



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 21, 2018 – 05:35 AM EST

PDB ID : 1TC1
Title : A 1.4 ANGSTROM CRYSTAL STRUCTURE FOR THE HYPOXANTHINE
PHOSPHORIBOSYLTRANSFERASE OF TRYPANOSOMA CRUZI
Authors : Focia, P.J.; Craig III, S.P.; Nieves-Alicea, R.; Fletterick, R.J.; Eakin, A.E.
Deposited on : 1998-09-30
Resolution : 1.41 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 ⓘ 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 : rb-20030736
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) : rb-20030736

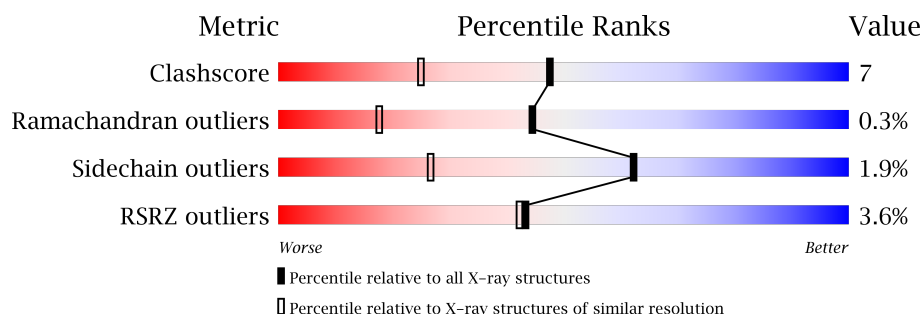
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.41 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))
Clashscore	112137	1955 (1.44-1.40)
Ramachandran outliers	110173	1908 (1.44-1.40)
Sidechain outliers	110143	1907 (1.44-1.40)
RSRZ outliers	101464	1845 (1.44-1.40)

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	220	
1	B	220	

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	FMB	B	901	-	-	-	X
3	MES	A	800	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MES	B	801	-	-	-	X

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3082 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.

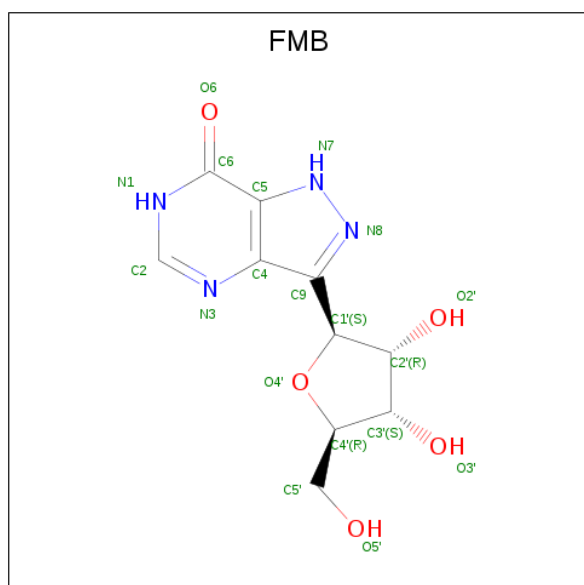
- Molecule 1 is a protein called PROTEIN (HYPOXANTHINE PHOSPHORIBOSYLTRANSFERASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	175	Total	C	N	O	S	0	0	0
			1407	914	235	251	7			
1	B	186	Total	C	N	O	S	0	0	0
			1483	959	246	271	7			

There are 5 discrepancies between the modelled and reference sequences:

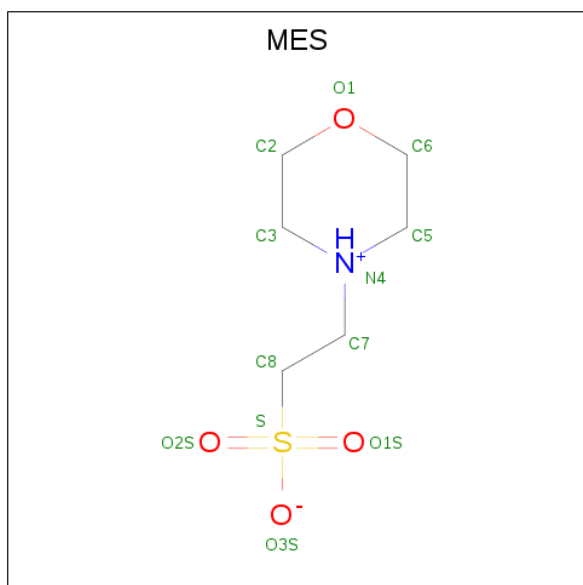
Chain	Residue	Modelled	Actual	Comment	Reference
A	23	LYS	MET	VARIANT	UNP Q27796
A	66	CYS	SER	VARIANT	UNP Q27796
B	23	LYS	MET	VARIANT	UNP Q27796
B	66	CYS	SER	VARIANT	UNP Q27796
B	86	LEU	VAL	VARIANT	UNP Q27796

