



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 09:24 PM UTC

PDB ID : 2C9M / pdb_00002c9m
Title : Structure of (SR) Calcium-ATPase in the Ca₂E1 state solved in a P1 crystal form.
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Deposited on : 2005-12-13
Resolution : 3.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

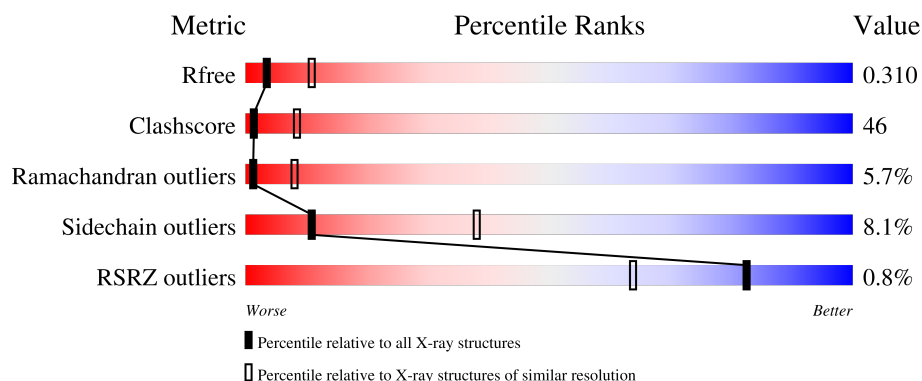
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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 $\leq 5\%$. 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	994	36% 53% 10% .
1	B	994	35% 53% 10% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15351 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 SARCOPLASMIC/ENDOPLASMIC RETICULUM CALCIUM ATPASE 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	994	Total	C	N	O	S	0	0	0
			7670	4876	1287	1450	57			
1	B	994	Total	C	N	O	S	0	0	0
			7670	4876	1287	1450	57			

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	4	Total	Ca	0	0
			4	4		
2	B	3	Total	Ca	0	0
			3	3		

- Molecule 3 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	K	0	0
			1	1		
3	B	1	Total	K	0	0
			1	1		

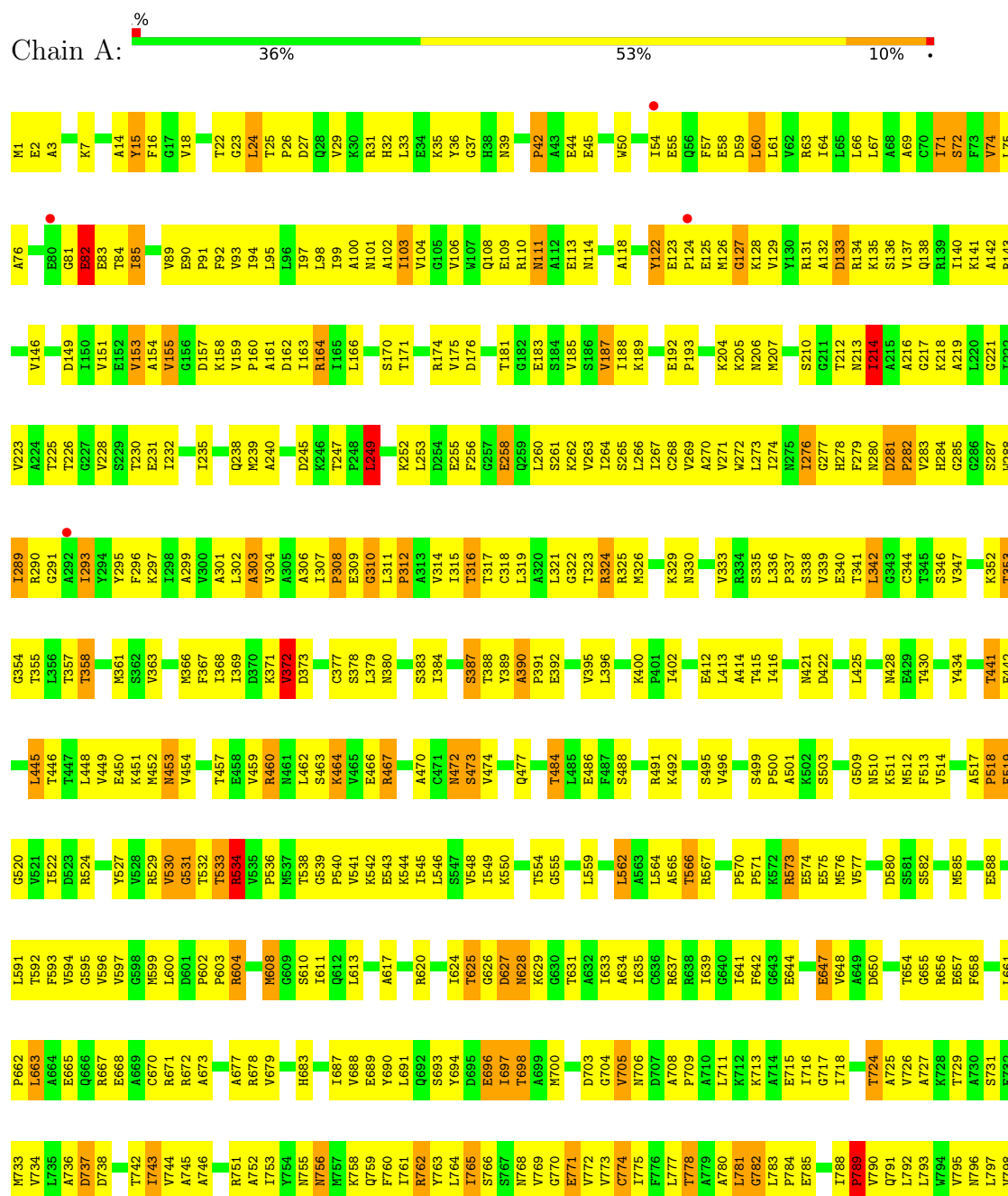
- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

