



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:36 PM UTC

PDB ID : 5YAA / pdb_00005yaa
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 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

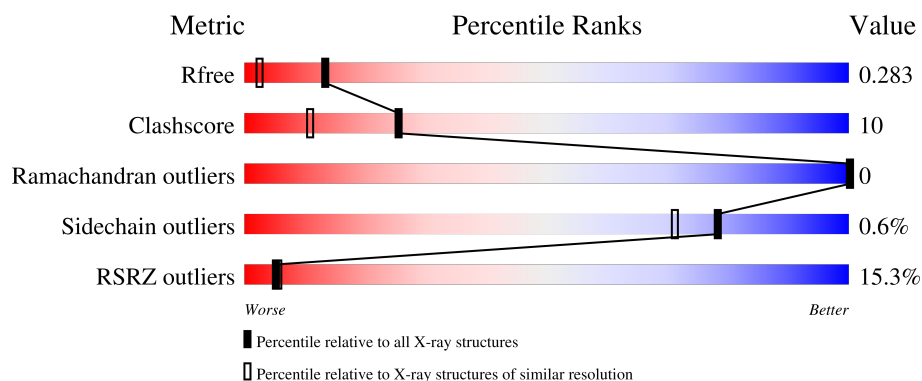
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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}	180053	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (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 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	163	
1	B	163	
1	C	163	
1	D	163	

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	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.

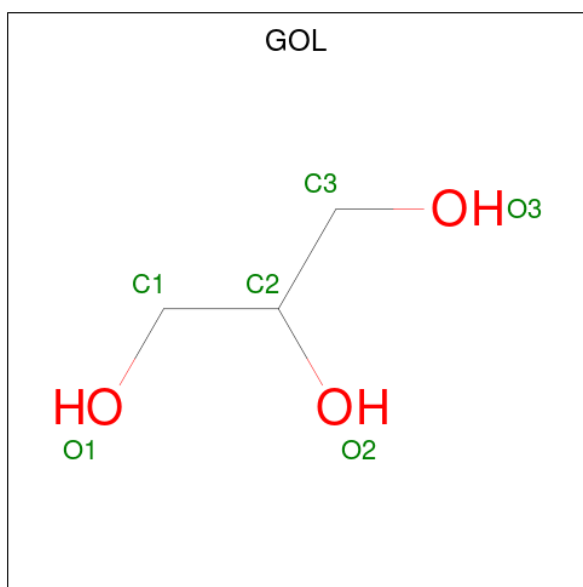
- Molecule 1 is a protein called Meiosis regulator and mRNA stability factor 1.

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 (CCD ID: GOL) (formula: C₃H₈O₃).



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	D	1	Total	C	O	0	0
			6	3	3		

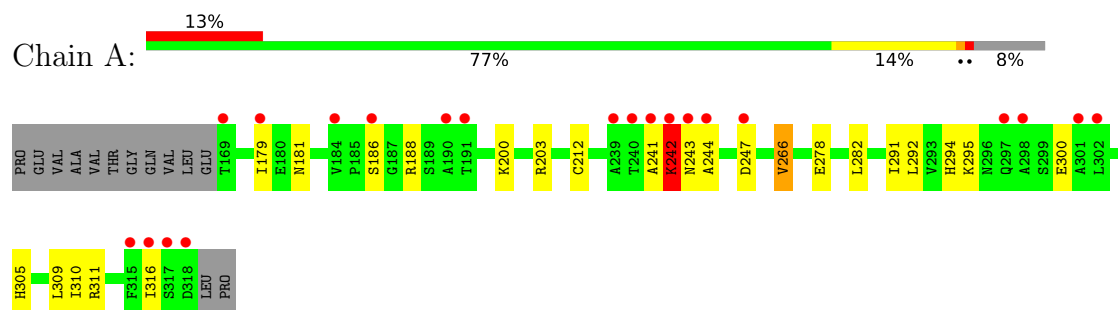
- Molecule 3 is water.

