Full wwPDB X-ray Structure Validation Report (i)

Sep 13, 2023 – 10:23 AM EDT

PDB ID	:	4Q3L
Title	:	Crystal structure of MGS-M2, an alpha/beta hydrolase enzyme from a Medee basin deep-sea metagenome library
Authors	:	Stogios, P.J.; Xu, X.; Cui, H.; Alcaide, M.; Ferrer, M.; Savchenko, A.
Deposited on	:	2014-04-11
Resolution	:	3.01 Å(reported)

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

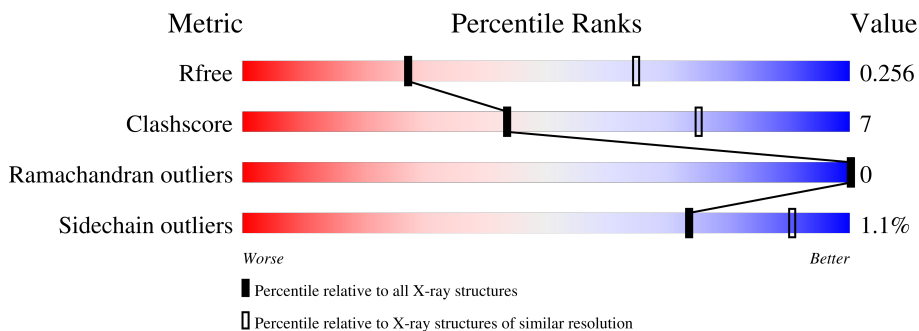|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 3.01 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	Percentile Ranks	Value
Rfree		0.256
Clashscore		7
Ramachandran outliers		0
Sidechain outliers		1.1%

Worse — *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2399 (3.04-3.00)
Clashscore	141614	2734 (3.04-3.00)
Ramachandran outliers	138981	2640 (3.04-3.00)
Sidechain outliers	138945	2643 (3.04-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 <=5%

Mol	Chain	Length	Quality of chain
1	A	297	76% · 15% · 7%
1	B	297	80% · 14% · 6%
1	C	297	78% · 15% · 6%
1	D	297	77% · 14% · 7%
1	E	297	81% · 11% · 7%
1	F	297	76% · 16% · 7%
1	G	297	75% · 18% · 6%

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Mol	Chain	Length	Quality of chain
1	H	297	

80%   13%   · 6%

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 18226 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-M2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	275	Total	C	N	O	S	0	0	0
			2223	1439	355	420	9			
1	B	280	Total	C	N	O	S	0	0	0
			2266	1469	361	427	9			
1	C	278	Total	C	N	O	S	0	0	0
			2243	1451	359	424	9			
1	D	275	Total	C	N	O	S	0	1	0
			2231	1444	358	420	9			
1	E	275	Total	C	N	O	S	0	0	0
			2223	1439	355	420	9			
1	F	275	Total	C	N	O	S	0	0	0
			2223	1439	355	420	9			
1	G	278	Total	C	N	O	S	0	0	0
			2243	1451	359	424	9			
1	H	280	Total	C	N	O	S	0	0	0
			2266	1469	361	427	9			

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

GOL

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	43	Total 43	O 43	0	0
3	B	33	Total 33	O 33	0	0
3	C	38	Total 38	O 38	0	0
3	D	37	Total 37	O 37	0	0
3	E	38	Total 41	O 41	0	3
3	F	30	Total 31	O 31	0	1
3	G	36	Total 36	O 36	0	0
3	H	37	Total 37	O 37	0	0