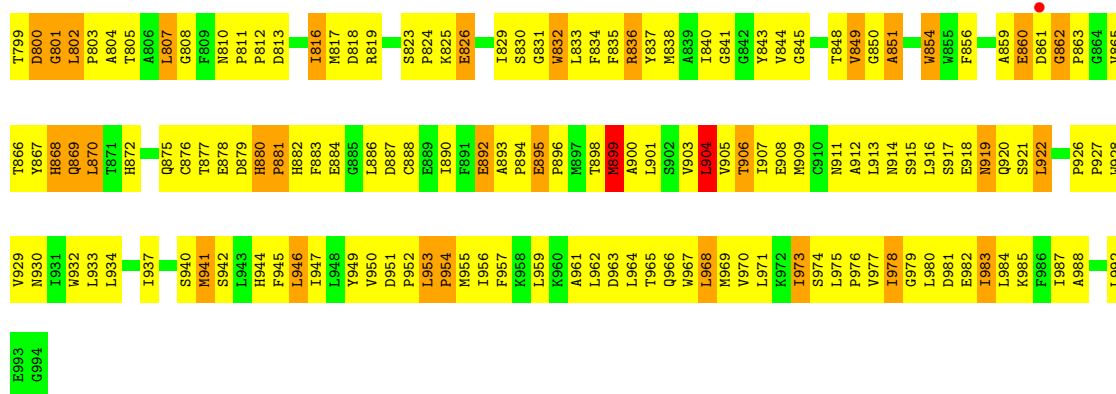
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		
4	B	1	Total	Cl	0	0
			1	1		

