



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:08 PM UTC

PDB ID : 9FN8 / pdb_00009fn8
Title : Crystal structure of human carboanhydrase XII with 4-benzyl-5,7,8-trifluoro-3,4-dihydro-2H-benzo[b][1,4]thiazine-6-sulfonamide 1,1-dioxide
Authors : Manakova, E.; Paketuryte, V.; Trumpickaite, G.; Smirnov, A.; Vaskevicius, A.
Deposited on : 2024-06-09
Resolution : 1.21 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

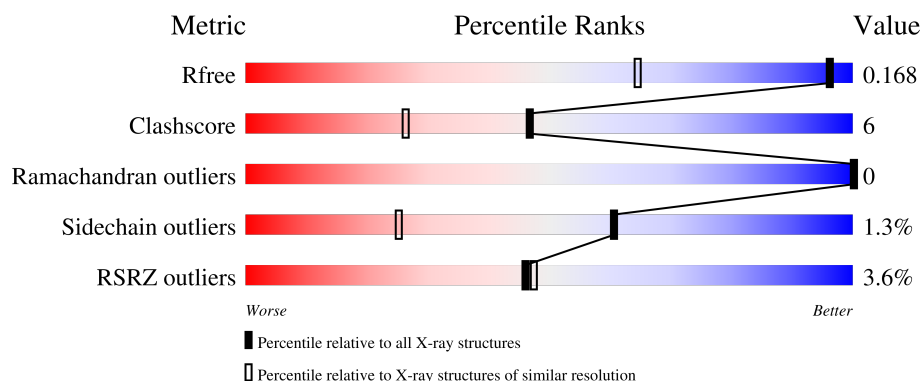
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.21 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	2002 (1.24-1.20)
Clashscore	190562	2061 (1.24-1.20)
Ramachandran outliers	187476	2009 (1.24-1.20)
Sidechain outliers	187428	2008 (1.24-1.20)
RSRZ outliers	180081	2000 (1.24-1.20)

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 $\leq 5\%$. 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	263	5% 88% 10% .
1	B	263	3% 88% 10% ..
1	C	263	3% 90% 9% .
1	D	263	3% 90% 8% ..

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	EDO	D	303	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10312 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 12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	259	Total	C	N	O	S	0	24	0
			2275	1442	388	436	9			
1	B	260	Total	C	N	O	S	0	19	0
			2231	1414	381	428	8			
1	C	260	Total	C	N	O	S	0	11	0
			2169	1376	372	413	8			
1	D	260	Total	C	N	O	S	4	18	0
			2225	1414	376	428	7			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP O43570
B	1	MET	-	initiating methionine	UNP O43570
C	1	MET	-	initiating methionine	UNP O43570
D	1	MET	-	initiating methionine	UNP O43570

- Molecule 2 is ZINC ION (CCD ID: 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		
2	C	1	Total	Zn	0	0
			1	1		
2	D	1	Total	Zn	0	0
			1	1		

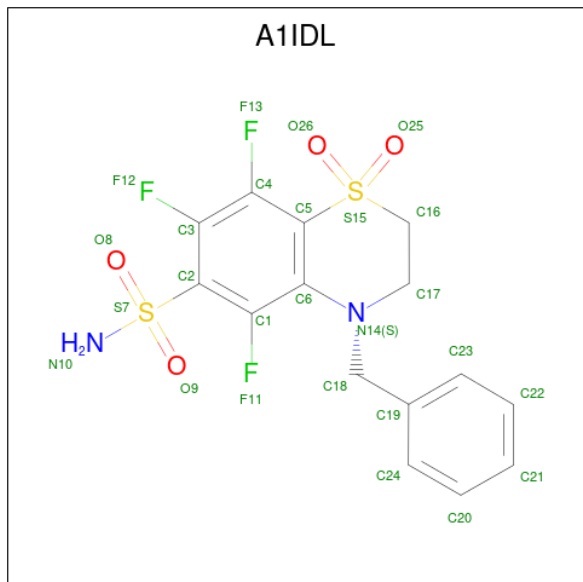
- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

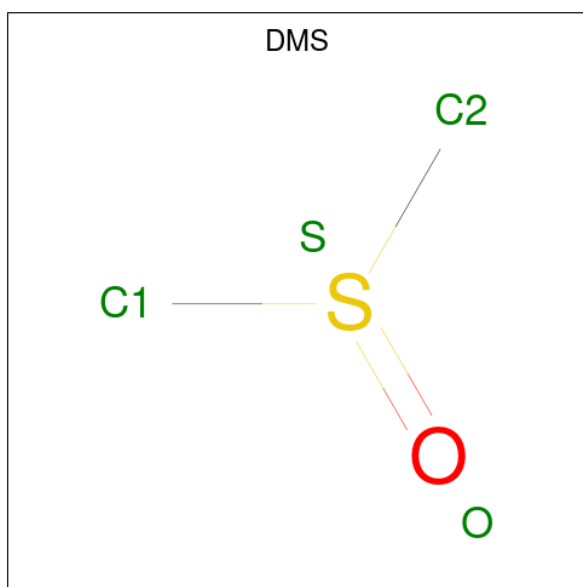
- Molecule 4 is 5,7,8-tris(fluoranyl)-1,1-bis(oxidanylidene)-4-(phenylmethyl)-2,3-dihydro-1 β -D-erythro-pyranose

{6},4-benzothiazine-6-sulfonamide (CCD ID: A1IDL) (formula: $C_{15}H_{13}F_3N_2O_4S_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	F	N	O	S	0	0
			26	15	3	2	4	2		
4	B	1	Total	C	F	N	O	S	0	0
			26	15	3	2	4	2		
4	C	1	Total	C	F	N	O	S	0	0
			26	15	3	2	4	2		
4	D	1	Total	C	F	N	O	S	0	0
			26	15	3	2	4	2		

- Molecule 5 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	D	1	Total	C	O	S	0	0
			4	2	1	1		

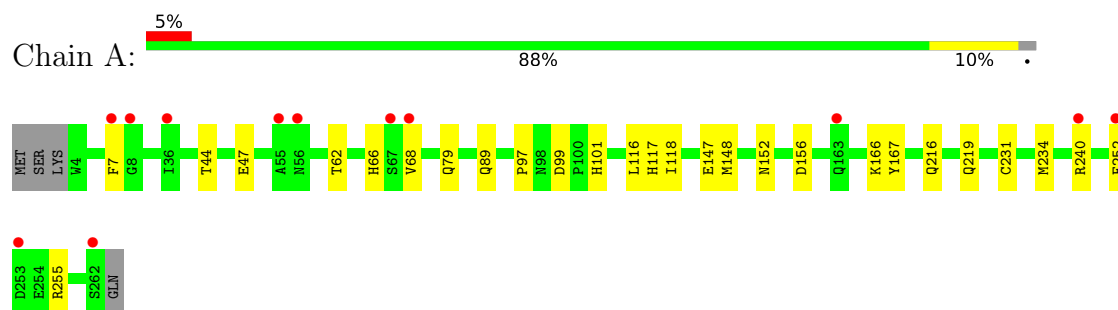
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	276	Total	O	0	4
			280	280		
6	B	335	Total	O	0	6
			341	341		
6	C	282	Total	O	0	5
			287	287		
6	D	335	Total	O	0	5
			340	340		