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

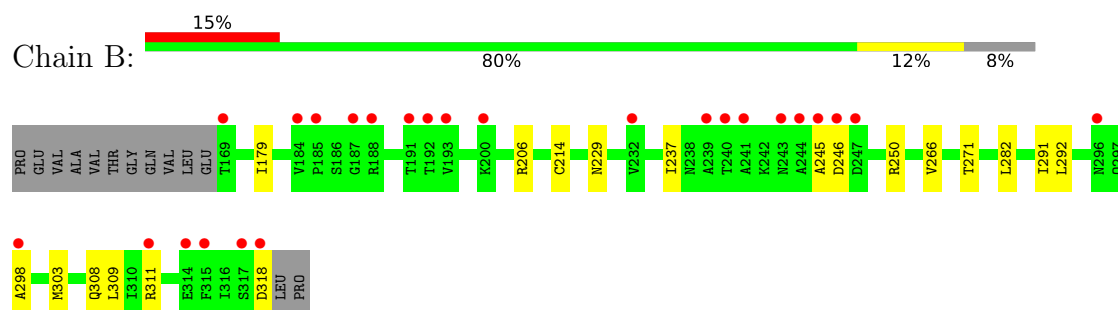
3 Residue-property plots [i](#)

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.

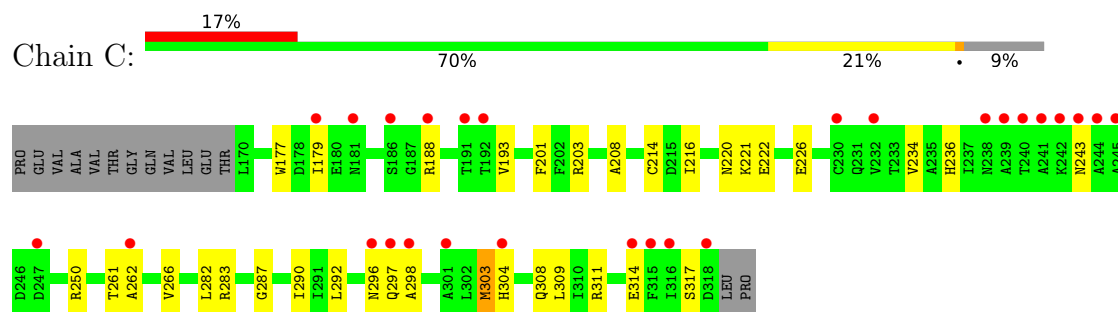
- Molecule 1: Meiosis regulator and mRNA stability factor 1



- Molecule 1: Meiosis regulator and mRNA stability factor 1

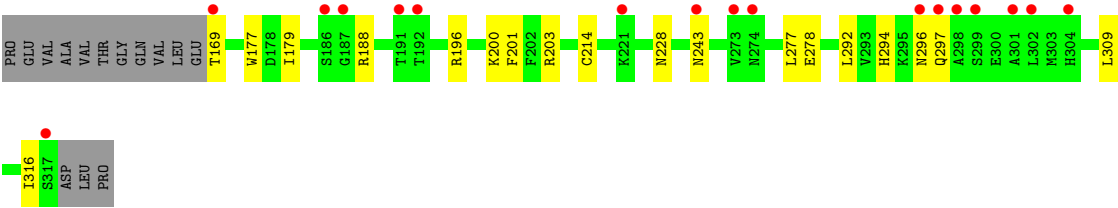


- Molecule 1: Meiosis regulator and mRNA stability factor 1



- Molecule 1: Meiosis regulator and mRNA stability factor 1





4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ 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	2861 reflections (5.07%)	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)	0.37 , 42.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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.*

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	0.55	1/1218 (0.1%)	0.75	2/1645 (0.1%)
1	B	0.37	0/1224	0.62	0/1653
1	C	0.50	1/1217 (0.1%)	0.69	2/1643 (0.1%)
1	D	0.41	0/1210	0.63	0/1634
All	All	0.46	2/4869 (0.0%)	0.67	4/6575 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	241	ALA	N-CA	-7.22	1.37	1.46
1	C	220	ASN	C-O	-5.90	1.16	1.23