3 Residue-property plots ⓘ

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. 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. 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.
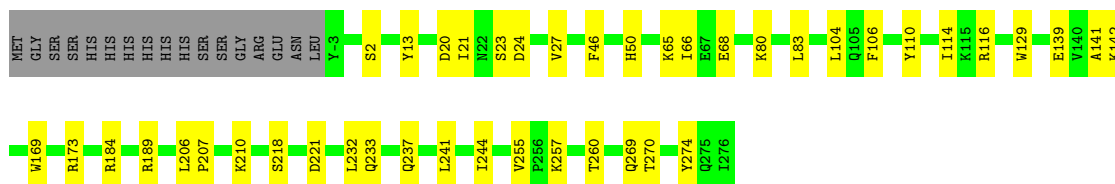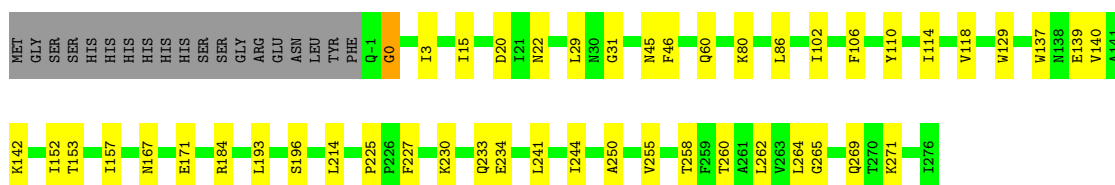
• Molecule 1: MGS-M2

Chain A:

• Molecule 1: MGS-M2

Chain B:

• Molecule 1: MGS-M2

Chain C:

• Molecule 1: MGS-M2

Chain D:

• Molecule 1: MGS-M2

Chain E:

81%   11%   7%

MET GLY SER HIS HIS HIS HIS HIS SER SER GLY ARG GLU ASN LEU TYR PHE GLN GLY VAL S2 Q7 E8 D20 I21 N22 I66 E77 K80 N81 F106 Y110 I114 K115 W137 K142 T153 I157 W169 R184 R192 L206

P207 S218 D221 Q237 I244 A250 S251 M252 Y253 E254 V255 P256 K257 T258 G265 Q269 I276

• Molecule 1: MGS-M2

Chain F:

76%   16%   7%

MET GLY SER HIS HIS HIS HIS HIS SER SER GLY ARG GLU ASN LEU TYR PHE GLN GLY VAL S2 I3 F4 T5 Y6 Q7 E8 L19 D20 I21 N22 S23 D24 V25 T36 N45 K48 V51 D56 M57 Q72 Q75 K80 I88 A89 Q90 Q105

F106 Y110 I114 K115 R116 M117 V118 V140 A141 I152 R184 L214 S218 D221 Q233 L236 A239 E240 L241 I244 V255 P256 K257 L262 G265 Q269 T270 D273 Y274 Q275 I276

• Molecule 1: MGS-M2

Chain G:

75%   18%   6%

MET GLY SER HIS HIS HIS HIS HIS SER SER GLY ARG GLU ASN LEU TYR PHE Q-1 S2 Y6 Q7 E8 K9 I15 L19 D20 S23 N30 G31 M34 F46 S47 K48 V51 Q60 S64 K80 L86 Q90 S97 Y98 F106

Y110 I114 K115 R116 M117 V118 W137 N138 E139 V140 A141 K142 I152 T153 K172 E175 L193 S196 L214 S218 D221 P225 P226 F227 Q233 L241 I244 V255 P256 K257 T260 A261 L262 G265 Q269 T270 K271 L272 D273 Y274 Q275

I276

• Molecule 1: MGS-M2

Chain H:

80%   13% • 6%

MET GLY SER HIS HIS HIS HIS HIS SER SER GLY ARG GLU ASN LEU Y-3 F-2 Q-1 F4 T5 Y6 D20 D24 G31 K37 D59 Q60 Y70 T71 Q72 K80 I96 Q105 F106 Y110 I114 W137 N138 E139 V140 A141 K142 Y149

