



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 12:27 pm GMT

PDB ID : 1RJ
Title : Structure of PPM1, a leucine carboxy methyltransferase involved in the regulation of protein phosphatase 2A activity
Authors : Leulliot, N.; Quevillon-Cheruel, S.; Sorel, I.; Li de La Sierra-Gallay, I.; Collinet, B.; Graille, M.; Blondeau, K.; Bettache, N.; Poupon, A.; Janin, J.; van Tilbeurgh, H.
Deposited on : 2003-11-19
Resolution : 1.80 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

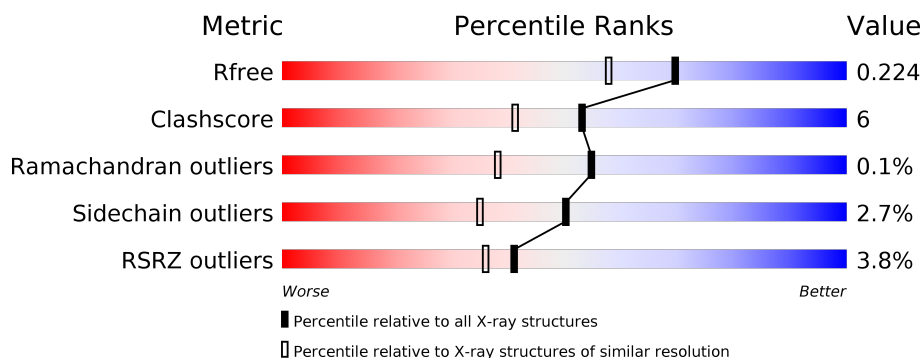
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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}	100719	4827 (1.80-1.80)
Clashscore	112137	5742 (1.80-1.80)
Ramachandran outliers	110173	5676 (1.80-1.80)
Sidechain outliers	110143	5675 (1.80-1.80)
RSRZ outliers	101464	4906 (1.80-1.80)

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. 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	334	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 98%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 2px;"> % 87% 10% .. </div> </div>
1	B	334	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 4%, orange 1%, yellow 1%, green 94%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 2px;"> 4% 87% 11% .. </div> </div>
1	C	334	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 5%, orange 1%, yellow 1%, green 93%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 2px;"> 5% 87% 11% . </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	BME	A	804	-	-	-	X
4	BME	A	807	-	-	-	X
4	BME	B	805	-	-	-	X
4	BME	B	808	-	-	-	X
4	BME	C	806	-	-	-	X
4	BME	C	809	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8873 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 carboxy methyl transferase for protein phosphatase 2A catalytic subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	328	Total	C	N	O	S	0	0	0
			2644	1681	451	494	18			
1	B	329	Total	C	N	O	S	0	1	0
			2660	1690	454	498	18			
1	C	333	Total	C	N	O	S	0	0	0
			2694	1711	466	499	18			

There are 18 discrepancies between the modelled and reference sequences:

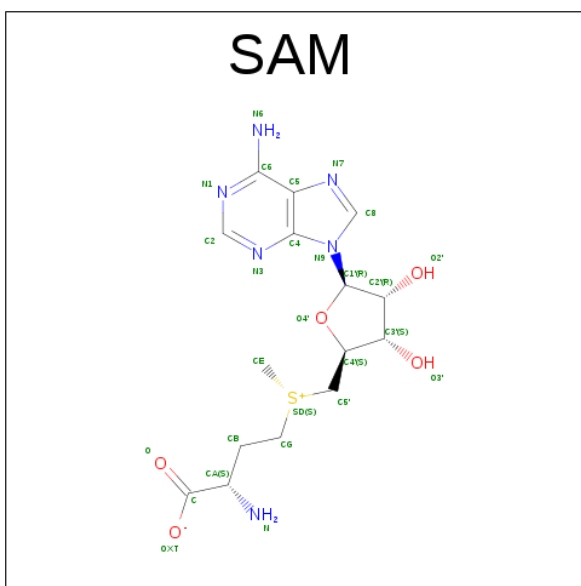
Chain	Residue	Modelled	Actual	Comment	Reference
A	329	HIS	-	EXPRESSION TAG	UNP Q04081
A	330	HIS	-	EXPRESSION TAG	UNP Q04081
A	331	HIS	-	EXPRESSION TAG	UNP Q04081
A	332	HIS	-	EXPRESSION TAG	UNP Q04081
A	333	HIS	-	EXPRESSION TAG	UNP Q04081
A	334	HIS	-	EXPRESSION TAG	UNP Q04081
B	329	HIS	-	EXPRESSION TAG	UNP Q04081
B	330	HIS	-	EXPRESSION TAG	UNP Q04081
B	331	HIS	-	EXPRESSION TAG	UNP Q04081
B	332	HIS	-	EXPRESSION TAG	UNP Q04081
B	333	HIS	-	EXPRESSION TAG	UNP Q04081
B	334	HIS	-	EXPRESSION TAG	UNP Q04081
C	329	HIS	-	EXPRESSION TAG	UNP Q04081
C	330	HIS	-	EXPRESSION TAG	UNP Q04081
C	331	HIS	-	EXPRESSION TAG	UNP Q04081
C	332	HIS	-	EXPRESSION TAG	UNP Q04081
C	333	HIS	-	EXPRESSION TAG	UNP Q04081
C	334	HIS	-	EXPRESSION TAG	UNP Q04081

