Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 07:23 am BST

PDB ID	:	5YAA
Title	:	Crystal structure of Marf1 NYN domain from Mus musculus
Authors	:	Yao, Q.Q.; Wu, B.X.; Ma, J.B.
Deposited on	:	2017-08-31
Resolution	:	1.75 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 ①) were used in the production of this report:

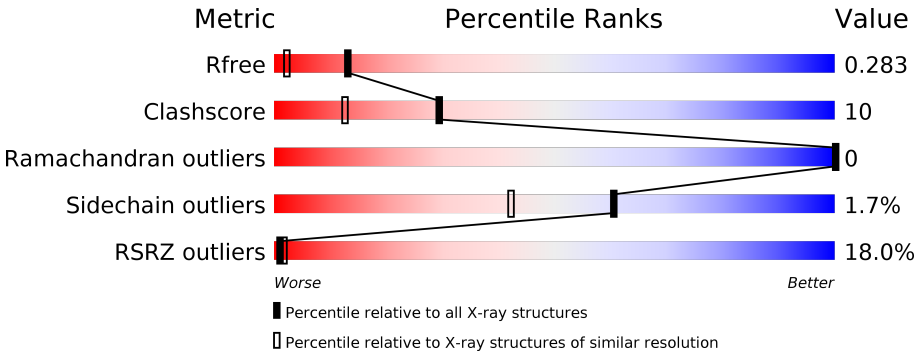
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA,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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.75 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	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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 <=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	163	15% 77% 13% • 8%
1	B	163	17% 79% 13% 8%
1	C	163	22% 71% 20% 9%
1	D	163	11% 79% 12% 9%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GOL	D	401	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5140 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.

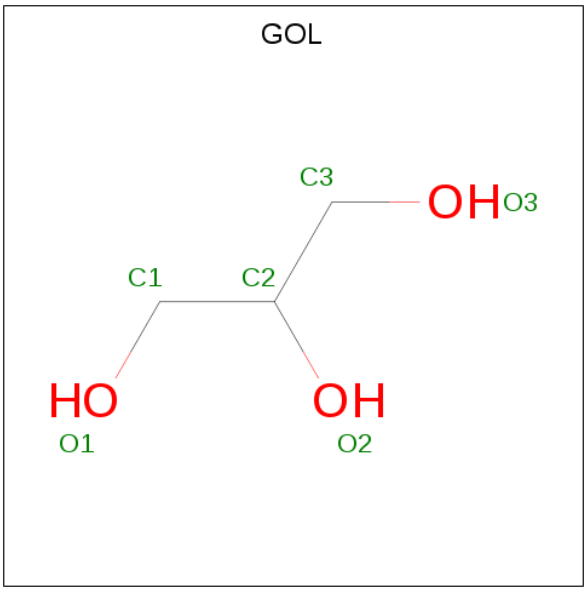
- Molecule 1 is a protein called Meiosis regulator and mRNA stability factor 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	150	Total	C	N	O	S	Se	0	0	0
			1197	747	224	220	4	2			
1	B	150	Total	C	N	O	S	Se	0	1	0
			1203	750	225	221	5	2			
1	C	149	Total	C	N	O	S	Se	0	1	0
			1196	746	224	219	5	2			
1	D	149	Total	C	N	O	S	Se	0	0	0
			1189	743	223	217	4	2			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	253	MSE	LEU	engineered mutation	UNP Q8BJ34
A	303	MSE	LEU	engineered mutation	UNP Q8BJ34
B	253	MSE	LEU	engineered mutation	UNP Q8BJ34
B	303	MSE	LEU	engineered mutation	UNP Q8BJ34
C	253	MSE	LEU	engineered mutation	UNP Q8BJ34
C	303	MSE	LEU	engineered mutation	UNP Q8BJ34
D	253	MSE	LEU	engineered mutation	UNP Q8BJ34
D	303	MSE	LEU	engineered mutation	UNP Q8BJ34

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 3 is water.

