Full wwPDB X-ray Structure Validation Report (i)

Sep 26, 2023 – 10:46 AM EDT

PDB ID	:	6CNL
Title	:	Crystal Structure of H105A PGAM5 Dodecamer
Authors	:	Ruiz, K.; Agnew, C.; Jura, N.
Deposited on	:	2018-03-08
Resolution	:	2.60 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

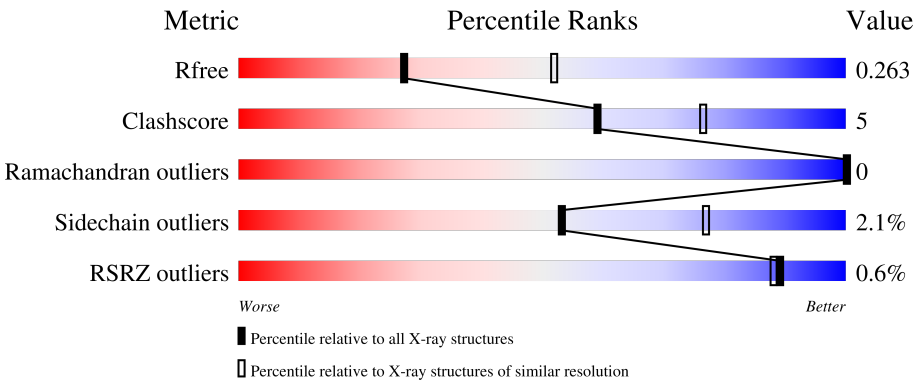
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% 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	223	74% 9% 17%
1	B	223	74% 10% • 16%
1	C	223	77% 8% 15%
1	D	223	75% 11% 14%
1	E	223	.% 75% 9% 16%

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Mol	Chain	Length	Quality of chain
1	F	223	73% 11% 16%
1	G	223	71% 13% 15%
1	H	223	.% 74% 9% 17%
1	I	223	.% 70% 12% 18%
1	J	223	.% 71% 10% • 17%
1	K	223	74% 10% 16%
1	L	223	72% 13% • 14%
2	M	14	64% 14% 21%
2	N	14	79% 21%
2	O	14	7% 57% 21% 21%
2	P	14	71% 7% 21%
2	Q	14	57% 14% 29%
2	R	14	57% 21% 21%
2	S	14	57% 21% 21%
2	T	14	71% 7% 21%
2	U	14	57% 21% 21%
2	V	14	57% 21% 21%
2	W	14	64% 14% 21%
2	X	14	7% 57% 14% 29%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 18873 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 Serine/threonine-protein phosphatase PGAM5, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	186	1459	922	271	261	5	0	0	0
			Total	C	N	O	S			
1	C	189	1475	935	269	266	5	0	0	0
			Total	C	N	O	S			
1	L	192	1478	932	271	270	5	0	0	0
			Total	C	N	O	S			
1	J	184	1397	887	249	256	5	0	0	0
			Total	C	N	O	S			
1	F	187	1462	925	270	262	5	0	0	0
			Total	C	N	O	S			
1	H	186	1458	921	266	266	5	0	0	0
			Total	C	N	O	S			
1	K	187	1444	914	268	257	5	0	1	0
			Total	C	N	O	S			
1	D	191	1479	938	269	267	5	0	0	0
			Total	C	N	O	S			
1	B	188	1458	922	265	266	5	0	0	0
			Total	C	N	O	S			
1	I	183	1410	892	258	255	5	0	0	0
			Total	C	N	O	S			
1	G	189	1461	923	268	265	5	0	0	0
			Total	C	N	O	S			
1	E	187	1463	925	269	264	5	0	0	0

There are 288 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	67	MET	-	initiating methionine	UNP Q96HS1
A	68	HIS	-	expression tag	UNP Q96HS1
A	69	HIS	-	expression tag	UNP Q96HS1
A	70	HIS	-	expression tag	UNP Q96HS1
A	71	HIS	-	expression tag	UNP Q96HS1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	72	HIS	-	expression tag	UNP Q96HS1
A	73	HIS	-	expression tag	UNP Q96HS1
A	74	SER	-	expression tag	UNP Q96HS1
A	75	SER	-	expression tag	UNP Q96HS1
A	76	GLY	-	expression tag	UNP Q96HS1
A	77	VAL	-	expression tag	UNP Q96HS1
A	78	ASP	-	expression tag	UNP Q96HS1
A	79	LEU	-	expression tag	UNP Q96HS1
A	80	GLY	-	expression tag	UNP Q96HS1
A	81	THR	-	expression tag	UNP Q96HS1
A	82	GLU	-	expression tag	UNP Q96HS1
A	83	ASN	-	expression tag	UNP Q96HS1
A	84	LEU	-	expression tag	UNP Q96HS1
A	85	TYR	-	expression tag	UNP Q96HS1
A	86	PHE	-	expression tag	UNP Q96HS1
A	87	GLN	-	expression tag	UNP Q96HS1
A	88	SER	-	expression tag	UNP Q96HS1
A	89	MET	-	expression tag	UNP Q96HS1
A	105	ALA	HIS	engineered mutation	UNP Q96HS1
C	67	MET	-	initiating methionine	UNP Q96HS1
C	68	HIS	-	expression tag	UNP Q96HS1
C	69	HIS	-	expression tag	UNP Q96HS1
C	70	HIS	-	expression tag	UNP Q96HS1
C	71	HIS	-	expression tag	UNP Q96HS1
C	72	HIS	-	expression tag	UNP Q96HS1
C	73	HIS	-	expression tag	UNP Q96HS1
C	74	SER	-	expression tag	UNP Q96HS1
C	75	SER	-	expression tag	UNP Q96HS1
C	76	GLY	-	expression tag	UNP Q96HS1
C	77	VAL	-	expression tag	UNP Q96HS1
C	78	ASP	-	expression tag	UNP Q96HS1
C	79	LEU	-	expression tag	UNP Q96HS1
C	80	GLY	-	expression tag	UNP Q96HS1
C	81	THR	-	expression tag	UNP Q96HS1
C	82	GLU	-	expression tag	UNP Q96HS1
C	83	ASN	-	expression tag	UNP Q96HS1
C	84	LEU	-	expression tag	UNP Q96HS1
C	85	TYR	-	expression tag	UNP Q96HS1
C	86	PHE	-	expression tag	UNP Q96HS1
C	87	GLN	-	expression tag	UNP Q96HS1
C	88	SER	-	expression tag	UNP Q96HS1
C	89	MET	-	expression tag	UNP Q96HS1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	105	ALA	HIS	engineered mutation	UNP Q96HS1
L	67	MET	-	initiating methionine	UNP Q96HS1
L	68	HIS	-	expression tag	UNP Q96HS1
L	69	HIS	-	expression tag	UNP Q96HS1
L	70	HIS	-	expression tag	UNP Q96HS1
L	71	HIS	-	expression tag	UNP Q96HS1
L	72	HIS	-	expression tag	UNP Q96HS1
L	73	HIS	-	expression tag	UNP Q96HS1
L	74	SER	-	expression tag	UNP Q96HS1
L	75	SER	-	expression tag	UNP Q96HS1
L	76	GLY	-	expression tag	UNP Q96HS1
L	77	VAL	-	expression tag	UNP Q96HS1
L	78	ASP	-	expression tag	UNP Q96HS1
L	79	LEU	-	expression tag	UNP Q96HS1
L	80	GLY	-	expression tag	UNP Q96HS1
L	81	THR	-	expression tag	UNP Q96HS1
L	82	GLU	-	expression tag	UNP Q96HS1
L	83	ASN	-	expression tag	UNP Q96HS1
L	84	LEU	-	expression tag	UNP Q96HS1
L	85	TYR	-	expression tag	UNP Q96HS1
L	86	PHE	-	expression tag	UNP Q96HS1
L	87	GLN	-	expression tag	UNP Q96HS1
L	88	SER	-	expression tag	UNP Q96HS1
L	89	MET	-	expression tag	UNP Q96HS1
L	105	ALA	HIS	engineered mutation	UNP Q96HS1
J	67	MET	-	initiating methionine	UNP Q96HS1
J	68	HIS	-	expression tag	UNP Q96HS1
J	69	HIS	-	expression tag	UNP Q96HS1
J	70	HIS	-	expression tag	UNP Q96HS1
J	71	HIS	-	expression tag	UNP Q96HS1
J	72	HIS	-	expression tag	UNP Q96HS1
J	73	HIS	-	expression tag	UNP Q96HS1
J	74	SER	-	expression tag	UNP Q96HS1
J	75	SER	-	expression tag	UNP Q96HS1
J	76	GLY	-	expression tag	UNP Q96HS1
J	77	VAL	-	expression tag	UNP Q96HS1
J	78	ASP	-	expression tag	UNP Q96HS1
J	79	LEU	-	expression tag	UNP Q96HS1
J	80	GLY	-	expression tag	UNP Q96HS1
J	81	THR	-	expression tag	UNP Q96HS1
J	82	GLU	-	expression tag	UNP Q96HS1
J	83	ASN	-	expression tag	UNP Q96HS1

