



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 02:01 AM UTC

PDB ID : 6XSR / pdb_00006xsr
Title : Crystal structure of GluA2 AMPA receptor in complex with trans-4-butylcyclohexane carboxylic acid (4-BCCA) inhibitor
Authors : Yelshanskaya, M.V.; Singh, A.K.; Sobolevsky, A.I.
Deposited on : 2020-07-16
Resolution : 4.25 Å(reported)

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

We welcome your comments at 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

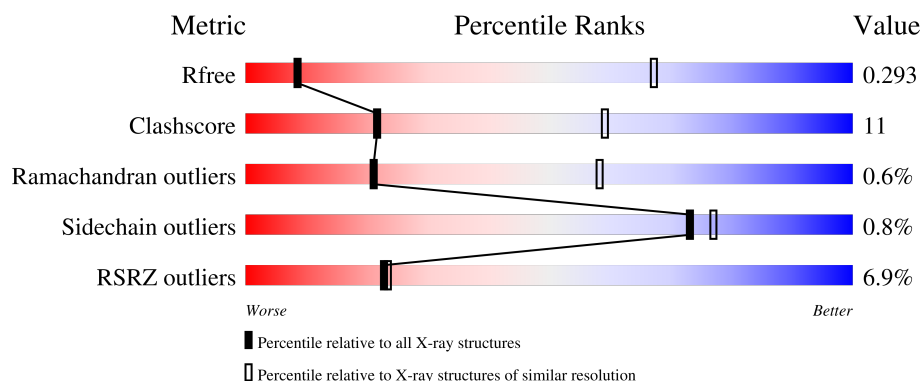
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.25 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1029 (4.62-3.90)
Clashscore	190562	1074 (4.62-3.90)
Ramachandran outliers	187476	1001 (4.62-3.88)
Sidechain outliers	187428	1021 (4.66-3.86)
RSRZ outliers	180081	1026 (4.62-3.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	808	5% 72% 23% 5%
1	B	808	9% 71% 24% • •
1	C	808	4% 70% 25% •
1	D	808	8% 77% 17% • •

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
2	NAG	B	901	-	-	X	-
3	V8G	A	902	-	-	X	-
3	V8G	C	902	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 23775 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 Glutamate receptor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	770	Total	C	N	O	S	0	0	0
			5912	3793	984	1108	27			
1	B	772	Total	C	N	O	S	0	0	0
			5954	3815	987	1124	28			
1	C	774	Total	C	N	O	S	0	0	0
			5918	3796	985	1111	26			
1	D	772	Total	C	N	O	S	0	0	0
			5909	3788	985	1110	26			

There are 44 discrepancies between the modelled and reference sequences:

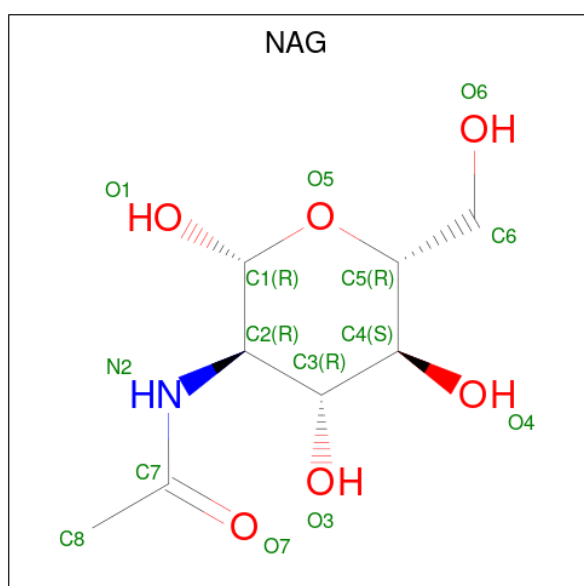
Chain	Residue	Modelled	Actual	Comment	Reference
A	241	GLU	ASN	conflict	UNP P19491
A	382	LEU	VAL	conflict	UNP P19491
A	?	-	LEU	deletion	UNP P19491
A	?	-	THR	deletion	UNP P19491
A	?	-	GLU	deletion	UNP P19491
A	?	-	LEU	deletion	UNP P19491
A	?	-	PRO	deletion	UNP P19491
A	?	-	SER	deletion	UNP P19491
A	384	GLU	GLY	conflict	UNP P19491
A	385	ASP	ASN	conflict	UNP P19491
A	392	GLN	ASN	conflict	UNP P19491
B	241	GLU	ASN	conflict	UNP P19491
B	382	LEU	VAL	conflict	UNP P19491
B	?	-	LEU	deletion	UNP P19491
B	?	-	THR	deletion	UNP P19491
B	?	-	GLU	deletion	UNP P19491
B	?	-	LEU	deletion	UNP P19491
B	?	-	PRO	deletion	UNP P19491
B	?	-	SER	deletion	UNP P19491
B	384	GLU	GLY	conflict	UNP P19491
B	385	ASP	ASN	conflict	UNP P19491

