



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 04:08 AM UTC

PDB ID : 4NAB / pdb_00004nab
Title : Structure of the (SR)Ca²⁺-ATPase mutant E309Q in the Ca²⁺-E1-MgAMPPCP form
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Deposited on : 2013-10-22
Resolution : 3.50 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
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

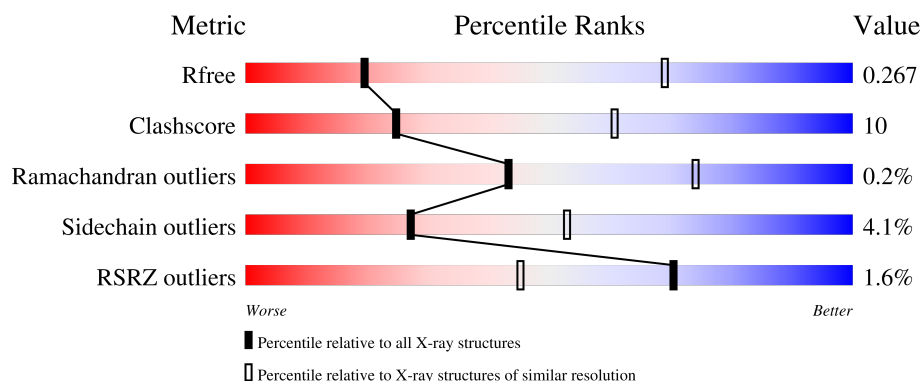
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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	1000	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6486 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	830	Total	C	N	O	S	0	0	0
			6427	4106	1067	1202	52			

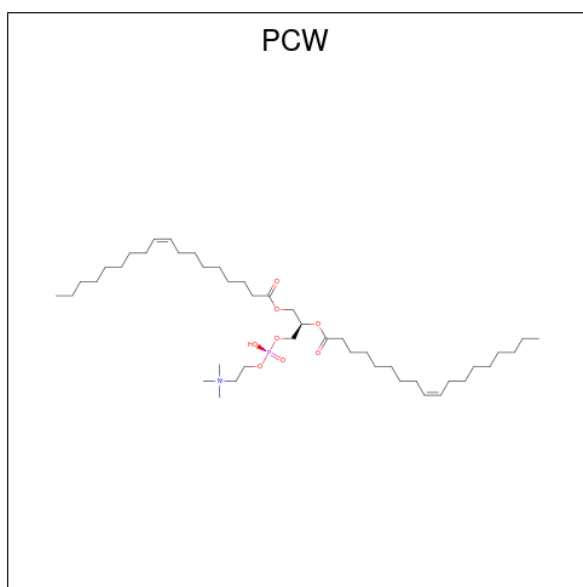
There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	309	GLN	GLU	engineered mutation	UNP P04191
A	995	GLY	-	expression tag	UNP P04191
A	996	GLY	-	expression tag	UNP P04191
A	997	LEU	-	expression tag	UNP P04191
A	998	VAL	-	expression tag	UNP P04191
A	999	PRO	-	expression tag	UNP P04191
A	1000	ARG	-	expression tag	UNP P04191

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Ca	0	0
			2	2		

- Molecule 3 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PCW) (formula: C₄₄H₈₅NO₈P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			54	44	1	8	1		

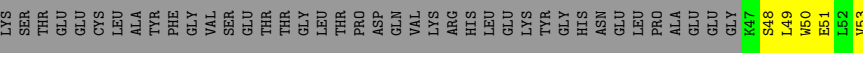
- Molecule 4 is POTASSIUM ION (CCD ID: K) (formula: K).

