



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 11:25 PM UTC

PDB ID : 7ZZS / pdb_00007zzs
Title : HDAC2 complexed with an inhibitory ligand
Authors : Cleasby, A.; Tisi, D.
Deposited on : 2022-05-26
Resolution : 1.88 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 ⓘ 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

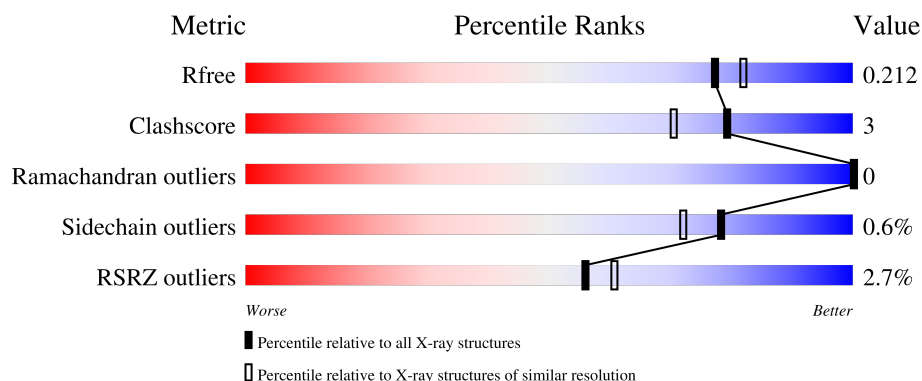
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.88 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	1220 (1.88-1.88)
Clashscore	190562	1234 (1.88-1.88)
Ramachandran outliers	187476	1222 (1.88-1.88)
Sidechain outliers	187428	1222 (1.88-1.88)
RSRZ outliers	180081	1220 (1.88-1.88)

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	5% 69% 5% 26%
1	B	498	70% 26%
1	C	498	5% 69% 5% 27%

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 9893 atoms, of which 223 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	0	0
			2968	1895	502	547	24			
1	B	367	Total	C	N	O	S	0	4	0
			2978	1906	500	545	27			
1	C	366	Total	C	N	O	S	0	1	0
			2956	1889	498	544	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

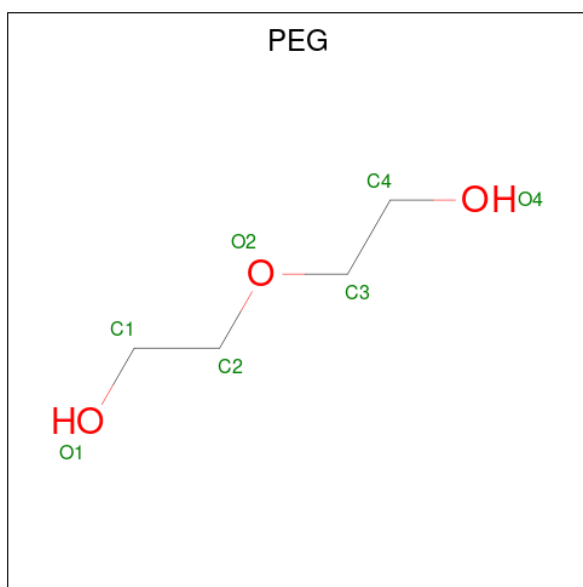
- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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).

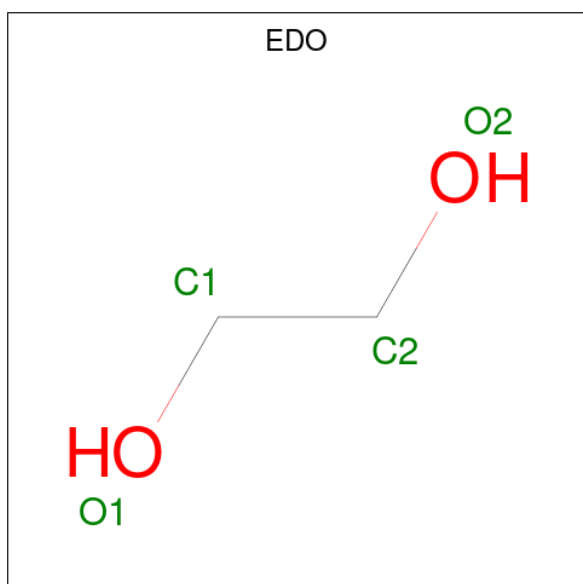
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Na 1 1	0	0
4	B	1	Total Na 1 1	0	0
4	C	1	Total Na 1 1	0	0

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



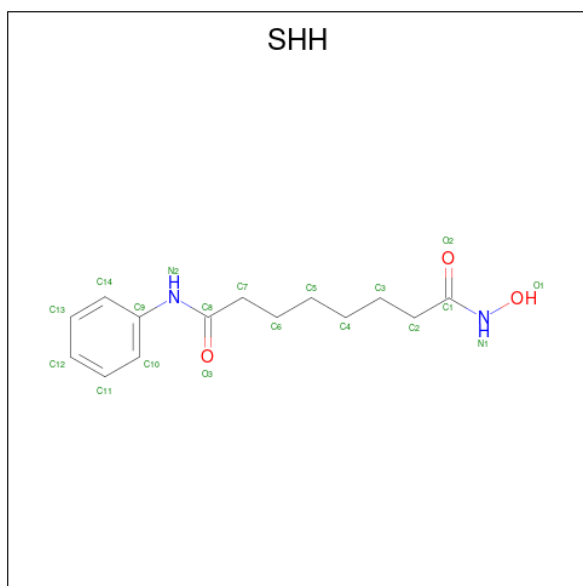
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	1	0
			17	4	10	3		
5	A	1	Total	C	H	O	1	0
			17	4	10	3		
5	A	1	Total	C	H	O	1	0
			17	4	10	3		
5	B	1	Total	C	H	O	1	0
			17	4	10	3		
5	C	1	Total	C	H	O	1	0
			17	4	10	3		

