wwPDB X-ray Structure Validation Summary Report (i)

Oct 9, 2023 – 04:42 AM EDT

PDB ID	:	6XSR
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 (i) 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 (i)) were used in the production of this report:

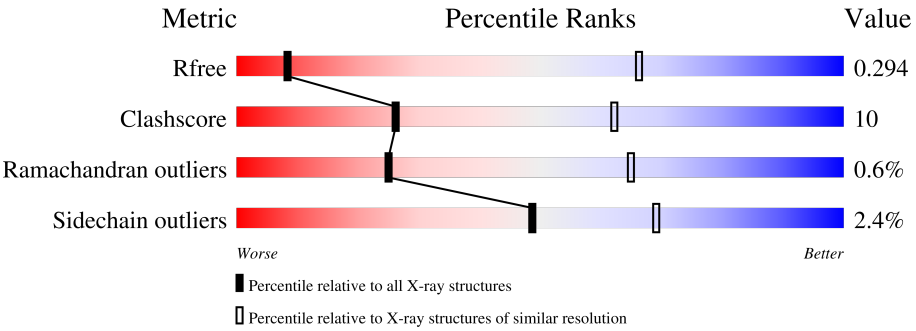
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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}	130704	1017 (4.72-3.78)
Clashscore	141614	1059 (4.72-3.80)
Ramachandran outliers	138981	1014 (4.72-3.80)
Sidechain outliers	138945	1018 (4.72-3.78)

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	808	72% 22% • 5%
1	B	808	70% 25% • •
1	C	808	71% 24% • •
1	D	808	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 (i)

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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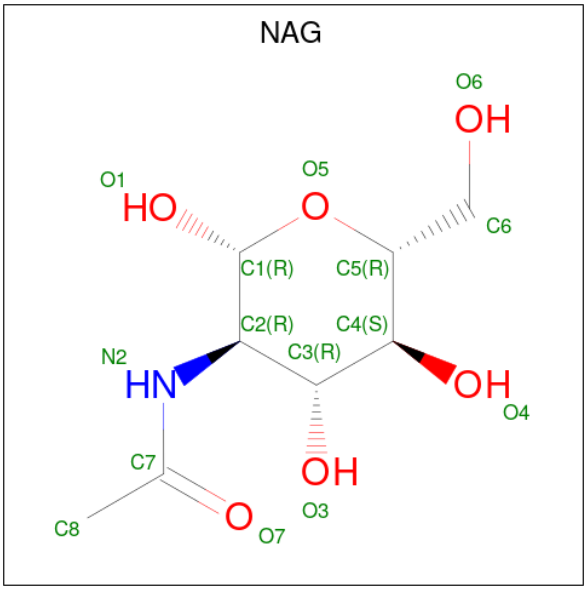
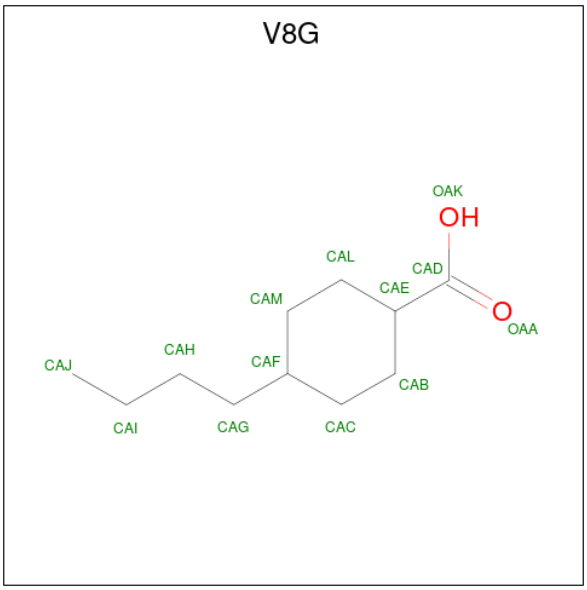
Chain	Residue	Modelled	Actual	Comment	Reference
B	392	GLN	ASN	conflict	UNP P19491
C	241	GLU	ASN	conflict	UNP P19491
C	382	LEU	VAL	conflict	UNP P19491
C	?	-	LEU	deletion	UNP P19491
C	?	-	THR	deletion	UNP P19491
C	?	-	GLU	deletion	UNP P19491
C	?	-	LEU	deletion	UNP P19491
C	?	-	PRO	deletion	UNP P19491
C	?	-	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 (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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



