Full wwPDB X-ray Structure Validation Report ⓘ

Jan 6, 2022 – 06:30 pm GMT

PDB ID	:	7Q0D
Title	:	Human carbonic anhydrase I in complex with Methyl 2-(benzenesulfonyl)-4-chloro-5-sulfamoylbenzoate
Authors	:	Paketuryte-Latve, V.; Smirnov, A.; Manakova, E.; Grazulis, S.
Deposited on	:	2021-10-14
Resolution	:	1.24 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 following versions of software and data (see references ⓘ) were used in the production of this report:

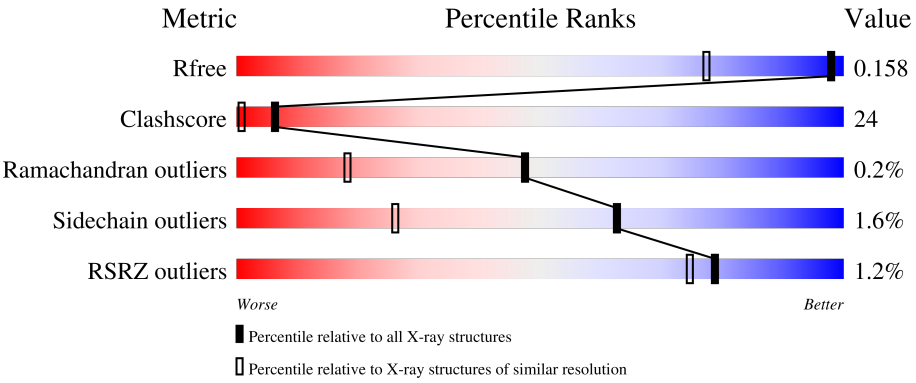
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.24
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.24

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

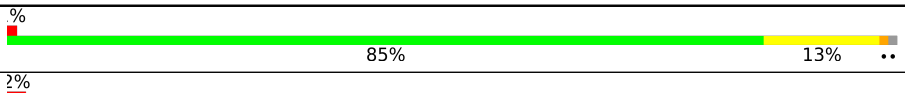
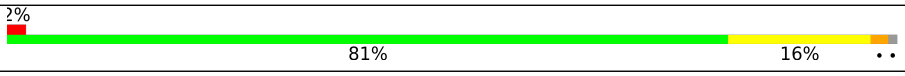
The reported resolution of this entry is 1.24 Å.

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	2024 (1.28-1.20)
Clashscore	141614	1007 (1.26-1.22)
Ramachandran outliers	138981	2053 (1.28-1.20)
Sidechain outliers	138945	2051 (1.28-1.20)
RSRZ outliers	127900	1987 (1.28-1.20)

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	261	
1	B	261	

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
3	84Z	A	302[A]	-	-	X	-
3	84Z	B	302[A]	-	-	X	-
4	EDO	A	305	-	-	X	-
4	EDO	A	311	-	-	X	-
4	EDO	A	312	-	-	X	-
4	EDO	A	314	-	-	X	-
4	EDO	A	315	-	-	-	X
4	EDO	B	311	-	-	X	-
4	EDO	B	314	-	-	X	-
4	EDO	B	315	-	-	-	X
4	EDO	B	316	-	-	X	-
4	EDO	B	317	-	-	X	-
5	ACT	A	306	-	-	X	-
5	ACT	A	307	-	-	X	-
5	ACT	B	305	-	-	X	-
6	PEG	A	308	-	-	X	-
6	PEG	A	310	-	-	X	X
6	PEG	B	303	-	-	X	-
6	PEG	B	306	-	-	X	-
6	PEG	B	308	-	-	X	-
6	PEG	B	309	-	-	X	-
6	PEG	B	310	-	-	X	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 5464 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

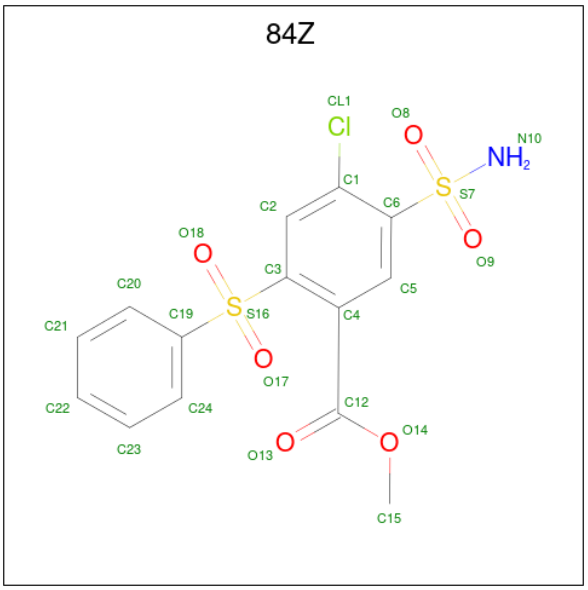
- Molecule 1 is a protein called Carbonic anhydrase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	258	Total	C	N	O	S	0	32	0
			2280	1438	393	446	3			
1	B	258	Total	C	N	O	S	0	14	0
			2114	1331	365	415	3			

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

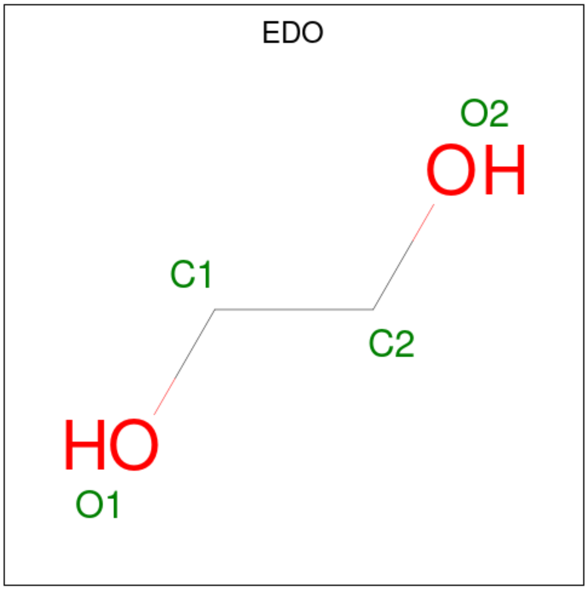
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		

- Molecule 3 is methyl 4-chloranyl-2-(phenylsulfonyl)-5-sulfamoyl-benzoate (three-letter code: 84Z) (formula: $C_{14}H_{12}ClNO_6S_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 48	C 28	Cl 2	N 2	O 12	S 4	0	1
3	B	1	Total 48	C 28	Cl 2	N 2	O 12	S 4	0	1

