Full wwPDB X-ray Structure Validation Report (i)

Aug 20, 2020 – 05:04 PM BST

PDB ID	:	6UB8
Title	:	Crystal structure of a GH128 (subgroup VI) exo-beta-1,3-glucanase from Aureobasidium namibiae (AnGH128_VI)
Authors	:	Santos, C.R.; Vieira, P.S.; Domingues, M.N.; Cordeiro, R.L.; Tomazini, A.; Murakami, M.T.
Deposited on	:	2019-09-11
Resolution	:	1.90 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

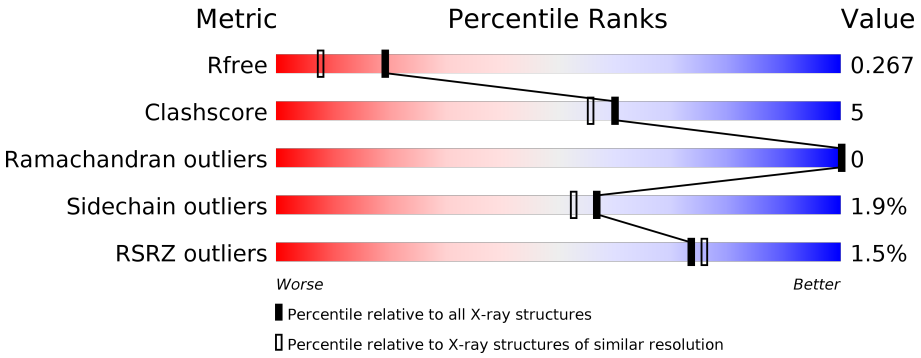
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 1.90 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 <=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	266	% 80% 12% • 6%
1	B	266	85% 8% 6%
1	C	266	% 83% 10% • 6%
1	D	266	% 83% 9% • 6%
1	E	266	84% 8% • 7%
1	F	266	83% 9% 7%

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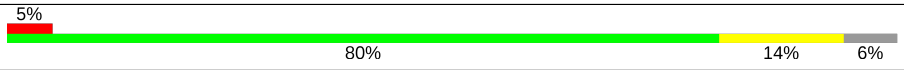
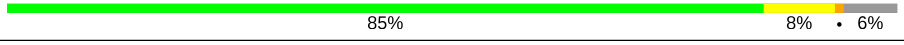
Mol	Chain	Length	Quality of chain
1	G	266	
1	H	266	
1	I	266	
1	J	266	

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	G	302	-	-	X	-
2	GOL	I	302	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 21733 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 Glyco_hydro_cc domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	249	Total	C	N	O	S	0	0	0
			2040	1305	354	365	16			
1	B	249	Total	C	N	O	S	0	1	0
			2047	1312	354	365	16			
1	C	249	Total	C	N	O	S	0	0	0
			2040	1305	354	365	16			
1	D	249	Total	C	N	O	S	0	0	0
			2040	1305	354	365	16			
1	E	248	Total	C	N	O	S	0	0	0
			2036	1303	353	364	16			
1	F	248	Total	C	N	O	S	0	0	0
			2036	1303	353	364	16			
1	G	249	Total	C	N	O	S	0	0	0
			2040	1305	354	365	16			
1	H	248	Total	C	N	O	S	0	0	0
			2036	1303	353	364	16			
1	I	249	Total	C	N	O	S	0	0	0
			2040	1305	354	365	16			
1	J	249	Total	C	N	O	S	0	0	0
			2040	1305	354	365	16			

There are 200 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP A0A074W9U7
A	-18	GLY	-	expression tag	UNP A0A074W9U7
A	-17	SER	-	expression tag	UNP A0A074W9U7
A	-16	SER	-	expression tag	UNP A0A074W9U7
A	-15	HIS	-	expression tag	UNP A0A074W9U7
A	-14	HIS	-	expression tag	UNP A0A074W9U7
A	-13	HIS	-	expression tag	UNP A0A074W9U7
A	-12	HIS	-	expression tag	UNP A0A074W9U7
A	-11	HIS	-	expression tag	UNP A0A074W9U7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	HIS	-	expression tag	UNP A0A074W9U7
A	-9	SER	-	expression tag	UNP A0A074W9U7
A	-8	SER	-	expression tag	UNP A0A074W9U7
A	-7	GLY	-	expression tag	UNP A0A074W9U7
A	-6	LEU	-	expression tag	UNP A0A074W9U7
A	-5	VAL	-	expression tag	UNP A0A074W9U7
A	-4	PRO	-	expression tag	UNP A0A074W9U7
A	-3	ALA	-	expression tag	UNP A0A074W9U7
A	-2	GLY	-	expression tag	UNP A0A074W9U7
A	-1	SER	-	expression tag	UNP A0A074W9U7
A	0	HIS	-	expression tag	UNP A0A074W9U7
B	-19	MET	-	initiating methionine	UNP A0A074W9U7
B	-18	GLY	-	expression tag	UNP A0A074W9U7
B	-17	SER	-	expression tag	UNP A0A074W9U7
B	-16	SER	-	expression tag	UNP A0A074W9U7
B	-15	HIS	-	expression tag	UNP A0A074W9U7
B	-14	HIS	-	expression tag	UNP A0A074W9U7
B	-13	HIS	-	expression tag	UNP A0A074W9U7
B	-12	HIS	-	expression tag	UNP A0A074W9U7
B	-11	HIS	-	expression tag	UNP A0A074W9U7
B	-10	HIS	-	expression tag	UNP A0A074W9U7
B	-9	SER	-	expression tag	UNP A0A074W9U7
B	-8	SER	-	expression tag	UNP A0A074W9U7
B	-7	GLY	-	expression tag	UNP A0A074W9U7
B	-6	LEU	-	expression tag	UNP A0A074W9U7
B	-5	VAL	-	expression tag	UNP A0A074W9U7
B	-4	PRO	-	expression tag	UNP A0A074W9U7
B	-3	ALA	-	expression tag	UNP A0A074W9U7
B	-2	GLY	-	expression tag	UNP A0A074W9U7
B	-1	SER	-	expression tag	UNP A0A074W9U7
B	0	HIS	-	expression tag	UNP A0A074W9U7
C	-19	MET	-	initiating methionine	UNP A0A074W9U7
C	-18	GLY	-	expression tag	UNP A0A074W9U7
C	-17	SER	-	expression tag	UNP A0A074W9U7
C	-16	SER	-	expression tag	UNP A0A074W9U7
C	-15	HIS	-	expression tag	UNP A0A074W9U7
C	-14	HIS	-	expression tag	UNP A0A074W9U7
C	-13	HIS	-	expression tag	UNP A0A074W9U7
C	-12	HIS	-	expression tag	UNP A0A074W9U7
C	-11	HIS	-	expression tag	UNP A0A074W9U7
C	-10	HIS	-	expression tag	UNP A0A074W9U7
C	-9	SER	-	expression tag	UNP A0A074W9U7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-8	SER	-	expression tag	UNP A0A074W9U7
C	-7	GLY	-	expression tag	UNP A0A074W9U7
C	-6	LEU	-	expression tag	UNP A0A074W9U7
C	-5	VAL	-	expression tag	UNP A0A074W9U7
C	-4	PRO	-	expression tag	UNP A0A074W9U7
C	-3	ALA	-	expression tag	UNP A0A074W9U7
C	-2	GLY	-	expression tag	UNP A0A074W9U7
C	-1	SER	-	expression tag	UNP A0A074W9U7
C	0	HIS	-	expression tag	UNP A0A074W9U7
D	-19	MET	-	initiating methionine	UNP A0A074W9U7
D	-18	GLY	-	expression tag	UNP A0A074W9U7
D	-17	SER	-	expression tag	UNP A0A074W9U7
D	-16	SER	-	expression tag	UNP A0A074W9U7
D	-15	HIS	-	expression tag	UNP A0A074W9U7
D	-14	HIS	-	expression tag	UNP A0A074W9U7
D	-13	HIS	-	expression tag	UNP A0A074W9U7
D	-12	HIS	-	expression tag	UNP A0A074W9U7
D	-11	HIS	-	expression tag	UNP A0A074W9U7
D	-10	HIS	-	expression tag	UNP A0A074W9U7
D	-9	SER	-	expression tag	UNP A0A074W9U7
D	-8	SER	-	expression tag	UNP A0A074W9U7
D	-7	GLY	-	expression tag	UNP A0A074W9U7
D	-6	LEU	-	expression tag	UNP A0A074W9U7
D	-5	VAL	-	expression tag	UNP A0A074W9U7
D	-4	PRO	-	expression tag	UNP A0A074W9U7
D	-3	ALA	-	expression tag	UNP A0A074W9U7
D	-2	GLY	-	expression tag	UNP A0A074W9U7
D	-1	SER	-	expression tag	UNP A0A074W9U7
D	0	HIS	-	expression tag	UNP A0A074W9U7
E	-19	MET	-	initiating methionine	UNP A0A074W9U7
E	-18	GLY	-	expression tag	UNP A0A074W9U7
E	-17	SER	-	expression tag	UNP A0A074W9U7
E	-16	SER	-	expression tag	UNP A0A074W9U7
E	-15	HIS	-	expression tag	UNP A0A074W9U7
E	-14	HIS	-	expression tag	UNP A0A074W9U7
E	-13	HIS	-	expression tag	UNP A0A074W9U7
E	-12	HIS	-	expression tag	UNP A0A074W9U7
E	-11	HIS	-	expression tag	UNP A0A074W9U7
E	-10	HIS	-	expression tag	UNP A0A074W9U7
E	-9	SER	-	expression tag	UNP A0A074W9U7
E	-8	SER	-	expression tag	UNP A0A074W9U7
E	-7	GLY	-	expression tag	UNP A0A074W9U7