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



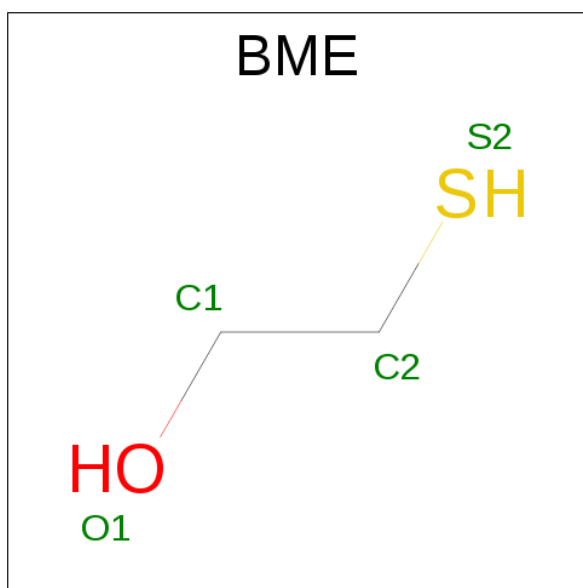
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is S-ADENOSYLMETHIONINE (three-letter code: SAM) (formula: $C_{15}H_{22}N_6O_5S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
3	B	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
3	C	1	Total	C	N	O	S	0	0
			27	15	6	5	1		

- Molecule 4 is BETA-MERCAPTOETHANOL (three-letter code: BME) (formula: C_2H_6OS).



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

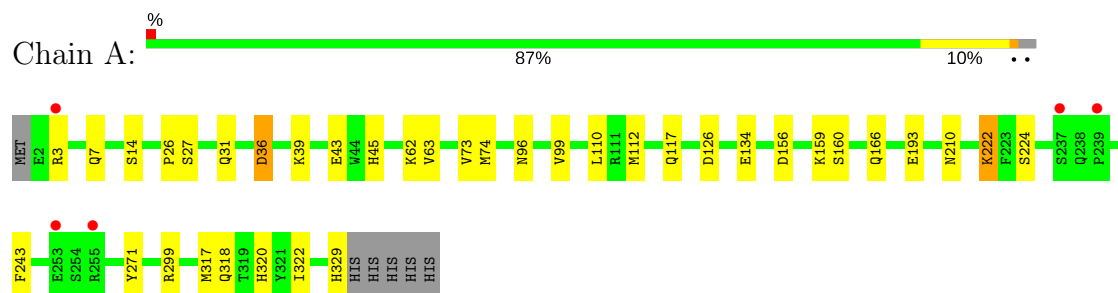
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	298	Total	O	0	0
			298	298		
5	B	247	Total	O	0	0
			247	247		
5	C	220	Total	O	0	0
			220	220		

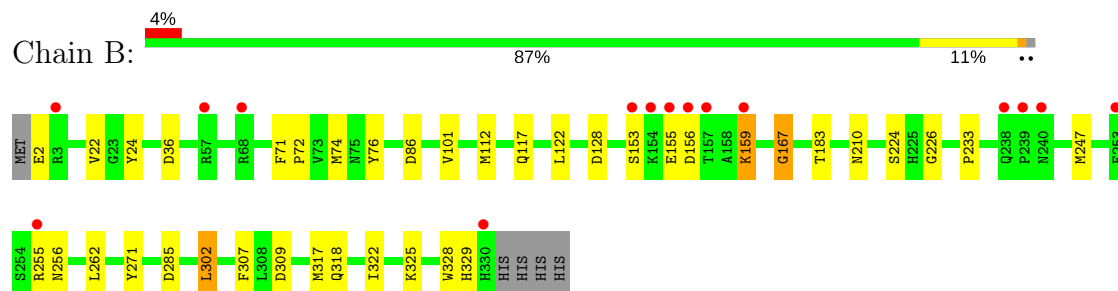
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

