



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 12:20 PM UTC

PDB ID : 5BWK / pdb_00005bwk
Title : 6.0 Å Crystal structure of a Get3-Get4-Get5 intermediate complex from *S.cerevisiae*
Authors : Gristick, H.B.; Chartron, J.W.; Clemons, W.M.
Deposited on : 2015-06-08
Resolution : 6.00 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

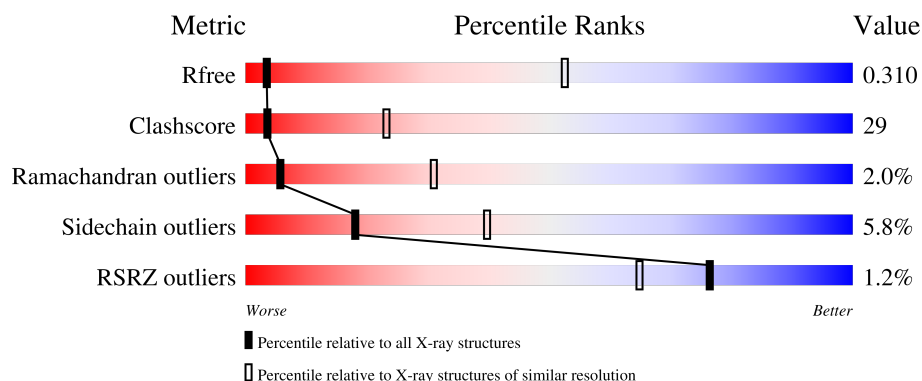
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 6.00 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}	180053	1143 (8.00-4.00)
Clashscore	190562	1210 (8.00-4.00)
Ramachandran outliers	187476	1034 (8.00-4.00)
Sidechain outliers	187428	1000 (8.00-4.00)
RSRZ outliers	180081	1136 (8.00-4.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	373	35% 39% 7% 18%
1	B	373	% 37% 38% 6% 18%
1	C	373	2% 36% 38% 8% 18%
1	D	373	% 37% 38% 6% 18%
1	M	373	% 36% 39% 6% 18%

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Mol	Chain	Length	Quality of chain
1	N	373	
1	O	373	
1	P	373	
2	E	319	
2	G	319	
2	I	319	
2	K	319	
2	Q	319	
2	S	319	
2	U	319	
2	W	319	
3	F	56	
3	H	56	
3	J	56	
3	L	56	
3	R	56	
3	T	56	
3	V	56	
3	X	56	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 41907 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 ATPase GET3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	304	Total	C	N	O	S	0	0	0
			2402	1522	399	464	17			
1	B	304	Total	C	N	O	S	0	0	0
			2402	1522	399	464	17			
1	D	304	Total	C	N	O	S	0	0	0
			2402	1522	399	464	17			
1	M	304	Total	C	N	O	S	0	0	0
			2402	1522	399	464	17			
1	N	304	Total	C	N	O	S	0	0	0
			2402	1522	399	464	17			
1	O	304	Total	C	N	O	S	0	0	0
			2402	1522	399	464	17			
1	P	304	Total	C	N	O	S	0	0	0
			2402	1522	399	464	17			
1	C	304	Total	C	N	O	S	0	0	0
			2402	1522	399	464	17			

There are 160 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	initiating methionine	UNP B3LGZ3
A	-17	GLY	-	expression tag	UNP B3LGZ3
A	-16	GLY	-	expression tag	UNP B3LGZ3
A	-15	SER	-	expression tag	UNP B3LGZ3
A	-14	HIS	-	expression tag	UNP B3LGZ3
A	-13	HIS	-	expression tag	UNP B3LGZ3
A	-12	HIS	-	expression tag	UNP B3LGZ3
A	-11	HIS	-	expression tag	UNP B3LGZ3
A	-10	HIS	-	expression tag	UNP B3LGZ3
A	-9	HIS	-	expression tag	UNP B3LGZ3
A	-8	GLY	-	expression tag	UNP B3LGZ3
A	-7	GLU	-	expression tag	UNP B3LGZ3
A	-6	ASN	-	expression tag	UNP B3LGZ3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	LEU	-	expression tag	UNP B3LGZ3
A	-4	TYR	-	expression tag	UNP B3LGZ3
A	-3	PHE	-	expression tag	UNP B3LGZ3
A	-2	GLN	-	expression tag	UNP B3LGZ3
A	-1	SER	-	expression tag	UNP B3LGZ3
A	0	VAL	-	expression tag	UNP B3LGZ3
A	1	ASP	-	expression tag	UNP B3LGZ3
B	-18	MET	-	initiating methionine	UNP B3LGZ3
B	-17	GLY	-	expression tag	UNP B3LGZ3
B	-16	GLY	-	expression tag	UNP B3LGZ3
B	-15	SER	-	expression tag	UNP B3LGZ3
B	-14	HIS	-	expression tag	UNP B3LGZ3
B	-13	HIS	-	expression tag	UNP B3LGZ3
B	-12	HIS	-	expression tag	UNP B3LGZ3
B	-11	HIS	-	expression tag	UNP B3LGZ3
B	-10	HIS	-	expression tag	UNP B3LGZ3
B	-9	HIS	-	expression tag	UNP B3LGZ3
B	-8	GLY	-	expression tag	UNP B3LGZ3
B	-7	GLU	-	expression tag	UNP B3LGZ3
B	-6	ASN	-	expression tag	UNP B3LGZ3
B	-5	LEU	-	expression tag	UNP B3LGZ3
B	-4	TYR	-	expression tag	UNP B3LGZ3
B	-3	PHE	-	expression tag	UNP B3LGZ3
B	-2	GLN	-	expression tag	UNP B3LGZ3
B	-1	SER	-	expression tag	UNP B3LGZ3
B	0	VAL	-	expression tag	UNP B3LGZ3
B	1	ASP	-	expression tag	UNP B3LGZ3
D	-18	MET	-	initiating methionine	UNP B3LGZ3
D	-17	GLY	-	expression tag	UNP B3LGZ3
D	-16	GLY	-	expression tag	UNP B3LGZ3
D	-15	SER	-	expression tag	UNP B3LGZ3
D	-14	HIS	-	expression tag	UNP B3LGZ3
D	-13	HIS	-	expression tag	UNP B3LGZ3
D	-12	HIS	-	expression tag	UNP B3LGZ3
D	-11	HIS	-	expression tag	UNP B3LGZ3
D	-10	HIS	-	expression tag	UNP B3LGZ3
D	-9	HIS	-	expression tag	UNP B3LGZ3
D	-8	GLY	-	expression tag	UNP B3LGZ3
D	-7	GLU	-	expression tag	UNP B3LGZ3
D	-6	ASN	-	expression tag	UNP B3LGZ3
D	-5	LEU	-	expression tag	UNP B3LGZ3
D	-4	TYR	-	expression tag	UNP B3LGZ3

