wwPDB X-ray Structure Validation Summary Report (i)

Feb 19, 2016 – 10:05 PM GMT

PDB ID	:	5BWK
Title	:	6.0 A 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

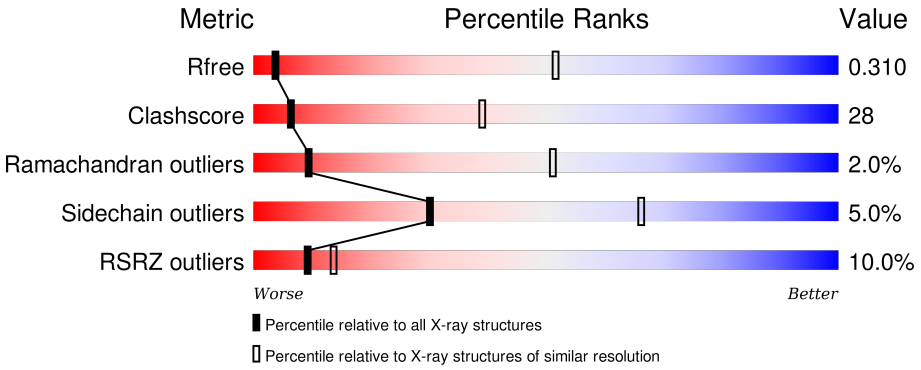
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance (i)

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}	91344	1002 (8.30-3.66)
Clashscore	102246	1050 (8.30-3.70)
Ramachandran outliers	100387	1023 (8.30-3.66)
Sidechain outliers	100360	1012 (8.30-3.64)
RSRZ outliers	91569	1001 (8.30-3.66)

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	373	9% 36% 40% 6% 18%
1	B	373	11% 39% 38% 5% 18%
1	C	373	11% 37% 39% 6% 18%
1	D	373	10% 39% 38% 5% 18%
1	M	373	8% 39% 36% 6% 18%

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Mol	Chain	Length	Quality of chain
1	N	373	8% 39% 36% 6% 18%
1	O	373	9% 37% 40% 5% 18%
1	P	373	7% 40% 36% 5% 18%
2	E	319	8% 61% 29% 9%
2	G	319	6% 61% 29% 9%
2	I	319	5% 62% 28% 9%
2	K	319	9% 62% 28% 9%
2	Q	319	8% 64% 26% 9%
2	S	319	8% 60% 30% 9%
2	U	319	6% 61% 29% 9%
2	W	319	8% 62% 28% 9%
3	F	56	16% 64% 32%
3	H	56	9% 63% 34%
3	J	56	9% 59% 38%
3	L	56	21% 63% 34%
3	R	56	13% 61% 36%
3	T	56	13% 63% 32%
3	V	56	14% 54% 43%
3	X	56	14% 61% 36%

2 Entry composition (i)

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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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 (three-letter code: ZN) (formula: Zn).

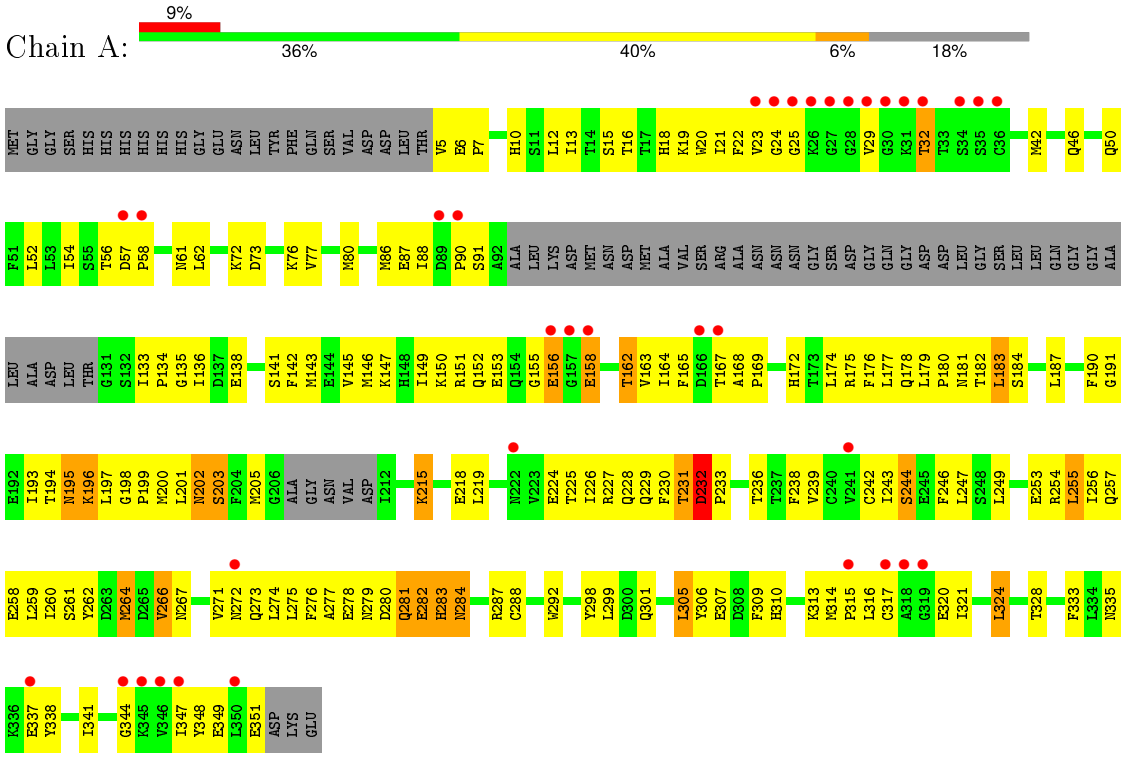
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	O	1	Total 1	Zn 1	0	0
4	A	1	Total 1	Zn 1	0	0
4	D	1	Total 1	Zn 1	0	0
4	M	1	Total 1	Zn 1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