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-6	LEU	-	expression tag	UNP A0A074W9U7
E	-5	VAL	-	expression tag	UNP A0A074W9U7
E	-4	PRO	-	expression tag	UNP A0A074W9U7
E	-3	ALA	-	expression tag	UNP A0A074W9U7
E	-2	GLY	-	expression tag	UNP A0A074W9U7
E	-1	SER	-	expression tag	UNP A0A074W9U7
E	0	HIS	-	expression tag	UNP A0A074W9U7
F	-19	MET	-	initiating methionine	UNP A0A074W9U7
F	-18	GLY	-	expression tag	UNP A0A074W9U7
F	-17	SER	-	expression tag	UNP A0A074W9U7
F	-16	SER	-	expression tag	UNP A0A074W9U7
F	-15	HIS	-	expression tag	UNP A0A074W9U7
F	-14	HIS	-	expression tag	UNP A0A074W9U7
F	-13	HIS	-	expression tag	UNP A0A074W9U7
F	-12	HIS	-	expression tag	UNP A0A074W9U7
F	-11	HIS	-	expression tag	UNP A0A074W9U7
F	-10	HIS	-	expression tag	UNP A0A074W9U7
F	-9	SER	-	expression tag	UNP A0A074W9U7
F	-8	SER	-	expression tag	UNP A0A074W9U7
F	-7	GLY	-	expression tag	UNP A0A074W9U7
F	-6	LEU	-	expression tag	UNP A0A074W9U7
F	-5	VAL	-	expression tag	UNP A0A074W9U7
F	-4	PRO	-	expression tag	UNP A0A074W9U7
F	-3	ALA	-	expression tag	UNP A0A074W9U7
F	-2	GLY	-	expression tag	UNP A0A074W9U7
F	-1	SER	-	expression tag	UNP A0A074W9U7
F	0	HIS	-	expression tag	UNP A0A074W9U7
G	-19	MET	-	initiating methionine	UNP A0A074W9U7
G	-18	GLY	-	expression tag	UNP A0A074W9U7
G	-17	SER	-	expression tag	UNP A0A074W9U7
G	-16	SER	-	expression tag	UNP A0A074W9U7
G	-15	HIS	-	expression tag	UNP A0A074W9U7
G	-14	HIS	-	expression tag	UNP A0A074W9U7
G	-13	HIS	-	expression tag	UNP A0A074W9U7
G	-12	HIS	-	expression tag	UNP A0A074W9U7
G	-11	HIS	-	expression tag	UNP A0A074W9U7
G	-10	HIS	-	expression tag	UNP A0A074W9U7
G	-9	SER	-	expression tag	UNP A0A074W9U7
G	-8	SER	-	expression tag	UNP A0A074W9U7
G	-7	GLY	-	expression tag	UNP A0A074W9U7
G	-6	LEU	-	expression tag	UNP A0A074W9U7
G	-5	VAL	-	expression tag	UNP A0A074W9U7

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-4	PRO	-	expression tag	UNP A0A074W9U7
G	-3	ALA	-	expression tag	UNP A0A074W9U7
G	-2	GLY	-	expression tag	UNP A0A074W9U7
G	-1	SER	-	expression tag	UNP A0A074W9U7
G	0	HIS	-	expression tag	UNP A0A074W9U7
H	-19	MET	-	initiating methionine	UNP A0A074W9U7
H	-18	GLY	-	expression tag	UNP A0A074W9U7
H	-17	SER	-	expression tag	UNP A0A074W9U7
H	-16	SER	-	expression tag	UNP A0A074W9U7
H	-15	HIS	-	expression tag	UNP A0A074W9U7
H	-14	HIS	-	expression tag	UNP A0A074W9U7
H	-13	HIS	-	expression tag	UNP A0A074W9U7
H	-12	HIS	-	expression tag	UNP A0A074W9U7
H	-11	HIS	-	expression tag	UNP A0A074W9U7
H	-10	HIS	-	expression tag	UNP A0A074W9U7
H	-9	SER	-	expression tag	UNP A0A074W9U7
H	-8	SER	-	expression tag	UNP A0A074W9U7
H	-7	GLY	-	expression tag	UNP A0A074W9U7
H	-6	LEU	-	expression tag	UNP A0A074W9U7
H	-5	VAL	-	expression tag	UNP A0A074W9U7
H	-4	PRO	-	expression tag	UNP A0A074W9U7
H	-3	ALA	-	expression tag	UNP A0A074W9U7
H	-2	GLY	-	expression tag	UNP A0A074W9U7
H	-1	SER	-	expression tag	UNP A0A074W9U7
H	0	HIS	-	expression tag	UNP A0A074W9U7
I	-19	MET	-	initiating methionine	UNP A0A074W9U7
I	-18	GLY	-	expression tag	UNP A0A074W9U7
I	-17	SER	-	expression tag	UNP A0A074W9U7
I	-16	SER	-	expression tag	UNP A0A074W9U7
I	-15	HIS	-	expression tag	UNP A0A074W9U7
I	-14	HIS	-	expression tag	UNP A0A074W9U7
I	-13	HIS	-	expression tag	UNP A0A074W9U7
I	-12	HIS	-	expression tag	UNP A0A074W9U7
I	-11	HIS	-	expression tag	UNP A0A074W9U7
I	-10	HIS	-	expression tag	UNP A0A074W9U7
I	-9	SER	-	expression tag	UNP A0A074W9U7
I	-8	SER	-	expression tag	UNP A0A074W9U7
I	-7	GLY	-	expression tag	UNP A0A074W9U7
I	-6	LEU	-	expression tag	UNP A0A074W9U7
I	-5	VAL	-	expression tag	UNP A0A074W9U7
I	-4	PRO	-	expression tag	UNP A0A074W9U7
I	-3	ALA	-	expression tag	UNP A0A074W9U7

