



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 02:26 am BST

PDB ID : 1Q40
Title : Crystal structure of the *C. albicans* Mtr2-Mex67 M domain complex
Authors : Senay, C.; Ferrari, P.; Rocher, C.; Rieger, K.J.; Winter, J.; Platel, D.; Bourne, Y.
Deposited on : 2003-08-01
Resolution : 1.95 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

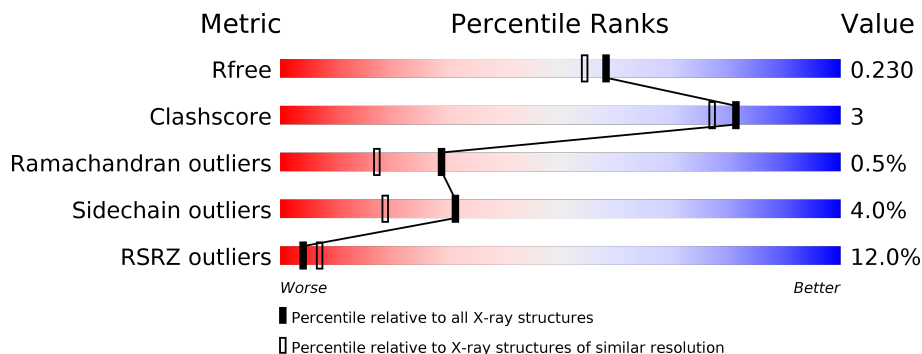
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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}	130704	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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 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	201	
1	C	201	
2	B	219	
2	D	219	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5862 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.

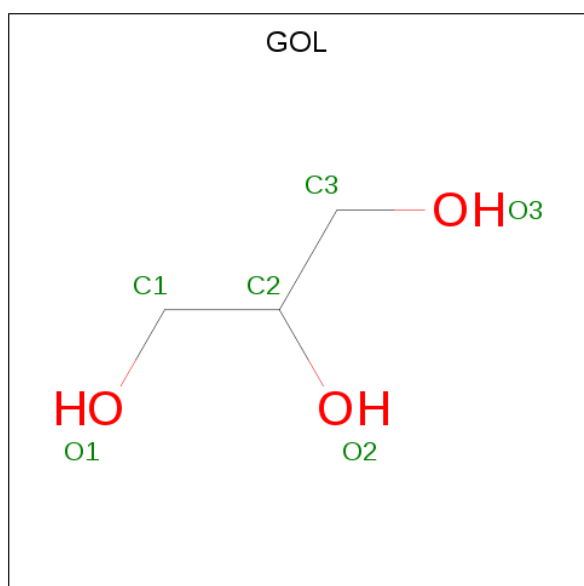
- Molecule 1 is a protein called MRNA TRANSPORT REGULATOR Mtr2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	N	O	S				Se
1	A	165	1311	835	222	251	1	2	0	0	0
1	C	164	1297	828	219	247	1	2	0	0	0

- Molecule 2 is a protein called mRNA export factor MEX67.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	Se			
2	B	186	1497	955	258	278	6	0	0	0
2	D	175	1408	899	239	264	6	0	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	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		

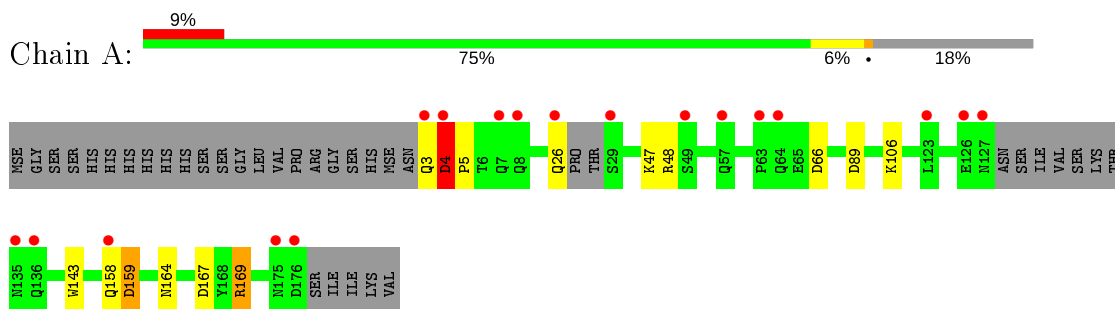
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	76	Total	O	0	0
			76	76		
4	B	84	Total	O	0	0
			84	84		
4	C	66	Total	O	0	0
			66	66		
4	D	105	Total	O	0	0
			105	105		

