



## wwPDB EM Map/Model Validation Report ⓘ

Apr 25, 2016 – 08:42 PM EDT

PDB ID : 5IOU  
EMDB ID: : EMD-8097  
Title : Cryo-EM structure of GluN1/GluN2B NMDA receptor in the glutamate/glycine-bound conformation  
Authors : Zhu, S.; Stein, A.R.; Yoshioka, C.; Lee, C.H.; Goehring, A.; Mchaourab, S.H.; Gouaux, E.  
Deposited on : 2016-03-09  
Resolution : 7.00 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

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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-20027257

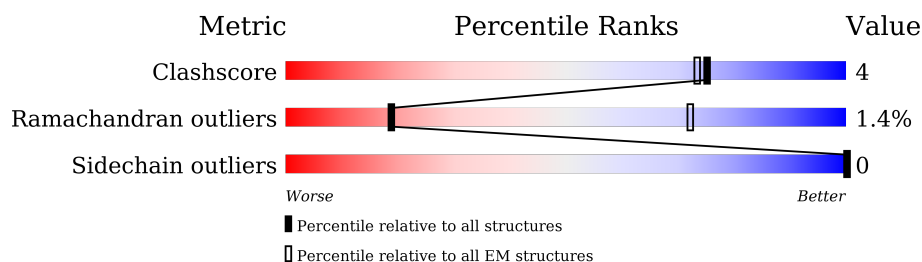
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 7.00 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  $\geq 3$ , 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	822	93% . . .
1	C	822	93% . .
2	B	825	88% 7% . .
2	D	825	88% 8% .

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15824 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	803	Total	C	N	O	0	0
			3963	2358	803	802		
1	C	803	Total	C	N	O	0	0
			3963	2358	803	802		

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	797	Total	C	N	O	0	0
			3934	2341	797	796		
2	D	797	Total	C	N	O	0	0
			3934	2341	797	796		

There are 48 discrepancies between the modelled and reference sequences:

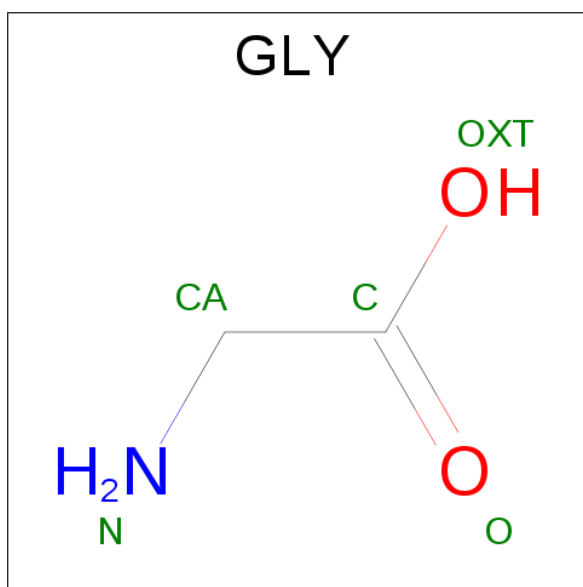
Chain	Residue	Modelled	Actual	Comment	Reference
B	20	SER	MET	engineered mutation	UNP A7XY94
B	21	ARG	GLY	engineered mutation	UNP A7XY94
B	22	ALA	CYS	engineered mutation	UNP A7XY94
B	64	GLU	ALA	engineered mutation	UNP A7XY94
B	69	GLN	ASN	engineered mutation	UNP A7XY94
B	343	ASP	ASN	engineered mutation	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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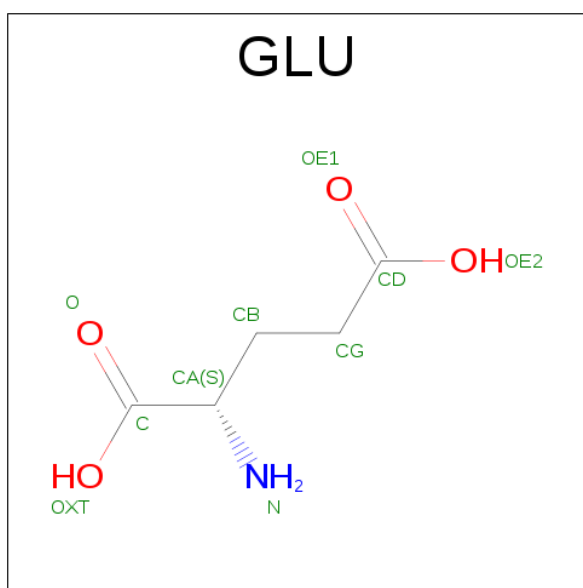
Chain	Residue	Modelled	Actual	Comment	Reference
B	640	ARG	GLU	engineered mutation	UNP A7XY94
B	641	ARG	GLU	engineered mutation	UNP A7XY94
D	20	SER	MET	engineered mutation	UNP A7XY94
D	21	ARG	GLY	engineered mutation	UNP A7XY94
D	22	ALA	CYS	engineered mutation	UNP A7XY94
D	64	GLU	ALA	engineered mutation	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

