wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 10:29 AM GMT

PDB ID	:	3LVH
Title	:	Crystal structure of a clathrin heavy chain and clathrin light chain complex
Authors	:	Wilbur, J.D.; Hwang, P.K.; Ybe, J.A.; Lane, M.; Sellers, B.D.; Jacobson, M.P.; Fletterick, R.J.; Brodsky, F.M.
Deposited on	:	2010-02-20
Resolution	:	9.00 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:

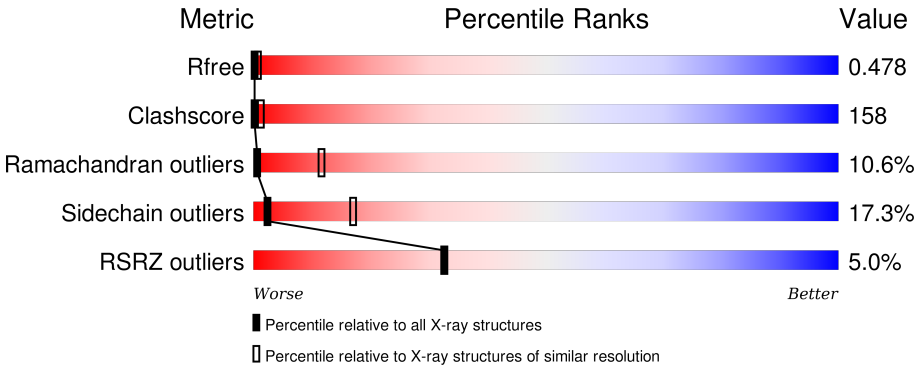
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 9.00 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	1015 (11.50-3.66)
Clashscore	102246	1064 (11.50-3.70)
Ramachandran outliers	100387	1036 (11.50-3.66)
Sidechain outliers	100360	1006 (11.50-3.66)
RSRZ outliers	91569	1014 (11.50-3.66)

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	624	8% 13% 51% 20% 5% 11%
1	B	624	% 12% 52% 20% 5% 11%
1	C	624	2% 13% 52% 20% 5% 11%
2	D	205	2% 9% 33% 11% • 45%
2	E	205	11% 9% 28% 9% • 50%

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Mol	Chain	Length	Quality of chain
2	F	205	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 16020 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	554	Total	C	N	O	S	0	0	0
			4550	2901	768	856	25			
1	B	554	Total	C	N	O	S	0	0	0
			4550	2901	768	856	25			
1	C	554	Total	C	N	O	S	0	0	0
			4550	2901	768	856	25			

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1052	MET	-	EXPRESSION TAG	UNP P49951
A	1053	GLY	-	EXPRESSION TAG	UNP P49951
A	1054	SER	-	EXPRESSION TAG	UNP P49951
A	1055	SER	-	EXPRESSION TAG	UNP P49951
A	1056	HIS	-	EXPRESSION TAG	UNP P49951
A	1057	HIS	-	EXPRESSION TAG	UNP P49951
A	1058	HIS	-	EXPRESSION TAG	UNP P49951
A	1059	HIS	-	EXPRESSION TAG	UNP P49951
A	1060	HIS	-	EXPRESSION TAG	UNP P49951
A	1061	HIS	-	EXPRESSION TAG	UNP P49951
A	1062	SER	-	EXPRESSION TAG	UNP P49951
A	1063	SER	-	EXPRESSION TAG	UNP P49951
A	1064	GLY	-	EXPRESSION TAG	UNP P49951
A	1065	LEU	-	EXPRESSION TAG	UNP P49951
A	1066	VAL	-	EXPRESSION TAG	UNP P49951
A	1067	PRO	-	EXPRESSION TAG	UNP P49951
A	1068	ARG	-	EXPRESSION TAG	UNP P49951
A	1069	GLY	-	EXPRESSION TAG	UNP P49951
A	1070	SER	-	EXPRESSION TAG	UNP P49951
A	1071	HIS	-	EXPRESSION TAG	UNP P49951
A	1072	MET	-	EXPRESSION TAG	UNP P49951
A	1073	LEU	-	EXPRESSION TAG	UNP P49951
B	1052	MET	-	EXPRESSION TAG	UNP P49951