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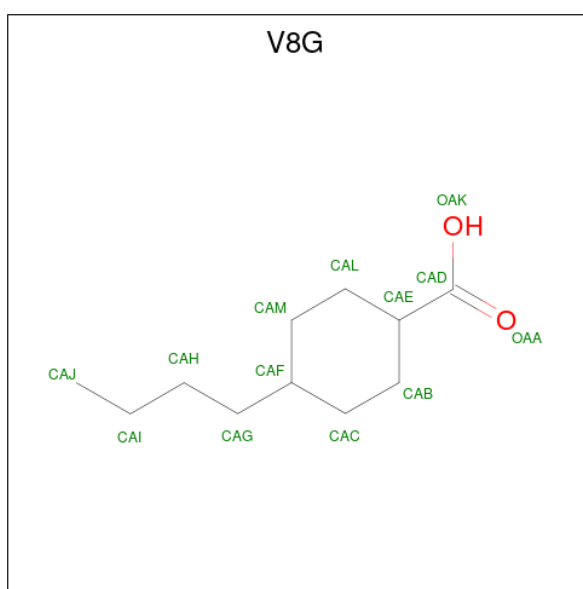
Chain	Residue	Modelled	Actual	Comment	Reference
B	392	GLN	ASN	conflict	UNP P19491
C	241	GLU	ASN	conflict	UNP P19491
C	382	LEU	VAL	conflict	UNP P19491
C	?	-	LEU	deletion	UNP P19491
C	?	-	THR	deletion	UNP P19491
C	?	-	GLU	deletion	UNP P19491
C	?	-	LEU	deletion	UNP P19491
C	?	-	PRO	deletion	UNP P19491
C	?	-	SER	deletion	UNP P19491
C	384	GLU	GLY	conflict	UNP P19491
C	385	ASP	ASN	conflict	UNP P19491
C	392	GLN	ASN	conflict	UNP P19491
D	241	GLU	ASN	conflict	UNP P19491
D	382	LEU	VAL	conflict	UNP P19491
D	?	-	LEU	deletion	UNP P19491
D	?	-	THR	deletion	UNP P19491
D	?	-	GLU	deletion	UNP P19491
D	?	-	LEU	deletion	UNP P19491
D	?	-	PRO	deletion	UNP P19491
D	?	-	SER	deletion	UNP P19491
D	384	GLU	GLY	conflict	UNP P19491
D	385	ASP	ASN	conflict	UNP P19491
D	392	GLN	ASN	conflict	UNP P19491

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).