3 Residue-property plots

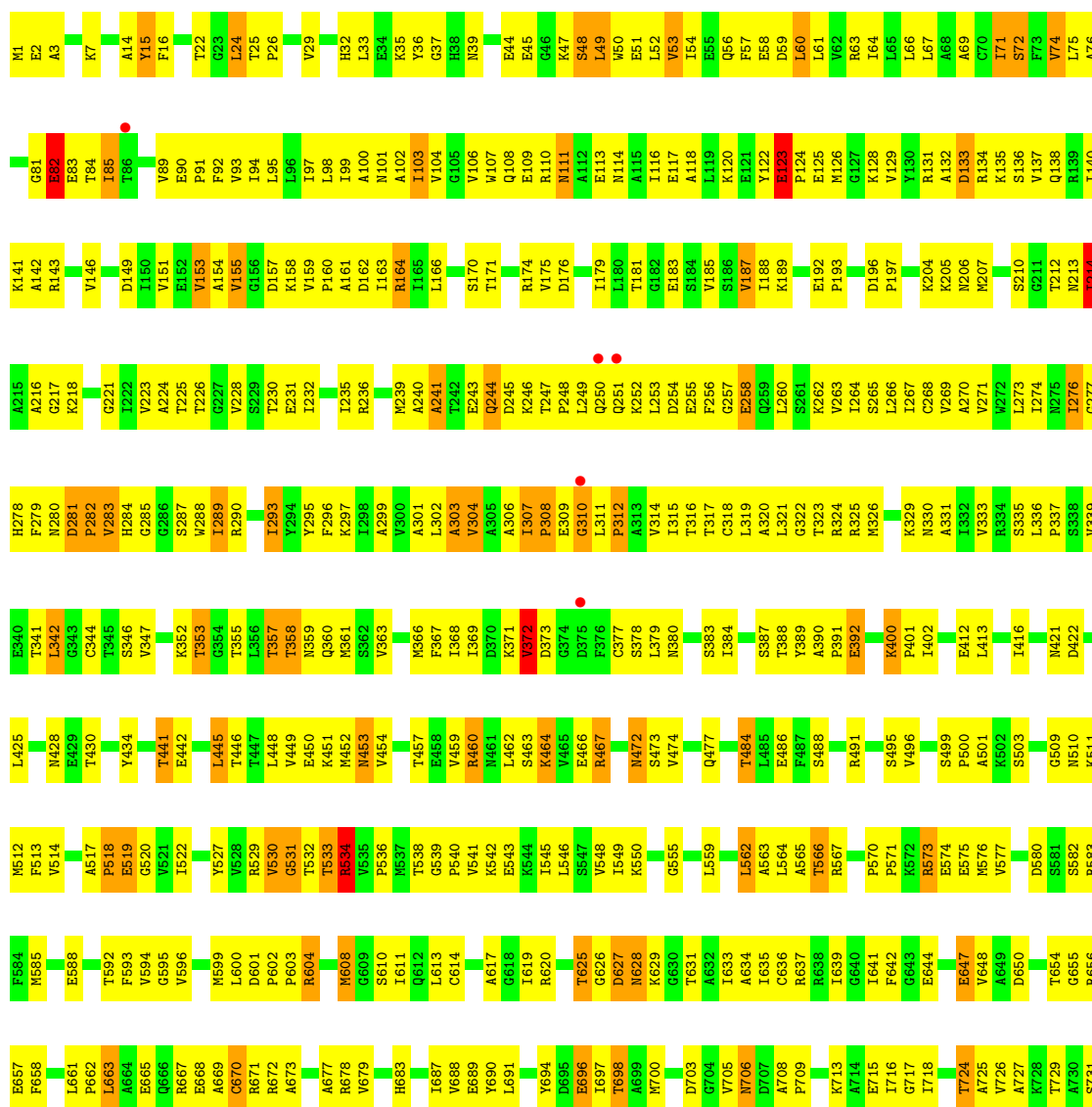
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: SARCOPLASMIC/ENDOPLASMIC RETICULUM CALCIUM ATPASE 1





● Molecule 1: SARCOPLASMIC/ENDOPLASMIC RETICULUM CALCIUM ATPASE 1



W832	T866	L792	E732
L933	Y867	L793	M733
L934	H868	M794	V734
	Q869	V795	L735
I937	L870	M796	A736
C938	T871	L797	D737
L939	H872	V798	D738
S940	F873	T799	N739
M941		D800	F740
S942	T877	G801	S741
L943		L802	T742
H944	P881		I743
F945	H882	M810	V744
L946	F883	P811	A745
F947	E884	D812	A746
L948	G885	D813	V747
Y949	L886	L814	E748
V950	D887		E749
D951	C888	M817	G750
P952	E889		R751
L953	I890	S823	A752
P954	F891		I753
M955	E892	E826	Y754
I956	A893	P827	N755
F957	P894		M756
K958	E895	S830	M757
L959	P896	G831	K758
K960	M897	W832	Q759
A961	T898	L833	F760
L962	M899	F834	I761
D963	A900	F835	R762
L964	L901	R836	Y763
T965	S902	R837	L764
Q966	V903	M838	I765
W967	L904	A839	S766
L968	V905	T840	S767
M969	T906	C841	N768
V970	I907	C842	V769
L971	E908	Y843	G770
K972	M909	W844	E771
I973	C910	G846	V772
S974	N911	A846	V773
L975	A912	A847	C774
P976	L913	T848	I775
V977	N914	W849	F776
I978	S915	G850	L777
G979	L916	A851	T778
L980	S917	A852	A779
D981	E918	A853	A780
E982	N919	W854	L781
I983	Q920	W855	G782
L984	S921	F856	L783
K985	L922	M857	F784
F986		Y858	E785
I987	P926	A859	A786
A988	P927		L787
	W928		I788
L992	V929	G862	P789
E993	V930	G863	V790
G994	I931	G864	Q791
		W865	

