



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 06:23 pm BST

PDB ID : 5LOB  
Title : Structure of the Ca<sup>2+</sup>-bound Rabphilin3A C2B- SNAP25 complex (C2 space group)  
Authors : Ferrer-Orta, C.; Verdaguer, N.  
Deposited on : 2016-08-09  
Resolution : 3.30 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

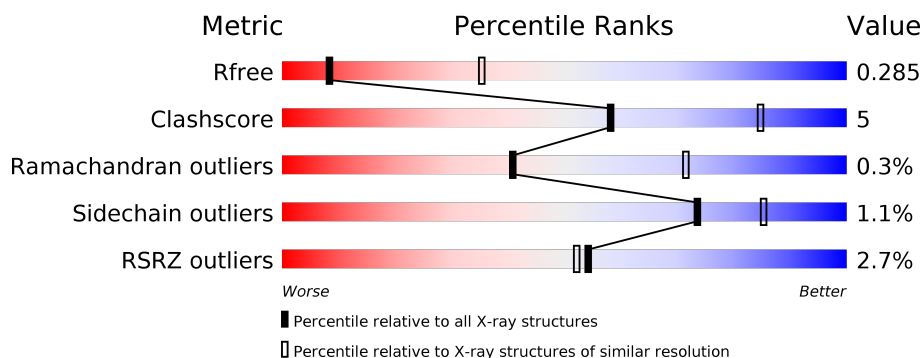
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	162	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="width: 78%; height: 10px; background-color: green;"></div> <div style="width: 6%; height: 10px; background-color: yellow;"></div> <div style="width: 15%; height: 10px; background-color: grey;"></div> </div>
1	B	162	<div> <div style="width: 7%; height: 10px; background-color: red;"></div> <div style="width: 69%; height: 10px; background-color: green;"></div> <div style="width: 17%; height: 10px; background-color: yellow;"></div> <div style="width: 14%; height: 10px; background-color: grey;"></div> </div>
1	C	162	<div> <div style="width: 72%; height: 10px; background-color: green;"></div> <div style="width: 13%; height: 10px; background-color: yellow;"></div> <div style="width: 15%; height: 10px; background-color: grey;"></div> </div>
2	D	100	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="width: 75%; height: 10px; background-color: green;"></div> <div style="width: 10%; height: 10px; background-color: yellow;"></div> <div style="width: 15%; height: 10px; background-color: grey;"></div> </div>
2	F	100	<div> <div style="width: 4%; height: 10px; background-color: red;"></div> <div style="width: 79%; height: 10px; background-color: green;"></div> <div style="width: 9%; height: 10px; background-color: yellow;"></div> <div style="width: 12%; height: 10px; background-color: grey;"></div> </div>
3	E	96	<div> <div style="width: 56%; height: 10px; background-color: green;"></div> <div style="width: 10%; height: 10px; background-color: yellow;"></div> <div style="width: 31%; height: 10px; background-color: grey;"></div> </div>

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Mol	Chain	Length	Quality of chain
3	G	96	 63% 11% 26%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	SO4	A	706	-	-	-	X
5	SO4	G	301	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5922 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
1	A	138	Total	C	N	O	S	0	0	0
			1124	721	196	201	6			
1	B	139	Total	C	N	O	S	0	0	0
			1133	726	197	204	6			
1	C	138	Total	C	N	O	S	0	0	0
			1124	721	196	201	6			

There are 51 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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	85	Total	C	N	O	S	0	0	0
			682	403	127	145	7			
2	F	88	Total	C	N	O	S	0	0	0
			694	412	128	147	7			

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-12	GLY	-	expression tag	PDB ?
D	-11	SER	-	expression tag	PDB ?

