



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 04:42 am GMT

PDB ID : 4Q3O  
Title : Crystal structure of MGS-MT1, an alpha/beta hydrolase enzyme from a Lake Matapan deep-sea metagenome library  
Authors : Stogios, P.J.; Xu, X.; Cui, H.; Alcaide, M.; Ferrer, M.; Savchenko, A.  
Deposited on : 2014-04-11  
Resolution : 1.74 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

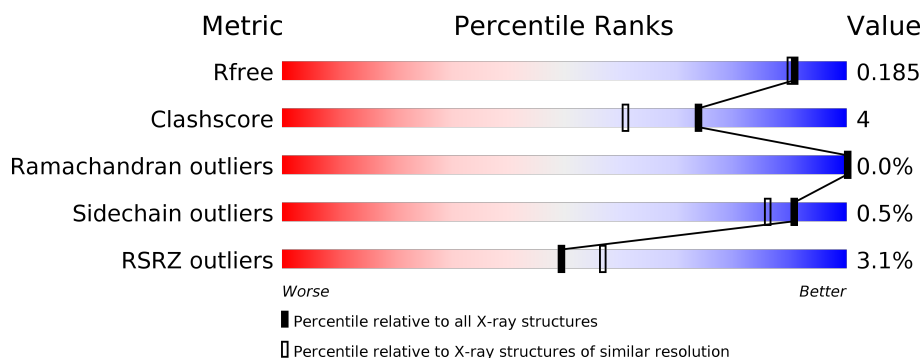
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.74 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))
$R_{free}$	100719	2694 (1.76-1.72)
Clashscore	112137	2854 (1.76-1.72)
Ramachandran outliers	110173	2824 (1.76-1.72)
Sidechain outliers	110143	2824 (1.76-1.72)
RSRZ outliers	101464	2705 (1.76-1.72)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	348	<div> <div>3%</div> <div> <div></div> <div>83%</div> <div>8%</div> <div>9%</div> </div> </div>
1	B	348	<div> <div>2%</div> <div> <div></div> <div>86%</div> <div>5%</div> <div>9%</div> </div> </div>
1	C	348	<div> <div>%</div> <div> <div></div> <div>83%</div> <div>7%</div> <div>9%</div> </div> </div>
1	D	348	<div> <div>%</div> <div> <div></div> <div>83%</div> <div>8%</div> <div>9%</div> </div> </div>
1	E	348	<div> <div>%</div> <div> <div></div> <div>85%</div> <div>6%</div> <div>9%</div> </div> </div>
1	F	348	<div> <div>4%</div> <div> <div></div> <div>84%</div> <div>7%</div> <div>9%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	348	
1	H	348	

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	CL	A	401	-	-	X	-
2	CL	B	401	-	-	-	X
2	CL	C	401	-	-	X	X
2	CL	E	401	-	-	X	X
3	MES	A	403	-	-	-	X
3	MES	A	404	-	-	X	X
3	MES	C	402	-	-	-	X
3	MES	G	402	-	-	-	X
3	MES	G	403	-	-	-	X
3	MES	H	401	-	-	-	X
3	MES	H	402	-	-	-	X
4	GOL	A	406	-	-	-	X
4	GOL	A	407	-	-	-	X
4	GOL	B	403	-	-	-	X
4	GOL	C	404	-	-	-	X
4	GOL	C	406	-	-	-	X
4	GOL	D	402	-	-	-	X
4	GOL	D	403	-	-	-	X
4	GOL	D	404	-	-	-	X
4	GOL	F	402	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 23319 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 MGS-MT1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	317	Total	C	N	O	S	0	5	0
			2501	1608	424	463	6			
1	B	317	Total	C	N	O	S	0	4	0
			2489	1602	418	463	6			
1	C	316	Total	C	N	O	S	0	4	0
			2486	1604	417	459	6			
1	D	316	Total	C	N	O	S	0	6	0
			2498	1610	423	459	6			
1	E	316	Total	C	N	O	S	0	5	0
			2490	1603	420	461	6			
1	F	316	Total	C	N	O	S	0	3	0
			2477	1595	417	459	6			
1	G	316	Total	C	N	O	S	0	4	0
			2487	1603	420	458	6			
1	H	316	Total	C	N	O	S	0	1	0
			2471	1590	417	457	7			

