



wwPDB X-ray Structure Validation Summary Report i

Feb 26, 2014 – 02:52 PM GMT

PDB ID : 3FGO
Title : Crystal Structure of the E2 magnesium fluoride complex of the (SR) Ca²⁺-ATPase with bound CPA and AMPPCP
Authors : Laursen, M.; Bublitz, M.; Moncoq, K.; Olesen, C.; Moller, J.V.; Young, H.S.; Nissen, P.; Morth, J.P.
Deposited on : 2008-12-08
Resolution : 2.50 Å(reported)

This is a wwPDB validation summary 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>

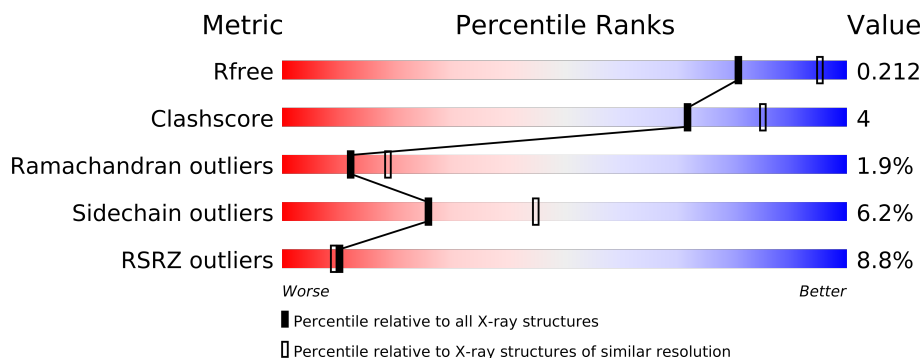
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.50 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}	66092	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (2.50-2.50)

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 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	A	994	
1	B	994	

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	MG	A	1002	-	X
2	MG	B	1002	-	X
3	MF4	A	1003	-	X
6	MN	A	1008	-	X
7	ACP	B	1007	-	X
8	ACT	A	3001	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
8	ACT	A	3002	-	X
8	ACT	B	3001	-	X
8	ACT	B	3002	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 15950 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 Sarcoplasmic/endoplasmicreticulum 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			

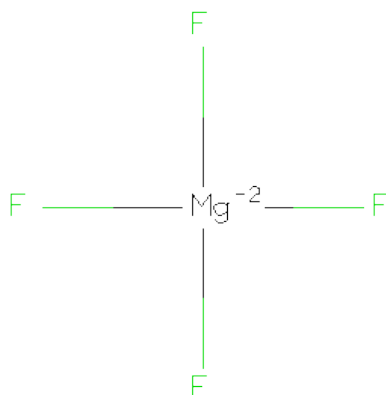
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	994	GLY	ASP	SEE REMARK 999	UNP P04191
B	994	GLY	ASP	SEE REMARK 999	UNP P04191

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is TETRAFLUOROMAGNESATE(2-) (three-letter code: MF4) (formula: F₄Mg).

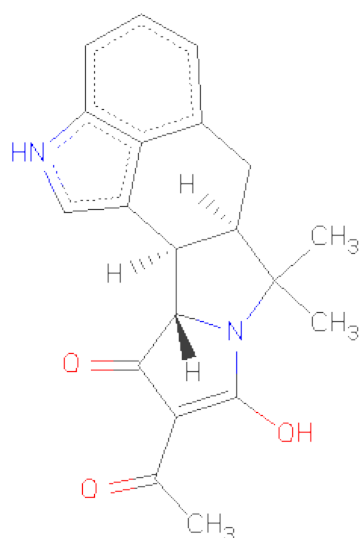


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	F	Mg	0	0
			5	4	1		
3	B	1	Total	F	Mg	0	0
			5	4	1		

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

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

- Molecule 5 is (6AR,11AS,11BR)-10-ACETYL-9-HYDROXY-7,7-DIMETHYL-2,6,6A,7,11A,11B-HEXAHYDRO-11H-PYRROLO[1',2':2,3]ISOINDOLO[4,5,6-CD]INDOL-11-ONE (three-letter code: CZA) (formula: C₂₀H₂₀N₂O₃).