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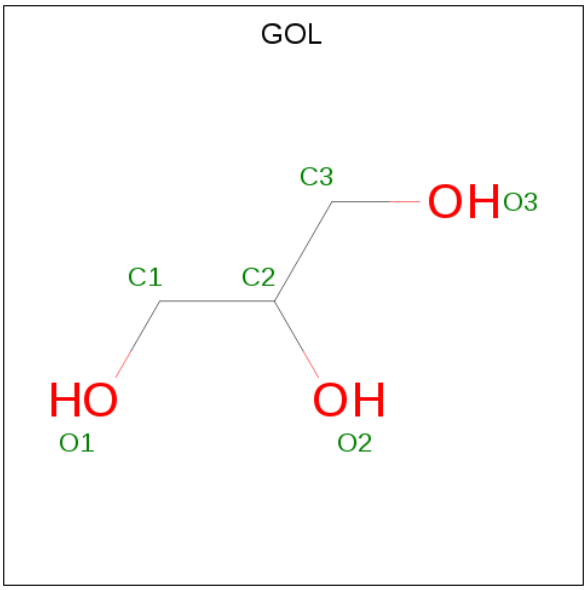
Chain	Residue	Modelled	Actual	Comment	Reference
I	-2	GLY	-	expression tag	UNP A0A074W9U7
I	-1	SER	-	expression tag	UNP A0A074W9U7
I	0	HIS	-	expression tag	UNP A0A074W9U7
J	-19	MET	-	initiating methionine	UNP A0A074W9U7
J	-18	GLY	-	expression tag	UNP A0A074W9U7
J	-17	SER	-	expression tag	UNP A0A074W9U7
J	-16	SER	-	expression tag	UNP A0A074W9U7
J	-15	HIS	-	expression tag	UNP A0A074W9U7
J	-14	HIS	-	expression tag	UNP A0A074W9U7
J	-13	HIS	-	expression tag	UNP A0A074W9U7
J	-12	HIS	-	expression tag	UNP A0A074W9U7
J	-11	HIS	-	expression tag	UNP A0A074W9U7
J	-10	HIS	-	expression tag	UNP A0A074W9U7
J	-9	SER	-	expression tag	UNP A0A074W9U7
J	-8	SER	-	expression tag	UNP A0A074W9U7
J	-7	GLY	-	expression tag	UNP A0A074W9U7
J	-6	LEU	-	expression tag	UNP A0A074W9U7
J	-5	VAL	-	expression tag	UNP A0A074W9U7
J	-4	PRO	-	expression tag	UNP A0A074W9U7
J	-3	ALA	-	expression tag	UNP A0A074W9U7
J	-2	GLY	-	expression tag	UNP A0A074W9U7
J	-1	SER	-	expression tag	UNP A0A074W9U7
J	0	HIS	-	expression tag	UNP A0A074W9U7

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



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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total C O 6 3 3	0	0
2	H	1	Total C O 6 3 3	0	0
2	H	1	Total C O 6 3 3	0	0
2	I	1	Total C O 6 3 3	0	0
2	I	1	Total C O 6 3 3	0	0
2	I	1	Total C O 6 3 3	0	0
2	I	1	Total C O 6 3 3	0	0
2	J	1	Total C O 6 3 3	0	0
2	J	1	Total C O 6 3 3	0	0
2	J	1	Total C O 6 3 3	0	0
2	J	1	Total C O 6 3 3	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	108	Total O 108 108	0	0
3	B	141	Total O 141 141	0	0
3	C	97	Total O 97 97	0	0
3	D	93	Total O 93 93	0	0
3	E	104	Total O 104 104	0	0
3	F	132	Total O 132 132	0	0
3	G	132	Total O 132 132	0	0
3	H	83	Total O 83 83	0	0

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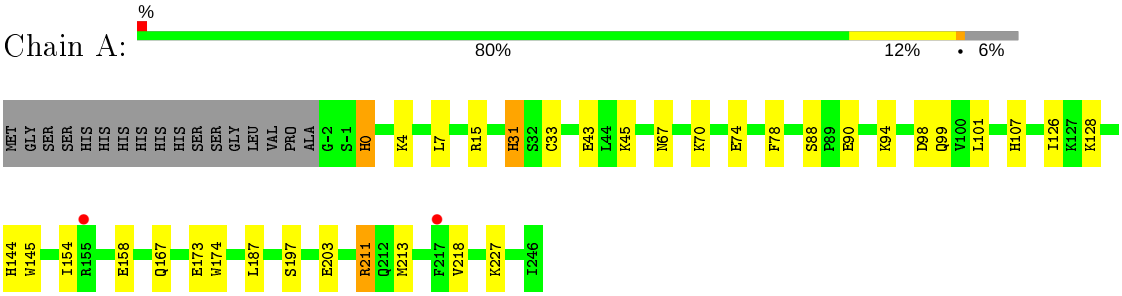
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	I	113	Total O 113 113	0	0
3	J	137	Total O 137 137	0	0

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.

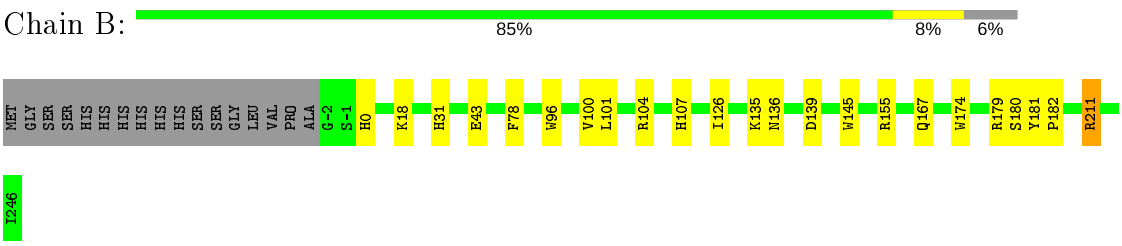
- Molecule 1: Glyco_hydro_cc domain-containing protein

Chain A:



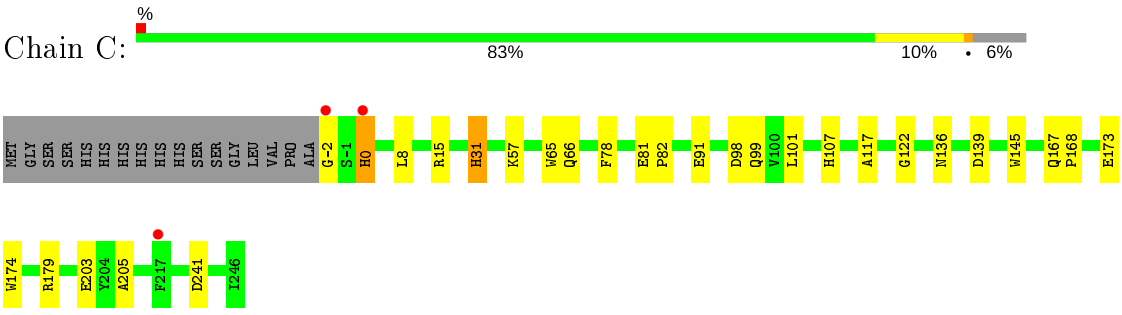
- Molecule 1: Glyco_hydro_cc domain-containing protein

Chain B:



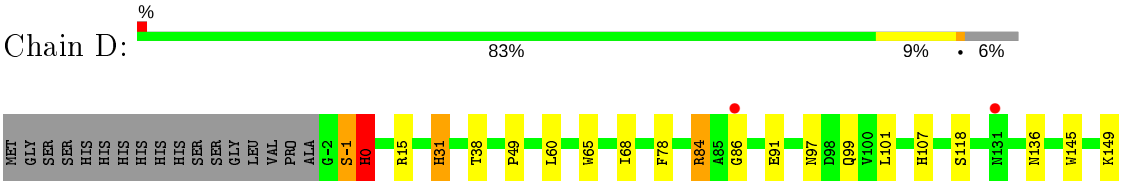
- Molecule 1: Glyco_hydro_cc domain-containing protein

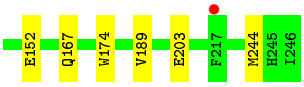
Chain C:



- Molecule 1: Glyco_hydro_cc domain-containing protein

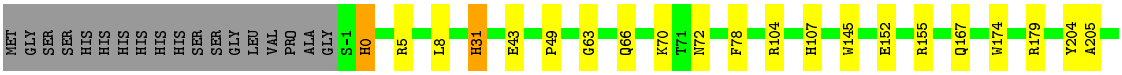
Chain D:

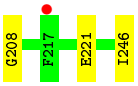




• Molecule 1: Glyco_hydro_cc domain-containing protein

Chain E:



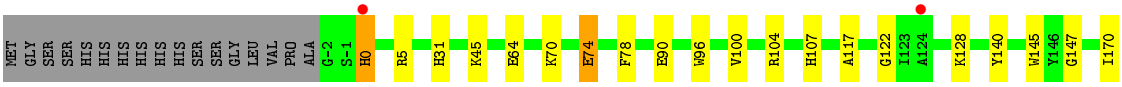


• Molecule 1: Glyco_hydro_cc domain-containing protein

Chain F:

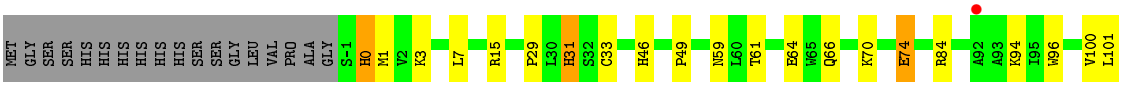
• Molecule 1: Glyco_hydro_cc domain-containing protein

