



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 4, 2022 – 08:19 PM EDT

PDB ID : 5UN1  
Title : Crystal structure of GluN1/GluN2B delta-ATD NMDA receptor  
Authors : Song, X.; Gouaux, E.  
Deposited on : 2017-01-30  
Resolution : 3.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : **FAILED**  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : **FAILED**  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.27

## 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.60 Å.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 20143 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 NR1-3a.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	424	Total	C	N	O	S	0	0	0
			2753	1727	499	512	15			
1	A	416	Total	C	N	O	S	0	0	0
			2643	1655	466	508	14			
1	E	412	Total	C	N	O	S	0	0	0
			2486	1549	448	477	12			
1	C	415	Total	C	N	O	S	0	0	0
			2591	1629	461	487	14			

There are 132 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	440	ASP	ASN	conflict	UNP C0KD15
G	469	ASP	ASN	conflict	UNP C0KD15
G	493	ALA	LYS	conflict	UNP C0KD15
G	494	ALA	LYS	conflict	UNP C0KD15
G	495	ALA	GLU	conflict	UNP C0KD15
G	?	-	LYS	deletion	UNP C0KD15
G	?	-	VAL	deletion	UNP C0KD15
G	?	-	ASN	deletion	UNP C0KD15
G	?	-	SER	deletion	UNP C0KD15
G	?	-	GLU	deletion	UNP C0KD15
G	?	-	GLU	deletion	UNP C0KD15
G	?	-	GLU	deletion	UNP C0KD15
G	?	-	GLU	deletion	UNP C0KD15
G	602	ARG	GLY	conflict	UNP C0KD15
G	609	LEU	ILE	conflict	UNP C0KD15
G	648	ARG	ASP	conflict	UNP C0KD15
G	761	GLU	ASN	conflict	UNP C0KD15
G	829	SER	-	expression tag	UNP C0KD15
G	830	ARG	-	expression tag	UNP C0KD15
G	831	ALA	-	expression tag	UNP C0KD15
G	832	GLU	-	expression tag	UNP C0KD15

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Chain	Residue	Modelled	Actual	Comment	Reference
G	833	ALA	-	expression tag	UNP C0KD15
G	834	LYS	-	expression tag	UNP C0KD15
G	835	ARG	-	expression tag	UNP C0KD15
G	836	MET	-	expression tag	UNP C0KD15
G	837	LYS	-	expression tag	UNP C0KD15
G	838	GLY	-	expression tag	UNP C0KD15
G	839	LEU	-	expression tag	UNP C0KD15
G	840	GLU	-	expression tag	UNP C0KD15
G	841	VAL	-	expression tag	UNP C0KD15
G	842	LEU	-	expression tag	UNP C0KD15
G	843	PHE	-	expression tag	UNP C0KD15
G	844	GLN	-	expression tag	UNP C0KD15
A	440	ASP	ASN	conflict	UNP C0KD15
A	469	ASP	ASN	conflict	UNP C0KD15
A	493	ALA	LYS	conflict	UNP C0KD15
A	494	ALA	LYS	conflict	UNP C0KD15
A	495	ALA	GLU	conflict	UNP C0KD15
A	?	-	LYS	deletion	UNP C0KD15
A	?	-	VAL	deletion	UNP C0KD15
A	?	-	ASN	deletion	UNP C0KD15
A	?	-	SER	deletion	UNP C0KD15
A	?	-	GLU	deletion	UNP C0KD15
A	?	-	GLU	deletion	UNP C0KD15
A	?	-	GLU	deletion	UNP C0KD15
A	?	-	GLU	deletion	UNP C0KD15
A	?	-	GLU	deletion	UNP C0KD15
A	602	ARG	GLY	conflict	UNP C0KD15
A	609	LEU	ILE	conflict	UNP C0KD15
A	648	ARG	ASP	conflict	UNP C0KD15
A	761	GLU	ASN	conflict	UNP C0KD15
A	829	SER	-	expression tag	UNP C0KD15
A	830	ARG	-	expression tag	UNP C0KD15
A	831	ALA	-	expression tag	UNP C0KD15
A	832	GLU	-	expression tag	UNP C0KD15
A	833	ALA	-	expression tag	UNP C0KD15
A	834	LYS	-	expression tag	UNP C0KD15
A	835	ARG	-	expression tag	UNP C0KD15
A	836	MET	-	expression tag	UNP C0KD15
A	837	LYS	-	expression tag	UNP C0KD15
A	838	GLY	-	expression tag	UNP C0KD15
A	839	LEU	-	expression tag	UNP C0KD15
A	840	GLU	-	expression tag	UNP C0KD15
A	841	VAL	-	expression tag	UNP C0KD15