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	66	Total	C	N	O	S	0	0	0
			530	313	100	112	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	71	Total	C	N	O	S	0	0	0
			525	308	101	112	4			

There are 38 discrepancies between the modelled and reference sequences:

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

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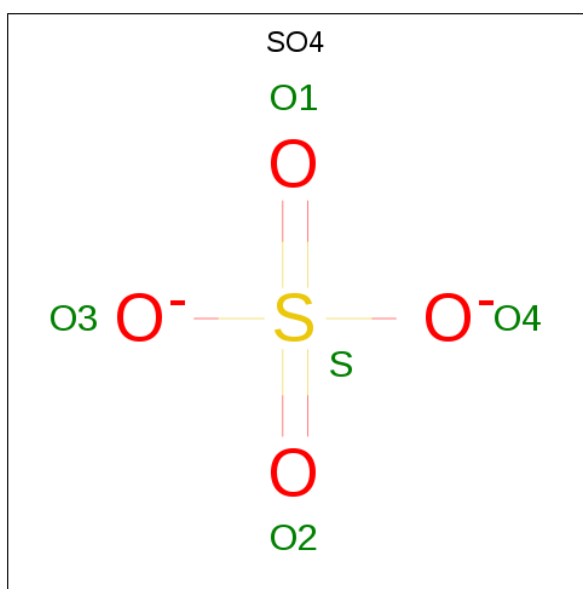
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Chain	Residue	Modelled	Actual	Comment	Reference
G	139	GLU	-	expression tag	PDB ?
G	140	PHE	-	expression tag	PDB ?

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	2	Total Ca 2 2	0	0
4	A	2	Total Ca 2 2	0	0
4	C	2	Total Ca 2 2	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O S 5 4 1	0	0
5	A	1	Total O S 5 4 1	0	0
5	A	1	Total O S 5 4 1	0	0
5	A	1	Total O S 5 4 1	0	0
5	B	1	Total O S 5 4 1	0	0

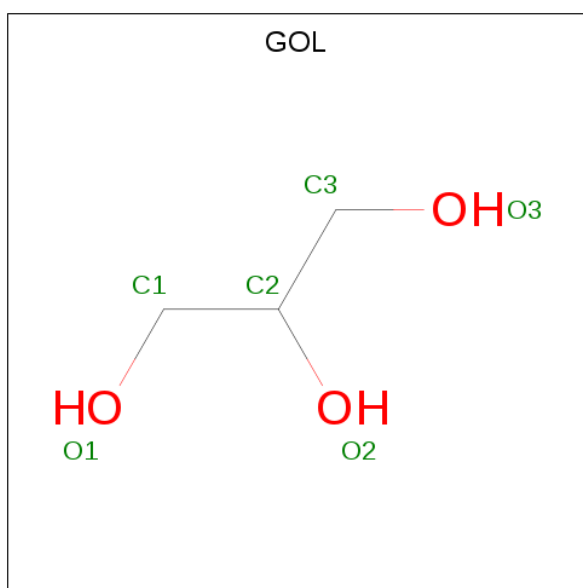
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	E	1	Total	O	S	0	0
			5	4	1		
5	F	1	Total	O	S	0	0
			5	4	1		
5	G	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

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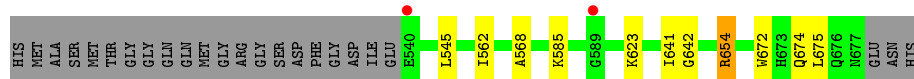
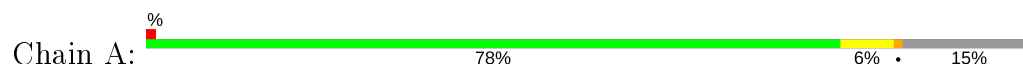
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	F	1	Total	C	O	0	0
			6	3	3		
6	G	1	Total	C	O	0	0
			6	3	3		
6	G	1	Total	C	O	0	0
			6	3	3		

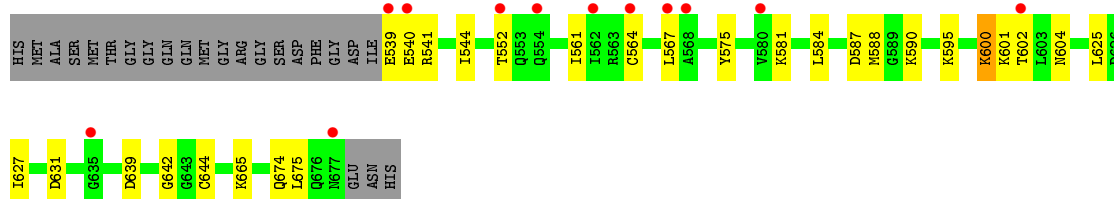
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