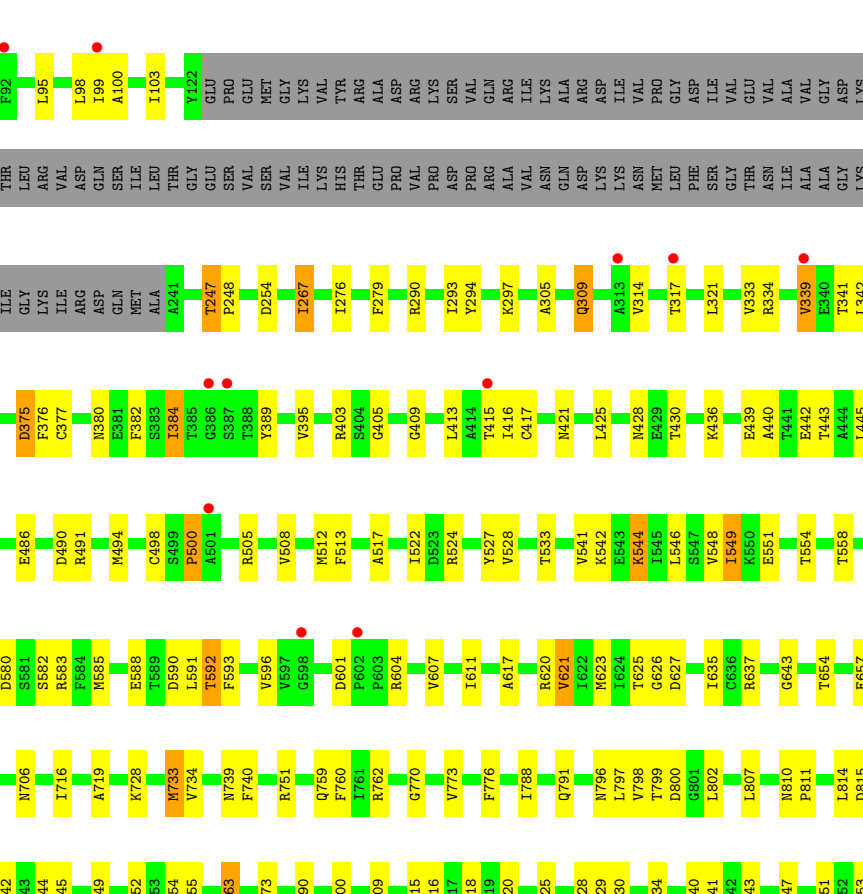
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	K	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	O	0	0
			2	2		

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.

- Chain A: 



Residue	Percentage
L971	61%
K972	61%
L973	61%
S974	61%
L975	61%
G979	61%
L980	61%
I983	61%
L987	61%
Y991	61%
G994	61%
GLY	61%
LEU	61%
VAL	61%
PRO	61%
ARG	61%
E826	61%
M838	61%
A839	61%
I840	61%
G841	61%
G842	61%
H843	61%
V844	61%
G845	61%
V849	61%
A852	61%
A853	61%
H854	61%
H855	61%
P863	61%
F873	61%
I880	61%
A900	61%
M909	61%
S915	61%
L916	61%
S917	61%
E918	61%
N919	61%
Q920	61%
M925	61%
W928	61%
V929	61%
N930	61%
L934	61%
S940	61%
M941	61%
L943	61%
I947	61%
D951	61%
P952	61%
L953	61%
K958	61%
Q966	61%
M969	61%
G970	61%
W976	61%
P671	61%
S672	61%
A677	61%
E680	61%
P681	61%
N706	61%
V716	61%
A719	61%
K728	61%
M733	61%
V734	61%
N739	61%
F740	61%
R751	61%
Q759	61%
F760	61%
R762	61%
G770	61%
V773	61%
F776	61%
I788	61%
Q791	61%
N796	61%
L797	61%
V798	61%
T799	61%
D800	61%
G801	61%
L802	61%
L807	61%
N810	61%
P811	61%
L814	61%
D815	61%
I816	61%
D817	61%
R819	61%
S823	61%
D568	61%
T569	61%
P570	61%
V577	61%
D580	61%
S581	61%
S582	61%
R583	61%
F584	61%
M585	61%
E588	61%
T589	61%
D590	61%
L591	61%
T592	61%
F593	61%
V596	61%
V597	61%
G598	61%
D601	61%
P602	61%
R603	61%
R604	61%
V607	61%
I611	61%
A617	61%
R620	61%
V621	61%
L622	61%
M623	61%
I624	61%
T625	61%
G626	61%
D627	61%
I635	61%
G636	61%
R637	61%
G643	61%
T654	61%
E657	61%
I658	61%
Q666	61%
A669	61%
P671	61%
S366	61%
F367	61%
I369	61%
D370	61%
D375	61%
F376	61%
C377	61%
N380	61%
E381	61%
F382	61%
S383	61%
I384	61%
T385	61%
G386	61%
S387	61%
Y389	61%
V395	61%
R403	61%
S404	61%
G405	61%
G409	61%
L413	61%
A414	61%
T415	61%
C417	61%
T533	61%
N421	61%
L425	61%
E543	61%
K544	61%
I545	61%
L546	61%
S547	61%
V548	61%
K550	61%
E551	61%
T554	61%
T558	61%
E567	61%
F568	61%
Q569	61%
A569	61%
L569	61%
L562	61%
C561	61%
T446	61%
L448	61%
N452	61%
L462	61%
T463	61%
V464	61%
T355	61%

