wwPDB X-ray Structure Validation Summary Report (i)

Sep 15, 2022 – 04:33 pm BST

PDB ID	:	7ZZU
Title	:	Inhibitory Ligand binding to HDAC2
Authors	:	Cleasby, A.; Tisi, D.
Deposited on	:	2022-05-26
Resolution	:	1.85 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:

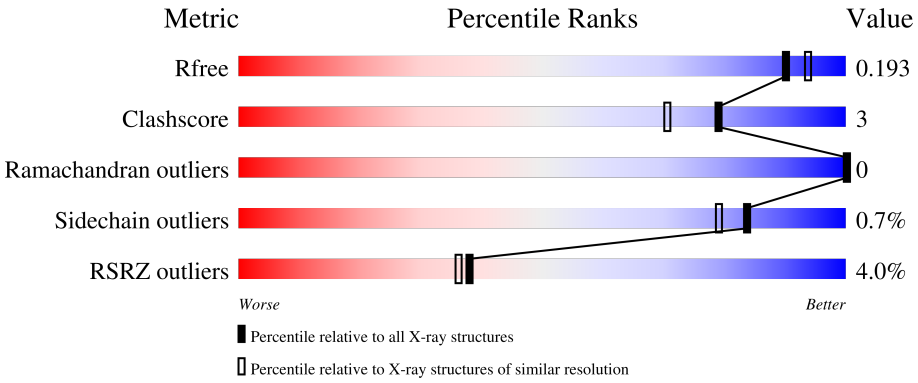
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.30
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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 1.85 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	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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	69% · 27%
1	B	498	% 69% 5% 26%
1	C	498	8% 68% 5% 27%

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	EDO	B	601	-	-	X	-

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 9784 atoms, of which 167 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	366	Total	C	N	O	S	0	14	0
			2996	1917	506	546	27			
1	B	371	Total	C	N	O	S	0	15	0
			3027	1936	511	554	26			
1	C	366	Total	C	N	O	S	0	11	0
			2974	1899	500	550	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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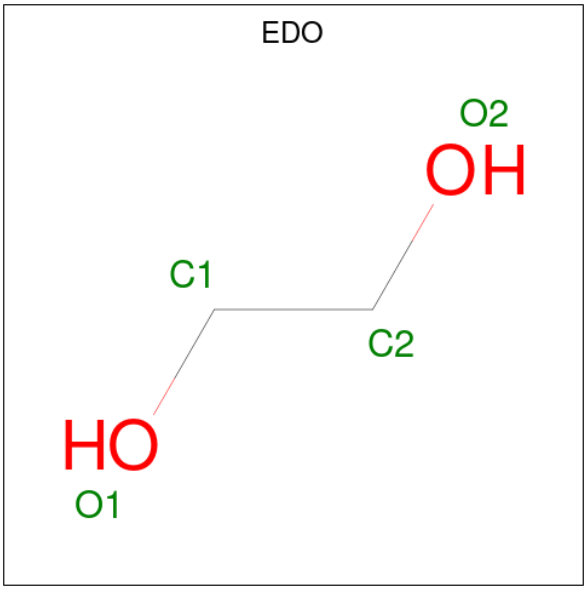
Chain	Residue	Modelled	Actual	Comment	Reference
C	496	GLY	-	expression tag	UNP Q92769
C	497	HIS	-	expression tag	UNP Q92769
C	498	HIS	-	expression tag	UNP Q92769
C	499	HIS	-	expression tag	UNP Q92769
C	500	HIS	-	expression tag	UNP Q92769
C	501	HIS	-	expression tag	UNP Q92769
C	502	HIS	-	expression tag	UNP Q92769

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C H O 10 2 6 2	1	0
2	A	1	Total C H O 10 2 6 2	1	0
2	A	1	Total C H O 10 2 6 2	1	0
2	A	1	Total C H O 10 2 6 2	1	0
2	A	1	Total C H O 10 2 6 2	1	0
2	B	1	Total C H O 10 2 6 2	1	0
2	B	1	Total C H O 10 2 6 2	1	0
2	B	1	Total C H O 10 2 6 2	1	0

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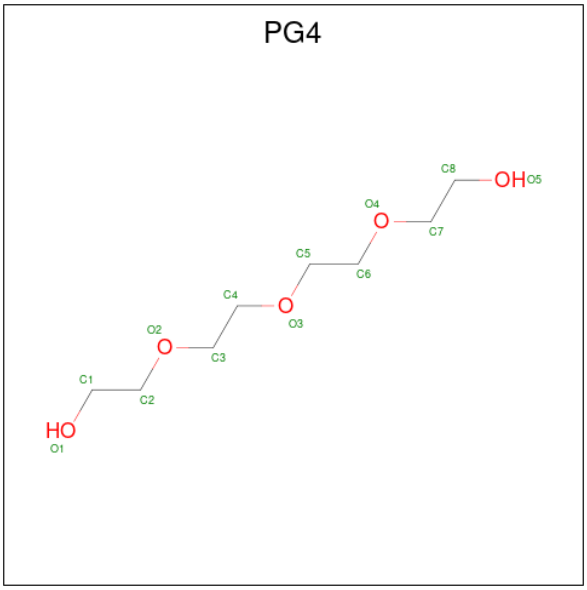
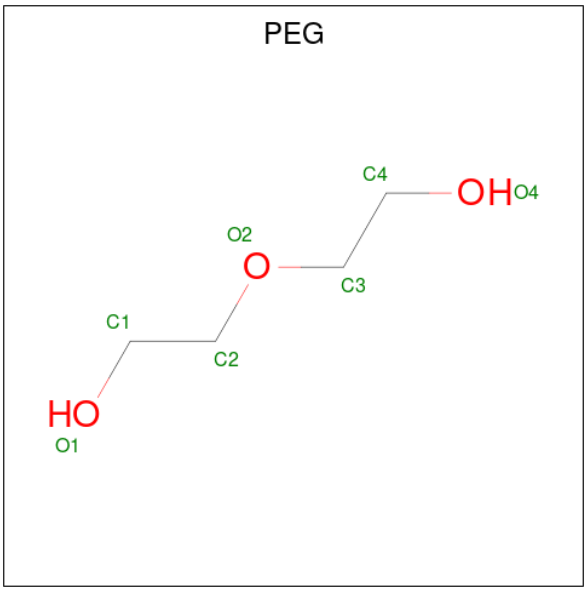
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	H	O	1	0
			10	2	6	2		