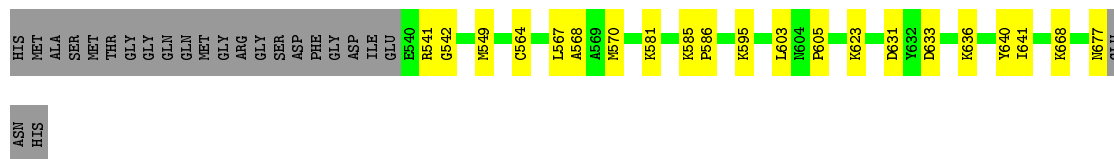
#### • Molecule 1: Rabphilin-3A



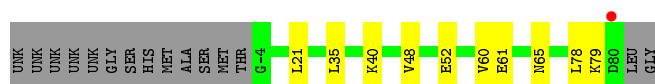
#### • Molecule 1: Rabphilin-3A



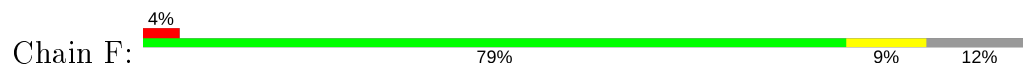
#### • Molecule 1: Rabphilin-3A

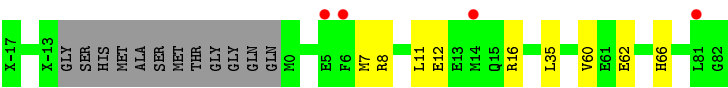


#### • Molecule 2: Synaptosomal-associated protein 25

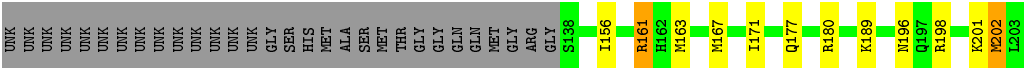


#### • Molecule 2: Synaptosomal-associated protein 25

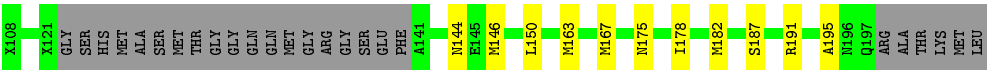




• Molecule 3: Synaptosomal-associated protein 25



• Molecule 3: Synaptosomal-associated protein 25



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	153.97Å 58.75Å 125.31Å 90.00° 103.24° 90.00°	Depositor
Resolution (Å)	42.53 – 3.30 42.53 – 3.30	Depositor EDS
% Data completeness (in resolution range)	77.2 (42.53-3.30) 77.3 (42.53-3.30)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.80 (at 3.32Å)	Xtriage
Refinement program	PHENIX (dev_2341: ???)	Depositor
R, $R_{free}$	0.240 , 0.286 0.239 , 0.285	Depositor DCC
$R_{free}$ test set	632 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	74.4	Xtriage
Anisotropy	0.400	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 54.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	5922	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.87% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, CA, SO4

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	0.24	0/1149	0.40	0/1539
1	B	0.23	0/1158	0.41	0/1551
1	C	0.24	0/1149	0.42	0/1539
2	D	0.22	0/683	0.33	0/905
2	F	0.22	0/670	0.34	0/887
3	E	0.23	0/531	0.35	0/706
3	G	0.25	0/455	0.37	0/607
All	All	0.23	0/5795	0.38	0/7734

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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	1124	0	1138	7	0
1	B	1133	0	1144	14	0
1	C	1124	0	1138	13	0
2	D	682	0	660	7	0
2	F	694	0	659	6	0
3	E	530	0	512	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	525	0	456	9	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
5	A	20	0	0	0	0
5	B	10	0	0	0	0
5	C	5	0	0	0	0
5	E	5	0	0	0	0
5	F	5	0	0	0	0
5	G	5	0	0	0	0
6	A	18	0	24	1	0
6	B	6	0	8	1	0
6	C	6	0	8	0	0
6	F	12	0	16	0	0
6	G	12	0	16	0	0
All	All	5922	0	5779	56	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 5.

