Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 09:59 PM GMT

PDB ID	:	1RJF
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.; de La Sierra-Gallay, I.L.; Collinet, B.; Graille, M.; Blondeau, K.; Bettache, N.; Poupon, A.; Janin, J.; van Tilbeurgh, H.
Deposited on	:	2003-11-19
Resolution	:	2.25 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

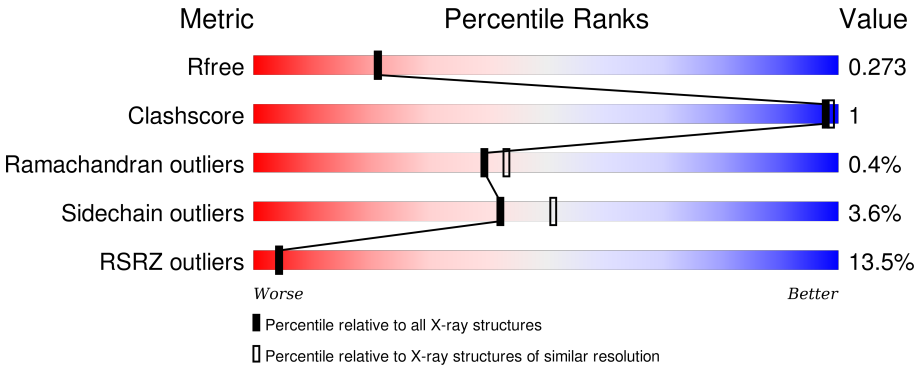
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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}	91344	1640 (2.28-2.24)
Clashscore	102246	1095 (2.26-2.26)
Ramachandran outliers	100387	1063 (2.26-2.26)
Sidechain outliers	100360	1063 (2.26-2.26)
RSRZ outliers	91569	1647 (2.28-2.24)

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 <=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	8% 90% 6% ·
1	B	334	11% 92% 6% ·
1	C	334	20% 89% 8% · ·

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
2	BME	A	335	-	-	-	X
2	BME	A	336	-	-	-	X
2	BME	B	335	-	-	-	X
2	BME	B	336	-	-	-	X
2	BME	C	335	-	-	-	X
3	GOL	A	337	-	-	-	X
3	GOL	A	338	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8150 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.

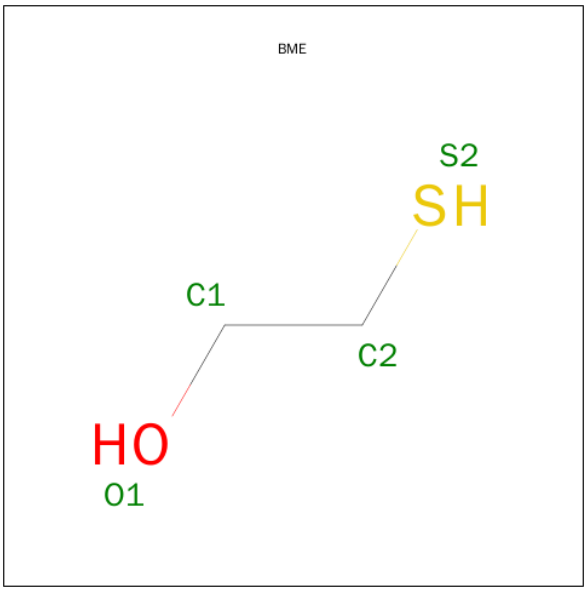
- Molecule 1 is a protein called carboxy methyl transferase for protein phosphatase 2A catalytic subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	321	Total	C	N	O	S	0	0	0
			2583	1644	439	482	18			
1	B	327	Total	C	N	O	S	0	1	0
			2640	1679	449	494	18			
1	C	325	Total	C	N	O	S	0	0	0
			2619	1665	448	488	18			

There are 18 discrepancies between the modelled and reference sequences:

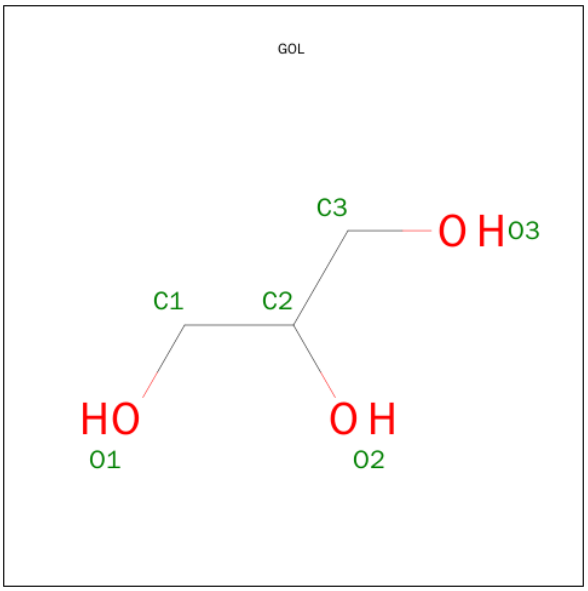
Chain	Residue	Modelled	Actual	Comment	Reference
A	329	HIS	-	EXPRESSION TAG	UNP Q04081
A	330	HIS	-	EXPRESSION TAG	UNP Q04081
A	331	HIS	-	EXPRESSION TAG	UNP Q04081
A	332	HIS	-	EXPRESSION TAG	UNP Q04081
A	333	HIS	-	EXPRESSION TAG	UNP Q04081
A	334	HIS	-	EXPRESSION TAG	UNP Q04081
B	329	HIS	-	EXPRESSION TAG	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 BETA-MERCAPTOETHANOL (three-letter code: BME) (formula: C_2H_6OS).



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

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0

- Molecule 4 is water.

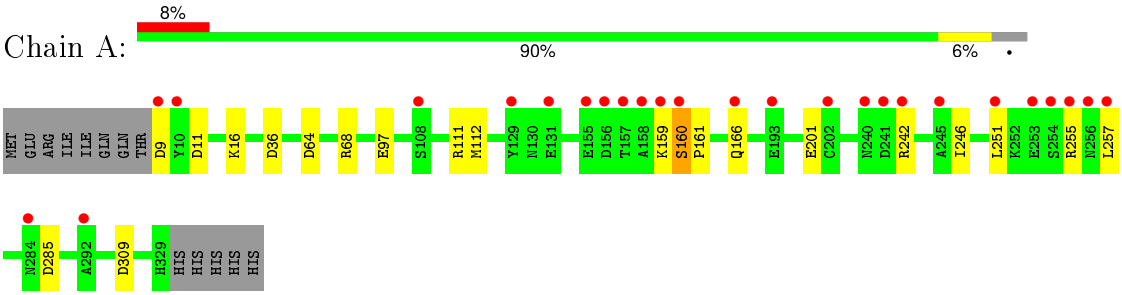
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	119	Total O 119 119	0	0
4	B	103	Total O 103 103	0	0
4	C	50	Total O 50 50	0	0

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 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.

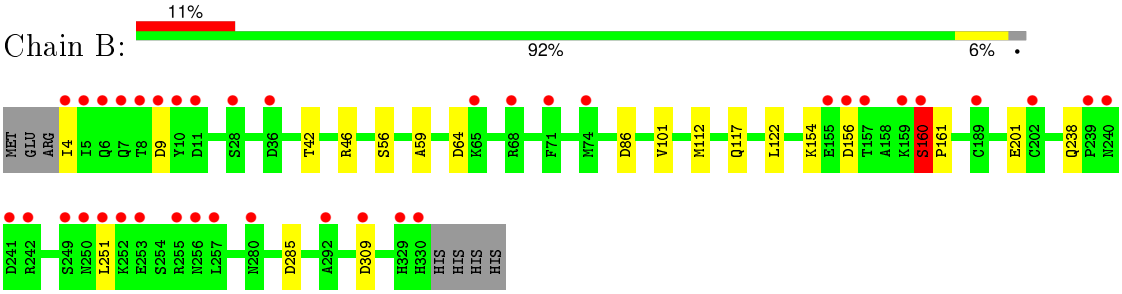
- Molecule 1: carboxy methyl transferase for protein phosphatase 2A catalytic subunit