- Molecule 3 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	1	0
			31	8	18	5		
3	B	1	Total	C	H	O	1	0
			31	8	18	5		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C H O 17 4 10 3	1	0
4	A	1	Total C H O 17 4 10 3	1	0
4	A	1	Total C H O 17 4 10 3	1	0
4	B	1	Total C H O 17 4 10 3	1	0
4	B	1	Total C H O 17 4 10 3	1	0
4	C	1	Total C H O 17 4 10 3	1	0

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

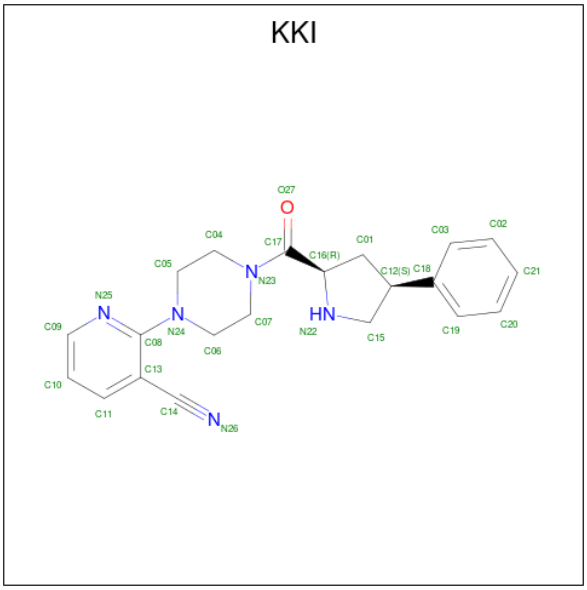
- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na).

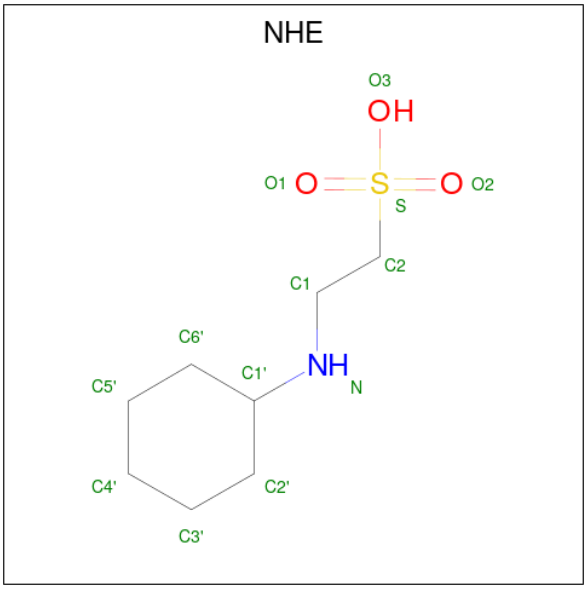
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Na 1 1	0	0
7	B	1	Total Na 1 1	0	0
7	C	1	Total Na 1 1	0	0

- Molecule 8 is 2-[4-[(2 {R},4 {S})-4-phenylpyrrolidin-2-yl]carbonylpiperazin-1-yl]pyridine-3-carbonitrile (three-letter code: KKI) (formula: $C_{21}H_{23}N_5O$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C N O 27 21 5 1	0	0
8	B	1	Total C N O 27 21 5 1	0	0
8	C	1	Total C N O 27 21 5 1	0	0

- Molecule 9 is 2-[N-CYCLOHEXYLAMINO]ETHANE SULFONIC ACID (three-letter code: NHE) (formula: $C_8H_{17}NO_3S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
9	A	1	Total	C	H	N	O	S	0	0
			30	8	17	1	3	1		

- Molecule 10 is water.

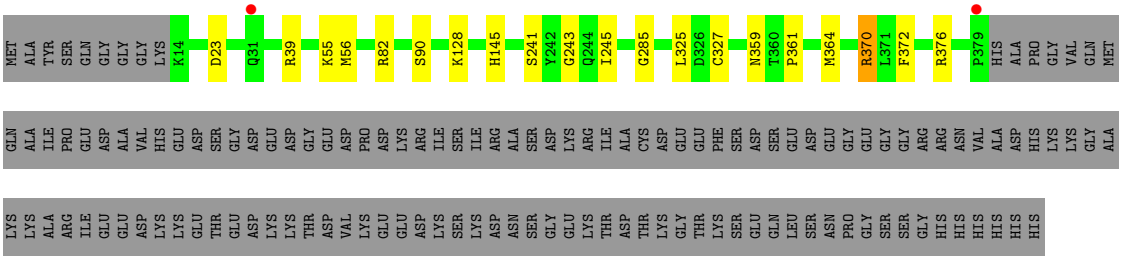
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	174	Total	O	0	0
			174	174		
10	B	157	Total	O	0	0
			157	157		
10	C	82	Total	O	0	0
			82	82		

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.