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



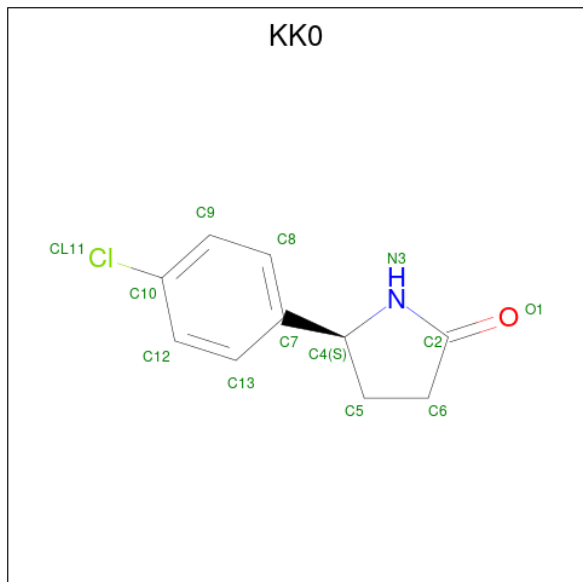
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C H O 10 2 6 2	1	0
6	B	1	Total C H O 10 2 6 2	1	0
6	B	1	Total C H O 10 2 6 2	1	0
6	B	1	Total C H O 10 2 6 2	1	0
6	B	1	Total C H O 10 2 6 2	1	0
6	B	1	Total C H O 10 2 6 2	1	0
6	C	1	Total C H O 10 2 6 2	1	0
6	C	1	Total C H O 10 2 6 2	1	0

- Molecule 7 is OCTANEDIOIC ACID HYDROXYAMIDE PHENYLAMIDE (CCD ID: SHH) (formula: $C_{14}H_{20}N_2O_3$).



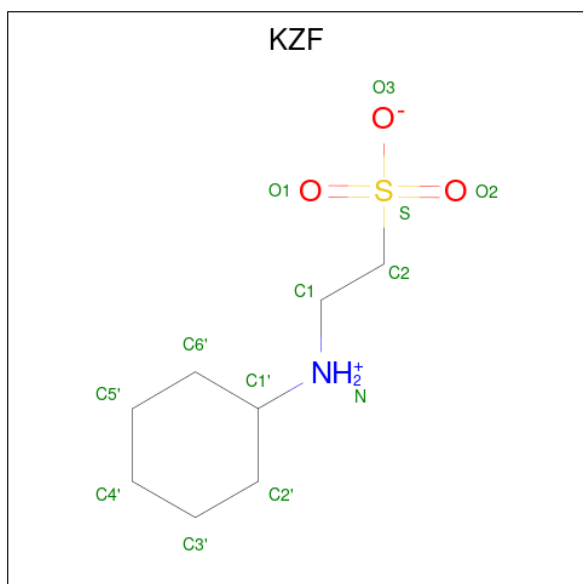
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C H N O 39 14 20 2 3	1	0
7	B	1	Total C H N O 39 14 20 2 3	1	0
7	C	1	Total C H N O 39 14 20 2 3	1	0

- Molecule 8 is (5 {S})-5-(4-chlorophenyl)pyrrolidin-2-one (CCD ID: KK0) (formula: $C_{10}H_{10}ClNO$) (labeled as "Ligand of Interest" by depositor).



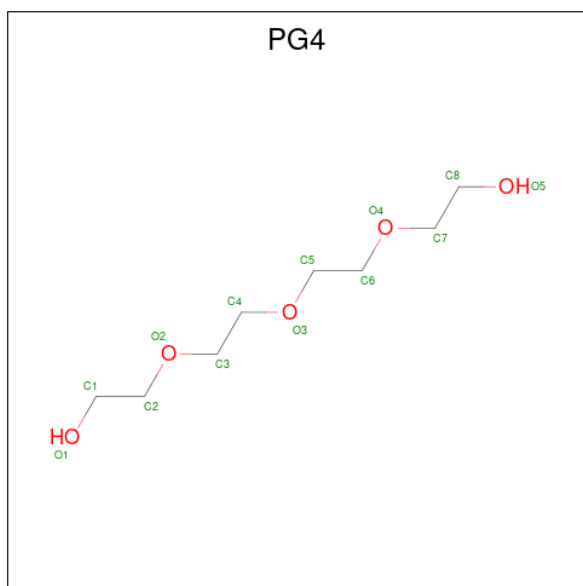
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
8	A	1	Total	C	Cl	H	N	O	0	0
			23	10	1	10	1	1		
8	B	1	Total	C	Cl	H	N	O	0	0
			23	10	1	10	1	1		
8	C	1	Total	C	Cl	H	N	O	0	0
			23	10	1	10	1	1		

- Molecule 9 is 2-(cyclohexylazanumyl)ethanesulfonate (CCD ID: KZF) (formula: $C_8H_{17}NO_3S$).