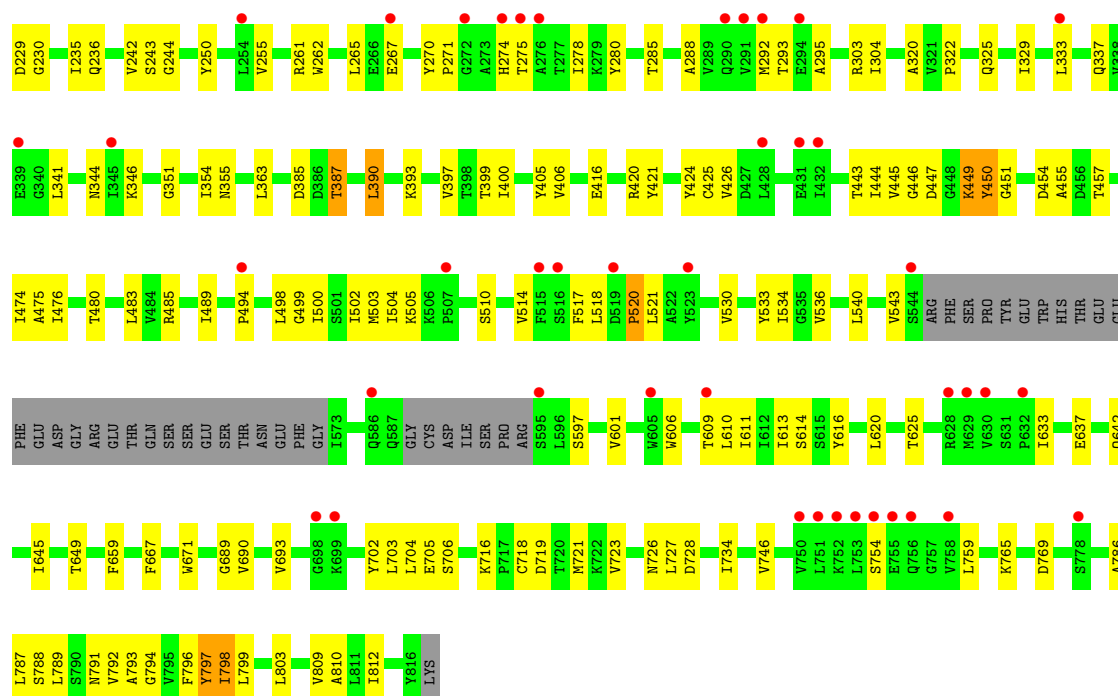


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		

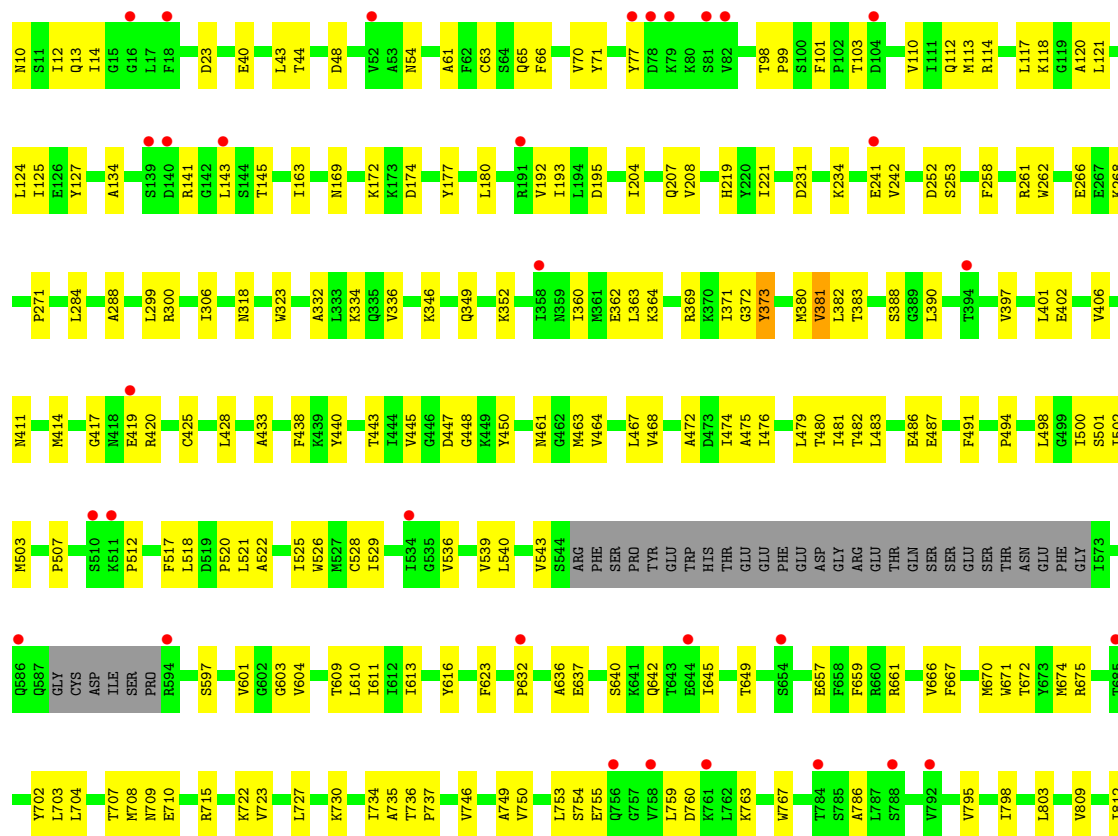
- Molecule 3 is trans-4-butylcyclohexane-1-carboxylic acid (CCD ID: V8G) (formula: $C_{11}H_{20}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	11	2		
3	C	1	Total	C	O	0	0
			13	11	2		