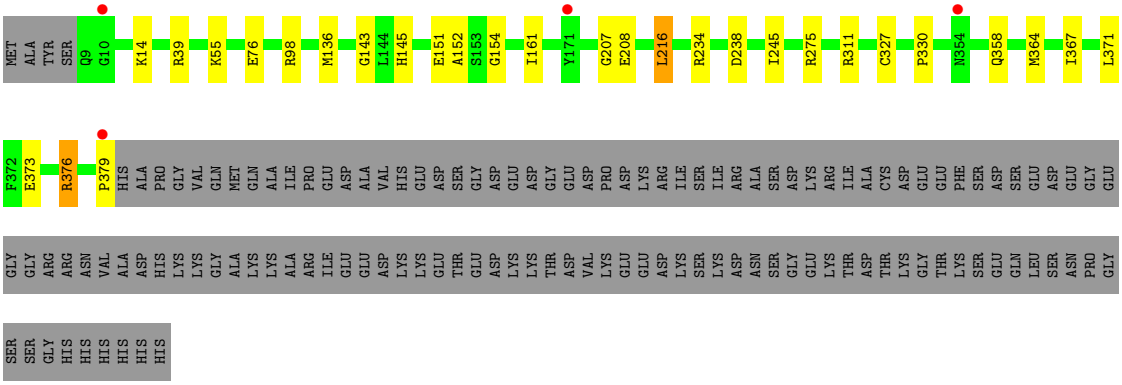
• Molecule 1: Histone deacetylase 2

Chain A:



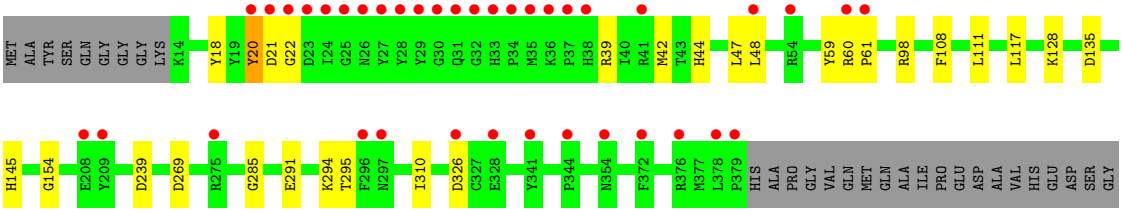
• Molecule 1: Histone deacetylase 2

Chain B:



• Molecule 1: Histone deacetylase 2

Chain C:



ASP GLU ASP GLY GLU ASP PRO ASP LYS ARG ILE SER ILE ARG ALA SER ASP LYS ARG ILE ALA CYS ASP GLU GLU PHE SER ASP SER GLU ASP GLU GLY GLU GLY GLY ARG ARG ASN VAL ALA ASP HIS LYS LYS GLY ALA LYS 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	92.35Å 98.35Å 139.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.45 – 1.85 48.40 – 1.85	Depositor EDS
% Data completeness (in resolution range)	98.6 (48.45-1.85) 98.6 (48.40-1.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.38 (at 1.86Å)	Xtriage
Refinement program	REFMAC 5.8.0232	Depositor
R, R_{free}	0.154 , 0.182 0.165 , 0.193	Depositor DCC
R_{free} test set	5334 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	18.9	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	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	0.96	EDS
Total number of atoms	9784	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.62% 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, EDO, ZN, NA, NHE, KKI, PG4, 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	0.53	0/3088	0.72	0/4167
1	B	0.53	0/3123	0.73	1/4214 (0.0%)
1	C	0.48	0/3057	0.65	1/4127 (0.0%)
All	All	0.51	0/9268	0.70	2/12508 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	B	0	4
1	C	0	3
All	All	0	12

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	B	238	ASP	CB-CG-OD1	5.82	123.53	118.30
1	C	269	ASP	CB-CG-OD2	-5.54	113.31	118.30

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	370[A]	ARG	Sidechain
1	A	370[B]	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	39	ARG	Sidechain
1	A	82[A]	ARG	Sidechain
1	A	82[B]	ARG	Sidechain

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	2996	0	2904	14	0
1	B	3027	0	2934	21	0
1	C	2974	0	2858	15	0
2	A	20	30	30	0	0
2	B	12	18	18	6	0
2	C	4	6	6	1	0
3	A	13	18	18	0	0
3	B	13	18	18	0	0
4	A	21	30	30	3	0
4	B	14	20	20	0	0
4	C	7	10	10	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
8	A	27	0	0	0	0
8	B	27	0	0	1	0
8	C	27	0	0	1	0
9	A	13	17	16	1	0
10	A	174	0	0	3	0
10	B	157	0	0	0	0
10	C	82	0	0	0	0
All	All	9617	167	8862	50	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.