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

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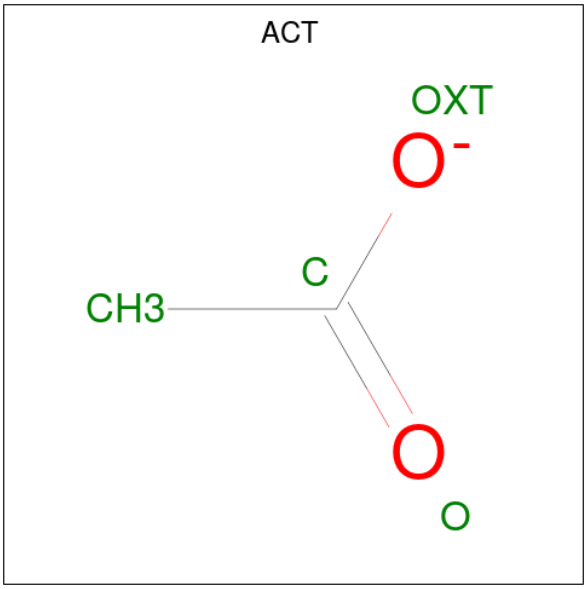
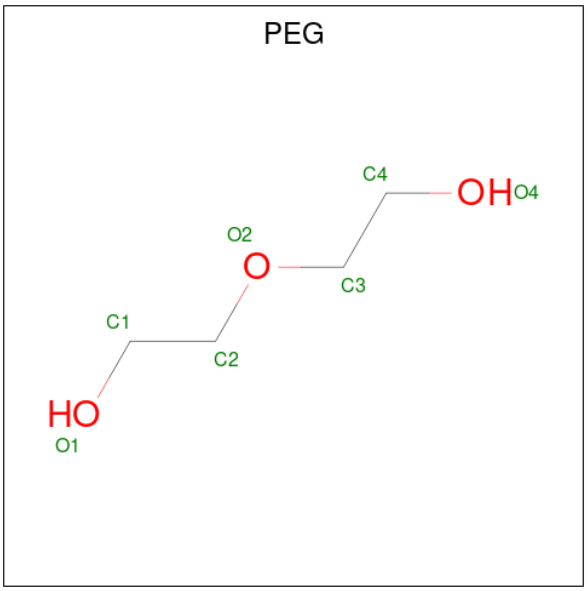
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 7 4 3	0	0
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 7 4 3	0	0
6	B	1	Total C O 7 4 3	0	0
6	B	1	Total C O 7 4 3	0	0
6	B	1	Total C O 7 4 3	0	0
6	B	1	Total C O 7 4 3	0	0
6	B	1	Total C O 7 4 3	0	0
6	B	1	Total C O 7 4 3	0	0

- Molecule 7 is water.

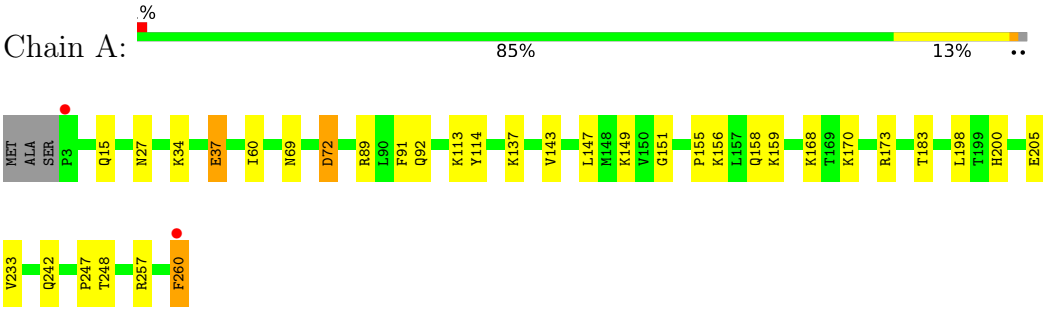
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	442	Total O 442 442	0	0
7	B	394	Total O 394 394	0	0

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.

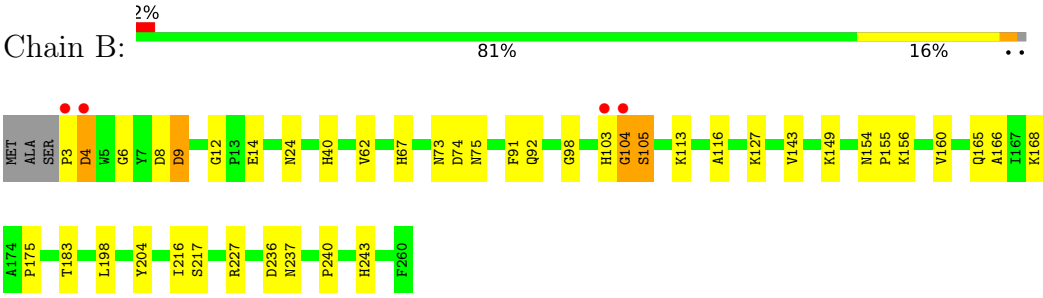
• Molecule 1: Carbonic anhydrase 1

Chain A:



• Molecule 1: Carbonic anhydrase 1

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	62.04Å 73.23Å 120.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	55.16 – 1.24 55.16 – 1.24	Depositor EDS
% Data completeness (in resolution range)	98.3 (55.16-1.24) 98.3 (55.16-1.24)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	3.50 (at 1.24Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.131 , 0.158 0.131 , 0.158	Depositor DCC
R_{free} test set	15031 reflections (9.90%)	wwPDB-VP
Wilson B-factor (Å^2)	10.7	Xtriage
Anisotropy	0.256	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	0.98	EDS
Total number of atoms	5464	wwPDB-VP
Average B, all atoms (Å^2)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.74% 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: PEG, ZN, ACT, EDO, 84Z

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	1.10	0/2343	1.05	0/3180
1	B	1.19	0/2175	1.13	2/2961 (0.1%)
All	All	1.14	0/4518	1.09	2/6141 (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	1

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	105	SER	N-CA-CB	8.47	123.21	110.50
1	B	105	SER	N-CA-C	-7.74	90.10	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	72[A]	ASP	Mainchain

CLOSE-CONTACTS INFOmissingINFO

5.2 Torsion angles (i)

5.2.1 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	287/261 (110%)	277 (96%)	10 (4%)	0	100 100
1	B	270/261 (103%)	259 (96%)	10 (4%)	1 (0%)	34 10
All	All	557/522 (107%)	536 (96%)	20 (4%)	1 (0%)	47 18

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	104	GLY

5.2.2 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	253/226 (112%)	247 (98%)	6 (2%)	49 11
1	B	230/226 (102%)	226 (98%)	4 (2%)	60 23
All	All	483/452 (107%)	473 (98%)	10 (2%)	62 15

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	37[A]	GLU
1	A	37[B]	GLU
1	A	168	LYS
1	A	260[A]	PHE

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Mol	Chain	Res	Type
1	A	260[B]	PHE
1	B	4	ASP
1	B	9	ASP
1	B	92[A]	GLN
1	B	92[B]	GLN

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	15	GLN
1	A	24	ASN
1	A	73	ASN
1	B	73	ASN

5.2.3 RNA

There are no RNA molecules in this entry.

5.3 Non-standard residues in protein, DNA, RNA chains

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

5.4 Carbohydrates

There are no monosaccharides in this entry.

