



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:53 AM UTC

PDB ID : 8A0B / pdb_00008a0b
Title : Inhibitor binding to HDAC2
Authors : Cleasby, A.; Tisi, D.
Deposited on : 2022-05-27
Resolution : 1.75 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

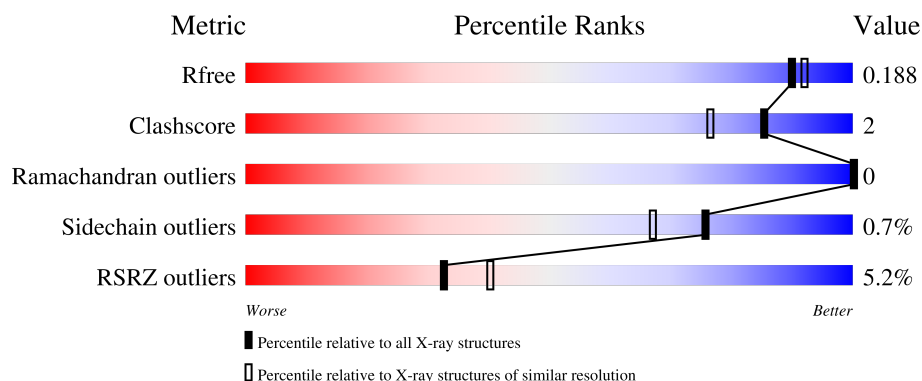
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1187 (1.74-1.74)
Clashscore	190562	1207 (1.74-1.74)
Ramachandran outliers	187476	1200 (1.74-1.74)
Sidechain outliers	187428	1200 (1.74-1.74)
RSRZ outliers	180081	1188 (1.74-1.74)

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	498	3% 69% • • 26%
1	B	498	2% 67% 6% • 26%
1	C	498	7% 69% • • 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 (CCD ID: 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 (CCD ID: 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 (CCD ID: NA) (formula: Na).

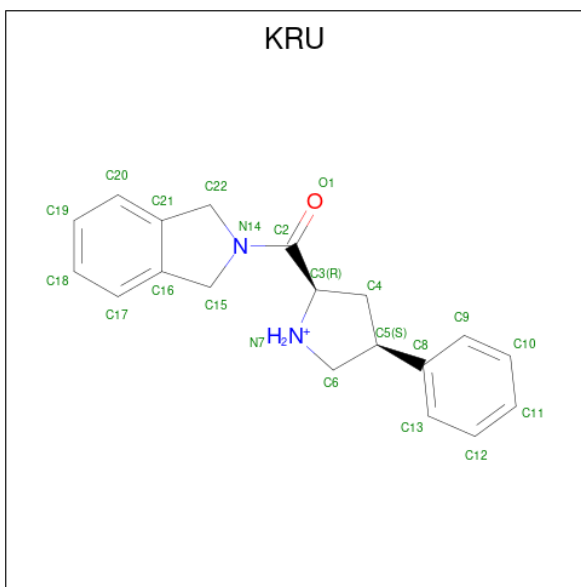
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Na 1 1	0	0
4	B	1	Total Na 1 1	0	0
4	C	1	Total Na 1 1	0	0

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



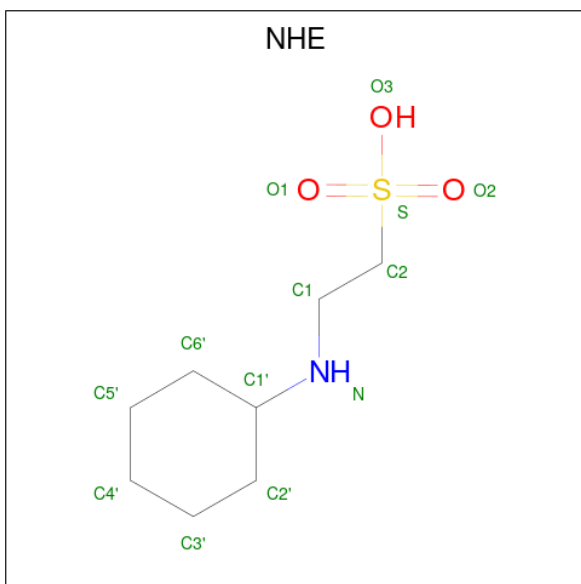
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		
5	B	1	Total	C	O	0	0
			7	4	3		
5	B	1	Total	C	O	0	0
			7	4	3		
5	B	1	Total	C	O	0	0
			7	4	3		
5	C	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is 1,3-dihydroisoindol-2-yl-[(2R,4S)-4-phenylpyrrolidin-1-ium-2-yl]methanone (CCD ID: KRU) (formula: C₁₉H₂₁N₂O) (labeled as "Ligand of Interest" by depositor).