The worst 5 of 50 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:370[A]:ARG:NH2	10:A:701:HOH:O	1.86	1.07
1:A:241:SER:HB3	1:A:364[B]:MET:SD	2.33	0.69
1:A:55:LYS:NZ	1:A:327:CYS:SG	2.70	0.65
1:B:55:LYS:NZ	1:B:327:CYS:SG	2.63	0.64
1:C:59:TYR:CG	1:C:128:LYS:HE3	2.38	0.58

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%)	366 (99%)	5 (1%)	0	100	100
1	B	377/498 (76%)	372 (99%)	5 (1%)	0	100	100
1	C	368/498 (74%)	363 (99%)	5 (1%)	0	100	100
All	All	1116/1494 (75%)	1101 (99%)	15 (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	323/425 (76%)	321 (99%)	2 (1%)	86 83
1	B	326/425 (77%)	321 (98%)	5 (2%)	65 53
1	C	320/425 (75%)	319 (100%)	1 (0%)	92 91
All	All	969/1275 (76%)	961 (99%)	8 (1%)	84 76

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	145	HIS
1	B	379	PRO
1	B	216[B]	LEU
1	B	216[A]	LEU
1	B	330	PRO

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

Mol	Chain	Res	Type
1	A	358	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 30 ligands modelled in this entry, 9 are monoatomic - leaving 21 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	$\#\|Z\| > 2$
3	PG4	A	603	-	12,12,12	0.45	0	11,11,11	0.35	0
4	PEG	B	602	-	6,6,6	0.34	0	5,5,5	0.57	0
2	EDO	A	605	-	3,3,3	0.45	0	2,2,2	0.26	0
8	KKI	C	606	5	29,30,30	0.39	0	34,41,41	0.52	0
2	EDO	B	604	-	3,3,3	0.41	0	2,2,2	0.34	0
2	EDO	C	602	-	3,3,3	0.55	0	2,2,2	0.20	0
4	PEG	B	605	-	6,6,6	0.47	0	5,5,5	0.20	0
2	EDO	A	608	-	3,3,3	0.42	0	2,2,2	0.31	0
2	EDO	B	606	-	3,3,3	0.46	0	2,2,2	0.24	0
4	PEG	A	604	-	6,6,6	0.38	0	5,5,5	0.28	0
8	KKI	B	610	5	29,30,30	0.41	0	34,41,41	0.67	0
2	EDO	B	601	-	3,3,3	0.41	0	2,2,2	0.55	0
4	PEG	A	606	-	6,6,6	0.42	0	5,5,5	0.42	0
4	PEG	A	607	-	6,6,6	0.53	0	5,5,5	1.06	0
2	EDO	A	602	-	3,3,3	0.46	0	2,2,2	0.18	0
4	PEG	C	601	-	6,6,6	0.42	0	5,5,5	0.34	0
3	PG4	B	603	-	12,12,12	0.46	0	11,11,11	0.31	0
9	NHE	A	614	-	13,13,13	0.56	0	16,17,17	0.55	0
8	KKI	A	613	5	29,30,30	0.42	0	34,41,41	0.69	0
2	EDO	A	609	-	3,3,3	0.39	0	2,2,2	0.39	0
2	EDO	A	601	-	3,3,3	0.41	0	2,2,2	0.35	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
3	PG4	A	603	-	-	0/10/10/10	-
4	PEG	B	602	-	-	1/4/4/4	-
2	EDO	A	605	-	-	0/1/1/1	-
8	KKI	C	606	5	-	0/17/37/37	0/4/4/4
2	EDO	B	604	-	-	1/1/1/1	-
2	EDO	C	602	-	-	1/1/1/1	-
4	PEG	B	605	-	-	2/4/4/4	-
2	EDO	A	608	-	-	1/1/1/1	-
2	EDO	B	606	-	-	1/1/1/1	-
4	PEG	A	604	-	-	0/4/4/4	-
8	KKI	B	610	5	-	0/17/37/37	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	B	601	-	-	0/1/1/1	-
4	PEG	A	606	-	-	2/4/4/4	-
4	PEG	A	607	-	-	4/4/4/4	-
2	EDO	A	602	-	-	1/1/1/1	-
4	PEG	C	601	-	-	0/4/4/4	-
3	PG4	B	603	-	-	4/10/10/10	-
9	NHE	A	614	-	-	0/7/15/15	0/1/1/1
8	KKI	A	613	5	-	0/17/37/37	0/4/4/4
2	EDO	A	609	-	-	0/1/1/1	-
2	EDO	A	601	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	605	PEG	O2-C3-C4-O4
4	A	607	PEG	O2-C3-C4-O4
4	B	602	PEG	O2-C3-C4-O4
4	A	606	PEG	O2-C3-C4-O4
2	B	606	EDO	O1-C1-C2-O2

There are no ring outliers.

