



Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 10:18 pm BST

PDB ID : 6EXE
Title : Crystal structure of DotM cytoplasmic domain (residues 153-380),R217E
Authors : Meir, A.; Waksman, G.
Deposited on : 2017-11-08
Resolution : 2.00 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

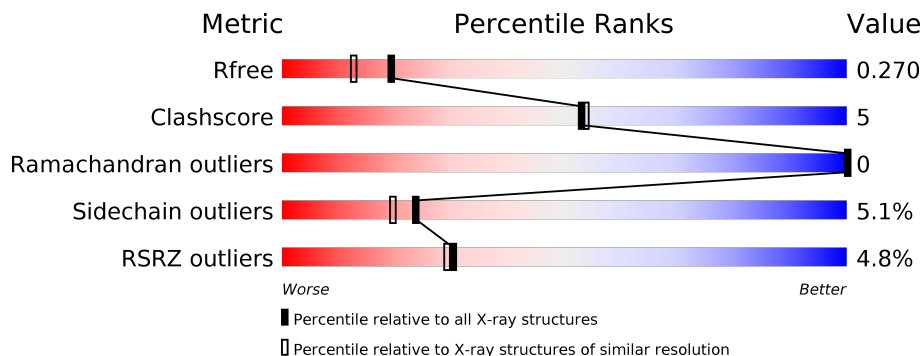
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	235	
1	B	235	

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	GOL	B	403	-	X	X	-
2	GOL	B	405	-	X	-	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3721 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 IcmP (DotM).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	219	1756	1120	307	316	13	0	0	0
1	B	223	1789	1140	313	323	13	0	1	0

There are 16 discrepancies between the modelled and reference sequences:

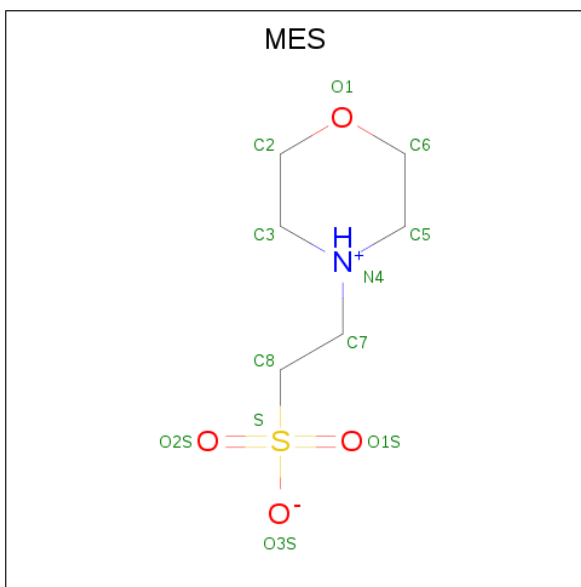
Chain	Residue	Modelled	Actual	Comment	Reference
A	146	GLY	-	expression tag	UNP Q5ZYC7
A	147	PRO	-	expression tag	UNP Q5ZYC7
A	148	SER	-	expression tag	UNP Q5ZYC7
A	149	GLY	-	expression tag	UNP Q5ZYC7
A	150	GLY	-	expression tag	UNP Q5ZYC7
A	151	GLY	-	expression tag	UNP Q5ZYC7
A	152	ALA	-	expression tag	UNP Q5ZYC7
A	217	GLU	ARG	engineered mutation	UNP Q5ZYC7
B	146	GLY	-	expression tag	UNP Q5ZYC7
B	147	PRO	-	expression tag	UNP Q5ZYC7
B	148	SER	-	expression tag	UNP Q5ZYC7
B	149	GLY	-	expression tag	UNP Q5ZYC7
B	150	GLY	-	expression tag	UNP Q5ZYC7
B	151	GLY	-	expression tag	UNP Q5ZYC7
B	152	ALA	-	expression tag	UNP Q5ZYC7
B	217	GLU	ARG	engineered mutation	UNP Q5ZYC7

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

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



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


- Molecule 4 is water.