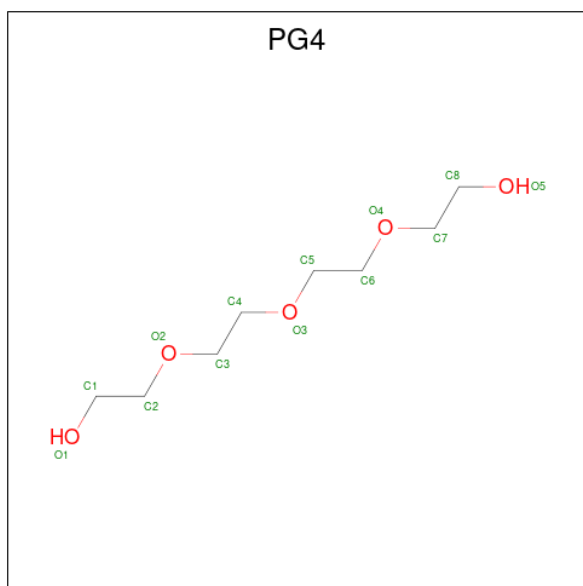
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total 43	C 19	H 21	N 2	O 1	0	0
6	B	1	Total 43	C 19	H 21	N 2	O 1	0	0
6	C	1	Total 43	C 19	H 21	N 2	O 1	0	0

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



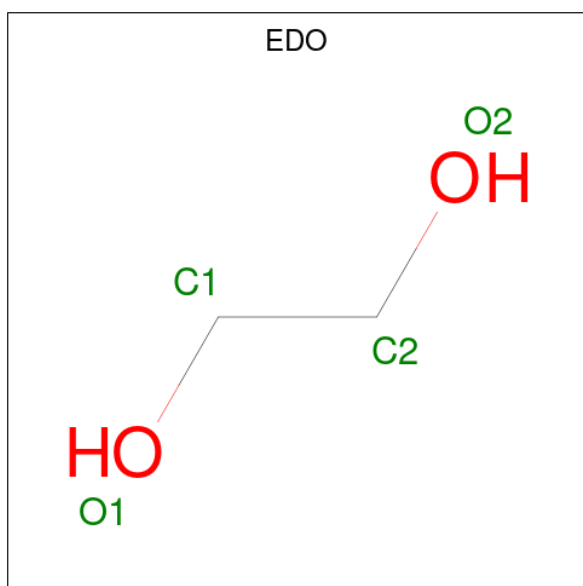
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	B	1	Total	C	N	O	S	0	0
			13	8	1	3	1		

- Molecule 8 is TETRAETHYLENE GLYCOL (CCD ID: 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 (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 10 is water.

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



4 Data and refinement statistics

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 67.17 – 1.75	Depositor EDS
% Data completeness (in resolution range)	96.9 (67.17-1.75) 96.9 (67.17-1.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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 (4.81%)	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)	0.36 , 45.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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.*

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: EDO, NA, PG4, NHE, ZN, KRU, CA, 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	1.00	2/3078 (0.1%)	1.00	6/4153 (0.1%)
1	B	1.07	8/3065 (0.3%)	1.01	12/4137 (0.3%)
1	C	0.89	2/3042 (0.1%)	0.94	2/4107 (0.0%)
All	All	0.99	12/9185 (0.1%)	0.99	20/12397 (0.2%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	56	MET	SD-CE	-7.73	1.60	1.79
1	B	199	MET	SD-CE	-7.69	1.60	1.79
1	A	56	MET	SD-CE	-7.68	1.60	1.79
1	A	199	MET	SD-CE	-7.53	1.60	1.79
1	B	103	GLU	CA-C	7.07	1.55	1.52
1	B	89	MET	SD-CE	-6.01	1.64	1.79
1	C	89	MET	SD-CE	-5.97	1.64	1.79
1	B	47	LEU	CB-CG	-5.90	1.41	1.53
1	B	66	ALA	CA-C	5.69	1.60	1.52
1	B	328	GLU	C-N	-5.43	1.27	1.33
1	C	245	ILE	CA-CB	5.40	1.62	1.54
1	B	258	GLN	CA-CB	5.20	1.56	1.52