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-3	PHE	-	expression tag	UNP B3LGZ3
D	-2	GLN	-	expression tag	UNP B3LGZ3
D	-1	SER	-	expression tag	UNP B3LGZ3
D	0	VAL	-	expression tag	UNP B3LGZ3
D	1	ASP	-	expression tag	UNP B3LGZ3
M	-18	MET	-	initiating methionine	UNP B3LGZ3
M	-17	GLY	-	expression tag	UNP B3LGZ3
M	-16	GLY	-	expression tag	UNP B3LGZ3
M	-15	SER	-	expression tag	UNP B3LGZ3
M	-14	HIS	-	expression tag	UNP B3LGZ3
M	-13	HIS	-	expression tag	UNP B3LGZ3
M	-12	HIS	-	expression tag	UNP B3LGZ3
M	-11	HIS	-	expression tag	UNP B3LGZ3
M	-10	HIS	-	expression tag	UNP B3LGZ3
M	-9	HIS	-	expression tag	UNP B3LGZ3
M	-8	GLY	-	expression tag	UNP B3LGZ3
M	-7	GLU	-	expression tag	UNP B3LGZ3
M	-6	ASN	-	expression tag	UNP B3LGZ3
M	-5	LEU	-	expression tag	UNP B3LGZ3
M	-4	TYR	-	expression tag	UNP B3LGZ3
M	-3	PHE	-	expression tag	UNP B3LGZ3
M	-2	GLN	-	expression tag	UNP B3LGZ3
M	-1	SER	-	expression tag	UNP B3LGZ3
M	0	VAL	-	expression tag	UNP B3LGZ3
M	1	ASP	-	expression tag	UNP B3LGZ3
N	-18	MET	-	initiating methionine	UNP B3LGZ3
N	-17	GLY	-	expression tag	UNP B3LGZ3
N	-16	GLY	-	expression tag	UNP B3LGZ3
N	-15	SER	-	expression tag	UNP B3LGZ3
N	-14	HIS	-	expression tag	UNP B3LGZ3
N	-13	HIS	-	expression tag	UNP B3LGZ3
N	-12	HIS	-	expression tag	UNP B3LGZ3
N	-11	HIS	-	expression tag	UNP B3LGZ3
N	-10	HIS	-	expression tag	UNP B3LGZ3
N	-9	HIS	-	expression tag	UNP B3LGZ3
N	-8	GLY	-	expression tag	UNP B3LGZ3
N	-7	GLU	-	expression tag	UNP B3LGZ3
N	-6	ASN	-	expression tag	UNP B3LGZ3
N	-5	LEU	-	expression tag	UNP B3LGZ3
N	-4	TYR	-	expression tag	UNP B3LGZ3
N	-3	PHE	-	expression tag	UNP B3LGZ3
N	-2	GLN	-	expression tag	UNP B3LGZ3

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Chain	Residue	Modelled	Actual	Comment	Reference
N	-1	SER	-	expression tag	UNP B3LGZ3
N	0	VAL	-	expression tag	UNP B3LGZ3
N	1	ASP	-	expression tag	UNP B3LGZ3
O	-18	MET	-	initiating methionine	UNP B3LGZ3
O	-17	GLY	-	expression tag	UNP B3LGZ3
O	-16	GLY	-	expression tag	UNP B3LGZ3
O	-15	SER	-	expression tag	UNP B3LGZ3
O	-14	HIS	-	expression tag	UNP B3LGZ3
O	-13	HIS	-	expression tag	UNP B3LGZ3
O	-12	HIS	-	expression tag	UNP B3LGZ3
O	-11	HIS	-	expression tag	UNP B3LGZ3
O	-10	HIS	-	expression tag	UNP B3LGZ3
O	-9	HIS	-	expression tag	UNP B3LGZ3
O	-8	GLY	-	expression tag	UNP B3LGZ3
O	-7	GLU	-	expression tag	UNP B3LGZ3
O	-6	ASN	-	expression tag	UNP B3LGZ3
O	-5	LEU	-	expression tag	UNP B3LGZ3
O	-4	TYR	-	expression tag	UNP B3LGZ3
O	-3	PHE	-	expression tag	UNP B3LGZ3
O	-2	GLN	-	expression tag	UNP B3LGZ3
O	-1	SER	-	expression tag	UNP B3LGZ3
O	0	VAL	-	expression tag	UNP B3LGZ3
O	1	ASP	-	expression tag	UNP B3LGZ3
P	-18	MET	-	initiating methionine	UNP B3LGZ3
P	-17	GLY	-	expression tag	UNP B3LGZ3
P	-16	GLY	-	expression tag	UNP B3LGZ3
P	-15	SER	-	expression tag	UNP B3LGZ3
P	-14	HIS	-	expression tag	UNP B3LGZ3
P	-13	HIS	-	expression tag	UNP B3LGZ3
P	-12	HIS	-	expression tag	UNP B3LGZ3
P	-11	HIS	-	expression tag	UNP B3LGZ3
P	-10	HIS	-	expression tag	UNP B3LGZ3
P	-9	HIS	-	expression tag	UNP B3LGZ3
P	-8	GLY	-	expression tag	UNP B3LGZ3
P	-7	GLU	-	expression tag	UNP B3LGZ3
P	-6	ASN	-	expression tag	UNP B3LGZ3
P	-5	LEU	-	expression tag	UNP B3LGZ3
P	-4	TYR	-	expression tag	UNP B3LGZ3
P	-3	PHE	-	expression tag	UNP B3LGZ3
P	-2	GLN	-	expression tag	UNP B3LGZ3
P	-1	SER	-	expression tag	UNP B3LGZ3
P	0	VAL	-	expression tag	UNP B3LGZ3

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Chain	Residue	Modelled	Actual	Comment	Reference
P	1	ASP	-	expression tag	UNP B3LGZ3
C	-18	MET	-	initiating methionine	UNP B3LGZ3
C	-17	GLY	-	expression tag	UNP B3LGZ3
C	-16	GLY	-	expression tag	UNP B3LGZ3
C	-15	SER	-	expression tag	UNP B3LGZ3
C	-14	HIS	-	expression tag	UNP B3LGZ3
C	-13	HIS	-	expression tag	UNP B3LGZ3
C	-12	HIS	-	expression tag	UNP B3LGZ3
C	-11	HIS	-	expression tag	UNP B3LGZ3
C	-10	HIS	-	expression tag	UNP B3LGZ3
C	-9	HIS	-	expression tag	UNP B3LGZ3
C	-8	GLY	-	expression tag	UNP B3LGZ3
C	-7	GLU	-	expression tag	UNP B3LGZ3
C	-6	ASN	-	expression tag	UNP B3LGZ3
C	-5	LEU	-	expression tag	UNP B3LGZ3
C	-4	TYR	-	expression tag	UNP B3LGZ3
C	-3	PHE	-	expression tag	UNP B3LGZ3
C	-2	GLN	-	expression tag	UNP B3LGZ3
C	-1	SER	-	expression tag	UNP B3LGZ3
C	0	VAL	-	expression tag	UNP B3LGZ3
C	1	ASP	-	expression tag	UNP B3LGZ3