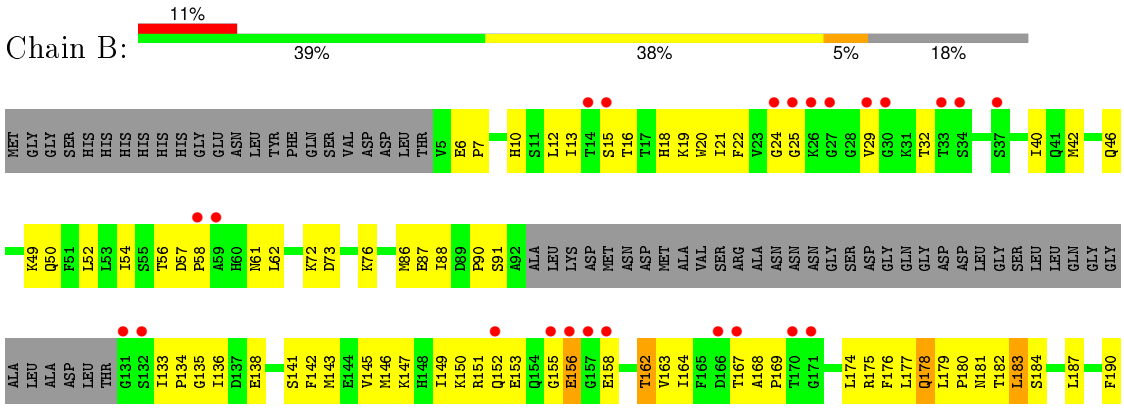
- Molecule 1: ATPase GET3

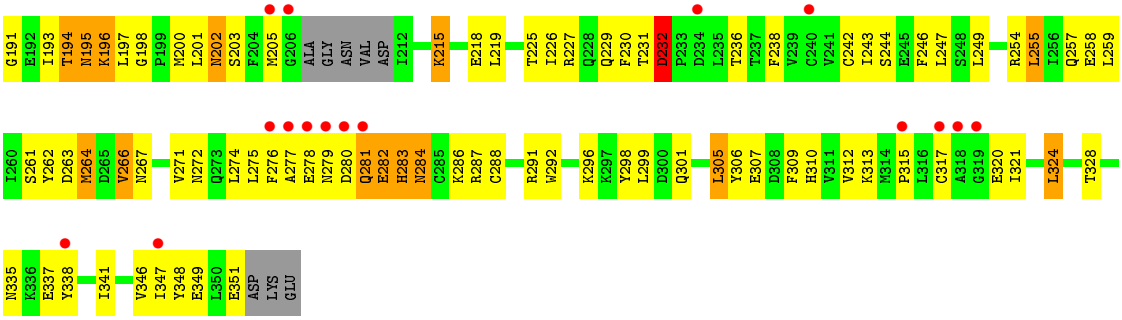
Chain A:



- Molecule 1: ATPase GET3

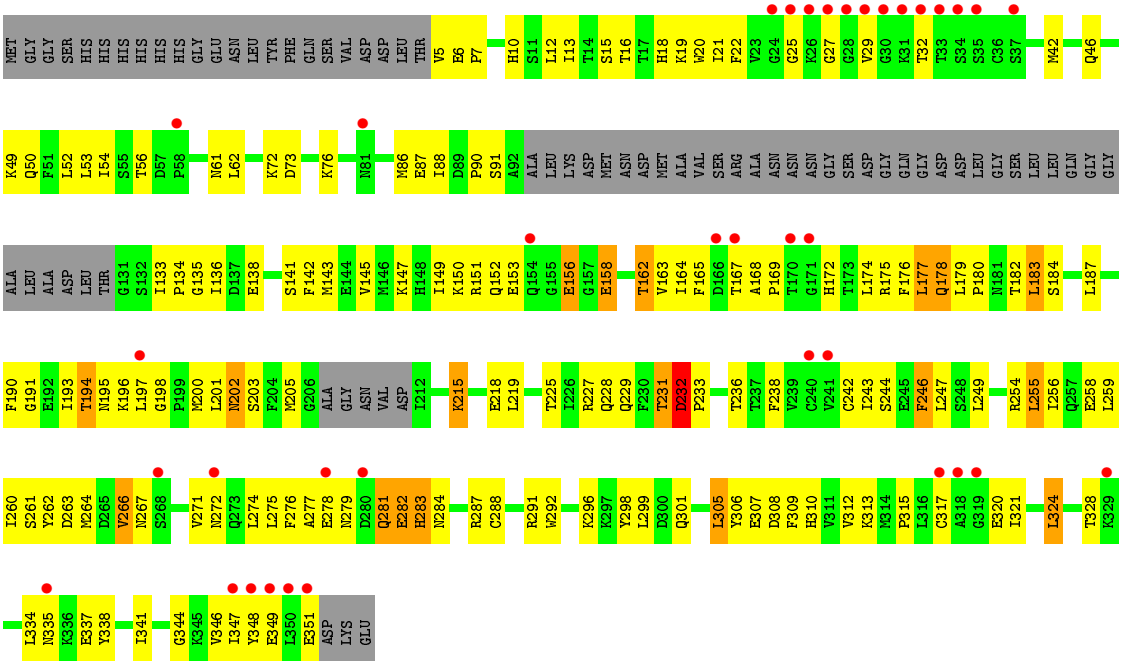
Chain B:





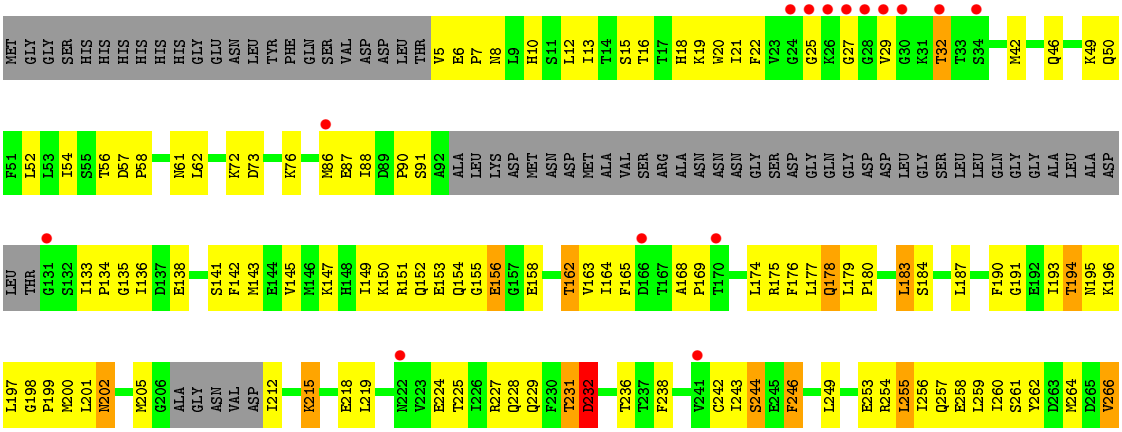
• Molecule 1: ATPase GET3

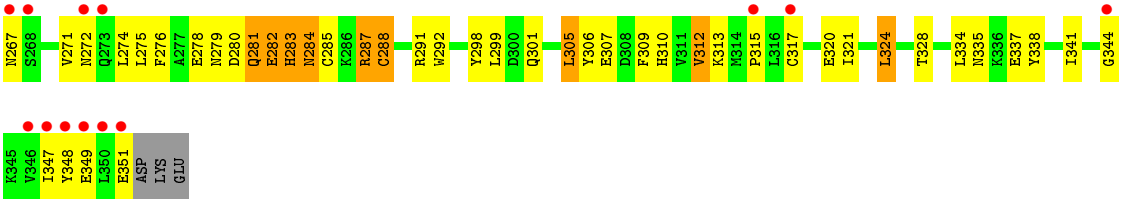
Chain D:



• Molecule 1: ATPase GET3

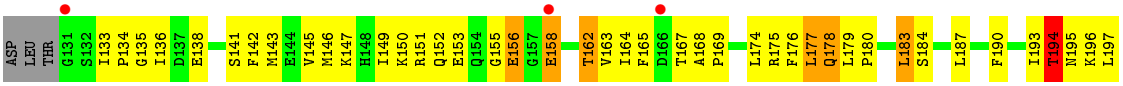
Chain M:

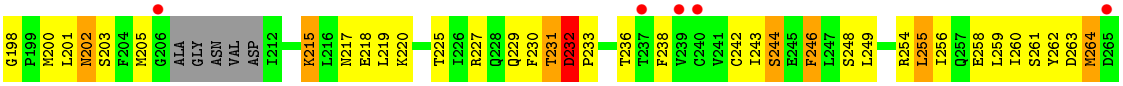


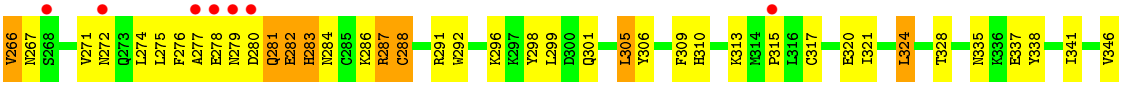


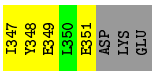
• Molecule 1: ATPase GET3

Chain N:



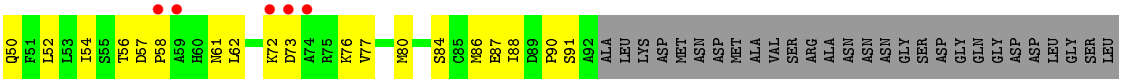


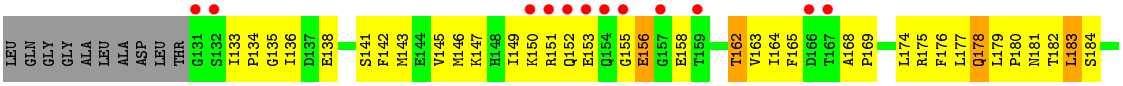


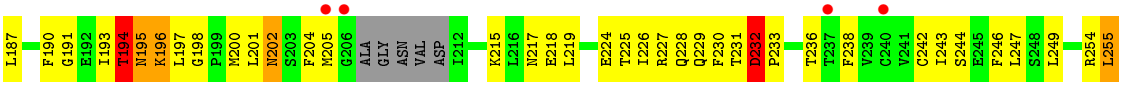


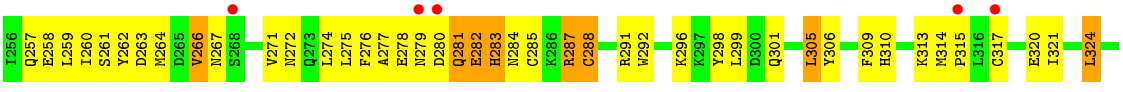
• Molecule 1: ATPase GET3

Chain O:



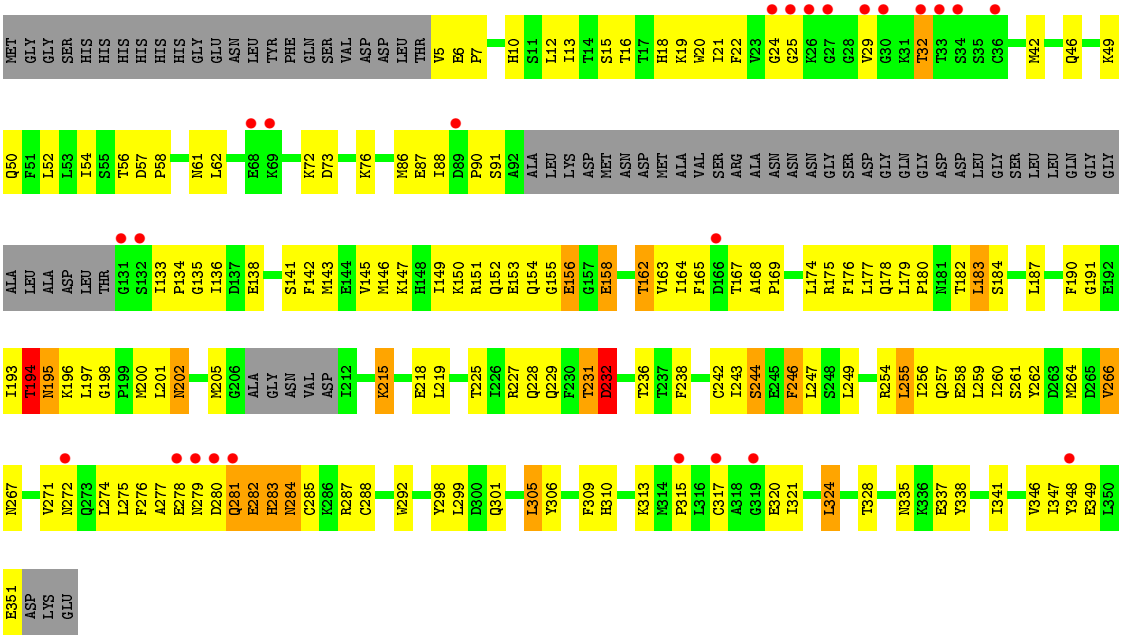






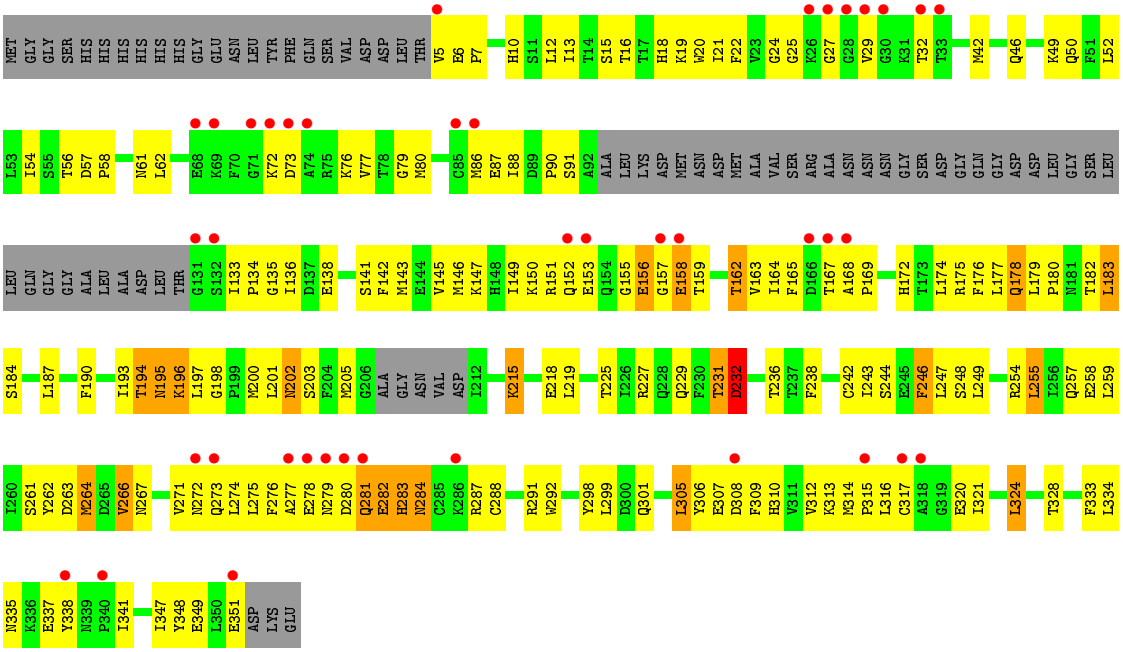
- Molecule 1: ATPase GET3

Chain P:



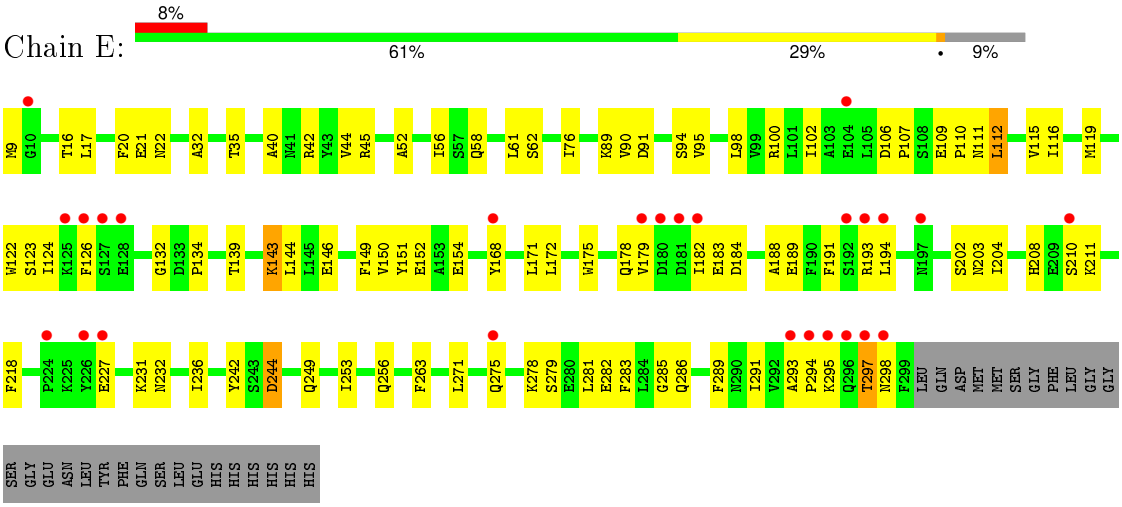
- Molecule 1: ATPase GET3

Chain C:



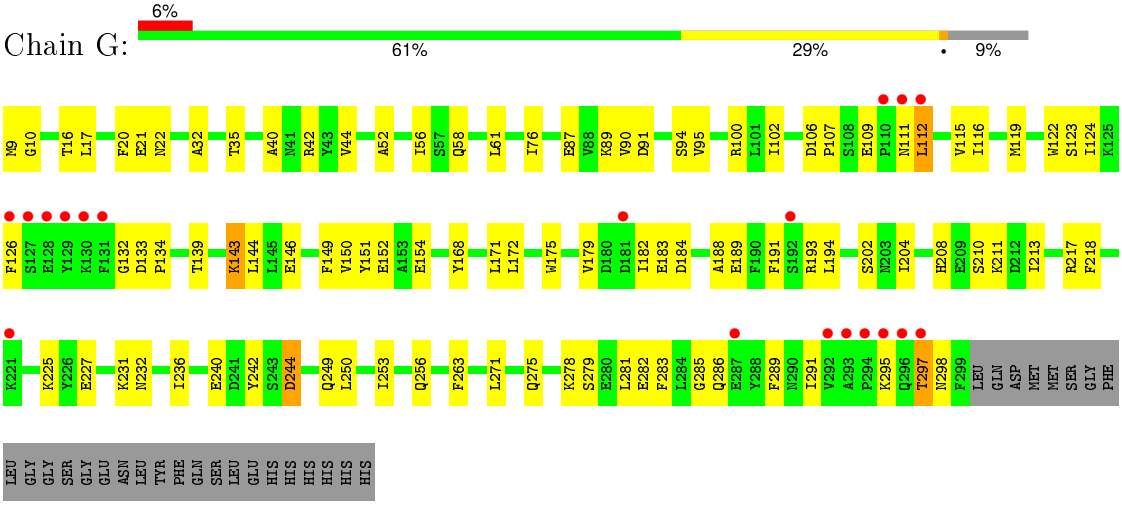
- Molecule 2: Golgi to ER traffic protein 4

