Full wwPDB X-ray Structure Validation Report (i)

Jan 4, 2024 – 07:35 am GMT

PDB ID	:	5LOW
Title	:	Structure of the Ca2+-bound Rabphilin 3A C2B domain SNAP25 complex (P21 space group)
Authors	:	Verdaguer, N.; Ferrer-Orta, C.
Deposited on	:	2016-08-10
Resolution	:	2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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:

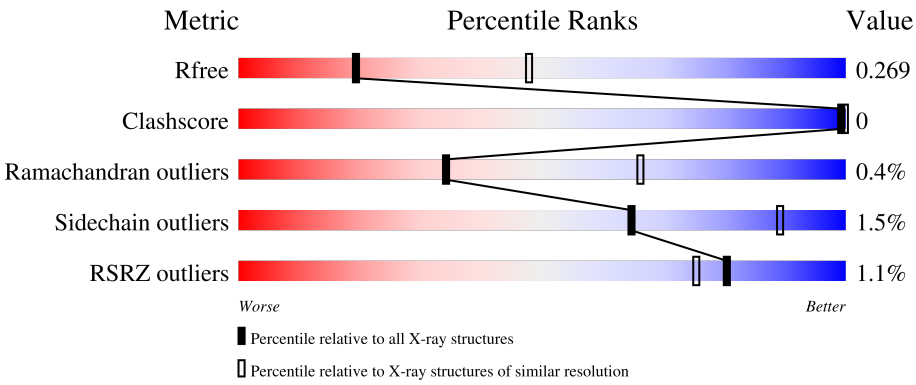
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.80 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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	162	86% • 12%
1	B	162	% 86% • 11%
1	C	162	88% • 11%
1	H	162	83% • 14%
1	I	162	% 88% • 10%

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Mol	Chain	Length	Quality of chain
1	J	162	%, 83%, 14%
2	D	95	%, 68%, 28%
2	F	95	%, 69%, 28%
2	K	95	%, 74%, 24%
2	M	95	%, 75%, 24%
3	E	82	%, 67%, 32%
3	G	82	2%, 70%, 27%
3	L	82	6%, 77%, 23%
3	N	82	73%, 27%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 11297 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 Rabphilin-3A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	142	1158	741	200	211	6	0	0	0
			Total	C	N	O	S			
1	B	144	1173	748	204	215	6	0	0	0
			Total	C	N	O	S			
1	C	144	1172	748	204	214	6	0	0	0
			Total	C	N	O	S			
1	H	140	1148	733	202	207	6	0	1	0
			Total	C	N	O	S			
1	I	145	1177	750	205	216	6	0	0	0
			Total	C	N	O	S			
1	J	140	1141	732	197	206	6	0	0	0

There are 102 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	519	HIS	-	expression tag	UNP P47709
A	520	MET	-	expression tag	UNP P47709
A	521	ALA	-	expression tag	UNP P47709
A	522	SER	-	expression tag	UNP P47709
A	523	MET	-	expression tag	UNP P47709
A	524	THR	-	expression tag	UNP P47709
A	525	GLY	-	expression tag	UNP P47709
A	526	GLY	-	expression tag	UNP P47709
A	527	GLN	-	expression tag	UNP P47709
A	528	GLN	-	expression tag	UNP P47709
A	529	MET	-	expression tag	UNP P47709
A	530	GLY	-	expression tag	UNP P47709
A	531	ARG	-	expression tag	UNP P47709
A	532	GLY	-	expression tag	UNP P47709
A	533	SER	-	expression tag	UNP P47709
A	534	ASP	-	expression tag	UNP P47709
A	535	PHE	-	expression tag	UNP P47709

