Full wwPDB X-ray Structure Validation Report ⓘ

Apr 7, 2025 – 11:42 AM EDT

PDB ID	:	9DA9 / pdb_00009da9
Title	:	Crystal structure of GluN1/GluN2A agonist-binding domains in complex with 7CKA and glutamate
Authors	:	Bosco, J.; Yates-Hansen, C.K.; McClelland, L.J.; Voronina, E.; Hansen, K.B.
Deposited on	:	2024-08-22
Resolution	:	2.05 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*
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:

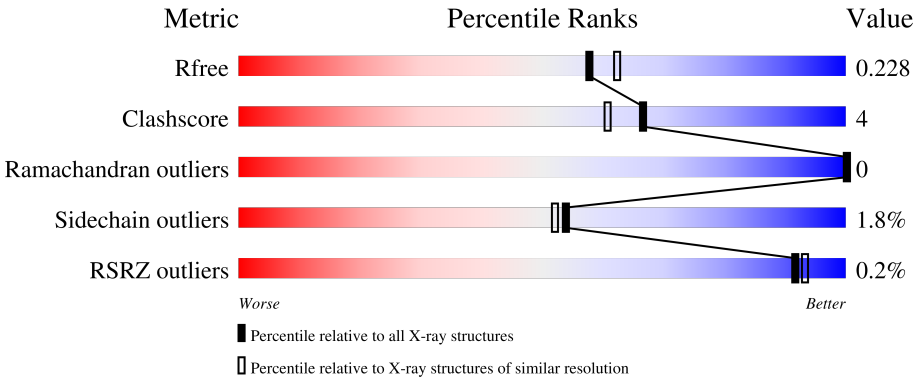
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

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 2.05 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}	164625	2096 (2.04-2.04)
Clashscore	180529	2229 (2.04-2.04)
Ramachandran outliers	177936	2217 (2.04-2.04)
Sidechain outliers	177891	2217 (2.04-2.04)
RSRZ outliers	164620	2096 (2.04-2.04)

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% 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	292	85% 10%
2	B	283	90% 8%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 9318 atoms, of which 4535 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 ionotropic, NMDA 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	280	4545	1447	2261	396	421	20	0	5	0

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP P35438
A	68	ILE	VAL	conflict	UNP P35438
A	?	-	GLU	deletion	UNP P35438
A	?	-	ILE	deletion	UNP P35438
A	?	-	PRO	deletion	UNP P35438
A	?	-	ARG	deletion	UNP P35438
A	?	-	SER	deletion	UNP P35438
A	?	-	THR	deletion	UNP P35438
A	?	-	LEU	deletion	UNP P35438
A	?	-	ASP	deletion	UNP P35438
A	?	-	SER	deletion	UNP P35438
A	?	-	PHE	deletion	UNP P35438
A	?	-	MET	deletion	UNP P35438
A	?	-	GLN	deletion	UNP P35438
A	?	-	PRO	deletion	UNP P35438
A	?	-	PHE	deletion	UNP P35438
A	?	-	GLN	deletion	UNP P35438
A	?	-	SER	deletion	UNP P35438
A	?	-	THR	deletion	UNP P35438
A	?	-	LEU	deletion	UNP P35438
A	?	-	TRP	deletion	UNP P35438
A	?	-	LEU	deletion	UNP P35438
A	?	-	LEU	deletion	UNP P35438
A	?	-	VAL	deletion	UNP P35438
A	?	-	GLY	deletion	UNP P35438
A	?	-	LEU	deletion	UNP P35438
A	?	-	SER	deletion	UNP P35438

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	VAL	deletion	UNP P35438
A	?	-	HIS	deletion	UNP P35438
A	?	-	VAL	deletion	UNP P35438
A	?	-	VAL	deletion	UNP P35438
A	?	-	ALA	deletion	UNP P35438
A	?	-	VAL	deletion	UNP P35438
A	?	-	MET	deletion	UNP P35438
A	?	-	LEU	deletion	UNP P35438
A	?	-	TYR	deletion	UNP P35438
A	?	-	LEU	deletion	UNP P35438
A	?	-	LEU	deletion	UNP P35438
A	?	-	ASP	deletion	UNP P35438
A	?	-	ARG	deletion	UNP P35438
A	?	-	PHE	deletion	UNP P35438
A	?	-	SER	deletion	UNP P35438
A	?	-	PRO	deletion	UNP P35438
A	?	-	PHE	deletion	UNP P35438
A	?	-	GLY	deletion	UNP P35438
A	?	-	ARG	deletion	UNP P35438
A	?	-	PHE	deletion	UNP P35438
A	?	-	LYS	deletion	UNP P35438
A	?	-	VAL	deletion	UNP P35438
A	?	-	ASN	deletion	UNP P35438
A	?	-	SER	deletion	UNP P35438
A	?	-	GLU	deletion	UNP P35438
A	?	-	GLU	deletion	UNP P35438
A	?	-	GLU	deletion	UNP P35438
A	?	-	GLU	deletion	UNP P35438
A	?	-	GLU	deletion	UNP P35438
A	?	-	ASP	deletion	UNP P35438
A	?	-	ALA	deletion	UNP P35438
A	?	-	LEU	deletion	UNP P35438
A	?	-	THR	deletion	UNP P35438
A	?	-	LEU	deletion	UNP P35438
A	?	-	SER	deletion	UNP P35438
A	?	-	SER	deletion	UNP P35438
A	?	-	ALA	deletion	UNP P35438
A	?	-	MET	deletion	UNP P35438
A	?	-	TRP	deletion	UNP P35438
A	?	-	PHE	deletion	UNP P35438
A	?	-	SER	deletion	UNP P35438
A	?	-	TRP	deletion	UNP P35438