Chain A:



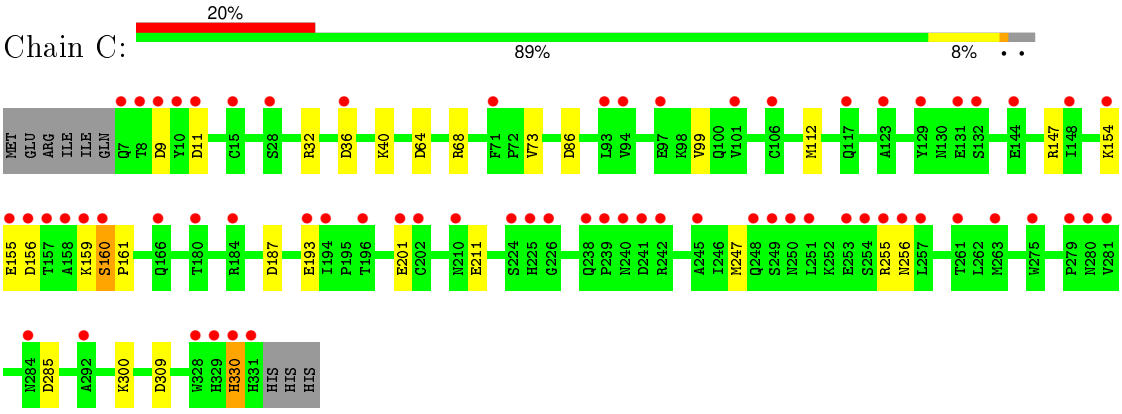
- Molecule 1: carboxy methyl transferase for protein phosphatase 2A catalytic subunit

Chain B:



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

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α, β, γ	112.39Å 112.39Å 162.85Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.25 28.18 – 2.25	Depositor EDS
% Data completeness (in resolution range)	97.6 (30.00-2.25) 97.6 (28.18-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.16 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.183 , 0.239 0.260 , 0.273	Depositor DCC
R_{free} test set	2738 reflections (5.35%)	DCC
Wilson B-factor (Å^2)	21.1	Xtriage
Anisotropy	0.033	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
Estimated twinning fraction	0.245 for h,-h-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 53873 reflections	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	8150	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.90% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: GOL, 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	0.31	1/2633 (0.0%)	0.59	5/3557 (0.1%)
1	B	0.31	1/2694 (0.0%)	0.60	6/3640 (0.2%)
1	C	0.31	1/2671 (0.0%)	0.60	9/3609 (0.2%)
All	All	0.31	3/7998 (0.0%)	0.60	20/10806 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	201	GLU	CD-OE2	7.57	1.33	1.25
1	A	201	GLU	CD-OE2	7.36	1.33	1.25
1	C	201	GLU	CD-OE2	6.93	1.33	1.25