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	167.01Å 55.79Å 161.79Å 90.00° 109.29° 90.00°	Depositor
Resolution (Å)	67.01 – 3.50 67.01 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (67.01-3.50) 99.9 (67.01-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.71 (at 3.49Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.216 , 0.266 0.229 , 0.267	Depositor DCC
R_{free} test set	920 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	122.1	Xtriage
Anisotropy	0.397	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 83.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6486	wwPDB-VP
Average B, all atoms (Å ²)	113.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.28% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.29	0/6550	0.74	4/8886 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	517	ALA	CA-C-N	6.38	127.81	119.84
1	A	517	ALA	C-N-CA	6.38	127.81	119.84
1	A	925	MET	CA-C-N	5.35	125.89	120.38
1	A	925	MET	C-N-CA	5.35	125.89	120.38

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	6427	0	6494	127	0
2	A	2	0	0	0	0
3	A	54	0	84	5	0
4	A	1	0	0	0	0
5	A	2	0	0	1	0
All	All	6486	0	6578	128	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 10.

The worst 5 of 128 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:A:681:PRO:HB3	1:A:706:ASN:HB3	1.70	0.74
1:A:528:VAL:HG21	1:A:541:VAL:HG11	1.71	0.73
1:A:486:GLU:O	1:A:491:ARG:NH2	2.23	0.71
1:A:770:GLY:HA3	1:A:844:VAL:HG23	1.74	0.69
1:A:512:MET:HB3	1:A:567:ARG:HB3	1.74	0.69

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	826/1000 (83%)	782 (95%)	42 (5%)	2 (0%)	43 74

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	863	PRO
1	A	500	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	703/844 (83%)	674 (96%)	29 (4%)	27 53

5 of 29 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	544	LYS
1	A	951	ASP
1	A	568	ASP
1	A	849	VAL
1	A	566	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	882	HIS
1	A	920	GLN
1	A	966	GLN
1	A	421	ASN
1	A	398	ASN

5.3.3 RNA ⓘ

There are no RNA molecules 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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	PCW	A	1103	-	53,53,53	0.99	1 (1%)	59,61,61	0.67	2 (3%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PCW	A	1103	-	-	35/57/57/57	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1103	PCW	O4P-C4	-2.51	1.34	1.44

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1103	PCW	C2-O2-C31	2.48	123.73	117.80
3	A	1103	PCW	O3-C11-O11	-2.08	118.43	123.63

There are no chirality outliers.