Chain E:



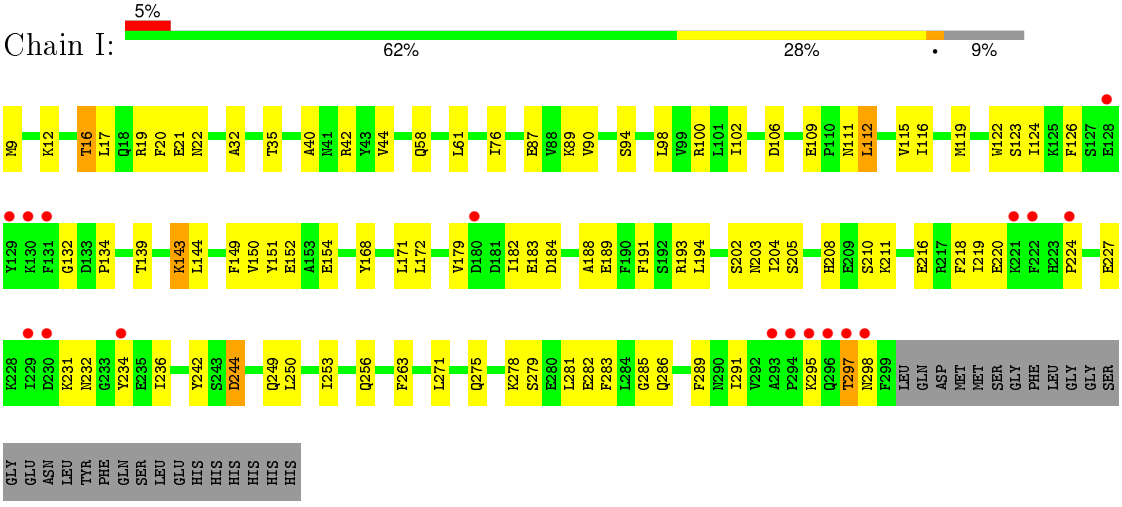
• Molecule 2: Golgi to ER traffic protein 4

Chain G:



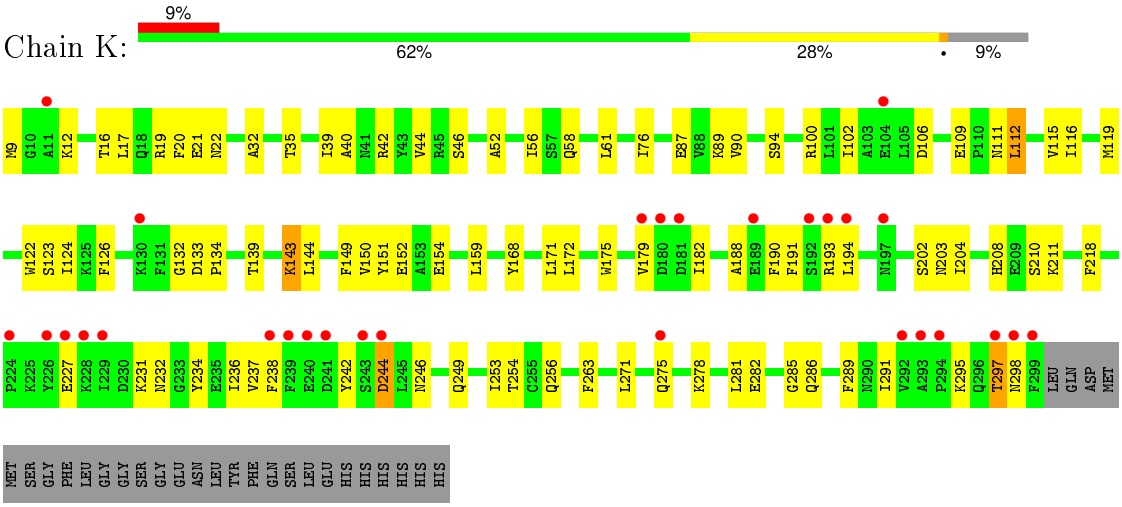
• Molecule 2: Golgi to ER traffic protein 4

Chain I:



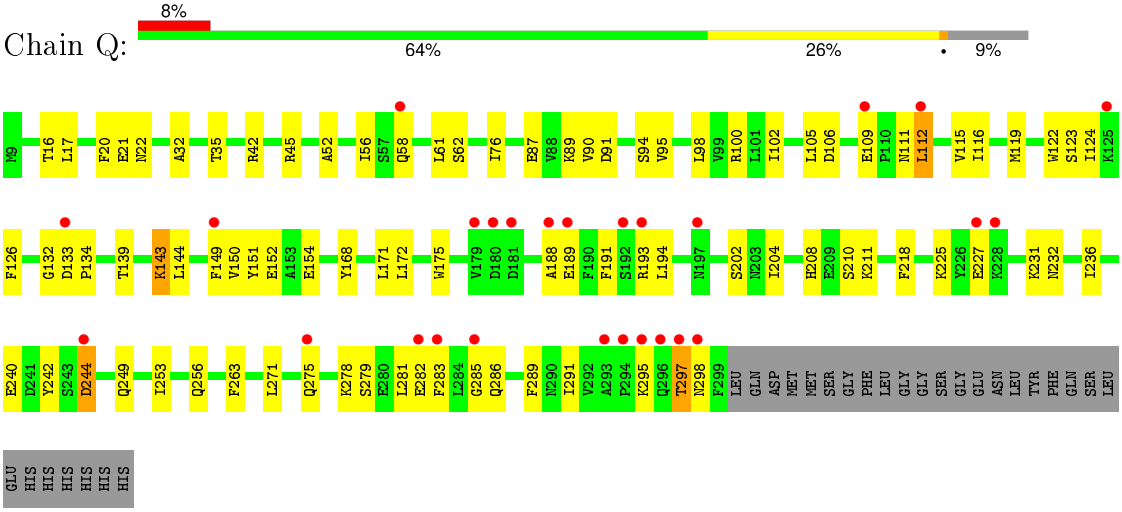
• Molecule 2: Golgi to ER traffic protein 4

