wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Mar 2, 2017 – 12:35 pm GMT

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PDB ID	:	5IPV
EMDB ID:	:	EMD-8106
Title	:	Cryo-EM structure of GluN1/GluN2B NMDA receptor in the DCKA/D-APV-bound conformation, state 1
Authors	:	Zhu, S.; Stein, A.R.; Yoshioka, C.; Lee, C.H.; Goehring, A.; McHaourab, S.H.; Gouaux, E.
Deposited on	:	2016-03-10
Resolution	:	9.25 Å(reported)

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 9.25 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.
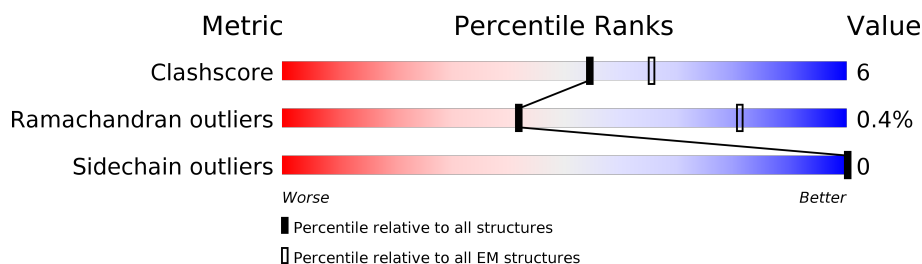
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	822	75% • 21%
1	C	822	76% • 21%
2	B	825	71% • 24%
2	D	825	71% • 25%

2 Entity composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 10209 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 N-methyl-D-aspartate receptor subunit NR1-8a.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	653	Total 2612	C 1306	N 653	O 653	0	0
1	C	653	Total 2612	C 1306	N 653	O 653	0	0

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	51	PHE	LYS	engineered mutation	UNP C0KD18
A	52	PHE	ARG	engineered mutation	UNP C0KD18
A	300	GLN	ASN	engineered mutation	UNP C0KD18
A	350	GLN	ASN	engineered mutation	UNP C0KD18
A	368	ASP	ASN	engineered mutation	UNP C0KD18
A	440	ASP	ASN	engineered mutation	UNP C0KD18
A	469	ASP	ASN	engineered mutation	UNP C0KD18
A	493	ALA	LYS	engineered mutation	UNP C0KD18
A	494	ALA	LYS	engineered mutation	UNP C0KD18
A	495	ALA	GLU	engineered mutation	UNP C0KD18
A	?	-	LYS	deletion	UNP C0KD18
A	?	-	VAL	deletion	UNP C0KD18
A	?	-	ASN	deletion	UNP C0KD18
A	?	-	SER	deletion	UNP C0KD18
A	?	-	GLU	deletion	UNP C0KD18
A	?	-	GLU	deletion	UNP C0KD18
A	?	-	GLU	deletion	UNP C0KD18
A	?	-	GLU	deletion	UNP C0KD18
A	602	ARG	GLY	engineered mutation	UNP C0KD18
A	609	LEU	ILE	engineered mutation	UNP C0KD18
A	648	ARG	ASP	engineered mutation	UNP C0KD18
A	761	GLU	ASN	engineered mutation	UNP C0KD18
A	829	SER	-	expression tag	UNP C0KD18
A	830	ARG	-	expression tag	UNP C0KD18
A	831	ALA	-	expression tag	UNP C0KD18
A	832	GLU	-	expression tag	UNP C0KD18