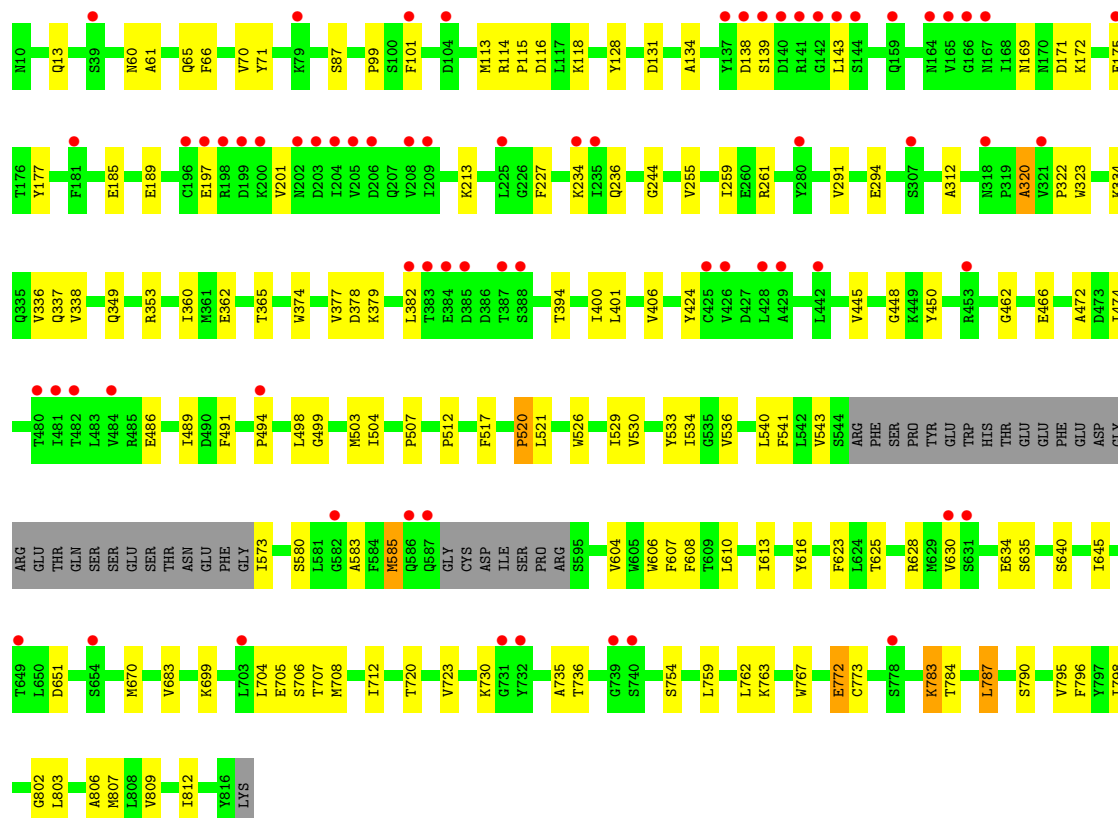
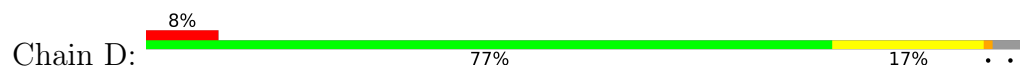