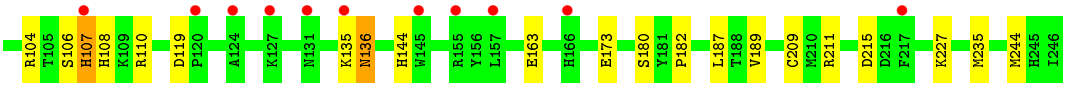
Chain G:



• Molecule 1: Glyco_hydro_cc domain-containing protein

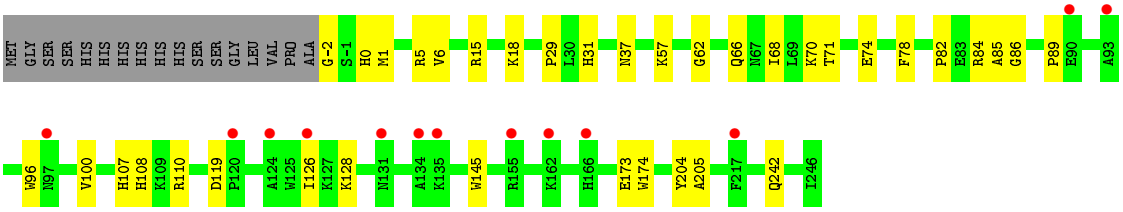
Chain H:





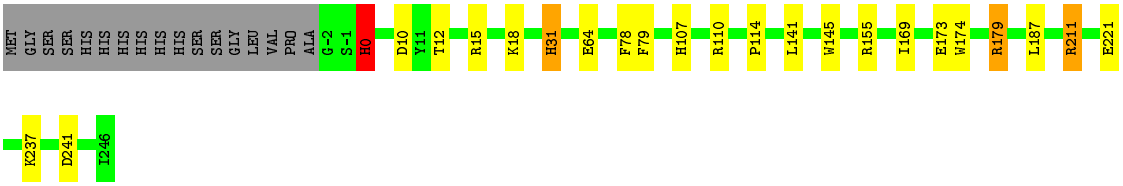
• Molecule 1: Glyco_hydro_cc domain-containing protein

Chain I:



- Molecule 1: Glyco_hydro_cc domain-containing protein

Chain J:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	117.99Å 151.86Å 166.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.21 – 1.90 48.16 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.3 (48.21-1.90) 99.3 (48.16-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.08 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.222 , 0.264 0.228 , 0.267	Depositor DCC
R_{free} test set	11663 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	28.6	Xtriage
Anisotropy	0.240	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 34.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	21733	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.48% of the height of the origin peak. No significant pseudotranslation is detected.*

[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	0.86	2/2108 (0.1%)	0.99	5/2864 (0.2%)
1	B	0.91	1/2120 (0.0%)	1.03	7/2880 (0.2%)
1	C	0.81	0/2108	0.97	5/2864 (0.2%)
1	D	0.83	1/2108 (0.0%)	0.95	2/2864 (0.1%)
1	E	0.86	2/2104 (0.1%)	1.01	5/2859 (0.2%)
1	F	0.88	1/2104 (0.0%)	1.02	5/2859 (0.2%)
1	G	0.88	0/2108	1.05	8/2864 (0.3%)
1	H	0.87	2/2104 (0.1%)	1.02	3/2859 (0.1%)
1	I	0.89	2/2108 (0.1%)	0.94	2/2864 (0.1%)
1	J	0.91	3/2108 (0.1%)	1.02	6/2864 (0.2%)
All	All	0.87	14/21080 (0.1%)	1.00	48/28641 (0.2%)

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	D	0	2
1	F	0	1
1	J	0	1
All	All	0	4

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	-2	GLY	N-CA	8.13	1.58	1.46
1	E	43	GLU	CD-OE2	6.92	1.33	1.25
1	A	74	GLU	CD-OE1	6.73	1.33	1.25
1	A	43	GLU	CD-OE2	6.07	1.32	1.25
1	E	208	GLY	C-O	6.05	1.33	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	163	GLU	CD-OE1	5.95	1.32	1.25
1	D	152	GLU	CD-OE2	5.94	1.32	1.25
1	B	43	GLU	CD-OE1	5.65	1.31	1.25
1	J	173	GLU	CD-OE1	5.62	1.31	1.25
1	F	152	GLU	CD-OE1	5.58	1.31	1.25
1	H	74	GLU	CD-OE2	5.37	1.31	1.25
1	J	64	GLU	CD-OE2	-5.06	1.20	1.25
1	I	173	GLU	CD-OE2	5.06	1.31	1.25
1	J	110	ARG	C-O	5.01	1.32	1.23

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	0	HIS	CA-CB-CG	11.44	133.04	113.60
1	E	104	ARG	NE-CZ-NH2	-9.61	115.50	120.30
1	B	104	ARG	NE-CZ-NH2	9.32	124.96	120.30
1	H	107	HIS	CB-CA-C	8.62	127.64	110.40
1	E	0	HIS	CA-CB-CG	8.44	127.94	113.60
1	A	15	ARG	NE-CZ-NH2	-8.40	116.10	120.30
1	C	0	HIS	CA-CB-CG	8.32	127.75	113.60
1	B	104	ARG	NE-CZ-NH1	-8.16	116.22	120.30
1	J	0	HIS	CA-CB-CG	7.45	126.26	113.60
1	E	104	ARG	NE-CZ-NH1	7.35	123.97	120.30
1	F	0	HIS	CA-CB-CG	7.21	125.85	113.60
1	C	15	ARG	NE-CZ-NH2	-6.91	116.85	120.30
1	D	0	HIS	CA-CB-CG	6.78	125.12	113.60
1	F	167	GLN	CB-CA-C	-6.77	96.86	110.40
1	A	0	HIS	CA-CB-CG	6.75	125.08	113.60
1	G	179	ARG	NE-CZ-NH2	-6.72	116.94	120.30
1	G	104	ARG	NE-CZ-NH1	-6.64	116.98	120.30
1	F	15	ARG	NE-CZ-NH2	-6.54	117.03	120.30
1	J	211	ARG	NE-CZ-NH2	-6.48	117.06	120.30
1	G	104	ARG	NE-CZ-NH2	6.30	123.45	120.30
1	C	179	ARG	NE-CZ-NH1	-6.19	117.20	120.30
1	G	179	ARG	NE-CZ-NH1	6.19	123.39	120.30
1	H	15	ARG	NE-CZ-NH2	-6.03	117.29	120.30
1	F	110	ARG	NE-CZ-NH1	5.97	123.28	120.30
1	G	228	ASP	CB-CG-OD2	-5.84	113.04	118.30
1	A	4	LYS	CB-CA-C	5.76	121.92	110.40
1	B	179	ARG	NE-CZ-NH1	5.71	123.15	120.30
1	G	0	HIS	ND1-CG-CD2	-5.62	98.14	106.00
1	H	0	HIS	CA-CB-CG	5.61	123.14	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	179	ARG	NE-CZ-NH2	-5.61	117.50	120.30
1	I	18	LYS	CB-CA-C	-5.57	99.26	110.40
1	D	15	ARG	NE-CZ-NH2	-5.55	117.53	120.30
1	J	15	ARG	NE-CZ-NH1	5.45	123.02	120.30
1	E	167	GLN	CB-CA-C	-5.45	99.51	110.40
1	A	211	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	J	211	ARG	CB-CG-CD	-5.43	97.47	111.60
1	C	98	ASP	CB-CA-C	-5.43	99.55	110.40
1	J	211	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	A	211	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	I	15	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	B	18	LYS	CB-CA-C	-5.14	100.11	110.40
1	B	211	ARG	NE-CZ-NH2	-5.11	117.74	120.30
1	B	211	ARG	NE-CZ-NH1	5.11	122.85	120.30
1	C	0	HIS	ND1-CG-CD2	-5.08	98.89	106.00
1	G	217	PHE	CB-CA-C	5.06	120.52	110.40
1	J	15	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	E	0	HIS	CB-CA-C	5.03	120.46	110.40
1	F	155	ARG	NE-CZ-NH2	-5.02	117.79	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	0	HIS	Peptide
1	D	86	GLY	Peptide
1	F	0	HIS	Peptide
1	J	0	HIS	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	2040	0	1966	21	0
1	B	2047	0	1971	15	0
1	C	2040	0	1966	21	0
1	D	2040	0	1966	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2036	0	1963	16	0
1	F	2036	0	1963	18	0
1	G	2040	0	1966	18	0
1	H	2036	0	1963	41	0
1	I	2040	0	1966	32	0
1	J	2040	0	1966	22	0
2	A	18	0	24	0	0
2	B	18	0	24	0	0
2	C	12	0	16	3	0
2	D	18	0	24	1	0
2	E	6	0	8	0	0
2	F	24	0	32	0	0
2	G	42	0	56	7	0
2	H	12	0	16	0	0
2	I	24	0	32	4	0
2	J	24	0	32	2	0
3	A	108	0	0	4	0
3	B	141	0	0	4	0
3	C	97	0	0	0	0
3	D	93	0	0	1	0
3	E	104	0	0	0	0
3	F	132	0	0	2	0
3	G	132	0	0	1	0
3	H	83	0	0	2	0
3	I	113	0	0	1	0
3	J	137	0	0	3	0
All	All	21733	0	19920	185	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 5.

