Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 12:25 AM GMT

PDB ID	:	2AAM
Title	:	Crystal structure of a putative glycosidase (tm1410) from thermotoga maritima at 2.20 A resolution
Authors	:	Joint Center for Structural Genomics (JCSG)
Deposited on	:	2005-07-13
Resolution	:	2.20 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
http://wwpdb.org/validation/2016/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:

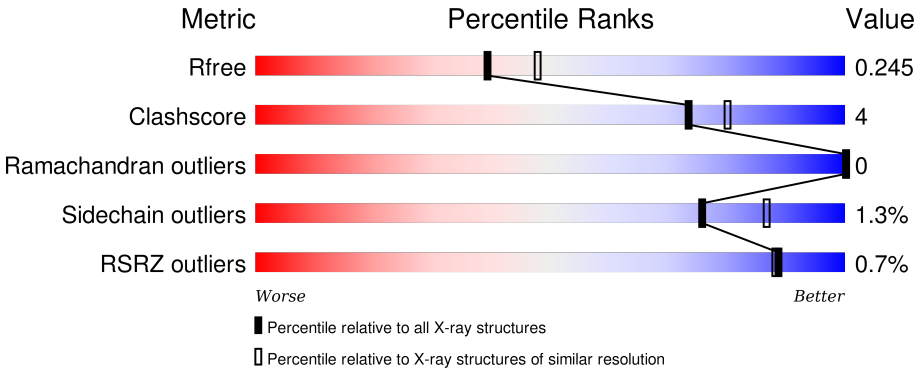
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.20 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}	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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. 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	309	86% 6% 8%
1	B	309	% 84% 8% • 7%
1	C	309	% 85% 6% • 7%
1	D	309	89% • 7%
1	E	309	% 86% 6% 7%

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Mol	Chain	Length	Quality of chain
1	F	309	87% 5% 7%

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	UNL	A	1	-	-	X	X
2	UNL	B	2	-	-	X	X
2	UNL	C	3	-	-	X	-
2	UNL	D	4	-	-	X	X
2	UNL	E	5	-	-	X	X
2	UNL	F	6	-	-	X	X
3	GOL	A	13	-	-	-	X
3	GOL	A	14	-	-	-	X
3	GOL	A	325	-	-	-	X
3	GOL	A	326	-	-	-	X
3	GOL	A	327	-	-	-	X
3	GOL	B	324	-	-	-	X
3	GOL	B	325	-	-	-	X
3	GOL	B	328	-	-	-	X
3	GOL	B	7	-	-	-	X
3	GOL	B	8	-	-	-	X
3	GOL	C	324	-	-	-	X
3	GOL	C	327	-	-	-	X
3	GOL	D	11	-	-	-	X
3	GOL	D	325	-	-	-	X
3	GOL	D	327	-	-	-	X
3	GOL	E	324	-	-	-	X
3	GOL	E	326	-	-	-	X
3	GOL	F	10	-	-	-	X
3	GOL	F	324	-	-	-	X
3	GOL	F	325	-	-	-	X
3	GOL	F	326	-	-	-	X
3	GOL	F	327	-	-	-	X
3	GOL	F	328	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15499 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 Hypothetical protein TM1410.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	285	Total	C	N	O	S	Se	0	8	0
			2381	1531	380	464	1	5			
1	B	287	Total	C	N	O	S	Se	0	6	0
			2390	1536	379	467	1	7			
1	C	286	Total	C	N	O	S	Se	0	3	0
			2377	1530	378	463	1	5			
1	D	286	Total	C	N	O	S	Se	0	0	0
			2360	1520	373	461	1	5			
1	E	287	Total	C	N	O	S	Se	0	1	0
			2372	1529	375	462	1	5			
1	F	286	Total	C	N	O	S	Se	0	3	0
			2369	1526	376	461	1	5			