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	155	PHE	CA-CB-CG	9.06	122.86	113.80
1	C	155	PHE	CA-CB-CG	8.89	122.69	113.80
1	A	372	PHE	CA-CB-CG	8.05	121.85	113.80
1	A	155	PHE	CA-CB-CG	8.04	121.84	113.80
1	B	372	PHE	CA-CB-CG	6.93	120.73	113.80
1	B	23	ASP	CA-CB-CG	-6.18	106.42	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	372	PHE	CA-CB-CG	5.88	119.68	113.80
1	B	66	ALA	CA-C-N	5.71	127.87	120.44
1	B	66	ALA	C-N-CA	5.71	127.87	120.44
1	B	328	GLU	N-CA-C	-5.65	101.07	110.17
1	A	349	HIS	CA-CB-CG	-5.58	108.22	113.80
1	A	39	ARG	CG-CD-NE	-5.47	99.96	112.00
1	A	279	PHE	CA-CB-CG	5.35	119.15	113.80
1	A	104	ASP	CA-CB-CG	5.32	117.92	112.60
1	B	104	ASP	CA-CB-CG	5.26	117.86	112.60
1	B	279	PHE	CA-CB-CG	5.22	119.02	113.80
1	B	39	ARG	CG-CD-NE	-5.15	100.66	112.00
1	B	349	HIS	CA-CB-CG	-5.06	108.74	113.80
1	B	296	PHE	CA-CB-CG	-5.04	108.75	113.80
1	B	179	ASP	CA-CB-CG	5.04	117.64	112.60

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	12	0
1	B	2981	0	2885	18	0
1	C	2959	0	2869	9	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	40	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.

All (40) 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:A:136[B]:MET:HE3	1:A:300:LEU:HD23	1.59	0.84
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
1:B:205:LYS:HD2	1:B:278[B]:CYS:SG	2.42	0.60
1:A:89:MET:HE3	1:A:96:MET:HE1	1.88	0.56
1:C:365:GLU:O	1:C:369:GLN:HG2	2.06	0.55
1:B:241:SER:HB3	1:B:364[B]:MET:SD	2.46	0.55
1:B:89:MET:HE3	1:B:96:MET:HE1	1.89	0.54
1:C:89:MET:HE3	1:C:96:MET:HE1	1.90	0.54
1:B:56:MET:HB3	1:B:325:LEU:HD21	1.89	0.54
5:C:604:PEG:H41	10:C:863:HOH:O	2.05	0.54
1:C:235:ASP:OD1	1:C:278:CYS:SG	2.63	0.52
1:A:205:LYS:CD	1:A:278[B]:CYS:SG	2.97	0.52
1:C:56:MET:HB3	1:C:325:LEU:HD21	1.92	0.52
1:A:113:GLU:OE1	1:B:131:ARG:NH2	2.43	0.52
1:A:56:MET:HB3	1:A:325:LEU:HD21	1.93	0.50
1:B:245:ILE:HG21	1:B:364[A]:MET:HE3	1.93	0.49
1:B:63:LYS:HE2	7:B:604:NHE:C3'	2.41	0.49
5:C:604:PEG:H22	10:C:863:HOH:O	2.13	0.49
1:C:369:GLN:O	1:C:373:GLU:HG3	2.12	0.49
1:C:44:HIS:O	1:C:48:LEU:HG	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:298:LEU:O	5:B:605:PEG:H22	2.13	0.48
1:B:63:LYS:HE2	7:B:604:NHE:H3'2	1.92	0.47
1:B:151:GLU:HG3	1:B:152:ALA:O	2.16	0.46
1:A:151:GLU:HG3	1:A:152:ALA:O	2.15	0.46
1:A:205:LYS:HD2	1:A:278[B]:CYS:HG	1.82	0.45
1:C:151:GLU:HG3	1:C:152:ALA:O	2.18	0.44
1:B:60:ARG:HD2	10:B:731:HOH:O	2.17	0.43
1:B:245:ILE:HG12	1:B:364[A]:MET:CE	2.48	0.43
1:A:136[B]:MET:CE	1:A:302:MET:SD	3.07	0.43
1:C:199[A]:MET:SD	1:C:253:VAL:HG13	2.58	0.42
1:B:359:ASN:HB3	1:B:364[A]:MET:SD	2.58	0.42
1:C:362:GLU:O	1:C:366:LYS:HG3	2.19	0.42
1:A:245:ILE:HG12	1:A:364:MET:CE	2.51	0.41
1:A:89:MET:CE	1:A:96:MET:HE1	2.51	0.41
1:A:240:GLU:O	1:A:244:GLN:HG3	2.21	0.41
1:B:89:MET:CE	1:B:96:MET:HE1	2.51	0.41