- Molecule 2 is a protein called Golgi to ER traffic protein 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	291	Total	C	N	O	S	0	0	0
			2406	1567	380	453	6			
2	G	291	Total	C	N	O	S	0	0	0
			2406	1567	380	453	6			
2	I	291	Total	C	N	O	S	0	0	0
			2406	1567	380	453	6			
2	K	291	Total	C	N	O	S	0	0	0
			2406	1567	380	453	6			
2	Q	291	Total	C	N	O	S	0	0	0
			2406	1567	380	453	6			
2	S	291	Total	C	N	O	S	0	0	0
			2406	1567	380	453	6			
2	U	291	Total	C	N	O	S	0	0	0
			2406	1567	380	453	6			
2	W	291	Total	C	N	O	S	0	0	0
			2406	1567	380	453	6			

There are 160 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	9	MET	-	initiating methionine	UNP Q12125
E	10	GLY	-	expression tag	UNP Q12125
E	258	ALA	LYS	conflict	UNP Q12125
E	260	ALA	LYS	conflict	UNP Q12125
E	312	GLY	-	expression tag	UNP Q12125
E	313	GLU	-	expression tag	UNP Q12125
E	314	ASN	-	expression tag	UNP Q12125
E	315	LEU	-	expression tag	UNP Q12125
E	316	TYR	-	expression tag	UNP Q12125
E	317	PHE	-	expression tag	UNP Q12125
E	318	GLN	-	expression tag	UNP Q12125
E	319	SER	-	expression tag	UNP Q12125
E	320	LEU	-	expression tag	UNP Q12125
E	321	GLU	-	expression tag	UNP Q12125
E	322	HIS	-	expression tag	UNP Q12125
E	323	HIS	-	expression tag	UNP Q12125
E	324	HIS	-	expression tag	UNP Q12125
E	325	HIS	-	expression tag	UNP Q12125
E	326	HIS	-	expression tag	UNP Q12125
E	327	HIS	-	expression tag	UNP Q12125
G	9	MET	-	initiating methionine	UNP Q12125
G	10	GLY	-	expression tag	UNP Q12125
G	258	ALA	LYS	conflict	UNP Q12125
G	260	ALA	LYS	conflict	UNP Q12125
G	312	GLY	-	expression tag	UNP Q12125
G	313	GLU	-	expression tag	UNP Q12125
G	314	ASN	-	expression tag	UNP Q12125
G	315	LEU	-	expression tag	UNP Q12125
G	316	TYR	-	expression tag	UNP Q12125
G	317	PHE	-	expression tag	UNP Q12125
G	318	GLN	-	expression tag	UNP Q12125
G	319	SER	-	expression tag	UNP Q12125
G	320	LEU	-	expression tag	UNP Q12125
G	321	GLU	-	expression tag	UNP Q12125
G	322	HIS	-	expression tag	UNP Q12125
G	323	HIS	-	expression tag	UNP Q12125
G	324	HIS	-	expression tag	UNP Q12125
G	325	HIS	-	expression tag	UNP Q12125
G	326	HIS	-	expression tag	UNP Q12125
G	327	HIS	-	expression tag	UNP Q12125
I	9	MET	-	initiating methionine	UNP Q12125
I	10	GLY	-	expression tag	UNP Q12125
I	258	ALA	LYS	conflict	UNP Q12125

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Chain	Residue	Modelled	Actual	Comment	Reference
I	260	ALA	LYS	conflict	UNP Q12125
I	312	GLY	-	expression tag	UNP Q12125
I	313	GLU	-	expression tag	UNP Q12125
I	314	ASN	-	expression tag	UNP Q12125
I	315	LEU	-	expression tag	UNP Q12125
I	316	TYR	-	expression tag	UNP Q12125
I	317	PHE	-	expression tag	UNP Q12125
I	318	GLN	-	expression tag	UNP Q12125
I	319	SER	-	expression tag	UNP Q12125
I	320	LEU	-	expression tag	UNP Q12125
I	321	GLU	-	expression tag	UNP Q12125
I	322	HIS	-	expression tag	UNP Q12125
I	323	HIS	-	expression tag	UNP Q12125
I	324	HIS	-	expression tag	UNP Q12125
I	325	HIS	-	expression tag	UNP Q12125
I	326	HIS	-	expression tag	UNP Q12125
I	327	HIS	-	expression tag	UNP Q12125
K	9	MET	-	initiating methionine	UNP Q12125
K	10	GLY	-	expression tag	UNP Q12125
K	258	ALA	LYS	conflict	UNP Q12125
K	260	ALA	LYS	conflict	UNP Q12125
K	312	GLY	-	expression tag	UNP Q12125
K	313	GLU	-	expression tag	UNP Q12125
K	314	ASN	-	expression tag	UNP Q12125
K	315	LEU	-	expression tag	UNP Q12125
K	316	TYR	-	expression tag	UNP Q12125
K	317	PHE	-	expression tag	UNP Q12125
K	318	GLN	-	expression tag	UNP Q12125
K	319	SER	-	expression tag	UNP Q12125
K	320	LEU	-	expression tag	UNP Q12125
K	321	GLU	-	expression tag	UNP Q12125
K	322	HIS	-	expression tag	UNP Q12125
K	323	HIS	-	expression tag	UNP Q12125
K	324	HIS	-	expression tag	UNP Q12125
K	325	HIS	-	expression tag	UNP Q12125
K	326	HIS	-	expression tag	UNP Q12125
K	327	HIS	-	expression tag	UNP Q12125
Q	9	MET	-	initiating methionine	UNP Q12125
Q	10	GLY	-	expression tag	UNP Q12125
Q	258	ALA	LYS	conflict	UNP Q12125
Q	260	ALA	LYS	conflict	UNP Q12125
Q	312	GLY	-	expression tag	UNP Q12125

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	313	GLU	-	expression tag	UNP Q12125
Q	314	ASN	-	expression tag	UNP Q12125
Q	315	LEU	-	expression tag	UNP Q12125
Q	316	TYR	-	expression tag	UNP Q12125
Q	317	PHE	-	expression tag	UNP Q12125
Q	318	GLN	-	expression tag	UNP Q12125
Q	319	SER	-	expression tag	UNP Q12125
Q	320	LEU	-	expression tag	UNP Q12125
Q	321	GLU	-	expression tag	UNP Q12125
Q	322	HIS	-	expression tag	UNP Q12125
Q	323	HIS	-	expression tag	UNP Q12125
Q	324	HIS	-	expression tag	UNP Q12125
Q	325	HIS	-	expression tag	UNP Q12125
Q	326	HIS	-	expression tag	UNP Q12125
Q	327	HIS	-	expression tag	UNP Q12125
S	9	MET	-	initiating methionine	UNP Q12125
S	10	GLY	-	expression tag	UNP Q12125
S	258	ALA	LYS	conflict	UNP Q12125
S	260	ALA	LYS	conflict	UNP Q12125
S	312	GLY	-	expression tag	UNP Q12125
S	313	GLU	-	expression tag	UNP Q12125
S	314	ASN	-	expression tag	UNP Q12125
S	315	LEU	-	expression tag	UNP Q12125
S	316	TYR	-	expression tag	UNP Q12125
S	317	PHE	-	expression tag	UNP Q12125
S	318	GLN	-	expression tag	UNP Q12125
S	319	SER	-	expression tag	UNP Q12125
S	320	LEU	-	expression tag	UNP Q12125
S	321	GLU	-	expression tag	UNP Q12125
S	322	HIS	-	expression tag	UNP Q12125
S	323	HIS	-	expression tag	UNP Q12125
S	324	HIS	-	expression tag	UNP Q12125
S	325	HIS	-	expression tag	UNP Q12125
S	326	HIS	-	expression tag	UNP Q12125
S	327	HIS	-	expression tag	UNP Q12125
U	9	MET	-	initiating methionine	UNP Q12125
U	10	GLY	-	expression tag	UNP Q12125
U	258	ALA	LYS	conflict	UNP Q12125
U	260	ALA	LYS	conflict	UNP Q12125
U	312	GLY	-	expression tag	UNP Q12125
U	313	GLU	-	expression tag	UNP Q12125
U	314	ASN	-	expression tag	UNP Q12125

