



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:24 PM UTC

PDB ID : 9R0U / pdb_00009r0u
Title : Three dimensional structure of human carbonic anhydrase XII in complex with sulfonamide
Authors : Eimonta, V.; Leitans, J.; Tars, K.
Deposited on : 2025-04-24
Resolution : 1.19 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

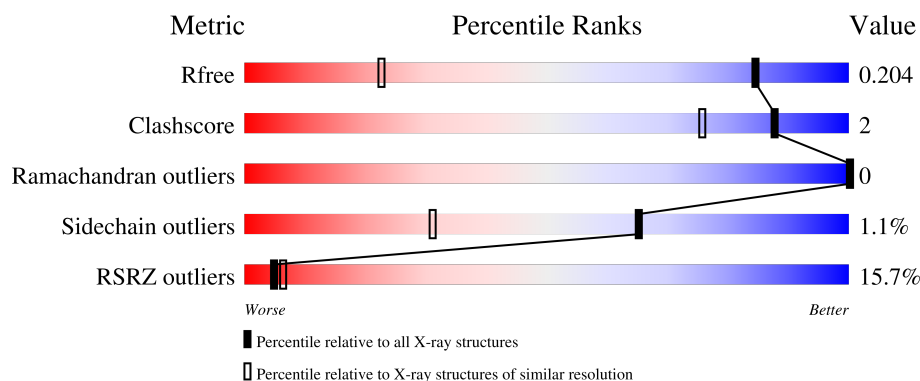
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.19 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	1216 (1.20-1.20)
Clashscore	190562	1265 (1.20-1.20)
Ramachandran outliers	187476	1226 (1.20-1.20)
Sidechain outliers	187428	1226 (1.20-1.20)
RSRZ outliers	180081	1214 (1.20-1.20)

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	14% 92% 7% .
1	B	263	31% 87% 11% ..
1	C	263	6% 95% . ..
1	D	263	12% 90% 9% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9350 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	0	0
			2084	1325	354	398	7			
1	B	260	Total	C	N	O	S	0	0	0
			2082	1325	352	398	7			
1	C	260	Total	C	N	O	S	0	0	0
			2082	1325	352	398	7			
1	D	260	Total	C	N	O	S	0	1	0
			2088	1329	353	399	7			

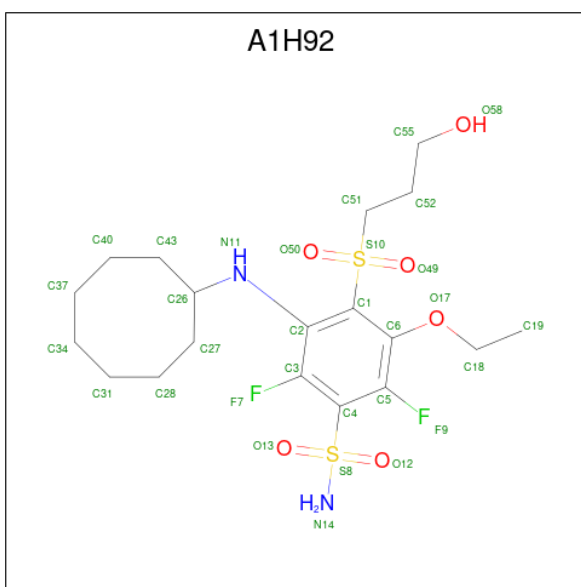
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	ALA	-	expression tag	UNP O43570
B	2	ALA	-	expression tag	UNP O43570
C	2	ALA	-	expression tag	UNP O43570
D	2	ALA	-	expression tag	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 3-(Cyclooctylamino)-5-ethoxy-2,6-difluoro-4-((3-hydroxypropyl)sulfonyl) benzenesulfonamide (CCD ID: A1H92) (formula: C₁₉H₃₀F₂N₂O₆S₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	S	0	0
			31	19	2	2	6	2		
3	B	1	Total	C	F	N	O	S	0	0
			31	19	2	2	6	2		
3	C	1	Total	C	F	N	O	S	0	0
			31	19	2	2	6	2		
3	D	1	Total	C	F	N	O	S	0	0
			31	19	2	2	6	2		

