



Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 06:11 pm BST

PDB ID : 6QTB
Title : Crystal structure of Rea1-MIDAS/Ytm1-UBL complex from *Chaetomium thermophilum*
Authors : Ahmed, Y.L.; Thoms, M.; Hurt, E.; Sinning, I.
Deposited on : 2019-02-22
Resolution : 1.89 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

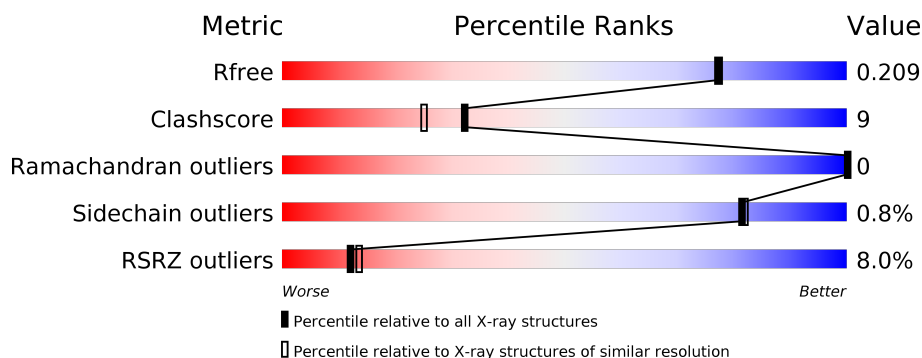
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.89 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	280	<div> <div>9%</div> <div> <div></div> <div>78%</div> <div>11%</div> <div>•</div> <div>9%</div> </div> </div>
1	D	280	<div> <div>9%</div> <div> <div></div> <div>78%</div> <div>10%</div> <div>•</div> <div>10%</div> </div> </div>
2	B	101	<div> <div>2%</div> <div> <div></div> <div>77%</div> <div>9%</div> <div></div> <div>14%</div> </div> </div>
2	E	101	<div> <div>3%</div> <div> <div></div> <div>77%</div> <div>9%</div> <div></div> <div>14%</div> </div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5794 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 Midasin,Midasin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	254	Total	C	N	O	S	0	0	0
			2005	1267	357	372	9			
1	D	251	Total	C	N	O	S	0	0	0
			1985	1258	351	367	9			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4689	MET	-	initiating methionine	UNP G0SHE6
A	4734	GLY	-	linker	UNP G0SHE6
A	4735	SER	-	linker	UNP G0SHE6
A	4773	GLY	-	linker	UNP G0SHE6
A	4998	GLY	-	expression tag	UNP G0SHE6
A	4999	SER	-	expression tag	UNP G0SHE6
A	5000	HIS	-	expression tag	UNP G0SHE6
A	5001	HIS	-	expression tag	UNP G0SHE6
A	5002	HIS	-	expression tag	UNP G0SHE6
A	5003	HIS	-	expression tag	UNP G0SHE6
A	5004	HIS	-	expression tag	UNP G0SHE6
A	5005	HIS	-	expression tag	UNP G0SHE6
D	4689	MET	-	initiating methionine	UNP G0SHE6
D	4734	GLY	-	linker	UNP G0SHE6
D	4772	SER	-	linker	UNP G0SHE6
D	4773	GLY	-	linker	UNP G0SHE6
D	4998	GLY	-	expression tag	UNP G0SHE6
D	4999	SER	-	expression tag	UNP G0SHE6
D	5000	HIS	-	expression tag	UNP G0SHE6
D	5001	HIS	-	expression tag	UNP G0SHE6
D	5002	HIS	-	expression tag	UNP G0SHE6
D	5003	HIS	-	expression tag	UNP G0SHE6
D	5004	HIS	-	expression tag	UNP G0SHE6
D	5005	HIS	-	expression tag	UNP G0SHE6

