



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Aug 21, 2017 – 04:46 PM EDT

PDB ID : 4BZI
EMDB ID: : EMD-2428
Title : The structure of the COPII coat assembled on membranes
Authors : Zanetti, G.; Prinz, S.; Daum, S.; Meister, A.; Schekman, R.; Bacia, K.; Briggs, J.A.G.
Deposited on : unknown
Resolution : 23.00 Å(reported)
Based on PDB ID : 1M2O

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

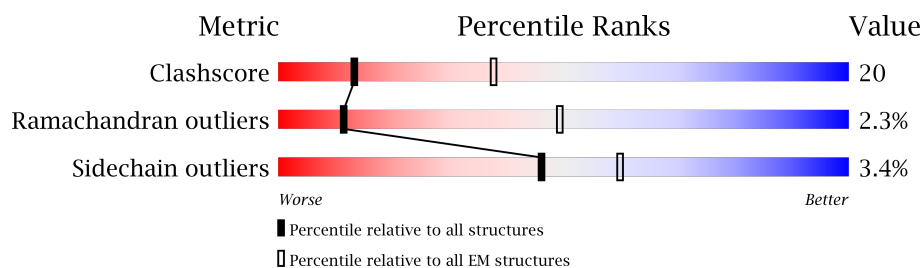
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 23.00 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)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	768	68% 25% • 5%
1	D	768	68% 25% • 5%
1	G	768	69% 25% • 5%
2	B	190	52% 31% • 14%
2	J	190	53% 31% • 14%
2	K	190	52% 32% • 14%
3	E	926	45% 31% • 21%
3	L	926	45% 31% • 21%
3	M	926	45% 32% • 21%

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Mol	Chain	Length	Quality of chain
4	F	926	99%
4	N	926	98%
4	O	926	98%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 39154 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 SEC23P.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	733	Total	C	N	O	S	0	0
			5780	3679	969	1109	23		
1	D	733	Total	C	N	O	S	0	0
			5780	3679	969	1109	23		
1	G	733	Total	C	N	O	S	0	0
			5780	3679	969	1109	23		

- Molecule 2 is a protein called SAR1P.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	164	Total	C	N	O	S	0	0
			1299	836	220	239	4		
2	J	164	Total	C	N	O	S	0	0
			1299	836	220	239	4		
2	K	164	Total	C	N	O	S	0	0
			1299	836	220	239	4		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	139	ALA	GLY	conflict	UNP C8ZIG2
J	139	ALA	GLY	conflict	UNP C8ZIG2
K	139	ALA	GLY	conflict	UNP C8ZIG2

- Molecule 3 is a protein called SEC24P.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	735	Total	C	N	O	S	0	0
			5823	3702	999	1084	38		
3	L	735	Total	C	N	O	S	0	0
			5823	3702	999	1084	38		
3	M	735	Total	C	N	O	S	0	0
			5823	3702	999	1084	38		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	408	THR	ALA	conflict	UNP C8ZAD6
E	865	VAL	ALA	conflict	UNP C8ZAD6
L	408	THR	ALA	conflict	UNP C8ZAD6
L	865	VAL	ALA	conflict	UNP C8ZAD6
M	408	THR	ALA	conflict	UNP C8ZAD6
M	865	VAL	ALA	conflict	UNP C8ZAD6

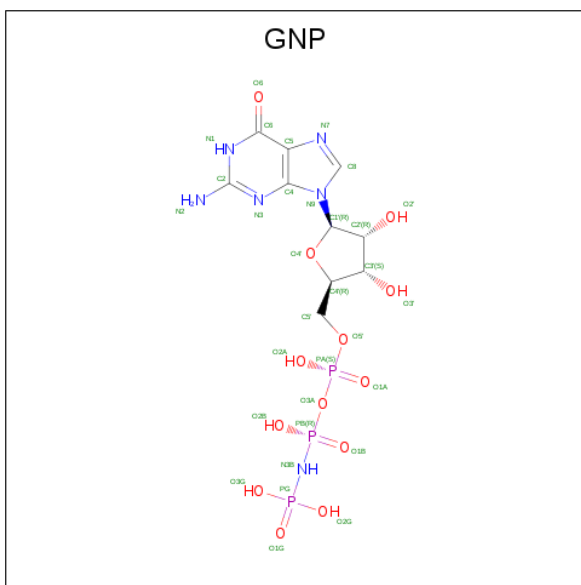
- Molecule 4 is a protein called SEC24P.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	F	13	Total	C	N	O	0	0
			109	70	19	20		
4	N	14	Total	C	N	O	0	0
			117	74	21	22		
4	O	14	Total	C	N	O	0	0
			117	74	21	22		