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Chain	Residue	Modelled	Actual	Comment	Reference
B	519	HIS	-	expression tag	UNP P47709
B	520	MET	-	expression tag	UNP P47709
B	521	ALA	-	expression tag	UNP P47709
B	522	SER	-	expression tag	UNP P47709
B	523	MET	-	expression tag	UNP P47709
B	524	THR	-	expression tag	UNP P47709
B	525	GLY	-	expression tag	UNP P47709
B	526	GLY	-	expression tag	UNP P47709
B	527	GLN	-	expression tag	UNP P47709
B	528	GLN	-	expression tag	UNP P47709
B	529	MET	-	expression tag	UNP P47709
B	530	GLY	-	expression tag	UNP P47709
B	531	ARG	-	expression tag	UNP P47709
B	532	GLY	-	expression tag	UNP P47709
B	533	SER	-	expression tag	UNP P47709
B	534	ASP	-	expression tag	UNP P47709
B	535	PHE	-	expression tag	UNP P47709
C	519	HIS	-	expression tag	UNP P47709
C	520	MET	-	expression tag	UNP P47709
C	521	ALA	-	expression tag	UNP P47709
C	522	SER	-	expression tag	UNP P47709
C	523	MET	-	expression tag	UNP P47709
C	524	THR	-	expression tag	UNP P47709
C	525	GLY	-	expression tag	UNP P47709
C	526	GLY	-	expression tag	UNP P47709
C	527	GLN	-	expression tag	UNP P47709
C	528	GLN	-	expression tag	UNP P47709
C	529	MET	-	expression tag	UNP P47709
C	530	GLY	-	expression tag	UNP P47709
C	531	ARG	-	expression tag	UNP P47709
C	532	GLY	-	expression tag	UNP P47709
C	533	SER	-	expression tag	UNP P47709
C	534	ASP	-	expression tag	UNP P47709
C	535	PHE	-	expression tag	UNP P47709
H	519	HIS	-	expression tag	UNP P47709
H	520	MET	-	expression tag	UNP P47709
H	521	ALA	-	expression tag	UNP P47709
H	522	SER	-	expression tag	UNP P47709
H	523	MET	-	expression tag	UNP P47709
H	524	THR	-	expression tag	UNP P47709
H	525	GLY	-	expression tag	UNP P47709
H	526	GLY	-	expression tag	UNP P47709

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Chain	Residue	Modelled	Actual	Comment	Reference
H	527	GLN	-	expression tag	UNP P47709
H	528	GLN	-	expression tag	UNP P47709
H	529	MET	-	expression tag	UNP P47709
H	530	GLY	-	expression tag	UNP P47709
H	531	ARG	-	expression tag	UNP P47709
H	532	GLY	-	expression tag	UNP P47709
H	533	SER	-	expression tag	UNP P47709
H	534	ASP	-	expression tag	UNP P47709
H	535	PHE	-	expression tag	UNP P47709
I	519	HIS	-	expression tag	UNP P47709
I	520	MET	-	expression tag	UNP P47709
I	521	ALA	-	expression tag	UNP P47709
I	522	SER	-	expression tag	UNP P47709
I	523	MET	-	expression tag	UNP P47709
I	524	THR	-	expression tag	UNP P47709
I	525	GLY	-	expression tag	UNP P47709
I	526	GLY	-	expression tag	UNP P47709
I	527	GLN	-	expression tag	UNP P47709
I	528	GLN	-	expression tag	UNP P47709
I	529	MET	-	expression tag	UNP P47709
I	530	GLY	-	expression tag	UNP P47709
I	531	ARG	-	expression tag	UNP P47709
I	532	GLY	-	expression tag	UNP P47709
I	533	SER	-	expression tag	UNP P47709
I	534	ASP	-	expression tag	UNP P47709
I	535	PHE	-	expression tag	UNP P47709
J	519	HIS	-	expression tag	UNP P47709
J	520	MET	-	expression tag	UNP P47709
J	521	ALA	-	expression tag	UNP P47709
J	522	SER	-	expression tag	UNP P47709
J	523	MET	-	expression tag	UNP P47709
J	524	THR	-	expression tag	UNP P47709
J	525	GLY	-	expression tag	UNP P47709
J	526	GLY	-	expression tag	UNP P47709
J	527	GLN	-	expression tag	UNP P47709
J	528	GLN	-	expression tag	UNP P47709
J	529	MET	-	expression tag	UNP P47709
J	530	GLY	-	expression tag	UNP P47709
J	531	ARG	-	expression tag	UNP P47709
J	532	GLY	-	expression tag	UNP P47709
J	533	SER	-	expression tag	UNP P47709
J	534	ASP	-	expression tag	UNP P47709

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Chain	Residue	Modelled	Actual	Comment	Reference
J	535	PHE	-	expression tag	UNP P47709

- Molecule 2 is a protein called Synaptosomal-associated protein 25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	D	68	557	332	101	118	6	0	0	0
			Total	C	N	O	S			
2	F	68	546	324	101	117	4	0	0	0
			Total	C	N	O	S			
2	K	72	582	345	106	125	6	0	0	0
			Total	C	N	O	S			
2	M	72	580	345	105	125	5	0	0	0

