



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 17, 2023 – 02:53 PM EST

PDB ID : 4U5F  
Title : Crystal structure of GluA2, con-ikot-ikot snail toxin, partial agonist KA and positive modulator (R,R)-2b complex, GluA2cryst2 construct  
Authors : Chen, L.; Gouaux, E.  
Deposited on : 2014-07-24  
Resolution : 3.70 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.

The types of validation reports are described at

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

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The following versions of software and data (see [references ⓘ](#)) 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 : 2.36  
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) : 2.36

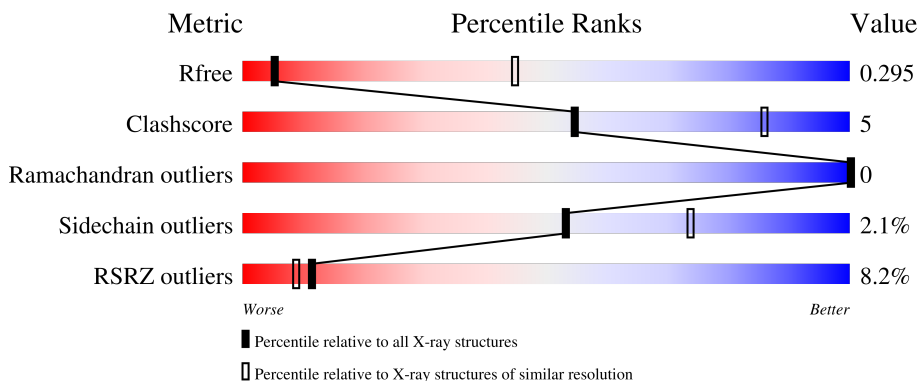
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.70 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	1049 (3.88-3.52)
Clashscore	141614	1027 (3.86-3.54)
Ramachandran outliers	138981	1069 (3.88-3.52)
Sidechain outliers	138945	1065 (3.88-3.52)
RSRZ outliers	127900	1578 (3.90-3.50)

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  $\geq 3$ , 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	814	<div style="display: flex; align-items: center;"> <div style="width: 7%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 78%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 11%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 10%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">7%      78%      11%      10%</p>
1	B	814	<div style="display: flex; align-items: center;"> <div style="width: 9%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 79%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 12%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 9%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">9%      79%      12%      9%</p>
1	C	814	<div style="display: flex; align-items: center;"> <div style="width: 7%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 80%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 11%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">7%      80%      11%      8%</p>
1	D	814	<div style="display: flex; align-items: center;"> <div style="width: 8%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 78%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 13%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 9%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">8%      78%      13%      9%</p>
2	E	90	<div style="display: flex; align-items: center;"> <div style="width: 0%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 71%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 23%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">%      71%      23%      6%</p>

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Mol	Chain	Length	Quality of chain
2	F	90	 <p>A horizontal bar chart showing the quality of chain. The bar is divided into four segments: a small red segment (2%), a large green segment (78%), a yellow segment (17%), and a small grey segment (6%).</p>

## 2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 23700 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
			Total	C	N	O	S			
1	A	735	5535	3562	903	1043	27	0	0	0
1	B	738	5618	3610	926	1055	27	0	0	0
1	C	747	5507	3531	908	1041	27	0	0	0
1	D	742	5578	3591	911	1049	27	0	0	0

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	184	GLY	LYS	engineered mutation	UNP P19491
A	237	GLU	ASN	engineered mutation	UNP P19491
A	?	-	LEU	deletion	UNP P19491
A	?	-	PRO	deletion	UNP P19491
A	385	ASP	ASN	engineered mutation	UNP P19491
A	392	GLN	ASN	engineered mutation	UNP P19491
A	?	-	ARG	deletion	UNP P19491
A	?	-	GLU	deletion	UNP P19491
A	?	-	THR	deletion	UNP P19491
A	?	-	GLN	deletion	UNP P19491
A	?	-	SER	deletion	UNP P19491
A	565	GLU	SER	engineered mutation	UNP P19491
A	589	ALA	CYS	engineered mutation	UNP P19491
A	815	ALA	CYS	engineered mutation	UNP P19491
A	818	ARG	SER	engineered mutation	UNP P19491
A	819	MET	ARG	engineered mutation	UNP P19491
A	820	LYS	ALA	engineered mutation	UNP P19491
A	821	LEU	GLU	engineered mutation	UNP P19491
A	822	VAL	ALA	engineered mutation	UNP P19491
A	823	PRO	LYS	engineered mutation	UNP P19491
A	?	-	MET	deletion	UNP P19491

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	LYS	deletion	UNP P19491
A	?	-	VAL	deletion	UNP P19491
B	184	GLY	LYS	engineered mutation	UNP P19491
B	237	GLU	ASN	engineered mutation	UNP P19491
B	?	-	LEU	deletion	UNP P19491
B	?	-	PRO	deletion	UNP P19491
B	385	ASP	ASN	engineered mutation	UNP P19491
B	392	GLN	ASN	engineered mutation	UNP P19491
B	?	-	ARG	deletion	UNP P19491
B	?	-	GLU	deletion	UNP P19491
B	?	-	THR	deletion	UNP P19491
B	?	-	GLN	deletion	UNP P19491
B	?	-	SER	deletion	UNP P19491
B	565	GLU	SER	engineered mutation	UNP P19491
B	589	ALA	CYS	engineered mutation	UNP P19491
B	815	ALA	CYS	engineered mutation	UNP P19491
B	818	ARG	SER	engineered mutation	UNP P19491
B	819	MET	ARG	engineered mutation	UNP P19491
B	820	LYS	ALA	engineered mutation	UNP P19491
B	821	LEU	GLU	engineered mutation	UNP P19491
B	822	VAL	ALA	engineered mutation	UNP P19491
B	823	PRO	LYS	engineered mutation	UNP P19491
B	?	-	MET	deletion	UNP P19491
B	?	-	LYS	deletion	UNP P19491
B	?	-	VAL	deletion	UNP P19491
C	184	GLY	LYS	engineered mutation	UNP P19491
C	237	GLU	ASN	engineered mutation	UNP P19491
C	?	-	LEU	deletion	UNP P19491
C	?	-	PRO	deletion	UNP P19491
C	385	ASP	ASN	engineered mutation	UNP P19491
C	392	GLN	ASN	engineered mutation	UNP P19491
C	?	-	ARG	deletion	UNP P19491
C	?	-	GLU	deletion	UNP P19491
C	?	-	THR	deletion	UNP P19491
C	?	-	GLN	deletion	UNP P19491
C	?	-	SER	deletion	UNP P19491
C	565	GLU	SER	engineered mutation	UNP P19491
C	589	ALA	CYS	engineered mutation	UNP P19491
C	815	ALA	CYS	engineered mutation	UNP P19491
C	818	ARG	SER	engineered mutation	UNP P19491
C	819	MET	ARG	engineered mutation	UNP P19491
C	820	LYS	ALA	engineered mutation	UNP P19491

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Chain	Residue	Modelled	Actual	Comment	Reference
C	821	LEU	GLU	engineered mutation	UNP P19491
C	822	VAL	ALA	engineered mutation	UNP P19491
C	823	PRO	LYS	engineered mutation	UNP P19491
C	?	-	MET	deletion	UNP P19491
C	?	-	LYS	deletion	UNP P19491
C	?	-	VAL	deletion	UNP P19491
D	184	GLY	LYS	engineered mutation	UNP P19491
D	237	GLU	ASN	engineered mutation	UNP P19491
D	?	-	LEU	deletion	UNP P19491
D	?	-	PRO	deletion	UNP P19491
D	385	ASP	ASN	engineered mutation	UNP P19491
D	392	GLN	ASN	engineered mutation	UNP P19491
D	?	-	ARG	deletion	UNP P19491
D	?	-	GLU	deletion	UNP P19491
D	?	-	THR	deletion	UNP P19491
D	?	-	GLN	deletion	UNP P19491
D	?	-	SER	deletion	UNP P19491
D	565	GLU	SER	engineered mutation	UNP P19491
D	589	ALA	CYS	engineered mutation	UNP P19491
D	815	ALA	CYS	engineered mutation	UNP P19491
D	818	ARG	SER	engineered mutation	UNP P19491
D	819	MET	ARG	engineered mutation	UNP P19491
D	820	LYS	ALA	engineered mutation	UNP P19491
D	821	LEU	GLU	engineered mutation	UNP P19491
D	822	VAL	ALA	engineered mutation	UNP P19491
D	823	PRO	LYS	engineered mutation	UNP P19491
D	?	-	MET	deletion	UNP P19491
D	?	-	LYS	deletion	UNP P19491
D	?	-	VAL	deletion	UNP P19491

- Molecule 2 is a protein called Con-ikot-ikot.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	85	Total	C	N	O	S	0	0	0
			641	387	113	125	16			
2	F	85	Total	C	N	O	S	0	0	0
			641	387	113	125	16			

There are 8 discrepancies between the modelled and reference sequences:

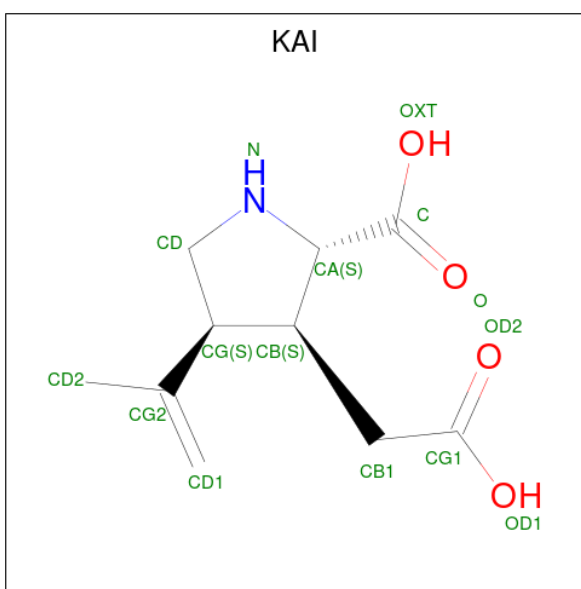
Chain	Residue	Modelled	Actual	Comment	Reference
E	-3	GLY	-	expression tag	UNP P0CB20

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-2	PRO	-	expression tag	UNP P0CB20
E	-1	GLY	-	expression tag	UNP P0CB20
E	0	SER	-	expression tag	UNP P0CB20
F	-3	GLY	-	expression tag	UNP P0CB20
F	-2	PRO	-	expression tag	UNP P0CB20
F	-1	GLY	-	expression tag	UNP P0CB20
F	0	SER	-	expression tag	UNP P0CB20

- Molecule 3 is 3-(CARBOXYMETHYL)-4-ISOPROPENYLPROLINE (three-letter code: KAI) (formula:  $C_{10}H_{15}NO_4$ ).



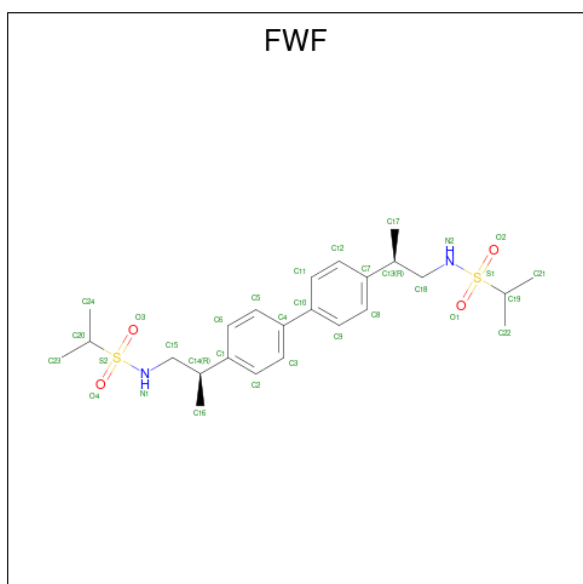
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	Total	C	N	O	0	0
			15	10	1	4		
3	B	1	Total	C	N	O	0	0
			15	10	1	4		
3	C	1	Total	C	N	O	0	0
			15	10	1	4		
3	D	1	Total	C	N	O	0	0
			15	10	1	4		

- 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
			Total	C	N	O		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is N,N'-[biphenyl-4,4'-diyl-di(2R)propane-2,1-diyl]dipropane-2-sulfonamide (three-letter code: FWF) (formula: C<sub>24</sub>H<sub>36</sub>N<sub>2</sub>O<sub>4</sub>S<sub>2</sub>).



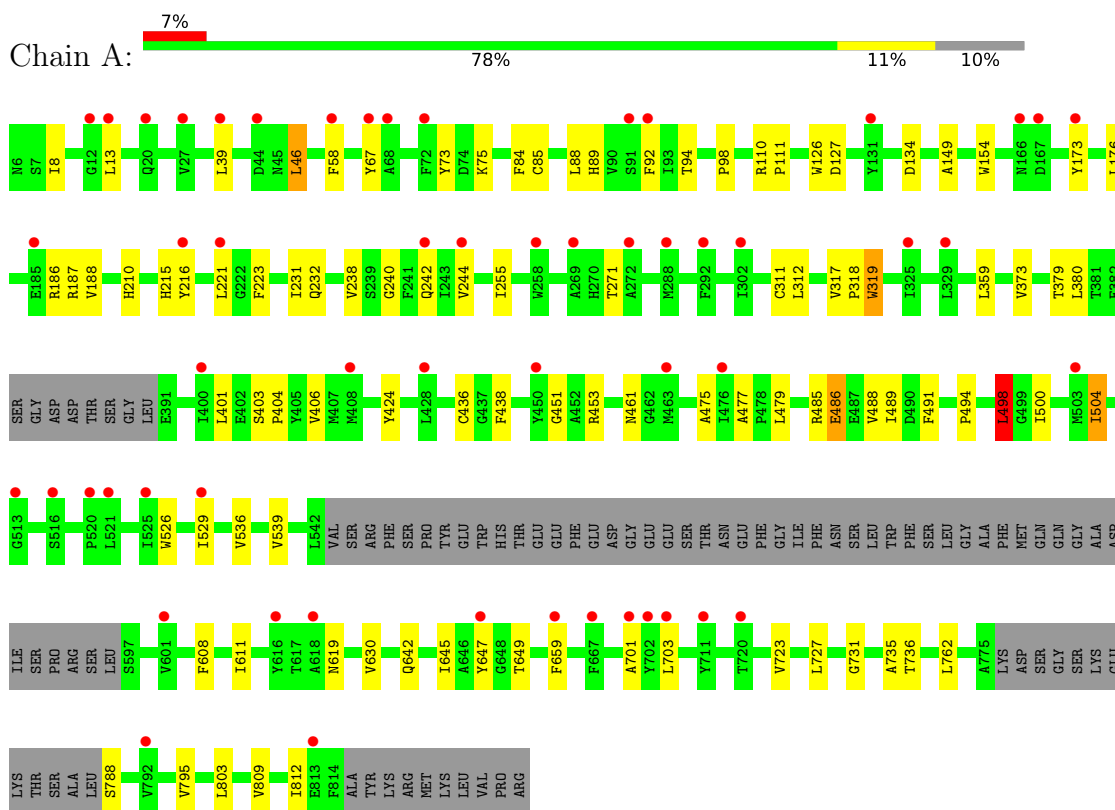


<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>					<b>ZeroOcc</b>	<b>AltConf</b>
5	B	1	Total	C	N	O	S	0	0
			32	24	2	4	2		
5	D	1	Total	C	N	O	S	0	0
			32	24	2	4	2		

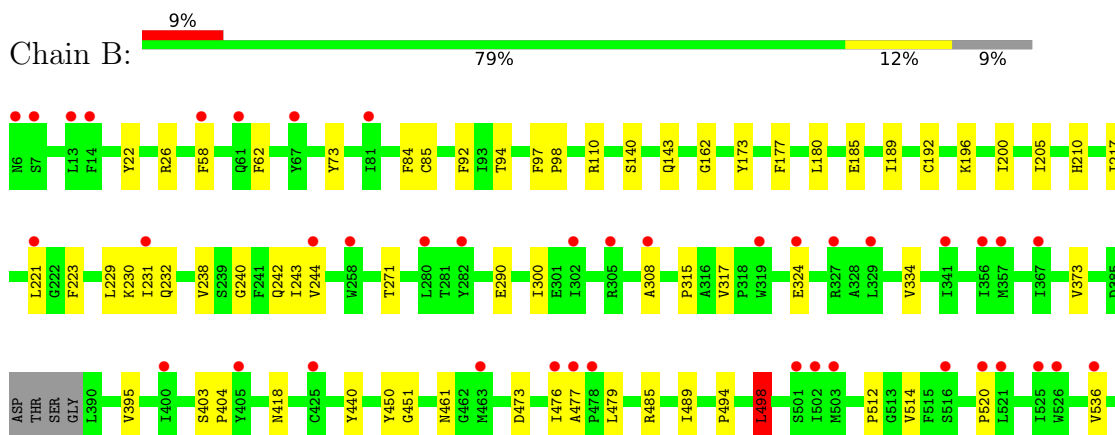
### 3 Residue-property plots [i](#)

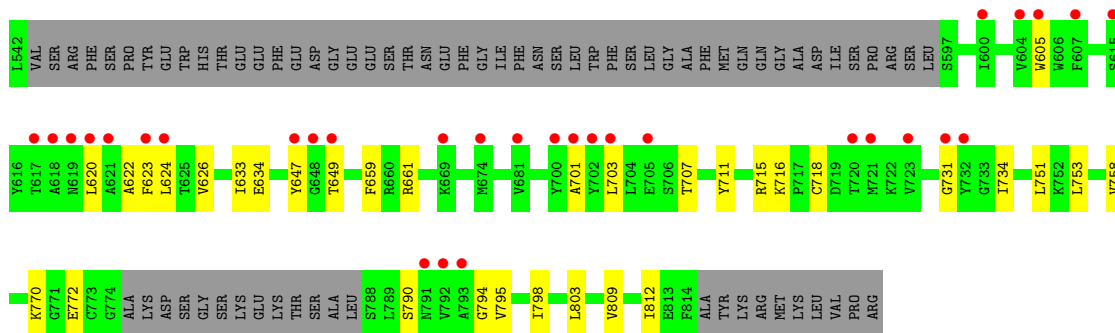
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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