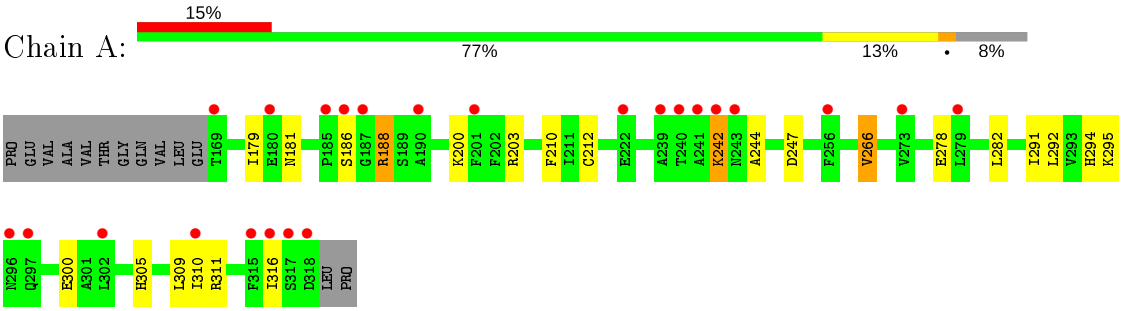
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	67	Total O 67 67	0	0
3	B	63	Total O 63 63	0	0
3	C	66	Total O 66 66	0	0
3	D	81	Total O 81 81	0	0

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 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.

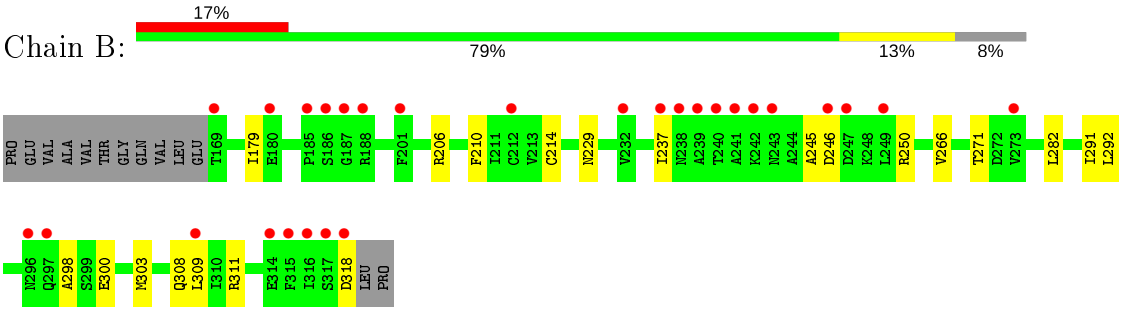
- Molecule 1: Meiosis regulator and mRNA stability factor 1

Chain A:



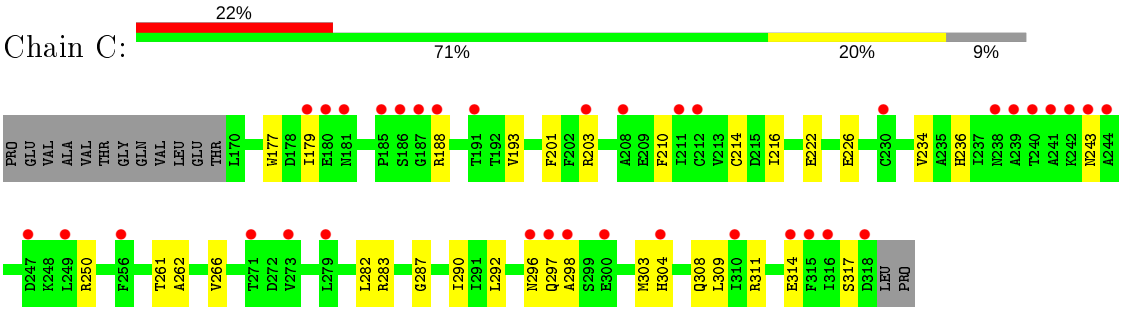
- Molecule 1: Meiosis regulator and mRNA stability factor 1

Chain B:



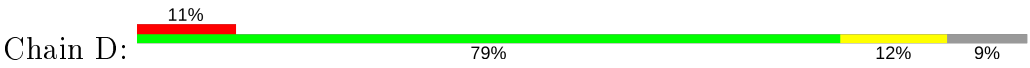
- Molecule 1: Meiosis regulator and mRNA stability factor 1