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Chain	Residue	Modelled	Actual	Comment	Reference
U	315	LEU	-	expression tag	UNP Q12125
U	316	TYR	-	expression tag	UNP Q12125
U	317	PHE	-	expression tag	UNP Q12125
U	318	GLN	-	expression tag	UNP Q12125
U	319	SER	-	expression tag	UNP Q12125
U	320	LEU	-	expression tag	UNP Q12125
U	321	GLU	-	expression tag	UNP Q12125
U	322	HIS	-	expression tag	UNP Q12125
U	323	HIS	-	expression tag	UNP Q12125
U	324	HIS	-	expression tag	UNP Q12125
U	325	HIS	-	expression tag	UNP Q12125
U	326	HIS	-	expression tag	UNP Q12125
U	327	HIS	-	expression tag	UNP Q12125
W	9	MET	-	initiating methionine	UNP Q12125
W	10	GLY	-	expression tag	UNP Q12125
W	258	ALA	LYS	conflict	UNP Q12125
W	260	ALA	LYS	conflict	UNP Q12125
W	312	GLY	-	expression tag	UNP Q12125
W	313	GLU	-	expression tag	UNP Q12125
W	314	ASN	-	expression tag	UNP Q12125
W	315	LEU	-	expression tag	UNP Q12125
W	316	TYR	-	expression tag	UNP Q12125
W	317	PHE	-	expression tag	UNP Q12125
W	318	GLN	-	expression tag	UNP Q12125
W	319	SER	-	expression tag	UNP Q12125
W	320	LEU	-	expression tag	UNP Q12125
W	321	GLU	-	expression tag	UNP Q12125
W	322	HIS	-	expression tag	UNP Q12125
W	323	HIS	-	expression tag	UNP Q12125
W	324	HIS	-	expression tag	UNP Q12125
W	325	HIS	-	expression tag	UNP Q12125
W	326	HIS	-	expression tag	UNP Q12125
W	327	HIS	-	expression tag	UNP Q12125

- Molecule 3 is a protein called Ubiquitin-like protein MDY2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	F	54	Total	C	N	O	0	0	0
			429	280	70	79			
3	H	54	Total	C	N	O	0	0	0
			430	280	70	80			
3	J	54	Total	C	N	O	0	0	0
			430	280	70	80			

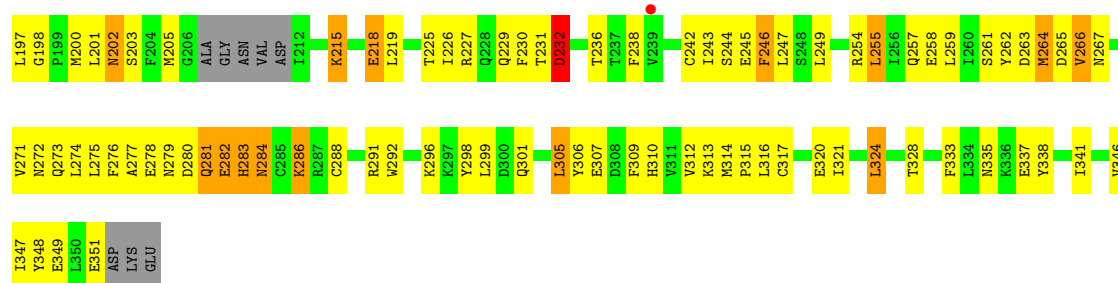
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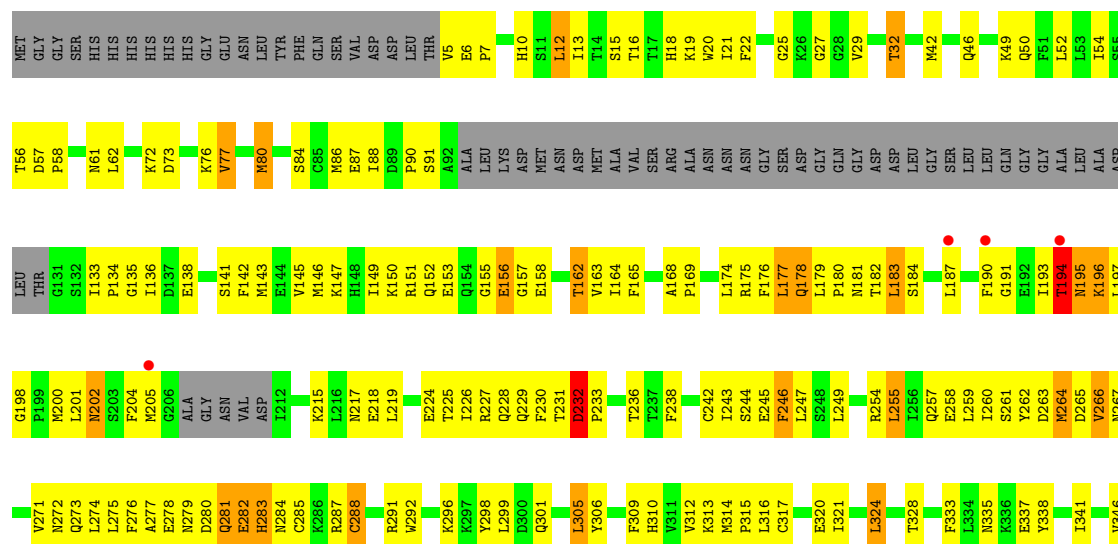
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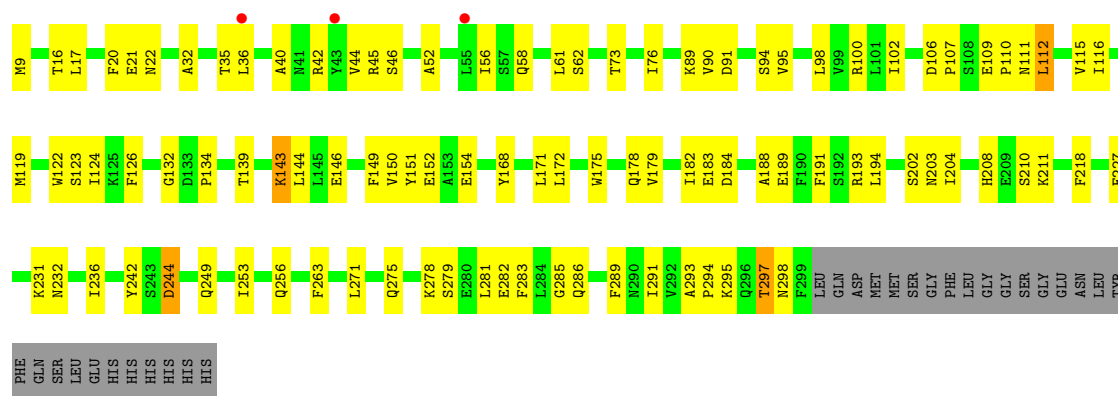
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	L	54	Total 430	C 280	N 70	O 80	0	0	0
3	R	54	Total 430	C 280	N 70	O 80	0	0	0
3	T	54	Total 430	C 280	N 70	O 80	0	0	0
3	V	54	Total 430	C 280	N 70	O 80	0	0	0
3	X	54	Total 430	C 280	N 70	O 80	0	0	0