R173 L193 S196 K204 S218 D221 Y222 L223 Q233 L241 I244 M252 V255 T258 G265 Q269 T270 K271 L272 Q275 I276

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	105.57Å 139.13Å 111.11Å 90.00° 89.94° 90.00°	Depositor
Resolution (Å)	31.67 – 3.01 31.67 – 3.01	Depositor EDS
% Data completeness (in resolution range)	99.2 (31.67-3.01) 80.4 (31.67-3.01)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.66 (at 3.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1631)	Depositor
R, R_{free}	0.201 , 0.255 0.203 , 0.256	Depositor DCC
R_{free} test set	1996 reflections (3.16%)	wwPDB-VP
Wilson B-factor (Å^2)	42.2	Xtriage
Anisotropy	0.475	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 100.0	EDS
L-test for twinning[2]	$< |L| > = 0.47, < L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.060 for -l,k,h 0.397 for h,-k,-l 0.069 for -l,-k,-h	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	18226	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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	0.29	0/2276	0.42	0/3090
1	B	0.25	0/2321	0.41	0/3151
1	C	0.22	0/2296	0.39	0/3117
1	D	0.28	0/2287	0.42	0/3104
1	E	0.26	0/2276	0.40	0/3090
1	F	0.28	0/2276	0.42	0/3090
1	G	0.30	0/2296	0.44	0/3117
1	H	0.26	0/2321	0.42	0/3151
All	All	0.27	0/18349	0.41	0/24910

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	C	0	1
1	H	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	0	GLY	Peptide
1	H	-3	TYR	Peptide

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	2223	0	2210	34	0
1	B	2266	0	2251	26	0
1	C	2243	0	2233	26	0
1	D	2231	0	2223	45	0
1	E	2223	0	2210	20	0
1	F	2223	0	2210	30	0
1	G	2243	0	2233	32	0
1	H	2266	0	2251	38	0
2	B	6	0	8	0	0
2	G	6	0	8	1	0
3	A	43	0	0	1	0
3	B	33	0	0	0	0
3	C	38	0	0	0	0
3	D	37	0	0	0	0
3	E	41	0	0	1	0
3	F	31	0	0	0	0
3	G	36	0	0	0	0
3	H	37	0	0	0	0
All	All	18226	0	17837	238	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 7.

