



Full wwPDB X-ray Structure Validation Report ⓘ

May 5, 2025 – 01:56 pm BST

PDB ID : 9F2O / pdb_00009f2o
Title : Structure of human carbonic anhydrase XII complexed with 3-(cyclooctylamino)-2,6-difluoro-4-((3-hydroxypropyl)sulfonyl)-5-methoxybenzenesulfonamide
Authors : Manakova, E.N.; Grazulis, S.; Paketuryte, V.; Smirnov, A.
Deposited on : 2024-04-23
Resolution : 1.12 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 Phenix2.0rc1
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

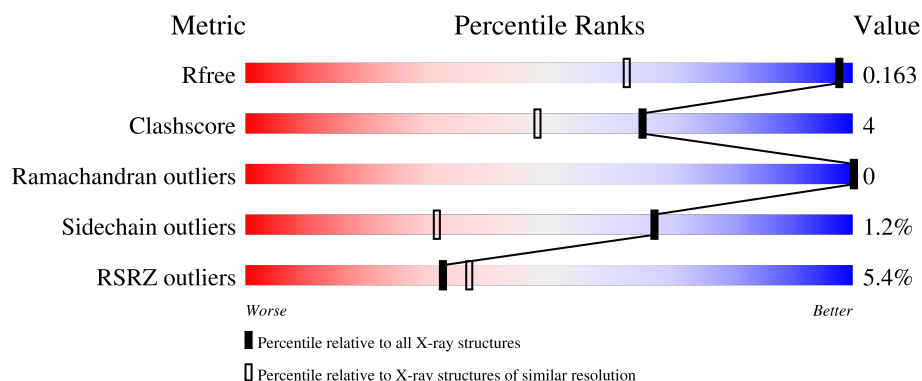
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


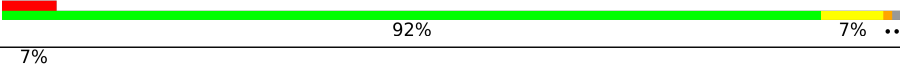
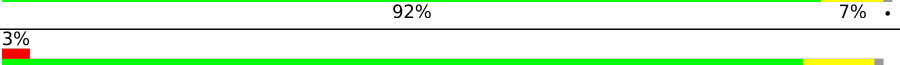

The reported resolution of this entry is 1.12 Å.

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}	164625	1652 (1.14-1.10)
Clashscore	180529	1870 (1.14-1.10)
Ramachandran outliers	177936	1828 (1.14-1.10)
Sidechain outliers	177891	1824 (1.14-1.10)
RSRZ outliers	164620	1652 (1.14-1.10)

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	 6% 89% 10% .
1	B	263	 6% 92% 7% ..
1	C	263	 7% 92% 7% .
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	302	-	-	X	-
6	PEG	B	306	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 10268 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	260	Total	C	N	O	S	0	17	0
			2206	1403	378	416	9			
1	B	261	Total	C	N	O	S	0	13	0
			2180	1386	366	420	8			
1	C	260	Total	C	N	O	S	0	15	0
			2186	1387	375	416	8			
1	D	260	Total	C	N	O	S	0	14	0
			2185	1391	368	418	8			

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).



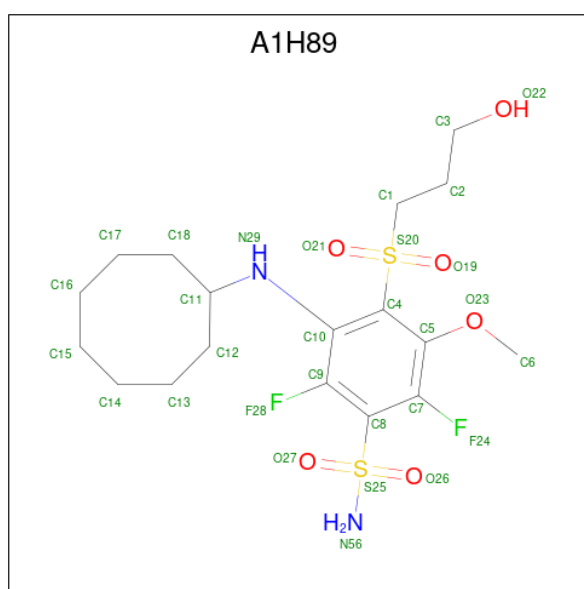
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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 3-(cyclooctylamino)-2,6-difluoro-4-((3-hydroxypropyl)sulfonyl)-5-methoxy benzenesulfonamide (CCD ID: A1H89) (formula: $C_{18}H_{28}F_2N_2O_6S_2$) (labeled as "Ligand of Interest" by depositor).



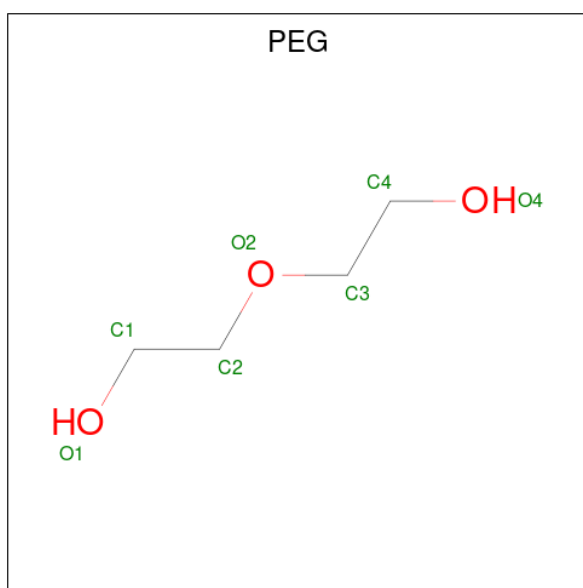
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	F	N	O	S	0	0
			30	18	2	2	6	2		
4	B	1	Total	C	F	N	O	S	0	0
			30	18	2	2	6	2		
4	C	1	Total	C	F	N	O	S	0	0
			30	18	2	2	6	2		
4	D	1	Total	C	F	N	O	S	0	0
			30	18	2	2	6	2		

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



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

- Molecule 6 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



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

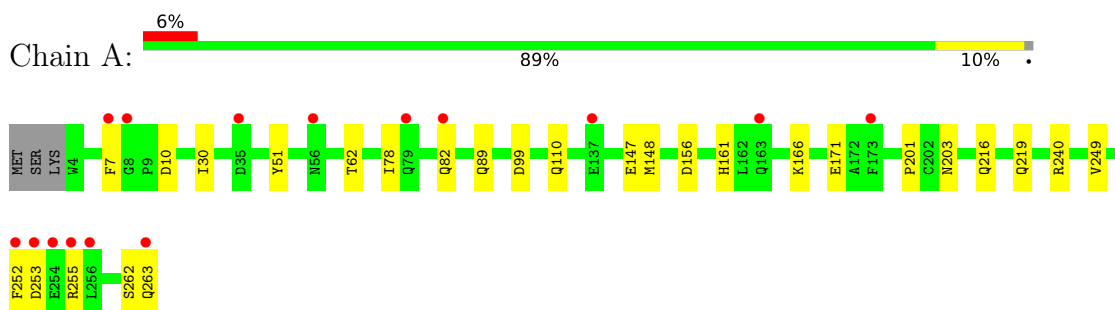
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	316	Total 319	O 319	0	3
7	B	338	Total 342	O 342	0	4
7	C	319	Total 322	O 322	0	3
7	D	319	Total 321	O 321	0	2

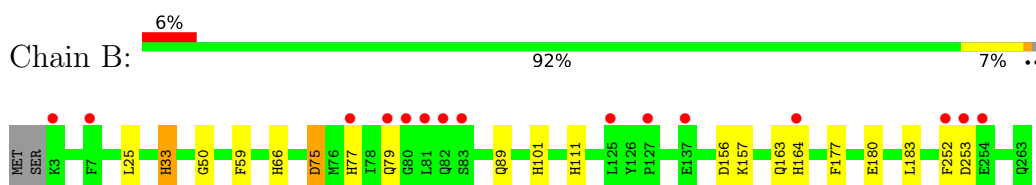
3 Residue-property plots [i](#)

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.