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	243	ASN	N-CA-C	-7.05	104.69	112.72
1	C	221	LYS	N-CA-C	5.46	117.23	111.28
1	A	242	LYS	N-CA-C	5.45	122.41	110.80
1	C	303	MSE	N-CA-C	5.23	117.72	111.71

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	1197	0	1180	20	1
1	B	1203	0	1184	22	1
1	C	1196	0	1177	32	1
1	D	1189	0	1176	19	0
2	A	18	0	24	4	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	6	0
3	B	63	0	0	7	1
3	C	66	0	0	10	2
3	D	81	0	0	8	1
All	All	5140	0	4821	93	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 (93) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:188:ARG:HH21	1:C:317:SER:C	2.10	0.59
1:D:196:ARG:O	1:D:200:LYS:HB2	2.01	0.59
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:A:181:ASN:O	1:A:295:LYS:NZ	2.37	0.56
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: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:305:HIS:HA	2:A:401:GOL:H11	1.90	0.53
1:B:237:ILE:O	1:B:237:ILE:HG13	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
2:A:402:GOL:O2	3:A:502:HOH:O	2.11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:208:ALA:C	3:C:526:HOH:O	2.65	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%)	129 (98%)	3 (2%)	44	24
1	B	133/141 (94%)	133 (100%)	0	100	100
1	C	132/141 (94%)	132 (100%)	0	100	100
1	D	131/141 (93%)	131 (100%)	0	100	100
All	All	528/564 (94%)	525 (99%)	3 (1%)	78	71

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	186	SER
1	A	242	LYS
1	A	266	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	308	GLN
1	C	296	ASN
1	C	297	GLN
1	D	294	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	B	401	-	5,5,5	0.34	0	5,5,5	0.21	0
2	GOL	B	402	-	5,5,5	0.36	0	5,5,5	0.34	0
2	GOL	C	403	-	5,5,5	0.40	0	5,5,5	0.30	0
2	GOL	C	406	-	5,5,5	0.37	0	5,5,5	0.46	0
2	GOL	C	401	-	5,5,5	0.32	0	5,5,5	0.76	0
2	GOL	C	404	-	5,5,5	0.27	0	5,5,5	0.21	0
2	GOL	C	402	-	5,5,5	0.32	0	5,5,5	0.52	0
2	GOL	A	403	-	5,5,5	0.35	0	5,5,5	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GOL	A	402	-	5,5,5	0.49	0	5,5,5	0.95	0
2	GOL	D	401	-	5,5,5	0.35	0	5,5,5	0.71	0
2	GOL	A	401	-	5,5,5	0.22	0	5,5,5	0.40	0
2	GOL	C	405	-	5,5,5	0.39	0	5,5,5	0.23	0
2	GOL	B	403	-	5,5,5	0.37	0	5,5,5	0.64	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	B	401	-	-	1/4/4/4	-
2	GOL	B	402	-	-	2/4/4/4	-
2	GOL	C	403	-	-	3/4/4/4	-
2	GOL	C	406	-	-	2/4/4/4	-
2	GOL	C	401	-	-	2/4/4/4	-
2	GOL	C	404	-	-	2/4/4/4	-
2	GOL	C	402	-	-	4/4/4/4	-
2	GOL	A	403	-	-	2/4/4/4	-
2	GOL	A	402	-	-	2/4/4/4	-
2	GOL	D	401	-	-	0/4/4/4	-
2	GOL	A	401	-	-	2/4/4/4	-
2	GOL	C	405	-	-	2/4/4/4	-
2	GOL	B	403	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (28) torsion outliers are listed below:

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

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

There are no ring outliers.

9 monomers are involved in 14 short contacts:

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

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, 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	148/163 (90%)	0.87	21 (14%) 6 7	9, 18, 37, 49	0
1	B	148/163 (90%)	1.10	25 (16%) 4 4	8, 20, 42, 54	1 (0%)
1	C	147/163 (90%)	1.18	27 (18%) 3 3	8, 20, 41, 51	1 (0%)
1	D	147/163 (90%)	0.87	17 (11%) 9 10	10, 18, 39, 51	0
All	All	590/652 (90%)	1.01	90 (15%) 5 5	8, 19, 40, 54	2 (0%)