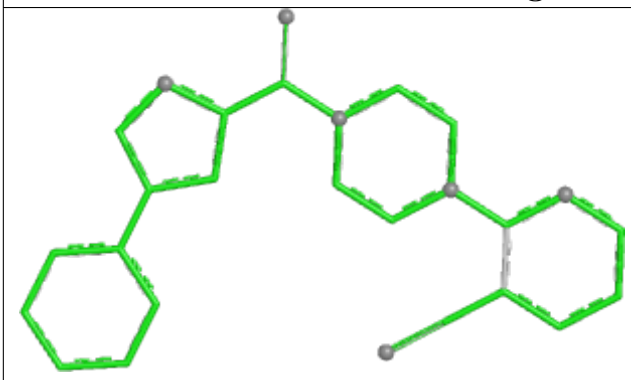
6 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	606	KKI	1	0
2	C	602	EDO	1	0
8	B	610	KKI	1	0
2	B	601	EDO	6	0
4	A	607	PEG	3	0
9	A	614	NHE	1	0

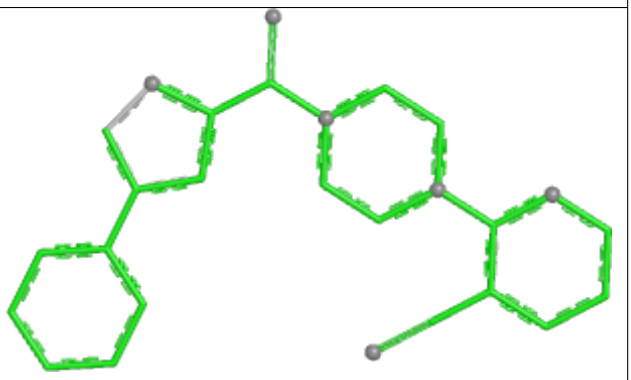
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