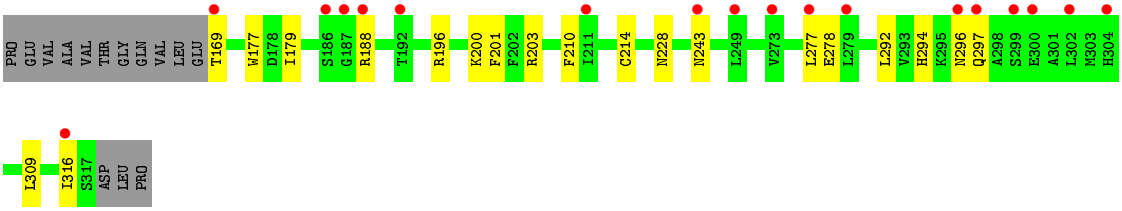
Chain C:



- Molecule 1: Meiosis regulator and mRNA stability factor 1

Chain D:




PRO
GLU
VAL
ALA
VAL
THR
GLY
GLN
VAL
LEU
GLU
T169
W177
D178
I179
S185
G187
R188
T192
R196
K200
F201
F202
R203
F210
I211
C214
N228
N243
L249
V273
L277
E278
L279
L292
V293
H294
K295
N296
Q297
A298
S299
E300
A301
L302
M303
H304
L309
I316
S317
ASP
LEU
PRO

4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	163.47Å 163.47Å 56.15Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.94 – 1.75 29.94 – 1.75	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.94-1.75) 99.8 (29.94-1.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.21 (at 1.75Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.232 , 0.283 0.233 , 0.283	Depositor DCC
R_{free} test set	2859 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	18.0	Xtriage
Anisotropy	0.258	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 52.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.034 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	5140	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 29.05 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.6575e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: 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	0.48	0/1218	0.68	0/1645
1	B	0.40	0/1224	0.61	0/1653
1	C	0.45	0/1217	0.63	0/1643
1	D	0.41	0/1210	0.61	0/1634
All	All	0.44	0/4869	0.63	0/6575

There are no bond length outliers.

There are no bond angle outliers.

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	1197	0	1180	21	1
1	B	1203	0	1184	22	1
1	C	1196	0	1177	31	1
1	D	1189	0	1176	19	0
2	A	18	0	24	3	0
2	B	18	0	24	0	0
2	C	36	0	48	8	0
2	D	6	0	8	3	1
3	A	67	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	63	0	0	7	1
3	C	66	0	0	9	2
3	D	81	0	0	8	1
All	All	5140	0	4821	92	4

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 10.