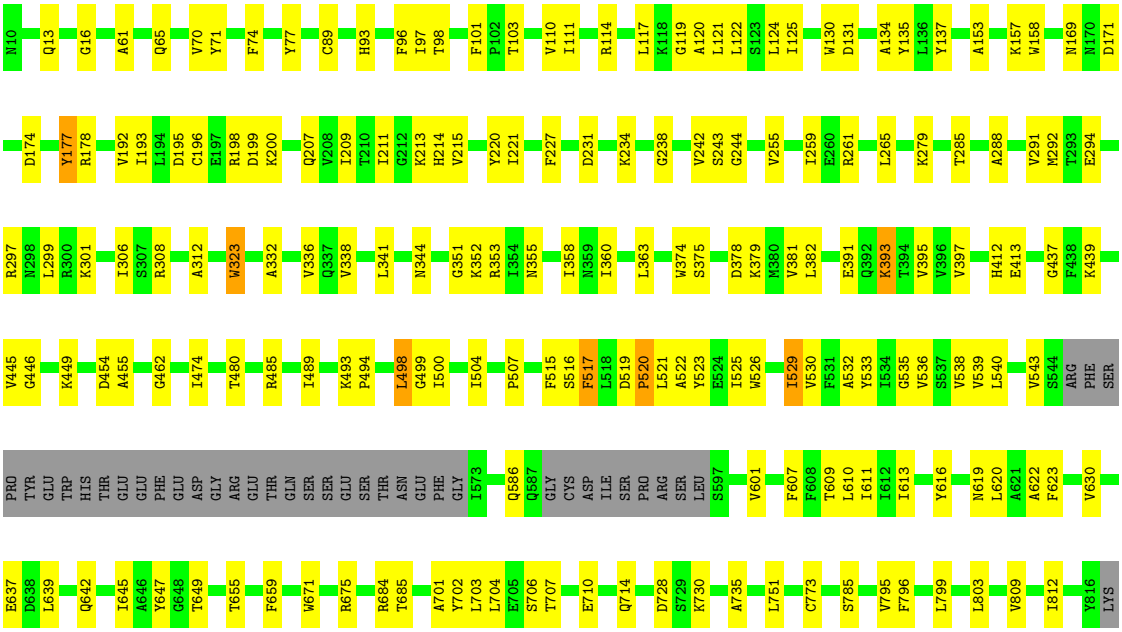
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 13 11 2	0	0
3	C	1	Total C O 13 11 2	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