- Molecule 2 is a protein called Ribosome biogenesis protein YTM1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	87	Total	C	N	O	S	0	0	0
			689	437	113	138	1			
2	E	87	Total	C	N	O	S	0	0	0
			689	437	113	138	1			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	MET	-	initiating methionine	UNP G0SFB5
B	-1	LYS	-	expression tag	UNP G0SFB5
B	0	HIS	-	expression tag	UNP G0SFB5
B	1	HIS	-	expression tag	UNP G0SFB5
B	2	HIS	-	expression tag	UNP G0SFB5
B	3	HIS	-	expression tag	UNP G0SFB5
B	4	HIS	-	expression tag	UNP G0SFB5
B	5	HIS	-	expression tag	UNP G0SFB5
B	6	PRO	-	expression tag	UNP G0SFB5
B	7	MET	-	expression tag	UNP G0SFB5
E	-2	MET	-	initiating methionine	UNP G0SFB5
E	-1	LYS	-	expression tag	UNP G0SFB5
E	0	HIS	-	expression tag	UNP G0SFB5
E	1	HIS	-	expression tag	UNP G0SFB5
E	2	HIS	-	expression tag	UNP G0SFB5
E	3	HIS	-	expression tag	UNP G0SFB5
E	4	HIS	-	expression tag	UNP G0SFB5
E	5	HIS	-	expression tag	UNP G0SFB5
E	6	PRO	-	expression tag	UNP G0SFB5
E	7	MET	-	expression tag	UNP G0SFB5

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

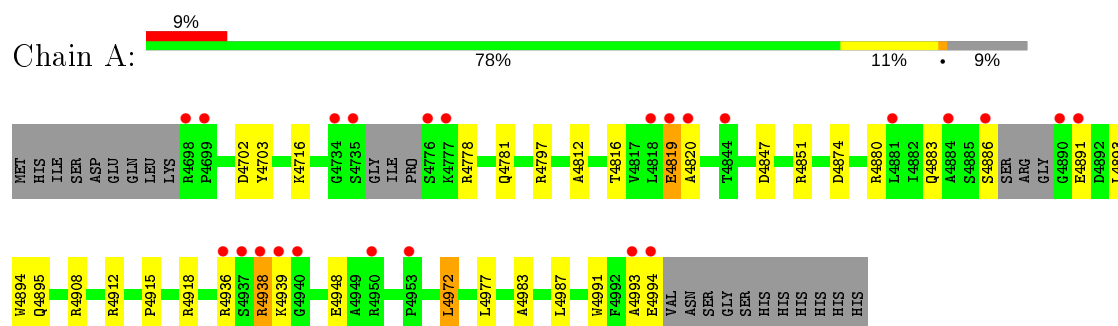
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	130	Total	O	0	0
			130	130		
5	B	71	Total	O	0	0
			71	71		
5	D	130	Total	O	0	0
			130	130		
5	E	75	Total	O	0	0
			75	75		

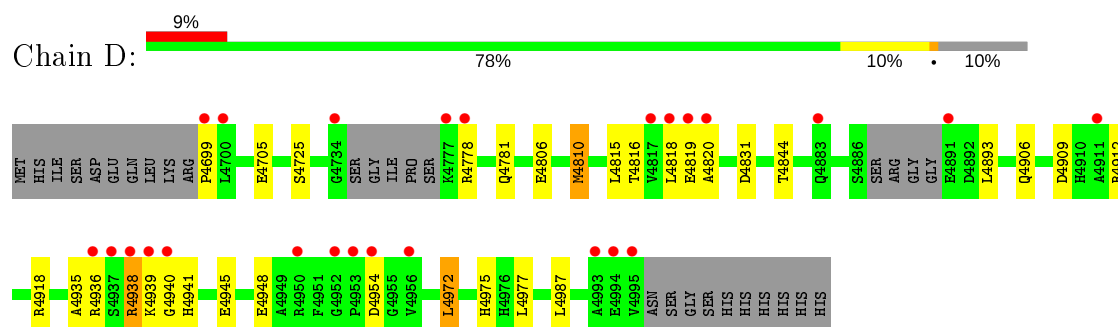
3 Residue-property plots [i](#)

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.