All (92) 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:298:ALA:HB3	1:B:303:MSE:CE	1.81	1.09
1:D:188:ARG:NH1	1:D:316:ILE:O	1.97	0.98
1:D:200:LYS:NZ	3:D:501:HOH:O	1.96	0.97
1:B:298:ALA:HB3	1:B:303:MSE:HE3	1.43	0.96
1:B:298:ALA:HB3	1:B:303:MSE:HE2	1.61	0.83
1:A:300:GLU:OE2	3:A:501:HOH:O	1.98	0.81
1:C:290:ILE:O	3:C:501:HOH:O	2.02	0.77
1:B:318:ASP:OD2	3:B:501:HOH:O	2.04	0.75
1:A:242:LYS:NZ	1:A:247:ASP:OD2	2.19	0.75
1:A:291:ILE:HG12	3:A:509:HOH:O	1.87	0.73
2:A:403:GOL:O1	2:C:406:GOL:O3	2.03	0.73
1:C:283:ARG:HH11	2:C:403:GOL:H32	1.53	0.73
1:B:298:ALA:CB	1:B:303:MSE:HE3	2.20	0.71
1:D:294:HIS:HE1	2:D:401:GOL:H2	1.56	0.70
1:A:179:ILE:HD11	1:A:212:CYS:HB3	1.73	0.70
2:A:403:GOL:HO1	2:C:406:GOL:HO3	1.37	0.69
1:B:237:ILE:HD11	1:B:245:ALA:HB2	1.74	0.69
1:A:203:ARG:NH2	3:A:504:HOH:O	2.25	0.68
1:C:298:ALA:HB3	1:C:303:MSE:HE2	1.75	0.68
1:B:291:ILE:HG12	3:B:533:HOH:O	1.94	0.68
1:C:250:ARG:NH1	3:C:502:HOH:O	2.27	0.67
1:B:291:ILE:HA	3:B:533:HOH:O	1.95	0.65
1:C:298:ALA:HB3	1:C:303:MSE:CE	2.26	0.65
1:D:278:GLU:OE2	3:D:502:HOH:O	2.14	0.65
1:D:179:ILE:HB	1:D:214:CYS:HB3	1.81	0.63
1:B:237:ILE:HD13	1:B:245:ALA:N	2.14	0.62
1:B:206:ARG:NH1	3:B:502:HOH:O	2.22	0.62
1:B:271:THR:HG23	1:B:298:ALA:HB2	1.80	0.62
1:B:308:GLN:HB2	3:B:533:HOH:O	2.02	0.59
1:D:196:ARG:O	1:D:200:LYS:HB2	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:179:ILE:CG2	1:B:214:CYS:HB3	2.33	0.58
1:A:291:ILE:HA	3:A:509:HOH:O	2.04	0.58
1:C:216:ILE:HD13	1:C:236:HIS:HB2	1.85	0.57
1:C:179:ILE:HG21	1:C:214:CYS:HB3	1.85	0.57
1:D:203:ARG:NH2	3:D:507:HOH:O	2.39	0.56
1:C:216:ILE:HD11	1:C:234:VAL:HG12	1.87	0.55
1:D:228:ASN:ND2	3:D:504:HOH:O	2.34	0.55
1:A:179:ILE:CD1	1:A:212:CYS:HB3	2.37	0.55
1:B:237:ILE:CD1	1:B:245:ALA:HB2	2.37	0.54
1:C:188:ARG:HH21	1:C:317:SER:C	2.10	0.54
1:A:311:ARG:HG3	1:C:311:ARG:HH12	1.71	0.54
1:C:311:ARG:NH2	3:C:508:HOH:O	2.40	0.54
1:B:246:ASP:O	1:B:250:ARG:HG3	2.08	0.53
1:B:292:LEU:HB3	1:B:309:LEU:HD23	1.89	0.53
1:D:294:HIS:CE1	2:D:401:GOL:H2	2.40	0.53
1:A:181:ASN:O	1:A:295:LYS:NZ	2.37	0.53
1:A:305:HIS:HA	2:A:401:GOL:H11	1.90	0.53
1:B:237:ILE:HG13	1:B:237:ILE:O	2.08	0.53
1:A:242:LYS:HE3	1:A:244:ALA:N	2.25	0.52
1:B:179:ILE:HG22	1:B:214:CYS:HB3	1.92	0.52
1:C:308:GLN:N	3:C:501:HOH:O	2.43	0.51
1:A:242:LYS:HE3	1:A:244:ALA:CA	2.40	0.51
1:C:296:ASN:ND2	1:C:297:GLN:HE21	2.09	0.50
1:C:243:ASN:HB3	3:C:507:HOH:O	2.12	0.50
2:C:401:GOL:H2	3:C:527:HOH:O	2.13	0.49
1:C:262:ALA:O	1:D:169:THR:HG21	2.13	0.49
1:B:237:ILE:HD13	1:B:245:ALA:CA	2.42	0.49
1:A:294:HIS:HE1	1:A:311:ARG:CZ	2.27	0.47
1:B:266:VAL:HG21	1:B:282:LEU:HD23	1.96	0.47
1:C:201:PHE:O	2:C:402:GOL:H12	2.15	0.47
1:C:203:ARG:HG3	3:C:564:HOH:O	2.14	0.46
1:D:296:ASN:HA	1:D:297:GLN:HA	1.64	0.46
1:C:287:GLY:O	2:C:401:GOL:H32	2.15	0.46
1:A:311:ARG:NE	1:C:311:ARG:HH22	2.13	0.46
1:C:266:VAL:HG21	1:C:282:LEU:HD23	1.98	0.46
1:C:179:ILE:CG2	1:C:214:CYS:HB3	2.46	0.45
2:C:401:GOL:H12	3:C:535:HOH:O	2.15	0.45
1:B:308:GLN:CB	3:B:533:HOH:O	2.60	0.45
1:A:311:ARG:HG3	1:C:311:ARG:NH1	2.31	0.45
1:A:188:ARG:HD2	1:A:316:ILE:O	2.18	0.44
1:A:200:LYS:NZ	1:A:310:ILE:HD12	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:VAL:HG11	1:A:282:LEU:HD23	2.00	0.43
1:C:177:TRP:CH2	1:C:193:VAL:HG11	2.53	0.43
1:C:292:LEU:HB3	1:C:309:LEU:HD23	2.00	0.43
1:D:297:GLN:HG2	2:D:401:GOL:H31	2.00	0.43
1:D:277:LEU:HA	3:D:516:HOH:O	2.19	0.43
1:C:298:ALA:O	1:C:303:MSE:HE3	2.18	0.43
1:D:177:TRP:CE2	1:D:179:ILE:HD13	2.54	0.43
1:B:229:ASN:ND2	3:B:503:HOH:O	2.37	0.42
1:D:292:LEU:HB3	1:D:309:LEU:HD23	2.00	0.42
1:C:261:THR:HB	1:D:169:THR:HG22	2.02	0.42
1:A:203:ARG:HB2	3:A:567:HOH:O	2.19	0.42
1:C:222:GLU:HG2	1:C:226:GLU:OE1	2.19	0.42
1:C:304:HIS:CE1	2:C:404:GOL:H12	2.55	0.41
1:C:214:CYS:O	1:C:236:HIS:HA	2.20	0.41
1:D:243:ASN:HA	3:D:565:HOH:O	2.21	0.41
1:A:292:LEU:HB3	1:A:309:LEU:HD23	2.03	0.41
1:A:200:LYS:HZ2	1:A:310:ILE:HD12	1.86	0.40
1:C:314:GLU:HB3	3:C:544:HOH:O	2.21	0.40
1:D:243:ASN:HB3	3:D:561:HOH:O	2.21	0.40
1:C:298:ALA:O	1:C:303:MSE:CE	2.70	0.40
1:D:201:PHE:HB3	3:D:542:HOH:O	2.22	0.40

