W O R L D W I D E

wwPDB

PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 19, 2016 – 08:16 PM GMT

PDB ID	:	4XZV
Title	:	Crystal Structure of SLMO1-TRIAP1 Complex
Authors	:	Miliara, X.; Garnett, J.A.; Matthews, S.J.
Deposited on	:	2015-02-05
Resolution	:	3.58 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

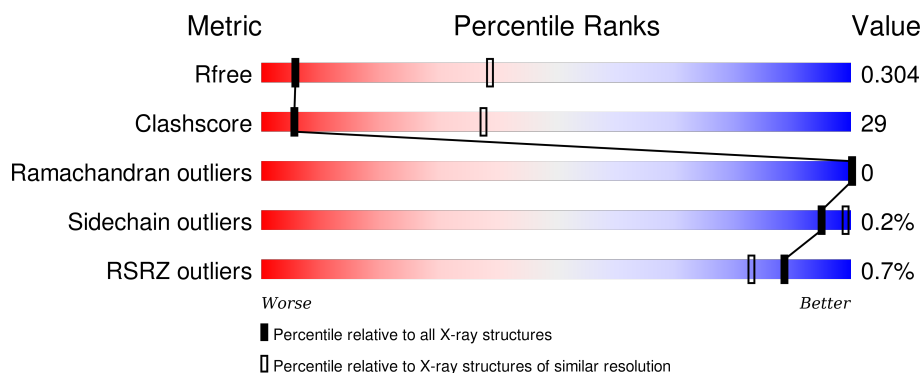|		
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
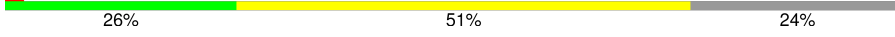*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.58 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		0.304
Clashscore		29
Ramachandran outliers		0
Sidechain outliers		0.2%
RSRZ outliers		0.7%

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$_{free}$	91344	1261 (3.76-3.40)
Clashscore	102246	1026 (3.72-3.44)
Ramachandran outliers	100387	1028 (3.74-3.42)
Sidechain outliers	100360	1028 (3.74-3.42)
RSRZ outliers	91569	1268 (3.76-3.40)

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	446	79% 14% 7%
1	C	446	79% 14% 7%
1	E	446	79% 13% 7%
1	G	446	80% 13% 7%
2	B	186	2% 26% 51% 24%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	D	186	2% 32% 44% 24%
2	F	186	% 29% 47% 24%
2	H	186	2% 26% 45% • 28%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 17248 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 Maltose-binding periplasmic protein,TP53-regulated inhibitor of apoptosis 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	416	Total	C	N	O	S	0	0	0
			3203	2054	525	613	11			
1	C	416	Total	C	N	O	S	0	0	0
			3203	2054	525	613	11			
1	E	413	Total	C	N	O	S	0	0	0
			3181	2040	522	608	11			
1	G	415	Total	C	N	O	S	0	0	0
			3194	2049	524	610	11			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP P0AEX9
A	82	ALA	ASP	conflict	UNP P0AEX9
A	83	ALA	LYS	conflict	UNP P0AEX9
A	172	ALA	GLU	conflict	UNP P0AEX9
A	173	ALA	ASN	conflict	UNP P0AEX9
A	239	ALA	LYS	conflict	UNP P0AEX9
A	359	ALA	GLU	conflict	UNP P0AEX9
A	362	ALA	LYS	conflict	UNP P0AEX9
A	363	ALA	ASP	conflict	UNP P0AEX9
A	367	ASN	-	linker	UNP P0AEX9
A	368	ALA	-	linker	UNP P0AEX9
A	369	ALA	-	linker	UNP P0AEX9
A	370	ALA	-	linker	UNP P0AEX9
C	0	MET	-	initiating methionine	UNP P0AEX9
C	82	ALA	ASP	conflict	UNP P0AEX9
C	83	ALA	LYS	conflict	UNP P0AEX9
C	172	ALA	GLU	conflict	UNP P0AEX9
C	173	ALA	ASN	conflict	UNP P0AEX9
C	239	ALA	LYS	conflict	UNP P0AEX9
C	359	ALA	GLU	conflict	UNP P0AEX9