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

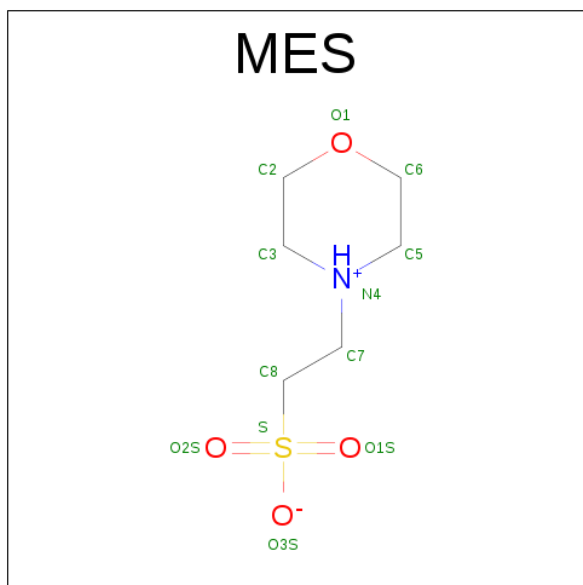
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	1	Total	Cl	0	0
			1	1		
2	D	1	Total	Cl	0	0
			1	1		
2	E	2	Total	Cl	0	0
			2	2		
2	B	1	Total	Cl	0	0
			1	1		
2	C	2	Total	Cl	0	0
			2	2		
2	A	2	Total	Cl	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	F	1	Total	Cl	0	0
			1	1		

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).



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

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	E	1	Total	C	O	0	0
			6	3	3		
4	F	1	Total	C	O	0	0
			6	3	3		
4	F	1	Total	C	O	0	0
			6	3	3		
4	G	1	Total	C	O	0	0
			6	3	3		

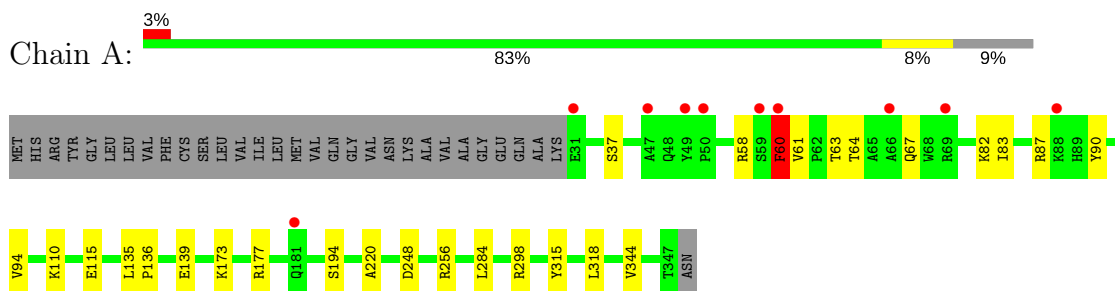
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	391	Total	O	0	16
			407	407		
5	B	435	Total	O	0	15
			450	450		
5	C	408	Total	O	0	18
			428	428		
5	D	391	Total	O	0	10
			401	401		
5	E	390	Total	O	0	15
			405	405		
5	F	384	Total	O	0	7
			391	391		
5	G	354	Total	O	0	12
			366	366		
5	H	332	Total	O	0	8
			340	340		

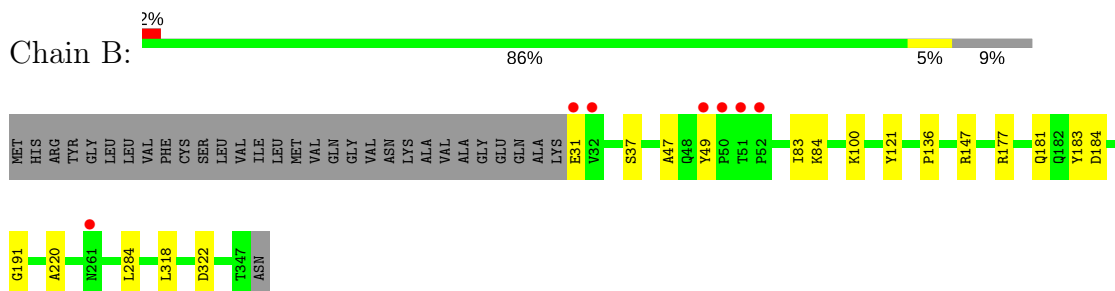
### 3 Residue-property plots [i](#)

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.

