



wwPDB EM Map/Model Validation Report ⓘ

Sep 29, 2016 – 02:13 PM EDT

PDB ID : 5KK2
EMDB ID: : EMD-8256
Title : Architecture of fully occupied GluA2 AMPA receptor - TARP complex elucidated by single particle cryo-electron microscopy
Authors : Zhao, Y.; Chen, S.; Yoshioka, C.; Bacongus, I.; Gouaux, E.
Deposited on : 2016-06-20
Resolution : 7.30 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 : unknown
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

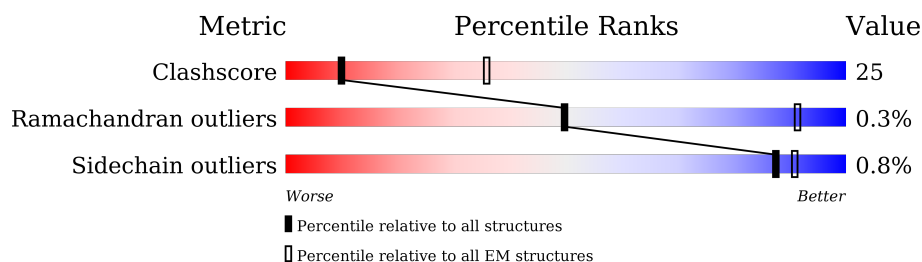
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 7.30 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)	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	889	31% 14% . 54%
1	B	889	32% 14% 54%
1	C	889	30% 15% 54%
1	D	889	32% 13% . 54%
2	E	323	38% 15% 46%
2	F	323	37% 14% 48%
2	G	323	37% 16% . 46%
2	H	323	39% 13% 48%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14639 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 Glutamate receptor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	408	Total	C	N	O	S	0	0
			2831	1822	453	538	18		
1	B	406	Total	C	N	O	S	0	0
			2810	1801	452	540	17		
1	C	406	Total	C	N	O	S	0	0
			2819	1812	452	536	19		
1	D	407	Total	C	N	O	S	0	0
			2829	1819	456	536	18		

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	586	ARG	GLN	variant	UNP P19491
A	848	ASP	-	insertion	UNP P19491
A	849	TYR	-	insertion	UNP P19491
A	850	LYS	-	insertion	UNP P19491
A	851	ASP	-	insertion	UNP P19491
A	852	ASP	-	insertion	UNP P19491
A	853	ASP	-	insertion	UNP P19491
A	854	ASP	TYR	conflict	UNP P19491
B	586	ARG	GLN	variant	UNP P19491
B	848	ASP	-	insertion	UNP P19491
B	849	TYR	-	insertion	UNP P19491
B	850	LYS	-	insertion	UNP P19491
B	851	ASP	-	insertion	UNP P19491
B	852	ASP	-	insertion	UNP P19491
B	853	ASP	-	insertion	UNP P19491
B	854	ASP	TYR	conflict	UNP P19491
C	586	ARG	GLN	variant	UNP P19491
C	848	ASP	-	insertion	UNP P19491
C	849	TYR	-	insertion	UNP P19491
C	850	LYS	-	insertion	UNP P19491
C	851	ASP	-	insertion	UNP P19491
C	852	ASP	-	insertion	UNP P19491

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Chain	Residue	Modelled	Actual	Comment	Reference
C	853	ASP	-	insertion	UNP P19491
C	854	ASP	TYR	conflict	UNP P19491
D	586	ARG	GLN	variant	UNP P19491
D	848	ASP	-	insertion	UNP P19491
D	849	TYR	-	insertion	UNP P19491
D	850	LYS	-	insertion	UNP P19491
D	851	ASP	-	insertion	UNP P19491
D	852	ASP	-	insertion	UNP P19491
D	853	ASP	-	insertion	UNP P19491
D	854	ASP	TYR	conflict	UNP P19491