All (56) 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)
3:E:196:ASN:ND2	3:G:146:MET:SD	2.65	0.70
1:B:539:GLU:O	1:B:674:GLN:NE2	2.27	0.68
2:D:21:LEU:HD21	3:G:195:ALA:HB1	1.79	0.65
1:A:654:ARG:HH11	1:A:674:GLN:H	1.45	0.65
2:D:60:VAL:HG22	2:F:35:LEU:HB3	1.80	0.64
1:B:600:LYS:H	1:B:600:LYS:HD3	1.65	0.62
1:C:564:CYS:HB2	1:C:605:PRO:HG2	1.81	0.62
3:E:189:LYS:HG3	3:G:150:LEU:HD13	1.83	0.60
2:D:40:LYS:HD2	3:E:156:ILE:HG23	1.83	0.60
1:C:586:PRO:HG2	1:C:623:LYS:HA	1.84	0.60
1:C:586:PRO:HB2	1:C:623:LYS:HD3	1.84	0.59
3:E:202:MET:HG2	2:F:11:LEU:HD11	1.85	0.58
2:F:62:GLU:O	2:F:66:HIS:ND1	2.34	0.58
1:C:549:MET:HB2	1:C:668:LYS:HA	1.84	0.57
1:C:585:LYS:HG3	1:C:586:PRO:HD3	1.87	0.57
1:C:633:ASP:HB3	1:C:636:LYS:HG3	1.86	0.57
3:E:171:ILE:HD13	3:G:167:MET:HB3	1.87	0.57
1:A:654:ARG:HD2	1:A:654:ARG:H	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:581:LYS:HG3	1:B:595:LYS:HG2	1.87	0.55
1:B:602:THR:HG22	1:B:604:ASN:H	1.73	0.53
3:E:161:ARG:NH2	3:G:175:ASN:O	2.42	0.53
1:B:564:CYS:HB3	1:B:567:LEU:HD21	1.91	0.52
1:B:631:ASP:HB3	1:B:639:ASP:HB2	1.90	0.52
1:A:568:ALA:HB3	1:A:641:ILE:HG23	1.92	0.52
1:C:581:LYS:HG3	1:C:595:LYS:HG2	1.92	0.50
1:C:631:ASP:HB2	1:C:641:ILE:HD11	1.94	0.50
3:E:161:ARG:NH2	3:G:175:ASN:OD1	2.44	0.50
1:A:585:LYS:HD3	1:A:623:LYS:HA	1.93	0.50
1:C:640:TYR:HE2	1:C:677:ASN:HA	1.78	0.49
1:B:627:ILE:O	1:B:644:CYS:N	2.44	0.49
1:C:541:ARG:HA	1:C:568:ALA:HB2	1.97	0.47
1:C:570:MET:HG3	1:C:641:ILE:HG12	1.96	0.47
3:G:163:MET:O	3:G:167:MET:N	2.43	0.46
1:C:542:GLY:HA3	1:C:567:LEU:HD23	1.98	0.46
2:F:7:MET:HB3	2:F:8:ARG:H	1.58	0.45
1:B:552:THR:HG21	1:B:665:LYS:HD2	1.98	0.45
1:B:642:GLY:HA3	1:B:675:LEU:HB3	1.98	0.45
2:D:35:LEU:HB3	2:F:60:VAL:HG22	1.99	0.45
1:B:590:LYS:HE3	6:B:705:GOL:H2	2.00	0.44
3:E:177:GLN:HG3	3:E:180:ARG:HH21	1.83	0.44
3:E:202:MET:N	3:E:202:MET:SD	2.91	0.44
3:E:163:MET:O	3:E:167:MET:HB2	2.18	0.44
1:B:544:ILE:HD11	1:B:561:ILE:HD12	1.99	0.43
1:A:545:LEU:HG	1:A:562:ILE:HD13	1.99	0.43
2:D:78:LEU:O	2:D:79:LYS:HD2	2.18	0.43
1:B:540:GLU:HG3	1:B:541:ARG:HG3	2.00	0.43
2:D:48:VAL:O	2:D:52:GLU:HG2	2.20	0.42
1:B:584:LEU:HB2	1:B:625:LEU:HD13	2.02	0.42
3:G:178:ILE:O	3:G:182:MET:HG3	2.20	0.42
1:B:575:TYR:CD2	1:B:601:LYS:HE2	2.55	0.41
1:A:672:TRP:HD1	6:A:708:GOL:H2	1.85	0.41
1:A:642:GLY:HA3	1:A:675:LEU:HB3	2.03	0.41
2:D:61:GLU:O	2:D:65:ASN:ND2	2.50	0.40
2:F:12:GLU:OE2	2:F:16:ARG:NH1	2.53	0.40
1:C:603:LEU:H	1:C:603:LEU:HD23	1.86	0.40
3:G:187:SER:HB3	3:G:191:ARG:HH12	1.87	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	136/162 (84%)	128 (94%)	8 (6%)	0	100	100
1	B	137/162 (85%)	125 (91%)	10 (7%)	2 (2%)	10	38
1	C	136/162 (84%)	125 (92%)	11 (8%)	0	100	100
2	D	83/100 (83%)	80 (96%)	3 (4%)	0	100	100
2	F	81/100 (81%)	76 (94%)	5 (6%)	0	100	100
3	E	64/96 (67%)	61 (95%)	3 (5%)	0	100	100
3	G	55/96 (57%)	55 (100%)	0	0	100	100
All	All	692/878 (79%)	650 (94%)	40 (6%)	2 (0%)	41	71