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	Zn 1	0	0
4	D	1	Total 1	Zn 1	0	0
4	M	1	Total 1	Zn 1	0	0
4	O	1	Total 1	Zn 1	0	0

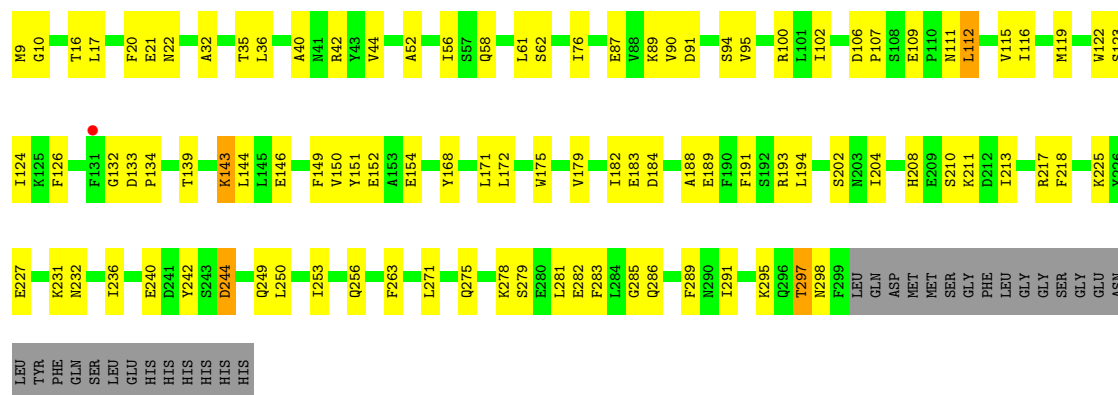






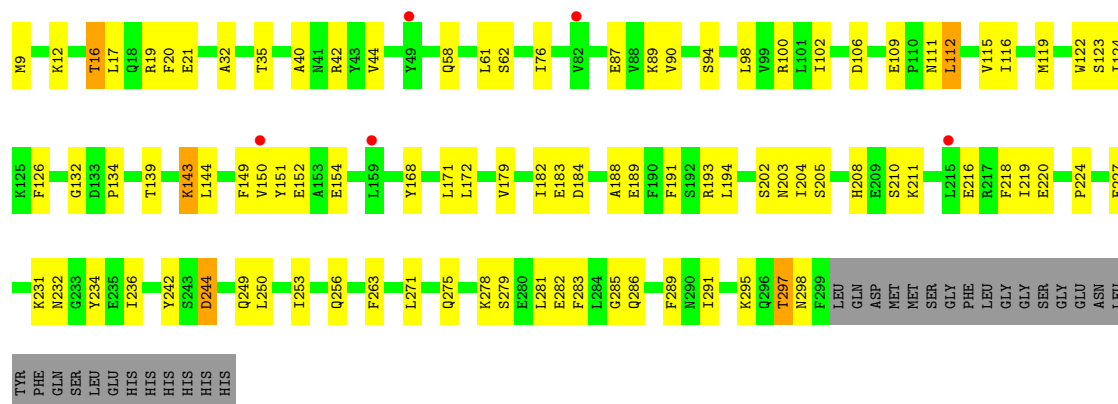
• Molecule 2: Golgi to ER traffic protein 4

Chain G: 60% 30% 9%



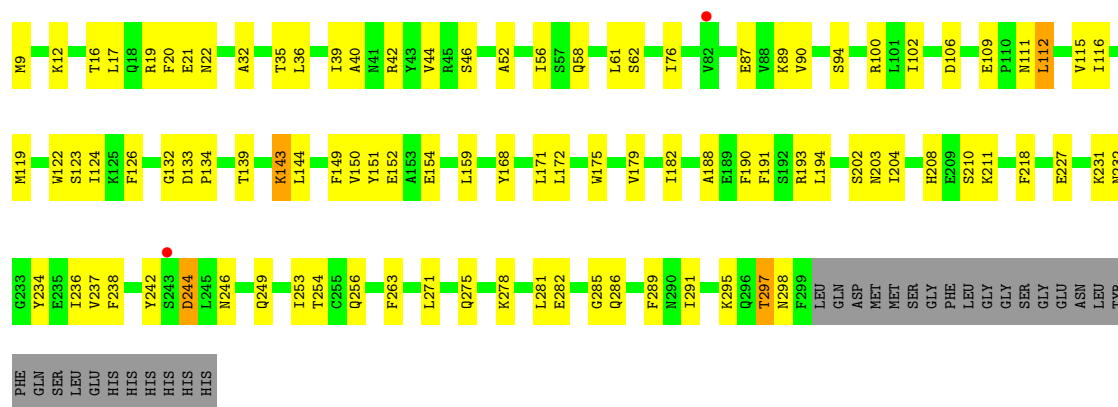
• Molecule 2: Golgi to ER traffic protein 4

