



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 16, 2024 – 04:23 PM EST

PDB ID : 3RL0
Title : Truncated SNARE complex with complexin (P1)
Authors : Kuemmel, D.; Reinisch, K.M.
Deposited on : 2011-04-19
Resolution : 3.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

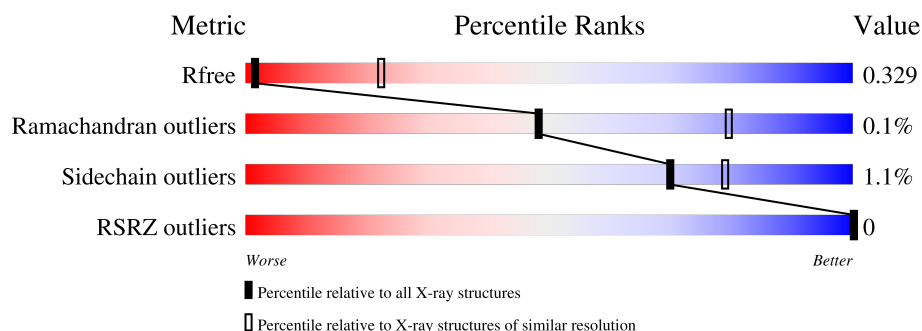
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 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.













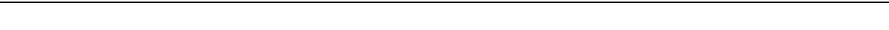

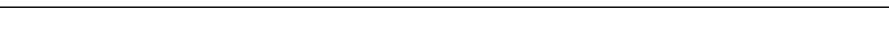
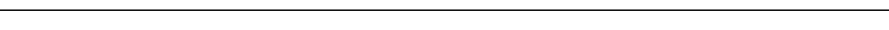





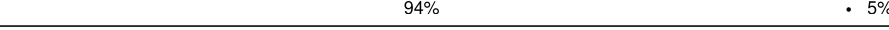

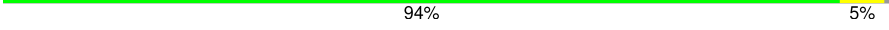
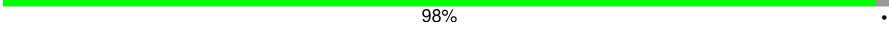
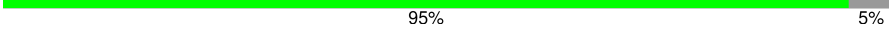

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	1025 (3.98-3.62)
Ramachandran outliers	177936	1044 (3.98-3.62)
Sidechain outliers	177891	1039 (3.98-3.62)
RSRZ outliers	164620	1025 (3.98-3.62)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	37	
1	E	37	
1	I	37	
1	M	37	
1	Q	37	
1	U	37	

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Mol	Chain	Length	Quality of chain
1	Y	37	 89% 5% 5%
1	c	37	 86% • • 8%
2	B	65	 88% • 9%
2	F	65	 92% • 6%
2	J	65	 91% 9%
2	N	65	 85% • 12%
2	R	65	 91% • 6%
2	V	65	 83% 6% 11%
2	Z	65	 85% 5% 11%
2	d	65	 89% • 9%
3	C	81	 83% 6% 11%
3	G	81	 84% 7% 9%
3	K	81	 81% 5% • 12%
3	O	81	 83% 5% • 11%
3	S	81	 80% 6% 14%
3	W	81	 81% 5% 14%
3	a	81	 81% 5% 14%
3	e	81	 83% 6% 11%
4	D	65	 94% • 5%
4	H	65	 91% • 6%
4	L	65	 94% 5% •
4	P	65	 98% •
4	T	65	 95% 5%
4	X	65	 95% • •
4	b	65	 91% • 6%

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Mol	Chain	Length	Quality of chain
4	f	65	<div><div></div><div>94%</div><div></div><div>• 5%</div></div>
5	g	63	<div><div></div><div>71%</div><div></div><div>• 25%</div></div>
5	h	63	<div><div></div><div>70%</div><div></div><div>• 27%</div></div>
5	i	63	<div><div></div><div>67%</div><div>5%</div><div>• 29%</div></div>
5	j	63	<div><div></div><div>70%</div><div></div><div>• 29%</div></div>
5	k	63	<div><div></div><div>71%</div><div></div><div>• 27%</div></div>
5	l	63	<div><div></div><div>73%</div><div></div><div>• 25%</div></div>
5	m	63	<div><div></div><div>70%</div><div></div><div>• 29%</div></div>
5	n	63	<div><div></div><div>70%</div><div></div><div>• 29%</div></div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 17672 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 Vesicle-associated membrane protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	35	Total	C	N	O	S	0	0	0
			283	169	56	57	1			
1	E	35	Total	C	N	O	S	3	0	0
			286	172	56	57	1			
1	I	34	Total	C	N	O	S	0	0	0
			278	166	55	56	1			
1	M	36	Total	C	N	O	S	3	0	0
			293	177	57	58	1			
1	Q	35	Total	C	N	O	S	3	0	0
			286	172	56	57	1			
1	U	35	Total	C	N	O	S	0	0	0
			286	172	56	57	1			
1	Y	35	Total	C	N	O	S	0	0	0
			286	172	56	57	1			
1	c	34	Total	C	N	O	S	4	0	0
			274	164	54	55	1			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	24	GLY	-	expression tag	UNP P63027
A	25	PRO	-	expression tag	UNP P63027
A	26	LEU	-	expression tag	UNP P63027
A	27	GLY	-	expression tag	UNP P63027
E	24	GLY	-	expression tag	UNP P63027
E	25	PRO	-	expression tag	UNP P63027
E	26	LEU	-	expression tag	UNP P63027
E	27	GLY	-	expression tag	UNP P63027
I	24	GLY	-	expression tag	UNP P63027
I	25	PRO	-	expression tag	UNP P63027
I	26	LEU	-	expression tag	UNP P63027
I	27	GLY	-	expression tag	UNP P63027
M	24	GLY	-	expression tag	UNP P63027

