wwPDB X-ray Structure Validation Summary Report (i)

Sep 15, 2022 – 04:32 pm BST

PDB ID	:	8A0B
Title	:	Inhibitor binding to HDAC2
Authors	:	Cleasby, A.; Tisi, D.
Deposited on	:	2022-05-27
Resolution	:	1.75 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

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

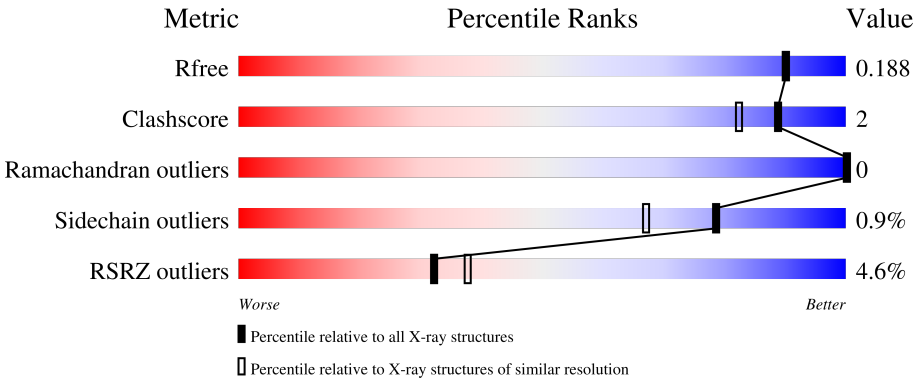
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.30
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.30

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 1.75 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	3764 (1.76-1.72)
Clashscore	141614	3923 (1.76-1.72)
Ramachandran outliers	138981	3878 (1.76-1.72)
Sidechain outliers	138945	3878 (1.76-1.72)
RSRZ outliers	127900	3705 (1.76-1.72)

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	498	% 71% . 26%
1	B	498	70% . 26%
1	C	498	9% 70% . 27%

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 9947 atoms, of which 63 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 Histone deacetylase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	369	Total	C	N	O	S	0	4	0
			2991	1911	506	548	26			
1	B	367	Total	C	N	O	S	0	4	0
			2981	1903	502	549	27			
1	C	366	Total	C	N	O	S	0	2	0
			2959	1891	498	545	25			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	493	GLY	-	expression tag	UNP Q92769
A	494	SER	-	expression tag	UNP Q92769
A	495	SER	-	expression tag	UNP Q92769
A	496	GLY	-	expression tag	UNP Q92769
A	497	HIS	-	expression tag	UNP Q92769
A	498	HIS	-	expression tag	UNP Q92769
A	499	HIS	-	expression tag	UNP Q92769
A	500	HIS	-	expression tag	UNP Q92769
A	501	HIS	-	expression tag	UNP Q92769
A	502	HIS	-	expression tag	UNP Q92769
B	493	GLY	-	expression tag	UNP Q92769
B	494	SER	-	expression tag	UNP Q92769
B	495	SER	-	expression tag	UNP Q92769
B	496	GLY	-	expression tag	UNP Q92769
B	497	HIS	-	expression tag	UNP Q92769
B	498	HIS	-	expression tag	UNP Q92769
B	499	HIS	-	expression tag	UNP Q92769
B	500	HIS	-	expression tag	UNP Q92769
B	501	HIS	-	expression tag	UNP Q92769
B	502	HIS	-	expression tag	UNP Q92769
C	493	GLY	-	expression tag	UNP Q92769
C	494	SER	-	expression tag	UNP Q92769
C	495	SER	-	expression tag	UNP Q92769

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Chain	Residue	Modelled	Actual	Comment	Reference
C	496	GLY	-	expression tag	UNP Q92769
C	497	HIS	-	expression tag	UNP Q92769
C	498	HIS	-	expression tag	UNP Q92769
C	499	HIS	-	expression tag	UNP Q92769
C	500	HIS	-	expression tag	UNP Q92769
C	501	HIS	-	expression tag	UNP Q92769
C	502	HIS	-	expression tag	UNP Q92769

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0
2	B	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0