• Molecule 1: Glutamate receptor 2





• Molecule 1: Glutamate receptor 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	92.79Å 110.40Å 600.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.91 – 4.25 48.91 – 4.25	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.91-4.25) 99.5 (48.91-4.25)	Depositor EDS
R_{merge}	0.45	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.89 (at 4.29Å)	Xtriage
Refinement program	PHENIX (1.16_3549)	Depositor
R, R_{free}	0.260 , 0.296 0.268 , 0.293	Depositor DCC
R_{free} test set	2226 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	217.9	Xtriage
Anisotropy	0.169	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 207.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	23775	wwPDB-VP
Average B, all atoms (Å ²)	259.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.30% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: V8G, NAG

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	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.20	0/6031	0.36	0/8167
1	B	0.25	3/6073 (0.0%)	0.41	1/8221 (0.0%)
1	C	0.15	0/6037	0.32	0/8180
1	D	0.25	0/6028	0.41	1/8165 (0.0%)
All	All	0.22	3/24169 (0.0%)	0.38	2/32733 (0.0%)

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	B	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	450	TYR	CA-C	7.00	1.61	1.52
1	B	449	LYS	C-N	6.30	1.42	1.33
1	B	450	TYR	N-CA	6.08	1.53	1.46

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	450	TYR	N-CA-C	9.27	124.82	109.06
1	D	628	ARG	N-CA-C	-5.08	104.63	111.54

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	449	LYS	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	5912	0	5783	143	0
1	B	5954	0	5844	161	1
1	C	5918	0	5758	145	1
1	D	5909	0	5755	111	0
2	A	14	0	13	2	0
2	B	14	0	13	15	0
2	C	14	0	13	0	0
2	D	14	0	13	1	0
3	A	13	0	0	12	0
3	C	13	0	0	9	0
All	All	23775	0	23192	509	1

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 11.

The worst 5 of 509 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:B:355:ASN:HD21	2:B:901:NAG:C1	1.06	1.60
1:A:355:ASN:HD21	2:A:901:NAG:C1	1.03	1.58
3:A:902:V8G:CAI	1:D:610:LEU:HD12	1.47	1.45
1:B:355:ASN:ND2	2:B:901:NAG:C1	1.73	1.44
1:A:355:ASN:ND2	2:A:901:NAG:C1	1.88	1.35

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:303:ARG:NH2	1:C:346:LYS:NZ[3_545]	1.53	0.67

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 X-ray entries followed by that with respect to entries of similar resolution.

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	764/808 (95%)	706 (92%)	54 (7%)	4 (0%)	24	62
1	B	766/808 (95%)	704 (92%)	58 (8%)	4 (0%)	24	62
1	C	768/808 (95%)	703 (92%)	58 (8%)	7 (1%)	14	49
1	D	766/808 (95%)	708 (92%)	54 (7%)	4 (0%)	24	62
All	All	3064/3232 (95%)	2821 (92%)	224 (7%)	19 (1%)	21	58

5 of 19 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	632	PRO
1	C	512	PRO
1	D	585	MET
1	A	507	PRO
1	B	798	ILE

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 X-ray entries followed by that with respect to entries of similar resolution.

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	613/691 (89%)	609 (99%)	4 (1%)	76	78
1	B	625/691 (90%)	617 (99%)	8 (1%)	61	71
1	C	609/691 (88%)	608 (100%)	1 (0%)	87	85
1	D	609/691 (88%)	602 (99%)	7 (1%)	65	73
All	All	2456/2764 (89%)	2436 (99%)	20 (1%)	73	77

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	625	THR
1	D	773	CYS
1	D	787	LEU
1	D	783	LYS
1	B	390	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	274	HIS
1	C	337	GLN
1	D	344	ASN
1	D	60	ASN
1	D	167	ASN