All (238) 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:F:7:GLN:OE1	1:F:8:GLU:N	1.87	1.08
1:A:8:GLU:N	1:A:8:GLU:OE1	2.00	0.94
1:E:7:GLN:O	1:E:8:GLU:HB2	1.68	0.91
1:D:250:ALA:HA	1:D:252:MET:HE1	1.58	0.85
1:A:20:ASP:OD1	1:A:22:ASN:HB3	1.79	0.82
1:H:-3:TYR:H3	1:H:-2:PHE:HD1	1.30	0.79
1:H:-3:TYR:N	1:H:-2:PHE:HB2	2.00	0.77
1:D:252:MET:CE	1:D:252:MET:H	1.99	0.76
1:D:250:ALA:C	1:D:252:MET:HE3	2.06	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:ARG:NH1	1:B:269:GLN:O	2.20	0.75
1:G:271:LYS:HD2	1:G:272:LEU:H	1.51	0.74
1:A:7:GLN:HB3	1:A:8:GLU:OE1	1.88	0.73
1:G:233:GLN:HG3	1:G:241:LEU:HB2	1.69	0.73
1:D:20:ASP:OD1	1:D:21:ILE:N	2.22	0.72
1:D:250:ALA:HA	1:D:252:MET:CE	2.20	0.70
1:H:-3:TYR:H3	1:H:-2:PHE:HB2	1.55	0.70
1:D:7:GLN:C	1:D:8:GLU:HG3	2.11	0.70
1:B:141:ALA:O	1:B:184:ARG:NH2	2.25	0.70
1:F:233:GLN:HG3	1:F:241:LEU:HB2	1.74	0.69
1:A:207:PRO:O	1:A:237:GLN:NE2	2.22	0.68
1:B:20:ASP:OD1	1:B:21:ILE:N	2.27	0.68
1:F:19:LEU:HD12	1:F:51:VAL:HG11	1.76	0.67
1:B:65:LYS:HZ2	1:B:189:ARG:HE	1.43	0.67
1:D:252:MET:H	1:D:252:MET:HE2	1.57	0.67
1:E:7:GLN:O	1:E:8:GLU:CB	2.39	0.66
1:A:8:GLU:H	1:A:8:GLU:CD	1.98	0.66
1:G:90:GLN:HG2	1:G:115:LYS:HG3	1.77	0.66
1:C:31:GLY:O	1:C:60:GLN:NE2	2.29	0.65
1:G:19:LEU:HD13	1:G:51:VAL:HG11	1.79	0.64
1:H:244:ILE:HG21	1:H:255:VAL:HG21	1.78	0.64
1:D:250:ALA:CA	1:D:252:MET:CE	2.75	0.64
1:H:-3:TYR:N	1:H:-2:PHE:HD1	1.96	0.64
1:H:233:GLN:HG3	1:H:241:LEU:HB2	1.80	0.64
1:F:273:ASP:OD1	1:F:274:TYR:N	2.33	0.61
1:G:6:TYR:CE1	1:G:7:GLN:HG2	2.36	0.61
1:H:-3:TYR:H3	1:H:-2:PHE:CB	2.13	0.61
1:A:21:ILE:N	1:A:21:ILE:HD13	2.15	0.61
1:C:230:LYS:NZ	1:C:234:GLU:OE2	2.31	0.61
1:C:0:GLY:HA2	1:C:3:ILE:HB	1.83	0.60
1:F:214:LEU:HD12	1:F:240:GLU:HB3	1.83	0.60
1:G:271:LYS:HD2	1:G:272:LEU:N	2.15	0.60
1:D:176:LEU:HD11	1:H:173:ARG:HG3	1.83	0.59
1:F:8:GLU:HA	1:F:8:GLU:OE1	2.01	0.59
1:E:207:PRO:O	1:E:237:GLN:NE2	2.35	0.58
1:E:253:TYR:HA	1:H:276:ILE:HD13	1.83	0.58
1:D:4:PHE:CE2	1:D:6:TYR:HB2	2.38	0.58
1:G:244:ILE:HG21	1:G:255:VAL:HG21	1.84	0.58
1:B:233:GLN:HG3	1:B:241:LEU:HB2	1.85	0.58
1:D:250:ALA:C	1:D:252:MET:CE	2.70	0.58
1:E:244:ILE:HG21	1:E:255:VAL:HG21	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:244:ILE:HG21	1:C:255:VAL:HG21	1.87	0.57
1:B:218:SER:HB2	1:B:221:ASP:HB2	1.86	0.57
1:G:118:VAL:HG22	1:G:214:LEU:HB3	1.86	0.57
1:F:244:ILE:HG21	1:F:255:VAL:HG21	1.87	0.57
1:A:21:ILE:HG22	1:A:21:ILE:O	2.04	0.56
1:B:269:GLN:NE2	1:B:274:TYR:OH	2.39	0.56
1:A:244:ILE:HG21	1:A:255:VAL:HG21	1.88	0.56
1:E:257:LYS:O	1:H:269:GLN:NE2	2.38	0.55
1:C:15:ILE:HD11	1:C:86:LEU:HD13	1.88	0.55