There are 102 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	15	MSE	-	MODIFIED RESIDUE	UNP Q9X1D0
A	16	GLY	-	LEADER SEQUENCE	UNP Q9X1D0
A	17	SER	-	LEADER SEQUENCE	UNP Q9X1D0
A	18	ASP	-	LEADER SEQUENCE	UNP Q9X1D0
A	19	LYS	-	LEADER SEQUENCE	UNP Q9X1D0
A	20	ILE	-	LEADER SEQUENCE	UNP Q9X1D0
A	22	HIS	-	LEADER SEQUENCE	UNP Q9X1D0
A	23	HIS	-	LEADER SEQUENCE	UNP Q9X1D0
A	24	HIS	-	LEADER SEQUENCE	UNP Q9X1D0
A	25	HIS	-	LEADER SEQUENCE	UNP Q9X1D0
A	26	HIS	-	LEADER SEQUENCE	UNP Q9X1D0
A	26	HIS	-	LEADER SEQUENCE	UNP Q9X1D0
A	32	MSE	MET	MODIFIED RESIDUE	UNP Q9X1D0
A	79	MSE	MET	MODIFIED RESIDUE	UNP Q9X1D0
A	179	MSE	MET	MODIFIED RESIDUE	UNP Q9X1D0
A	197	MSE	MET	MODIFIED RESIDUE	UNP Q9X1D0
A	302	MSE	MET	MODIFIED RESIDUE	UNP Q9X1D0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	15	MSE	-	MODIFIED RESIDUE	UNP Q9X1D0
B	16	GLY	-	LEADER SEQUENCE	UNP Q9X1D0
B	17	SER	-	LEADER SEQUENCE	UNP Q9X1D0
B	18	ASP	-	LEADER SEQUENCE	UNP Q9X1D0
B	19	LYS	-	LEADER SEQUENCE	UNP Q9X1D0
B	20	ILE	-	LEADER SEQUENCE	UNP Q9X1D0
B	22	HIS	-	LEADER SEQUENCE	UNP Q9X1D0
B	23	HIS	-	LEADER SEQUENCE	UNP Q9X1D0
B	24	HIS	-	LEADER SEQUENCE	UNP Q9X1D0
B	25	HIS	-	LEADER SEQUENCE	UNP Q9X1D0
B	26	HIS	-	LEADER SEQUENCE	UNP Q9X1D0
B	26	HIS	-	LEADER SEQUENCE	UNP Q9X1D0
B	32	MSE	MET	MODIFIED RESIDUE	UNP Q9X1D0
B	79	MSE	MET	MODIFIED RESIDUE	UNP Q9X1D0
B	179	MSE	MET	MODIFIED RESIDUE	UNP Q9X1D0
B	197	MSE	MET	MODIFIED RESIDUE	UNP Q9X1D0
B	302	MSE	MET	MODIFIED RESIDUE	UNP Q9X1D0
C	15	MSE	-	MODIFIED RESIDUE	UNP Q9X1D0
C	16	GLY	-	LEADER SEQUENCE	UNP Q9X1D0
C	17	SER	-	LEADER SEQUENCE	UNP Q9X1D0
C	18	ASP	-	LEADER SEQUENCE	UNP Q9X1D0
C	19	LYS	-	LEADER SEQUENCE	UNP Q9X1D0
C	20	ILE	-	LEADER SEQUENCE	UNP Q9X1D0
C	22	HIS	-	LEADER SEQUENCE	UNP Q9X1D0
C	23	HIS	-	LEADER SEQUENCE	UNP Q9X1D0
C	24	HIS	-	LEADER SEQUENCE	UNP Q9X1D0
C	25	HIS	-	LEADER SEQUENCE	UNP Q9X1D0
C	26	HIS	-	LEADER SEQUENCE	UNP Q9X1D0
C	26	HIS	-	LEADER SEQUENCE	UNP Q9X1D0
C	32	MSE	MET	MODIFIED RESIDUE	UNP Q9X1D0
C	79	MSE	MET	MODIFIED RESIDUE	UNP Q9X1D0
C	179	MSE	MET	MODIFIED RESIDUE	UNP Q9X1D0
C	197	MSE	MET	MODIFIED RESIDUE	UNP Q9X1D0
C	302	MSE	MET	MODIFIED RESIDUE	UNP Q9X1D0
D	15	MSE	-	MODIFIED RESIDUE	UNP Q9X1D0
D	16	GLY	-	LEADER SEQUENCE	UNP Q9X1D0
D	17	SER	-	LEADER SEQUENCE	UNP Q9X1D0
D	18	ASP	-	LEADER SEQUENCE	UNP Q9X1D0
D	19	LYS	-	LEADER SEQUENCE	UNP Q9X1D0
D	20	ILE	-	LEADER SEQUENCE	UNP Q9X1D0
D	22	HIS	-	LEADER SEQUENCE	UNP Q9X1D0
D	23	HIS	-	LEADER SEQUENCE	UNP Q9X1D0

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Chain	Residue	Modelled	Actual	Comment	Reference
D	24	HIS	-	LEADER SEQUENCE	UNP Q9X1D0
D	25	HIS	-	LEADER SEQUENCE	UNP Q9X1D0
D	26	HIS	-	LEADER SEQUENCE	UNP Q9X1D0
D	26	HIS	-	LEADER SEQUENCE	UNP Q9X1D0
D	32	MSE	MET	MODIFIED RESIDUE	UNP Q9X1D0
D	79	MSE	MET	MODIFIED RESIDUE	UNP Q9X1D0
D	179	MSE	MET	MODIFIED RESIDUE	UNP Q9X1D0
D	197	MSE	MET	MODIFIED RESIDUE	UNP Q9X1D0
D	302	MSE	MET	MODIFIED RESIDUE	UNP Q9X1D0
E	15	MSE	-	MODIFIED RESIDUE	UNP Q9X1D0
E	16	GLY	-	LEADER SEQUENCE	UNP Q9X1D0
E	17	SER	-	LEADER SEQUENCE	UNP Q9X1D0
E	18	ASP	-	LEADER SEQUENCE	UNP Q9X1D0
E	19	LYS	-	LEADER SEQUENCE	UNP Q9X1D0
E	20	ILE	-	LEADER SEQUENCE	UNP Q9X1D0
E	22	HIS	-	LEADER SEQUENCE	UNP Q9X1D0
E	23	HIS	-	LEADER SEQUENCE	UNP Q9X1D0
E	24	HIS	-	LEADER SEQUENCE	UNP Q9X1D0
E	25	HIS	-	LEADER SEQUENCE	UNP Q9X1D0
E	26	HIS	-	LEADER SEQUENCE	UNP Q9X1D0
E	26	HIS	-	LEADER SEQUENCE	UNP Q9X1D0
E	32	MSE	MET	MODIFIED RESIDUE	UNP Q9X1D0
E	79	MSE	MET	MODIFIED RESIDUE	UNP Q9X1D0
E	179	MSE	MET	MODIFIED RESIDUE	UNP Q9X1D0
E	197	MSE	MET	MODIFIED RESIDUE	UNP Q9X1D0
E	302	MSE	MET	MODIFIED RESIDUE	UNP Q9X1D0
F	15	MSE	-	MODIFIED RESIDUE	UNP Q9X1D0
F	16	GLY	-	LEADER SEQUENCE	UNP Q9X1D0
F	17	SER	-	LEADER SEQUENCE	UNP Q9X1D0
F	18	ASP	-	LEADER SEQUENCE	UNP Q9X1D0
F	19	LYS	-	LEADER SEQUENCE	UNP Q9X1D0
F	20	ILE	-	LEADER SEQUENCE	UNP Q9X1D0
F	22	HIS	-	LEADER SEQUENCE	UNP Q9X1D0
F	23	HIS	-	LEADER SEQUENCE	UNP Q9X1D0
F	24	HIS	-	LEADER SEQUENCE	UNP Q9X1D0
F	25	HIS	-	LEADER SEQUENCE	UNP Q9X1D0
F	26	HIS	-	LEADER SEQUENCE	UNP Q9X1D0
F	26	HIS	-	LEADER SEQUENCE	UNP Q9X1D0
F	32	MSE	MET	MODIFIED RESIDUE	UNP Q9X1D0
F	79	MSE	MET	MODIFIED RESIDUE	UNP Q9X1D0
F	179	MSE	MET	MODIFIED RESIDUE	UNP Q9X1D0
F	197	MSE	MET	MODIFIED RESIDUE	UNP Q9X1D0