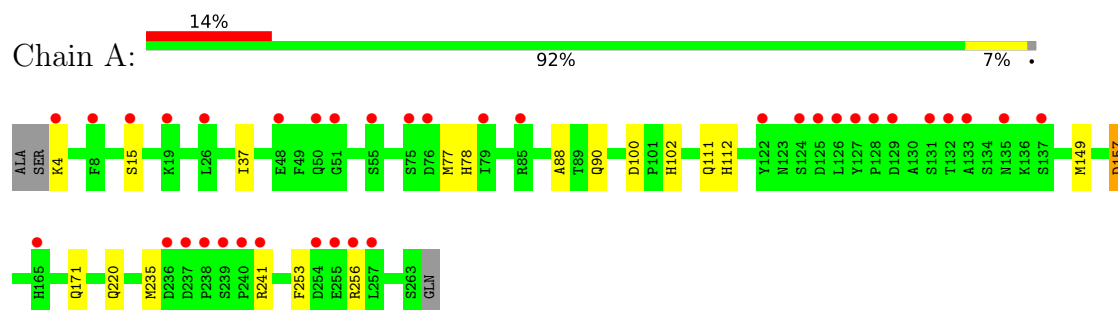
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	224	Total	O	0	0
			224	224		
4	B	195	Total	O	0	0
			195	195		
4	C	250	Total	O	0	0
			250	250		
4	D	217	Total	O	0	0
			217	217		

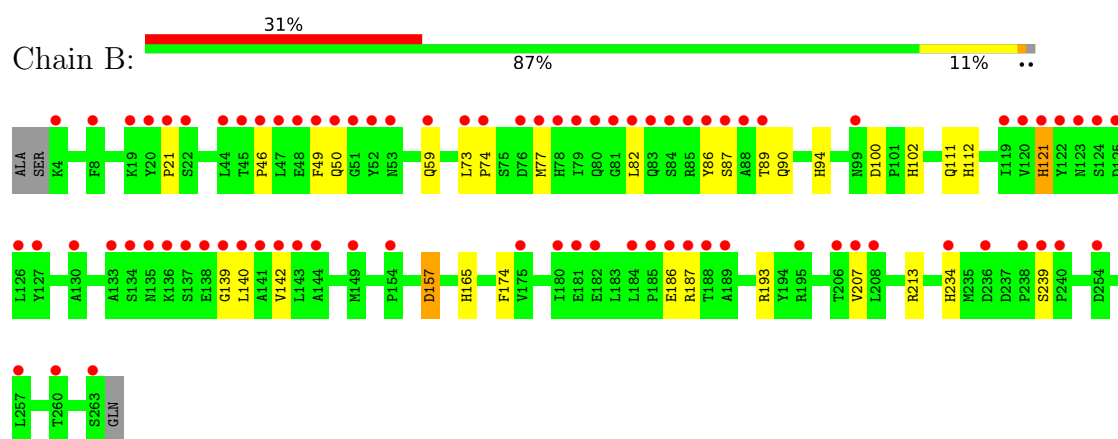
3 Residue-property plots [i](#)

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.