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Chain	Residue	Modelled	Actual	Comment	Reference
A	842	LEU	-	expression tag	UNP C0KD15
A	843	PHE	-	expression tag	UNP C0KD15
A	844	GLN	-	expression tag	UNP C0KD15
E	440	ASP	ASN	conflict	UNP C0KD15
E	469	ASP	ASN	conflict	UNP C0KD15
E	493	ALA	LYS	conflict	UNP C0KD15
E	494	ALA	LYS	conflict	UNP C0KD15
E	495	ALA	GLU	conflict	UNP C0KD15
E	?	-	LYS	deletion	UNP C0KD15
E	?	-	VAL	deletion	UNP C0KD15
E	?	-	ASN	deletion	UNP C0KD15
E	?	-	SER	deletion	UNP C0KD15
E	?	-	GLU	deletion	UNP C0KD15
E	?	-	GLU	deletion	UNP C0KD15
E	?	-	GLU	deletion	UNP C0KD15
E	?	-	GLU	deletion	UNP C0KD15
E	602	ARG	GLY	conflict	UNP C0KD15
E	609	LEU	ILE	conflict	UNP C0KD15
E	648	ARG	ASP	conflict	UNP C0KD15
E	761	GLU	ASN	conflict	UNP C0KD15
E	829	SER	-	expression tag	UNP C0KD15
E	830	ARG	-	expression tag	UNP C0KD15
E	831	ALA	-	expression tag	UNP C0KD15
E	832	GLU	-	expression tag	UNP C0KD15
E	833	ALA	-	expression tag	UNP C0KD15
E	834	LYS	-	expression tag	UNP C0KD15
E	835	ARG	-	expression tag	UNP C0KD15
E	836	MET	-	expression tag	UNP C0KD15
E	837	LYS	-	expression tag	UNP C0KD15
E	838	GLY	-	expression tag	UNP C0KD15
E	839	LEU	-	expression tag	UNP C0KD15
E	840	GLU	-	expression tag	UNP C0KD15
E	841	VAL	-	expression tag	UNP C0KD15
E	842	LEU	-	expression tag	UNP C0KD15
E	843	PHE	-	expression tag	UNP C0KD15
E	844	GLN	-	expression tag	UNP C0KD15
C	440	ASP	ASN	conflict	UNP C0KD15
C	469	ASP	ASN	conflict	UNP C0KD15
C	493	ALA	LYS	conflict	UNP C0KD15
C	494	ALA	LYS	conflict	UNP C0KD15
C	495	ALA	GLU	conflict	UNP C0KD15
C	?	-	LYS	deletion	UNP C0KD15

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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	VAL	deletion	UNP C0KD15
C	?	-	ASN	deletion	UNP C0KD15
C	?	-	SER	deletion	UNP C0KD15
C	?	-	GLU	deletion	UNP C0KD15
C	?	-	GLU	deletion	UNP C0KD15
C	?	-	GLU	deletion	UNP C0KD15
C	?	-	GLU	deletion	UNP C0KD15
C	602	ARG	GLY	conflict	UNP C0KD15
C	609	LEU	ILE	conflict	UNP C0KD15
C	648	ARG	ASP	conflict	UNP C0KD15
C	761	GLU	ASN	conflict	UNP C0KD15
C	829	SER	-	expression tag	UNP C0KD15
C	830	ARG	-	expression tag	UNP C0KD15
C	831	ALA	-	expression tag	UNP C0KD15
C	832	GLU	-	expression tag	UNP C0KD15
C	833	ALA	-	expression tag	UNP C0KD15
C	834	LYS	-	expression tag	UNP C0KD15
C	835	ARG	-	expression tag	UNP C0KD15
C	836	MET	-	expression tag	UNP C0KD15
C	837	LYS	-	expression tag	UNP C0KD15
C	838	GLY	-	expression tag	UNP C0KD15
C	839	LEU	-	expression tag	UNP C0KD15
C	840	GLU	-	expression tag	UNP C0KD15
C	841	VAL	-	expression tag	UNP C0KD15
C	842	LEU	-	expression tag	UNP C0KD15
C	843	PHE	-	expression tag	UNP C0KD15
C	844	GLN	-	expression tag	UNP C0KD15

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	397	Total	C	N	O	S	0	0	0
			2328	1452	427	440	9			
2	H	409	Total	C	N	O	S	0	0	0
			2382	1460	443	466	13			
2	F	416	Total	C	N	O	S	0	0	0
			2319	1436	430	445	8			
2	D	405	Total	C	N	O	S	0	0	0
			2413	1502	439	461	11			