- Molecule 3 is GLYCINE (three-letter code: GLY) (formula:  $C_2H_5NO_2$ ).



Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	0
			5	2	1	2	
3	C	1	Total	C	N	O	0
			5	2	1	2	

- Molecule 4 is GLUTAMIC ACID (three-letter code: GLU) (formula: C<sub>5</sub>H<sub>9</sub>NO<sub>4</sub>).



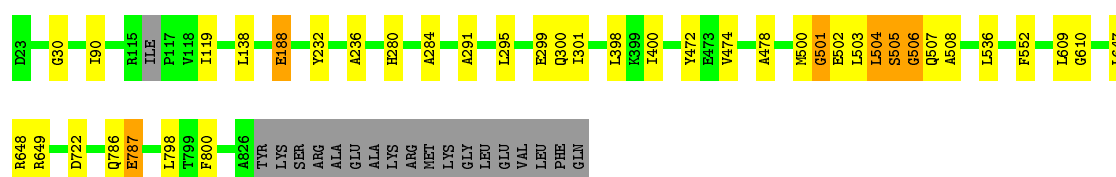
Mol	Chain	Residues	Atoms				AltConf
4	B	1	Total	C	N	O	0
			10	5	1	4	
4	D	1	Total	C	N	O	0
			10	5	1	4	

### 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 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.

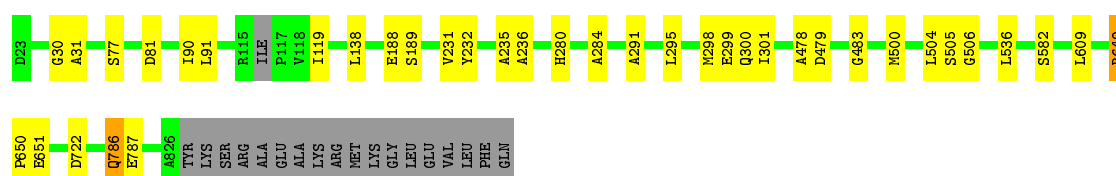
- Molecule 1: N-methyl-D-aspartate receptor subunit NR1-8a

Chain A:  93%




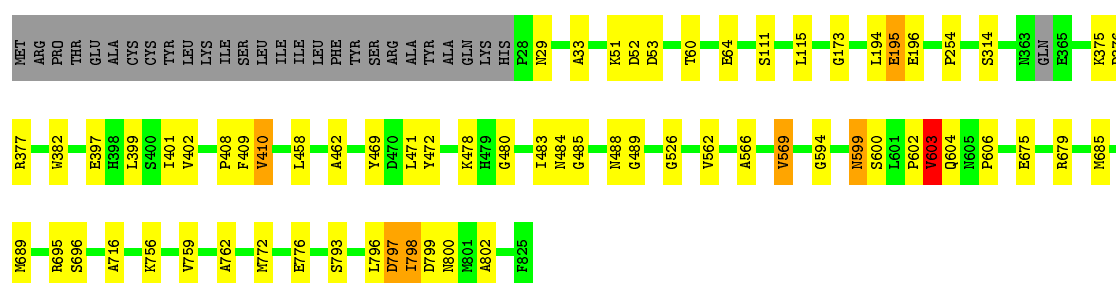
- Molecule 1: N-methyl-D-aspartate receptor subunit NR1-8a