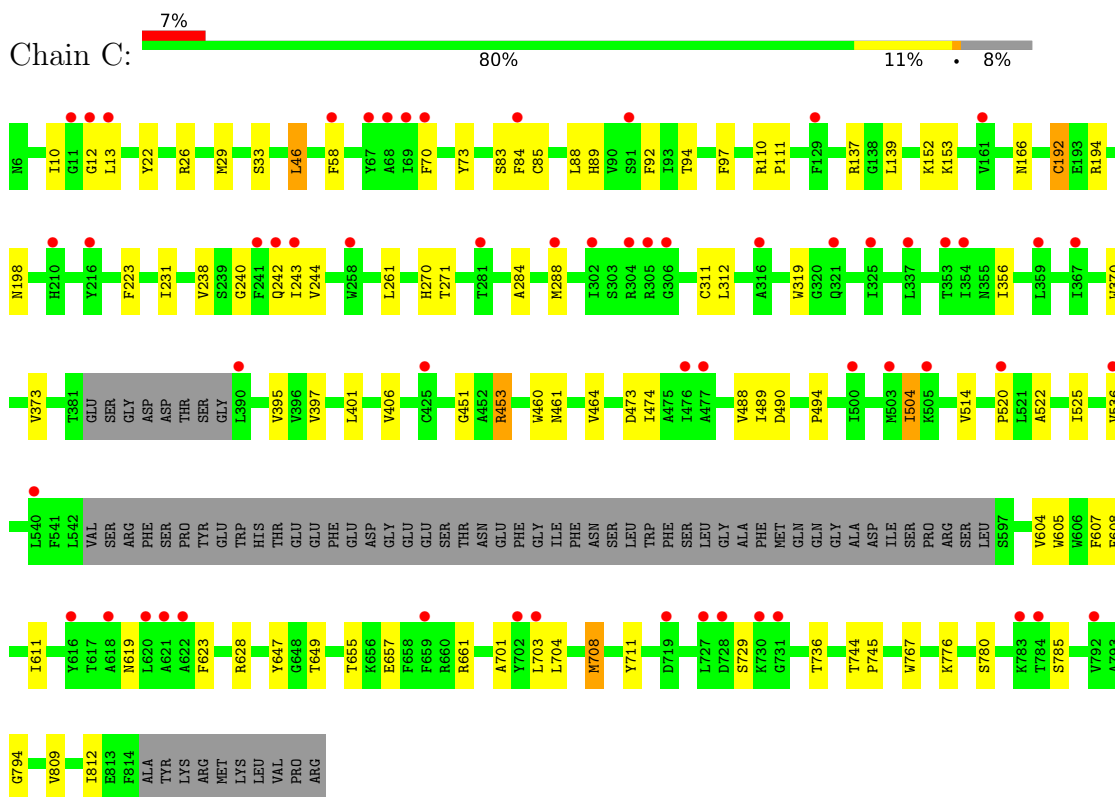


- Molecule 1: Glutamate receptor 2

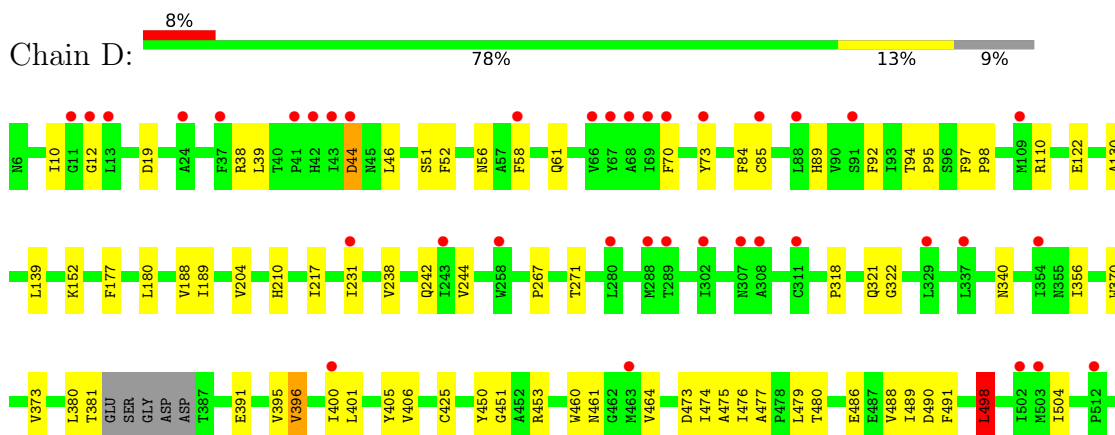


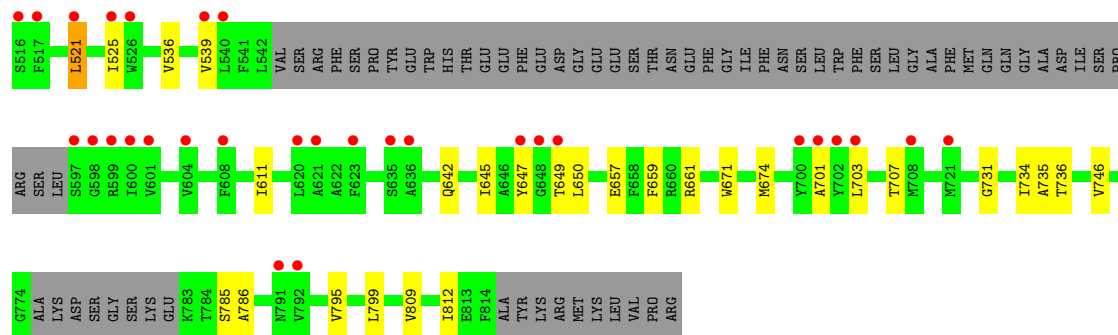


- Molecule 1: Glutamate receptor 2



- Molecule 1: Glutamate receptor 2

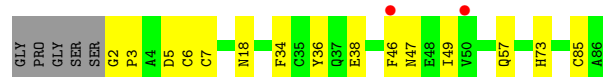
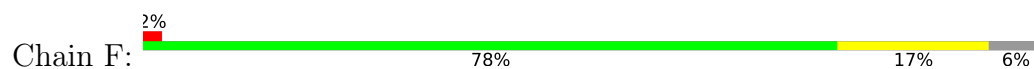




- Molecule 2: Con-ikot-ikot



- Molecule 2: Con-ikot-ikot



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	160.29Å 365.42Å 108.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 3.70 146.79 – 3.70	Depositor EDS
% Data completeness (in resolution range)	93.5 (19.99-3.70) 93.4 (146.79-3.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.14 (at 3.67Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, $R_{free}$	0.250 , 0.286 0.259 , 0.295	Depositor DCC
$R_{free}$ test set	3270 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	122.1	Xtrriage
Anisotropy	0.058	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.22 , 85.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.25$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	23700	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	175.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.79% 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.

## 5 Model quality [i](#)

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

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

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	0.23	0/5651	0.42	1/7684 (0.0%)
1	B	0.24	0/5734	0.42	1/7782 (0.0%)
1	C	0.23	0/5620	0.41	0/7653
1	D	0.24	0/5694	0.42	1/7746 (0.0%)
2	E	0.25	0/651	0.44	0/873
2	F	0.25	0/651	0.43	0/873
All	All	0.24	0/24001	0.42	3/32611 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	498	LEU	CA-CB-CG	5.29	127.46	115.30
1	A	498	LEU	CA-CB-CG	5.13	127.11	115.30
1	D	498	LEU	CA-CB-CG	5.12	127.09	115.30

There are no chirality outliers.

There are no planarity outliers.

### 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	5535	0	5296	57	0
1	B	5618	0	5428	58	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	5507	0	5175	59	0
1	D	5578	0	5336	66	0
2	E	641	0	593	14	0
2	F	641	0	593	11	0
3	A	15	0	13	1	0
3	B	15	0	13	2	0
3	C	15	0	13	2	0
3	D	15	0	13	1	0
4	A	14	0	13	0	0
4	B	14	0	13	0	0
4	C	14	0	13	0	0
4	D	14	0	13	1	0
5	B	32	0	36	4	0
5	D	32	0	36	1	0
All	All	23700	0	22597	240	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 5.