All (185) 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:H:107:HIS:CE1	1:I:0:HIS:NE2	2.09	1.21
1:A:107:HIS:HE2	1:G:0:HIS:CE1	1.59	1.20
1:C:0:HIS:CE1	1:D:107:HIS:HE2	1.58	1.19
1:C:107:HIS:HE2	1:D:0:HIS:CE1	1.63	1.15
1:E:0:HIS:CE1	1:J:107:HIS:NE2	2.18	1.12
1:A:107:HIS:NE2	1:G:0:HIS:CE1	2.15	1.12
1:B:107:HIS:NE2	1:F:0:HIS:CE1	2.20	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:484:HOH:O	1:G:74:GLU:HG3	1.56	1.06
1:H:0:HIS:CE1	1:I:107:HIS:NE2	2.32	0.98
1:H:135:LYS:C	1:H:136:ASN:HD22	1.66	0.97
1:C:107:HIS:NE2	1:D:0:HIS:CE1	2.32	0.97
1:H:107:HIS:CE1	1:I:0:HIS:CE1	2.52	0.97
1:C:0:HIS:CE1	1:D:107:HIS:NE2	2.33	0.97
1:E:107:HIS:NE2	1:J:0:HIS:CE1	2.38	0.92
1:H:107:HIS:NE2	1:I:0:HIS:NE2	2.17	0.91
1:J:141:LEU:HD23	1:J:169:ILE:CD1	2.08	0.83
1:A:0:HIS:CE1	1:G:107:HIS:NE2	2.48	0.82
2:G:301:GOL:O1	2:G:303:GOL:H11	1.78	0.82
1:J:141:LEU:HD23	1:J:169:ILE:HD11	1.61	0.82
1:D:38:THR:HG22	1:D:68:ILE:HD11	1.62	0.80
1:H:107:HIS:HE1	1:I:0:HIS:NE2	1.76	0.78
1:B:0:HIS:CE1	1:F:107:HIS:NE2	2.53	0.76
1:C:66:GLN:NE2	1:D:-1:SER:OG	2.18	0.76
1:H:107:HIS:CE1	1:I:0:HIS:HE2	1.88	0.72
1:C:57:LYS:NZ	1:C:91:GLU:OE2	2.22	0.71
1:H:136:ASN:N	1:H:136:ASN:HD22	1.91	0.69
1:C:0:HIS:NE2	1:D:107:HIS:NE2	2.38	0.69
1:A:211:ARG:HD3	3:A:454:HOH:O	1.93	0.68
1:B:107:HIS:CE1	1:F:0:HIS:CE1	2.83	0.67
1:A:0:HIS:CE1	1:G:107:HIS:CE1	2.83	0.67
1:G:45:LYS:HE3	3:G:414:HOH:O	1.95	0.66
1:A:0:HIS:HE1	1:G:107:HIS:NE2	1.89	0.66
1:H:59:ASN:HA	1:H:64:GLU:HG2	1.78	0.65
1:B:211:ARG:HD3	3:B:403:HOH:O	1.95	0.65
1:E:63:GLY:HA3	1:F:1:MET:HE2	1.81	0.63
1:A:145:TRP:O	1:A:174:TRP:HA	2.00	0.62
1:A:107:HIS:CE1	1:G:0:HIS:CE1	2.87	0.62
1:D:84:ARG:HG3	1:D:84:ARG:HH11	1.64	0.61
1:H:0:HIS:CE1	1:I:107:HIS:CE1	2.88	0.61
1:G:64:GLU:OE2	2:G:302:GOL:H2	2.01	0.61
1:H:107:HIS:NE2	1:I:0:HIS:CE1	2.66	0.60
1:C:241:ASP:OD2	2:C:302:GOL:O3	2.20	0.60
1:H:0:HIS:HE1	1:I:107:HIS:NE2	1.93	0.60
1:G:145:TRP:CH2	1:G:147:GLY:HA3	2.36	0.60
1:B:0:HIS:CE1	1:F:107:HIS:CE1	2.90	0.59
1:F:187:LEU:HD23	1:F:187:LEU:C	2.23	0.59
1:E:0:HIS:CE1	1:J:107:HIS:CE1	2.92	0.58
1:I:37:ASN:OD1	2:I:302:GOL:H31	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:ASN:HA	1:A:70:LYS:HE3	1.87	0.56
1:H:59:ASN:HA	1:H:64:GLU:CG	2.36	0.54
1:E:31:HIS:O	1:E:49:PRO:HD2	2.07	0.54
1:E:63:GLY:HA3	1:F:1:MET:CE	2.38	0.53
1:F:149:LYS:HE3	3:F:498:HOH:O	2.08	0.53
1:J:155:ARG:NH1	3:J:401:HOH:O	2.24	0.53
1:I:96:TRP:HA	1:I:100:VAL:HB	1.88	0.53
1:E:107:HIS:NE2	1:J:0:HIS:ND1	2.57	0.53
2:G:301:GOL:C1	2:G:303:GOL:H11	2.38	0.53
1:D:38:THR:CG2	1:D:68:ILE:HD11	2.35	0.52
1:A:94:LYS:HE2	1:A:98:ASP:OD2	2.08	0.52
1:C:101:LEU:HD11	1:C:136:ASN:HB3	1.91	0.52
1:I:84:ARG:NH1	1:I:119:ASP:OD2	2.41	0.52
1:H:84:ARG:NH2	1:H:119:ASP:OD2	2.42	0.52
2:G:302:GOL:H32	1:I:1:MET:CE	2.39	0.52
1:F:186:GLY:HA2	1:F:246:ILE:HD11	1.91	0.52
1:B:101:LEU:HD11	1:B:136:ASN:HB3	1.92	0.52
1:C:101:LEU:HD11	1:C:136:ASN:CB	2.40	0.51
1:J:141:LEU:HB3	1:J:169:ILE:HD13	1.91	0.51
1:C:107:HIS:NE2	1:D:0:HIS:NE2	2.50	0.51
1:H:144:HIS:CD2	1:H:173:GLU:HB2	2.46	0.51
1:H:180:SER:OG	1:H:182:PRO:HD2	2.12	0.50
1:H:31:HIS:O	1:H:49:PRO:HD2	2.12	0.50
1:H:101:LEU:HD11	1:H:136:ASN:CB	2.42	0.50
1:E:145:TRP:O	1:E:174:TRP:HA	2.12	0.50
1:G:90:GLU:OE2	1:G:128:LYS:HE3	2.11	0.49
1:G:117:ALA:O	1:G:122:GLY:HA3	2.11	0.49
1:I:145:TRP:O	1:I:174:TRP:HA	2.12	0.49
1:G:145:TRP:O	1:G:174:TRP:HA	2.13	0.49
1:A:144:HIS:HA	1:A:173:GLU:O	2.13	0.49
1:J:141:LEU:HD23	1:J:169:ILE:HD12	1.95	0.49
1:B:139:ASP:O	1:B:167:GLN:HB2	2.13	0.49
1:F:145:TRP:O	1:F:174:TRP:HA	2.13	0.48
1:J:145:TRP:O	1:J:174:TRP:HA	2.13	0.48
1:D:84:ARG:HG3	1:D:84:ARG:NH1	2.28	0.48
1:C:173:GLU:OE1	2:C:301:GOL:H31	2.14	0.48
1:B:155:ARG:NH2	3:B:406:HOH:O	2.41	0.48
1:H:106:SER:OG	1:H:107:HIS:HD2	1.96	0.48
1:E:0:HIS:NE2	1:J:107:HIS:NE2	2.56	0.48
1:J:241:ASP:OD2	2:J:301:GOL:O1	2.28	0.48
1:A:90:GLU:OE2	1:A:128:LYS:HE2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:68:ILE:O	1:I:71:THR:HG22	2.14	0.47
1:J:211:ARG:HD3	3:J:416:HOH:O	2.13	0.47
1:H:209:CYS:SG	1:H:235:MET:HE2	2.53	0.47
1:A:187:LEU:C	1:A:187:LEU:HD23	2.34	0.47
1:D:60:LEU:O	1:D:99:GLN:NE2	2.48	0.47
1:H:3:LYS:HG2	1:H:29:PRO:HA	1.95	0.47
1:C:145:TRP:O	1:C:174:TRP:HA	2.15	0.47
1:E:5:ARG:HG2	1:E:204:TYR:CE1	2.49	0.47
1:F:142:GLY:HA2	1:F:170:ILE:O	2.14	0.47
1:H:136:ASN:ND2	1:H:136:ASN:N	2.62	0.47
1:H:187:LEU:C	1:H:187:LEU:HD23	2.35	0.47
1:B:107:HIS:NE2	1:F:0:HIS:NE2	2.60	0.47
1:A:227:LYS:HE2	3:A:490:HOH:O	2.14	0.47
1:A:154:ILE:O	1:A:158:GLU:HG3	2.15	0.47
1:H:101:LEU:HD11	1:H:136:ASN:HB3	1.96	0.47
1:D:101:LEU:HD11	1:D:136:ASN:CB	2.45	0.46