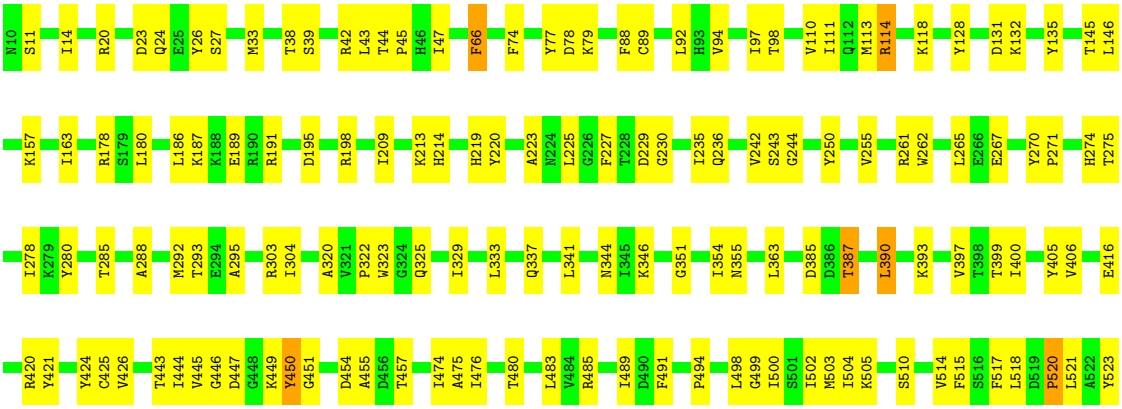
- Molecule 1: Glutamate receptor 2

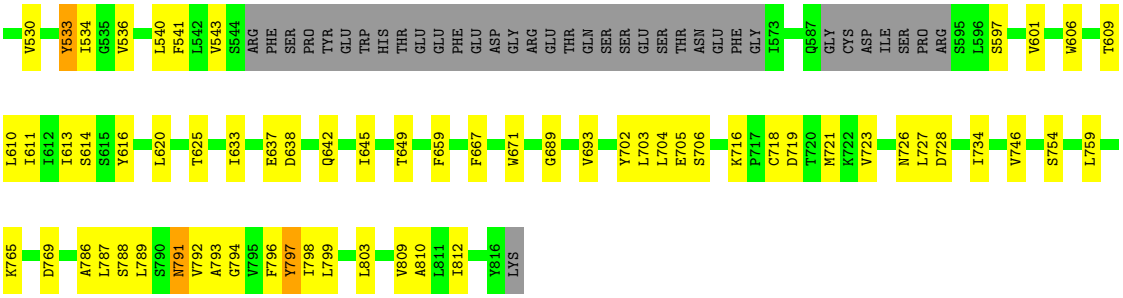
Chain A:



- Molecule 1: Glutamate receptor 2

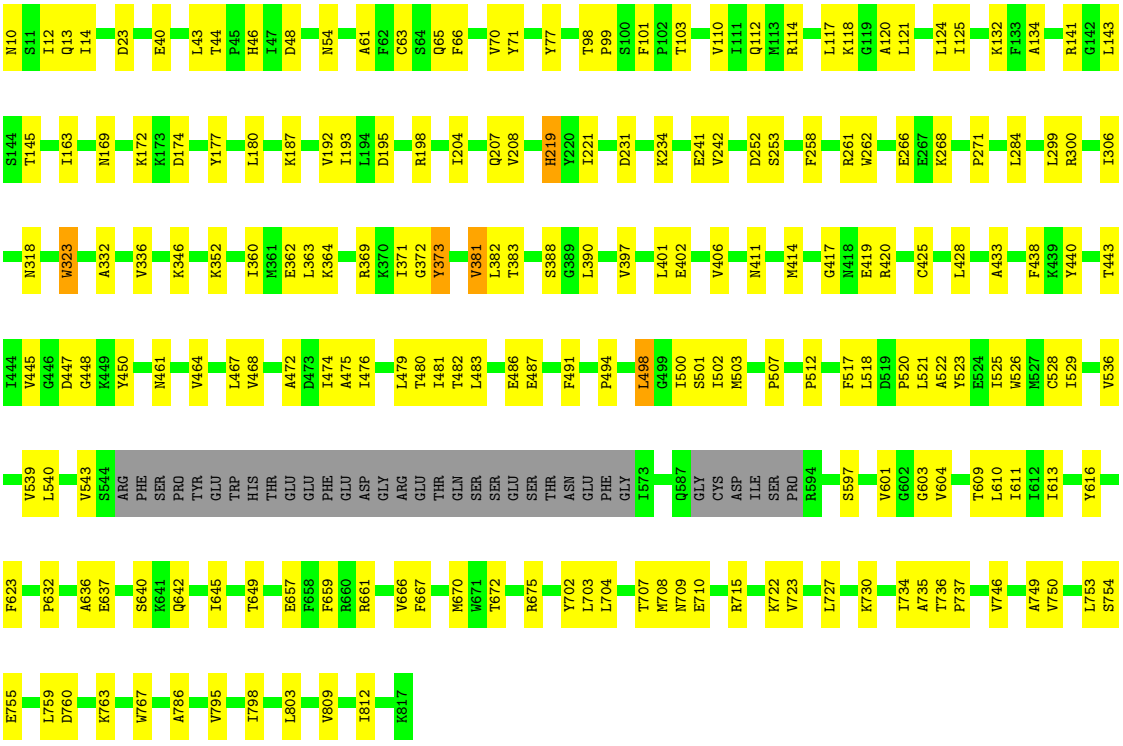
Chain B:





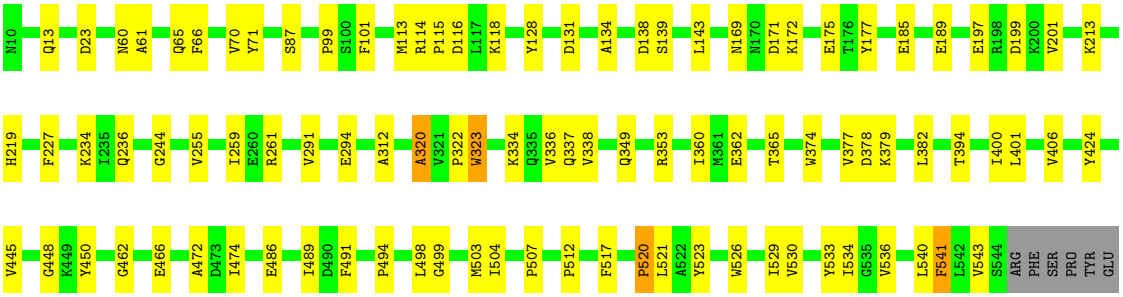
• Molecule 1: Glutamate receptor 2

Chain C:



• Molecule 1: Glutamate receptor 2

Chain D:




TRP HIS THR GLU GLU PHE GLU ASP GLY ARG GLU THR GLN SER SER GLU SER THR ASN GLU PHE GLY I573 S580 A583 F584 M585 Q586 Q587 GLY CYS ASP ILE SER PRO ARG S595 V604 W605 W606 F607 F608 T609 L610 I613 Y616 F623 L624 T625 V630 E634 S635
S640 I645 D651 M670 V683 K699 E705 S706 T707 M708 I712 T720 V723 K730 A735 T736 S754 L759 L762 K763 W767 E772 C773 K783 T784 L787 S790 V795 F796 Y797 I798 G802 L803 A806 M807 L808 V809
I812 Y816 LYS

4 Data and refinement statistics (i)

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) 99.6 (48.91-4.25)	Depositor EDS
R_{merge}	0.45	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.89 (at 4.29Å)	Xtriage
Refinement program	PHENIX (1.16_3549)	Depositor
R, R_{free}	0.260 , 0.296 0.262 , 0.294	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)	0.22 , 167.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.86	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.27	0/6031	0.43	0/8167
1	B	0.28	0/6073	0.45	1/8221 (0.0%)
1	C	0.26	0/6037	0.42	0/8180
1	D	0.28	0/6028	0.44	0/8165
All	All	0.27	0/24169	0.44	1/32733 (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

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	450	TYR	N-CA-C	5.12	124.82	111.00

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 (i)

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	135	0
1	B	5954	0	5844	156	1
1	C	5918	0	5758	141	1
1	D	5909	0	5755	108	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	489	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 10.

The worst 5 of 489 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 (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 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%)	29	68
1	B	766/808 (95%)	704 (92%)	58 (8%)	4 (0%)	29	68
1	C	768/808 (95%)	703 (92%)	58 (8%)	7 (1%)	17	56
1	D	766/808 (95%)	708 (92%)	54 (7%)	4 (0%)	29	68
All	All	3064/3232 (95%)	2821 (92%)	224 (7%)	19 (1%)	25	65

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 (i)

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%)	600 (98%)	13 (2%)	53	72
1	B	625/691 (90%)	600 (96%)	25 (4%)	31	57
1	C	609/691 (88%)	602 (99%)	7 (1%)	73	85
1	D	609/691 (88%)	595 (98%)	14 (2%)	50	70
All	All	2456/2764 (89%)	2397 (98%)	59 (2%)	49	69

5 of 59 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	447	ASP
1	D	772	GLU
1	B	541	PHE
1	D	635	SER
1	D	394	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	355	ASN
1	C	337	GLN
1	D	60	ASN
1	B	24	GLN
1	A	355	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 monosaccharides 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	0.71	0	16,16,16	1.11	1 (6%)
2	NAG	B	901	-	14,14,15	0.34	0	17,19,21	0.52	0
2	NAG	D	901	1	14,14,15	0.35	0	17,19,21	0.51	0
3	V8G	C	902	-	13,13,13	0.72	0	16,16,16	1.11	1 (6%)
2	NAG	A	901	-	14,14,15	0.48	0	17,19,21	0.50	0
2	NAG	C	901	-	14,14,15	0.29	0	17,19,21	0.59	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	B	901	-	-	0/6/23/26	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	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(^{o})	Ideal(^{o})
3	A	902	V8G	OAK-CAD-CAE	2.22	120.03	114.21
3	C	902	V8G	OAK-CAD-CAE	2.20	119.95	114.21
2	C	901	NAG	C1-O5-C5	2.02	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