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLY	deletion	UNP P35438
A	?	-	VAL	deletion	UNP P35438
A	?	-	LEU	deletion	UNP P35438
A	?	-	LEU	deletion	UNP P35438
A	?	-	ASN	deletion	UNP P35438
A	?	-	SER	deletion	UNP P35438
A	?	-	GLY	deletion	UNP P35438
A	?	-	ILE	deletion	UNP P35438
A	?	-	GLY	deletion	UNP P35438
A	?	-	GLU	deletion	UNP P35438
A	?	-	GLY	deletion	UNP P35438
A	?	-	ALA	deletion	UNP P35438
A	?	-	PRO	deletion	UNP P35438
A	?	-	ARG	deletion	UNP P35438
A	?	-	SER	deletion	UNP P35438
A	?	-	PHE	deletion	UNP P35438
A	?	-	SER	deletion	UNP P35438
A	?	-	ALA	deletion	UNP P35438
A	?	-	ARG	deletion	UNP P35438
A	?	-	ILE	deletion	UNP P35438
A	?	-	LEU	deletion	UNP P35438
A	?	-	GLY	deletion	UNP P35438
A	?	-	MET	deletion	UNP P35438
A	?	-	VAL	deletion	UNP P35438
A	?	-	TRP	deletion	UNP P35438
A	?	-	ALA	deletion	UNP P35438
A	?	-	GLY	deletion	UNP P35438
A	?	-	PHE	deletion	UNP P35438
A	?	-	ALA	deletion	UNP P35438
A	?	-	MET	deletion	UNP P35438
A	?	-	ILE	deletion	UNP P35438
A	?	-	ILE	deletion	UNP P35438
A	?	-	VAL	deletion	UNP P35438
A	?	-	ALA	deletion	UNP P35438
A	?	-	SER	deletion	UNP P35438
A	?	-	TYR	deletion	UNP P35438
A	?	-	THR	deletion	UNP P35438
A	?	-	ALA	deletion	UNP P35438
A	?	-	ASN	deletion	UNP P35438
A	?	-	LEU	deletion	UNP P35438
A	?	-	ALA	deletion	UNP P35438
A	?	-	ALA	deletion	UNP P35438

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	PHE	deletion	UNP P35438
A	?	-	LEU	deletion	UNP P35438
A	?	-	VAL	deletion	UNP P35438
A	?	-	LEU	deletion	UNP P35438
A	?	-	ASP	deletion	UNP P35438
A	?	-	ARG	deletion	UNP P35438
A	?	-	PRO	deletion	UNP P35438
A	153	GLY	GLU	conflict	UNP P35438
A	154	THR	GLU	conflict	UNP P35438

- Molecule 2 is a protein called Glutamate receptor ionotropic, NMDA 2A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	280	Total	C	H	N	O	S	0	9	0
			4534	1438	2262	389	423	22			

There are 123 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	4	SER	-	expression tag	UNP Q00959
B	?	-	SER	deletion	UNP Q00959
B	?	-	ASN	deletion	UNP Q00959
B	?	-	GLY	deletion	UNP Q00959
B	?	-	THR	deletion	UNP Q00959
B	?	-	VAL	deletion	UNP Q00959
B	?	-	SER	deletion	UNP Q00959
B	?	-	PRO	deletion	UNP Q00959
B	?	-	SER	deletion	UNP Q00959
B	?	-	ALA	deletion	UNP Q00959
B	?	-	PHE	deletion	UNP Q00959
B	?	-	LEU	deletion	UNP Q00959
B	?	-	GLU	deletion	UNP Q00959
B	?	-	PRO	deletion	UNP Q00959
B	?	-	PHE	deletion	UNP Q00959
B	?	-	SER	deletion	UNP Q00959
B	?	-	ALA	deletion	UNP Q00959
B	?	-	SER	deletion	UNP Q00959
B	?	-	VAL	deletion	UNP Q00959
B	?	-	TRP	deletion	UNP Q00959
B	?	-	VAL	deletion	UNP Q00959
B	?	-	MET	deletion	UNP Q00959
B	?	-	MET	deletion	UNP Q00959