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-12	GLY	-	expression tag	UNP P60881
D	-11	SER	-	expression tag	UNP P60881
D	-10	HIS	-	expression tag	UNP P60881
D	-9	MET	-	expression tag	UNP P60881
D	-8	ALA	-	expression tag	UNP P60881
D	-7	SER	-	expression tag	UNP P60881
D	-6	MET	-	expression tag	UNP P60881
D	-5	THR	-	expression tag	UNP P60881
D	-4	GLY	-	expression tag	UNP P60881
D	-3	GLY	-	expression tag	UNP P60881
D	-2	GLN	-	expression tag	UNP P60881
D	-1	GLN	-	expression tag	UNP P60881
D	0	MET	-	expression tag	UNP P60881
D	1	GLY	-	expression tag	UNP P60881
D	2	ARG	-	expression tag	UNP P60881
D	3	GLY	-	expression tag	UNP P60881
D	4	SER	-	expression tag	UNP P60881
D	5	GLU	-	expression tag	UNP P60881
D	6	PHE	-	expression tag	UNP P60881
F	-12	GLY	-	expression tag	UNP P60881
F	-11	SER	-	expression tag	UNP P60881
F	-10	HIS	-	expression tag	UNP P60881
F	-9	MET	-	expression tag	UNP P60881
F	-8	ALA	-	expression tag	UNP P60881
F	-7	SER	-	expression tag	UNP P60881

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-6	MET	-	expression tag	UNP P60881
F	-5	THR	-	expression tag	UNP P60881
F	-4	GLY	-	expression tag	UNP P60881
F	-3	GLY	-	expression tag	UNP P60881
F	-2	GLN	-	expression tag	UNP P60881
F	-1	GLN	-	expression tag	UNP P60881
F	0	MET	-	expression tag	UNP P60881
F	1	GLY	-	expression tag	UNP P60881
F	2	ARG	-	expression tag	UNP P60881
F	3	GLY	-	expression tag	UNP P60881
F	4	SER	-	expression tag	UNP P60881
F	5	GLU	-	expression tag	UNP P60881
F	6	PHE	-	expression tag	UNP P60881
K	-12	GLY	-	expression tag	UNP P60881
K	-11	SER	-	expression tag	UNP P60881
K	-10	HIS	-	expression tag	UNP P60881
K	-9	MET	-	expression tag	UNP P60881
K	-8	ALA	-	expression tag	UNP P60881
K	-7	SER	-	expression tag	UNP P60881
K	-6	MET	-	expression tag	UNP P60881
K	-5	THR	-	expression tag	UNP P60881
K	-4	GLY	-	expression tag	UNP P60881
K	-3	GLY	-	expression tag	UNP P60881
K	-2	GLN	-	expression tag	UNP P60881
K	-1	GLN	-	expression tag	UNP P60881
K	0	MET	-	expression tag	UNP P60881
K	1	GLY	-	expression tag	UNP P60881
K	2	ARG	-	expression tag	UNP P60881
K	3	GLY	-	expression tag	UNP P60881
K	4	SER	-	expression tag	UNP P60881
K	5	GLU	-	expression tag	UNP P60881
K	6	PHE	-	expression tag	UNP P60881
M	-12	GLY	-	expression tag	UNP P60881
M	-11	SER	-	expression tag	UNP P60881
M	-10	HIS	-	expression tag	UNP P60881
M	-9	MET	-	expression tag	UNP P60881
M	-8	ALA	-	expression tag	UNP P60881
M	-7	SER	-	expression tag	UNP P60881
M	-6	MET	-	expression tag	UNP P60881
M	-5	THR	-	expression tag	UNP P60881
M	-4	GLY	-	expression tag	UNP P60881
M	-3	GLY	-	expression tag	UNP P60881

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Chain	Residue	Modelled	Actual	Comment	Reference
M	-2	GLN	-	expression tag	UNP P60881
M	-1	GLN	-	expression tag	UNP P60881
M	0	MET	-	expression tag	UNP P60881
M	1	GLY	-	expression tag	UNP P60881
M	2	ARG	-	expression tag	UNP P60881
M	3	GLY	-	expression tag	UNP P60881
M	4	SER	-	expression tag	UNP P60881
M	5	GLU	-	expression tag	UNP P60881
M	6	PHE	-	expression tag	UNP P60881