1:G:245:HIS:HE1	2:G:301:GOL:O1	1.99	0.46
1:E:107:HIS:CE1	1:J:0:HIS:ND1	2.83	0.46
1:E:179:ARG:O	1:E:221:GLU:HG3	2.16	0.46
1:H:59:ASN:HD22	1:H:64:GLU:CG	2.29	0.46
1:H:215:ASP:HB2	3:H:642:HOH:O	2.16	0.46
1:H:189:VAL:HG22	1:H:244:MET:HB3	1.98	0.46
1:D:65:TRP:CZ2	1:D:99:GLN:HG2	2.52	0.45
1:F:211:ARG:HD2	1:F:227:LYS:O	2.16	0.45
1:H:96:TRP:HA	1:H:100:VAL:HB	1.99	0.45
1:H:74:GLU:HB3	1:I:74:GLU:HG2	1.98	0.45
2:G:302:GOL:H32	1:I:1:MET:HE2	1.98	0.45
1:G:211:ARG:HD2	1:G:227:LYS:O	2.15	0.45
1:H:211:ARG:HD2	1:H:227:LYS:O	2.17	0.45
1:A:101:LEU:HD23	1:A:101:LEU:HA	1.77	0.45
1:C:8:LEU:HG	1:C:205:ALA:HB1	1.98	0.44
1:H:66:GLN:O	1:H:70:LYS:HG3	2.17	0.44
1:B:101:LEU:HD11	1:B:136:ASN:CB	2.47	0.44
1:C:81:GLU:N	1:C:82:PRO:CD	2.80	0.44
1:I:6:VAL:HB	1:I:205:ALA:HB2	1.99	0.44
1:D:145:TRP:O	1:D:174:TRP:HA	2.18	0.44
1:H:110:ARG:NH2	1:I:108:HIS:O	2.48	0.44
1:A:45:LYS:CE	3:A:413:HOH:O	2.65	0.44
1:I:82:PRO:HA	1:I:85:ALA:HB3	2.00	0.44
1:H:209:CYS:SG	1:H:235:MET:CE	3.06	0.43
2:C:302:GOL:O2	2:I:302:GOL:H12	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:117:ALA:O	1:C:122:GLY:HA3	2.18	0.43
1:J:179:ARG:O	1:J:221:GLU:HG3	2.18	0.43
1:E:72:ASN:OD1	1:J:31:HIS:HB2	2.18	0.43
1:E:8:LEU:HG	1:E:205:ALA:HB1	2.00	0.43
1:F:149:LYS:CE	3:F:498:HOH:O	2.63	0.43
1:B:181:TYR:HB3	1:B:182:PRO:HD3	2.01	0.43
1:E:152:GLU:OE1	1:E:155:ARG:NH2	2.44	0.43
1:I:37:ASN:OD1	2:I:302:GOL:C3	2.65	0.43
3:B:500:HOH:O	1:E:66:GLN:HG2	2.19	0.43
1:C:31:HIS:NE2	1:C:203:GLU:OE1	2.50	0.43
1:D:167:GLN:NE2	3:D:510:HOH:O	2.49	0.43
1:I:37:ASN:HD21	2:I:302:GOL:H11	1.83	0.43
1:C:139:ASP:O	1:C:168:PRO:HD2	2.19	0.43
1:F:8:LEU:HG	1:F:205:ALA:HB1	2.00	0.43
1:I:126:ILE:HD12	1:I:126:ILE:HA	1.82	0.43
1:D:31:HIS:O	1:D:49:PRO:HD2	2.19	0.42
1:F:35:ASN:C	1:F:35:ASN:OD1	2.57	0.42
1:C:107:HIS:CE1	1:D:0:HIS:CE1	3.05	0.42
1:J:79:PHE:O	1:J:114:PRO:HA	2.19	0.42
1:H:107:HIS:HE1	1:I:0:HIS:CD2	2.34	0.42
1:H:135:LYS:C	1:H:136:ASN:ND2	2.51	0.42
1:H:110:ARG:HG3	1:I:110:ARG:CZ	2.49	0.42
1:I:66:GLN:HB3	1:I:70:LYS:HE3	2.01	0.42
1:I:86:GLY:HA2	3:I:491:HOH:O	2.17	0.42
1:I:89:PRO:HG2	1:I:128:LYS:HD3	2.00	0.42
1:A:31:HIS:NE2	1:A:203:GLU:OE1	2.49	0.42
1:G:140:TYR:HB3	1:G:170:ILE:HG13	2.02	0.42
1:G:5:ARG:HG2	1:G:204:TYR:CE1	2.54	0.42
1:H:106:SER:OG	1:H:107:HIS:CD2	2.71	0.42
1:I:5:ARG:HG2	1:I:204:TYR:CE1	2.53	0.42
1:J:18:LYS:HG3	3:J:502:HOH:O	2.20	0.42
2:G:302:GOL:H32	1:I:1:MET:HE3	2.01	0.42
1:B:135:LYS:HB2	3:B:485:HOH:O	2.19	0.42
1:I:29:PRO:HG3	1:I:242:GLN:HB2	2.00	0.42
1:H:104:ARG:O	1:H:108:HIS:HA	2.20	0.42
1:J:78:PHE:HD2	1:J:114:PRO:HD3	1.85	0.42
1:B:145:TRP:O	1:B:174:TRP:HA	2.20	0.41
1:F:181:TYR:N	1:F:182:PRO:CD	2.84	0.41
1:D:189:VAL:HG22	1:D:244:MET:HB3	2.02	0.41
1:D:31:HIS:NE2	1:D:203:GLU:OE1	2.50	0.41
1:C:-2:GLY:HA2	1:I:62:GLY:HA2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:96:TRP:HA	1:G:100:VAL:HB	2.02	0.41
1:B:126:ILE:HD12	1:B:126:ILE:HA	1.88	0.41
1:B:96:TRP:HA	1:B:100:VAL:HB	2.03	0.41
1:A:126:ILE:HA	1:A:126:ILE:HD12	1.87	0.41
2:D:402:GOL:C1	1:H:1:MET:HE2	2.51	0.41
1:J:10:ASP:OD2	1:J:12:THR:HG23	2.21	0.41
1:A:7:LEU:O	1:A:33:CYS:HA	2.21	0.40
1:J:187:LEU:C	1:J:187:LEU:HD23	2.41	0.40
1:J:237:LYS:HG2	2:J:301:GOL:O1	2.21	0.40
1:C:65:TRP:CZ2	1:C:99:GLN:HG2	2.56	0.40
1:F:5:ARG:HG2	1:F:204:TYR:CE1	2.56	0.40
1:A:213:MET:HE3	1:A:218:VAL:HG23	2.02	0.40
1:H:7:LEU:O	1:H:33:CYS:HA	2.21	0.40
1:H:46:HIS:HA	3:H:604:HOH:O	2.21	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	247/266 (93%)	235 (95%)	12 (5%)	0	100	100
1	B	248/266 (93%)	241 (97%)	7 (3%)	0	100	100
1	C	247/266 (93%)	238 (96%)	9 (4%)	0	100	100
1	D	247/266 (93%)	236 (96%)	11 (4%)	0	100	100
1	E	246/266 (92%)	233 (95%)	13 (5%)	0	100	100
1	F	246/266 (92%)	236 (96%)	10 (4%)	0	100	100
1	G	247/266 (93%)	237 (96%)	10 (4%)	0	100	100
1	H	246/266 (92%)	238 (97%)	8 (3%)	0	100	100
1	I	247/266 (93%)	237 (96%)	10 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	J	247/266 (93%)	237 (96%)	10 (4%)	0	100	100
All	All	2468/2660 (93%)	2368 (96%)	100 (4%)	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	221/235 (94%)	215 (97%)	6 (3%)	44	38
1	B	222/235 (94%)	219 (99%)	3 (1%)	67	65
1	C	221/235 (94%)	218 (99%)	3 (1%)	67	65
1	D	221/235 (94%)	213 (96%)	8 (4%)	35	26
1	E	221/235 (94%)	217 (98%)	4 (2%)	59	55
1	F	221/235 (94%)	218 (99%)	3 (1%)	67	65
1	G	221/235 (94%)	217 (98%)	4 (2%)	59	55
1	H	221/235 (94%)	217 (98%)	4 (2%)	59	55
1	I	221/235 (94%)	218 (99%)	3 (1%)	67	65
1	J	221/235 (94%)	218 (99%)	3 (1%)	67	65
All	All	2211/2350 (94%)	2170 (98%)	41 (2%)	57	53