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
5	G	1	Total	Zn	0
			1	1	
5	D	1	Total	Zn	0
			1	1	
5	E	1	Total	Zn	0
			1	1	
5	A	1	Total	Zn	0
			1	1	
5	L	1	Total	Zn	0
			1	1	
5	M	1	Total	Zn	0
			1	1	

- Molecule 6 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: C₁₀H₁₇N₆O₁₃P₃).



Mol	Chain	Residues	Atoms					AltConf
6	B	1	Total 32	C 10	N 6	O 13	P 3	0
6	J	1	Total 32	C 10	N 6	O 13	P 3	0
6	K	1	Total 32	C 10	N 6	O 13	P 3	0

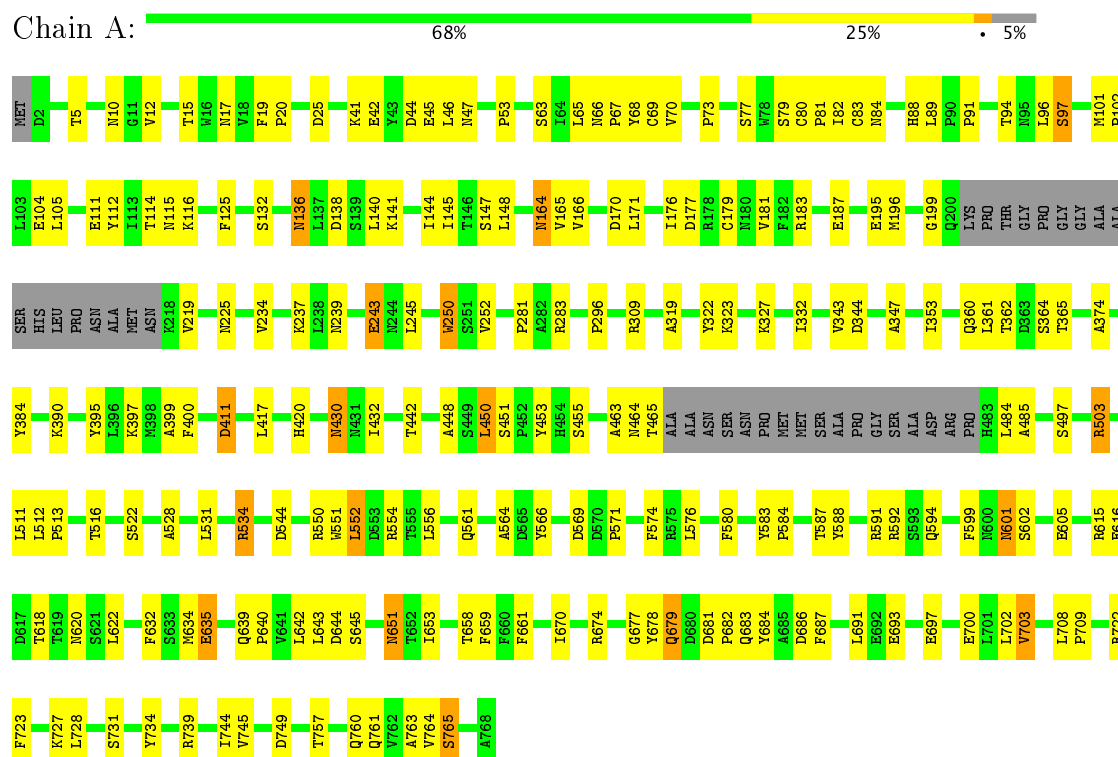
- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
7	B	1	Total Mg 1 1	0
7	J	1	Total Mg 1 1	0
7	K	1	Total Mg 1 1	0