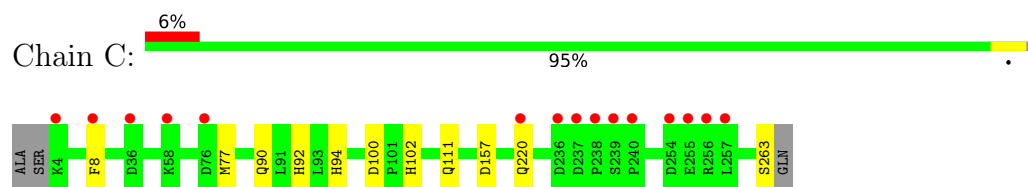
• Molecule 1: Carbonic anhydrase 12



• Molecule 1: Carbonic anhydrase 12

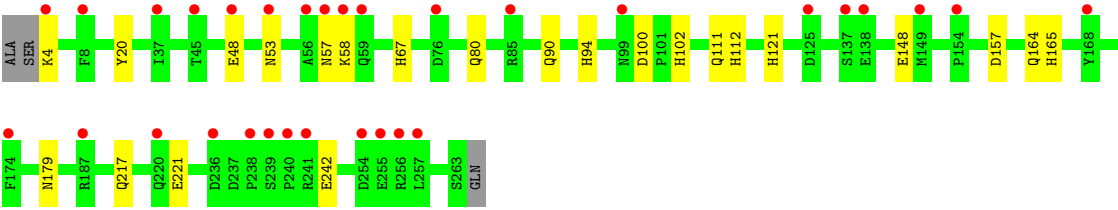


• Molecule 1: Carbonic anhydrase 12



• Molecule 1: Carbonic anhydrase 12





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	46.59Å 67.12Å 80.46Å 81.54° 84.30° 86.47°	Depositor
Resolution (Å)	47.64 – 1.19 47.64 – 1.19	Depositor EDS
% Data completeness (in resolution range)	95.2 (47.64-1.19) 95.2 (47.64-1.19)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.89 (at 1.19Å)	Xtriage
Refinement program	REFMAC 5.8.0350	Depositor
R, R_{free}	0.166 , 0.194 (Not available) , 0.204	Depositor DCC
R_{free} test set	14632 reflections (4.76%)	wwPDB-VP
Wilson B-factor (Å ²)	7.2	Xtriage
Anisotropy	0.384	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 36.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9350	wwPDB-VP
Average B, all atoms (Å ²)	21.0	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 56.32 % 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 2.7826e-05. 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: A1H92, 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	0.76	4/2147 (0.2%)	0.96	0/2926
1	B	1.09	14/2145 (0.7%)	1.11	5/2923 (0.2%)
1	C	0.78	2/2145 (0.1%)	1.00	3/2923 (0.1%)
1	D	1.01	8/2154 (0.4%)	1.06	2/2935 (0.1%)
All	All	0.92	28/8591 (0.3%)	1.04	10/11707 (0.1%)

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	2
1	B	0	1
All	All	0	3

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	221	GLU	CD-OE1	16.04	1.55	1.25
1	D	242	GLU	CD-OE1	14.08	1.52	1.25
1	B	46	PRO	C-O	13.27	1.39	1.23
1	D	221	GLU	CD-OE2	12.36	1.48	1.25
1	B	82	LEU	C-O	10.47	1.38	1.24
1	B	50	GLN	C-O	10.17	1.35	1.23
1	B	239	SER	C-O	9.59	1.35	1.24
1	B	49	PHE	C-O	9.27	1.34	1.23
1	B	186	GLU	CD-OE1	7.35	1.39	1.25
1	B	139	GLY	C-O	6.88	1.33	1.23
1	C	94	HIS	CE1-NE2	6.63	1.39	1.32
1	B	86	TYR	C-O	6.60	1.31	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	21	PRO	C-O	6.47	1.32	1.24
1	B	94	HIS	CE1-NE2	6.17	1.38	1.32
1	A	78	HIS	CE1-NE2	6.09	1.38	1.32
1	B	112	HIS	CE1-NE2	6.06	1.38	1.32
1	B	121	HIS	CE1-NE2	5.91	1.38	1.32
1	D	112	HIS	CE1-NE2	5.90	1.38	1.32
1	D	121	HIS	CE1-NE2	5.86	1.38	1.32
1	D	67	HIS	CE1-NE2	5.82	1.38	1.32
1	A	15	SER	CB-OG	5.78	1.53	1.42
1	D	94	HIS	CE1-NE2	5.75	1.38	1.32
1	A	112	HIS	CE1-NE2	5.27	1.37	1.32
1	A	157	ASP	CG-OD1	5.23	1.35	1.25
1	B	234	HIS	CE1-NE2	5.20	1.37	1.32
1	D	57	ASN	CG-ND2	5.18	1.44	1.33
1	B	157	ASP	CG-OD1	5.08	1.35	1.25
1	C	92	HIS	CE1-NE2	5.07	1.37	1.32

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	8	PHE	CA-CB-CG	6.40	120.20	113.80
1	B	46	PRO	CB-CA-C	6.23	119.50	111.46
1	B	73	LEU	O-C-N	6.10	127.05	121.80
1	B	89	THR	CA-CB-OG1	-5.46	101.40	109.60
1	B	73	LEU	CA-C-O	-5.45	114.31	120.46
1	C	263	SER	CA-C-O	-5.42	111.58	120.80
1	D	112	HIS	CB-CG-CD2	-5.25	124.37	131.20
1	C	77	MET	N-CA-CB	-5.22	102.18	110.06
1	B	49	PHE	O-C-N	5.11	129.16	122.87
1	D	112	HIS	N-CA-CB	5.11	117.77	110.06

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	241	ARG	Sidechain
1	A	256	ARG	Sidechain
1	B	213	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2084	0	1968	10	0
1	B	2082	0	1968	13	0
1	C	2082	0	1968	8	0
1	D	2088	0	1976	12	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	31	0	0	0	0
3	B	31	0	0	0	0
3	C	31	0	0	0	0
3	D	31	0	0	0	0
4	A	224	0	0	0	0
4	B	195	0	0	1	0
4	C	250	0	0	0	0
4	D	217	0	0	1	0
All	All	9350	0	7880	33	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 2.