5.5 Ligand geometry

Of 34 ligands modelled in this entry, 2 are monoatomic - leaving 32 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	$\#\|Z\|>2$
4	EDO	A	314	-	3,3,3	0.46	0	2,2,2	0.34	0
4	EDO	A	304	-	3,3,3	0.46	0	2,2,2	0.33	0
4	EDO	B	317	-	3,3,3	0.46	0	2,2,2	0.34	0
4	EDO	A	312	-	3,3,3	0.46	0	2,2,2	0.34	0
5	ACT	B	305	-	1,3,3	1.29	0	0,3,3	-	-
6	PEG	B	307	-	6,6,6	0.43	0	5,5,5	0.31	0
4	EDO	B	312	-	3,3,3	0.46	0	2,2,2	0.34	0
6	PEG	B	310	-	6,6,6	0.43	0	5,5,5	0.31	0
4	EDO	A	305	-	3,3,3	0.46	0	2,2,2	0.34	0
6	PEG	B	306	-	6,6,6	0.43	0	5,5,5	0.31	0
4	EDO	A	313	-	3,3,3	0.46	0	2,2,2	0.34	0
4	EDO	B	314	-	3,3,3	0.46	0	2,2,2	0.34	0
4	EDO	A	311	-	3,3,3	0.45	0	2,2,2	0.33	0
3	84Z	A	302[A]	2	25,25,25	2.65	8 (32%)	38,38,38	3.31	21 (55%)
3	84Z	B	302[A]	2	25,25,25	2.57	10 (40%)	38,38,38	2.79	18 (47%)
6	PEG	B	309	-	6,6,6	0.43	0	5,5,5	0.31	0
5	ACT	A	306	-	1,3,3	1.33	0	0,3,3	-	-
6	PEG	B	303	-	6,6,6	0.43	0	5,5,5	0.32	0
4	EDO	A	315	-	3,3,3	0.46	0	2,2,2	0.34	0
4	EDO	B	316	-	3,3,3	0.46	0	2,2,2	0.34	0
3	84Z	A	302[B]	2	25,25,25	2.08	7 (28%)	38,38,38	2.45	12 (31%)
3	84Z	B	302[B]	1,2	25,25,25	2.65	6 (24%)	38,38,38	1.76	11 (28%)
6	PEG	A	308	-	6,6,6	0.43	0	5,5,5	0.31	0
4	EDO	B	315	-	3,3,3	0.46	0	2,2,2	0.33	0
4	EDO	B	311	-	3,3,3	0.46	0	2,2,2	0.34	0
4	EDO	B	313	-	3,3,3	0.46	0	2,2,2	0.34	0
6	PEG	B	308	-	6,6,6	0.43	0	5,5,5	0.31	0
5	ACT	A	307	-	1,3,3	1.39	0	0,3,3	-	-
6	PEG	A	309	-	3,3,6	0.44	0	2,2,5	0.34	0
6	PEG	A	310	-	6,6,6	0.43	0	5,5,5	0.31	0
4	EDO	A	303	-	3,3,3	0.46	0	2,2,2	0.34	0
4	EDO	B	304	-	3,3,3	0.46	0	2,2,2	0.34	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
4	EDO	A	314	-	-	0/1/1/1	-
4	EDO	A	304	-	-	1/1/1/1	-
4	EDO	B	317	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	A	312	-	-	1/1/1/1	-
6	PEG	B	307	-	-	4/4/4/4	-
4	EDO	B	312	-	-	1/1/1/1	-
6	PEG	B	310	-	-	2/4/4/4	-
4	EDO	A	305	-	-	1/1/1/1	-
6	PEG	B	306	-	-	3/4/4/4	-
4	EDO	A	313	-	-	0/1/1/1	-
4	EDO	B	314	-	-	0/1/1/1	-
4	EDO	A	311	-	-	1/1/1/1	-
3	84Z	A	302[A]	2	-	0/24/24/24	0/2/2/2
3	84Z	B	302[A]	2	-	2/24/24/24	0/2/2/2
6	PEG	B	309	-	-	2/4/4/4	-
6	PEG	B	303	-	-	2/4/4/4	-
4	EDO	A	315	-	-	1/1/1/1	-
4	EDO	B	316	-	-	0/1/1/1	-
3	84Z	A	302[B]	2	-	7/24/24/24	0/2/2/2
3	84Z	B	302[B]	1,2	-	4/24/24/24	0/2/2/2
6	PEG	A	308	-	-	0/4/4/4	-
4	EDO	B	315	-	-	1/1/1/1	-
4	EDO	B	311	-	-	0/1/1/1	-
4	EDO	B	313	-	-	0/1/1/1	-
6	PEG	B	308	-	-	2/4/4/4	-
6	PEG	A	309	-	-	1/1/1/4	-
6	PEG	A	310	-	-	1/4/4/4	-
4	EDO	A	303	-	-	0/1/1/1	-
4	EDO	B	304	-	-	0/1/1/1	-

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	302[A]	84Z	C19-S16	-7.46	1.65	1.77
3	B	302[B]	84Z	C4-C3	6.70	1.47	1.40
3	B	302[B]	84Z	O18-S16	6.38	1.55	1.44
3	B	302[A]	84Z	S7-N10	6.08	1.72	1.60
3	B	302[B]	84Z	C3-S16	6.05	1.86	1.78
3	A	302[A]	84Z	O18-S16	6.01	1.55	1.44
3	B	302[A]	84Z	O9-S7	4.95	1.52	1.43
3	A	302[A]	84Z	C2-C3	-4.92	1.31	1.39
3	A	302[B]	84Z	C5-C4	-4.46	1.32	1.39
3	B	302[A]	84Z	C19-S16	-4.32	1.70	1.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	302[A]	84Z	O18-S16	4.21	1.51	1.44
3	B	302[A]	84Z	O17-S16	4.13	1.51	1.44
3	B	302[B]	84Z	C6-S7	4.07	1.82	1.77
3	A	302[B]	84Z	C19-S16	-4.00	1.70	1.77
3	A	302[A]	84Z	C4-C12	-3.91	1.41	1.50
3	A	302[B]	84Z	O14-C15	-3.81	1.36	1.45
3	B	302[A]	84Z	O14-C15	-3.64	1.36	1.45
3	A	302[B]	84Z	C2-C1	-3.64	1.32	1.38
3	A	302[A]	84Z	O14-C15	-3.03	1.38	1.45
3	A	302[B]	84Z	S7-N10	-2.92	1.54	1.60
3	B	302[A]	84Z	C2-C3	-2.83	1.34	1.39
3	A	302[B]	84Z	O18-S16	2.73	1.49	1.44
3	B	302[A]	84Z	O8-S7	2.71	1.48	1.43
3	A	302[B]	84Z	C6-S7	-2.63	1.74	1.77
3	A	302[A]	84Z	C4-C3	2.61	1.43	1.40
3	A	302[A]	84Z	O14-C12	2.35	1.38	1.33
3	A	302[A]	84Z	C2-C1	-2.25	1.35	1.38
3	B	302[A]	84Z	C5-C6	-2.25	1.35	1.39
3	B	302[A]	84Z	C4-C12	-2.22	1.45	1.50
3	B	302[B]	84Z	C24-C19	2.16	1.42	1.38
3	B	302[B]	84Z	C2-C1	2.13	1.42	1.38