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1053	GLY	-	EXPRESSION TAG	UNP P49951
B	1054	SER	-	EXPRESSION TAG	UNP P49951
B	1055	SER	-	EXPRESSION TAG	UNP P49951
B	1056	HIS	-	EXPRESSION TAG	UNP P49951
B	1057	HIS	-	EXPRESSION TAG	UNP P49951
B	1058	HIS	-	EXPRESSION TAG	UNP P49951
B	1059	HIS	-	EXPRESSION TAG	UNP P49951
B	1060	HIS	-	EXPRESSION TAG	UNP P49951
B	1061	HIS	-	EXPRESSION TAG	UNP P49951
B	1062	SER	-	EXPRESSION TAG	UNP P49951
B	1063	SER	-	EXPRESSION TAG	UNP P49951
B	1064	GLY	-	EXPRESSION TAG	UNP P49951
B	1065	LEU	-	EXPRESSION TAG	UNP P49951
B	1066	VAL	-	EXPRESSION TAG	UNP P49951
B	1067	PRO	-	EXPRESSION TAG	UNP P49951
B	1068	ARG	-	EXPRESSION TAG	UNP P49951
B	1069	GLY	-	EXPRESSION TAG	UNP P49951
B	1070	SER	-	EXPRESSION TAG	UNP P49951
B	1071	HIS	-	EXPRESSION TAG	UNP P49951
B	1072	MET	-	EXPRESSION TAG	UNP P49951
B	1073	LEU	-	EXPRESSION TAG	UNP P49951
C	1052	MET	-	EXPRESSION TAG	UNP P49951
C	1053	GLY	-	EXPRESSION TAG	UNP P49951
C	1054	SER	-	EXPRESSION TAG	UNP P49951
C	1055	SER	-	EXPRESSION TAG	UNP P49951
C	1056	HIS	-	EXPRESSION TAG	UNP P49951
C	1057	HIS	-	EXPRESSION TAG	UNP P49951
C	1058	HIS	-	EXPRESSION TAG	UNP P49951
C	1059	HIS	-	EXPRESSION TAG	UNP P49951
C	1060	HIS	-	EXPRESSION TAG	UNP P49951
C	1061	HIS	-	EXPRESSION TAG	UNP P49951
C	1062	SER	-	EXPRESSION TAG	UNP P49951
C	1063	SER	-	EXPRESSION TAG	UNP P49951
C	1064	GLY	-	EXPRESSION TAG	UNP P49951
C	1065	LEU	-	EXPRESSION TAG	UNP P49951
C	1066	VAL	-	EXPRESSION TAG	UNP P49951
C	1067	PRO	-	EXPRESSION TAG	UNP P49951
C	1068	ARG	-	EXPRESSION TAG	UNP P49951
C	1069	GLY	-	EXPRESSION TAG	UNP P49951
C	1070	SER	-	EXPRESSION TAG	UNP P49951
C	1071	HIS	-	EXPRESSION TAG	UNP P49951
C	1072	MET	-	EXPRESSION TAG	UNP P49951

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1073	LEU	-	EXPRESSION TAG	UNP P49951

- Molecule 2 is a protein called Clathrin light chain B.

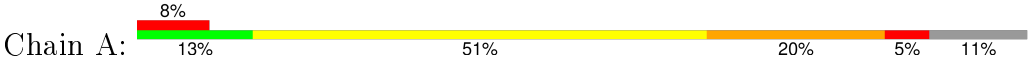
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	113	Total	C	N	O	S	0	0	0
			811	489	160	161	1			
2	E	102	Total	C	N	O	S	0	0	0
			753	455	149	148	1			
2	F	112	Total	C	N	O	S	0	0	0
			806	486	159	160	1			