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Chain	Residue	Modelled	Actual	Comment	Reference
M	25	PRO	-	expression tag	UNP P63027
M	26	LEU	-	expression tag	UNP P63027
M	27	GLY	-	expression tag	UNP P63027
Q	24	GLY	-	expression tag	UNP P63027
Q	25	PRO	-	expression tag	UNP P63027
Q	26	LEU	-	expression tag	UNP P63027
Q	27	GLY	-	expression tag	UNP P63027
U	24	GLY	-	expression tag	UNP P63027
U	25	PRO	-	expression tag	UNP P63027
U	26	LEU	-	expression tag	UNP P63027
U	27	GLY	-	expression tag	UNP P63027
Y	24	GLY	-	expression tag	UNP P63027
Y	25	PRO	-	expression tag	UNP P63027
Y	26	LEU	-	expression tag	UNP P63027
Y	27	GLY	-	expression tag	UNP P63027
c	24	GLY	-	expression tag	UNP P63027
c	25	PRO	-	expression tag	UNP P63027
c	26	LEU	-	expression tag	UNP P63027
c	27	GLY	-	expression tag	UNP P63027

- Molecule 2 is a protein called Syntaxin-1A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	59	Total	C	N	O	S	8	0	0
			481	297	81	98	5			
2	F	61	Total	C	N	O	S	10	0	0
			496	305	83	103	5			
2	J	59	Total	C	N	O	S	0	0	0
			481	297	81	98	5			
2	N	57	Total	C	N	O	S	15	0	0
			468	289	79	95	5			
2	R	61	Total	C	N	O	S	8	0	0
			496	305	83	103	5			
2	V	58	Total	C	N	O	S	16	0	0
			475	294	80	96	5			
2	Z	58	Total	C	N	O	S	6	0	0
			474	292	80	97	5			
2	d	59	Total	C	N	O	S	12	0	0
			481	297	81	98	5			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	189	GLY	-	expression tag	UNP P32851
B	190	SER	-	expression tag	UNP P32851
F	189	GLY	-	expression tag	UNP P32851
F	190	SER	-	expression tag	UNP P32851
J	189	GLY	-	expression tag	UNP P32851
J	190	SER	-	expression tag	UNP P32851
N	189	GLY	-	expression tag	UNP P32851
N	190	SER	-	expression tag	UNP P32851
R	189	GLY	-	expression tag	UNP P32851
R	190	SER	-	expression tag	UNP P32851
V	189	GLY	-	expression tag	UNP P32851
V	190	SER	-	expression tag	UNP P32851
Z	189	GLY	-	expression tag	UNP P32851
Z	190	SER	-	expression tag	UNP P32851
d	189	GLY	-	expression tag	UNP P32851
d	190	SER	-	expression tag	UNP P32851

- Molecule 3 is a protein called Synaptosomal-associated protein 25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	72	Total	C	N	O	S	20	0	0
			587	348	109	125	5			
3	G	74	Total	C	N	O	S	28	0	0
			603	358	111	129	5			
3	K	71	Total	C	N	O	S	23	0	0
			576	342	105	124	5			
3	O	72	Total	C	N	O	S	22	0	0
			583	346	109	123	5			
3	S	70	Total	C	N	O	S	8	0	0
			568	338	103	122	5			
3	W	70	Total	C	N	O	S	18	0	0
			570	336	106	123	5			
3	a	70	Total	C	N	O	S	10	0	0
			568	338	103	122	5			
3	e	72	Total	C	N	O	S	33	0	0
			587	348	109	125	5			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	3	GLY	-	expression tag	UNP P60880
C	4	SER	-	expression tag	UNP P60880
C	5	HIS	-	expression tag	UNP P60880