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	302[A]	84Z	O18-S16-C19	9.96	119.20	107.97
3	A	302[A]	84Z	O17-S16-O18	-7.86	104.21	119.23
3	A	302[A]	84Z	C23-C24-C19	7.09	126.31	118.95
3	A	302[B]	84Z	O18-S16-C19	7.03	115.90	107.97
3	A	302[B]	84Z	O17-S16-C19	-6.52	100.62	107.97
3	B	302[A]	84Z	O18-S16-C19	6.41	115.20	107.97
3	B	302[A]	84Z	O17-S16-O18	-6.21	107.37	119.23
3	A	302[A]	84Z	C22-C23-C24	-5.20	112.26	120.19
3	A	302[B]	84Z	C24-C19-S16	-5.13	112.98	119.52
3	B	302[A]	84Z	C19-S16-C3	5.12	112.51	105.28
3	A	302[B]	84Z	C20-C19-S16	4.77	125.60	119.52
3	B	302[A]	84Z	C1-C6-S7	-4.32	118.00	123.49
3	B	302[A]	84Z	O8-S7-C6	-4.30	100.98	107.29
3	B	302[A]	84Z	C5-C6-C1	4.29	122.83	118.27
3	A	302[A]	84Z	O18-S16-C3	4.22	114.99	107.96
3	B	302[A]	84Z	C4-C5-C6	-4.12	116.40	122.02
3	A	302[A]	84Z	O8-S7-C6	-4.10	101.27	107.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	302[A]	84Z	C1-C2-C3	-4.09	116.89	120.60
3	A	302[A]	84Z	C5-C6-S7	4.03	123.16	118.34
3	B	302[A]	84Z	O14-C12-C4	3.83	118.65	112.30
3	A	302[B]	84Z	O17-S16-C3	3.73	114.18	107.96
3	B	302[B]	84Z	C20-C19-C24	3.63	125.51	120.44
3	B	302[A]	84Z	C6-S7-N10	3.56	114.84	108.28
3	B	302[B]	84Z	O17-S16-O18	-3.40	112.74	119.23
3	A	302[A]	84Z	O17-S16-C19	-3.37	104.17	107.97
3	A	302[B]	84Z	C19-S16-C3	-3.30	100.61	105.28
3	B	302[B]	84Z	C2-C3-S16	3.18	121.55	116.71
3	B	302[A]	84Z	O9-S7-O8	-3.13	113.62	118.76
3	A	302[A]	84Z	C20-C19-S16	3.10	123.47	119.52
3	B	302[A]	84Z	C15-O14-C12	3.07	121.75	115.83
3	A	302[B]	84Z	O14-C12-C4	-3.04	107.25	112.30
3	A	302[A]	84Z	O9-S7-N10	2.98	111.79	107.36
3	B	302[A]	84Z	C5-C4-C3	2.92	120.56	117.62
3	B	302[B]	84Z	C2-C3-C4	-2.85	117.52	120.24
3	A	302[A]	84Z	C5-C4-C3	2.80	120.44	117.62
3	B	302[B]	84Z	O18-S16-C19	2.79	111.12	107.97
3	A	302[A]	84Z	C1-C6-S7	-2.70	120.07	123.49
3	B	302[A]	84Z	C2-C3-C4	2.68	122.80	120.24
3	A	302[A]	84Z	O14-C12-C4	2.67	116.73	112.30
3	B	302[B]	84Z	C19-S16-C3	2.64	109.01	105.28
3	A	302[B]	84Z	C22-C21-C20	2.63	124.20	120.19
3	A	302[A]	84Z	C21-C22-C23	2.62	124.80	119.93
3	B	302[B]	84Z	C23-C24-C19	-2.54	116.32	118.95
3	A	302[A]	84Z	C4-C5-C6	-2.53	118.57	122.02
3	B	302[B]	84Z	C21-C20-C19	-2.41	116.45	118.95
3	A	302[A]	84Z	O17-S16-C3	-2.40	103.96	107.96
3	A	302[A]	84Z	C5-C4-C12	-2.37	113.71	118.41
3	A	302[B]	84Z	C23-C24-C19	2.33	121.37	118.95
3	A	302[B]	84Z	O9-S7-N10	2.33	110.81	107.36
3	B	302[B]	84Z	O9-S7-C6	-2.28	103.95	107.29
3	A	302[A]	84Z	C19-S16-C3	2.26	108.47	105.28
3	A	302[A]	84Z	C2-C1-CL1	-2.25	114.85	118.49
3	A	302[B]	84Z	C21-C22-C23	-2.23	115.78	119.93
3	A	302[A]	84Z	O14-C12-O13	2.19	127.75	123.45
3	A	302[B]	84Z	C5-C6-S7	2.16	120.92	118.34
3	B	302[A]	84Z	C5-C4-C12	-2.16	114.12	118.41
3	A	302[A]	84Z	C22-C21-C20	-2.13	116.95	120.19
3	B	302[B]	84Z	O9-S7-N10	2.11	110.49	107.36
3	B	302[A]	84Z	C20-C19-S16	-2.11	116.83	119.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	302[A]	84Z	O18-S16-C3	-2.08	104.49	107.96
3	B	302[B]	84Z	C24-C19-S16	-2.03	116.94	119.52
3	B	302[A]	84Z	C24-C19-S16	2.02	122.09	119.52

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	302[B]	84Z	C4-C12-O14-C15
3	A	302[B]	84Z	O13-C12-O14-C15
3	B	302[A]	84Z	C4-C12-O14-C15
6	A	310	PEG	C1-C2-O2-C3
3	B	302[A]	84Z	O13-C12-O14-C15
4	A	311	EDO	O1-C1-C2-O2
4	A	315	EDO	O1-C1-C2-O2
4	B	315	EDO	O1-C1-C2-O2
6	B	303	PEG	O1-C1-C2-O2
6	B	306	PEG	O2-C3-C4-O4
6	B	308	PEG	O1-C1-C2-O2
6	B	308	PEG	O2-C3-C4-O4
6	A	309	PEG	O2-C3-C4-O4
6	B	309	PEG	C4-C3-O2-C2
6	B	307	PEG	C4-C3-O2-C2
6	B	309	PEG	C1-C2-O2-C3
3	A	302[B]	84Z	O14-C12-C4-C3
6	B	303	PEG	C4-C3-O2-C2
3	A	302[B]	84Z	O14-C12-C4-C5
6	B	307	PEG	O1-C1-C2-O2
6	B	310	PEG	C4-C3-O2-C2
6	B	307	PEG	O2-C3-C4-O4
4	A	305	EDO	O1-C1-C2-O2
6	B	306	PEG	C4-C3-O2-C2
3	B	302[B]	84Z	O14-C12-C4-C3
3	A	302[B]	84Z	O13-C12-C4-C3
3	B	302[B]	84Z	O13-C12-C4-C3
3	B	302[B]	84Z	O14-C12-C4-C5
6	B	307	PEG	C1-C2-O2-C3
6	B	306	PEG	C1-C2-O2-C3
3	A	302[B]	84Z	C2-C3-S16-O17
4	B	312	EDO	O1-C1-C2-O2
3	A	302[B]	84Z	C4-C3-S16-O18
3	B	302[B]	84Z	O13-C12-C4-C5

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Mol	Chain	Res	Type	Atoms
6	B	310	PEG	O2-C3-C4-O4
4	A	304	EDO	O1-C1-C2-O2
4	A	312	EDO	O1-C1-C2-O2

There are no ring outliers.

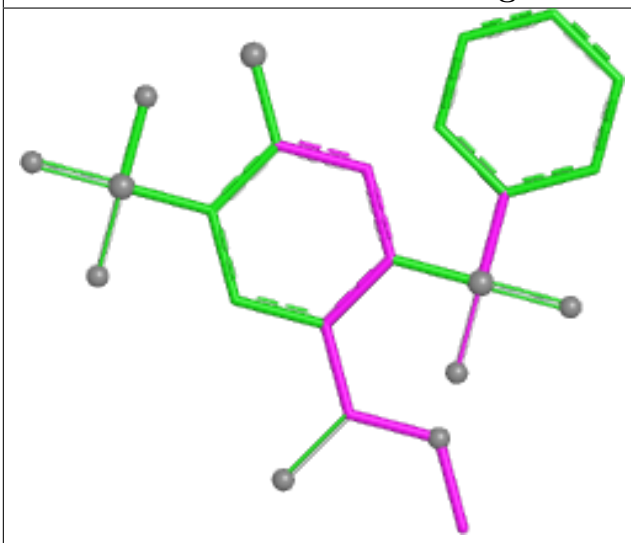
28 monomers are involved in 164 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	314	EDO	5	0
4	B	317	EDO	4	0
4	A	312	EDO	10	0
5	B	305	ACT	4	0
6	B	307	PEG	3	0
4	B	312	EDO	2	0
6	B	310	PEG	7	0
4	A	305	EDO	6	0
6	B	306	PEG	5	0
4	A	313	EDO	2	0
4	B	314	EDO	4	0
4	A	311	EDO	5	0
3	A	302[A]	84Z	8	0
3	B	302[A]	84Z	9	0
6	B	309	PEG	16	0
5	A	306	ACT	5	0
6	B	303	PEG	10	0
4	A	315	EDO	2	0
4	B	316	EDO	4	0
3	A	302[B]	84Z	5	0
3	B	302[B]	84Z	5	0
6	A	308	PEG	10	0
4	B	315	EDO	3	0
4	B	311	EDO	5	0
6	B	308	PEG	6	0
5	A	307	ACT	6	0
6	A	309	PEG	3	0
6	A	310	PEG	13	0