There are 128 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	486	VAL	THR	conflict	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	conflict	UNP A7XY94
B	640	ARG	GLU	conflict	UNP A7XY94
B	641	ARG	GLU	conflict	UNP A7XY94
B	826	TYR	-	expression tag	UNP A7XY94
B	827	LYS	-	expression tag	UNP A7XY94
B	828	SER	-	expression tag	UNP A7XY94
B	829	ARG	-	expression tag	UNP A7XY94
B	830	ALA	-	expression tag	UNP A7XY94
B	831	GLU	-	expression tag	UNP A7XY94
B	832	ALA	-	expression tag	UNP A7XY94
B	833	LYS	-	expression tag	UNP A7XY94
B	834	ARG	-	expression tag	UNP A7XY94
B	835	MET	-	expression tag	UNP A7XY94
B	836	LYS	-	expression tag	UNP A7XY94
B	837	GLY	-	expression tag	UNP A7XY94
B	838	LEU	-	expression tag	UNP A7XY94
B	839	GLU	-	expression tag	UNP A7XY94
B	840	VAL	-	expression tag	UNP A7XY94
B	841	LEU	-	expression tag	UNP A7XY94
B	842	PHE	-	expression tag	UNP A7XY94
B	843	GLN	-	expression tag	UNP A7XY94
H	486	VAL	THR	conflict	UNP A7XY94
H	?	-	ARG	deletion	UNP A7XY94
H	?	-	CYS	deletion	UNP A7XY94
H	?	-	LEU	deletion	UNP A7XY94
H	?	-	ALA	deletion	UNP A7XY94
H	?	-	ASP	deletion	UNP A7XY94
H	?	-	GLY	deletion	UNP A7XY94
H	?	-	ARG	deletion	UNP A7XY94
H	?	-	GLU	deletion	UNP A7XY94
H	?	-	PRO	deletion	UNP A7XY94
H	?	-	GLY	deletion	UNP A7XY94

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Chain	Residue	Modelled	Actual	Comment	Reference
H	601	LEU	VAL	conflict	UNP A7XY94
H	640	ARG	GLU	conflict	UNP A7XY94
H	641	ARG	GLU	conflict	UNP A7XY94
H	826	TYR	-	expression tag	UNP A7XY94
H	827	LYS	-	expression tag	UNP A7XY94
H	828	SER	-	expression tag	UNP A7XY94
H	829	ARG	-	expression tag	UNP A7XY94
H	830	ALA	-	expression tag	UNP A7XY94
H	831	GLU	-	expression tag	UNP A7XY94
H	832	ALA	-	expression tag	UNP A7XY94
H	833	LYS	-	expression tag	UNP A7XY94
H	834	ARG	-	expression tag	UNP A7XY94
H	835	MET	-	expression tag	UNP A7XY94
H	836	LYS	-	expression tag	UNP A7XY94
H	837	GLY	-	expression tag	UNP A7XY94
H	838	LEU	-	expression tag	UNP A7XY94
H	839	GLU	-	expression tag	UNP A7XY94
H	840	VAL	-	expression tag	UNP A7XY94
H	841	LEU	-	expression tag	UNP A7XY94
H	842	PHE	-	expression tag	UNP A7XY94
H	843	GLN	-	expression tag	UNP A7XY94
F	486	VAL	THR	conflict	UNP A7XY94
F	?	-	ARG	deletion	UNP A7XY94
F	?	-	CYS	deletion	UNP A7XY94
F	?	-	LEU	deletion	UNP A7XY94
F	?	-	ALA	deletion	UNP A7XY94
F	?	-	ASP	deletion	UNP A7XY94
F	?	-	GLY	deletion	UNP A7XY94
F	?	-	ARG	deletion	UNP A7XY94
F	?	-	GLU	deletion	UNP A7XY94
F	?	-	PRO	deletion	UNP A7XY94
F	?	-	GLY	deletion	UNP A7XY94
F	601	LEU	VAL	conflict	UNP A7XY94
F	640	ARG	GLU	conflict	UNP A7XY94
F	641	ARG	GLU	conflict	UNP A7XY94
F	826	TYR	-	expression tag	UNP A7XY94
F	827	LYS	-	expression tag	UNP A7XY94
F	828	SER	-	expression tag	UNP A7XY94
F	829	ARG	-	expression tag	UNP A7XY94
F	830	ALA	-	expression tag	UNP A7XY94
F	831	GLU	-	expression tag	UNP A7XY94
F	832	ALA	-	expression tag	UNP A7XY94