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Chain	Residue	Modelled	Actual	Comment	Reference
J	84	LEU	-	expression tag	UNP Q96HS1
J	85	TYR	-	expression tag	UNP Q96HS1
J	86	PHE	-	expression tag	UNP Q96HS1
J	87	GLN	-	expression tag	UNP Q96HS1
J	88	SER	-	expression tag	UNP Q96HS1
J	89	MET	-	expression tag	UNP Q96HS1
J	105	ALA	HIS	engineered mutation	UNP Q96HS1
F	67	MET	-	initiating methionine	UNP Q96HS1
F	68	HIS	-	expression tag	UNP Q96HS1
F	69	HIS	-	expression tag	UNP Q96HS1
F	70	HIS	-	expression tag	UNP Q96HS1
F	71	HIS	-	expression tag	UNP Q96HS1
F	72	HIS	-	expression tag	UNP Q96HS1
F	73	HIS	-	expression tag	UNP Q96HS1
F	74	SER	-	expression tag	UNP Q96HS1
F	75	SER	-	expression tag	UNP Q96HS1
F	76	GLY	-	expression tag	UNP Q96HS1
F	77	VAL	-	expression tag	UNP Q96HS1
F	78	ASP	-	expression tag	UNP Q96HS1
F	79	LEU	-	expression tag	UNP Q96HS1
F	80	GLY	-	expression tag	UNP Q96HS1
F	81	THR	-	expression tag	UNP Q96HS1
F	82	GLU	-	expression tag	UNP Q96HS1
F	83	ASN	-	expression tag	UNP Q96HS1
F	84	LEU	-	expression tag	UNP Q96HS1
F	85	TYR	-	expression tag	UNP Q96HS1
F	86	PHE	-	expression tag	UNP Q96HS1
F	87	GLN	-	expression tag	UNP Q96HS1
F	88	SER	-	expression tag	UNP Q96HS1
F	89	MET	-	expression tag	UNP Q96HS1
F	105	ALA	HIS	engineered mutation	UNP Q96HS1
H	67	MET	-	initiating methionine	UNP Q96HS1
H	68	HIS	-	expression tag	UNP Q96HS1
H	69	HIS	-	expression tag	UNP Q96HS1
H	70	HIS	-	expression tag	UNP Q96HS1
H	71	HIS	-	expression tag	UNP Q96HS1
H	72	HIS	-	expression tag	UNP Q96HS1
H	73	HIS	-	expression tag	UNP Q96HS1
H	74	SER	-	expression tag	UNP Q96HS1
H	75	SER	-	expression tag	UNP Q96HS1
H	76	GLY	-	expression tag	UNP Q96HS1
H	77	VAL	-	expression tag	UNP Q96HS1

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Chain	Residue	Modelled	Actual	Comment	Reference
H	78	ASP	-	expression tag	UNP Q96HS1
H	79	LEU	-	expression tag	UNP Q96HS1
H	80	GLY	-	expression tag	UNP Q96HS1
H	81	THR	-	expression tag	UNP Q96HS1
H	82	GLU	-	expression tag	UNP Q96HS1
H	83	ASN	-	expression tag	UNP Q96HS1
H	84	LEU	-	expression tag	UNP Q96HS1
H	85	TYR	-	expression tag	UNP Q96HS1
H	86	PHE	-	expression tag	UNP Q96HS1
H	87	GLN	-	expression tag	UNP Q96HS1
H	88	SER	-	expression tag	UNP Q96HS1
H	89	MET	-	expression tag	UNP Q96HS1
H	105	ALA	HIS	engineered mutation	UNP Q96HS1
K	67	MET	-	initiating methionine	UNP Q96HS1
K	68	HIS	-	expression tag	UNP Q96HS1
K	69	HIS	-	expression tag	UNP Q96HS1
K	70	HIS	-	expression tag	UNP Q96HS1
K	71	HIS	-	expression tag	UNP Q96HS1
K	72	HIS	-	expression tag	UNP Q96HS1
K	73	HIS	-	expression tag	UNP Q96HS1
K	74	SER	-	expression tag	UNP Q96HS1
K	75	SER	-	expression tag	UNP Q96HS1
K	76	GLY	-	expression tag	UNP Q96HS1
K	77	VAL	-	expression tag	UNP Q96HS1
K	78	ASP	-	expression tag	UNP Q96HS1
K	79	LEU	-	expression tag	UNP Q96HS1
K	80	GLY	-	expression tag	UNP Q96HS1
K	81	THR	-	expression tag	UNP Q96HS1
K	82	GLU	-	expression tag	UNP Q96HS1
K	83	ASN	-	expression tag	UNP Q96HS1
K	84	LEU	-	expression tag	UNP Q96HS1
K	85	TYR	-	expression tag	UNP Q96HS1
K	86	PHE	-	expression tag	UNP Q96HS1
K	87	GLN	-	expression tag	UNP Q96HS1
K	88	SER	-	expression tag	UNP Q96HS1
K	89	MET	-	expression tag	UNP Q96HS1
K	105	ALA	HIS	engineered mutation	UNP Q96HS1
D	67	MET	-	initiating methionine	UNP Q96HS1
D	68	HIS	-	expression tag	UNP Q96HS1
D	69	HIS	-	expression tag	UNP Q96HS1
D	70	HIS	-	expression tag	UNP Q96HS1
D	71	HIS	-	expression tag	UNP Q96HS1