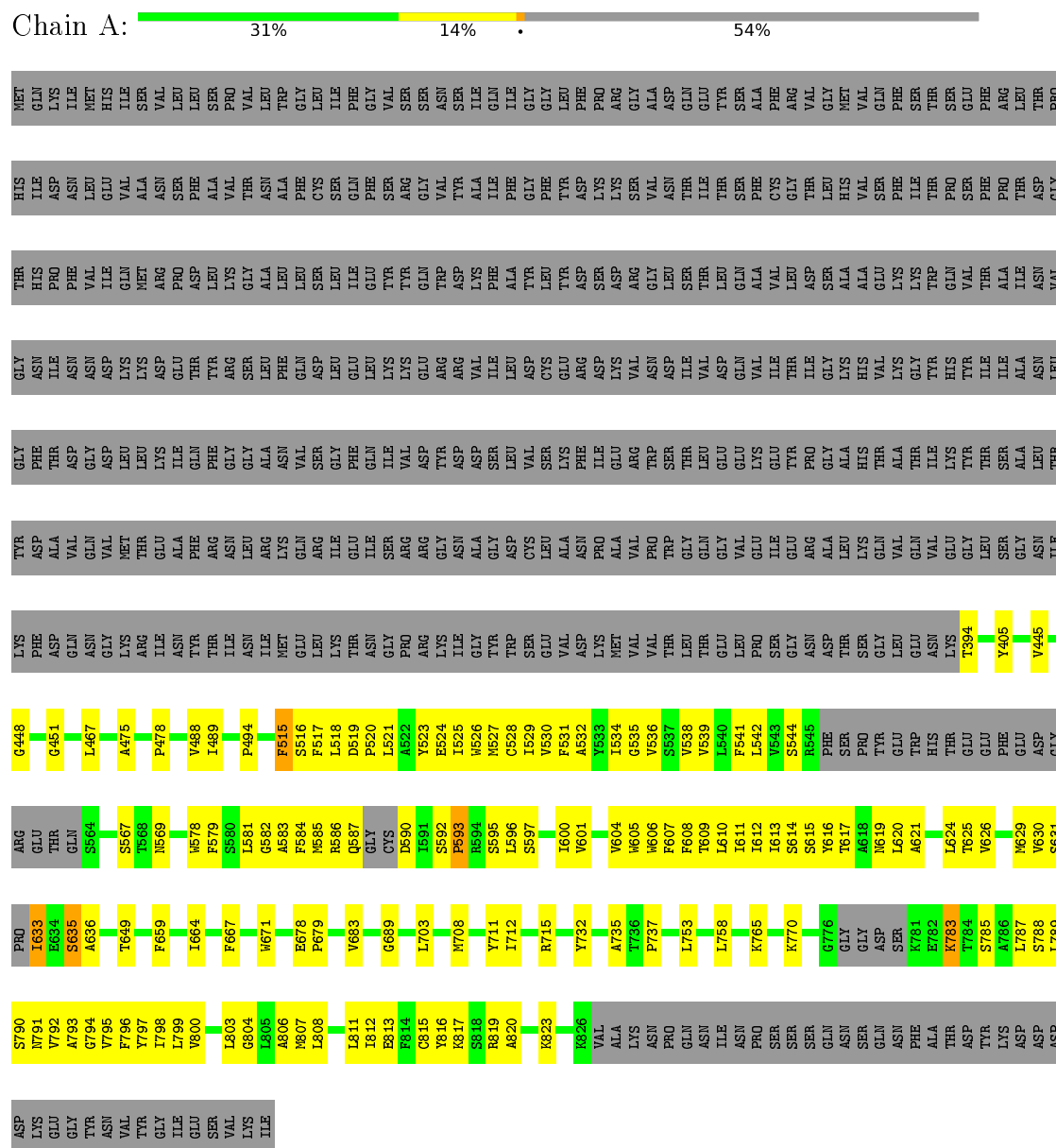
- Molecule 2 is a protein called Voltage-dependent calcium channel gamma-2 subunit.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	E	173	Total	C	N	O	0	0
			850	504	173	173		
2	F	167	Total	C	N	O	0	0
			820	486	167	167		
2	G	174	Total	C	N	O	0	0
			855	507	174	174		
2	H	168	Total	C	N	O	0	0
			825	489	168	168		


