



wwPDB EM Map/Model Validation Report ⓘ

Sep 16, 2016 – 10:21 AM EDT

PDB ID : 5GJW
EMDB ID: : EMD-9515
Title : Structure of the mammalian voltage-gated calcium channel Cav1.1 complex
for ClassII map
Authors : Wu, J.P.; Yan, Z.; Li, Z.Q.; Zhou, Q.; Yan, N.
Deposited on : 2016-07-02
Resolution : 3.90 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could
stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027939

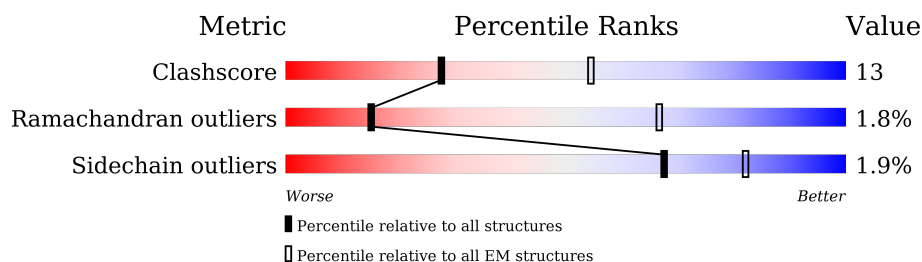
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	1873	
2	B	106	
3	C	199	
4	E	222	
5	F	1106	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 21561 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Voltage-dependent L-type calcium channel subunit alpha-1S.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1291	Total	C	N	O	S	0	0
			10261	6745	1687	1759	70		

- Molecule 2 is a protein called Voltage-dependent L-type calcium channel subunit beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	100	Total	C	N	O	S	0	0
			710	455	125	129	1		

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	69	SER	-	expression tag	UNP P19517
B	70	LEU	-	expression tag	UNP P19517
B	71	GLU	-	expression tag	UNP P19517
B	72	VAL	-	expression tag	UNP P19517
B	73	LEU	-	expression tag	UNP P19517
B	74	PHE	-	expression tag	UNP P19517
B	75	GLN	-	expression tag	UNP P19517
B	76	GLY	-	expression tag	UNP P19517
B	77	PRO	-	expression tag	UNP P19517
B	78	HIS	-	expression tag	UNP P19517
B	79	MET	-	expression tag	UNP P19517

- Molecule 3 is a protein called Voltage-dependent L-type calcium channel subunit beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	178	Total	C	N	O	S	0	0
			1367	876	232	254	5		

- Molecule 4 is a protein called Voltage-dependent calcium channel gamma-1 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	166	Total	C	N	O	S	0	0
			1304	860	213	213	18		

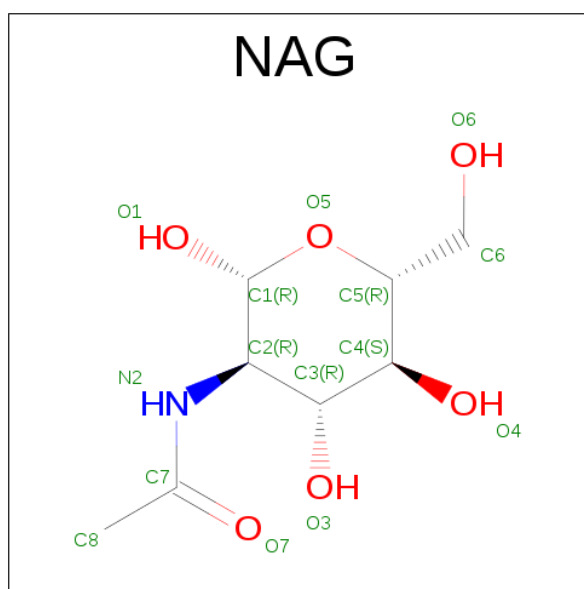
- Molecule 5 is a protein called Voltage-dependent calcium channel subunit alpha-2/delta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	942	Total	C	N	O	S	2	0
			7572	4812	1278	1452	30		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	1075	ETA	GLY	See sequence details	UNP P13806