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Chain	Residue	Modelled	Actual	Comment	Reference
A	833	ALA	-	expression tag	UNP C0KD18
A	834	LYS	-	expression tag	UNP C0KD18
A	835	ARG	-	expression tag	UNP C0KD18
A	836	MET	-	expression tag	UNP C0KD18
A	837	LYS	-	expression tag	UNP C0KD18
A	838	GLY	-	expression tag	UNP C0KD18
A	839	LEU	-	expression tag	UNP C0KD18
A	840	GLU	-	expression tag	UNP C0KD18
A	841	VAL	-	expression tag	UNP C0KD18
A	842	LEU	-	expression tag	UNP C0KD18
A	843	PHE	-	expression tag	UNP C0KD18
A	844	GLN	-	expression tag	UNP C0KD18
C	51	PHE	LYS	engineered mutation	UNP C0KD18
C	52	PHE	ARG	engineered mutation	UNP C0KD18
C	300	GLN	ASN	engineered mutation	UNP C0KD18
C	350	GLN	ASN	engineered mutation	UNP C0KD18
C	368	ASP	ASN	engineered mutation	UNP C0KD18
C	440	ASP	ASN	engineered mutation	UNP C0KD18
C	469	ASP	ASN	engineered mutation	UNP C0KD18
C	493	ALA	LYS	engineered mutation	UNP C0KD18
C	494	ALA	LYS	engineered mutation	UNP C0KD18
C	495	ALA	GLU	engineered mutation	UNP C0KD18
C	?	-	LYS	deletion	UNP C0KD18
C	?	-	VAL	deletion	UNP C0KD18
C	?	-	ASN	deletion	UNP C0KD18
C	?	-	SER	deletion	UNP C0KD18
C	?	-	GLU	deletion	UNP C0KD18
C	?	-	GLU	deletion	UNP C0KD18
C	?	-	GLU	deletion	UNP C0KD18
C	?	-	GLU	deletion	UNP C0KD18
C	602	ARG	GLY	engineered mutation	UNP C0KD18
C	609	LEU	ILE	engineered mutation	UNP C0KD18
C	648	ARG	ASP	engineered mutation	UNP C0KD18
C	761	GLU	ASN	engineered mutation	UNP C0KD18
C	829	SER	-	expression tag	UNP C0KD18
C	830	ARG	-	expression tag	UNP C0KD18
C	831	ALA	-	expression tag	UNP C0KD18
C	832	GLU	-	expression tag	UNP C0KD18
C	833	ALA	-	expression tag	UNP C0KD18
C	834	LYS	-	expression tag	UNP C0KD18
C	835	ARG	-	expression tag	UNP C0KD18
C	836	MET	-	expression tag	UNP C0KD18

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Chain	Residue	Modelled	Actual	Comment	Reference
C	837	LYS	-	expression tag	UNP C0KD18
C	838	GLY	-	expression tag	UNP C0KD18
C	839	LEU	-	expression tag	UNP C0KD18
C	840	GLU	-	expression tag	UNP C0KD18
C	841	VAL	-	expression tag	UNP C0KD18
C	842	LEU	-	expression tag	UNP C0KD18
C	843	PHE	-	expression tag	UNP C0KD18
C	844	GLN	-	expression tag	UNP C0KD18

- Molecule 2 is a protein called Ionotropic glutamate receptor subunit NR2B.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	B	623	Total 2493	C 1247	N 623	O 623	0	0
2	D	622	Total 2492	C 1248	N 622	O 622	0	0

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	20	SER	MET	engineered mutation	UNP A7XY94
B	21	ARG	GLY	engineered mutation	UNP A7XY94
B	22	ALA	CYS	engineered mutation	UNP A7XY94
B	64	GLU	ALA	engineered mutation	UNP A7XY94
B	69	GLN	ASN	engineered mutation	UNP A7XY94
B	343	ASP	ASN	engineered mutation	UNP A7XY94
B	?	-	LYS	deletion	UNP A7XY94
B	?	-	TYR	deletion	UNP A7XY94
B	?	-	TYR	deletion	UNP A7XY94
B	?	-	VAL	deletion	UNP A7XY94
B	486	VAL	THR	engineered mutation	UNP A7XY94
B	?	-	ARG	deletion	UNP A7XY94
B	?	-	CYS	deletion	UNP A7XY94
B	?	-	LEU	deletion	UNP A7XY94
B	?	-	ALA	deletion	UNP A7XY94
B	?	-	ASP	deletion	UNP A7XY94
B	?	-	GLY	deletion	UNP A7XY94
B	?	-	ARG	deletion	UNP A7XY94
B	?	-	GLU	deletion	UNP A7XY94
B	?	-	PRO	deletion	UNP A7XY94
B	?	-	GLY	deletion	UNP A7XY94
B	601	LEU	VAL	engineered mutation	UNP A7XY94