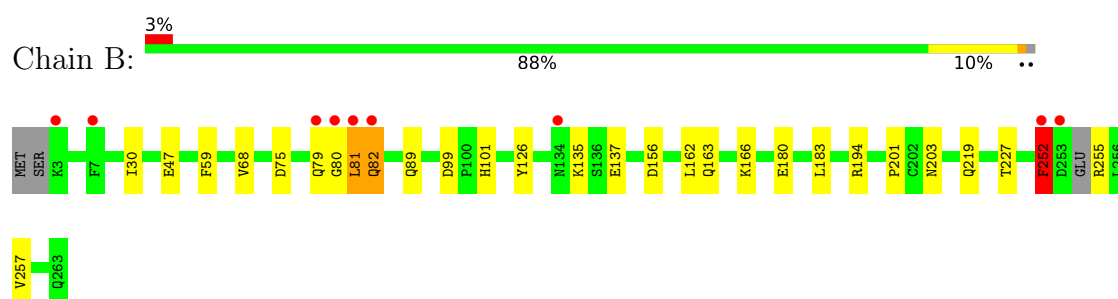
3 Residue-property plots [i](#)

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.

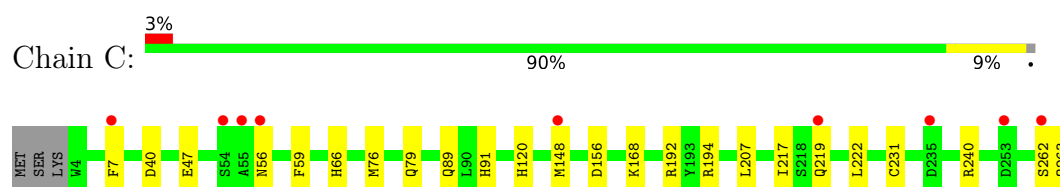
- Molecule 1: Carbonic anhydrase 12



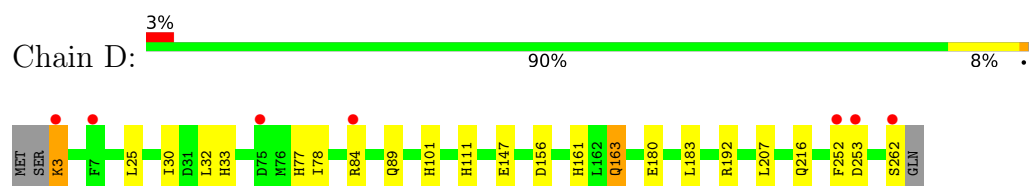
- Molecule 1: Carbonic anhydrase 12



- Molecule 1: Carbonic anhydrase 12



- Molecule 1: Carbonic anhydrase 12



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	77.52Å 74.08Å 91.84Å 90.00° 108.84° 90.00°	Depositor
Resolution (Å)	73.37 – 1.21 73.37 – 1.21	Depositor EDS
% Data completeness (in resolution range)	96.8 (73.37-1.21) 96.8 (73.37-1.21)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 1.21Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.136 , 0.170 0.140 , 0.168	Depositor DCC
R_{free} test set	28812 reflections (9.65%)	wwPDB-VP
Wilson B-factor (Å ²)	12.3	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 40.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	10312	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 41.27 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.4196e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DMS, A1IDL, EDO, ZN

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	0.69	0/2342	1.02	1/3187 (0.0%)
1	B	0.73	0/2302	1.06	9/3130 (0.3%)
1	C	0.76	2/2235 (0.1%)	1.04	3/3042 (0.1%)
1	D	0.74	2/2300 (0.1%)	0.98	1/3132 (0.0%)
All	All	0.73	4/9179 (0.0%)	1.03	14/12491 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	66	HIS	CE1-NE2	6.77	1.39	1.32
1	C	91	HIS	CE1-NE2	5.88	1.38	1.32
1	D	101	HIS	CE1-NE2	5.78	1.38	1.32
1	D	161	HIS	CE1-NE2	5.73	1.38	1.32

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	75	ASP	CA-CB-CG	7.43	120.03	112.60
1	B	81	LEU	CA-C-N	-7.38	110.90	120.65
1	B	81	LEU	C-N-CA	-7.38	110.90	120.65
1	B	252	PHE	CA-C-N	6.32	133.07	121.70
1	B	252	PHE	C-N-CA	6.32	133.07	121.70
1	A	66	HIS	N-CA-C	-6.31	105.23	113.12
1	C	59	PHE	CA-CB-CG	-6.27	107.53	113.80
1	C	40	ASP	CA-CB-CG	6.25	118.85	112.60
1	B	82	GLN	N-CA-C	-5.79	104.66	110.97
1	B	59	PHE	CA-CB-CG	-5.36	108.44	113.80
1	B	219	GLN	CB-CG-CD	5.15	121.36	112.60
1	D	163	GLN	CB-CG-CD	5.13	121.33	112.60
1	C	120	HIS	CA-CB-CG	5.12	118.92	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	80	GLY	O-C-N	5.05	129.26	122.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2275	0	2151	34	0
1	B	2231	0	2107	20	0
1	C	2169	0	2059	20	0
1	D	2225	0	2099	21	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	28	0	42	4	0
3	B	4	0	6	0	0
3	C	8	0	12	0	0
3	D	12	0	18	7	0
4	A	26	0	0	0	0
4	B	26	0	0	0	0
4	C	26	0	0	0	0
4	D	26	0	0	0	0
5	D	4	0	6	1	0
6	A	280	0	0	5	0
6	B	341	0	0	4	0
6	C	287	0	0	4	0
6	D	340	0	0	8	0
All	All	10312	0	8500	100	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 6.