- Molecule 6 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	N	O	0
			14	8	1	5	
6	F	1	Total	C	N	O	0
			308	176	22	110	
6	F	1	Total	C	N	O	0
			308	176	22	110	
6	F	1	Total	C	N	O	0
			308	176	22	110	
6	F	1	Total	C	N	O	0
			308	176	22	110	

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Mol	Chain	Residues	Atoms				AltConf
6	F	1	Total	C	N	O	0
			308	176	22	110	
6	F	1	Total	C	N	O	0
			308	176	22	110	
6	F	1	Total	C	N	O	0
			308	176	22	110	
6	F	1	Total	C	N	O	0
			308	176	22	110	
6	F	1	Total	C	N	O	0
			308	176	22	110	
6	F	1	Total	C	N	O	0
			308	176	22	110	
6	F	1	Total	C	N	O	0
			308	176	22	110	
6	F	1	Total	C	N	O	0
			308	176	22	110	
6	F	1	Total	C	N	O	0
			308	176	22	110	
6	F	1	Total	C	N	O	0
			308	176	22	110	
6	F	1	Total	C	N	O	0
			308	176	22	110	
6	F	1	Total	C	N	O	0
			308	176	22	110	
6	F	1	Total	C	N	O	0
			308	176	22	110	
6	F	1	Total	C	N	O	0
			308	176	22	110	
6	F	1	Total	C	N	O	0
			308	176	22	110	
6	F	1	Total	C	N	O	0
			308	176	22	110	
6	F	1	Total	C	N	O	0
			308	176	22	110	
6	F	1	Total	C	N	O	0
			308	176	22	110	

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

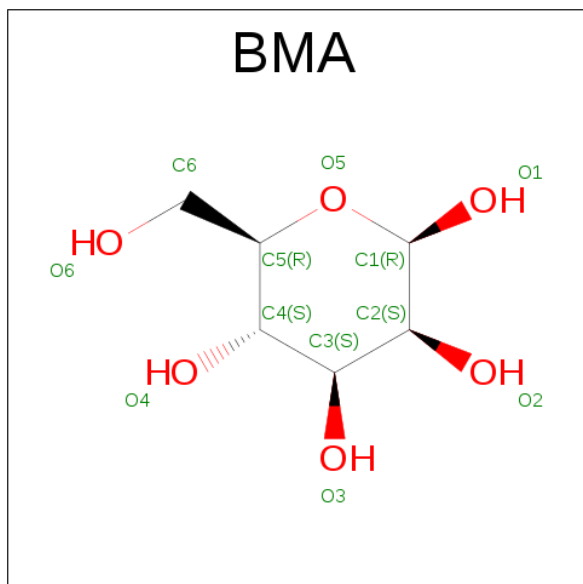
Mol	Chain	Residues	Atoms		AltConf
7	A	2	Total	Ca	0
			2	2	

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Mol	Chain	Residues	Atoms		AltConf
7	F	1	Total	Ca	0
			1	1	

- Molecule 8 is BETA-D-MANNOSE (three-letter code: BMA) (formula: $C_6H_{12}O_6$).