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	PHE	deletion	UNP Q00959
B	?	-	VAL	deletion	UNP Q00959
B	?	-	MET	deletion	UNP Q00959
B	?	-	LEU	deletion	UNP Q00959
B	?	-	LEU	deletion	UNP Q00959
B	?	-	ILE	deletion	UNP Q00959
B	?	-	VAL	deletion	UNP Q00959
B	?	-	SER	deletion	UNP Q00959
B	?	-	ALA	deletion	UNP Q00959
B	?	-	ILE	deletion	UNP Q00959
B	?	-	ALA	deletion	UNP Q00959
B	?	-	VAL	deletion	UNP Q00959
B	?	-	PHE	deletion	UNP Q00959
B	?	-	VAL	deletion	UNP Q00959
B	?	-	PHE	deletion	UNP Q00959
B	?	-	GLU	deletion	UNP Q00959
B	?	-	TYR	deletion	UNP Q00959
B	?	-	PHE	deletion	UNP Q00959
B	?	-	SER	deletion	UNP Q00959
B	?	-	PRO	deletion	UNP Q00959
B	?	-	VAL	deletion	UNP Q00959
B	?	-	GLY	deletion	UNP Q00959
B	?	-	TYR	deletion	UNP Q00959
B	?	-	ASN	deletion	UNP Q00959
B	?	-	ARG	deletion	UNP Q00959
B	?	-	ASN	deletion	UNP Q00959
B	?	-	LEU	deletion	UNP Q00959
B	?	-	ALA	deletion	UNP Q00959
B	?	-	LYS	deletion	UNP Q00959
B	?	-	GLY	deletion	UNP Q00959
B	?	-	LYS	deletion	UNP Q00959
B	?	-	ALA	deletion	UNP Q00959
B	?	-	PRO	deletion	UNP Q00959
B	?	-	HIS	deletion	UNP Q00959
B	?	-	GLY	deletion	UNP Q00959
B	?	-	PRO	deletion	UNP Q00959
B	?	-	SER	deletion	UNP Q00959
B	?	-	PHE	deletion	UNP Q00959
B	?	-	THR	deletion	UNP Q00959
B	?	-	ILE	deletion	UNP Q00959
B	?	-	GLY	deletion	UNP Q00959
B	?	-	LYS	deletion	UNP Q00959

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	ALA	deletion	UNP Q00959
B	?	-	ILE	deletion	UNP Q00959
B	?	-	TRP	deletion	UNP Q00959
B	?	-	LEU	deletion	UNP Q00959
B	?	-	LEU	deletion	UNP Q00959
B	?	-	TRP	deletion	UNP Q00959
B	?	-	GLY	deletion	UNP Q00959
B	?	-	LEU	deletion	UNP Q00959
B	?	-	VAL	deletion	UNP Q00959
B	?	-	PHE	deletion	UNP Q00959
B	?	-	ASN	deletion	UNP Q00959
B	?	-	ASN	deletion	UNP Q00959
B	?	-	SER	deletion	UNP Q00959
B	?	-	VAL	deletion	UNP Q00959
B	?	-	PRO	deletion	UNP Q00959
B	?	-	VAL	deletion	UNP Q00959
B	?	-	GLN	deletion	UNP Q00959
B	?	-	ASN	deletion	UNP Q00959
B	?	-	PRO	deletion	UNP Q00959
B	?	-	LYS	deletion	UNP Q00959
B	?	-	GLY	deletion	UNP Q00959
B	?	-	THR	deletion	UNP Q00959
B	?	-	THR	deletion	UNP Q00959
B	?	-	SER	deletion	UNP Q00959
B	?	-	LYS	deletion	UNP Q00959
B	?	-	ILE	deletion	UNP Q00959
B	?	-	MET	deletion	UNP Q00959
B	?	-	VAL	deletion	UNP Q00959
B	?	-	SER	deletion	UNP Q00959
B	?	-	VAL	deletion	UNP Q00959
B	?	-	TRP	deletion	UNP Q00959
B	?	-	ALA	deletion	UNP Q00959
B	?	-	PHE	deletion	UNP Q00959
B	?	-	PHE	deletion	UNP Q00959
B	?	-	ALA	deletion	UNP Q00959
B	?	-	VAL	deletion	UNP Q00959
B	?	-	ILE	deletion	UNP Q00959
B	?	-	PHE	deletion	UNP Q00959
B	?	-	LEU	deletion	UNP Q00959
B	?	-	ALA	deletion	UNP Q00959
B	?	-	SER	deletion	UNP Q00959
B	?	-	TYR	deletion	UNP Q00959