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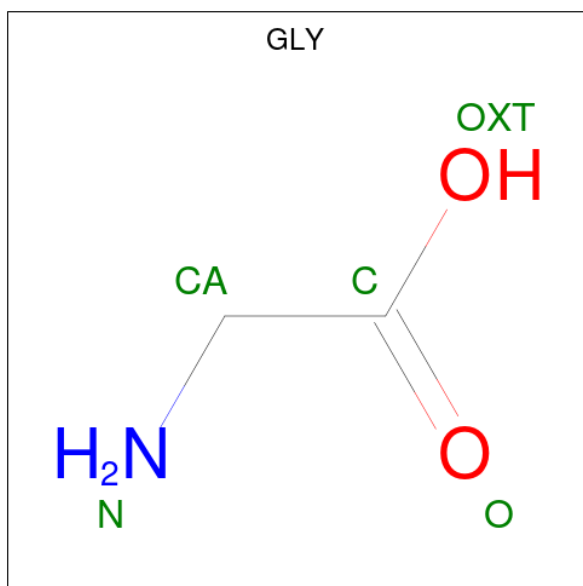
Chain	Residue	Modelled	Actual	Comment	Reference
F	833	LYS	-	expression tag	UNP A7XY94
F	834	ARG	-	expression tag	UNP A7XY94
F	835	MET	-	expression tag	UNP A7XY94
F	836	LYS	-	expression tag	UNP A7XY94
F	837	GLY	-	expression tag	UNP A7XY94
F	838	LEU	-	expression tag	UNP A7XY94
F	839	GLU	-	expression tag	UNP A7XY94
F	840	VAL	-	expression tag	UNP A7XY94
F	841	LEU	-	expression tag	UNP A7XY94
F	842	PHE	-	expression tag	UNP A7XY94
F	843	GLN	-	expression tag	UNP A7XY94
D	486	VAL	THR	conflict	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	conflict	UNP A7XY94
D	640	ARG	GLU	conflict	UNP A7XY94
D	641	ARG	GLU	conflict	UNP A7XY94
D	826	TYR	-	expression tag	UNP A7XY94
D	827	LYS	-	expression tag	UNP A7XY94
D	828	SER	-	expression tag	UNP A7XY94
D	829	ARG	-	expression tag	UNP A7XY94
D	830	ALA	-	expression tag	UNP A7XY94
D	831	GLU	-	expression tag	UNP A7XY94
D	832	ALA	-	expression tag	UNP A7XY94
D	833	LYS	-	expression tag	UNP A7XY94
D	834	ARG	-	expression tag	UNP A7XY94
D	835	MET	-	expression tag	UNP A7XY94
D	836	LYS	-	expression tag	UNP A7XY94
D	837	GLY	-	expression tag	UNP A7XY94
D	838	LEU	-	expression tag	UNP A7XY94
D	839	GLU	-	expression tag	UNP A7XY94
D	840	VAL	-	expression tag	UNP A7XY94
D	841	LEU	-	expression tag	UNP A7XY94
D	842	PHE	-	expression tag	UNP A7XY94

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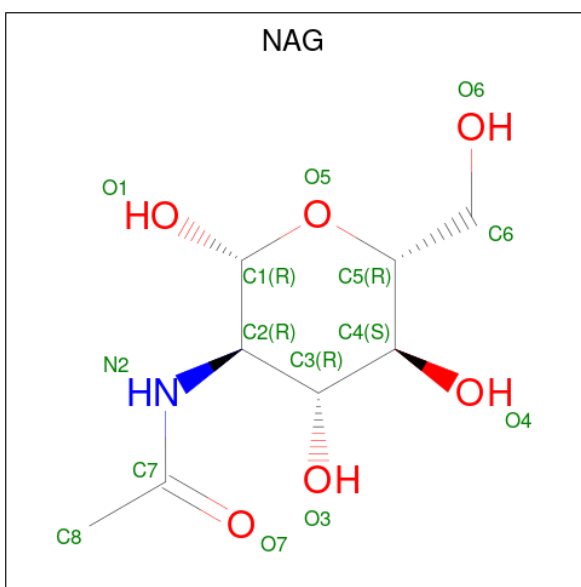
Chain	Residue	Modelled	Actual	Comment	Reference
D	843	GLN	-	expression tag	UNP A7XY94

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



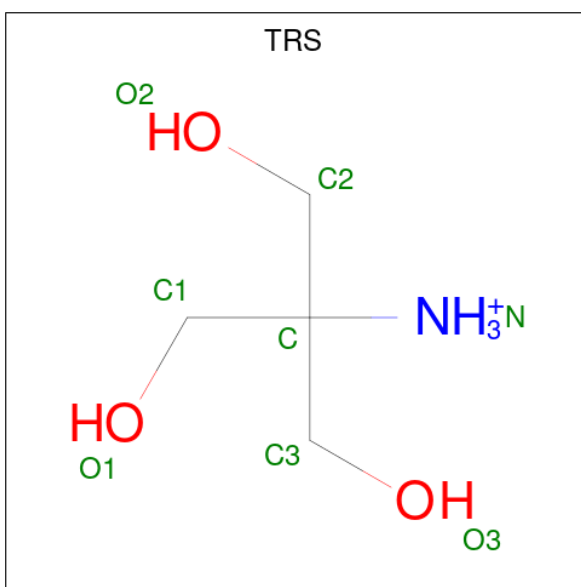
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	G	1	Total	C	N	O	0	0
			5	2	1	2		
3	A	1	Total	C	N	O	0	0
			5	2	1	2		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



