



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 8, 2023 – 07:52 am GMT

PDB ID : 8BST
Title : Crystal structure of the kainate receptor GluK3-H523A ligand binding domain in complex with kainate at 2.7Å resolution
Authors : Venskutonyte, R.; Frydenvang, K.; Kastrup, J.S.
Deposited on : 2022-11-26
Resolution : 2.70 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

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 : 1.8.4, 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

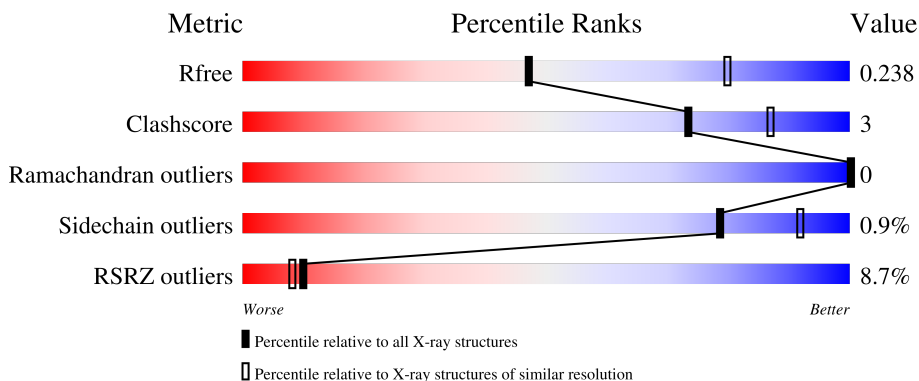
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	258	 7% 90% 8% .
1	B	258	 7% 85% 13% .
1	C	258	 15% 84% 9% 6%
1	D	258	 4% 88% 8% .

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	ACT	D	901	-	-	-	X

2 Entry composition i

There are 9 unique types of molecules in this entry. The entry contains 8240 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 ionotropic, kainate 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	252	2012	1286	336	378	12	0	2	0
1	B	253	2027	1296	339	380	12	0	3	0
1	C	242	1939	1242	320	366	11	0	1	0
1	D	247	1974	1265	326	372	11	0	1	0

There are 24 discrepancies between the modelled and reference sequences:

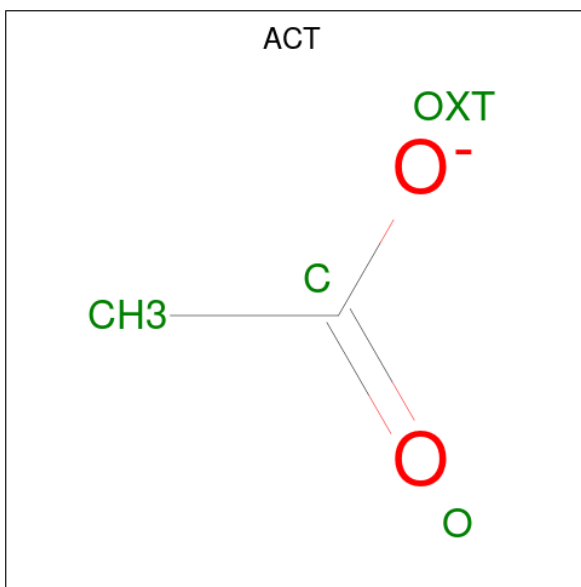
Chain	Residue	Modelled	Actual	Comment	Reference
A	429	GLY	-	expression tag	UNP P42264
A	430	PRO	-	expression tag	UNP P42264
A	431	GLY	-	expression tag	UNP P42264
A	523	ALA	HIS	engineered mutation	UNP P42264
A	547	GLY	-	linker	UNP P42264
A	548	THR	-	linker	UNP P42264
B	429	GLY	-	expression tag	UNP P42264
B	430	PRO	-	expression tag	UNP P42264
B	431	GLY	-	expression tag	UNP P42264
B	523	ALA	HIS	engineered mutation	UNP P42264
B	547	GLY	-	linker	UNP P42264
B	548	THR	-	linker	UNP P42264
C	429	GLY	-	expression tag	UNP P42264
C	430	PRO	-	expression tag	UNP P42264
C	431	GLY	-	expression tag	UNP P42264
C	523	ALA	HIS	engineered mutation	UNP P42264
C	667	GLY	-	linker	UNP P42264
C	668	THR	-	linker	UNP P42264
D	429	GLY	-	expression tag	UNP P42264
D	430	PRO	-	expression tag	UNP P42264
D	431	GLY	-	expression tag	UNP P42264

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Chain	Residue	Modelled	Actual	Comment	Reference
D	523	ALA	HIS	engineered mutation	UNP P42264
D	547	GLY	-	linker	UNP P42264
D	548	THR	-	linker	UNP P42264

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	4	Total Zn 4 4	0	2
3	B	6	Total Zn 6 6	0	6

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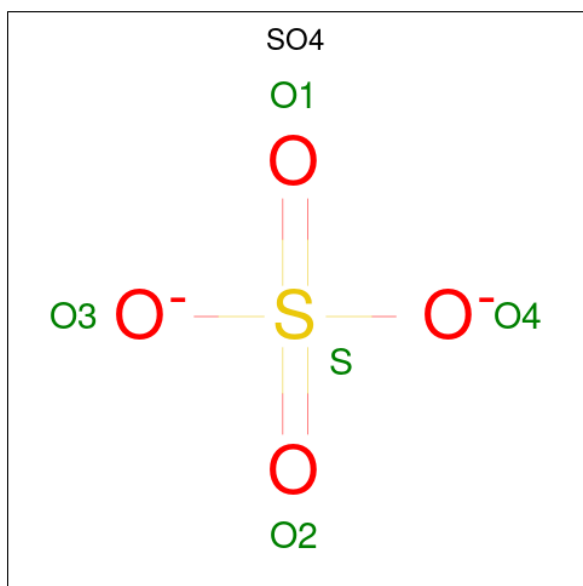
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	2	Total	Zn	0	1
			2	2		
3	D	1	Total	Zn	0	0
			1	1		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Cl	0	0
			2	2		
4	B	2	Total	Cl	0	0
			2	2		
4	C	1	Total	Cl	0	0
			1	1		
4	D	2	Total	Cl	0	0
			2	2		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



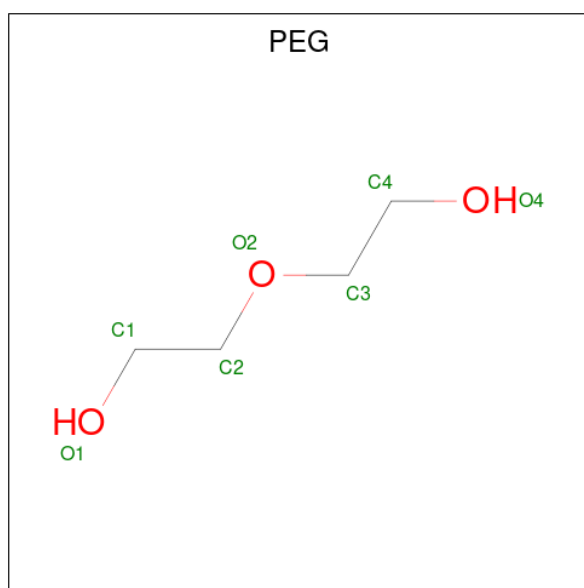
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		

