wwPDB X-ray Structure Validation Summary Report (i)

Feb 15, 2024 – 12:55 PM EST

PDB ID	:	3QIL
Title	:	Crystal structure analysis of the clathrin trimerization domain
Authors	:	Ybe, J.A.; Mishra, S.; Nix, J.
Deposited on	:	2011-01-27
Resolution	:	3.92 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 (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 (i)) were used in the production of this report:

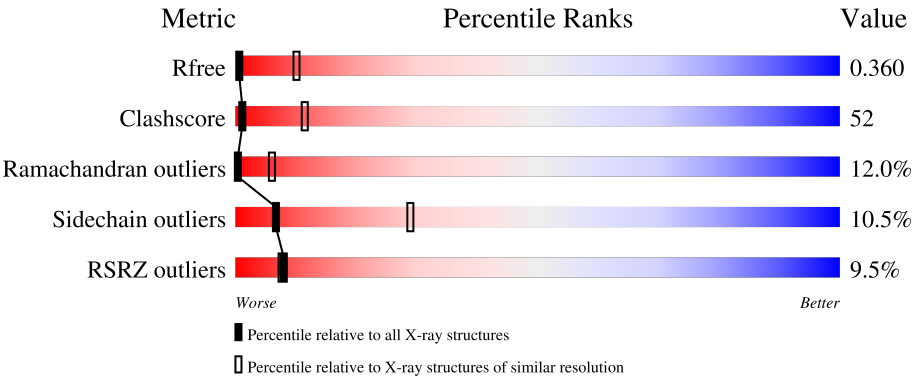
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.92 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	1019 (4.18-3.66)
Clashscore	141614	1016 (4.16-3.68)
Ramachandran outliers	138981	1039 (4.18-3.66)
Sidechain outliers	138945	1032 (4.18-3.66)
RSRZ outliers	127900	1002 (4.20-3.64)

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	125	4% 41% 41% 16%
1	B	125	13% 24% 43% 10% 22%
1	C	125	12% 32% 49% 18%
1	D	125	2% 40% 42% 14%
1	E	125	12% 32% 35% 10% 22%

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Mol	Chain	Length	Quality of chain
1	F	125	13% 30% 54% 14%
1	G	125	3% 42% 40% 16%
1	H	125	10% 26% 42% 9% 22%
1	I	125	13% 35% 47% 16%
1	J	125	7% 45% 39% 13%
1	K	125	8% 26% 41% 10% 22%
1	L	125	13% 33% 50% 16%
1	M	125	5% 42% 40% 15%
1	N	125	10% 29% 38% 10% 22%
1	O	125	13% 29% 55% 14%
1	P	125	4% 43% 40% 14%
1	Q	125	6% 32% 35% 10% 22%
1	R	125	13% 28% 54% 17%
1	S	125	4% 44% 37% 18%
1	T	125	13% 21% 47% 10% 22%
1	U	125	10% 30% 54% 14%
1	V	125	2% 44% 37% 17%
1	W	125	10% 27% 40% 10% 22%
1	X	125	13% 33% 51% 14%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 23032 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 Clathrin heavy chain 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	125	Total	C	N	O	S	0	0	0
			1034	655	175	195	9			
1	B	97	Total	C	N	O	S	0	0	0
			811	519	127	158	7			
1	C	125	Total	C	N	O	S	0	0	0
			1034	655	175	195	9			
1	D	125	Total	C	N	O	S	0	0	0
			1034	655	175	195	9			
1	E	97	Total	C	N	O	S	0	0	0
			811	519	127	158	7			
1	F	125	Total	C	N	O	S	0	0	0
			1034	655	175	195	9			
1	G	125	Total	C	N	O	S	0	0	0
			1034	655	175	195	9			
1	H	97	Total	C	N	O	S	0	0	0
			811	519	127	158	7			
1	I	125	Total	C	N	O	S	0	0	0
			1034	655	175	195	9			
1	J	125	Total	C	N	O	S	0	0	0
			1034	655	175	195	9			
1	K	97	Total	C	N	O	S	0	0	0
			811	519	127	158	7			
1	L	125	Total	C	N	O	S	0	0	0
			1034	655	175	195	9			
1	M	125	Total	C	N	O	S	0	0	0
			1034	655	175	195	9			
1	N	97	Total	C	N	O	S	0	0	0
			811	519	127	158	7			
1	O	125	Total	C	N	O	S	0	0	0
			1034	655	175	195	9			
1	P	125	Total	C	N	O	S	0	0	0
			1034	655	175	195	9			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	97	Total	C	N	O	S	0	0	0
			811	519	127	158	7			
1	R	125	Total	C	N	O	S	0	0	0
			1034	655	175	195	9			
1	S	125	Total	C	N	O	S	0	0	0
			1034	655	175	195	9			
1	T	97	Total	C	N	O	S	0	0	0
			811	519	127	158	7			
1	U	125	Total	C	N	O	S	0	0	0
			1034	655	175	195	9			
1	V	125	Total	C	N	O	S	0	0	0
			1034	655	175	195	9			
1	W	97	Total	C	N	O	S	0	0	0
			811	519	127	158	7			
1	X	125	Total	C	N	O	S	0	0	0
			1034	655	175	195	9			

There are 552 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1500	MET	-	expression tag	UNP P49951
A	1501	GLY	-	expression tag	UNP P49951
A	1502	SER	-	expression tag	UNP P49951
A	1503	SER	-	expression tag	UNP P49951
A	1504	HIS	-	expression tag	UNP P49951
A	1505	HIS	-	expression tag	UNP P49951
A	1506	HIS	-	expression tag	UNP P49951
A	1507	HIS	-	expression tag	UNP P49951
A	1508	HIS	-	expression tag	UNP P49951
A	1509	HIS	-	expression tag	UNP P49951
A	1510	SER	-	expression tag	UNP P49951
A	1511	SER	-	expression tag	UNP P49951
A	1512	GLY	-	expression tag	UNP P49951
A	1513	LEU	-	expression tag	UNP P49951
A	1514	VAL	-	expression tag	UNP P49951
A	1515	PRO	-	expression tag	UNP P49951
A	1516	ARG	-	expression tag	UNP P49951
A	1517	GLY	-	expression tag	UNP P49951
A	1518	SER	-	expression tag	UNP P49951
A	1519	HIS	-	expression tag	UNP P49951
A	1520	MET	-	expression tag	UNP P49951
A	1528	ALA	CYS	engineered mutation	UNP P49951
A	1585	LEU	THR	engineered mutation	UNP P49951

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1500	MET	-	expression tag	UNP P49951
B	1501	GLY	-	expression tag	UNP P49951
B	1502	SER	-	expression tag	UNP P49951
B	1503	SER	-	expression tag	UNP P49951
B	1504	HIS	-	expression tag	UNP P49951
B	1505	HIS	-	expression tag	UNP P49951
B	1506	HIS	-	expression tag	UNP P49951
B	1507	HIS	-	expression tag	UNP P49951
B	1508	HIS	-	expression tag	UNP P49951
B	1509	HIS	-	expression tag	UNP P49951
B	1510	SER	-	expression tag	UNP P49951
B	1511	SER	-	expression tag	UNP P49951
B	1512	GLY	-	expression tag	UNP P49951
B	1513	LEU	-	expression tag	UNP P49951
B	1514	VAL	-	expression tag	UNP P49951
B	1515	PRO	-	expression tag	UNP P49951
B	1516	ARG	-	expression tag	UNP P49951
B	1517	GLY	-	expression tag	UNP P49951
B	1518	SER	-	expression tag	UNP P49951
B	1519	HIS	-	expression tag	UNP P49951
B	1520	MET	-	expression tag	UNP P49951
B	1528	ALA	CYS	engineered mutation	UNP P49951
B	1585	LEU	THR	engineered mutation	UNP P49951
C	1500	MET	-	expression tag	UNP P49951
C	1501	GLY	-	expression tag	UNP P49951
C	1502	SER	-	expression tag	UNP P49951
C	1503	SER	-	expression tag	UNP P49951
C	1504	HIS	-	expression tag	UNP P49951
C	1505	HIS	-	expression tag	UNP P49951
C	1506	HIS	-	expression tag	UNP P49951
C	1507	HIS	-	expression tag	UNP P49951
C	1508	HIS	-	expression tag	UNP P49951
C	1509	HIS	-	expression tag	UNP P49951
C	1510	SER	-	expression tag	UNP P49951
C	1511	SER	-	expression tag	UNP P49951
C	1512	GLY	-	expression tag	UNP P49951
C	1513	LEU	-	expression tag	UNP P49951
C	1514	VAL	-	expression tag	UNP P49951
C	1515	PRO	-	expression tag	UNP P49951
C	1516	ARG	-	expression tag	UNP P49951
C	1517	GLY	-	expression tag	UNP P49951
C	1518	SER	-	expression tag	UNP P49951