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	362	ALA	LYS	conflict	UNP P0AEX9
C	363	ALA	ASP	conflict	UNP P0AEX9
C	367	ASN	-	linker	UNP P0AEX9
C	368	ALA	-	linker	UNP P0AEX9
C	369	ALA	-	linker	UNP P0AEX9
C	370	ALA	-	linker	UNP P0AEX9
E	0	MET	-	initiating methionine	UNP P0AEX9
E	82	ALA	ASP	conflict	UNP P0AEX9
E	83	ALA	LYS	conflict	UNP P0AEX9
E	172	ALA	GLU	conflict	UNP P0AEX9
E	173	ALA	ASN	conflict	UNP P0AEX9
E	239	ALA	LYS	conflict	UNP P0AEX9
E	359	ALA	GLU	conflict	UNP P0AEX9
E	362	ALA	LYS	conflict	UNP P0AEX9
E	363	ALA	ASP	conflict	UNP P0AEX9
E	367	ASN	-	linker	UNP P0AEX9
E	368	ALA	-	linker	UNP P0AEX9
E	369	ALA	-	linker	UNP P0AEX9
E	370	ALA	-	linker	UNP P0AEX9
G	0	MET	-	initiating methionine	UNP P0AEX9
G	82	ALA	ASP	conflict	UNP P0AEX9
G	83	ALA	LYS	conflict	UNP P0AEX9
G	172	ALA	GLU	conflict	UNP P0AEX9
G	173	ALA	ASN	conflict	UNP P0AEX9
G	239	ALA	LYS	conflict	UNP P0AEX9
G	359	ALA	GLU	conflict	UNP P0AEX9
G	362	ALA	LYS	conflict	UNP P0AEX9
G	363	ALA	ASP	conflict	UNP P0AEX9
G	367	ASN	-	linker	UNP P0AEX9
G	368	ALA	-	linker	UNP P0AEX9
G	369	ALA	-	linker	UNP P0AEX9
G	370	ALA	-	linker	UNP P0AEX9

- Molecule 2 is a protein called Protein slowmo homolog 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	142	Total	C	N	O	S	0	0	0
			1112	706	194	206	6			
2	D	141	Total	C	N	O	S	0	0	0
			1105	701	193	205	6			
2	F	142	Total	C	N	O	S	0	0	0
			1112	706	194	206	6			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	133	1046	664	185	192	5	0	0	0

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-13	MET	-	initiating methionine	UNP Q96N28
B	-12	ALA	-	expression tag	UNP Q96N28
B	-11	HIS	-	expression tag	UNP Q96N28
B	-10	HIS	-	expression tag	UNP Q96N28
B	-9	HIS	-	expression tag	UNP Q96N28
B	-8	HIS	-	expression tag	UNP Q96N28
B	-7	HIS	-	expression tag	UNP Q96N28
B	-6	HIS	-	expression tag	UNP Q96N28
B	-5	VAL	-	expression tag	UNP Q96N28
B	-4	ASP	-	expression tag	UNP Q96N28
B	-3	ASP	-	expression tag	UNP Q96N28
B	-2	ASP	-	expression tag	UNP Q96N28
B	-1	ASP	-	expression tag	UNP Q96N28
B	0	LYS	-	expression tag	UNP Q96N28
D	-13	MET	-	initiating methionine	UNP Q96N28
D	-12	ALA	-	expression tag	UNP Q96N28
D	-11	HIS	-	expression tag	UNP Q96N28
D	-10	HIS	-	expression tag	UNP Q96N28
D	-9	HIS	-	expression tag	UNP Q96N28
D	-8	HIS	-	expression tag	UNP Q96N28
D	-7	HIS	-	expression tag	UNP Q96N28
D	-6	HIS	-	expression tag	UNP Q96N28
D	-5	VAL	-	expression tag	UNP Q96N28
D	-4	ASP	-	expression tag	UNP Q96N28
D	-3	ASP	-	expression tag	UNP Q96N28
D	-2	ASP	-	expression tag	UNP Q96N28
D	-1	ASP	-	expression tag	UNP Q96N28
D	0	LYS	-	expression tag	UNP Q96N28
F	-13	MET	-	initiating methionine	UNP Q96N28
F	-12	ALA	-	expression tag	UNP Q96N28
F	-11	HIS	-	expression tag	UNP Q96N28
F	-10	HIS	-	expression tag	UNP Q96N28
F	-9	HIS	-	expression tag	UNP Q96N28
F	-8	HIS	-	expression tag	UNP Q96N28
F	-7	HIS	-	expression tag	UNP Q96N28
F	-6	HIS	-	expression tag	UNP Q96N28