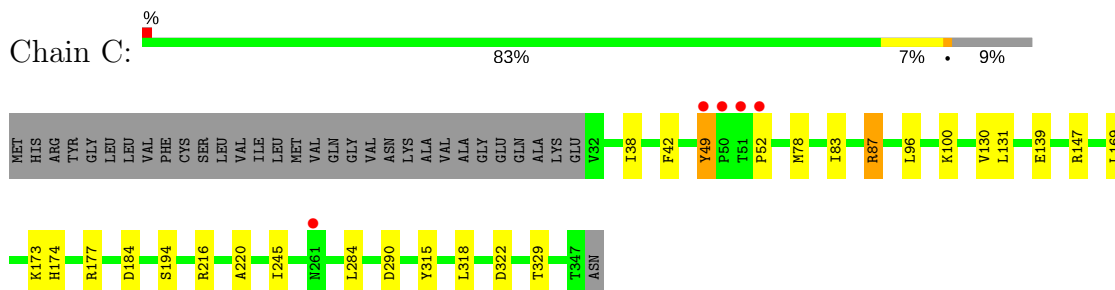
#### • Molecule 1: MGS-MT1



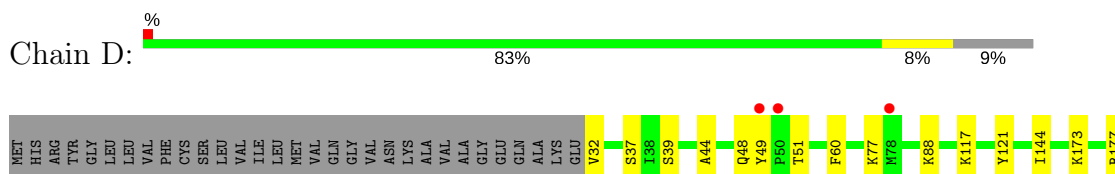
#### • Molecule 1: MGS-MT1



#### • Molecule 1: MGS-MT1



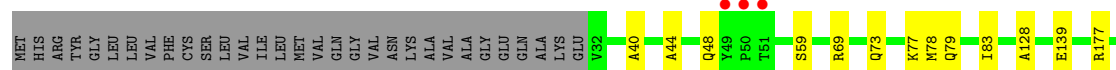
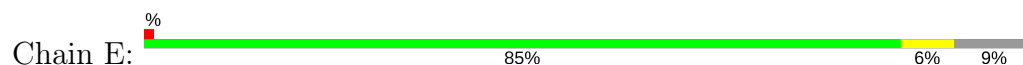
#### • Molecule 1: MGS-MT1



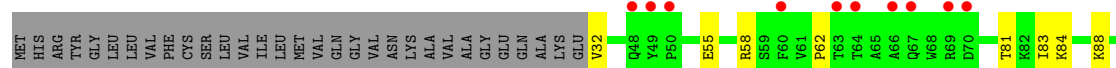
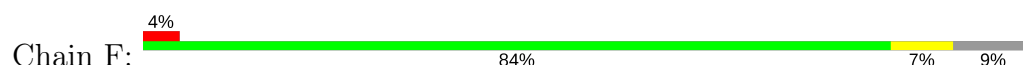




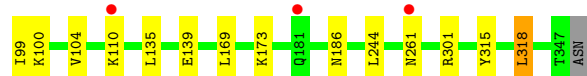
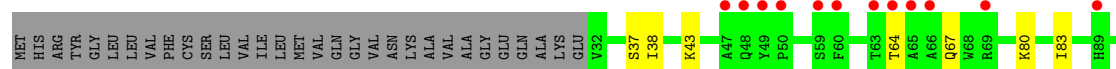
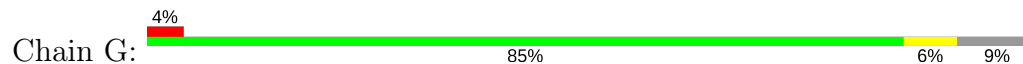
## ● Molecule 1: MGS-MT1