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%)	319 (99%)	2 (1%)	78	71
1	B	321/425 (76%)	319 (99%)	2 (1%)	78	71
1	C	318/425 (75%)	315 (99%)	3 (1%)	70	59
All	All	960/1275 (75%)	953 (99%)	7 (1%)	76	67

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	151	GLU
1	A	155	PHE
1	B	151	GLU
1	B	155	PHE
1	C	151	GLU
1	C	155	PHE
1	C	245	ILE

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

Mol	Chain	Res	Type
1	A	297	ASN
1	B	95	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](#)

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	$\# Z > 2$
8	PG4	B	606	-	12,12,12	0.33	0	11,11,11	0.40	0
5	PEG	B	607	-	6,6,6	0.18	0	5,5,5	0.28	0
6	KRU	B	609	2	25,25,25	0.62	1 (4%)	28,35,35	0.53	0
5	PEG	B	605	-	6,6,6	0.24	0	5,5,5	0.32	0
9	EDO	C	605	-	3,3,3	0.61	0	2,2,2	0.33	0
5	PEG	C	604	-	6,6,6	0.43	0	5,5,5	0.19	0
6	KRU	A	605	2	25,25,25	0.70	1 (4%)	28,35,35	0.51	0
5	PEG	B	608	-	6,6,6	0.52	0	5,5,5	0.34	0
5	PEG	A	604	-	6,6,6	0.25	0	5,5,5	0.17	0
6	KRU	C	606	2	25,25,25	0.43	0	28,35,35	0.48	0
7	NHE	B	604	-	13,13,13	0.59	0	16,17,17	1.04	1 (6%)

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
8	PG4	B	606	-	-	1/10/10/10	-
5	PEG	B	607	-	-	1/4/4/4	-
6	KRU	B	609	2	-	0/12/29/29	0/4/4/4
5	PEG	B	605	-	-	1/4/4/4	-
9	EDO	C	605	-	-	0/1/1/1	-
5	PEG	C	604	-	-	1/4/4/4	-
6	KRU	A	605	2	-	0/12/29/29	0/4/4/4
5	PEG	B	608	-	-	2/4/4/4	-

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	605	KRU	C6-C5	-2.40	1.51	1.54
6	B	609	KRU	C6-C5	-2.23	1.52	1.54

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	604	NHE	C3'-C2'-C1'	2.99	116.45	111.09

There are no chirality outliers.

All (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
7	B	604	NHE	C1-C2-S-O1
5	A	604	PEG	O2-C3-C4-O4
8	B	606	PG4	O3-C5-C6-O4
5	C	604	PEG	O1-C1-C2-O2
5	B	605	PEG	O1-C1-C2-O2
7	B	604	NHE	C1-C2-S-O3
5	B	608	PEG	C1-C2-O2-C3