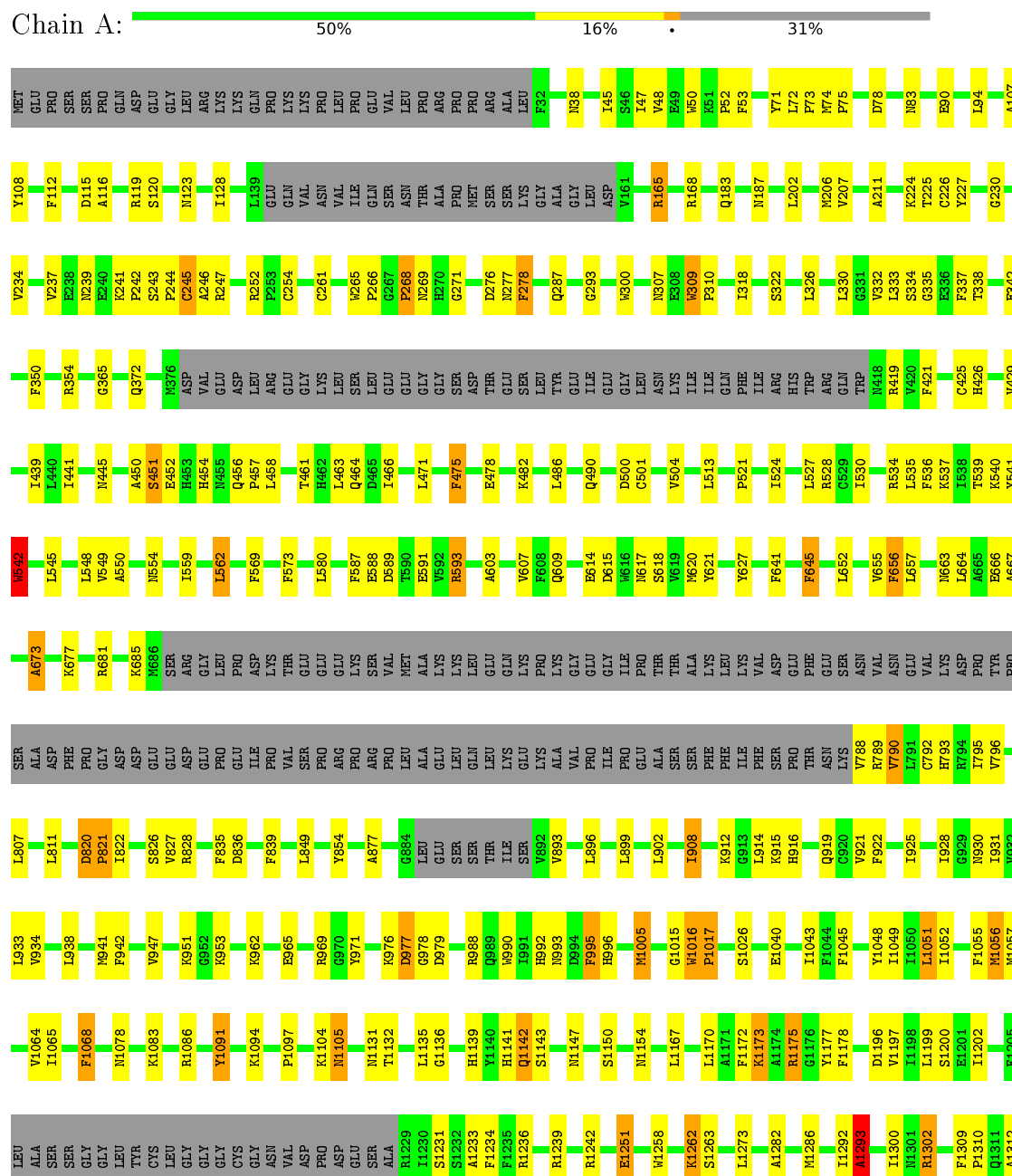


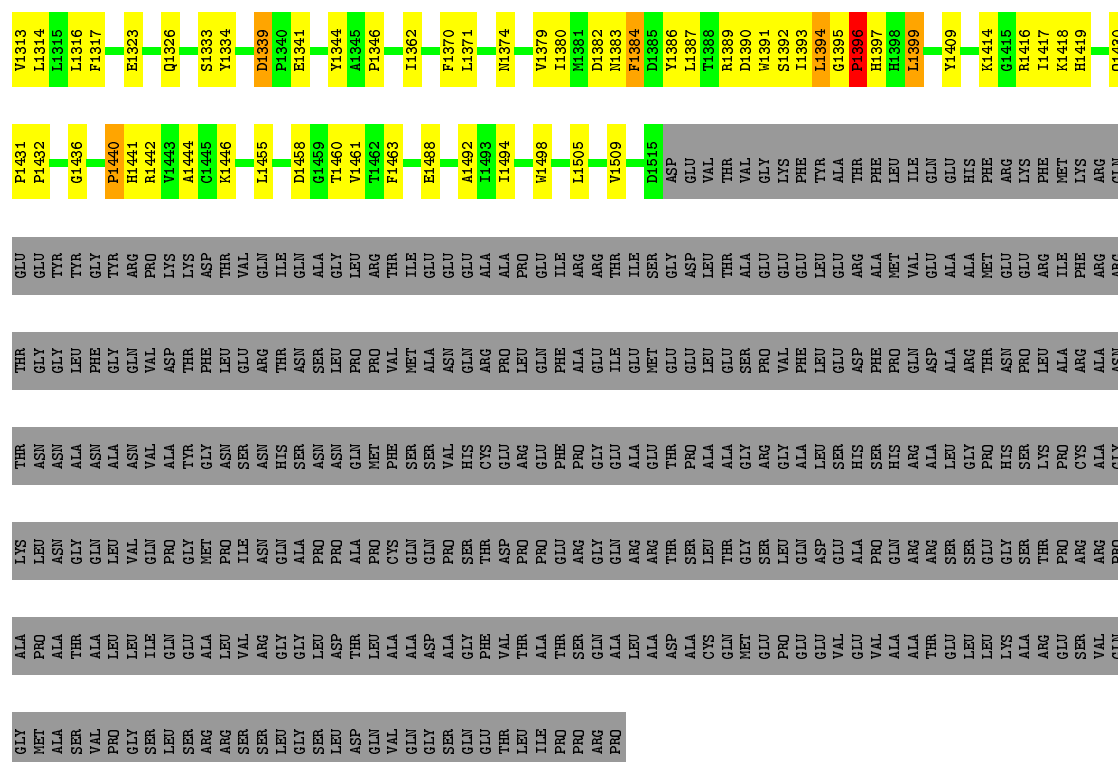
Mol	Chain	Residues	Atoms			AltConf
8	F	1	Total	C	O	0
			22	12	10	
8	F	1	Total	C	O	0
			22	12	10	