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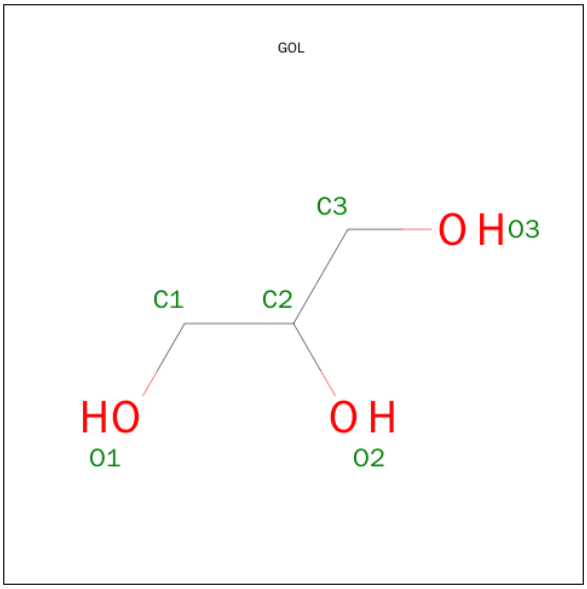
Chain	Residue	Modelled	Actual	Comment	Reference
F	302	MSE	MET	MODIFIED RESIDUE	UNP Q9X1D0

- Molecule 2 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total O 17 17	0	0
2	E	1	Total O 17 17	0	0
2	B	1	Total O 17 17	0	0
2	C	1	Total O 17 17	0	0
2	A	1	Total O 17 17	0	0
2	F	1	Total O 17 17	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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

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

- Molecule 4 is water.

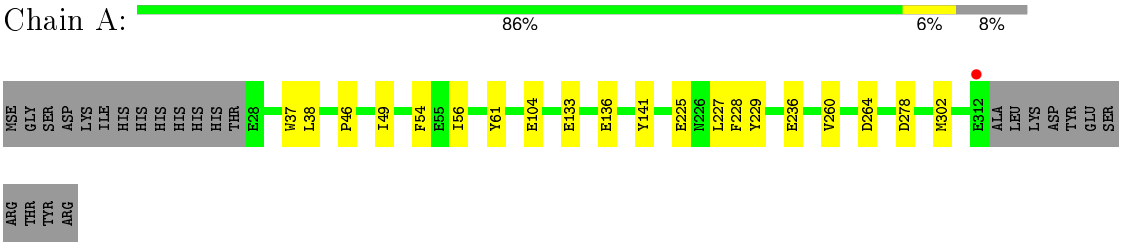
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	155	Total O 155 155	0	0
4	B	134	Total O 134 134	0	0
4	C	136	Total O 136 136	0	0
4	D	162	Total O 162 162	0	0
4	E	159	Total O 159 159	0	0
4	F	180	Total O 180 180	0	0

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 errors 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.

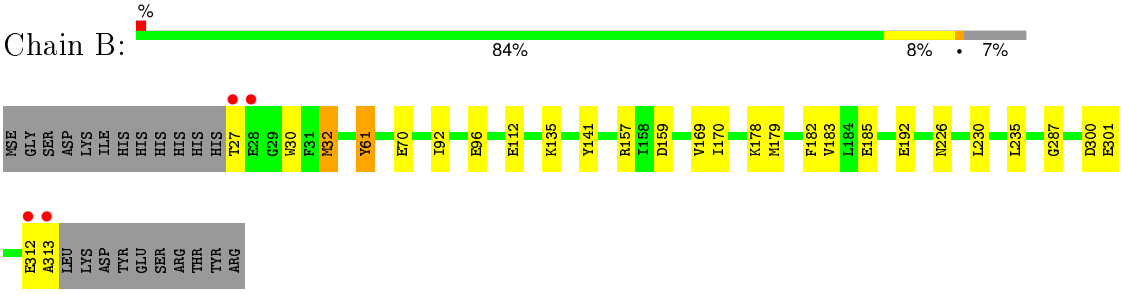
- Molecule 1: Hypothetical protein TM1410

Chain A:



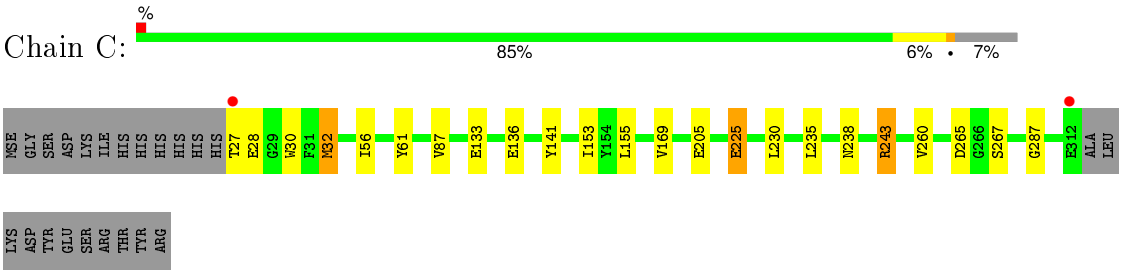
- Molecule 1: Hypothetical protein TM1410

Chain B:



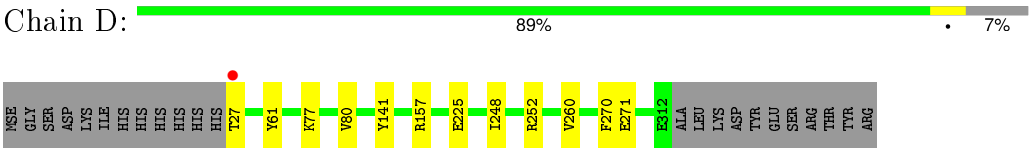
- Molecule 1: Hypothetical protein TM1410

Chain C:



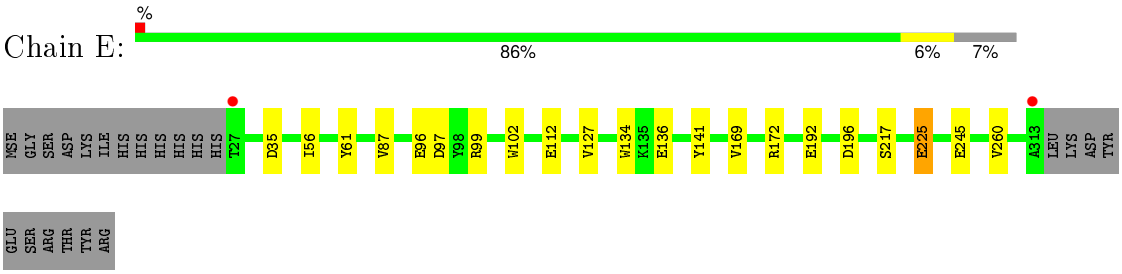
- Molecule 1: Hypothetical protein TM1410

Chain D:



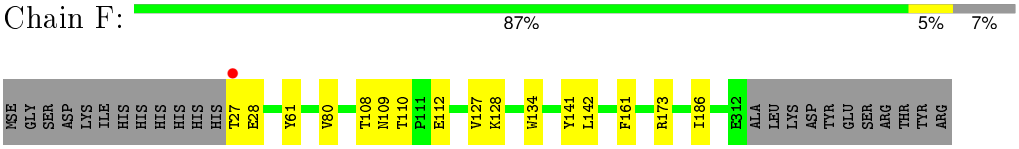
- Molecule 1: Hypothetical protein TM1410

Chain E:



• Molecule 1: Hypothetical protein TM1410

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	194.93Å 84.62Å 195.01Å 90.00° 119.90° 90.00°	Depositor
Resolution (Å)	28.59 – 2.20 28.59 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.4 (28.59-2.20) 97.1 (28.59-2.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.84 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.216 , 0.239 0.227 , 0.245	Depositor DCC
R_{free} test set	13743 reflections (5.32%)	DCC
Wilson B-factor (Å^2)	31.3	Xtriage
Anisotropy	0.189	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
Estimated twinning fraction	0.236 for -h-l,k,h 0.236 for l,k,-h-l 0.117 for h,-k,-h-l 0.116 for -h-l,-k,l 0.116 for l,-k,h	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.36$, $< L^2 > = 0.19$	Xtriage
Outliers	0 of 272052 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	15499	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.14% 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, 0.375 respectively for untwinned datasets, and 0.333, 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, UNL

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	0.73	0/2481	0.75	1/3358 (0.0%)
1	B	0.78	2/2481 (0.1%)	0.79	2/3358 (0.1%)
1	C	0.83	4/2454 (0.2%)	0.81	2/3324 (0.1%)
1	D	0.79	1/2420 (0.0%)	0.77	2/3281 (0.1%)
1	E	0.82	3/2436 (0.1%)	0.79	2/3303 (0.1%)
1	F	0.76	0/2444	0.76	1/3311 (0.0%)
All	All	0.78	10/14716 (0.1%)	0.78	10/19935 (0.1%)

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	B	0	1
1	C	0	2
1	F	0	2
All	All	0	5

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	267	SER	CB-OG	8.69	1.53	1.42
1	C	225	GLU	CB-CG	-6.72	1.39	1.52
1	E	225	GLU	CB-CG	-6.46	1.39	1.52
1	E	192	GLU	CD-OE2	5.87	1.32	1.25
1	B	192	GLU	CG-CD	5.59	1.60	1.51
1	B	192	GLU	CD-OE2	5.35	1.31	1.25
1	D	270	PHE	CG-CD1	5.21	1.46	1.38
1	E	136	GLU	CD-OE2	5.15	1.31	1.25
1	C	32[A]	MSE	SE-CE	-5.11	1.65	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	32[B]	MSE	SE-CE	-5.11	1.65	1.95

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	157	ARG	NE-CZ-NH2	-10.17	115.22	120.30
1	D	157	ARG	NE-CZ-NH1	8.78	124.69	120.30
1	E	172	ARG	NE-CZ-NH2	-8.44	116.08	120.30
1	C	243	ARG	NE-CZ-NH1	7.90	124.25	120.30
1	E	172	ARG	NE-CZ-NH1	7.06	123.83	120.30
1	B	32[A]	MSE	CB-CG-SE	5.87	130.31	112.70
1	B	32[B]	MSE	CB-CG-SE	5.87	130.31	112.70
1	F	173	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	C	265	ASP	CB-CA-C	-5.37	99.67	110.40
1	A	264	ASP	CB-CG-OD1	5.11	122.90	118.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	27	THR	Peptide
1	C	27	THR	Peptide
1	C	28	GLU	Peptide
1	F	27	THR	Peptide
1	F	28	GLU	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	2381	0	2232	14	0
1	B	2390	0	2248	22	0
1	C	2377	0	2239	18	0
1	D	2360	0	2217	4	0
1	E	2372	0	2238	9	0
1	F	2369	0	2236	9	0
2	A	17	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	17	0	0	9	0
2	C	17	0	0	7	0
2	D	17	0	0	7	0
2	E	17	0	0	7	0
2	F	17	0	0	7	0
3	A	42	0	56	1	0
3	B	60	0	80	0	0
3	C	24	0	32	0	0
3	D	30	0	40	0	0
3	E	24	0	32	0	0
3	F	42	0	56	1	0
4	A	155	0	0	3	0
4	B	134	0	0	4	0
4	C	136	0	0	3	0
4	D	162	0	0	0	0
4	E	159	0	0	2	0
4	F	180	0	0	0	0
All	All	15499	0	13706	115	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.