All (33) 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:111:GLN:NE2	1:B:111:GLN:NE2	2.25	0.84
1:C:111:GLN:NE2	1:D:111:GLN:NE2	2.35	0.74
1:A:111:GLN:HE21	1:B:111:GLN:NE2	1.84	0.72
1:A:111:GLN:NE2	1:B:111:GLN:HE21	1.89	0.69
1:A:111:GLN:HE21	1:B:111:GLN:HE22	1.41	0.68
1:C:111:GLN:HE21	1:D:111:GLN:HE22	1.45	0.64
1:A:111:GLN:HE22	1:B:111:GLN:HE21	1.46	0.63
1:C:111:GLN:HE21	1:D:111:GLN:NE2	1.98	0.62
1:B:165:HIS:HD2	4:B:572:HOH:O	1.83	0.61
1:B:142:VAL:HG23	1:B:207:VAL:HG11	1.84	0.58
1:A:149:MET:HE2	1:A:220:GLN:HE21	1.70	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:GLN:HG3	1:B:174:PHE:CD1	2.40	0.55
1:C:111:GLN:NE2	1:D:111:GLN:HE21	2.03	0.54
1:C:220:GLN:HA	1:C:220:GLN:HE21	1.74	0.53
1:A:171:GLN:HE22	1:A:235:MET:HE3	1.74	0.52
1:B:140:LEU:HB2	1:B:207:VAL:HG22	1.90	0.52
1:D:164[B]:GLN:NE2	1:D:165:HIS:CE1	2.79	0.51
1:D:100:ASP:OD1	1:D:102:HIS:HD2	1.94	0.50
1:A:100:ASP:OD1	1:A:102:HIS:HD2	1.95	0.50
1:D:58:LYS:HE2	4:D:573:HOH:O	2.11	0.49
1:A:37:ILE:HD12	1:A:253:PHE:CD2	2.48	0.49
1:C:100:ASP:OD1	1:C:102:HIS:HD2	1.96	0.49
1:B:100:ASP:OD1	1:B:102:HIS:HD2	1.96	0.48
1:B:187:ARG:HH11	1:B:187:ARG:HG3	1.79	0.47
1:C:111:GLN:HE22	1:D:111:GLN:HE21	1.63	0.47
1:C:220:GLN:HA	1:C:220:GLN:NE2	2.29	0.47
1:D:4:LYS:HD2	1:D:20:TYR:OH	2.15	0.46
1:B:87:SER:O	1:B:121:HIS:HA	2.15	0.46
1:D:48:GLU:HB2	1:D:80:GLN:HB3	2.00	0.44
1:D:53:ASN:HA	1:D:179:ASN:HA	2.00	0.42
1:D:148:GLU:O	1:D:217:GLN:HA	2.20	0.41
1:A:77:MET:HB2	1:A:88:ALA:HB3	2.03	0.41
1:B:74:PRO:O	1:B:77:MET:HB3	2.20	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	258/263 (98%)	253 (98%)	5 (2%)	0	100	100
1	B	258/263 (98%)	251 (97%)	7 (3%)	0	100	100
1	C	258/263 (98%)	253 (98%)	5 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	259/263 (98%)	254 (98%)	5 (2%)	0	100	100
All	All	1033/1052 (98%)	1011 (98%)	22 (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	231/234 (99%)	228 (99%)	3 (1%)	61	25
1	B	231/234 (99%)	228 (99%)	3 (1%)	61	25
1	C	231/234 (99%)	229 (99%)	2 (1%)	70	40
1	D	232/234 (99%)	230 (99%)	2 (1%)	70	40
All	All	925/936 (99%)	915 (99%)	10 (1%)	65	31