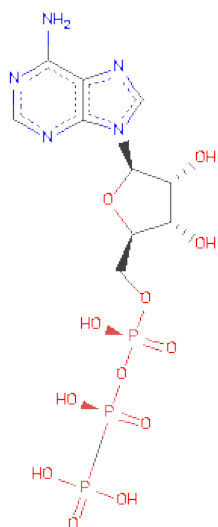


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			25	20	2	3		
5	B	1	Total	C	N	O	0	0
			25	20	2	3		

- Molecule 6 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

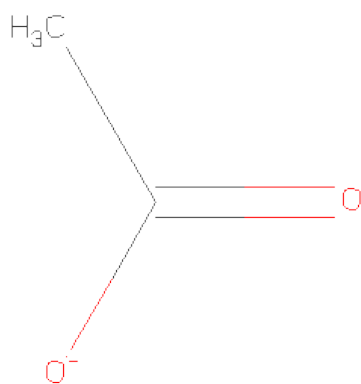
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Mn	0	0
			1	1		
6	A	2	Total	Mn	0	0
			2	2		

- Molecule 7 is PHOSPHOMETHYLPHOSPHONICACID ADENYLATE ESTER (three-letter code: ACP) (formula: C₁₁H₁₈N₅O₁₂P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	P	0	0
			31	11	5	12	3		
7	B	1	Total	C	N	O	P	0	0
			31	11	5	12	3		

- Molecule 8 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			4	2	2		
8	A	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			4	2	2		
8	B	1	Total	C	O	0	0
			4	2	2		

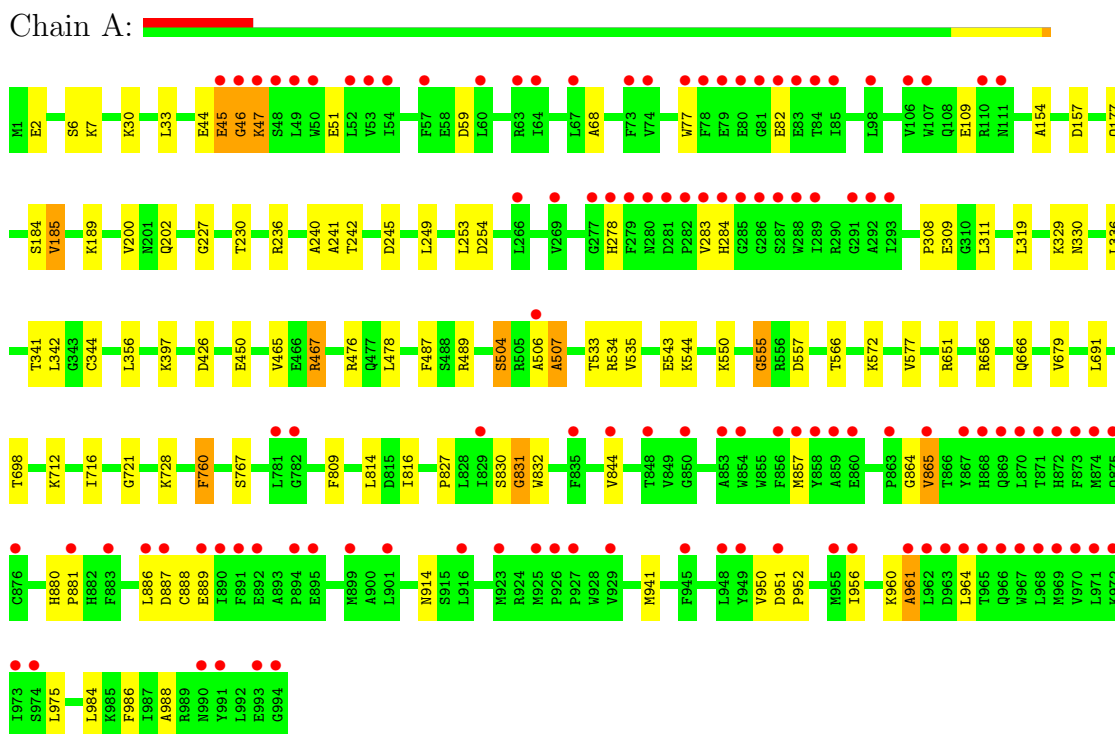
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	263	Total	O	0	0
			263	263		
9	B	202	Total	O	0	0
			202	202		