All (115) 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)
2:E:5:UNL:O10	2:E:5:UNL:O6	1.53	1.27
2:B:2:UNL:O2	2:B:2:UNL:O4	1.53	1.26
2:C:3:UNL:O16	2:C:3:UNL:O14	1.54	1.25
2:C:3:UNL:O8	2:C:3:UNL:O7	1.55	1.24
2:D:4:UNL:O4	2:D:4:UNL:O2	1.54	1.24
2:E:5:UNL:O8	2:E:5:UNL:O7	1.55	1.24
2:F:6:UNL:O7	2:F:6:UNL:O8	1.55	1.24
2:D:4:UNL:O14	2:D:4:UNL:O10	1.55	1.24
2:A:1:UNL:O14	2:A:1:UNL:O10	1.56	1.24
2:A:1:UNL:O8	2:A:1:UNL:O7	1.56	1.24
2:D:4:UNL:O14	2:D:4:UNL:O16	1.55	1.23
2:E:5:UNL:O16	2:E:5:UNL:O14	1.57	1.23
2:B:2:UNL:O14	2:B:2:UNL:O10	1.54	1.23
2:C:3:UNL:O11	2:C:3:UNL:O10	1.54	1.23
2:B:2:UNL:O14	2:B:2:UNL:O16	1.53	1.23
2:F:6:UNL:O14	2:F:6:UNL:O10	1.56	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:6:UNL:O10	2:F:6:UNL:O11	1.57	1.22
2:C:3:UNL:O6	2:C:3:UNL:O4	1.57	1.22
2:D:4:UNL:O10	2:D:4:UNL:O11	1.55	1.22
2:F:6:UNL:O6	2:F:6:UNL:O7	1.55	1.22
2:B:2:UNL:O11	2:B:2:UNL:O10	1.54	1.22
2:B:2:UNL:O7	2:B:2:UNL:O6	1.57	1.22
2:D:4:UNL:O7	2:D:4:UNL:O6	1.54	1.22
2:E:5:UNL:O4	2:E:5:UNL:O6	1.57	1.22
2:F:6:UNL:O6	2:F:6:UNL:O4	1.56	1.22
2:A:1:UNL:O10	2:A:1:UNL:O6	1.56	1.22
2:C:3:UNL:O10	2:C:3:UNL:O14	1.54	1.22
2:D:4:UNL:O6	2:D:4:UNL:O4	1.56	1.22
2:B:2:UNL:O4	2:B:2:UNL:O6	1.56	1.21
2:E:5:UNL:O7	2:E:5:UNL:O6	1.57	1.21
2:A:1:UNL:O7	2:A:1:UNL:O6	1.57	1.21
2:A:1:UNL:O6	2:A:1:UNL:O4	1.57	1.21
2:E:5:UNL:O14	2:E:5:UNL:O10	1.57	1.20
2:B:2:UNL:O8	2:B:2:UNL:O7	1.55	1.20
2:D:4:UNL:O10	2:D:4:UNL:O6	1.55	1.20
2:A:1:UNL:O14	2:A:1:UNL:O16	1.55	1.20
2:F:6:UNL:O10	2:F:6:UNL:O6	1.56	1.20
2:A:1:UNL:O10	2:A:1:UNL:O11	1.56	1.20
2:B:2:UNL:O10	2:B:2:UNL:O6	1.55	1.19
2:C:3:UNL:O6	2:C:3:UNL:O7	1.56	1.19
2:F:6:UNL:O14	2:F:6:UNL:O16	1.56	1.19
2:E:5:UNL:O11	2:E:5:UNL:O10	1.54	1.17
2:C:3:UNL:O6	2:C:3:UNL:O10	1.56	1.16
1:A:38:LEU:HD22	1:A:302[A]:MSE:HE3	1.58	0.85
1:B:179[A]:MSE:HE2	1:B:183:VAL:HG23	1.63	0.79
1:A:49:ILE:HA	1:A:302[A]:MSE:HE1	1.63	0.78
1:B:112[A]:GLU:HG2	1:C:133[A]:GLU:HG3	1.66	0.77
1:B:135:LYS:NZ	1:B:185:GLU:OE2	2.17	0.76
1:D:27:THR:HG21	1:D:252:ARG:HG2	1.69	0.73
1:B:169:VAL:HA	4:C:415:HOH:O	1.93	0.67
4:A:404:HOH:O	1:F:109:ASN:HB2	1.95	0.65
1:A:38:LEU:HD22	1:A:302[A]:MSE:CE	2.25	0.65
1:C:32[A]:MSE:CE	1:C:287:GLY:HA2	2.27	0.64
1:A:104:GLU:HG2	4:A:367:HOH:O	1.99	0.63
1:B:30:TRP:HB2	1:B:32[B]:MSE:HE3	1.82	0.62
1:B:32[B]:MSE:HE2	1:B:287:GLY:HA2	1.83	0.59
1:A:133[B]:GLU:HG3	1:F:112:GLU:HG2	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:30:TRP:CB	1:C:32[A]:MSE:HE3	2.34	0.58
3:A:14:GOL:O1	4:A:475:HOH:O	2.17	0.57
1:D:77:LYS:HA	1:D:80:VAL:HG22	1.87	0.56
1:C:205:GLU:OE2	1:C:243:ARG:HD2	2.05	0.56
1:C:56:ILE:HD11	1:C:87:VAL:HG21	1.88	0.56
1:B:112[A]:GLU:HG2	1:C:133[A]:GLU:CG	2.35	0.55
1:A:38:LEU:CD2	1:A:302[A]:MSE:HE3	2.32	0.54
1:A:54:PHE:CD2	1:A:302[A]:MSE:HE2	2.43	0.54