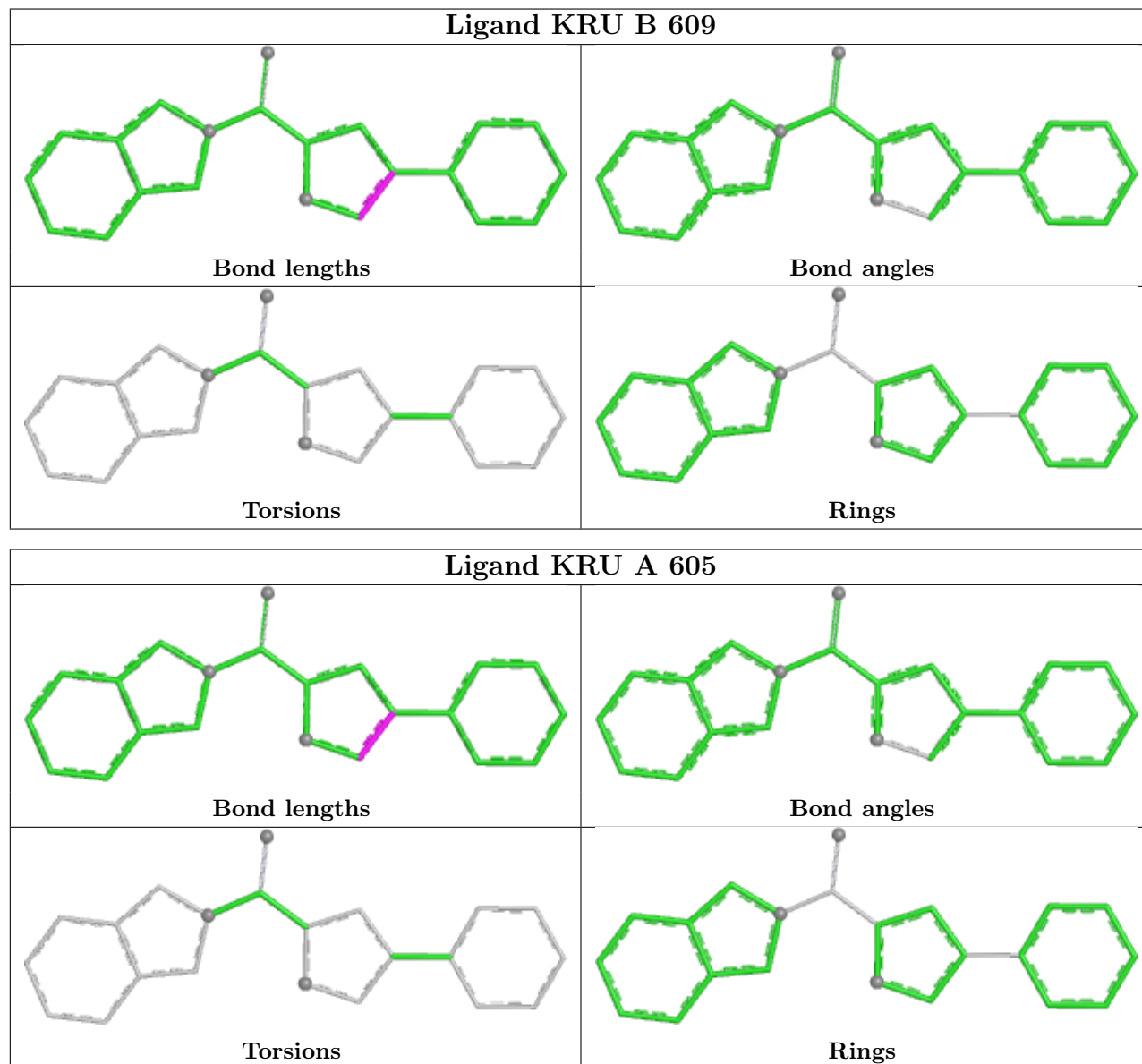
There are no ring outliers.