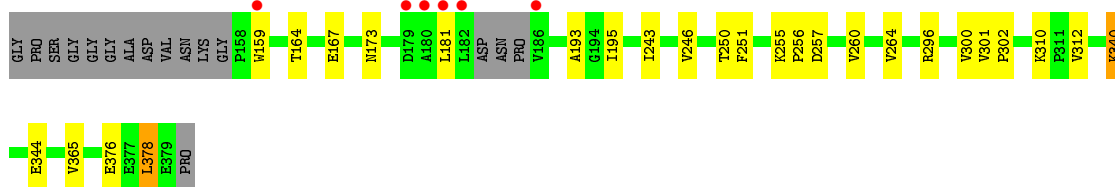
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	68	Total	O	0	0
			68	68		
4	B	66	Total	O	0	0
			66	66		

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.

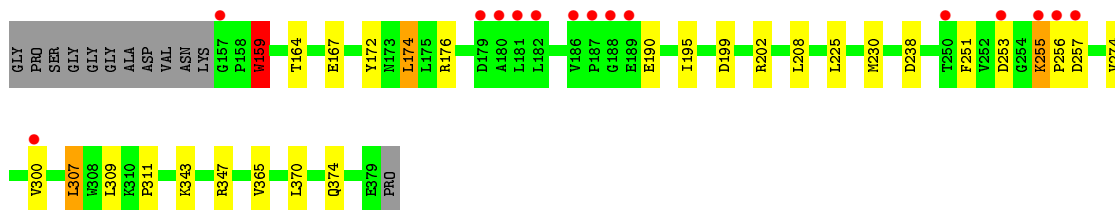
- Molecule 1: IcmP (DotM)

Chain A: 



- Molecule 1: IcmP (DotM)

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	118.28 Å 118.28 Å 66.57 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	53.45 – 2.00 44.21 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.4 (53.45-2.00) 99.4 (44.21-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.18	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.13 (at 2.00 Å)	Xtrriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.223 , 0.264 0.229 , 0.270	Depositor DCC
R_{free} test set	1749 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	33.9	Xtrriage
Anisotropy	0.104	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 56.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.052 for h,-h-k,-l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3721	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.85% 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, 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	0.80	0/1794	0.92	0/2424
1	B	0.83	3/1832 (0.2%)	0.89	2/2479 (0.1%)
All	All	0.82	3/3626 (0.1%)	0.90	2/4903 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	159	TRP	CB-CG	-7.46	1.36	1.50
1	B	159	TRP	CG-CD1	-7.02	1.26	1.36
1	B	159	TRP	CG-CD2	-5.26	1.34	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	202	ARG	NE-CZ-NH1	5.33	122.96	120.30
1	B	347	ARG	NE-CZ-NH1	5.01	122.81	120.30

There are no chirality outliers.

There are no planarity outliers.

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	1756	0	1768	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1789	0	1801	25	0
2	A	6	0	8	3	0
2	B	24	0	30	11	0
3	B	12	0	13	0	0
4	A	68	0	0	0	0
4	B	66	0	0	1	0
All	All	3721	0	3620	39	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 5.