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Voltage-dependent L-type calcium channel subunit alpha-1S





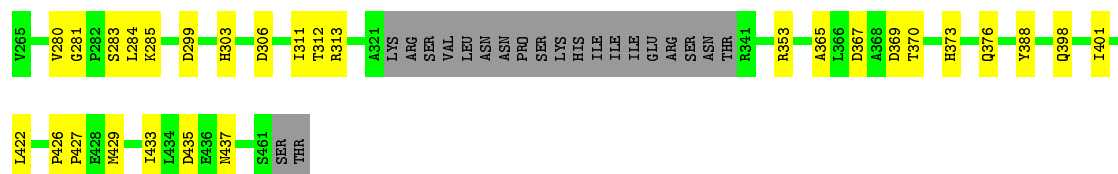
• Molecule 2: Voltage-dependent L-type calcium channel subunit beta-1

Chain B: 83% 11% 6%



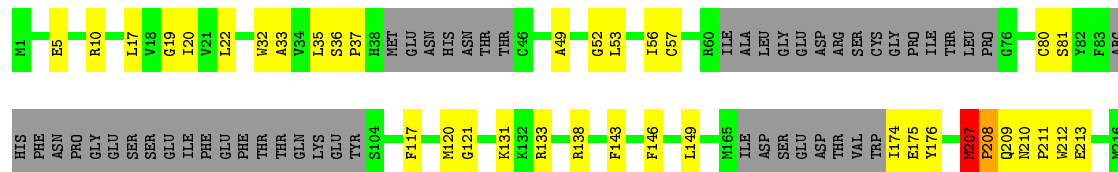
• Molecule 3: Voltage-dependent L-type calcium channel subunit beta-1