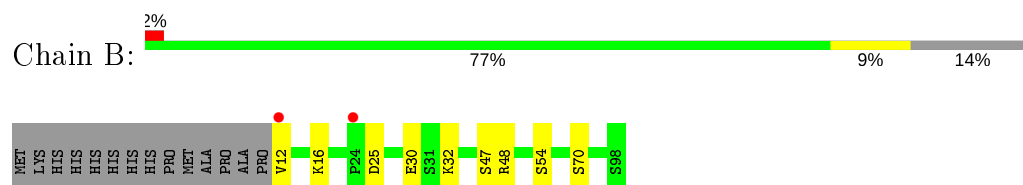
- Molecule 1: Midasin,Midasin



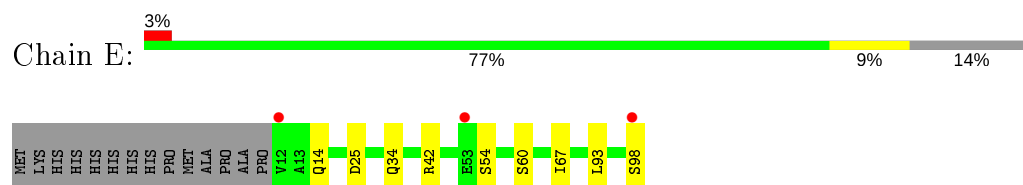
- Molecule 1: Midasin,Midasin



- Molecule 2: Ribosome biogenesis protein YTM1



- Molecule 2: Ribosome biogenesis protein YTM1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	75.55Å 83.18Å 77.69Å 90.00° 117.72° 90.00°	Depositor
Resolution (Å)	36.58 – 1.89 39.61 – 1.84	Depositor EDS
% Data completeness (in resolution range)	98.1 (36.58-1.89) 99.0 (39.61-1.84)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 1.84Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.190 , 0.213 0.187 , 0.209	Depositor DCC
R_{free} test set	3768 reflections (5.15%)	wwPDB-VP
Wilson B-factor (Å ²)	28.6	Xtriage
Anisotropy	0.270	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 54.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.018 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5794	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.59% 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: GOL, 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	0.78	0/2041	0.86	3/2761 (0.1%)
1	D	0.82	1/2021 (0.0%)	0.86	2/2735 (0.1%)
2	B	0.85	0/699	0.84	0/947
2	E	0.87	0/699	0.86	1/947 (0.1%)
All	All	0.82	1/5460 (0.0%)	0.86	6/7390 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	4810	MET	CB-CG	5.42	1.68	1.51

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4972	LEU	CB-CG-CD2	-8.73	96.16	111.00
1	D	4972	LEU	CB-CG-CD2	-7.77	97.79	111.00
1	A	4819	GLU	CA-CB-CG	-6.62	98.85	113.40
1	D	4831	ASP	CB-CG-OD1	6.45	124.11	118.30
1	A	4908	ARG	CD-NE-CZ	6.14	132.19	123.60
2	E	42	ARG	NE-CZ-NH1	-5.05	117.78	120.30

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	2005	0	2002	31	0
1	D	1985	0	1986	46	0
2	B	689	0	699	10	0
2	E	689	0	699	10	0
3	A	1	0	0	0	0
3	D	1	0	0	0	0
4	A	6	0	8	2	0
4	D	6	0	8	0	0
4	E	6	0	8	1	0
5	A	130	0	0	13	0
5	B	71	0	0	5	0
5	D	130	0	0	13	0
5	E	75	0	0	5	0
All	All	5794	0	5410	95	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 9.