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	64.95Å 81.28Å 131.01Å 97.64° 99.94° 95.22°	Depositor
Resolution (Å)	15.00 – 3.00 15.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	80.4 (15.00-3.00) 79.7 (15.00-3.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.40 (at 2.99Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.266 , 0.317 0.262 , 0.310	Depositor DCC
R_{free} test set	1158 reflections (2.56%)	wwPDB-VP
Wilson B-factor (Å ²)	75.2	Xtriage
Anisotropy	0.441	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 49.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	15351	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.63% 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

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

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	0.62	0/7811	1.10	51/10592 (0.5%)
1	B	0.60	0/7811	1.08	54/10592 (0.5%)
All	All	0.61	0/15622	1.09	105/21184 (0.5%)

There are no bond length outliers.

The worst 5 of 105 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	870	LEU	N-CA-C	-9.76	100.47	112.38
1	A	922	LEU	N-CA-C	-9.54	101.64	113.18
1	A	869	GLN	N-CA-C	-9.50	102.29	112.93
1	A	159	VAL	CA-C-N	9.23	128.88	119.56
1	A	159	VAL	C-N-CA	9.23	128.88	119.56

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	7670	0	7764	684	0
1	B	7670	0	7766	725	0
2	A	4	0	0	0	0
2	B	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	1	0	0	1	0
4	B	1	0	0	0	0
All	All	15351	0	15530	1409	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 46.

The worst 5 of 1409 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:830:SER:HB3	1:B:833:LEU:HB2	1.40	1.03
1:A:372:VAL:HG13	1:A:377:CYS:HB3	1.44	0.99
1:A:263:VAL:HG12	1:A:267:ILE:HD11	1.44	0.97
1:B:941:MET:HE3	1:B:941:MET:HA	1.44	0.97
1:B:372:VAL:HG13	1:B:377:CYS:HB3	1.46	0.97

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	992/994 (100%)	785 (79%)	152 (15%)	55 (6%)	1	8
1	B	992/994 (100%)	774 (78%)	160 (16%)	58 (6%)	1	8
All	All	1984/1988 (100%)	1559 (79%)	312 (16%)	113 (6%)	1	8

5 of 113 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	85	ILE
1	A	205	LYS
1	A	283	VAL
1	A	518	PRO
1	A	519	GLU

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	840/840 (100%)	770 (92%)	70 (8%)	10	37
1	B	840/840 (100%)	774 (92%)	66 (8%)	11	39
All	All	1680/1680 (100%)	1544 (92%)	136 (8%)	11	38

5 of 136 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	706	ASN
1	B	756	ASN
1	B	907	ILE
1	A	737	ASP
1	A	724	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 41 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	472	ASN
1	B	791	GLN
1	B	477	GLN
1	B	706	ASN
1	B	882	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 11 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.

No monomer is involved in short contacts.

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	994/994 (100%)	-0.13	5 (0%) 87 72	24, 73, 138, 174	0
1	B	994/994 (100%)	-0.02	10 (1%) 79 59	24, 77, 138, 175	0
All	All	1988/1988 (100%)	-0.07	15 (0%) 82 64	24, 75, 138, 175	0

The worst 5 of 15 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	864	GLY	3.2
1	A	124	PRO	3.1
1	B	767	SER	2.8
1	A	861	ASP	2.7
1	B	86	THR	2.6

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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. The B-factors column lists the minimum, median, 95th 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	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	K	A	997	1/1	0.68	0.20	91,91,91,91	0
3	K	B	997	1/1	0.79	0.17	69,69,69,69	0
2	CA	A	998	1/1	0.86	0.08	64,64,64,64	0
2	CA	B	995	1/1	0.89	0.07	70,70,70,70	0
4	CL	B	999	1/1	0.91	0.07	40,40,40,40	0
2	CA	B	998	1/1	0.93	0.11	84,84,84,84	0
2	CA	A	999	1/1	0.94	0.10	83,83,83,83	0
2	CA	B	996	1/1	0.94	0.14	52,52,52,52	0
2	CA	A	995	1/1	0.96	0.07	49,49,49,49	0
4	CL	A	1000	1/1	0.96	0.05	56,56,56,56	0
2	CA	A	996	1/1	0.96	0.12	39,39,39,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.