All (240) 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:C:611:ILE:HG21	1:D:795:VAL:HG21	1.69	0.74
1:A:232:GLN:HA	1:A:359:LEU:HD21	1.72	0.71
1:B:661:ARG:HG2	1:B:661:ARG:HH11	1.56	0.70
1:A:187:ARG:NH2	2:E:67:ASN:OD1	2.23	0.70
1:C:464:VAL:HG13	1:C:489:ILE:HD11	1.72	0.70
1:D:122:GLU:OE1	1:D:152:LYS:NZ	2.26	0.69
1:D:476:ILE:HG12	1:D:734:ILE:HD12	1.76	0.67
1:A:453:ARG:NH1	2:E:38:GLU:OE2	2.27	0.67
1:D:44:ASP:OD1	1:D:44:ASP:N	2.27	0.66
1:C:356:ILE:HD11	1:C:370:TRP:HB2	1.75	0.66
1:D:488:VAL:HG23	1:D:489:ILE:HG12	1.78	0.66
1:D:356:ILE:HD11	1:D:370:TRP:HB2	1.78	0.66
1:A:231:ILE:HD12	1:A:238:VAL:HG21	1.78	0.66
1:A:379:THR:HG22	1:A:380:LEU:H	1.62	0.63
1:C:312:LEU:O	1:D:56:ASN:ND2	2.28	0.63
1:D:231:ILE:HD12	1:D:238:VAL:HG21	1.80	0.63
1:A:536:VAL:HG22	1:B:803:LEU:HD21	1.81	0.62
1:D:486:GLU:HG2	1:D:491:PHE:HD2	1.64	0.62
1:B:162:GLY:HA2	1:B:196:LYS:HE2	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:901:FWF:N2	1:C:494:PRO:O	2.27	0.60
1:D:475:ALA:HB3	1:D:735:ALA:HB3	1.83	0.60
1:C:13:LEU:HD23	1:C:46:LEU:HD21	1.84	0.59
1:C:649:THR:HG22	1:C:703:LEU:HB2	1.85	0.58
1:A:611:ILE:HG12	1:B:795:VAL:HG11	1.86	0.57
1:D:657:GLU:OE1	1:D:661:ARG:NH1	2.37	0.57
1:A:494:PRO:O	5:D:901:FWF:N1	2.31	0.57
1:D:451:GLY:HA2	1:D:461:ASN:O	2.04	0.57
1:C:194:ARG:O	1:C:198:ASN:ND2	2.38	0.57
1:A:242:GLN:HE21	1:A:244:VAL:H	1.53	0.56
1:A:486:GLU:HG2	1:A:491:PHE:HD2	1.71	0.56
1:A:642:GLN:HE22	1:A:645:ILE:HB	1.71	0.56
1:A:649:THR:HG22	1:A:703:LEU:HB2	1.86	0.56
2:E:47:ASN:ND2	2:E:85:CYS:O	2.26	0.56
1:B:395:VAL:HG13	1:B:473:ASP:HB2	1.88	0.55
1:D:649:THR:HG22	1:D:703:LEU:HB2	1.88	0.55
2:E:80:SER:HB3	2:F:5:ASP:HB2	1.88	0.55
1:C:488:VAL:HG23	1:C:489:ILE:HG13	1.89	0.55
1:D:453:ARG:NH2	1:D:460:TRP:HE1	2.06	0.54
1:B:514:VAL:HG13	1:B:794:GLY:HA3	1.90	0.54
1:C:73:TYR:CE2	1:C:94:THR:HG21	2.43	0.54
1:B:649:THR:HG22	1:B:703:LEU:HB2	1.90	0.53
1:A:803:LEU:HB3	1:D:539:VAL:HG21	1.90	0.53
1:D:97:PHE:HA	1:D:110:ARG:HD2	1.90	0.53
1:A:795:VAL:HG21	1:D:611:ILE:HG21	1.89	0.53
1:A:803:LEU:HD21	1:D:536:VAL:HG22	1.91	0.53
1:A:126:TRP:CG	1:A:187:ARG:HD3	2.43	0.53
1:B:711:TYR:OH	1:B:715:ARG:NH1	2.42	0.53
5:B:901:FWF:H8	1:C:729:SER:HB2	1.91	0.53
1:A:88:LEU:HD11	1:A:311:CYS:HB2	1.90	0.53
1:C:231:ILE:HD12	1:C:238:VAL:HG21	1.91	0.53
1:D:489:ILE:HG22	1:D:490:ASP:H	1.74	0.52
1:B:494:PRO:O	5:B:901:FWF:N1	2.35	0.52
1:D:396:VAL:HG23	1:D:473:ASP:H	1.73	0.52
1:C:453:ARG:NH2	2:F:38:GLU:OE2	2.42	0.52
1:B:58:PHE:CE2	1:B:84:PHE:HB3	2.44	0.52
1:B:97:PHE:HA	1:B:110:ARG:HD2	1.90	0.52
1:B:221:LEU:HB3	1:B:243:ILE:HB	1.92	0.52
1:C:655:THR:OG1	3:C:901:KAI:OD2	2.22	0.51
2:E:5:ASP:HB3	2:E:8:ARG:HB3	1.93	0.51
1:C:401:LEU:HD23	1:C:406:VAL:HG12	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:204:VAL:HG12	1:D:210:HIS:HB3	1.92	0.51
1:C:522:ALA:HB3	1:C:525:ILE:HG13	1.92	0.51
2:E:21:LEU:HD21	2:E:32:VAL:HA	1.92	0.51
1:C:489:ILE:HG22	1:C:490:ASP:H	1.75	0.51
1:D:58:PHE:CE2	1:D:84:PHE:HB3	2.46	0.51
1:D:73:TYR:CE2	1:D:94:THR:HG21	2.46	0.51
1:C:704:LEU:HD12	1:C:708:MET:HB2	1.93	0.50
1:A:504:ILE:HD11	1:A:723:VAL:HG21	1.94	0.50
1:A:58:PHE:CE2	1:A:84:PHE:HB3	2.47	0.50
1:A:67:TYR:HD1	1:A:319:TRP:HH2	1.60	0.50
1:A:401:LEU:HD23	1:A:406:VAL:HG12	1.94	0.50
1:A:453:ARG:NH2	2:E:37:GLN:OE1	2.41	0.50
1:A:647:TYR:HB3	1:A:701:ALA:HB3	1.95	0.49
1:C:522:ALA:H	1:C:525:ILE:HD12	1.77	0.49
1:D:242:GLN:HE21	1:D:244:VAL:H	1.60	0.49
1:D:395:VAL:HG13	1:D:473:ASP:HB2	1.93	0.49
1:B:809:VAL:HA	1:B:812:ILE:HG12	1.94	0.49
1:B:140:SER:HA	1:B:143:GLN:HE21	1.77	0.49
1:B:477:ALA:O	1:B:479:LEU:N	2.45	0.49
1:B:73:TYR:CE2	1:B:94:THR:HG21	2.48	0.49
1:C:261:LEU:O	1:C:270:HIS:ND1	2.45	0.48
1:C:139:LEU:HD12	1:D:139:LEU:HD12	1.96	0.48
1:B:498:LEU:HD13	1:B:731:GLY:HA2	1.95	0.48
1:C:488:VAL:HG12	2:F:34:PHE:HD2	1.79	0.48
1:A:424:TYR:CE2	1:A:762:LEU:HB3	2.49	0.48
1:D:474:ILE:HG13	1:D:736:THR:HG22	1.95	0.48
1:C:514:VAL:HG13	1:C:794:GLY:HA3	1.95	0.48
1:B:85:CYS:SG	1:B:92:PHE:HB2	2.53	0.48
1:D:659:PHE:CE2	1:D:703:LEU:HD13	2.49	0.48
1:C:88:LEU:HD11	1:C:311:CYS:HB2	1.96	0.48
2:F:36:TYR:CG	2:F:57:GLN:HG3	2.48	0.47
1:B:223:PHE:CD1	1:B:240:GLY:HA3	2.48	0.47
1:C:647:TYR:HB3	1:C:701:ALA:HB3	1.95	0.47
1:D:642:GLN:HE22	1:D:645:ILE:HB	1.79	0.47
1:D:809:VAL:HA	1:D:812:ILE:HG12	1.97	0.47
1:C:152:LYS:HG3	1:C:153:LYS:H	1.79	0.47
1:A:13:LEU:HD23	1:A:46:LEU:HD21	1.97	0.47
1:A:608:PHE:O	1:A:611:ILE:HG13	2.14	0.47
1:B:315:PRO:HB2	1:B:317:VAL:O	2.15	0.47
1:B:622:ALA:O	1:B:626:VAL:HG23	2.14	0.47
1:C:619:ASN:HD21	1:D:786:ALA:HB3	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:451:GLY:HA2	1:A:461:ASN:O	2.14	0.47
2:E:36:TYR:CG	2:E:57:GLN:HG3	2.50	0.47
1:D:477:ALA:O	1:D:479:LEU:N	2.45	0.47
1:B:177:PHE:HA	1:B:180:LEU:HB2	1.97	0.47
1:D:189:ILE:HG12	1:D:217:ILE:HB	1.96	0.47
2:F:18:ASN:HB2	2:F:73:HIS:CE1	2.50	0.46
1:A:73:TYR:CE2	1:A:94:THR:HG21	2.50	0.46
1:C:284:ALA:O	1:C:288:MET:HG3	2.15	0.46
1:C:223:PHE:CD1	1:C:240:GLY:HA3	2.50	0.46
2:E:83:ASN:ND2	2:E:85:CYS:SG	2.86	0.46
1:B:315:PRO:C	1:B:317:VAL:H	2.19	0.46
1:B:22:TYR:CE2	1:B:26:ARG:HD2	2.51	0.46
1:D:98:PRO:HD3	1:D:110:ARG:HD2	1.98	0.46
1:A:111:PRO:HD2	1:A:221:LEU:HD11	1.98	0.46
1:D:318:PRO:HG2	1:D:321:GLN:HG2	1.96	0.46
1:D:400:ILE:HG21	1:D:450:TYR:CZ	2.50	0.46
2:F:36:TYR:CE1	2:F:57:GLN:HB2	2.51	0.46
1:C:628:ARG:NH1	1:C:785:SER:O	2.49	0.45