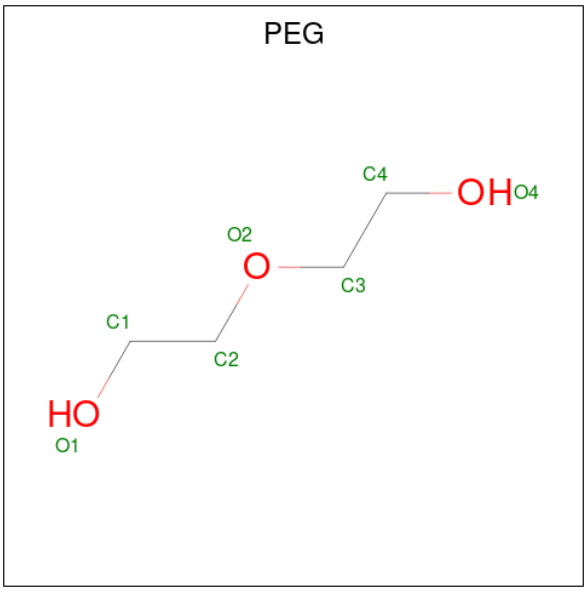
- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Ca 1 1	0	0
3	B	1	Total Ca 1 1	0	0
3	C	1	Total Ca 1 1	0	0

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

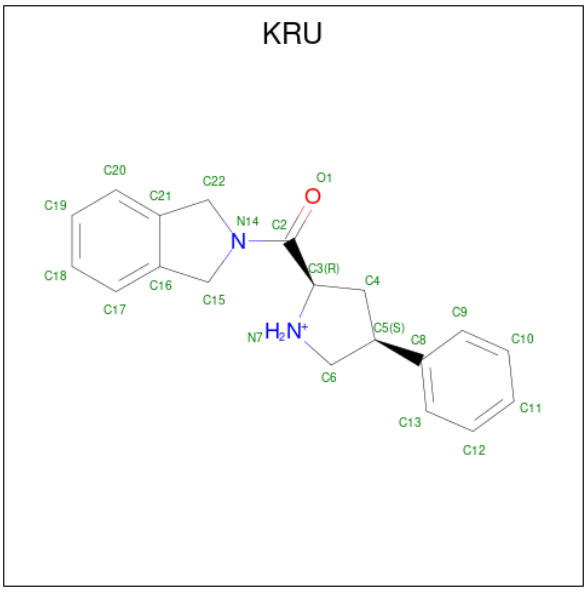
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Na 1 1	0	0
4	B	1	Total Na 1 1	0	0
4	C	1	Total Na 1 1	0	0

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



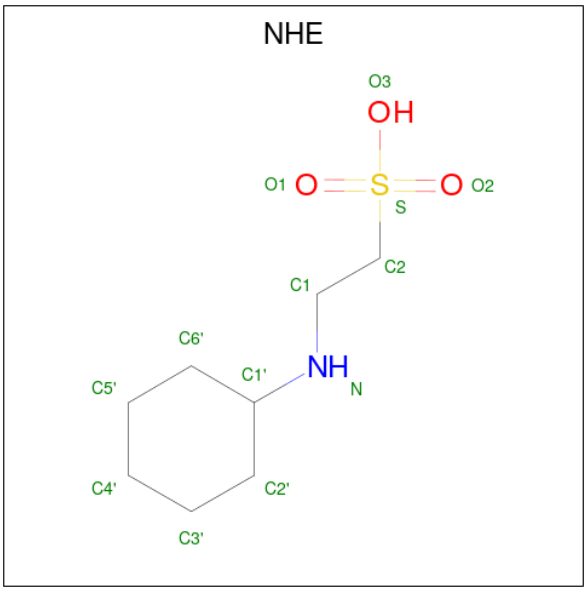
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 7 4 3	0	0
5	B	1	Total C O 7 4 3	0	0
5	B	1	Total C O 7 4 3	0	0
5	B	1	Total C O 7 4 3	0	0
5	C	1	Total C O 7 4 3	0	0

- Molecule 6 is 1,3-dihydroisoindol-2-yl-[(2R,4S)-4-phenylpyrrolidin-1-ium-2-yl]metha none (three-letter code: KRU) (formula: $C_{19}H_{21}N_2O$) (labeled as "Ligand of Interest" by depositor).



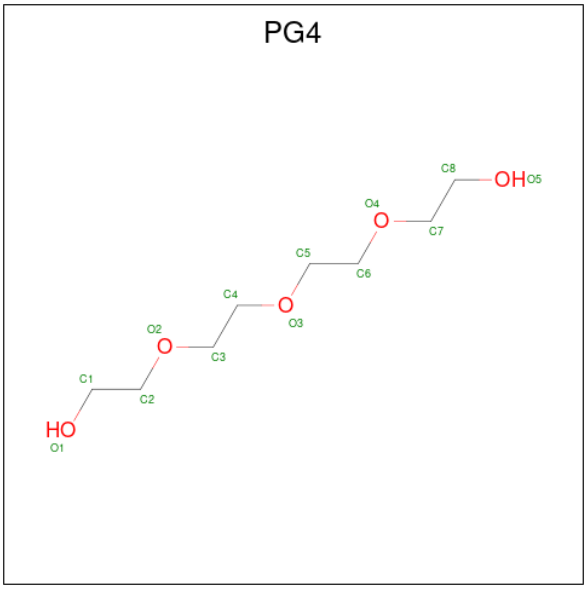
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	H	N	O	0	0
			43	19	21	2	1		
6	B	1	Total	C	H	N	O	0	0
			43	19	21	2	1		
6	C	1	Total	C	H	N	O	0	0
			43	19	21	2	1		

- Molecule 7 is 2-[N-CYCLOHEXYLAMINO]ETHANE SULFONIC ACID (three-letter code: NHE) (formula: $C_8H_{17}NO_3S$).