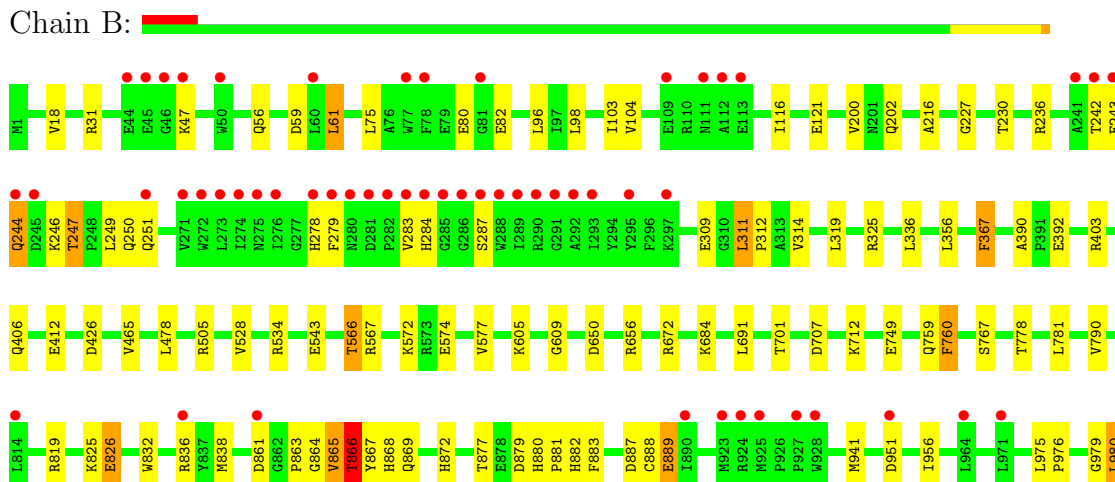
3 Residue-property plots

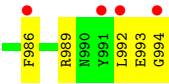
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ($\text{RSRZ} > 2$). 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/endoplasmicreticulum calcium ATPase 1



- Molecule 1: Sarcoplasmic/endoplasmicreticulum calcium ATPase 1





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	101.43Å 108.87Å 274.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.93 – 2.50 45.97 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.6 (24.93-2.50) 97.6 (45.97-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.60 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.174 , 0.217 0.169 , 0.212	Depositor DCC
R_{free} test set	3074 reflections (2.98%)	DCC
Wilson B-factor (Å ²)	52.0	Xtriage
Anisotropy	0.216	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 53.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 103184 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	15950	wwPDB-VP
Average B, all atoms (Å ²)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.34% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, K, MN, ACP, MF4, ACT, CZA

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	0.50	0/7811	0.64	3/10592 (0.0%)
1	B	0.49	0/7811	0.64	1/10592 (0.0%)
All	All	0.50	0/15622	0.64	4/21184 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

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	B	567	ARG	NE-CZ-NH2	-6.60	117.00	120.30
1	A	467	ARG	NE-CZ-NH1	-6.45	117.08	120.30
1	A	476	ARG	NE-CZ-NH1	-5.62	117.49	120.30
1	A	476	ARG	CG-CD-NE	-5.32	100.62	111.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	555	GLY	Peptide

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	7670	0	0	29	0
1	B	7670	0	0	40	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	25	0	20	1	0
5	B	25	0	20	2	0
6	A	2	0	0	0	0
6	B	1	0	0	0	0
7	A	31	0	14	2	0
7	B	31	0	14	0	0
8	A	8	0	6	2	0
8	B	8	0	6	3	0
9	A	263	0	0	4	0
9	B	202	0	0	2	0
All	All	15950	0	80	69	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.

The worst 5 of 69 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:227:GLY:O	8:A:3002:ACT:H3	1.92	0.69
1:B:672:ARG:NH1	9:B:1199:HOH:O	2.32	0.61
1:B:574:GLU:N	1:B:574:GLU:OE2	2.34	0.60
1:B:869:GLN:NE2	1:B:882:HIS:O	2.34	0.60
1:A:450:GLU:OE2	1:A:467:ARG:NH1	2.37	0.57

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	A	992/994 (100%)	892 (90%)	77 (8%)	23 (2%)	10	14
1	B	992/994 (100%)	898 (90%)	80 (8%)	14 (1%)	16	27
All	All	1984/1988 (100%)	1790 (90%)	157 (8%)	37 (2%)	12	19

5 of 37 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	45	GLU
1	A	82	GLU
1	A	504	SER
1	A	507	ALA
1	A	961	ALA

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%)	786 (94%)	54 (6%)	25	43
1	B	840/840 (100%)	790 (94%)	50 (6%)	27	47
All	All	1680/1680 (100%)	1576 (94%)	104 (6%)	26	45

5 of 104 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	886	LEU
1	B	75	LEU
1	B	861	ASP
1	A	914	ASN

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Mol	Chain	Res	Type
1	A	975	LEU