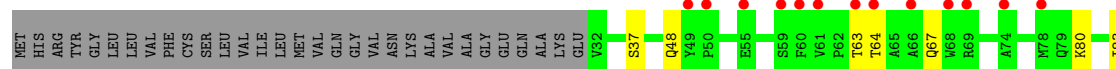
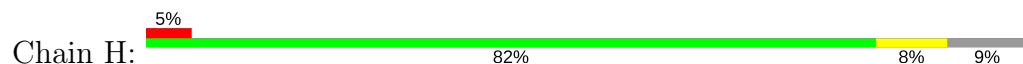
## ● Molecule 1: MGS-MT1



## ● Molecule 1: MGS-MT1



## ● Molecule 1: MGS-MT1



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	189.45Å 131.40Å 112.44Å 90.00° 103.55° 90.00°	Depositor
Resolution (Å)	19.72 – 1.74 19.72 – 1.74	Depositor EDS
% Data completeness (in resolution range)	99.5 (19.72-1.74) 93.1 (19.72-1.74)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.37 (at 1.74Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, $R_{free}$	0.145 , 0.185 0.145 , 0.185	Depositor DCC
$R_{free}$ test set	13722 reflections (5.05%)	DCC
Wilson B-factor (Å <sup>2</sup> )	15.8	Xtriage
Anisotropy	0.184	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 67.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	23319	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	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 48.87 % 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 8.0897e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, CL

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	0.72	0/2579	0.73	0/3512
1	B	0.77	0/2564	0.80	0/3493
1	C	0.74	1/2562 (0.0%)	0.76	2/3491 (0.1%)
1	D	0.75	0/2579	0.75	0/3512
1	E	0.72	0/2568	0.72	0/3498
1	F	0.72	0/2549	0.72	0/3473
1	G	0.66	0/2562	0.71	0/3490
1	H	0.66	0/2537	0.68	1/3457 (0.0%)
All	All	0.72	1/20500 (0.0%)	0.74	3/27926 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	49	TYR	CB-CG	-5.58	1.43	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	290	ASP	CB-CG-OD1	5.11	122.89	118.30
1	H	301	ARG	NE-CZ-NH1	-5.06	117.77	120.30
1	C	87	ARG	NE-CZ-NH2	-5.02	117.79	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	60	PHE	Peptide

## 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	2501	0	2512	23	0
1	B	2489	0	2495	14	0
1	C	2486	0	2495	20	0
1	D	2498	0	2521	22	0
1	E	2490	0	2501	14	0
1	F	2477	0	2484	17	0
1	G	2487	0	2503	16	0
1	H	2471	0	2472	20	0
2	A	2	0	0	2	0
2	B	1	0	0	0	0
2	C	2	0	0	2	0
2	D	1	0	0	0	0
2	E	2	0	0	3	0
2	F	1	0	0	1	0
2	G	1	0	0	1	0
3	A	24	0	24	9	0
3	B	12	0	12	1	0
3	C	24	0	24	1	0
3	D	12	0	12	0	0
3	G	24	0	24	6	0
3	H	24	0	24	2	0
4	A	18	0	24	2	0
4	B	6	0	8	0	0
4	C	18	0	24	1	0
4	D	30	0	40	0	0
4	E	12	0	16	0	0
4	F	12	0	16	0	0
4	G	6	0	8	0	0
5	A	407	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	450	0	0	2	0
5	C	428	0	0	6	0
5	D	401	0	0	8	0
5	E	405	0	0	6	0
5	F	391	0	0	8	0
5	G	366	0	0	6	0
5	H	340	0	0	5	0
All	All	23319	0	20239	152	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 4.