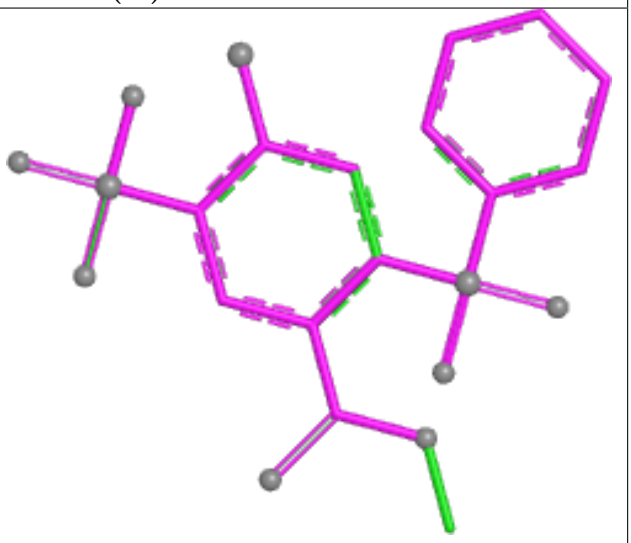
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

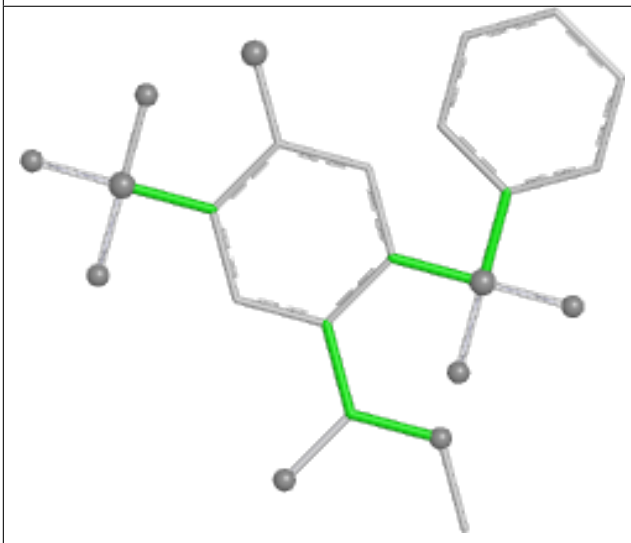
Ligand 84Z A 302 (A)



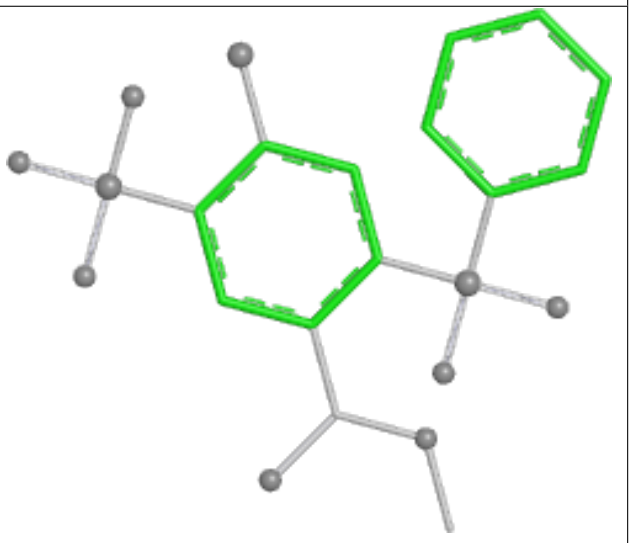
Bond lengths



Bond angles

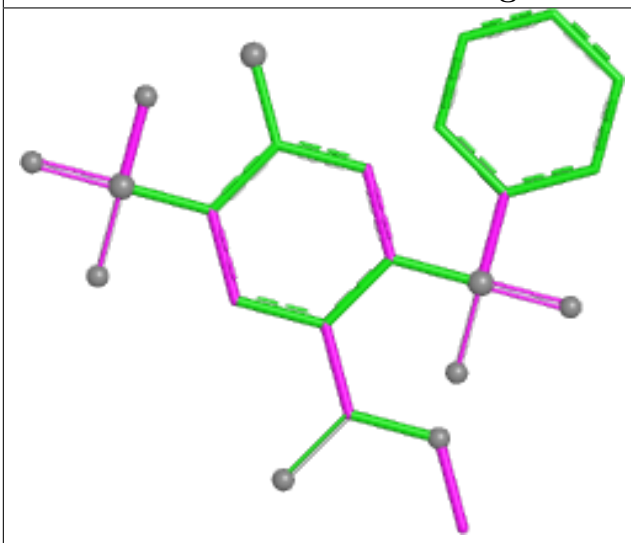


Torsions

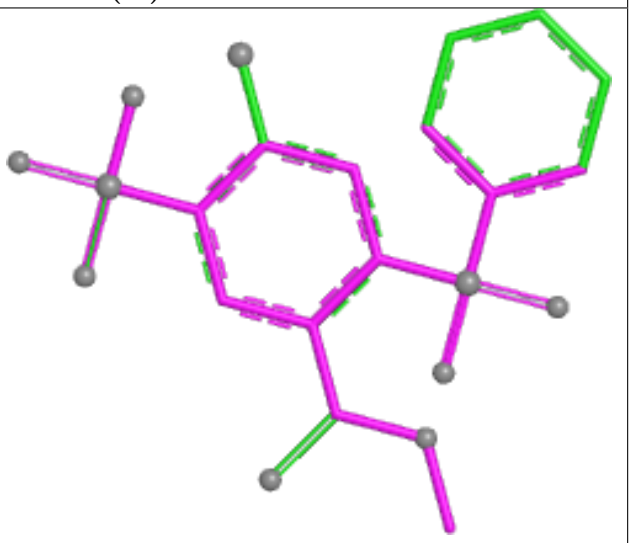


Rings

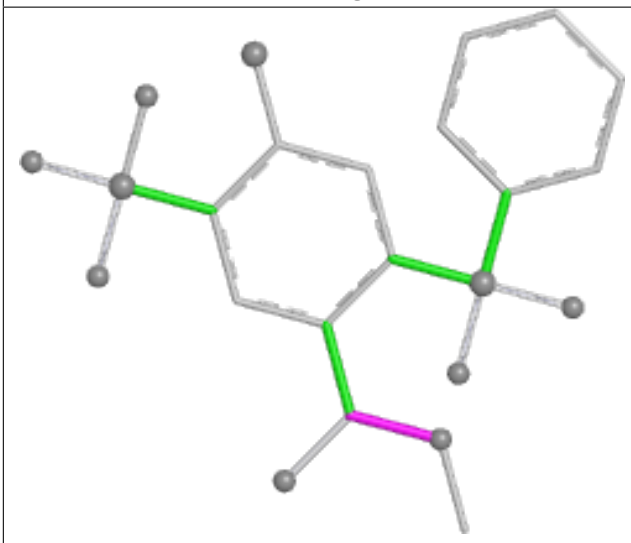
Ligand 84Z B 302 (A)