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 oligosaccharides 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	V8G	A	902	-	13,13,13	0.73	0	16,16,16	1.08	1 (6%)
2	NAG	D	901	1	14,14,15	0.38	0	17,19,21	0.53	0
3	V8G	C	902	-	13,13,13	0.74	0	16,16,16	1.08	1 (6%)
2	NAG	A	901	-	14,14,15	0.51	0	17,19,21	0.51	0
2	NAG	B	901	-	14,14,15	0.36	0	17,19,21	0.54	0
2	NAG	C	901	-	14,14,15	0.31	0	17,19,21	0.61	1 (5%)

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	V8G	A	902	-	-	3/8/18/18	0/1/1/1
2	NAG	D	901	1	-	0/6/23/26	0/1/1/1
3	V8G	C	902	-	-	3/8/18/18	0/1/1/1
2	NAG	A	901	-	-	0/6/23/26	0/1/1/1
2	NAG	B	901	-	-	0/6/23/26	0/1/1/1
2	NAG	C	901	-	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	902	V8G	OAK-CAD-CAE	2.26	120.03	114.16
3	C	902	V8G	OAK-CAD-CAE	2.23	119.95	114.16
2	C	901	NAG	C1-O5-C5	2.05	114.93	112.19

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

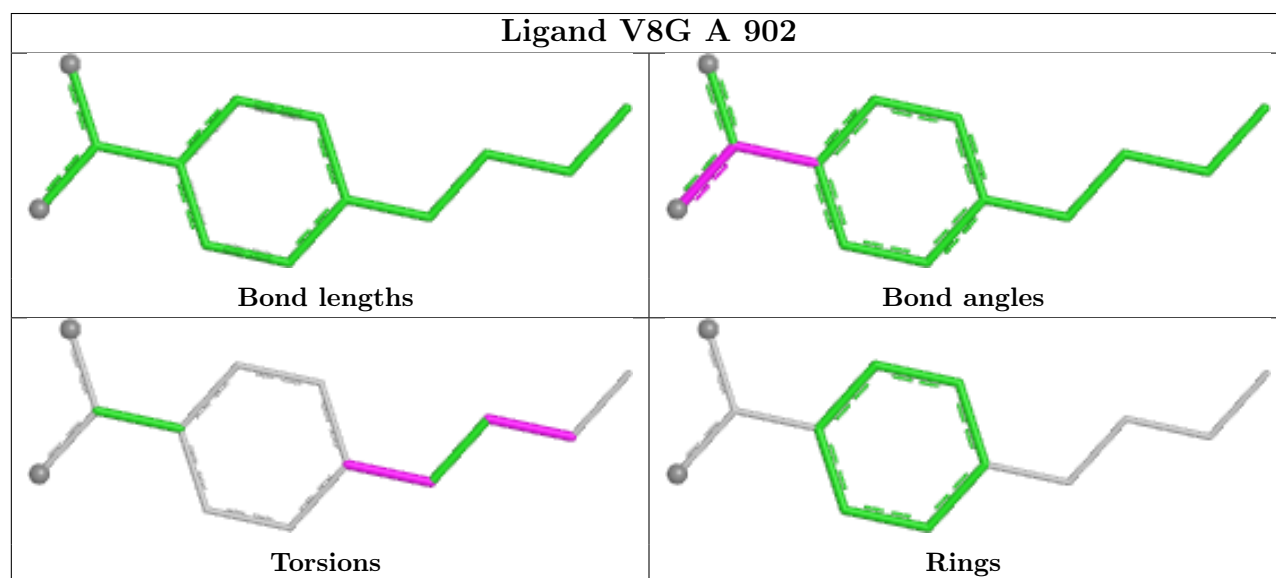
Mol	Chain	Res	Type	Atoms
3	A	902	V8G	CAC-CAF-CAG-CAH
3	C	902	V8G	CAC-CAF-CAG-CAH
3	A	902	V8G	CAG-CAH-CAI-CAJ
3	C	902	V8G	CAG-CAH-CAI-CAJ
3	A	902	V8G	CAM-CAF-CAG-CAH

