



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:28 PM UTC

PDB ID : 3UPY / pdb_00003upy
Title : Crystal structure of the Brucella abortus enzyme catalyzing the first committed step of the methylerythritol 4-phosphate pathway.
Authors : Calisto, B.M.; Perez-Gil, J.; Fita, I.; Rodriguez-Concepcion, M.
Deposited on : 2011-11-18
Resolution : 1.80 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

<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
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

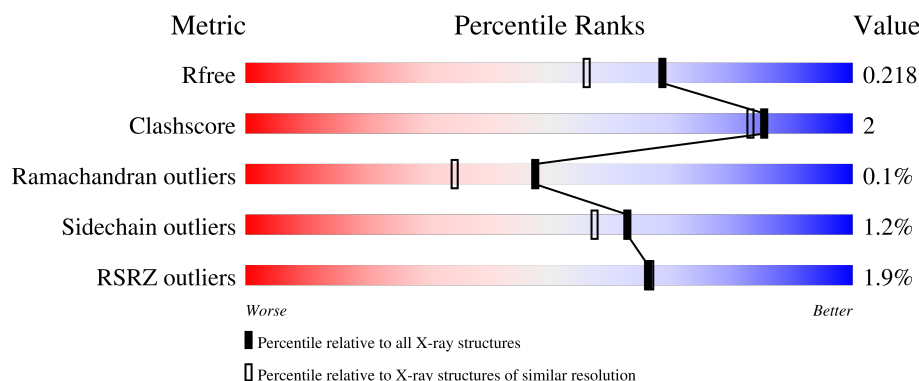
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

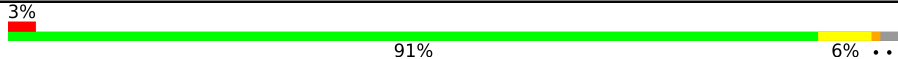
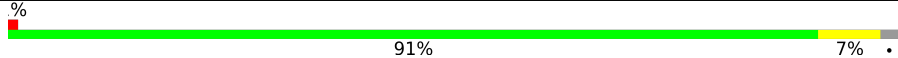
The reported resolution of this entry is 1.80 Å.

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}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (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 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	445	
1	B	445	

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
3	FOM	A	447	-	X	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7224 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 Oxidoreductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	436	Total	C	N	O	S	0	9	0
			3292	2068	575	629	20			
1	B	436	Total	C	N	O	S	0	4	0
			3264	2049	571	625	19			

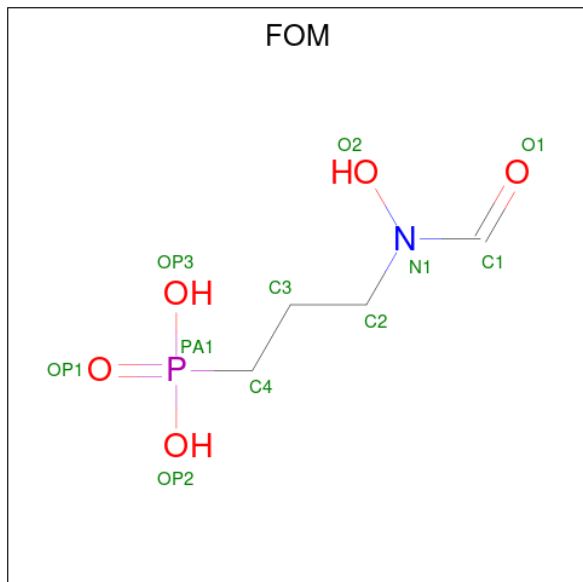
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	438	LEU	-	expression tag	UNP Q2YIM3
A	439	GLU	-	expression tag	UNP Q2YIM3
A	440	HIS	-	expression tag	UNP Q2YIM3
A	441	HIS	-	expression tag	UNP Q2YIM3
A	442	HIS	-	expression tag	UNP Q2YIM3
A	443	HIS	-	expression tag	UNP Q2YIM3
A	444	HIS	-	expression tag	UNP Q2YIM3
A	445	HIS	-	expression tag	UNP Q2YIM3
B	438	LEU	-	expression tag	UNP Q2YIM3
B	439	GLU	-	expression tag	UNP Q2YIM3
B	440	HIS	-	expression tag	UNP Q2YIM3
B	441	HIS	-	expression tag	UNP Q2YIM3
B	442	HIS	-	expression tag	UNP Q2YIM3
B	443	HIS	-	expression tag	UNP Q2YIM3
B	444	HIS	-	expression tag	UNP Q2YIM3
B	445	HIS	-	expression tag	UNP Q2YIM3