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1519	HIS	-	expression tag	UNP P49951
C	1520	MET	-	expression tag	UNP P49951
C	1528	ALA	CYS	engineered mutation	UNP P49951
C	1585	LEU	THR	engineered mutation	UNP P49951
D	1500	MET	-	expression tag	UNP P49951
D	1501	GLY	-	expression tag	UNP P49951
D	1502	SER	-	expression tag	UNP P49951
D	1503	SER	-	expression tag	UNP P49951
D	1504	HIS	-	expression tag	UNP P49951
D	1505	HIS	-	expression tag	UNP P49951
D	1506	HIS	-	expression tag	UNP P49951
D	1507	HIS	-	expression tag	UNP P49951
D	1508	HIS	-	expression tag	UNP P49951
D	1509	HIS	-	expression tag	UNP P49951
D	1510	SER	-	expression tag	UNP P49951
D	1511	SER	-	expression tag	UNP P49951
D	1512	GLY	-	expression tag	UNP P49951
D	1513	LEU	-	expression tag	UNP P49951
D	1514	VAL	-	expression tag	UNP P49951
D	1515	PRO	-	expression tag	UNP P49951
D	1516	ARG	-	expression tag	UNP P49951
D	1517	GLY	-	expression tag	UNP P49951
D	1518	SER	-	expression tag	UNP P49951
D	1519	HIS	-	expression tag	UNP P49951
D	1520	MET	-	expression tag	UNP P49951
D	1528	ALA	CYS	engineered mutation	UNP P49951
D	1585	LEU	THR	engineered mutation	UNP P49951
E	1500	MET	-	expression tag	UNP P49951
E	1501	GLY	-	expression tag	UNP P49951
E	1502	SER	-	expression tag	UNP P49951
E	1503	SER	-	expression tag	UNP P49951
E	1504	HIS	-	expression tag	UNP P49951
E	1505	HIS	-	expression tag	UNP P49951
E	1506	HIS	-	expression tag	UNP P49951
E	1507	HIS	-	expression tag	UNP P49951
E	1508	HIS	-	expression tag	UNP P49951
E	1509	HIS	-	expression tag	UNP P49951
E	1510	SER	-	expression tag	UNP P49951
E	1511	SER	-	expression tag	UNP P49951
E	1512	GLY	-	expression tag	UNP P49951
E	1513	LEU	-	expression tag	UNP P49951
E	1514	VAL	-	expression tag	UNP P49951

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Chain	Residue	Modelled	Actual	Comment	Reference
E	1515	PRO	-	expression tag	UNP P49951
E	1516	ARG	-	expression tag	UNP P49951
E	1517	GLY	-	expression tag	UNP P49951
E	1518	SER	-	expression tag	UNP P49951
E	1519	HIS	-	expression tag	UNP P49951
E	1520	MET	-	expression tag	UNP P49951
E	1528	ALA	CYS	engineered mutation	UNP P49951
E	1585	LEU	THR	engineered mutation	UNP P49951
F	1500	MET	-	expression tag	UNP P49951
F	1501	GLY	-	expression tag	UNP P49951
F	1502	SER	-	expression tag	UNP P49951
F	1503	SER	-	expression tag	UNP P49951
F	1504	HIS	-	expression tag	UNP P49951
F	1505	HIS	-	expression tag	UNP P49951
F	1506	HIS	-	expression tag	UNP P49951
F	1507	HIS	-	expression tag	UNP P49951
F	1508	HIS	-	expression tag	UNP P49951
F	1509	HIS	-	expression tag	UNP P49951
F	1510	SER	-	expression tag	UNP P49951
F	1511	SER	-	expression tag	UNP P49951
F	1512	GLY	-	expression tag	UNP P49951
F	1513	LEU	-	expression tag	UNP P49951
F	1514	VAL	-	expression tag	UNP P49951
F	1515	PRO	-	expression tag	UNP P49951
F	1516	ARG	-	expression tag	UNP P49951
F	1517	GLY	-	expression tag	UNP P49951
F	1518	SER	-	expression tag	UNP P49951
F	1519	HIS	-	expression tag	UNP P49951
F	1520	MET	-	expression tag	UNP P49951
F	1528	ALA	CYS	engineered mutation	UNP P49951
F	1585	LEU	THR	engineered mutation	UNP P49951
G	1500	MET	-	expression tag	UNP P49951
G	1501	GLY	-	expression tag	UNP P49951
G	1502	SER	-	expression tag	UNP P49951
G	1503	SER	-	expression tag	UNP P49951
G	1504	HIS	-	expression tag	UNP P49951
G	1505	HIS	-	expression tag	UNP P49951
G	1506	HIS	-	expression tag	UNP P49951
G	1507	HIS	-	expression tag	UNP P49951
G	1508	HIS	-	expression tag	UNP P49951
G	1509	HIS	-	expression tag	UNP P49951
G	1510	SER	-	expression tag	UNP P49951

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Chain	Residue	Modelled	Actual	Comment	Reference
G	1511	SER	-	expression tag	UNP P49951
G	1512	GLY	-	expression tag	UNP P49951
G	1513	LEU	-	expression tag	UNP P49951
G	1514	VAL	-	expression tag	UNP P49951
G	1515	PRO	-	expression tag	UNP P49951
G	1516	ARG	-	expression tag	UNP P49951
G	1517	GLY	-	expression tag	UNP P49951
G	1518	SER	-	expression tag	UNP P49951
G	1519	HIS	-	expression tag	UNP P49951
G	1520	MET	-	expression tag	UNP P49951
G	1528	ALA	CYS	engineered mutation	UNP P49951
G	1585	LEU	THR	engineered mutation	UNP P49951
H	1500	MET	-	expression tag	UNP P49951
H	1501	GLY	-	expression tag	UNP P49951
H	1502	SER	-	expression tag	UNP P49951
H	1503	SER	-	expression tag	UNP P49951
H	1504	HIS	-	expression tag	UNP P49951
H	1505	HIS	-	expression tag	UNP P49951
H	1506	HIS	-	expression tag	UNP P49951
H	1507	HIS	-	expression tag	UNP P49951
H	1508	HIS	-	expression tag	UNP P49951
H	1509	HIS	-	expression tag	UNP P49951
H	1510	SER	-	expression tag	UNP P49951
H	1511	SER	-	expression tag	UNP P49951
H	1512	GLY	-	expression tag	UNP P49951
H	1513	LEU	-	expression tag	UNP P49951
H	1514	VAL	-	expression tag	UNP P49951
H	1515	PRO	-	expression tag	UNP P49951
H	1516	ARG	-	expression tag	UNP P49951
H	1517	GLY	-	expression tag	UNP P49951
H	1518	SER	-	expression tag	UNP P49951
H	1519	HIS	-	expression tag	UNP P49951
H	1520	MET	-	expression tag	UNP P49951
H	1528	ALA	CYS	engineered mutation	UNP P49951
H	1585	LEU	THR	engineered mutation	UNP P49951
I	1500	MET	-	expression tag	UNP P49951
I	1501	GLY	-	expression tag	UNP P49951
I	1502	SER	-	expression tag	UNP P49951
I	1503	SER	-	expression tag	UNP P49951
I	1504	HIS	-	expression tag	UNP P49951
I	1505	HIS	-	expression tag	UNP P49951
I	1506	HIS	-	expression tag	UNP P49951

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Chain	Residue	Modelled	Actual	Comment	Reference
I	1507	HIS	-	expression tag	UNP P49951
I	1508	HIS	-	expression tag	UNP P49951
I	1509	HIS	-	expression tag	UNP P49951
I	1510	SER	-	expression tag	UNP P49951
I	1511	SER	-	expression tag	UNP P49951
I	1512	GLY	-	expression tag	UNP P49951
I	1513	LEU	-	expression tag	UNP P49951
I	1514	VAL	-	expression tag	UNP P49951
I	1515	PRO	-	expression tag	UNP P49951
I	1516	ARG	-	expression tag	UNP P49951
I	1517	GLY	-	expression tag	UNP P49951
I	1518	SER	-	expression tag	UNP P49951
I	1519	HIS	-	expression tag	UNP P49951
I	1520	MET	-	expression tag	UNP P49951
I	1528	ALA	CYS	engineered mutation	UNP P49951
I	1585	LEU	THR	engineered mutation	UNP P49951
J	1500	MET	-	expression tag	UNP P49951
J	1501	GLY	-	expression tag	UNP P49951
J	1502	SER	-	expression tag	UNP P49951
J	1503	SER	-	expression tag	UNP P49951
J	1504	HIS	-	expression tag	UNP P49951
J	1505	HIS	-	expression tag	UNP P49951
J	1506	HIS	-	expression tag	UNP P49951
J	1507	HIS	-	expression tag	UNP P49951
J	1508	HIS	-	expression tag	UNP P49951
J	1509	HIS	-	expression tag	UNP P49951
J	1510	SER	-	expression tag	UNP P49951
J	1511	SER	-	expression tag	UNP P49951
J	1512	GLY	-	expression tag	UNP P49951
J	1513	LEU	-	expression tag	UNP P49951
J	1514	VAL	-	expression tag	UNP P49951
J	1515	PRO	-	expression tag	UNP P49951
J	1516	ARG	-	expression tag	UNP P49951
J	1517	GLY	-	expression tag	UNP P49951
J	1518	SER	-	expression tag	UNP P49951
J	1519	HIS	-	expression tag	UNP P49951
J	1520	MET	-	expression tag	UNP P49951
J	1528	ALA	CYS	engineered mutation	UNP P49951
J	1585	LEU	THR	engineered mutation	UNP P49951
K	1500	MET	-	expression tag	UNP P49951
K	1501	GLY	-	expression tag	UNP P49951
K	1502	SER	-	expression tag	UNP P49951