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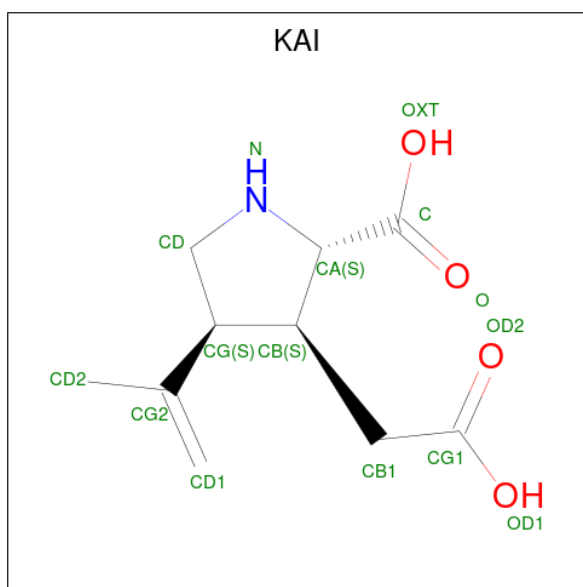
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O S 5 4 1	0	0
5	B	1	Total O S 5 4 1	0	0
5	B	1	Total O S 5 4 1	0	0
5	C	1	Total O S 5 4 1	0	0
5	C	1	Total O S 5 4 1	0	0
5	C	1	Total O S 5 4 1	0	0
5	D	1	Total O S 5 4 1	0	0

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



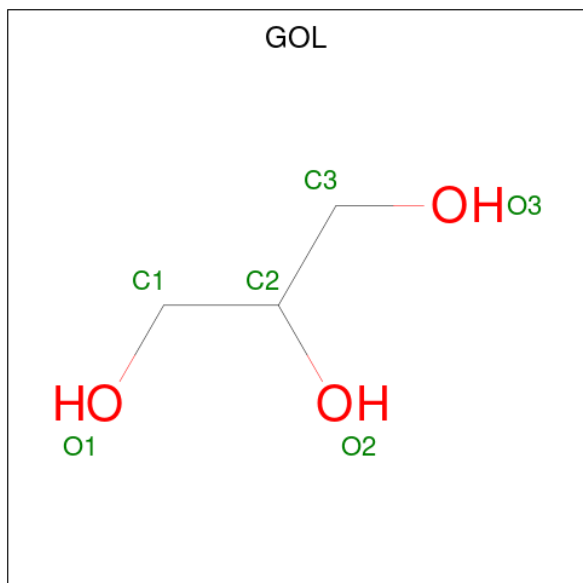
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 7 4 3	0	0

- Molecule 7 is 3-(CARBOXYMETHYL)-4-ISOPROPENYLPROLINE (three-letter code: KAI) (formula: C₁₀H₁₅NO₄) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		
8	D	1	Total	C	O	0	0
			6	3	3		

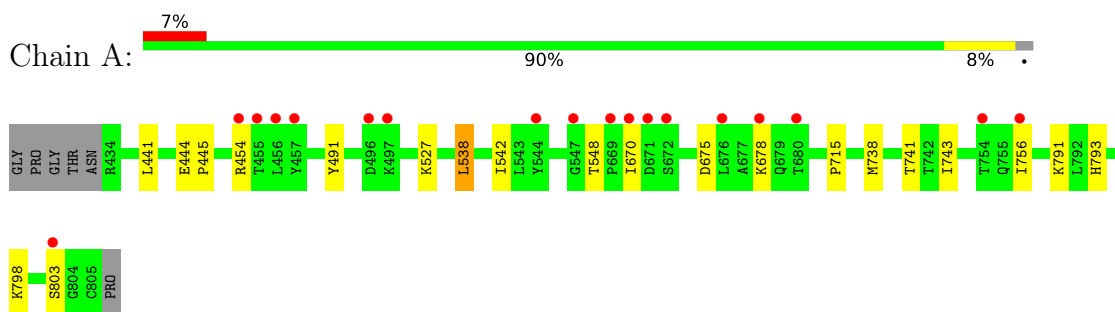
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	24	Total	O	0	0
			24	24		
9	B	27	Total	O	0	0
			27	27		
9	C	17	Total	O	0	0
			17	17		
9	D	29	Total	O	0	1
			29	29		

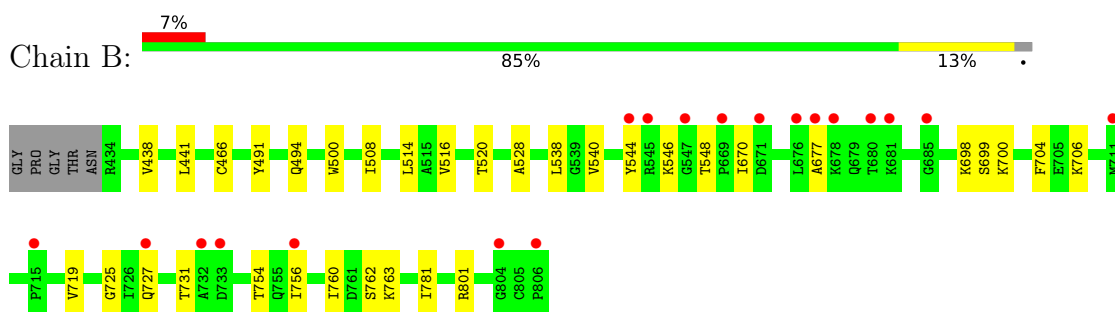
3 Residue-property plots [i](#)

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.

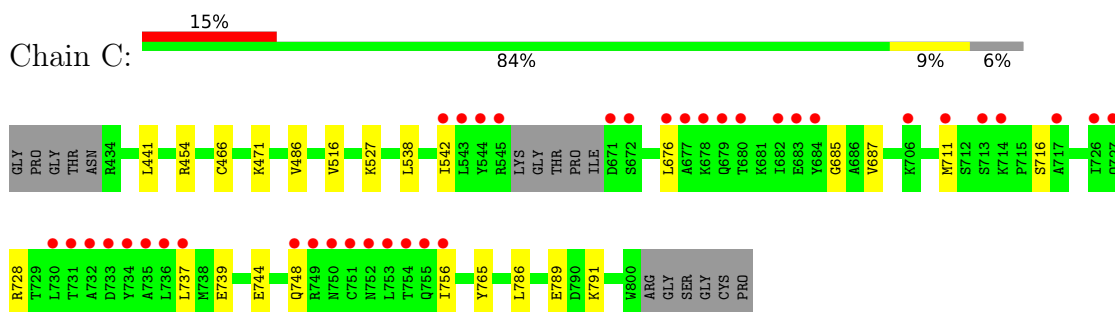
- Molecule 1: Glutamate receptor ionotropic, kainate 3



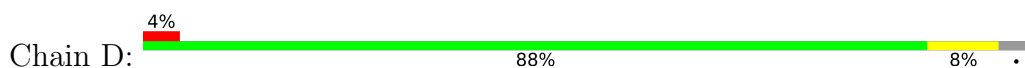
- Molecule 1: Glutamate receptor ionotropic, kainate 3

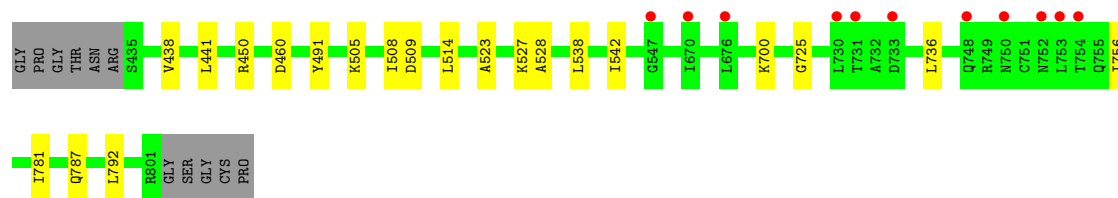


- Molecule 1: Glutamate receptor ionotropic, kainate 3



- Molecule 1: Glutamate receptor ionotropic, kainate 3





4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	69.41Å 101.60Å 83.41Å 90.00° 111.99° 90.00°	Depositor
Resolution (Å)	39.88 – 2.70 42.46 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.5 (39.88-2.70) 99.6 (42.46-2.70)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.95 (at 2.69Å)	Xtrriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.204 , 0.238 0.204 , 0.238	Depositor DCC
R_{free} test set	1469 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	44.8	Xtrriage
Anisotropy	0.819	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 43.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	0.043 for h,-k,-h-l	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8240	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.85% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, ZN, KAI, CL, ACT, GOL, PEG