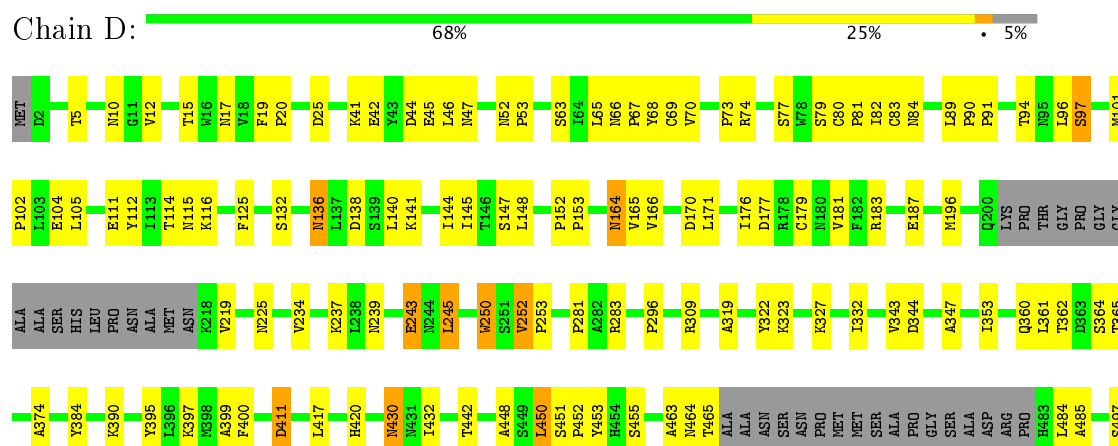
3 Residue-property plots

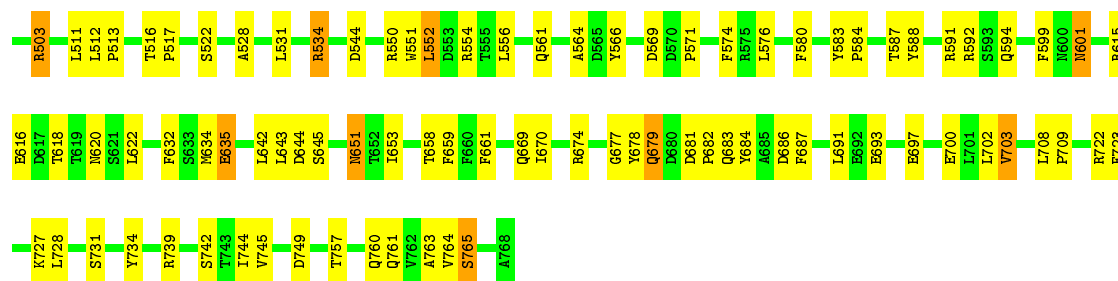
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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. 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: SEC23P