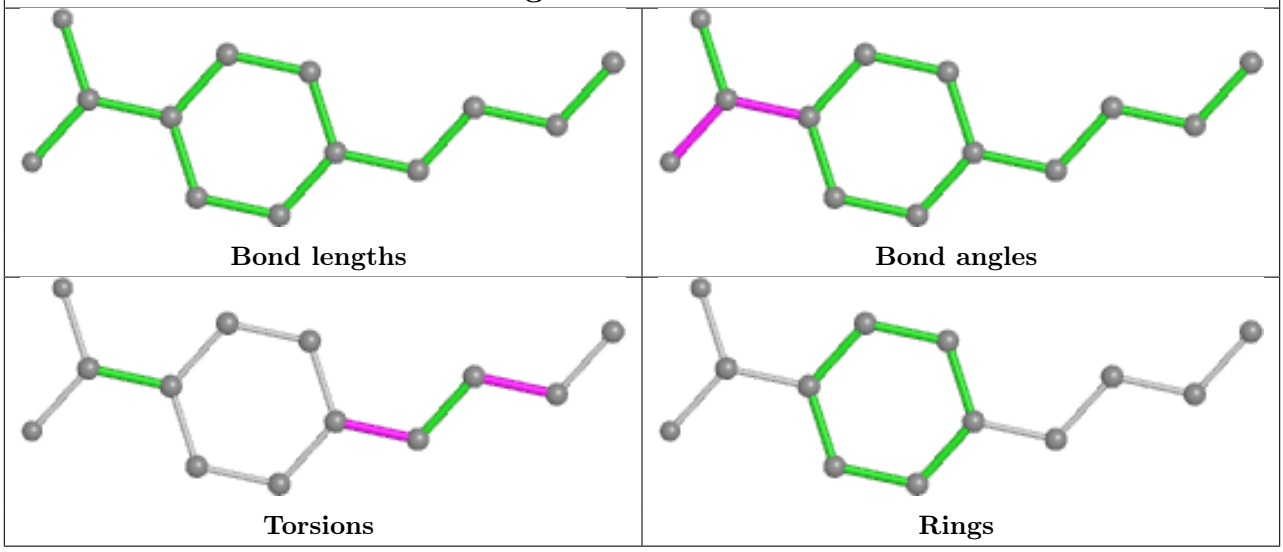
There are no ring outliers.

5 monomers are involved in 39 short contacts:

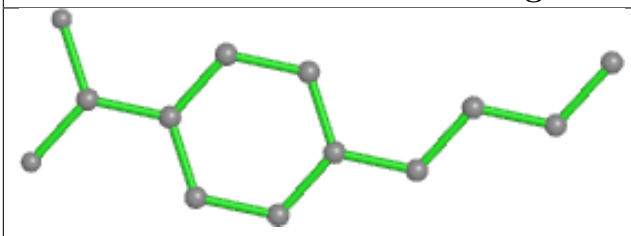
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	902	V8G	12	0
2	B	901	NAG	15	0
2	D	901	NAG	1	0
3	C	902	V8G	9	0
2	A	901	NAG	2	0

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 then 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.