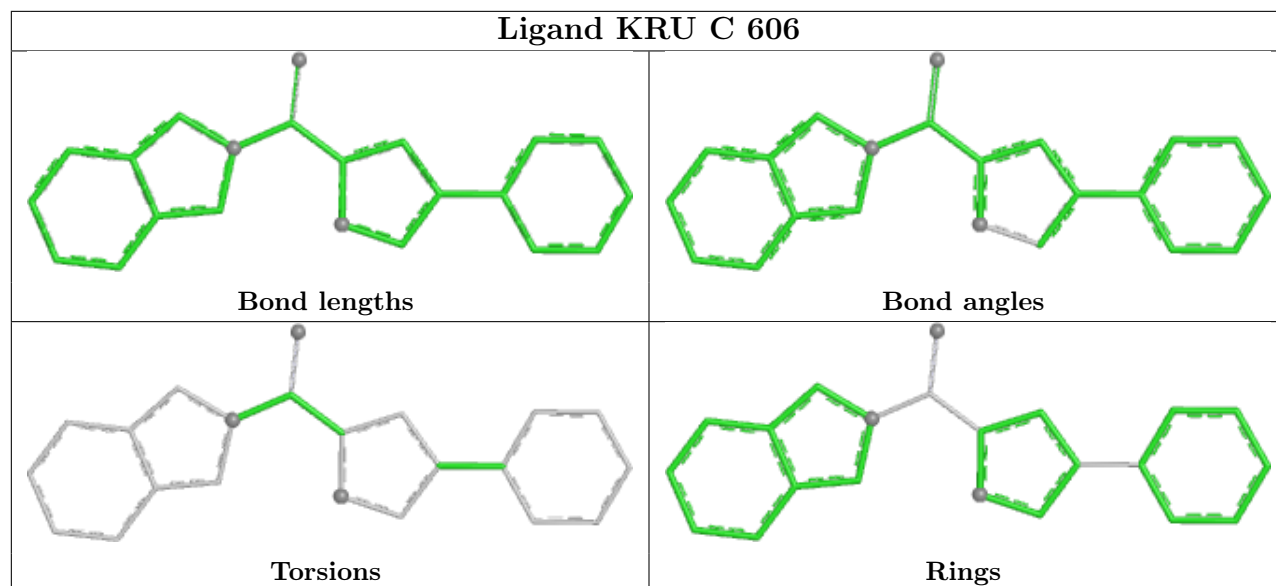
3 monomers are involved in 8 short contacts:

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 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	369/498 (74%)	0.08	14 (3%)	44 53	15, 26, 45, 67	4 (1%)
1	B	367/498 (73%)	0.01	10 (2%)	56 64	13, 25, 44, 57	4 (1%)
1	C	366/498 (73%)	0.94	33 (9%)	15 20	18, 37, 56, 69	2 (0%)
All	All	1102/1494 (73%)	0.34	57 (5%)	33 40	13, 29, 52, 69	10 (0%)

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	11	GLY	4.8
1	C	379	PRO	4.3
1	C	62	HIS	3.9
1	C	341	TYR	3.5
1	C	378	LEU	3.5
1	B	327	CYS	3.2
1	C	52	LEU	3.2
1	C	28	TYR	3.2
1	A	54	ARG	3.2
1	A	90	SER	3.1
1	A	102	GLY	3.1
1	B	341	TYR	3.1
1	C	24	ILE	3.0
1	C	375	LEU	3.0
1	C	58	ILE	2.9
1	A	341	TYR	2.9
1	C	372	PHE	2.8
1	C	245	ILE	2.8
1	C	352	PRO	2.7
1	A	171	TYR	2.7
1	A	379	PRO	2.7
1	C	310	ILE	2.6
1	C	48	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	54	ARG	2.5
1	C	38	HIS	2.5
1	B	15	LYS	2.5
1	C	61	PRO	2.5
1	C	19	TYR	2.5
1	A	354	ASN	2.4
1	C	107	VAL	2.4
1	C	102	GLY	2.4
1	A	244	GLN	2.4
1	A	208	GLU	2.4
1	C	25	GLY	2.3
1	C	32	GLY	2.3
1	C	60	ARG	2.3
1	B	171	TYR	2.3
1	C	20	TYR	2.3
1	C	329	ILE	2.3
1	B	93	SER	2.3
1	C	14	LYS	2.3
1	B	208	GLU	2.3
1	A	92	TYR	2.3
1	C	59	TYR	2.3
1	C	283	VAL	2.3
1	A	82	ARG	2.2
1	C	93	SER	2.1
1	B	245	ILE	2.1
1	C	47	LEU	2.1
1	C	344	PRO	2.1
1	B	372	PHE	2.1
1	C	29	TYR	2.1
1	C	92	TYR	2.1
1	A	216	LEU	2.0
1	A	295	THR	2.0
1	B	98	ARG	2.0
1	C	94	LYS	2.0

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 oligosaccharides in this entry.