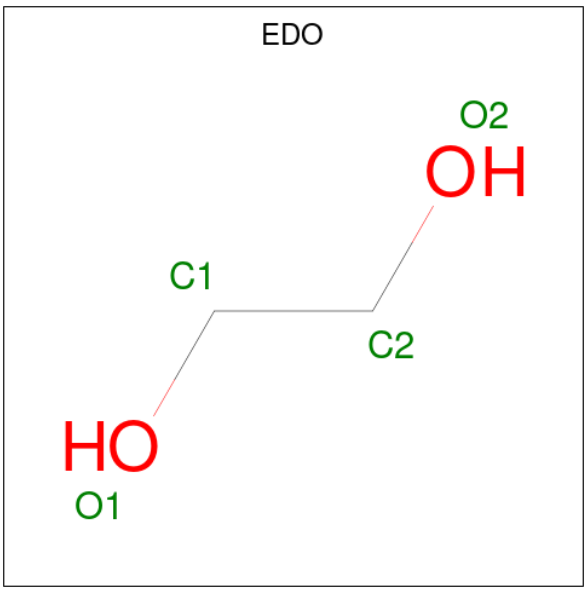
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	B	1	Total	C	N	O	S	0	0
			13	8	1	3	1		

- Molecule 8 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			13	8	5		

- Molecule 9 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	C	1	Total C O 4 2 2	0	0

- Molecule 10 is water.

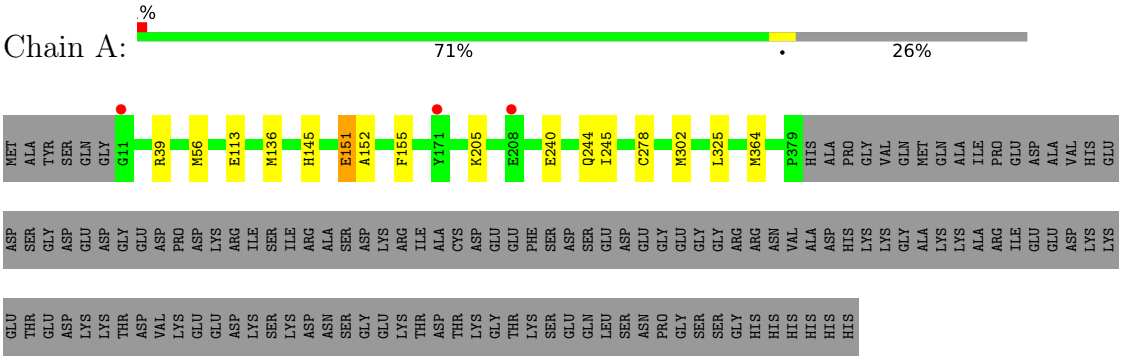
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	309	Total O 309 309	0	0
10	B	321	Total O 321 321	0	0
10	C	183	Total O 183 183	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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.

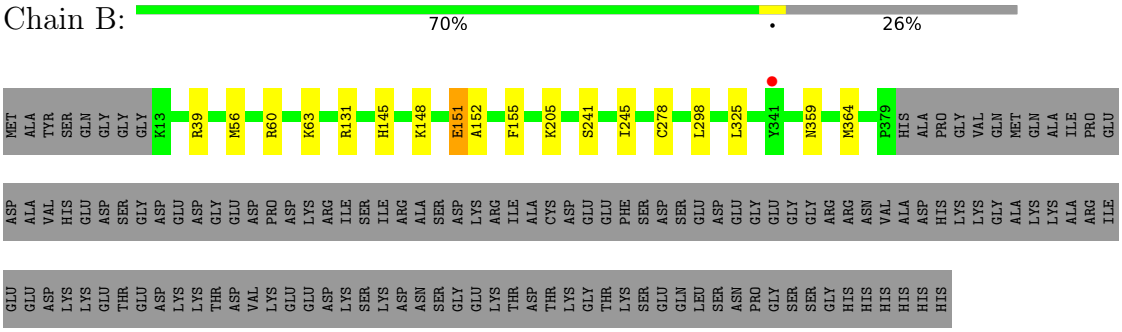
• Molecule 1: Histone deacetylase 2

Chain A:



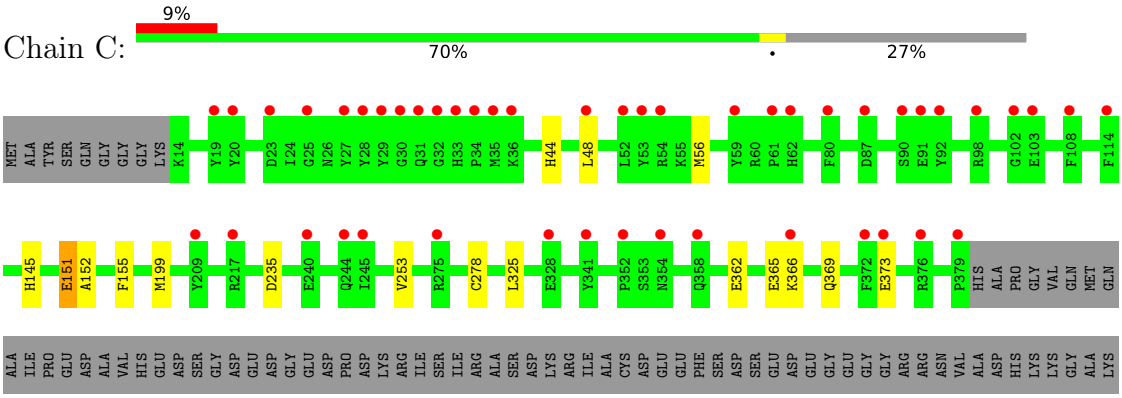
• Molecule 1: Histone deacetylase 2

Chain B:



• Molecule 1: Histone deacetylase 2

Chain C:



LYS ALA ARG ILE GLU GLU ASP LYS LYS GLU THR GLU ASP LYS LYS THR ASP VAL LYS GLU GLU ASP LYS SER LYS ASP ASN SER GLY GLU LYS THR ASP THR LYS GLY THR LYS SER GLU GLN LEU SER ASN PRO GLY SER SER GLY HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	92.22Å 98.02Å 139.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	67.17 – 1.75 80.18 – 1.75	Depositor EDS
% Data completeness (in resolution range)	96.9 (67.17-1.75) 96.9 (80.18-1.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.07 (at 1.75Å)	Xtriage
Refinement program	BUSTER 2.11.8 (16-JUL-2021)	Depositor
R, R_{free}	0.165 , 0.188 0.170 , 0.188	Depositor DCC
R_{free} test set	6193 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	24.7	Xtriage
Anisotropy	0.453	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	9947	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.49% 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: CA, PEG, KRU, NA, EDO, NHE, ZN, PG4

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	0.68	0/3078	0.68	1/4153 (0.0%)
1	B	0.74	0/3065	0.70	1/4137 (0.0%)
1	C	0.59	0/3042	0.64	0/4107
All	All	0.67	0/9185	0.67	2/12397 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	39	ARG	CG-CD-NE	-5.64	99.96	111.80
1	B	39	ARG	CG-CD-NE	-5.30	100.66	111.80

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	2991	0	2907	10	0
1	B	2981	0	2885	15	0
1	C	2959	0	2869	8	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
5	A	7	0	10	0	0
5	B	21	0	30	1	0
5	C	7	0	10	2	0
6	A	22	21	0	0	0
6	B	22	21	0	0	0
6	C	22	21	0	0	0
7	B	13	0	16	5	0
8	B	13	0	18	0	0
9	C	4	0	6	0	0
10	A	309	0	0	0	0
10	B	321	0	0	2	0
10	C	183	0	0	2	0
All	All	9884	63	8751	34	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 2.

The worst 5 of 34 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:63:LYS:HE3	7:B:604:NHE:H3'2	1.49	0.94
1:B:63:LYS:CE	7:B:604:NHE:H3'2	2.06	0.85
1:B:148:LYS:HE3	10:B:725:HOH:O	1.96	0.66
1:B:63:LYS:CE	7:B:604:NHE:C3'	2.77	0.61
1:A:205:LYS:HD2	1:A:278[B]:CYS:SG	2.41	0.60

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	371/498 (74%)	367 (99%)	4 (1%)	0	100	100
1	B	369/498 (74%)	364 (99%)	5 (1%)	0	100	100
1	C	366/498 (74%)	361 (99%)	5 (1%)	0	100	100
All	All	1106/1494 (74%)	1092 (99%)	14 (1%)	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	321/425 (76%)	318 (99%)	3 (1%)	78	67
1	B	321/425 (76%)	318 (99%)	3 (1%)	78	67
1	C	318/425 (75%)	315 (99%)	3 (1%)	78	67
All	All	960/1275 (75%)	951 (99%)	9 (1%)	78	67