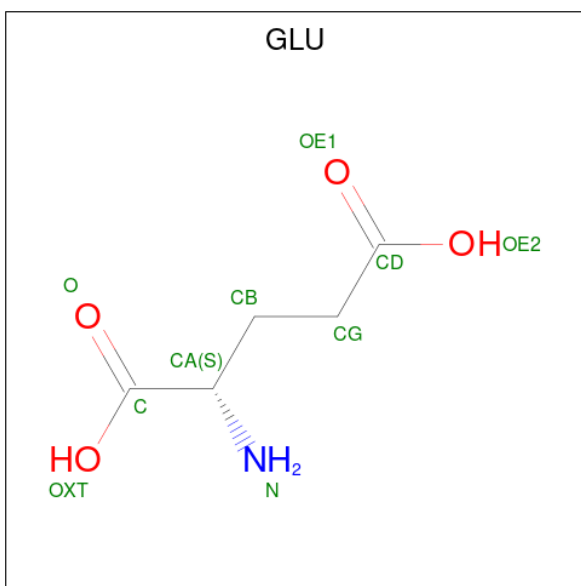
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	G	1	Total	C	N	O	0	0
			15	8	1	6		
4	B	1	Total	C	N	O	0	0
			15	8	1	6		
4	H	1	Total	C	N	O	0	0
			15	8	1	6		
4	F	1	Total	C	N	O	0	0
			15	8	1	6		
4	D	1	Total	C	N	O	0	0
			15	8	1	6		
4	D	1	Total	C	N	O	0	0
			15	8	1	6		

- Molecule 5 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula:  $C_4H_{12}NO_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	G	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 6 is GLUTAMIC ACID (three-letter code: GLU) (formula: C<sub>5</sub>H<sub>9</sub>NO<sub>4</sub>).



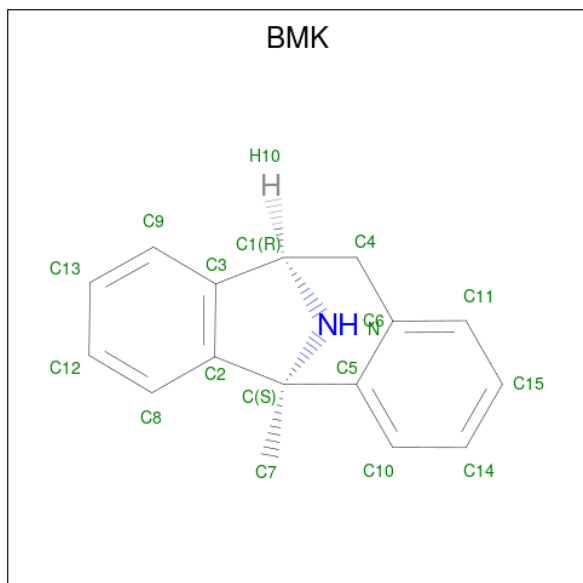
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	G	1	Total	C	N	O	0	0
			10	5	1	4		
6	G	1	Total	C	N	O	0	0
			10	5	1	4		
6	B	1	Total	C	N	O	0	0
			10	5	1	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	H	1	Total	C	N	O	0	0
			10	5	1	4		
6	D	1	Total	C	N	O	0	0
			10	5	1	4		

- Molecule 7 is (5S,10R)-5-methyl-10,11-dihydro-5H-5,10-epiminodibenzo[a,d][7]annulene (three-letter code: BMK) (formula: C<sub>16</sub>H<sub>15</sub>N).

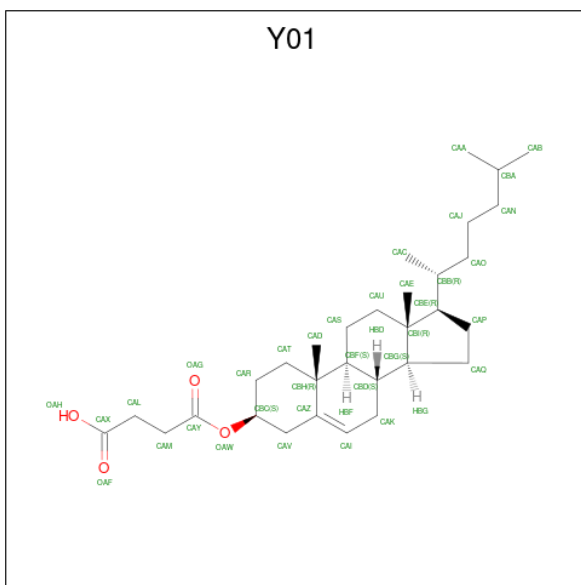


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	G	1	Total	C	N		0	0
			17	16	1			
7	B	1	Total	C	N		0	0
			17	16	1			

- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Mg	0	0
			1	1		

- Molecule 9 is CHOLESTEROL HEMISUCCINATE (three-letter code: Y01) (formula: C<sub>31</sub>H<sub>50</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	E	1	Total	C	O	0	0
			35	31	4		

MolProbit and EDS failed to run properly - this section is therefore empty.