All (100) 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:116[B]:LEU:CD2	1:A:118[B]:ILE:HD11	1.87	1.04
1:C:148:MET:HA	1:C:148:MET:HE2	1.46	0.96
1:A:7:PHE:HZ	1:A:240:ARG:HD2	1.33	0.93
1:A:116[B]:LEU:HD21	1:A:118[B]:ILE:HD11	1.50	0.93
1:A:118[B]:ILE:HD12	1:A:118[B]:ILE:N	1.86	0.90
1:C:148:MET:HB3	6:C:631:HOH:O	1.75	0.86
1:B:255:ARG:CD	6:B:410:HOH:O	2.26	0.82
1:B:255:ARG:HD2	6:B:410:HOH:O	1.79	0.81
1:C:148:MET:HE3	1:C:222:LEU:HD22	1.63	0.80
1:A:166:LYS:HE3	1:A:167:TYR:CZ	2.18	0.79
1:B:201[A]:PRO:HG2	1:B:203[A]:ASN:OD1	1.82	0.79
3:D:303:EDO:H12	6:D:410:HOH:O	1.81	0.79
1:A:117:HIS:C	1:A:118[B]:ILE:HD12	2.08	0.77
1:A:116[B]:LEU:CD2	1:A:118[B]:ILE:CD1	2.65	0.74
1:D:77[A]:HIS:CE1	1:D:84:ARG:NH1	2.56	0.74
1:A:166:LYS:HE3	1:A:167:TYR:CE2	2.26	0.70
1:A:44[A]:THR:HG23	6:A:410:HOH:O	1.90	0.70
1:D:77[A]:HIS:CE1	1:D:84:ARG:HH11	2.09	0.70
1:A:7:PHE:CZ	1:A:240:ARG:HD2	2.22	0.69
1:A:118[B]:ILE:N	1:A:118[B]:ILE:CD1	2.55	0.69
1:C:148:MET:SD	1:C:219:GLN:HA	2.33	0.69
1:B:137:GLU:HG2	1:B:194:ARG:HH12	1.58	0.68
1:A:97:PRO:HB3	3:A:307:EDO:H12	1.75	0.68
1:A:116[B]:LEU:HD23	1:A:118[B]:ILE:HD11	1.75	0.68
1:B:163[A]:GLN:O	1:B:166[A]:LYS:HG3	1.94	0.67
1:C:148:MET:HE1	1:C:222:LEU:HB2	1.77	0.67
1:D:163:GLN:HB2	6:D:519:HOH:O	1.95	0.66
1:A:116[B]:LEU:HD23	1:A:118[B]:ILE:CD1	2.25	0.65
1:B:180[A]:GLU:HG3	1:B:183:LEU:HD12	1.77	0.65
1:A:148:MET:SD	1:A:219[A]:GLN:HG3	2.38	0.64
1:A:252:PHE:CE1	1:A:255[B]:ARG:HD2	2.35	0.62
1:A:116[B]:LEU:HD21	1:A:118[B]:ILE:CD1	2.29	0.61
1:B:227:THR:HB	3:D:304:EDO:H11	1.83	0.61
1:A:231[A]:CYS:SG	1:A:240:ARG:HB3	2.40	0.61
1:D:111:HIS:NE2	3:D:303:EDO:C2	2.65	0.59
1:D:111:HIS:NE2	3:D:303:EDO:H21	2.17	0.59
1:B:162:LEU:HD12	6:B:623:HOH:O	2.03	0.59
1:A:47[B]:GLU:HB3	1:A:79:GLN:HB3	1.85	0.58
1:B:81:LEU:O	1:B:82:GLN:C	2.40	0.58
1:B:68[A]:VAL:O	1:B:68[A]:VAL:HG13	2.03	0.57
1:C:219:GLN:HG3	6:C:553:HOH:O	2.03	0.57
1:A:231[A]:CYS:SG	1:A:240:ARG:CB	2.93	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:148:MET:HE2	1:C:148:MET:CA	2.29	0.56
1:C:148:MET:CE	1:C:222:LEU:HB2	2.36	0.56
1:A:7:PHE:CE2	6:A:520:HOH:O	2.53	0.56
1:A:148:MET:SD	1:A:219[A]:GLN:CG	2.94	0.55
1:A:62[A]:THR:O	1:A:68[A]:VAL:HA	2.07	0.55
1:B:82:GLN:OE1	1:B:82:GLN:N	2.39	0.55
1:B:137:GLU:CG	1:B:194:ARG:HH12	2.20	0.54
3:D:303:EDO:C1	6:D:410:HOH:O	2.45	0.54
3:D:303:EDO:C2	6:D:410:HOH:O	2.57	0.53
3:A:304:EDO:C1	6:A:414:HOH:O	2.56	0.52
1:B:81:LEU:O	1:B:82:GLN:O	2.27	0.52
1:D:30[B]:ILE:HD11	1:D:32:LEU:HD21	1.91	0.52
1:D:147[A]:GLU:HG3	1:D:216:GLN:HG2	1.92	0.51
1:D:77[A]:HIS:CD2	1:D:84:ARG:HD3	2.46	0.51
1:C:219:GLN:NE2	6:C:402:HOH:O	2.34	0.51
1:D:30[B]:ILE:HD11	1:D:32:LEU:CD2	2.40	0.51
1:D:25:LEU:HB3	6:D:417:HOH:O	2.11	0.51
1:B:99:ASP:OD1	1:B:101[B]:HIS:HD2	1.94	0.50
1:D:253:ASP:CB	6:D:417:HOH:O	2.59	0.50
3:A:304:EDO:H11	6:A:414:HOH:O	2.12	0.48
1:D:30[B]:ILE:CD1	1:D:32:LEU:HD23	2.43	0.48
1:C:168:LYS:HB2	1:C:231[B]:CYS:O	2.13	0.47
1:A:166:LYS:HE3	1:A:167:TYR:OH	2.13	0.47
1:B:47:GLU:HB2	1:B:79:GLN:HB3	1.97	0.47
1:C:148:MET:CE	1:C:222:LEU:HD22	2.40	0.47
1:C:148:MET:HE1	1:C:217:ILE:HG13	1.96	0.47
1:C:192:ARG:HD2	1:C:207[B]:LEU:HD11	1.97	0.47
1:A:44[A]:THR:HG22	3:A:302:EDO:H11	1.97	0.46
1:B:252:PHE:CE2	1:B:257:VAL:HG23	2.50	0.46
1:C:148:MET:HA	1:C:148:MET:CE	2.29	0.46
1:B:137:GLU:HG2	1:B:194:ARG:NH1	2.29	0.46
1:D:30[B]:ILE:CD1	1:D:32:LEU:CD2	2.93	0.46
1:D:180[B]:GLU:CD	6:D:407:HOH:O	2.59	0.46
1:C:47:GLU:HB2	1:C:79:GLN:HB3	1.98	0.45
1:A:231[A]:CYS:SG	1:A:240:ARG:HB2	2.56	0.45
1:C:262:SER:OG	1:C:263:GLN:N	2.49	0.45
1:A:147:GLU:O	1:A:216[B]:GLN:HA	2.17	0.44
1:C:194[B]:ARG:HD2	1:C:207[B]:LEU:HD12	2.00	0.44
1:D:111:HIS:NE2	3:D:303:EDO:H22	2.32	0.44
1:A:152:ASN:HB2	1:A:216[A]:GLN:O	2.18	0.44
1:D:180[A]:GLU:HG3	1:D:183:LEU:HD12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231[A]:CYS:SG	1:A:240:ARG:NH1	2.91	0.43
1:A:166:LYS:CE	1:A:167:TYR:CE2	3.00	0.43
1:B:126:TYR:CE1	1:B:135:LYS:HG3	2.53	0.43
1:C:56:ASN:OD1	1:C:56:ASN:C	2.61	0.43
1:D:3:LYS:CE	6:D:401:HOH:O	2.67	0.43
1:B:30:ILE:HD13	1:B:252:PHE:CE1	2.54	0.43
1:D:33:HIS:HE1	1:D:252[B]:PHE:CE2	2.37	0.42
1:D:192:ARG:HD2	1:D:207:LEU:HD11	2.01	0.42
1:D:262:SER:O	5:D:306:DMS:H11	2.20	0.42
1:A:234[A]:MET:HE2	1:A:234[A]:MET:HB3	1.75	0.42
1:C:7:PHE:CE2	1:C:240:ARG:CD	3.02	0.42
1:A:99:ASP:OD1	1:A:101:HIS:HD2	2.03	0.42
1:A:148:MET:SD	1:A:219[A]:GLN:HG2	2.60	0.42
1:A:219[A]:GLN:HG3	6:A:532:HOH:O	2.19	0.41
1:C:219:GLN:HG2	6:C:402:HOH:O	2.19	0.41
1:B:180[B]:GLU:CD	6:B:411:HOH:O	2.64	0.41