- Molecule 2 is FORMYCIN B (three-letter code: FMB) (formula: C₁₀H₁₂N₄O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			10	5	4	1		
2	B	1	Total	C	N	O	0	0
			10	5	4	1		

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

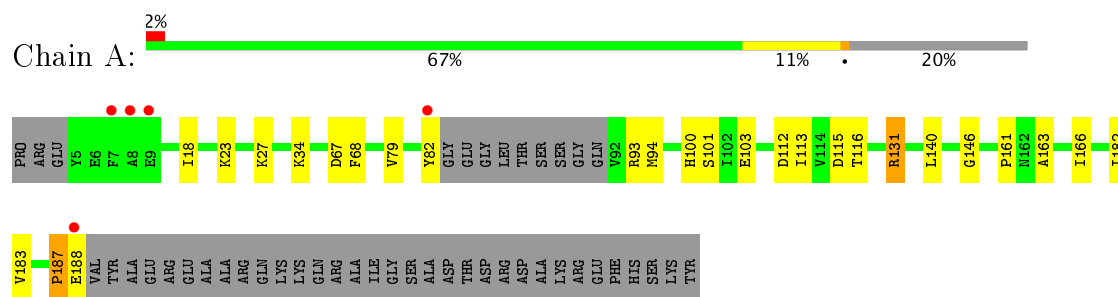
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	68	Total	O	0	0
			68	68		
4	B	80	Total	O	0	0
			80	80		

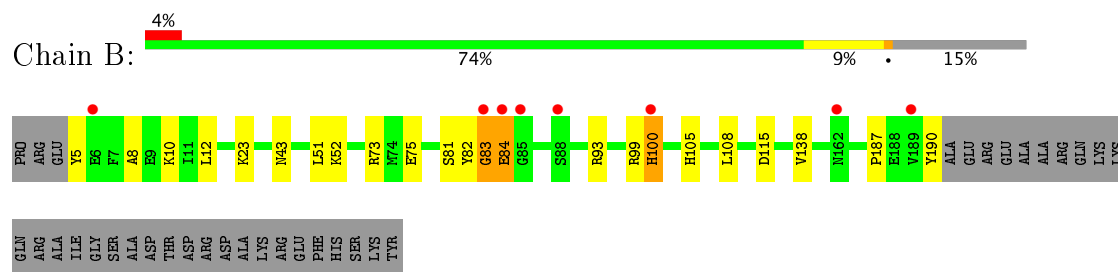
3 Residue-property plots [i](#)

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: PROTEIN (HYPOXANTHINE PHOSPHORIBOSYLTRANSFERASE)



- Molecule 1: PROTEIN (HYPOXANTHINE PHOSPHORIBOSYLTRANSFERASE)



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	39.50Å 94.09Å 52.12Å 90.00° 94.75° 90.00°	Depositor
Resolution (Å)	6.00 – 1.41 10.01 – 1.41	Depositor EDS
% Data completeness (in resolution range)	98.0 (6.00-1.41) 97.5 (10.01-1.41)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.52 (at 1.41Å)	Xtriage
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.198 , 0.228 0.200 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	13.5	Xtriage
Anisotropy	0.186	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.56 , 73.6	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	0.96	EDS
Total number of atoms	3082	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.43% 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: FMB, MES

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	2/1436 (0.1%)	0.76	3/1947 (0.2%)
1	B	0.62	0/1514	0.77	2/2055 (0.1%)
All	All	0.61	2/2950 (0.1%)	0.77	5/4002 (0.1%)

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	187	PRO	C-N	9.93	1.56	1.34
1	A	82	TYR	C-O	-5.08	1.13	1.23

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	187	PRO	O-C-N	7.16	134.15	122.70
1	B	81	SER	O-C-N	6.70	133.42	122.70
1	A	187	PRO	CA-C-N	-6.04	103.92	117.20
1	B	81	SER	CA-C-N	-5.62	104.83	117.20
1	A	187	PRO	C-N-CA	5.20	134.69	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	187	PRO	Peptide

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	1407	0	1414	23	0
1	B	1483	0	1477	17	0
2	A	10	0	3	0	0
2	B	10	0	3	1	0
3	A	12	0	13	2	0
3	B	12	0	13	1	0
4	A	68	0	0	0	0
4	B	80	0	0	1	0
All	All	3082	0	2923	41	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 7.