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 3 is 3-[FORMYL(HYDROXY)AMINO]PROPYLPHOSPHONIC ACID (CCD ID: FOM) (formula: $C_4H_{10}NO_5P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			11	4	1	5	1		

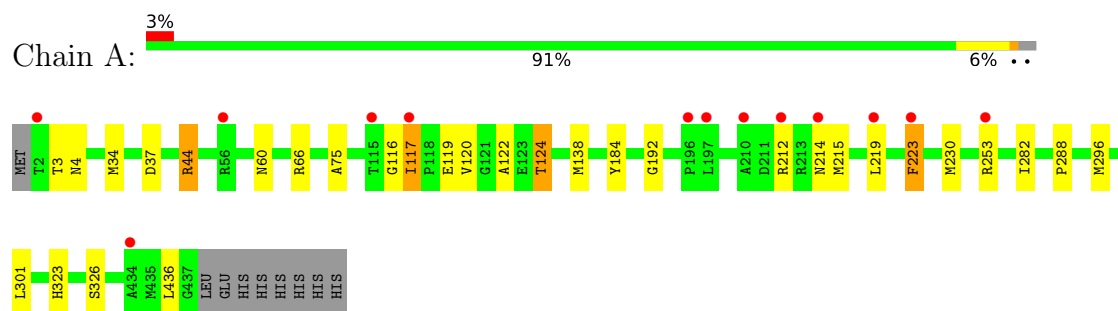
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	297	Total	O	0	0
			297	297		
4	B	358	Total	O	0	0
			358	358		

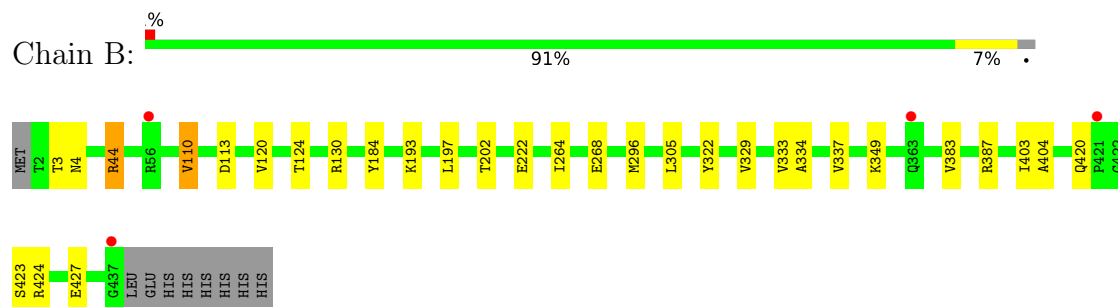
3 Residue-property plots [i](#)

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.

• Molecule 1: Oxidoreductase



• Molecule 1: Oxidoreductase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	49.39Å 63.38Å 79.33Å 68.79° 75.54° 72.07°	Depositor
Resolution (Å)	39.55 – 1.80 39.55 – 1.80	Depositor EDS
% Data completeness (in resolution range)	93.5 (39.55-1.80) 93.7 (39.55-1.80)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.163 , 0.204 0.181 , 0.218	Depositor DCC
R_{free} test set	3657 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	17.3	Xtriage
Anisotropy	0.074	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 28.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7224	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.06% 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: FOM, MG

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	1.30	9/3367 (0.3%)	1.09	2/4569 (0.0%)
1	B	1.25	8/3328 (0.2%)	1.08	7/4517 (0.2%)
All	All	1.28	17/6695 (0.3%)	1.09	9/9086 (0.1%)