All (95) 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:D:4936:ARG:HA	1:D:4938:ARG:CD	1.81	1.11
2:E:34:GLN:NE2	5:E:201:HOH:O	1.81	1.10
1:D:4935:ALA:O	1:D:4938:ARG:HD3	1.59	1.01
1:D:4815:LEU:O	5:D:5201:HOH:O	1.85	0.93
1:D:4705:GLU:OE1	5:D:5202:HOH:O	1.87	0.92
1:D:4936:ARG:HA	1:D:4938:ARG:HD3	1.50	0.90
1:D:4699:PRO:O	5:D:5203:HOH:O	1.92	0.87
1:D:4936:ARG:HA	1:D:4938:ARG:NE	1.90	0.87
1:A:4936:ARG:NH2	5:A:5204:HOH:O	2.10	0.84
1:A:4994:GLU:N	5:A:5202:HOH:O	2.10	0.84
1:A:4702:ASP:OD1	5:A:5201:HOH:O	1.95	0.83
1:D:4945:GLU:OE2	5:D:5204:HOH:O	1.98	0.82
1:D:4818:LEU:N	5:D:5201:HOH:O	2.06	0.81
1:A:4936:ARG:NH1	5:A:5204:HOH:O	2.16	0.79
1:D:4906:GLN:HE22	2:E:14:GLN:H	1.32	0.77
1:D:4819:GLU:HG3	1:D:4820:ALA:H	1.48	0.77
1:A:4797:ARG:HE	1:A:4938:ARG:HH12	1.34	0.75
1:D:4948:GLU:OE2	5:D:5205:HOH:O	2.05	0.75
1:A:4797:ARG:HE	1:A:4938:ARG:NH1	1.84	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4880:ARG:HH21	1:A:4895:GLN:HE22	1.34	0.73
2:E:54:SER:HB3	5:E:222:HOH:O	1.89	0.72
1:A:4936:ARG:CZ	5:A:5204:HOH:O	2.35	0.72
2:E:34:GLN:CD	5:E:201:HOH:O	2.15	0.71
1:D:4936:ARG:CA	1:D:4938:ARG:NE	2.53	0.71
1:A:4936:ARG:NH2	5:A:5206:HOH:O	2.22	0.71
1:D:4936:ARG:CA	1:D:4938:ARG:HD3	2.24	0.68
2:B:48:ARG:NH1	5:B:101:HOH:O	1.73	0.68
1:A:4948:GLU:OE2	5:A:5203:HOH:O	2.10	0.68
1:D:4816:THR:HG22	1:D:4844:THR:HG23	1.76	0.67
1:D:4806:GLU:OE1	5:D:5206:HOH:O	2.15	0.64
1:D:4954:ASP:OD2	1:D:4954:ASP:N	2.24	0.64
4:A:5102:GOL:H12	5:A:5232:HOH:O	1.98	0.64
1:D:4936:ARG:NH2	5:D:5206:HOH:O	2.06	0.63
1:D:4816:THR:CG2	1:D:4844:THR:HG23	2.29	0.62
1:A:4883:GLN:OE1	1:A:4891:GLU:HG3	1.99	0.62
1:D:4936:ARG:CA	1:D:4938:ARG:CD	2.71	0.61
1:D:4939:LYS:HZ3	1:D:4941:HIS:CE1	2.19	0.59
1:D:4936:ARG:HB2	1:D:4938:ARG:CZ	2.32	0.59
1:D:4810:MET:HE3	1:D:4977:LEU:HD22	1.87	0.57
1:D:4819:GLU:CG	1:D:4820:ALA:H	2.17	0.56
1:A:4883:GLN:OE1	1:A:4891:GLU:CG	2.53	0.56
1:A:4781:GLN:HG3	1:A:4893:LEU:HD11	1.86	0.55
1:A:4716:LYS:HZ2	1:A:4977:LEU:HD12	1.72	0.55
1:D:4939:LYS:NZ	1:D:4941:HIS:HE1	2.05	0.55
1:D:4816:THR:C	5:D:5201:HOH:O	2.46	0.54
2:B:16:LYS:NZ	5:B:104:HOH:O	2.25	0.54
1:A:4880:ARG:HH21	1:A:4895:GLN:NE2	2.06	0.54
1:D:4699:PRO:HG2	5:D:5203:HOH:O	2.08	0.53
2:E:98:SER:HA	5:E:227:HOH:O	2.07	0.53
2:E:25:ASP:N	2:E:25:ASP:OD1	2.24	0.52
1:A:4991:TRP:C	5:A:5202:HOH:O	2.47	0.52
1:D:4781:GLN:HG3	1:D:4893:LEU:HD11	1.93	0.51
1:A:4703:TYR:OH	1:A:4847:ASP:OD1	2.22	0.51