3 Residue-property plots

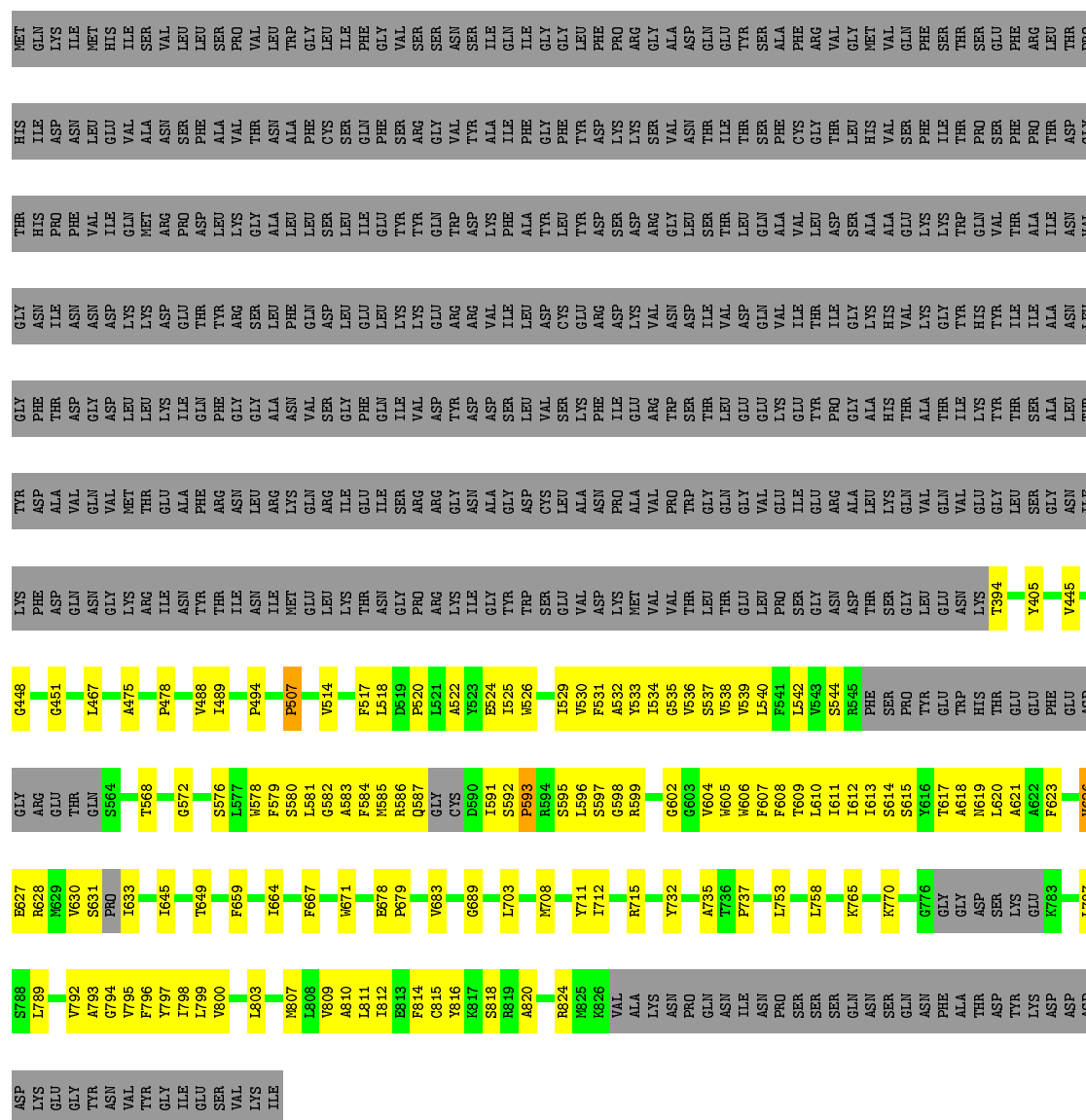
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric 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: Glutamate receptor 2