1:B:112[B]:GLU:HG2	1:C:133[B]:GLU:OE1	2.08	0.53
1:C:30:TRP:HB2	1:C:32[A]:MSE:HE3	1.90	0.53
1:B:170:ILE:HD11	1:B:178:LYS:HD2	1.90	0.53
1:C:169:VAL:HA	4:E:391:HOH:O	2.09	0.53
1:C:32[A]:MSE:HE3	1:C:287:GLY:HA2	1.91	0.53
1:C:225:GLU:O	1:C:243:ARG:NH2	2.43	0.51
1:F:110:THR:HG21	3:F:327:GOL:C3	2.41	0.50
1:D:248:ILE:O	1:D:252:ARG:HG3	2.11	0.50
1:C:32[A]:MSE:HE2	1:C:287:GLY:HA2	1.93	0.49
1:B:92:ILE:HD12	1:B:179[A]:MSE:HE1	1.94	0.49
1:A:229:TYR:OH	1:A:278:ASP:OD2	2.26	0.49
1:B:230:LEU:HB2	1:B:235:LEU:HD21	1.95	0.49
1:C:136:GLU:O	4:C:415:HOH:O	2.20	0.48
1:B:179[A]:MSE:HE3	1:B:182:PHE:HB3	1.94	0.48
1:C:32[A]:MSE:HE2	1:C:287:GLY:CA	2.43	0.48
1:B:96:GLU:OE2	4:B:423:HOH:O	2.20	0.48
1:C:153:ILE:HD12	1:C:155:LEU:HD21	1.96	0.47
4:B:348:HOH:O	1:E:169:VAL:HA	2.14	0.46
1:B:157[B]:ARG:NH1	1:B:159:ASP:OD1	2.49	0.46
1:B:32[B]:MSE:CE	1:B:287:GLY:HA2	2.44	0.46
1:B:301[B]:GLU:HG3	4:B:340:HOH:O	2.15	0.46
1:C:230:LEU:HB2	1:C:235:LEU:HD21	1.97	0.46
1:B:301[A]:GLU:HG3	4:B:340:HOH:O	2.16	0.46
1:E:56:ILE:HD11	1:E:87:VAL:HG21	1.98	0.45
1:F:127:VAL:HG21	1:F:134:TRP:CE2	2.52	0.45
1:D:225:GLU:HA	1:D:260:VAL:O	2.17	0.45
1:A:54:PHE:HD2	1:A:302[A]:MSE:HE2	1.79	0.45
1:E:35:ASP:O	1:E:35:ASP:OD1	2.35	0.44
2:B:2:UNL:O16	2:B:2:UNL:O15	2.35	0.44
1:A:227:LEU:HD23	1:A:228:PHE:CE2	2.53	0.44
1:E:225:GLU:HA	1:E:260:VAL:O	2.17	0.43
1:C:238:ASN:HB2	4:C:335:HOH:O	2.17	0.43
1:F:142:LEU:HD11	1:F:186:ILE:HG23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:TRP:CB	1:B:32[B]:MSE:HE3	2.48	0.43
1:A:37:TRP:HB2	1:A:56:ILE:HG23	2.00	0.42
1:E:196:ASP:OD1	1:E:196:ASP:N	2.35	0.42
1:A:136:GLU:OE1	1:F:128:LYS:NZ	2.36	0.42
1:B:312:GLU:O	1:B:313:ALA:CB	2.68	0.42
1:E:127:VAL:HG21	1:E:134:TRP:CE2	2.55	0.41
1:A:133[B]:GLU:CG	1:F:112:GLU:HG2	2.50	0.41
1:E:97:ASP:HA	1:E:102:TRP:CE3	2.55	0.41
1:F:108[A]:THR:HG23	1:F:109:ASN:OD1	2.20	0.41
1:E:245:GLU:OE1	4:E:411:HOH:O	2.22	0.41
1:B:61:TYR:CE2	1:B:70:GLU:HG2	2.56	0.41
1:E:96:GLU:HB2	1:E:99:ARG:HG2	2.02	0.40
1:C:225:GLU:HA	1:C:260:VAL:O	2.21	0.40
1:A:225:GLU:HA	1:A:260:VAL:O	2.20	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	291/309 (94%)	282 (97%)	9 (3%)	0	100	100
1	B	291/309 (94%)	282 (97%)	9 (3%)	0	100	100
1	C	287/309 (93%)	282 (98%)	5 (2%)	0	100	100
1	D	284/309 (92%)	276 (97%)	8 (3%)	0	100	100
1	E	286/309 (93%)	280 (98%)	6 (2%)	0	100	100
1	F	287/309 (93%)	279 (97%)	8 (3%)	0	100	100
All	All	1726/1854 (93%)	1681 (97%)	45 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	258/268 (96%)	254 (98%)	4 (2%)	70 82
1	B	259/268 (97%)	255 (98%)	4 (2%)	72 84
1	C	256/268 (96%)	254 (99%)	2 (1%)	86 93
1	D	251/268 (94%)	248 (99%)	3 (1%)	78 88
1	E	253/268 (94%)	249 (98%)	4 (2%)	70 82
1	F	255/268 (95%)	252 (99%)	3 (1%)	78 88
All	All	1532/1608 (95%)	1512 (99%)	20 (1%)	76 87