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Chain	Residue	Modelled	Actual	Comment	Reference
D	72	HIS	-	expression tag	UNP Q96HS1
D	73	HIS	-	expression tag	UNP Q96HS1
D	74	SER	-	expression tag	UNP Q96HS1
D	75	SER	-	expression tag	UNP Q96HS1
D	76	GLY	-	expression tag	UNP Q96HS1
D	77	VAL	-	expression tag	UNP Q96HS1
D	78	ASP	-	expression tag	UNP Q96HS1
D	79	LEU	-	expression tag	UNP Q96HS1
D	80	GLY	-	expression tag	UNP Q96HS1
D	81	THR	-	expression tag	UNP Q96HS1
D	82	GLU	-	expression tag	UNP Q96HS1
D	83	ASN	-	expression tag	UNP Q96HS1
D	84	LEU	-	expression tag	UNP Q96HS1
D	85	TYR	-	expression tag	UNP Q96HS1
D	86	PHE	-	expression tag	UNP Q96HS1
D	87	GLN	-	expression tag	UNP Q96HS1
D	88	SER	-	expression tag	UNP Q96HS1
D	89	MET	-	expression tag	UNP Q96HS1
D	105	ALA	HIS	engineered mutation	UNP Q96HS1
B	67	MET	-	initiating methionine	UNP Q96HS1
B	68	HIS	-	expression tag	UNP Q96HS1
B	69	HIS	-	expression tag	UNP Q96HS1
B	70	HIS	-	expression tag	UNP Q96HS1
B	71	HIS	-	expression tag	UNP Q96HS1
B	72	HIS	-	expression tag	UNP Q96HS1
B	73	HIS	-	expression tag	UNP Q96HS1
B	74	SER	-	expression tag	UNP Q96HS1
B	75	SER	-	expression tag	UNP Q96HS1
B	76	GLY	-	expression tag	UNP Q96HS1
B	77	VAL	-	expression tag	UNP Q96HS1
B	78	ASP	-	expression tag	UNP Q96HS1
B	79	LEU	-	expression tag	UNP Q96HS1
B	80	GLY	-	expression tag	UNP Q96HS1
B	81	THR	-	expression tag	UNP Q96HS1
B	82	GLU	-	expression tag	UNP Q96HS1
B	83	ASN	-	expression tag	UNP Q96HS1
B	84	LEU	-	expression tag	UNP Q96HS1
B	85	TYR	-	expression tag	UNP Q96HS1
B	86	PHE	-	expression tag	UNP Q96HS1
B	87	GLN	-	expression tag	UNP Q96HS1
B	88	SER	-	expression tag	UNP Q96HS1
B	89	MET	-	expression tag	UNP Q96HS1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	105	ALA	HIS	engineered mutation	UNP Q96HS1
I	67	MET	-	initiating methionine	UNP Q96HS1
I	68	HIS	-	expression tag	UNP Q96HS1
I	69	HIS	-	expression tag	UNP Q96HS1
I	70	HIS	-	expression tag	UNP Q96HS1
I	71	HIS	-	expression tag	UNP Q96HS1
I	72	HIS	-	expression tag	UNP Q96HS1
I	73	HIS	-	expression tag	UNP Q96HS1
I	74	SER	-	expression tag	UNP Q96HS1
I	75	SER	-	expression tag	UNP Q96HS1
I	76	GLY	-	expression tag	UNP Q96HS1
I	77	VAL	-	expression tag	UNP Q96HS1
I	78	ASP	-	expression tag	UNP Q96HS1
I	79	LEU	-	expression tag	UNP Q96HS1
I	80	GLY	-	expression tag	UNP Q96HS1
I	81	THR	-	expression tag	UNP Q96HS1
I	82	GLU	-	expression tag	UNP Q96HS1
I	83	ASN	-	expression tag	UNP Q96HS1
I	84	LEU	-	expression tag	UNP Q96HS1
I	85	TYR	-	expression tag	UNP Q96HS1
I	86	PHE	-	expression tag	UNP Q96HS1
I	87	GLN	-	expression tag	UNP Q96HS1
I	88	SER	-	expression tag	UNP Q96HS1
I	89	MET	-	expression tag	UNP Q96HS1
I	105	ALA	HIS	engineered mutation	UNP Q96HS1
G	67	MET	-	initiating methionine	UNP Q96HS1
G	68	HIS	-	expression tag	UNP Q96HS1
G	69	HIS	-	expression tag	UNP Q96HS1
G	70	HIS	-	expression tag	UNP Q96HS1
G	71	HIS	-	expression tag	UNP Q96HS1
G	72	HIS	-	expression tag	UNP Q96HS1
G	73	HIS	-	expression tag	UNP Q96HS1
G	74	SER	-	expression tag	UNP Q96HS1
G	75	SER	-	expression tag	UNP Q96HS1
G	76	GLY	-	expression tag	UNP Q96HS1
G	77	VAL	-	expression tag	UNP Q96HS1
G	78	ASP	-	expression tag	UNP Q96HS1
G	79	LEU	-	expression tag	UNP Q96HS1
G	80	GLY	-	expression tag	UNP Q96HS1
G	81	THR	-	expression tag	UNP Q96HS1
G	82	GLU	-	expression tag	UNP Q96HS1
G	83	ASN	-	expression tag	UNP Q96HS1

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Chain	Residue	Modelled	Actual	Comment	Reference
G	84	LEU	-	expression tag	UNP Q96HS1
G	85	TYR	-	expression tag	UNP Q96HS1
G	86	PHE	-	expression tag	UNP Q96HS1
G	87	GLN	-	expression tag	UNP Q96HS1
G	88	SER	-	expression tag	UNP Q96HS1
G	89	MET	-	expression tag	UNP Q96HS1
G	105	ALA	HIS	engineered mutation	UNP Q96HS1
E	67	MET	-	initiating methionine	UNP Q96HS1
E	68	HIS	-	expression tag	UNP Q96HS1
E	69	HIS	-	expression tag	UNP Q96HS1
E	70	HIS	-	expression tag	UNP Q96HS1
E	71	HIS	-	expression tag	UNP Q96HS1
E	72	HIS	-	expression tag	UNP Q96HS1
E	73	HIS	-	expression tag	UNP Q96HS1
E	74	SER	-	expression tag	UNP Q96HS1
E	75	SER	-	expression tag	UNP Q96HS1
E	76	GLY	-	expression tag	UNP Q96HS1
E	77	VAL	-	expression tag	UNP Q96HS1
E	78	ASP	-	expression tag	UNP Q96HS1
E	79	LEU	-	expression tag	UNP Q96HS1
E	80	GLY	-	expression tag	UNP Q96HS1
E	81	THR	-	expression tag	UNP Q96HS1
E	82	GLU	-	expression tag	UNP Q96HS1
E	83	ASN	-	expression tag	UNP Q96HS1
E	84	LEU	-	expression tag	UNP Q96HS1
E	85	TYR	-	expression tag	UNP Q96HS1
E	86	PHE	-	expression tag	UNP Q96HS1
E	87	GLN	-	expression tag	UNP Q96HS1
E	88	SER	-	expression tag	UNP Q96HS1
E	89	MET	-	expression tag	UNP Q96HS1
E	105	ALA	HIS	engineered mutation	UNP Q96HS1

- Molecule 2 is a protein called PGAM5 Multimerization Motif Peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	M	11	101	63	20	18	0	0	0
			Total	C	N	O			
2	O	11	101	63	20	18	0	0	0
			Total	C	N	O			
2	X	10	92	58	19	15	0	0	0
			Total	C	N	O			
2	V	11	101	63	20	18	0	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	R	11	101	63	20	18	0	0	0
2	T	11	101	63	20	18	0	0	0
2	W	11	101	63	20	18	0	0	0
2	P	11	101	63	20	18	0	0	0
2	N	11	101	63	20	18	0	0	0
2	U	11	101	63	20	18	0	0	0
2	S	11	101	63	20	18	0	0	0
2	Q	10	97	61	19	17	0	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
3	A	1	1	1	0	0
3	C	5	5	5	0	0
3	L	2	2	2	0	0
3	J	2	2	2	0	0
3	F	4	4	4	0	0
3	H	2	2	2	0	0
3	K	1	1	1	0	0
3	D	3	3	3	0	0
3	B	2	2	2	0	0
3	I	3	3	3	0	0
3	G	3	3	3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	2	Total Mg 2 2	0	0
3	P	1	Total Mg 1 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	16	Total O 16 16	0	0
4	C	16	Total O 16 16	0	0
4	L	19	Total O 19 19	0	0
4	J	10	Total O 10 10	0	0
4	F	23	Total O 23 23	0	0
4	H	12	Total O 12 12	0	0
4	K	12	Total O 12 12	0	0
4	D	17	Total O 17 17	0	0
4	B	16	Total O 16 16	0	0
4	I	14	Total O 14 14	0	0
4	G	11	Total O 11 11	0	0
4	E	21	Total O 21 21	0	0
4	M	1	Total O 1 1	0	0
4	O	3	Total O 3 3	0	0
4	X	1	Total O 1 1	0	0
4	V	1	Total O 1 1	0	0
4	R	1	Total O 1 1	0	0

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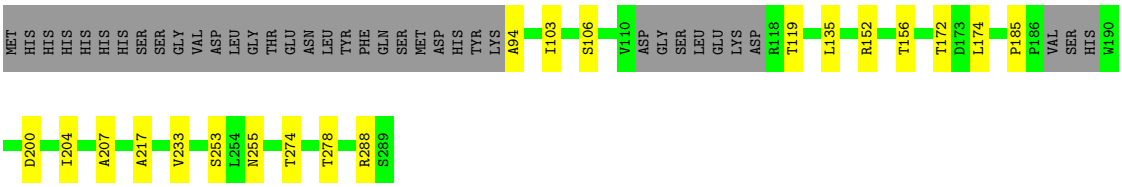
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	P	1	1	1	0	0
			Total	O		
4	N	1	1	1	0	0
			Total	O		
4	U	1	1	1	0	0
			Total	O		
4	Q	2	2	2	0	0

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.