6.4 Ligands ⓘ

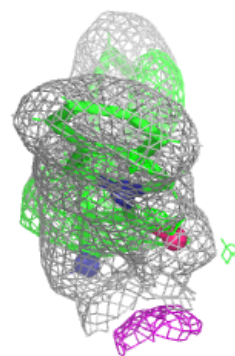
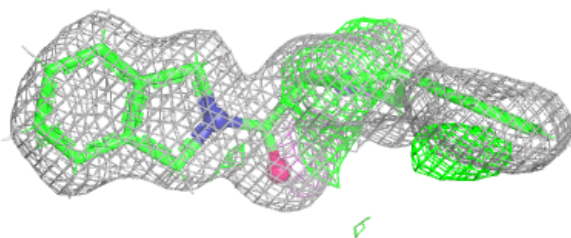
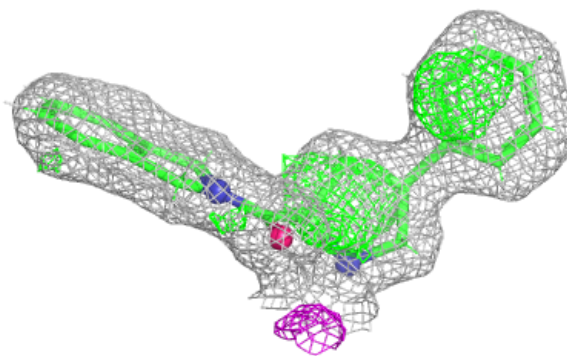
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	PEG	A	604	7/7	0.74	0.19	56,57,59,59	0
5	PEG	B	608	7/7	0.75	0.24	52,53,54,55	0
9	EDO	C	605	4/4	0.77	0.20	61,62,62,62	0
7	NHE	B	604	13/13	0.86	0.17	29,31,38,39	13
5	PEG	B	607	7/7	0.86	0.17	49,49,51,51	0
5	PEG	B	605	7/7	0.87	0.15	44,47,52,53	0
5	PEG	C	604	7/7	0.89	0.13	41,43,46,48	0
8	PG4	B	606	13/13	0.90	0.14	40,44,46,47	0
6	KRU	C	606	22/22	0.93	0.10	15,18,24,24	43
6	KRU	A	605	22/22	0.97	0.05	19,22,28,28	0
6	KRU	B	609	22/22	0.97	0.05	18,20,26,27	0
4	NA	C	603	1/1	0.98	0.12	30,30,30,30	0
3	CA	B	602	1/1	0.99	0.11	28,28,28,28	0
3	CA	C	602	1/1	0.99	0.20	35,35,35,35	0
4	NA	A	603	1/1	0.99	0.02	27,27,27,27	0
2	ZN	B	601	1/1	1.00	0.04	19,19,19,19	0
2	ZN	C	601	1/1	1.00	0.05	27,27,27,27	0
4	NA	B	603	1/1	1.00	0.02	26,26,26,26	0
3	CA	A	602	1/1	1.00	0.09	28,28,28,28	0
2	ZN	A	601	1/1	1.00	0.05	21,21,21,21	0

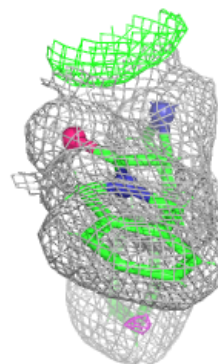
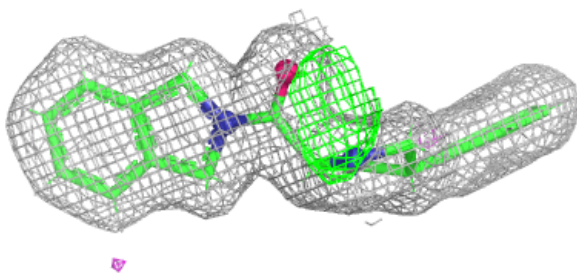
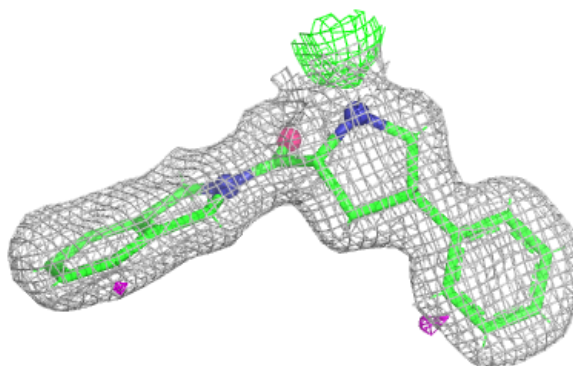
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