Chain C: 75% 14% 11%



• Molecule 4: Voltage-dependent calcium channel gamma-1 subunit

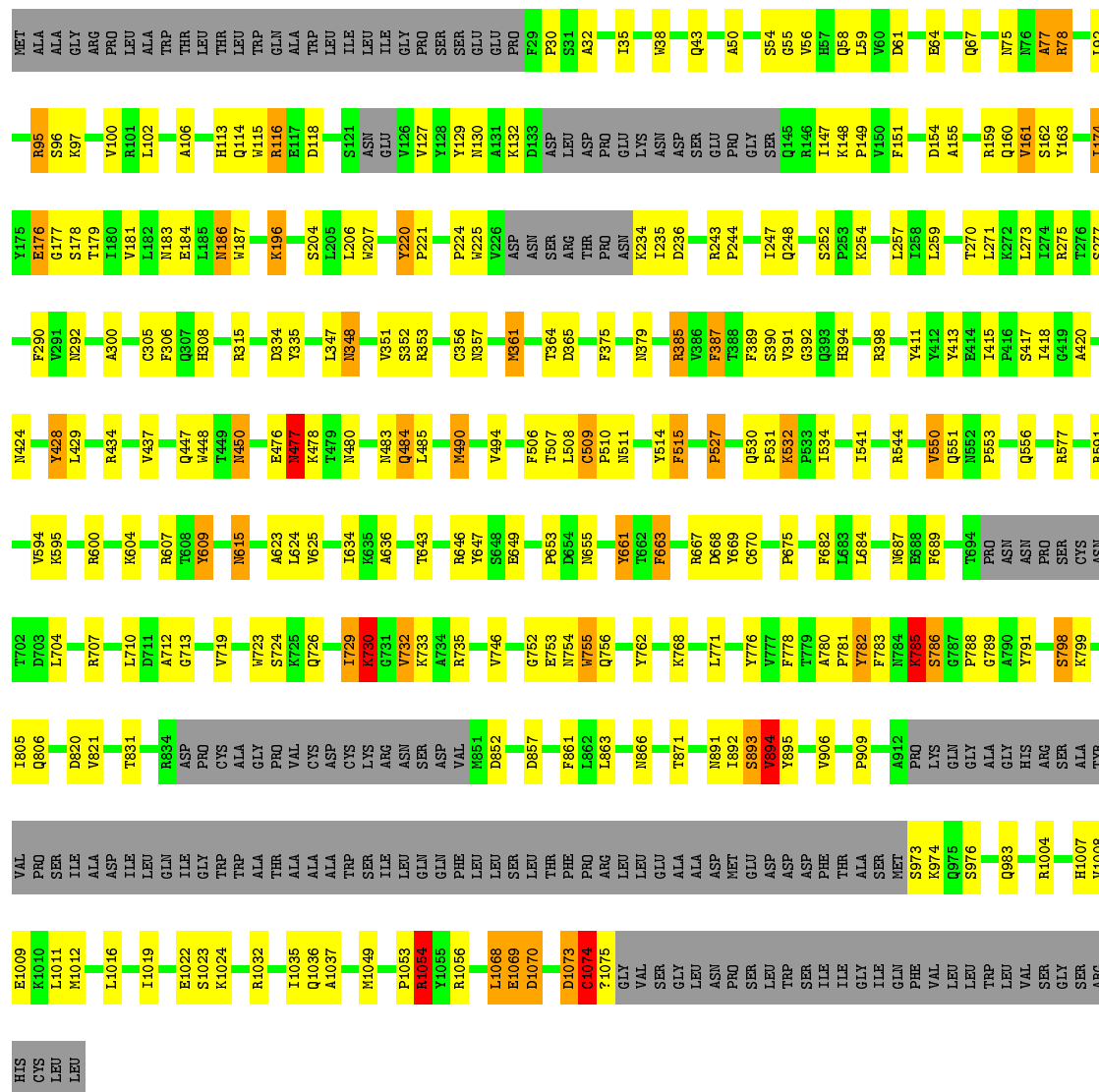
Chain E: 58% 16% 25%



ASP
ALA
GLU
PRO
GLU
HIS

- Molecule 5: Voltage-dependent calcium channel subunit alpha-2/delta-1

Chain F:  61% 20% 15%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	123274	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	Depositor

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 2$	RMSZ	# $ Z > 2$
1	A	0.55	4/10507 (0.0%)	0.69	9/14255 (0.1%)
2	B	0.31	0/723	0.52	0/979
3	C	0.31	0/1394	0.49	0/1892
4	E	0.40	0/1336	0.69	3/1802 (0.2%)
5	F	0.67	4/7729 (0.1%)	0.87	30/10474 (0.3%)
All	All	0.57	8/21689 (0.0%)	0.75	42/29402 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	16
3	C	0	2
4	E	0	2
5	F	0	18
All	All	0	38

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	527	PRO	N-CD	6.29	1.56	1.47
1	A	1339	ASP	C-N	-6.17	1.22	1.34
1	A	242	PRO	N-CD	5.98	1.56	1.47
5	F	515	PHE	CB-CG	-5.76	1.41	1.51
1	A	1017	PRO	N-CD	5.42	1.55	1.47

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	33	ALA	CB-CA-C	-9.85	95.32	110.10
5	F	413	TYR	CB-CA-C	-9.32	91.77	110.40
5	F	661	TYR	N-CA-C	-9.06	86.55	111.00
5	F	390	SER	CB-CA-C	8.99	127.17	110.10
5	F	300	ALA	CB-CA-C	8.87	123.40	110.10

There are no chirality outliers.