1:D:106:PHE:HD2	1:D:114:ILE:HD11	1.72	0.55
1:A:155:PRO:O	1:B:129:TRP:NE1	2.33	0.55
1:B:80:LYS:HD2	1:B:110:TYR:CZ	2.42	0.54
1:D:72:GLN:OE1	1:D:105:GLN:NE2	2.40	0.54
1:D:233:GLN:HG3	1:D:241:LEU:HB2	1.89	0.54
1:G:218:SER:HB2	1:G:221:ASP:HB2	1.89	0.54
1:D:7:GLN:OE1	1:D:7:GLN:HA	2.07	0.53
1:D:250:ALA:CA	1:D:252:MET:HE1	2.34	0.53
1:E:106:PHE:HD2	1:E:114:ILE:HD11	1.74	0.53
1:A:4:PHE:CE2	1:A:6:TYR:HB2	2.43	0.53
1:C:233:GLN:HG3	1:C:241:LEU:HB2	1.89	0.53
1:A:275:GLN:N	1:A:275:GLN:OE1	2.41	0.53
1:E:169:TRP:NE1	1:H:276:ILE:OXT	2.35	0.53
1:A:106:PHE:HD2	1:A:114:ILE:HD11	1.74	0.53
1:F:45:ASN:ND2	1:G:274:TYR:OH	2.42	0.52
1:F:106:PHE:HD2	1:F:114:ILE:HD11	1.74	0.52
1:A:21:ILE:N	1:A:21:ILE:CD1	2.73	0.52
1:B:24:ASP:OD2	1:B:50:HIS:ND1	2.42	0.52
1:D:174:LYS:HG2	1:H:37:LYS:HE2	1.91	0.52
1:G:9:LYS:HB3	1:G:64:SER:HB2	1.90	0.52
1:B:104:LEU:HD11	1:B:232:LEU:HD11	1.92	0.52
1:D:80:LYS:HD2	1:D:110:TYR:CZ	2.45	0.52
1:G:31:GLY:O	1:G:60:GLN:NE2	2.43	0.52
1:F:270:THR:OG1	1:G:48:LYS:NZ	2.38	0.51
1:F:118:VAL:HG22	1:F:214:LEU:HB3	1.92	0.51
1:D:252:MET:CE	1:D:252:MET:N	2.73	0.51
1:C:106:PHE:HD2	1:C:114:ILE:HD11	1.75	0.51
1:G:97:SER:OG	1:G:98:TYR:N	2.44	0.51
1:G:214:LEU:HD21	1:G:262:LEU:HD22	1.92	0.50
1:B:139:GLU:HA	1:B:142:LYS:HD3	1.92	0.50
1:H:271:LYS:HD2	1:H:272:LEU:H	1.75	0.50
1:B:244:ILE:HG21	1:B:255:VAL:HG21	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:29:LEU:HD23	1:C:102:ILE:HB	1.94	0.50
1:B:27:VAL:HG21	1:B:83:LEU:HD21	1.92	0.50
1:D:40:ASP:OD1	1:D:54:ARG:NH1	2.39	0.50
1:G:172:LYS:O	1:G:175:GLU:HG2	2.10	0.50
1:C:214:LEU:HD21	1:C:262:LEU:HD22	1.93	0.50
1:D:7:GLN:O	1:D:8:GLU:HG3	2.12	0.50
1:D:176:LEU:HD21	1:H:173:ARG:HE	1.77	0.50
1:F:21:ILE:CD1	1:F:21:ILE:N	2.75	0.50
1:C:129:TRP:NE1	1:D:155:PRO:O	2.34	0.49
1:A:25:VAL:HG11	1:A:88:ILE:HD13	1.94	0.49
1:G:80:LYS:HD3	1:G:110:TYR:CZ	2.48	0.49
1:H:-3:TYR:C	1:H:-2:PHE:CD1	2.85	0.49
1:B:210:LYS:HD2	1:B:237:GLN:NE2	2.28	0.49
1:D:220:GLU:OE1	1:D:222:TYR:OH	2.21	0.49
1:E:157:ILE:HG22	1:E:250:ALA:HB2	1.94	0.49
1:G:6:TYR:CD1	1:G:7:GLN:N	2.81	0.49
1:B:106:PHE:HD2	1:B:114:ILE:HD11	1.78	0.49
1:C:139:GLU:HA	1:C:142:LYS:HD3	1.94	0.49
1:B:65:LYS:NZ	1:B:189:ARG:HE	2.09	0.49
1:C:271:LYS:HB3	1:C:271:LYS:HE3	1.57	0.49
1:H:-3:TYR:N	1:H:-2:PHE:CB	2.73	0.48
1:D:77:GLU:O	1:D:81:ASN:ND2	2.46	0.48
1:H:72:GLN:OE1	1:H:105:GLN:NE2	2.47	0.48
1:C:20:ASP:OD1	1:C:22:ASN:HB3	2.13	0.48
1:F:90:GLN:HG2	1:F:115:LYS:HG2	1.95	0.48
1:D:250:ALA:CA	1:D:252:MET:HE3	2.42	0.48
1:D:20:ASP:OD2	1:D:22:ASN:HB3	2.14	0.48
1:G:116:ARG:HE	2:G:301:GOL:H2	1.78	0.48
