



wwPDB EM Map/Model Validation Report ⓘ

Apr 25, 2016 – 08:36 PM EDT

PDB ID : 5IOV
EMDB ID: : EMD-8098
Title : Cryo-EM structure of GluN1/GluN2B NMDA receptor in the glutamate/glycine/Ro25-6981-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 : 7.50 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-20027257

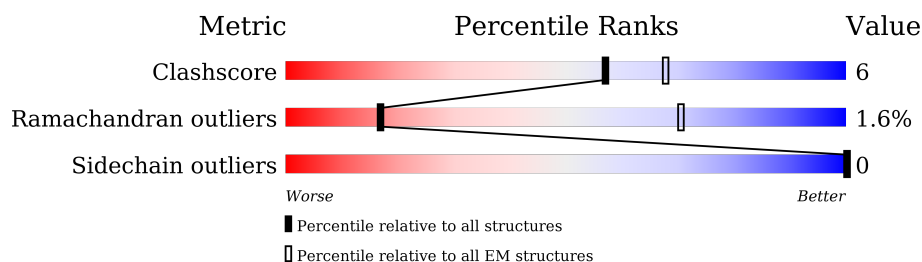
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 7.50 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	822	91% 6% .
1	C	822	92% 5% ..
2	B	825	88% 8% ..
2	D	825	88% 8% ..

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
4	QEM	B	901	-	-	X	-
4	QEM	D	901	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15879 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	798	Total	C	N	O	0	0
			3939	2344	798	797		
2	D	797	Total	C	N	O	0	0
			3934	2341	797	796		

There are 48 discrepancies between the modelled and reference sequences:

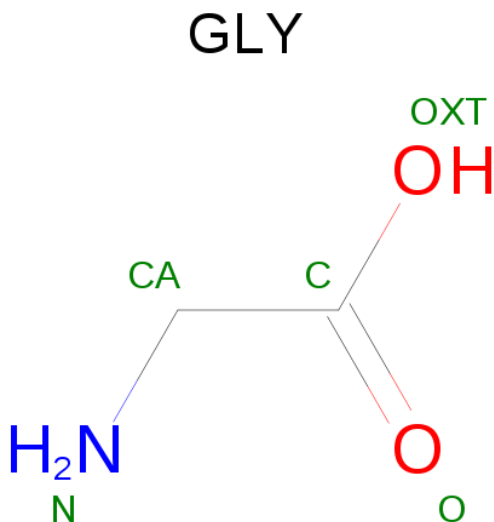
Chain	Residue	Modelled	Actual	Comment	Reference
B	20	SER	MET	engineered mutation	UNP A7XY94
B	21	ARG	GLY	engineered mutation	UNP A7XY94
B	22	ALA	CYS	engineered mutation	UNP A7XY94
B	64	GLU	ALA	engineered mutation	UNP A7XY94
B	69	GLN	ASN	engineered mutation	UNP A7XY94
B	343	ASP	ASN	engineered mutation	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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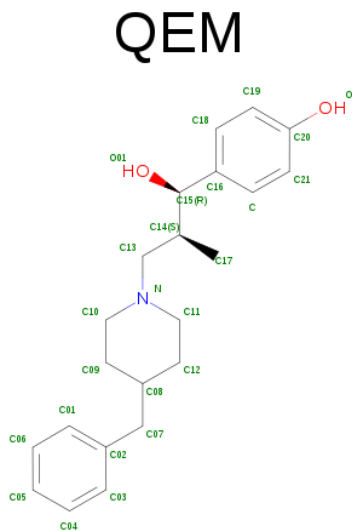
Chain	Residue	Modelled	Actual	Comment	Reference
B	640	ARG	GLU	engineered mutation	UNP A7XY94
B	641	ARG	GLU	engineered mutation	UNP A7XY94
D	20	SER	MET	engineered mutation	UNP A7XY94
D	21	ARG	GLY	engineered mutation	UNP A7XY94
D	22	ALA	CYS	engineered mutation	UNP A7XY94
D	64	GLU	ALA	engineered mutation	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: C₂H₅NO₂).



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

- Molecule 4 is 4-[(1R,2S)-3-(4-benzylpiperidin-1-yl)-1-hydroxy-2-methylpropyl]phenol (three-letter code: QEM) (formula: C₂₂H₂₉NO₂).