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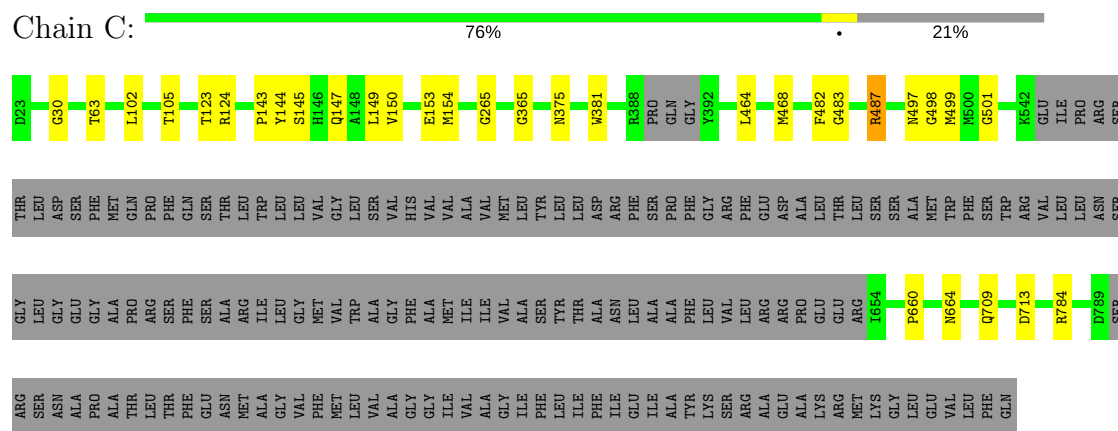| Chain	Residue	Modelled	Actual	Comment	Reference
B	640	ARG	GLU	engineered mutation	UNP A7XY94
B	641	ARG	GLU	engineered mutation	UNP A7XY94
D	20	SER	MET	engineered mutation	UNP A7XY94
D	21	ARG	GLY	engineered mutation	UNP A7XY94
D	22	ALA	CYS	engineered mutation	UNP A7XY94
D	64	GLU	ALA	engineered mutation	UNP A7XY94
D	69	GLN	ASN	engineered mutation	UNP A7XY94
D	343	ASP	ASN	engineered mutation	UNP A7XY94
D	?	-	LYS	deletion	UNP A7XY94
D	?	-	TYR	deletion	UNP A7XY94
D	?	-	TYR	deletion	UNP A7XY94
D	?	-	VAL	deletion	UNP A7XY94
D	486	VAL	THR	engineered mutation	UNP A7XY94
D	?	-	ARG	deletion	UNP A7XY94
D	?	-	CYS	deletion	UNP A7XY94
D	?	-	LEU	deletion	UNP A7XY94
D	?	-	ALA	deletion	UNP A7XY94
D	?	-	ASP	deletion	UNP A7XY94
D	?	-	GLY	deletion	UNP A7XY94
D	?	-	ARG	deletion	UNP A7XY94
D	?	-	GLU	deletion	UNP A7XY94
D	?	-	PRO	deletion	UNP A7XY94
D	?	-	GLY	deletion	UNP A7XY94
D	601	LEU	VAL	engineered mutation	UNP A7XY94
D	640	ARG	GLU	engineered mutation	UNP A7XY94
D	641	ARG	GLU	engineered mutation	UNP A7XY94

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 the various outlier classes 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.
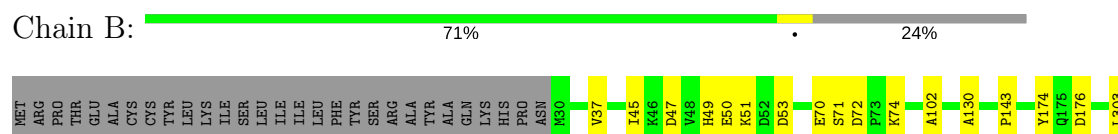
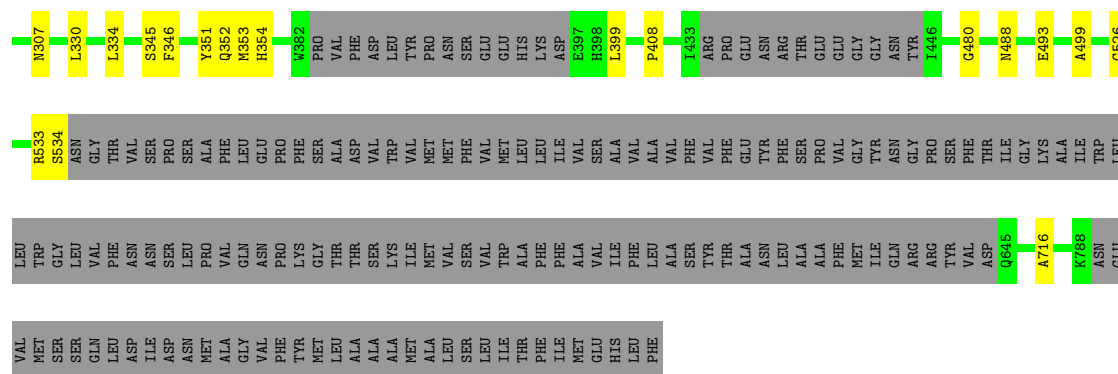• Molecule 1: N-methyl-D-aspartate receptor subunit NR1-8a