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

- Molecule 10 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



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

- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	239	Total	O		
			239	239	0	0
11	B	225	Total	O		
			225	225	0	0
11	C	106	Total	O		
			106	106	0	0

LYS	THR	ASP	VAL	GLU	GLU	ASP	LYS	SER	SER	LYS	ASP	ASN	SER	SER	GLY	GLU	LYS	THR	ASP	THR	LYS	GLY	THR	LYS	SER	GLU	GLN	SER	ASN	PRO	GLY	SER	SER	GLY	GLY	GLY	ARG	ARG	ASN	VAL	ALA	ASP	HIS	LYS	LYS	GLY	ALA	LYS	LYS	ALA	ARG	THR	GLU	GLU	ASP	LYS																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																									
ASP	GLY	GLU	ASP	PRO	LYS	ASP	ARG	ILE	SER	ILE	ALA	ALA	CYS	ASP	GLY	GLU	GLU	PHE	SER	SER	ASP	SER	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY</

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	92.50Å 98.66Å 139.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.49 – 1.88 48.49 – 1.88	Depositor EDS
% Data completeness (in resolution range)	99.3 (48.49-1.88) 99.3 (48.49-1.88)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.60 (at 1.88Å)	Xtriage
Refinement program	REFMAC 5.8.0232	Depositor
R, R_{free}	0.166 , 0.207 0.177 , 0.212	Depositor DCC
R_{free} test set	5136 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	31.4	Xtriage
Anisotropy	0.533	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 47.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	9893	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.71% 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: PG4, EDO, KZF, NA, ZN, PEG, SHH, KK0, CA

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	0.78	0/3045	0.93	2/4110 (0.0%)
1	B	0.79	0/3067	0.94	1/4139 (0.0%)
1	C	0.78	0/3036	0.87	0/4099
All	All	0.78	0/9148	0.92	3/12348 (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	4
1	B	0	3
1	C	0	1
All	All	0	8

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	47	LEU	N-CA-CB	-9.37	96.34	110.12
1	A	349	HIS	CA-CB-CG	-7.92	105.88	113.80
1	A	294	LYS	CB-CA-C	-5.29	100.84	110.63

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	131	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	39	ARG	Sidechain
1	A	41	ARG	Sidechain
1	A	54	ARG	Sidechain
1	B	39	ARG	Sidechain

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	2968	0	2874	17	0
1	B	2978	0	2902	16	0
1	C	2956	0	2864	13	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	21	30	30	0	0
5	B	7	10	10	0	0
5	C	7	10	10	0	0
6	A	4	6	6	0	0
6	B	20	30	30	0	0
6	C	8	12	12	0	0
7	A	19	20	19	1	0
7	B	19	20	19	1	0
7	C	19	20	19	1	0
8	A	13	10	0	0	0
8	B	13	10	0	0	0
8	C	13	10	0	1	0
9	B	13	17	0	0	0
10	B	13	18	18	0	0
11	A	239	0	0	3	0
11	B	225	0	0	1	0
11	C	106	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	9670	223	8813	48	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 48 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:245[A]:ILE:HG21	1:B:364[A]:MET:HE3	1.21	1.10
1:B:245[A]:ILE:HG21	1:B:364[A]:MET:CE	1.93	0.98
1:A:136:MET:HE1	1:A:324:ALA:O	1.85	0.76
1:A:16:VAL:HG22	1:A:136:MET:HE3	1.67	0.74
1:A:14:LYS:HB2	1:A:136:MET:HE2	1.69	0.73

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	367/498 (74%)	363 (99%)	4 (1%)	0	100	100
1	B	369/498 (74%)	363 (98%)	6 (2%)	0	100	100
1	C	365/498 (73%)	358 (98%)	7 (2%)	0	100	100
All	All	1101/1494 (74%)	1084 (98%)	17 (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	317/425 (75%)	317 (100%)	0	100	100
1	B	321/425 (76%)	319 (99%)	2 (1%)	78	72
1	C	317/425 (75%)	313 (99%)	4 (1%)	61	50
All	All	955/1275 (75%)	949 (99%)	6 (1%)	78	72