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	404	ALA	C-O	-7.46	1.17	1.24
1	A	117	ILE	CA-C	6.56	1.58	1.53
1	A	223	PHE	C-O	-6.24	1.16	1.24
1	A	192	GLY	N-CA	6.18	1.50	1.44
1	B	222	GLU	C-N	-5.66	1.26	1.33
1	B	403	ILE	CA-CB	5.62	1.60	1.54
1	A	223	PHE	CA-C	5.49	1.59	1.52
1	B	124	THR	CA-CB	5.45	1.62	1.53
1	B	322	TYR	N-CA	5.39	1.52	1.45
1	B	264	ILE	CA-C	5.38	1.58	1.52
1	A	122	ALA	CA-CB	-5.30	1.45	1.53
1	B	383	VAL	N-CA	5.26	1.52	1.46
1	A	75	ALA	C-O	5.26	1.30	1.23
1	A	116	GLY	N-CA	5.13	1.53	1.45
1	B	334	ALA	CA-C	5.13	1.59	1.52
1	A	230	MET	CA-C	5.10	1.59	1.52
1	A	75	ALA	CA-CB	5.07	1.60	1.53

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	222	GLU	CA-C-N	6.87	129.72	120.65
1	B	222	GLU	C-N-CA	6.87	129.72	120.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	202	THR	CA-C-N	-5.51	113.94	119.56
1	B	202	THR	C-N-CA	-5.51	113.94	119.56
1	A	119	GLU	N-CA-C	-5.24	105.57	111.28
1	B	329	VAL	N-CA-CB	5.20	113.77	110.50
1	B	424	ARG	N-CA-C	-5.14	105.68	111.28
1	B	337	VAL	N-CA-C	5.00	115.23	110.53
1	A	215	MET	N-CA-C	5.00	117.13	110.53

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	3292	0	3361	18	0
1	B	3264	0	3332	12	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	11	0	7	0	0
4	A	297	0	0	2	0
4	B	358	0	0	3	0
All	All	7224	0	6700	29	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 2.

All (29) 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:288[A]:PRO:O	1:A:323[A]:HIS:CD2	2.15	0.97
1:A:288[A]:PRO:O	1:A:323[A]:HIS:HD2	1.48	0.93
1:B:110[A]:VAL:HG11	1:B:333:VAL:HG13	1.64	0.78
1:A:34[B]:MET:HA	1:A:34[B]:MET:HE2	1.70	0.74
1:A:120:VAL:O	1:A:124:THR:HG23	1.92	0.70
1:A:34[B]:MET:CE	1:A:37:ASP:OD2	2.40	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:ASN:ND2	4:A:489:HOH:O	2.29	0.65
1:A:34[B]:MET:HE2	1:A:37:ASP:OD2	2.04	0.57
1:A:34[B]:MET:HE1	1:A:37:ASP:OD2	2.04	0.56
1:A:219:LEU:O	1:A:223:PHE:CG	2.59	0.55
1:A:138:MET:HE1	1:A:326[A]:SER:OG	2.06	0.54
1:B:420:GLN:HG3	4:B:610:HOH:O	2.08	0.53
1:A:253:ARG:HA	1:A:282:ILE:O	2.10	0.51
1:A:3:THR:O	1:A:4:ASN:HB2	2.13	0.49
1:B:423:SER:O	1:B:427:GLU:HG3	2.13	0.48
1:A:44:ARG:CZ	1:A:44:ARG:HB3	2.44	0.47
1:B:110[B]:VAL:HG21	1:B:333:VAL:HG13	1.97	0.45
1:B:113:ASP:OD2	1:B:120:VAL:HG12	2.17	0.44
1:B:184:TYR:CD2	1:B:296:MET:HE1	2.53	0.44
1:B:193:LYS:HE2	1:B:197:LEU:CD2	2.47	0.44
1:B:3:THR:O	1:B:4:ASN:HB2	2.17	0.44
1:A:117:ILE:CG2	1:A:120:VAL:HG23	2.48	0.43
1:A:66:ARG:NH2	4:A:492:HOH:O	2.39	0.42
1:B:193:LYS:HE2	1:B:197:LEU:HD21	2.01	0.42
1:A:436:LEU:HD23	1:A:436:LEU:HA	1.87	0.41
1:A:184:TYR:CD2	1:A:296:MET:HE1	2.56	0.41
1:A:301:LEU:HD11	1:B:44:ARG:HD2	2.03	0.41
1:B:387:ARG:NH2	4:B:773:HOH:O	2.54	0.41
1:B:130:ARG:NH2	4:B:611:HOH:O	2.54	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	443/445 (100%)	435 (98%)	7 (2%)	1 (0%)	43	31
1	B	438/445 (98%)	428 (98%)	10 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	881/890 (99%)	863 (98%)	17 (2%)	1 (0%)	48 34