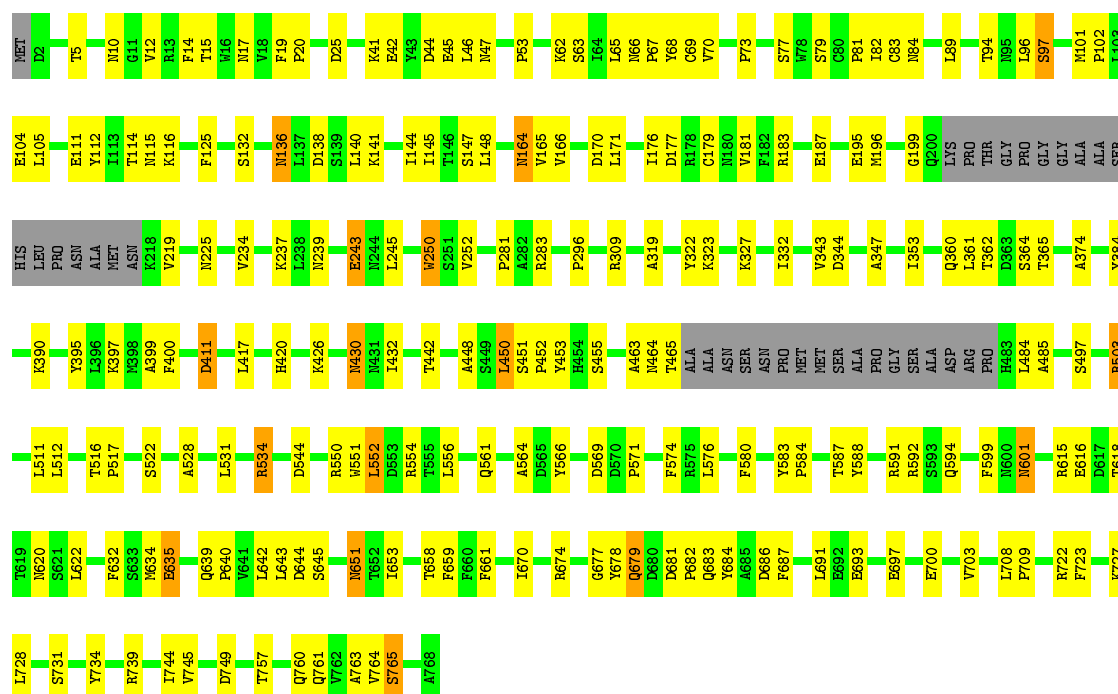
• Molecule 1: SEC23P





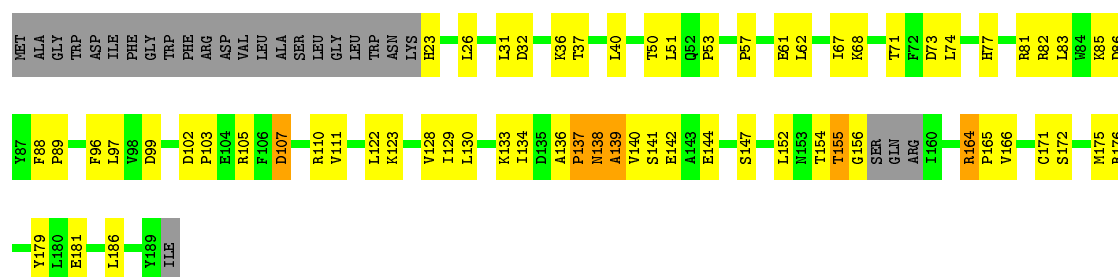
• Molecule 1: SEC23P

Chain G: 69% 25% 5%



• Molecule 2: SAR1P

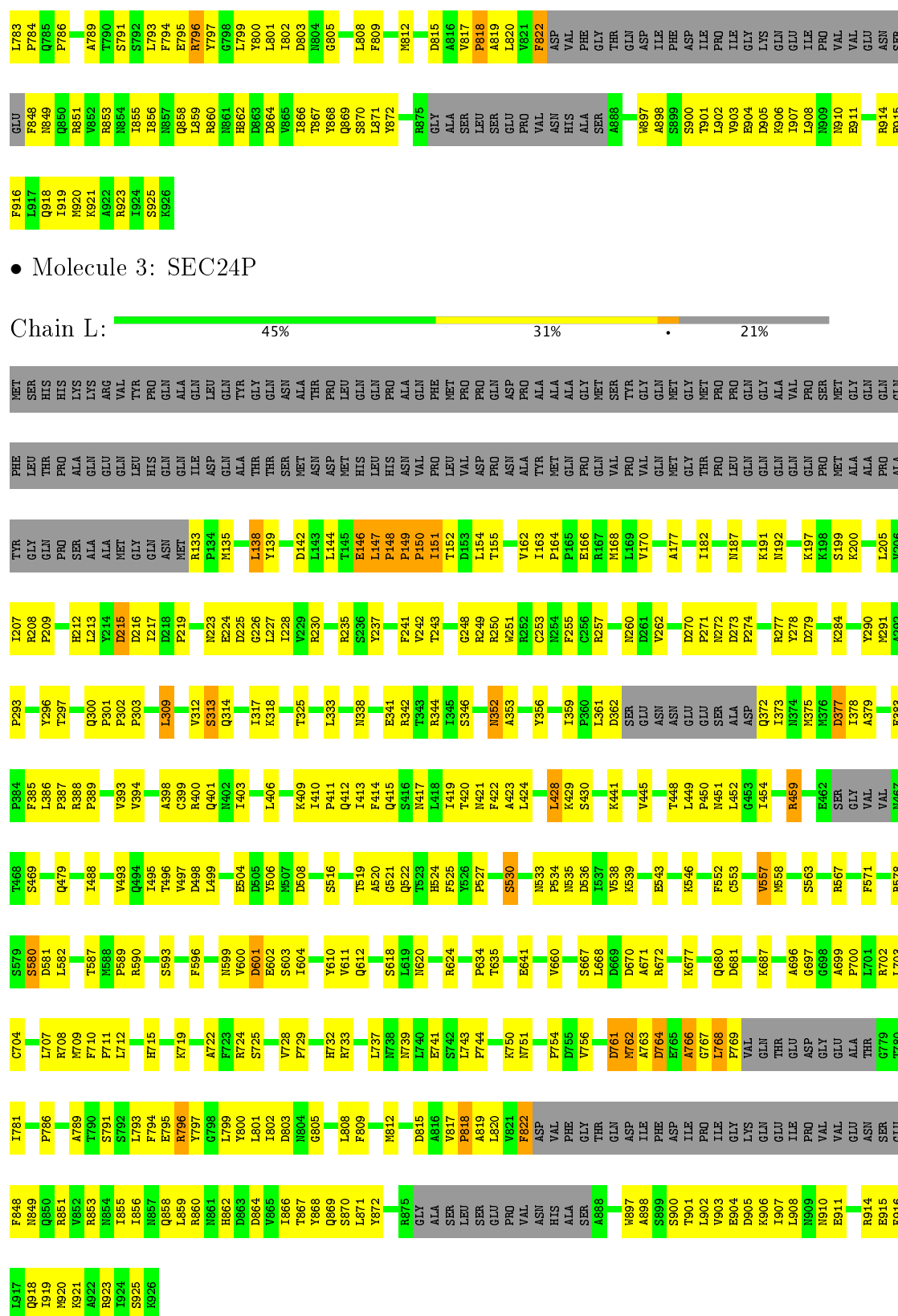
Chain B: 52% 31% 14%



• Molecule 2: SAR1P

Chain J: 53% 31% 14%





• Molecule 3: SEC24P

Chain M: 45% 32% 21%

TYR	GLY	P209	Y296	E383	SER	A696	GLN	GLN	K906
LEU	THR	E212	T297	F384	GLY	G697	THR	GLU	I907
GLN	PRO	L213		F385	VAL	G698	GLU	ILE	I908
HIS	ALA				VAL	A699	ASP	PRO	N909
LYS	GLN	Y214	Q300	L386	TYR	P700	GLY	VAL	N910
ARG	GLU	D215	P301	P387	LEU	L701	GLY	VAL	E911
VAL	GLN	D216	P302	R388	ALA	R702	ALA	GLU	
THR	LEU	I217	P303	R389	THR	L703	THR	ASN	R914
PRO	HIS	D218	C307	N390	GLY	C704	GLY	GLY	E915
GLN	GLN	P219	F308	N391	THR		THR	ASN	F916
ALA	ASN	P220	L309	M392	GLN	L707	GLN	GLU	L917
GLN	ILE			V393	THR	R708	THR	GLN	Q918
LEU	ASP	N223	V312	V394	GLY	R709	GLY	ALA	N919
GLN	ASP	E224	S313	A398	THR	F710	THR	GLN	R920
GLN	GLN	D225	Q314	C399	THR	L711	THR	GLN	R921
TYR	ALA	G226	Q314	R400	THR	L712	THR	GLN	A922
GLY	THR	L227	I317	R401	THR	H715	THR	GLN	R923
GLN	THR	D228	K318	Q401	THR	S716	THR	GLN	N924
ASN	SER	Y229		M402	THR	L717	THR	GLN	I925
ALA	ALA	R230		L403	THR	L718	THR	GLN	S926
ALA	ASN			L406	THR	F719	THR	GLN	
PRO	ASP	R235		L406	THR	K719	THR	GLN	
LEU	MET	Y237		L410	THR	A722	THR	GLN	
GLN	HIS			N411	THR	F723	THR	GLN	