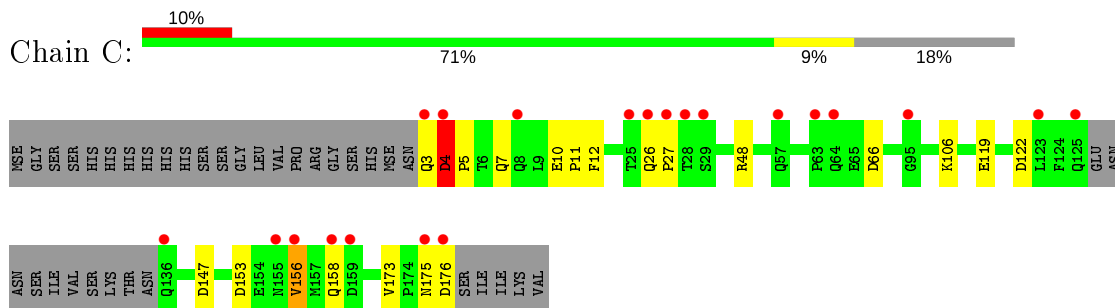
3 Residue-property plots [i](#)

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.

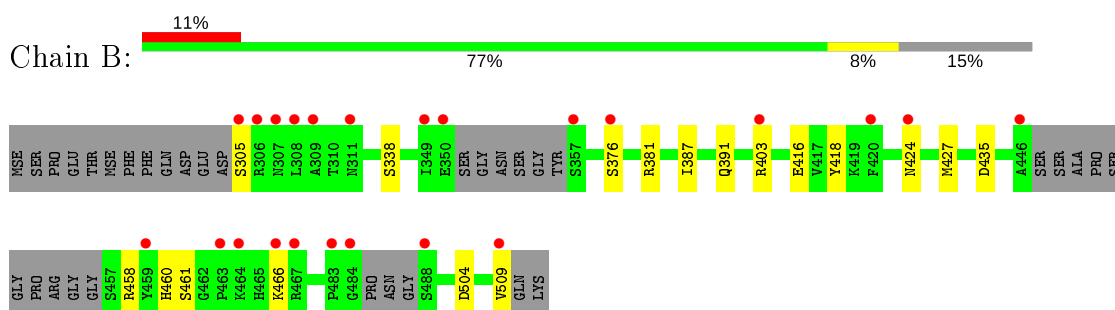
- Molecule 1: MRNA TRANSPORT REGULATOR Mtr2



- Molecule 1: MRNA TRANSPORT REGULATOR Mtr2

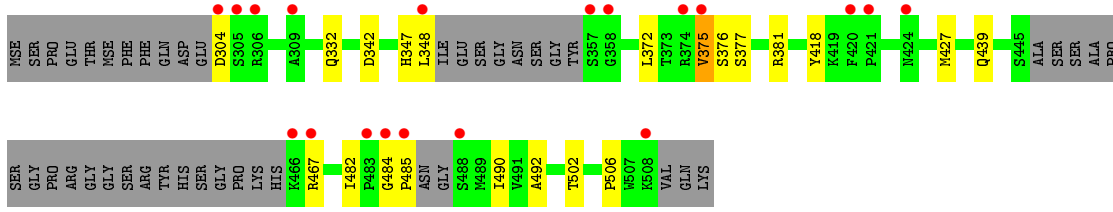


- Molecule 2: mRNA export factor MEX67



- Molecule 2: mRNA export factor MEX67





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	70.41Å 54.08Å 109.75Å 90.00° 96.12° 90.00°	Depositor
Resolution (Å)	12.00 – 1.95 11.99 – 1.95	Depositor EDS
% Data completeness (in resolution range)	91.7 (12.00-1.95) 91.7 (11.99-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.01 (at 1.94Å)	Xtrriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.177 , 0.219 0.195 , 0.230	Depositor DCC
R_{free} test set	1092 reflections (1.99%)	wwPDB-VP
Wilson B-factor (Å ²)	27.9	Xtrriage
Anisotropy	0.025	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 57.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5862	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.00% 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 i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: GOL

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	0.43	0/1341	0.74	3/1819 (0.2%)
1	C	0.44	0/1328	0.76	6/1804 (0.3%)
2	B	0.42	0/1525	0.66	2/2048 (0.1%)
2	D	0.45	0/1433	0.72	1/1925 (0.1%)
All	All	0.44	0/5627	0.72	12/7596 (0.2%)

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
2	D	0	1

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	C	66	ASP	CB-CG-OD2	6.49	124.14	118.30
1	C	4	ASP	CB-CG-OD2	6.07	123.76	118.30
1	C	122	ASP	CB-CG-OD2	6.07	123.76	118.30
1	C	27	PRO	N-CA-CB	5.72	110.17	103.30
1	A	66	ASP	CB-CG-OD2	5.53	123.27	118.30
1	C	153	ASP	CB-CG-OD2	5.51	123.26	118.30
2	D	342	ASP	CB-CG-OD2	5.46	123.22	118.30
2	B	435	ASP	CB-CG-OD2	5.44	123.20	118.30
2	B	504	ASP	CB-CG-OD2	5.39	123.15	118.30
1	A	159	ASP	CB-CG-OD2	5.31	123.08	118.30
1	A	169	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	C	147	ASP	CB-CG-OD2	5.20	122.98	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	375	VAL	Peptide