Chain K:



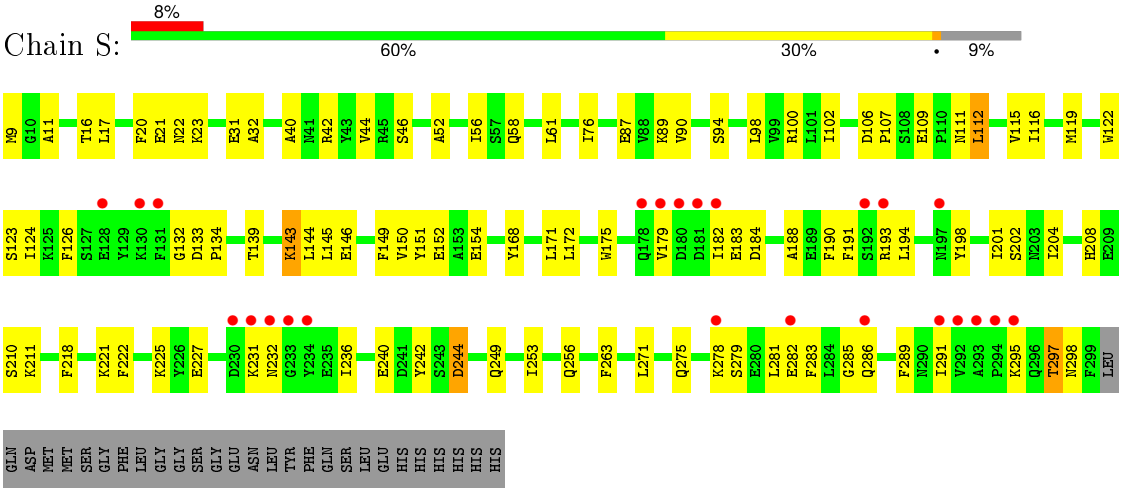
• Molecule 2: Golgi to ER traffic protein 4

Chain Q:



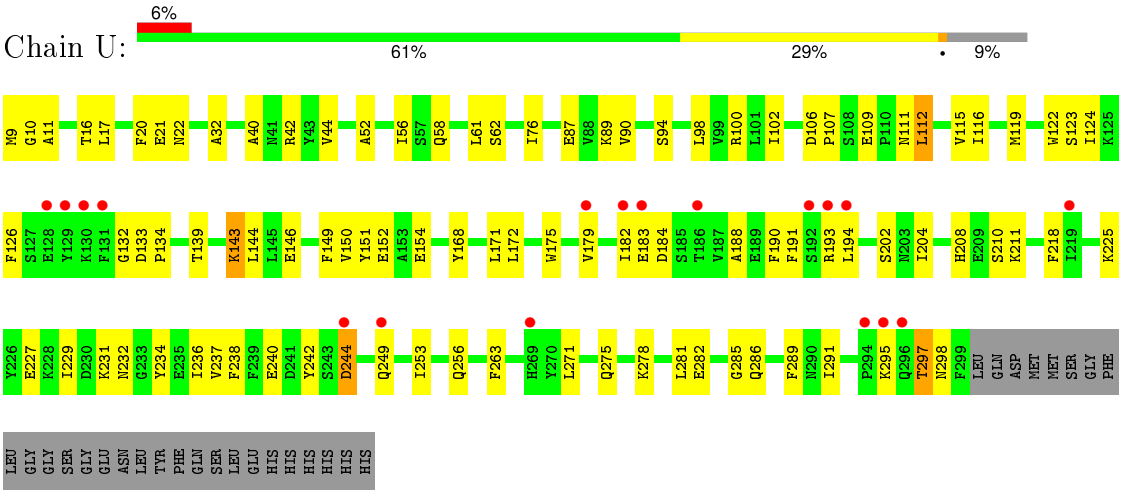
• Molecule 2: Golgi to ER traffic protein 4

Chain S:



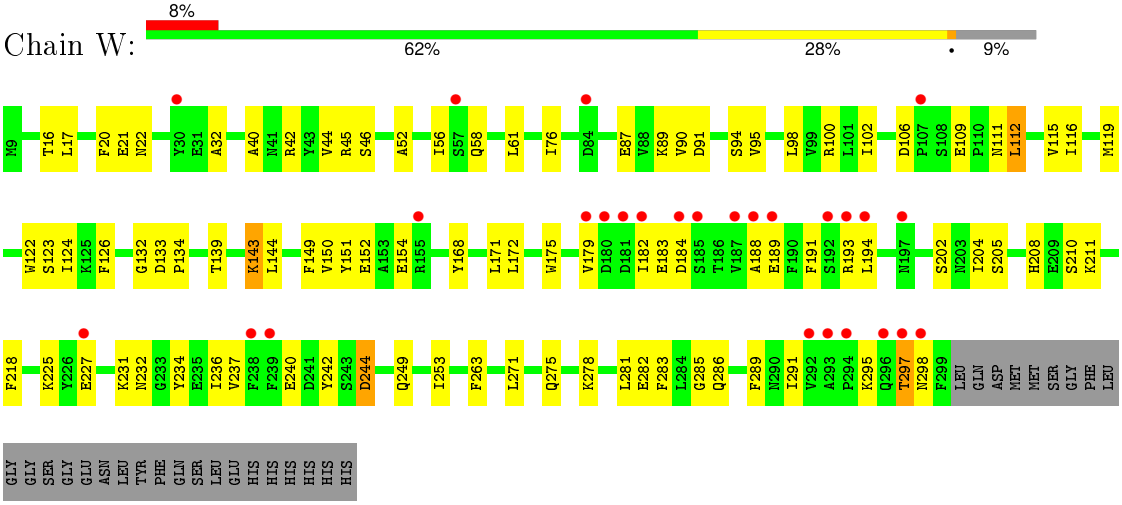
• Molecule 2: Golgi to ER traffic protein 4