### 3 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	181.57Å 108.47Å 182.46Å 90.00° 111.44° 90.00°	Depositor
Resolution (Å)	49.99 – 3.60	Depositor
% Data completeness (in resolution range)	91.0 (49.99-3.60)	Depositor
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.70 (at 3.41Å)	Xtriage
Refinement program	PHENIX (dev_2597: ???)	Depositor
R, $R_{free}$	0.288 , 0.316	Depositor
Wilson B-factor (Å <sup>2</sup> )	104.5	Xtriage
Anisotropy	0.060	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.34$ , $\langle L^2 \rangle = 0.17$	Xtriage
Estimated twinning fraction	0.117 for l,-k,h	Xtriage
Total number of atoms	20143	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	133.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.85% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 4 Model quality [i](#)

### 4.1 Standard geometry [i](#)

MolProbity failed to run properly - this section is therefore empty.

### 4.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section is therefore empty.

### 4.3 Torsion angles [i](#)

#### 4.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section is therefore empty.

#### 4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

#### 4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

### 4.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 4.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 4.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 1 is monoatomic - leaving 17 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
3	GLY	A	902	-	1,4,4	0.06	0	0,4,4	-	-
6	GLU	H	1001	-	2,9,9	0.59	0	2,11,11	1.03	0
6	GLU	G	1004	-	2,9,9	0.19	0	2,11,11	0.68	0
5	TRS	G	1003	-	7,7,7	0.39	0	9,9,9	0.55	0
4	NAG	H	1002	-	15,15,15	0.13	0	21,21,21	0.12	0
6	GLU	G	1006	-	2,9,9	0.26	0	2,11,11	0.39	0
7	BMK	G	1005	-	17,20,20	2.33	4 (23%)	20,31,31	1.40	3 (15%)
3	GLY	G	1001	-	1,4,4	0.06	0	0,4,4	-	-
4	NAG	B	1002	-	15,15,15	0.18	0	21,21,21	0.27	0
4	NAG	G	1002	-	15,15,15	0.22	0	21,21,21	0.21	0
4	NAG	D	1001	-	15,15,15	0.12	0	21,21,21	0.16	0
4	NAG	D	1003	-	15,15,15	0.09	0	21,21,21	0.13	0
6	GLU	D	1002	-	2,9,9	0.24	0	2,11,11	1.12	0
6	GLU	B	1001	-	2,9,9	0.42	0	2,11,11	0.65	0
9	Y01	E	1001	-	35,38,38	8.36	26 (74%)	54,57,57	2.81	25 (46%)
4	NAG	F	1001	-	15,15,15	0.14	0	21,21,21	0.13	0
7	BMK	B	1003	-	17,20,20	2.36	4 (23%)	20,31,31	1.41	3 (15%)

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	902	-	-	0/0/2/2	-
6	GLU	H	1001	-	-	2/3/9/9	-
6	GLU	G	1004	-	-	1/3/9/9	-
5	TRS	G	1003	-	-	6/9/9/9	-
4	NAG	H	1002	-	-	2/6/26/26	0/1/1/1
6	GLU	G	1006	-	-	0/3/9/9	-
7	BMK	G	1005	-	-	-	0/5/4/4
3	GLY	G	1001	-	-	0/0/2/2	-
4	NAG	B	1002	-	-	1/6/26/26	0/1/1/1
4	NAG	G	1002	-	-	2/6/26/26	0/1/1/1
4	NAG	D	1001	-	-	2/6/26/26	0/1/1/1
4	NAG	D	1003	-	-	2/6/26/26	0/1/1/1
6	GLU	D	1002	-	-	1/3/9/9	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GLU	B	1001	-	-	1/3/9/9	-
9	Y01	E	1001	-	-	8/17/77/77	0/4/4/4
4	NAG	F	1001	-	-	2/6/26/26	0/1/1/1
7	BMK	B	1003	-	-	-	0/5/4/4