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	-5	VAL	-	expression tag	UNP Q96N28
F	-4	ASP	-	expression tag	UNP Q96N28
F	-3	ASP	-	expression tag	UNP Q96N28
F	-2	ASP	-	expression tag	UNP Q96N28
F	-1	ASP	-	expression tag	UNP Q96N28
F	0	LYS	-	expression tag	UNP Q96N28
H	-13	MET	-	initiating methionine	UNP Q96N28
H	-12	ALA	-	expression tag	UNP Q96N28
H	-11	HIS	-	expression tag	UNP Q96N28
H	-10	HIS	-	expression tag	UNP Q96N28
H	-9	HIS	-	expression tag	UNP Q96N28
H	-8	HIS	-	expression tag	UNP Q96N28
H	-7	HIS	-	expression tag	UNP Q96N28
H	-6	HIS	-	expression tag	UNP Q96N28
H	-5	VAL	-	expression tag	UNP Q96N28
H	-4	ASP	-	expression tag	UNP Q96N28
H	-3	ASP	-	expression tag	UNP Q96N28
H	-2	ASP	-	expression tag	UNP Q96N28
H	-1	ASP	-	expression tag	UNP Q96N28
H	0	LYS	-	expression tag	UNP Q96N28

- Molecule 3 is ALPHA-D-GLUCOSE (three-letter code: GLC) (formula: $C_6H_{12}O_6$).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 12	C 6	O 6	0	0

Continued on next page...

Continued from previous page...

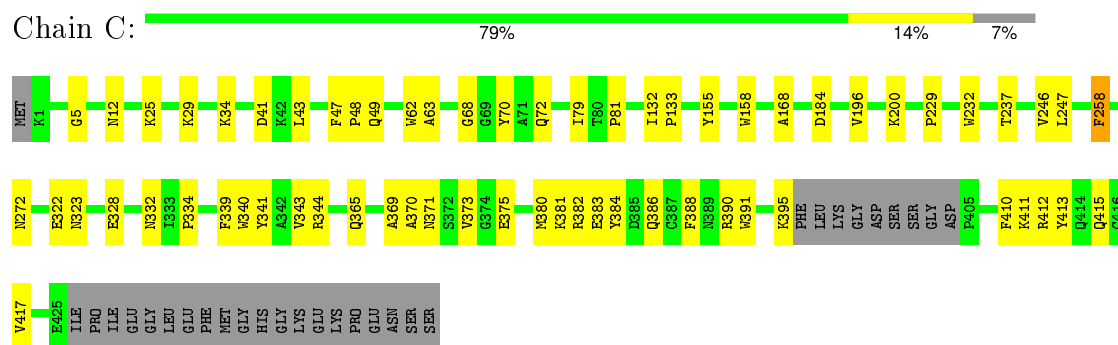| Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 11	C 6	O 5	0	0
3	C	1	Total 12	C 6	O 6	0	0
3	C	1	Total 11	C 6	O 5	0	0
3	E	1	Total 12	C 6	O 6	0	0
3	E	1	Total 11	C 6	O 5	0	0
3	G	1	Total 12	C 6	O 6	0	0
3	G	1	Total 11	C 6	O 5	0	0