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	151	GLU
1	C	155	PHE
1	B	145	HIS
1	B	151	GLU
1	B	155	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 20 ligands modelled in this entry, 9 are monoatomic - leaving 11 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	$\#\|Z\| > 2$
5	PEG	B	608	-	6,6,6	0.52	0	5,5,5	0.34	0
6	KRU	B	609	2	25,25,25	0.57	1 (4%)	28,35,35	0.49	0
5	PEG	A	604	-	6,6,6	0.25	0	5,5,5	0.18	0
6	KRU	C	606	2	25,25,25	0.41	0	28,35,35	0.49	0
5	PEG	B	605	-	6,6,6	0.24	0	5,5,5	0.33	0
5	PEG	B	607	-	6,6,6	0.18	0	5,5,5	0.28	0
5	PEG	C	604	-	6,6,6	0.43	0	5,5,5	0.19	0
9	EDO	C	605	-	3,3,3	0.66	0	2,2,2	0.31	0
6	KRU	A	605	2	25,25,25	0.65	1 (4%)	28,35,35	0.49	0
7	NHE	B	604	-	13,13,13	0.57	0	16,17,17	1.04	1 (6%)
8	PG4	B	606	-	12,12,12	0.33	0	11,11,11	0.40	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
5	PEG	B	608	-	-	2/4/4/4	-
6	KRU	B	609	2	-	0/12/29/29	0/4/4/4
5	PEG	A	604	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	KRU	C	606	2	-	0/12/29/29	0/4/4/4
5	PEG	B	605	-	-	1/4/4/4	-
5	PEG	B	607	-	-	1/4/4/4	-
5	PEG	C	604	-	-	1/4/4/4	-
9	EDO	C	605	-	-	0/1/1/1	-
6	KRU	A	605	2	-	0/12/29/29	0/4/4/4
7	NHE	B	604	-	-	2/7/15/15	0/1/1/1
8	PG4	B	606	-	-	1/10/10/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	605	KRU	C6-C5	-2.29	1.51	1.54
6	B	609	KRU	C6-C5	-2.12	1.52	1.54

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B	604	NHE	C3'-C2'-C1'	2.84	116.45	111.11

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	607	PEG	O2-C3-C4-O4
5	B	608	PEG	O2-C3-C4-O4
5	A	604	PEG	O1-C1-C2-O2
5	A	604	PEG	O2-C3-C4-O4
7	B	604	NHE	C1-C2-S-O1

There are no ring outliers.

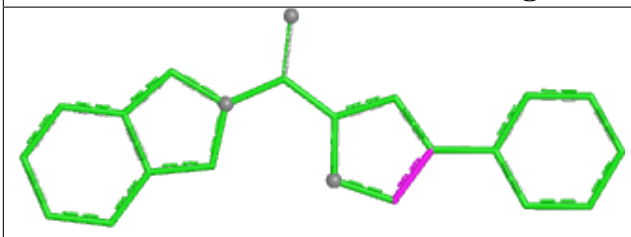
3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	605	PEG	1	0
5	C	604	PEG	2	0
7	B	604	NHE	5	0

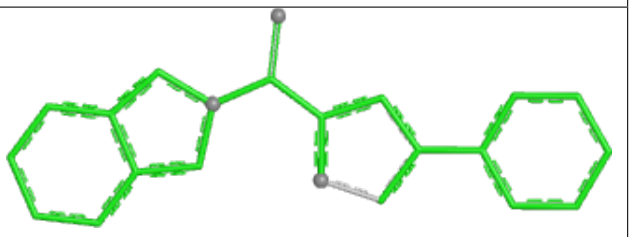
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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.