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	588	MET
1	B	587	ASP

### 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	121/139 (87%)	120 (99%)	1 (1%)	81	89
1	B	122/139 (88%)	121 (99%)	1 (1%)	81	89
1	C	121/139 (87%)	121 (100%)	0	100	100
2	D	74/81 (91%)	74 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	73/81 (90%)	73 (100%)	0	100	100
3	E	58/68 (85%)	54 (93%)	4 (7%)	15	44
3	G	50/68 (74%)	49 (98%)	1 (2%)	55	76
All	All	619/715 (87%)	612 (99%)	7 (1%)	73	85

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	654	ARG
1	B	600	LYS
3	E	161	ARG
3	E	198	ARG
3	E	201	LYS
3	E	202	MET
3	G	144	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
3	E	196	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 25 ligands modelled in this entry, 6 are monoatomic - leaving 19 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
5	SO4	C	703	4	4,4,4	0.13	0	6,6,6	0.07	0
5	SO4	A	703	4	4,4,4	0.14	0	6,6,6	0.06	0
5	SO4	B	703	-	4,4,4	0.15	0	6,6,6	0.06	0
6	GOL	A	709	-	5,5,5	0.38	0	5,5,5	0.21	0
6	GOL	B	705	-	5,5,5	0.37	0	5,5,5	0.26	0
5	SO4	B	704	-	4,4,4	0.14	0	6,6,6	0.05	0
6	GOL	F	103	-	5,5,5	0.36	0	5,5,5	0.20	0
5	SO4	A	705	-	4,4,4	0.14	0	6,6,6	0.05	0
6	GOL	C	704	-	5,5,5	0.37	0	5,5,5	0.29	0
6	GOL	F	102	-	5,5,5	0.36	0	5,5,5	0.22	0
5	SO4	E	301	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	A	706	-	4,4,4	0.14	0	6,6,6	0.05	0
6	GOL	A	707	-	5,5,5	0.35	0	5,5,5	0.26	0
6	GOL	G	303	-	5,5,5	0.38	0	5,5,5	0.26	0
5	SO4	A	704	-	4,4,4	0.14	0	6,6,6	0.05	0
6	GOL	G	302	-	5,5,5	0.36	0	5,5,5	0.30	0
5	SO4	G	301	-	4,4,4	0.15	0	6,6,6	0.04	0
6	GOL	A	708	-	5,5,5	0.38	0	5,5,5	0.29	0
5	SO4	F	101	-	4,4,4	0.14	0	6,6,6	0.05	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
6	GOL	A	709	-	-	2/4/4/4	-
6	GOL	B	705	-	-	2/4/4/4	-
6	GOL	F	102	-	-	2/4/4/4	-
6	GOL	G	303	-	-	2/4/4/4	-
6	GOL	C	704	-	-	2/4/4/4	-
6	GOL	A	708	-	-	2/4/4/4	-
6	GOL	F	103	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	A	707	-	-	2/4/4/4	-
6	GOL	G	302	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	705	GOL	O1-C1-C2-C3
6	C	704	GOL	O1-C1-C2-C3
6	A	708	GOL	O1-C1-C2-C3
6	G	302	GOL	O1-C1-C2-C3
6	F	102	GOL	O1-C1-C2-C3
6	G	303	GOL	O1-C1-C2-C3
6	A	707	GOL	O1-C1-C2-C3
6	F	103	GOL	O1-C1-C2-C3
6	A	709	GOL	O1-C1-C2-C3
6	F	103	GOL	O1-C1-C2-O2
6	A	708	GOL	O1-C1-C2-O2
6	F	102	GOL	O1-C1-C2-O2
6	G	303	GOL	O1-C1-C2-O2
6	A	709	GOL	O1-C1-C2-O2
6	B	705	GOL	O1-C1-C2-O2
6	C	704	GOL	O1-C1-C2-O2
6	G	302	GOL	O1-C1-C2-O2
6	A	707	GOL	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	705	GOL	1	0
6	A	708	GOL	1	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	G	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	G	117:UNK	C	118:UNK	N	4.83