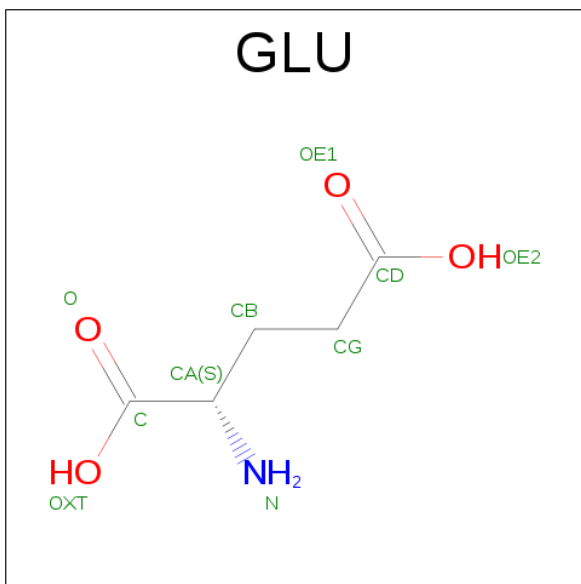
Mol	Chain	Residues	Atoms				AltConf
4	B	1	Total	C	N	O	0
			25	22	1	2	

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Mol	Chain	Residues	Atoms				AltConf
4	D	1	Total	C	N	O	0
			25	22	1	2	

- Molecule 5 is GLUTAMIC ACID (three-letter code: GLU) (formula: $C_5H_9NO_4$).

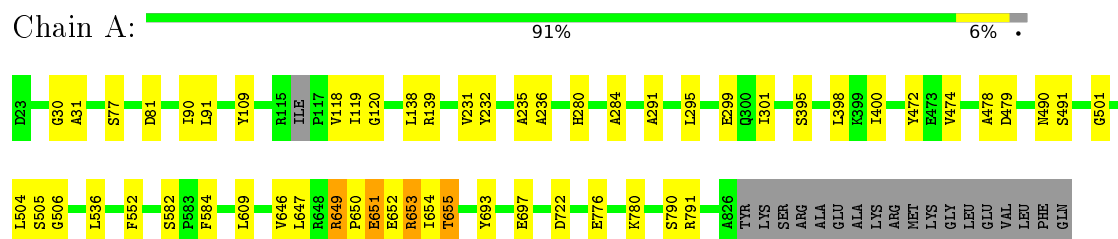


Mol	Chain	Residues	Atoms				AltConf
5	B	1	Total	C	N	O	0
			10	5	1	4	
5	D	1	Total	C	N	O	0
			10	5	1	4	

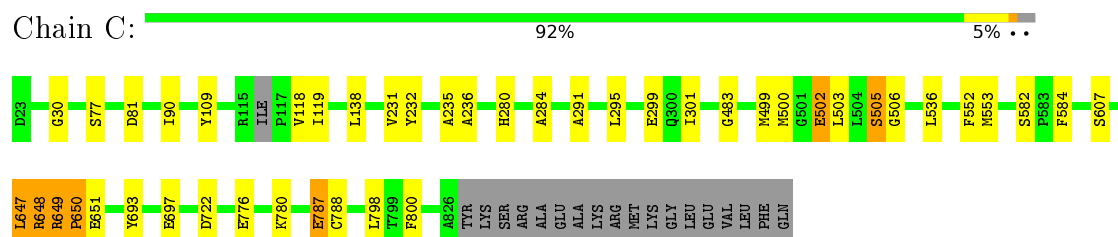
3 Residue-property plots

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.

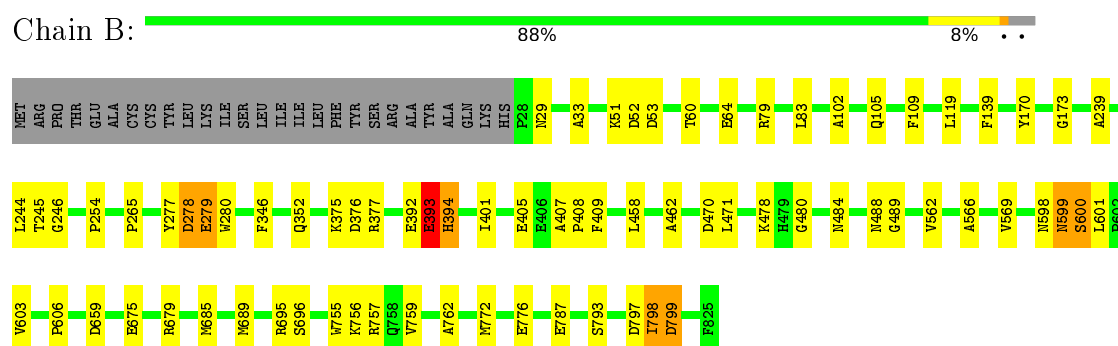
- Molecule 1: N-methyl-D-aspartate receptor subunit NR1-8a



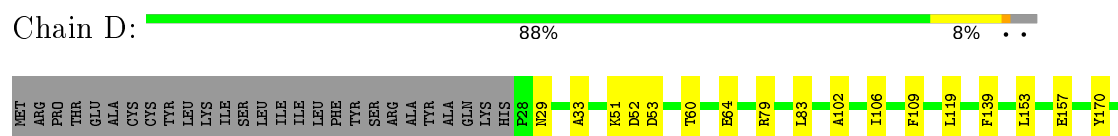
- Molecule 1: N-methyl-D-aspartate receptor subunit NR1-8a