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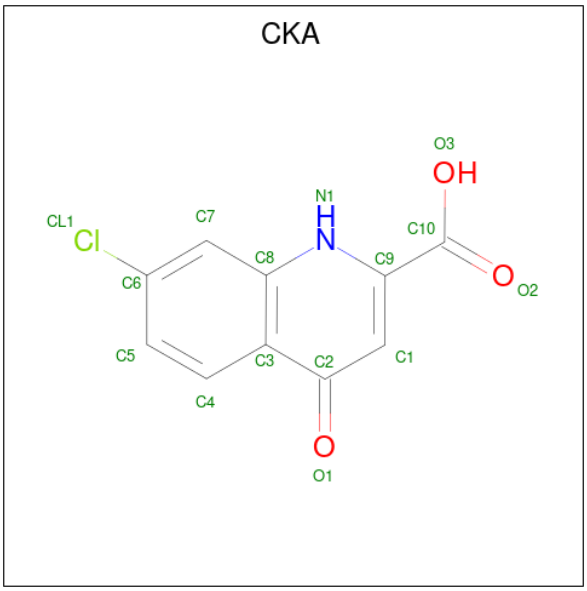
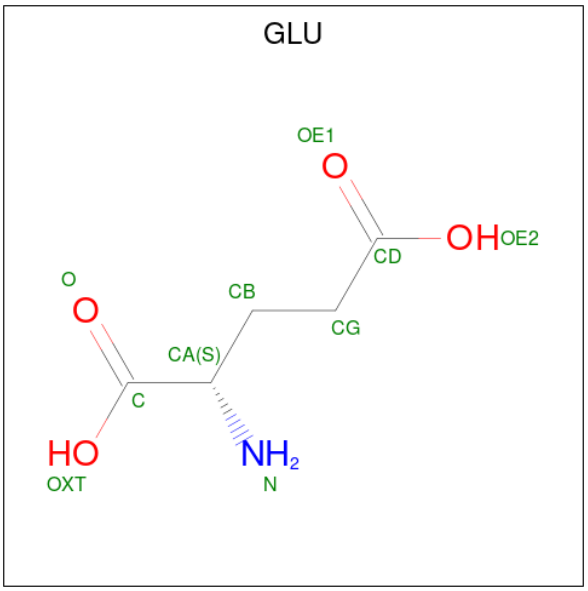
Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	THR	deletion	UNP Q00959
B	?	-	ALA	deletion	UNP Q00959
B	?	-	ASN	deletion	UNP Q00959
B	?	-	LEU	deletion	UNP Q00959
B	?	-	ALA	deletion	UNP Q00959
B	?	-	ALA	deletion	UNP Q00959
B	?	-	PHE	deletion	UNP Q00959
B	?	-	MET	deletion	UNP Q00959
B	?	-	ILE	deletion	UNP Q00959
B	?	-	GLN	deletion	UNP Q00959
B	?	-	GLU	deletion	UNP Q00959
B	?	-	GLU	deletion	UNP Q00959
B	?	-	PHE	deletion	UNP Q00959
B	143	GLY	VAL	conflict	UNP Q00959
B	144	THR	ASP	conflict	UNP Q00959
B	242	THR	SER	conflict	UNP Q00959

- Molecule 3 is 7-Chlorokynurenic acid (CCD ID: CKA) (formula: $C_{10}H_6ClNO_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	Cl	H	N	O		
3	A	1	20	10	1	5	1	3	0	0

- Molecule 4 is GLUTAMIC ACID (CCD ID: GLU) (formula: $C_5H_9NO_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	H	N	O	0	0
			17	5	7	1	4		

- Molecule 5 is water.

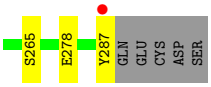
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	84	Total	O	0	0
			84	84		
5	B	118	Total	O	0	0
			118	118		

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 ionotropic, NMDA 1

Chain A:



- Molecule 2: Glutamate receptor ionotropic, NMDA 2A

Chain B:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	54.24Å 87.34Å 135.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.97 – 2.05 33.97 – 2.05	Depositor EDS
% Data completeness (in resolution range)	99.4 (33.97-2.05) 99.3 (33.97-2.05)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.45 (at 2.05Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.168 , 0.228 0.168 , 0.228	Depositor DCC
R_{free} test set	2064 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	37.3	Xtriage
Anisotropy	0.293	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 29.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	9318	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.68% 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: CKA

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	0.60	0/2333	0.72	0/3145
2	B	0.61	0/2316	0.72	0/3129
All	All	0.61	0/4649	0.72	0/6274

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2284	2261	2257	18	1
2	B	2272	2262	2254	15	1
3	A	15	5	5	0	0
4	B	10	7	5	1	0
5	A	84	0	0	1	0
5	B	118	0	0	1	0
All	All	4783	4535	4521	33	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 4.