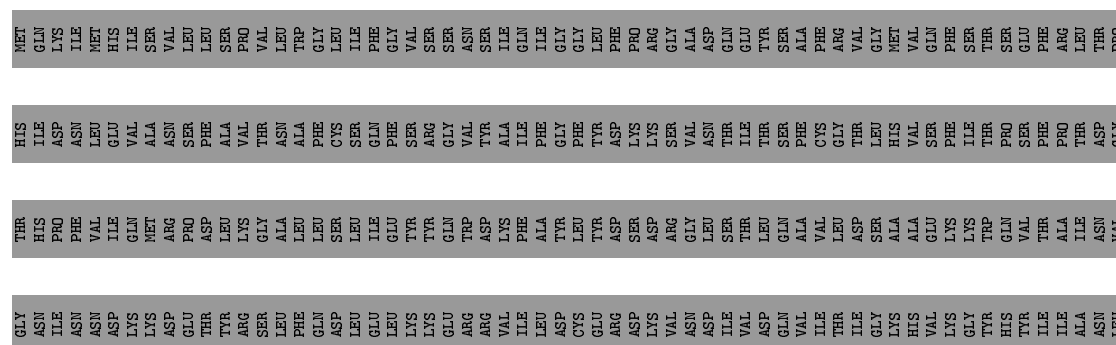
- Molecule 1: Glutamate receptor 2

Chain B:  32% 14% 54%

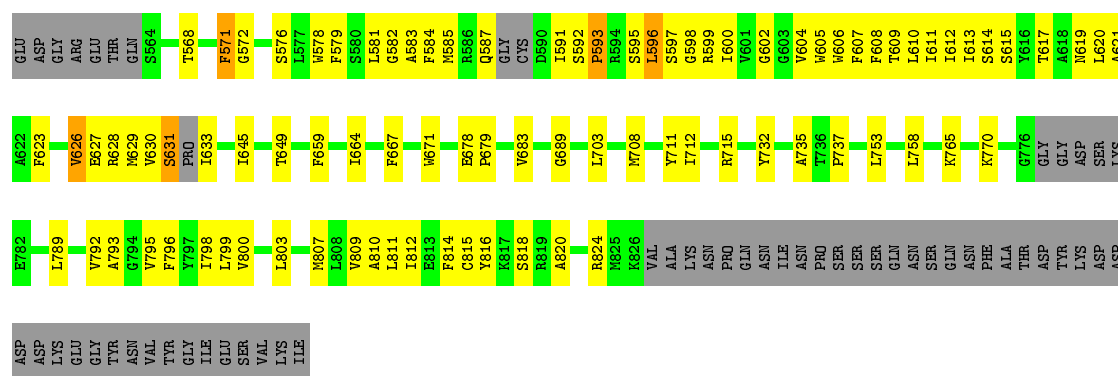


- Molecule 1: Glutamate receptor 2

Chain C: 30% 15% 54%

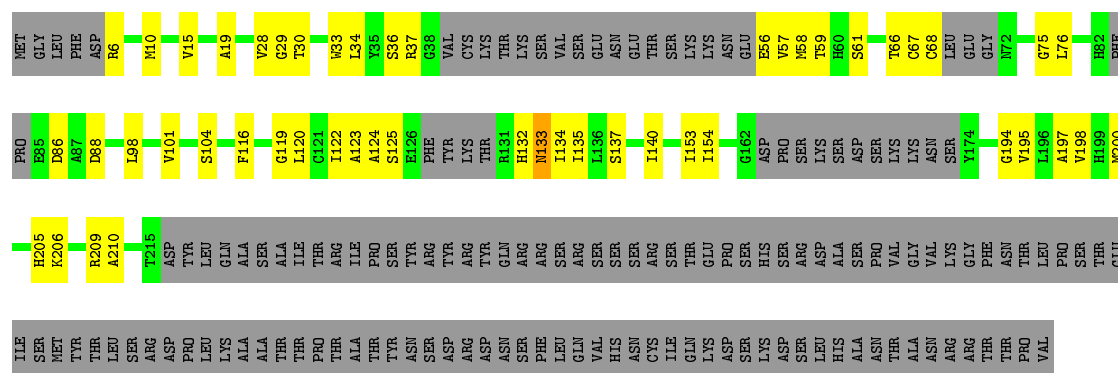






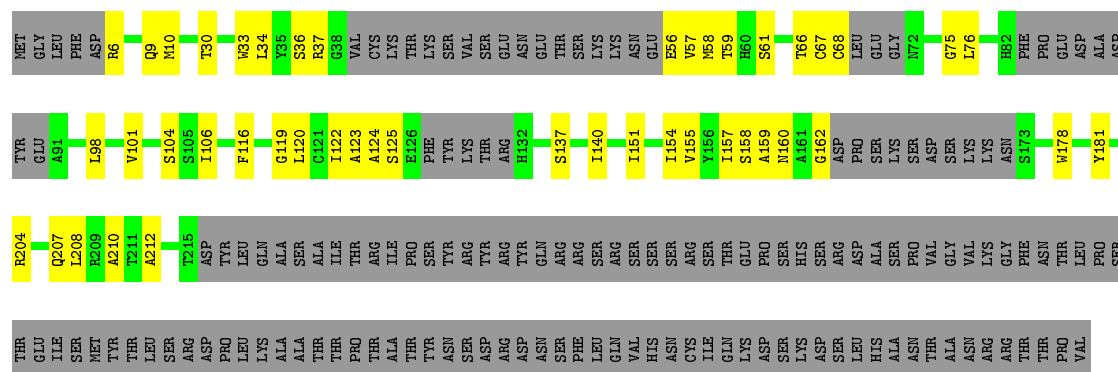
• Molecule 2: Voltage-dependent calcium channel gamma-2 subunit

Chain E: 38% 15% 46%