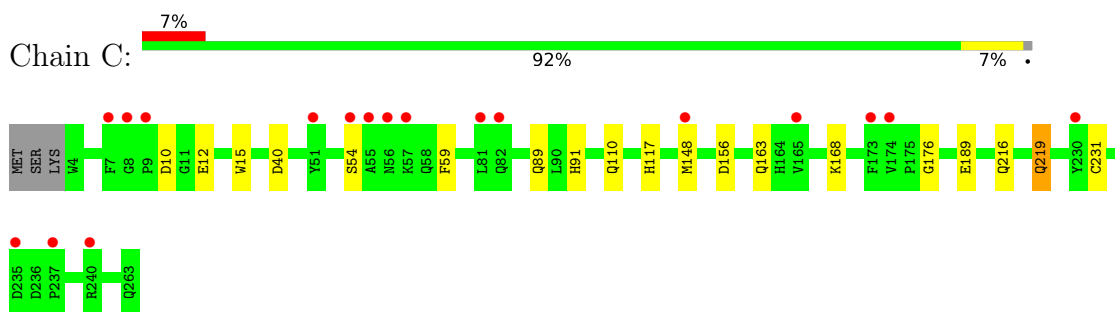
- Molecule 1: Carbonic anhydrase 12



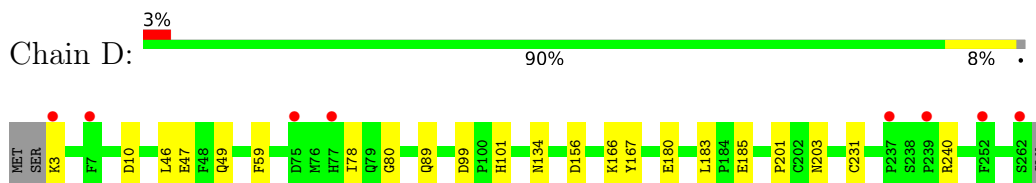
- Molecule 1: Carbonic anhydrase 12



- 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	77.39Å 73.95Å 91.36Å 90.00° 108.88° 90.00°	Depositor
Resolution (Å)	56.26 – 1.12 56.26 – 1.12	Depositor EDS
% Data completeness (in resolution range)	96.2 (56.26-1.12) 96.2 (56.26-1.12)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 1.12Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.136 , 0.164 0.141 , 0.163	Depositor DCC
R_{free} test set	37162 reflections (10.02%)	wwPDB-VP
Wilson B-factor (Å ²)	11.1	Xtriage
Anisotropy	0.099	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 41.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	10268	wwPDB-VP
Average B, all atoms (Å ²)	16.0	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 37.95 % 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 3.9683e-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: PEG, EDO, DMS, A1H89, 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	0.71	1/2291 (0.0%)	1.01	4/3114 (0.1%)
1	B	0.75	2/2263 (0.1%)	1.07	7/3078 (0.2%)
1	C	0.74	0/2268	1.04	6/3083 (0.2%)
1	D	0.75	0/2268	0.98	2/3087 (0.1%)
All	All	0.74	3/9090 (0.0%)	1.03	19/12362 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	66	HIS	CD2-NE2	-5.29	1.32	1.37
1	B	33	HIS	CE1-NE2	-5.17	1.27	1.32
1	A	161	HIS	CE1-NE2	5.12	1.37	1.32

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	75	ASP	CA-CB-CG	7.45	120.05	112.60
1	B	164	HIS	CA-CB-CG	-6.88	106.92	113.80
1	B	252[A]	PHE	CA-CB-CG	-6.56	107.24	113.80
1	B	252[B]	PHE	CA-CB-CG	-6.56	107.24	113.80
1	A	262	SER	N-CA-C	-5.81	106.84	114.04
1	A	253	ASP	CA-CB-CG	5.67	118.27	112.60
1	D	185	GLU	CB-CG-CD	5.63	122.17	112.60
1	C	10	ASP	CA-C-N	5.54	129.59	121.67
1	C	10	ASP	C-N-CA	5.54	129.59	121.67
1	D	59	PHE	CA-CB-CG	-5.46	108.34	113.80
1	C	91	HIS	CA-CB-CG	-5.41	108.39	113.80
1	C	59	PHE	CA-CB-CG	-5.40	108.40	113.80
1	A	10	ASP	CA-C-N	5.34	129.31	121.67
1	A	10	ASP	C-N-CA	5.34	129.31	121.67

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	117	HIS	ND1-CG-CD2	5.28	111.38	106.10
1	B	111	HIS	CB-CA-C	-5.26	100.64	109.53
1	C	40	ASP	CA-CB-CG	5.17	117.77	112.60
1	B	163	GLN	OE1-CD-NE2	-5.11	117.49	122.60
1	B	59	PHE	CA-CB-CG	-5.04	108.76	113.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2206	0	2119	19	0
1	B	2180	0	2068	15	0
1	C	2186	0	2091	11	0
1	D	2185	0	2075	20	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	16	0	24	0	0
3	B	12	0	17	1	0
3	C	20	0	30	0	0
3	D	20	0	30	5	0
4	A	30	0	0	0	0
4	B	30	0	0	0	0
4	C	30	0	0	0	0
4	D	30	0	0	0	0
5	A	4	0	6	2	0
5	C	4	0	6	1	0
6	B	7	0	10	6	0
7	A	319	0	0	4	0
7	B	342	0	0	6	0
7	C	322	0	0	2	0
7	D	321	0	0	0	0
All	All	10268	0	8476	65	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 4.