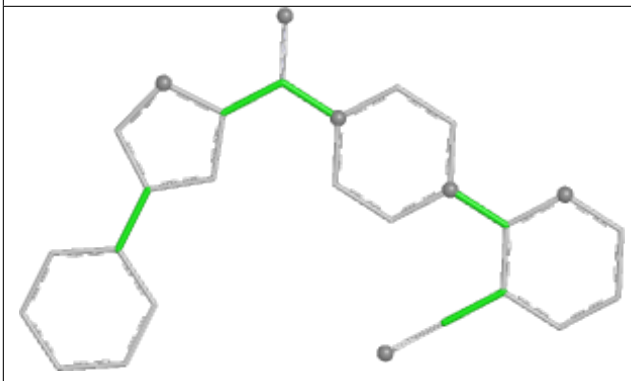
Ligand KKI C 606



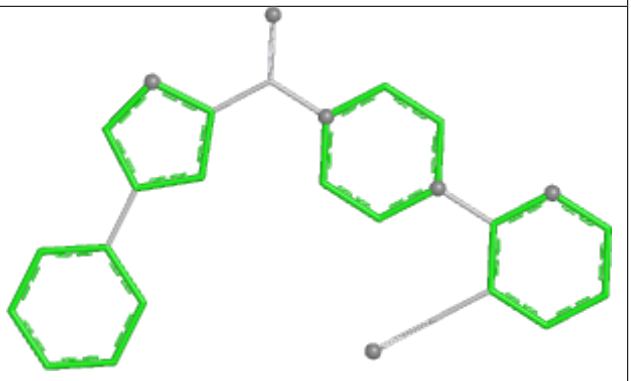
Bond lengths



Bond angles

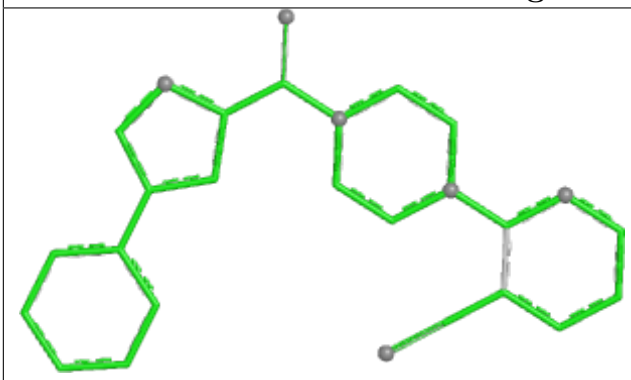


Torsions

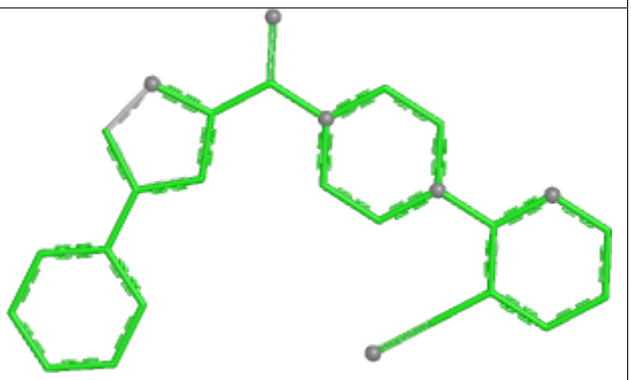


Rings

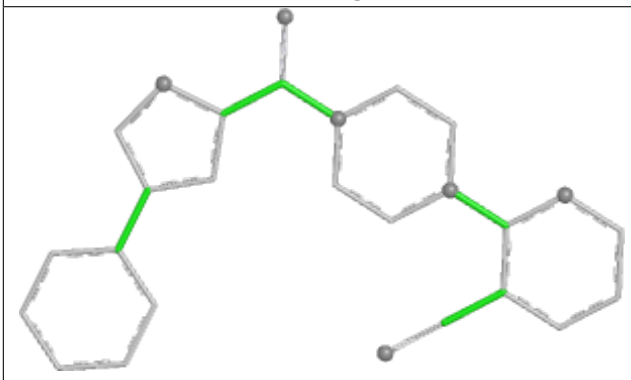
Ligand KKI B 610



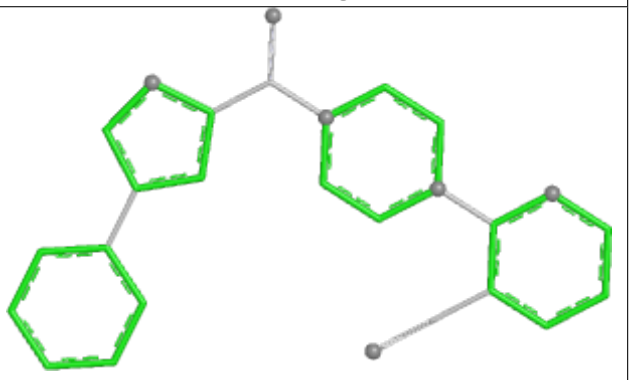
Bond lengths



Bond angles

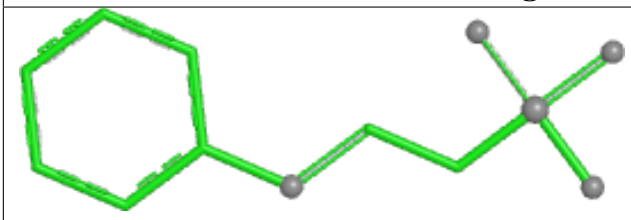


Torsions

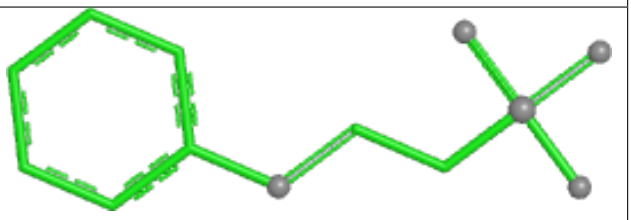


Rings

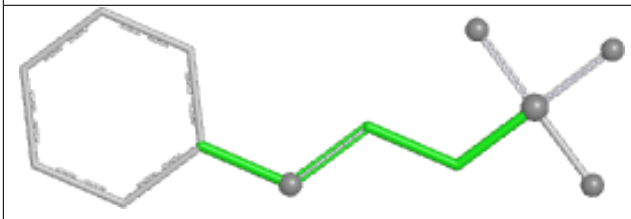
Ligand NHE A 614



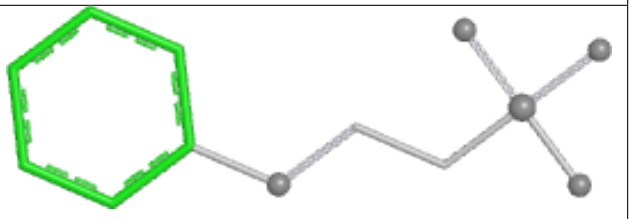
Bond lengths



Bond angles

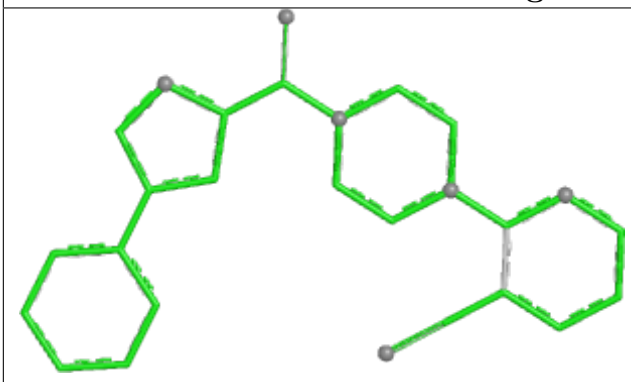


Torsions

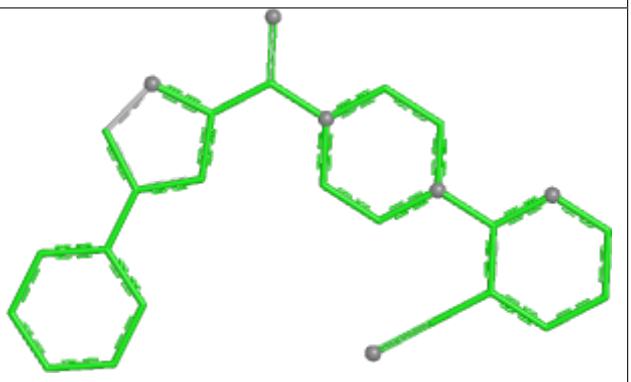


Rings

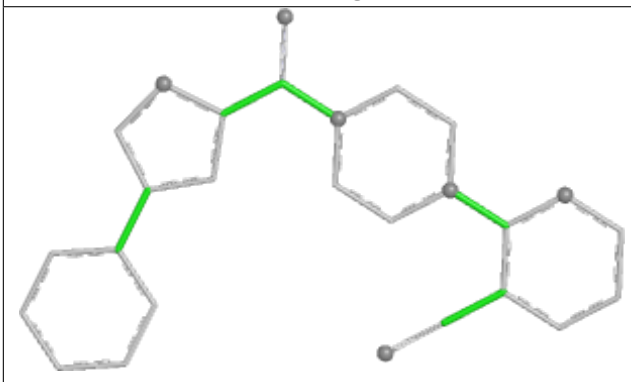
Ligand KKI A 613



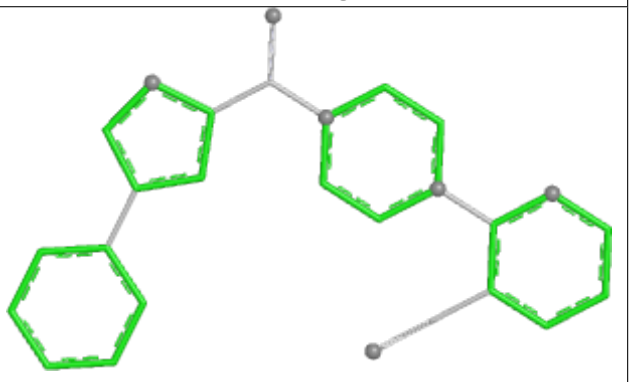
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	366/498 (73%)	-0.22	2 (0%) 91 91	8, 19, 38, 59	3 (0%)
1	B	371/498 (74%)	-0.18	4 (1%) 80 81	10, 20, 39, 67	3 (0%)
1	C	366/498 (73%)	0.43	38 (10%) 6 6	15, 30, 61, 84	3 (0%)
All	All	1103/1494 (73%)	0.01	44 (3%) 38 36	8, 22, 47, 84	9 (0%)

The worst 5 of 44 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	32	GLY	8.3
1	C	31	GLN	6.9
1	C	34	PRO	5.7
1	C	28	TYR	5.7
1	C	29	TYR	4.7

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

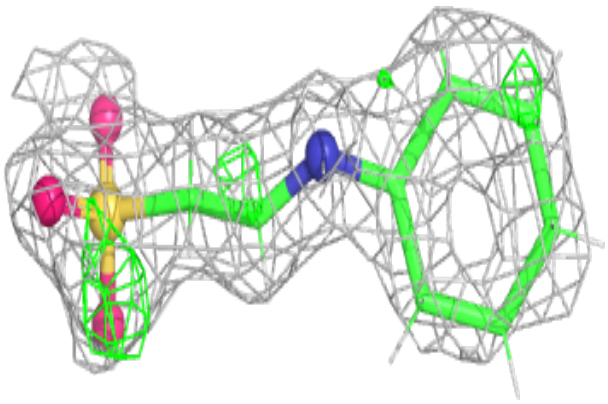