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	11	ASP	CB-CG-OD2	5.29	123.06	118.30
1	C	285	ASP	CB-CG-OD2	5.26	123.04	118.30
1	B	9	ASP	CB-CG-OD2	5.25	123.02	118.30
1	C	9	ASP	CB-CG-OD2	5.20	122.98	118.30
1	B	285	ASP	CB-CG-OD2	5.17	122.95	118.30
1	A	64	ASP	CB-CG-OD2	5.16	122.95	118.30
1	A	285	ASP	CB-CG-OD2	5.16	122.94	118.30
1	A	9	ASP	CB-CG-OD2	5.13	122.92	118.30
1	A	11	ASP	CB-CG-OD2	5.12	122.91	118.30
1	C	64	ASP	CB-CG-OD2	5.12	122.91	118.30
1	A	309	ASP	CB-CG-OD2	5.11	122.90	118.30
1	B	64	ASP	CB-CG-OD2	5.11	122.90	118.30
1	C	309	ASP	CB-CG-OD2	5.10	122.89	118.30
1	C	156	ASP	CB-CG-OD2	5.07	122.86	118.30
1	B	309	ASP	CB-CG-OD2	5.06	122.86	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	187	ASP	CB-CG-OD2	5.05	122.85	118.30
1	C	36	ASP	CB-CG-OD2	5.05	122.84	118.30
1	B	86	ASP	CB-CG-OD2	5.04	122.84	118.30
1	C	86	ASP	CB-CG-OD2	5.03	122.83	118.30
1	B	156	ASP	CB-CG-OD2	5.03	122.82	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	2583	0	2608	6	0
1	B	2640	0	2663	7	0
1	C	2619	0	2637	5	0
2	A	8	0	12	0	0
2	B	8	0	12	0	0
2	C	8	0	12	0	0
3	A	12	0	16	0	0
4	A	119	0	0	0	0
4	B	103	0	0	0	0
4	C	50	0	0	0	0
All	All	8150	0	7960	17	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 1.

All (17) 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:160:SER:CB	1:A:161:PRO:CD	2.80	0.59
1:C:160:SER:HB2	1:C:161:PRO:CD	2.40	0.52
1:C:160:SER:CB	1:C:161:PRO:CD	2.88	0.51
1:A:160:SER:HB3	1:A:161:PRO:HD3	1.93	0.50
1:A:160:SER:CB	1:A:161:PRO:HD3	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:330:HIS:CD2	1:C:330:HIS:C	2.85	0.49
1:A:160:SER:HB2	1:A:161:PRO:CD	2.42	0.49
1:C:160:SER:CB	1:C:161:PRO:HD2	2.45	0.47
1:B:160:SER:HB2	1:B:161:PRO:HD3	1.97	0.46
1:B:160:SER:CB	1:B:161:PRO:HD3	2.46	0.46
1:B:101:VAL:HG23	1:B:122:LEU:HD11	1.99	0.45
1:A:242:ARG:O	1:A:246:ILE:HD12	2.17	0.45
1:B:160:SER:CB	1:B:161:PRO:CD	2.96	0.43
1:A:36:ASP:H	1:B:117:GLN:HE22	1.66	0.43
1:B:42:THR:O	1:B:46:ARG:HG3	2.20	0.42
1:B:56:SER:HB3	1:B:59:ALA:HB3	2.02	0.41
1:C:160:SER:HB2	1:C:161:PRO:HD2	2.03	0.40

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	319/334 (96%)	304 (95%)	14 (4%)	1 (0%)	46	52
1	B	326/334 (98%)	314 (96%)	11 (3%)	1 (0%)	46	52
1	C	323/334 (97%)	308 (95%)	13 (4%)	2 (1%)	30	30
All	All	968/1002 (97%)	926 (96%)	38 (4%)	4 (0%)	39	43

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	160	SER
1	C	160	SER
1	C	256	ASN
1	B	160	SER

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	290/303 (96%)	280 (97%)	10 (3%)	44	54
1	B	297/303 (98%)	291 (98%)	6 (2%)	63	73
1	C	294/303 (97%)	278 (95%)	16 (5%)	27	29
All	All	881/909 (97%)	849 (96%)	32 (4%)	42	51

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	LYS
1	A	68	ARG
1	A	97	GLU
1	A	111	ARG
1	A	112	MET
1	A	159	LYS
1	A	166	GLN
1	A	251	LEU
1	A	255	ARG
1	A	257	LEU
1	B	4	ILE
1	B	112	MET
1	B	154	LYS
1	B	160	SER
1	B	238	GLN
1	B	251	LEU
1	C	32	ARG
1	C	40	LYS
1	C	68	ARG
1	C	73	VAL
1	C	99	VAL
1	C	112	MET
1	C	147	ARG
1	C	154	LYS
1	C	155	GLU
1	C	159	LYS