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	281/263 (107%)	275 (98%)	6 (2%)	0	100	100
1	B	275/263 (105%)	268 (98%)	7 (2%)	0	100	100
1	C	269/263 (102%)	265 (98%)	4 (2%)	0	100	100
1	D	276/263 (105%)	270 (98%)	6 (2%)	0	100	100
All	All	1101/1052 (105%)	1078 (98%)	23 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	255/235 (108%)	253 (99%)	2 (1%)	73	44
1	B	250/235 (106%)	247 (99%)	3 (1%)	63	28
1	C	243/235 (103%)	240 (99%)	3 (1%)	63	28
1	D	250/235 (106%)	245 (98%)	5 (2%)	48	12
All	All	998/940 (106%)	985 (99%)	13 (1%)	61	25

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	89	GLN
1	A	156	ASP
1	B	89	GLN
1	B	156	ASP
1	B	252	PHE
1	C	76	MET
1	C	89	GLN
1	C	156	ASP
1	D	3	LYS
1	D	78[A]	ILE
1	D	78[B]	ILE
1	D	89	GLN
1	D	156	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	ASN
1	A	110	GLN
1	A	111	HIS
1	A	164	HIS
1	A	250	GLN
1	B	13	ASN

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Mol	Chain	Res	Type
1	B	77	HIS
1	B	111	HIS
1	B	250	GLN
1	C	13	ASN
1	C	250	GLN
1	C	263	GLN
1	D	13	ASN
1	D	250	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 22 ligands modelled in this entry, 4 are monoatomic - leaving 18 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	EDO	B	302	-	3,3,3	0.36	0	2,2,2	0.92	0
4	A1IDL	A	309	2	27,28,28	1.07	1 (3%)	35,44,44	1.08	2 (5%)
3	EDO	D	303	-	3,3,3	0.46	0	2,2,2	1.37	0
3	EDO	A	302	-	3,3,3	0.12	0	2,2,2	0.14	0
3	EDO	A	307	-	3,3,3	0.32	0	2,2,2	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	A1IDL	B	303	2	27,28,28	1.05	1 (3%)	35,44,44	1.19	5 (14%)
3	EDO	D	304	-	3,3,3	0.48	0	2,2,2	0.73	0
3	EDO	A	303	-	3,3,3	0.43	0	2,2,2	0.69	0
3	EDO	A	308	-	3,3,3	0.17	0	2,2,2	0.26	0
4	A1IDL	C	304	2	27,28,28	0.95	1 (3%)	35,44,44	1.35	2 (5%)
4	A1IDL	D	305	2	27,28,28	1.17	2 (7%)	35,44,44	1.66	9 (25%)
3	EDO	A	304	-	3,3,3	0.45	0	2,2,2	0.17	0
3	EDO	A	306	-	3,3,3	0.41	0	2,2,2	0.21	0
5	DMS	D	306	-	3,3,3	0.32	0	3,3,3	0.25	0
3	EDO	C	302	-	3,3,3	0.59	0	2,2,2	0.44	0
3	EDO	D	302	-	3,3,3	0.54	0	2,2,2	0.83	0
3	EDO	A	305	-	3,3,3	0.69	0	2,2,2	0.64	0
3	EDO	C	303	-	3,3,3	0.44	0	2,2,2	0.62	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	EDO	B	302	-	-	1/1/1/1	-
4	A1IDL	A	309	2	-	4/10/26/26	0/2/3/3
3	EDO	D	303	-	-	1/1/1/1	-
3	EDO	A	302	-	-	0/1/1/1	-
3	EDO	A	307	-	-	0/1/1/1	-
4	A1IDL	B	303	2	-	4/10/26/26	0/2/3/3
3	EDO	D	304	-	-	1/1/1/1	-
3	EDO	A	303	-	-	0/1/1/1	-
3	EDO	A	308	-	-	0/1/1/1	-
4	A1IDL	C	304	2	-	4/10/26/26	0/2/3/3
4	A1IDL	D	305	2	-	3/10/26/26	0/2/3/3
3	EDO	A	304	-	-	1/1/1/1	-
3	EDO	A	306	-	-	0/1/1/1	-
3	EDO	C	302	-	-	0/1/1/1	-
3	EDO	D	302	-	-	0/1/1/1	-
3	EDO	A	305	-	-	1/1/1/1	-
3	EDO	C	303	-	-	0/1/1/1	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	303	A1IDL	S7-N10	3.94	1.68	1.60
4	C	304	A1IDL	S7-N10	3.82	1.67	1.60
4	A	309	A1IDL	S7-N10	3.81	1.67	1.60
4	D	305	A1IDL	S7-N10	-2.55	1.55	1.60
4	D	305	A1IDL	C4-C5	-2.37	1.35	1.39

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	304	A1IDL	O25-S15-C16	-5.16	103.10	109.69
4	A	309	A1IDL	O25-S15-C16	-3.51	105.20	109.69
4	D	305	A1IDL	C20-C24-C19	-3.43	115.79	120.61
4	B	303	A1IDL	O25-S15-C16	-3.41	105.33	109.69
4	D	305	A1IDL	C21-C20-C24	3.24	124.23	120.24
4	C	304	A1IDL	O25-S15-O26	3.07	120.24	117.69
4	D	305	A1IDL	C1-C2-C3	-2.95	114.64	116.65
4	B	303	A1IDL	C19-C18-N14	2.78	118.62	114.13
4	B	303	A1IDL	O25-S15-O26	2.74	119.97	117.69
4	D	305	A1IDL	O8-S7-N10	2.66	111.19	107.35
4	D	305	A1IDL	O9-S7-N10	2.62	111.14	107.35
4	D	305	A1IDL	O26-S15-C16	2.52	112.91	109.69
4	A	309	A1IDL	C19-C18-N14	2.47	118.12	114.13
4	D	305	A1IDL	F11-C1-C6	-2.33	115.92	119.64
4	B	303	A1IDL	F11-C1-C2	-2.26	116.69	120.76
4	D	305	A1IDL	C3-C2-S7	2.07	126.38	121.34
4	B	303	A1IDL	C3-C2-S7	2.03	126.29	121.34
4	D	305	A1IDL	F11-C1-C2	-2.03	117.11	120.76

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	309	A1IDL	C3-C2-S7-O9
4	A	309	A1IDL	C3-C2-S7-N10
4	A	309	A1IDL	C1-C2-S7-O9
4	B	303	A1IDL	C3-C2-S7-N10
4	C	304	A1IDL	C3-C2-S7-O9
4	C	304	A1IDL	C3-C2-S7-N10
4	C	304	A1IDL	C1-C2-S7-O9
4	D	305	A1IDL	C3-C2-S7-N10
3	D	304	EDO	O1-C1-C2-O2
4	B	303	A1IDL	C3-C2-S7-O9