Chain I: 2% 62% 28% 9%

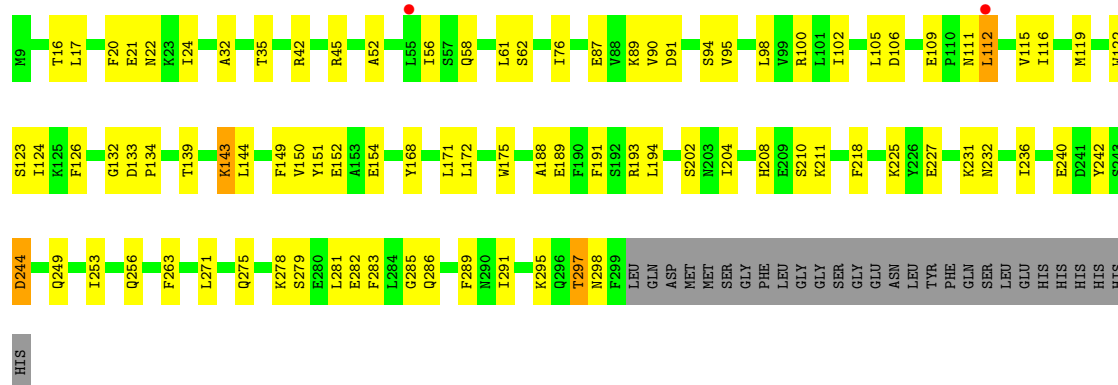


• Molecule 2: Golgi to ER traffic protein 4

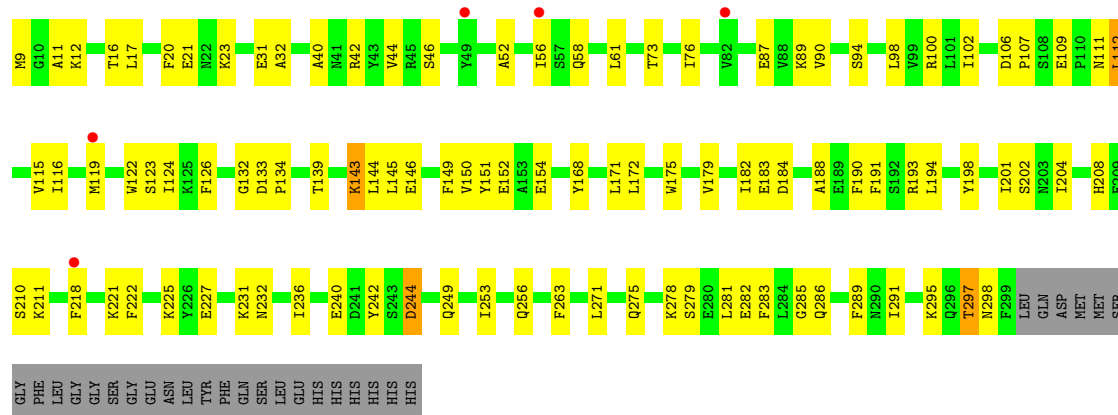
Chain K: 61% 29% 9%



• Molecule 2: Golgi to ER traffic protein 4

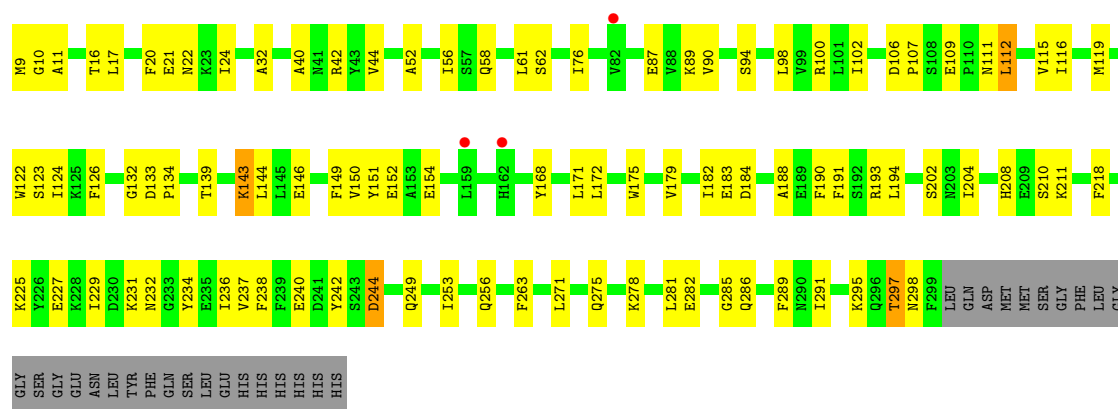


• Molecule 2: Golgi to ER traffic protein 4

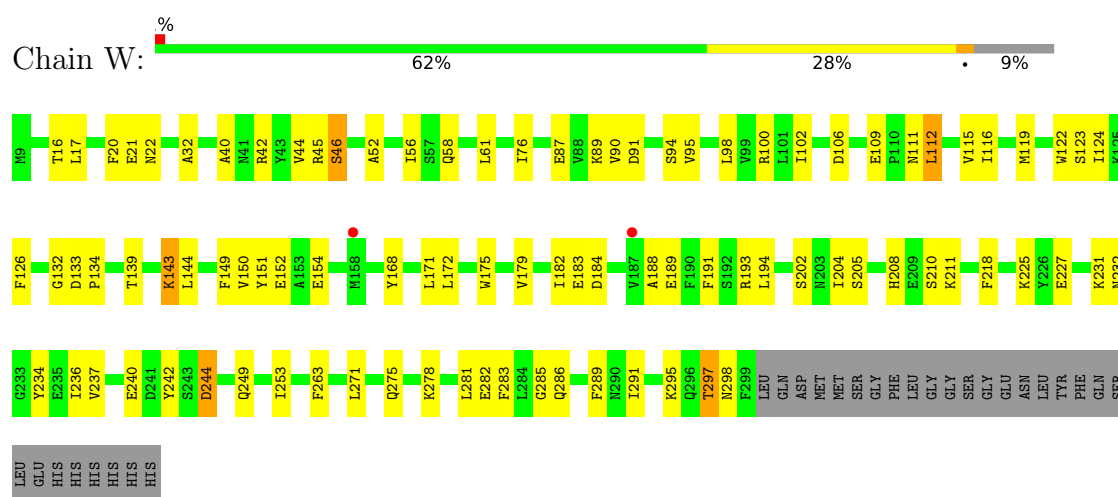


• Molecule 2: Golgi to ER traffic protein 4

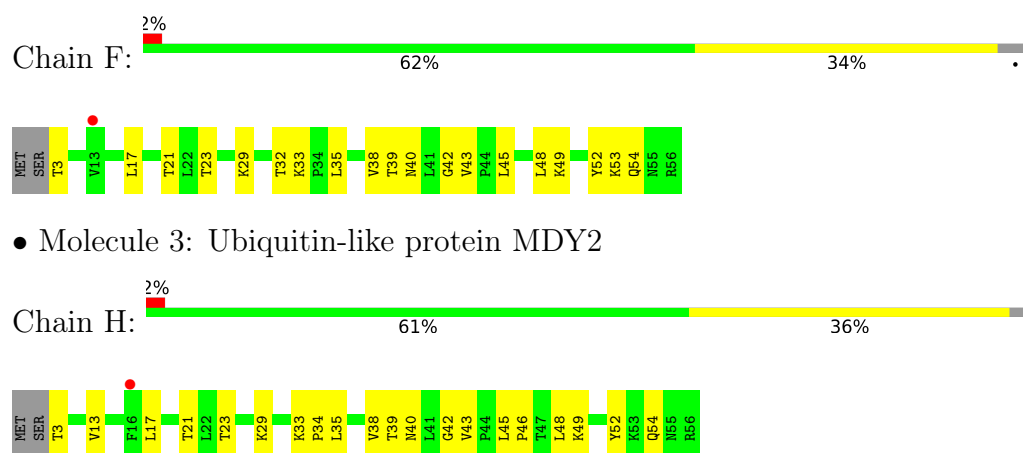




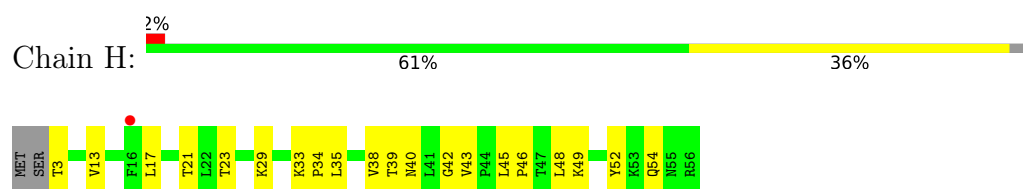
• Molecule 2: Golgi to ER traffic protein 4