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Mol	Chain	Res	Type
1	C	193	GLU
1	C	211	GLU
1	C	247	MET
1	C	255	ARG
1	C	300	LYS
1	C	330	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	117	GLN
1	A	166	GLN
1	A	177	ASN
1	A	209	ASN
1	B	117	GLN
1	B	130	ASN
1	B	177	ASN
1	B	209	ASN
1	B	210	ASN
1	C	177	ASN
1	C	209	ASN
1	C	330	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry

8 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	$\#\|Z\| > 2$
2	BME	A	335	-	3,3,3	0.27	0	2,2,2	0.17	0
2	BME	A	336	-	3,3,3	0.28	0	2,2,2	0.17	0
3	GOL	A	337	-	5,5,5	0.34	0	5,5,5	0.26	0
3	GOL	A	338	-	5,5,5	0.34	0	5,5,5	0.17	0
2	BME	B	335	-	3,3,3	0.26	0	2,2,2	0.16	0
2	BME	B	336	-	3,3,3	0.29	0	2,2,2	0.11	0
2	BME	C	335	-	3,3,3	0.28	0	2,2,2	0.17	0
2	BME	C	336	-	3,3,3	0.25	0	2,2,2	0.16	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
2	BME	A	335	-	-	0/1/1/1	0/0/0/0
2	BME	A	336	-	-	0/1/1/1	0/0/0/0
3	GOL	A	337	-	-	0/4/4/4	0/0/0/0
3	GOL	A	338	-	-	0/4/4/4	0/0/0/0
2	BME	B	335	-	-	0/1/1/1	0/0/0/0
2	BME	B	336	-	-	0/1/1/1	0/0/0/0
2	BME	C	335	-	-	0/1/1/1	0/0/0/0
2	BME	C	336	-	-	0/1/1/1	0/0/0/0

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

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^{th} 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	321/334 (96%)	0.77	26 (8%) 15 16	16, 24, 49, 75	0
1	B	327/334 (97%)	0.83	38 (11%) 6 6	17, 27, 59, 79	0
1	C	325/334 (97%)	1.30	67 (20%) 1 1	27, 42, 75, 91	0
All	All	973/1002 (97%)	0.97	131 (13%) 4 4	16, 30, 65, 91	0