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Mol	Chain	Res	Type	Atoms
3	B	302	EDO	O1-C1-C2-O2
3	D	303	EDO	O1-C1-C2-O2
4	C	304	A1IDL	C19-C18-N14-C6
4	D	305	A1IDL	C19-C18-N14-C6
4	B	303	A1IDL	C1-C2-S7-O9
3	A	305	EDO	O1-C1-C2-O2
4	D	305	A1IDL	C1-C2-S7-O8
3	A	304	EDO	O1-C1-C2-O2
4	A	309	A1IDL	C19-C18-N14-C6
4	B	303	A1IDL	C19-C18-N14-C6

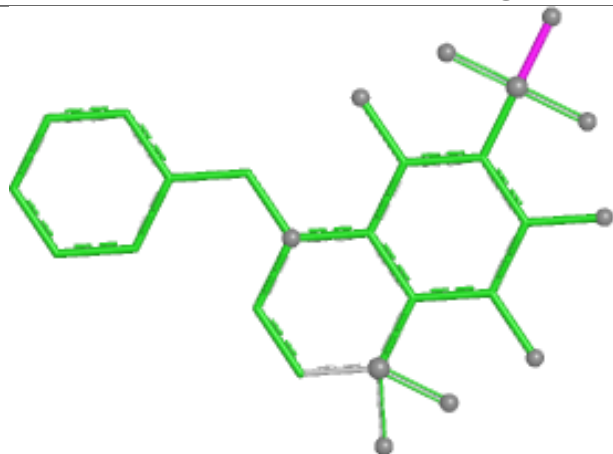
There are no ring outliers.

6 monomers are involved in 12 short contacts:

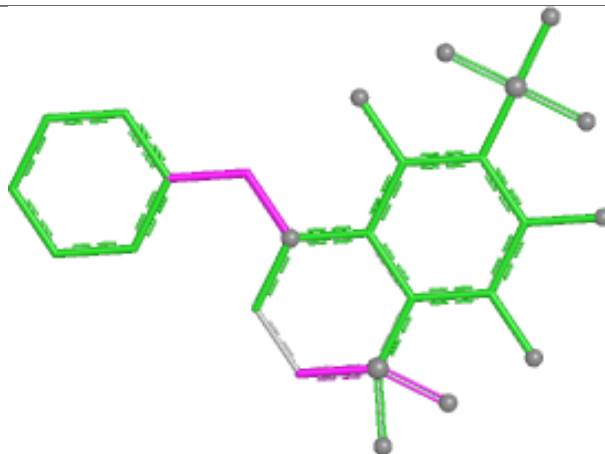
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	303	EDO	6	0
3	A	302	EDO	1	0
3	A	307	EDO	1	0
3	D	304	EDO	1	0
3	A	304	EDO	2	0
5	D	306	DMS	1	0

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.