All (33) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:ARG:NH1	1:A:101:SER:OG	2.26	0.69
2:B:256:LYS:NZ	5:B:401:HOH:O	2.28	0.65
1:A:56:ARG:NH1	5:A:402:HOH:O	2.36	0.54
1:A:165:ARG:HD3	1:A:194:MET:HE3	1.90	0.53
1:A:165:ARG:HD3	1:A:194:MET:CE	2.39	0.53
2:B:140:VAL:HG21	2:B:234:ILE:HD11	1.91	0.53
2:B:110[B]:MET:CE	2:B:247:ILE:HG21	2.40	0.52
2:B:116:THR:HG1	4:B:301:GLU:N	2.08	0.51
1:A:41:LYS:HD3	1:A:62[B]:CYS:SG	2.50	0.51
1:A:4:THR:HG23	1:A:5:ARG:H	1.76	0.51
1:A:144:GLN:OE1	1:A:224:ASP:OD2	2.31	0.48
2:B:284:CYS:O	2:B:285:HIS:ND1	2.47	0.48
2:B:140:VAL:CG2	2:B:234:ILE:HD11	2.43	0.48
2:B:22:VAL:HG22	2:B:59[B]:CYS:SG	2.53	0.48
2:B:110[B]:MET:HE3	2:B:247:ILE:HG21	1.97	0.46
1:A:190:GLU:H	1:A:190:GLU:CD	2.19	0.45
1:A:233:SER:HB3	1:A:287:TYR:HD2	1.81	0.45
1:A:30:GLU:O	1:A:30:GLU:HG3	2.17	0.45
2:B:69:LYS:NZ	2:B:271:GLU:OE1	2.35	0.44
1:A:149:LEU:HD21	1:A:238:LEU:HD13	2.01	0.42
2:B:186:HIS:O	2:B:190:THR:HG23	2.18	0.42
1:A:164:LEU:HD22	1:A:173:TYR:CD1	2.55	0.42
2:B:39[B]:CYS:SG	2:B:82:LEU:HG	2.59	0.42
1:A:31:GLU:OE1	1:A:41:LYS:NZ	2.45	0.42
1:A:28[B]:CYS:HB3	1:A:41:LYS:HD3	2.01	0.42
1:A:215:ASP:HB2	1:A:217:LYS:HE3	2.02	0.42
2:B:110[A]:MET:HA	2:B:248:ALA:O	2.20	0.42
2:B:32[A]:CYS:HB3	2:B:36:THR:OG1	2.20	0.41
1:A:97:ARG:NH2	1:A:103:LYS:HA	2.36	0.41
2:B:225:ARG:HE	2:B:225:ARG:HB3	1.78	0.41
1:A:23:MET:SD	1:A:29:LYS:HD3	2.60	0.40
1:A:4:THR:HG23	1:A:5:ARG:N	2.37	0.40
2:B:146:VAL:HG23	2:B:234:ILE:HG13	2.02	0.40

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:A:186:ARG:HH21	2:B:142:ARG:O[3_444]	1.52	0.08

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	281/292 (96%)	270 (96%)	11 (4%)	0	100	100
2	B	287/283 (101%)	276 (96%)	11 (4%)	0	100	100
All	All	568/575 (99%)	546 (96%)	22 (4%)	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	254/260 (98%)	247 (97%)	7 (3%)	38	34
2	B	254/248 (102%)	252 (99%)	2 (1%)	79	80
All	All	508/508 (100%)	499 (98%)	9 (2%)	54	52

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ARG
1	A	48	ASN
1	A	97	ARG
1	A	152	LYS
1	A	177	LYS
1	A	265	SER
1	A	278	GLU
2	B	152	LYS

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Mol	Chain	Res	Type
2	B	191	ARG

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

Mol	Chain	Res	Type
2	B	155	GLN

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)

2 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	GLU	B	301	-	8,9,9	1.69	2 (25%)	8,11,11	1.26	1 (12%)
3	CKA	A	301	-	16,16,16	1.53	3 (18%)	21,23,23	1.23	2 (9%)

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	GLU	B	301	-	-	2/9/9/9	-
3	CKA	A	301	-	-	0/4/4/4	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	301	CKA	C9-C10	4.20	1.58	1.48
4	B	301	GLU	CG-CD	3.77	1.59	1.50
3	A	301	CKA	C9-N1	2.62	1.38	1.35
3	A	301	CKA	C3-C2	-2.38	1.44	1.48
4	B	301	GLU	OXT-C	-2.26	1.23	1.30

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	301	CKA	C5-C6-C7	2.60	124.93	121.53
4	B	301	GLU	OE1-CD-CG	-2.60	114.86	123.09
3	A	301	CKA	O2-C10-C9	-2.09	116.78	121.01

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	301	GLU	OE1-CD-CG-CB
4	B	301	GLU	OE2-CD-CG-CB

There are no ring outliers.