3 Residue-property plots ⓘ

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.
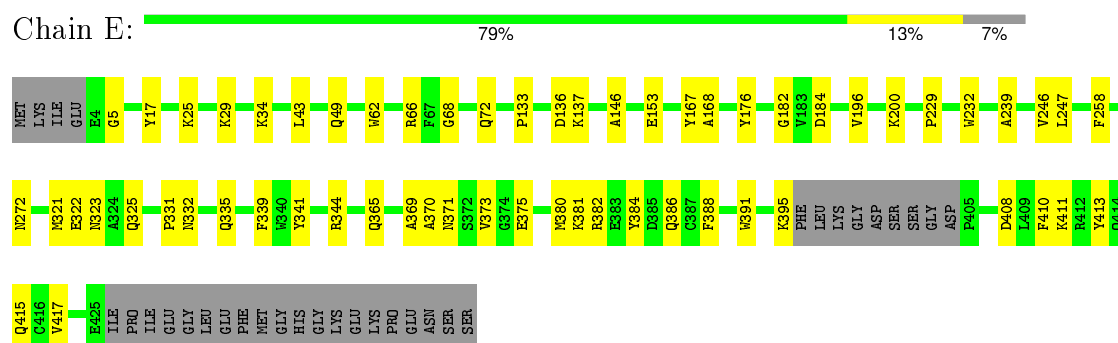
- Molecule 1: Maltose-binding periplasmic protein,TP53-regulated inhibitor of apoptosis 1
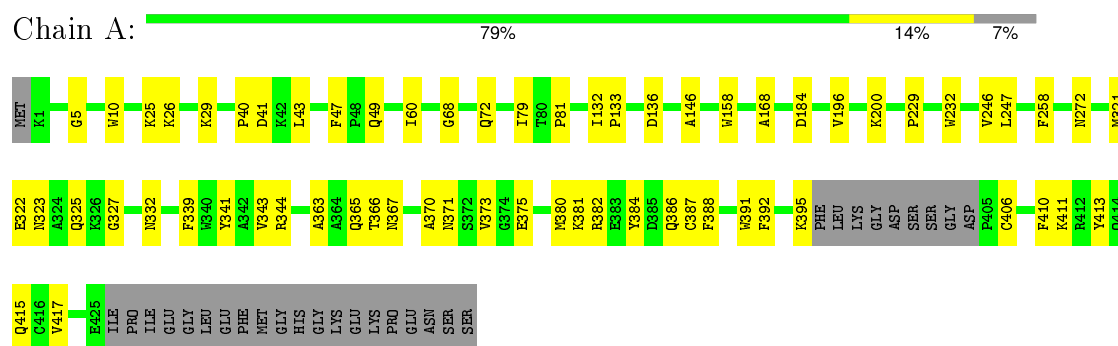
- Molecule 1: Maltose-binding periplasmic protein,TP53-regulated inhibitor of apoptosis 1
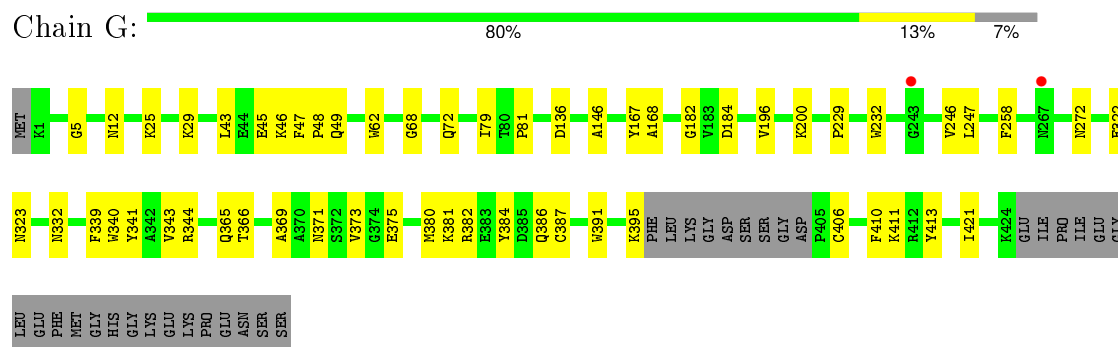