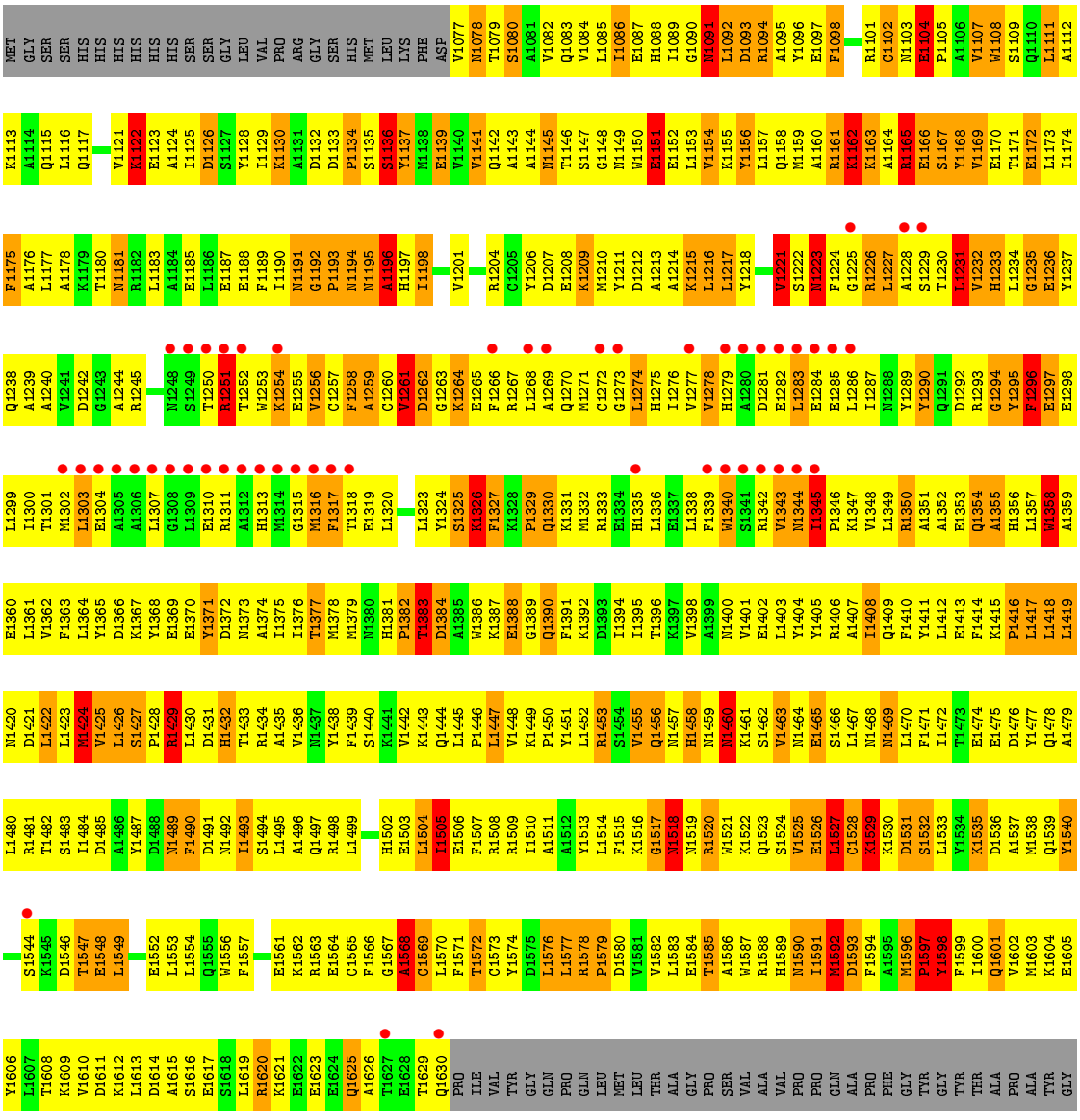
3 Residue-property plots (i)