All (39) 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:TRP:HH2	2:B:403:GOL:HO1	0.94	0.87
1:A:246:VAL:O	1:A:250:THR:OG1	1.92	0.87
1:B:230:MET:HG2	1:B:274:VAL:HG21	1.69	0.74
1:B:159:TRP:CZ3	2:B:403:GOL:H12	2.25	0.71
1:B:159:TRP:HH2	2:B:403:GOL:O1	1.73	0.67
1:A:164:THR:HG23	1:A:167:GLU:H	1.63	0.64
1:B:159:TRP:CH2	2:B:403:GOL:H12	2.35	0.61
1:B:159:TRP:CH2	2:B:403:GOL:C1	2.86	0.59
1:A:257:ASP:O	1:A:260:VAL:HG12	2.03	0.57
1:A:159:TRP:CZ3	1:B:256:PRO:HD3	2.40	0.57
1:B:300:VAL:HA	2:B:404:GOL:H31	1.88	0.56
1:B:159:TRP:HZ3	2:B:403:GOL:C3	2.21	0.53
1:A:301:VAL:N	2:A:401:GOL:O1	2.37	0.53
1:A:300:VAL:HA	2:A:401:GOL:O1	2.10	0.52
1:B:255[B]:LYS:HD2	1:B:256:PRO:CD	2.40	0.52
1:B:159:TRP:CH2	1:B:311:PRO:HG3	2.44	0.52
1:B:195:ILE:HD11	1:B:365:VAL:HG21	1.94	0.50
1:A:159:TRP:CZ3	1:B:251:PHE:HA	2.48	0.49
1:A:195:ILE:HD11	1:A:365:VAL:HG21	1.96	0.48
1:A:340:LYS:O	1:A:344:GLU:HG3	2.14	0.48
1:A:250:THR:HB	1:A:256:PRO:HA	1.97	0.47
1:B:159:TRP:CH2	2:B:403:GOL:O1	2.57	0.47
1:B:176:ARG:NH2	2:B:402:GOL:O1	2.48	0.46
1:B:159:TRP:CZ3	2:B:403:GOL:C1	2.96	0.45
1:A:164:THR:HG22	1:A:167:GLU:CD	2.36	0.45
1:A:193:ALA:HB2	1:A:378:LEU:HD21	1.98	0.45
1:B:172:TYR:O	1:B:174:LEU:HD13	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:ILE:HD11	1:A:264:VAL:HG21	1.99	0.44
1:A:164:THR:HG22	1:A:167:GLU:CG	2.48	0.44
1:A:251:PHE:CD2	1:B:307:LEU:HD21	2.53	0.43
1:A:296:ARG:NE	2:A:401:GOL:H11	2.34	0.43
1:A:159:TRP:CH2	1:B:256:PRO:HG3	2.53	0.42
1:B:164:THR:HG22	1:B:167:GLU:CG	2.49	0.42
1:B:159:TRP:HZ3	2:B:403:GOL:H32	1.83	0.42
1:B:164:THR:HG21	4:B:554:HOH:O	2.19	0.42
1:A:300:VAL:HG22	1:A:302:PRO:HD3	2.02	0.41
1:B:225:LEU:CD1	1:B:309:LEU:HD22	2.51	0.41
1:B:370:LEU:HB3	1:B:374:GLN:HB2	2.03	0.40
1:B:255[B]:LYS:HD2	1:B:256:PRO:HD3	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	215/235 (92%)	205 (95%)	10 (5%)	0	100	100
1	B	222/235 (94%)	212 (96%)	10 (4%)	0	100	100
All	All	437/470 (93%)	417 (95%)	20 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	185/195 (95%)	177 (96%)	8 (4%)	29	26
1	B	189/195 (97%)	177 (94%)	12 (6%)	18	13
All	All	374/390 (96%)	354 (95%)	20 (5%)	24	18

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	173	ASN
1	A	181	LEU
1	A	255	LYS
1	A	310	LYS
1	A	312	VAL
1	A	340	LYS
1	A	376	GLU
1	A	378	LEU
1	B	159	TRP
1	B	174	LEU
1	B	190	GLU
1	B	199	ASP
1	B	208	LEU
1	B	238	ASP
1	B	253	ASP
1	B	255[A]	LYS
1	B	255[B]	LYS
1	B	257	ASP
1	B	307	LEU
1	B	343	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	173	ASN
1	A	234	ASN
1	A	269	GLN
1	B	234	ASN
1	B	321	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](#)

6 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	B	401	-	12,12,12	2.07	1 (8%)	14,16,16	2.03	3 (21%)
2	GOL	B	403	-	5,5,5	2.67	1 (20%)	5,5,5	4.31	4 (80%)
2	GOL	B	404	-	5,5,5	0.34	0	5,5,5	0.63	0
2	GOL	B	402	-	5,5,5	0.71	0	5,5,5	0.49	0
2	GOL	A	401	-	5,5,5	0.84	0	5,5,5	1.92	2 (40%)
2	GOL	B	405	-	5,5,5	2.92	1 (20%)	5,5,5	2.23	3 (60%)