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	PRO
1	A	61	TYR
1	A	141	TYR
1	A	236	GLU
1	B	61	TYR
1	B	141	TYR
1	B	226	ASN
1	B	300	ASP
1	C	61	TYR
1	C	141	TYR
1	D	61	TYR
1	D	141	TYR
1	D	271	GLU
1	E	61	TYR
1	E	112	GLU
1	E	141	TYR
1	E	217	SER
1	F	61	TYR
1	F	141	TYR
1	F	161	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no

such sidechains identified.

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 carbohydrates in this entry.

5.6 Ligand geometry

Of 43 ligands modelled in this entry, 6 are unknown - leaving 37 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	GOL	A	12	-	5,5,5	0.43	0	5,5,5	0.93	0
3	GOL	A	13	-	5,5,5	0.45	0	5,5,5	0.57	0
3	GOL	A	14	-	5,5,5	0.29	0	5,5,5	0.61	0
3	GOL	A	324	-	5,5,5	0.38	0	5,5,5	0.34	0
3	GOL	A	325	-	5,5,5	0.59	0	5,5,5	0.42	0
3	GOL	A	326	-	5,5,5	0.59	0	5,5,5	0.59	0
3	GOL	A	327	-	5,5,5	0.38	0	5,5,5	0.26	0
3	GOL	B	324	-	5,5,5	0.53	0	5,5,5	0.40	0
3	GOL	B	325	-	5,5,5	0.45	0	5,5,5	0.46	0
3	GOL	B	326	-	5,5,5	0.31	0	5,5,5	0.33	0
3	GOL	B	327	-	5,5,5	0.45	0	5,5,5	0.16	0
3	GOL	B	328	-	5,5,5	0.37	0	5,5,5	0.45	0
3	GOL	B	329	-	5,5,5	0.33	0	5,5,5	0.35	0
3	GOL	B	330	-	5,5,5	0.44	0	5,5,5	0.43	0
3	GOL	B	331	-	5,5,5	0.34	0	5,5,5	0.20	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	GOL	B	7	-	5,5,5	0.34	0	5,5,5	0.77	0
3	GOL	B	8	-	5,5,5	0.33	0	5,5,5	0.37	0
3	GOL	C	324	-	5,5,5	0.24	0	5,5,5	0.85	0
3	GOL	C	325	-	5,5,5	0.36	0	5,5,5	0.24	0
3	GOL	C	326	-	5,5,5	0.58	0	5,5,5	0.36	0
3	GOL	C	327	-	5,5,5	0.47	0	5,5,5	0.88	0
3	GOL	D	11	-	5,5,5	0.39	0	5,5,5	0.63	0
3	GOL	D	324	-	5,5,5	0.40	0	5,5,5	0.57	0
3	GOL	D	325	-	5,5,5	0.45	0	5,5,5	0.50	0
3	GOL	D	326	-	5,5,5	0.38	0	5,5,5	0.22	0
3	GOL	D	327	-	5,5,5	0.36	0	5,5,5	0.59	0
3	GOL	E	324	-	5,5,5	0.53	0	5,5,5	0.29	0
3	GOL	E	325	-	5,5,5	0.45	0	5,5,5	0.46	0
3	GOL	E	326	-	5,5,5	0.32	0	5,5,5	0.41	0
3	GOL	E	9	-	5,5,5	0.28	0	5,5,5	0.63	0
3	GOL	F	10	-	5,5,5	0.32	0	5,5,5	0.44	0
3	GOL	F	324	-	5,5,5	0.56	0	5,5,5	0.62	0
3	GOL	F	325	-	5,5,5	0.40	0	5,5,5	0.45	0
3	GOL	F	326	-	5,5,5	0.31	0	5,5,5	0.48	0
3	GOL	F	327	-	5,5,5	0.48	0	5,5,5	0.70	0
3	GOL	F	328	-	5,5,5	0.43	0	5,5,5	0.29	0
3	GOL	F	329	-	5,5,5	0.38	0	5,5,5	0.36	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
3	GOL	A	12	-	-	0/4/4/4	0/0/0/0
3	GOL	A	13	-	-	0/4/4/4	0/0/0/0
3	GOL	A	14	-	-	0/4/4/4	0/0/0/0
3	GOL	A	324	-	-	0/4/4/4	0/0/0/0
3	GOL	A	325	-	-	0/4/4/4	0/0/0/0
3	GOL	A	326	-	-	0/4/4/4	0/0/0/0
3	GOL	A	327	-	-	0/4/4/4	0/0/0/0
3	GOL	B	324	-	-	0/4/4/4	0/0/0/0
3	GOL	B	325	-	-	0/4/4/4	0/0/0/0
3	GOL	B	326	-	-	0/4/4/4	0/0/0/0
3	GOL	B	327	-	-	0/4/4/4	0/0/0/0
3	GOL	B	328	-	-	0/4/4/4	0/0/0/0
3	GOL	B	329	-	-	0/4/4/4	0/0/0/0
3	GOL	B	330	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	B	331	-	-	0/4/4/4	0/0/0/0
3	GOL	B	7	-	-	0/4/4/4	0/0/0/0
3	GOL	B	8	-	-	0/4/4/4	0/0/0/0
3	GOL	C	324	-	-	0/4/4/4	0/0/0/0
3	GOL	C	325	-	-	0/4/4/4	0/0/0/0
3	GOL	C	326	-	-	0/4/4/4	0/0/0/0
3	GOL	C	327	-	-	0/4/4/4	0/0/0/0
3	GOL	D	11	-	-	0/4/4/4	0/0/0/0
3	GOL	D	324	-	-	0/4/4/4	0/0/0/0
3	GOL	D	325	-	-	0/4/4/4	0/0/0/0
3	GOL	D	326	-	-	0/4/4/4	0/0/0/0
3	GOL	D	327	-	-	0/4/4/4	0/0/0/0
3	GOL	E	324	-	-	0/4/4/4	0/0/0/0
3	GOL	E	325	-	-	0/4/4/4	0/0/0/0
3	GOL	E	326	-	-	0/4/4/4	0/0/0/0
3	GOL	E	9	-	-	0/4/4/4	0/0/0/0
3	GOL	F	10	-	-	0/4/4/4	0/0/0/0
3	GOL	F	324	-	-	0/4/4/4	0/0/0/0
3	GOL	F	325	-	-	0/4/4/4	0/0/0/0
3	GOL	F	326	-	-	0/4/4/4	0/0/0/0
3	GOL	F	327	-	-	0/4/4/4	0/0/0/0
3	GOL	F	328	-	-	0/4/4/4	0/0/0/0
3	GOL	F	329	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	14	GOL	1	0
3	F	327	GOL	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	280/309 (90%)	-0.31	1 (0%)	93	93	34, 40, 45, 59	0
1	B	282/309 (91%)	-0.21	4 (1%)	78	77	33, 40, 45, 62	0
1	C	281/309 (90%)	-0.23	2 (0%)	89	88	35, 40, 45, 61	0
1	D	281/309 (90%)	-0.27	1 (0%)	93	93	35, 40, 44, 65	0
1	E	282/309 (91%)	-0.25	2 (0%)	89	88	34, 40, 46, 68	0
1	F	281/309 (90%)	-0.23	1 (0%)	93	93	35, 40, 45, 66	0
All	All	1687/1854 (90%)	-0.25	11 (0%)	89	88	33, 40, 45, 68	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	27	THR	10.1
1	B	27	THR	8.2
1	D	27	THR	6.7
1	E	27	THR	6.3
1	B	313	ALA	5.0
1	E	313	ALA	3.9
1	A	312	GLU	2.5
1	C	312	GLU	2.4
1	C	27	THR	2.2
1	B	312	GLU	2.1
1	B	28	GLU	2.1