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Chain	Residue	Modelled	Actual	Comment	Reference
K	1503	SER	-	expression tag	UNP P49951
K	1504	HIS	-	expression tag	UNP P49951
K	1505	HIS	-	expression tag	UNP P49951
K	1506	HIS	-	expression tag	UNP P49951
K	1507	HIS	-	expression tag	UNP P49951
K	1508	HIS	-	expression tag	UNP P49951
K	1509	HIS	-	expression tag	UNP P49951
K	1510	SER	-	expression tag	UNP P49951
K	1511	SER	-	expression tag	UNP P49951
K	1512	GLY	-	expression tag	UNP P49951
K	1513	LEU	-	expression tag	UNP P49951
K	1514	VAL	-	expression tag	UNP P49951
K	1515	PRO	-	expression tag	UNP P49951
K	1516	ARG	-	expression tag	UNP P49951
K	1517	GLY	-	expression tag	UNP P49951
K	1518	SER	-	expression tag	UNP P49951
K	1519	HIS	-	expression tag	UNP P49951
K	1520	MET	-	expression tag	UNP P49951
K	1528	ALA	CYS	engineered mutation	UNP P49951
K	1585	LEU	THR	engineered mutation	UNP P49951
L	1500	MET	-	expression tag	UNP P49951
L	1501	GLY	-	expression tag	UNP P49951
L	1502	SER	-	expression tag	UNP P49951
L	1503	SER	-	expression tag	UNP P49951
L	1504	HIS	-	expression tag	UNP P49951
L	1505	HIS	-	expression tag	UNP P49951
L	1506	HIS	-	expression tag	UNP P49951
L	1507	HIS	-	expression tag	UNP P49951
L	1508	HIS	-	expression tag	UNP P49951
L	1509	HIS	-	expression tag	UNP P49951
L	1510	SER	-	expression tag	UNP P49951
L	1511	SER	-	expression tag	UNP P49951
L	1512	GLY	-	expression tag	UNP P49951
L	1513	LEU	-	expression tag	UNP P49951
L	1514	VAL	-	expression tag	UNP P49951
L	1515	PRO	-	expression tag	UNP P49951
L	1516	ARG	-	expression tag	UNP P49951
L	1517	GLY	-	expression tag	UNP P49951
L	1518	SER	-	expression tag	UNP P49951
L	1519	HIS	-	expression tag	UNP P49951
L	1520	MET	-	expression tag	UNP P49951
L	1528	ALA	CYS	engineered mutation	UNP P49951

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Chain	Residue	Modelled	Actual	Comment	Reference
L	1585	LEU	THR	engineered mutation	UNP P49951
M	1500	MET	-	expression tag	UNP P49951
M	1501	GLY	-	expression tag	UNP P49951
M	1502	SER	-	expression tag	UNP P49951
M	1503	SER	-	expression tag	UNP P49951
M	1504	HIS	-	expression tag	UNP P49951
M	1505	HIS	-	expression tag	UNP P49951
M	1506	HIS	-	expression tag	UNP P49951
M	1507	HIS	-	expression tag	UNP P49951
M	1508	HIS	-	expression tag	UNP P49951
M	1509	HIS	-	expression tag	UNP P49951
M	1510	SER	-	expression tag	UNP P49951
M	1511	SER	-	expression tag	UNP P49951
M	1512	GLY	-	expression tag	UNP P49951
M	1513	LEU	-	expression tag	UNP P49951
M	1514	VAL	-	expression tag	UNP P49951
M	1515	PRO	-	expression tag	UNP P49951
M	1516	ARG	-	expression tag	UNP P49951
M	1517	GLY	-	expression tag	UNP P49951
M	1518	SER	-	expression tag	UNP P49951
M	1519	HIS	-	expression tag	UNP P49951
M	1520	MET	-	expression tag	UNP P49951
M	1528	ALA	CYS	engineered mutation	UNP P49951
M	1585	LEU	THR	engineered mutation	UNP P49951
N	1500	MET	-	expression tag	UNP P49951
N	1501	GLY	-	expression tag	UNP P49951
N	1502	SER	-	expression tag	UNP P49951
N	1503	SER	-	expression tag	UNP P49951
N	1504	HIS	-	expression tag	UNP P49951
N	1505	HIS	-	expression tag	UNP P49951
N	1506	HIS	-	expression tag	UNP P49951
N	1507	HIS	-	expression tag	UNP P49951
N	1508	HIS	-	expression tag	UNP P49951
N	1509	HIS	-	expression tag	UNP P49951
N	1510	SER	-	expression tag	UNP P49951
N	1511	SER	-	expression tag	UNP P49951
N	1512	GLY	-	expression tag	UNP P49951
N	1513	LEU	-	expression tag	UNP P49951
N	1514	VAL	-	expression tag	UNP P49951
N	1515	PRO	-	expression tag	UNP P49951
N	1516	ARG	-	expression tag	UNP P49951
N	1517	GLY	-	expression tag	UNP P49951

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Chain	Residue	Modelled	Actual	Comment	Reference
N	1518	SER	-	expression tag	UNP P49951
N	1519	HIS	-	expression tag	UNP P49951
N	1520	MET	-	expression tag	UNP P49951
N	1528	ALA	CYS	engineered mutation	UNP P49951
N	1585	LEU	THR	engineered mutation	UNP P49951
O	1500	MET	-	expression tag	UNP P49951
O	1501	GLY	-	expression tag	UNP P49951
O	1502	SER	-	expression tag	UNP P49951
O	1503	SER	-	expression tag	UNP P49951
O	1504	HIS	-	expression tag	UNP P49951
O	1505	HIS	-	expression tag	UNP P49951
O	1506	HIS	-	expression tag	UNP P49951
O	1507	HIS	-	expression tag	UNP P49951
O	1508	HIS	-	expression tag	UNP P49951
O	1509	HIS	-	expression tag	UNP P49951
O	1510	SER	-	expression tag	UNP P49951
O	1511	SER	-	expression tag	UNP P49951
O	1512	GLY	-	expression tag	UNP P49951
O	1513	LEU	-	expression tag	UNP P49951
O	1514	VAL	-	expression tag	UNP P49951
O	1515	PRO	-	expression tag	UNP P49951
O	1516	ARG	-	expression tag	UNP P49951
O	1517	GLY	-	expression tag	UNP P49951
O	1518	SER	-	expression tag	UNP P49951
O	1519	HIS	-	expression tag	UNP P49951
O	1520	MET	-	expression tag	UNP P49951
O	1528	ALA	CYS	engineered mutation	UNP P49951
O	1585	LEU	THR	engineered mutation	UNP P49951
P	1500	MET	-	expression tag	UNP P49951
P	1501	GLY	-	expression tag	UNP P49951
P	1502	SER	-	expression tag	UNP P49951
P	1503	SER	-	expression tag	UNP P49951
P	1504	HIS	-	expression tag	UNP P49951
P	1505	HIS	-	expression tag	UNP P49951
P	1506	HIS	-	expression tag	UNP P49951
P	1507	HIS	-	expression tag	UNP P49951
P	1508	HIS	-	expression tag	UNP P49951
P	1509	HIS	-	expression tag	UNP P49951
P	1510	SER	-	expression tag	UNP P49951
P	1511	SER	-	expression tag	UNP P49951
P	1512	GLY	-	expression tag	UNP P49951
P	1513	LEU	-	expression tag	UNP P49951

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Chain	Residue	Modelled	Actual	Comment	Reference
P	1514	VAL	-	expression tag	UNP P49951
P	1515	PRO	-	expression tag	UNP P49951
P	1516	ARG	-	expression tag	UNP P49951
P	1517	GLY	-	expression tag	UNP P49951
P	1518	SER	-	expression tag	UNP P49951
P	1519	HIS	-	expression tag	UNP P49951
P	1520	MET	-	expression tag	UNP P49951
P	1528	ALA	CYS	engineered mutation	UNP P49951
P	1585	LEU	THR	engineered mutation	UNP P49951
Q	1500	MET	-	expression tag	UNP P49951
Q	1501	GLY	-	expression tag	UNP P49951
Q	1502	SER	-	expression tag	UNP P49951
Q	1503	SER	-	expression tag	UNP P49951
Q	1504	HIS	-	expression tag	UNP P49951
Q	1505	HIS	-	expression tag	UNP P49951
Q	1506	HIS	-	expression tag	UNP P49951
Q	1507	HIS	-	expression tag	UNP P49951
Q	1508	HIS	-	expression tag	UNP P49951
Q	1509	HIS	-	expression tag	UNP P49951
Q	1510	SER	-	expression tag	UNP P49951
Q	1511	SER	-	expression tag	UNP P49951
Q	1512	GLY	-	expression tag	UNP P49951
Q	1513	LEU	-	expression tag	UNP P49951
Q	1514	VAL	-	expression tag	UNP P49951
Q	1515	PRO	-	expression tag	UNP P49951
Q	1516	ARG	-	expression tag	UNP P49951
Q	1517	GLY	-	expression tag	UNP P49951
Q	1518	SER	-	expression tag	UNP P49951
Q	1519	HIS	-	expression tag	UNP P49951
Q	1520	MET	-	expression tag	UNP P49951
Q	1528	ALA	CYS	engineered mutation	UNP P49951
Q	1585	LEU	THR	engineered mutation	UNP P49951
R	1500	MET	-	expression tag	UNP P49951
R	1501	GLY	-	expression tag	UNP P49951
R	1502	SER	-	expression tag	UNP P49951
R	1503	SER	-	expression tag	UNP P49951
R	1504	HIS	-	expression tag	UNP P49951
R	1505	HIS	-	expression tag	UNP P49951
R	1506	HIS	-	expression tag	UNP P49951
R	1507	HIS	-	expression tag	UNP P49951
R	1508	HIS	-	expression tag	UNP P49951
R	1509	HIS	-	expression tag	UNP P49951