Chain U:



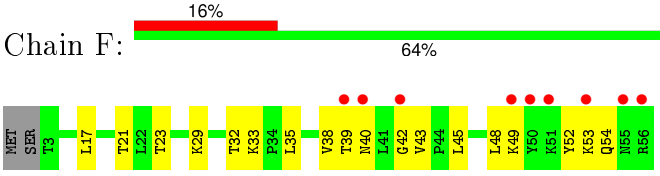
• Molecule 2: Golgi to ER traffic protein 4

Chain W:



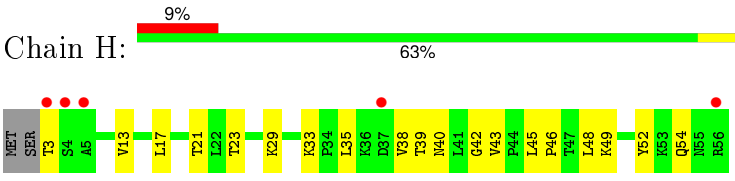
• Molecule 3: Ubiquitin-like protein MDY2

Chain F:



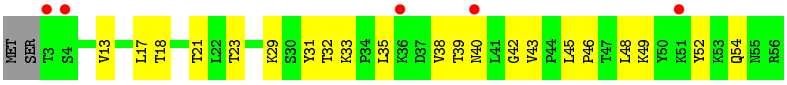
• Molecule 3: Ubiquitin-like protein MDY2

Chain H:



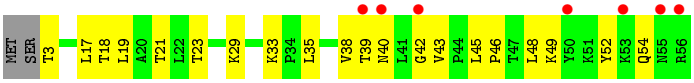
• Molecule 3: Ubiquitin-like protein MDY2

Chain J:

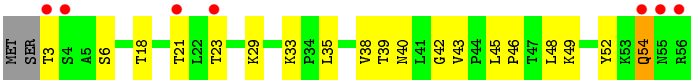


• Molecule 3: Ubiquitin-like protein MDY2

• Molecule 3: Ubiquitin-like protein MDY2



• Molecule 3: Ubiquitin-like protein MDY2



• Molecule 3: Ubiquitin-like protein MDY2

• Molecule 3: Ubiquitin-like protein MDY2

4 Data and refinement statistics (i)

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 29.99 – 6.00	Depositor EDS
% Data completeness (in resolution range)	96.5 (30.00-6.00) 96.5 (29.99-6.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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	No test flags present.	DCC
Wilson B-factor (Å^2)	359.5	Xtriage
Anisotropy	0.210	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.23 , 262.4	EDS
Estimated twinning fraction	0.035 for h,-k,-h-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.26$	Xtriage
Outliers	0 of 18379 reflections	Xtriage
F_o,F_c correlation	0.85	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.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.47	0/3294
1	B	0.26	0/2444	0.47	0/3294
1	C	0.26	0/2444	0.47	0/3294
1	D	0.26	0/2444	0.47	0/3294
1	M	0.26	0/2444	0.47	0/3294
1	N	0.26	0/2444	0.47	0/3294
1	O	0.26	0/2444	0.47	0/3294
1	P	0.26	0/2444	0.47	0/3294
2	E	0.27	0/2465	0.41	0/3330
2	G	0.27	0/2465	0.41	0/3330
2	I	0.27	0/2465	0.41	0/3330
2	K	0.27	0/2465	0.41	0/3330
2	Q	0.27	0/2465	0.41	0/3330
2	S	0.27	0/2465	0.41	0/3330
2	U	0.27	0/2465	0.41	0/3330
2	W	0.27	0/2465	0.41	0/3330
3	F	0.26	0/440	0.44	0/597
3	H	0.26	0/441	0.44	0/597
3	J	0.26	0/441	0.45	0/597
3	L	0.26	0/441	0.44	0/597
3	R	0.26	0/441	0.44	0/597
3	T	0.26	0/441	0.44	0/597
3	V	0.26	0/441	0.44	0/597
3	X	0.26	0/441	0.44	0/597
All	All	0.27	0/42799	0.44	0/57768

There are no bond length outliers.

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	2402	0	2388	195	0
1	B	2402	0	2387	214	0
1	C	2402	0	2387	263	0
1	D	2402	0	2387	194	1
1	M	2402	0	2387	226	0
1	N	2402	0	2386	246	1
1	O	2402	0	2387	246	0
1	P	2402	0	2386	213	0
2	E	2406	0	2339	93	0
2	G	2406	0	2339	104	0
2	I	2406	0	2339	107	0
2	K	2406	0	2339	97	0
2	Q	2406	0	2339	87	0
2	S	2406	0	2339	94	0
2	U	2406	0	2339	103	0
2	W	2406	0	2339	92	0
3	F	429	0	452	30	0
3	H	430	0	452	25	0
3	J	430	0	452	33	0
3	L	430	0	452	27	0
3	R	430	0	452	25	0
3	T	430	0	452	25	0
3	V	430	0	452	37	0
3	X	430	0	452	28	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	2311	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 28.