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Chain	Residue	Modelled	Actual	Comment	Reference
C	6	MET	-	expression tag	UNP P60880
C	83	TRP	-	expression tag	UNP P60880
G	3	GLY	-	expression tag	UNP P60880
G	4	SER	-	expression tag	UNP P60880
G	5	HIS	-	expression tag	UNP P60880
G	6	MET	-	expression tag	UNP P60880
G	83	TRP	-	expression tag	UNP P60880
K	3	GLY	-	expression tag	UNP P60880
K	4	SER	-	expression tag	UNP P60880
K	5	HIS	-	expression tag	UNP P60880
K	6	MET	-	expression tag	UNP P60880
K	83	TRP	-	expression tag	UNP P60880
O	3	GLY	-	expression tag	UNP P60880
O	4	SER	-	expression tag	UNP P60880
O	5	HIS	-	expression tag	UNP P60880
O	6	MET	-	expression tag	UNP P60880
O	83	TRP	-	expression tag	UNP P60880
S	3	GLY	-	expression tag	UNP P60880
S	4	SER	-	expression tag	UNP P60880
S	5	HIS	-	expression tag	UNP P60880
S	6	MET	-	expression tag	UNP P60880
S	83	TRP	-	expression tag	UNP P60880
W	3	GLY	-	expression tag	UNP P60880
W	4	SER	-	expression tag	UNP P60880
W	5	HIS	-	expression tag	UNP P60880
W	6	MET	-	expression tag	UNP P60880
W	83	TRP	-	expression tag	UNP P60880
a	3	GLY	-	expression tag	UNP P60880
a	4	SER	-	expression tag	UNP P60880
a	5	HIS	-	expression tag	UNP P60880
a	6	MET	-	expression tag	UNP P60880
a	83	TRP	-	expression tag	UNP P60880
e	3	GLY	-	expression tag	UNP P60880
e	4	SER	-	expression tag	UNP P60880
e	5	HIS	-	expression tag	UNP P60880
e	6	MET	-	expression tag	UNP P60880
e	83	TRP	-	expression tag	UNP P60880

- Molecule 4 is a protein called Synaptosomal-associated protein 25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	62	Total	C	N	O	S	2	0	0
			488	284	95	105	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	61	Total	C	N	O	S	7	0	0
			481	280	94	103	4			
4	L	64	Total	C	N	O	S	7	0	0
			505	295	98	107	5			
4	P	64	Total	C	N	O	S	4	0	0
			505	295	98	107	5			
4	T	62	Total	C	N	O	S	0	0	0
			484	281	94	105	4			
4	X	63	Total	C	N	O	S	7	0	0
			497	290	97	106	4			
4	b	61	Total	C	N	O	S	9	0	0
			481	280	94	103	4			
4	f	62	Total	C	N	O	S	6	0	0
			481	279	94	105	3			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	139	GLY	-	expression tag	UNP P60880
D	140	SER	-	expression tag	UNP P60880
H	139	GLY	-	expression tag	UNP P60880
H	140	SER	-	expression tag	UNP P60880
L	139	GLY	-	expression tag	UNP P60880
L	140	SER	-	expression tag	UNP P60880
P	139	GLY	-	expression tag	UNP P60880
P	140	SER	-	expression tag	UNP P60880
T	139	GLY	-	expression tag	UNP P60880
T	140	SER	-	expression tag	UNP P60880
X	139	GLY	-	expression tag	UNP P60880
X	140	SER	-	expression tag	UNP P60880
b	139	GLY	-	expression tag	UNP P60880
b	140	SER	-	expression tag	UNP P60880
f	139	GLY	-	expression tag	UNP P60880
f	140	SER	-	expression tag	UNP P60880

- Molecule 5 is a protein called Complexin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	g	47	Total	C	N	O	Se	0	0	0
			379	230	72	75	2			
5	h	46	Total	C	N	O	Se	0	0	0
			375	228	71	74	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	i	45	Total 369	C 225	N 70	O 72	Se 2	7	0	0
5	j	45	Total 369	C 225	N 70	O 72	Se 2	10	0	0
5	k	46	Total 375	C 228	N 71	O 74	Se 2	6	0	0
5	l	47	Total 379	C 230	N 72	O 75	Se 2	0	0	0
5	m	45	Total 369	C 225	N 70	O 72	Se 2	10	0	0
5	n	45	Total 369	C 225	N 70	O 72	Se 2	9	0	0