All (65) 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)
5:A:307:DMS:H11	7:A:533:HOH:O	1.53	1.06
1:D:47[B]:GLU:CG	1:D:49[B]:GLN:HE21	1.72	1.02
1:D:47[B]:GLU:HG2	1:D:49[B]:GLN:HE21	1.31	0.95
1:A:62[B]:THR:HG22	1:A:171:GLU:HG2	1.52	0.91
1:D:134:ASN:HB3	3:D:302:EDO:H22	1.58	0.85
1:A:201[B]:PRO:HG2	1:A:203:ASN:OD1	1.75	0.84
1:A:7:PHE:CE2	1:A:240[B]:ARG:CZ	2.65	0.80
1:D:47[B]:GLU:CG	1:D:49[B]:GLN:NE2	2.48	0.77
1:D:80:GLY:O	3:D:304:EDO:H21	1.87	0.73
1:D:166[A]:LYS:HE2	1:D:167:TYR:CZ	2.24	0.73
1:C:189:GLU:OE2	1:C:189:GLU:CG	2.38	0.72
1:A:7:PHE:CZ	1:A:240[B]:ARG:NE	2.59	0.70
1:D:166[A]:LYS:HE2	1:D:167:TYR:OH	1.91	0.69
1:A:263:GLN:NE2	7:A:401:HOH:O	2.25	0.69
1:B:75:ASP:HB2	6:B:306:PEG:H11	1.75	0.68
1:C:216:GLN:HG3	7:C:648:HOH:O	1.93	0.68
1:A:148[A]:MET:HE3	1:A:219:GLN:HB3	1.74	0.68
1:D:47[B]:GLU:HG3	1:D:49[B]:GLN:HE21	1.58	0.66
1:A:7:PHE:CZ	1:A:240[B]:ARG:CZ	2.79	0.66
1:B:75:ASP:HB2	6:B:306:PEG:C1	2.26	0.65
1:C:189:GLU:CG	1:C:189:GLU:OE1	2.44	0.65
1:A:99:ASP:OD2	1:B:33:HIS:HE1	1.83	0.62
1:D:47[B]:GLU:HG2	1:D:49[B]:GLN:NE2	2.10	0.62
1:A:7:PHE:CE2	1:A:240[B]:ARG:NH2	2.68	0.62
1:B:180[A]:GLU:HG3	1:B:183:LEU:HD12	1.82	0.61
1:A:30:ILE:HA	1:A:249[B]:VAL:HG13	1.82	0.60
1:C:189:GLU:OE2	1:C:189:GLU:OE1	2.20	0.60
1:A:252:PHE:CE1	1:A:255[A]:ARG:HD2	2.38	0.58
1:D:201[A]:PRO:HG2	3:D:302:EDO:H11	1.84	0.58
1:A:148[A]:MET:HE1	7:A:414:HOH:O	2.04	0.58
1:C:168:LYS:HB2	1:C:231[B]:CYS:O	2.04	0.58
1:D:180[A]:GLU:HG3	1:D:183:LEU:HD12	1.86	0.57
1:C:148:MET:SD	1:C:219[B]:GLN:HG2	2.45	0.57
1:D:47[B]:GLU:HG2	1:D:49[B]:GLN:HG2	1.88	0.56
1:B:79:GLN:HA	7:B:415:HOH:O	2.06	0.55
1:D:231[B]:CYS:SG	1:D:240:ARG:HB2	2.46	0.55
1:A:148[A]:MET:CE	1:A:219:GLN:HB3	2.39	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:TYR:OH	1:A:78[A]:ILE:HD11	2.09	0.52
1:D:201[B]:PRO:HG3	3:D:302:EDO:H11	1.91	0.51
1:D:3:LYS:NZ	1:D:10:ASP:OD2	2.42	0.51
1:B:50:GLY:HA2	6:B:306:PEG:H41	1.94	0.49
1:D:203[B]:ASN:HD21	3:D:302:EDO:C2	2.26	0.49
1:A:82:GLN:CD	1:C:163:GLN:HE22	2.21	0.48
1:D:47[B]:GLU:HG3	1:D:49[B]:GLN:NE2	2.25	0.48
1:C:216:GLN:HG3	7:C:611:HOH:O	2.15	0.47
1:B:101:HIS:ND1	7:B:401:HOH:O	2.24	0.47
1:B:157[B]:LYS:HD3	1:B:177:PHE:CG	2.50	0.46
3:B:304:EDO:H21	7:B:524:HOH:O	2.16	0.45
1:B:75:ASP:HB2	6:B:306:PEG:H12	1.96	0.45
1:C:110:GLN:HB3	5:C:308:DMS:H21	1.99	0.45
1:A:148[A]:MET:HE3	1:A:219:GLN:CB	2.44	0.45
1:A:110:GLN:HB3	5:A:307:DMS:H23	1.98	0.45
1:D:47[B]:GLU:OE2	1:D:49[B]:GLN:NE2	2.50	0.44
1:B:75:ASP:O	6:B:306:PEG:H11	2.18	0.44
1:B:180[B]:GLU:CD	7:B:410:HOH:O	2.62	0.43
1:B:25:LEU:HB3	7:B:407:HOH:O	2.18	0.43
1:C:54[A]:SER:O	1:C:176:GLY:HA3	2.18	0.42
1:C:12:GLU:HA	1:C:15:TRP:CE2	2.54	0.42
1:D:46:LEU:HD22	1:D:78[B]:ILE:CG2	2.50	0.42
1:A:201[B]:PRO:HG3	7:A:538:HOH:O	2.19	0.41
1:B:253:ASP:CB	7:B:407:HOH:O	2.67	0.41
1:B:75:ASP:CB	6:B:306:PEG:H11	2.48	0.41
1:D:99:ASP:OD1	1:D:101:HIS:HD2	2.05	0.40
1:B:157[B]:LYS:HD3	1:B:177:PHE:CB	2.51	0.40
1:A:147:GLU:O	1:A:216[B]:GLN:HA	2.22	0.40

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	275/263 (105%)	268 (98%)	7 (2%)	0	100	100
1	B	272/263 (103%)	268 (98%)	4 (2%)	0	100	100
1	C	273/263 (104%)	266 (97%)	7 (3%)	0	100	100
1	D	272/263 (103%)	266 (98%)	6 (2%)	0	100	100
All	All	1092/1052 (104%)	1068 (98%)	24 (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	249/235 (106%)	246 (99%)	3 (1%)	67	31
1	B	246/235 (105%)	243 (99%)	3 (1%)	67	31
1	C	246/235 (105%)	242 (98%)	4 (2%)	58	21
1	D	246/235 (105%)	244 (99%)	2 (1%)	79	50
All	All	987/940 (105%)	975 (99%)	12 (1%)	67	31

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	89	GLN
1	A	156	ASP
1	A	166	LYS
1	B	77	HIS
1	B	89	GLN
1	B	156	ASP
1	C	89	GLN
1	C	156	ASP
1	C	219[A]	GLN
1	C	219[B]	GLN
1	D	89	GLN
1	D	156	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	ASN
1	A	110	GLN
1	B	250	GLN
1	C	13	ASN
1	C	250	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 28 ligands modelled in this entry, 4 are monoatomic - leaving 24 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	D	302	-	3,3,3	1.15	0	2,2,2	2.02	1 (50%)
4	A1H89	C	307	2	29,31,31	1.04	1 (3%)	37,45,45	1.45	8 (21%)
3	EDO	D	305	-	3,3,3	0.08	0	2,2,2	0.52	0
3	EDO	C	306	-	3,3,3	0.54	0	2,2,2	0.91	0
3	EDO	B	303	-	3,3,3	0.87	0	2,2,2	0.82	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	D	304	-	3,3,3	0.74	0	2,2,2	0.93	0
6	PEG	B	306	-	6,6,6	0.32	0	5,5,5	0.36	0
3	EDO	D	306	-	3,3,3	0.53	0	2,2,2	0.85	0
3	EDO	A	305	-	3,3,3	0.22	0	2,2,2	0.21	0
3	EDO	C	305	-	3,3,3	0.28	0	2,2,2	0.82	0
3	EDO	C	303	-	3,3,3	0.31	0	2,2,2	0.35	0
5	DMS	C	308	-	3,3,3	0.34	0	3,3,3	0.27	0
4	A1H89	B	305	2	29,31,31	1.51	4 (13%)	37,45,45	1.41	6 (16%)
3	EDO	C	304	-	3,3,3	0.17	0	2,2,2	0.50	0
4	A1H89	D	307	2	29,31,31	1.37	2 (6%)	37,45,45	1.40	6 (16%)
5	DMS	A	307	-	3,3,3	0.41	0	3,3,3	0.28	0
3	EDO	B	302	-	3,3,3	0.64	0	2,2,2	0.51	0
3	EDO	A	303	-	3,3,3	0.20	0	2,2,2	0.47	0
4	A1H89	A	306	2	29,31,31	1.17	3 (10%)	37,45,45	1.19	4 (10%)
3	EDO	D	303	-	3,3,3	0.06	0	2,2,2	0.38	0
3	EDO	A	302	-	3,3,3	0.35	0	2,2,2	0.36	0
3	EDO	B	304	-	3,3,3	0.72	0	2,2,2	1.45	1 (50%)
3	EDO	C	302	-	3,3,3	0.57	0	2,2,2	0.42	0
3	EDO	A	304	-	3,3,3	0.17	0	2,2,2	0.16	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	D	302	-	-	1/1/1/1	-
4	A1H89	C	307	2	-	8/23/33/33	0/2/2/2
3	EDO	D	305	-	-	0/1/1/1	-
3	EDO	C	306	-	-	0/1/1/1	-
3	EDO	B	303	-	-	0/1/1/1	-
3	EDO	D	304	-	-	0/1/1/1	-
6	PEG	B	306	-	-	3/4/4/4	-
3	EDO	D	306	-	-	0/1/1/1	-
3	EDO	A	305	-	-	1/1/1/1	-
3	EDO	C	305	-	-	1/1/1/1	-
3	EDO	C	303	-	-	0/1/1/1	-
4	A1H89	B	305	2	-	8/23/33/33	0/2/2/2
3	EDO	C	304	-	-	0/1/1/1	-
4	A1H89	D	307	2	-	7/23/33/33	0/2/2/2
3	EDO	B	302	-	-	1/1/1/1	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	A	303	-	-	0/1/1/1	-
4	A1H89	A	306	2	-	7/23/33/33	0/2/2/2
3	EDO	D	303	-	-	0/1/1/1	-
3	EDO	A	302	-	-	0/1/1/1	-
3	EDO	B	304	-	-	1/1/1/1	-
3	EDO	C	302	-	-	0/1/1/1	-
3	EDO	A	304	-	-	0/1/1/1	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	305	A1H89	C18-C11	-5.09	1.44	1.52
4	D	307	A1H89	C18-C11	-5.08	1.44	1.52
4	A	306	A1H89	C18-C11	-3.45	1.46	1.52
4	C	307	A1H89	C18-C11	-3.42	1.46	1.52
4	A	306	A1H89	S25-N56	-3.18	1.54	1.60
4	B	305	A1H89	S25-N56	-2.23	1.56	1.60
4	B	305	A1H89	C17-C18	-2.19	1.43	1.52
4	B	305	A1H89	C13-C12	-2.19	1.44	1.52
4	A	306	A1H89	O23-C5	-2.18	1.34	1.38
4	D	307	A1H89	C16-C17	2.13	1.63	1.52