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	E	56	450	263	86	97	4	0	0	0
			Total	C	N	O	S			
3	G	60	476	278	93	101	4	0	0	0
			Total	C	N	O	S			
3	L	63	503	296	97	105	5	0	0	0
			Total	C	N	O	S			
3	N	60	486	286	93	103	4	0	0	0

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	122	GLY	-	expression tag	UNP P60881
E	123	SER	-	expression tag	UNP P60881
E	124	HIS	-	expression tag	UNP P60881
E	125	MET	-	expression tag	UNP P60881
E	126	ALA	-	expression tag	UNP P60881
E	127	SER	-	expression tag	UNP P60881
E	128	MET	-	expression tag	UNP P60881
E	129	THR	-	expression tag	UNP P60881
E	130	GLY	-	expression tag	UNP P60881
E	131	GLY	-	expression tag	UNP P60881
E	132	GLN	-	expression tag	UNP P60881
E	133	GLN	-	expression tag	UNP P60881
E	134	MET	-	expression tag	UNP P60881
E	135	GLY	-	expression tag	UNP P60881
E	136	ARG	-	expression tag	UNP P60881
E	137	GLY	-	expression tag	UNP P60881
E	138	SER	-	expression tag	UNP P60881

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Chain	Residue	Modelled	Actual	Comment	Reference
E	139	GLU	-	expression tag	UNP P60881
E	140	PHE	-	expression tag	UNP P60881
G	122	GLY	-	expression tag	UNP P60881
G	123	SER	-	expression tag	UNP P60881
G	124	HIS	-	expression tag	UNP P60881
G	125	MET	-	expression tag	UNP P60881
G	126	ALA	-	expression tag	UNP P60881
G	127	SER	-	expression tag	UNP P60881
G	128	MET	-	expression tag	UNP P60881
G	129	THR	-	expression tag	UNP P60881
G	130	GLY	-	expression tag	UNP P60881
G	131	GLY	-	expression tag	UNP P60881
G	132	GLN	-	expression tag	UNP P60881
G	133	GLN	-	expression tag	UNP P60881
G	134	MET	-	expression tag	UNP P60881
G	135	GLY	-	expression tag	UNP P60881
G	136	ARG	-	expression tag	UNP P60881
G	137	GLY	-	expression tag	UNP P60881
G	138	SER	-	expression tag	UNP P60881
G	139	GLU	-	expression tag	UNP P60881
G	140	PHE	-	expression tag	UNP P60881
L	122	GLY	-	expression tag	UNP P60881
L	123	SER	-	expression tag	UNP P60881
L	124	HIS	-	expression tag	UNP P60881
L	125	MET	-	expression tag	UNP P60881
L	126	ALA	-	expression tag	UNP P60881
L	127	SER	-	expression tag	UNP P60881
L	128	MET	-	expression tag	UNP P60881
L	129	THR	-	expression tag	UNP P60881
L	130	GLY	-	expression tag	UNP P60881
L	131	GLY	-	expression tag	UNP P60881
L	132	GLN	-	expression tag	UNP P60881
L	133	GLN	-	expression tag	UNP P60881
L	134	MET	-	expression tag	UNP P60881
L	135	GLY	-	expression tag	UNP P60881
L	136	ARG	-	expression tag	UNP P60881
L	137	GLY	-	expression tag	UNP P60881
L	138	SER	-	expression tag	UNP P60881
L	139	GLU	-	expression tag	UNP P60881
L	140	PHE	-	expression tag	UNP P60881
N	122	GLY	-	expression tag	UNP P60881
N	123	SER	-	expression tag	UNP P60881