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	0.24	0/2057	0.46	0/2769
1	B	0.24	0/2077	0.47	0/2796
1	C	0.24	0/1978	0.46	0/2662
1	D	0.24	0/2015	0.46	0/2714
All	All	0.24	0/8127	0.46	0/10941

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 [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	2012	0	2033	14	0
1	B	2027	0	2047	17	0
1	C	1939	0	1957	15	0
1	D	1974	0	1999	11	0
2	A	8	0	6	0	0
2	B	4	0	3	0	0
2	C	4	0	3	0	0
2	D	8	0	6	0	0
3	A	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	6	0	0	0	0
3	C	2	0	0	0	0
3	D	1	0	0	0	0
4	A	2	0	0	1	0
4	B	2	0	0	0	0
4	C	1	0	0	0	0
4	D	2	0	0	0	0
5	A	20	0	0	0	0
5	B	10	0	0	0	0
5	C	15	0	0	1	0
5	D	5	0	0	0	0
6	A	7	0	10	0	0
7	A	15	0	13	0	0
7	B	15	0	13	0	0
7	C	15	0	13	1	0
7	D	15	0	13	0	0
8	A	6	0	8	0	0
8	B	18	0	24	2	0
8	D	6	0	8	0	0
9	A	24	0	0	0	0
9	B	27	0	0	0	0
9	C	17	0	0	0	0
9	D	29	0	0	0	0
All	All	8240	0	8156	53	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 3.

All (53) 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:789:GLU:HB2	1:C:791:LYS:HE3	1.76	0.67
1:A:791:LYS:HE2	1:D:700:LYS:HE2	1.76	0.67
1:B:677:ALA:HB1	1:B:706:LYS:HD2	1.77	0.66
1:C:542:ILE:HD13	1:C:676:LEU:HD12	1.78	0.65
1:A:548:THR:HG22	1:A:670:ILE:H	1.61	0.62
1:A:675:ASP:HA	1:A:678:LYS:HE2	1.81	0.62
1:A:798:LYS:HG2	1:C:471:LYS:HD3	1.81	0.60
1:C:542:ILE:HG12	1:C:737:LEU:HD13	1.87	0.56
1:B:466:CYS:HB3	1:B:516:VAL:HG12	1.88	0.54
1:C:527:LYS:HG2	1:D:781:ILE:HD13	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:542:ILE:HB	1:A:756:ILE:HB	1.90	0.54
1:D:542:ILE:HB	1:D:756:ILE:HB	1.91	0.53
1:A:441:LEU:HD11	1:A:491:TYR:CZ	2.45	0.52
1:C:786:LEU:HD23	1:C:791:LYS:HD2	1.92	0.52
1:A:527:LYS:HG2	1:B:781:ILE:HD13	1.92	0.51
1:B:544:TYR:HE2	1:B:548:THR:HG21	1.77	0.50
1:B:670:ILE:HG22	1:B:756:ILE:HG21	1.94	0.50
1:C:441:LEU:HB3	1:C:486:VAL:HG12	1.94	0.49
1:C:685:GLY:HA2	1:C:711:MET:HG2	1.95	0.49
1:A:738:MET:HE3	1:A:743:ILE:HG12	1.94	0.49
1:D:450:ARG:NH1	1:D:460:ASP:OD1	2.46	0.49
1:D:508:ILE:HD11	1:D:528:ALA:HB1	1.95	0.48
1:C:739:GLU:OE1	1:C:765:TYR:OH	2.20	0.48
1:A:793[B]:HIS:HD2	8:B:915:GOL:H12	1.79	0.47
1:A:793[B]:HIS:CD2	8:B:915:GOL:H31	2.50	0.47
1:D:441:LEU:HD11	1:D:491:TYR:CZ	2.49	0.47
1:B:727:GLN:HE21	1:B:731:THR:HG23	1.81	0.46
1:B:441:LEU:HD11	1:B:491:TYR:CZ	2.50	0.46
1:C:716:SER:C	1:C:728:ARG:HH12	2.18	0.46
1:B:508:ILE:HD11	1:B:528:ALA:HB1	1.99	0.45
1:C:687:VAL:HG11	7:C:908:KAI:HD23	1.99	0.45
1:C:542:ILE:HB	1:C:756:ILE:HB	1.99	0.45
1:A:670:ILE:HG22	1:A:756:ILE:HG21	1.98	0.45
1:C:466:CYS:HB3	1:C:516:VAL:HG12	1.98	0.44
1:D:505:LYS:NZ	1:D:509:ASP:OD1	2.47	0.44
1:D:523:ALA:O	1:D:527:LYS:HG3	2.18	0.43
1:D:787:GLN:HG3	1:D:792:LEU:HD12	1.99	0.43
1:D:438:VAL:HG22	1:D:514:LEU:HB2	2.01	0.43
1:A:715:PRO:HD2	4:A:908:CL:CL	2.55	0.43
1:B:698:LYS:HE3	1:B:698:LYS:HB3	1.87	0.43
1:B:699:SER:O	1:B:700:LYS:HD3	2.19	0.42
1:B:704:PHE:CZ	1:B:760:ILE:HG23	2.54	0.42
1:C:454:ARG:NH2	5:C:905:SO4:O1	2.44	0.41
1:B:438:VAL:HG22	1:B:514:LEU:HB2	2.02	0.41
1:B:520:THR:HG21	1:B:763:LYS:HD2	2.02	0.41
1:B:546:LYS:HG2	1:B:754:THR:HB	2.02	0.41
1:D:725:GLY:HA3	1:D:736:LEU:HD22	2.03	0.41
1:C:744:GLU:O	1:C:748:GLN:HG3	2.21	0.41
1:A:444:GLU:HA	1:A:445:PRO:HA	1.90	0.41
1:B:719:VAL:HG11	1:B:725:GLY:HA2	2.03	0.41
1:B:540:VAL:HG23	1:B:763:LYS:HE2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:538:LEU:HB3	1:A:741:THR:HG23	2.04	0.40
1:B:494:GLN:HG3	1:B:500:TRP:CE2	2.57	0.40

There are no symmetry-related clashes.