1:A:485:ARG:O	1:A:489:ILE:HG13	2.15	0.45
1:C:657:GLU:O	1:C:661:ARG:HG3	2.15	0.45
2:E:58:MET:O	2:E:62:ARG:HG2	2.16	0.45
1:A:134:ASP:N	1:A:134:ASP:OD1	2.50	0.45
1:A:317:VAL:HA	1:A:318:PRO:HD3	1.81	0.45
1:A:475:ALA:HB3	1:A:735:ALA:HB3	1.98	0.45
1:B:62:PHE:CZ	1:B:308:ALA:HB1	2.52	0.45
1:B:536:VAL:HG21	1:B:605:TRP:CE3	2.52	0.45
1:B:716:LYS:HA	1:B:718:CYS:H	1.82	0.45
1:D:340:ASN:ND2	4:D:903:NAG:O5	2.50	0.45
1:C:22:TYR:CE2	1:C:26:ARG:HD2	2.51	0.45
1:C:520:PRO:O	1:C:619:ASN:ND2	2.49	0.45
1:D:401:LEU:HD23	1:D:406:VAL:HG12	1.97	0.45
1:A:126:TRP:CD2	1:A:187:ARG:HD3	2.52	0.45
1:A:216:TYR:HB2	1:A:238:VAL:HG22	1.99	0.45
1:B:498:LEU:HB3	1:B:707:THR:HG23	1.99	0.45
1:A:539:VAL:HG21	1:B:803:LEU:HB3	1.98	0.45
1:D:130:ALA:HB3	1:D:188:VAL:HG22	1.99	0.44
1:A:488:VAL:HG12	2:E:34:PHE:HD2	1.82	0.44
1:D:177:PHE:HA	1:D:180:LEU:HB2	1.99	0.44
1:B:242:GLN:HE21	1:B:244:VAL:H	1.65	0.44
1:B:290:GLU:HG3	1:B:334:VAL:HG11	1.99	0.44
1:B:647:TYR:HB3	1:B:701:ALA:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:10:ILE:HD13	1:D:39:LEU:HD23	2.00	0.44
1:D:85:CYS:SG	1:D:92:PHE:HB2	2.58	0.44
1:D:734:ILE:HG21	1:D:746:VAL:HG11	1.99	0.44
1:D:498:LEU:HD13	1:D:731:GLY:HA2	1.98	0.44
2:F:47:ASN:ND2	2:F:85:CYS:O	2.47	0.44
1:A:500:ILE:HB	1:A:727:LEU:HB2	2.00	0.44
1:C:84:PHE:CE1	1:D:52:PHE:HA	2.53	0.44
1:B:173:TYR:HE1	1:B:200:ILE:HG12	1.83	0.44
1:B:451:GLY:HA2	1:B:461:ASN:O	2.18	0.44
1:D:89:HIS:HB3	1:D:322:GLY:HA3	1.99	0.44
1:D:498:LEU:HB3	1:D:707:THR:HG23	2.00	0.44
1:B:300:ILE:HG21	1:B:324:GLU:HG2	1.99	0.44
1:C:242:GLN:HE21	1:C:244:VAL:H	1.66	0.44
1:C:623:PHE:CZ	1:D:785:SER:HA	2.52	0.44
1:B:520:PRO:HG2	1:B:620:LEU:HD13	2.00	0.43
1:A:223:PHE:CD1	1:A:240:GLY:HA3	2.54	0.43
3:C:901:KAI:HD2	3:C:901:KAI:HD12	1.70	0.43
1:A:611:ILE:HD13	1:B:795:VAL:HG21	2.01	0.43
1:A:788:SER:O	1:D:525:ILE:HD11	2.18	0.43
1:B:485:ARG:O	1:B:489:ILE:HG13	2.18	0.43
1:D:521:LEU:HG	1:D:525:ILE:HD12	2.00	0.43
1:A:8:ILE:HB	1:A:39:LEU:HD23	2.00	0.43
1:B:418:ASN:ND2	1:B:440:TYR:O	2.50	0.43
1:D:19:ASP:HB3	1:D:267:PRO:HB2	2.01	0.43
1:A:403:SER:HA	1:A:404:PRO:HA	1.72	0.43
1:D:405:TYR:HB3	1:D:425:CYS:SG	2.59	0.43
1:D:650:LEU:HD13	3:D:902:KAI:HD23	1.99	0.43
1:B:450:TYR:CE2	3:B:902:KAI:HD1	2.53	0.43
1:C:711:TYR:HB2	1:C:767:TRP:NE1	2.34	0.43
1:B:98:PRO:HD3	1:B:110:ARG:HD2	2.00	0.43
1:B:403:SER:HA	1:B:404:PRO:HA	1.75	0.43
1:A:98:PRO:HD3	1:A:110:ARG:HD2	2.00	0.43
1:B:210:HIS:HE1	1:D:210:HIS:HE1	1.67	0.43
1:C:97:PHE:HA	1:C:110:ARG:HD2	2.00	0.43
1:A:477:ALA:O	1:A:479:LEU:N	2.49	0.42
1:C:604:VAL:HG12	1:D:799:LEU:HD12	2.00	0.42
1:D:460:TRP:NE1	1:D:488:VAL:HG11	2.34	0.42
1:B:661:ARG:HG2	1:B:661:ARG:NH1	2.29	0.42
1:C:83:SER:HB3	1:D:51:SER:HB2	2.00	0.42
1:A:186:ARG:O	1:A:188:VAL:HG23	2.18	0.42
1:D:671:TRP:HA	1:D:674:MET:HE2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:ALA:HA	1:A:154:TRP:HB2	2.01	0.42
1:B:189:ILE:HG12	1:B:217:ILE:HB	2.01	0.42
1:B:659:PHE:CE2	1:B:703:LEU:HD13	2.54	0.42
2:E:80:SER:HB2	2:F:3:PRO:HG2	2.01	0.42
2:F:6:CYS:HB3	2:F:46:PHE:HE2	1.83	0.42
1:C:243:ILE:HG23	1:C:244:VAL:HG23	2.01	0.42
1:B:229:LEU:HD23	1:B:232:GLN:OE1	2.20	0.42
1:C:58:PHE:CE2	1:C:84:PHE:HB3	2.54	0.42
1:C:809:VAL:HA	1:C:812:ILE:HG12	2.00	0.42
1:A:489:ILE:HD13	1:A:735:ALA:HB1	2.01	0.42
1:C:474:ILE:HG13	1:C:736:THR:HG22	2.01	0.42
1:D:464:VAL:HG13	1:D:489:ILE:HG13	2.02	0.42
1:D:647:TYR:HB3	1:D:701:ALA:HB3	2.02	0.42
2:E:13:CYS:HB2	2:E:52:CYS:HB2	1.90	0.42
1:B:753:LEU:HD22	1:B:758:VAL:HG11	2.02	0.42
1:A:436:CYS:HB2	1:A:438:PHE:CE2	2.55	0.42
2:F:2:GLY:HA2	2:F:3:PRO:HD3	1.90	0.42
1:A:173:TYR:HA	1:A:176:LEU:HB3	2.02	0.42
1:A:809:VAL:HA	1:A:812:ILE:HG12	2.01	0.42
3:A:901:KAI:HD12	3:A:901:KAI:HD2	1.71	0.42
1:C:395:VAL:HG13	1:C:473:ASP:HB2	2.02	0.42
1:C:451:GLY:HA2	1:C:461:ASN:O	2.20	0.42
2:E:26:GLY:H	2:E:28:GLU:CD	2.23	0.42
1:A:619:ASN:HA	1:B:624:LEU:HD13	2.01	0.41
1:A:526:TRP:O	1:A:529:ILE:HG22	2.20	0.41
1:B:205:ILE:CD1	1:B:230:LYS:HB3	2.50	0.41
1:A:85:CYS:SG	1:A:92:PHE:HB2	2.61	0.41
1:A:127:ASP:OD1	1:A:127:ASP:N	2.53	0.41
1:B:795:VAL:HA	1:B:798:ILE:HG22	2.02	0.41
3:B:902:KAI:HD2	3:B:902:KAI:HD12	1.69	0.41
1:C:85:CYS:SG	1:C:92:PHE:HB2	2.60	0.41
1:B:476:ILE:HG12	1:B:734:ILE:HG23	2.02	0.41
1:B:751:LEU:HA	5:B:901:FWF:H34	2.01	0.41
1:C:137:ARG:HH22	1:C:192:CYS:C	2.24	0.41
1:C:536:VAL:HG21	1:C:605:TRP:CE3	2.55	0.41
1:C:460:TRP:CE2	1:C:488:VAL:HG11	2.56	0.41
1:B:231:ILE:HD12	1:B:238:VAL:HG21	2.02	0.41
1:B:716:LYS:HA	1:B:718:CYS:N	2.35	0.41
1:C:110:ARG:HA	1:C:111:PRO:HD3	1.85	0.41
1:C:504:ILE:HD13	1:C:504:ILE:H	1.85	0.41
1:C:607:PHE:O	1:C:611:ILE:HG12	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:642:GLN:OE1	1:D:645:ILE:N	2.37	0.41
1:A:659:PHE:CE2	1:A:703:LEU:HD13	2.56	0.41
1:B:770:LYS:HE2	1:B:770:LYS:HB3	1.84	0.41
1:C:608:PHE:CD1	1:D:799:LEU:HD22	2.56	0.41
1:C:776:LYS:O	1:C:780:SER:N	2.52	0.41
1:D:12:GLY:HA2	1:D:70:PHE:O	2.21	0.41
1:D:380:LEU:HG	1:D:381:THR:HG23	2.03	0.41
1:D:44:ASP:OD1	1:D:61:GLN:NE2	2.54	0.40
1:B:512:PRO:HB2	1:B:790:SER:HB2	2.03	0.40
1:C:12:GLY:HA2	1:C:70:PHE:O	2.21	0.40
1:C:744:THR:HB	1:C:745:PRO:HD3	2.03	0.40
1:D:94:THR:HA	1:D:95:PRO:HD3	1.90	0.40
1:B:205:ILE:HG23	1:B:210:HIS:CE1	2.56	0.40
1:C:29:MET:O	1:C:33:SER:HB3	2.22	0.40
1:C:661:ARG:NH2	2:F:49:ILE:HA	2.36	0.40
1:A:498:LEU:HD13	1:A:731:GLY:HA2	2.03	0.40