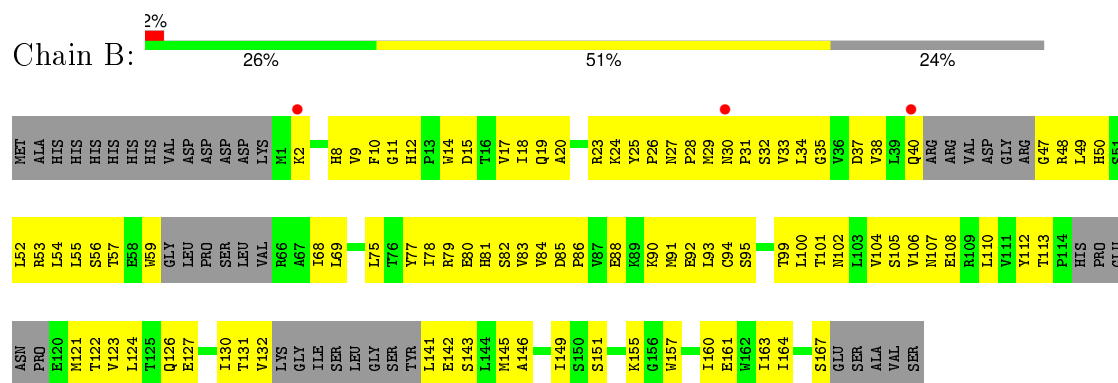- Molecule 1: Maltose-binding periplasmic protein,TP53-regulated inhibitor of apoptosis 1