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	214	ASN

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	350/351 (100%)	347 (99%)	3 (1%)	70 67
1	B	346/351 (99%)	340 (98%)	6 (2%)	53 45
All	All	696/702 (99%)	687 (99%)	9 (1%)	63 54

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	ARG
1	A	124	THR
1	A	212	ARG
1	B	44	ARG
1	B	110[A]	VAL
1	B	110[B]	VAL
1	B	268	GLU
1	B	305	LEU
1	B	349	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	ASN
1	A	99	ASN
1	A	153	GLN

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Mol	Chain	Res	Type
1	A	194	ASN
1	A	266	GLN
1	A	398	GLN
1	B	41	GLN
1	B	60	ASN
1	B	99	ASN
1	B	194	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 3 ligands modelled in this entry, 2 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	FOM	A	447	2	10,10,10	3.81	3 (30%)	11,13,13	2.47	7 (63%)

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	FOM	A	447	2	-	3/7/9/9	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	447	FOM	O2-N1	-11.19	1.26	1.39
3	A	447	FOM	PA1-OP1	3.14	1.56	1.50
3	A	447	FOM	C1-N1	-2.37	1.30	1.34

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	447	FOM	OP3-PA1-C4	-4.41	96.38	106.91
3	A	447	FOM	OP2-PA1-C4	-3.06	99.59	106.91
3	A	447	FOM	OP3-PA1-OP2	3.03	116.58	107.96
3	A	447	FOM	O2-N1-C2	2.76	120.20	113.81
3	A	447	FOM	C4-C3-C2	-2.73	105.04	111.33
3	A	447	FOM	PA1-C4-C3	-2.62	111.72	114.94
3	A	447	FOM	O1-C1-N1	-2.04	120.27	125.49

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	447	FOM	C3-C2-N1-O2
3	A	447	FOM	C2-C3-C4-PA1
3	A	447	FOM	N1-C2-C3-C4

There are no ring outliers.

No monomer is involved in short contacts.

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	436/445 (97%)	-0.10	13 (2%) 52 52	6, 18, 34, 48	9 (2%)
1	B	436/445 (97%)	-0.27	4 (0%) 81 81	6, 16, 29, 51	4 (0%)
All	All	872/890 (97%)	-0.18	17 (1%) 66 66	6, 17, 32, 51	13 (1%)

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	437	GLY	4.6
1	B	421	PRO	3.9
1	A	214	ASN	3.8
1	A	223	PHE	3.6
1	A	117	ILE	3.3
1	A	2	THR	2.9
1	A	115	THR	2.8
1	A	212	ARG	2.7
1	A	253	ARG	2.6
1	A	196	PRO	2.6
1	A	219	LEU	2.6
1	A	56	ARG	2.5
1	A	434	ALA	2.3
1	A	210	ALA	2.2
1	A	197	LEU	2.1
1	B	56	ARG	2.1
1	B	363	GLN	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 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($\text{\AA}^2$)	Q<0.9
3	FOM	A	447	11/11	0.91	0.11	13,23,26,26	11
2	MG	A	446	1/1	0.99	0.07	2,2,2,2	0
2	MG	B	446	1/1	1.00	0.02	6,6,6,6	0

6.5 Other polymers [i](#)

There are no such residues in this entry.