:NH2[2_556]	2.07	0.13
1:A:1045:THR:OG1	1:A:1116:ASP:OD1[2_555]	2.19	0.01

## 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.

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	327/354 (92%)	256 (78%)	57 (17%)	14 (4%)	4	48
1	B	327/354 (92%)	258 (79%)	55 (17%)	14 (4%)	4	48
1	C	327/354 (92%)	256 (78%)	57 (17%)	14 (4%)	4	48
1	D	327/354 (92%)	256 (78%)	57 (17%)	14 (4%)	4	48
1	E	327/354 (92%)	256 (78%)	57 (17%)	14 (4%)	4	48
All	All	1635/1770 (92%)	1282 (78%)	283 (17%)	70 (4%)	4	48

5 of 70 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1202	ARG
1	A	1244	GLU
1	B	2202	ARG
1	B	2244	GLU
1	C	3202	ARG

### 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	A	311/332 (94%)	282 (91%)	29 (9%)	13	56
1	B	311/332 (94%)	282 (91%)	29 (9%)	13	56
1	C	311/332 (94%)	282 (91%)	29 (9%)	13	56
1	D	311/332 (94%)	282 (91%)	29 (9%)	13	56
1	E	311/332 (94%)	282 (91%)	29 (9%)	13	56
All	All	1555/1660 (94%)	1410 (91%)	145 (9%)	13	56

5 of 145 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	3184	LEU
1	C	3281	SER

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Mol	Chain	Res	Type
1	E	5239	VAL
1	C	3200	LEU
1	C	3220	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	3033	ASN
1	C	3095	GLN
1	D	4217	ASN
1	B	2314	ASN
1	E	5033	ASN

### 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 ⓘ

Of 13 ligands modelled in this entry, 13 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	331/354 (93%)	0.25	10 (3%) 48 29	37, 137, 197, 200	0
1	B	331/354 (93%)	0.19	11 (3%) 44 28	37, 120, 183, 200	0
1	C	331/354 (93%)	0.41	16 (4%) 29 19	45, 132, 195, 200	0
1	D	331/354 (93%)	0.13	8 (2%) 56 35	49, 143, 197, 200	0
1	E	331/354 (93%)	0.29	15 (4%) 32 21	54, 151, 199, 200	0
All	All	1655/1770 (93%)	0.25	60 (3%) 38 26	37, 137, 197, 200	0

The worst 5 of 60 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2315	PHE	6.3
1	C	3032	MET	4.2
1	C	3041	GLU	4.2
1	C	3042	PHE	3.7
1	E	5245	LYS	3.6

### 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 ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	CA	B	6102	1/1	0.83	15.54	114,114,114,114	0
2	CA	A	6211	1/1	0.69	6.33	125,125,125,125	0
2	CA	B	6212	1/1	0.42	5.86	125,125,125,125	0
2	CA	E	6215	1/1	0.29	3.41	125,125,125,125	0
2	CA	D	6214	1/1	0.34	3.36	125,125,125,125	0
2	CA	B	6201	1/1	0.43	2.09	133,133,133,133	0
2	CA	C	6213	1/1	0.22	0.26	125,125,125,125	0
2	CA	C	6202	1/1	0.21	-0.34	133,133,133,133	0
2	CA	D	6204	1/1	0.17	-1.14	133,133,133,133	0
2	CA	D	6203	1/1	0.14	-1.15	133,133,133,133	0
2	CA	A	6205	1/1	0.07	-2.74	133,133,133,133	0
2	CA	A	6301	1/1	0.13	-3.06	97,97,97,97	1
2	CA	A	6101	1/1	0.74	-	157,157,157,157	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.