1:A:80:LYS:HD3	1:A:110:TYR:CZ	2.49	0.48
1:G:106:PHE:HD2	1:G:114:ILE:HD11	1.79	0.48
1:A:233:GLN:HG3	1:A:241:LEU:HB2	1.96	0.47
1:E:218:SER:HB2	1:E:221:ASP:HB2	1.95	0.47
1:F:141:ALA:O	1:F:184:ARG:NH2	2.48	0.47
1:F:4:PHE:CE2	1:F:6:TYR:HB2	2.49	0.47
1:F:269:GLN:NE2	1:G:257:LYS:O	2.48	0.47
1:A:218:SER:HB2	1:A:221:ASP:HB2	1.97	0.47
1:H:-3:TYR:H2	1:H:-2:PHE:HB2	1.78	0.47
1:A:213:THR:O	1:A:240:GLU:N	2.42	0.47
1:A:7:GLN:HB3	1:A:8:GLU:H	1.64	0.47
1:F:25:VAL:HG11	1:F:88:ILE:HD13	1.97	0.47
1:G:30:ASN:HB3	1:G:34:MET:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:139:GLU:HA	1:H:142:LYS:HE3	1.96	0.47
1:F:236:LEU:HB2	1:F:239:ALA:HB2	1.97	0.46
1:F:218:SER:HB2	1:F:221:ASP:HB2	1.97	0.46
1:A:265:GLY:O	1:A:269:GLN:HG3	2.14	0.46
1:B:65:LYS:HZ3	1:B:189:ARG:HH21	1.61	0.46
1:C:118:VAL:HG22	1:C:214:LEU:HB3	1.97	0.46
1:B:257:LYS:HB2	1:D:240:GLU:OE1	2.16	0.46
1:C:193:LEU:O	1:C:196:SER:OG	2.31	0.46
1:A:140:VAL:HG21	1:A:152:ILE:HD13	1.98	0.46
1:F:80:LYS:HD3	1:F:110:TYR:CZ	2.50	0.46
1:C:45:ASN:HD22	1:C:260:THR:HG21	1.80	0.46
1:C:46:PHE:HA	1:C:264:LEU:HD21	1.97	0.46
1:A:59:ASP:CG	1:A:192:ARG:HH21	2.18	0.45
1:B:169:TRP:CZ2	1:B:173:ARG:HD2	2.51	0.45
1:G:6:TYR:CD1	1:G:7:GLN:HG2	2.51	0.45
1:A:137:TRP:CE2	1:A:153:THR:HG22	2.52	0.45
1:A:153:THR:O	1:A:157:ILE:HG12	2.17	0.45
1:A:271:LYS:NZ	3:A:319:HOH:O	2.40	0.45
1:H:-3:TYR:HA	1:H:-1:GLN:H	1.82	0.45
1:G:137:TRP:CE2	1:G:153:THR:HG22	2.52	0.45
1:H:59:ASP:OD2	1:H:70:TYR:OH	2.30	0.45
1:C:167:ASN:O	1:C:171:GLU:HG2	2.17	0.45
1:D:271:LYS:HD2	1:D:272:LEU:H	1.82	0.45
1:E:142:LYS:HA	1:E:184:ARG:HH22	1.82	0.44
1:F:57:MET:HB3	1:F:75:GLN:OE1	2.17	0.44
1:H:31:GLY:O	1:H:60:GLN:NE2	2.50	0.44
1:D:140:VAL:HG21	1:D:152:ILE:HD13	1.99	0.44
1:H:193:LEU:O	1:H:196:SER:OG	2.31	0.44
1:D:251:SER:N	1:D:252:MET:CE	2.80	0.44
1:A:218:SER:HB3	1:A:247:CYS:O	2.18	0.44
1:E:265:GLY:O	1:E:269:GLN:HG3	2.17	0.44
1:H:-2:PHE:O	1:H:-1:GLN:HG3	2.17	0.44
1:B:66:ILE:HG22	1:B:68:GLU:H	1.83	0.44
1:H:139:GLU:O	1:H:142:LYS:HG2	2.17	0.44
1:A:225:PRO:HB2	1:A:227:PHE:CD2	2.52	0.44
1:C:244:ILE:HD12	1:C:258:THR:HG21	2.00	0.44
1:D:152:ILE:HG13	1:D:153:THR:HG23	1.99	0.44
1:E:80:LYS:HD3	1:E:110:TYR:CZ	2.53	0.44
1:A:7:GLN:OE1	1:A:7:GLN:HA	2.17	0.44
1:C:265:GLY:O	1:C:269:GLN:HG3	2.18	0.44
1:H:96:ILE:CD1	1:H:252:MET:SD	3.06	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:137:TRP:HH2	1:H:223:LEU:HD21	1.82	0.44
1:A:9:LYS:HB3	1:A:64:SER:HB2	1.99	0.43
1:E:21:ILE:O	1:E:21:ILE:HG22	2.17	0.43
1:D:8:GLU:C	1:D:9:LYS:HG2	2.38	0.43
1:G:265:GLY:O	1:G:269:GLN:HG3	2.17	0.43