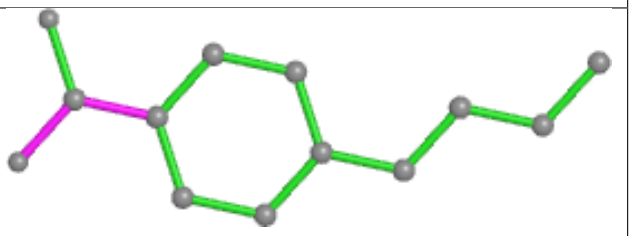
Ligand V8G A 902



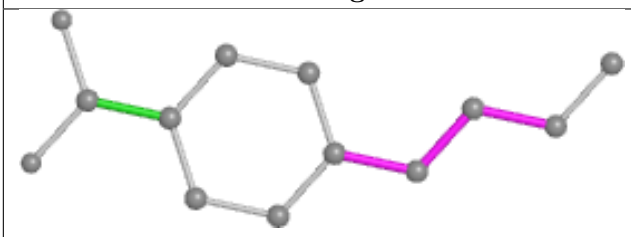
Ligand V8G C 902



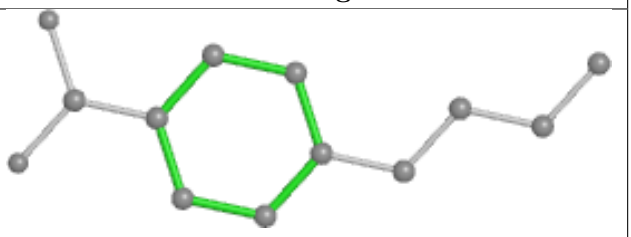
Bond lengths



Bond angles



Torsions



Rings

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.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

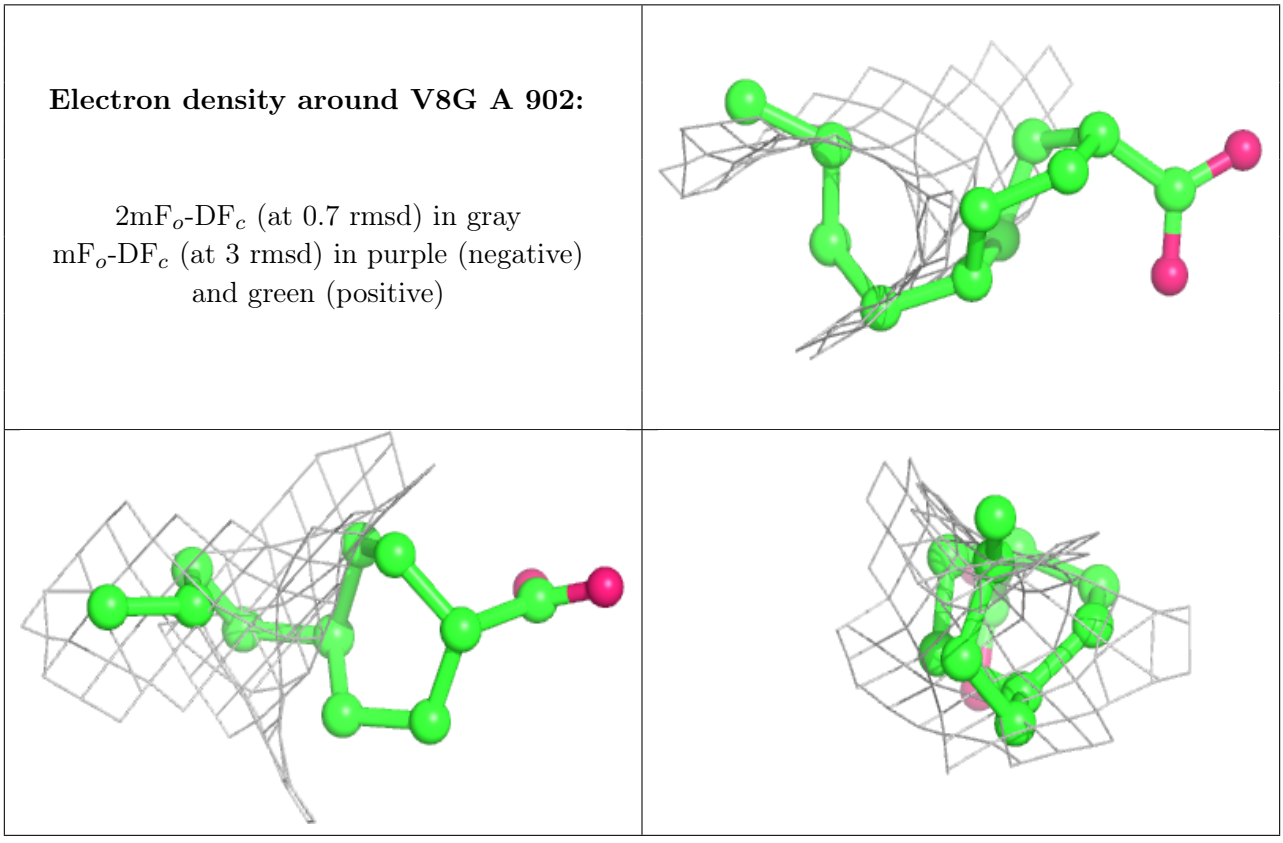
6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

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.