Chain C:  93%




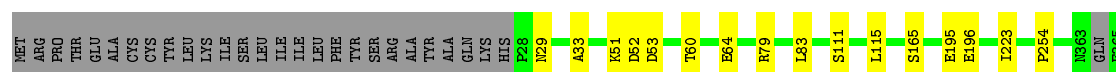
- Molecule 2: Ionotropic glutamate receptor subunit NR2B

Chain B:  88% 7%



- Molecule 2: Ionotropic glutamate receptor subunit NR2B

Chain D:  88% 8%







## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	116968	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)	2500	Depositor
Maximum defocus (nm)	4000	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	0.24	0/3961	0.76	11/5512 (0.2%)
1	C	0.25	0/3961	0.73	20/5512 (0.4%)
2	B	0.24	0/3932	0.66	13/5472 (0.2%)
2	D	0.24	0/3932	0.63	15/5472 (0.3%)
All	All	0.24	0/15786	0.70	59/21968 (0.3%)

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	1
1	C	0	1
All	All	0	2

There are no bond length outliers.

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	609	LEU	CB-CA-C	-19.65	72.86	110.20
1	A	504	LEU	CB-CA-C	-18.71	74.65	110.20
2	B	600	SER	N-CA-CB	-16.88	85.19	110.50
2	B	599	ASN	CB-CA-C	-16.64	77.11	110.40
1	A	786	GLN	CB-CA-C	-16.41	77.58	110.40
1	C	299	GLU	N-CA-C	15.78	153.59	111.00
1	A	188	GLU	N-CA-C	15.70	153.38	111.00
1	C	504	LEU	CB-CA-C	-15.60	80.56	110.20
1	A	505	SER	N-CA-CB	-13.54	90.18	110.50
1	C	505	SER	N-CA-CB	-13.08	90.89	110.50
1	C	299	GLU	N-CA-CB	-12.47	88.16	110.60
2	D	794	SER	N-CA-CB	-11.07	93.89	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	786	GLN	N-CA-C	10.98	140.64	111.00
1	C	189	SER	N-CA-CB	10.96	126.95	110.50
1	A	188	GLU	C-N-CA	10.56	148.10	121.70
1	A	300	GLN	N-CA-CB	-10.09	92.45	110.60
2	D	196	GLU	N-CA-CB	-10.05	92.51	110.60
2	B	196	GLU	N-CA-CB	-10.01	92.58	110.60
1	A	188	GLU	CB-CA-C	-9.82	90.75	110.40
1	C	298	MET	N-CA-C	-9.74	84.70	111.00
1	C	188	GLU	N-CA-C	9.63	137.01	111.00
2	D	794	SER	N-CA-C	9.48	136.60	111.00
2	D	195	GLU	N-CA-C	-8.95	86.84	111.00
2	B	195	GLU	N-CA-C	-8.91	86.95	111.00
2	B	798	ILE	N-CA-C	-8.67	87.59	111.00
2	D	793	SER	N-CA-C	-8.50	88.04	111.00
1	C	787	GLU	N-CA-CB	-8.49	95.31	110.60
1	C	189	SER	N-CA-C	-7.54	90.65	111.00
1	C	478	ALA	CB-CA-C	-7.37	99.04	110.10
2	B	797	ASP	CB-CA-C	7.27	124.94	110.40
1	C	582	SER	N-CA-CB	-7.21	99.68	110.50
2	B	797	ASP	N-CA-C	-7.13	91.74	111.00
1	C	299	GLU	CB-CA-C	-7.08	96.24	110.40
1	A	610	GLY	N-CA-C	7.03	130.68	113.10
2	D	394	HIS	N-CA-C	6.97	129.82	111.00
1	C	504	LEU	N-CA-C	6.89	129.59	111.00
2	D	394	HIS	CB-CA-C	-6.79	96.81	110.40
2	D	695	ARG	CB-CA-C	6.79	123.98	110.40
1	C	786	GLN	CB-CA-C	-6.73	96.94	110.40
2	D	696	SER	N-CA-CB	-6.71	100.44	110.50
1	C	478	ALA	N-CA-C	6.69	129.06	111.00
2	B	604	GLN	N-CA-CB	-6.65	98.64	110.60
2	D	604	GLN	N-CA-CB	-6.63	98.66	110.60
1	C	479	ASP	N-CA-CB	6.54	122.37	110.60
2	D	395	LYS	N-CA-CB	6.50	122.30	110.60
2	D	484	ASN	N-CA-C	-6.33	93.90	111.00
1	C	786	GLN	O-C-N	-6.10	112.94	122.70
2	B	695	ARG	CB-CA-C	5.94	122.28	110.40
2	B	696	SER	N-CA-CB	-5.90	101.65	110.50
1	C	300	GLN	N-CA-CB	-5.89	99.99	110.60
1	C	300	GLN	N-CA-C	-5.89	95.10	111.00
1	A	787	GLU	N-CA-CB	5.85	121.14	110.60
1	C	188	GLU	CB-CA-C	-5.82	98.75	110.40
2	D	603	VAL	N-CA-C	-5.78	95.41	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	603	VAL	N-CA-C	-5.76	95.46	111.00
2	B	196	GLU	N-CA-C	5.48	125.79	111.00
2	B	569	VAL	CB-CA-C	5.47	121.80	111.40
2	D	196	GLU	N-CA-C	5.44	125.68	111.00
2	D	395	LYS	N-CA-C	-5.32	96.64	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	188	GLU	Peptide
1	C	786	GLN	Mainchain