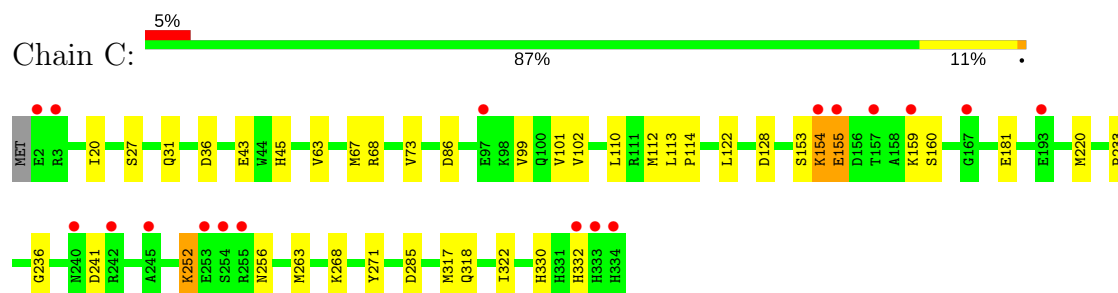
- Molecule 1: carboxy methyl transferase for protein phosphatase 2A catalytic subunit



- Molecule 1: carboxy methyl transferase for protein phosphatase 2A catalytic subunit



- Molecule 1: carboxy methyl transferase for protein phosphatase 2A catalytic subunit



4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	110.68Å 110.68Å 165.88Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	52.70 – 1.80 52.50 – 1.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (52.70-1.80) 100.0 (52.50-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.30 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.178 , 0.215 0.190 , 0.224	Depositor DCC
R_{free} test set	5424 reflections (5.38%)	DCC
Wilson B-factor (Å ²)	12.8	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 27.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.239 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8873	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.95% 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: SO4, SAM, BME

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	0.61	0/2694	0.77	3/3639 (0.1%)
1	B	0.60	0/2714	0.77	3/3666 (0.1%)
1	C	0.55	0/2749	0.75	4/3714 (0.1%)
All	All	0.59	0/8157	0.76	10/11019 (0.1%)

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	285	ASP	CB-CG-OD2	6.54	124.18	118.30
1	C	285	ASP	CB-CG-OD2	6.33	124.00	118.30
1	A	36	ASP	CB-CG-OD2	6.14	123.83	118.30
1	A	126	ASP	CB-CG-OD1	6.04	123.73	118.30
1	A	156	ASP	CB-CG-OD2	5.63	123.37	118.30

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	2644	0	2670	40	0
1	B	2660	0	2680	31	0
1	C	2694	0	2705	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	5	0	0	1	0
3	A	27	0	22	0	0
3	B	27	0	22	0	0
3	C	27	0	22	0	0
4	A	8	0	10	0	0
4	B	8	0	10	1	0
4	C	8	0	10	1	0
5	A	298	0	0	15	0
5	B	247	0	0	9	1
5	C	220	0	0	12	0
All	All	8873	0	8151	101	1

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 6.

The worst 5 of 101 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:159:LYS:O	5:B:1008:HOH:O	1.69	1.09
1:A:73:VAL:CG2	5:A:977:HOH:O	2.09	0.99
1:A:317:MET:HE2	1:A:318:GLN:HE21	1.35	0.90
1:A:73:VAL:HG12	1:A:317:MET:HE1	1.52	0.89
1:A:317:MET:CE	1:A:318:GLN:HE21	1.87	0.86

All (1) 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	Interatomic distance (Å)	Clash overlap (Å)
5:B:1035:HOH:O	5:B:1037:HOH:O[6_664]	2.16	0.04

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	326/334 (98%)	320 (98%)	6 (2%)	0	100	100
1	B	328/334 (98%)	322 (98%)	5 (2%)	1 (0%)	44	29
1	C	331/334 (99%)	324 (98%)	7 (2%)	0	100	100
All	All	985/1002 (98%)	966 (98%)	18 (2%)	1 (0%)	55	38

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	167	GLY

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	297/303 (98%)	290 (98%)	7 (2%)	54	40
1	B	299/303 (99%)	291 (97%)	8 (3%)	50	35
1	C	302/303 (100%)	293 (97%)	9 (3%)	46	30
All	All	898/909 (99%)	874 (97%)	24 (3%)	50	35

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	210	ASN
1	B	302	LEU
1	C	252	LYS
1	B	255	ARG
1	B	256	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	210	ASN
1	B	318	GLN

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Mol	Chain	Res	Type
1	C	329	HIS
1	B	225	HIS
1	A	166	GLN

5.3.3 RNA [i](#)

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

10 ligands are modelled in this entry.