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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^{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	LLDF	B-factors(Å^2)	Q<0.9
3	GOL	C	327	6/6	0.78	0.35	21.07	60,61,62,64	0
3	GOL	B	8	6/6	0.87	0.26	18.58	64,66,66,67	0
3	GOL	E	326	6/6	0.90	0.29	18.27	72,72,72,73	0
2	UNL	D	4	17/-	0.90	0.21	12.47	51,58,64,67	0
3	GOL	B	325	6/6	0.79	0.27	12.25	49,55,55,56	0
3	GOL	D	327	6/6	0.84	0.33	11.94	77,77,78,78	0
3	GOL	A	13	6/6	0.74	0.27	10.33	63,66,68,68	0
3	GOL	F	328	6/6	0.75	0.27	9.58	68,69,69,69	0
3	GOL	F	326	6/6	0.87	0.38	9.24	64,65,65,66	0
3	GOL	D	11	6/6	0.93	0.19	9.24	45,51,55,59	0
3	GOL	D	325	6/6	0.89	0.26	9.23	53,56,57,60	0
3	GOL	B	328	6/6	0.88	0.28	8.79	68,71,71,72	0
3	GOL	F	10	6/6	0.91	0.17	8.39	38,47,51,51	0
3	GOL	B	324	6/6	0.93	0.21	7.56	56,60,63,64	0
3	GOL	F	327	6/6	0.88	0.22	7.40	60,62,63,64	0
2	UNL	F	6	17/-	0.85	0.20	7.33	54,59,62,64	0
2	UNL	A	1	17/-	0.85	0.22	7.23	51,56,62,62	0
3	GOL	C	324	6/6	0.68	0.41	7.15	73,74,76,76	0
2	UNL	B	2	17/-	0.88	0.17	6.93	45,53,59,60	0
3	GOL	A	327	6/6	0.85	0.34	5.51	66,67,68,69	0
3	GOL	A	14	6/6	0.94	0.16	4.85	41,49,51,55	0
2	UNL	E	5	17/-	0.86	0.16	4.78	44,57,61,62	0
3	GOL	F	324	6/6	0.89	0.15	3.88	52,53,55,58	0
3	GOL	A	326	6/6	0.78	0.23	3.53	64,66,67,67	0
3	GOL	E	324	6/6	0.92	0.28	3.00	50,53,54,60	0
3	GOL	A	325	6/6	0.94	0.16	2.73	56,59,60,61	0
3	GOL	F	325	6/6	0.72	0.29	2.65	65,69,70,71	0
3	GOL	B	7	6/6	0.93	0.16	2.35	37,47,50,54	0
3	GOL	B	326	6/6	0.79	0.24	1.95	64,68,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	GOL	D	326	6/6	0.88	0.20	1.16	69,71,72,72	0
2	UNL	C	3	17/-	0.85	0.23	0.93	65,67,73,73	0
3	GOL	C	325	6/6	0.96	0.12	-0.01	42,52,55,57	0
3	GOL	E	9	6/6	0.95	0.11	-0.09	40,43,47,47	0
3	GOL	A	12	6/6	0.89	0.21	-	45,48,49,49	0
3	GOL	B	329	6/6	0.90	0.30	-	70,73,74,75	0
3	GOL	A	324	6/6	0.79	0.30	-	68,69,72,74	0
3	GOL	B	327	6/6	0.84	0.45	-	76,77,78,80	0
3	GOL	B	331	6/6	0.89	0.37	-	65,65,67,67	0
3	GOL	B	330	6/6	0.84	0.33	-	66,67,68,69	0
3	GOL	E	325	6/6	0.92	0.23	-	52,54,56,56	0
3	GOL	F	329	6/6	0.74	0.37	-	62,65,67,67	0
3	GOL	C	326	6/6	0.91	0.20	-	59,62,62,62	0
3	GOL	D	324	6/6	0.89	0.21	-	60,64,65,67	0

6.5 Other polymers (i)

There are no such residues in this entry.