## 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	3963	0	1808	19	0
1	C	3963	0	1809	12	0
2	B	3934	0	1748	31	0
2	D	3934	0	1748	28	0
3	A	5	0	2	0	0
3	C	5	0	2	0	0
4	B	10	0	5	0	0
4	D	10	0	5	0	0
All	All	15824	0	7127	90	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 4.

All (90) 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:B:594:GLY:O	2:B:599:ASN:CA	1.66	1.40
1:C:649:ARG:O	1:C:651:GLU:N	1.74	1.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:594:GLY:C	2:B:599:ASN:HA	1.81	1.01
2:B:594:GLY:O	2:B:599:ASN:HA	0.82	0.99
1:A:503:LEU:O	1:A:508:ALA:HB3	1.65	0.96
1:A:400:ILE:O	1:A:474:VAL:HA	1.67	0.94
2:B:594:GLY:O	2:B:599:ASN:N	2.02	0.92
2:D:29:ASN:HA	2:D:60:THR:O	1.70	0.91
2:B:29:ASN:HA	2:B:60:THR:O	1.70	0.90
1:A:119:ILE:HA	1:A:138:LEU:O	1.76	0.85
1:C:119:ILE:HA	1:C:138:LEU:O	1.77	0.85
2:B:409:PHE:O	2:B:410:VAL:CB	2.35	0.74
1:A:398:LEU:O	1:A:472:TYR:HA	1.88	0.74
2:D:399:LEU:O	2:D:469:TYR:HA	1.90	0.71
2:B:796:LEU:O	2:B:797:ASP:C	2.31	0.69
2:B:799:ASP:O	2:B:802:ALA:N	2.26	0.69
1:A:647:LEU:O	1:A:649:ARG:N	2.26	0.69
2:B:480:GLY:HA2	2:B:488:ASN:O	1.93	0.67
2:D:480:GLY:HA2	2:D:488:ASN:O	1.96	0.65
2:D:755:TRP:O	2:D:757:ARG:N	2.32	0.63
1:C:30:GLY:O	1:C:90:ILE:HA	1.99	0.62
2:D:401:ILE:O	2:D:471:LEU:HA	2.01	0.61
2:B:399:LEU:O	2:B:469:TYR:HA	2.00	0.61
1:A:647:LEU:C	1:A:649:ARG:H	2.05	0.59
1:A:30:GLY:O	1:A:90:ILE:HA	2.03	0.59
1:A:500:MET:O	1:A:502:GLU:N	2.37	0.58
2:D:480:GLY:HA2	2:D:489:GLY:HA3	1.85	0.57
2:D:562:VAL:O	2:D:566:ALA:CB	2.53	0.57
2:B:480:GLY:HA2	2:B:489:GLY:HA3	1.86	0.56
1:A:536:LEU:HA	1:A:722:ASP:HA	1.89	0.54
2:B:562:VAL:O	2:B:566:ALA:CB	2.56	0.54
2:B:796:LEU:O	2:B:798:ILE:N	2.40	0.54
1:C:536:LEU:HA	1:C:722:ASP:HA	1.89	0.53
2:D:598:ASN:O	2:D:600:SER:N	2.42	0.53
1:A:291:ALA:O	1:A:295:LEU:CB	2.57	0.53
2:B:562:VAL:O	2:B:566:ALA:HB3	2.08	0.53
1:C:483:GLY:HA2	1:C:500:MET:H	1.73	0.52
2:B:401:ILE:O	2:B:471:LEU:HA	2.09	0.52
2:B:375:LYS:O	2:B:377:ARG:N	2.42	0.52
2:B:458:LEU:O	2:B:462:ALA:HB2	2.10	0.52
2:D:562:VAL:O	2:D:566:ALA:HB3	2.10	0.52
2:D:458:LEU:O	2:D:462:ALA:HB2	2.11	0.51
2:D:33:ALA:HA	2:D:64:GLU:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:505:SER:C	1:A:507:GLN:H	2.14	0.51