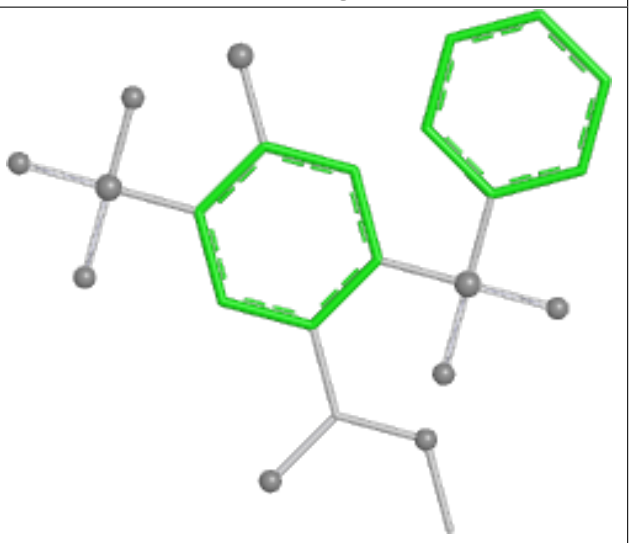
Bond lengths



Bond angles

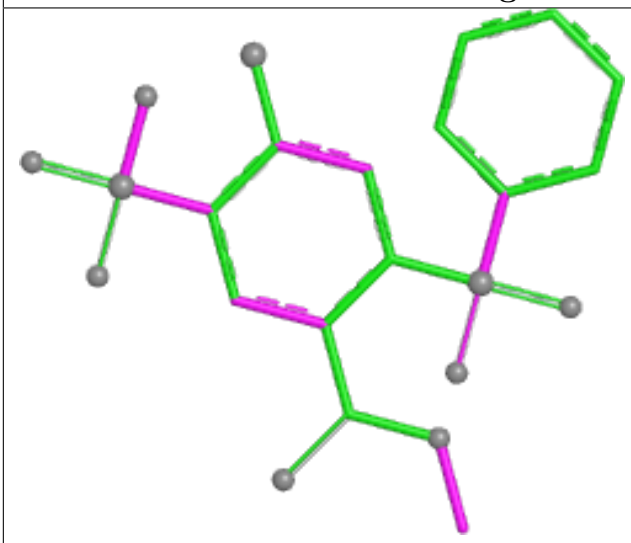


Torsions

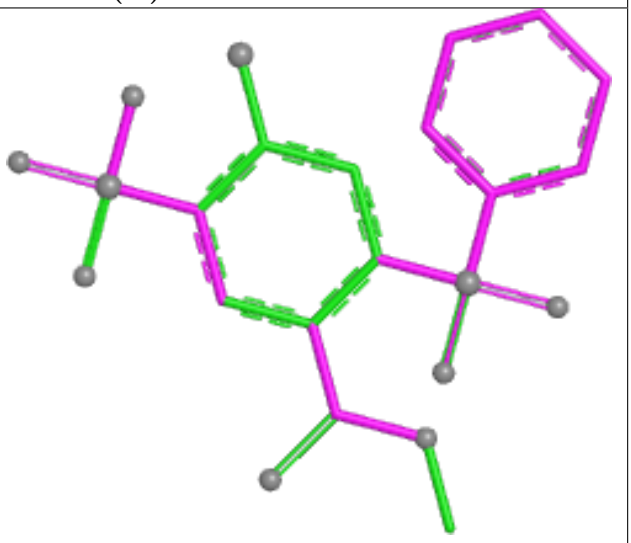


Rings

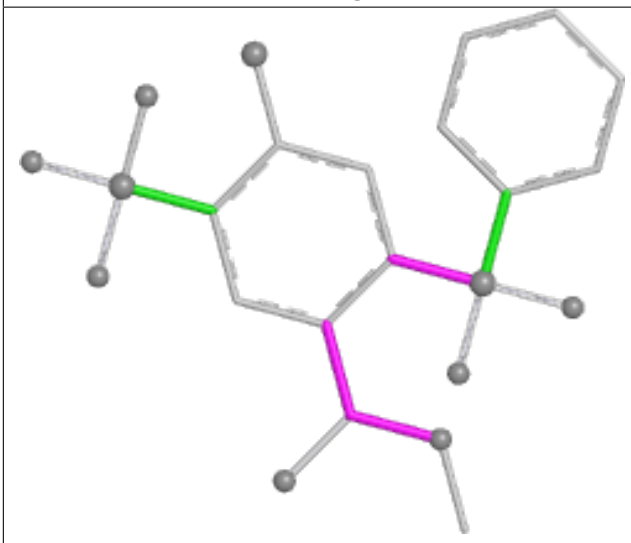
Ligand 84Z A 302 (B)