All (41) 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:163:ALA:HB2	1:A:188:GLU:HG3	1.25	1.11
1:B:84:GLU:HG2	1:B:84:GLU:O	1.55	1.04
1:A:163:ALA:CB	1:A:188:GLU:HG3	2.02	0.88
1:B:73:ARG:HD3	1:B:100:HIS:HD2	1.41	0.86
1:B:73:ARG:HD3	1:B:100:HIS:CD2	2.17	0.78
1:A:27:LYS:HE2	1:A:68:PHE:HZ	1.56	0.71
1:B:82:TYR:O	1:B:83:GLY:O	2.09	0.70
1:B:99:ARG:HB2	1:B:100:HIS:CE1	2.30	0.67
1:A:27:LYS:HE2	1:A:68:PHE:CZ	2.30	0.67
1:B:115:ASP:OD2	2:B:901:FMB:N8	2.29	0.65
1:A:103:GLU:HG3	1:A:131:ARG:HB2	1.83	0.58
1:B:84:GLU:O	1:B:84:GLU:CG	2.44	0.57
1:B:43:ASN:OD1	1:B:105:HIS:HD2	1.89	0.56
1:B:5:TYR:HB3	1:B:8:ALA:HB3	1.89	0.55
1:B:82:TYR:C	1:B:83:GLY:O	2.44	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:LYS:HE2	1:A:68:PHE:CE2	2.43	0.54
1:A:163:ALA:HB2	1:A:188:GLU:CG	2.18	0.52
1:A:161:PRO:HG3	1:A:188:GLU:HG2	1.91	0.51
1:A:131:ARG:CB	1:A:131:ARG:HH11	2.23	0.51
1:A:100:HIS:HD2	1:A:101:SER:O	1.94	0.50
1:B:187:PRO:HA	1:B:190:TYR:CE1	2.47	0.49
1:A:113:ILE:HG22	3:A:800:MES:H62	1.95	0.48
1:A:131:ARG:HB3	1:A:131:ARG:HH11	1.78	0.47
1:B:82:TYR:O	1:B:83:GLY:C	2.52	0.47
1:A:131:ARG:HB3	1:A:131:ARG:NH1	2.29	0.47
1:A:161:PRO:CG	1:A:188:GLU:HG2	2.46	0.46
1:A:113:ILE:CG2	3:A:800:MES:H62	2.46	0.46
1:A:18:ILE:HD11	1:A:182:ILE:HG13	1.98	0.46
1:A:166:ILE:HG13	1:A:183:VAL:HG22	1.97	0.45
1:A:93:ARG:HD3	1:A:93:ARG:N	2.31	0.45
1:A:79:VAL:HG12	1:A:94:MET:SD	2.56	0.45
1:B:23:LYS:HG2	4:B:981:HOH:O	2.15	0.45
1:B:10:LYS:HD2	1:B:12:LEU:HD23	2.00	0.44
1:A:112:ASP:O	1:A:140:LEU:HB3	2.17	0.43
1:A:116:THR:HA	1:A:146:GLY:O	2.19	0.42
3:B:801:MES:H82	3:B:801:MES:H31	1.85	0.42
1:B:51:LEU:HB3	1:B:52:LYS:HA	2.02	0.41
1:B:75:GLU:OE2	1:B:100:HIS:CD2	2.74	0.41
1:A:163:ALA:HB2	1:A:188:GLU:HA	2.02	0.41
1:A:23:LYS:HE3	1:A:67:ASP:OD2	2.21	0.40
1:B:108:LEU:HG	1:B:138:VAL:HG12	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	171/220 (78%)	165 (96%)	6 (4%)	0	100	100
1	B	184/220 (84%)	179 (97%)	4 (2%)	1 (0%)	32	9
All	All	355/440 (81%)	344 (97%)	10 (3%)	1 (0%)	44	18

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	83	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	152/193 (79%)	149 (98%)	3 (2%)	60	24
1	B	160/193 (83%)	157 (98%)	3 (2%)	62	27
All	All	312/386 (81%)	306 (98%)	6 (2%)	62	27