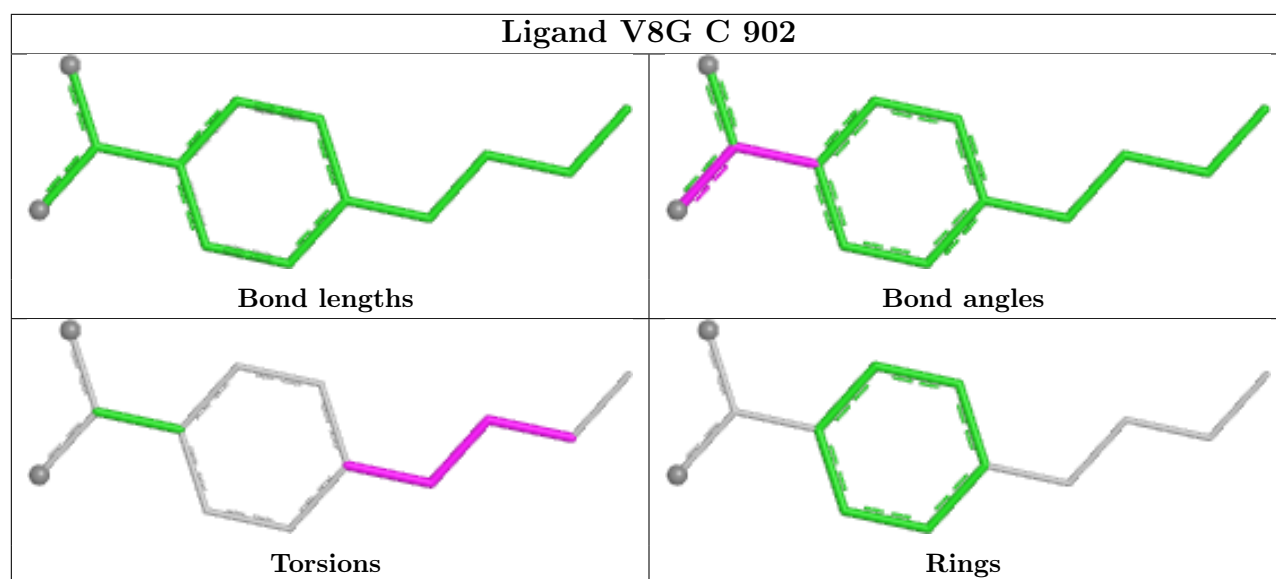
There are no ring outliers.

5 monomers are involved in 39 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	902	V8G	12	0
2	D	901	NAG	1	0
3	C	902	V8G	9	0
2	A	901	NAG	2	0
2	B	901	NAG	15	0

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.





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.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	770/808 (95%)	0.18	43 (5%)	30	28	159, 239, 367, 393	0
1	B	772/808 (95%)	0.38	69 (8%)	15	18	154, 222, 377, 407	0
1	C	774/808 (95%)	0.19	32 (4%)	41	35	178, 258, 368, 408	0
1	D	772/808 (95%)	0.39	68 (8%)	15	19	191, 287, 378, 395	0
All	All	3088/3232 (95%)	0.29	212 (6%)	23	23	154, 248, 374, 408	0

The worst 5 of 212 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	309	ARG	12.6
1	D	200	LYS	10.8
1	D	139	SER	9.8
1	D	197	GLU	7.3
1	B	630	VAL	7.2

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

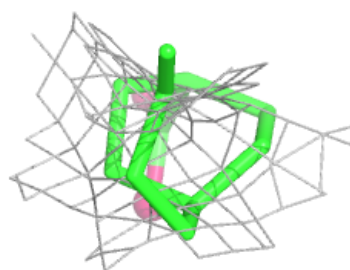
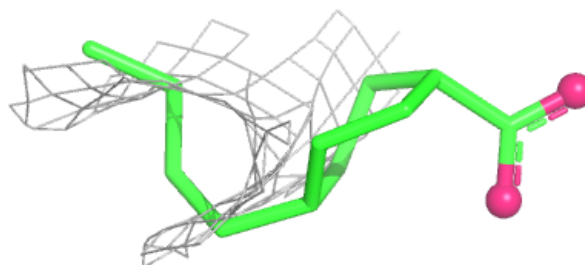
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