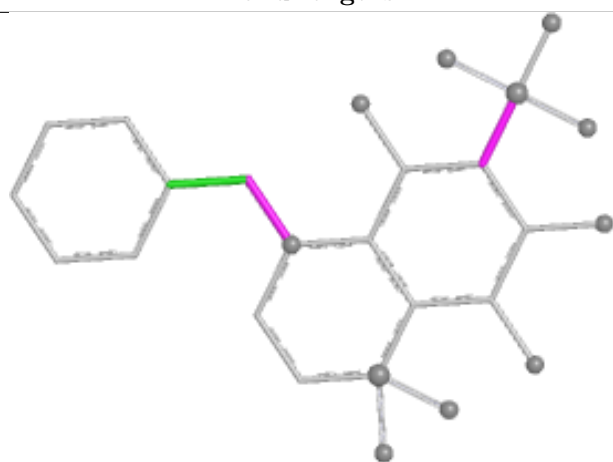
Ligand A1IDL A 309



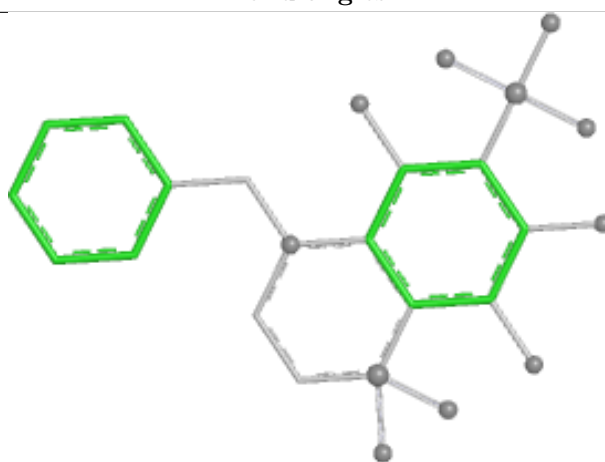
Bond lengths



Bond angles

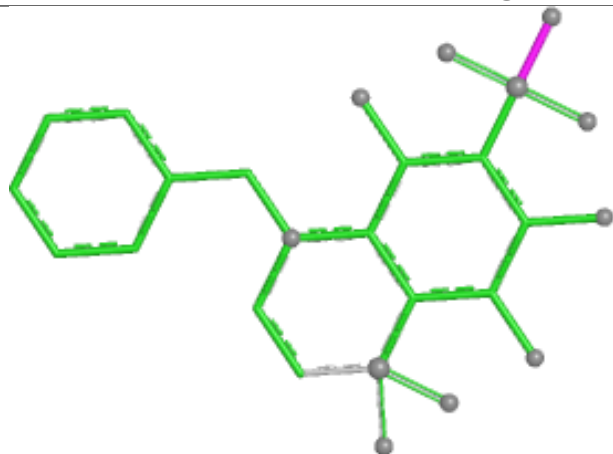


Torsions

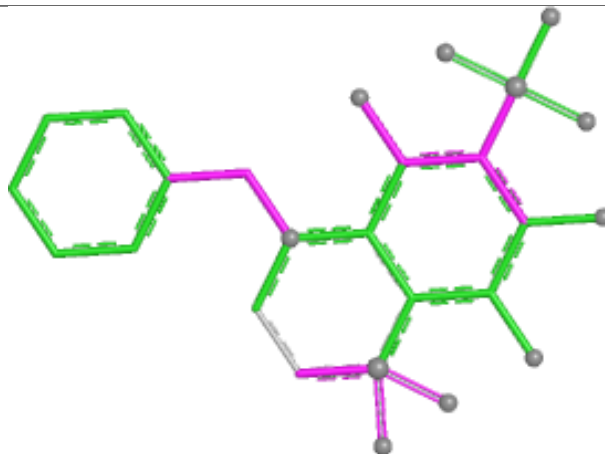


Rings

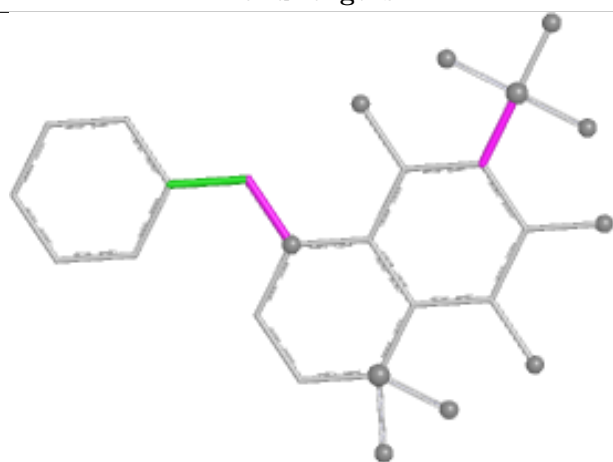
Ligand A1IDL B 303



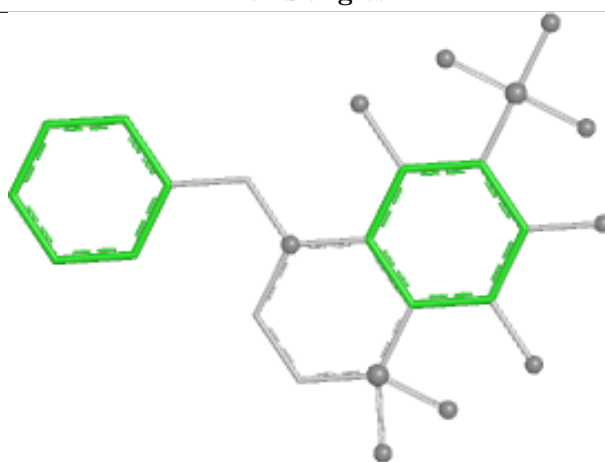
Bond lengths



Bond angles

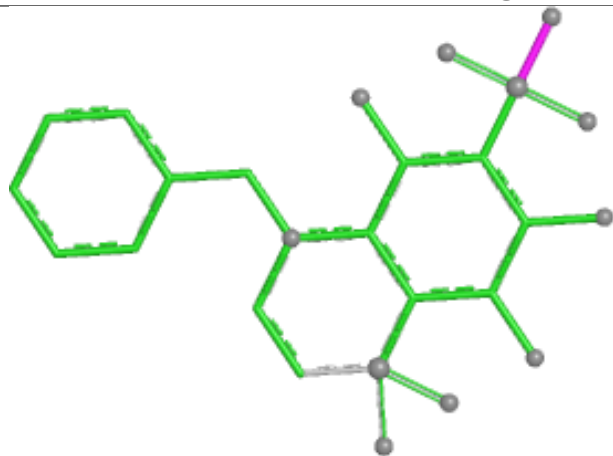


Torsions

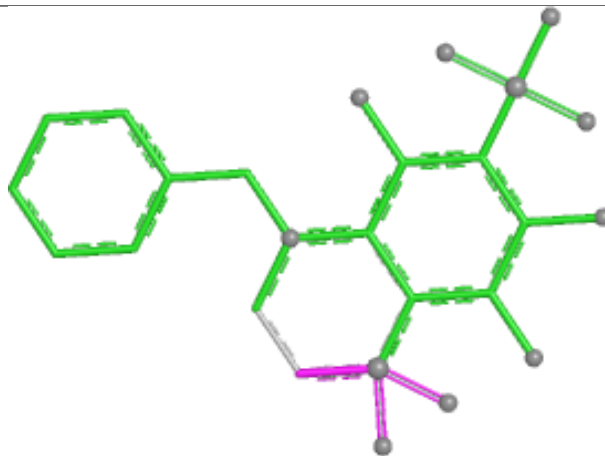


Rings

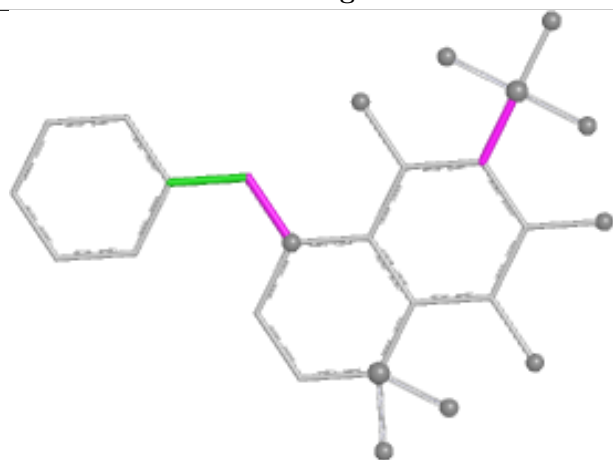
Ligand A1IDL C 304



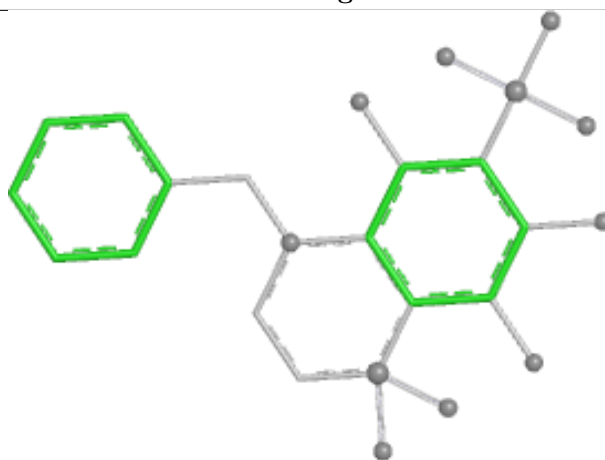
Bond lengths



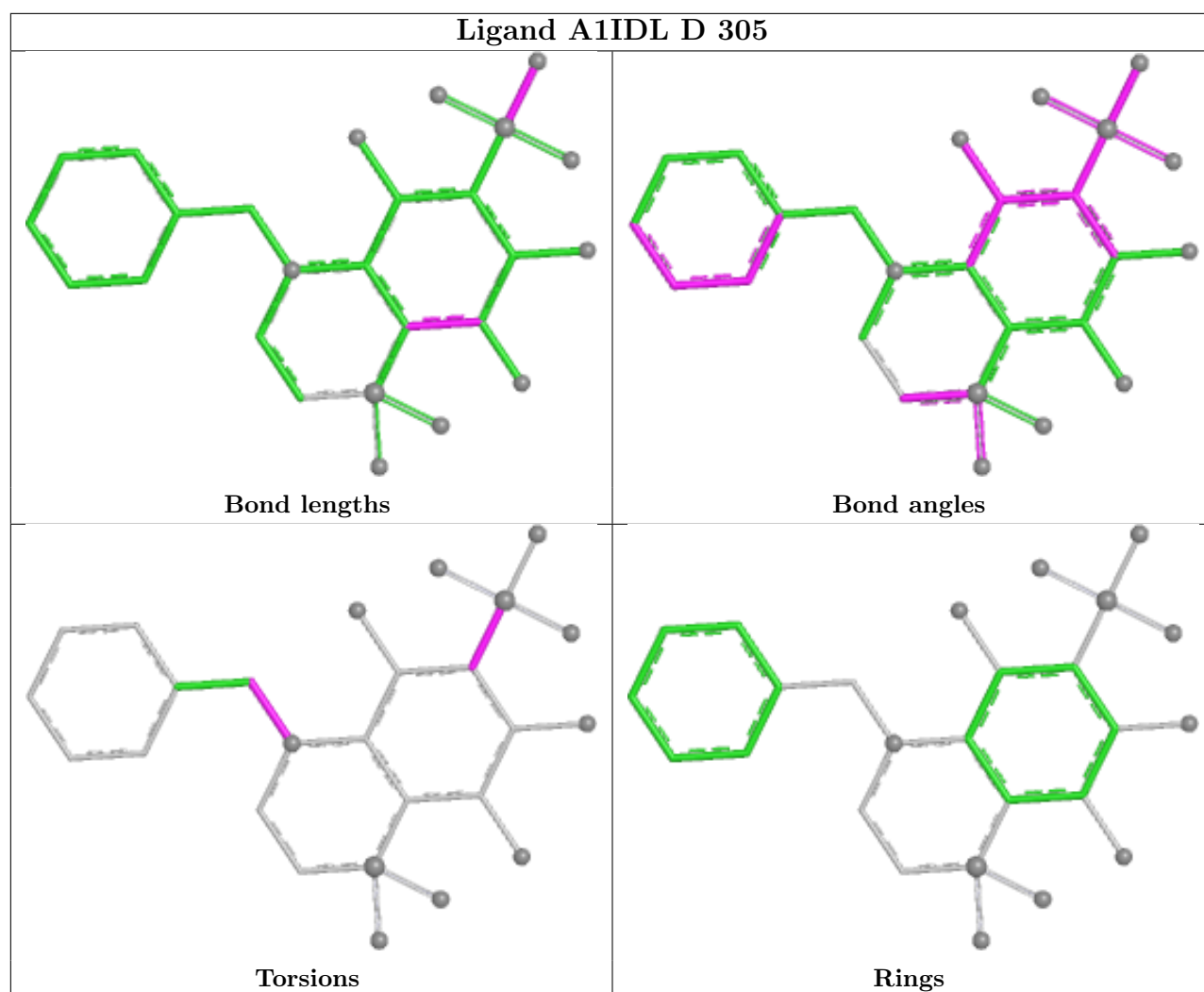
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	259/263 (98%)	0.03	12 (4%) 37 40	5, 16, 33, 64	24 (9%)
1	B	260/263 (98%)	-0.19	9 (3%) 47 48	5, 13, 29, 47	19 (7%)
1	C	260/263 (98%)	0.06	9 (3%) 47 48	6, 17, 35, 48	13 (5%)
1	D	260/263 (98%)	-0.24	7 (2%) 56 57	5, 13, 25, 38	19 (7%)
All	All	1039/1052 (98%)	-0.09	37 (3%) 46 47	5, 14, 31, 64	75 (7%)

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	252	PHE	9.3
1	A	7	PHE	6.6
1	C	235	ASP	6.6
1	C	7	PHE	6.4
1	B	82	GLN	5.3
1	D	252[A]	PHE	4.7
1	B	81	LEU	4.1
1	D	262	SER	4.1
1	B	3	LYS	3.8
1	C	148	MET	3.8
1	A	67	SER	3.8
1	D	75	ASP	3.7
1	D	3	LYS	3.5
1	A	253	ASP	3.3
1	B	253	ASP	3.3
1	C	56	ASN	3.0
1	C	219	GLN	3.0
1	B	79	GLN	2.9
1	C	55	ALA	2.9
1	C	262	SER	2.8
1	A	8	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	253	ASP	2.7
1	B	134[A]	ASN	2.6