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	307	A1H89	C7-C8-C9	-3.81	114.00	116.67
4	B	305	A1H89	O19-S20-O21	-3.22	114.67	118.44
4	D	307	A1H89	C7-C8-C9	-3.21	114.42	116.67
4	C	307	A1H89	O19-S20-O21	-3.16	114.75	118.44
4	B	305	A1H89	O27-S25-C8	-3.05	102.77	107.30
4	B	305	A1H89	C10-C9-C8	2.92	126.90	121.81
4	C	307	A1H89	O26-S25-N56	2.85	111.59	107.36
4	B	305	A1H89	F28-C9-C8	-2.65	115.73	120.70
4	A	306	A1H89	O27-S25-C8	-2.65	103.36	107.30
4	A	306	A1H89	F24-C7-C5	-2.65	115.64	119.39
4	B	305	A1H89	C17-C18-C11	2.64	126.46	116.21
4	D	307	A1H89	C10-C9-C8	2.64	126.41	121.81
4	A	306	A1H89	O19-S20-O21	-2.63	115.36	118.44
4	B	305	A1H89	O26-S25-N56	2.62	111.25	107.36
4	D	307	A1H89	O26-S25-N56	2.57	111.17	107.36
4	A	306	A1H89	O26-S25-N56	2.51	111.09	107.36
4	D	307	A1H89	O27-S25-C8	-2.48	103.62	107.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	307	A1H89	F28-C9-C8	-2.46	116.09	120.70
4	C	307	A1H89	C10-C9-C8	2.36	125.92	121.81
4	C	307	A1H89	F24-C7-C5	-2.24	116.22	119.39
4	C	307	A1H89	C7-C5-C4	2.23	121.13	116.88
4	C	307	A1H89	O23-C5-C4	-2.17	117.70	120.89
3	D	302	EDO	O1-C1-C2	2.16	127.45	111.91
4	D	307	A1H89	O19-S20-O21	-2.12	115.95	118.44
3	B	304	EDO	O1-C1-C2	2.05	126.62	111.91
4	C	307	A1H89	C5-C7-C8	2.02	124.24	121.47

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	306	A1H89	C7-C8-S25-N56
4	A	306	A1H89	C7-C8-S25-O26
4	A	306	A1H89	C10-C4-S20-O21
4	A	306	A1H89	C10-C4-S20-O19
4	B	305	A1H89	C7-C8-S25-N56
4	B	305	A1H89	C7-C8-S25-O26
4	B	305	A1H89	C10-C4-S20-O21
4	B	305	A1H89	C10-C4-S20-C1
4	B	305	A1H89	C10-C4-S20-O19
4	C	307	A1H89	C7-C8-S25-N56
4	C	307	A1H89	C7-C8-S25-O26
4	C	307	A1H89	C10-C4-S20-O21
4	C	307	A1H89	C10-C4-S20-O19
4	D	307	A1H89	C7-C8-S25-N56
4	D	307	A1H89	C7-C8-S25-O26
4	D	307	A1H89	C10-C4-S20-O21
4	D	307	A1H89	C10-C4-S20-C1
4	D	307	A1H89	C10-C4-S20-O19
6	B	306	PEG	O2-C3-C4-O4
3	D	302	EDO	O1-C1-C2-O2
6	B	306	PEG	O1-C1-C2-O2
6	B	306	PEG	C4-C3-O2-C2
4	A	306	A1H89	C9-C8-S25-O26
4	B	305	A1H89	C9-C8-S25-O26
4	C	307	A1H89	C9-C8-S25-O26
3	B	302	EDO	O1-C1-C2-O2
3	C	305	EDO	O1-C1-C2-O2
4	A	306	A1H89	C9-C8-S25-N56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	B	305	A1H89	C9-C8-S25-N56
4	C	307	A1H89	C9-C8-S25-N56
4	D	307	A1H89	C9-C8-S25-N56
3	B	304	EDO	O1-C1-C2-O2
4	A	306	A1H89	C18-C11-N29-C10
4	B	305	A1H89	C18-C11-N29-C10
4	C	307	A1H89	C18-C11-N29-C10
4	D	307	A1H89	C18-C11-N29-C10
3	A	305	EDO	O1-C1-C2-O2
4	C	307	A1H89	C10-C4-S20-C1