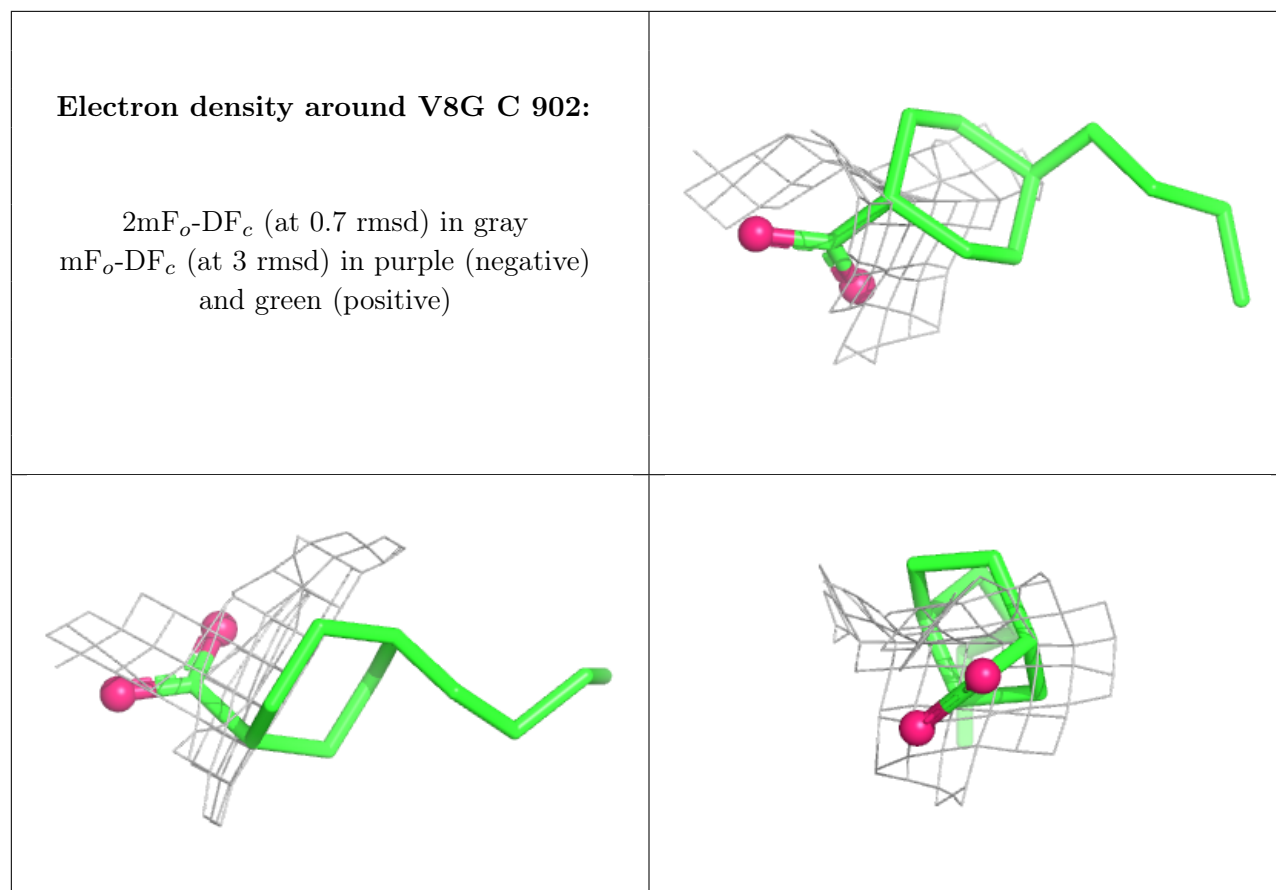
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	B	901	14/15	0.56	0.15	196,196,199,200	0
2	NAG	D	901	14/15	0.60	0.16	269,269,270,272	0
2	NAG	A	901	14/15	0.70	0.17	255,255,257,262	0
2	NAG	C	901	14/15	0.78	0.18	416,416,418,424	0
3	V8G	A	902	13/13	0.86	0.12	331,331,331,331	0
3	V8G	C	902	13/13	0.92	0.11	341,341,341,341	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around V8G A 902:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.