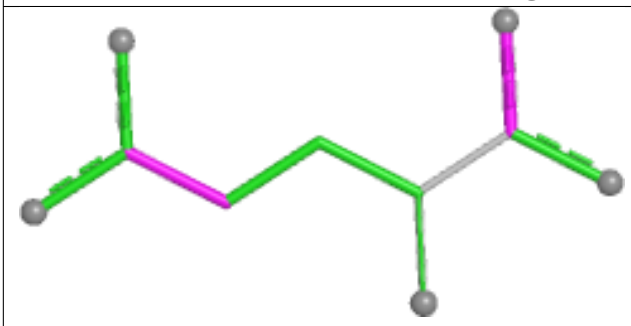
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	301	GLU	1	0

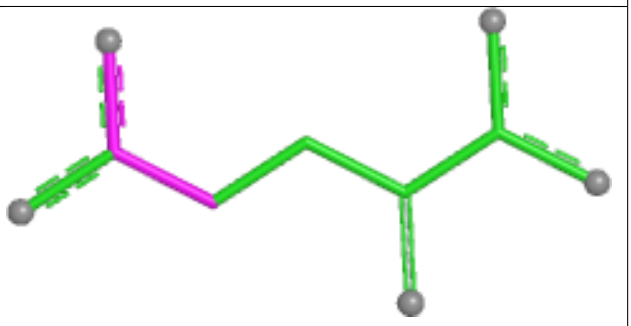
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