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	E	1001	Y01	CBD-CBG	-27.67	1.00	1.53
9	E	1001	Y01	CAU-CAS	-17.07	1.17	1.53
9	E	1001	Y01	CAU-CBI	-16.27	1.24	1.54
9	E	1001	Y01	CAK-CBD	-15.32	1.27	1.53
9	E	1001	Y01	CBH-CAZ	-11.69	1.29	1.52
9	E	1001	Y01	CAQ-CAP	10.34	1.82	1.54
9	E	1001	Y01	CBI-CBE	9.93	1.73	1.55
9	E	1001	Y01	CBH-CBF	8.70	1.70	1.56
9	E	1001	Y01	CBD-CBF	-8.55	1.37	1.53
9	E	1001	Y01	CAQ-CBG	8.17	1.71	1.54
9	E	1001	Y01	CAK-CAI	8.15	1.67	1.50
9	E	1001	Y01	CAT-CBH	7.05	1.67	1.54
9	E	1001	Y01	CBB-CBE	-6.83	1.42	1.54
7	B	1003	BMK	C6-C5	6.74	1.49	1.40
7	G	1005	BMK	C6-C5	6.61	1.49	1.40
9	E	1001	Y01	CBI-CBG	5.92	1.66	1.55
7	B	1003	BMK	C3-C2	5.30	1.46	1.39
7	G	1005	BMK	C3-C2	5.13	1.46	1.39
9	E	1001	Y01	CAR-CBC	-4.83	1.38	1.51
9	E	1001	Y01	CAP-CBE	4.35	1.63	1.54
9	E	1001	Y01	CAI-CAZ	3.92	1.41	1.33
9	E	1001	Y01	OAW-CAY	3.82	1.45	1.34
9	E	1001	Y01	CAO-CBB	3.67	1.63	1.54
9	E	1001	Y01	CAV-CAZ	3.17	1.58	1.51
7	B	1003	BMK	C3-C1	-3.05	1.47	1.51
7	G	1005	BMK	C3-C1	-2.87	1.47	1.51
9	E	1001	Y01	CAC-CBB	2.83	1.60	1.53
7	G	1005	BMK	C-C5	-2.83	1.48	1.53
7	B	1003	BMK	C-C5	-2.55	1.49	1.53
9	E	1001	Y01	CAE-CBI	2.52	1.58	1.54
9	E	1001	Y01	OAW-CBC	2.36	1.52	1.46
9	E	1001	Y01	CAV-CBC	2.20	1.57	1.52
9	E	1001	Y01	CAM-CAY	2.09	1.56	1.50
9	E	1001	Y01	CAS-CBF	2.07	1.57	1.53

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	E	1001	Y01	CAC-CBB-CBE	6.89	123.47	112.92
9	E	1001	Y01	CAS-CBF-CBH	-5.81	105.43	113.08
9	E	1001	Y01	CBH-CAZ-CAI	-5.79	114.05	122.90
9	E	1001	Y01	CAT-CBH-CAZ	5.64	119.07	108.75
9	E	1001	Y01	CAE-CBI-CBG	-5.19	102.03	111.71
9	E	1001	Y01	CBF-CBD-CBG	5.16	116.00	109.09
9	E	1001	Y01	OAW-CAY-CAM	5.09	122.47	111.50
9	E	1001	Y01	CAK-CAI-CAZ	-5.04	115.75	125.06
9	E	1001	Y01	CAK-CBD-CBF	4.10	114.68	109.71
9	E	1001	Y01	CAM-CAL-CAX	-4.08	105.83	112.67
9	E	1001	Y01	CAD-CBH-CBF	-3.81	107.14	111.68
7	G	1005	BMK	C13-C9-C3	-3.72	116.29	121.01
7	B	1003	BMK	C13-C9-C3	-3.57	116.48	121.01
9	E	1001	Y01	CBG-CBI-CBE	3.36	104.06	100.07
7	B	1003	BMK	C3-C1-N	-3.32	98.90	101.85
9	E	1001	Y01	CAU-CBI-CBG	3.24	112.29	107.27
9	E	1001	Y01	CAS-CAU-CBI	3.09	118.08	112.78
9	E	1001	Y01	CAC-CBB-CAO	-2.77	106.02	110.36
9	E	1001	Y01	CAV-CAZ-CAI	-2.61	116.84	120.61
9	E	1001	Y01	CAD-CBH-CAT	-2.56	105.39	109.43
9	E	1001	Y01	CBI-CBE-CBB	2.55	123.48	119.49
7	G	1005	BMK	C3-C1-N	-2.49	99.64	101.85
9	E	1001	Y01	CAQ-CBG-CBI	-2.42	100.93	103.84
9	E	1001	Y01	CAK-CBD-CBG	2.36	114.33	110.91
9	E	1001	Y01	CAP-CBE-CBI	-2.28	101.09	103.84
9	E	1001	Y01	OAW-CBC-CAR	2.17	113.58	108.33
7	G	1005	BMK	C12-C8-C2	-2.15	116.05	119.96
7	B	1003	BMK	C12-C8-C2	-2.08	116.18	119.96
9	E	1001	Y01	OAW-CAY-OAG	-2.05	118.76	123.70
9	E	1001	Y01	CAV-CAZ-CBH	-2.05	113.70	116.42
9	E	1001	Y01	CAE-CBI-CBE	-2.01	107.97	111.71

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	G	1003	TRS	C3-C-C1-O1
5	G	1003	TRS	C2-C-C3-O3
6	B	1001	GLU	CA-CB-CG-CD
6	H	1001	GLU	N-CA-CB-CG
6	H	1001	GLU	C-CA-CB-CG