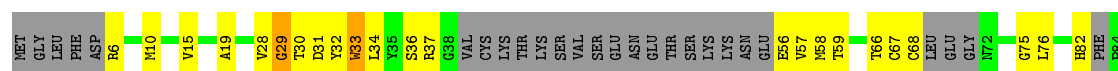
• Molecule 2: Voltage-dependent calcium channel gamma-2 subunit

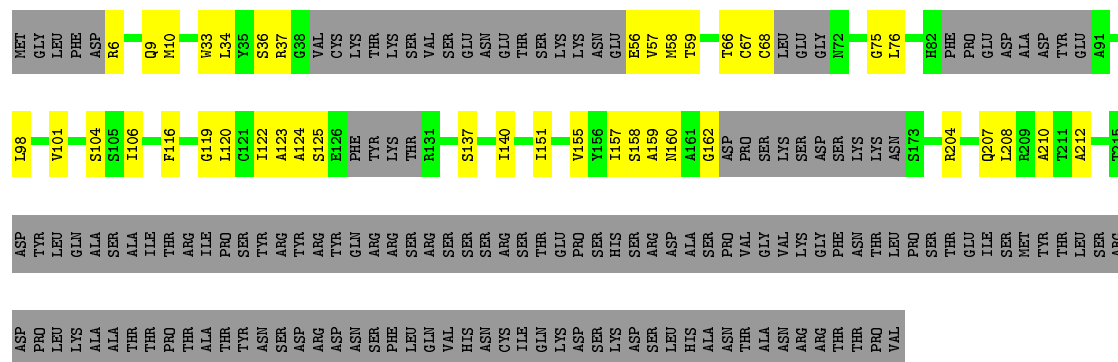
Chain F: 37% 14% 48%



• Molecule 2: Voltage-dependent calcium channel gamma-2 subunit

Chain G: 37% 16% 46%





4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	26297	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