GLN	HIS	P241		Q412	THR	R724	THR	GLN	
ALA	ASN	V242		L413	THR	S725	THR	GLN	
GLN	VAL	T243		F414	THR		THR	GLN	
PRO	PRO	I151		Q415	THR	V610	THR	GLN	
PHE	LEU	T152		S416	THR	V611	THR	GLN	
MET	LEU	D153		N417	THR	Q612	THR	GLN	
PRO	VAL	R249		L418	THR	H732	THR	GLN	
PRO	ASP	R250		S346	THR	R733	THR	GLN	
GLN	PRO	W251		L419	THR	L737	THR	GLN	
ASP	ASN	C252		T420	THR	N738	THR	GLN	
ALA	ALA	R253		N421	THR	L740	THR	GLN	
ALA	TYR	N254		F422	THR	E741	THR	GLN	
ALA	MET	R255		L423	THR	S742	THR	GLN	
ALA	GLN	C256		L424	THR	L743	THR	GLN	
GLY	PRO	R257		L428	THR	P744	THR	GLN	
MET	GLN	N260		K429	THR		THR	GLN	
SER	VAL	D261		P534	THR	E641	THR	GLN	
TYR	VAL	V262		S430	THR	V680	THR	GLN	
GLY	VAL	A177		L435	THR	N750	THR	GLN	
GLN	MET	D270		SER	THR	N751	THR	GLN	
MET	GLY	P271		GLU	THR	P754	THR	GLN	
GLY	THR	N272		ASN	THR	D755	THR	GLN	
MET	THR	D273		ASN	THR	V756	THR	GLN	
PRO	PRO	N187		GLU	THR		THR	GLN	
PRO	LEU	P274		GLU	THR	D670	THR	GLN	
GLN	GLN			SER	THR	A671	THR	GLN	
GLY	GLN	R277		ALA	THR	R672	THR	GLN	
ALA	GLN	Y278		L449	THR		THR	GLN	
VAL	GLN	D279		P450	THR	M762	THR	GLN	
GLN	GLN	K197		N451	THR	A763	THR	GLN	
PRO	GLN	K198		L452	THR	D764	THR	GLN	
SER	PRO	S199		K374	THR	E765	THR	GLN	
MET	MET	K200		N375	THR	A766	THR	GLN	
GLY	ALA	L205		K376	THR	G767	THR	GLN	
GLN	PRO	A292		L378	THR	L768	THR	GLN	
GLN	ALA	R208		R459	THR	P769	THR	GLN	
				E462	THR	VAL	THR	GLN	