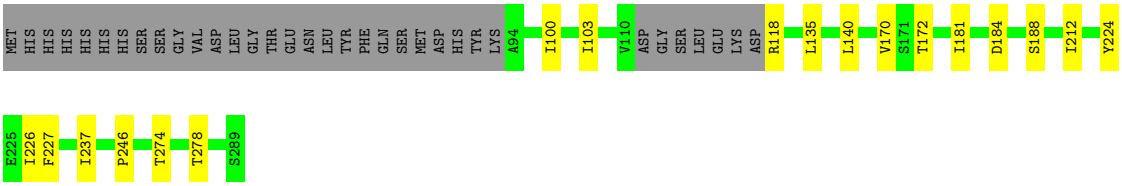
• Molecule 1: Serine/threonine-protein phosphatase PGAM5, mitochondrial

Chain A:



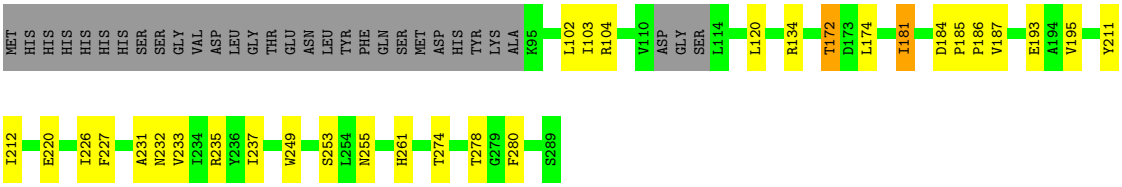
• Molecule 1: Serine/threonine-protein phosphatase PGAM5, mitochondrial

Chain C:



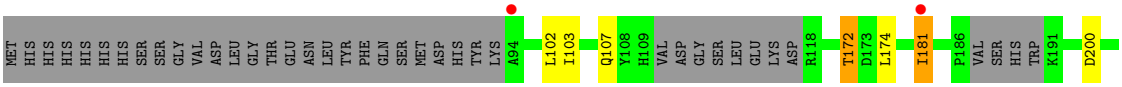
• Molecule 1: Serine/threonine-protein phosphatase PGAM5, mitochondrial

Chain L:



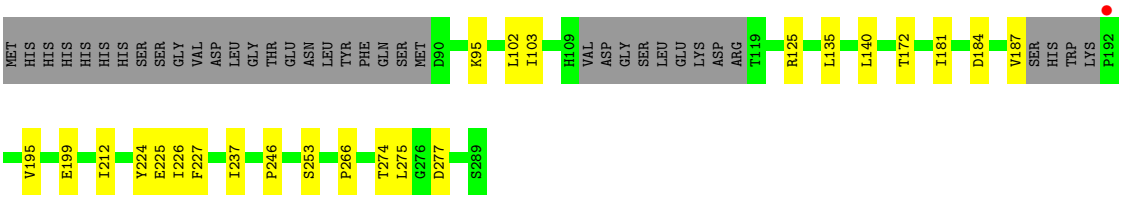
• Molecule 1: Serine/threonine-protein phosphatase PGAM5, mitochondrial

Chain J:



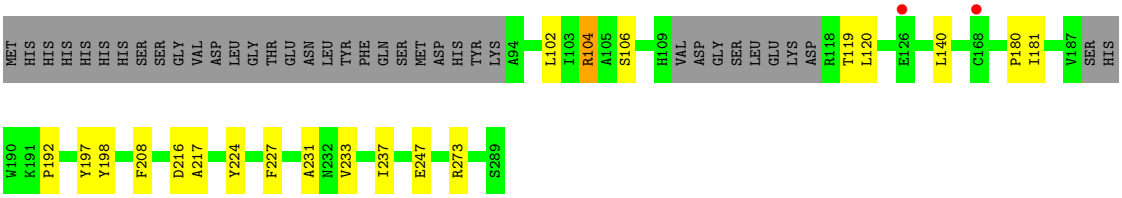
• Molecule 1: Serine/threonine-protein phosphatase PGAM5, mitochondrial

Chain F:



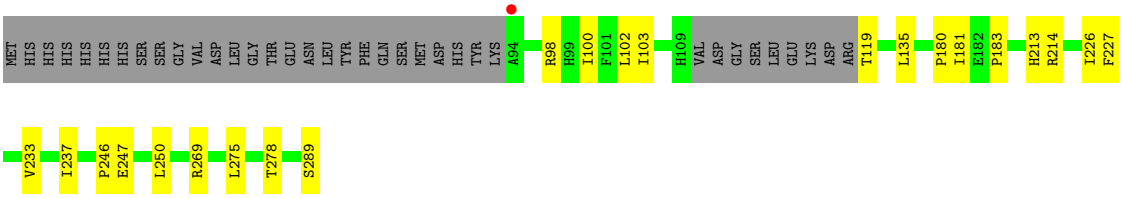
• Molecule 1: Serine/threonine-protein phosphatase PGAM5, mitochondrial

Chain H:



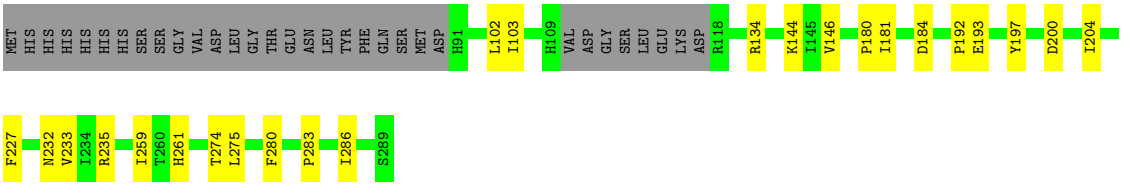
• Molecule 1: Serine/threonine-protein phosphatase PGAM5, mitochondrial

Chain K:



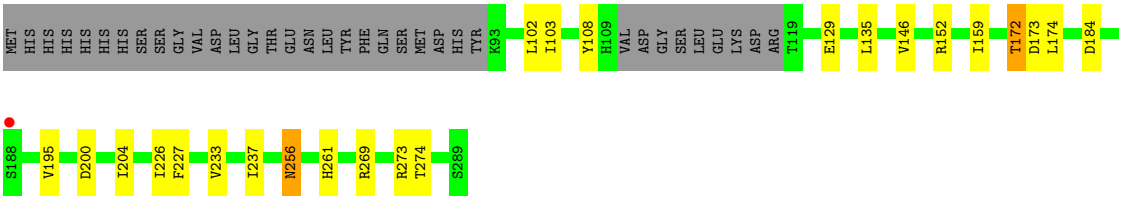
• Molecule 1: Serine/threonine-protein phosphatase PGAM5, mitochondrial

Chain D:



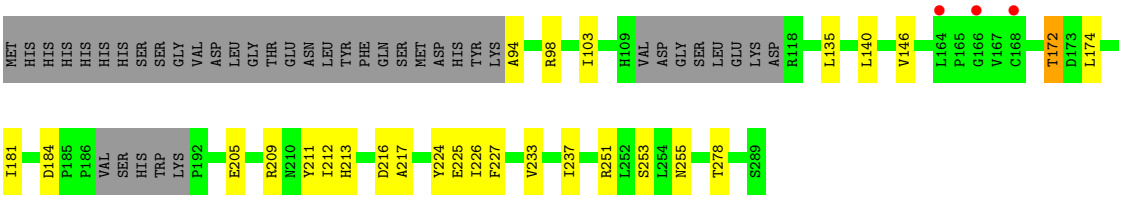
• Molecule 1: Serine/threonine-protein phosphatase PGAM5, mitochondrial

Chain B:



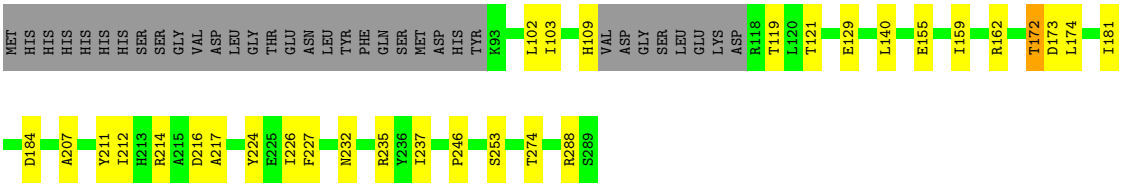
• Molecule 1: Serine/threonine-protein phosphatase PGAM5, mitochondrial

Chain I:



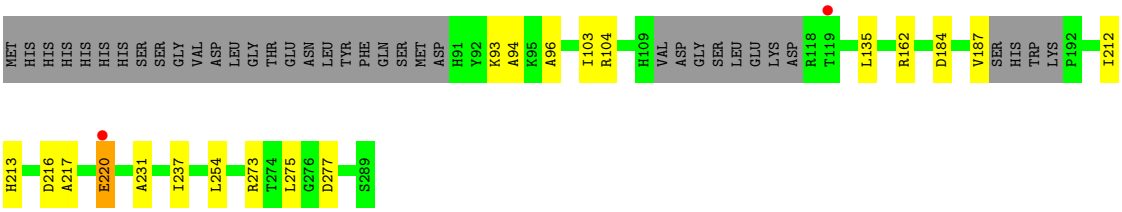
• Molecule 1: Serine/threonine-protein phosphatase PGAM5, mitochondrial

Chain G:



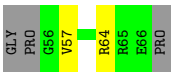
• Molecule 1: Serine/threonine-protein phosphatase PGAM5, mitochondrial

Chain E:



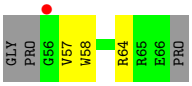
• Molecule 2: PGAM5 Multimerization Motif Peptide

Chain M:



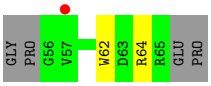
• Molecule 2: PGAM5 Multimerization Motif Peptide

Chain O:



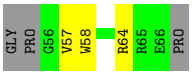
• Molecule 2: PGAM5 Multimerization Motif Peptide

Chain X:



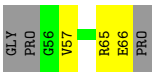
• Molecule 2: PGAM5 Multimerization Motif Peptide

Chain V:



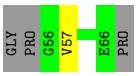
• Molecule 2: PGAM5 Multimerization Motif Peptide

Chain R:



• Molecule 2: PGAM5 Multimerization Motif Peptide

Chain T:

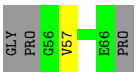


• Molecule 2: PGAM5 Multimerization Motif Peptide

Chain W:

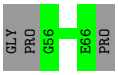
• Molecule 2: PGAM5 Multimerization Motif Peptide

Chain P:



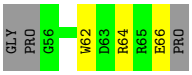
• Molecule 2: PGAM5 Multimerization Motif Peptide

Chain N:



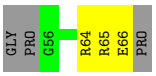
• Molecule 2: PGAM5 Multimerization Motif Peptide

Chain U:



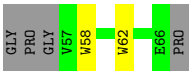
• Molecule 2: PGAM5 Multimerization Motif Peptide

Chain S:



• Molecule 2: PGAM5 Multimerization Motif Peptide

Chain Q:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	49.37Å 242.54Å 272.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.60 – 2.60 49.70 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.5 (48.60-2.60) 99.8 (49.70-2.60)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.81 (at 2.61Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.223 , 0.264 0.226 , 0.263	Depositor DCC
R_{free} test set	5091 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	35.9	Xtriage
Anisotropy	0.441	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 56.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	18873	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% 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 (i)

5.1 Standard geometry (i)

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

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	0.28	0/1491	0.52	0/2027
1	B	0.28	0/1491	0.53	0/2030
1	C	0.28	0/1509	0.52	0/2052
1	D	0.28	0/1513	0.50	0/2059
1	E	0.39	1/1495 (0.1%)	0.57	0/2029
1	F	0.28	0/1494	0.51	0/2027
1	G	0.28	0/1493	0.51	0/2030
1	H	0.30	0/1490	0.52	0/2025
1	I	0.29	0/1440	0.50	0/1957
1	J	0.30	0/1427	0.51	0/1946
1	K	0.28	0/1479	0.51	0/2013
1	L	0.30	0/1509	0.53	0/2053
2	M	0.24	0/105	0.56	0/143
2	N	0.22	0/105	0.64	0/143
2	O	0.27	0/105	0.50	0/143
2	P	0.21	0/105	0.55	0/143
2	Q	0.24	0/101	0.46	0/138
2	R	0.24	0/105	0.66	0/143
2	S	0.32	0/105	0.48	0/143
2	T	0.21	0/105	0.52	0/143
2	U	0.26	0/105	0.50	0/143
2	V	0.28	0/105	0.64	0/143
2	W	0.23	0/105	0.47	0/143
2	X	0.23	0/96	0.58	0/131
All	All	0.29	1/19078 (0.0%)	0.52	0/25947

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	220	GLU	CB-CG	-7.68	1.37	1.52

There are no bond angle outliers.