There are no symmetry-related clashes.

## 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	727/814 (89%)	705 (97%)	22 (3%)	0	100	100
1	B	730/814 (90%)	712 (98%)	18 (2%)	0	100	100
1	C	741/814 (91%)	720 (97%)	21 (3%)	0	100	100
1	D	734/814 (90%)	711 (97%)	23 (3%)	0	100	100
2	E	83/90 (92%)	79 (95%)	4 (5%)	0	100	100
2	F	83/90 (92%)	80 (96%)	3 (4%)	0	100	100
All	All	3098/3436 (90%)	3007 (97%)	91 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	561/693 (81%)	546 (97%)	15 (3%)	44	68
1	B	576/693 (83%)	567 (98%)	9 (2%)	62	80
1	C	541/693 (78%)	529 (98%)	12 (2%)	52	72
1	D	564/693 (81%)	553 (98%)	11 (2%)	55	74
2	E	73/76 (96%)	72 (99%)	1 (1%)	67	82
2	F	73/76 (96%)	72 (99%)	1 (1%)	67	82
All	All	2388/2924 (82%)	2339 (98%)	49 (2%)	53	74

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	LEU
1	A	75	LYS
1	A	89	HIS
1	A	210	HIS
1	A	215	HIS
1	A	255	ILE
1	A	271	THR
1	A	312	LEU
1	A	319	TRP
1	A	373	VAL
1	A	486	GLU
1	A	498	LEU
1	A	504	ILE
1	A	630	VAL
1	A	736	THR
1	B	185	GLU
1	B	192	CYS
1	B	271	THR
1	B	373	VAL

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Mol	Chain	Res	Type
1	B	498	LEU
1	B	623	PHE
1	B	633	ILE
1	B	634	GLU
1	B	772	GLU
1	C	10	ILE
1	C	46	LEU
1	C	89	HIS
1	C	166	ASN
1	C	192	CYS
1	C	271	THR
1	C	319	TRP
1	C	373	VAL
1	C	397	VAL
1	C	453	ARG
1	C	504	ILE
1	C	708	MET
1	D	38	ARG
1	D	44	ASP
1	D	46	LEU
1	D	271	THR
1	D	373	VAL
1	D	391	GLU
1	D	396	VAL
1	D	480	THR
1	D	498	LEU
1	D	504	ILE
1	D	521	LEU
2	E	23	ARG
2	F	7	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	619	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](#)

10 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
4	NAG	C	902	1	14,14,15	0.24	0	17,19,21	0.45	0
3	KAI	C	901	-	13,15,15	1.05	0	14,21,21	0.95	0
3	KAI	B	902	-	13,15,15	1.01	0	14,21,21	0.90	0
5	FWF	B	901	-	31,33,33	1.45	2 (6%)	38,48,48	2.90	3 (7%)
4	NAG	A	902	1	14,14,15	0.45	0	17,19,21	0.60	0
3	KAI	D	902	-	13,15,15	1.12	1 (7%)	14,21,21	0.94	0
4	NAG	B	903	1	14,14,15	0.29	0	17,19,21	0.37	0
3	KAI	A	901	-	13,15,15	1.05	0	14,21,21	0.85	0
5	FWF	D	901	-	31,33,33	1.44	2 (6%)	38,48,48	3.24	4 (10%)
4	NAG	D	903	1	14,14,15	0.37	0	17,19,21	0.62	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
4	NAG	C	902	1	-	0/6/23/26	0/1/1/1
3	KAI	C	901	-	-	2/12/25/25	0/1/1/1
3	KAI	B	902	-	-	2/12/25/25	0/1/1/1
5	FWF	B	901	-	-	7/32/36/36	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	902	1	-	2/6/23/26	0/1/1/1
3	KAI	D	902	-	-	2/12/25/25	0/1/1/1
4	NAG	B	903	1	-	2/6/23/26	0/1/1/1
3	KAI	A	901	-	-	0/12/25/25	0/1/1/1
5	FWF	D	901	-	-	2/32/36/36	0/2/2/2
4	NAG	D	903	1	-	2/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	901	FWF	C19-S1	-5.59	1.66	1.78
5	B	901	FWF	C19-S1	-5.58	1.66	1.78
5	B	901	FWF	C20-S2	-5.46	1.66	1.78
5	D	901	FWF	C20-S2	-5.34	1.67	1.78
3	D	902	KAI	CB-CA	-2.05	1.51	1.54

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	901	FWF	O2-S1-O1	-13.58	109.05	119.24
5	D	901	FWF	O4-S2-O3	-13.20	109.34	119.24
5	B	901	FWF	O4-S2-O3	-12.65	109.75	119.24
5	B	901	FWF	O2-S1-O1	-11.18	110.85	119.24
5	D	901	FWF	O1-S1-N2	2.68	111.00	107.76
5	B	901	FWF	O4-S2-N1	2.32	110.56	107.76
5	D	901	FWF	O4-S2-N1	2.24	110.46	107.76

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	901	FWF	C22-C19-S1-O1
4	B	903	NAG	C4-C5-C6-O6
4	B	903	NAG	O5-C5-C6-O6
4	A	902	NAG	C4-C5-C6-O6
4	A	902	NAG	O5-C5-C6-O6
4	D	903	NAG	C4-C5-C6-O6
5	D	901	FWF	C18-C13-C7-C12
4	D	903	NAG	O5-C5-C6-O6
5	B	901	FWF	C21-C19-S1-O1

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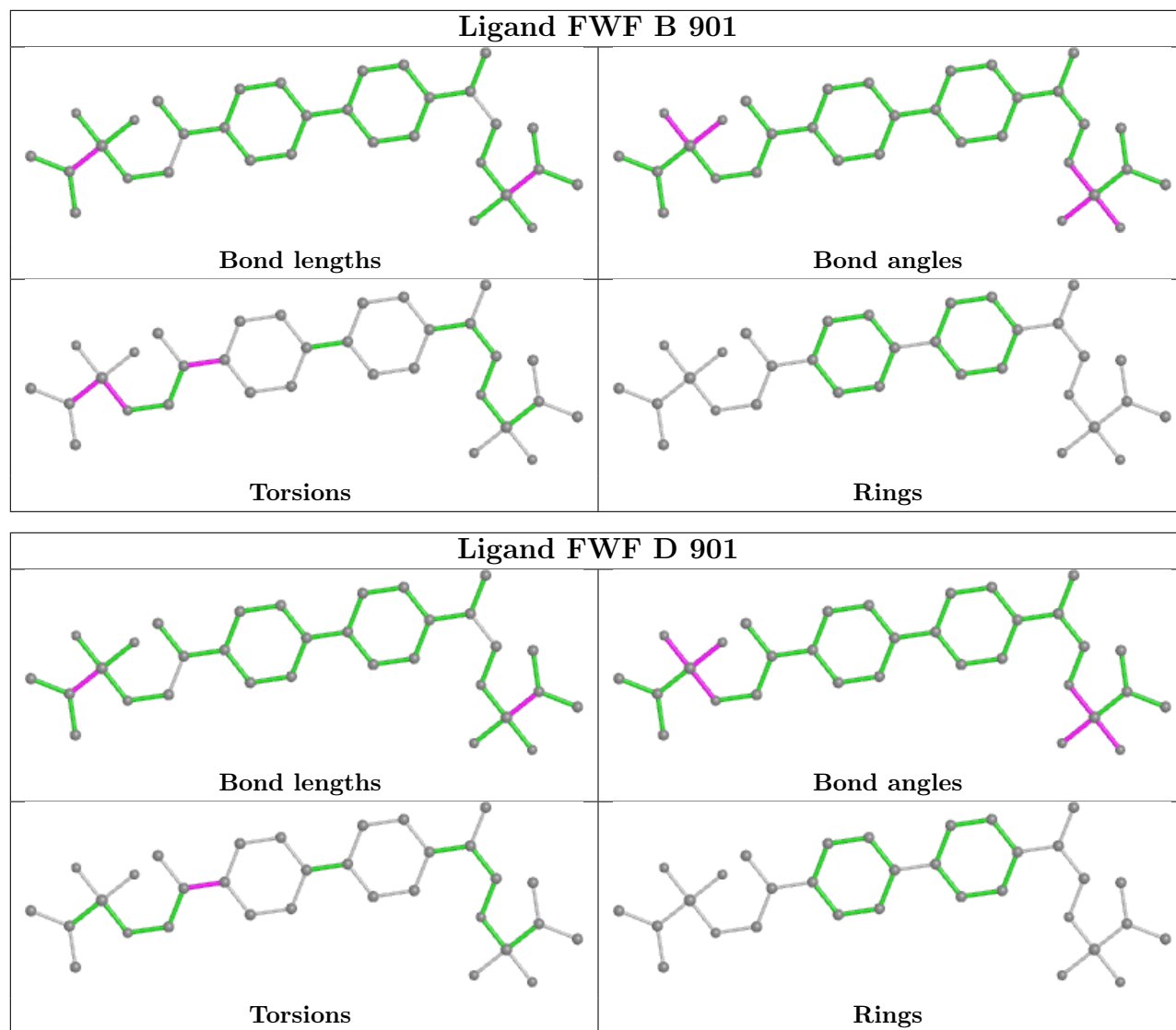
Mol	Chain	Res	Type	Atoms
5	B	901	FWF	C21-C19-S1-O2
3	C	901	KAI	O-C-CA-N
3	C	901	KAI	OXT-C-CA-N
3	D	902	KAI	OXT-C-CA-N
5	D	901	FWF	C18-C13-C7-C8
3	B	902	KAI	CB-CB1-CG1-OD1
3	B	902	KAI	CB-CB1-CG1-OD2
5	B	901	FWF	C18-N2-S1-C19
3	D	902	KAI	O-C-CA-N
5	B	901	FWF	C18-C13-C7-C8
5	B	901	FWF	C18-C13-C7-C12
5	B	901	FWF	C22-C19-S1-O2

There are no ring outliers.