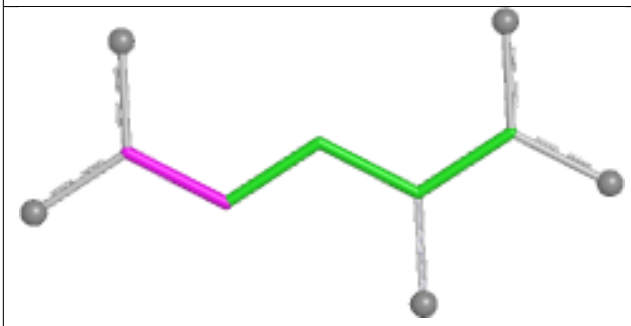
Ligand GLU B 301



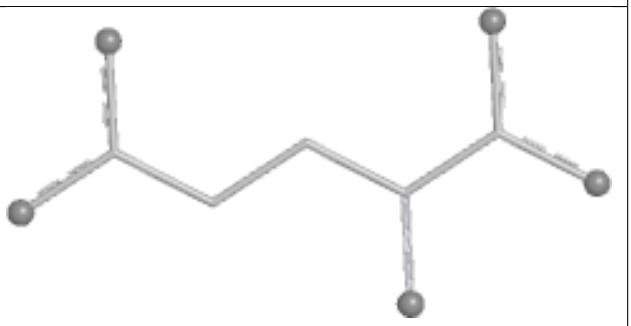
Bond lengths



Bond angles

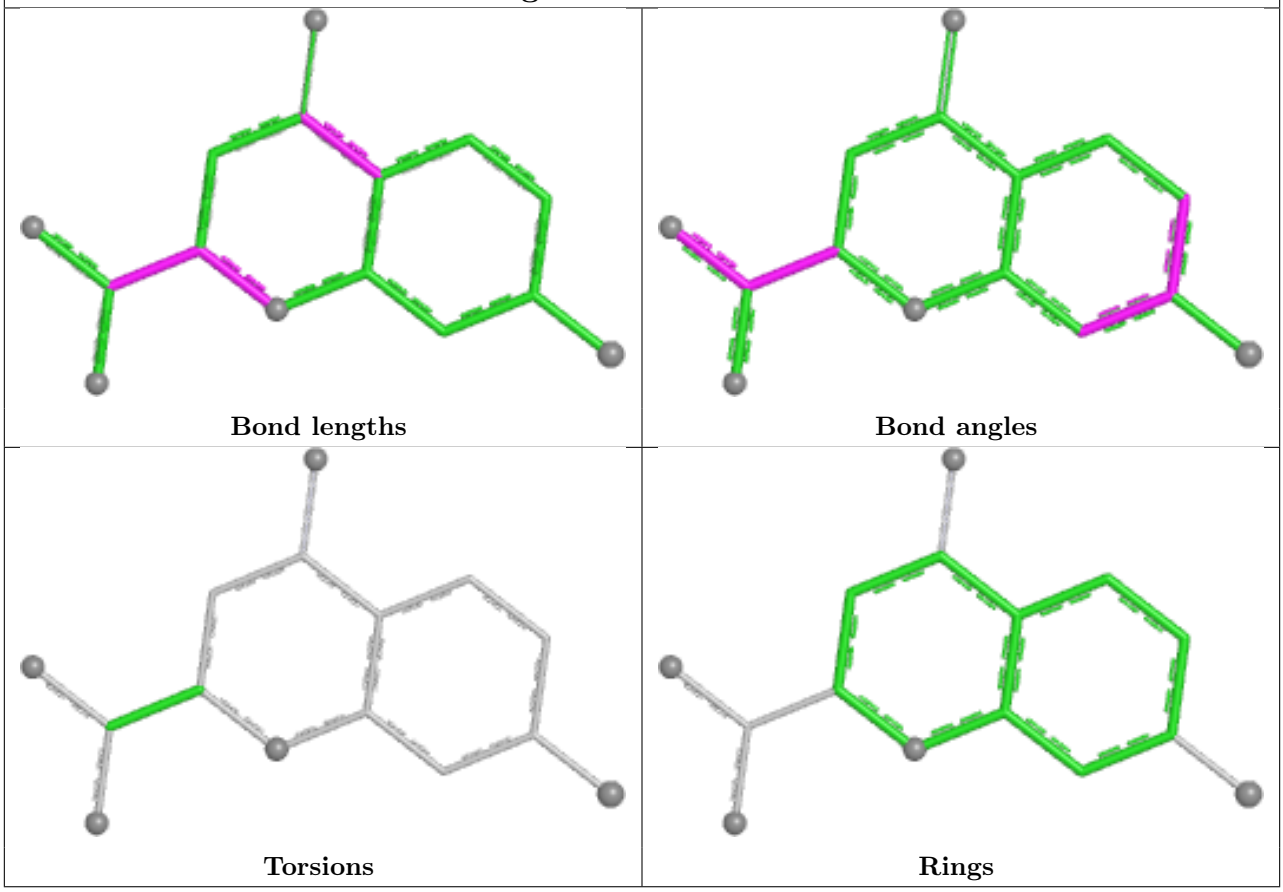


Torsions



Rings

Ligand CKA A 301



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^{th} 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	280/292 (95%)	-0.26	1 (0%) 89 90	18, 49, 85, 123	5 (1%)
2	B	280/283 (98%)	-0.34	0 100 100	17, 44, 77, 105	9 (3%)
All	All	560/575 (97%)	-0.30	1 (0%) 92 93	17, 47, 83, 123	14 (2%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	287	TYR	4.2

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

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^{th} 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.

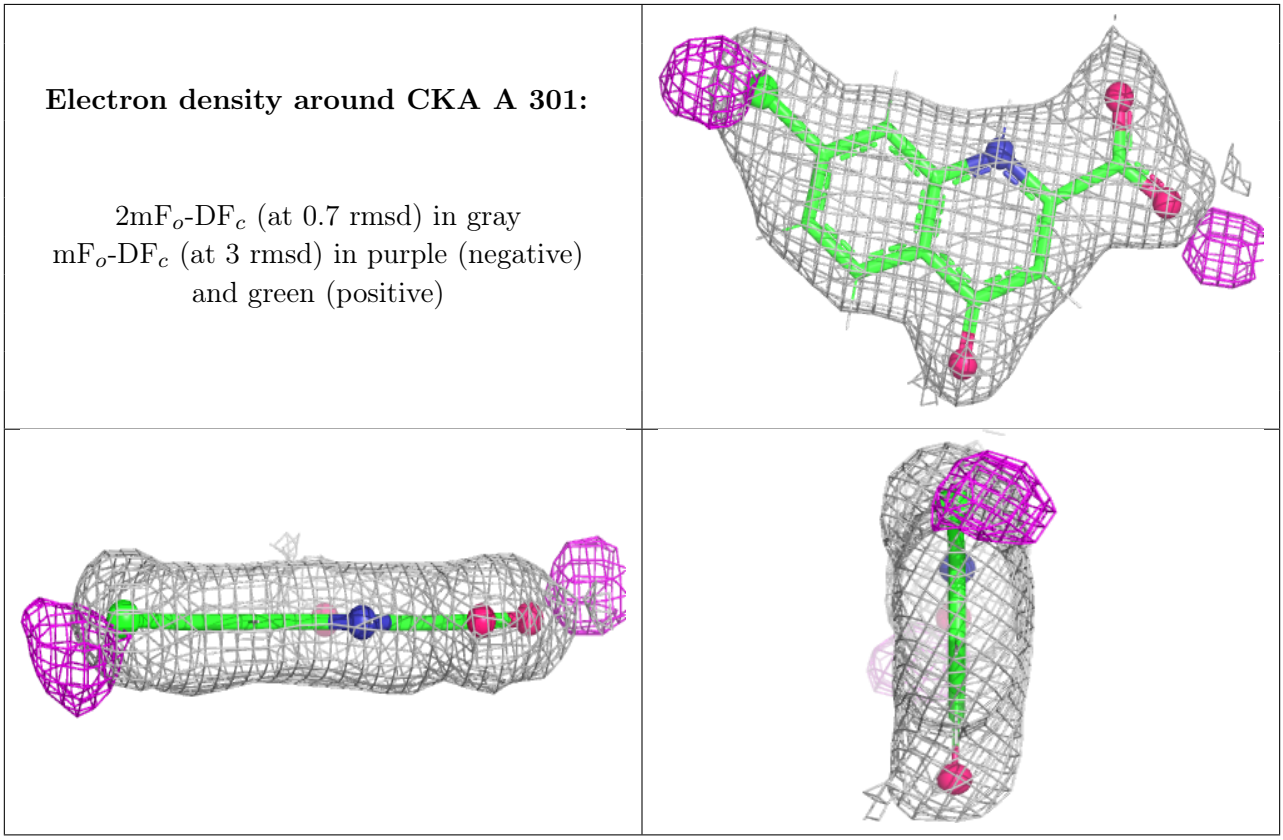
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	CKA	A	301	15/15	0.94	0.07	32,39,47,49	0
4	GLU	B	301	10/10	0.97	0.06	27,36,48,48	0