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
g	21	GLY	-	expression tag	UNP O14810
g	22	PRO	-	expression tag	UNP O14810
g	23	LEU	-	expression tag	UNP O14810
g	24	GLY	-	expression tag	UNP O14810
g	25	SER	-	expression tag	UNP O14810
g	27	LEU	ASP	engineered mutation	UNP O14810
g	34	MSE	GLU	engineered mutation	UNP O14810
g	37	ALA	ARG	engineered mutation	UNP O14810
h	21	GLY	-	expression tag	UNP O14810
h	22	PRO	-	expression tag	UNP O14810
h	23	LEU	-	expression tag	UNP O14810
h	24	GLY	-	expression tag	UNP O14810
h	25	SER	-	expression tag	UNP O14810
h	27	LEU	ASP	engineered mutation	UNP O14810
h	34	MSE	GLU	engineered mutation	UNP O14810
h	37	ALA	ARG	engineered mutation	UNP O14810
i	21	GLY	-	expression tag	UNP O14810
i	22	PRO	-	expression tag	UNP O14810
i	23	LEU	-	expression tag	UNP O14810
i	24	GLY	-	expression tag	UNP O14810
i	25	SER	-	expression tag	UNP O14810
i	27	LEU	ASP	engineered mutation	UNP O14810
i	34	MSE	GLU	engineered mutation	UNP O14810
i	37	ALA	ARG	engineered mutation	UNP O14810
j	21	GLY	-	expression tag	UNP O14810
j	22	PRO	-	expression tag	UNP O14810
j	23	LEU	-	expression tag	UNP O14810

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Chain	Residue	Modelled	Actual	Comment	Reference
j	24	GLY	-	expression tag	UNP O14810
j	25	SER	-	expression tag	UNP O14810
j	27	LEU	ASP	engineered mutation	UNP O14810
j	34	MSE	GLU	engineered mutation	UNP O14810
j	37	ALA	ARG	engineered mutation	UNP O14810
k	21	GLY	-	expression tag	UNP O14810
k	22	PRO	-	expression tag	UNP O14810
k	23	LEU	-	expression tag	UNP O14810
k	24	GLY	-	expression tag	UNP O14810
k	25	SER	-	expression tag	UNP O14810
k	27	LEU	ASP	engineered mutation	UNP O14810
k	34	MSE	GLU	engineered mutation	UNP O14810
k	37	ALA	ARG	engineered mutation	UNP O14810
l	21	GLY	-	expression tag	UNP O14810
l	22	PRO	-	expression tag	UNP O14810
l	23	LEU	-	expression tag	UNP O14810
l	24	GLY	-	expression tag	UNP O14810
l	25	SER	-	expression tag	UNP O14810
l	27	LEU	ASP	engineered mutation	UNP O14810
l	34	MSE	GLU	engineered mutation	UNP O14810
l	37	ALA	ARG	engineered mutation	UNP O14810
m	21	GLY	-	expression tag	UNP O14810
m	22	PRO	-	expression tag	UNP O14810
m	23	LEU	-	expression tag	UNP O14810
m	24	GLY	-	expression tag	UNP O14810
m	25	SER	-	expression tag	UNP O14810
m	27	LEU	ASP	engineered mutation	UNP O14810
m	34	MSE	GLU	engineered mutation	UNP O14810
m	37	ALA	ARG	engineered mutation	UNP O14810
n	21	GLY	-	expression tag	UNP O14810
n	22	PRO	-	expression tag	UNP O14810
n	23	LEU	-	expression tag	UNP O14810
n	24	GLY	-	expression tag	UNP O14810
n	25	SER	-	expression tag	UNP O14810
n	27	LEU	ASP	engineered mutation	UNP O14810
n	34	MSE	GLU	engineered mutation	UNP O14810
n	37	ALA	ARG	engineered mutation	UNP O14810

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.

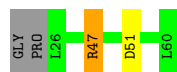
- Molecule 1: Vesicle-associated membrane protein 2

Chain A:  89% . . 5%




- Molecule 1: Vesicle-associated membrane protein 2

Chain E:  89% . . 5%




- Molecule 1: Vesicle-associated membrane protein 2

Chain I:  86% 5% 8%




- Molecule 1: Vesicle-associated membrane protein 2

Chain M:  89% 5% . .




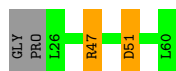
- Molecule 1: Vesicle-associated membrane protein 2

Chain Q:  86% 8% 5%



- Molecule 1: Vesicle-associated membrane protein 2

Chain U:  89% 5% 5%



- Molecule 1: Vesicle-associated membrane protein 2

Chain Y: 89% 5% 5%



- Molecule 1: Vesicle-associated membrane protein 2

Chain c: 86% • • 8%



- Molecule 2: Syntaxin-1A

Chain B: 88% • 9%



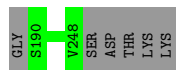
- Molecule 2: Syntaxin-1A

Chain F: 92% • 6%



- Molecule 2: Syntaxin-1A

Chain J: 91% • 9%



- Molecule 2: Syntaxin-1A

Chain N: 85% • 12%

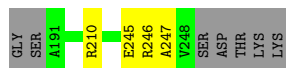
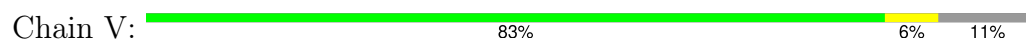