5 of 35 torsion outliers are listed below:

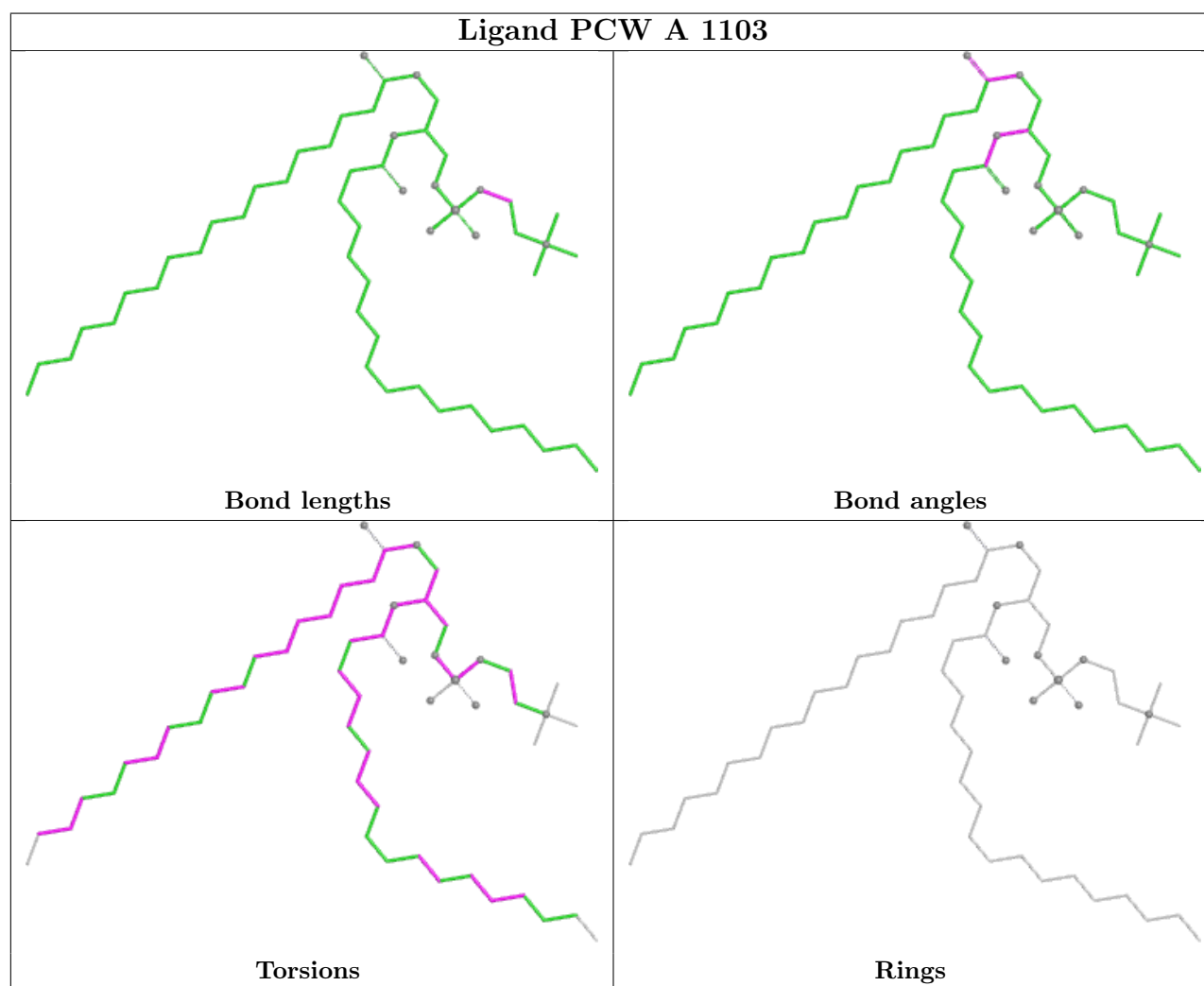
Mol	Chain	Res	Type	Atoms
3	A	1103	PCW	C1-O3P-P-O1P
3	A	1103	PCW	C1-O3P-P-O4P
3	A	1103	PCW	C4-O4P-P-O1P
3	A	1103	PCW	C4-O4P-P-O2P
3	A	1103	PCW	C4-O4P-P-O3P

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1103	PCW	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

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 [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	830/1000 (83%)	-0.16	13 (1%)	70 45	46, 104, 185, 277	0

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	602	PRO	4.3
1	A	339	VAL	3.6
1	A	561	CYS	3.0
1	A	598	GLY	2.8
1	A	360	GLN	2.7

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.