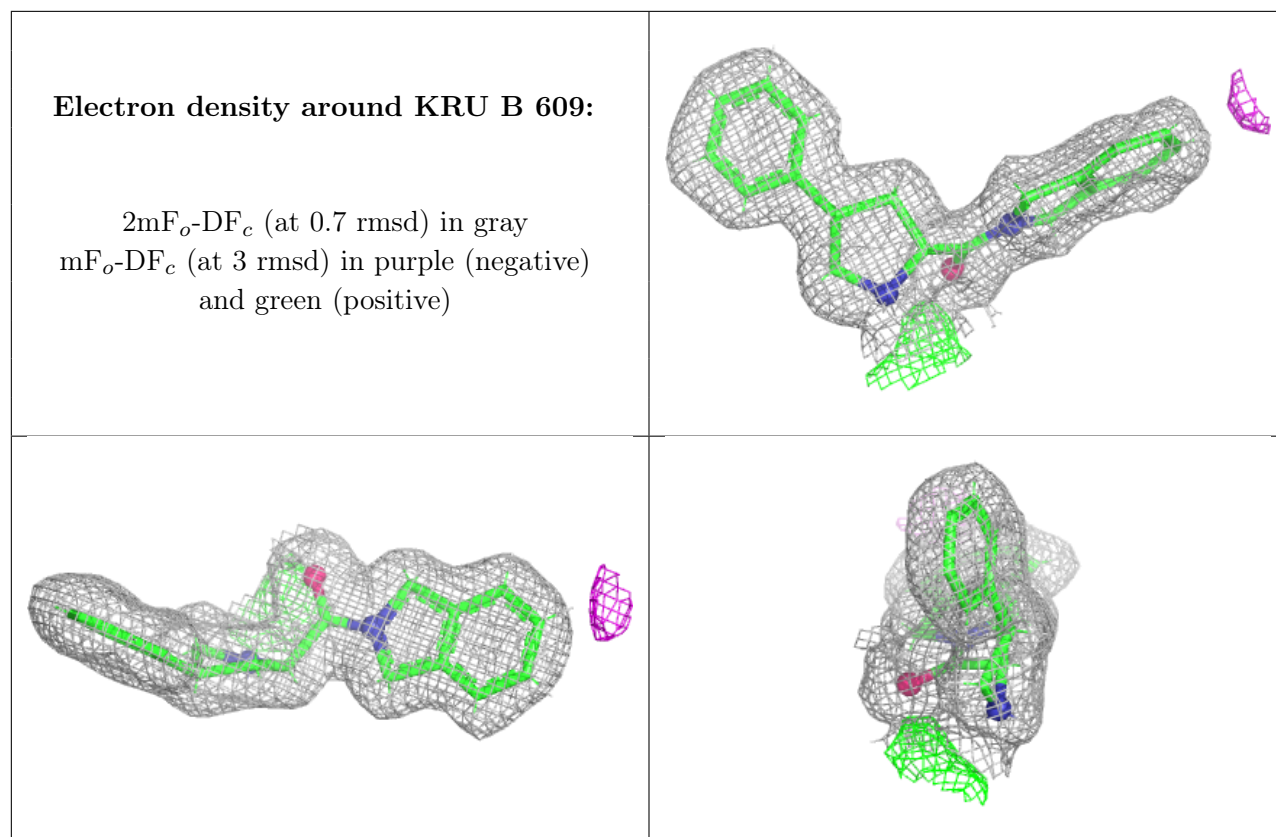
Electron density around KRU C 606:

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

**Electron density around KRU 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.