All (4) 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)
1:B:311:ARG:NH1	2:D:401:GOL:O1[3_555]	2.04	0.16
1:A:278:GLU:OE2	1:C:250:ARG:NH2[1_554]	2.08	0.12
3:B:502:HOH:O	3:C:552:HOH:O[5_444]	2.16	0.04
3:C:555:HOH:O	3:D:546:HOH:O[8_544]	2.18	0.02

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	148/163 (91%)	144 (97%)	4 (3%)	0	100	100
1	B	149/163 (91%)	146 (98%)	3 (2%)	0	100	100
1	C	148/163 (91%)	145 (98%)	3 (2%)	0	100	100
1	D	147/163 (90%)	143 (97%)	4 (3%)	0	100	100
All	All	592/652 (91%)	578 (98%)	14 (2%)	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	132/141 (94%)	127 (96%)	5 (4%)	33	11
1	B	133/141 (94%)	131 (98%)	2 (2%)	65	49
1	C	132/141 (94%)	131 (99%)	1 (1%)	81	72
1	D	131/141 (93%)	130 (99%)	1 (1%)	81	72
All	All	528/564 (94%)	519 (98%)	9 (2%)	60	42

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

Mol	Chain	Res	Type
1	A	186	SER
1	A	188	ARG
1	A	210	PHE
1	A	242	LYS
1	A	266	VAL
1	B	210	PHE
1	B	300	GLU
1	C	210	PHE
1	D	210	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such

sidechains are listed below:

Mol	Chain	Res	Type
1	C	296	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 carbohydrates in this entry.