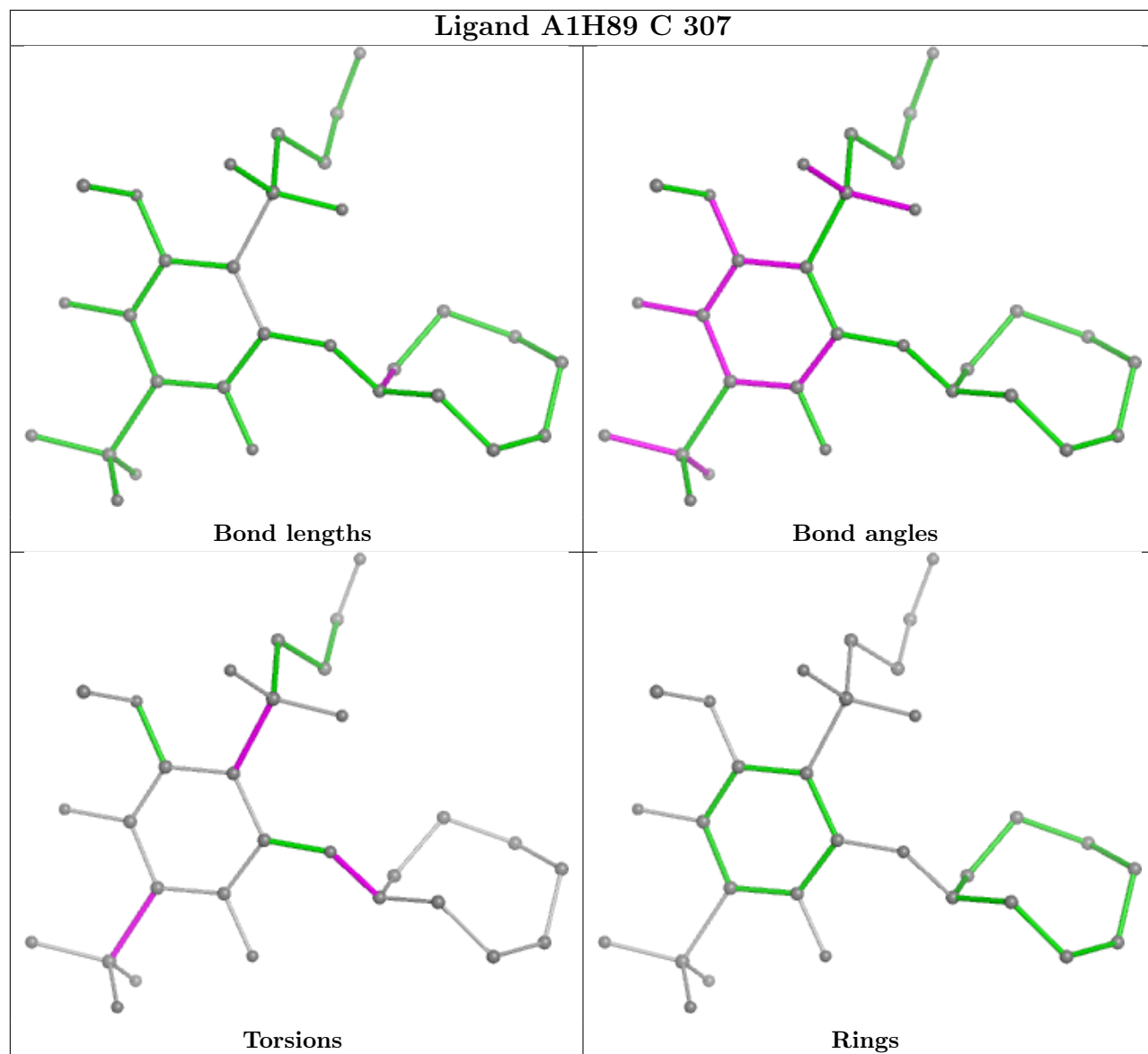
There are no ring outliers.

6 monomers are involved in 15 short contacts:

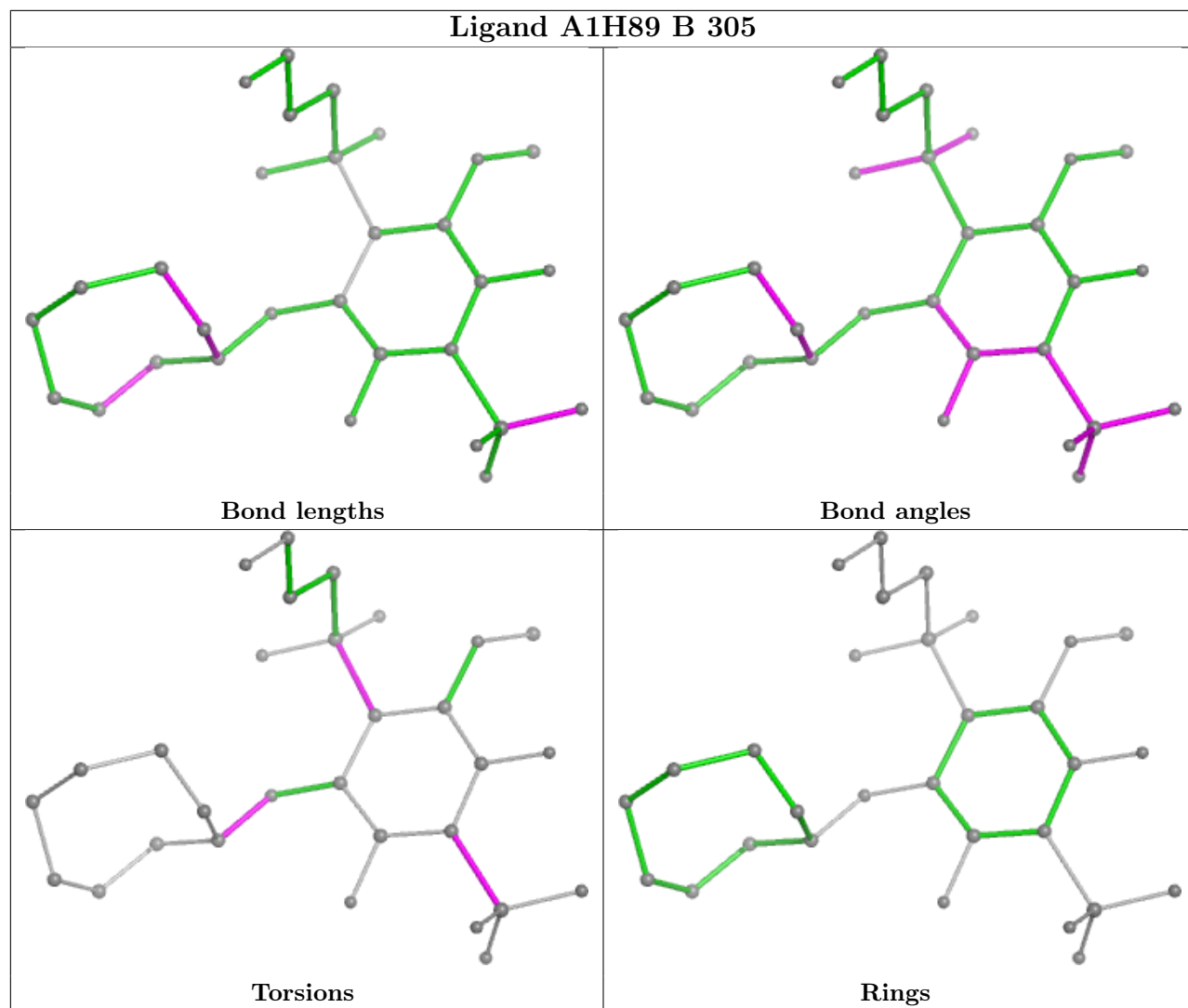
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	302	EDO	4	0
3	D	304	EDO	1	0
6	B	306	PEG	6	0
5	C	308	DMS	1	0
5	A	307	DMS	2	0
3	B	304	EDO	1	0

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.