The worst 5 of 152 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)
3:A:404:MES:H71	1:B:37:SER:HB2	1.42	0.98
2:A:401:CL:CL	5:A:859:HOH:O	2.25	0.90
2:E:401:CL:CL	5:E:827:HOH:O	2.30	0.86
2:C:401:CL:CL	5:C:739:HOH:O	2.32	0.83
1:C:78:MET:SD	5:C:719:HOH:O	2.36	0.81

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	320/348 (92%)	309 (97%)	11 (3%)	0	100	100
1	B	319/348 (92%)	309 (97%)	10 (3%)	0	100	100
1	C	318/348 (91%)	309 (97%)	9 (3%)	0	100	100
1	D	320/348 (92%)	308 (96%)	12 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	319/348 (92%)	307 (96%)	12 (4%)	0	100	100
1	F	317/348 (91%)	302 (95%)	14 (4%)	1 (0%)	44	24
1	G	318/348 (91%)	304 (96%)	14 (4%)	0	100	100
1	H	315/348 (90%)	301 (96%)	14 (4%)	0	100	100
All	All	2546/2784 (92%)	2449 (96%)	96 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	184	ASP

### 5.3.2 Protein sidechains ⓘ

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	271/291 (93%)	270 (100%)	1 (0%)	93	89
1	B	270/291 (93%)	269 (100%)	1 (0%)	93	89
1	C	269/291 (92%)	268 (100%)	1 (0%)	93	89
1	D	271/291 (93%)	270 (100%)	1 (0%)	93	89
1	E	270/291 (93%)	268 (99%)	2 (1%)	87	78
1	F	268/291 (92%)	267 (100%)	1 (0%)	93	89
1	G	269/291 (92%)	268 (100%)	1 (0%)	93	89
1	H	266/291 (91%)	264 (99%)	2 (1%)	85	75
All	All	2154/2328 (92%)	2144 (100%)	10 (0%)	91	86

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	78	MET
1	E	279	PHE
1	G	318	LEU

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Mol	Chain	Res	Type
1	D	279	PHE
1	F	279	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	187	HIS
1	H	187	HIS
1	G	261	ASN
1	B	300	ASN
1	G	67	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 37 ligands modelled in this entry, 10 are monoatomic - leaving 27 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	$\# Z  > 2$
3	MES	A	403	-	12,12,12	2.03	2 (16%)	14,16,16	3.15	5 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	MES	A	404	-	12,12,12	2.26	1 (8%)	14,16,16	3.53	8 (57%)
4	GOL	A	405	-	5,5,5	0.49	0	5,5,5	0.44	0
4	GOL	A	406	-	5,5,5	0.35	0	5,5,5	0.23	0
4	GOL	A	407	-	5,5,5	0.92	0	5,5,5	0.67	0
3	MES	B	402	-	12,12,12	1.81	1 (8%)	14,16,16	2.59	3 (21%)
4	GOL	B	403	-	5,5,5	0.38	0	5,5,5	0.80	0
3	MES	C	402	-	12,12,12	2.09	1 (8%)	14,16,16	2.45	5 (35%)
3	MES	C	403	-	12,12,12	1.75	1 (8%)	14,16,16	2.38	5 (35%)
4	GOL	C	404	-	5,5,5	0.42	0	5,5,5	0.23	0
4	GOL	C	405	-	5,5,5	0.28	0	5,5,5	0.43	0
4	GOL	C	406	-	5,5,5	0.45	0	5,5,5	0.48	0
3	MES	D	401	-	12,12,12	1.83	1 (8%)	14,16,16	3.21	4 (28%)
4	GOL	D	402	-	5,5,5	0.52	0	5,5,5	0.78	0
4	GOL	D	403	-	5,5,5	0.33	0	5,5,5	1.56	1 (20%)
4	GOL	D	404	-	5,5,5	0.39	0	5,5,5	0.50	0
4	GOL	D	405	-	5,5,5	0.33	0	5,5,5	0.47	0
4	GOL	D	406	-	5,5,5	0.29	0	5,5,5	0.21	0
4	GOL	E	403	-	5,5,5	0.31	0	5,5,5	0.38	0
4	GOL	E	404	-	5,5,5	0.50	0	5,5,5	0.47	0
4	GOL	F	402	-	5,5,5	0.18	0	5,5,5	0.79	0
4	GOL	F	403	-	5,5,5	0.38	0	5,5,5	0.76	0
3	MES	G	402	-	12,12,12	2.04	2 (16%)	14,16,16	2.82	7 (50%)
3	MES	G	403	-	12,12,12	1.79	1 (8%)	14,16,16	3.01	4 (28%)
4	GOL	G	404	-	5,5,5	0.44	0	5,5,5	0.94	0
3	MES	H	401	-	12,12,12	2.16	2 (16%)	14,16,16	2.33	5 (35%)
3	MES	H	402	-	12,12,12	1.93	1 (8%)	14,16,16	3.63	7 (50%)