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.

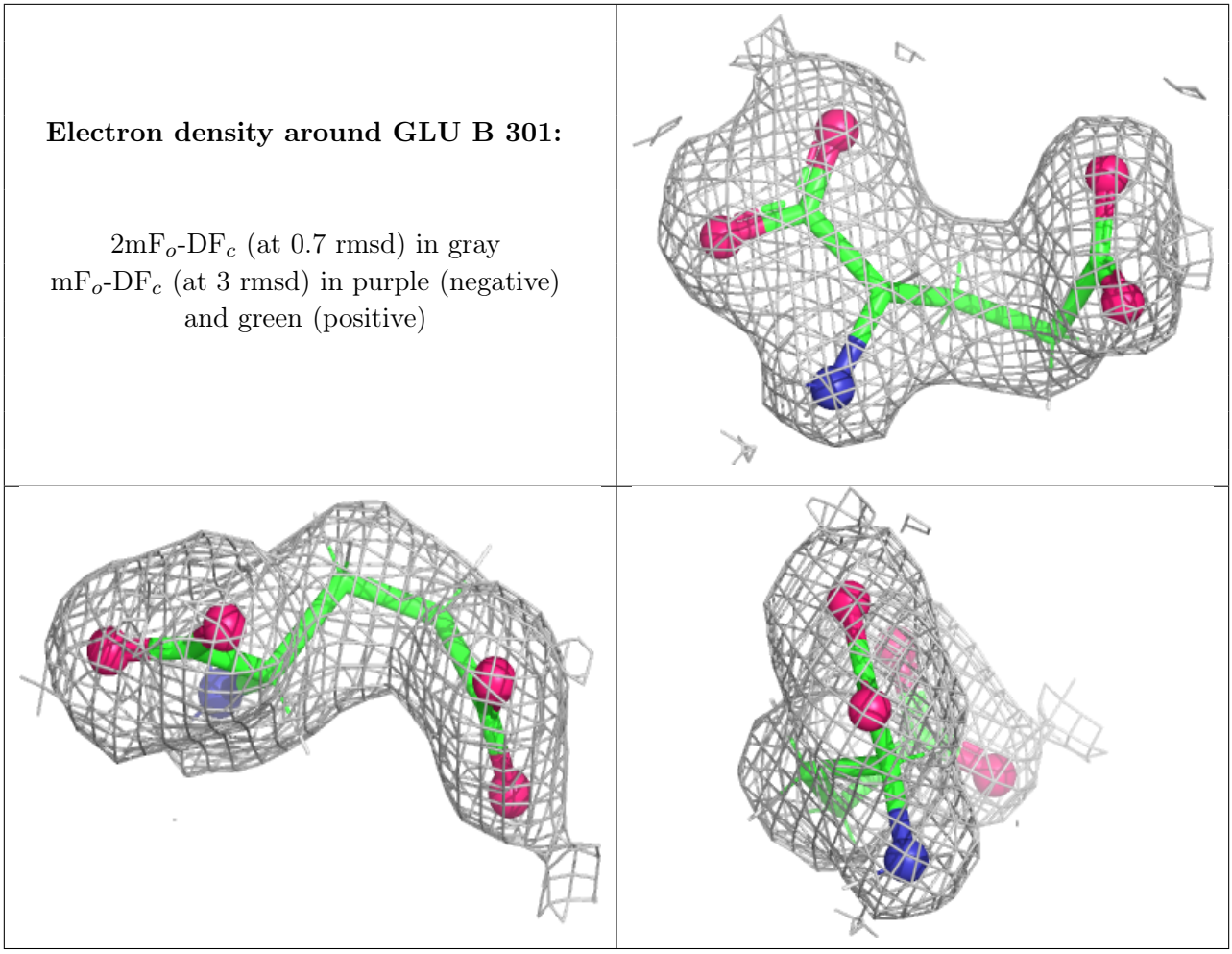
Electron density around CKA A 301:

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



Electron density around GLU B 301:

$2mF_o$-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

There are no such residues in this entry.