Chain A:

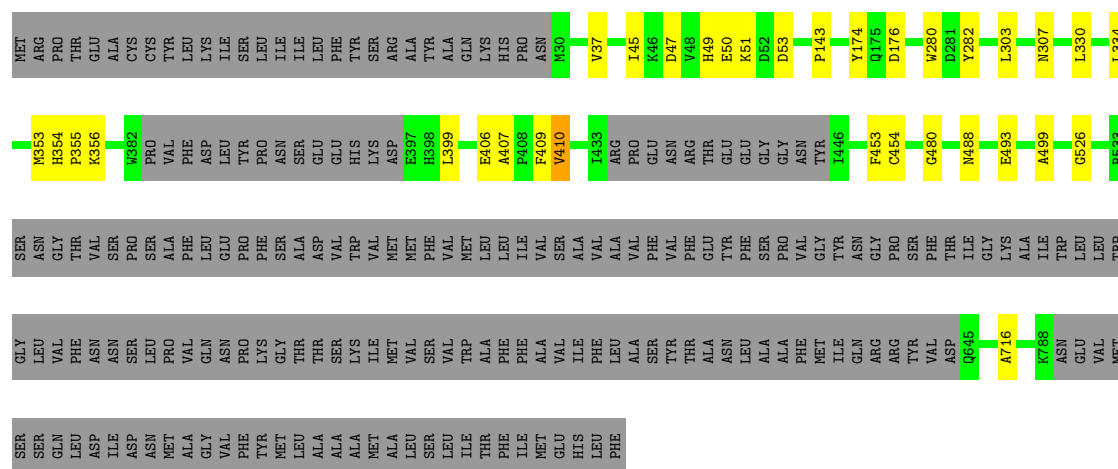• Molecule 1: N-methyl-D-aspartate receptor subunit NR1-8a

Chain C:

• Molecule 2: Ionotropic glutamate receptor subunit NR2B

Chain B:

N307 L330 L334 S345 F346 Y351 Q352 M353 H354 W382 PRO VAL PHE ASP LEU TYR PRO ASN SER GLU GLU HIS LYS ASP E397 H398 L399 P408 I433 ARG PRO GLU ASN ARG THR GLU GLU GLY GLY ASN TYR I446 G480 N488 E493 A499 G526

R533 S534 ASN GLY THR VAL SER PRO SER ALA PHE LEU GLU PRO PHE SER ALA ASP VAL TRP VAL MET PHE VAL MET LEU LEU ILE VAL SER ALA VAL ALA VAL PHE VAL PHE GLU TYR PHE SER PRO VAL GLY TYR ASN GLY PRO SER PHE THR ILE GLY LYS ALA ILE TRP LEU

LEU TRP GLY LEU VAL PHE ASN ASN SER LEU PRO VAL GLN ASN PRO LYS GLY THR THR SER LYS ILE MET VAL SER VAL TRP ALA PHE PHE ALA VAL ILE PHE LEU ALA SER TYR THR ALA ASN LEU ALA ALA PHE MET ILE GLN ARG ARG TYR VAL ASP Q645 A716 K788 ASN GLU

VAL MET SER SER GLN LEU ASP ILE ASP ASN MET ALA GLY VAL PHE TYR MET LEU ALA ALA ALA MET ALA LEU SER LEU ILE THR PHE ILE MET GLU HIS LEU PHE