The worst 5 of 2311 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: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
1:M:138:GLU:HG2	1:M: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%)	4 35
1	B	298/373 (80%)	257 (86%)	29 (10%)	12 (4%)	4 35
1	C	298/373 (80%)	257 (86%)	29 (10%)	12 (4%)	4 35
1	D	298/373 (80%)	257 (86%)	29 (10%)	12 (4%)	4 35
1	M	298/373 (80%)	257 (86%)	32 (11%)	9 (3%)	5 42
1	N	298/373 (80%)	257 (86%)	30 (10%)	11 (4%)	4 37
1	O	298/373 (80%)	260 (87%)	26 (9%)	12 (4%)	4 35
1	P	298/373 (80%)	257 (86%)	29 (10%)	12 (4%)	4 35
2	E	289/319 (91%)	269 (93%)	19 (7%)	1 (0%)	46 83
2	G	289/319 (91%)	270 (93%)	18 (6%)	1 (0%)	46 83
2	I	289/319 (91%)	269 (93%)	19 (7%)	1 (0%)	46 83
2	K	289/319 (91%)	269 (93%)	18 (6%)	2 (1%)	26 71
2	Q	289/319 (91%)	268 (93%)	20 (7%)	1 (0%)	46 83

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	S	289/319 (91%)	271 (94%)	17 (6%)	1 (0%)	46 83
2	U	289/319 (91%)	271 (94%)	16 (6%)	2 (1%)	26 71
2	W	289/319 (91%)	268 (93%)	19 (7%)	2 (1%)	26 71
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%)	9 51

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 (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	272/325 (84%)	252 (93%)	20 (7%)	17 54
1	B	272/325 (84%)	251 (92%)	21 (8%)	16 53
1	C	272/325 (84%)	251 (92%)	21 (8%)	16 53
1	D	272/325 (84%)	252 (93%)	20 (7%)	17 54
1	M	272/325 (84%)	252 (93%)	20 (7%)	17 54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	N	272/325 (84%)	251 (92%)	21 (8%)	16 53
1	O	272/325 (84%)	252 (93%)	20 (7%)	17 54
1	P	272/325 (84%)	253 (93%)	19 (7%)	19 56
2	E	260/284 (92%)	253 (97%)	7 (3%)	52 79
2	G	260/284 (92%)	254 (98%)	6 (2%)	58 83
2	I	260/284 (92%)	254 (98%)	6 (2%)	58 83
2	K	260/284 (92%)	254 (98%)	6 (2%)	58 83
2	Q	260/284 (92%)	253 (97%)	7 (3%)	52 79
2	S	260/284 (92%)	254 (98%)	6 (2%)	58 83
2	U	260/284 (92%)	253 (97%)	7 (3%)	52 79
2	W	260/284 (92%)	254 (98%)	6 (2%)	58 83
3	F	50/52 (96%)	48 (96%)	2 (4%)	38 71
3	H	50/52 (96%)	47 (94%)	3 (6%)	24 61
3	J	50/52 (96%)	48 (96%)	2 (4%)	38 71
3	L	50/52 (96%)	47 (94%)	3 (6%)	24 61
3	R	50/52 (96%)	47 (94%)	3 (6%)	24 61
3	T	50/52 (96%)	47 (94%)	3 (6%)	24 61
3	V	50/52 (96%)	47 (94%)	3 (6%)	24 61
3	X	50/52 (96%)	47 (94%)	3 (6%)	24 61
All	All	4656/5288 (88%)	4421 (95%)	235 (5%)	30 66

5 of 235 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	266	VAL
1	N	287	ARG
1	C	194	THR
1	M	287	ARG
1	N	178	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 161 such sidechains are listed below:

Mol	Chain	Res	Type
1	M	229	GLN

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Mol	Chain	Res	Type
1	N	281	GLN
1	C	82	ASN
1	M	284	ASN
1	N	18	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	304/373 (81%)	0.39	35 (11%) 6 11	355, 355, 355, 355	0
1	B	304/373 (81%)	0.61	40 (13%) 4 10	362, 362, 362, 362	0
1	C	304/373 (81%)	0.48	40 (13%) 4 10	364, 364, 364, 364	0
1	D	304/373 (81%)	0.57	37 (12%) 5 11	347, 347, 347, 347	0
1	M	304/373 (81%)	0.34	28 (9%) 11 15	357, 357, 357, 357	0
1	N	304/373 (81%)	0.50	31 (10%) 9 13	350, 350, 350, 350	0
1	O	304/373 (81%)	0.47	35 (11%) 6 11	355, 355, 355, 355	0
1	P	304/373 (81%)	0.42	25 (8%) 14 18	353, 353, 353, 353	0
2	E	291/319 (91%)	0.58	26 (8%) 12 16	294, 363, 363, 363	1 (0%)
2	G	291/319 (91%)	0.38	19 (6%) 22 23	298, 367, 367, 367	1 (0%)
2	I	291/319 (91%)	0.30	17 (5%) 26 27	287, 354, 354, 354	1 (0%)
2	K	291/319 (91%)	0.58	29 (9%) 9 14	302, 372, 372, 372	1 (0%)
2	Q	291/319 (91%)	0.51	27 (9%) 11 15	291, 359, 359, 359	1 (0%)
2	S	291/319 (91%)	0.46	24 (8%) 14 18	295, 364, 364, 364	1 (0%)
2	U	291/319 (91%)	0.47	18 (6%) 24 24	298, 368, 368, 368	1 (0%)
2	W	291/319 (91%)	0.56	27 (9%) 11 15	303, 374, 374, 374	1 (0%)
3	F	54/56 (96%)	0.84	9 (16%) 2 8	373, 373, 373, 373	0
3	H	54/56 (96%)	0.47	5 (9%) 11 15	379, 379, 379, 379	0
3	J	54/56 (96%)	0.61	5 (9%) 11 15	370, 370, 370, 370	0
3	L	54/56 (96%)	1.22	12 (22%) 1 6	386, 386, 386, 386	0
3	R	54/56 (96%)	0.59	7 (12%) 5 10	371, 371, 371, 371	0
3	T	54/56 (96%)	0.58	7 (12%) 5 10	380, 380, 380, 380	0
3	V	54/56 (96%)	0.65	8 (14%) 3 9	384, 384, 384, 384	0
3	X	54/56 (96%)	0.84	8 (14%) 3 9	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%)	0.50	519 (9%)	9	14	287, 362, 379, 386	8 (0%)

The worst 5 of 519 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	30	GLY	8.2
1	D	24	GLY	7.8
1	D	30	GLY	7.2
1	B	317	CYS	7.1
1	N	26	LYS	6.8

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 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
4	ZN	A	500	1/1	0.95	0.23	-0.55	354,354,354,354	0
4	ZN	D	501	1/1	0.88	0.09	-2.20	363,363,363,363	0
4	ZN	M	401	1/1	0.93	0.07	-2.59	356,356,356,356	0
4	ZN	O	401	1/1	0.93	0.14	-2.61	354,354,354,354	0

6.5 Other polymers (i)

There are no such residues in this entry.