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	90	SER
1	C	326	ASP
1	C	368	LYS
1	B	328	GLU
1	B	60	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	297	ASN
1	A	358	GLN
1	C	38	HIS
1	C	62	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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
5	PEG	A	606	-	6,6,6	0.49	0	5,5,5	0.46	0
9	KZF	B	604	-	13,13,13	0.60	0	16,17,17	0.54	0
10	PG4	B	607	-	12,12,12	0.54	0	11,11,11	0.24	0
7	SHH	A	607	2	19,19,19	0.81	0	21,22,22	1.01	1 (4%)
6	EDO	B	611	-	3,3,3	0.46	0	2,2,2	0.34	0
8	KK0	B	613	-	14,14,14	0.27	0	18,19,19	0.88	1 (5%)
6	EDO	C	605	-	3,3,3	0.44	0	2,2,2	0.25	0
6	EDO	B	605	-	3,3,3	0.40	0	2,2,2	0.39	0
6	EDO	B	612	-	3,3,3	0.44	0	2,2,2	0.42	0
5	PEG	B	609	-	6,6,6	0.46	0	5,5,5	0.28	0
6	EDO	B	608	-	3,3,3	0.39	0	2,2,2	0.37	0
8	KK0	C	608	-	14,14,14	0.26	0	18,19,19	0.48	0
5	PEG	A	604	-	6,6,6	0.41	0	5,5,5	0.30	0
7	SHH	B	610	2	19,19,19	0.76	0	21,22,22	0.83	0
6	EDO	B	606	-	3,3,3	0.41	0	2,2,2	0.40	0
5	PEG	C	606	-	6,6,6	0.51	0	5,5,5	0.23	0
7	SHH	C	607	2	19,19,19	0.65	0	21,22,22	0.96	2 (9%)
5	PEG	A	608	-	6,6,6	0.40	0	5,5,5	0.30	0
8	KK0	A	609	-	14,14,14	0.26	0	18,19,19	0.68	1 (5%)
6	EDO	C	604	-	3,3,3	0.40	0	2,2,2	0.42	0
6	EDO	A	605	-	3,3,3	0.47	0	2,2,2	0.31	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	A	606	-	-	3/4/4/4	-
9	KZF	B	604	-	-	3/7/15/15	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	PG4	B	607	-	-	1/10/10/10	-
7	SHH	A	607	2	-	2/15/15/15	0/1/1/1
6	EDO	B	611	-	-	0/1/1/1	-
8	KK0	B	613	-	-	0/4/13/13	0/2/2/2
6	EDO	C	605	-	-	0/1/1/1	-
6	EDO	B	605	-	-	1/1/1/1	-
6	EDO	B	612	-	-	1/1/1/1	-
5	PEG	B	609	-	-	1/4/4/4	-
6	EDO	B	608	-	-	0/1/1/1	-
8	KK0	C	608	-	-	0/4/13/13	0/2/2/2
5	PEG	A	604	-	-	1/4/4/4	-
7	SHH	B	610	2	-	2/15/15/15	0/1/1/1
6	EDO	B	606	-	-	1/1/1/1	-
5	PEG	C	606	-	-	0/4/4/4	-
7	SHH	C	607	2	-	3/15/15/15	0/1/1/1
5	PEG	A	608	-	-	1/4/4/4	-
8	KK0	A	609	-	-	0/4/13/13	0/2/2/2
6	EDO	C	604	-	-	0/1/1/1	-
6	EDO	A	605	-	-	0/1/1/1	-

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	613	KK0	C7-C4-N3	-3.25	109.09	112.81
8	A	609	KK0	C7-C4-N3	-2.44	110.02	112.81
7	A	607	SHH	C7-C8-N2	2.15	118.33	114.59
7	C	607	SHH	O1-N1-C1	2.13	122.93	119.79
7	C	607	SHH	O3-C8-C7	-2.01	118.37	122.02

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

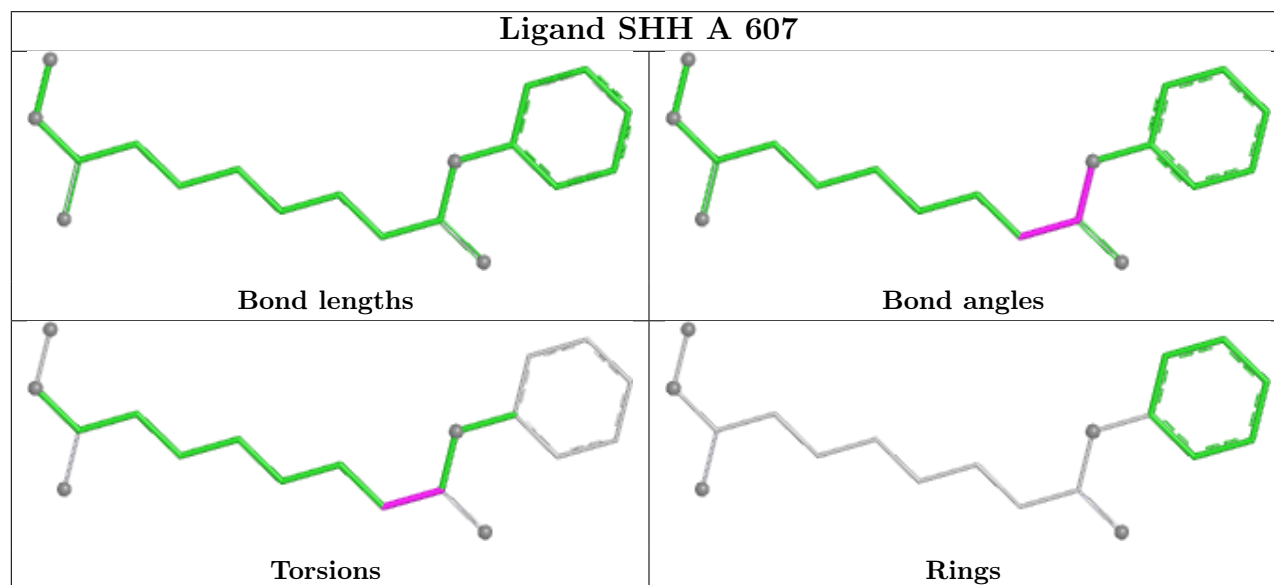
Mol	Chain	Res	Type	Atoms
5	A	606	PEG	O1-C1-C2-O2
5	A	604	PEG	O1-C1-C2-O2
6	B	605	EDO	O1-C1-C2-O2
6	B	606	EDO	O1-C1-C2-O2
9	B	604	KZF	C1-C2-S-O3