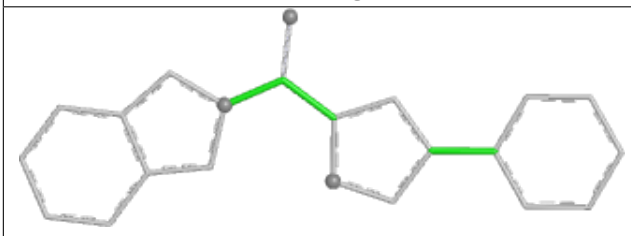
Ligand KRU B 609



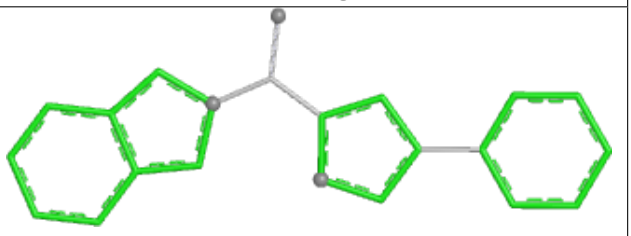
Bond lengths



Bond angles

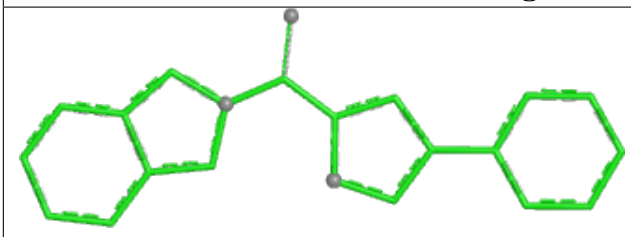


Torsions

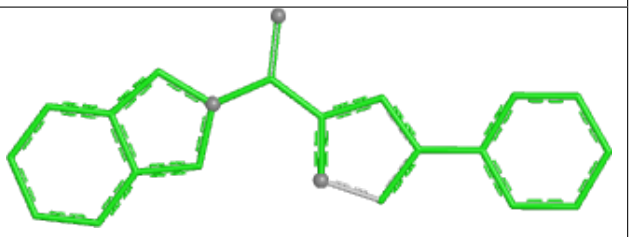


Rings

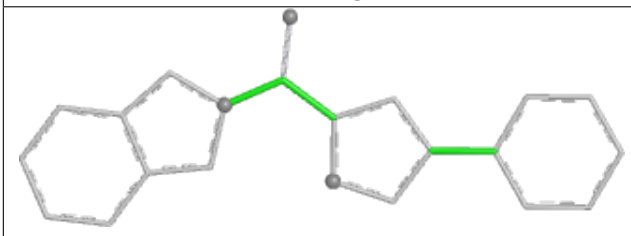
Ligand KRU C 606



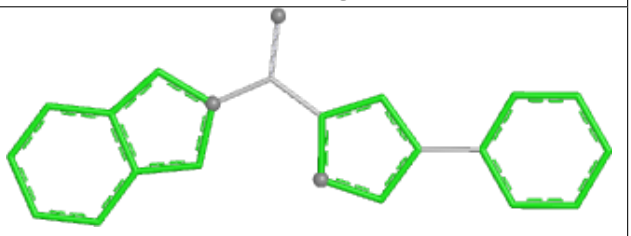
Bond lengths



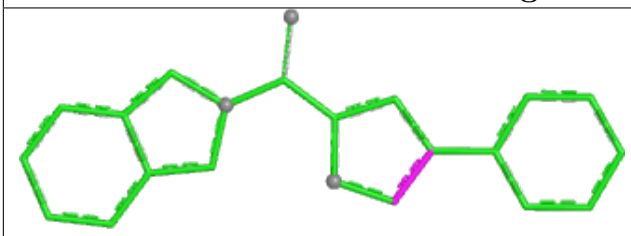
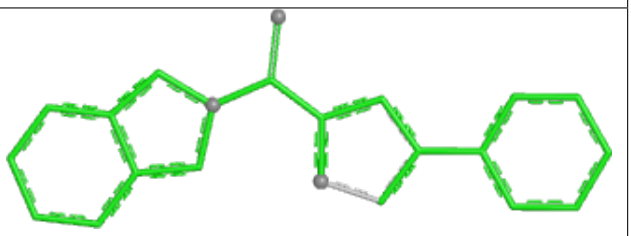
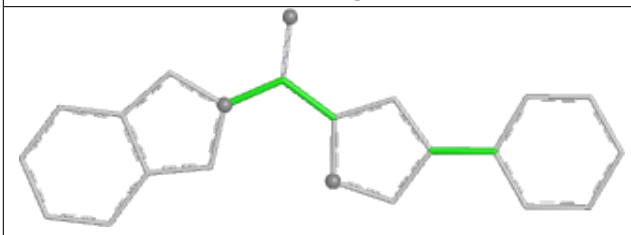
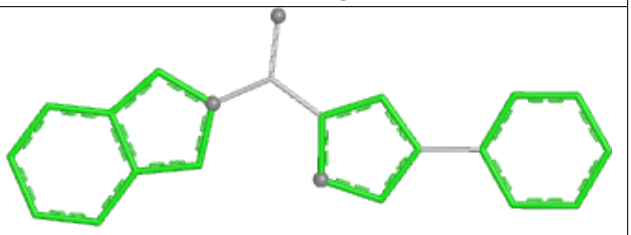
Bond angles