5.6 Ligand geometry

13 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	GOL	C	402	-	5,5,5	0.32	0	5,5,5	0.50	0
2	GOL	C	406	-	5,5,5	0.37	0	5,5,5	0.42	0
2	GOL	B	403	-	5,5,5	0.37	0	5,5,5	0.58	0
2	GOL	A	403	-	5,5,5	0.35	0	5,5,5	0.47	0
2	GOL	C	403	-	5,5,5	0.39	0	5,5,5	0.28	0
2	GOL	C	404	-	5,5,5	0.27	0	5,5,5	0.19	0
2	GOL	B	402	-	5,5,5	0.36	0	5,5,5	0.33	0
2	GOL	B	401	-	5,5,5	0.33	0	5,5,5	0.18	0
2	GOL	C	401	-	5,5,5	0.32	0	5,5,5	0.71	0
2	GOL	A	401	-	5,5,5	0.22	0	5,5,5	0.37	0
2	GOL	D	401	-	5,5,5	0.35	0	5,5,5	0.65	0
2	GOL	C	405	-	5,5,5	0.39	0	5,5,5	0.21	0
2	GOL	A	402	-	5,5,5	0.47	0	5,5,5	0.90	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	GOL	C	402	-	-	4/4/4/4	-
2	GOL	C	406	-	-	2/4/4/4	-
2	GOL	B	403	-	-	4/4/4/4	-
2	GOL	A	403	-	-	2/4/4/4	-
2	GOL	C	403	-	-	4/4/4/4	-
2	GOL	C	404	-	-	3/4/4/4	-
2	GOL	B	402	-	-	2/4/4/4	-
2	GOL	B	401	-	-	1/4/4/4	-
2	GOL	C	401	-	-	2/4/4/4	-
2	GOL	A	401	-	-	2/4/4/4	-
2	GOL	D	401	-	-	0/4/4/4	-
2	GOL	C	405	-	-	2/4/4/4	-
2	GOL	A	402	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	402	GOL	O1-C1-C2-C3
2	C	406	GOL	C1-C2-C3-O3
2	C	404	GOL	C1-C2-C3-O3
2	C	401	GOL	C1-C2-C3-O3
2	C	405	GOL	O1-C1-C2-C3
2	A	402	GOL	O1-C1-C2-O2
2	A	402	GOL	O1-C1-C2-C3
2	C	402	GOL	C1-C2-C3-O3
2	B	403	GOL	O1-C1-C2-C3
2	B	403	GOL	C1-C2-C3-O3
2	C	403	GOL	O1-C1-C2-C3
2	B	402	GOL	O1-C1-C2-C3
2	A	401	GOL	C1-C2-C3-O3
2	B	403	GOL	O2-C2-C3-O3
2	C	404	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
2	C	402	GOL	O1-C1-C2-O2
2	C	406	GOL	O2-C2-C3-O3
2	C	401	GOL	O2-C2-C3-O3
2	C	403	GOL	O1-C1-C2-O2
2	C	403	GOL	O2-C2-C3-O3
2	C	402	GOL	O2-C2-C3-O3
2	B	403	GOL	O1-C1-C2-O2
2	C	405	GOL	O1-C1-C2-O2
2	A	403	GOL	O1-C1-C2-C3
2	B	402	GOL	O1-C1-C2-O2
2	A	401	GOL	O2-C2-C3-O3
2	B	401	GOL	O1-C1-C2-C3
2	A	403	GOL	O1-C1-C2-O2
2	C	403	GOL	C1-C2-C3-O3
2	C	404	GOL	O1-C1-C2-C3

There are no ring outliers.

8 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	402	GOL	1	0
2	C	406	GOL	2	0
2	A	403	GOL	2	0
2	C	403	GOL	1	0
2	C	404	GOL	1	0
2	C	401	GOL	3	0
2	A	401	GOL	1	0
2	D	401	GOL	3	1

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	148/163 (90%)	1.24	24 (16%)	1 2	9, 18, 37, 49	0
1	B	148/163 (90%)	1.44	28 (18%)	1 1	9, 20, 42, 54	0
1	C	147/163 (90%)	1.58	36 (24%)	0 0	11, 20, 41, 51	0
1	D	147/163 (90%)	1.19	18 (12%)	4 6	10, 18, 39, 51	0
All	All	590/652 (90%)	1.36	106 (17%)	1 2	9, 19, 40, 54	0

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	240	THR	10.2
1	A	186	SER	8.6
1	C	242	LYS	8.6
1	A	169	THR	7.9
1	C	241	ALA	7.8
1	B	169	THR	6.4
1	D	169	THR	6.1
1	A	316	ILE	6.1
1	C	186	SER	6.0
1	B	239	ALA	5.8
1	A	240	THR	5.6
1	B	240	THR	5.5
1	C	297	GLN	5.3
1	C	318	ASP	5.2
1	A	243	ASN	5.2
1	D	186	SER	5.0
1	C	244	ALA	5.0
1	C	243	ASN	4.9
1	D	243	ASN	4.8
1	B	188	ARG	4.8
1	D	297	GLN	4.7