- Molecule 2: Syntaxin-1A

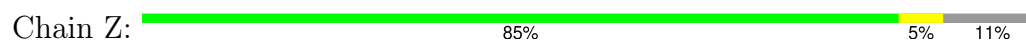
Chain R: 91% • 6%



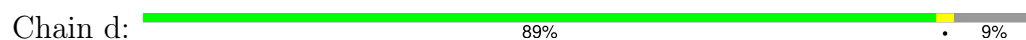
- Molecule 2: Syntaxin-1A



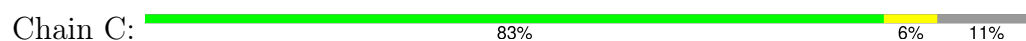
- Molecule 2: Syntaxin-1A



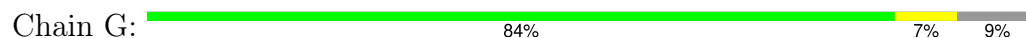
- Molecule 2: Syntaxin-1A



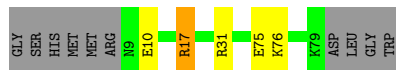
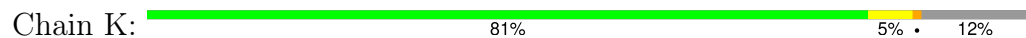
- Molecule 3: Synaptosomal-associated protein 25



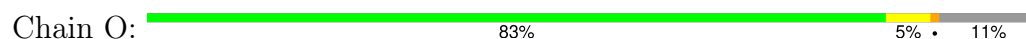
- Molecule 3: Synaptosomal-associated protein 25

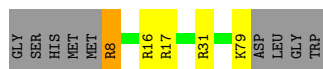


- Molecule 3: Synaptosomal-associated protein 25

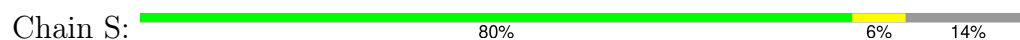


- Molecule 3: Synaptosomal-associated protein 25

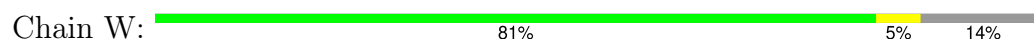




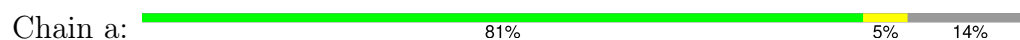
- Molecule 3: Synaptosomal-associated protein 25



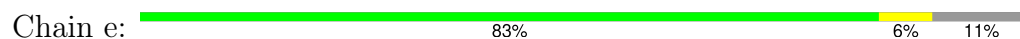
- Molecule 3: Synaptosomal-associated protein 25



- Molecule 3: Synaptosomal-associated protein 25



- Molecule 3: Synaptosomal-associated protein 25



- Molecule 4: Synaptosomal-associated protein 25

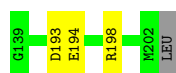


- Molecule 4: Synaptosomal-associated protein 25



- Molecule 4: Synaptosomal-associated protein 25





- Molecule 4: Synaptosomal-associated protein 25

Chain P: 98% .



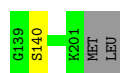
- Molecule 4: Synaptosomal-associated protein 25

Chain T: 95% 5%



- Molecule 4: Synaptosomal-associated protein 25

Chain X: 95% . .



- Molecule 4: Synaptosomal-associated protein 25

Chain b: 91% . 6%



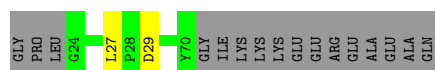
- Molecule 4: Synaptosomal-associated protein 25

Chain f: 94% . 5%



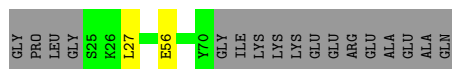
- Molecule 5: Complexin-1

Chain g: 71% . 25%



- Molecule 5: Complexin-1

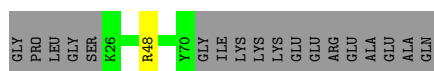
Chain h: 70% . 27%



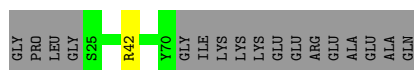
● Molecule 5: Complexin-1



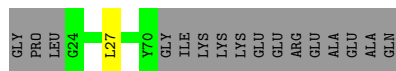
● Molecule 5: Complexin-1



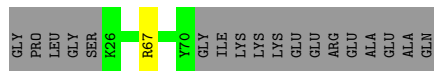
● Molecule 5: Complexin-1



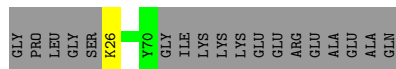
● Molecule 5: Complexin-1



● Molecule 5: Complexin-1



● Molecule 5: Complexin-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	53.74Å 127.36Å 142.72Å 107.49° 90.01° 90.05°	Depositor
Resolution (Å)	30.00 – 3.80 30.00 – 3.80	Depositor EDS
% Data completeness (in resolution range)	97.2 (30.00-3.80) 97.0 (30.00-3.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.83 (at 3.75Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.306 , 0.345 0.290 , 0.329	Depositor DCC
R_{free} test set	1872 reflections (5.42%)	wwPDB-VP
Wilson B-factor (Å ²)	76.4	Xtriage
Anisotropy	1.209	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 680.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.409 for h,-k,-l	Xtriage
Reported twinning fraction	0.470 for h,-h-k,-l	Depositor
Outliers	0 of 34379 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	17672	wwPDB-VP
Average B, all atoms (Å ²)	116.0	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 24.77 % 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 3.5978e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