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	A	403	-	-	0/6/14/14	0/1/1/1
3	MES	A	404	-	-	0/6/14/14	0/1/1/1
4	GOL	A	405	-	-	0/4/4/4	0/0/0/0
4	GOL	A	406	-	-	0/4/4/4	0/0/0/0
4	GOL	A	407	-	-	0/4/4/4	0/0/0/0
3	MES	B	402	-	-	0/6/14/14	0/1/1/1
4	GOL	B	403	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MES	C	402	-	-	0/6/14/14	0/1/1/1
3	MES	C	403	-	-	0/6/14/14	0/1/1/1
4	GOL	C	404	-	-	0/4/4/4	0/0/0/0
4	GOL	C	405	-	-	0/4/4/4	0/0/0/0
4	GOL	C	406	-	-	0/4/4/4	0/0/0/0
3	MES	D	401	-	-	0/6/14/14	0/1/1/1
4	GOL	D	402	-	-	0/4/4/4	0/0/0/0
4	GOL	D	403	-	-	0/4/4/4	0/0/0/0
4	GOL	D	404	-	-	0/4/4/4	0/0/0/0
4	GOL	D	405	-	-	0/4/4/4	0/0/0/0
4	GOL	D	406	-	-	0/4/4/4	0/0/0/0
4	GOL	E	403	-	-	0/4/4/4	0/0/0/0
4	GOL	E	404	-	-	0/4/4/4	0/0/0/0
4	GOL	F	402	-	-	0/4/4/4	0/0/0/0
4	GOL	F	403	-	-	0/4/4/4	0/0/0/0
3	MES	G	402	-	-	0/6/14/14	0/1/1/1
3	MES	G	403	-	-	0/6/14/14	0/1/1/1
4	GOL	G	404	-	-	0/4/4/4	0/0/0/0
3	MES	H	401	-	-	0/6/14/14	0/1/1/1
3	MES	H	402	-	-	0/6/14/14	0/1/1/1

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	404	MES	C8-S	-7.45	1.66	1.77
3	C	402	MES	C8-S	-6.97	1.67	1.77
3	H	401	MES	C8-S	-6.76	1.67	1.77
3	H	402	MES	C8-S	-6.44	1.67	1.77
3	G	402	MES	C8-S	-6.39	1.67	1.77

The worst 5 of 54 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	402	MES	O1S-S-C8	-5.68	101.92	106.79
3	C	402	MES	C2-C3-N4	-3.23	105.58	110.11
3	G	402	MES	C6-C5-N4	-3.20	105.62	110.11
4	D	403	GOL	C3-C2-C1	-3.15	99.01	111.52
3	H	401	MES	C6-C5-N4	-3.04	105.84	110.11

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	403	MES	2	0
3	A	404	MES	7	0
4	A	405	GOL	1	0
4	A	406	GOL	1	0
3	B	402	MES	1	0
3	C	403	MES	1	0
4	C	404	GOL	1	0
3	G	402	MES	4	0
3	G	403	MES	2	0
3	H	401	MES	1	0
3	H	402	MES	1	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	317/348 (91%)	-0.25	10 (3%) 48 55	8, 16, 44, 103	0
1	B	317/348 (91%)	-0.47	7 (2%) 62 70	8, 14, 32, 94	0
1	C	316/348 (90%)	-0.43	5 (1%) 72 80	9, 15, 33, 86	0
1	D	316/348 (90%)	-0.47	4 (1%) 77 83	8, 16, 31, 71	0
1	E	316/348 (90%)	-0.38	4 (1%) 77 83	9, 17, 35, 83	0
1	F	316/348 (90%)	-0.24	14 (4%) 35 41	8, 17, 49, 88	0
1	G	316/348 (90%)	-0.22	15 (4%) 32 38	9, 19, 48, 84	0
1	H	316/348 (90%)	0.07	19 (6%) 23 27	11, 22, 49, 105	0
All	All	2530/2784 (90%)	-0.30	78 (3%) 49 57	8, 17, 42, 105	0