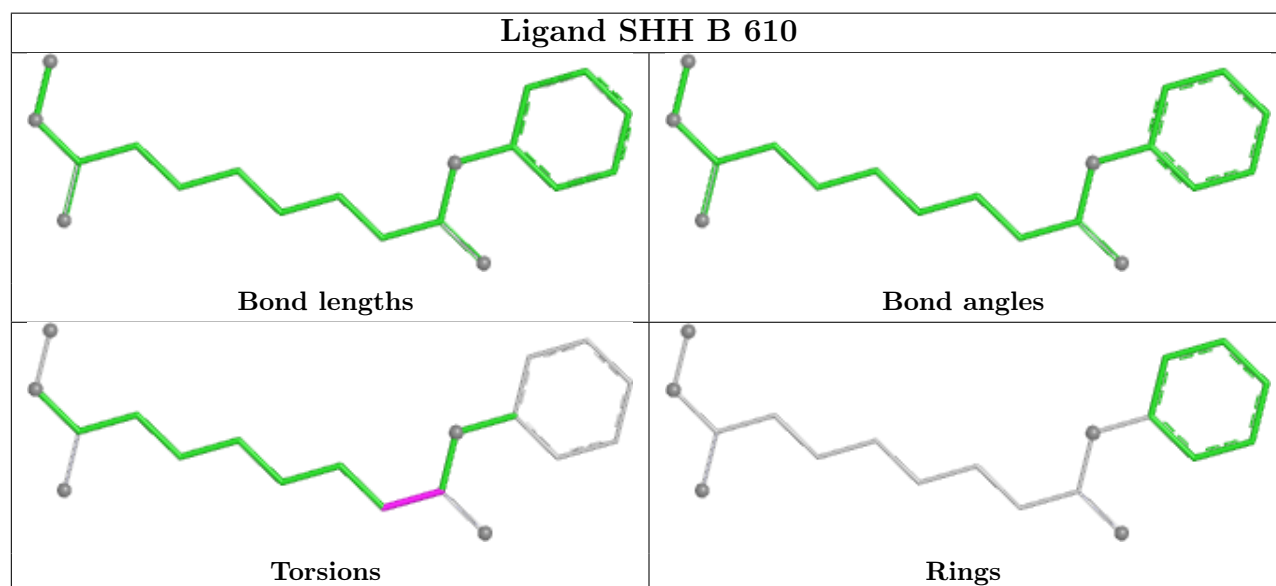
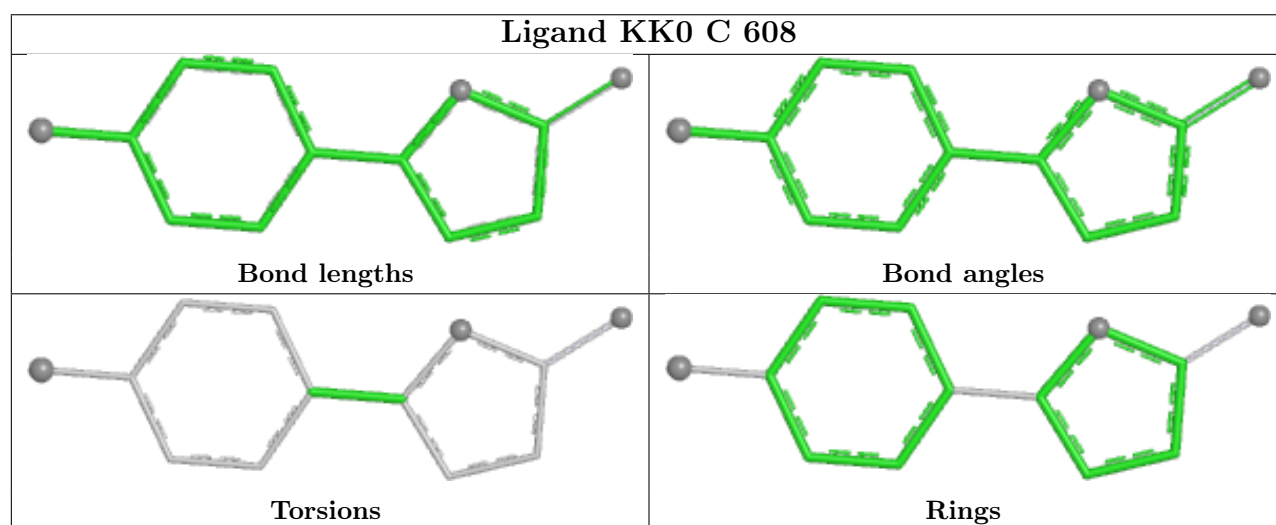
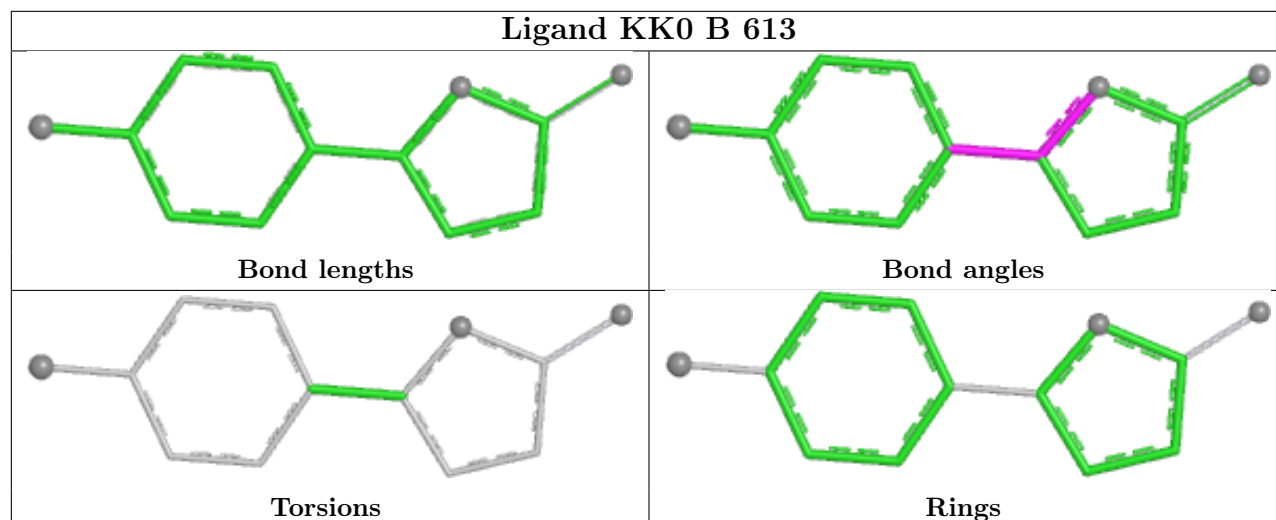
There are no ring outliers.