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	1459	0	1439	11	0
1	B	1458	0	1422	19	0
1	C	1475	0	1454	9	0
1	D	1479	0	1445	13	0
1	E	1463	0	1444	17	0
1	F	1462	0	1449	15	0
1	G	1461	0	1409	18	0
1	H	1458	0	1432	12	0
1	I	1410	0	1382	19	0
1	J	1397	0	1344	17	0
1	K	1444	0	1416	12	0
1	L	1478	0	1439	20	0
2	M	101	0	84	3	0
2	N	101	0	84	0	0
2	O	101	0	84	3	0
2	P	101	0	84	1	0
2	Q	97	0	81	2	0
2	R	101	0	84	2	0
2	S	101	0	84	3	0
2	T	101	0	84	1	0
2	U	101	0	84	3	0
2	V	101	0	84	3	0
2	W	101	0	84	2	0
2	X	92	0	78	1	0
3	A	1	0	0	0	0
3	B	2	0	0	0	0
3	C	5	0	0	0	0
3	D	3	0	0	0	0
3	E	2	0	0	0	0
3	F	4	0	0	0	0
3	G	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	2	0	0	0	0
3	I	3	0	0	0	0
3	J	2	0	0	0	0
3	K	1	0	0	0	0
3	L	2	0	0	0	0
3	P	1	0	0	0	0
4	A	16	0	0	0	0
4	B	16	0	0	0	0
4	C	16	0	0	1	0
4	D	17	0	0	0	0
4	E	21	0	0	0	0
4	F	23	0	0	1	0
4	G	11	0	0	0	0
4	H	12	0	0	0	0
4	I	14	0	0	1	0
4	J	10	0	0	0	0
4	K	12	0	0	0	0
4	L	19	0	0	0	0
4	M	1	0	0	0	0
4	N	1	0	0	0	0
4	O	3	0	0	0	0
4	P	1	0	0	0	0
4	Q	2	0	0	0	0
4	R	1	0	0	0	0
4	U	1	0	0	0	0
4	V	1	0	0	0	0
4	X	1	0	0	0	0
All	All	18873	0	18074	174	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 (174) 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:G:129:GLU:OE2	1:G:162:ARG:NH2	2.06	0.89
1:F:199:GLU:OE2	2:S:65:ARG:NH1	2.10	0.84
1:E:94:ALA:N	1:E:220:GLU:OE2	2.13	0.81
1:A:204:ILE:HD12	1:A:233:VAL:HG22	1.64	0.78
1:K:103:ILE:HD13	1:K:226:ILE:HG23	1.66	0.77
1:A:152:ARG:O	1:A:156:THR:HG23	1.87	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:ILE:HD12	1:B:233:VAL:HG22	1.69	0.73
1:B:102:LEU:HD23	1:B:227:PHE:HB2	1.70	0.73
1:J:102:LEU:HD23	1:J:227:PHE:HB2	1.71	0.73
1:D:283:PRO:HA	1:D:286:ILE:HD12	1.70	0.72
1:G:103:ILE:HD13	1:G:226:ILE:HG23	1.72	0.72
2:U:62:TRP:O	2:U:64:ARG:NH2	2.25	0.70
1:H:102:LEU:HD23	1:H:227:PHE:HB2	1.74	0.69
1:B:103:ILE:HD11	1:B:135:LEU:HD11	1.74	0.69
1:F:184:ASP:OD1	2:Q:58:TRP:N	2.25	0.69
1:L:103:ILE:HD13	1:L:226:ILE:HG23	1.75	0.69
1:L:186:PRO:O	1:K:269:ARG:NH1	2.29	0.66
1:D:204:ILE:HD12	1:D:233:VAL:HG22	1.77	0.65
1:K:183:PRO:HG3	1:K:250:LEU:HD12	1.76	0.65
1:L:195:VAL:HG22	2:M:64:ARG:O	1.97	0.64
1:E:103:ILE:CD1	1:E:135:LEU:HD11	2.27	0.64
1:E:94:ALA:O	1:E:220:GLU:OE2	2.15	0.64
1:I:94:ALA:N	4:I:401:HOH:O	2.30	0.63
1:C:181:ILE:HD11	1:C:246:PRO:HB2	1.80	0.63
1:A:253:SER:OG	1:B:273:ARG:NH2	2.31	0.63
1:D:102:LEU:HD23	1:D:227:PHE:HB2	1.81	0.63
1:J:204:ILE:HD12	1:J:233:VAL:HG22	1.79	0.62
1:F:125:ARG:NH1	4:F:401:HOH:O	2.31	0.62
1:J:200:ASP:O	1:J:204:ILE:HG12	2.00	0.62
1:A:106:SER:H	1:A:156:THR:HG21	1.66	0.61
1:B:184:ASP:OD2	2:M:57:VAL:HA	2.02	0.60
1:G:216:ASP:OD1	1:G:217:ALA:N	2.35	0.59
1:L:184:ASP:OD2	2:W:57:VAL:HA	2.03	0.59
1:L:195:VAL:CG2	2:M:64:ARG:O	2.51	0.58
1:I:135:LEU:HD13	1:I:226:ILE:HD13	1.86	0.57
1:C:103:ILE:CD1	1:C:135:LEU:HD11	2.35	0.57
1:C:184:ASP:OD2	2:P:57:VAL:HA	2.04	0.56
2:R:65:ARG:O	2:R:66:GLU:HB2	2.05	0.56
1:A:200:ASP:O	1:A:204:ILE:HG12	2.05	0.56
1:G:181:ILE:HD11	1:G:246:PRO:HB2	1.88	0.56
1:I:98:ARG:NH2	1:I:225:GLU:OE2	2.34	0.56
1:B:108:TYR:CD2	1:B:152:ARG:HD2	2.41	0.56
1:L:172:THR:HG22	1:L:174:LEU:H	1.71	0.55
1:F:195:VAL:HG22	2:S:64:ARG:O	2.06	0.55
2:X:62:TRP:O	2:X:64:ARG:NH1	2.38	0.55
1:E:216:ASP:OD1	1:E:217:ALA:N	2.39	0.55
1:K:102:LEU:HD23	1:K:227:PHE:HB2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:102:LEU:HD23	1:F:227:PHE:HB2	1.90	0.54
1:F:103:ILE:HD13	1:F:226:ILE:HG23	1.87	0.54
1:D:200:ASP:O	1:D:204:ILE:HG12	2.08	0.54
1:B:200:ASP:O	1:B:204:ILE:HG12	2.07	0.54
1:B:103:ILE:CD1	1:B:135:LEU:HD11	2.36	0.54
1:E:184:ASP:OD2	2:R:57:VAL:HA	2.07	0.54
1:K:233:VAL:O	1:K:237:ILE:HG12	2.09	0.52
1:J:103:ILE:HD13	1:J:226:ILE:HG23	1.91	0.52
1:I:184:ASP:OD2	2:V:58:TRP:N	2.36	0.52
1:I:216:ASP:OD1	1:I:217:ALA:N	2.43	0.52
1:H:198:TYR:HB2	2:U:64:ARG:HD3	1.91	0.52
1:E:104:ARG:NH1	1:E:254:LEU:O	2.43	0.51
1:F:253:SER:HB3	1:E:273:ARG:HA	1.92	0.51
1:B:256:ASN:OD1	1:B:256:ASN:N	2.41	0.50
1:A:174:LEU:HB3	1:A:207:ALA:HB2	1.94	0.50
1:D:184:ASP:OD2	2:O:58:TRP:N	2.34	0.50
1:I:103:ILE:CD1	1:I:135:LEU:HD11	2.42	0.50
1:C:212:ILE:HG13	1:C:237:ILE:HG23	1.94	0.49
1:C:140:LEU:HD22	1:C:224:TYR:CD2	2.47	0.49
1:J:233:VAL:O	1:J:237:ILE:HG12	2.12	0.49
2:V:64:ARG:HD2	2:V:64:ARG:N	2.27	0.49
1:J:255:ASN:HB2	1:J:278:THR:HG21	1.95	0.49
1:F:212:ILE:HG13	1:F:237:ILE:HG23	1.95	0.49
1:G:129:GLU:OE2	1:G:159:ILE:HG23	2.13	0.49
1:G:212:ILE:HG13	1:G:237:ILE:HG23	1.93	0.49
1:E:93:LYS:CB	1:E:220:GLU:CD	2.81	0.49
1:I:103:ILE:HD11	1:I:135:LEU:HD11	1.95	0.49
1:C:118:ARG:N	4:C:402:HOH:O	2.47	0.48
1:D:232:ASN:OD1	1:D:235:ARG:NH2	2.46	0.48
1:B:261:HIS:CB	1:B:274:THR:HG22	2.44	0.48
1:G:172:THR:HG22	1:G:174:LEU:H	1.78	0.48
1:A:255:ASN:HB2	1:A:278:THR:HG21	1.96	0.48
1:H:208:PHE:HB2	1:H:237:ILE:HD13	1.96	0.48
1:J:181:ILE:HD12	1:J:247:GLU:HA	1.95	0.47
1:I:172:THR:HG22	1:I:174:LEU:H	1.78	0.47
1:C:100:ILE:HG23	1:C:227:PHE:CD1	2.49	0.47
1:L:181:ILE:CD1	1:L:249:TRP:CD1	2.97	0.47
1:G:232:ASN:OD1	1:G:235:ARG:NH2	2.47	0.47
1:H:233:VAL:O	1:H:237:ILE:HG12	2.15	0.47
1:G:119:THR:OG1	1:G:155:GLU:OE2	2.25	0.47
1:L:220:GLU:CD	1:L:220:GLU:H	2.19	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:134:ARG:HG2	1:D:280:PHE:CD2	2.50	0.47
1:D:180:PRO:O	1:D:181:ILE:HG23	2.16	0.46
1:E:93:LYS:CB	1:E:220:GLU:OE2	2.63	0.46
1:L:172:THR:HG21	1:L:211:TYR:OH	2.14	0.46
1:C:135:LEU:HD13	1:C:226:ILE:HD13	1.97	0.46
1:A:103:ILE:CD1	1:A:135:LEU:HD11	2.46	0.46
1:K:100:ILE:HG23	1:K:227:PHE:CD1	2.51	0.46
1:F:135:LEU:HD13	1:F:226:ILE:HD13	1.98	0.46
1:L:261:HIS:CB	1:L:274:THR:HG22	2.46	0.45
1:E:103:ILE:HD11	1:E:135:LEU:HD11	1.96	0.45
1:E:104:ARG:NE	1:E:231:ALA:HB2	2.31	0.45