- Molecule 2: Ionotropic glutamate receptor subunit NR2B



- Molecule 2: Ionotropic glutamate receptor subunit NR2B



G173	D176	K180	Q243	P254	M363	GLN	E365	R375	D376	R377	M382	S391	E392	E393	L399	S400	I401	V402	A407	L458	I461	A462	V465	K466	F467	T468	Y469	D470	L471	Y472	K478	H479	G480	I484	I488	G489	G526	Y562	A566	
V569	T584	A588	M598	M599	S600	V603	P606	D659	M685	M689	S696	A716	I755	K756	R757	Q758	V759	A762	M772	E776	S793	D797	I798	D799	F825															

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	87851	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)	1500	Depositor
Maximum defocus (nm)	3500	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: QEM

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	0.78	16/5512 (0.3%)
1	C	0.24	0/3961	0.71	12/5512 (0.2%)
2	B	0.26	1/3938 (0.0%)	0.63	12/5482 (0.2%)
2	D	0.24	0/3932	0.62	13/5472 (0.2%)
All	All	0.24	1/15792 (0.0%)	0.69	53/21978 (0.2%)

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
2	B	0	2
2	D	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	393	GLU	C-N	-5.53	1.21	1.34

The worst 5 of 53 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	490	ASN	CB-CA-C	-18.72	72.96	110.40
1	A	584	PHE	CB-CA-C	-16.49	77.42	110.40
1	C	584	PHE	CB-CA-C	-16.31	77.78	110.40
1	A	790	SER	CB-CA-C	-15.48	80.69	110.10
1	A	504	LEU	CB-CA-C	-15.04	81.62	110.20

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	393	GLU	Mainchain,Peptide
2	D	756	LYS	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	3963	0	1809	29	0
1	C	3963	0	1808	23	0
2	B	3939	0	1750	41	0
2	D	3934	0	1746	50	0
3	A	5	0	2	0	0
3	C	5	0	2	0	0
4	B	25	0	29	11	0
4	D	25	0	29	11	0
5	B	10	0	5	0	0
5	D	10	0	5	0	0
All	All	15879	0	7185	143	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 143 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:109:TYR:CB	4:B:901:QEM:C01	2.14	1.25
1:C:649:ARG:O	1:C:651:GLU:N	1.72	1.23
2:B:109:PHE:CB	4:B:901:QEM:H04	1.76	1.14
2:D:102:ALA:HB1	4:D:901:QEM:H09A	1.32	1.10
2:D:462:ALA:HA	2:D:465:VAL:CB	1.81	1.10

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%)	684 (86%)	106 (13%)	9 (1%)	17	63
1	C	799/822 (97%)	681 (85%)	110 (14%)	8 (1%)	19	65
2	B	796/825 (96%)	666 (84%)	110 (14%)	20 (2%)	7	46
2	D	793/825 (96%)	678 (86%)	100 (13%)	15 (2%)	10	52
All	All	3187/3294 (97%)	2709 (85%)	426 (13%)	52 (2%)	17	56

5 of 52 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	651	GLU
1	A	655	THR
1	C	506	GLY
1	C	649	ARG
1	C	650	PRO

5.3.2 Protein sidechains [i](#)

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

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](#)

6 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	QEM	B	901	-	27,27,27	1.00	1 (3%)	34,36,36	1.29	5 (14%)
5	GLU	B	902	-	3,9,9	0.33	0	3,11,11	0.11	0
3	GLY	C	1001	-	1,4,4	0.51	0	0,4,4	0.00	-
4	QEM	D	901	-	27,27,27	0.85	1 (3%)	34,36,36	1.15	3 (8%)
5	GLU	D	902	-	3,9,9	0.32	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	QEM	B	901	-	-	0/16/26/26	0/3/3/3
5	GLU	B	902	-	-	0/3/9/9	0/0/0/0
3	GLY	C	1001	-	-	0/0/2/2	0/0/0/0
4	QEM	D	901	-	-	0/16/26/26	0/3/3/3
5	GLU	D	902	-	-	0/3/9/9	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	901	QEM	C06-C01	-2.71	1.33	1.38
4	D	901	QEM	O-C20	2.01	1.41	1.37

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	901	QEM	C14-C13-N	-2.81	109.06	115.33
4	B	901	QEM	C14-C13-N	-2.73	109.23	115.33
4	B	901	QEM	C09-C08-C07	-2.72	105.57	111.86
4	B	901	QEM	C18-C16-C15	-2.03	117.63	120.72
4	D	901	QEM	C12-C11-N	2.24	114.72	110.97

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	901	QEM	11	0
4	D	901	QEM	11	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.