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	LYS
1	A	115	ASP
1	A	131	ARG
1	B	84	GLU
1	B	93	ARG
1	B	100	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	100	HIS
1	B	105	HIS
1	B	162	ASN

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](#)

4 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	MES	A	800	-	12,12,12	8.43	8 (66%)	14,16,16	3.17	5 (35%)
2	FMB	A	900	-	11,11,21	1.34	2 (18%)	4,15,31	2.73	3 (75%)
3	MES	B	801	-	12,12,12	8.62	8 (66%)	14,16,16	2.67	4 (28%)
2	FMB	B	901	-	11,11,21	1.17	1 (9%)	4,15,31	2.55	2 (50%)

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	MES	A	800	-	-	0/6/14/14	0/1/1/1
2	FMB	A	900	-	-	0/0/0/22	0/2/2/3
3	MES	B	801	-	-	0/6/14/14	0/1/1/1
2	FMB	B	901	-	-	0/0/0/22	0/2/2/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	801	MES	C8-S	-23.20	1.42	1.77
3	A	800	MES	C8-S	-22.18	1.44	1.77
3	B	801	MES	C7-C8	-4.62	1.38	1.52
3	A	800	MES	C7-C8	-4.61	1.38	1.52
3	A	800	MES	C7-N4	-3.61	1.39	1.47
3	B	801	MES	C7-N4	-3.10	1.40	1.47
3	A	800	MES	C3-C2	-2.78	1.39	1.50
3	B	801	MES	C3-C2	-2.71	1.39	1.50
3	A	800	MES	C5-N4	-2.57	1.40	1.47
3	B	801	MES	C5-N4	-2.10	1.41	1.47
2	A	900	FMB	C9-C4	2.01	1.45	1.40
2	A	900	FMB	O6-C6	2.63	1.31	1.24
2	B	901	FMB	O6-C6	2.96	1.32	1.24
3	B	801	MES	O3S-S	8.55	1.76	1.47
3	A	800	MES	O3S-S	8.96	1.77	1.47
3	B	801	MES	O2S-S	10.33	1.75	1.45
3	A	800	MES	O1S-S	10.54	1.75	1.45
3	A	800	MES	O2S-S	10.62	1.76	1.45
3	B	801	MES	O1S-S	11.14	1.77	1.45

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	900	FMB	C2-N3-C4	-3.22	111.89	115.27
2	B	901	FMB	C2-N3-C4	-3.15	111.97	115.27
3	A	800	MES	O3S-S-O2S	-2.80	104.96	111.37
3	B	801	MES	O3S-S-O2S	-2.43	105.80	111.37
3	A	800	MES	O3S-S-O1S	-2.29	106.12	111.37
2	A	900	FMB	N3-C2-N1	-2.20	126.94	128.86
2	B	901	FMB	C2-N1-C6	3.57	121.88	115.91
3	A	800	MES	O2S-S-C8	3.60	109.88	106.79
2	A	900	FMB	C2-N1-C6	3.66	122.02	115.91
3	B	801	MES	O1S-S-C8	4.92	111.02	106.79
3	B	801	MES	O2S-S-C8	5.01	111.09	106.79
3	A	800	MES	O1S-S-C8	5.24	111.29	106.79
3	B	801	MES	O3S-S-C8	5.67	113.03	106.06
3	A	800	MES	O3S-S-C8	8.78	116.85	106.06

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	800	MES	2	0
3	B	801	MES	1	0
2	B	901	FMB	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	175/220 (79%)	-0.04	5 (2%) 52 51	8, 15, 28, 39	0
1	B	186/220 (84%)	0.06	8 (4%) 36 35	8, 15, 29, 38	0
All	All	361/440 (82%)	0.01	13 (3%) 43 42	8, 15, 29, 39	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	84	GLU	8.1
1	A	82	TYR	7.8
1	B	83	GLY	6.4
1	B	88	SER	5.0
1	A	188	GLU	4.4
1	B	6	GLU	3.3
1	B	85	GLY	3.1
1	B	100	HIS	2.9
1	B	162	ASN	2.8
1	A	9	GLU	2.5
1	A	8	ALA	2.4
1	A	7	PHE	2.2
1	B	189	VAL	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, 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(Å ²)	Q<0.9
3	MES	A	800	12/12	0.87	0.28	8.18	17,34,44,45	0
3	MES	B	801	12/12	0.91	0.21	5.23	17,31,41,42	0
2	FMB	B	901	10/19	0.57	0.21	4.62	55,57,59,59	0
2	FMB	A	900	10/19	0.83	0.10	0.39	21,24,27,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.