2:B:33:ALA:HA	2:B:64:GLU:O	2.11	0.51
2:B:772:MET:O	2:B:776:GLU:CB	2.59	0.51
2:D:772:MET:O	2:D:776:GLU:CB	2.58	0.51
1:A:500:MET:C	1:A:502:GLU:N	2.64	0.51
2:D:685:MET:O	2:D:689:MET:CB	2.60	0.50
1:C:291:ALA:O	1:C:295:LEU:CB	2.59	0.50
2:D:375:LYS:O	2:D:376:ASP:C	2.50	0.49
2:B:685:MET:O	2:B:689:MET:CB	2.60	0.49
2:B:799:ASP:O	2:B:800:ASN:C	2.50	0.49
2:D:602:PRO:O	2:D:603:VAL:C	2.52	0.48
1:A:504:LEU:C	1:A:506:GLY:H	2.17	0.48
1:C:280:HIS:O	1:C:284:ALA:HB2	2.14	0.47
2:B:602:PRO:O	2:B:603:VAL:C	2.52	0.47
1:C:232:TYR:O	1:C:236:ALA:HB2	2.14	0.47
2:B:194:LEU:C	2:B:195:GLU:O	2.48	0.47
1:A:232:TYR:O	1:A:236:ALA:HB2	2.15	0.47
1:A:280:HIS:O	1:A:284:ALA:HB2	2.15	0.46
2:D:51:LYS:O	2:D:53:ASP:N	2.48	0.46
2:D:483:ILE:O	2:D:484:ASN:C	2.54	0.46
2:B:51:LYS:O	2:B:53:ASP:N	2.48	0.45
2:D:165:SER:O	2:D:223:ILE:HA	2.17	0.45
2:D:759:VAL:O	2:D:762:ALA:HB3	2.16	0.45
1:C:31:ALA:HA	1:C:91:LEU:H	1.82	0.45
2:D:458:LEU:O	2:D:462:ALA:CB	2.65	0.45
2:B:458:LEU:O	2:B:462:ALA:CB	2.65	0.44
2:D:584:THR:O	2:D:588:ALA:HB2	2.17	0.44
2:B:483:ILE:O	2:B:485:GLY:N	2.50	0.44
1:A:500:MET:O	1:A:501:GLY:C	2.55	0.44
2:B:759:VAL:O	2:B:762:ALA:HB3	2.18	0.44
2:B:402:VAL:HA	2:B:472:TYR:O	2.18	0.43
2:D:79:ARG:O	2:D:83:LEU:CB	2.66	0.43
1:A:798:LEU:O	1:A:800:PHE:N	2.45	0.43
2:D:800:ASN:O	2:D:803:GLY:N	2.53	0.42
1:C:232:TYR:O	1:C:236:ALA:CB	2.68	0.42
2:D:402:VAL:HA	2:D:472:TYR:O	2.20	0.42
1:C:231:VAL:O	1:C:235:ALA:HB3	2.20	0.41
2:D:526:GLY:O	2:D:716:ALA:N	2.53	0.41
2:D:111:SER:O	2:D:115:LEU:N	2.48	0.41
2:D:675:GLU:O	2:D:679:ARG:CB	2.68	0.41
2:B:675:GLU:O	2:B:679:ARG:CB	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:TYR:O	1:A:236:ALA:CB	2.69	0.41
2:B:526:GLY:O	2:B:716:ALA:N	2.54	0.41
2:D:391:SER:C	2:D:393:GLU:N	2.73	0.40
2:B:111:SER:O	2:B:115:LEU:N	2.47	0.40
1:A:505:SER:O	1:A:507:GLN:N	2.54	0.40
1:C:77:SER:O	1:C:81:ASP:CB	2.69	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 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	799/822 (97%)	685 (86%)	106 (13%)	8 (1%)	19	65
1	C	799/822 (97%)	688 (86%)	106 (13%)	5 (1%)	30	74
2	B	793/825 (96%)	676 (85%)	101 (13%)	16 (2%)	9	51
2	D	793/825 (96%)	676 (85%)	103 (13%)	14 (2%)	11	53
All	All	3184/3294 (97%)	2725 (86%)	416 (13%)	43 (1%)	19	58