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Chain	Residue	Modelled	Actual	Comment	Reference
R	1510	SER	-	expression tag	UNP P49951
R	1511	SER	-	expression tag	UNP P49951
R	1512	GLY	-	expression tag	UNP P49951
R	1513	LEU	-	expression tag	UNP P49951
R	1514	VAL	-	expression tag	UNP P49951
R	1515	PRO	-	expression tag	UNP P49951
R	1516	ARG	-	expression tag	UNP P49951
R	1517	GLY	-	expression tag	UNP P49951
R	1518	SER	-	expression tag	UNP P49951
R	1519	HIS	-	expression tag	UNP P49951
R	1520	MET	-	expression tag	UNP P49951
R	1528	ALA	CYS	engineered mutation	UNP P49951
R	1585	LEU	THR	engineered mutation	UNP P49951
S	1500	MET	-	expression tag	UNP P49951
S	1501	GLY	-	expression tag	UNP P49951
S	1502	SER	-	expression tag	UNP P49951
S	1503	SER	-	expression tag	UNP P49951
S	1504	HIS	-	expression tag	UNP P49951
S	1505	HIS	-	expression tag	UNP P49951
S	1506	HIS	-	expression tag	UNP P49951
S	1507	HIS	-	expression tag	UNP P49951
S	1508	HIS	-	expression tag	UNP P49951
S	1509	HIS	-	expression tag	UNP P49951
S	1510	SER	-	expression tag	UNP P49951
S	1511	SER	-	expression tag	UNP P49951
S	1512	GLY	-	expression tag	UNP P49951
S	1513	LEU	-	expression tag	UNP P49951
S	1514	VAL	-	expression tag	UNP P49951
S	1515	PRO	-	expression tag	UNP P49951
S	1516	ARG	-	expression tag	UNP P49951
S	1517	GLY	-	expression tag	UNP P49951
S	1518	SER	-	expression tag	UNP P49951
S	1519	HIS	-	expression tag	UNP P49951
S	1520	MET	-	expression tag	UNP P49951
S	1528	ALA	CYS	engineered mutation	UNP P49951
S	1585	LEU	THR	engineered mutation	UNP P49951
T	1500	MET	-	expression tag	UNP P49951
T	1501	GLY	-	expression tag	UNP P49951
T	1502	SER	-	expression tag	UNP P49951
T	1503	SER	-	expression tag	UNP P49951
T	1504	HIS	-	expression tag	UNP P49951
T	1505	HIS	-	expression tag	UNP P49951

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Chain	Residue	Modelled	Actual	Comment	Reference
T	1506	HIS	-	expression tag	UNP P49951
T	1507	HIS	-	expression tag	UNP P49951
T	1508	HIS	-	expression tag	UNP P49951
T	1509	HIS	-	expression tag	UNP P49951
T	1510	SER	-	expression tag	UNP P49951
T	1511	SER	-	expression tag	UNP P49951
T	1512	GLY	-	expression tag	UNP P49951
T	1513	LEU	-	expression tag	UNP P49951
T	1514	VAL	-	expression tag	UNP P49951
T	1515	PRO	-	expression tag	UNP P49951
T	1516	ARG	-	expression tag	UNP P49951
T	1517	GLY	-	expression tag	UNP P49951
T	1518	SER	-	expression tag	UNP P49951
T	1519	HIS	-	expression tag	UNP P49951
T	1520	MET	-	expression tag	UNP P49951
T	1528	ALA	CYS	engineered mutation	UNP P49951
T	1585	LEU	THR	engineered mutation	UNP P49951
U	1500	MET	-	expression tag	UNP P49951
U	1501	GLY	-	expression tag	UNP P49951
U	1502	SER	-	expression tag	UNP P49951
U	1503	SER	-	expression tag	UNP P49951
U	1504	HIS	-	expression tag	UNP P49951
U	1505	HIS	-	expression tag	UNP P49951
U	1506	HIS	-	expression tag	UNP P49951
U	1507	HIS	-	expression tag	UNP P49951
U	1508	HIS	-	expression tag	UNP P49951
U	1509	HIS	-	expression tag	UNP P49951
U	1510	SER	-	expression tag	UNP P49951
U	1511	SER	-	expression tag	UNP P49951
U	1512	GLY	-	expression tag	UNP P49951
U	1513	LEU	-	expression tag	UNP P49951
U	1514	VAL	-	expression tag	UNP P49951
U	1515	PRO	-	expression tag	UNP P49951
U	1516	ARG	-	expression tag	UNP P49951
U	1517	GLY	-	expression tag	UNP P49951
U	1518	SER	-	expression tag	UNP P49951
U	1519	HIS	-	expression tag	UNP P49951
U	1520	MET	-	expression tag	UNP P49951
U	1528	ALA	CYS	engineered mutation	UNP P49951
U	1585	LEU	THR	engineered mutation	UNP P49951
V	1500	MET	-	expression tag	UNP P49951
V	1501	GLY	-	expression tag	UNP P49951

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Chain	Residue	Modelled	Actual	Comment	Reference
V	1502	SER	-	expression tag	UNP P49951
V	1503	SER	-	expression tag	UNP P49951
V	1504	HIS	-	expression tag	UNP P49951
V	1505	HIS	-	expression tag	UNP P49951
V	1506	HIS	-	expression tag	UNP P49951
V	1507	HIS	-	expression tag	UNP P49951
V	1508	HIS	-	expression tag	UNP P49951
V	1509	HIS	-	expression tag	UNP P49951
V	1510	SER	-	expression tag	UNP P49951
V	1511	SER	-	expression tag	UNP P49951
V	1512	GLY	-	expression tag	UNP P49951
V	1513	LEU	-	expression tag	UNP P49951
V	1514	VAL	-	expression tag	UNP P49951
V	1515	PRO	-	expression tag	UNP P49951
V	1516	ARG	-	expression tag	UNP P49951
V	1517	GLY	-	expression tag	UNP P49951
V	1518	SER	-	expression tag	UNP P49951
V	1519	HIS	-	expression tag	UNP P49951
V	1520	MET	-	expression tag	UNP P49951
V	1528	ALA	CYS	engineered mutation	UNP P49951
V	1585	LEU	THR	engineered mutation	UNP P49951
W	1500	MET	-	expression tag	UNP P49951
W	1501	GLY	-	expression tag	UNP P49951
W	1502	SER	-	expression tag	UNP P49951
W	1503	SER	-	expression tag	UNP P49951
W	1504	HIS	-	expression tag	UNP P49951
W	1505	HIS	-	expression tag	UNP P49951
W	1506	HIS	-	expression tag	UNP P49951
W	1507	HIS	-	expression tag	UNP P49951
W	1508	HIS	-	expression tag	UNP P49951
W	1509	HIS	-	expression tag	UNP P49951
W	1510	SER	-	expression tag	UNP P49951
W	1511	SER	-	expression tag	UNP P49951
W	1512	GLY	-	expression tag	UNP P49951
W	1513	LEU	-	expression tag	UNP P49951
W	1514	VAL	-	expression tag	UNP P49951
W	1515	PRO	-	expression tag	UNP P49951
W	1516	ARG	-	expression tag	UNP P49951
W	1517	GLY	-	expression tag	UNP P49951
W	1518	SER	-	expression tag	UNP P49951
W	1519	HIS	-	expression tag	UNP P49951
W	1520	MET	-	expression tag	UNP P49951

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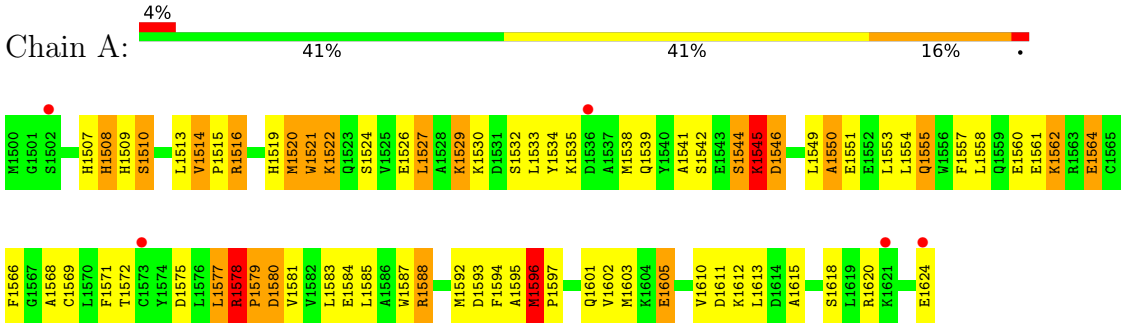
Chain	Residue	Modelled	Actual	Comment	Reference
W	1528	ALA	CYS	engineered mutation	UNP P49951
W	1585	LEU	THR	engineered mutation	UNP P49951
X	1500	MET	-	expression tag	UNP P49951
X	1501	GLY	-	expression tag	UNP P49951
X	1502	SER	-	expression tag	UNP P49951
X	1503	SER	-	expression tag	UNP P49951
X	1504	HIS	-	expression tag	UNP P49951
X	1505	HIS	-	expression tag	UNP P49951
X	1506	HIS	-	expression tag	UNP P49951
X	1507	HIS	-	expression tag	UNP P49951
X	1508	HIS	-	expression tag	UNP P49951
X	1509	HIS	-	expression tag	UNP P49951
X	1510	SER	-	expression tag	UNP P49951
X	1511	SER	-	expression tag	UNP P49951
X	1512	GLY	-	expression tag	UNP P49951
X	1513	LEU	-	expression tag	UNP P49951
X	1514	VAL	-	expression tag	UNP P49951
X	1515	PRO	-	expression tag	UNP P49951
X	1516	ARG	-	expression tag	UNP P49951
X	1517	GLY	-	expression tag	UNP P49951
X	1518	SER	-	expression tag	UNP P49951
X	1519	HIS	-	expression tag	UNP P49951
X	1520	MET	-	expression tag	UNP P49951
X	1528	ALA	CYS	engineered mutation	UNP P49951
X	1585	LEU	THR	engineered mutation	UNP P49951

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.