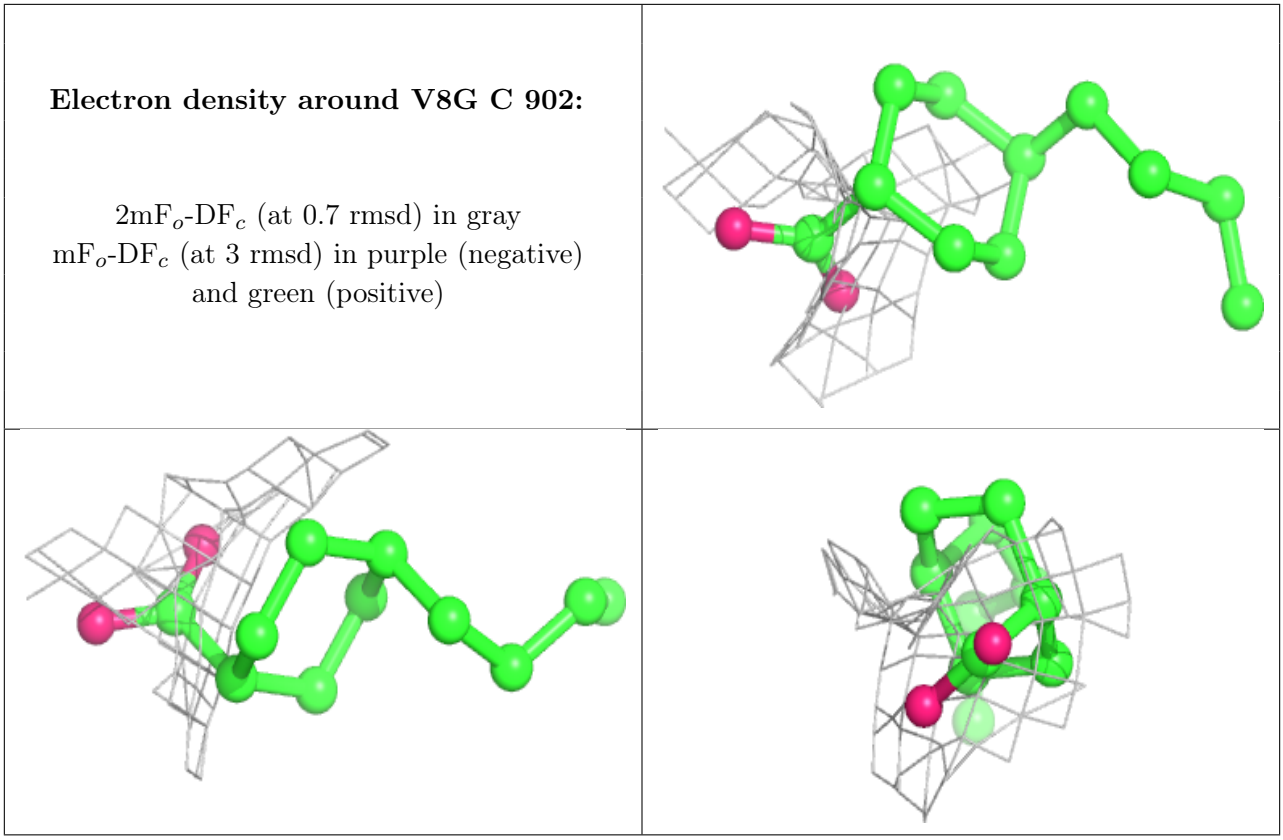
Electron density around V8G A 902:

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



Electron density around V8G C 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)

Unable to reproduce the depositors R factor - this section is therefore empty.