7 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	901	KAI	2	0
3	B	902	KAI	2	0
5	B	901	FWF	4	0
3	D	902	KAI	1	0
3	A	901	KAI	1	0
5	D	901	FWF	1	0
4	D	903	NAG	1	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

### 6.1 Protein, DNA and RNA chains

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	735/814 (90%)	0.46	55 (7%) 14 10	90, 162, 261, 344	0
1	B	738/814 (90%)	0.52	72 (9%) 7 6	100, 169, 267, 342	0
1	C	747/814 (91%)	0.42	58 (7%) 13 9	110, 186, 277, 329	0
1	D	742/814 (91%)	0.52	68 (9%) 9 6	85, 164, 256, 325	0
2	E	85/90 (94%)	0.30	1 (1%) 79 69	110, 141, 185, 254	0
2	F	85/90 (94%)	0.41	2 (2%) 59 47	127, 159, 209, 246	0
All	All	3132/3436 (91%)	0.47	256 (8%) 11 9	85, 169, 264, 344	0

All (256) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	68	ALA	8.0
1	B	791	ASN	6.9
1	D	12	GLY	6.9
1	C	390	LEU	6.2
1	A	167	ASP	6.0
1	C	67	TYR	5.9
1	C	618	ALA	5.7
1	A	792	VAL	5.3
1	D	68	ALA	5.2
1	B	702	TYR	5.2
1	D	11	GLY	5.1
1	C	91	SER	5.0
1	D	621	ALA	4.9
1	C	305	ARG	4.8
1	B	792	VAL	4.8
1	A	67	TYR	4.8
1	D	792	VAL	4.7
1	A	520	PRO	4.7
1	D	516	SER	4.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	D	597	SER	4.6
1	D	702	TYR	4.5
1	B	305	ARG	4.4
1	C	731	GLY	4.4
1	C	302	ILE	4.2
1	D	525	ILE	4.1
1	D	791	ASN	4.1
1	D	620	LEU	4.1
1	D	601	VAL	4.1
1	B	67	TYR	4.1
1	B	700	TYR	3.9
1	D	648	GLY	3.9
1	C	540	LEU	3.9
1	B	647	TYR	3.8
1	B	703	LEU	3.8
1	C	13	LEU	3.8
1	A	13	LEU	3.8
1	A	302	ILE	3.8
1	C	702	TYR	3.7
1	C	620	LEU	3.7
1	B	502	ILE	3.7
1	D	600	ILE	3.7
1	D	647	TYR	3.7
1	D	701	ALA	3.7
1	D	67	TYR	3.7
1	D	649	THR	3.7
1	A	166	ASN	3.6
1	B	58	PHE	3.6
1	A	12	GLY	3.5
1	B	721	MET	3.5
1	C	477	ALA	3.5
1	C	476	ILE	3.5
1	B	619	ASN	3.5
1	B	701	ALA	3.5
1	B	476	ILE	3.5
1	D	302	ILE	3.5
1	D	517	PHE	3.5
1	B	503	MET	3.4
1	C	12	GLY	3.4
1	A	242	GLN	3.4
1	A	701	ALA	3.4
1	D	69	ILE	3.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	D	503	MET	3.4
1	C	11	GLY	3.4
2	F	46	PHE	3.3
1	B	620	LEU	3.3
1	C	353	THR	3.3
1	C	354	ILE	3.3
1	C	727	LEU	3.3
1	C	258	TRP	3.2
1	D	635	SER	3.2
1	B	648	GLY	3.2
1	A	702	TYR	3.1
1	B	6	ASN	3.1
1	D	700	TYR	3.1
1	A	720	THR	3.1
1	D	598	GLY	3.1
1	C	500	ILE	3.1
1	A	329	LEU	3.1
1	B	341	ILE	3.0
1	B	367	ILE	3.0
1	B	732	TYR	3.0
1	A	325	ILE	3.0
1	D	13	LEU	3.0
1	D	329	LEU	3.0
1	B	624	LEU	3.0
1	A	400	ILE	2.9
1	C	792	VAL	2.9
1	B	617	THR	2.9
1	B	674	MET	2.9
1	C	304	ARG	2.9
1	B	607	PHE	2.8
1	A	813	GLU	2.8
1	D	540	LEU	2.8
1	D	66	VAL	2.8
1	A	292	PHE	2.8
1	D	311	CYS	2.8
1	D	521	LEU	2.8
1	A	703	LEU	2.7
1	D	289	THR	2.7
1	B	478	PRO	2.7
1	C	783	LYS	2.7
1	D	354	ILE	2.7
1	D	502	ILE	2.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	302	ILE	2.7
1	C	621	ALA	2.7
1	B	604	VAL	2.7
1	D	41	PRO	2.7
1	A	58	PHE	2.7
1	C	321	GLN	2.7
1	B	425	CYS	2.7
1	C	337	LEU	2.7
1	C	325	ILE	2.6
1	C	241	PHE	2.6
1	A	408	MET	2.6
1	A	503	MET	2.6
1	C	520	PRO	2.6
1	D	539	VAL	2.6
2	F	50	VAL	2.6
1	A	244	VAL	2.6
2	E	57	GLN	2.6
1	B	61	GLN	2.6
1	A	68	ALA	2.6
1	B	731	GLY	2.6
1	A	450	TYR	2.6
1	B	13	LEU	2.6
1	D	58	PHE	2.5
1	C	69	ILE	2.5
1	B	308	ALA	2.5
1	C	242	GLN	2.5
1	C	622	ALA	2.5
1	B	516	SER	2.5
1	B	258	TRP	2.5
1	A	221	LEU	2.5
1	D	70	PHE	2.5
1	D	337	LEU	2.5
1	A	476	ILE	2.5
1	B	615	SER	2.5
1	B	329	LEU	2.5
1	B	477	ALA	2.5
1	C	359	LEU	2.5
1	A	618	ALA	2.5
1	A	516	SER	2.5
1	B	282	TYR	2.5
1	A	269	ALA	2.5
1	B	356	ILE	2.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	505	LYS	2.5
1	D	623	PHE	2.5
1	A	288	MET	2.4
1	C	728	ASP	2.4
1	D	703	LEU	2.4
1	A	463	MET	2.4
1	C	58	PHE	2.4
1	D	512	PRO	2.4
1	D	288	MET	2.4
1	C	703	LEU	2.4
1	C	730	LYS	2.4
1	B	357	MET	2.4
1	C	616	TYR	2.4
1	D	91	SER	2.4
1	A	272	ALA	2.3
1	D	42	HIS	2.3
1	C	210	HIS	2.3
1	B	649	THR	2.3
1	C	161	VAL	2.3
1	D	280	LEU	2.3
1	A	72	PHE	2.3
1	C	216	TYR	2.3
1	B	521	LEU	2.3
1	B	720	THR	2.3
1	A	27	VAL	2.3
1	B	221	LEU	2.3
1	C	536	VAL	2.3
1	A	44	ASP	2.3
1	C	503	MET	2.3
1	B	231	ILE	2.3
1	D	88	LEU	2.3
1	A	513	GLY	2.3
1	D	109	MET	2.3
1	C	316	ALA	2.3
1	C	719	ASP	2.3
1	C	288	MET	2.3
1	B	244	VAL	2.3
1	B	324	GLU	2.2
1	C	306	GLY	2.2
1	B	280	LEU	2.2
1	B	463	MET	2.2
1	A	616	TYR	2.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	84	PHE	2.2
1	D	608	PHE	2.2
1	C	784	THR	2.2
1	C	367	ILE	2.2
1	C	243	ILE	2.2
1	D	24	ALA	2.2
1	D	463	MET	2.2
1	B	526	TRP	2.2
1	B	669	LYS	2.2
1	B	7	SER	2.2
1	D	43	ILE	2.2
1	B	520	PRO	2.2
1	A	525	ILE	2.2
1	A	601	VAL	2.2
1	B	501	SER	2.2
1	B	705	GLU	2.2
1	B	14	PHE	2.2
1	D	44	ASP	2.2
1	B	81	ILE	2.2
1	D	599	ARG	2.2
1	B	327	ARG	2.2
1	D	526	TRP	2.2
1	B	618	ALA	2.1
1	B	525	ILE	2.1
1	C	129	PHE	2.1
1	D	400	ILE	2.1
1	A	258	TRP	2.1
1	D	307	ASN	2.1
1	D	73	TYR	2.1
1	A	659	PHE	2.1
1	B	319	TRP	2.1
1	A	521	LEU	2.1
1	B	536	VAL	2.1
1	D	721	MET	2.1
1	A	667	PHE	2.1
1	C	70	PHE	2.1
1	D	231	ILE	2.1
1	D	243	ILE	2.1
1	A	39	LEU	2.1
1	B	605	TRP	2.1
1	B	621	ALA	2.1
1	A	131	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	425	CYS	2.1
1	D	604	VAL	2.1
1	A	185	GLU	2.1
1	A	428	LEU	2.1
1	A	216	TYR	2.1
1	C	281	THR	2.1
1	D	85	CYS	2.1
1	A	20	GLN	2.1
1	D	308	ALA	2.1
1	A	173	TYR	2.1
1	B	600	ILE	2.1
1	C	659	PHE	2.0
1	B	793	ALA	2.0
1	B	405	TYR	2.0
1	B	623	PHE	2.0
1	D	37	PHE	2.0
1	D	258	TRP	2.0
1	B	681	VAL	2.0
1	D	636	ALA	2.0
1	A	711	TYR	2.0
1	D	708	MET	2.0
1	A	91	SER	2.0
1	A	529	ILE	2.0
1	B	400	ILE	2.0
1	A	647	TYR	2.0
1	B	723	VAL	2.0
1	A	92	PHE	2.0