The worst 5 of 78 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	50	PRO	8.1
1	H	60	PHE	7.5
1	E	49	TYR	7.3
1	G	60	PHE	6.5
1	H	64	THR	6.5

### 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 ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	MES	A	404	12/12	0.87	0.26	22.46	12,34,44,45	12
4	GOL	B	403	6/6	0.86	0.15	17.40	29,40,42,48	6
3	MES	G	402	12/12	0.89	0.24	15.99	14,52,59,60	12
3	MES	H	401	12/12	0.88	0.25	14.04	10,40,52,54	12
2	CL	C	401	1/1	0.74	0.15	12.83	54,54,54,54	0
4	GOL	D	404	6/6	0.84	0.18	12.38	35,52,59,60	0
3	MES	G	403	12/12	0.93	0.16	9.04	26,52,60,62	12
4	GOL	D	402	6/6	0.88	0.13	8.51	34,51,54,54	0
3	MES	A	403	12/12	0.95	0.14	7.55	13,37,55,58	12
2	CL	E	401	1/1	0.84	0.12	7.42	55,55,55,55	0
4	GOL	F	402	6/6	0.81	0.17	6.88	34,53,60,62	6
4	GOL	C	404	6/6	0.82	0.22	5.29	38,52,58,61	0
3	MES	C	402	12/12	0.95	0.12	4.40	19,35,49,49	12
3	MES	H	402	12/12	0.96	0.12	4.39	19,37,51,52	12
4	GOL	A	406	6/6	0.67	0.27	4.36	41,55,58,62	0
4	GOL	C	406	6/6	0.93	0.11	3.61	27,29,31,40	6
4	GOL	D	403	6/6	0.77	0.13	3.53	42,46,58,62	0
4	GOL	A	407	6/6	0.96	0.10	3.29	13,17,26,41	6
2	CL	B	401	1/1	0.82	0.08	2.31	55,55,55,55	0
2	CL	F	401	1/1	0.95	0.06	1.91	49,49,49,49	0
4	GOL	E	404	6/6	0.90	0.15	1.90	36,44,52,56	0
4	GOL	D	406	6/6	0.94	0.10	1.63	20,23,33,41	0
2	CL	A	401	1/1	0.96	0.08	1.61	45,45,45,45	1
2	CL	G	401	1/1	0.91	0.08	1.54	53,53,53,53	0
4	GOL	C	405	6/6	0.83	0.14	1.36	27,36,39,43	6
4	GOL	G	404	6/6	0.96	0.10	1.17	15,22,36,43	0
4	GOL	F	403	6/6	0.96	0.08	1.00	14,16,26,33	0
2	CL	E	402	1/1	0.99	0.04	-2.54	14,14,14,14	0
2	CL	D	407	1/1	0.99	0.03	-3.12	13,13,13,13	0
2	CL	C	407	1/1	1.00	0.04	-3.72	13,13,13,13	0
2	CL	A	402	1/1	1.00	0.02	-4.82	13,13,13,13	0
4	GOL	D	405	6/6	0.61	0.36	-	79,80,80,81	0
3	MES	C	403	12/12	0.82	0.19	-	19,26,34,36	12
4	GOL	E	403	6/6	0.77	0.29	-	46,57,58,62	6

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	MES	D	401	12/12	0.85	0.17	-	18,25,37,38	12
4	GOL	A	405	6/6	0.86	0.17	-	36,42,47,47	6
3	MES	B	402	12/12	0.81	0.23	-	18,27,32,34	12

## 6.5 Other polymers [i](#)

There are no such residues in this entry.