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	252/258 (98%)	248 (98%)	4 (2%)	0	100	100
1	B	254/258 (98%)	247 (97%)	7 (3%)	0	100	100
1	C	239/258 (93%)	234 (98%)	5 (2%)	0	100	100
1	D	246/258 (95%)	242 (98%)	4 (2%)	0	100	100
All	All	991/1032 (96%)	971 (98%)	20 (2%)	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	218/220 (99%)	215 (99%)	3 (1%)	67	86
1	B	220/220 (100%)	217 (99%)	3 (1%)	67	86
1	C	210/220 (96%)	209 (100%)	1 (0%)	88	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	214/220 (97%)	213 (100%)	1 (0%)	88	96
All	All	862/880 (98%)	854 (99%)	8 (1%)	78	92

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	454	ARG
1	A	538	LEU
1	A	803	SER
1	B	538	LEU
1	B	762	SER
1	B	801	ARG
1	C	538	LEU
1	D	538	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	727	GLN
1	B	785	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 46 ligands modelled in this entry, 20 are monoatomic - leaving 26 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ACT	A	901	-	3,3,3	1.26	0	3,3,3	1.41	0
2	ACT	D	901	3	3,3,3	1.31	0	3,3,3	1.51	0
5	SO4	D	906	-	4,4,4	0.14	0	6,6,6	0.04	0
2	ACT	D	902	-	3,3,3	1.30	0	3,3,3	1.38	0
6	PEG	A	913	-	6,6,6	0.12	0	5,5,5	0.08	0
8	GOL	D	908	-	5,5,5	0.91	0	5,5,5	0.99	0
2	ACT	A	902	-	3,3,3	1.28	0	3,3,3	1.37	0
8	GOL	B	914	-	5,5,5	0.90	0	5,5,5	1.00	0
7	KAI	C	908	-	13,15,15	1.42	2 (15%)	14,21,21	0.98	0
7	KAI	A	914	-	13,15,15	1.40	2 (15%)	14,21,21	1.01	0
8	GOL	A	915	-	5,5,5	0.89	0	5,5,5	1.05	0
5	SO4	C	905	-	4,4,4	0.14	0	6,6,6	0.05	0
8	GOL	B	915	-	5,5,5	0.93	0	5,5,5	0.97	0
7	KAI	D	907	-	13,15,15	1.41	3 (23%)	14,21,21	1.06	0
2	ACT	B	901	-	3,3,3	1.33	0	3,3,3	1.52	0
2	ACT	C	901	-	3,3,3	1.26	0	3,3,3	1.54	0
5	SO4	A	910	3	4,4,4	0.14	0	6,6,6	0.04	0
5	SO4	A	912	-	4,4,4	0.44	0	6,6,6	0.05	0
5	SO4	A	911	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	B	910	-	4,4,4	0.15	0	6,6,6	0.04	0
5	SO4	C	906	-	4,4,4	0.14	0	6,6,6	0.05	0
8	GOL	B	913	-	5,5,5	0.91	0	5,5,5	1.07	0
5	SO4	A	909	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	B	911	3	4,4,4	0.13	0	6,6,6	0.05	0
5	SO4	C	907	-	4,4,4	0.13	0	6,6,6	0.05	0
7	KAI	B	912	-	13,15,15	1.43	2 (15%)	14,21,21	0.97	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
6	PEG	A	913	-	-	1/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	KAI	A	914	-	-	0/12/25/25	0/1/1/1
8	GOL	D	908	-	-	0/4/4/4	-
8	GOL	A	915	-	-	0/4/4/4	-
8	GOL	B	914	-	-	0/4/4/4	-
8	GOL	B	915	-	-	0/4/4/4	-
8	GOL	B	913	-	-	0/4/4/4	-
7	KAI	D	907	-	-	0/12/25/25	0/1/1/1
7	KAI	C	908	-	-	4/12/25/25	0/1/1/1
7	KAI	B	912	-	-	2/12/25/25	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	912	KAI	CA-C	2.62	1.56	1.52
7	C	908	KAI	CA-C	2.58	1.56	1.52
7	D	907	KAI	CA-C	2.58	1.56	1.52
7	A	914	KAI	CA-C	2.56	1.56	1.52
7	A	914	KAI	CB1-CB	2.09	1.57	1.53
7	C	908	KAI	CB1-CB	2.07	1.57	1.53
7	D	907	KAI	CB1-CB	2.07	1.57	1.53
7	B	912	KAI	CB1-CB	2.04	1.56	1.53
7	D	907	KAI	CD-N	2.00	1.54	1.47

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

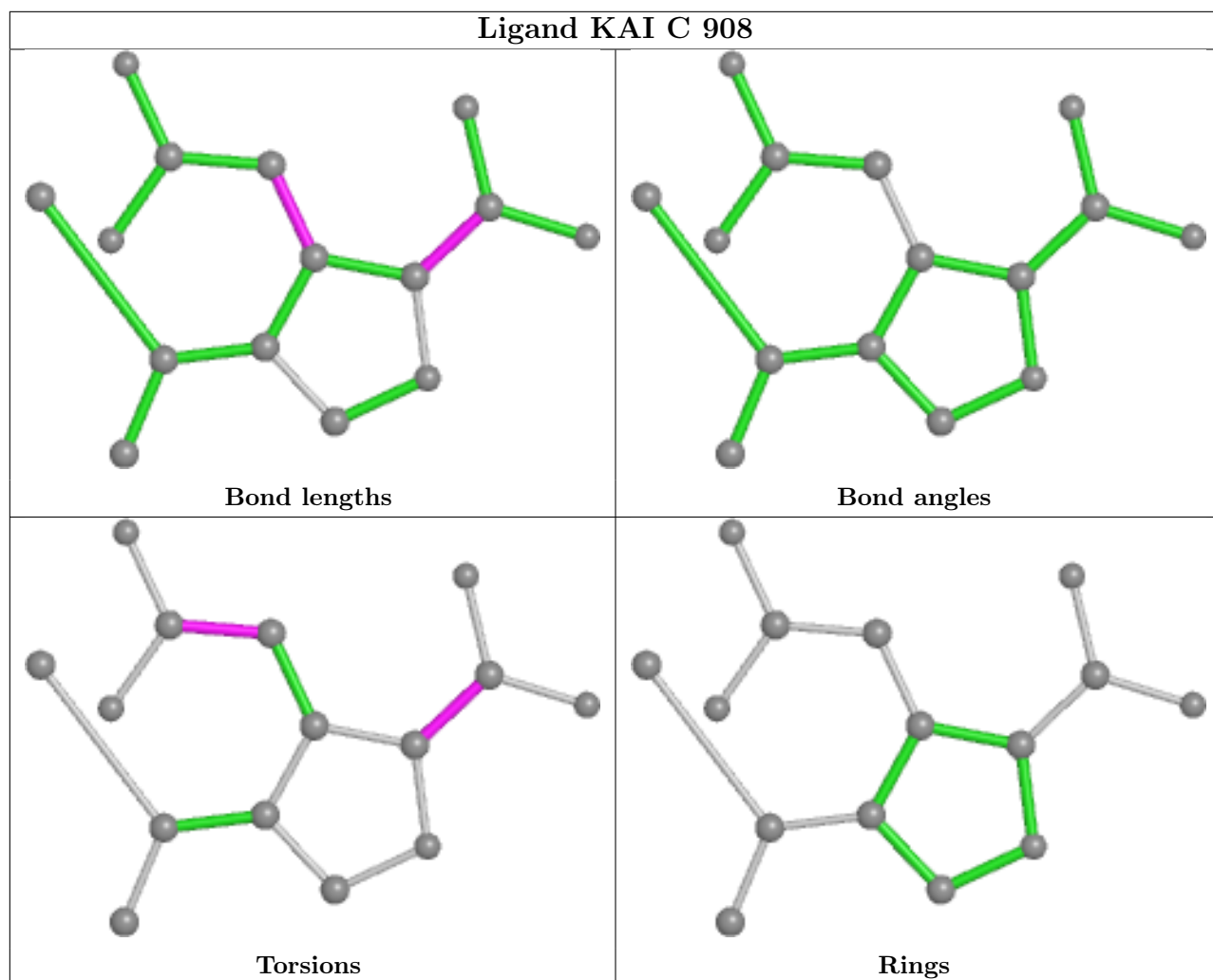
Mol	Chain	Res	Type	Atoms
6	A	913	PEG	C4-C3-O2-C2
7	B	912	KAI	CB-CB1-CG1-OD1
7	B	912	KAI	CB-CB1-CG1-OD2
7	C	908	KAI	CB-CB1-CG1-OD1
7	C	908	KAI	O-C-CA-CB
7	C	908	KAI	OXT-C-CA-CB
7	C	908	KAI	CB-CB1-CG1-OD2