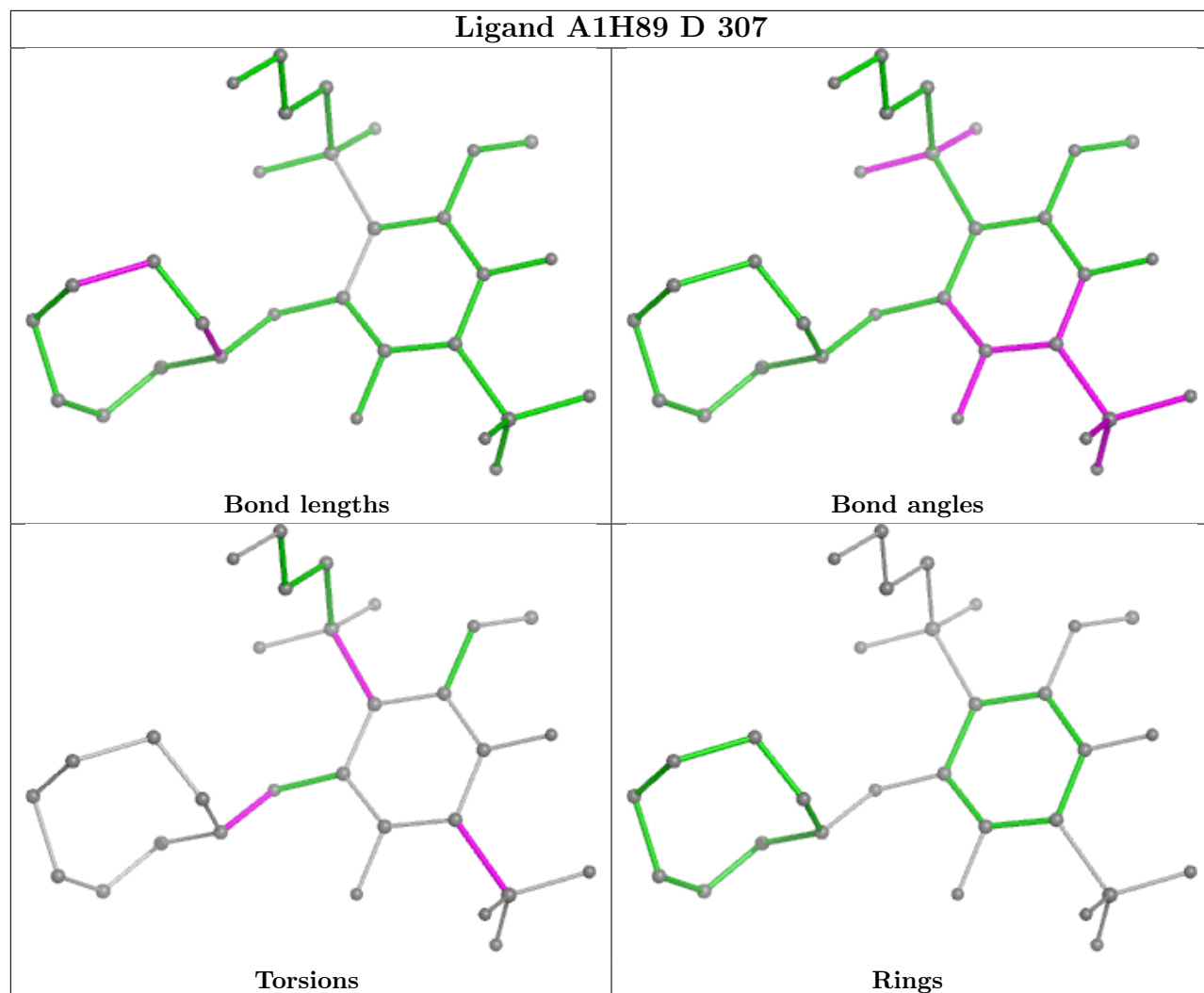
Ligand A1H89 C 307

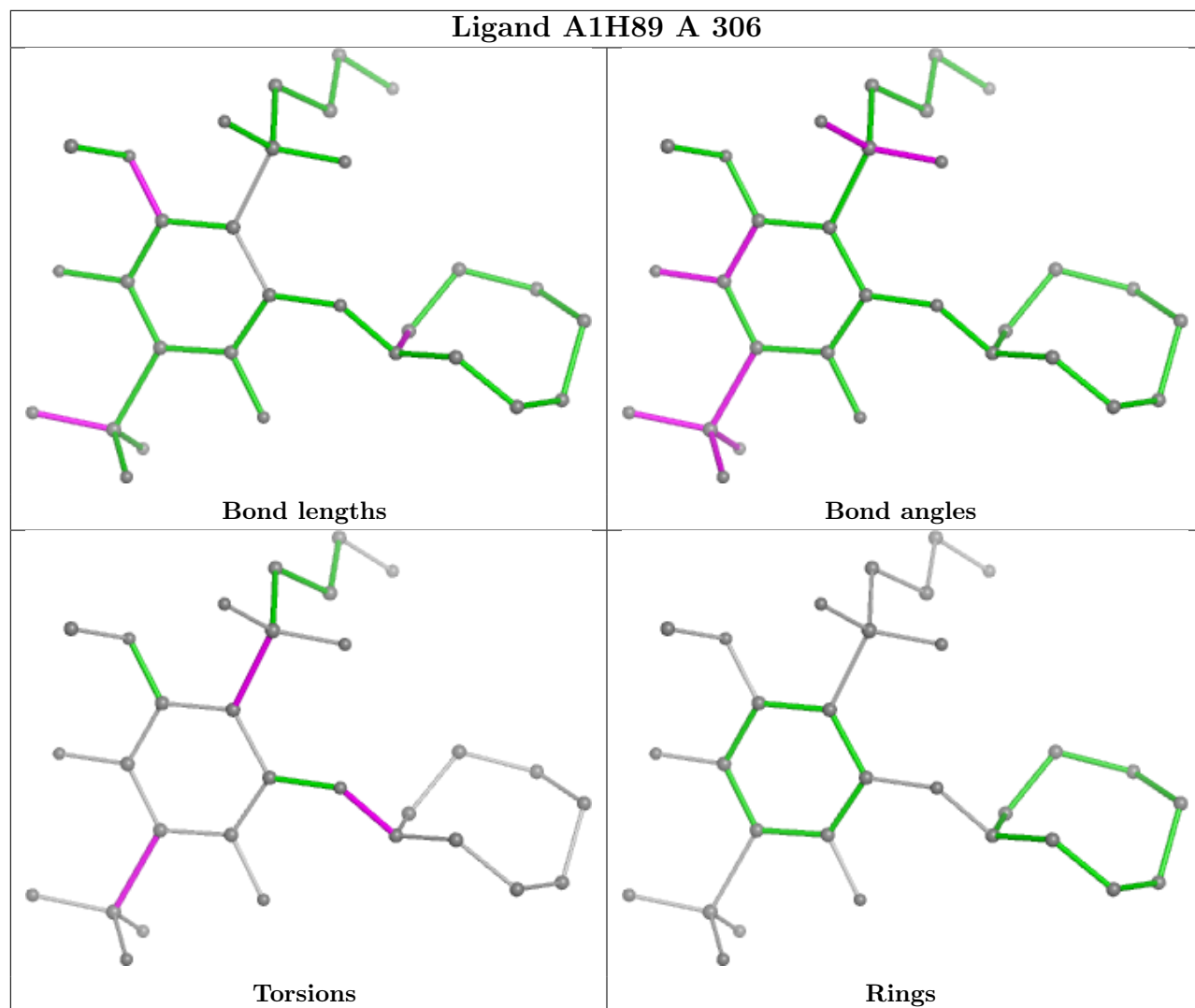


Ligand A1H89 B 305



Ligand A1H89 D 307





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	260/263 (98%)	0.40	15 (5%)	30 35	5, 14, 29, 40	17 (6%)
1	B	261/263 (99%)	0.15	15 (5%)	30 35	5, 11, 25, 38	13 (4%)
1	C	260/263 (98%)	0.65	18 (6%)	24 29	6, 15, 30, 41	17 (6%)
1	D	260/263 (98%)	0.08	8 (3%)	51 56	5, 12, 24, 40	14 (5%)
All	All	1041/1052 (98%)	0.32	56 (5%)	32 37	5, 13, 27, 41	61 (5%)