- Molecule 1: Maltose-binding periplasmic protein,TP53-regulated inhibitor of apoptosis 1
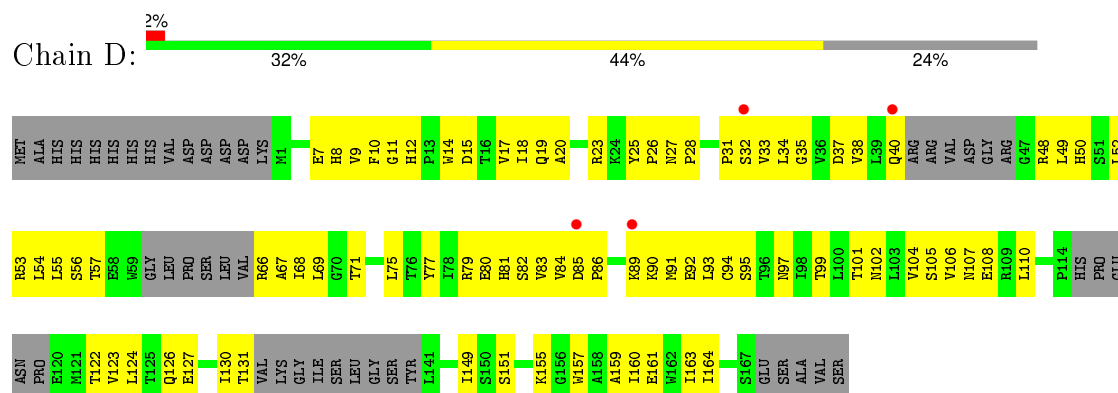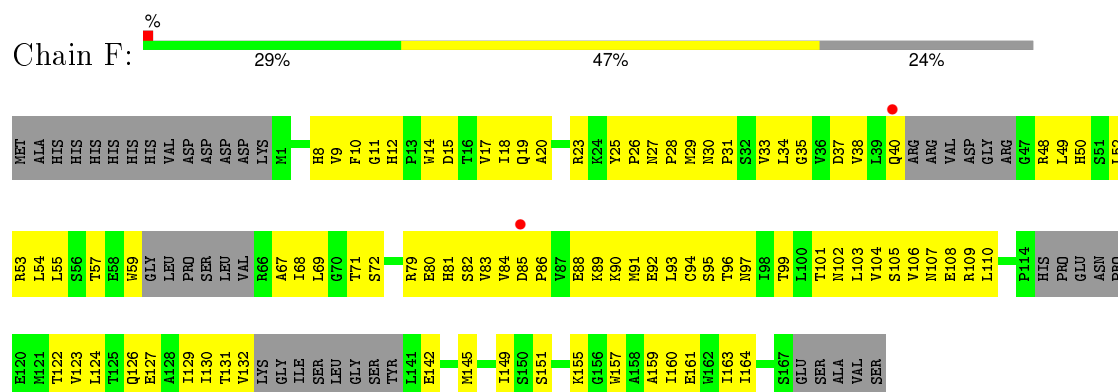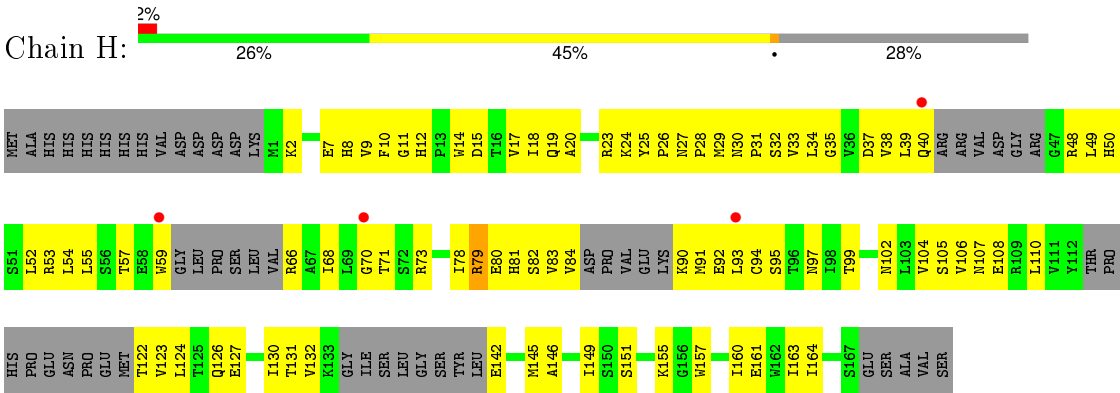
Chain G:

• Molecule 2: Protein slowmo homolog 1

Chain B:

• Molecule 2: Protein slowmo homolog 1

Chain D:

• Molecule 2: Protein slowmo homolog 1

Chain F:

● Molecule 2: Protein slowmo homolog 1

Chain H:

4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	79.62Å 80.68Å 98.02Å 87.25° 85.62° 89.92°	Depositor
Resolution (Å)	97.62 – 3.58 97.62 – 3.58	Depositor EDS
% Data completeness (in resolution range)	98.9 (97.62-3.58) 97.4 (97.62-3.58)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	2.67 (at 3.58Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.273 , 0.309 0.270 , 0.304	Depositor DCC
R_{free} test set	1499 reflections (5.59%)	DCC
Wilson B-factor (Å^2)	93.4	Xtriage
Anisotropy	0.271	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.23 , 113.3	EDS
Estimated twinning fraction	0.026 for -k,-h,-l	Xtriage
L-test for twinning [2]	$< \mid L \mid > = 0.47, < L^2 > = 0.29$	Xtriage
Outliers	0 of 28326 reflections	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	17248	wwPDB-VP
Average B, all atoms (Å^2)	181.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.36% of the height of the origin peak. No significant pseudotranslation is detected.*