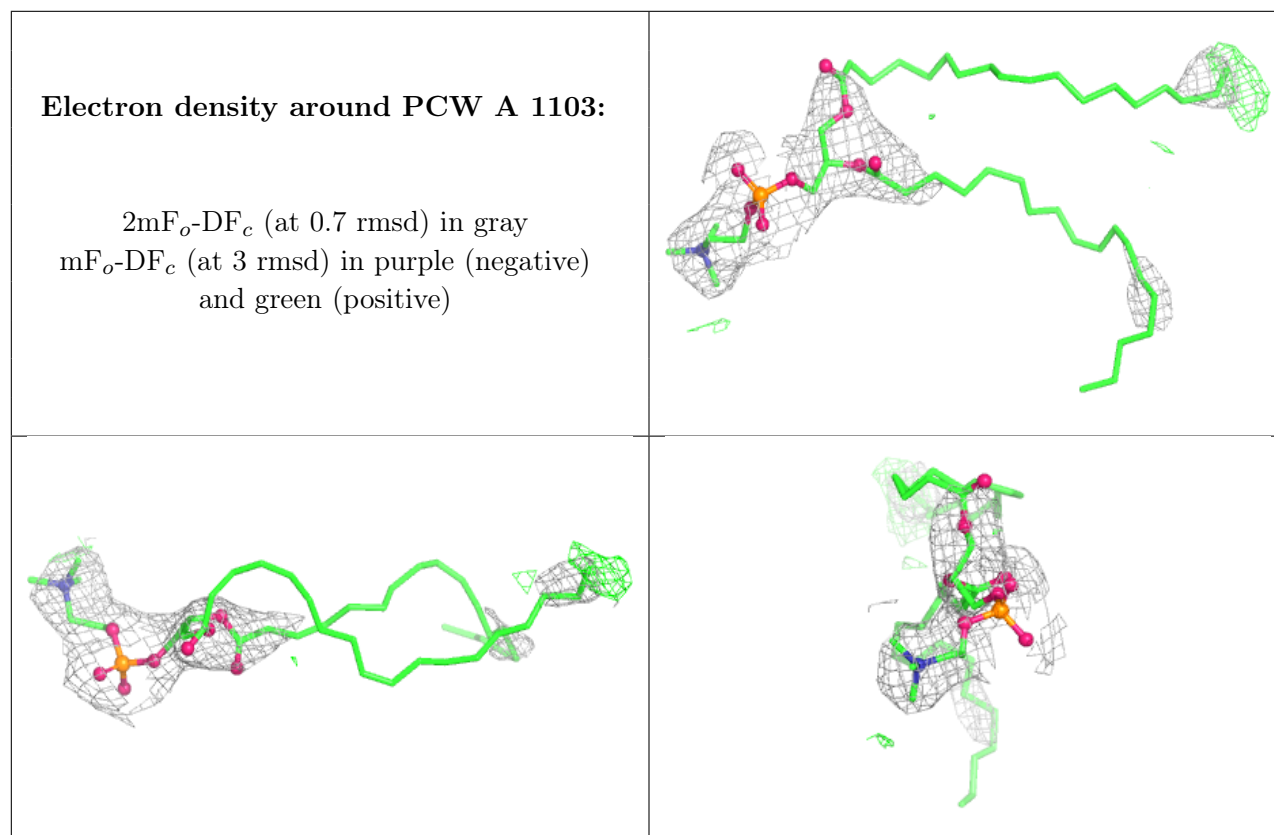
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q < 0.9
3	PCW	A	1103	54/54	0.88	0.22	54,101,131,135	0
4	K	A	1104	1/1	0.95	0.06	149,149,149,149	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CA	A	1102	1/1	0.98	0.07	50,50,50,50	0
2	CA	A	1101	1/1	0.99	0.04	69,69,69,69	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.