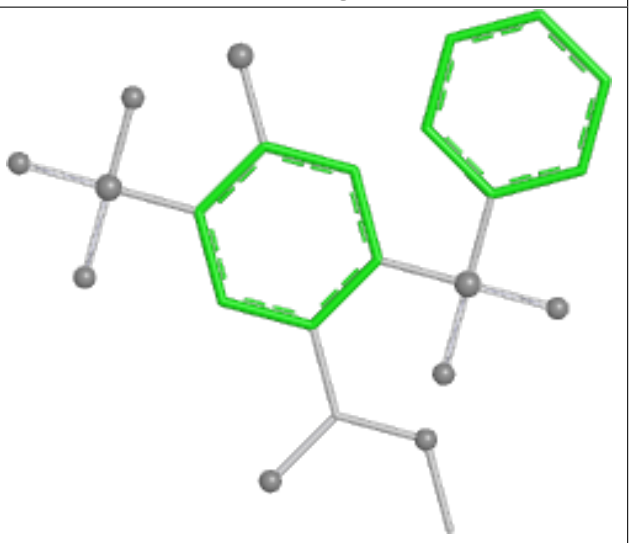
Bond lengths



Bond angles

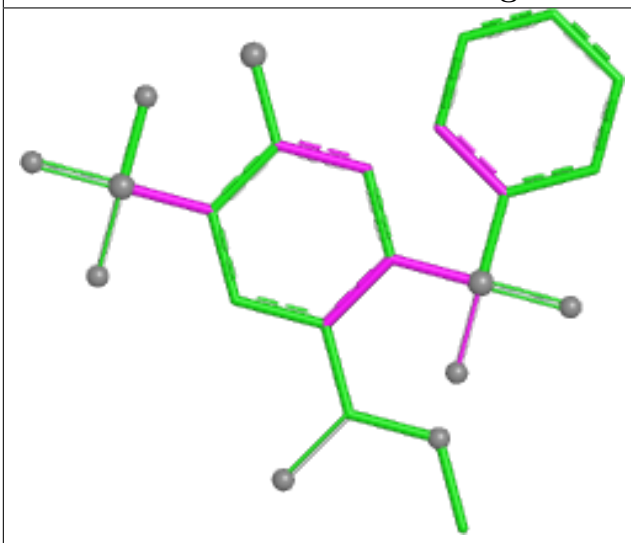


Torsions

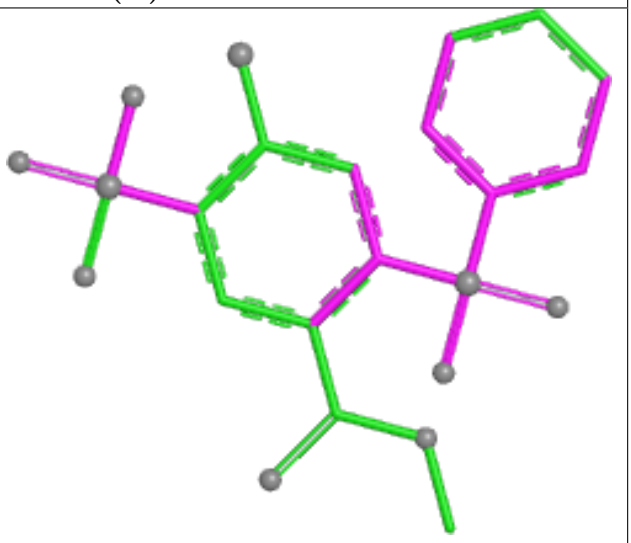


Rings

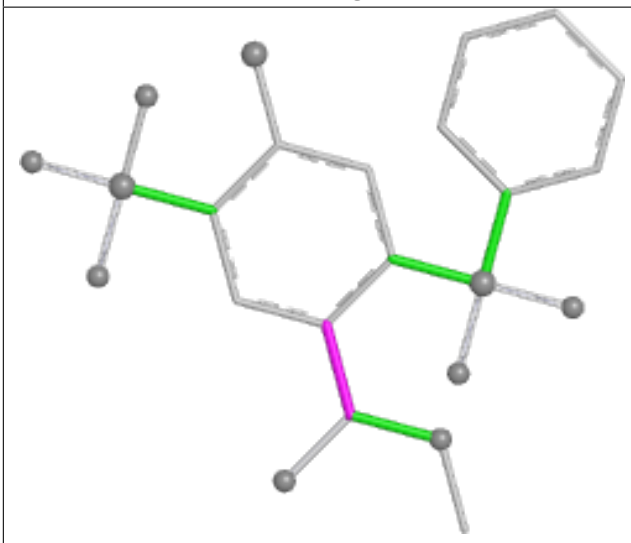
Ligand 84Z B 302 (B)



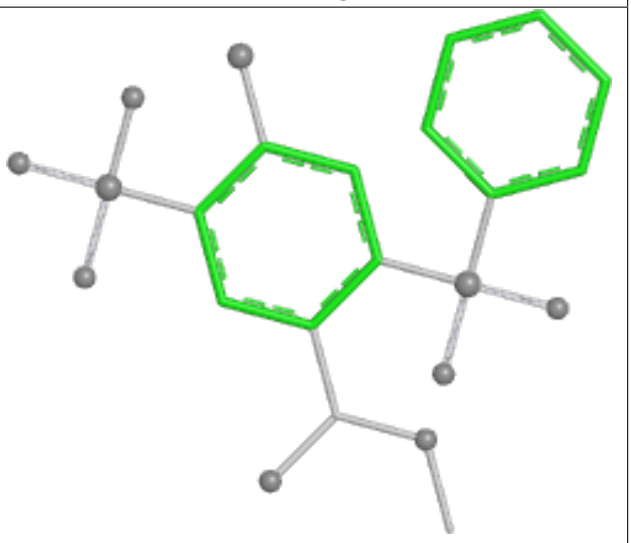
Bond lengths



Bond angles



Torsions



Rings

5.6 Other polymers

There are no such residues in this entry.

5.7 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	258/261 (98%)	-0.40	2 (0%)	86	83	7, 12, 23, 39	0
1	B	258/261 (98%)	-0.49	4 (1%)	72	67	8, 14, 30, 66	0
All	All	516/522 (98%)	-0.44	6 (1%)	79	74	7, 13, 26, 66	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	3	PRO	6.6
1	B	104	GLY	5.7
1	A	260[A]	PHE	4.7
1	A	3	PRO	3.8
1	B	4	ASP	3.2
1	B	103[A]	HIS	2.6

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

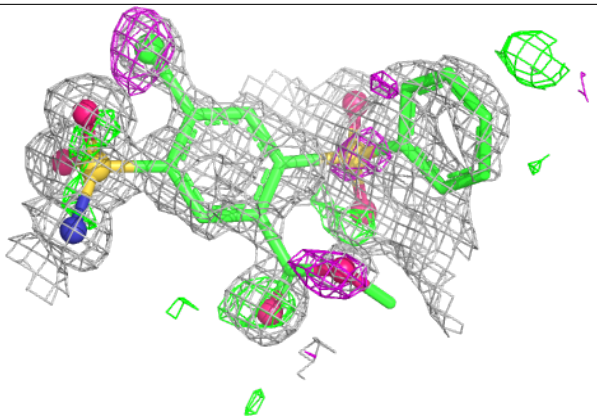
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

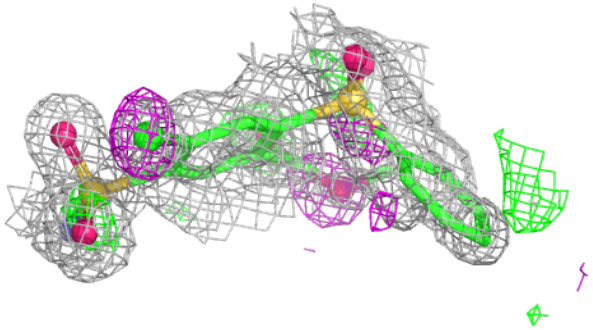
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	PEG	A	310	7/7	0.49	0.47	20,20,20,20	0
6	PEG	B	310	7/7	0.57	0.40	20,20,20,20	0
4	EDO	B	312	4/4	0.62	0.29	40,42,49,51	0
4	EDO	B	316	4/4	0.68	0.26	20,20,20,20	0
6	PEG	B	306	7/7	0.71	0.40	52,63,76,90	0
6	PEG	B	309	7/7	0.72	0.36	20,20,20,20	0
4	EDO	A	315	4/4	0.74	0.47	23,24,27,27	0
6	PEG	A	308	7/7	0.75	0.22	26,31,48,56	0
6	PEG	A	309	4/7	0.75	0.34	47,86,93,98	0
5	ACT	A	306	4/4	0.77	0.21	23,31,33,40	0
4	EDO	B	315	4/4	0.77	0.41	20,20,25,26	0
6	PEG	B	303	7/7	0.77	0.28	24,27,45,97	0
4	EDO	B	317	4/4	0.78	0.31	20,20,20,20	0
5	ACT	B	305	4/4	0.79	0.12	17,23,26,34	0
4	EDO	A	304	4/4	0.81	0.30	27,32,33,55	0
4	EDO	B	311	4/4	0.81	0.21	25,29,39,52	0
4	EDO	A	314	4/4	0.81	0.46	23,26,29,30	0
4	EDO	A	312	4/4	0.82	0.21	18,20,30,37	0
4	EDO	B	314	4/4	0.84	0.19	29,30,37,37	0
6	PEG	B	308	7/7	0.89	0.15	20,23,42,53	0
4	EDO	A	311	4/4	0.89	0.32	21,25,27,28	0
5	ACT	A	307	4/4	0.89	0.30	27,28,31,35	0
4	EDO	B	313	4/4	0.90	0.18	21,25,31,36	0
6	PEG	B	307	7/7	0.92	0.17	20,34,48,66	0
4	EDO	A	313	4/4	0.93	0.19	17,21,23,25	0
4	EDO	A	303	4/4	0.93	0.10	21,28,35,35	0
4	EDO	B	304	4/4	0.96	0.07	19,20,22,33	0
4	EDO	A	305	4/4	0.96	0.18	19,22,28,33	0
3	84Z	B	302[A]	24/24	0.97	0.12	9,16,23,29	24
3	84Z	B	302[B]	24/24	0.97	0.12	8,11,20,21	24
3	84Z	A	302[A]	24/24	0.99	0.09	11,14,22,691	24
3	84Z	A	302[B]	24/24	0.99	0.09	5,15,33,38	24
2	ZN	A	301	1/1	1.00	0.04	7,7,7,7	0
2	ZN	B	301	1/1	1.00	0.04	8,8,8,8	0