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	HIS
1	A	78	PHE
1	A	88	SER
1	A	99	GLN
1	A	167	GLN
1	A	197	SER
1	B	31	HIS
1	B	78	PHE

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Mol	Chain	Res	Type
1	B	180	SER
1	C	31	HIS
1	C	78	PHE
1	C	167	GLN
1	D	-1	SER
1	D	31	HIS
1	D	78	PHE
1	D	84	ARG
1	D	91	GLU
1	D	97	ASN
1	D	118	SER
1	D	149	LYS
1	E	31	HIS
1	E	70	LYS
1	E	78	PHE
1	E	246	ILE
1	F	78	PHE
1	F	135	LYS
1	F	246	ILE
1	G	31	HIS
1	G	70	LYS
1	G	74	GLU
1	G	78	PHE
1	H	31	HIS
1	H	61	THR
1	H	94	LYS
1	H	136	ASN
1	I	31	HIS
1	I	57	LYS
1	I	78	PHE
1	J	0	HIS
1	J	31	HIS
1	J	179	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	0	HIS
1	B	0	HIS
1	B	66	GLN
1	C	66	GLN
1	C	97	ASN

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Mol	Chain	Res	Type
1	C	167	GLN
1	D	0	HIS
1	D	58	ASN
1	E	0	HIS
1	F	0	HIS
1	G	0	HIS
1	G	223	GLN
1	H	0	HIS
1	H	107	HIS
1	H	136	ASN
1	J	0	HIS
1	J	223	GLN

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

33 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	301	-	5,5,5	0.17	0	5,5,5	0.50	0
2	GOL	A	301	-	5,5,5	0.12	0	5,5,5	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	GOL	C	301	-	5,5,5	0.18	0	5,5,5	0.39	0
2	GOL	G	306	-	5,5,5	0.14	0	5,5,5	0.38	0
2	GOL	I	303	-	5,5,5	0.28	0	5,5,5	0.82	0
2	GOL	D	403	-	5,5,5	0.12	0	5,5,5	0.31	0
2	GOL	A	303	-	5,5,5	0.13	0	5,5,5	0.25	0
2	GOL	F	302	-	5,5,5	0.14	0	5,5,5	0.35	0
2	GOL	J	301	-	5,5,5	0.11	0	5,5,5	0.48	0
2	GOL	I	301	-	5,5,5	0.49	0	5,5,5	0.94	0
2	GOL	E	301	-	5,5,5	0.14	0	5,5,5	0.53	0
2	GOL	D	401	-	5,5,5	0.32	0	5,5,5	1.17	1 (20%)
2	GOL	C	302	-	5,5,5	0.44	0	5,5,5	0.67	0
2	GOL	A	302	-	5,5,5	0.30	0	5,5,5	0.32	0
2	GOL	I	304	-	5,5,5	0.39	0	5,5,5	0.66	0
2	GOL	F	304	-	5,5,5	0.19	0	5,5,5	0.36	0
2	GOL	H	502	-	5,5,5	0.22	0	5,5,5	0.39	0
2	GOL	J	302	-	5,5,5	0.13	0	5,5,5	0.32	0
2	GOL	G	304	-	5,5,5	0.17	0	5,5,5	0.27	0
2	GOL	J	304	-	5,5,5	0.26	0	5,5,5	0.50	0
2	GOL	I	302	-	5,5,5	0.28	0	5,5,5	0.63	0
2	GOL	D	402	-	5,5,5	0.24	0	5,5,5	0.32	0
2	GOL	F	303	-	5,5,5	0.27	0	5,5,5	0.43	0
2	GOL	G	303	-	5,5,5	0.20	0	5,5,5	0.60	0
2	GOL	G	307	-	5,5,5	0.20	0	5,5,5	0.51	0
2	GOL	H	501	-	5,5,5	0.26	0	5,5,5	0.41	0
2	GOL	B	302	-	5,5,5	0.24	0	5,5,5	0.53	0
2	GOL	F	301	-	5,5,5	0.24	0	5,5,5	0.61	0
2	GOL	G	301	-	5,5,5	0.35	0	5,5,5	0.46	0
2	GOL	G	302	-	5,5,5	0.37	0	5,5,5	1.03	0
2	GOL	G	305	-	5,5,5	0.13	0	5,5,5	0.43	0
2	GOL	J	303	-	5,5,5	0.08	0	5,5,5	0.49	0
2	GOL	B	303	-	5,5,5	0.16	0	5,5,5	0.41	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	301	-	-	0/4/4/4	-
2	GOL	A	301	-	-	0/4/4/4	-
2	GOL	C	301	-	-	4/4/4/4	-
2	GOL	G	306	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	I	303	-	-	2/4/4/4	-
2	GOL	D	403	-	-	4/4/4/4	-
2	GOL	A	303	-	-	2/4/4/4	-
2	GOL	F	302	-	-	2/4/4/4	-
2	GOL	J	301	-	-	4/4/4/4	-
2	GOL	I	301	-	-	2/4/4/4	-
2	GOL	E	301	-	-	3/4/4/4	-
2	GOL	D	401	-	-	4/4/4/4	-
2	GOL	C	302	-	-	0/4/4/4	-
2	GOL	A	302	-	-	0/4/4/4	-
2	GOL	I	304	-	-	0/4/4/4	-
2	GOL	F	304	-	-	0/4/4/4	-
2	GOL	H	502	-	-	2/4/4/4	-
2	GOL	J	302	-	-	2/4/4/4	-
2	GOL	G	304	-	-	2/4/4/4	-
2	GOL	J	304	-	-	4/4/4/4	-
2	GOL	I	302	-	-	4/4/4/4	-
2	GOL	D	402	-	-	0/4/4/4	-
2	GOL	F	303	-	-	0/4/4/4	-
2	GOL	G	303	-	-	3/4/4/4	-
2	GOL	G	307	-	-	2/4/4/4	-
2	GOL	H	501	-	-	0/4/4/4	-
2	GOL	B	302	-	-	2/4/4/4	-
2	GOL	F	301	-	-	0/4/4/4	-
2	GOL	G	301	-	-	1/4/4/4	-
2	GOL	G	302	-	-	4/4/4/4	-
2	GOL	G	305	-	-	0/4/4/4	-
2	GOL	J	303	-	-	2/4/4/4	-
2	GOL	B	303	-	-	3/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	401	GOL	O2-C2-C1	2.17	118.69	109.12

There are no chirality outliers.