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 ⓘ

Of 17 ligands modelled in this entry, 7 are monoatomic - leaving 10 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	MF4	A	1003	1	0,4,4	0.00	-	0,6,6	0.00	-
5	CZA	A	1005	6	29,29,29	1.46	5 (17%)	47,48,48	2.63	10 (21%)
7	ACP	A	1007	-	33,33,33	3.92	9 (27%)	52,52,52	2.65	10 (19%)
8	ACT	A	3001	-	1,3,3	3.11	1 (100%)	0,3,3	0.00	-
8	ACT	A	3002	-	1,3,3	1.66	0	0,3,3	0.00	-
3	MF4	B	1003	1	0,4,4	0.00	-	0,6,6	0.00	-
5	CZA	B	1005	6	29,29,29	1.47	6 (20%)	47,48,48	2.53	9 (19%)
7	ACP	B	1007	-	33,33,33	4.16	8 (24%)	52,52,52	2.37	13 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	ACT	B	3001	-	1,3,3	2.74	1 (100%)	0,3,3	0.00	-
8	ACT	B	3002	-	1,3,3	1.86	0	0,3,3	0.00	-

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	MF4	A	1003	1	-	0/0/0/0	0/0/0/0
5	CZA	A	1005	6	-	0/4/52/52	0/0/5/5
7	ACP	A	1007	-	-	0/20/38/38	0/1/3/3
8	ACT	A	3001	-	-	0/0/0/0	0/0/0/0
8	ACT	A	3002	-	-	0/0/0/0	0/0/0/0
3	MF4	B	1003	1	-	0/0/0/0	0/0/0/0
5	CZA	B	1005	6	-	0/4/52/52	0/0/5/5
7	ACP	B	1007	-	-	0/20/38/38	0/1/3/3
8	ACT	B	3001	-	-	0/0/0/0	0/0/0/0
8	ACT	B	3002	-	-	0/0/0/0	0/0/0/0

The worst 5 of 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	1007	ACP	PG-C3B	-16.93	1.65	1.79
7	A	1007	ACP	PG-C3B	-16.65	1.65	1.79
7	B	1007	ACP	PB-C3B	-13.04	1.68	1.79
7	A	1007	ACP	PB-C3B	-11.33	1.70	1.79
7	B	1007	ACP	C8-N9	5.02	1.44	1.36

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1005	CZA	C7-C15-C14	-11.45	118.76	124.56
5	A	1005	CZA	C7-C15-C14	-11.29	118.84	124.56
7	A	1007	ACP	PB-C3B-PG	11.19	133.72	117.62
7	B	1007	ACP	PB-C3B-PG	8.42	129.73	117.62
7	B	1007	ACP	PA-O3A-PB	7.94	155.60	131.74

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, 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%)	0.40	117 (11%) 5 5	27, 62, 204, 387	0
1	B	994/994 (100%)	0.14	59 (5%) 22 22	31, 66, 161, 261	0
All	All	1988/1988 (100%)	0.27	176 (8%) 10 9	27, 64, 186, 387	0

The worst 5 of 176 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	283	VAL	14.8
1	A	284	HIS	10.9
1	A	891	PHE	10.5
1	A	280	ASN	10.3
1	B	288	TRP	9.2

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, 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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
8	ACT	B	3001	4/4	0.28	12.11	50,68,69,75	0
6	MN	A	1008	1/1	0.24	6.83	149,149,149,149	1
7	ACP	B	1007	31/31	0.23	3.96	33,75,151,385	31
2	MG	B	1002	1/1	0.25	3.42	36,36,36,36	0
8	ACT	A	3002	4/4	0.18	2.97	38,52,53,58	0
3	MF4	A	1003	5/5	0.25	2.94	33,40,42,47	0
2	MG	A	1002	1/1	0.22	2.37	36,36,36,36	0
8	ACT	B	3002	4/4	0.17	2.05	55,57,60,61	0
8	ACT	A	3001	4/4	0.17	2.04	52,64,64,71	0
3	MF4	B	1003	5/5	0.21	1.76	33,33,36,52	0
4	K	B	1004	1/1	0.22	1.57	95,95,95,95	0
7	ACP	A	1007	31/31	0.18	1.50	38,59,118,420	31
4	K	A	1004	1/1	0.18	0.90	87,87,87,87	0
6	MN	B	1006	1/1	0.14	0.54	96,96,96,96	0
5	CZA	B	1005	25/25	0.14	-0.47	74,86,99,101	0
5	CZA	A	1005	25/25	0.14	-0.55	110,122,127,177	0
6	MN	A	1006	1/1	0.08	-1.79	103,103,103,103	0

6.5 Other polymers ⓘ

There are no such residues in this entry.