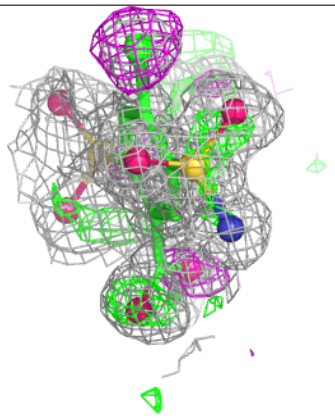
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 84Z B 302 (A):

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

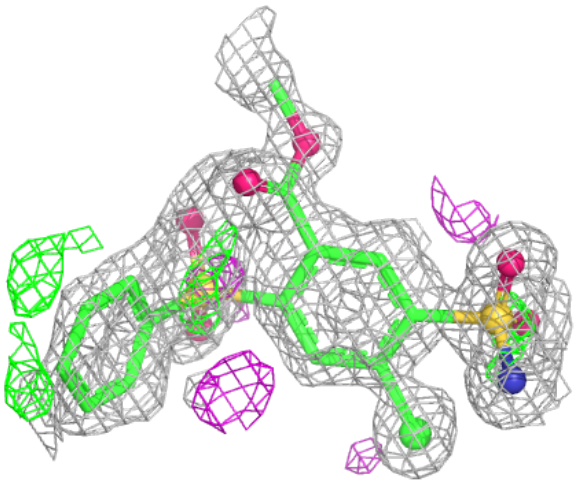


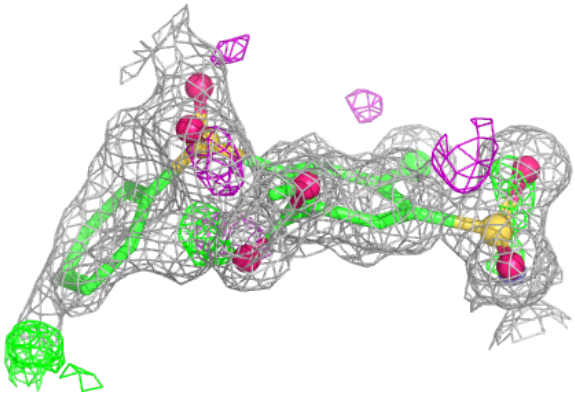


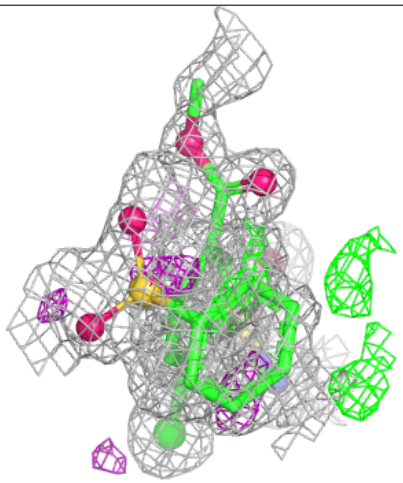


Electron density around 84Z B 302 (B):

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

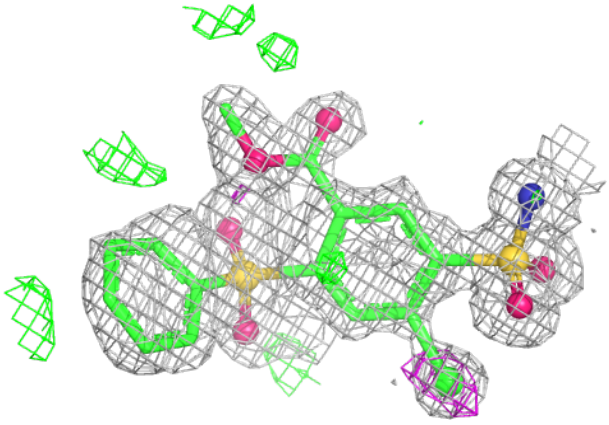


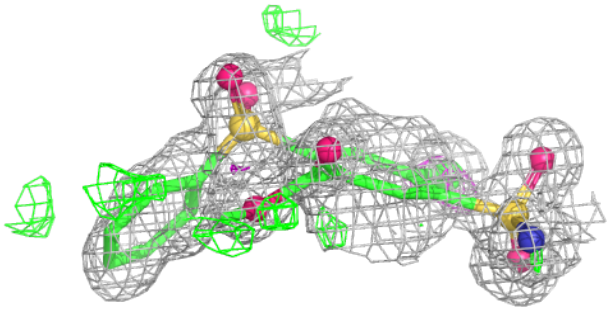


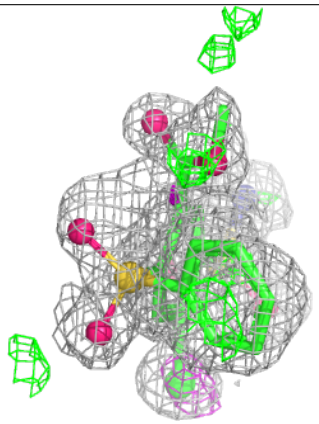


Electron density around 84Z A 302 (A):

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

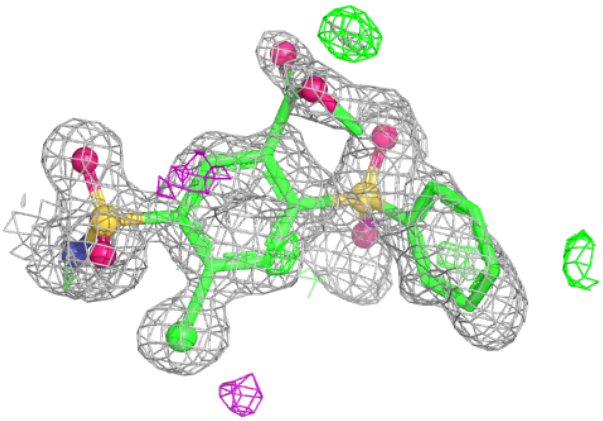


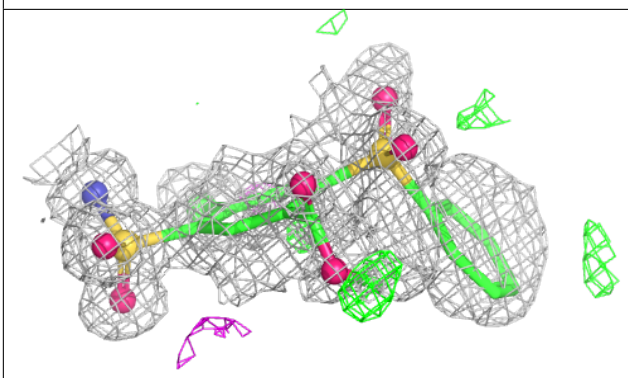


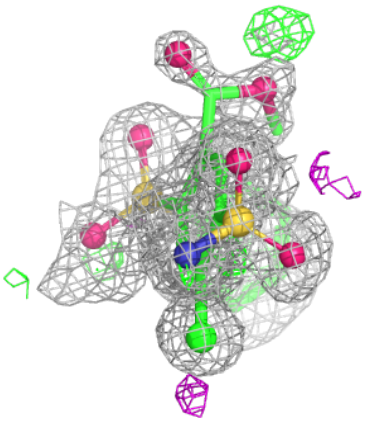


Electron density around 84Z A 302 (B):

$2mF_o$-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.