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

Mol	Chain	Res	Type
1	A	4	LYS
1	A	90	GLN
1	A	157	ASP
1	B	90	GLN
1	B	157	ASP
1	B	193	ARG
1	C	90	GLN
1	C	157	ASP
1	D	90	GLN
1	D	157	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	112	HIS
1	A	171	GLN
1	A	220	GLN
1	A	251	GLN
1	B	14	ASN
1	B	39	GLN
1	B	57	ASN
1	B	59	GLN
1	B	99	ASN
1	B	111	GLN
1	B	165	HIS
1	B	220	GLN
1	C	57	ASN
1	C	111	GLN
1	C	234	HIS
1	C	251	GLN
1	D	14	ASN
1	D	78	HIS
1	D	80	GLN
1	D	102	HIS
1	D	111	GLN
1	D	165	HIS
1	D	204	ASN
1	D	234	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	A1H92	D	302	2	32,32,32	1.90	9 (28%)	38,46,46	1.67	9 (23%)
3	A1H92	C	302	2	32,32,32	1.76	8 (25%)	38,46,46	1.70	8 (21%)
3	A1H92	B	302	2	32,32,32	2.03	10 (31%)	38,46,46	2.04	9 (23%)
3	A1H92	A	302	2	32,32,32	2.19	13 (40%)	38,46,46	1.98	7 (18%)

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	A1H92	D	302	2	-	7/24/34/34	0/2/2/2
3	A1H92	C	302	2	-	8/24/34/34	0/2/2/2
3	A1H92	B	302	2	-	7/24/34/34	0/2/2/2
3	A1H92	A	302	2	-	9/24/34/34	0/2/2/2

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	302	A1H92	C4-S8	-5.73	1.69	1.78
3	A	302	A1H92	C4-S8	-5.05	1.70	1.78
3	A	302	A1H92	C5-C4	4.79	1.47	1.39
3	D	302	A1H92	C4-S8	-4.78	1.71	1.78
3	C	302	A1H92	C4-S8	-4.61	1.71	1.78
3	B	302	A1H92	C3-C4	4.14	1.46	1.39
3	A	302	A1H92	C51-S10	-4.02	1.70	1.77
3	A	302	A1H92	C6-C1	3.83	1.46	1.40
3	D	302	A1H92	C51-S10	-3.78	1.70	1.77
3	D	302	A1H92	C6-C1	3.55	1.45	1.40
3	D	302	A1H92	C3-C4	3.50	1.45	1.39
3	C	302	A1H92	C3-C4	3.45	1.45	1.39
3	A	302	A1H92	C3-C4	3.39	1.45	1.39
3	C	302	A1H92	S8-N14	-3.37	1.53	1.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	302	A1H92	C51-S10	-3.34	1.71	1.77
3	B	302	A1H92	C2-C3	3.33	1.44	1.39
3	B	302	A1H92	O12-S8	3.31	1.49	1.43
3	A	302	A1H92	C2-C3	3.20	1.44	1.39
3	D	302	A1H92	S8-N14	-3.15	1.54	1.60
3	A	302	A1H92	F7-C3	-3.08	1.30	1.34
3	B	302	A1H92	F7-C3	-2.85	1.30	1.34
3	C	302	A1H92	C6-C1	2.83	1.44	1.40
3	B	302	A1H92	S8-N14	-2.73	1.55	1.60
3	A	302	A1H92	S8-N14	-2.71	1.55	1.60
3	B	302	A1H92	C1-S10	-2.65	1.67	1.81
3	A	302	A1H92	C1-S10	-2.65	1.67	1.81
3	A	302	A1H92	O17-C6	-2.53	1.33	1.39
3	B	302	A1H92	C5-C4	2.47	1.43	1.39
3	D	302	A1H92	C2-C3	2.47	1.43	1.39
3	C	302	A1H92	C2-C1	2.39	1.47	1.40
3	B	302	A1H92	C6-C5	2.30	1.43	1.39
3	A	302	A1H92	O49-S10	-2.27	1.41	1.44
3	C	302	A1H92	C1-S10	-2.27	1.69	1.81
3	D	302	A1H92	C1-S10	-2.24	1.69	1.81
3	A	302	A1H92	C2-C1	2.17	1.46	1.40
3	B	302	A1H92	O17-C6	-2.14	1.34	1.39
3	D	302	A1H92	F7-C3	-2.07	1.32	1.34
3	D	302	A1H92	C2-C1	2.06	1.46	1.40
3	A	302	A1H92	O12-S8	2.01	1.47	1.43
3	C	302	A1H92	O17-C6	-2.00	1.35	1.39