1	D	84	ARG	2.5
1	A	56	ASN	2.5
1	A	163[A]	GLN	2.4
1	D	7	PHE	2.4
1	B	7	PHE	2.3
1	A	262	SER	2.2
1	A	36	ILE	2.2
1	A	55	ALA	2.2
1	A	68[A]	VAL	2.2
1	B	80	GLY	2.2
1	A	240	ARG	2.1
1	C	54[A]	SER	2.1
1	A	252	PHE	2.1
1	C	253	ASP	2.0

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(Å ²)	Q<0.9
5	DMS	D	306	4/4	0.73	0.22	42,69,79,82	0
3	EDO	A	304	4/4	0.76	0.15	31,32,38,63	0
3	EDO	D	303	4/4	0.80	0.13	23,25,27,33	0
3	EDO	D	304	4/4	0.86	0.14	24,31,37,61	0
3	EDO	B	302	4/4	0.89	0.12	26,29,37,47	0
3	EDO	A	305	4/4	0.89	0.12	27,30,38,40	0
3	EDO	D	302	4/4	0.90	0.11	23,24,24,29	0

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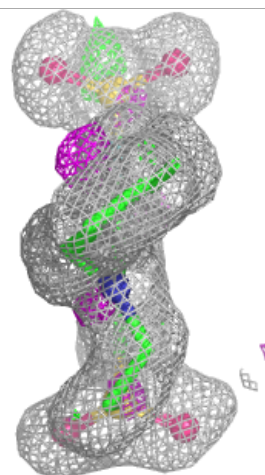
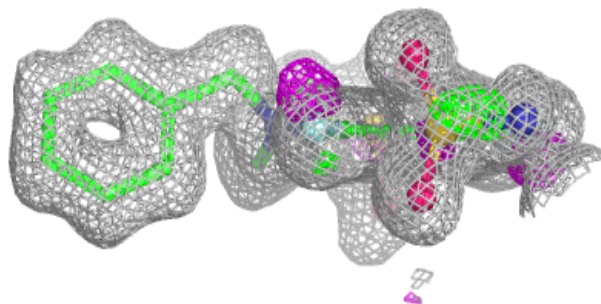
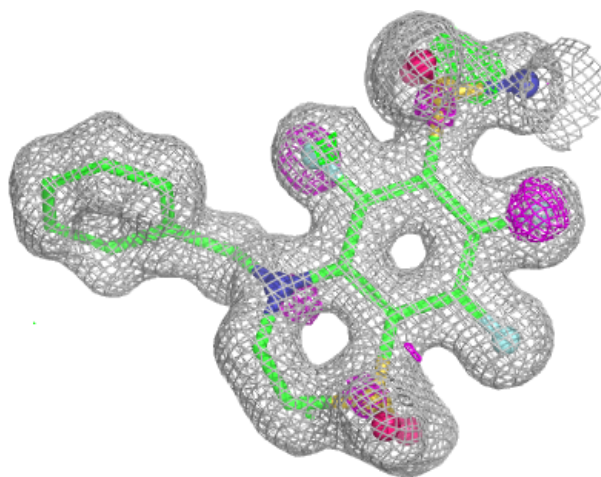
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	EDO	A	306	4/4	0.91	0.10	25,28,28,32	0
3	EDO	A	308	4/4	0.92	0.10	28,32,33,40	0
3	EDO	C	303	4/4	0.92	0.09	38,45,49,53	0
3	EDO	C	302	4/4	0.93	0.10	18,23,25,27	0
3	EDO	A	303	4/4	0.93	0.09	21,23,25,26	0
3	EDO	A	302	4/4	0.96	0.08	20,29,42,51	0
4	A1IDL	A	309	26/26	0.98	0.06	10,15,24,26	0
4	A1IDL	C	304	26/26	0.98	0.06	11,14,21,25	0
3	EDO	A	307	4/4	0.98	0.07	20,22,42,44	0
4	A1IDL	D	305	26/26	0.99	0.04	9,13,19,22	0
4	A1IDL	B	303	26/26	0.99	0.05	9,13,22,23	0
2	ZN	C	301	1/1	1.00	0.01	10,10,10,10	0
2	ZN	D	301	1/1	1.00	0.01	8,8,8,8	0
2	ZN	A	301	1/1	1.00	0.00	9,9,9,9	0
2	ZN	B	301	1/1	1.00	0.00	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.