---

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< \mid L \mid >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GLC

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	0.57	0/3279	0.71	1/4454 (0.0%)
1	C	0.57	0/3279	0.72	0/4454
1	E	0.50	0/3257	0.67	0/4424
1	G	0.48	0/3270	0.67	0/4442
2	B	0.59	0/1131	0.87	1/1536 (0.1%)
2	D	0.58	0/1124	0.82	0/1526
2	F	0.50	0/1131	0.78	0/1536
2	H	0.50	0/1062	0.77	1/1438 (0.1%)
All	All	0.54	0/17533	0.72	3/23810 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	79	ARG	NE-CZ-NH1	5.65	123.12	120.30
1	A	41	ASP	CB-CG-OD1	5.31	123.08	118.30
2	B	30	ASN	C-N-CD	5.03	138.97	128.40

There are no chirality outliers.

There are no planarity outliers.

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	3203	0	3125	101	0
1	C	3203	0	3123	93	0
1	E	3181	0	3101	80	0
1	G	3194	0	3117	84	0
2	B	1112	0	1122	187	0
2	D	1105	0	1113	168	0
2	F	1112	0	1122	176	0
2	H	1046	0	1059	151	0
3	A	23	0	21	0	0
3	C	23	0	21	3	0
3	E	23	0	21	1	0
3	G	23	0	21	0	0
All	All	17248	0	16966	1006	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 29.

The worst 5 of 1006 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:D:18:ILE:HD12	2:D:91:MET:CE	1.43	1.45
1:A:387:CYS:SG	1:A:406:CYS:SG	1.44	1.43
2:B:48:ARG:HB3	2:B:85:ASP:CG	1.40	1.42
2:H:18:ILE:HD12	2:H:91:MET:CE	1.55	1.35
2:F:18:ILE:HD12	2:F:91:MET:CE	1.58	1.32

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	412/446 (92%)	402 (98%)	10 (2%)	0	100	100

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	412/446 (92%)	399 (97%)	13 (3%)	0	100	100
1	E	409/446 (92%)	399 (98%)	10 (2%)	0	100	100
1	G	411/446 (92%)	400 (97%)	11 (3%)	0	100	100
2	B	132/186 (71%)	123 (93%)	9 (7%)	0	100	100
2	D	131/186 (70%)	123 (94%)	8 (6%)	0	100	100
2	F	132/186 (71%)	124 (94%)	8 (6%)	0	100	100
2	H	121/186 (65%)	111 (92%)	10 (8%)	0	100	100
All	All	2160/2528 (85%)	2081 (96%)	79 (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	323/353 (92%)	322 (100%)	1 (0%)	94	99
1	C	323/353 (92%)	322 (100%)	1 (0%)	94	99
1	E	321/353 (91%)	320 (100%)	1 (0%)	94	99
1	G	322/353 (91%)	321 (100%)	1 (0%)	94	99
2	B	125/167 (75%)	125 (100%)	0	100	100
2	D	124/167 (74%)	124 (100%)	0	100	100
2	F	125/167 (75%)	125 (100%)	0	100	100
2	H	117/167 (70%)	117 (100%)	0	100	100
All	All	1780/2080 (86%)	1776 (100%)	4 (0%)	95	99

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	258	PHE
1	C	258	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	258	PHE
1	G	258	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	97	ASN
1	E	415	GLN
2	H	50	HIS
1	E	49	GLN
1	E	272	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

8 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	#$|Z| > 2$
3	GLC	A	501	3	12,12,12	0.91	0	17,17,17	2.10	7 (41%)