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: Clathrin heavy chain 1

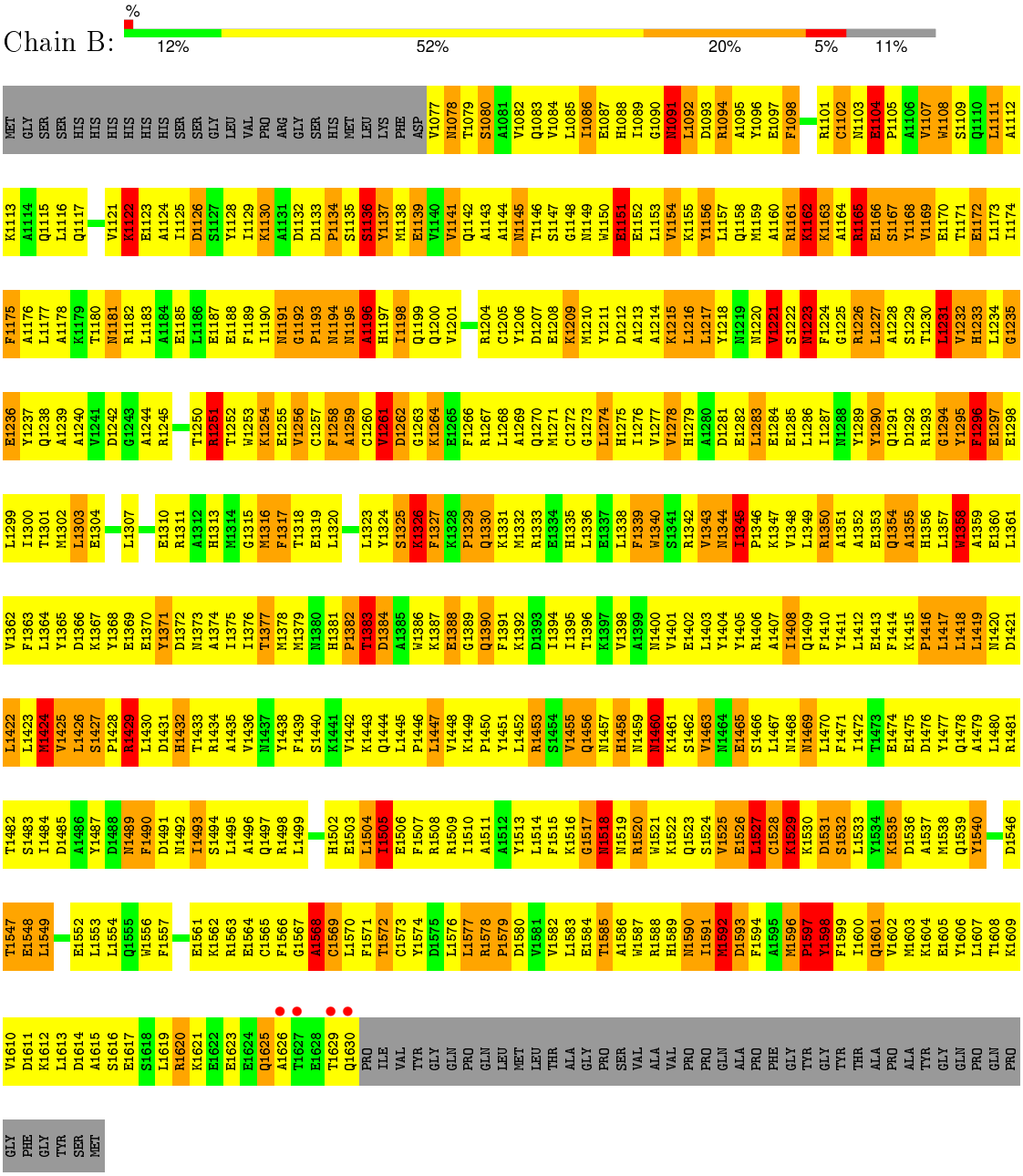
Chain A:





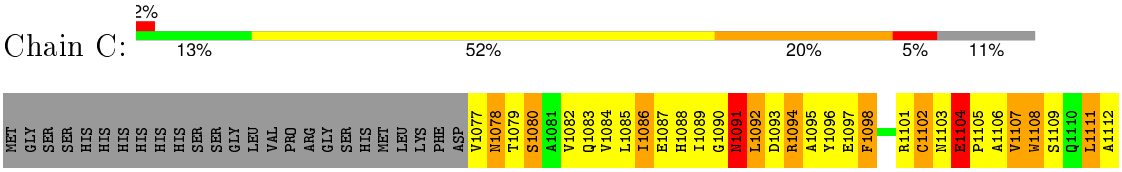
- Molecule 1: Clathrin heavy chain 1

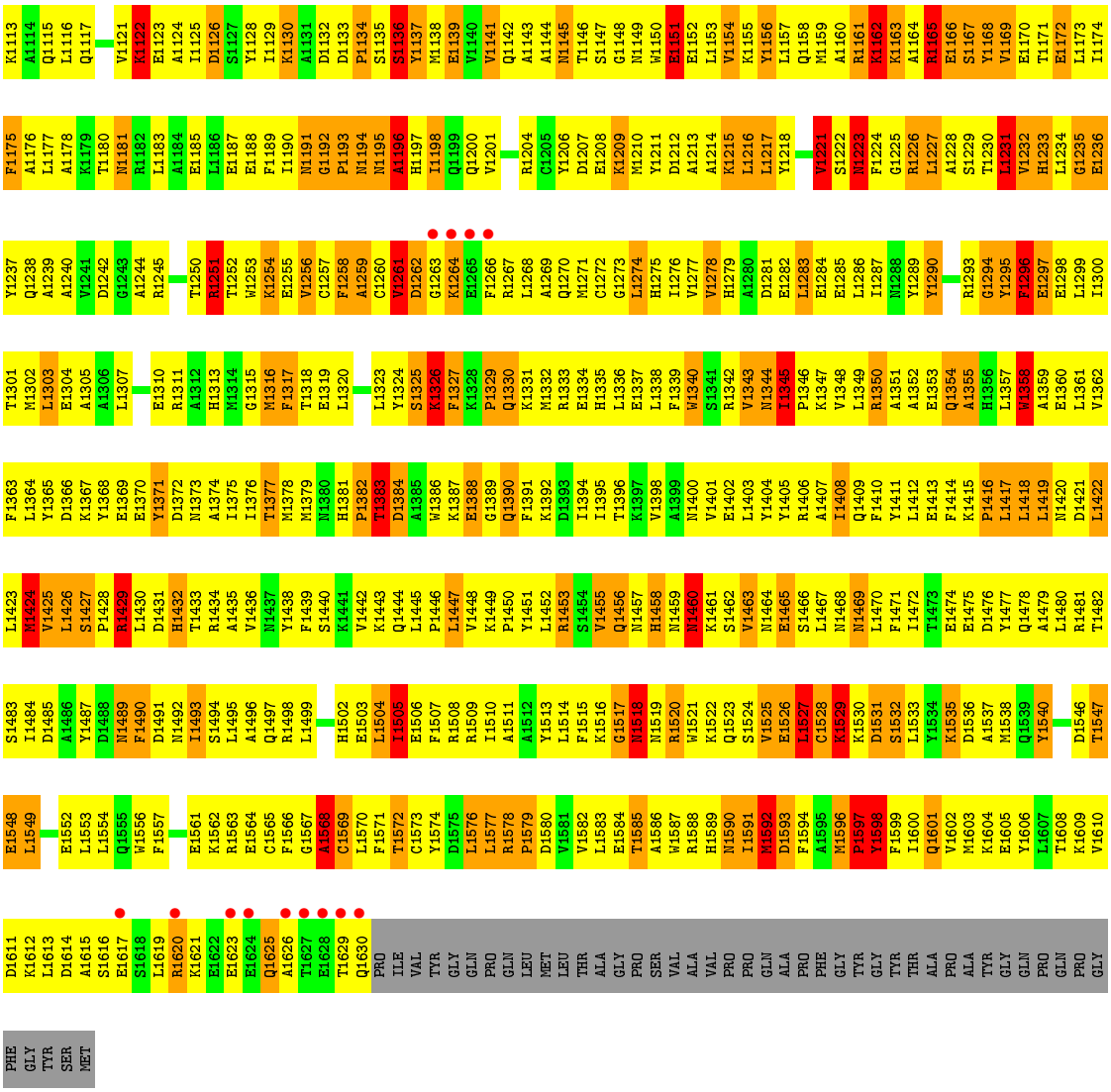
Chain B:



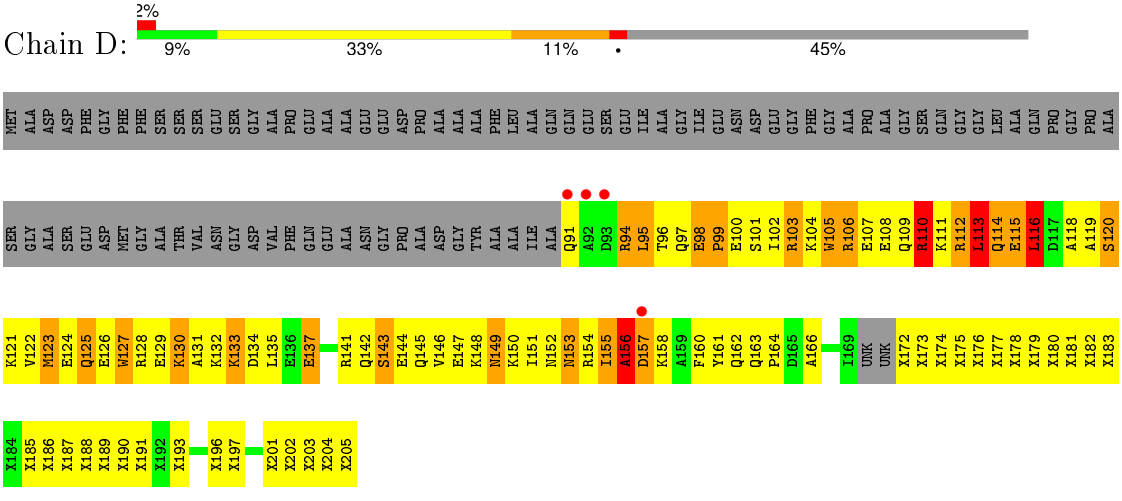
- Molecule 1: Clathrin heavy chain 1

Chain C:



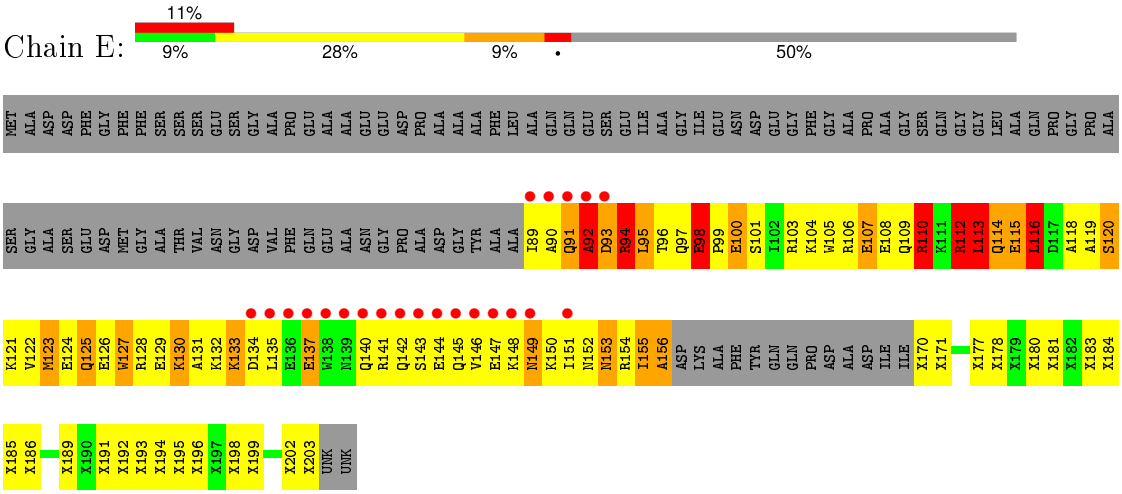


• Molecule 2: Clathrin light chain B



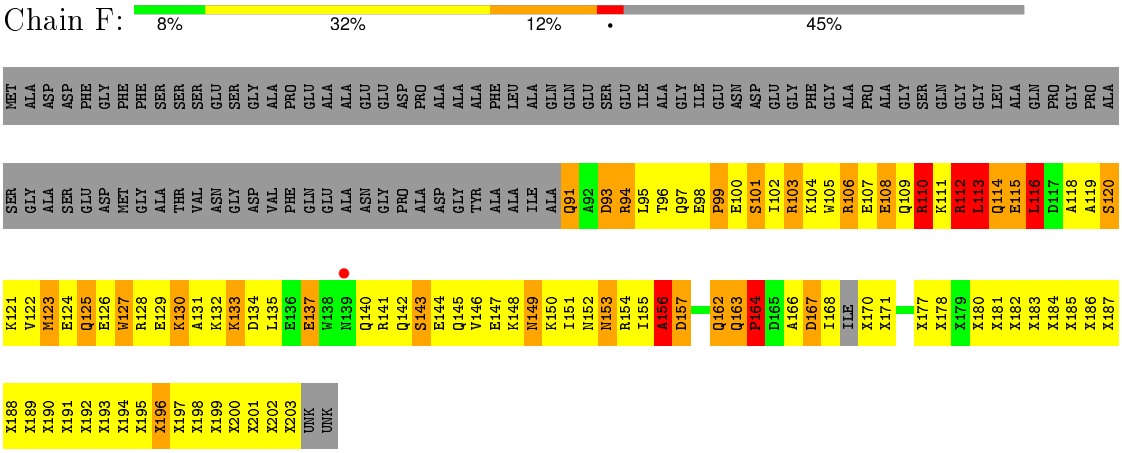
• Molecule 2: Clathrin light chain B

Chain E:



- Molecule 2: Clathrin light chain B

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α, β, γ	229.71Å 229.71Å 512.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	500.00 – 9.00 86.66 – 9.00	Depositor EDS
% Data completeness (in resolution range)	78.7 (500.00-9.00) 78.9 (86.66-9.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.18	Depositor
$< I/\sigma(I) >$ [1]	1.66 (at 8.41Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.473 , 0.487 0.483 , 0.478	Depositor DCC
R_{free} test set	430 reflections (5.33%)	DCC
Wilson B-factor (Å^2)	604.9	Xtriage
Anisotropy	0.404	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.09 , -10.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.38$, $< L^2 > = 0.21$	Xtriage
Outliers	1 of 8529 reflections (0.012%)	Xtriage
F_o,F_c correlation	0.69	EDS
Total number of atoms	16020	wwPDB-VP
Average B, all atoms (Å^2)	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.04% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.48	3/4645 (0.1%)	1.41	104/6276 (1.7%)
1	B	0.36	2/4645 (0.0%)	1.38	101/6276 (1.6%)
1	C	0.36	2/4645 (0.0%)	1.38	101/6276 (1.6%)
2	D	0.74	0/647	1.15	8/866 (0.9%)
2	E	0.69	0/589	1.24	5/785 (0.6%)
2	F	0.77	0/642	1.20	8/859 (0.9%)
All	All	0.46	7/15813 (0.0%)	1.37	327/21338 (1.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	7
1	B	0	6
1	C	0	6
2	F	0	1
All	All	0	20

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1196	ALA	C-N	-21.36	0.84	1.34
1	C	1136	SER	C-N	-13.41	1.03	1.34
1	B	1136	SER	C-N	-13.39	1.03	1.34
1	A	1136	SER	C-N	-13.36	1.03	1.34
1	B	1592	MET	C-N	-10.33	1.10	1.34

The worst 5 of 327 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	1136	SER	C-N-CA	22.64	178.31	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1136	SER	C-N-CA	22.63	178.27	121.70
1	A	1136	SER	C-N-CA	22.58	178.15	121.70
1	A	1196	ALA	CB-CA-C	21.84	142.86	110.10
1	C	1196	ALA	CB-CA-C	21.79	142.78	110.10

There are no chirality outliers.