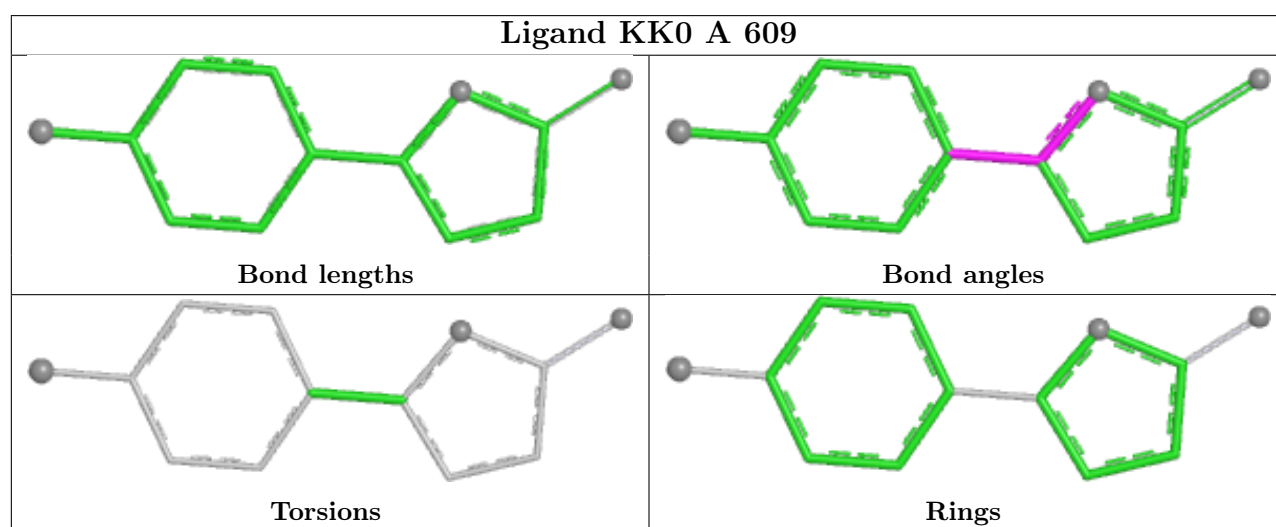
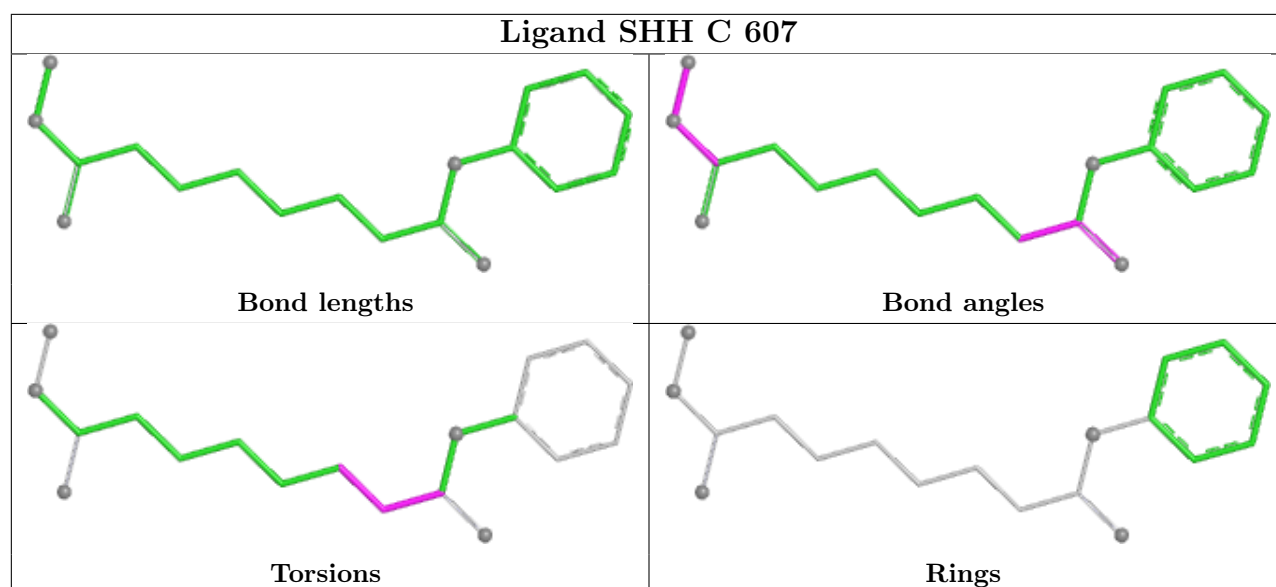
4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	607	SHH	1	0
8	C	608	KK0	1	0
7	B	610	SHH	1	0
7	C	607	SHH	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 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	-0.13	3 (0%) 82 86	24, 34, 55, 72	0
1	B	367/498 (73%)	-0.11	0 100 100	17, 34, 58, 75	4 (1%)
1	C	366/498 (73%)	0.93	27 (7%) 20 23	35, 54, 78, 93	1 (0%)
All	All	1102/1494 (73%)	0.23	30 (2%) 56 61	17, 40, 71, 93	5 (0%)