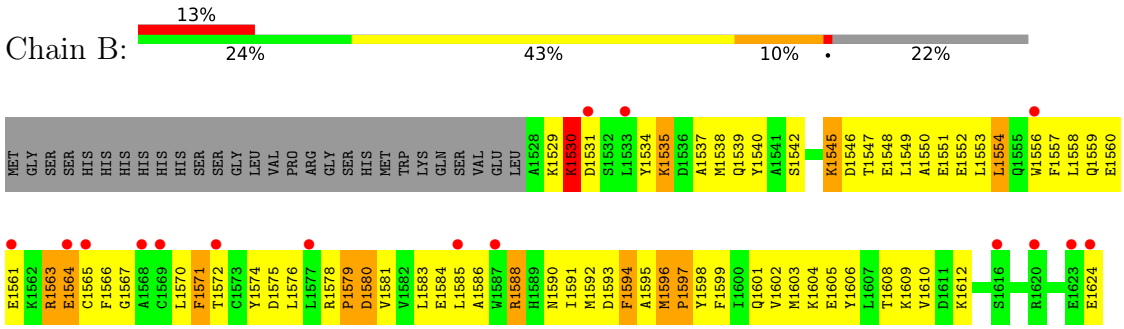
• Molecule 1: Clathrin heavy chain 1

Chain A:



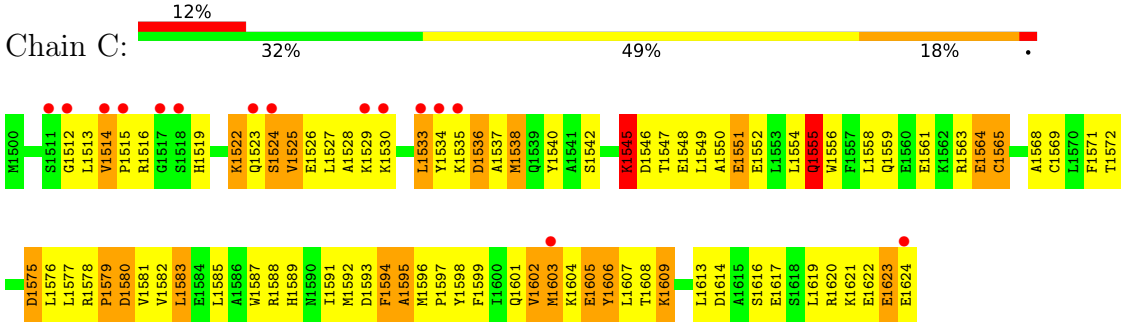
• Molecule 1: Clathrin heavy chain 1

Chain B:



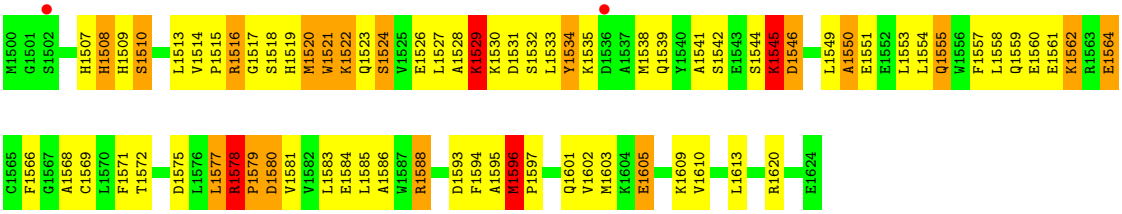
• Molecule 1: Clathrin heavy chain 1

Chain C:

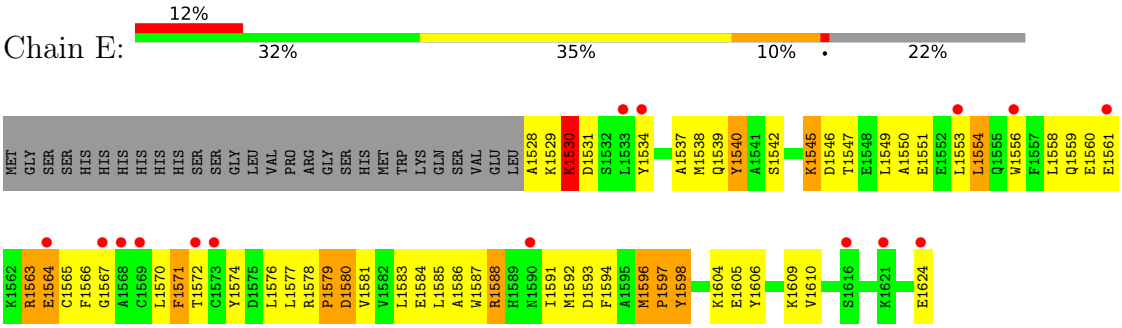


• Molecule 1: Clathrin heavy chain 1

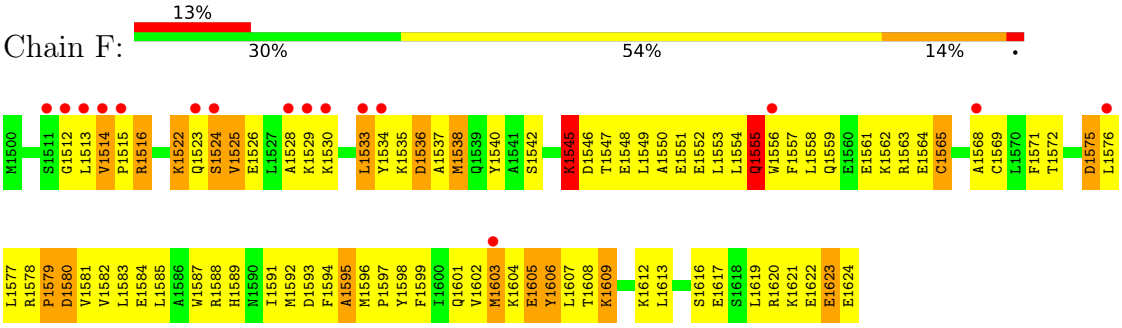
Chain D:



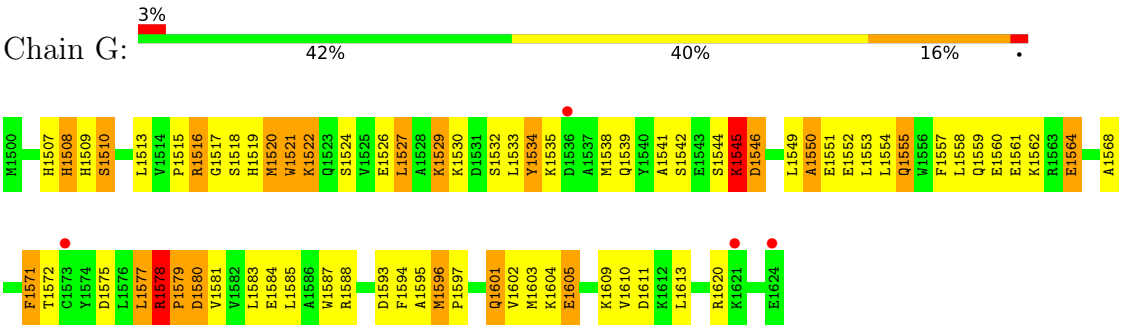
• Molecule 1: Clathrin heavy chain 1



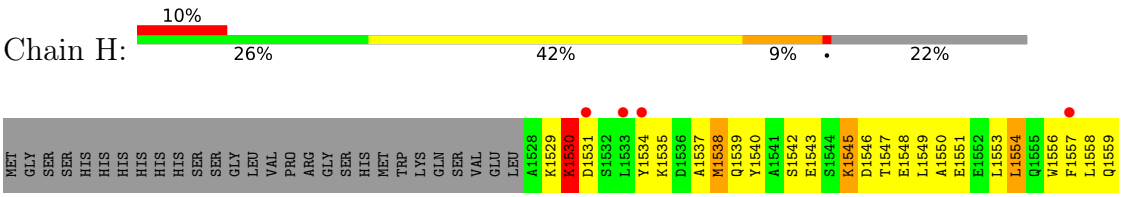
• Molecule 1: Clathrin heavy chain 1

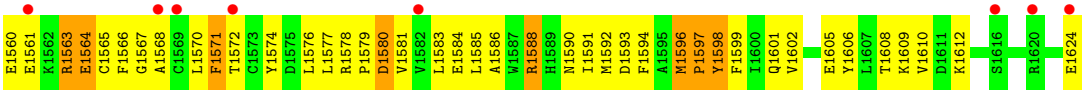


• Molecule 1: Clathrin heavy chain 1



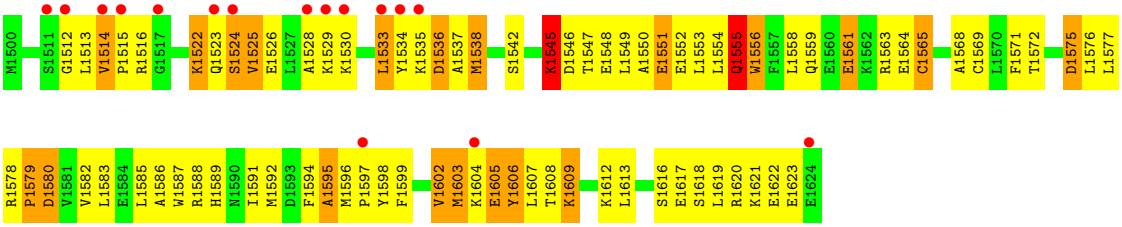
• Molecule 1: Clathrin heavy chain 1





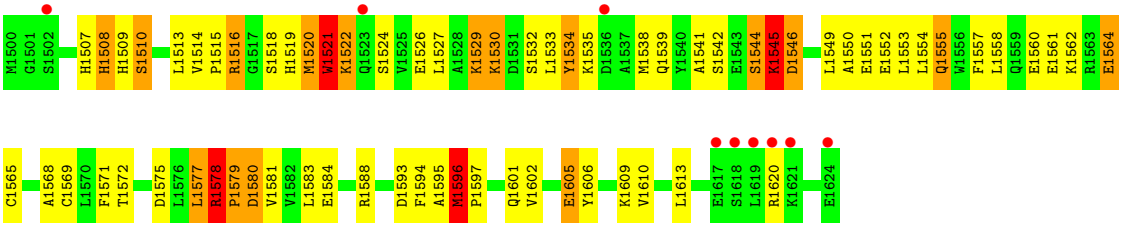
• Molecule 1: Clathrin heavy chain 1

Chain I:



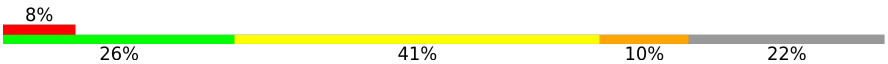
• Molecule 1: Clathrin heavy chain 1

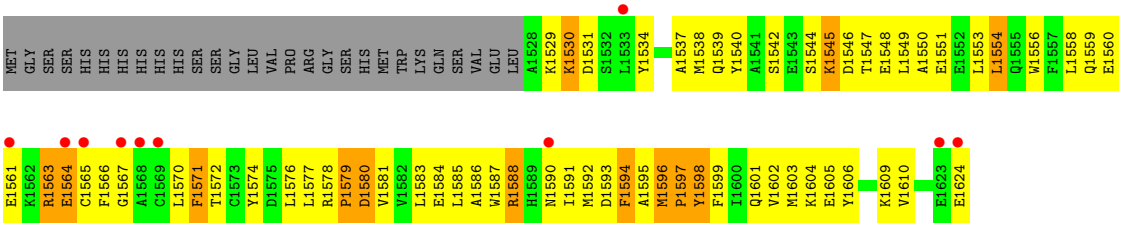
Chain J:



• Molecule 1: Clathrin heavy chain 1

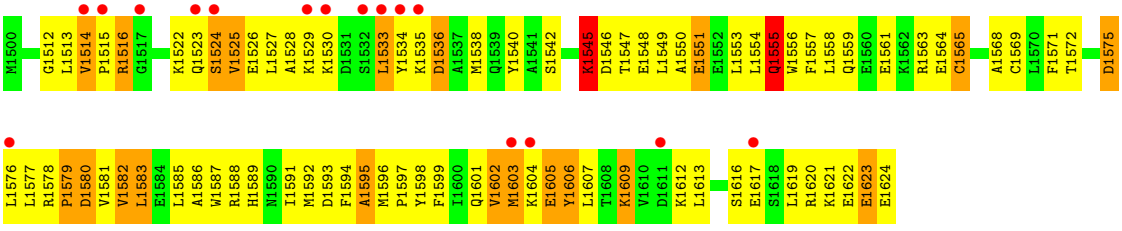
Chain K:



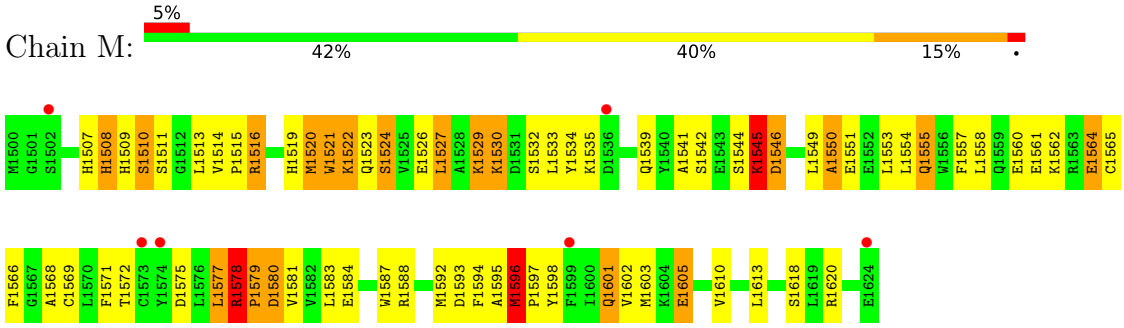


• Molecule 1: Clathrin heavy chain 1

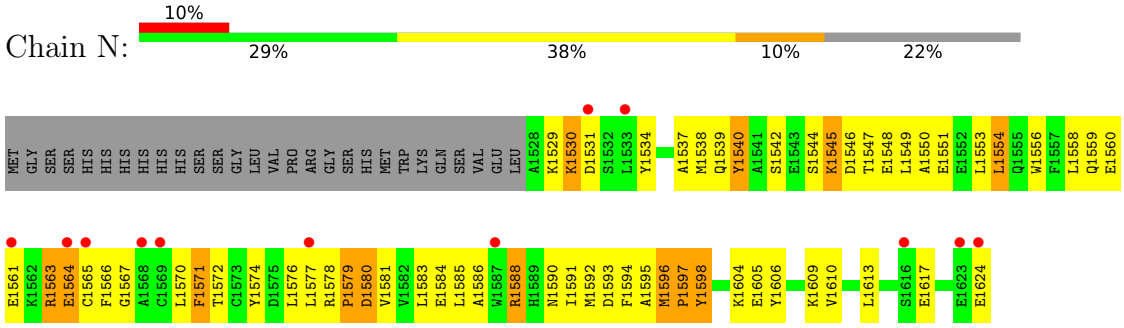
Chain L:



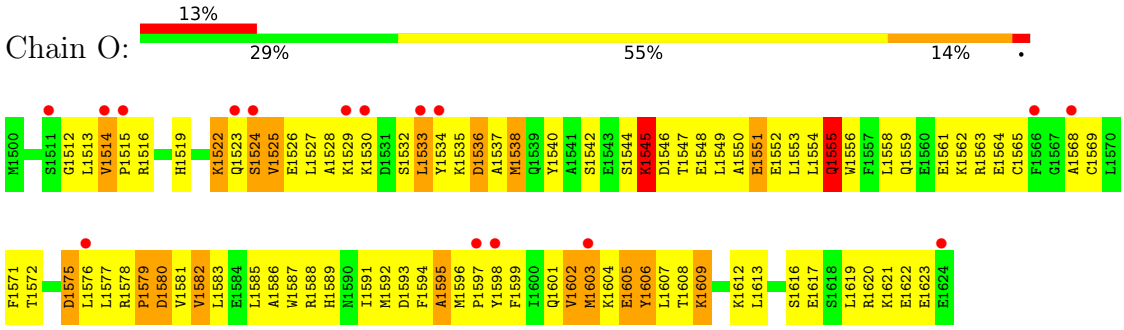
• Molecule 1: Clathrin heavy chain 1



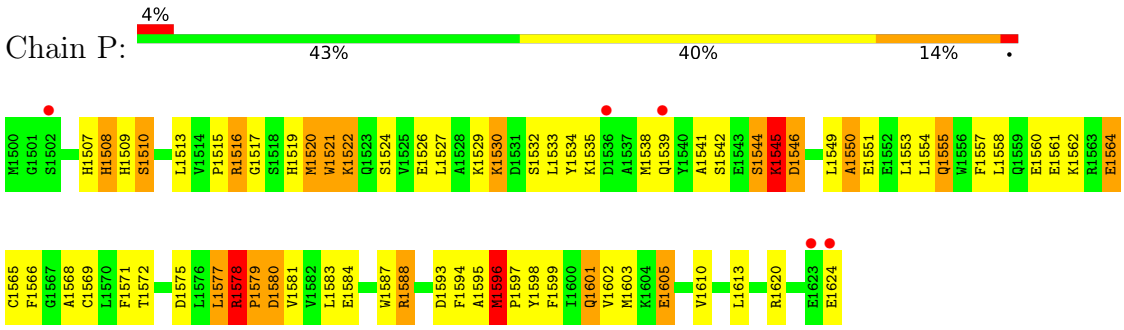
• Molecule 1: Clathrin heavy chain 1



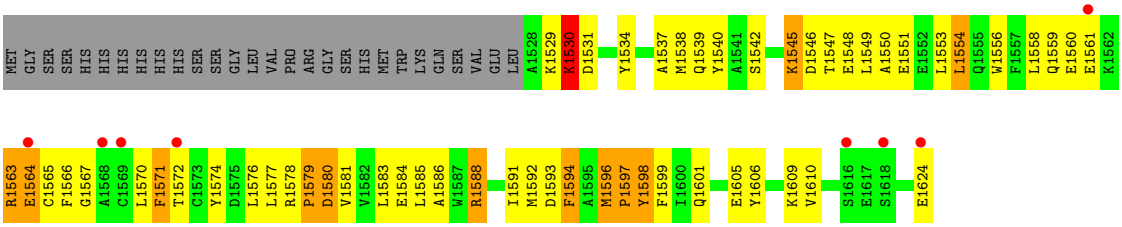
• Molecule 1: Clathrin heavy chain 1



• Molecule 1: Clathrin heavy chain 1

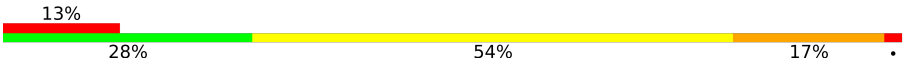


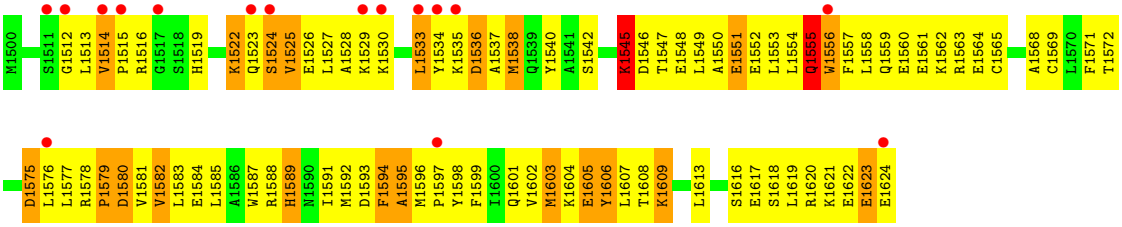
• Molecule 1: Clathrin heavy chain 1



• Molecule 1: Clathrin heavy chain 1

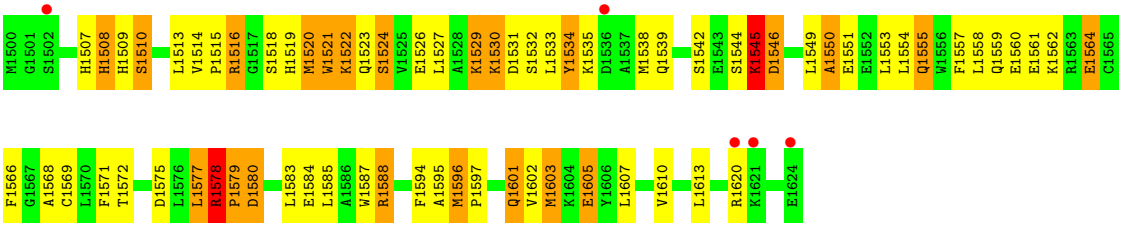
Chain R:





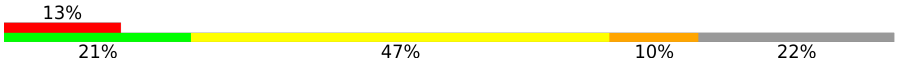
• Molecule 1: Clathrin heavy chain 1

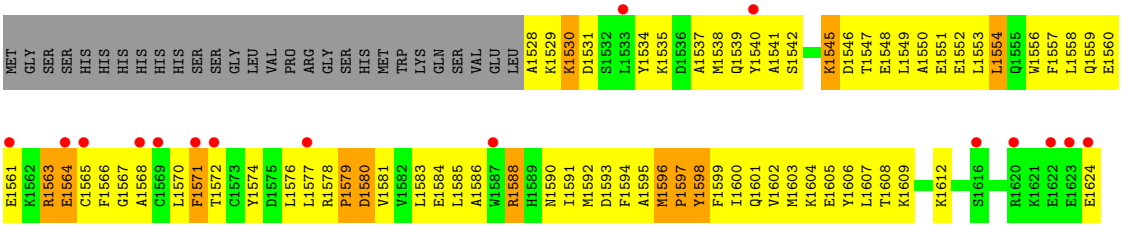
Chain S:



• Molecule 1: Clathrin heavy chain 1

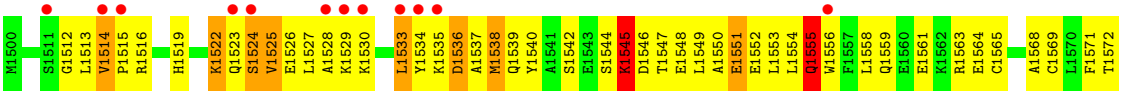
Chain T:





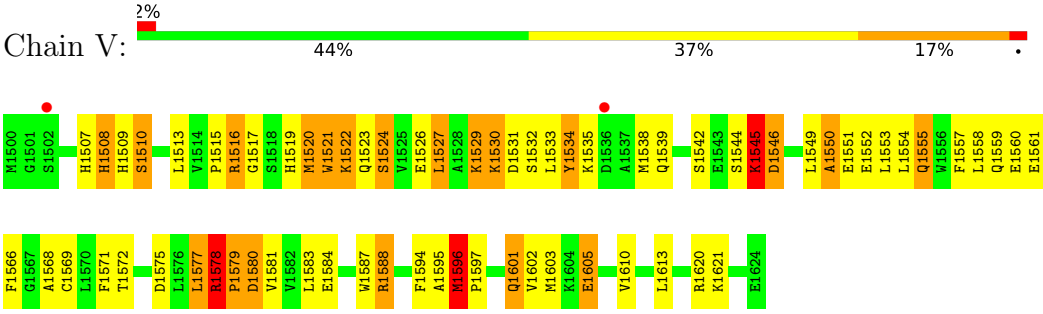
• Molecule 1: Clathrin heavy chain 1

Chain U:



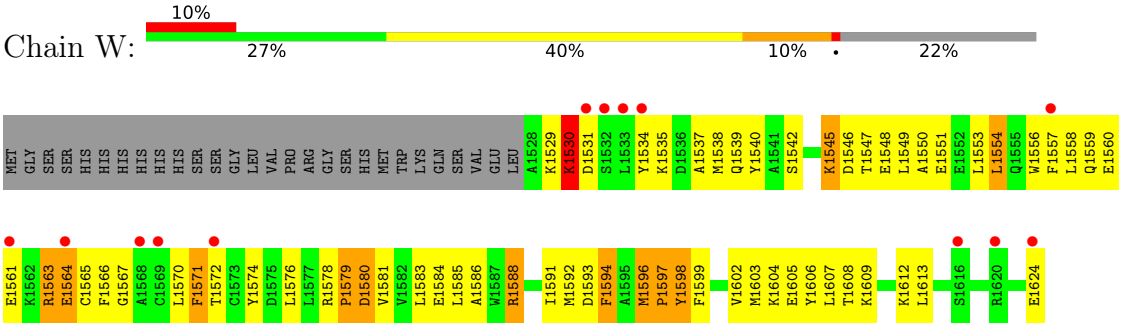
• Molecule 1: Clathrin heavy chain 1

Chain V:



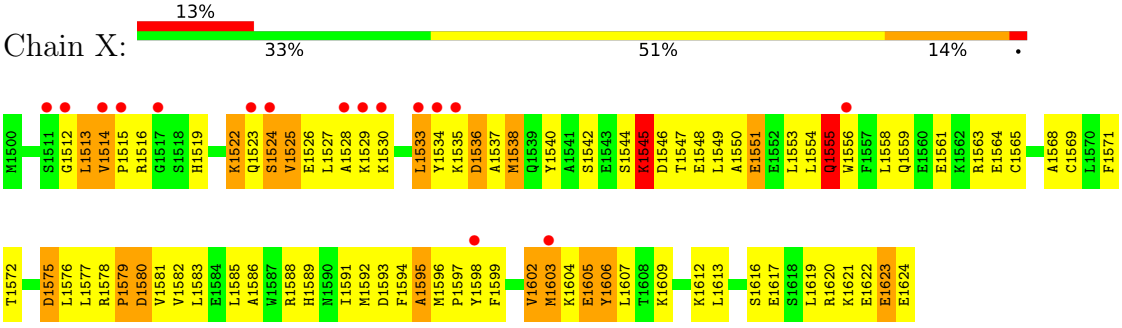
• Molecule 1: Clathrin heavy chain 1

Chain W:



• Molecule 1: Clathrin heavy chain 1

Chain X:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	255.78Å 255.78Å 312.99Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	54.58 – 3.92 48.34 – 3.92	Depositor EDS
% Data completeness (in resolution range)	86.1 (54.58-3.92) 89.0 (48.34-3.92)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.68 (at 3.88Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.339 , 0.386 0.343 , 0.360	Depositor DCC
R_{free} test set	6653 reflections (9.74%)	wwPDB-VP
Wilson B-factor (Å^2)	134.3	Xtriage
Anisotropy	0.011	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 500.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.458 for -2/3*h-1/3*k+2/3*l,-1/3*h-2/3*k-2/3*l,2/3*h-2/3*k+1/3*l 0.458 for -h,1/3*h-1/3*k+2/3*l,2/3*h+4/3*k+1/3*l 0.458 for -1/3*h+1/3*k-2/3*l,-k,-4/3*h-2/3*k+1/3*l 0.458 for -h,2/3*h+1/3*k-2/3*l,-2/3*h-4/3*k-1/3*l 0.458 for 1/3*h+2/3*k+2/3*l,-k,4/3*h+2/3*k-1/3*l 0.458 for -1/3*h-2/3*k-2/3*l,-2/3*h-1/3*k+2/3*l,-2/3*h+2/3*k-1/3*l 0.458 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	23032	wwPDB-VP
Average B, all atoms (Å^2)	277.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% 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)

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	0.85	2/1060 (0.2%)	0.89	1/1424 (0.1%)
1	B	0.70	0/827	0.73	0/1110
1	C	0.74	3/1060 (0.3%)	0.75	0/1424
1	D	0.81	1/1060 (0.1%)	0.90	2/1424 (0.1%)
1	E	0.82	1/827 (0.1%)	0.79	0/1110
1	F	0.71	1/1060 (0.1%)	0.76	0/1424
1	G	0.80	0/1060	0.87	2/1424 (0.1%)
1	H	0.77	0/827	0.81	0/1110
1	I	0.81	3/1060 (0.3%)	0.78	0/1424
1	J	0.82	2/1060 (0.2%)	0.88	0/1424
1	K	0.75	1/827 (0.1%)	0.74	0/1110
1	L	0.76	0/1060	0.82	1/1424 (0.1%)
1	M	0.81	0/1060	0.89	2/1424 (0.1%)
1	N	0.74	0/827	0.74	0/1110
1	O	0.73	0/1060	0.79	0/1424
1	P	0.84	2/1060 (0.2%)	0.89	2/1424 (0.1%)
1	Q	0.76	0/827	0.76	0/1110
1	R	0.74	0/1060	0.75	0/1424
1	S	0.82	0/1060	0.85	0/1424
1	T	0.74	1/827 (0.1%)	0.74	0/1110
1	U	0.74	1/1060 (0.1%)	0.76	0/1424
1	V	0.83	0/1060	0.89	1/1424 (0.1%)
1	W	0.72	0/827	0.73	0/1110
1	X	0.77	1/1060 (0.1%)	0.76	0/1424
All	All	0.78	19/23576 (0.1%)	0.81	11/31664 (0.0%)