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	302	A1H92	O49-S10-O50	-6.17	111.84	118.45
3	A	302	A1H92	O49-S10-O50	-6.12	111.89	118.45
3	A	302	A1H92	C3-C4-C5	-6.10	112.48	116.65
3	B	302	A1H92	C3-C4-C5	-5.97	112.56	116.65
3	C	302	A1H92	C3-C4-C5	-5.31	113.02	116.65
3	D	302	A1H92	C3-C4-C5	-5.06	113.19	116.65
3	C	302	A1H92	O49-S10-O50	-4.82	113.28	118.45
3	D	302	A1H92	O49-S10-O50	-4.46	113.67	118.45
3	A	302	A1H92	C6-C5-C4	3.46	126.20	121.36
3	B	302	A1H92	O12-S8-C4	-3.36	102.34	107.28
3	B	302	A1H92	C5-C6-C1	3.31	123.32	116.95
3	C	302	A1H92	F7-C3-C4	-3.07	115.24	120.76

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	302	A1H92	F9-C5-C6	-3.01	114.82	119.39
3	B	302	A1H92	C3-C2-C1	2.96	121.18	115.97
3	A	302	A1H92	O12-S8-C4	-2.90	103.01	107.28
3	D	302	A1H92	O13-S8-C4	-2.83	103.12	107.28
3	D	302	A1H92	F7-C3-C4	-2.68	115.93	120.76
3	B	302	A1H92	O50-S10-C51	2.64	112.50	108.18
3	A	302	A1H92	C3-C2-C1	2.55	120.46	115.97
3	B	302	A1H92	F7-C3-C4	-2.51	116.25	120.76
3	C	302	A1H92	F9-C5-C6	-2.48	115.63	119.39
3	B	302	A1H92	C2-C1-C6	-2.48	114.86	119.42
3	C	302	A1H92	C6-C5-C4	2.40	124.72	121.36
3	B	302	A1H92	O13-S8-N14	2.39	110.79	107.35
3	A	302	A1H92	F7-C3-C4	-2.32	116.59	120.76
3	D	302	A1H92	C5-C6-C1	2.31	121.38	116.95
3	D	302	A1H92	C2-C3-C4	2.29	125.73	121.81
3	C	302	A1H92	C5-C6-C1	2.28	121.34	116.95
3	C	302	A1H92	C2-C3-C4	2.18	125.55	121.81
3	D	302	A1H92	C6-C5-C4	2.12	124.32	121.36
3	D	302	A1H92	F9-C5-C6	-2.11	116.18	119.39
3	C	302	A1H92	O13-S8-C4	-2.06	104.24	107.28
3	D	302	A1H92	O13-S8-N14	2.04	110.30	107.35

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	302	A1H92	C2-C1-S10-O50
3	A	302	A1H92	C2-C1-S10-O49
3	A	302	A1H92	C2-C1-S10-C51
3	A	302	A1H92	C5-C4-S8-O13
3	A	302	A1H92	C5-C4-S8-N14
3	B	302	A1H92	C2-C1-S10-O50
3	B	302	A1H92	C2-C1-S10-O49
3	B	302	A1H92	C2-C1-S10-C51
3	B	302	A1H92	C5-C4-S8-O13
3	B	302	A1H92	C5-C4-S8-N14
3	C	302	A1H92	C2-C1-S10-O50
3	C	302	A1H92	C2-C1-S10-O49
3	C	302	A1H92	C2-C1-S10-C51
3	C	302	A1H92	C5-C4-S8-N14
3	C	302	A1H92	C5-C4-S8-O12
3	D	302	A1H92	C2-C1-S10-O50

Continued on next page...

Continued from previous page...

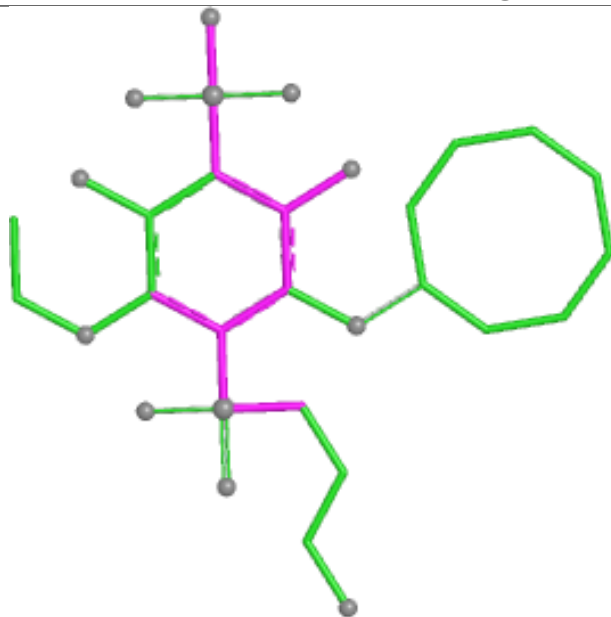
Mol	Chain	Res	Type	Atoms
3	D	302	A1H92	C2-C1-S10-O49
3	D	302	A1H92	C5-C4-S8-N14
3	D	302	A1H92	C5-C4-S8-O12
3	A	302	A1H92	C3-C4-S8-O13
3	B	302	A1H92	C3-C4-S8-N14
3	B	302	A1H92	C3-C4-S8-O13
3	C	302	A1H92	C3-C4-S8-O12
3	D	302	A1H92	C3-C4-S8-O12
3	A	302	A1H92	C19-C18-O17-C6
3	A	302	A1H92	C3-C4-S8-N14
3	C	302	A1H92	C3-C4-S8-N14
3	D	302	A1H92	C3-C4-S8-N14
3	C	302	A1H92	C43-C26-N11-C2
3	D	302	A1H92	C2-C1-S10-C51
3	A	302	A1H92	C3-C2-N11-C26