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	B	401	-	-	6/6/14/14	0/1/1/1
2	GOL	B	403	-	-	3/4/4/4	-
2	GOL	B	404	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	B	402	-	-	2/4/4/4	-
2	GOL	A	401	-	-	2/4/4/4	-
2	GOL	B	405	-	-	3/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	401	MES	C8-S	-6.61	1.68	1.77
2	B	405	GOL	O2-C2	-6.03	1.25	1.43
2	B	403	GOL	O2-C2	-5.75	1.26	1.43

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	403	GOL	O2-C2-C3	-6.80	79.17	109.12
3	B	401	MES	O1S-S-C8	5.61	113.67	106.92
2	B	403	GOL	C3-C2-C1	5.00	131.16	111.70
2	B	403	GOL	O2-C2-C1	-3.52	93.60	109.12
2	A	401	GOL	O2-C2-C1	-3.41	94.11	109.12
3	B	401	MES	O2S-S-C8	3.39	111.00	106.92
2	B	405	GOL	O2-C2-C1	-3.25	94.81	109.12
2	B	403	GOL	O3-C3-C2	-3.02	95.70	110.20
3	B	401	MES	O2S-S-O1S	-2.64	104.81	113.95
2	B	405	GOL	C3-C2-C1	2.53	121.53	111.70
2	A	401	GOL	O2-C2-C3	2.17	118.69	109.12
2	B	405	GOL	O2-C2-C3	-2.09	99.90	109.12

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	401	MES	C8-C7-N4-C3
3	B	401	MES	C8-C7-N4-C5
3	B	401	MES	N4-C7-C8-S
3	B	401	MES	C7-C8-S-O1S
2	B	404	GOL	O1-C1-C2-C3
2	B	402	GOL	C1-C2-C3-O3
2	A	401	GOL	C1-C2-C3-O3
2	B	405	GOL	C1-C2-C3-O3
2	B	405	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
2	B	402	GOL	O2-C2-C3-O3
2	B	403	GOL	O1-C1-C2-C3
2	B	404	GOL	C1-C2-C3-O3
2	B	405	GOL	O1-C1-C2-C3
3	B	401	MES	C7-C8-S-O3S
2	B	403	GOL	O1-C1-C2-O2
2	B	404	GOL	O2-C2-C3-O3
2	A	401	GOL	O2-C2-C3-O3
2	B	404	GOL	O1-C1-C2-O2
3	B	401	MES	C7-C8-S-O2S
2	B	403	GOL	O2-C2-C3-O3

There are no ring outliers.

4 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	403	GOL	9	0
2	B	404	GOL	1	0
2	B	402	GOL	1	0
2	A	401	GOL	3	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	219/235 (93%)	0.10	6 (2%) 54 53	20, 41, 70, 108	0
1	B	223/235 (94%)	0.11	15 (6%) 17 17	21, 43, 82, 99	0
All	All	442/470 (94%)	0.11	21 (4%) 30 29	20, 42, 80, 108	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	182	LEU	6.9
1	B	256	PRO	5.6
1	A	181	LEU	5.6
1	A	180	ALA	5.2
1	B	180	ALA	4.0
1	A	179	ASP	3.9
1	B	181	LEU	3.7
1	B	253	ASP	3.7
1	B	188	GLY	3.7
1	B	182	LEU	3.4
1	B	300	VAL	3.3
1	B	157	GLY	3.0
1	B	187	PRO	3.0
1	B	189	GLU	2.9
1	B	186	VAL	2.9
1	B	257	ASP	2.6
1	B	179	ASP	2.5
1	A	186	VAL	2.5
1	A	159	TRP	2.4
1	B	255[A]	LYS	2.4
1	B	250	THR	2.1

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(\AA^2)	Q<0.9
3	MES	B	401	12/12	0.75	0.22	86,90,105,107	0
2	GOL	B	402	6/6	0.76	0.18	39,43,49,54	0
2	GOL	A	401	6/6	0.88	0.19	46,50,56,63	0
2	GOL	B	404	6/6	0.89	0.23	53,59,71,83	0
2	GOL	B	405	6/6	0.89	0.23	14,32,37,37	0
2	GOL	B	403	6/6	0.96	0.25	19,37,49,51	0

6.5 Other polymers [i](#)

There are no such residues in this entry.