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

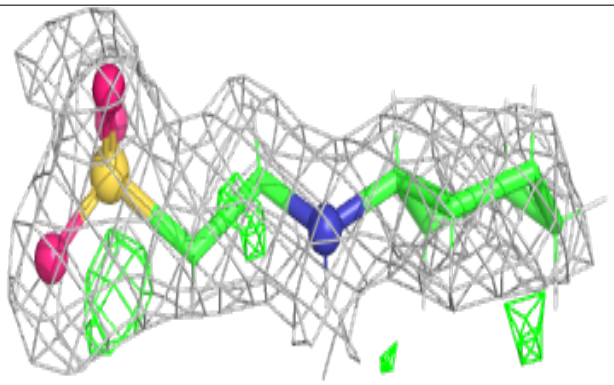
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	EDO	B	606	4/4	0.68	0.16	30,48,51,52	1
3	PG4	B	603	13/13	0.80	0.18	30,55,65,66	1
2	EDO	A	601	4/4	0.81	0.16	20,54,56,56	1
2	EDO	A	605	4/4	0.81	0.11	30,42,49,50	1
4	PEG	A	606	7/7	0.81	0.30	30,48,52,55	1
2	EDO	A	602	4/4	0.82	0.11	20,45,48,50	1
4	PEG	B	605	7/7	0.82	0.18	30,54,62,62	1
4	PEG	A	607	7/7	0.85	0.32	20,29,39,43	1
3	PG4	A	603	13/13	0.86	0.14	30,40,47,52	1
2	EDO	C	602	4/4	0.87	0.22	20,43,46,47	1
2	EDO	A	608	4/4	0.87	0.12	30,47,54,58	1
4	PEG	C	601	7/7	0.87	0.13	20,42,47,47	1
2	EDO	B	604	4/4	0.88	0.07	30,45,49,50	1
9	NHE	A	614	13/13	0.89	0.16	20,24,33,38	30
4	PEG	B	602	7/7	0.90	0.15	20,46,52,59	1
4	PEG	A	604	7/7	0.92	0.14	30,36,38,38	1
2	EDO	A	609	4/4	0.93	0.09	30,42,49,54	1
2	EDO	B	601	4/4	0.94	0.18	20,26,28,29	1
8	KKI	C	606	27/27	0.95	0.11	10,21,32,34	27
8	KKI	A	613	27/27	0.96	0.10	10,16,24,27	0
8	KKI	B	610	27/27	0.97	0.10	10,15,24,26	0
7	NA	B	609	1/1	0.99	0.13	11,11,11,11	0
7	NA	C	605	1/1	0.99	0.12	14,14,14,14	0
7	NA	A	612	1/1	1.00	0.20	9,9,9,9	0
5	ZN	A	610	1/1	1.00	0.09	9,9,9,9	0
5	ZN	B	607	1/1	1.00	0.10	11,11,11,11	0
5	ZN	C	603	1/1	1.00	0.05	17,17,17,17	0
6	CA	A	611	1/1	1.00	0.09	11,11,11,11	0
6	CA	B	608	1/1	1.00	0.10	12,12,12,12	0
6	CA	C	604	1/1	1.00	0.05	19,19,19,19	0