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	0.69	0/282	0.67	1/376 (0.3%)
1	E	0.69	0/285	0.67	1/380 (0.3%)
1	I	0.68	0/277	0.66	0/369
1	M	0.67	0/293	0.76	2/391 (0.5%)
1	Q	0.73	1/285 (0.4%)	0.70	1/380 (0.3%)
1	U	0.95	2/285 (0.7%)	1.48	6/380 (1.6%)
1	Y	0.67	0/285	0.65	0/380
1	c	0.68	0/273	0.67	2/364 (0.5%)
2	B	0.53	0/486	0.54	0/652
2	F	0.55	1/501 (0.2%)	0.55	0/673
2	J	0.49	0/486	0.55	0/652
2	N	0.76	2/473 (0.4%)	0.52	0/634
2	R	0.57	1/501 (0.2%)	0.54	0/673
2	V	0.78	3/480 (0.6%)	0.64	2/644 (0.3%)
2	Z	0.60	1/479 (0.2%)	0.51	0/642
2	d	0.55	1/486 (0.2%)	0.56	0/652
3	C	0.87	4/587 (0.7%)	0.88	4/780 (0.5%)
3	G	0.93	6/603 (1.0%)	1.00	5/802 (0.6%)
3	K	0.89	4/576 (0.7%)	1.05	8/766 (1.0%)
3	O	1.04	6/583 (1.0%)	1.35	6/775 (0.8%)
3	S	0.78	4/568 (0.7%)	0.88	3/755 (0.4%)
3	W	0.80	3/570 (0.5%)	0.77	1/758 (0.1%)
3	a	0.75	3/568 (0.5%)	0.72	1/755 (0.1%)
3	e	0.96	5/587 (0.9%)	0.80	3/780 (0.4%)
4	D	0.56	1/488 (0.2%)	0.59	1/651 (0.2%)
4	H	0.63	1/481 (0.2%)	0.62	1/641 (0.2%)
4	L	0.60	1/505 (0.2%)	0.73	2/672 (0.3%)
4	P	0.45	0/505	0.51	0/672
4	T	0.46	0/484	0.50	0/647
4	X	0.53	0/497	0.50	0/662
4	b	0.45	0/481	0.57	1/641 (0.2%)
4	f	0.55	1/481 (0.2%)	0.51	0/644
5	g	0.44	0/379	0.56	0/496
5	h	0.50	0/375	0.57	0/491

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
5	i	1.01	2/369 (0.5%)	0.66	0/483
5	j	0.41	0/369	0.56	0/483
5	k	0.45	0/375	0.50	0/491
5	l	0.45	0/379	0.55	0/496
5	m	0.68	1/369 (0.3%)	0.68	1/483 (0.2%)
5	n	0.56	1/369 (0.3%)	0.57	0/483
All	All	0.69	55/17705 (0.3%)	0.72	52/23549 (0.2%)

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
3	O	0	1
5	g	0	1
5	h	0	1
5	l	0	1
All	All	0	4

The worst 5 of 55 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	8	ARG	CD-NE	14.24	1.70	1.46
3	e	73	GLU	CB-CG	13.64	1.78	1.52
5	i	26	LYS	CB-CG	-12.71	1.18	1.52
3	C	79	LYS	CB-CG	-12.00	1.20	1.52
3	O	16	ARG	CB-CG	10.65	1.81	1.52

The worst 5 of 52 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	31	ARG	NE-CZ-NH1	-22.07	109.26	120.30
3	O	31	ARG	NE-CZ-NH2	17.14	128.87	120.30
1	U	47	ARG	NE-CZ-NH1	14.08	127.34	120.30
3	G	80	ASP	CB-CG-OD1	13.59	130.53	118.30
1	U	51	ASP	CB-CG-OD2	13.38	130.34	118.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	O	8	ARG	Sidechain
5	g	27	LEU	Peptide
5	h	27	LEU	Peptide
5	l	27	LEU	Peptide