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	0.33	0/2879	0.53	1/3933 (0.0%)
1	B	0.33	0/2857	0.53	2/3906 (0.1%)
1	C	0.32	0/2866	0.54	2/3913 (0.1%)
1	D	0.34	0/2877	0.56	4/3930 (0.1%)
2	E	0.39	0/844	0.66	2/1163 (0.2%)
2	F	0.39	0/814	0.65	2/1121 (0.2%)
2	G	0.37	0/849	0.72	2/1170 (0.2%)
2	H	0.39	0/819	0.65	2/1128 (0.2%)
All	All	0.34	0/14805	0.57	17/20264 (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	2
1	B	0	1
1	C	0	3
1	D	0	1
2	E	0	1
2	F	0	1
2	G	0	1
2	H	0	1
All	All	0	11

There are no bond length outliers.

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	29	GLY	N-CA-C	-11.01	85.56	113.10
1	D	571	PHE	CB-CA-C	-10.68	89.03	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	451	GLY	N-CA-C	-9.20	90.10	113.10
1	B	451	GLY	N-CA-C	-9.16	90.19	113.10
1	C	451	GLY	N-CA-C	-8.78	91.16	113.10

There are no chirality outliers.

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	515	PHE	Peptide
1	A	593	PRO	Peptide
1	B	593	PRO	Peptide
1	C	505	LYS	Mainchain
1	C	515	PHE	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	2831	0	2571	152	0
1	B	2810	0	2535	163	0
1	C	2819	0	2569	149	0
1	D	2829	0	2573	144	0
2	E	850	0	417	38	0
2	F	820	0	402	34	0
2	G	855	0	419	41	0
2	H	825	0	404	27	0
All	All	14639	0	11890	674	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 25.

The worst 5 of 674 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:D:583:ALA:HB1	1:D:605:TRP:NE1	1.48	1.29

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:631:SER:C	1:A:633:ILE:CD1	2.05	1.24
1:B:544:SER:O	1:B:568:THR:CB	1.89	1.19
1:D:814:PHE:O	1:D:818:SER:OG	1.60	1.18
1:B:814:PHE:O	1:B:818:SER:OG	1.60	1.15

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	398/889 (45%)	350 (88%)	47 (12%)	1 (0%)	46	83
1	B	396/889 (44%)	357 (90%)	37 (9%)	2 (0%)	34	77
1	C	396/889 (44%)	348 (88%)	48 (12%)	0	100	100
1	D	397/889 (45%)	358 (90%)	37 (9%)	2 (0%)	34	77
2	E	161/323 (50%)	136 (84%)	24 (15%)	1 (1%)	30	74
2	F	155/323 (48%)	131 (84%)	24 (16%)	0	100	100
2	G	162/323 (50%)	137 (85%)	25 (15%)	0	100	100
2	H	156/323 (48%)	134 (86%)	22 (14%)	0	100	100
All	All	2221/4848 (46%)	1951 (88%)	264 (12%)	6 (0%)	50	83

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	571	PHE
1	A	783	LYS
1	B	507	PRO
2	E	133	ASN
1	B	626	VAL

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	258/761 (34%)	255 (99%)	3 (1%)	78	90
1	B	255/761 (34%)	254 (100%)	1 (0%)	93	96
1	C	258/761 (34%)	256 (99%)	2 (1%)	86	94
1	D	258/761 (34%)	256 (99%)	2 (1%)	86	94
All	All	1029/3044 (34%)	1021 (99%)	8 (1%)	87	94

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	394	THR
1	D	631	SER
1	C	635	SER
1	A	635	SER
1	C	394	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 carbohydrates 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.