Torsions



Rings

Ligand KRU A 605	
 Bond lengths	 Bond angles
 Torsions	 Rings

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	369/498 (74%)	-0.03	3 (0%) 86 90	19, 26, 45, 67	0
1	B	367/498 (73%)	-0.07	1 (0%) 94 95	16, 25, 44, 57	0
1	C	366/498 (73%)	0.66	47 (12%) 3 4	25, 37, 56, 69	0
All	All	1102/1494 (73%)	0.19	51 (4%) 32 38	16, 29, 52, 69	0

The worst 5 of 51 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	379	PRO	7.7
1	C	32	GLY	6.1
1	C	341	TYR	5.7
1	C	31	GLN	5.1
1	C	48	LEU	5.1

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

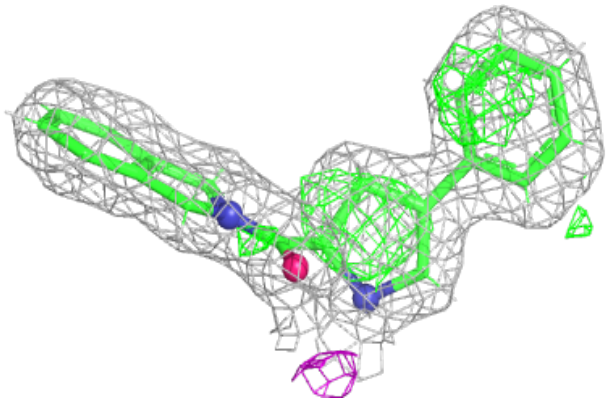
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

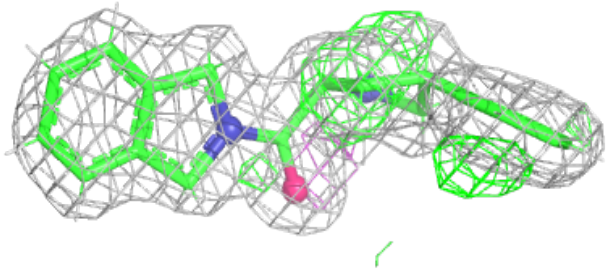
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	EDO	C	605	4/4	0.56	0.15	61,62,62,62	0
5	PEG	B	608	7/7	0.71	0.19	52,53,54,55	0
5	PEG	A	604	7/7	0.79	0.16	56,57,59,59	0
5	PEG	B	605	7/7	0.84	0.14	44,47,52,53	0
8	PG4	B	606	13/13	0.85	0.14	40,44,46,47	0
7	NHE	B	604	13/13	0.86	0.17	29,31,38,39	13
5	PEG	C	604	7/7	0.88	0.11	41,43,46,48	0
5	PEG	B	607	7/7	0.88	0.13	49,49,51,51	0
6	KRU	C	606	22/22	0.93	0.18	15,18,24,24	43
6	KRU	B	609	22/22	0.97	0.09	18,20,26,27	0
6	KRU	A	605	22/22	0.98	0.07	19,22,28,28	0
4	NA	C	603	1/1	0.98	0.10	30,30,30,30	0
3	CA	C	602	1/1	0.99	0.10	35,35,35,35	0
4	NA	A	603	1/1	0.99	0.07	27,27,27,27	0
4	NA	B	603	1/1	0.99	0.06	26,26,26,26	0
2	ZN	A	601	1/1	1.00	0.14	21,21,21,21	0
2	ZN	B	601	1/1	1.00	0.13	19,19,19,19	0
2	ZN	C	601	1/1	1.00	0.04	27,27,27,27	0
3	CA	A	602	1/1	1.00	0.04	28,28,28,28	0
3	CA	B	602	1/1	1.00	0.05	28,28,28,28	0

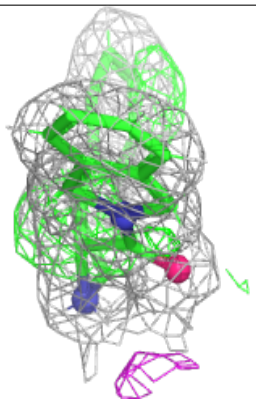
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around KRU C 606:

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

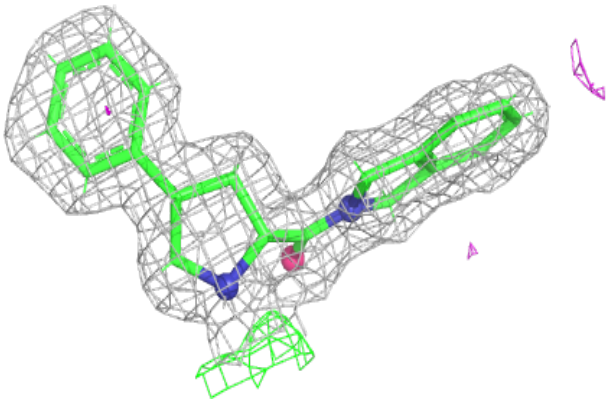


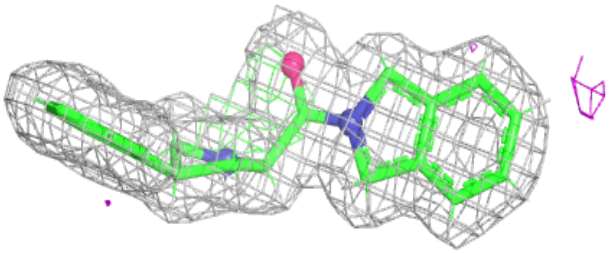


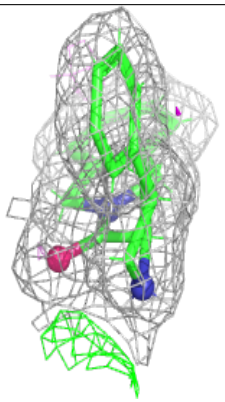


Electron density around KRU B 609:

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

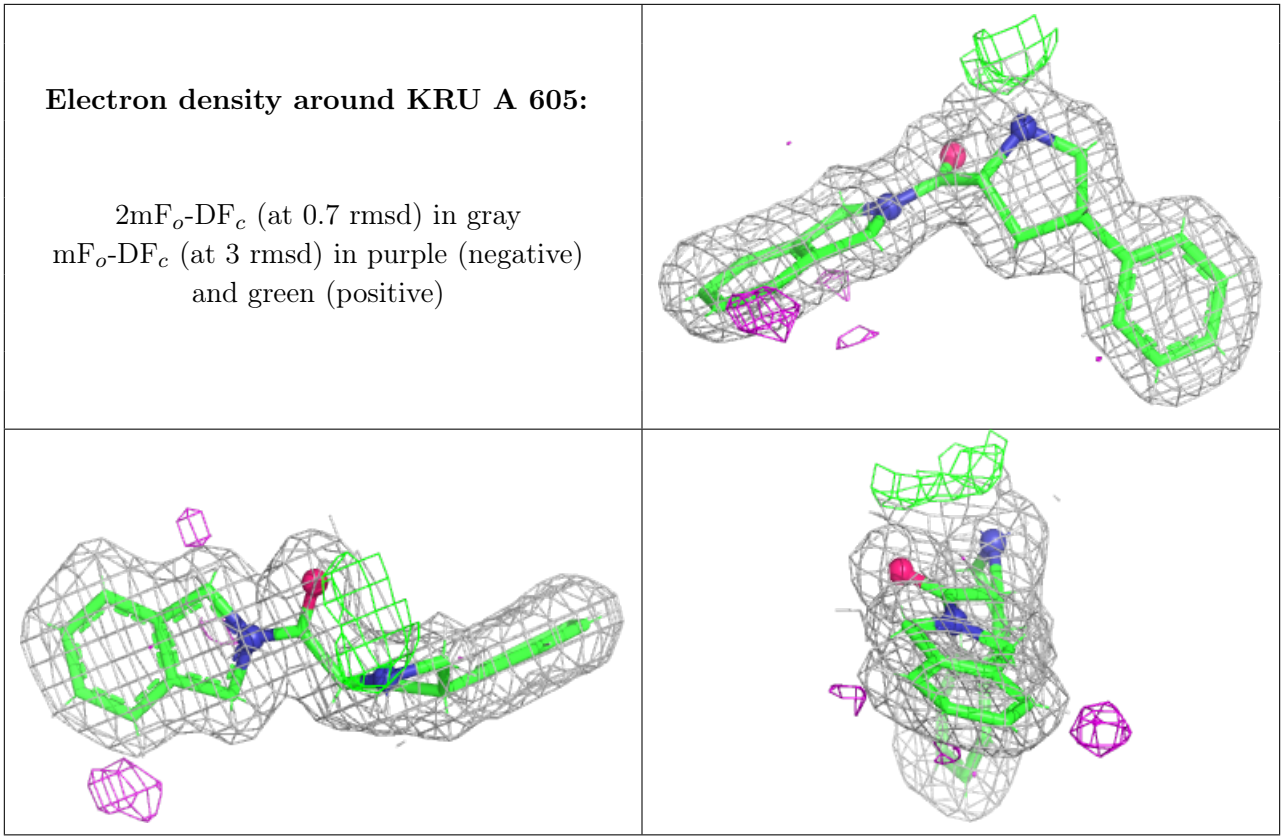






Electron density around KRU A 605:

$2mF_o$-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.