5.2 Too-close contacts [i](#)

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	1311	0	1252	8	0
1	C	1297	0	1241	9	0
2	B	1497	0	1484	7	0
2	D	1408	0	1395	11	0
3	A	6	0	8	0	0
3	B	6	0	8	0	0
3	C	6	0	8	0	0
4	A	76	0	0	0	0
4	B	84	0	0	0	2
4	C	66	0	0	0	0
4	D	105	0	0	0	2
All	All	5862	0	5396	28	2

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 3.

All (28) 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:3:GLN:N	2:B:381:ARG:HE	1.67	0.93
1:A:3:GLN:N	2:B:381:ARG:NE	2.36	0.74
2:D:482:ILE:HD12	2:D:492:ALA:HB2	1.72	0.70
2:D:418:TYR:OH	2:D:427:MSE:HE2	1.95	0.66
1:C:3:GLN:N	2:D:381:ARG:HE	1.99	0.61
2:B:387:ILE:H	2:B:391:GLN:NE2	2.02	0.58
1:A:47:LYS:NZ	1:A:164:ASN:HD21	2.02	0.57
2:D:484:GLY:N	2:D:485:PRO:HD3	2.20	0.56
2:B:418:TYR:OH	2:B:427:MSE:HE3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:372:LEU:HA	2:D:375:VAL:HG12	1.91	0.52
2:D:484:GLY:N	2:D:485:PRO:CD	2.74	0.51
2:D:372:LEU:HD23	2:D:375:VAL:CG1	2.41	0.50
1:C:4:ASP:HB3	1:C:5:PRO:HD3	1.93	0.49
1:C:4:ASP:CB	1:C:5:PRO:HD3	2.44	0.47
1:A:4:ASP:CB	1:A:5:PRO:HD3	2.44	0.47
1:A:47:LYS:HZ1	1:A:164:ASN:HD21	1.60	0.47
1:C:3:GLN:N	1:C:7:GLN:OE1	2.48	0.46
2:B:460:HIS:HD2	2:B:461:SER:O	1.97	0.46
1:C:3:GLN:N	2:D:381:ARG:NE	2.62	0.45
2:D:332:GLN:HG2	2:D:490:ILE:HD12	1.98	0.45
1:C:10:GLU:HB3	1:C:11:PRO:HD3	1.99	0.44
2:D:439:GLN:OE1	2:D:467:ARG:NH2	2.51	0.44
1:A:167:ASP:OD2	2:B:416:GLU:OE2	2.36	0.43
1:C:175:ASN:O	1:C:176:ASP:CB	2.68	0.41
1:A:89:ASP:OD2	2:B:338:SER:OG	2.37	0.41
1:A:106:LYS:HD3	1:A:143:TRP:CD2	2.57	0.40
1:C:173:VAL:HG23	2:D:506:PRO:HB3	2.02	0.40
1:C:12:PHE:HB2	1:C:156:VAL:HG13	2.03	0.40

All (2) 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)
4:B:920:HOH:O	4:D:609:HOH:O[2_647]	1.46	0.74
4:B:920:HOH:O	4:D:523:HOH:O[2_647]	2.08	0.12

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	159/201 (79%)	155 (98%)	3 (2%)	1 (1%)	25 14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	160/201 (80%)	155 (97%)	4 (2%)	1 (1%)	25	14
2	B	178/219 (81%)	176 (99%)	2 (1%)	0	100	100
2	D	167/219 (76%)	160 (96%)	6 (4%)	1 (1%)	25	14
All	All	664/840 (79%)	646 (97%)	15 (2%)	3 (0%)	29	17

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	4	ASP
2	D	347	HIS
1	A	4	ASP

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	146/179 (82%)	140 (96%)	6 (4%)	30	18
1	C	144/179 (80%)	137 (95%)	7 (5%)	25	12
2	B	169/187 (90%)	162 (96%)	7 (4%)	30	18
2	D	160/187 (86%)	155 (97%)	5 (3%)	40	28
All	All	619/732 (85%)	594 (96%)	25 (4%)	31	19

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ASP
1	A	26	GLN
1	A	48	ARG
1	A	158	GLN
1	A	159	ASP
1	A	169	ARG
2	B	305	SER
2	B	376	SER