The worst 5 of 30 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	378	LEU	3.8
1	C	379	PRO	3.6
1	C	375	LEU	3.4
1	C	216	LEU	3.0
1	C	14	LYS	3.0

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

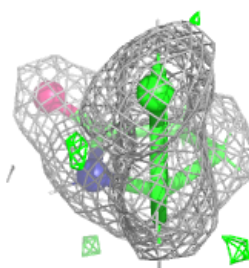
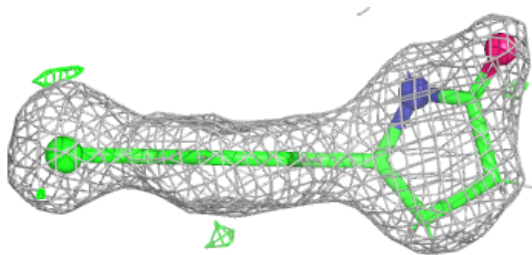
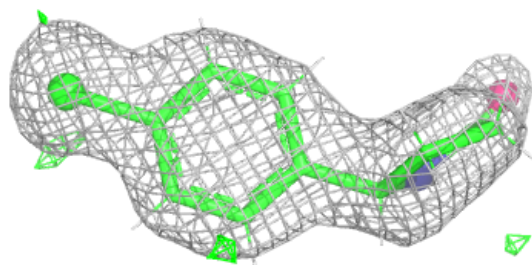
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	PEG	A	606	7/7	0.81	0.13	47,54,58,60	1
6	EDO	C	605	4/4	0.83	0.10	53,64,71,84	1
6	EDO	B	612	4/4	0.84	0.13	53,69,70,72	1
5	PEG	A	604	7/7	0.84	0.15	53,82,89,92	1
5	PEG	C	606	7/7	0.85	0.13	53,59,61,61	1
9	KZF	B	604	13/13	0.85	0.12	47,52,61,73	0
6	EDO	C	604	4/4	0.86	0.10	53,69,72,74	1
6	EDO	B	606	4/4	0.86	0.13	53,69,75,78	1
5	PEG	B	609	7/7	0.86	0.13	53,67,76,78	1
6	EDO	A	605	4/4	0.88	0.12	53,68,71,74	1
6	EDO	B	611	4/4	0.89	0.10	53,61,63,66	1
8	KK0	C	608	13/13	0.90	0.12	29,37,43,48	23
7	SHH	C	607	19/19	0.90	0.11	40,61,79,82	1
6	EDO	B	608	4/4	0.91	0.10	53,58,62,64	1
10	PG4	B	607	13/13	0.91	0.10	40,55,66,69	1
5	PEG	A	608	7/7	0.93	0.09	46,52,60,64	1
6	EDO	B	605	4/4	0.93	0.08	52,55,60,63	1
7	SHH	A	607	19/19	0.93	0.12	24,42,54,57	1
7	SHH	B	610	19/19	0.93	0.10	28,41,58,61	1
8	KK0	A	609	13/13	0.95	0.07	23,28,33,42	0
8	KK0	B	613	13/13	0.96	0.07	20,24,26,37	23
4	NA	C	603	1/1	0.97	0.12	40,40,40,40	0
3	CA	C	602	1/1	0.97	0.20	55,55,55,55	0
4	NA	A	603	1/1	0.98	0.05	34,34,34,34	0
4	NA	B	603	1/1	0.98	0.04	37,37,37,37	0
3	CA	B	602	1/1	0.99	0.11	40,40,40,40	0
3	CA	A	602	1/1	0.99	0.09	37,37,37,37	0
2	ZN	A	601	1/1	1.00	0.04	25,25,25,25	0
2	ZN	B	601	1/1	1.00	0.02	24,24,24,24	0
2	ZN	C	601	1/1	1.00	0.08	41,41,41,41	0

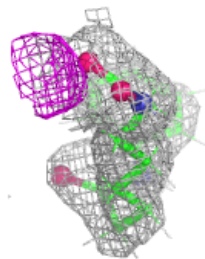
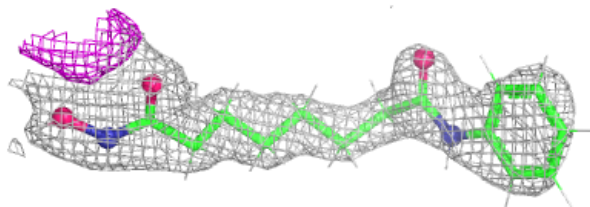
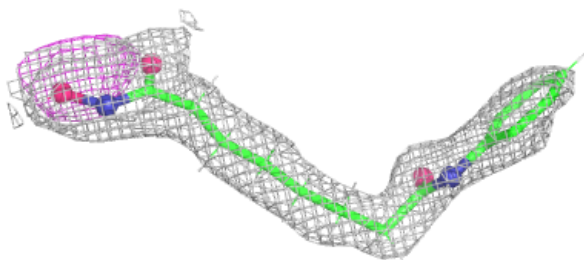
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around KK0 C 608:

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

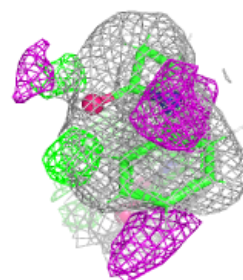
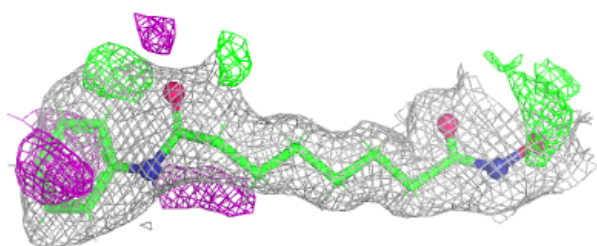
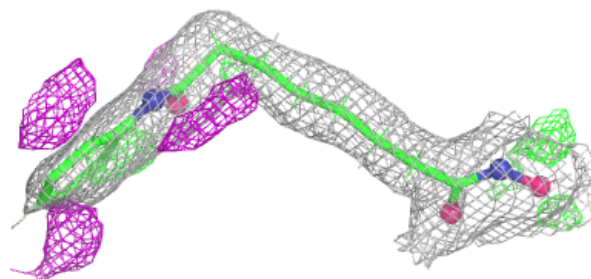
**Electron density around SHH C 607:**

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

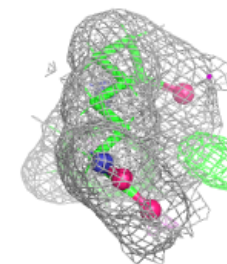
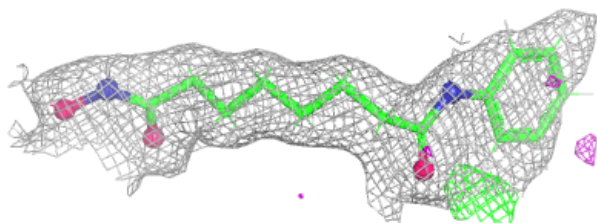
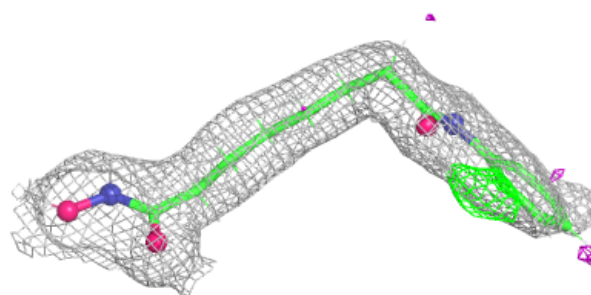


Electron density around SHH A 607:

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

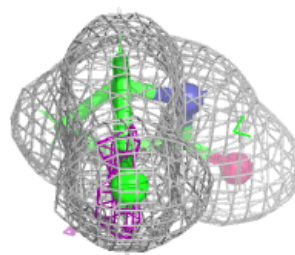
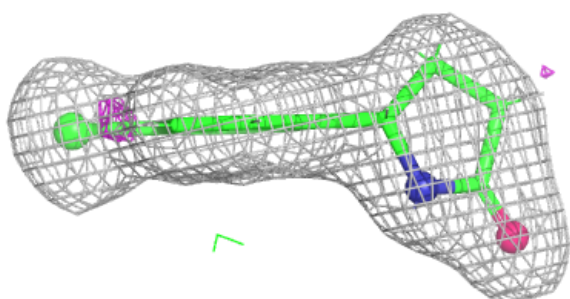
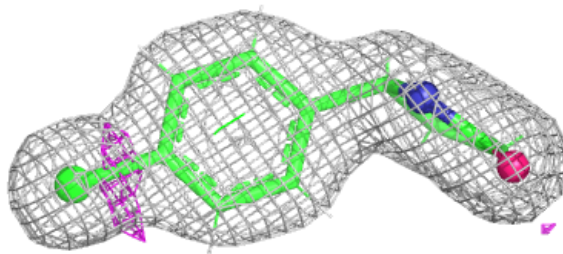
**Electron density around SHH B 610:**

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

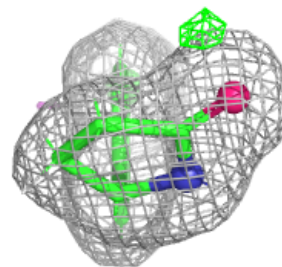
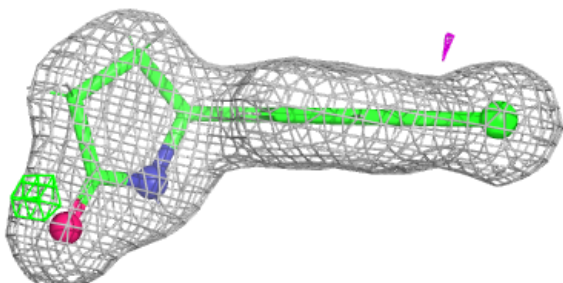
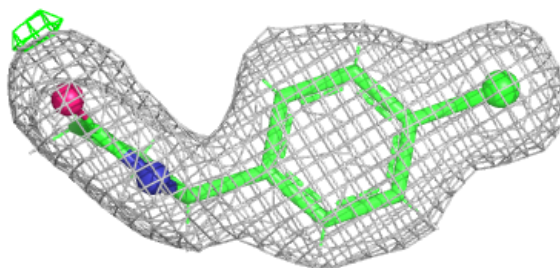


Electron density around KK0 A 609:

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

**Electron density around KK0 B 613:**

$2mF_o-DF_c$ (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.