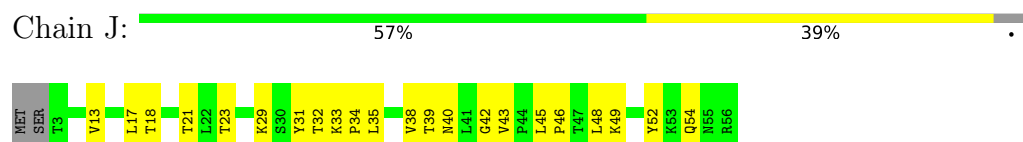
• Molecule 3: Ubiquitin-like protein MDY2



• Molecule 3: Ubiquitin-like protein MDY2

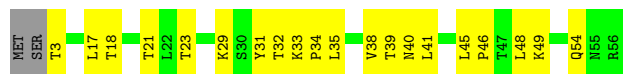


• Molecule 3: Ubiquitin-like protein MDY2



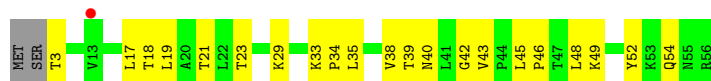
- Molecule 3: Ubiquitin-like protein MDY2

Chain L:  61% 36% .



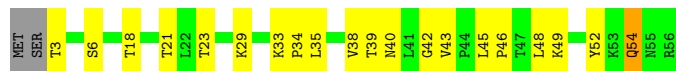
- Molecule 3: Ubiquitin-like protein MDY2

Chain R:  2% 59% 38% .



- Molecule 3: Ubiquitin-like protein MDY2

Chain T:  61% 34% . .



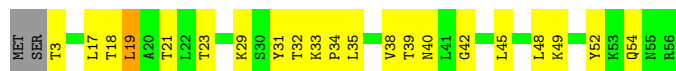
- Molecule 3: Ubiquitin-like protein MDY2

Chain V:  52% 45% .



- Molecule 3: Ubiquitin-like protein MDY2

Chain X:  59% 36% . .



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	152.43Å 127.33Å 210.26Å 90.00° 110.23° 90.00°	Depositor
Resolution (Å)	30.00 – 6.00 30.00 – 6.00	Depositor EDS
% Data completeness (in resolution range)	96.5 (30.00-6.00) 95.7 (30.00-6.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 6.07Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.274 , 0.302 0.277 , 0.310	Depositor DCC
R_{free} test set	917 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å ²)	359.5	Xtriage
Anisotropy	0.210	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 370.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.035 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	41907	wwPDB-VP
Average B, all atoms (Å ²)	361.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 20.29 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.9806e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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:
ZN

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	0.26	0/2444	0.78	1/3294 (0.0%)
1	B	0.27	0/2444	0.78	1/3294 (0.0%)
1	C	0.27	0/2444	0.79	1/3294 (0.0%)
1	D	0.27	0/2444	0.78	1/3294 (0.0%)
1	M	0.27	0/2444	0.78	1/3294 (0.0%)
1	N	0.27	0/2444	0.79	1/3294 (0.0%)
1	O	0.27	0/2444	0.79	1/3294 (0.0%)
1	P	0.27	0/2444	0.79	1/3294 (0.0%)
2	E	0.27	0/2465	0.72	1/3330 (0.0%)
2	G	0.27	0/2465	0.72	1/3330 (0.0%)
2	I	0.27	0/2465	0.71	0/3330
2	K	0.27	0/2465	0.71	1/3330 (0.0%)
2	Q	0.27	0/2465	0.72	1/3330 (0.0%)
2	S	0.27	0/2465	0.71	0/3330
2	U	0.27	0/2465	0.71	1/3330 (0.0%)
2	W	0.27	0/2465	0.71	1/3330 (0.0%)
3	F	0.29	0/440	0.70	0/597
3	H	0.29	0/441	0.72	0/597
3	J	0.29	0/441	0.72	0/597
3	L	0.29	0/441	0.72	0/597
3	R	0.30	0/441	0.72	0/597
3	T	0.30	0/441	0.72	0/597
3	V	0.30	0/441	0.71	0/597
3	X	0.30	0/441	0.72	0/597
All	All	0.27	0/42799	0.75	14/57768 (0.0%)

There are no bond length outliers.

The worst 5 of 14 bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	157	GLY	N-CA-C	-8.05	104.97	113.58
1	C	157	GLY	N-CA-C	-8.05	104.97	113.58
1	B	157	GLY	N-CA-C	-7.88	105.14	113.58
1	P	157	GLY	N-CA-C	-7.83	105.21	113.58
1	M	157	GLY	N-CA-C	-7.82	105.22	113.58

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	2402	0	2388	212	0
1	B	2402	0	2387	231	0
1	C	2402	0	2387	276	0
1	D	2402	0	2387	210	1
1	M	2402	0	2387	244	0
1	N	2402	0	2386	263	1
1	O	2402	0	2387	262	0
1	P	2402	0	2386	227	0
2	E	2406	0	2339	95	0
2	G	2406	0	2339	107	0
2	I	2406	0	2339	109	0
2	K	2406	0	2339	98	0
2	Q	2406	0	2339	88	0
2	S	2406	0	2339	97	0
2	U	2406	0	2339	104	0
2	W	2406	0	2339	92	0
3	F	429	0	452	30	0
3	H	430	0	452	26	0
3	J	430	0	452	34	0
3	L	430	0	452	28	0
3	R	430	0	452	26	0
3	T	430	0	452	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	V	430	0	452	38	0
3	X	430	0	452	30	0
4	A	1	0	0	0	0
4	D	1	0	0	0	0
4	M	1	0	0	0	0
4	O	1	0	0	0	0
All	All	41907	0	41423	2446	1

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 2446 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:B:143:MET:CE	1:C:201:LEU:HB3	1.70	1.20
1:N:147:LYS:HZ1	1:O:197:LEU:HD13	1.13	1.12
1:D:180:PRO:HG2	1:D:229:GLN:HE21	1.13	1.11
1:P:138:GLU:HG2	1:P:175:ARG:HB3	1.33	1.10
1:A:138:GLU:HG2	1:A:175:ARG:HB3	1.35	1.09

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:156:GLU:OE1	1:N:220:LYS:NZ[1_655]	2.19	0.01