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	252[A]	PHE	6.3
1	C	7	PHE	6.3
1	B	81	LEU	5.7
1	C	235	ASP	5.4
1	A	7	PHE	5.4
1	C	55	ALA	5.2
1	B	80	GLY	5.0
1	D	3	LYS	4.8
1	D	75	ASP	3.9
1	A	8	GLY	3.9
1	C	57	LYS	3.8
1	C	173	PHE	3.7
1	A	253	ASP	3.5
1	D	262	SER	3.4
1	C	174	VAL	3.3
1	D	237	PRO	3.2
1	C	54[A]	SER	3.1
1	A	256	LEU	3.0
1	C	8	GLY	3.0
1	D	252[A]	PHE	2.9
1	A	255[A]	ARG	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	56	ASN	2.8
1	D	77	HIS	2.8
1	A	263	GLN	2.8
1	B	137	GLU	2.7
1	C	237	PRO	2.7
1	A	35	ASP	2.7
1	B	253	ASP	2.7
1	A	252	PHE	2.6
1	A	173	PHE	2.6
1	B	127	PRO	2.5
1	C	165	VAL	2.5
1	C	51	TYR	2.4
1	B	3	LYS	2.4
1	B	7	PHE	2.4
1	B	77	HIS	2.4
1	A	56	ASN	2.3
1	B	79	GLN	2.3
1	C	240	ARG	2.3
1	B	254	GLU	2.3
1	D	7	PHE	2.3
1	C	82	GLN	2.3
1	C	230	TYR	2.3
1	C	81	LEU	2.2
1	B	125	LEU	2.2
1	B	83	SER	2.2
1	A	82	GLN	2.2
1	A	163[A]	GLN	2.1
1	A	137	GLU	2.1
1	B	164	HIS	2.1
1	C	9	PRO	2.1
1	D	239	PRO	2.1
1	A	79	GLN	2.1
1	B	82	GLN	2.1
1	C	148	MET	2.0
1	A	254	GLU	2.0

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

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

6.3 Carbohydrates

There are no 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, 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.

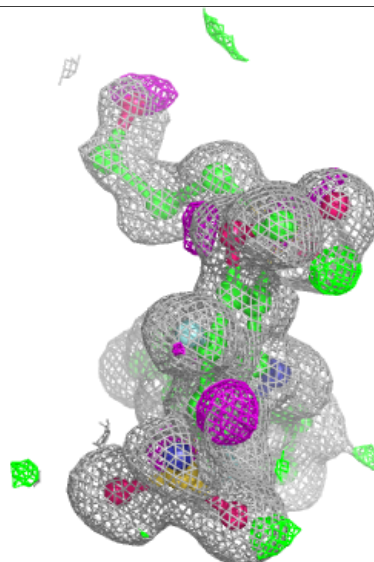
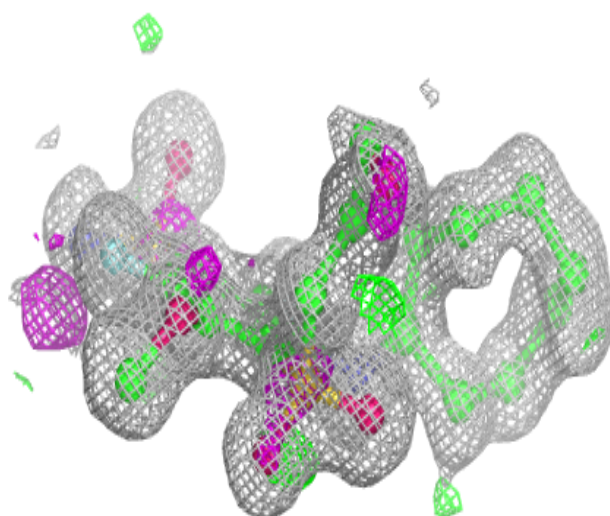
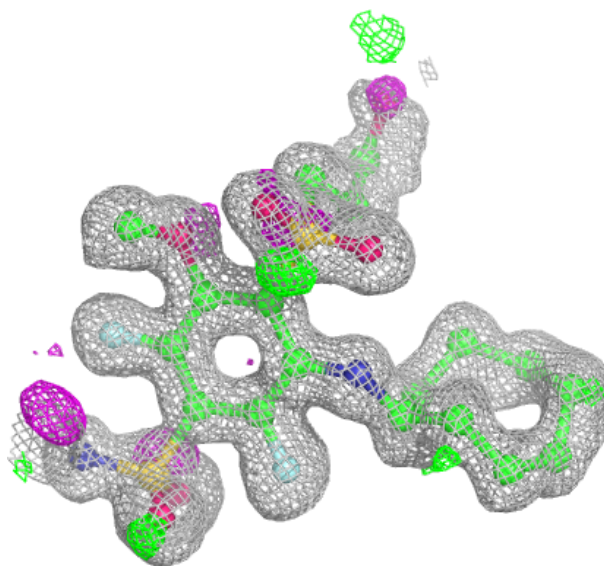
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	EDO	D	305	4/4	0.62	0.24	31,35,38,41	0
5	DMS	C	308	4/4	0.79	0.18	38,38,48,58	0
5	DMS	A	307	4/4	0.81	0.17	41,45,47,53	0
3	EDO	D	303	4/4	0.83	0.12	24,29,35,48	0
3	EDO	C	306	4/4	0.84	0.13	27,31,33,44	0
6	PEG	B	306	7/7	0.85	0.15	27,35,42,45	0
3	EDO	D	306	4/4	0.87	0.16	26,26,32,35	0
3	EDO	B	302	4/4	0.87	0.13	22,22,30,36	0
3	EDO	C	305	4/4	0.88	0.13	23,25,32,36	0
3	EDO	D	304	4/4	0.90	0.11	21,22,23,27	0
3	EDO	B	304	4/4	0.90	0.10	17,19,25,32	0
3	EDO	D	302	4/4	0.93	0.13	22,22,36,36	0
3	EDO	C	303	4/4	0.93	0.10	21,22,25,26	0
3	EDO	C	304	4/4	0.94	0.09	16,20,21,22	0
3	EDO	A	305	4/4	0.95	0.10	16,21,30,34	0
3	EDO	A	304	4/4	0.96	0.10	10,12,16,17	0
3	EDO	A	303	4/4	0.96	0.07	23,23,25,25	0
3	EDO	B	303	4/4	0.97	0.06	16,16,16,16	0
3	EDO	C	302	4/4	0.97	0.07	15,15,17,17	0
4	A1H89	C	307	30/30	0.98	0.07	9,13,23,34	0
3	EDO	A	302	4/4	0.98	0.06	18,22,23,23	0
4	A1H89	B	305	30/30	0.99	0.05	7,11,19,26	0
4	A1H89	A	306	30/30	0.99	0.06	8,12,21,27	0
4	A1H89	D	307	30/30	0.99	0.05	7,11,18,26	0
2	ZN	A	301	1/1	1.00	0.01	8,8,8,8	0
2	ZN	B	301	1/1	1.00	0.01	6,6,6,6	0
2	ZN	C	301	1/1	1.00	0.01	9,9,9,9	0
2	ZN	D	301	1/1	1.00	0.01	7,7,7,7	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.

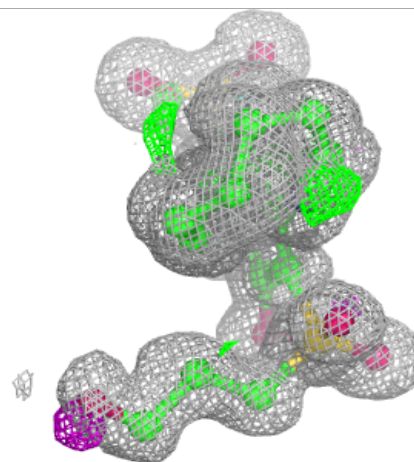
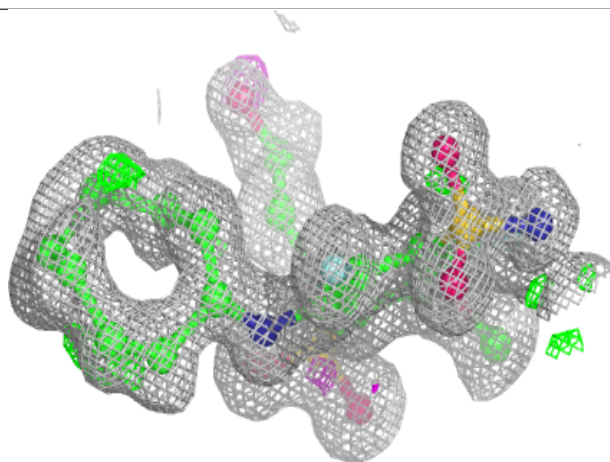
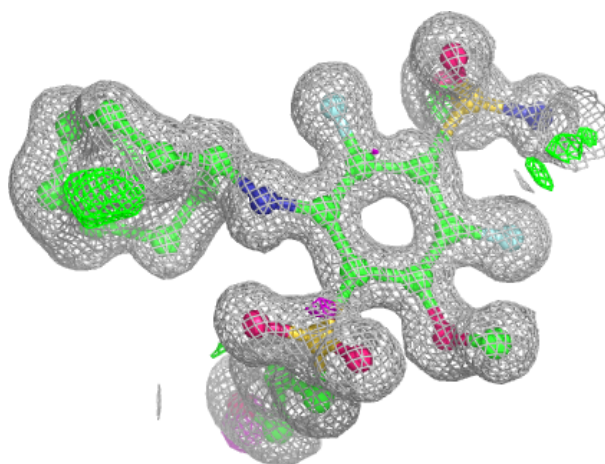
Electron density around A1H89 C 307:

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



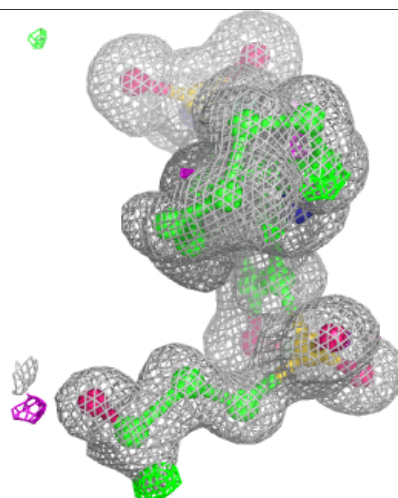
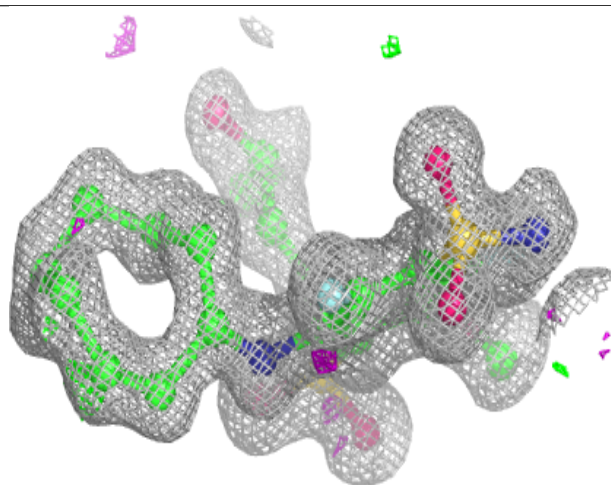
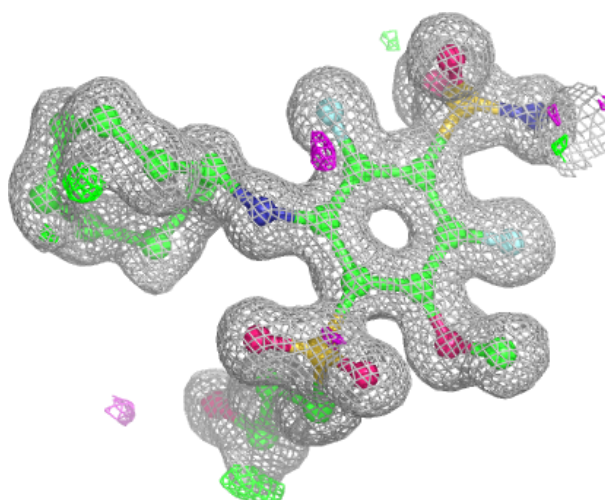
Electron density around A1H89 B 305:

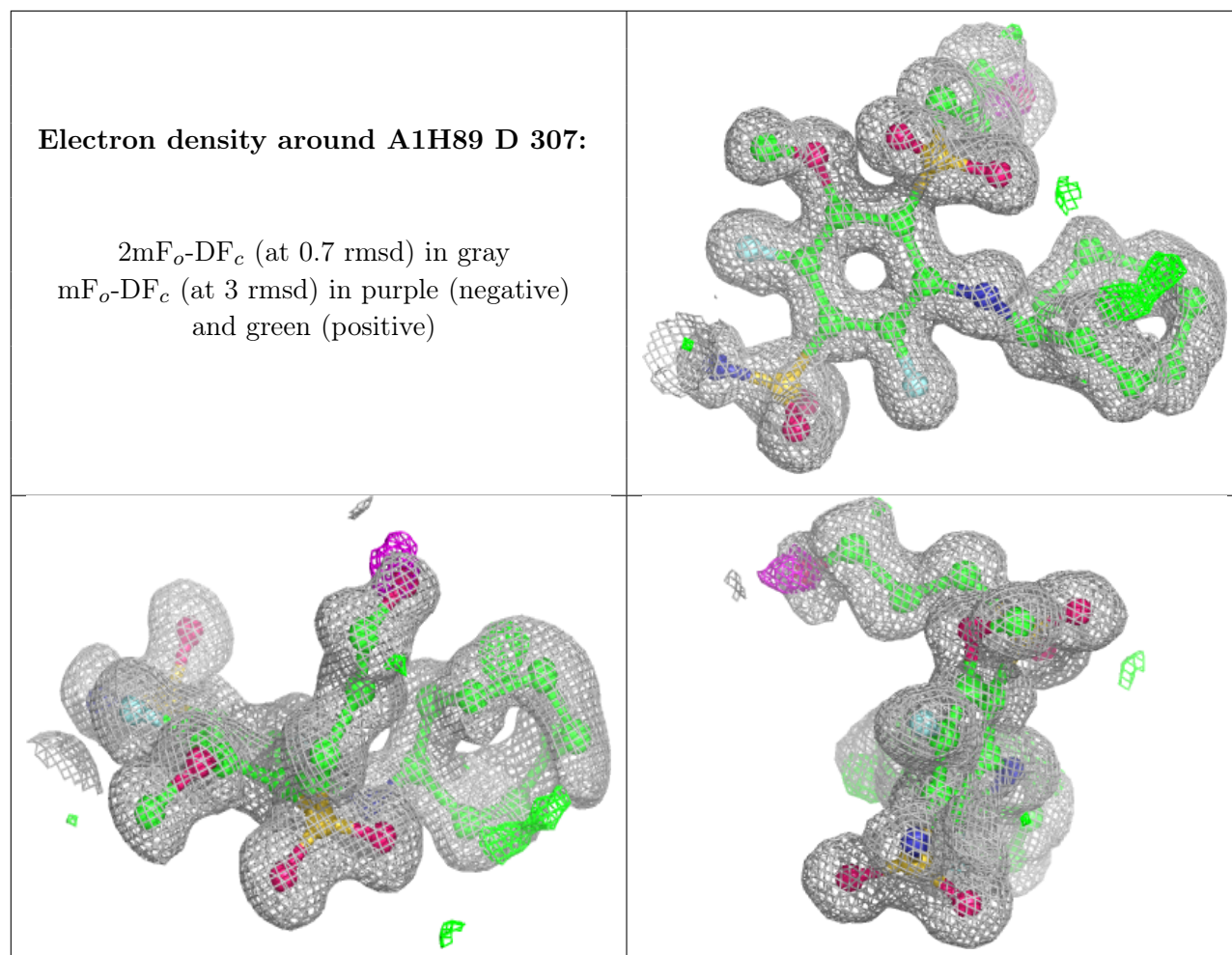
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around A1H89 A 306:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.