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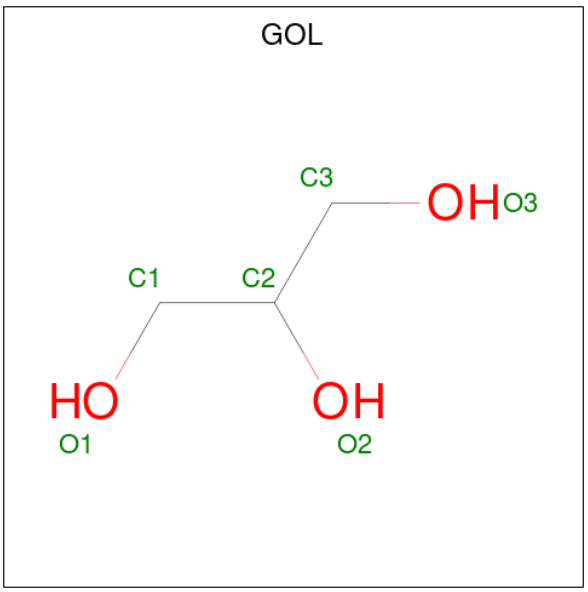
Chain	Residue	Modelled	Actual	Comment	Reference
N	124	HIS	-	expression tag	UNP P60881
N	125	MET	-	expression tag	UNP P60881
N	126	ALA	-	expression tag	UNP P60881
N	127	SER	-	expression tag	UNP P60881
N	128	MET	-	expression tag	UNP P60881
N	129	THR	-	expression tag	UNP P60881
N	130	GLY	-	expression tag	UNP P60881
N	131	GLY	-	expression tag	UNP P60881
N	132	GLN	-	expression tag	UNP P60881
N	133	GLN	-	expression tag	UNP P60881
N	134	MET	-	expression tag	UNP P60881
N	135	GLY	-	expression tag	UNP P60881
N	136	ARG	-	expression tag	UNP P60881
N	137	GLY	-	expression tag	UNP P60881
N	138	SER	-	expression tag	UNP P60881
N	139	GLU	-	expression tag	UNP P60881
N	140	PHE	-	expression tag	UNP P60881

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	6	3	3	0	0
4	B	1	6	3	3	0	0
4	C	1	6	3	3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	K	1	6	3	3	0	0
			Total	C	O		
4	M	1	6	3	3	0	0
			Total	C	O		
4	M	1	6	3	3	0	0
			Total	C	O		
4	N	1	6	3	3	0	0

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
5	A	2	2	2	0	0
			Total	Ca		
5	B	2	2	2	0	0
			Total	Ca		
5	C	2	2	2	0	0
			Total	Ca		
5	H	2	2	2	0	0
			Total	Ca		
5	I	2	2	2	0	0
			Total	Ca		
5	J	2	2	2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	8	8	8	0	0
			Total	O		
6	B	9	9	9	0	0
			Total	O		
6	C	8	8	8	0	0
			Total	O		
6	D	4	4	4	0	0
			Total	O		
6	E	4	4	4	0	0
			Total	O		
6	F	4	4	4	0	0
			Total	O		
6	G	6	6	6	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	H	6	6	6	0	0
			Total	O		
6	I	7	7	7	0	0
			Total	O		
6	J	16	16	16	0	0
			Total	O		
6	K	4	4	4	0	0
			Total	O		
6	L	6	6	6	0	0
			Total	O		
6	M	8	8	8	0	0
			Total	O		
6	N	4	4	4	0	0

3 Residue-property plots (i)

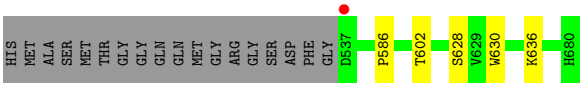
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Rabphilin-3A

Chain A:

• Molecule 1: Rabphilin-3A

Chain B:



• Molecule 1: Rabphilin-3A

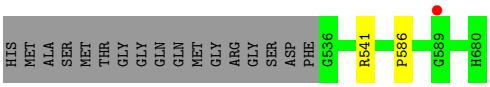
Chain C:

• Molecule 1: Rabphilin-3A

Chain H:

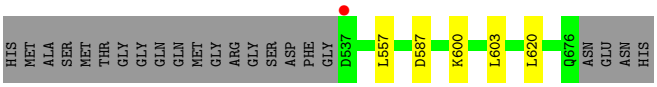
• Molecule 1: Rabphilin-3A

Chain I:



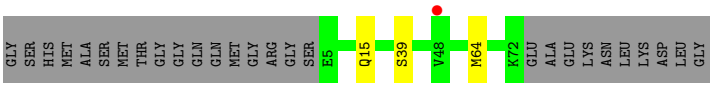
• Molecule 1: Rabphilin-3A

Chain J:



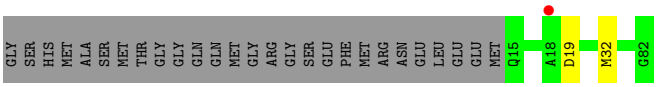
• Molecule 2: Synaptosomal-associated protein 25

Chain D:



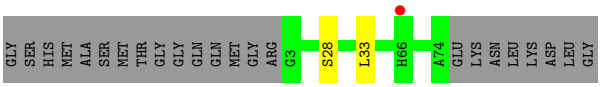
• Molecule 2: Synaptosomal-associated protein 25