There are no ring outliers.

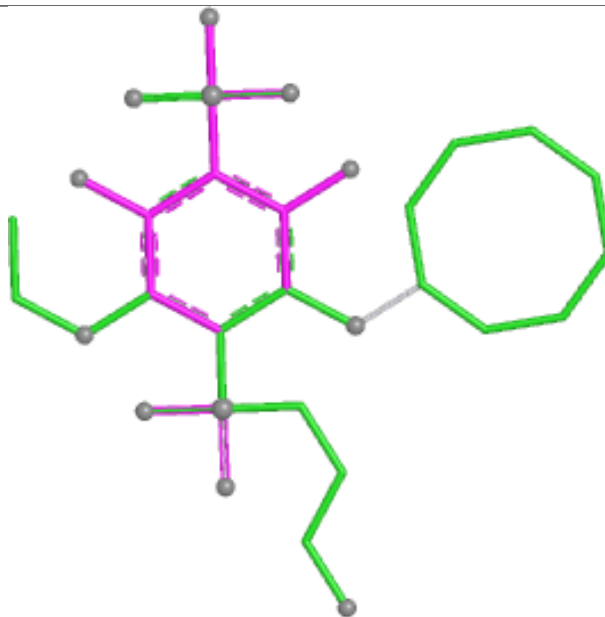
No monomer is involved in short contacts.

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.