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	1544	SER	CA-CB	6.89	1.63	1.52
1	I	1586	ALA	CA-CB	-6.60	1.38	1.52
1	A	1514	VAL	CA-CB	-6.34	1.41	1.54
1	K	1537	ALA	CA-CB	6.26	1.65	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	1544	SER	CA-CB	6.06	1.62	1.52

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	1565	CYS	CA-CB-SG	7.19	126.94	114.00
1	M	1527	LEU	CB-CG-CD2	-5.96	100.87	111.00
1	G	1527	LEU	CB-CG-CD2	-5.73	101.26	111.00
1	P	1544	SER	CA-CB-OG	5.71	126.62	111.20
1	P	1517	GLY	N-CA-C	5.41	126.63	113.10

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	1034	0	991	87	0
1	B	811	0	788	85	0
1	C	1034	0	991	112	0
1	D	1034	0	991	97	1
1	E	811	0	788	98	0
1	F	1034	0	991	143	0
1	G	1034	0	991	93	0
1	H	811	0	788	97	0
1	I	1034	0	991	105	0
1	J	1034	0	991	81	0
1	K	811	0	788	102	0
1	L	1034	0	991	153	0
1	M	1034	0	991	85	0
1	N	811	0	788	96	0
1	O	1034	0	991	130	0
1	P	1034	0	991	87	0
1	Q	811	0	788	78	0
1	R	1034	0	991	124	0
1	S	1034	0	991	99	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	T	811	0	788	128	0
1	U	1034	0	991	143	1
1	V	1034	0	991	97	0
1	W	811	0	788	106	0
1	X	1034	0	991	114	0
All	All	23032	0	22160	2357	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 52.

The worst 5 of 2357 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:T:1604:LYS:HD3	1:U:1612:LYS:NZ	1.44	1.31
1:L:1533:LEU:HD12	1:V:1588:ARG:NH2	1.58	1.18
1:E:1546:ASP:H	1:E:1550:ALA:HB2	1.07	1.16
1:V:1572:THR:HA	1:V:1578:ARG:NH2	1.60	1.16
1:M:1593:ASP:HA	1:O:1587:TRP:CZ3	1.82	1.14

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:1588:ARG:NH1	1:U:1533:LEU:CG[3_655]	2.17	0.03

5.3 Torsion angles

5.3.1 Protein backbone

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	123/125 (98%)	77 (63%)	29 (24%)	17 (14%)	0 4
1	B	95/125 (76%)	60 (63%)	28 (30%)	7 (7%)	1 16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	123/125 (98%)	78 (63%)	28 (23%)	17 (14%)	0 4
1	D	123/125 (98%)	76 (62%)	29 (24%)	18 (15%)	0 4
1	E	95/125 (76%)	61 (64%)	28 (30%)	6 (6%)	1 19
1	F	123/125 (98%)	78 (63%)	29 (24%)	16 (13%)	0 5
1	G	123/125 (98%)	77 (63%)	29 (24%)	17 (14%)	0 4
1	H	95/125 (76%)	61 (64%)	27 (28%)	7 (7%)	1 16
1	I	123/125 (98%)	76 (62%)	31 (25%)	16 (13%)	0 5
1	J	123/125 (98%)	74 (60%)	31 (25%)	18 (15%)	0 4
1	K	95/125 (76%)	59 (62%)	29 (30%)	7 (7%)	1 16
1	L	123/125 (98%)	80 (65%)	26 (21%)	17 (14%)	0 4
1	M	123/125 (98%)	75 (61%)	31 (25%)	17 (14%)	0 4
1	N	95/125 (76%)	62 (65%)	27 (28%)	6 (6%)	1 19
1	O	123/125 (98%)	78 (63%)	28 (23%)	17 (14%)	0 4
1	P	123/125 (98%)	77 (63%)	29 (24%)	17 (14%)	0 4
1	Q	95/125 (76%)	59 (62%)	29 (30%)	7 (7%)	1 16
1	R	123/125 (98%)	79 (64%)	27 (22%)	17 (14%)	0 4
1	S	123/125 (98%)	78 (63%)	27 (22%)	18 (15%)	0 4
1	T	95/125 (76%)	61 (64%)	28 (30%)	6 (6%)	1 19
1	U	123/125 (98%)	77 (63%)	30 (24%)	16 (13%)	0 5
1	V	123/125 (98%)	77 (63%)	27 (22%)	19 (15%)	0 3
1	W	95/125 (76%)	59 (62%)	29 (30%)	7 (7%)	1 16
1	X	123/125 (98%)	78 (63%)	29 (24%)	16 (13%)	0 5
All	All	2728/3000 (91%)	1717 (63%)	685 (25%)	326 (12%)	0 6

5 of 326 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1508	HIS
1	A	1516	ARG
1	A	1545	LYS
1	A	1578	ARG
1	A	1605	GLU

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	113/113 (100%)	103 (91%)	10 (9%)	10	36
1	B	88/113 (78%)	78 (89%)	10 (11%)	5	26
1	C	113/113 (100%)	99 (88%)	14 (12%)	4	24
1	D	113/113 (100%)	102 (90%)	11 (10%)	8	31
1	E	88/113 (78%)	79 (90%)	9 (10%)	7	30
1	F	113/113 (100%)	101 (89%)	12 (11%)	6	29
1	G	113/113 (100%)	101 (89%)	12 (11%)	6	29
1	H	88/113 (78%)	79 (90%)	9 (10%)	7	30
1	I	113/113 (100%)	101 (89%)	12 (11%)	6	29
1	J	113/113 (100%)	102 (90%)	11 (10%)	8	31
1	K	88/113 (78%)	79 (90%)	9 (10%)	7	30
1	L	113/113 (100%)	100 (88%)	13 (12%)	5	26
1	M	113/113 (100%)	101 (89%)	12 (11%)	6	29
1	N	88/113 (78%)	80 (91%)	8 (9%)	9	35
1	O	113/113 (100%)	100 (88%)	13 (12%)	5	26
1	P	113/113 (100%)	102 (90%)	11 (10%)	8	31
1	Q	88/113 (78%)	79 (90%)	9 (10%)	7	30
1	R	113/113 (100%)	100 (88%)	13 (12%)	5	26
1	S	113/113 (100%)	102 (90%)	11 (10%)	8	31
1	T	88/113 (78%)	78 (89%)	10 (11%)	5	26
1	U	113/113 (100%)	101 (89%)	12 (11%)	6	29
1	V	113/113 (100%)	101 (89%)	12 (11%)	6	29
1	W	88/113 (78%)	78 (89%)	10 (11%)	5	26
1	X	113/113 (100%)	101 (89%)	12 (11%)	6	29
All	All	2512/2712 (93%)	2247 (90%)	265 (10%)	7	29

5 of 265 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	V	1520	MET
1	V	1562	LYS
1	X	1555	GLN
1	I	1606	TYR
1	I	1556	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 72 such sidechains are listed below:

Mol	Chain	Res	Type
1	U	1519	HIS
1	X	1590	ASN
1	U	1539	GLN
1	W	1559	GLN
1	I	1559	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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, 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	125/125 (100%)	-0.12	5 (4%) 38 31	1, 194, 535, 658	0
1	B	97/125 (77%)	0.58	16 (16%) 1 2	65, 222, 595, 778	0
1	C	125/125 (100%)	0.63	15 (12%) 4 5	30, 257, 615, 873	0
1	D	125/125 (100%)	-0.16	2 (1%) 72 62	1, 195, 535, 658	0
1	E	97/125 (77%)	0.53	15 (15%) 2 2	68, 222, 595, 779	0
1	F	125/125 (100%)	0.40	16 (12%) 3 4	36, 256, 615, 873	0
1	G	125/125 (100%)	-0.14	4 (3%) 47 37	1, 195, 535, 658	0
1	H	97/125 (77%)	0.51	12 (12%) 4 5	69, 222, 595, 778	0
1	I	125/125 (100%)	0.47	16 (12%) 3 4	28, 256, 615, 873	0
1	J	125/125 (100%)	-0.06	9 (7%) 15 12	1, 195, 535, 658	0
1	K	97/125 (77%)	0.25	10 (10%) 6 6	69, 222, 595, 778	0
1	L	125/125 (100%)	0.62	16 (12%) 3 4	30, 257, 615, 873	0
1	M	125/125 (100%)	-0.05	6 (4%) 30 26	7, 195, 535, 658	0
1	N	97/125 (77%)	0.44	12 (12%) 4 5	70, 222, 595, 778	0
1	O	125/125 (100%)	0.37	16 (12%) 3 4	27, 256, 615, 873	0
1	P	125/125 (100%)	0.02	5 (4%) 38 31	14, 194, 536, 658	0
1	Q	97/125 (77%)	0.29	8 (8%) 11 10	68, 221, 595, 778	0
1	R	125/125 (100%)	0.57	16 (12%) 3 4	24, 257, 615, 873	0
1	S	125/125 (100%)	-0.16	5 (4%) 38 31	5, 194, 535, 658	0
1	T	97/125 (77%)	0.49	16 (16%) 1 2	69, 222, 595, 778	0
1	U	125/125 (100%)	0.39	12 (9%) 8 7	37, 256, 615, 873	0
1	V	125/125 (100%)	-0.21	2 (1%) 72 62	1, 194, 535, 658	0
1	W	97/125 (77%)	0.46	13 (13%) 3 3	70, 221, 595, 778	0
1	X	125/125 (100%)	0.40	16 (12%) 3 4	32, 257, 615, 873	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
All	All	2776/3000 (92%)	0.26	263 (9%)	8	7	1, 218, 595, 873	0

The worst 5 of 263 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	1515	PRO	14.5
1	I	1515	PRO	13.6
1	C	1515	PRO	13.3
1	F	1515	PRO	12.3
1	E	1568	ALA	11.7

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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.