All (131) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	240	ASN	10.2
1	B	5	ILE	8.7
1	C	330	HIS	8.2
1	C	251	LEU	7.6
1	C	331	HIS	7.1
1	B	253	GLU	6.4
1	C	240	ASN	5.9
1	C	257	LEU	5.8
1	C	249	SER	5.3
1	C	7	GLN	5.2
1	B	156	ASP	5.0
1	C	8	THR	5.0
1	B	4	ILE	4.9
1	A	255	ARG	4.9
1	C	255	ARG	4.8
1	A	160	SER	4.7
1	B	6	GLN	4.7
1	A	257	LEU	4.7
1	A	256	ASN	4.4
1	A	242	ARG	4.3
1	B	7	GLN	4.3
1	A	9	ASP	4.3
1	C	225	HIS	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	329	HIS	4.0
1	A	129	TYR	4.0
1	C	280	ASN	4.0
1	B	330	HIS	4.0
1	C	224	SER	3.8
1	C	329	HIS	3.8
1	C	160	SER	3.7
1	A	10	TYR	3.6
1	A	202	CYS	3.6
1	B	240	ASN	3.6
1	A	155	GLU	3.6
1	C	148	ILE	3.6
1	B	249	SER	3.6
1	A	251	LEU	3.5
1	C	157	THR	3.4
1	C	154	LYS	3.4
1	B	202	CYS	3.4
1	C	129	TYR	3.4
1	B	242	ARG	3.4
1	C	156	ASP	3.3
1	A	254	SER	3.3
1	C	10	TYR	3.2
1	B	157	THR	3.2
1	B	239	PRO	3.1
1	C	131	GLU	3.1
1	C	256	ASN	3.0
1	C	159	LYS	3.0
1	C	250	ASN	3.0
1	A	131	GLU	3.0
1	A	253	GLU	3.0
1	C	238	GLN	2.9
1	C	248	GLN	2.9
1	B	159	LYS	2.9
1	B	71	PHE	2.9
1	B	255	ARG	2.9
1	C	242	ARG	2.9
1	C	144	GLU	2.9
1	B	251	LEU	2.9
1	A	156	ASP	2.8
1	A	193	GLU	2.8
1	C	36	ASP	2.8
1	C	28	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	256	ASN	2.8
1	B	8	THR	2.7
1	B	68	ARG	2.7
1	A	166	GLN	2.7
1	C	279	PRO	2.7
1	B	280	ASN	2.6
1	B	252	LYS	2.6
1	C	180	THR	2.6
1	C	132	SER	2.6
1	C	292	ALA	2.6
1	A	157	THR	2.6
1	C	254	SER	2.5
1	C	328	TRP	2.5
1	C	97	GLU	2.5
1	B	160	SER	2.5
1	C	239	PRO	2.5
1	B	257	LEU	2.5
1	A	284	ASN	2.5
1	C	158	ALA	2.5
1	B	74	MET	2.5
1	A	159	LYS	2.4
1	B	189	CYS	2.4
1	C	245	ALA	2.4
1	C	275	TRP	2.4
1	C	253	GLU	2.4
1	C	166	GLN	2.4
1	B	65	LYS	2.4
1	B	9	ASP	2.4
1	C	94	VAL	2.3
1	B	155	GLU	2.3
1	B	250	ASN	2.3
1	C	193	GLU	2.3
1	C	9	ASP	2.3
1	C	202	CYS	2.3
1	C	263	MET	2.3
1	A	241	ASP	2.3
1	B	241	ASP	2.3
1	C	101	VAL	2.3
1	C	210	ASN	2.3
1	C	261	THR	2.3
1	C	194	ILE	2.3
1	C	93	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	117	GLN	2.2
1	A	158	ALA	2.2
1	C	155	GLU	2.2
1	C	281	VAL	2.2
1	C	184	ARG	2.2
1	C	11	ASP	2.2
1	A	292	ALA	2.2
1	C	123	ALA	2.2
1	C	241	ASP	2.2
1	C	226	GLY	2.2
1	C	201	GLU	2.2
1	C	15	CYS	2.2
1	C	196	THR	2.1
1	A	245	ALA	2.1
1	C	71	PHE	2.1
1	A	108	SER	2.1
1	B	10	TYR	2.1
1	B	11	ASP	2.1
1	B	292	ALA	2.0
1	B	309	ASP	2.0
1	C	284	ASN	2.0
1	B	36	ASP	2.0
1	C	106	CYS	2.0
1	B	28	SER	2.0

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, 95^{th} 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(Å^2)	Q<0.9
3	GOL	A	337	6/6	0.55	0.40	7.77	51,54,56,56	0
2	BME	B	335	4/4	0.63	0.38	5.46	33,40,40,43	0
2	BME	B	336	4/4	0.60	0.43	5.29	53,58,58,60	0
2	BME	A	335	4/4	0.62	0.35	3.87	31,42,42,49	0
3	GOL	A	338	6/6	0.53	0.27	3.10	63,64,65,65	0
2	BME	A	336	4/4	0.72	0.29	2.72	44,47,48,49	0
2	BME	C	335	4/4	0.54	0.45	2.07	47,54,55,57	0
2	BME	C	336	4/4	0.56	0.27	1.74	45,46,48,50	0

6.5 Other polymers (i)

There are no such residues in this entry.