Chain F:



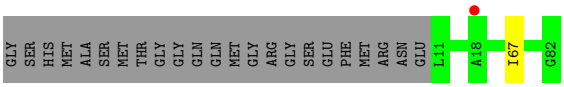
• Molecule 2: Synaptosomal-associated protein 25

Chain K:



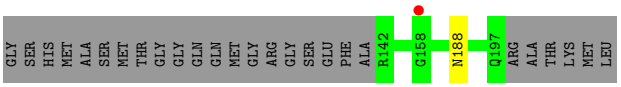
• Molecule 2: Synaptosomal-associated protein 25

Chain M:



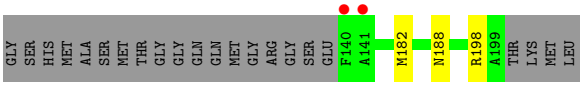
• Molecule 3: Synaptosomal-associated protein 25

Chain E:



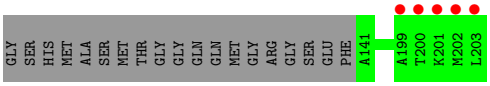
• Molecule 3: Synaptosomal-associated protein 25

Chain G:



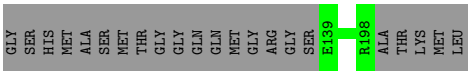
• Molecule 3: Synaptosomal-associated protein 25

Chain L:



• Molecule 3: Synaptosomal-associated protein 25

Chain N:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	60.08Å 239.50Å 71.49Å 90.00° 114.92° 90.00°	Depositor
Resolution (Å)	45.03 – 2.80 45.03 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.1 (45.03-2.80) 98.1 (45.03-2.80)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.27 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.238 , 0.269 0.240 , 0.269	Depositor DCC
R_{free} test set	2212 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	48.7	Xtriage
Anisotropy	0.181	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 9.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	0.408 for h,-k,-h-l	Xtriage
Reported twinning fraction	0.537 for H, K, L 0.463 for -H, -K, H+L	Depositor
Outliers	0 of 43903 reflections	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	11297	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.48% 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)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, GOL

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	0.35	0/1183	0.51	1/1585 (0.1%)
1	B	0.34	0/1199	0.50	0/1607
1	C	0.34	0/1198	0.48	0/1607
1	H	0.35	0/1173	0.49	0/1572
1	I	0.35	0/1203	0.49	0/1612
1	J	0.34	0/1166	0.48	0/1562
2	D	0.36	0/558	0.52	0/741
2	F	0.36	0/546	0.52	0/725
2	K	0.37	0/583	0.53	0/775
2	M	0.36	0/580	0.54	0/770
3	E	0.37	0/450	0.55	0/600
3	G	0.38	0/476	0.61	0/635
3	L	0.37	0/503	0.54	0/670
3	N	0.38	0/487	0.54	0/649
All	All	0.35	0/11305	0.51	1/15110 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	585	LYS	C-N-CD	-5.32	108.89	120.60

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	1158	0	1165	0	0
1	B	1173	0	1167	1	0
1	C	1172	0	1167	0	0
1	H	1148	0	1151	1	0
1	I	1177	0	1170	0	0
1	J	1141	0	1153	1	0
2	D	557	0	537	1	0
2	F	546	0	535	1	0
2	K	582	0	557	1	0
2	M	580	0	567	1	0
3	E	450	0	429	0	0
3	G	476	0	454	0	0
3	L	503	0	492	0	0
3	N	486	0	462	0	0
4	A	6	0	8	0	0
4	B	6	0	8	0	0
4	C	6	0	8	0	0
4	K	6	0	8	0	0
4	M	12	0	16	0	0
4	N	6	0	8	0	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
5	C	2	0	0	0	0
5	H	2	0	0	0	0
5	I	2	0	0	0	0
5	J	2	0	0	0	0
6	A	8	0	0	0	0
6	B	9	0	0	0	0
6	C	8	0	0	0	0
6	D	4	0	0	0	0
6	E	4	0	0	0	0
6	F	4	0	0	0	0
6	G	6	0	0	0	0
6	H	6	0	0	0	0
6	I	7	0	0	0	0
6	J	16	0	0	0	0
6	K	4	0	0	0	0
6	L	6	0	0	0	0
6	M	8	0	0	0	0
6	N	4	0	0	0	0
All	All	11297	0	11062	5	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 0.