1:A:210:LYS:HB3	1:A:210:LYS:HE3	1.73	0.43
1:C:225:PRO:HB2	1:C:227:PHE:CD1	2.53	0.43
1:D:16:ASP:HB2	1:D:52:LEU:HB3	2.00	0.43
1:H:80:LYS:HD2	1:H:110:TYR:CZ	2.54	0.43
1:C:137:TRP:CE2	1:C:153:THR:HG22	2.54	0.43
1:D:6:TYR:CE2	1:D:7:GLN:HB2	2.53	0.43
1:H:106:PHE:HD2	1:H:114:ILE:HD11	1.84	0.43
1:D:244:ILE:HG21	1:D:255:VAL:HG21	2.01	0.43
1:F:265:GLY:O	1:F:269:GLN:HG3	2.18	0.43
1:D:14:GLU:OE2	1:D:54:ARG:NH2	2.52	0.43
1:B:2:SER:HB2	1:B:13:TYR:O	2.18	0.43
1:D:20:ASP:CG	1:D:22:ASN:H	2.22	0.43
1:D:8:GLU:HB2	1:D:9:LYS:HG2	2.00	0.42
1:D:22:ASN:OD1	1:D:22:ASN:O	2.36	0.42
1:D:131:LYS:HE2	1:D:135:ASP:OD2	2.19	0.42
1:E:77:GLU:O	1:E:81:ASN:ND2	2.42	0.42
1:F:116:ARG:NH1	1:F:269:GLN:O	2.46	0.42
1:H:-3:TYR:HA	1:H:-1:GLN:N	2.34	0.42
1:D:7:GLN:O	1:D:9:LYS:HG3	2.19	0.42
1:F:72:GLN:OE1	1:F:105:GLN:NE2	2.52	0.42
1:H:218:SER:HB2	1:H:221:ASP:HB2	2.01	0.42
1:H:265:GLY:O	1:H:269:GLN:HG3	2.19	0.42
1:E:115:LYS:NZ	3:E:329:HOH:O	2.50	0.42
1:F:21:ILE:N	1:F:21:ILE:HD13	2.35	0.42
1:G:139:GLU:HA	1:G:142:LYS:HD3	2.02	0.42
1:H:244:ILE:HD12	1:H:258:THR:HG21	2.01	0.42
1:C:142:LYS:C	1:C:184:ARG:HH22	2.23	0.42
1:D:137:TRP:CE2	1:D:153:THR:HG22	2.55	0.42
1:D:218:SER:HB2	1:D:221:ASP:HB2	2.02	0.42
1:H:204:LYS:HB3	1:H:204:LYS:HE3	1.87	0.42
1:A:157:ILE:HG22	1:A:250:ALA:HB2	2.02	0.42
1:H:141:ALA:HB2	1:H:149:TYR:CE1	2.55	0.42
1:F:140:VAL:HG21	1:F:152:ILE:HD13	2.01	0.41
1:F:257:LYS:O	1:G:269:GLN:NE2	2.52	0.41
1:B:20:ASP:O	1:B:23:SER:HB2	2.21	0.41
1:C:140:VAL:HG21	1:C:152:ILE:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:244:ILE:HD12	1:E:258:THR:HG21	2.03	0.41
1:E:66:ILE:O	1:E:192:ARG:NE	2.54	0.41
1:G:15:ILE:HD11	1:G:86:LEU:HD13	2.02	0.41
1:C:80:LYS:HD3	1:C:110:TYR:CZ	2.55	0.41
1:A:57:MET:HB3	1:A:75:GLN:OE1	2.21	0.41
1:C:157:ILE:HG22	1:C:250:ALA:HB2	2.03	0.41
1:E:206:LEU:HB2	1:E:207:PRO:HD3	2.02	0.41
1:F:214:LEU:HD21	1:F:262:LEU:HB3	2.03	0.41
1:G:225:PRO:HB2	1:G:227:PHE:CD1	2.56	0.41
1:H:137:TRP:CH2	1:H:223:LEU:HD21	2.56	0.41
1:B:169:TRP:CE2	1:B:173:ARG:HD2	2.56	0.40
1:F:36:THR:HG23	1:F:56:ASP:OD1	2.21	0.40
1:B:46:PHE:HE1	1:B:260:THR:HG23	1.85	0.40
1:G:140:VAL:HG21	1:G:152:ILE:HD13	2.03	0.40
1:H:4:PHE:CE2	1:H:6:TYR:HB2	2.55	0.40
1:F:48:LYS:HD2	1:F:48:LYS:HA	1.84	0.40
1:H:275:GLN:HA	1:H:275:GLN:OE1	2.22	0.40
1:A:184:ARG:HD2	1:A:184:ARG:HA	1.93	0.40
1:A:226:PRO:O	1:A:230:LYS:HG2	2.21	0.40
1:E:137:TRP:CE2	1:E:153:THR:HG22	2.57	0.40
1:G:193:LEU:O	1:G:196:SER:OG	2.34	0.40
1:B:206:LEU:HB2	1:B:207:PRO:HD3	2.04	0.40
1:D:206:LEU:HB2	1:D:207:PRO:HD3	2.04	0.40
1:G:46:PHE:HE1	1:G:260:THR:HG23	1.87	0.40