1:H:140:LEU:HD22	1:H:224:TYR:CE2	2.51	0.45
1:B:129:GLU:OE1	1:B:159:ILE:HG23	2.17	0.45
1:J:107:GLN:HA	1:J:256:ASN:OD1	2.16	0.45
1:I:140:LEU:HD22	1:I:224:TYR:CE2	2.51	0.45
1:J:261:HIS:CB	1:J:274:THR:HG22	2.46	0.45
1:H:104:ARG:HD2	1:H:231:ALA:HB2	1.99	0.45
1:B:233:VAL:O	1:B:237:ILE:HG12	2.17	0.45
1:G:172:THR:HG21	1:G:211:TYR:OH	2.17	0.45
1:G:174:LEU:HB3	1:G:207:ALA:HB2	1.99	0.45
1:H:181:ILE:HD12	1:H:247:GLU:HG3	1.99	0.44
1:L:212:ILE:HG13	1:L:237:ILE:HG23	1.98	0.44
1:E:96:ALA:HB2	1:E:220:GLU:C	2.38	0.44
1:D:184:ASP:OD2	2:O:57:VAL:HA	2.18	0.44
1:G:184:ASP:OD2	2:T:57:VAL:HA	2.17	0.44
1:G:214:ARG:NH1	2:S:66:GLU:OE1	2.50	0.44
1:D:146:VAL:O	1:D:227:PHE:HA	2.18	0.43
1:E:93:LYS:C	1:E:220:GLU:OE2	2.56	0.43
1:L:102:LEU:HD23	1:L:227:PHE:HB2	2.00	0.43
1:I:212:ILE:HG13	1:I:237:ILE:HG23	2.00	0.43
1:L:104:ARG:NE	1:L:231:ALA:HB2	2.34	0.43
1:F:172:THR:HA	1:G:173:ASP:OD2	2.19	0.43
1:G:102:LEU:HD23	1:G:227:PHE:HB2	2.01	0.43
1:L:261:HIS:HB3	1:L:274:THR:HG22	2.00	0.43
1:K:181:ILE:HD11	1:K:246:PRO:HB2	2.01	0.43
1:I:172:THR:HG21	1:I:211:TYR:OH	2.18	0.43
1:K:214:ARG:NH1	2:W:66:GLU:OE1	2.44	0.42
1:F:140:LEU:HD22	1:F:224:TYR:CE2	2.54	0.42
1:D:192:PRO:HG2	1:D:197:TYR:CZ	2.54	0.42
1:G:140:LEU:HD22	1:G:224:TYR:CE2	2.54	0.42
1:L:184:ASP:OD1	1:L:185:PRO:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:103:ILE:HA	1:J:258:SER:O	2.19	0.42
1:H:216:ASP:OD1	1:H:217:ALA:N	2.52	0.42
1:I:255:ASN:HB2	1:I:278:THR:HG21	2.01	0.42
1:F:95:LYS:HB3	1:F:266:PRO:HB3	2.02	0.42
1:B:146:VAL:O	1:B:227:PHE:HA	2.19	0.42
1:D:103:ILE:CD1	1:D:259:ILE:HG12	2.49	0.42
1:A:185:PRO:HB2	1:B:269:ARG:NH1	2.33	0.42
1:J:172:THR:HG22	1:J:174:LEU:H	1.85	0.42
1:K:181:ILE:HD12	1:K:247:GLU:HG3	2.02	0.42
1:I:184:ASP:OD2	2:V:57:VAL:HA	2.20	0.42
1:F:181:ILE:HD11	1:F:246:PRO:HB2	2.02	0.42
1:H:192:PRO:HG2	1:H:197:TYR:CZ	2.54	0.42
1:I:233:VAL:O	1:I:237:ILE:HG12	2.20	0.42
1:L:232:ASN:OD1	1:L:235:ARG:NH2	2.53	0.41
1:J:255:ASN:O	1:J:258:SER:OG	2.21	0.41
1:F:275:LEU:HB3	1:E:275:LEU:HB3	2.01	0.41
1:C:172:THR:HA	1:B:173:ASP:OD2	2.20	0.41
1:H:180:PRO:O	1:H:181:ILE:HG23	2.21	0.41
1:H:106:SER:HB2	1:H:120:LEU:HD22	2.02	0.41
1:J:242:LEU:O	1:I:251:ARG:NH1	2.52	0.41
1:K:135:LEU:HD13	1:K:226:ILE:HD13	2.02	0.41
1:K:98:ARG:HD3	1:K:213:HIS:O	2.20	0.41
1:E:212:ILE:HG13	1:E:237:ILE:HG23	2.01	0.41
1:J:256:ASN:N	1:J:256:ASN:HD22	2.18	0.41
1:B:195:VAL:CG2	2:O:64:ARG:O	2.69	0.41
1:I:205:GLU:O	1:I:209:ARG:HG3	2.21	0.41
1:G:109:HIS:CE1	1:G:121:THR:HG22	2.55	0.41
1:A:288:ARG:HD3	1:B:273:ARG:NH2	2.36	0.41
1:L:233:VAL:O	1:L:237:ILE:HG12	2.21	0.41
1:D:261:HIS:HB3	1:D:274:THR:HG22	2.02	0.41
1:B:172:THR:HG22	1:B:174:LEU:H	1.86	0.41
1:E:213:HIS:HA	2:Q:62:TRP:CH2	2.55	0.41
1:K:180:PRO:O	1:K:181:ILE:HG23	2.21	0.41
1:A:94:ALA:HA	1:A:217:ALA:HA	2.04	0.40
1:J:212:ILE:HG13	1:J:237:ILE:HG23	2.03	0.40
1:F:277:ASP:OD1	1:E:277:ASP:OD1	2.39	0.40
1:H:273:ARG:HD2	1:G:288:ARG:HD3	2.03	0.40
1:L:181:ILE:HD12	1:L:249:TRP:CD1	2.57	0.40
1:L:255:ASN:HB2	1:L:278:THR:HG21	2.03	0.40
1:B:135:LEU:HD13	1:B:226:ILE:HD13	2.03	0.40
1:L:134:ARG:HG2	1:L:280:PHE:CD2	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:273:ARG:HG3	1:I:253:SER:HB3	2.04	0.40
1:I:146:VAL:O	1:I:227:PHE:HA	2.21	0.40
1:I:213:HIS:HA	2:U:62:TRP:CH2	2.56	0.40
1:J:258:SER:HB3	1:J:276:GLY:HA2	2.04	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	180/223 (81%)	178 (99%)	2 (1%)	0	100	100
1	B	184/223 (82%)	180 (98%)	4 (2%)	0	100	100
1	C	185/223 (83%)	181 (98%)	4 (2%)	0	100	100
1	D	187/223 (84%)	179 (96%)	8 (4%)	0	100	100
1	E	181/223 (81%)	179 (99%)	2 (1%)	0	100	100
1	F	181/223 (81%)	179 (99%)	2 (1%)	0	100	100
1	G	185/223 (83%)	183 (99%)	2 (1%)	0	100	100
1	H	180/223 (81%)	176 (98%)	4 (2%)	0	100	100
1	I	177/223 (79%)	175 (99%)	2 (1%)	0	100	100
1	J	178/223 (80%)	175 (98%)	3 (2%)	0	100	100
1	K	184/223 (82%)	180 (98%)	4 (2%)	0	100	100
1	L	188/223 (84%)	184 (98%)	4 (2%)	0	100	100
2	M	9/14 (64%)	8 (89%)	1 (11%)	0	100	100
2	N	9/14 (64%)	8 (89%)	1 (11%)	0	100	100
2	O	9/14 (64%)	9 (100%)	0	0	100	100
2	P	9/14 (64%)	8 (89%)	1 (11%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	Q	8/14 (57%)	7 (88%)	1 (12%)	0	100	100
2	R	9/14 (64%)	9 (100%)	0	0	100	100
2	S	9/14 (64%)	8 (89%)	1 (11%)	0	100	100
2	T	9/14 (64%)	8 (89%)	1 (11%)	0	100	100
2	U	9/14 (64%)	7 (78%)	2 (22%)	0	100	100
2	V	9/14 (64%)	7 (78%)	2 (22%)	0	100	100
2	W	9/14 (64%)	9 (100%)	0	0	100	100
2	X	8/14 (57%)	8 (100%)	0	0	100	100
All	All	2296/2844 (81%)	2245 (98%)	51 (2%)	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	152/193 (79%)	149 (98%)	3 (2%)	55	78
1	B	151/193 (78%)	149 (99%)	2 (1%)	69	86
1	C	154/193 (80%)	150 (97%)	4 (3%)	46	72
1	D	152/193 (79%)	149 (98%)	3 (2%)	55	78
1	E	153/193 (79%)	151 (99%)	2 (1%)	69	86
1	F	153/193 (79%)	150 (98%)	3 (2%)	55	78
1	G	148/193 (77%)	145 (98%)	3 (2%)	55	78
1	H	153/193 (79%)	151 (99%)	2 (1%)	69	86
1	I	145/193 (75%)	143 (99%)	2 (1%)	67	85
1	J	141/193 (73%)	136 (96%)	5 (4%)	36	62
1	K	147/193 (76%)	143 (97%)	4 (3%)	44	71
1	L	152/193 (79%)	146 (96%)	6 (4%)	32	58
2	M	10/12 (83%)	10 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	N	10/12 (83%)	10 (100%)	0	100	100
2	O	10/12 (83%)	10 (100%)	0	100	100
2	P	10/12 (83%)	10 (100%)	0	100	100
2	Q	10/12 (83%)	10 (100%)	0	100	100
2	R	10/12 (83%)	10 (100%)	0	100	100
2	S	10/12 (83%)	10 (100%)	0	100	100
2	T	10/12 (83%)	10 (100%)	0	100	100
2	U	10/12 (83%)	9 (90%)	1 (10%)	7	14
2	V	10/12 (83%)	10 (100%)	0	100	100
2	W	10/12 (83%)	10 (100%)	0	100	100
2	X	9/12 (75%)	9 (100%)	0	100	100
All	All	1920/2460 (78%)	1880 (98%)	40 (2%)	53	77