All (5) 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)
2:D:64:MET:SD	2:F:32:MET:SD	3.12	0.47
1:H:557:LEU:HD22	1:H:620:LEU:HD11	1.97	0.46
1:J:557:LEU:HD22	1:J:620:LEU:HD11	2.00	0.43
2:K:28:SER:O	2:M:67:ILE:HD11	2.19	0.42
1:B:628:SER:HG	1:B:630:TRP:HE1	1.70	0.40

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 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	140/162 (86%)	130 (93%)	9 (6%)	1 (1%)	22	53
1	B	142/162 (88%)	130 (92%)	11 (8%)	1 (1%)	22	53
1	C	142/162 (88%)	134 (94%)	7 (5%)	1 (1%)	22	53
1	H	139/162 (86%)	127 (91%)	11 (8%)	1 (1%)	22	53
1	I	143/162 (88%)	131 (92%)	11 (8%)	1 (1%)	22	53
1	J	138/162 (85%)	127 (92%)	11 (8%)	0	100	100
2	D	66/95 (70%)	66 (100%)	0	0	100	100
2	F	66/95 (70%)	65 (98%)	1 (2%)	0	100	100
2	K	70/95 (74%)	68 (97%)	2 (3%)	0	100	100
2	M	70/95 (74%)	67 (96%)	3 (4%)	0	100	100
3	E	54/82 (66%)	54 (100%)	0	0	100	100
3	G	58/82 (71%)	56 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	L	61/82 (74%)	58 (95%)	3 (5%)	0	100	100
3	N	58/82 (71%)	56 (97%)	2 (3%)	0	100	100
All	All	1347/1680 (80%)	1269 (94%)	73 (5%)	5 (0%)	34	66

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	586	PRO
1	B	586	PRO
1	H	586	PRO
1	C	538	ILE
1	I	586	PRO

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	125/139 (90%)	124 (99%)	1 (1%)	81	94
1	B	126/139 (91%)	124 (98%)	2 (2%)	62	88
1	C	126/139 (91%)	126 (100%)	0	100	100
1	H	123/139 (88%)	119 (97%)	4 (3%)	38	72
1	I	126/139 (91%)	125 (99%)	1 (1%)	81	94
1	J	123/139 (88%)	120 (98%)	3 (2%)	49	81
2	D	61/81 (75%)	59 (97%)	2 (3%)	38	72
2	F	60/81 (74%)	59 (98%)	1 (2%)	60	87
2	K	64/81 (79%)	63 (98%)	1 (2%)	62	88
2	M	64/81 (79%)	64 (100%)	0	100	100
3	E	50/68 (74%)	49 (98%)	1 (2%)	55	84
3	G	51/68 (75%)	48 (94%)	3 (6%)	19	49
3	L	55/68 (81%)	55 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	N	53/68 (78%)	53 (100%)	0	100	100
All	All	1207/1430 (84%)	1188 (98%)	19 (2%)	65	88

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	636	LYS
1	B	602	THR
1	B	636	LYS
2	D	15	GLN
2	D	39	SER
3	E	188	ASN
2	F	19	ASP
3	G	182	MET
3	G	188	ASN
3	G	198	ARG
1	H	541[A]	ARG
1	H	541[B]	ARG
1	H	600	LYS
1	H	636	LYS
1	I	541	ARG
1	J	587	ASP
1	J	600	LYS
1	J	603	LEU
2	K	33	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	554	GLN
2	D	34	GLN
3	E	188	ASN
2	F	20	GLN
1	H	604	ASN
3	L	149	ASN
2	M	53	GLN
3	N	175	ASN

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)

Of 19 ligands modelled in this entry, 12 are monoatomic - leaving 7 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	$\#\|Z\| > 2$
4	GOL	B	701	-	5,5,5	0.31	0	5,5,5	0.13	0
4	GOL	M	102	-	5,5,5	0.30	0	5,5,5	0.19	0
4	GOL	M	101	-	5,5,5	0.35	0	5,5,5	0.18	0
4	GOL	K	101	-	5,5,5	0.33	0	5,5,5	0.28	0
4	GOL	N	301	-	5,5,5	0.27	0	5,5,5	0.22	0
4	GOL	A	701	-	5,5,5	0.32	0	5,5,5	0.17	0
4	GOL	C	701	-	5,5,5	0.30	0	5,5,5	0.26	0