All (60) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	403	GOL	O1-C1-C2-C3
2	F	302	GOL	O1-C1-C2-C3
2	J	301	GOL	C1-C2-C3-O3
2	D	401	GOL	O1-C1-C2-C3
2	H	502	GOL	C1-C2-C3-O3
2	H	502	GOL	O2-C2-C3-O3
2	J	302	GOL	C1-C2-C3-O3
2	J	302	GOL	O2-C2-C3-O3
2	G	304	GOL	O1-C1-C2-C3
2	J	304	GOL	O1-C1-C2-C3
2	I	302	GOL	O1-C1-C2-C3
2	I	302	GOL	C1-C2-C3-O3
2	G	303	GOL	O1-C1-C2-C3
2	G	307	GOL	O1-C1-C2-C3
2	B	302	GOL	C1-C2-C3-O3
2	B	302	GOL	O2-C2-C3-O3
2	G	302	GOL	C1-C2-C3-O3
2	J	303	GOL	O1-C1-C2-C3
2	B	303	GOL	C1-C2-C3-O3
2	A	303	GOL	O2-C2-C3-O3
2	J	301	GOL	O2-C2-C3-O3
2	G	304	GOL	O1-C1-C2-O2
2	J	304	GOL	O1-C1-C2-O2
2	C	301	GOL	O1-C1-C2-C3
2	C	301	GOL	C1-C2-C3-O3
2	G	306	GOL	O1-C1-C2-C3
2	D	403	GOL	C1-C2-C3-O3
2	A	303	GOL	C1-C2-C3-O3
2	J	301	GOL	O1-C1-C2-C3
2	E	301	GOL	O1-C1-C2-C3
2	D	401	GOL	C1-C2-C3-O3
2	J	304	GOL	C1-C2-C3-O3
2	G	302	GOL	O1-C1-C2-C3
2	C	301	GOL	O1-C1-C2-O2
2	F	302	GOL	O1-C1-C2-O2
2	E	301	GOL	O1-C1-C2-O2
2	D	401	GOL	O2-C2-C3-O3
2	J	304	GOL	O2-C2-C3-O3
2	I	302	GOL	O1-C1-C2-O2
2	I	302	GOL	O2-C2-C3-O3
2	J	303	GOL	O1-C1-C2-O2
2	B	303	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
2	D	401	GOL	O1-C1-C2-O2
2	G	303	GOL	O1-C1-C2-O2
2	G	307	GOL	O1-C1-C2-O2
2	G	302	GOL	O2-C2-C3-O3
2	G	303	GOL	C1-C2-C3-O3
2	C	301	GOL	O2-C2-C3-O3
2	J	301	GOL	O1-C1-C2-O2
2	I	303	GOL	O2-C2-C3-O3
2	E	301	GOL	O2-C2-C3-O3
2	I	303	GOL	C1-C2-C3-O3
2	D	403	GOL	O2-C2-C3-O3
2	I	301	GOL	O1-C1-C2-C3
2	G	301	GOL	O1-C1-C2-C3
2	B	303	GOL	O1-C1-C2-C3
2	G	306	GOL	O1-C1-C2-O2
2	D	403	GOL	O1-C1-C2-O2
2	I	301	GOL	O1-C1-C2-O2
2	G	302	GOL	O1-C1-C2-O2

There are no ring outliers.

8 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	301	GOL	1	0
2	J	301	GOL	2	0
2	C	302	GOL	2	0
2	I	302	GOL	4	0
2	D	402	GOL	1	0
2	G	303	GOL	2	0
2	G	301	GOL	3	0
2	G	302	GOL	4	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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	249/266 (93%)	-0.05	2 (0%) 86 87	26, 37, 54, 67	0
1	B	249/266 (93%)	-0.15	0 100 100	24, 30, 42, 58	0
1	C	249/266 (93%)	0.02	3 (1%) 79 81	27, 37, 58, 67	0
1	D	249/266 (93%)	0.00	3 (1%) 79 81	28, 38, 59, 71	0
1	E	248/266 (93%)	-0.06	1 (0%) 92 93	28, 35, 47, 66	0
1	F	248/266 (93%)	-0.10	1 (0%) 92 93	25, 33, 44, 59	0
1	G	249/266 (93%)	-0.19	2 (0%) 86 87	23, 31, 45, 51	0
1	H	248/266 (93%)	0.43	12 (4%) 30 33	29, 41, 57, 64	0
1	I	249/266 (93%)	0.23	13 (5%) 27 30	24, 35, 57, 73	0
1	J	249/266 (93%)	-0.14	0 100 100	24, 31, 47, 70	0
All	All	2487/2660 (93%)	-0.00	37 (1%) 73 76	23, 35, 55, 73	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	217	PHE	4.5
1	I	135	LYS	4.5
1	I	93	ALA	4.2
1	G	124	ALA	4.0
1	H	157	LEU	3.5
1	I	131	ASN	3.4
1	D	217	PHE	3.4
1	I	217	PHE	3.3
1	H	92	ALA	3.1
1	H	135	LYS	3.0
1	I	166	HIS	2.9
1	H	120	PRO	2.9
1	C	0	HIS	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	155	ARG	2.7
1	H	107	HIS	2.6
1	I	120	PRO	2.5
1	H	131	ASN	2.5
1	E	217	PHE	2.5
1	H	127	LYS	2.4
1	I	126	ILE	2.4
1	I	124	ALA	2.4
1	H	155	ARG	2.4
1	H	217	PHE	2.4
1	H	124	ALA	2.4
1	I	90	GLU	2.3
1	I	134	ALA	2.3
1	F	0	HIS	2.3
1	D	131	ASN	2.2
1	H	145	TRP	2.2
1	G	0	HIS	2.1
1	H	166	HIS	2.1
1	I	97	ASN	2.1
1	C	-2	GLY	2.1
1	A	217	PHE	2.1
1	I	155	ARG	2.1
1	I	162	LYS	2.1
1	D	86	GLY	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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GOL	I	304	6/6	0.75	0.28	46,48,49,49	0
2	GOL	A	303	6/6	0.76	0.20	60,66,69,69	0
2	GOL	J	303	6/6	0.78	0.23	54,54,55,56	0
2	GOL	I	301	6/6	0.79	0.16	37,42,42,44	0
2	GOL	I	302	6/6	0.81	0.16	52,54,55,55	0
2	GOL	G	304	6/6	0.82	0.20	54,56,58,60	0
2	GOL	F	304	6/6	0.83	0.21	61,62,62,63	0
2	GOL	G	303	6/6	0.86	0.16	43,44,45,50	0
2	GOL	J	304	6/6	0.87	0.16	41,46,48,52	0
2	GOL	C	301	6/6	0.87	0.18	56,57,58,62	0
2	GOL	B	303	6/6	0.88	0.12	45,46,48,48	0
2	GOL	D	403	6/6	0.89	0.14	60,62,66,66	0
2	GOL	J	302	6/6	0.89	0.14	50,52,55,59	0
2	GOL	B	302	6/6	0.89	0.14	39,44,45,45	0
2	GOL	E	301	6/6	0.89	0.13	40,41,42,43	0
2	GOL	I	303	6/6	0.89	0.17	42,45,45,48	0
2	GOL	C	302	6/6	0.90	0.12	40,40,41,41	0
2	GOL	H	502	6/6	0.90	0.12	39,41,43,48	0
2	GOL	G	305	6/6	0.91	0.19	55,56,56,56	0
2	GOL	G	307	6/6	0.91	0.14	50,54,55,56	0
2	GOL	G	301	6/6	0.91	0.15	30,32,34,35	0
2	GOL	H	501	6/6	0.92	0.17	46,48,52,54	0
2	GOL	D	401	6/6	0.93	0.11	32,35,39,42	0
2	GOL	D	402	6/6	0.93	0.13	43,46,48,49	0
2	GOL	F	302	6/6	0.93	0.13	41,47,47,48	0
2	GOL	F	301	6/6	0.93	0.16	41,45,47,49	0
2	GOL	F	303	6/6	0.94	0.12	31,34,36,37	0
2	GOL	G	306	6/6	0.94	0.13	40,47,49,51	0
2	GOL	J	301	6/6	0.95	0.14	38,40,43,50	0
2	GOL	A	302	6/6	0.95	0.08	30,33,34,36	0
2	GOL	G	302	6/6	0.96	0.13	30,31,31,31	0
2	GOL	A	301	6/6	0.96	0.09	31,32,32,32	0
2	GOL	B	301	6/6	0.97	0.09	31,33,34,34	0

6.5 Other polymers (i)

There are no such residues in this entry.