● Molecule 2: Ionotropic glutamate receptor subunit NR2B

Chain D:

71%   •   25%

MET ARG PRO THR GLU ALA CYS CYS TYR LEU LYS ILE SER LEU LEU ILE LEU LEU PHE TYR SER ARG ALA ALA TYR ALA GLN LYS HIS PRO ASN M30 V37 I45 K46 D47 V48 H49 E50 K51 D52 D53 P143 Y174 Q175 D176 W280 D281 Y282 L303 N307 L330 L334

M353 H354 P355 K356 W382 PRO VAL PHE ASP LEU TYR PRO ASN SER GLU GLU HIS LYS ASP E397 H398 L399 E406 A407 P408 F409 V410 I433 ARG PRO GLU ASN ARG THR GLU GLU GLY GLY ASN TYR I446 F453 C454 G480 N488 E493 A499 G526 R533

SER ASN GLY THR VAL SER PRO SER ALA PHE LEU GLU PRO PHE SER ALA ASP VAL TRP VAL MET PHE VAL MET LEU LEU ILE VAL SER ALA VAL ALA VAL PHE VAL PHE GLU TYR PHE SER PRO VAL GLY TYR ASN GLY PRO SER PHE THR ILE GLY LYS ALA ILE TRP LEU LEU TRP

GLY LEU VAL PHE ASN ASN SER LEU PRO VAL GLN ASN PRO LYS GLY THR THR SER LYS ILE MET VAL SER VAL TRP ALA PHE PHE ALA VAL ILE PHE LEU ALA SER TYR THR ALA ASN LEU ALA ALA PHE MET ILE GLN ARG ARG TYR VAL ASP Q645 A716 K788 ASN GLU VAL MET

SER SER GLN LEU ASP ILE ASP ASN MET ALA GLY VAL PHE TYR MET LEU ALA ALA ALA MET ALA LEU SER LEU ILE THR PHE ILE MET GLU HIS LEU PHE

4 Experimental information ⓘ

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	393513	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 $(e^-/\text{Å}^2)$	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	0.28	0/2609	0.70	5/3256 (0.2%)
1	C	0.30	0/2609	0.97	5/3256 (0.2%)
2	B	0.32	0/2489	0.71	4/3105 (0.1%)
2	D	0.32	0/2489	0.70	4/3107 (0.1%)
All	All	0.30	0/10196	0.78	18/12724 (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	C	0	1

There are no bond length outliers.

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	784	ARG	O-C-N	23.06	159.59	122.70
1	C	784	ARG	C-N-CA	-20.77	69.79	121.70
1	C	487	ARG	N-CA-C	19.94	164.83	111.00
1	C	784	ARG	CA-C-N	-19.45	74.41	117.20
1	A	784	ARG	N-CA-C	11.99	143.36	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	487	ARG	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	2612	0	699	30	0
1	C	2612	0	699	14	0
2	B	2493	0	685	31	0
2	D	2492	0	688	21	0
All	All	10209	0	2771	81	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 6.

The worst 5 of 81 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:79:CYS:CA	2:B:74:LYS:CA	1.77	1.62
2:B:345:SER:O	2:B:353:MET:N	1.79	1.15
1:A:79:CYS:CA	2:B:74:LYS:N	2.17	1.07
2:D:409:PHE:CB	2:D:454:CYS:H	1.68	1.06
1:A:133:ILE:CA	2:B:130:ALA:CA	2.36	1.04

There are no symmetry-related clashes.

5.3   Torsion angles ⓘ

5.3.1   Protein backbone ⓘ

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	647/822 (79%)	614 (95%)	29 (4%)	4 (1%)	28	71
1	C	647/822 (79%)	617 (95%)	28 (4%)	2 (0%)	44	81

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	615/825 (74%)	582 (95%)	31 (5%)	2 (0%)	44	81
2	D	614/825 (74%)	578 (94%)	33 (5%)	3 (0%)	32	74
All	All	2523/3294 (77%)	2391 (95%)	121 (5%)	11 (0%)	42	77

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	141	VAL
1	A	142	PRO
1	A	143	PRO
2	B	143	PRO
2	B	408	PRO

5.3.2   Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	
2	D	1/727 (0%)	1 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

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 ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.