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	SAM	A	801	-	21,29,29	1.02	2 (9%)	17,42,42	2.70	2 (11%)
4	BME	A	804	1	3,3,3	0.26	0	2,2,2	1.54	1 (50%)
4	BME	A	807	1	3,3,3	0.35	0	2,2,2	0.45	0
3	SAM	B	802	-	21,29,29	1.08	2 (9%)	17,42,42	2.71	3 (17%)
4	BME	B	805	1	3,3,3	0.16	0	2,2,2	1.03	0
4	BME	B	808	1	3,3,3	0.28	0	2,2,2	0.08	0
2	SO4	C	335	-	4,4,4	0.28	0	6,6,6	0.23	0
3	SAM	C	803	-	21,29,29	1.15	2 (9%)	17,42,42	2.67	1 (5%)
4	BME	C	806	1	3,3,3	0.43	0	2,2,2	0.83	0
4	BME	C	809	-	3,3,3	0.39	0	2,2,2	0.30	0

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	SAM	A	801	-	-	0/8/33/33	0/3/3/3
4	BME	A	804	1	-	0/1/1/1	0/0/0/0
4	BME	A	807	1	-	0/1/1/1	0/0/0/0
3	SAM	B	802	-	-	0/8/33/33	0/3/3/3
4	BME	B	805	1	-	0/1/1/1	0/0/0/0
4	BME	B	808	1	-	0/1/1/1	0/0/0/0
2	SO4	C	335	-	-	0/0/0/0	0/0/0/0
3	SAM	C	803	-	-	0/8/33/33	0/3/3/3
4	BME	C	806	1	-	0/1/1/1	0/0/0/0
4	BME	C	809	-	-	0/1/1/1	0/0/0/0

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	802	SAM	C2-N1	2.12	1.37	1.33
3	A	801	SAM	C2-N1	2.71	1.39	1.33
3	C	803	SAM	C2-N1	2.84	1.39	1.33
3	A	801	SAM	C2-N3	3.01	1.37	1.32
3	C	803	SAM	C2-N3	3.21	1.37	1.32

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	801	SAM	N3-C2-N1	-10.42	119.78	128.86
3	C	803	SAM	N3-C2-N1	-10.34	119.85	128.86
3	B	802	SAM	N3-C2-N1	-10.09	120.07	128.86
3	B	802	SAM	C4-C5-N7	-2.83	106.68	109.41
3	B	802	SAM	C4'-O4'-C1'	-2.33	107.28	109.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	805	BME	1	0
2	C	335	SO4	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	806	BME	1	0

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	328/334 (98%)	-0.31	5 (1%) 74 70	5, 10, 26, 39	0
1	B	329/334 (98%)	-0.19	15 (4%) 33 28	5, 11, 32, 43	0
1	C	333/334 (99%)	-0.03	18 (5%) 26 22	9, 17, 39, 50	0
All	All	990/1002 (98%)	-0.18	38 (3%) 41 36	5, 13, 33, 50	0

The worst 5 of 38 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	239	PRO	5.4
1	B	155	GLU	4.2
1	C	240	ASN	4.1
1	C	334	HIS	4.1
1	B	156	ASP	4.0

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 carbohydrates 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. 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	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	BME	B	805	4/4	0.94	0.13	19.13	13,18,20,26	0
4	BME	A	807	4/4	0.96	0.33	6.50	29,31,32,34	0
4	BME	A	804	4/4	0.94	0.15	6.22	13,20,20,28	0
4	BME	C	806	4/4	0.97	0.17	5.50	24,30,32,36	0
4	BME	C	809	4/4	0.80	0.23	3.98	39,40,40,42	0
4	BME	B	808	4/4	0.91	0.21	2.52	35,37,37,38	0
3	SAM	A	801	27/27	0.98	0.08	-0.17	4,6,7,10	0
3	SAM	C	803	27/27	0.97	0.08	-0.18	8,12,14,17	0
2	SO4	C	335	5/5	0.96	0.15	-0.22	22,23,23,24	0
3	SAM	B	802	27/27	0.99	0.06	-0.81	5,7,8,10	0

6.5 Other polymers [i](#)

There are no such residues in this entry.