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	241	ALA	6.1
1	C	244	ALA	5.1
1	C	240	THR	4.8
1	D	298	ALA	4.4
1	A	169	THR	4.3
1	D	299	SER	4.2
1	A	243	ASN	4.1
1	A	241	ALA	4.1
1	B	243	ASN	4.1
1	C	243	ASN	4.0
1	B	318	ASP	4.0
1	A	186	SER	3.9
1	B	241	ALA	3.9
1	B	169	THR	3.8
1	C	242	LYS	3.8
1	B	239	ALA	3.8
1	D	243	ASN	3.8
1	C	191	THR	3.7
1	D	186	SER	3.5
1	A	317	SER	3.3
1	D	297	GLN	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	188	ARG	3.3
1	B	191	THR	3.2
1	A	318	ASP	3.2
1	C	192	THR	3.2
1	A	239	ALA	3.2
1	C	301	ALA	3.1
1	D	169	THR	3.1
1	C	247	ASP	3.0
1	B	240	THR	3.0
1	A	298	ALA	3.0
1	B	315	PHE	2.9
1	D	304	HIS	2.9
1	C	316	ILE	2.9
1	D	296	ASN	2.9
1	B	232	VAL	2.9
1	C	181	ASN	2.9
1	D	317	SER	2.8
1	C	179	ILE	2.8
1	B	245	ALA	2.8
1	B	192	THR	2.8
1	D	221	LYS	2.8
1	B	244	ALA	2.7
1	B	246	ASP	2.7
1	C	315	PHE	2.7
1	C	318	ASP	2.7
1	D	191	THR	2.6
1	D	192	THR	2.6
1	C	245	ALA	2.6
1	C	296	ASN	2.6
1	C	297	GLN	2.5
1	A	242	LYS	2.5
1	B	314	GLU	2.5
1	C	298	ALA	2.5
1	B	298	ALA	2.5
1	B	184	VAL	2.4
1	B	200	LYS	2.4
1	D	302	LEU	2.4
1	A	301	ALA	2.4
1	C	188	ARG	2.4
1	A	302	LEU	2.4
1	C	304	HIS	2.4
1	C	186	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	262	ALA	2.3
1	A	297	GLN	2.3
1	B	311	ARG	2.3
1	B	296	ASN	2.3
1	A	191	THR	2.2
1	A	244	ALA	2.2
1	C	239	ALA	2.2
1	C	238	ASN	2.2
1	B	317	SER	2.2
1	B	187	GLY	2.2
1	B	193	VAL	2.2
1	D	273	VAL	2.2
1	A	240	THR	2.2
1	C	232	VAL	2.2
1	D	187	GLY	2.2
1	B	247	ASP	2.1
1	A	179	ILE	2.1
1	C	314	GLU	2.1
1	A	316	ILE	2.1
1	A	190	ALA	2.1
1	D	301	ALA	2.1
1	C	230	CYS	2.1
1	A	247	ASP	2.1
1	B	185	PRO	2.0
1	D	274	ASN	2.0
1	A	315	PHE	2.0
1	A	184	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 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(Å ²)	Q<0.9
2	GOL	A	403	6/6	0.55	0.23	42,47,49,54	0
2	GOL	A	402	6/6	0.68	0.20	21,24,34,35	0
2	GOL	C	405	6/6	0.71	0.17	24,32,36,42	0
2	GOL	C	402	6/6	0.74	0.19	22,25,31,33	0
2	GOL	C	403	6/6	0.74	0.16	29,30,31,36	0
2	GOL	C	401	6/6	0.74	0.17	23,28,32,36	0
2	GOL	B	402	6/6	0.75	0.16	28,33,35,40	0
2	GOL	B	403	6/6	0.75	0.20	15,27,31,35	0
2	GOL	D	401	6/6	0.80	0.13	41,41,43,45	0
2	GOL	C	406	6/6	0.81	0.13	32,35,36,37	0
2	GOL	C	404	6/6	0.83	0.13	21,27,32,37	0
2	GOL	B	401	6/6	0.87	0.11	22,27,30,32	0
2	GOL	A	401	6/6	0.89	0.14	17,26,30,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.