1:D:4918:ARG:NH2	5:D:5207:HOH:O	2.11	0.51
1:A:4874:ASP:OD2	5:A:5205:HOH:O	2.20	0.50
1:D:4935:ALA:O	1:D:4938:ARG:CD	2.47	0.49
1:D:4936:ARG:O	1:D:4938:ARG:NE	2.42	0.48
1:D:4938:ARG:C	1:D:4940:GLY:H	2.17	0.48
1:D:4939:LYS:NZ	1:D:4941:HIS:CE1	2.81	0.48
1:D:4906:GLN:OE1	4:E:101:GOL:H2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4812:ALA:O	1:A:4816:THR:HG23	2.14	0.48
1:A:4716:LYS:NZ	1:A:4977:LEU:HD12	2.29	0.47
1:D:4906:GLN:HE22	2:E:14:GLN:N	2.07	0.47
2:B:47:SER:OG	2:B:48:ARG:NH2	2.48	0.46
1:D:4941:HIS:CD2	2:E:34:GLN:HE21	2.34	0.46
1:D:4909:ASP:HA	1:D:4912:ARG:HG3	1.98	0.46
2:B:12:VAL:HG22	2:B:12:VAL:O	2.16	0.46
2:B:32:LYS:HD3	2:B:54:SER:O	2.16	0.46
1:A:4972:LEU:HD21	1:A:4987:LEU:CD1	2.46	0.46
2:B:48:ARG:NH2	5:B:107:HOH:O	2.49	0.45
1:A:4778:ARG:HD3	1:A:4894:TRP:CE2	2.52	0.45
2:B:25:ASP:CG	5:B:103:HOH:O	2.55	0.45
1:A:4939:LYS:HE2	2:B:30:GLU:OE2	2.17	0.45
1:A:4918:ARG:NH2	5:A:5216:HOH:O	2.51	0.44
1:A:4912:ARG:O	1:A:4915:PRO:HD2	2.17	0.44
4:A:5102:GOL:H11	5:A:5223:HOH:O	2.17	0.44
1:D:4936:ARG:HB2	1:D:4938:ARG:NH2	2.33	0.44
1:D:4936:ARG:C	1:D:4938:ARG:NE	2.71	0.44
1:A:4883:GLN:HA	1:A:4883:GLN:NE2	2.33	0.43
1:A:4972:LEU:HD22	1:A:4983:ALA:HB1	2.01	0.43
1:D:4918:ARG:NE	5:D:5207:HOH:O	2.45	0.42
1:D:4725:SER:HB2	1:D:4818:LEU:HD21	2.01	0.42
1:D:4815:LEU:C	5:D:5201:HOH:O	2.46	0.42
2:E:60:SER:OG	5:E:202:HOH:O	2.21	0.42
2:B:48:ARG:NE	5:B:102:HOH:O	2.05	0.42
1:D:4935:ALA:HB2	1:D:4975:HIS:HB3	2.00	0.42
1:A:4851:ARG:HA	1:A:4851:ARG:HD3	1.65	0.41
1:D:4936:ARG:C	1:D:4938:ARG:HE	2.24	0.41
1:D:4972:LEU:HD21	1:D:4987:LEU:CD1	2.50	0.41
1:A:4880:ARG:NH2	1:A:4895:GLN:HE22	2.11	0.41
1:A:4993:ALA:N	5:A:5202:HOH:O	2.52	0.41
2:B:25:ASP:N	2:B:25:ASP:OD1	2.43	0.40
1:D:4972:LEU:HD23	1:D:4972:LEU:HA	1.90	0.40
1:A:4819:GLU:HG2	1:A:4820:ALA:N	2.34	0.40
2:E:67:ILE:HG12	2:E:93:LEU:CD2	2.52	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	248/280 (89%)	241 (97%)	7 (3%)	0	100	100
1	D	245/280 (88%)	237 (97%)	8 (3%)	0	100	100
2	B	85/101 (84%)	82 (96%)	3 (4%)	0	100	100
2	E	85/101 (84%)	83 (98%)	2 (2%)	0	100	100
All	All	663/762 (87%)	643 (97%)	20 (3%)	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	217/240 (90%)	215 (99%)	2 (1%)	78	79
1	D	215/240 (90%)	213 (99%)	2 (1%)	78	79
2	B	81/93 (87%)	80 (99%)	1 (1%)	71	70
2	E	81/93 (87%)	81 (100%)	0	100	100
All	All	594/666 (89%)	589 (99%)	5 (1%)	81	82