## 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 monosaccharides in this entry.

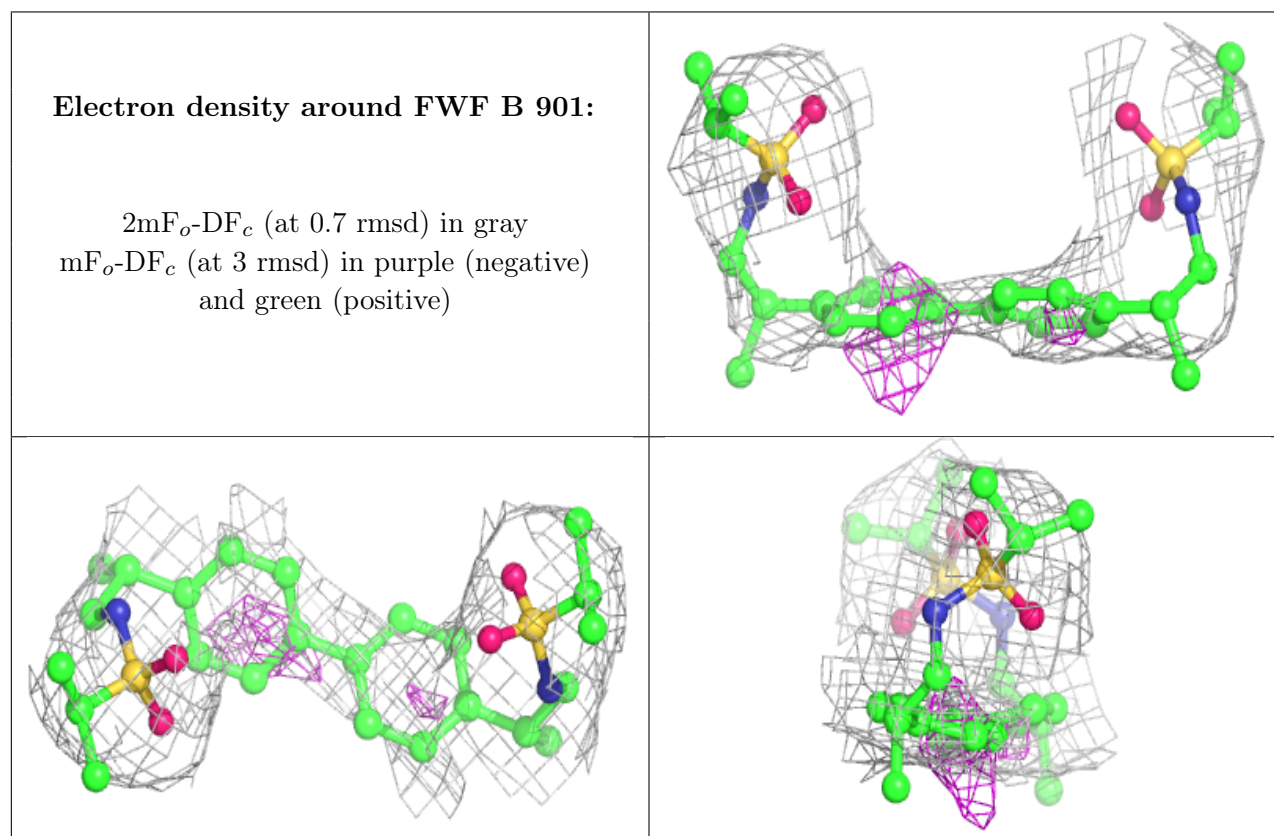
## 6.4 Ligands [i](#)

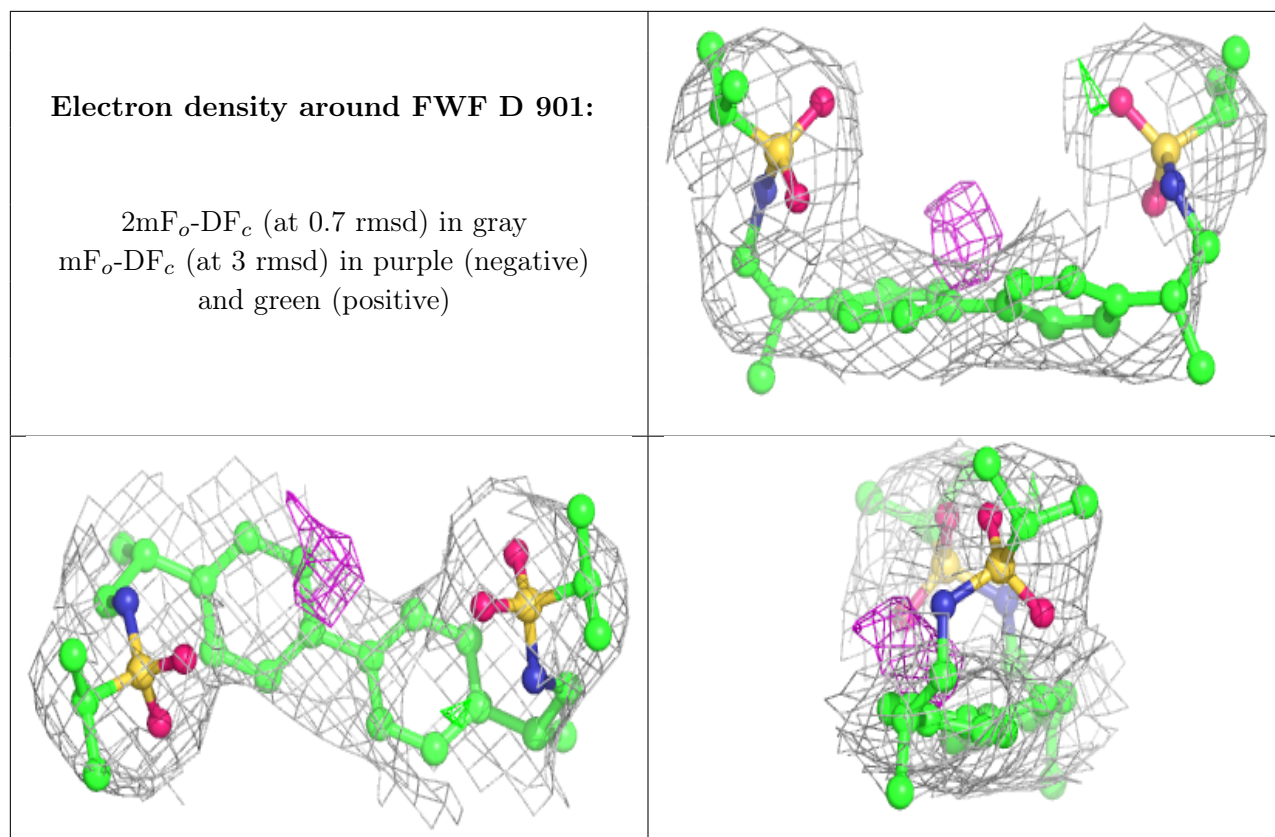
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95<sup>th</sup> 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(Å <sup>2</sup> )	Q<0.9
4	NAG	D	903	14/15	0.84	0.23	177,232,493,493	0
4	NAG	A	902	14/15	0.85	0.39	94,128,159,163	0
4	NAG	C	902	14/15	0.88	0.33	74,144,189,208	0
4	NAG	B	903	14/15	0.88	0.20	127,191,223,243	0
3	KAI	B	902	15/15	0.91	0.63	115,136,171,184	0
3	KAI	C	901	15/15	0.94	0.33	108,133,171,178	0
3	KAI	D	902	15/15	0.94	0.38	74,99,152,153	0
3	KAI	A	901	15/15	0.95	0.29	79,113,128,134	0
5	FWF	B	901	32/32	0.95	0.52	95,136,149,159	0
5	FWF	D	901	32/32	0.95	0.46	62,116,163,189	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.





## 6.5 Other polymers [i](#)

There are no such residues in this entry.