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	33/37 (89%)	33 (100%)	0	0	100	100
1	E	33/37 (89%)	32 (97%)	1 (3%)	0	100	100
1	I	32/37 (86%)	32 (100%)	0	0	100	100
1	M	34/37 (92%)	34 (100%)	0	0	100	100
1	Q	33/37 (89%)	33 (100%)	0	0	100	100
1	U	33/37 (89%)	32 (97%)	1 (3%)	0	100	100
1	Y	33/37 (89%)	33 (100%)	0	0	100	100
1	c	32/37 (86%)	32 (100%)	0	0	100	100
2	B	57/65 (88%)	57 (100%)	0	0	100	100
2	F	59/65 (91%)	58 (98%)	1 (2%)	0	100	100
2	J	57/65 (88%)	56 (98%)	1 (2%)	0	100	100
2	N	55/65 (85%)	55 (100%)	0	0	100	100
2	R	59/65 (91%)	58 (98%)	1 (2%)	0	100	100
2	V	56/65 (86%)	56 (100%)	0	0	100	100
2	Z	56/65 (86%)	55 (98%)	0	1 (2%)	7	34
2	d	57/65 (88%)	56 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	70/81 (86%)	68 (97%)	2 (3%)	0	100	100
3	G	72/81 (89%)	71 (99%)	1 (1%)	0	100	100
3	K	69/81 (85%)	69 (100%)	0	0	100	100
3	O	70/81 (86%)	69 (99%)	1 (1%)	0	100	100
3	S	68/81 (84%)	66 (97%)	2 (3%)	0	100	100
3	W	68/81 (84%)	66 (97%)	2 (3%)	0	100	100
3	a	68/81 (84%)	67 (98%)	1 (2%)	0	100	100
3	e	70/81 (86%)	68 (97%)	2 (3%)	0	100	100
4	D	60/65 (92%)	60 (100%)	0	0	100	100
4	H	59/65 (91%)	59 (100%)	0	0	100	100
4	L	62/65 (95%)	62 (100%)	0	0	100	100
4	P	62/65 (95%)	62 (100%)	0	0	100	100
4	T	60/65 (92%)	60 (100%)	0	0	100	100
4	X	61/65 (94%)	61 (100%)	0	0	100	100
4	b	59/65 (91%)	59 (100%)	0	0	100	100
4	f	60/65 (92%)	60 (100%)	0	0	100	100
5	g	45/63 (71%)	41 (91%)	4 (9%)	0	100	100
5	h	44/63 (70%)	40 (91%)	3 (7%)	1 (2%)	5	30
5	i	43/63 (68%)	42 (98%)	1 (2%)	0	100	100
5	j	43/63 (68%)	42 (98%)	1 (2%)	0	100	100
5	k	44/63 (70%)	41 (93%)	3 (7%)	0	100	100
5	l	45/63 (71%)	41 (91%)	4 (9%)	0	100	100
5	m	43/63 (68%)	41 (95%)	2 (5%)	0	100	100
5	n	43/63 (68%)	41 (95%)	2 (5%)	0	100	100
All	All	2107/2488 (85%)	2068 (98%)	37 (2%)	2 (0%)	48	79

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	Z	191	ALA
5	h	56	GLU

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	32/34 (94%)	30 (94%)	2 (6%)	15	40
1	E	33/34 (97%)	31 (94%)	2 (6%)	15	41
1	I	32/34 (94%)	30 (94%)	2 (6%)	15	40
1	M	34/34 (100%)	32 (94%)	2 (6%)	16	41
1	Q	33/34 (97%)	31 (94%)	2 (6%)	15	41
1	U	33/34 (97%)	31 (94%)	2 (6%)	15	41
1	Y	33/34 (97%)	31 (94%)	2 (6%)	15	41
1	c	31/34 (91%)	29 (94%)	2 (6%)	14	39
2	B	54/59 (92%)	54 (100%)	0	100	100
2	F	56/59 (95%)	56 (100%)	0	100	100
2	J	54/59 (92%)	54 (100%)	0	100	100
2	N	52/59 (88%)	52 (100%)	0	100	100
2	R	56/59 (95%)	55 (98%)	1 (2%)	54	71
2	V	53/59 (90%)	53 (100%)	0	100	100
2	Z	53/59 (90%)	53 (100%)	0	100	100
2	d	54/59 (92%)	54 (100%)	0	100	100
3	C	65/72 (90%)	65 (100%)	0	100	100
3	G	67/72 (93%)	67 (100%)	0	100	100
3	K	64/72 (89%)	64 (100%)	0	100	100
3	O	64/72 (89%)	64 (100%)	0	100	100
3	S	63/72 (88%)	62 (98%)	1 (2%)	58	73
3	W	63/72 (88%)	62 (98%)	1 (2%)	58	73
3	a	63/72 (88%)	63 (100%)	0	100	100
3	e	65/72 (90%)	65 (100%)	0	100	100
4	D	53/56 (95%)	53 (100%)	0	100	100
4	H	52/56 (93%)	52 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	L	55/56 (98%)	55 (100%)	0	100	100
4	P	55/56 (98%)	55 (100%)	0	100	100
4	T	52/56 (93%)	52 (100%)	0	100	100
4	X	54/56 (96%)	53 (98%)	1 (2%)	52	69
4	b	52/56 (93%)	52 (100%)	0	100	100
4	f	51/56 (91%)	51 (100%)	0	100	100
5	g	36/46 (78%)	35 (97%)	1 (3%)	38	59
5	h	36/46 (78%)	36 (100%)	0	100	100
5	i	35/46 (76%)	34 (97%)	1 (3%)	37	58
5	j	35/46 (76%)	35 (100%)	0	100	100
5	k	36/46 (78%)	36 (100%)	0	100	100
5	l	36/46 (78%)	36 (100%)	0	100	100
5	m	35/46 (76%)	35 (100%)	0	100	100
5	n	35/46 (76%)	35 (100%)	0	100	100
All	All	1915/2136 (90%)	1893 (99%)	22 (1%)	70	79