Mol	Type	Chain	Res	Link	Bond lengths				Bond angles			
					Counts	RMSZ	$\#|Z| > 2$		Counts	RMSZ	$\#|Z| > 2$	
3	GLC	A	502	3	11,11,12	0.93	0		15,15,17	1.55	4 (26%)	
3	GLC	C	501	3	12,12,12	0.75	0		17,17,17	2.35	6 (35%)	
3	GLC	C	502	3	11,11,12	0.97	1 (9%)		15,15,17	1.18	2 (13%)	
3	GLC	E	501	3	12,12,12	0.56	0		17,17,17	2.18	3 (17%)	
3	GLC	E	502	3	11,11,12	0.52	0		15,15,17	1.10	1 (6%)	
3	GLC	G	501	3	12,12,12	0.69	0		17,17,17	2.13	6 (35%)	
3	GLC	G	502	3	11,11,12	0.61	0		15,15,17	1.09	1 (6%)	

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	GLC	A	501	3	-	0/2/22/22	0/1/1/1
3	GLC	A	502	3	-	0/2/19/22	0/1/1/1
3	GLC	C	501	3	-	0/2/22/22	0/1/1/1
3	GLC	C	502	3	-	0/2/19/22	0/1/1/1
3	GLC	E	501	3	-	0/2/22/22	0/1/1/1
3	GLC	E	502	3	-	0/2/19/22	0/1/1/1
3	GLC	G	501	3	-	0/2/22/22	0/1/1/1
3	GLC	G	502	3	-	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	502	GLC	O5-C1	-2.29	1.40	1.43

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	501	GLC	O4-C4-C3	-3.47	102.54	110.36
3	C	501	GLC	O4-C4-C3	-3.16	103.23	110.36
3	A	502	GLC	O5-C5-C4	-2.51	105.97	110.13
3	C	501	GLC	O1-C1-O5	-2.43	103.56	110.33
3	G	501	GLC	O4-C4-C3	-2.42	104.91	110.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	502	GLC	3	0
3	E	502	GLC	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 ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	416/446 (93%)	-0.79	0	100	100	67, 125, 193, 260	0
1	C	416/446 (93%)	-0.66	0	100	100	80, 136, 205, 262	0
1	E	413/446 (92%)	-0.39	0	100	100	131, 193, 285, 377	0
1	G	415/446 (93%)	-0.40	2 (0%)	91	88	134, 195, 270, 323	0
2	B	142/186 (76%)	-0.06	3 (2%)	67	57	123, 190, 264, 315	0
2	D	141/186 (75%)	-0.09	4 (2%)	56	46	120, 195, 273, 313	0
2	F	142/186 (76%)	0.00	2 (1%)	78	69	195, 232, 290, 332	0
2	H	133/186 (71%)	0.13	4 (3%)	54	43	196, 259, 302, 326	0
All	All	2218/2528 (87%)	-0.42	15 (0%)	89	83	67, 176, 274, 377	0

The worst 5 of 15 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	40	GLN	3.9
2	B	40	GLN	3.5
2	H	40	GLN	3.0
2	D	85	ASP	2.8
2	H	59	TRP	2.7

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	GLC	C	501	12/12	0.97	0.15	0.69	48,61,68,80	0
3	GLC	A	502	11/12	0.97	0.11	-0.59	35,36,43,50	0
3	GLC	E	501	12/12	0.94	0.16	-0.64	89,98,110,112	0
3	GLC	A	501	12/12	0.98	0.11	-0.93	36,41,46,54	0
3	GLC	G	501	12/12	0.97	0.13	-0.97	74,81,90,92	0
3	GLC	C	502	11/12	0.98	0.10	-1.05	35,41,48,56	0
3	GLC	G	502	11/12	0.96	0.12	-1.22	67,80,86,89	0
3	GLC	E	502	11/12	0.97	0.09	-1.85	68,82,96,107	0

6.5 Other polymers (i)

There are no such residues in this entry.