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Mol	Chain	Res	Type	RSRZ
1	C	239	ALA	4.7
1	B	186	SER	4.6
1	B	243	ASN	4.6
1	D	299	SER	4.5
1	D	296	ASN	4.4
1	B	242	LYS	4.4
1	B	318	ASP	4.3
1	B	241	ALA	4.2
1	A	297	GLN	4.2
1	A	318	ASP	4.1
1	D	187	GLY	4.0
1	A	317	SER	3.9
1	A	239	ALA	3.9
1	A	241	ALA	3.7
1	B	316	ILE	3.7
1	C	212[A]	CYS	3.6
1	D	188	ARG	3.6
1	C	211	ILE	3.6
1	B	314	GLU	3.5
1	D	304	HIS	3.5
1	C	296	ASN	3.5
1	C	187	GLY	3.4
1	C	316	ILE	3.4
1	B	296	ASN	3.4
1	C	247	ASP	3.4
1	B	212[A]	CYS	3.4
1	D	273	VAL	3.3
1	B	297	GLN	3.3
1	C	279	LEU	3.3
1	B	315	PHE	3.2
1	C	203	ARG	3.2
1	B	238	ASN	3.1
1	C	181	ASN	3.1
1	D	300	GLU	3.1
1	D	316	ILE	3.1
1	C	315	PHE	3.0
1	C	179	ILE	2.9
1	B	232	VAL	2.9
1	B	180	GLU	2.8
1	C	180	GLU	2.8
1	B	185	PRO	2.8
1	C	249	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	211	ILE	2.7
1	A	302	LEU	2.7
1	D	249	LEU	2.7
1	A	185	PRO	2.7
1	C	185	PRO	2.7
1	C	314	GLU	2.6
1	A	296	ASN	2.6
1	B	246	ASP	2.5
1	A	315	PHE	2.5
1	A	242	LYS	2.5
1	A	180	GLU	2.5
1	C	271	THR	2.5
1	C	304	HIS	2.5
1	D	279	LEU	2.5
1	C	230	CYS	2.4
1	C	238	ASN	2.4
1	C	191	THR	2.4
1	B	273	VAL	2.3
1	C	256	PHE	2.3
1	D	192	THR	2.3
1	B	249	LEU	2.3
1	B	237	ILE	2.3
1	C	310	ILE	2.2
1	A	187	GLY	2.2
1	A	190	ALA	2.2
1	C	298	ALA	2.2
1	C	273	VAL	2.2
1	D	302	LEU	2.2
1	A	222	GLU	2.2
1	B	187	GLY	2.2
1	B	201	PHE	2.2
1	A	256	PHE	2.1
1	C	188	ARG	2.1
1	B	309	LEU	2.1
1	A	310	ILE	2.1
1	B	317	SER	2.1
1	A	201	PHE	2.1
1	C	208	ALA	2.0
1	B	247	ASP	2.0
1	A	273	VAL	2.0
1	C	300	GLU	2.0
1	A	279	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	277	LEU	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, 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	B-factors(Å^2)	Q<0.9
2	GOL	C	403	6/6	0.61	0.29	29,30,31,36	0
2	GOL	A	402	6/6	0.62	0.35	21,24,34,35	0
2	GOL	B	402	6/6	0.65	0.26	28,33,35,40	0
2	GOL	A	403	6/6	0.69	0.30	42,47,49,54	0
2	GOL	C	401	6/6	0.70	0.30	23,28,32,36	0
2	GOL	C	402	6/6	0.70	0.22	22,25,31,33	0
2	GOL	B	403	6/6	0.72	0.34	15,27,31,35	0
2	GOL	C	405	6/6	0.73	0.32	24,32,36,42	0
2	GOL	C	404	6/6	0.77	0.17	21,27,32,37	0
2	GOL	C	406	6/6	0.80	0.34	32,35,36,37	0
2	GOL	A	401	6/6	0.85	0.20	17,26,30,36	0
2	GOL	D	401	6/6	0.86	0.20	41,41,43,45	0
2	GOL	B	401	6/6	0.88	0.17	22,27,30,32	0

6.5 Other polymers (i)

There are no such residues in this entry.