• Molecule 4: SEC24P

Chain F: ..

99%

MET	SER	F61	GLN	GLN	K906
SER	HIS	L62	ILE	THR	I907
HIS	PRO	Q66	PRO	GLU	G998
LYS	ALA	E67	ASP	GLY	A699
ARG	VAL	Q68	GLY	GLY	P700
VAL	GLN	L69	ALA	ALA	L701
THR	THR	Q72	ASN	THR	R702
PRO	GLN	I73	GLY	THR	L703
GLN	ALA	ASP	GLU	GLY	C704
ALA	GLN	GLN	GLU	THR	L707
LEU	ASN	THR	GLN	THR	R708
GLN	ALA	THR	GLN	THR	R709
LYS	LEU	THR	GLN	THR	F710
LYS	LEU	THR	GLN	THR	L711
LYS	TYR	SER	TYR	THR	L712
LYS	PRO	MET	GLY	THR	H715
GLN	ILE	ASN	GLN	THR	S716
ASP	ASP	ASP	ASN	THR	L717
LEU	LEU	LEU	ALA	THR	L718
THR	LEU	LEU	ALA	THR	F719
LEU	GLU	LEU	GLU	THR	K719
VAL	VAL	VAL	LEU	THR	A722
ARG	PRO	PRO	VAL	THR	F723
PRO	PRO	PRO	PRO	THR	R724
TYR	PRO	PRO	LEU	THR	S725
GLN	ILE	ILE	VAL	THR	
GLN	GLN	GLN	VAL	THR	V610
PHE	GLN	GLN	VAL	THR	V611
ASP	THR	THR	ASP	THR	Q612
PRO	LEU	LEU	PRO	THR	H732
PRO	LEU	LEU	ASN	THR	R733
ALA	ALA	ALA	ALA	THR	L737
ALA	ALA	ALA	ALA	THR	N738
GLY	GLY	GLY	GLY	THR	L740
MET	MET	MET	MET	THR	E741
GLY	GLY	GLY	GLY	THR	S742
VAL	VAL	VAL	VAL	THR	L743
ARG	ARG	ARG	ARG	THR	P744
ILE	ILE	ILE	ILE	THR	
VAL	VAL	VAL	VAL	THR	K750
ARG	ARG	ARG	ARG	THR	N751
ILE	ILE	ILE	ILE	THR	
VAL	VAL	VAL	VAL	THR	P754
ARG	ARG	ARG	ARG	THR	D755
CTYS	CTYS	CTYS	CTYS	THR	V756
ARG	ARG	ARG	ARG	THR	
CTYS	CTYS	CTYS	CTYS	THR	D761
				THR	M762
				THR	A763
				THR	D764
				THR	E765
				THR	A766
				THR	G767
				THR	L768
				THR	P769
				THR	VAL