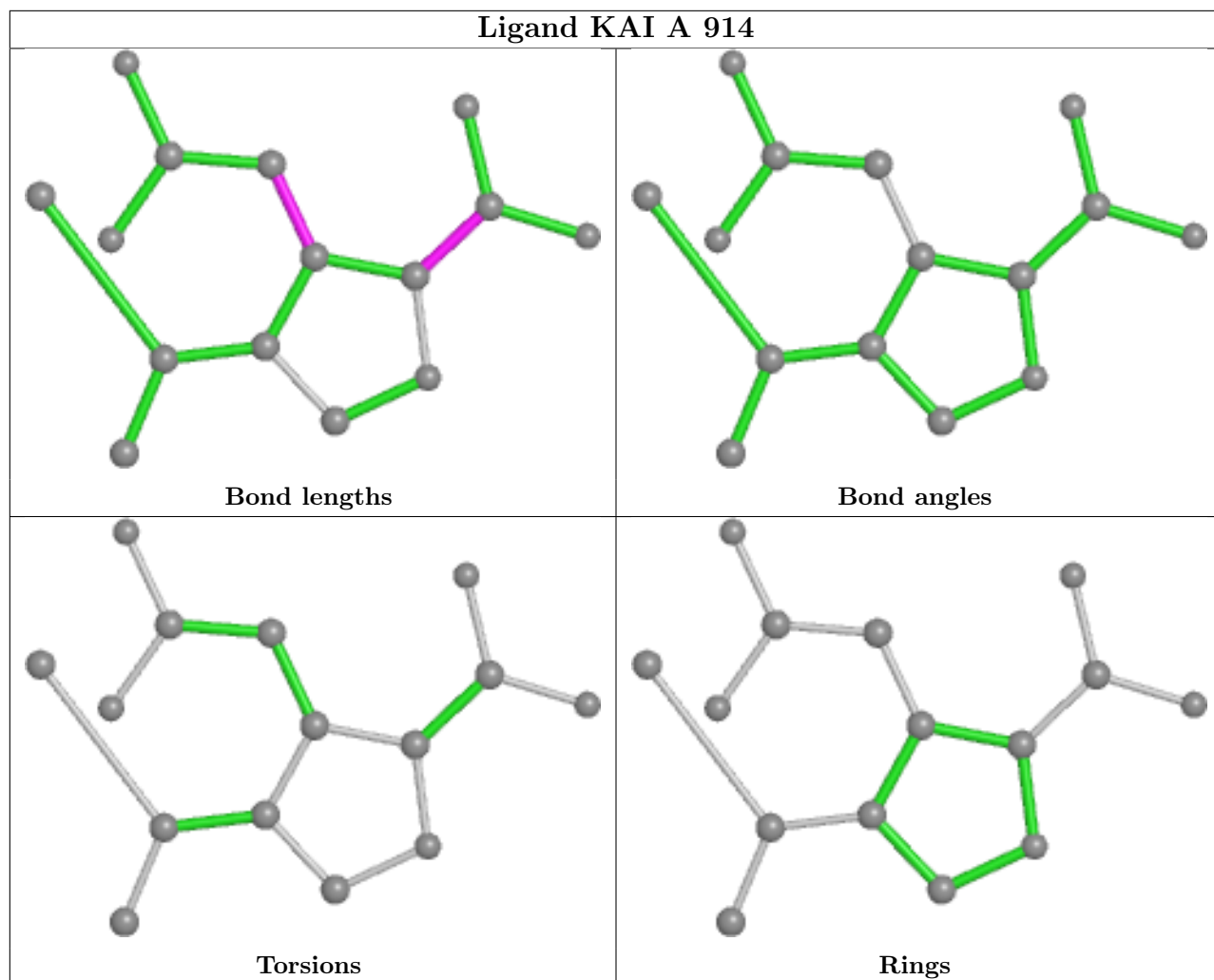
There are no ring outliers.

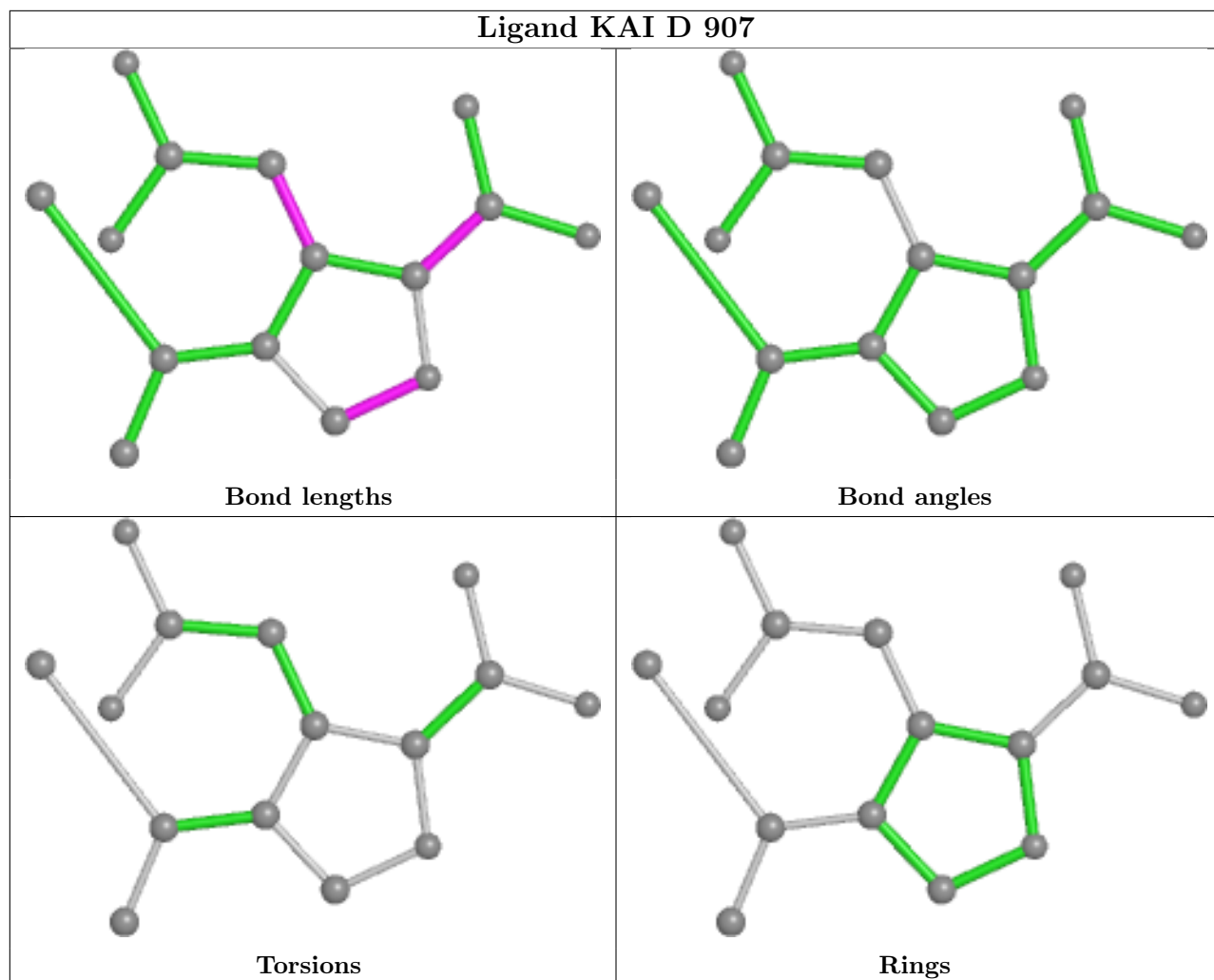
3 monomers are involved in 4 short contacts:

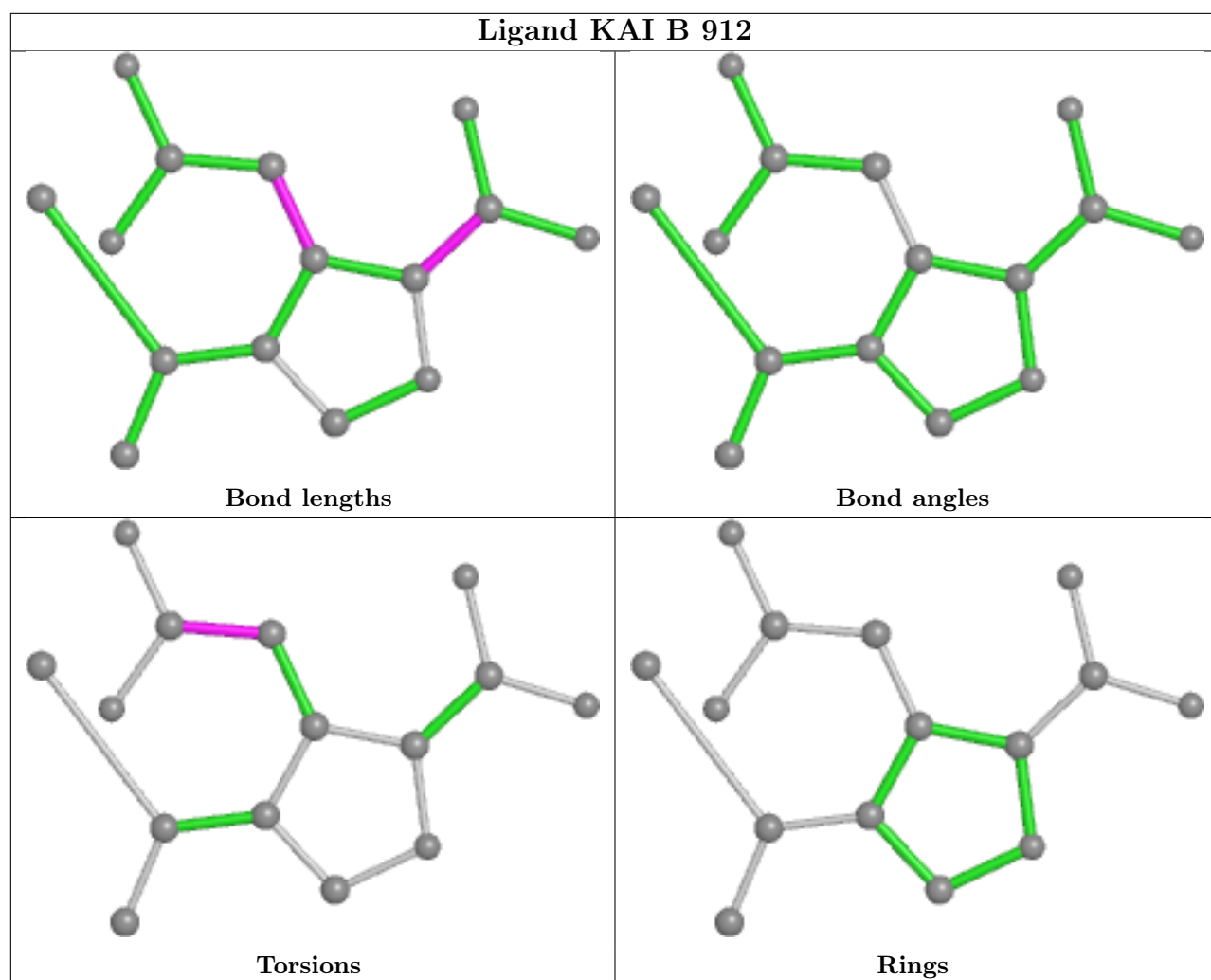
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	908	KAI	1	0
5	C	905	SO4	1	0
8	B	915	GOL	2	0

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 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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	252/258 (97%)	0.42	18 (7%) 16 14	30, 48, 96, 117	0
1	B	253/258 (98%)	0.40	19 (7%) 14 12	28, 50, 95, 118	0
1	C	242/258 (93%)	0.81	38 (15%) 2 1	31, 58, 119, 158	0
1	D	247/258 (95%)	0.34	11 (4%) 33 31	36, 54, 89, 110	0
All	All	994/1032 (96%)	0.49	86 (8%) 10 8	28, 53, 104, 158	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	544	TYR	7.1
1	C	730	LEU	6.1
1	C	733	ASP	6.0
1	C	735	ALA	5.6
1	C	734	TYR	5.0
1	C	714	LYS	4.9
1	C	679	GLN	4.6
1	C	752	ASN	4.6
1	C	753	LEU	4.3
1	C	756	ILE	4.3
1	C	755	GLN	4.3
1	C	682	ILE	4.3
1	C	545	ARG	4.2
1	C	713	SER	4.2
1	C	676	LEU	4.1
1	A	497	LYS	4.0
1	C	680	THR	4.0
1	C	678	LYS	4.0
1	C	732	ALA	3.9
1	B	545	ARG	3.8
1	A	669	PRO	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	750	ASN	3.7
1	A	547	GLY	3.6
1	A	676	LEU	3.5
1	D	547	GLY	3.4
1	D	750	ASN	3.4
1	B	669	PRO	3.4
1	B	547	GLY	3.4
1	A	754	THR	3.3
1	A	670	ILE	3.3
1	B	677	ALA	3.2
1	A	496	ASP	3.2
1	D	753	LEU	3.2
1	B	544	TYR	3.2
1	C	542	ILE	3.2
1	C	731	THR	3.1
1	C	726	ILE	3.1
1	D	731	THR	3.1
1	B	678	LYS	3.1
1	D	752	ASN	3.1
1	C	748	GLN	3.1
1	D	748	GLN	3.0
1	A	756	ILE	3.0
1	C	717	ALA	3.0
1	A	544	TYR	2.8
1	B	806	PRO	2.8
1	C	543	LEU	2.8
1	A	803	SER	2.8
1	B	715	PRO	2.7
1	C	684	TYR	2.7
1	A	672	SER	2.7
1	B	671	ASP	2.7
1	C	677	ALA	2.6
1	B	733	ASP	2.6
1	A	457	TYR	2.6
1	B	732	ALA	2.6
1	C	706	LYS	2.6
1	B	685	GLY	2.6
1	C	751	CYS	2.6
1	C	754	THR	2.5
1	D	730	LEU	2.5
1	D	670	ILE	2.5
1	B	804	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	749	ARG	2.4
1	C	711	MET	2.4
1	B	756	ILE	2.4
1	D	733	ASP	2.3
1	A	455	THR	2.3
1	A	678	LYS	2.3
1	A	671	ASP	2.3
1	A	454	ARG	2.3
1	C	727	GLN	2.2
1	A	680	THR	2.2
1	C	671	ASP	2.2
1	B	680	THR	2.2
1	C	683	GLU	2.2
1	A	456	LEU	2.1
1	C	737	LEU	2.1
1	B	681	LYS	2.1
1	C	736	LEU	2.1
1	B	711	MET	2.1
1	B	727	GLN	2.1
1	C	672	SER	2.0
1	D	676	LEU	2.0
1	D	754	THR	2.0
1	B	676	LEU	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