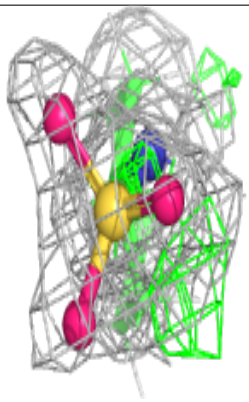
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NHE A 614:

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

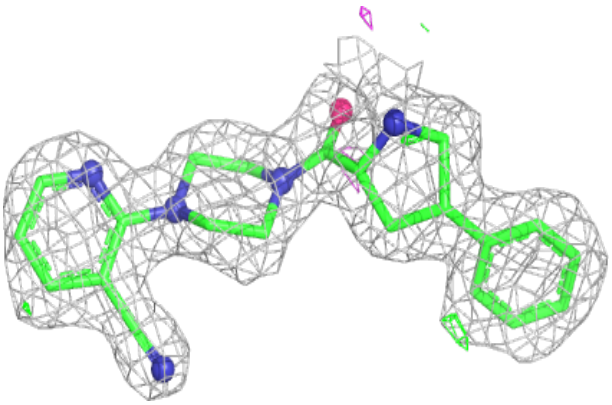


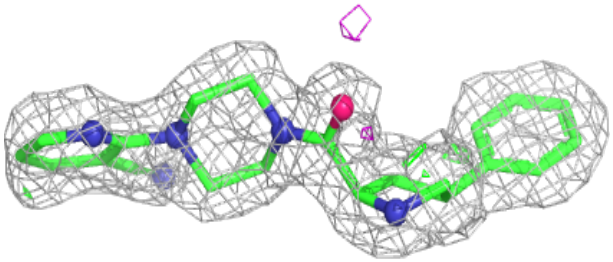


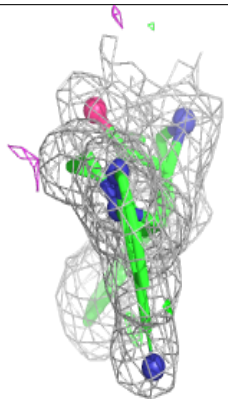


Electron density around KKI C 606:

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

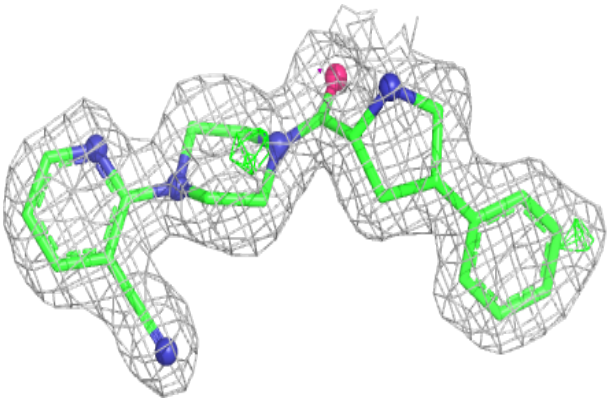


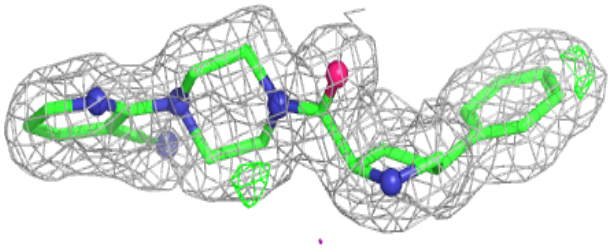


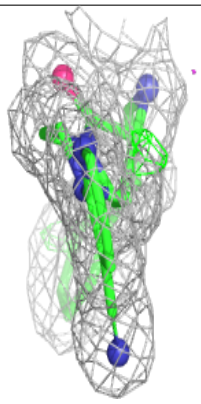


Electron density around KKI A 613:

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

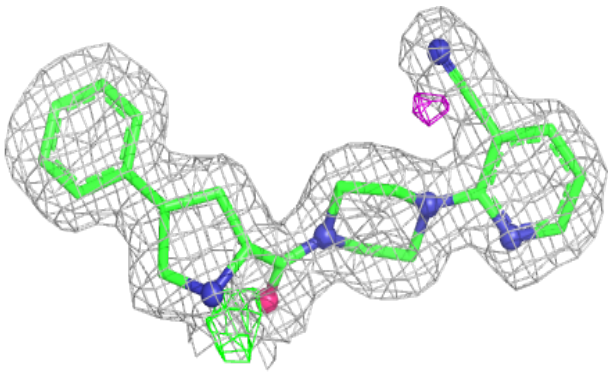


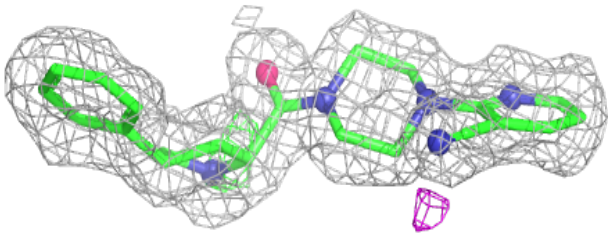


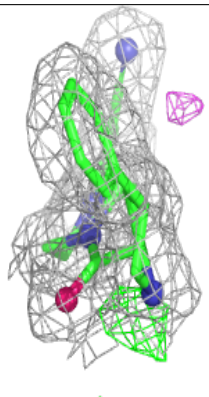


Electron density around KKI B 610:

$2mF_o$-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.