[illegible]

- Molecule 4: SEC24P

Chain N: 98%

[illegible]

[illegible]

- Molecule 4: SEC24P

Chain 0: 98%

[illegible]

[illegible]

4 Experimental information

Property	Value	Source
Reconstruction method	TOMOGRAPHY	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of tilted images used	15000	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	EACH TILTED IMAGE WITHIN TOMOGRAM	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	80	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	3200	Depositor
Magnification	19500	Depositor
Image detector	GATAN MULTISCAN	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A	0.38	0/5915	0.62	0/8052
1	D	0.38	0/5915	0.62	0/8052
1	G	0.38	0/5915	0.62	0/8052
2	B	0.34	0/1327	0.61	0/1800
2	J	0.34	0/1327	0.61	0/1800
2	K	0.34	0/1327	0.61	0/1800
3	E	0.39	0/5943	0.68	1/8064 (0.0%)
3	L	0.39	0/5943	0.68	1/8064 (0.0%)
3	M	0.39	0/5943	0.68	1/8064 (0.0%)
4	F	0.35	0/111	0.47	0/150
4	N	0.35	0/118	0.47	0/158
4	O	0.35	0/118	0.48	0/158
All	All	0.38	0/39902	0.64	3/54214 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	768	LEU	CA-CB-CG	5.33	127.56	115.30
3	M	768	LEU	CA-CB-CG	5.33	127.56	115.30
3	L	768	LEU	CA-CB-CG	5.32	127.55	115.30

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	5780	0	5663	201	0
1	D	5780	0	5663	205	0
1	G	5780	0	5663	193	0
2	B	1299	0	1288	65	0
2	J	1299	0	1288	59	0
2	K	1299	0	1288	61	0
3	E	5823	0	5853	291	0
3	L	5823	0	5853	293	0
3	M	5823	0	5853	301	0
4	F	109	0	105	14	0
4	N	117	0	110	14	0
4	O	117	0	110	12	0
5	A	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	G	1	0	0	0	0
5	L	1	0	0	0	0
5	M	1	0	0	0	0
6	B	32	0	13	5	0
6	J	32	0	13	4	0
6	K	32	0	13	5	0
7	B	1	0	0	0	0
7	J	1	0	0	0	0
7	K	1	0	0	0	0
All	All	39154	0	38776	1589	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 20.