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	298/373 (80%)	257 (86%)	29 (10%)	12 (4%)	2 18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	298/373 (80%)	257 (86%)	29 (10%)	12 (4%)	2	18
1	C	298/373 (80%)	257 (86%)	29 (10%)	12 (4%)	2	18
1	D	298/373 (80%)	257 (86%)	29 (10%)	12 (4%)	2	18
1	M	298/373 (80%)	257 (86%)	32 (11%)	9 (3%)	3	22
1	N	298/373 (80%)	257 (86%)	30 (10%)	11 (4%)	2	19
1	O	298/373 (80%)	260 (87%)	26 (9%)	12 (4%)	2	18
1	P	298/373 (80%)	257 (86%)	29 (10%)	12 (4%)	2	18
2	E	289/319 (91%)	269 (93%)	19 (7%)	1 (0%)	36	72
2	G	289/319 (91%)	270 (93%)	18 (6%)	1 (0%)	36	72
2	I	289/319 (91%)	269 (93%)	19 (7%)	1 (0%)	36	72
2	K	289/319 (91%)	269 (93%)	18 (6%)	2 (1%)	18	56
2	Q	289/319 (91%)	268 (93%)	20 (7%)	1 (0%)	36	72
2	S	289/319 (91%)	271 (94%)	17 (6%)	1 (0%)	36	72
2	U	289/319 (91%)	271 (94%)	16 (6%)	2 (1%)	18	56
2	W	289/319 (91%)	268 (93%)	19 (7%)	2 (1%)	18	56
3	F	52/56 (93%)	46 (88%)	6 (12%)	0	100	100
3	H	52/56 (93%)	46 (88%)	6 (12%)	0	100	100
3	J	52/56 (93%)	46 (88%)	6 (12%)	0	100	100
3	L	52/56 (93%)	46 (88%)	6 (12%)	0	100	100
3	R	52/56 (93%)	46 (88%)	6 (12%)	0	100	100
3	T	52/56 (93%)	46 (88%)	6 (12%)	0	100	100
3	V	52/56 (93%)	46 (88%)	6 (12%)	0	100	100
3	X	52/56 (93%)	46 (88%)	6 (12%)	0	100	100
All	All	5112/5984 (85%)	4582 (90%)	427 (8%)	103 (2%)	6	31

5 of 103 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	232	ASP
1	A	282	GLU
1	A	283	HIS
1	B	282	GLU
1	B	283	HIS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	272/325 (84%)	247 (91%)	25 (9%)	8	27
1	B	272/325 (84%)	245 (90%)	27 (10%)	7	24
1	C	272/325 (84%)	248 (91%)	24 (9%)	9	28
1	D	272/325 (84%)	250 (92%)	22 (8%)	11	31
1	M	272/325 (84%)	249 (92%)	23 (8%)	10	29
1	N	272/325 (84%)	247 (91%)	25 (9%)	8	27
1	O	272/325 (84%)	248 (91%)	24 (9%)	9	28
1	P	272/325 (84%)	247 (91%)	25 (9%)	8	27
2	E	260/284 (92%)	253 (97%)	7 (3%)	39	60
2	G	260/284 (92%)	254 (98%)	6 (2%)	44	64
2	I	260/284 (92%)	254 (98%)	6 (2%)	44	64
2	K	260/284 (92%)	254 (98%)	6 (2%)	44	64
2	Q	260/284 (92%)	253 (97%)	7 (3%)	39	60
2	S	260/284 (92%)	254 (98%)	6 (2%)	44	64
2	U	260/284 (92%)	253 (97%)	7 (3%)	39	60
2	W	260/284 (92%)	254 (98%)	6 (2%)	44	64
3	F	50/52 (96%)	47 (94%)	3 (6%)	17	39
3	H	50/52 (96%)	47 (94%)	3 (6%)	17	39
3	J	50/52 (96%)	48 (96%)	2 (4%)	28	49
3	L	50/52 (96%)	47 (94%)	3 (6%)	17	39
3	R	50/52 (96%)	47 (94%)	3 (6%)	17	39
3	T	50/52 (96%)	47 (94%)	3 (6%)	17	39
3	V	50/52 (96%)	47 (94%)	3 (6%)	17	39
3	X	50/52 (96%)	46 (92%)	4 (8%)	11	31
All	All	4656/5288 (88%)	4386 (94%)	270 (6%)	18	40

5 of 270 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	U	244	ASP
2	W	46	SER
1	C	264	MET
2	I	244	ASP
2	I	21	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 167 such sidechains are listed below:

Mol	Chain	Res	Type
1	O	335	ASN
2	U	275	GLN
1	P	46	GLN
1	P	301	GLN
1	C	46	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 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 ⓘ

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(Å ²)	Q<0.9
1	A	304/373 (81%)	-0.35	1 (0%) 90 82	355, 355, 355, 355	0
1	B	304/373 (81%)	-0.23	4 (1%) 75 63	362, 362, 362, 362	0
1	C	304/373 (81%)	-0.11	7 (2%) 61 52	364, 364, 364, 364	0
1	D	304/373 (81%)	-0.18	4 (1%) 75 63	347, 347, 347, 347	0
1	M	304/373 (81%)	-0.33	2 (0%) 84 73	357, 357, 357, 357	0
1	N	304/373 (81%)	-0.03	10 (3%) 49 44	350, 350, 350, 350	0
1	O	304/373 (81%)	-0.20	4 (1%) 75 63	355, 355, 355, 355	0
1	P	304/373 (81%)	-0.22	2 (0%) 84 73	353, 353, 353, 353	0
2	E	291/319 (91%)	-0.30	3 (1%) 79 68	294, 363, 363, 363	1 (0%)
2	G	291/319 (91%)	-0.33	1 (0%) 90 82	298, 367, 367, 367	1 (0%)
2	I	291/319 (91%)	-0.24	5 (1%) 69 58	287, 354, 354, 354	1 (0%)
2	K	291/319 (91%)	-0.32	2 (0%) 84 73	302, 372, 372, 372	1 (0%)
2	Q	291/319 (91%)	-0.22	2 (0%) 84 73	291, 359, 359, 359	1 (0%)
2	S	291/319 (91%)	-0.25	5 (1%) 69 58	295, 364, 364, 364	1 (0%)
2	U	291/319 (91%)	-0.29	3 (1%) 79 68	298, 368, 368, 368	1 (0%)
2	W	291/319 (91%)	-0.27	2 (0%) 84 73	303, 374, 374, 374	1 (0%)
3	F	54/56 (96%)	-0.40	1 (1%) 66 56	373, 373, 373, 373	0
3	H	54/56 (96%)	-0.34	1 (1%) 66 56	379, 379, 379, 379	0
3	J	54/56 (96%)	-0.38	0 100 100	370, 370, 370, 370	0
3	L	54/56 (96%)	-0.33	0 100 100	386, 386, 386, 386	0
3	R	54/56 (96%)	-0.34	1 (1%) 66 56	371, 371, 371, 371	0
3	T	54/56 (96%)	-0.16	0 100 100	380, 380, 380, 380	0
3	V	54/56 (96%)	-0.50	0 100 100	384, 384, 384, 384	0
3	X	54/56 (96%)	-0.33	0 100 100	386, 386, 386, 386	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	5192/5984 (86%)	-0.25	60 (1%) 76 65	287, 362, 379, 386	8 (0%)

The worst 5 of 60 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	N	225	THR	5.2
1	N	228	GLN	5.0
2	S	82	VAL	4.3
2	W	187	VAL	4.1
1	N	194	THR	4.1

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 oligosaccharides 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
4	ZN	A	500	1/1	0.94	0.15	354,354,354,354	0
4	ZN	D	501	1/1	0.94	0.08	363,363,363,363	0
4	ZN	O	401	1/1	0.96	0.07	354,354,354,354	0
4	ZN	M	401	1/1	0.99	0.03	356,356,356,356	0

6.5 Other polymers [i](#)

There are no such residues in this entry.