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	119	THR
1	A	172	THR
1	A	274	THR
1	C	170	VAL
1	C	188	SER
1	C	274	THR
1	C	278	THR
1	L	120	LEU
1	L	172	THR
1	L	181	ILE
1	L	187	VAL
1	L	193	GLU
1	L	253	SER
1	J	172	THR
1	J	181	ILE
1	J	229	CYS
1	J	256	ASN
1	J	275	LEU
1	F	187	VAL
1	F	225	GLU
1	F	274	THR
1	H	104	ARG

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Mol	Chain	Res	Type
1	H	119	THR
1	K	119	THR
1	K	275	LEU
1	K	278	THR
1	K	289	SER
1	D	144	LYS
1	D	193	GLU
1	D	275	LEU
1	B	172	THR
1	B	256	ASN
1	I	172	THR
1	I	181	ILE
1	G	172	THR
1	G	253	SER
1	G	274	THR
1	E	162	ARG
1	E	187	VAL
2	U	66	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	256	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 31 ligands modelled in this entry, 31 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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(Å^2)	Q<0.9
1	A	186/223 (83%)	-0.20	0 100 100	22, 31, 49, 56	0
1	B	188/223 (84%)	-0.14	1 (0%) 91 89	22, 32, 54, 66	0
1	C	189/223 (84%)	-0.19	0 100 100	20, 30, 45, 56	1 (0%)
1	D	191/223 (85%)	-0.12	0 100 100	22, 33, 53, 61	0
1	E	187/223 (83%)	-0.12	2 (1%) 80 78	21, 31, 44, 56	1 (0%)
1	F	187/223 (83%)	-0.19	1 (0%) 91 89	21, 31, 45, 60	2 (1%)
1	G	189/223 (84%)	-0.12	0 100 100	26, 37, 54, 62	0
1	H	186/223 (83%)	0.03	2 (1%) 80 78	25, 37, 52, 59	0
1	I	183/223 (82%)	0.07	3 (1%) 72 68	26, 37, 53, 66	0
1	J	184/223 (82%)	-0.02	2 (1%) 80 78	26, 38, 51, 64	0
1	K	187/223 (83%)	-0.09	1 (0%) 91 89	25, 35, 52, 66	0
1	L	192/223 (86%)	-0.18	0 100 100	22, 33, 53, 67	0
2	M	11/14 (78%)	-0.11	0 100 100	28, 31, 49, 51	0
2	N	11/14 (78%)	-0.05	0 100 100	26, 32, 48, 52	0
2	O	11/14 (78%)	0.40	1 (9%) 9 6	27, 31, 48, 55	0
2	P	11/14 (78%)	-0.11	0 100 100	26, 31, 45, 52	0
2	Q	10/14 (71%)	-0.25	0 100 100	27, 32, 43, 52	0
2	R	11/14 (78%)	-0.12	0 100 100	28, 34, 44, 53	0
2	S	11/14 (78%)	0.06	0 100 100	36, 38, 55, 61	0
2	T	11/14 (78%)	-0.02	0 100 100	31, 37, 47, 56	0
2	U	11/14 (78%)	-0.04	0 100 100	35, 41, 55, 56	0
2	V	11/14 (78%)	0.17	0 100 100	37, 39, 50, 55	0
2	W	11/14 (78%)	0.12	0 100 100	33, 42, 52, 52	0
2	X	10/14 (71%)	0.14	1 (10%) 7 4	32, 37, 54, 54	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
All	All	2379/2844 (83%)	-0.10	14 (0%)	89	88	20, 34, 52, 67	4 (0%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	94	ALA	3.4
1	F	192	PRO	3.0
1	E	119	THR	2.6
1	I	168	CYS	2.6
1	J	181	ILE	2.5
2	O	56	GLY	2.5
1	K	94	ALA	2.4
1	E	220	GLU	2.4
1	B	188	SER	2.4
1	H	126	GLU	2.2
1	I	164	LEU	2.2
2	X	57	VAL	2.1
1	H	168	CYS	2.1
1	I	166	GLY	2.1

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, 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	B-factors(Å^2)	Q<0.9
3	MG	H	302	1/1	0.77	0.28	41,41,41,41	0
3	MG	J	302	1/1	0.80	0.30	39,39,39,39	0
3	MG	I	301	1/1	0.81	0.16	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MG	F	302	1/1	0.82	0.55	41,41,41,41	0
3	MG	G	301	1/1	0.83	0.20	55,55,55,55	0
3	MG	C	301	1/1	0.86	0.26	58,58,58,58	0
3	MG	D	302	1/1	0.90	0.12	30,30,30,30	0
3	MG	B	301	1/1	0.90	0.25	50,50,50,50	0
3	MG	D	303	1/1	0.91	0.15	40,40,40,40	0
3	MG	G	303	1/1	0.91	0.73	52,52,52,52	0
3	MG	F	301	1/1	0.94	0.17	13,13,13,13	0
3	MG	L	302	1/1	0.94	0.17	26,26,26,26	0
3	MG	L	301	1/1	0.94	0.14	21,21,21,21	0
3	MG	F	303	1/1	0.95	0.17	32,32,32,32	0
3	MG	I	302	1/1	0.95	0.10	17,17,17,17	0
3	MG	F	304	1/1	0.95	0.11	29,29,29,29	0
3	MG	C	305	1/1	0.95	0.28	31,31,31,31	0
3	MG	P	101	1/1	0.95	0.21	30,30,30,30	0
3	MG	C	302	1/1	0.96	0.21	27,27,27,27	0
3	MG	J	301	1/1	0.97	0.09	20,20,20,20	0
3	MG	E	301	1/1	0.97	0.10	32,32,32,32	0
3	MG	D	301	1/1	0.97	0.13	16,16,16,16	0
3	MG	C	303	1/1	0.98	0.13	13,13,13,13	0
3	MG	C	304	1/1	0.98	0.17	36,36,36,36	0
3	MG	G	302	1/1	0.98	0.13	13,13,13,13	0
3	MG	H	301	1/1	0.98	0.08	18,18,18,18	0
3	MG	A	301	1/1	0.98	0.11	15,15,15,15	0
3	MG	K	301	1/1	0.98	0.17	14,14,14,14	0
3	MG	I	303	1/1	0.99	0.27	39,39,39,39	0
3	MG	E	302	1/1	0.99	0.14	21,21,21,21	0
3	MG	B	302	1/1	0.99	0.18	11,11,11,11	0

6.5 Other polymers (i)

There are no such residues in this entry.