All (43) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	648	ARG
1	C	649	ARG
1	C	650	PRO
2	B	376	ASP
2	B	410	VAL
2	D	408	PRO
2	D	756	LYS
1	A	552	PHE
1	A	787	GLU

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Mol	Chain	Res	Type
2	B	254	PRO
2	B	397	GLU
2	B	484	ASN
2	D	254	PRO
2	D	409	PHE
2	D	599	ASN
1	A	478	ALA
1	A	501	GLY
2	B	52	ASP
2	B	478	LYS
2	B	603	VAL
2	B	606	PRO
2	B	756	LYS
2	D	52	ASP
2	D	478	LYS
2	D	598	ASN
2	D	606	PRO
1	C	609	LEU
2	B	314	SER
2	B	793	SER
2	D	569	VAL
2	D	603	VAL
1	A	301	ILE
1	C	301	ILE
2	D	392	GLU
1	A	299	GLU
1	A	506	GLY
2	B	382	TRP
2	D	382	TRP
2	D	405	GLU
2	B	173	GLY
2	B	569	VAL
1	C	506	GLY
2	B	408	PRO

### 5.3.2 Protein sidechains ⓘ

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

### 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 ⓘ

4 ligands are 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	$\# Z  > 2$
3	GLY	A	901	-	1,4,4	0.50	0	0,4,4	0.00	-
4	GLU	B	2001	-	3,9,9	0.33	0	3,11,11	0.11	0
3	GLY	C	1001	-	1,4,4	0.50	0	0,4,4	0.00	-
4	GLU	D	901	-	3,9,9	0.33	0	3,11,11	0.12	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
3	GLY	A	901	-	-	0/0/2/2	0/0/0/0
4	GLU	B	2001	-	-	0/3/9/9	0/0/0/0
3	GLY	C	1001	-	-	0/0/2/2	0/0/0/0
4	GLU	D	901	-	-	0/3/9/9	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.

No monomer is involved in short contacts.

## 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.