5 of 20 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1136	SER	Mainchain
1	A	1196	ALA	Mainchain,Peptide
1	A	1223	ASN	Peptide
1	A	1326	LYS	Peptide
1	A	1429	ARG	Peptide

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	4550	0	4457	1578	23
1	B	4550	0	4456	1511	40
1	C	4550	0	4461	1420	30
2	D	811	0	641	286	0
2	E	753	0	615	220	0
2	F	806	0	640	345	35
All	All	16020	0	15270	4959	70

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 158.

The worst 5 of 4959 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:C:1253:TRP:CZ3	1:C:1276:ILE:HG22	1.19	1.67
1:A:1253:TRP:CZ3	1:A:1276:ILE:HG22	1.19	1.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1253:TRP:CZ3	1:B:1276:ILE:HG22	1.19	1.67
2:E:203:UNK:C	2:E:203:UNK:CA	1.76	1.62
1:B:1108:TRP:CH2	1:B:1129:ILE:HB	1.34	1.61

The worst 5 of 70 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:B:1198:ILE:N	2:F:103:ARG:NH1[5_545]	0.57	1.63
1:B:1199:GLN:N	2:F:103:ARG:NH2[5_545]	0.64	1.56
1:A:1097:GLU:OE1	1:C:1094:ARG:CG[8_465]	0.90	1.30
1:A:1097:GLU:CD	1:C:1094:ARG:CG[8_465]	0.92	1.28
1:B:1198:ILE:CD1	2:F:103:ARG:CB[5_545]	0.98	1.22

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	552/624 (88%)	332 (60%)	164 (30%)	56 (10%)	1 14
1	B	552/624 (88%)	332 (60%)	166 (30%)	54 (10%)	1 14
1	C	552/624 (88%)	332 (60%)	166 (30%)	54 (10%)	1 14
2	D	77/205 (38%)	50 (65%)	16 (21%)	11 (14%)	0 6
2	E	66/205 (32%)	35 (53%)	21 (32%)	10 (15%)	0 5
2	F	76/205 (37%)	42 (55%)	20 (26%)	14 (18%)	0 4
All	All	1875/2487 (75%)	1123 (60%)	553 (30%)	199 (11%)	0 11

5 of 199 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1086	ILE

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Mol	Chain	Res	Type
1	A	1122	LYS
1	A	1193	PRO
1	A	1231	LEU
1	A	1251	ARG

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	486/541 (90%)	410 (84%)	76 (16%)	3 21
1	B	486/541 (90%)	409 (84%)	77 (16%)	3 21
1	C	486/541 (90%)	410 (84%)	76 (16%)	3 21
2	D	62/128 (48%)	45 (73%)	17 (27%)	0 4
2	E	61/128 (48%)	42 (69%)	19 (31%)	0 2
2	F	62/128 (48%)	42 (68%)	20 (32%)	0 2
All	All	1643/2007 (82%)	1358 (83%)	285 (17%)	2 17

5 of 285 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1422	LEU
1	C	1111	LEU
2	E	153	ASN
1	B	1460	ASN
1	B	1574	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 71 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1381	HIS
1	B	1489	ASN
2	D	149	ASN
1	B	1390	GLN

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Mol	Chain	Res	Type
1	B	1457	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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	554/624 (88%)	0.10	51 (9%) 11 16	50, 50, 132, 133	0
1	B	554/624 (88%)	-0.24	4 (0%) 89 85	50, 50, 132, 133	0
1	C	554/624 (88%)	-0.34	13 (2%) 64 59	50, 50, 132, 133	0
2	D	79/205 (38%)	0.23	4 (5%) 32 32	298, 298, 298, 298	0
2	E	68/205 (33%)	1.51	22 (32%) 1 5	314, 314, 314, 314	0
2	F	78/205 (38%)	-0.12	1 (1%) 79 73	339, 339, 339, 339	0
All	All	1887/2487 (75%)	-0.08	95 (5%) 32 32	50, 50, 314, 339	0

The worst 5 of 95 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1313	HIS	7.4
1	A	1306	ALA	6.9
1	A	1312	ALA	6.9
1	A	1341	SER	6.5
1	A	1279	HIS	6.5

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.