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4886	SER
1	A	4938	ARG

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Mol	Chain	Res	Type
2	B	70	SER
1	D	4778	ARG
1	D	4938	ARG

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

Mol	Chain	Res	Type
1	A	4895	GLN
1	D	4906	GLN
1	D	4941	HIS
2	E	34	GLN

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](#)

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 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	$\# Z > 2$
4	GOL	D	5102	-	5,5,5	0.93	0	5,5,5	0.91	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	A	5102	-	5,5,5	0.79	0	5,5,5	1.24	1 (20%)
4	GOL	E	101	-	5,5,5	0.79	0	5,5,5	1.02	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
4	GOL	D	5102	-	-	2/4/4/4	-
4	GOL	A	5102	-	-	1/4/4/4	-
4	GOL	E	101	-	-	2/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	5102	GOL	C3-C2-C1	-2.23	103.03	111.70

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	5102	GOL	O2-C2-C3-O3
4	D	5102	GOL	C1-C2-C3-O3
4	E	101	GOL	C1-C2-C3-O3
4	E	101	GOL	O2-C2-C3-O3
4	A	5102	GOL	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	5102	GOL	2	0
4	E	101	GOL	1	0

5.7 Other polymers [i](#)

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	254/280 (90%)	0.40	24 (9%) 8 9	20, 35, 78, 91	0
1	D	251/280 (89%)	0.35	25 (9%) 7 8	19, 34, 77, 93	0
2	B	87/101 (86%)	-0.12	2 (2%) 60 63	21, 33, 55, 84	0
2	E	87/101 (86%)	-0.20	3 (3%) 45 48	20, 31, 54, 65	0
All	All	679/762 (89%)	0.24	54 (7%) 12 13	19, 34, 75, 93	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	4938	ARG	10.5
1	A	4939	LYS	8.6
1	A	4940	GLY	8.3
2	B	12	VAL	6.7
1	D	4953	PRO	5.7
1	A	4698	ARG	5.6
1	D	4820	ALA	5.4
1	D	4940	GLY	5.2
1	A	4993	ALA	5.0
1	D	4734	GLY	5.0
1	A	4735	SER	4.8
1	A	4776	SER	4.6
2	B	24	PRO	4.6
2	E	12	VAL	4.5
1	D	4993	ALA	4.3
1	A	4819	GLU	4.3
1	A	4886	SER	4.3
1	A	4938	ARG	4.2
1	A	4820	ALA	4.1
1	A	4891	GLU	4.1
1	A	4734	GLY	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	4890	GLY	3.7
1	A	4953	PRO	3.6
1	D	4817	VAL	3.5
1	D	4777	LYS	3.4
1	D	4936	ARG	3.3
1	D	4891	GLU	3.2
1	A	4936	ARG	3.2
1	D	4778	ARG	3.2
1	A	4818	LEU	3.2
1	A	4937	SER	3.2
1	D	4994	GLU	3.1
1	A	4699	PRO	3.1
1	D	4937	SER	3.0
1	A	4777	LYS	3.0
1	D	4819	GLU	2.8
1	D	4939	LYS	2.8
1	A	4884	ALA	2.8
1	D	4954	ASP	2.7
1	D	4952	GLY	2.7
1	A	4881	LEU	2.7
1	D	4911	ALA	2.6
1	D	4956	VAL	2.6
1	D	4995	VAL	2.5
1	A	4994	GLU	2.5
1	D	4699	PRO	2.5
2	E	98	SER	2.3
1	D	4883	GLN	2.2
1	D	4700	LEU	2.2
1	D	4950	ARG	2.2
1	A	4950	ARG	2.1
1	A	4844	THR	2.1
2	E	53	GLU	2.1
1	D	4818	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

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
4	GOL	A	5102	6/6	0.72	0.15	56,66,69,69	0
4	GOL	E	101	6/6	0.86	0.22	54,69,70,72	0
4	GOL	D	5102	6/6	0.92	0.14	48,67,70,73	0
3	MG	A	5101	1/1	0.99	0.09	23,23,23,23	0
3	MG	D	5101	1/1	1.00	0.10	21,21,21,21	0

6.5 Other polymers [i](#)

There are no such residues in this entry.