5 of 38 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	268	PRO	Peptide
1	A	276	ASP	Peptide
1	A	309	TRP	Peptide
1	A	38	ASN	Peptide
1	A	450	ALA	Peptide

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	10261	0	10238	316	0
2	B	710	0	633	6	0
3	C	1367	0	1343	17	0
4	E	1304	0	1330	33	0
5	F	7572	0	7411	185	0
6	A	14	0	13	0	0
6	F	308	0	276	2	0
7	A	2	0	0	0	0
7	F	1	0	0	0	0
8	F	22	0	20	0	0
All	All	21561	0	21264	543	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 13.

The worst 5 of 543 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:ASN:ND2	1:A:621:TYR:CE2	1.84	1.43
1:A:1380:ILE:CG2	1:A:1384:PHE:CE2	2.14	1.31
5:F:531:PRO:O	5:F:532:LYS:HG3	1.14	1.25
1:A:664:LEU:CD2	1:A:1065:ILE:HD12	1.69	1.23
1:A:1380:ILE:HG21	1:A:1384:PHE:CE2	1.75	1.17

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1279/1873 (68%)	1099 (86%)	163 (13%)	17 (1%)	15	59
2	B	98/106 (92%)	91 (93%)	7 (7%)	0	100	100
3	C	174/199 (87%)	168 (97%)	6 (3%)	0	100	100
4	E	156/222 (70%)	143 (92%)	13 (8%)	0	100	100
5	F	930/1106 (84%)	752 (81%)	148 (16%)	30 (3%)	5	43
All	All	2637/3506 (75%)	2253 (85%)	337 (13%)	47 (2%)	15	54

5 of 47 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	F	348	ASN
5	F	351	VAL
5	F	477	ASN
5	F	478	LYS
5	F	532	LYS

5.3.2 Protein sidechains [i](#)

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

entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1081/1628 (66%)	1059 (98%)	22 (2%)	63	86
2	B	59/91 (65%)	58 (98%)	1 (2%)	68	88
3	C	143/179 (80%)	143 (100%)	0	100	100
4	E	141/192 (73%)	140 (99%)	1 (1%)	88	94
5	F	838/974 (86%)	818 (98%)	20 (2%)	57	82
All	All	2262/3064 (74%)	2218 (98%)	44 (2%)	67	86

5 of 44 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1302	ARG
5	F	78	ARG
5	F	1024	LYS
1	A	1384	PHE
2	B	115	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1326	GLN
5	F	130	ASN
5	F	716	ASN
1	A	1383	ASN
4	E	160	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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	ETA	F	1075	5	3,3,3	0.48	0	2,2,2	0.54	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
5	ETA	F	1075	5	-	0/1/1/1	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	1075	ETA	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 28 ligands modelled in this entry, 3 are monoatomic - leaving 25 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected

value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	NAG	A	1901	1	14,14,15	0.32	0	15,19,21	0.88	1 (6%)
6	NAG	F	1202	5,6	14,14,15	0.41	0	15,19,21	1.03	1 (6%)
6	NAG	F	1203	6	14,14,15	0.38	0	15,19,21	0.65	1 (6%)
6	NAG	F	1204	5	14,14,15	0.21	0	15,19,21	0.40	0
6	NAG	F	1205	5,6	14,14,15	0.77	1 (7%)	15,19,21	0.90	0
6	NAG	F	1206	6	14,14,15	0.59	0	15,19,21	0.57	0
6	NAG	F	1207	5	14,14,15	0.52	0	15,19,21	0.30	0
8	BMA	F	1208	6	11,11,12	0.69	0	15,15,17	1.08	2 (13%)
6	NAG	F	1209	8,6	14,14,15	0.41	0	15,19,21	0.49	0
6	NAG	F	1210	5,6	14,14,15	0.71	1 (7%)	15,19,21	0.48	0
6	NAG	F	1211	5,6	14,14,15	0.39	0	15,19,21	1.01	1 (6%)
6	NAG	F	1212	8,6	14,14,15	0.32	0	15,19,21	0.40	0
8	BMA	F	1213	6	11,11,12	1.12	2 (18%)	15,15,17	1.33	2 (13%)
6	NAG	F	1214	5	14,14,15	0.23	0	15,19,21	0.42	0
6	NAG	F	1215	5	14,14,15	0.26	0	15,19,21	0.32	0
6	NAG	F	1216	5,6	14,14,15	0.41	0	15,19,21	0.61	0
6	NAG	F	1217	6	14,14,15	0.50	0	15,19,21	0.43	0
6	NAG	F	1218	5,6	14,14,15	0.25	0	15,19,21	1.03	1 (6%)
6	NAG	F	1219	6	14,14,15	0.61	0	15,19,21	0.87	1 (6%)
6	NAG	F	1220	5	14,14,15	0.34	0	15,19,21	0.27	0
6	NAG	F	1221	5	14,14,15	0.42	0	15,19,21	0.35	0
6	NAG	F	1222	5	14,14,15	0.46	0	15,19,21	0.67	1 (6%)
6	NAG	F	1223	6	14,14,15	0.29	0	15,19,21	0.65	1 (6%)
6	NAG	F	1224	6	14,14,15	0.90	1 (7%)	15,19,21	2.38	2 (13%)
6	NAG	F	1225	5,6	14,14,15	0.41	0	15,19,21	0.69	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	NAG	A	1901	1	-	0/6/23/26	0/1/1/1
6	NAG	F	1202	5,6	-	0/6/23/26	0/1/1/1
6	NAG	F	1203	6	-	0/6/23/26	0/1/1/1
6	NAG	F	1204	5	-	0/6/23/26	0/1/1/1
6	NAG	F	1205	5,6	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	F	1206	6	-	0/6/23/26	0/1/1/1
6	NAG	F	1207	5	-	0/6/23/26	0/1/1/1
8	BMA	F	1208	6	-	0/2/19/22	0/1/1/1
6	NAG	F	1209	8,6	-	0/6/23/26	0/1/1/1
6	NAG	F	1210	5,6	-	0/6/23/26	0/1/1/1
6	NAG	F	1211	5,6	-	0/6/23/26	0/1/1/1
6	NAG	F	1212	8,6	-	0/6/23/26	0/1/1/1
8	BMA	F	1213	6	-	0/2/19/22	0/1/1/1
6	NAG	F	1214	5	-	0/6/23/26	0/1/1/1
6	NAG	F	1215	5	-	0/6/23/26	0/1/1/1
6	NAG	F	1216	5,6	-	0/6/23/26	0/1/1/1
6	NAG	F	1217	6	-	0/6/23/26	0/1/1/1
6	NAG	F	1218	5,6	-	0/6/23/26	0/1/1/1
6	NAG	F	1219	6	-	0/6/23/26	0/1/1/1
6	NAG	F	1220	5	-	0/6/23/26	0/1/1/1
6	NAG	F	1221	5	-	0/6/23/26	0/1/1/1
6	NAG	F	1222	5	-	0/6/23/26	0/1/1/1
6	NAG	F	1223	6	-	0/6/23/26	0/1/1/1
6	NAG	F	1224	6	-	0/6/23/26	0/1/1/1
6	NAG	F	1225	5,6	-	0/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	1224	NAG	O5-C1	-2.93	1.38	1.43
6	F	1210	NAG	O5-C1	-2.31	1.39	1.43
8	F	1213	BMA	C2-C3	2.21	1.55	1.52
6	F	1205	NAG	C1-C2	2.57	1.56	1.52
8	F	1213	BMA	C1-C2	2.67	1.58	1.52

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	F	1208	BMA	O2-C2-C3	-2.12	105.91	110.19
6	F	1224	NAG	C8-C7-N2	2.01	119.95	116.10
6	F	1203	NAG	C1-O5-C5	2.23	115.42	112.14
6	F	1223	NAG	C1-O5-C5	2.24	115.44	112.14
6	F	1222	NAG	C1-O5-C5	2.41	115.69	112.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	F	1205	NAG	2	0
6	F	1206	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.