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
4	GOL	B	701	-	-	2/4/4/4	-
4	GOL	M	102	-	-	0/4/4/4	-
4	GOL	M	101	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	K	101	-	-	4/4/4/4	-
4	GOL	N	301	-	-	0/4/4/4	-
4	GOL	A	701	-	-	2/4/4/4	-
4	GOL	C	701	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	701	GOL	C1-C2-C3-O3
4	M	101	GOL	C1-C2-C3-O3
4	B	701	GOL	O1-C1-C2-O2
4	M	101	GOL	O2-C2-C3-O3
4	B	701	GOL	O1-C1-C2-C3
4	A	701	GOL	O2-C2-C3-O3
4	K	101	GOL	O2-C2-C3-O3
4	K	101	GOL	O1-C1-C2-C3
4	K	101	GOL	O1-C1-C2-O2
4	K	101	GOL	C1-C2-C3-O3

There are no ring outliers.

No monomer is involved in short contacts.

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	142/162 (87%)	-0.03	0	100	100	34, 47, 56, 66	0
1	B	144/162 (88%)	0.03	1 (0%)	87	84	41, 49, 57, 69	0
1	C	144/162 (88%)	-0.03	0	100	100	39, 46, 51, 69	0
1	H	140/162 (86%)	-0.01	0	100	100	37, 48, 57, 61	0
1	I	145/162 (89%)	0.06	1 (0%)	87	84	43, 51, 65, 73	0
1	J	140/162 (86%)	0.03	1 (0%)	87	84	38, 44, 55, 64	0
2	D	68/95 (71%)	0.10	1 (1%)	73	68	31, 39, 55, 57	0
2	F	68/95 (71%)	-0.16	1 (1%)	73	68	32, 38, 59, 63	0
2	K	72/95 (75%)	0.13	1 (1%)	75	70	34, 41, 70, 74	0
2	M	72/95 (75%)	-0.10	1 (1%)	75	70	36, 42, 67, 69	0
3	E	56/82 (68%)	-0.01	1 (1%)	68	61	32, 41, 48, 50	0
3	G	60/82 (73%)	-0.08	2 (3%)	46	36	33, 38, 65, 74	0
3	L	63/82 (76%)	0.20	5 (7%)	12	7	36, 44, 77, 82	0
3	N	60/82 (73%)	-0.22	0	100	100	34, 39, 53, 55	0
All	All	1374/1680 (81%)	-0.00	15 (1%)	80	75	31, 46, 61, 82	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	589	GLY	3.6
3	L	202	MET	3.3
3	L	201	LYS	3.2
3	L	200	THR	2.3
3	E	158	GLY	2.3
3	G	140	PHE	2.3
2	M	18	ALA	2.2
3	L	203	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	537	ASP	2.1
2	K	66	HIS	2.1
2	F	18	ALA	2.1
3	G	141	ALA	2.1
3	L	199	ALA	2.1
1	J	537	ASP	2.1
2	D	48	VAL	2.0

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)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	CA	B	702	1/1	0.79	0.14	55,55,55,55	0
5	CA	C	703	1/1	0.80	0.13	65,65,65,65	0
4	GOL	B	701	6/6	0.84	0.26	65,65,66,66	0
5	CA	H	702	1/1	0.87	0.15	72,72,72,72	0
5	CA	B	703	1/1	0.88	0.13	58,58,58,58	0
5	CA	I	702	1/1	0.88	0.17	54,54,54,54	0
5	CA	J	701	1/1	0.89	0.12	73,73,73,73	0
4	GOL	N	301	6/6	0.90	0.19	47,47,47,48	0
5	CA	H	701	1/1	0.91	0.14	52,52,52,52	0
4	GOL	M	101	6/6	0.92	0.20	40,41,41,41	0
4	GOL	M	102	6/6	0.93	0.14	42,42,42,42	0
4	GOL	K	101	6/6	0.93	0.15	40,40,40,41	0
4	GOL	C	701	6/6	0.93	0.14	62,63,63,63	0
4	GOL	A	701	6/6	0.94	0.18	29,29,30,30	0
5	CA	J	702	1/1	0.94	0.14	48,48,48,48	0
5	CA	A	703	1/1	0.95	0.12	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	CA	A	702	1/1	0.96	0.11	64,64,64,64	0
5	CA	C	702	1/1	0.97	0.16	55,55,55,55	0
5	CA	I	701	1/1	0.98	0.17	58,58,58,58	0

6.5 Other polymers (i)

There are no such residues in this entry.