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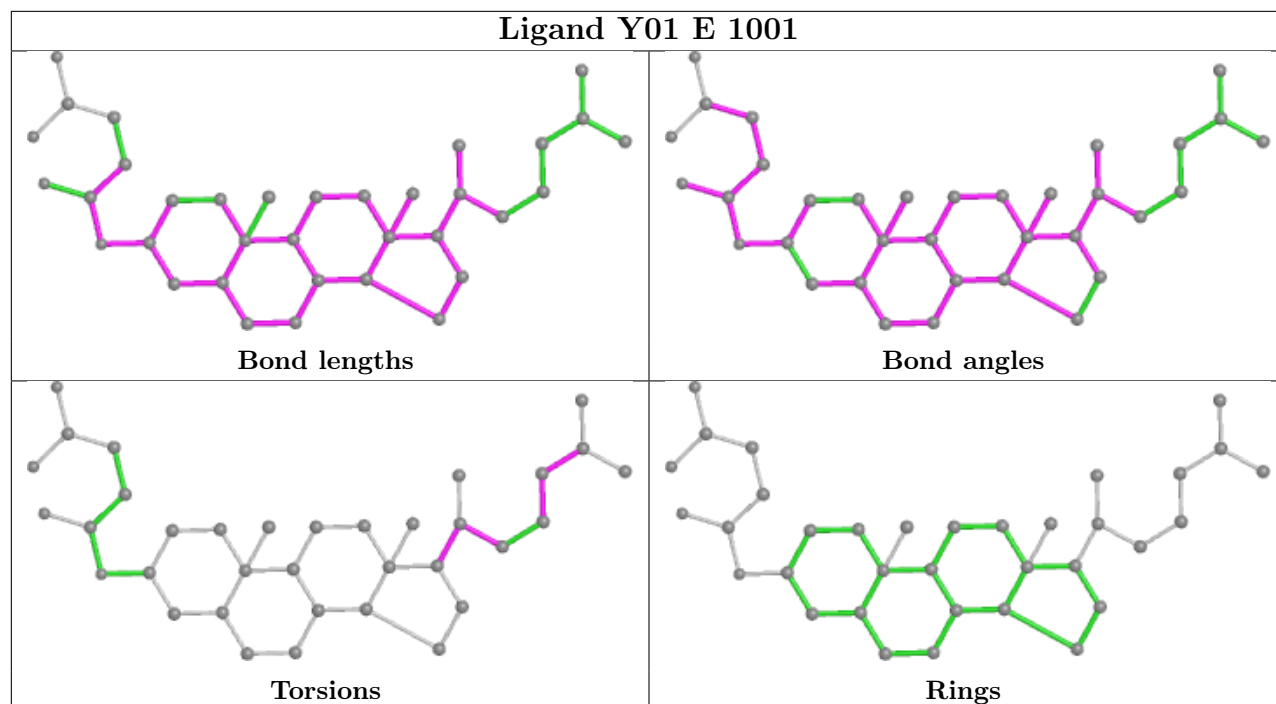
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Mol	Chain	Res	Type	Atoms
6	D	1002	GLU	CA-CB-CG-CD
9	E	1001	Y01	CAO-CBB-CBE-CAP
9	E	1001	Y01	CAO-CBB-CBE-CBI
9	E	1001	Y01	CAC-CBB-CBE-CBI
9	E	1001	Y01	CAC-CBB-CBE-CAP
4	G	1002	NAG	O5-C5-C6-O6
4	H	1002	NAG	O5-C5-C6-O6
4	D	1003	NAG	C4-C5-C6-O6
9	E	1001	Y01	CAJ-CAO-CBB-CBE
4	D	1003	NAG	O5-C5-C6-O6
9	E	1001	Y01	CAO-CAJ-CAN-CBA
4	F	1001	NAG	O5-C5-C6-O6
4	B	1002	NAG	O5-C5-C6-O6
4	H	1002	NAG	C4-C5-C6-O6
4	G	1002	NAG	C4-C5-C6-O6
4	D	1001	NAG	O5-C5-C6-O6
5	G	1003	TRS	C2-C-C1-O1
5	G	1003	TRS	C1-C-C3-O3
4	F	1001	NAG	C4-C5-C6-O6
5	G	1003	TRS	N-C-C1-O1
5	G	1003	TRS	N-C-C3-O3
9	E	1001	Y01	CAJ-CAO-CBB-CAC
4	D	1001	NAG	C1-C2-N2-C7
6	G	1004	GLU	CA-CB-CG-CD
9	E	1001	Y01	CAJ-CAN-CBA-CAB

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



#### 4.7 Other polymers [i](#)

There are no such residues in this entry.

#### 4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 5 Fit of model and data

### 5.1 Protein, DNA and RNA chains

EDS failed to run properly - this section is therefore empty.

### 5.2 Non-standard residues in protein, DNA, RNA chains

EDS failed to run properly - this section is therefore empty.

### 5.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

### 5.4 Ligands

EDS failed to run properly - this section is therefore empty.

### 5.5 Other polymers

EDS failed to run properly - this section is therefore empty.