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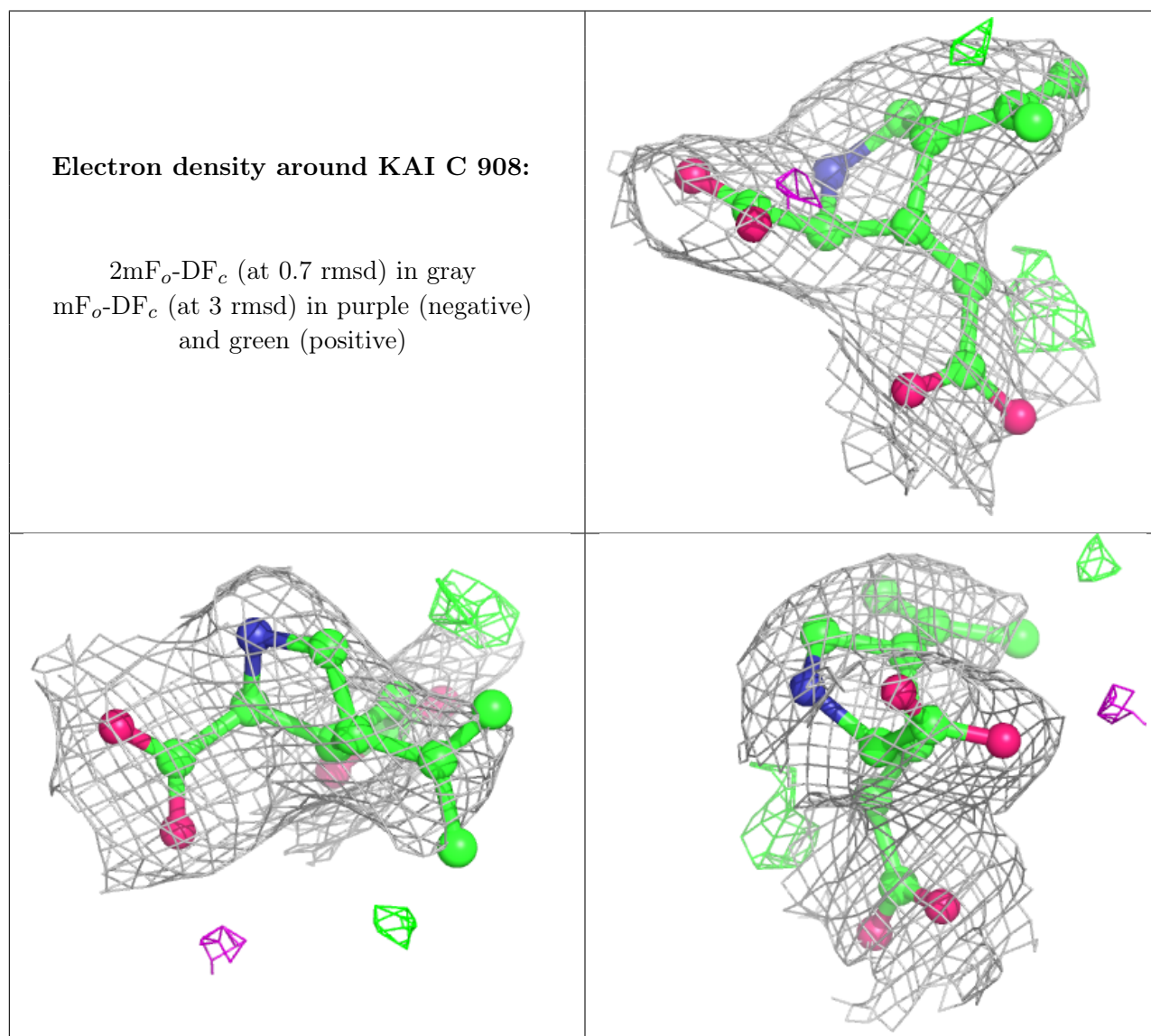
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	ZN	B	907[B]	1/1	0.45	0.16	79,79,79,79	1
3	ZN	C	902[A]	1/1	0.59	0.16	64,64,64,64	1
3	ZN	D	903	1/1	0.63	0.14	93,93,93,93	1
6	PEG	A	913	7/7	0.64	0.36	52,56,64,67	0
3	ZN	B	906[B]	1/1	0.67	0.37	51,51,51,51	1
2	ACT	D	901	4/4	0.72	0.62	54,60,67,68	4
2	ACT	C	901	4/4	0.74	0.29	56,61,64,64	0
5	SO4	C	907	5/5	0.77	0.36	57,60,63,64	5
3	ZN	B	902[A]	1/1	0.77	0.13	84,84,84,84	1
2	ACT	A	902	4/4	0.81	0.24	53,54,61,63	0
3	ZN	B	904[B]	1/1	0.81	0.12	72,72,72,72	1
3	ZN	A	906[B]	1/1	0.82	0.44	43,43,43,43	1
5	SO4	A	909	5/5	0.82	0.27	71,82,91,121	0
5	SO4	B	911	5/5	0.83	0.32	55,57,62,68	5
4	CL	A	907	1/1	0.83	0.18	56,56,56,56	0
5	SO4	A	912	5/5	0.83	0.21	75,78,86,87	5
8	GOL	A	915	6/6	0.85	0.41	54,57,60,61	6
7	KAI	C	908	15/15	0.86	0.23	39,48,55,66	0
4	CL	C	904	1/1	0.86	0.15	48,48,48,48	0
8	GOL	B	915	6/6	0.86	0.22	52,58,60,62	0
3	ZN	C	903	1/1	0.87	0.09	90,90,90,90	1
8	GOL	B	914	6/6	0.87	0.30	53,56,61,62	0
2	ACT	B	901	4/4	0.87	0.21	44,50,51,51	0
8	GOL	D	908	6/6	0.88	0.23	51,52,55,57	0
4	CL	A	908	1/1	0.89	0.15	89,89,89,89	0
3	ZN	B	905[A]	1/1	0.89	0.36	72,72,72,72	1
4	CL	B	909	1/1	0.90	0.47	74,74,74,74	0
5	SO4	B	910	5/5	0.90	0.21	47,51,59,68	5
5	SO4	A	910	5/5	0.90	0.14	60,66,73,81	5
8	GOL	B	913	6/6	0.90	0.25	42,48,53,54	0
5	SO4	C	906	5/5	0.90	0.27	46,60,61,64	5
5	SO4	A	911	5/5	0.90	0.22	50,55,61,67	5
5	SO4	D	906	5/5	0.90	0.17	75,77,82,98	0
3	ZN	B	903[A]	1/1	0.91	0.19	94,94,94,94	1
4	CL	D	904	1/1	0.91	0.15	55,55,55,55	0
4	CL	B	908	1/1	0.92	0.12	42,42,42,42	0
7	KAI	A	914	15/15	0.92	0.24	36,38,48,51	0
2	ACT	D	902	4/4	0.93	0.22	42,49,55,57	0
7	KAI	B	912	15/15	0.93	0.22	34,40,47,48	0
7	KAI	D	907	15/15	0.94	0.20	29,40,43,52	0
2	ACT	A	901	4/4	0.94	0.14	44,46,47,57	0