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	138/162 (85%)	0.23	2 (1%) 75 75	47, 71, 118, 196	0
1	B	139/162 (85%)	0.65	12 (8%) 10 10	49, 79, 140, 175	0
1	C	138/162 (85%)	0.05	0 100 100	49, 74, 119, 182	0
2	D	85/100 (85%)	0.13	1 (1%) 79 78	45, 75, 119, 167	0
2	F	83/100 (83%)	0.37	4 (4%) 30 28	40, 74, 132, 178	0
3	E	66/96 (68%)	0.29	0 100 100	41, 82, 146, 185	0
3	G	57/96 (59%)	0.08	0 100 100	45, 65, 95, 120	0
All	All	706/878 (80%)	0.27	19 (2%) 54 52	40, 74, 132, 196	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	589	GLY	8.1
1	B	540	GLU	5.9
1	B	677	ASN	4.1
2	F	6	PHE	4.0
2	F	14	MET	3.2
2	F	81	LEU	3.2
1	B	552	THR	3.2
1	B	580	VAL	2.9
1	B	602	THR	2.9
2	F	5	GLU	2.8
1	B	564	CYS	2.8
1	B	562	ILE	2.7
2	D	80	ASP	2.7
1	B	539	GLU	2.5
1	A	540	GLU	2.4
1	B	567	LEU	2.2
1	B	635	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	568	ALA	2.1
1	B	554	GLN	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 carbohydrates 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
6	GOL	A	709	6/6	0.61	0.26	71,79,82,83	0
6	GOL	F	103	6/6	0.64	0.26	64,72,73,75	0
5	SO4	A	706	5/5	0.70	0.42	164,165,165,165	0
5	SO4	G	301	5/5	0.71	0.50	174,174,175,176	0
5	SO4	E	301	5/5	0.77	0.25	134,134,135,135	0
6	GOL	B	705	6/6	0.80	0.28	47,60,63,63	0
5	SO4	A	705	5/5	0.81	0.36	71,72,74,76	5
6	GOL	C	704	6/6	0.83	0.16	61,64,71,72	0
5	SO4	C	703	5/5	0.84	0.17	151,151,153,154	0
6	GOL	G	302	6/6	0.84	0.29	69,72,77,80	0
6	GOL	F	102	6/6	0.84	0.33	73,78,86,87	0
5	SO4	B	704	5/5	0.86	0.15	129,129,130,131	0
6	GOL	A	707	6/6	0.86	0.24	79,88,90,91	0
6	GOL	A	708	6/6	0.87	0.32	63,72,79,84	6
5	SO4	F	101	5/5	0.87	0.21	122,122,123,125	5
5	SO4	A	704	5/5	0.89	0.49	48,50,52,60	5
5	SO4	A	703	5/5	0.90	0.19	115,116,118,119	0
6	GOL	G	303	6/6	0.90	0.25	52,68,71,77	0
5	SO4	B	703	5/5	0.94	0.17	66,70,76,84	0
4	CA	B	702	1/1	0.97	0.08	57,57,57,57	0
4	CA	B	701	1/1	0.98	0.04	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	CA	C	702	1/1	0.98	0.05	56,56,56,56	0
4	CA	A	702	1/1	0.98	0.10	58,58,58,58	0
4	CA	A	701	1/1	0.98	0.10	46,46,46,46	0
4	CA	C	701	1/1	0.99	0.09	56,56,56,56	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.