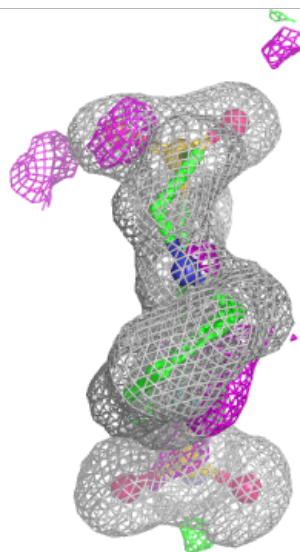
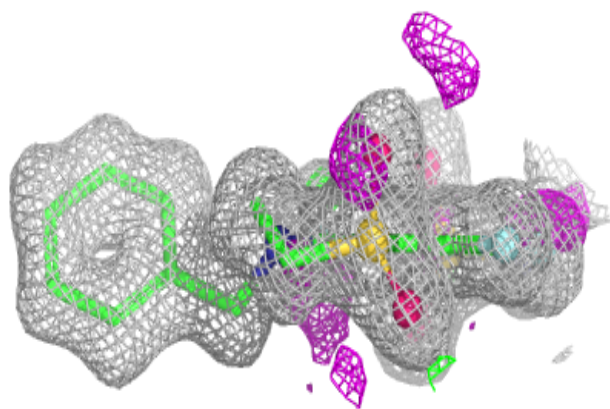
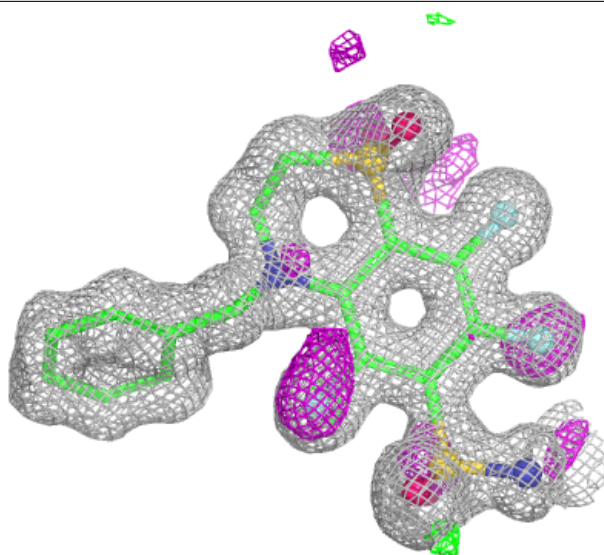
Electron density around A1IDL A 309:

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



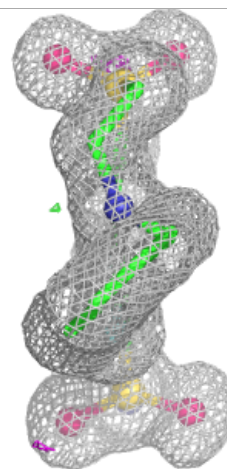
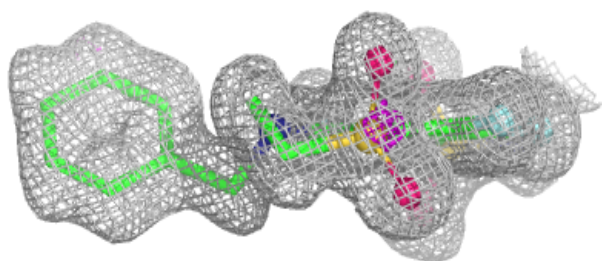
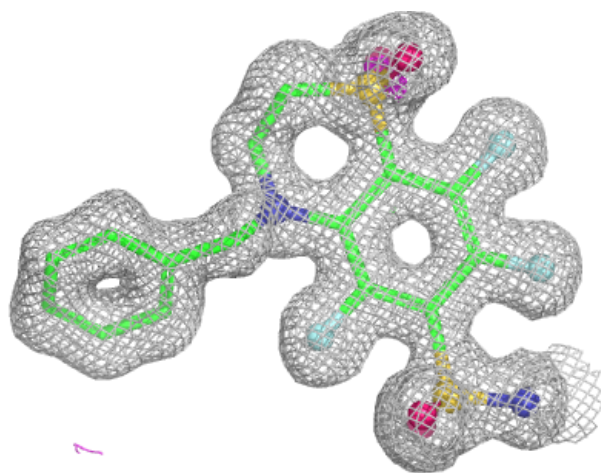
Electron density around A1IDL C 304:

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



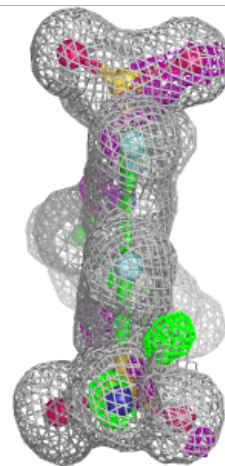
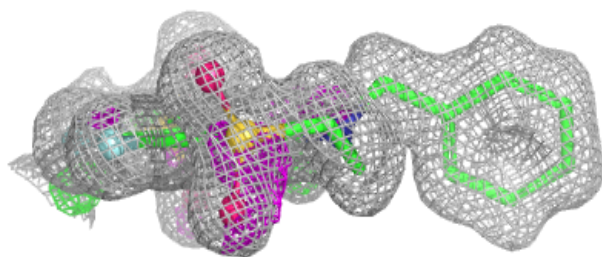
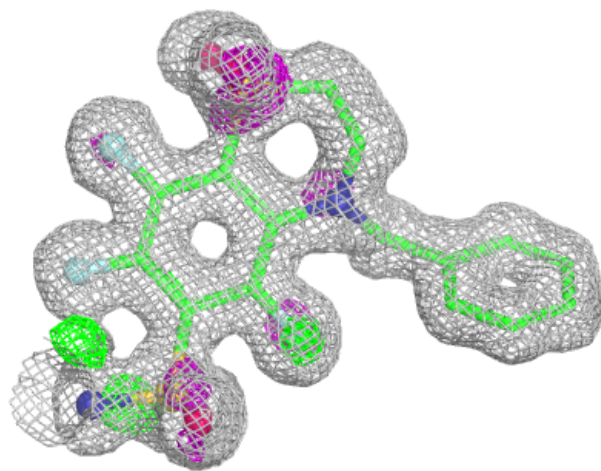
Electron density around A1IDL D 305:

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



Electron density around A1IDL B 303:

$2mF_o-DF_c$ (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.