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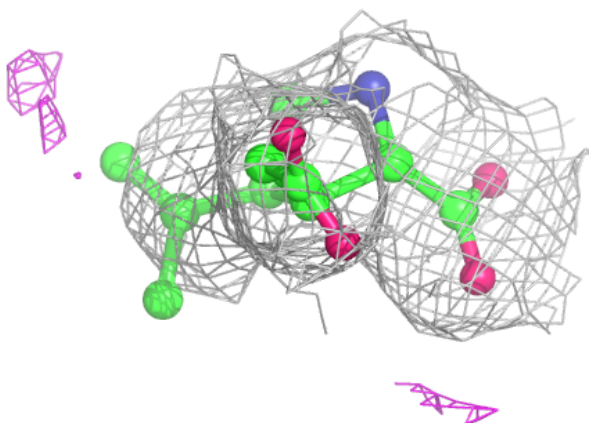
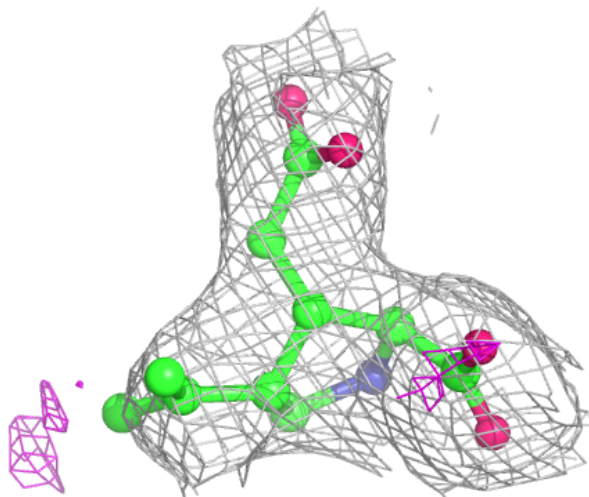
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	CL	D	905	1/1	0.95	0.17	46,46,46,46	0
3	ZN	A	904	1/1	0.96	0.18	68,68,68,68	1
5	SO4	C	905	5/5	0.97	0.13	53,59,70,71	0
3	ZN	A	905	1/1	0.97	0.04	87,87,87,87	1
3	ZN	A	903[A]	1/1	0.98	0.10	41,41,41,41	1

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.



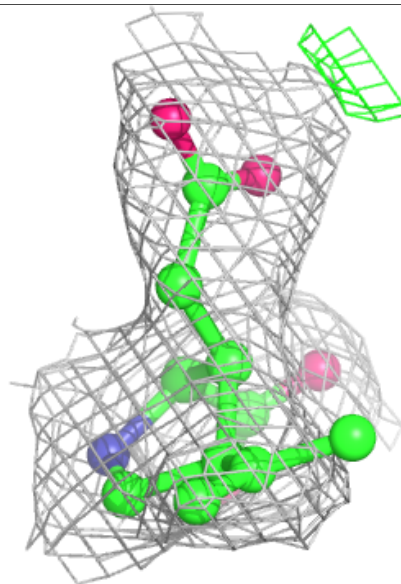
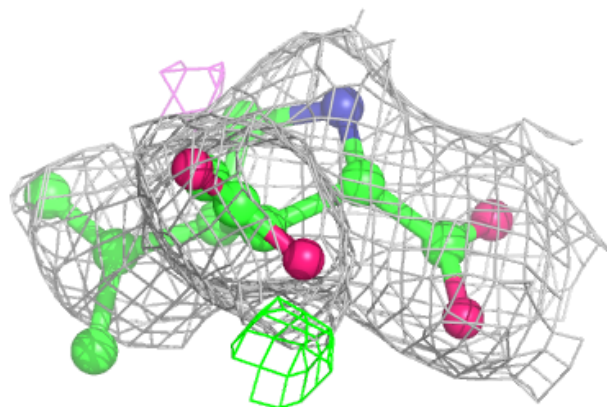
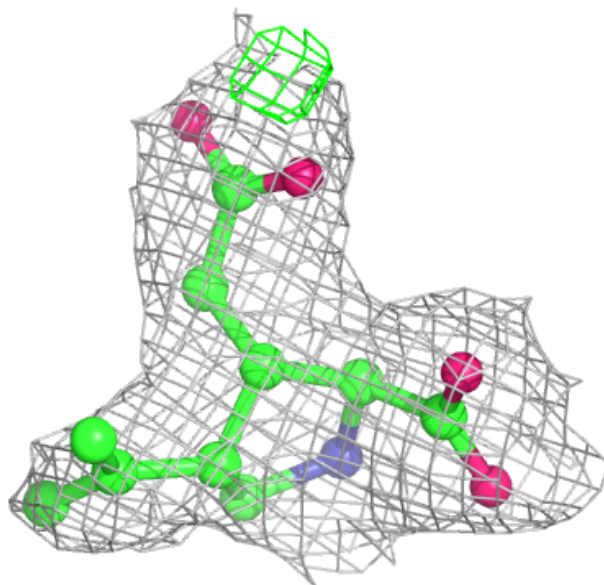
Electron density around KAI A 914:

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



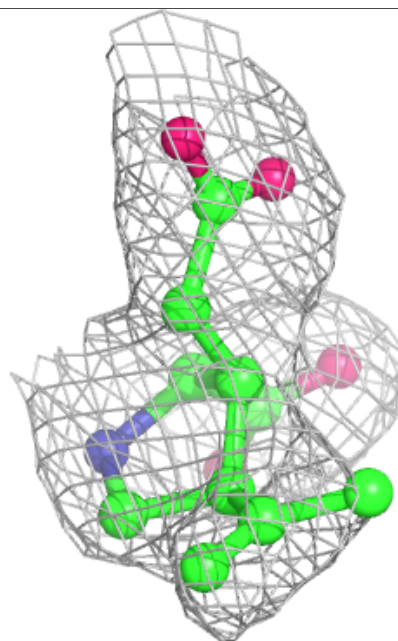
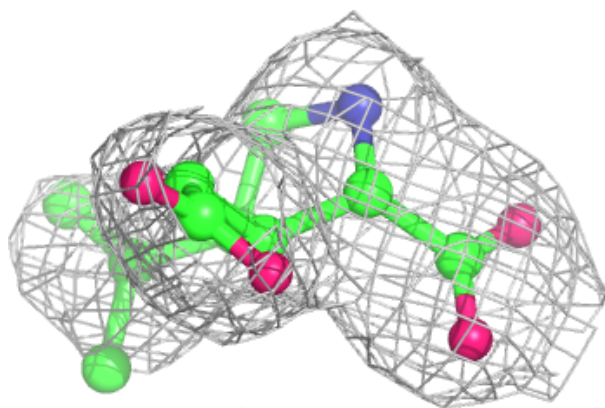
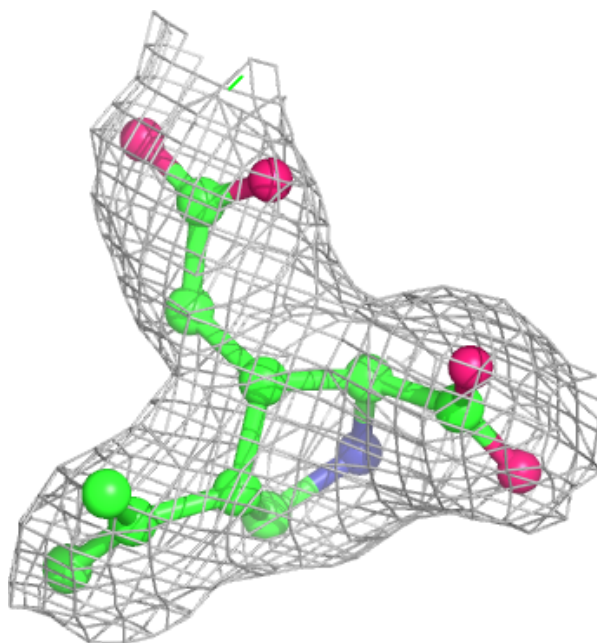
Electron density around KAI B 912:

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



Electron density around KAI D 907:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.