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	W	16	ARG
1	Y	51	ASP
1	Y	47	ARG
1	c	47	ARG
1	M	47	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
4	T	159	ASN
4	X	159	ASN
4	f	152	GLN
4	X	152	GLN
2	Z	226	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	35/37 (94%)	-0.89	0 100 100	73, 99, 132, 137	0
1	E	35/37 (94%)	-0.71	0 100 100	70, 94, 115, 128	1 (2%)
1	I	34/37 (91%)	-0.93	0 100 100	64, 90, 126, 135	0
1	M	36/37 (97%)	-0.80	0 100 100	61, 89, 127, 132	1 (2%)
1	Q	35/37 (94%)	-0.77	0 100 100	68, 92, 114, 126	1 (2%)
1	U	35/37 (94%)	-0.85	0 100 100	70, 95, 117, 132	0
1	Y	35/37 (94%)	-0.80	0 100 100	60, 90, 129, 136	0
1	c	34/37 (91%)	-0.81	0 100 100	52, 94, 134, 146	1 (2%)
2	B	59/65 (90%)	-0.76	0 100 100	61, 111, 143, 151	2 (3%)
2	F	61/65 (93%)	-0.72	0 100 100	50, 103, 132, 143	2 (3%)
2	J	59/65 (90%)	-0.68	0 100 100	76, 106, 145, 148	0
2	N	57/65 (87%)	-0.82	0 100 100	36, 99, 133, 138	3 (5%)
2	R	61/65 (93%)	-0.74	0 100 100	59, 102, 130, 135	2 (3%)
2	V	58/65 (89%)	-0.69	0 100 100	39, 107, 136, 139	3 (5%)
2	Z	58/65 (89%)	-0.70	0 100 100	49, 102, 138, 140	1 (1%)
2	d	59/65 (90%)	-0.64	0 100 100	41, 113, 161, 167	2 (3%)
3	C	72/81 (88%)	-0.66	0 100 100	53, 113, 145, 149	4 (5%)
3	G	74/81 (91%)	-0.90	0 100 100	51, 107, 135, 138	7 (9%)
3	K	71/81 (87%)	-0.80	0 100 100	83, 115, 158, 170	6 (8%)
3	O	72/81 (88%)	-0.88	0 100 100	40, 104, 134, 138	5 (6%)
3	S	70/81 (86%)	-0.75	0 100 100	64, 108, 134, 136	2 (2%)
3	W	70/81 (86%)	-0.64	0 100 100	52, 111, 141, 148	4 (5%)
3	a	70/81 (86%)	-0.79	0 100 100	49, 107, 139, 162	2 (2%)
3	e	72/81 (88%)	-0.73	0 100 100	73, 120, 181, 189	8 (11%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
4	D	62/65 (95%)	-0.73	0	100 100	102, 120, 149, 159 1 (1%)
4	H	61/65 (93%)	-0.81	0	100 100	79, 113, 137, 145 2 (3%)
4	L	64/65 (98%)	-0.77	0	100 100	87, 117, 159, 185 2 (3%)
4	P	64/65 (98%)	-0.96	0	100 100	90, 112, 150, 165 1 (1%)
4	T	62/65 (95%)	-0.77	0	100 100	97, 113, 137, 145 0
4	X	63/65 (96%)	-0.78	0	100 100	88, 115, 147, 157 2 (3%)
4	b	61/65 (93%)	-0.84	0	100 100	86, 111, 149, 167 2 (3%)
4	f	62/65 (95%)	-0.83	0	100 100	75, 126, 186, 206 1 (1%)
5	g	45/63 (71%)	-0.87	0	100 100	88, 129, 147, 157 0
5	h	44/63 (69%)	-0.75	0	100 100	92, 151, 164, 170 0
5	i	43/63 (68%)	-0.94	0	100 100	59, 120, 129, 139 2 (4%)
5	j	43/63 (68%)	-0.78	0	100 100	50, 153, 168, 178 2 (4%)
5	k	44/63 (69%)	-0.87	0	100 100	77, 153, 182, 191 1 (2%)
5	l	45/63 (71%)	-0.96	0	100 100	93, 122, 134, 135 0
5	m	43/63 (68%)	-0.73	0	100 100	47, 141, 153, 160 2 (4%)
5	n	43/63 (68%)	-0.86	0	100 100	48, 142, 155, 157 2 (4%)
All	All	2171/2488 (87%)	-0.79	0	100 100	36, 113, 156, 206 77 (3%)

There are no RSRZ outliers to report.

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.