The worst 5 of 1589 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:A:91:PRO:HB3	1:D:669:GLN:NE2	1.18	1.43
1:A:91:PRO:CB	1:D:669:GLN:HE21	1.35	1.38
1:D:183:ARG:NH1	3:L:383:GLU:HB2	1.53	1.22
1:G:183:ARG:NH1	3:M:383:GLU:HB2	1.53	1.22
1:A:183:ARG:NH1	3:E:383:GLU:HB2	1.53	1.21

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	727/768 (95%)	687 (94%)	35 (5%)	5 (1%)	25	68
1	D	727/768 (95%)	688 (95%)	34 (5%)	5 (1%)	25	68
1	G	727/768 (95%)	688 (95%)	34 (5%)	5 (1%)	25	68
2	B	160/190 (84%)	142 (89%)	13 (8%)	5 (3%)	5	37
2	J	160/190 (84%)	142 (89%)	13 (8%)	5 (3%)	5	37
2	K	160/190 (84%)	142 (89%)	13 (8%)	5 (3%)	5	37
3	E	723/926 (78%)	640 (88%)	55 (8%)	28 (4%)	3	31
3	L	723/926 (78%)	641 (89%)	54 (8%)	28 (4%)	3	31
3	M	723/926 (78%)	641 (89%)	54 (8%)	28 (4%)	3	31
4	F	11/926 (1%)	10 (91%)	1 (9%)	0	100	100
4	N	11/926 (1%)	10 (91%)	1 (9%)	0	100	100
4	O	11/926 (1%)	10 (91%)	1 (9%)	0	100	100
All	All	4863/8430 (58%)	4441 (91%)	308 (6%)	114 (2%)	11	43

5 of 114 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	703	VAL
2	B	139	ALA
2	B	155	THR
1	D	703	VAL
3	E	147	LEU

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 PDB entries followed by that with respect to all EM entries.

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	644/668 (96%)	616 (96%)	28 (4%)	33	64
1	D	644/668 (96%)	616 (96%)	28 (4%)	33	64
1	G	644/668 (96%)	616 (96%)	28 (4%)	33	64
2	B	138/159 (87%)	136 (99%)	2 (1%)	71	86
2	J	138/159 (87%)	136 (99%)	2 (1%)	71	86
2	K	138/159 (87%)	136 (99%)	2 (1%)	71	86
3	E	660/819 (81%)	640 (97%)	20 (3%)	46	72
3	L	660/819 (81%)	640 (97%)	20 (3%)	46	72
3	M	660/819 (81%)	640 (97%)	20 (3%)	46	72
4	F	12/817 (2%)	12 (100%)	0	100	100
4	N	13/817 (2%)	13 (100%)	0	100	100
4	O	13/817 (2%)	13 (100%)	0	100	100
All	All	4364/7389 (59%)	4214 (97%)	150 (3%)	46	69

5 of 150 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	E	428	LEU
1	G	166	VAL
3	M	377	ASP
3	E	557	VAL
3	E	822	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 97 such sidechains are listed below:

Mol	Chain	Res	Type
3	E	535	ASN
1	G	233	GLN
3	M	533	ASN
3	E	732	HIS
1	G	47	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 ⓘ

Of 12 ligands modelled in this entry, 9 are monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
6	GNP	B	1190	7	27,34,34	2.26	7 (25%)	26,54,54	1.67	4 (15%)
6	GNP	J	1190	7	27,34,34	2.26	7 (25%)	26,54,54	1.67	4 (15%)
6	GNP	K	1190	7	27,34,34	2.26	7 (25%)	26,54,54	1.66	4 (15%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GNP	B	1190	7	-	0/16/38/38	0/3/3/3
6	GNP	J	1190	7	-	0/16/38/38	0/3/3/3
6	GNP	K	1190	7	-	0/16/38/38	0/3/3/3

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	K	1190	GNP	C4-N9	-7.18	1.38	1.47
6	J	1190	GNP	C4-N9	-7.18	1.38	1.47
6	B	1190	GNP	C4-N9	-7.13	1.38	1.47
6	B	1190	GNP	PB-O2B	-4.08	1.45	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	J	1190	GNP	PB-O2B	-4.06	1.45	1.56

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	K	1190	GNP	O3G-PG-O1G	-4.24	102.63	113.41
6	B	1190	GNP	O3G-PG-O1G	-4.23	102.65	113.41
6	J	1190	GNP	O3G-PG-O1G	-4.23	102.66	113.41
6	J	1190	GNP	O6-C6-N1	-2.86	118.89	122.70
6	B	1190	GNP	O6-C6-N1	-2.85	118.90	122.70

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	1190	GNP	5	0
6	J	1190	GNP	4	0
6	K	1190	GNP	5	0

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.