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Mol	Chain	Res	Type
2	B	403	ARG
2	B	424	ASN
2	B	458	ARG
2	B	466	LYS
2	B	509	VAL
1	C	4	ASP
1	C	26	GLN
1	C	48	ARG
1	C	106	LYS
1	C	119	GLU
1	C	156	VAL
1	C	158	GLN
2	D	304	ASP
2	D	348	LEU
2	D	376	SER
2	D	377	SER
2	D	502	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	34	ASN
1	A	64	GLN
1	A	136	GLN
1	A	164	ASN
2	B	391	GLN
2	B	460	HIS
1	C	64	GLN
1	C	125	GLN
1	C	149	ASN
2	D	311	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](#)

3 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	GOL	B	903	-	5,5,5	0.36	0	5,5,5	0.36	0
3	GOL	A	901	-	5,5,5	0.37	0	5,5,5	0.26	0
3	GOL	C	902	-	5,5,5	0.42	0	5,5,5	0.43	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	GOL	B	903	-	-	3/4/4/4	-
3	GOL	A	901	-	-	1/4/4/4	-
3	GOL	C	902	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	903	GOL	C1-C2-C3-O3
3	C	902	GOL	C1-C2-C3-O3
3	B	903	GOL	O2-C2-C3-O3
3	C	902	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
3	B	903	GOL	O1-C1-C2-C3
3	A	901	GOL	O1-C1-C2-C3

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

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	163/201 (81%)	0.38	18 (11%) 5 9	22, 36, 60, 76	0
1	C	162/201 (80%)	0.36	21 (12%) 3 5	25, 36, 57, 67	0
2	B	180/219 (82%)	0.55	23 (12%) 3 6	20, 37, 71, 98	0
2	D	169/219 (77%)	0.42	19 (11%) 5 8	21, 31, 62, 75	0
All	All	674/840 (80%)	0.43	81 (12%) 4 7	20, 35, 64, 98	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	485	PRO	11.2
1	A	127	ASN	8.1
2	D	357	SER	7.8
1	A	135	ASN	6.8
2	D	348	LEU	6.3
2	D	484	GLY	6.1
2	B	309	ALA	5.6
2	D	466	LYS	5.5
2	D	375	VAL	5.3
1	C	64	GLN	5.1
2	B	350	GLU	5.0
1	C	27	PRO	4.8
2	B	484	GLY	4.6
1	C	26	GLN	4.6
2	B	459	TYR	4.6
1	A	3	GLN	4.4
2	B	509	VAL	4.4
2	D	358	GLY	4.4
2	B	357	SER	4.4
1	A	175	ASN	4.3
1	C	125	GLN	4.3

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Mol	Chain	Res	Type	RSRZ
1	C	159	ASP	4.2
1	C	3	GLN	4.2
2	D	374	ARG	4.2
1	A	176	ASP	4.1
2	B	307	ASN	4.1
2	D	488	SER	4.1
1	A	29	SER	4.0
1	C	95	GLY	4.0
2	B	308	LEU	4.0
2	D	483	PRO	3.9
1	A	63	PRO	3.9
1	C	136	GLN	3.8
2	D	304	ASP	3.7
1	C	25	THR	3.7
2	B	446	ALA	3.7
1	C	4	ASP	3.6
2	B	463	PRO	3.5
2	B	466	LYS	3.5
1	A	136	GLN	3.4
1	C	158	GLN	3.4
2	D	305	SER	3.3
2	B	306	ARG	3.2
2	B	467	ARG	3.1
2	B	483	PRO	3.1
1	C	175	ASN	3.0
2	B	488	SER	3.0
1	C	28	THR	3.0
1	A	4	ASP	2.9
2	D	306	ARG	2.9
1	A	64	GLN	2.9
1	A	126	GLU	2.8
1	C	8	GLN	2.8
2	B	424	ASN	2.8
2	B	420	PHE	2.8
1	C	63	PRO	2.8
2	B	403	ARG	2.7
1	C	176	ASP	2.7
2	D	420	PHE	2.6
1	C	156	VAL	2.6
2	D	421	PRO	2.6
1	A	49	SER	2.6
2	B	311	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	464	LYS	2.5
2	D	508	LYS	2.5
2	D	424	ASN	2.5
1	A	57	GLN	2.5
2	B	376	SER	2.4
1	C	29	SER	2.3
1	A	158	GLN	2.3
2	B	349	ILE	2.2
1	A	123	LEU	2.1
1	C	155	ASN	2.1
1	A	26	GLN	2.1
2	D	309	ALA	2.1
1	A	8	GLN	2.1
1	A	7	GLN	2.1
2	D	467	ARG	2.0
1	C	57	GLN	2.0
1	C	123	LEU	2.0
2	B	305	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. 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(Å ²)	Q<0.9
3	GOL	A	901	6/6	0.83	0.20	39,43,44,48	0
3	GOL	C	902	6/6	0.87	0.16	42,46,47,49	0
3	GOL	B	903	6/6	0.96	0.11	37,39,40,40	0

6.5 Other polymers

There are no such residues in this entry.