There are no symmetry-related clashes.

5.3　Torsion angles ⓘ

5.3.1　Protein backbone ⓘ

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	273/297 (92%)	263 (96%)	10 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	278/297 (94%)	270 (97%)	8 (3%)	0	100	100
1	C	276/297 (93%)	266 (96%)	10 (4%)	0	100	100
1	D	274/297 (92%)	260 (95%)	14 (5%)	0	100	100
1	E	273/297 (92%)	261 (96%)	12 (4%)	0	100	100
1	F	273/297 (92%)	260 (95%)	13 (5%)	0	100	100
1	G	276/297 (93%)	267 (97%)	9 (3%)	0	100	100
1	H	278/297 (94%)	266 (96%)	12 (4%)	0	100	100
All	All	2201/2376 (93%)	2113 (96%)	88 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	247/266 (93%)	244 (99%)	3 (1%)	71	89
1	B	251/266 (94%)	250 (100%)	1 (0%)	91	97
1	C	249/266 (94%)	249 (100%)	0	100	100
1	D	248/266 (93%)	245 (99%)	3 (1%)	71	89
1	E	247/266 (93%)	244 (99%)	3 (1%)	71	89
1	F	247/266 (93%)	244 (99%)	3 (1%)	71	89
1	G	249/266 (94%)	245 (98%)	4 (2%)	62	86
1	H	251/266 (94%)	247 (98%)	4 (2%)	62	86
All	All	1989/2128 (94%)	1968 (99%)	21 (1%)	73	90

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	21	ILE

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Mol	Chain	Res	Type
1	A	23	SER
1	B	270	THR
1	D	8	GLU
1	D	9	LYS
1	D	252	MET
1	E	20	ASP
1	E	22	ASN
1	E	252	MET
1	F	21	ILE
1	F	22	ASN
1	F	23	SER
1	G	2	SER
1	G	20	ASP
1	G	23	SER
1	G	172	LYS
1	H	20	ASP
1	H	24	ASP
1	H	37	LYS
1	H	252	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	269	GLN
1	B	121	ASN
1	B	237	GLN
1	B	269	GLN
1	C	81	ASN
1	C	121	ASN
1	D	81	ASN
1	D	121	ASN
1	D	269	GLN
1	E	121	ASN
1	E	151	HIS
1	F	105	GLN
1	F	121	ASN
1	G	62	GLN
1	G	121	ASN
1	H	121	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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

2 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	G	301	-	5,5,5	0.37	0	5,5,5	0.29	0
2	GOL	B	301	-	5,5,5	0.36	0	5,5,5	0.30	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	G	301	-	-	2/4/4/4	-
2	GOL	B	301	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	301	GOL	O1-C1-C2-C3
2	G	301	GOL	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	301	GOL	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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.