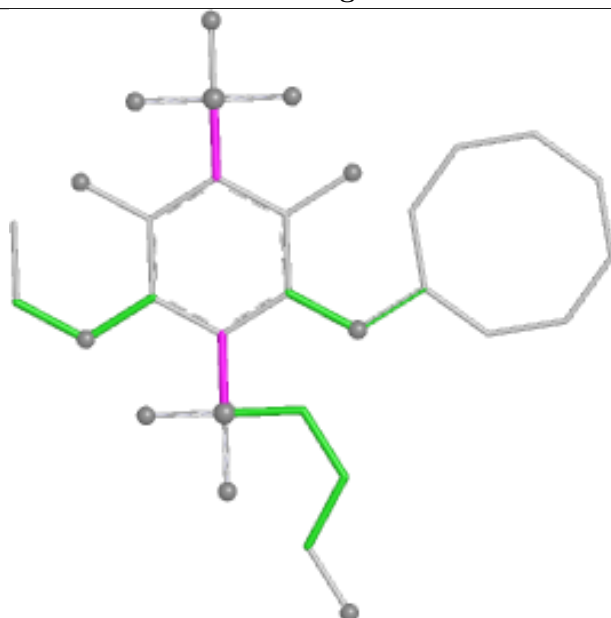
Ligand A1H92 D 302



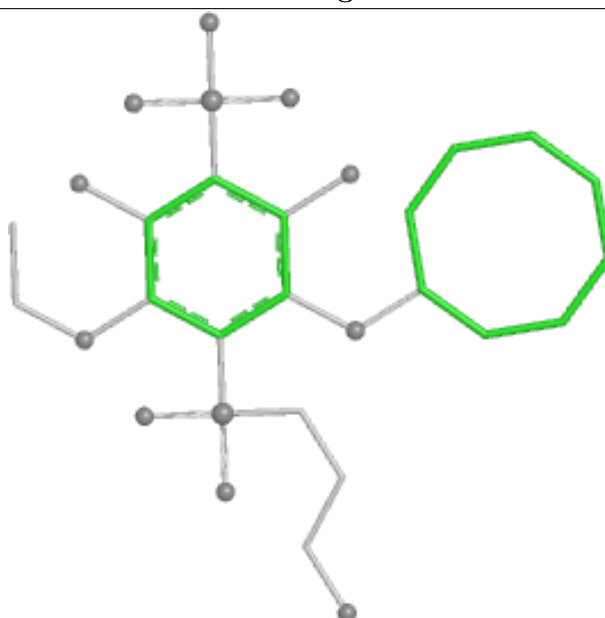
Bond lengths



Bond angles

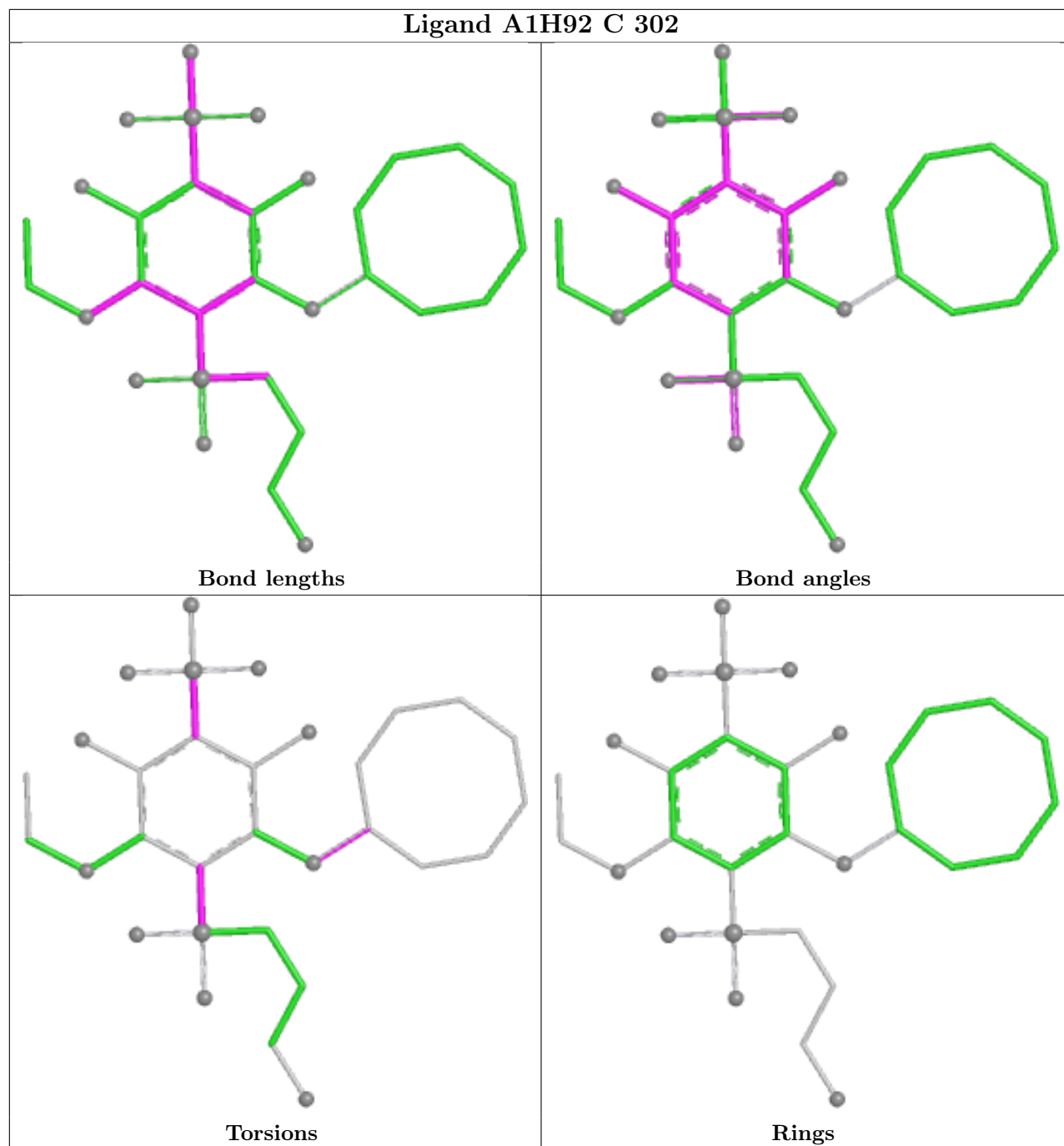


Torsions

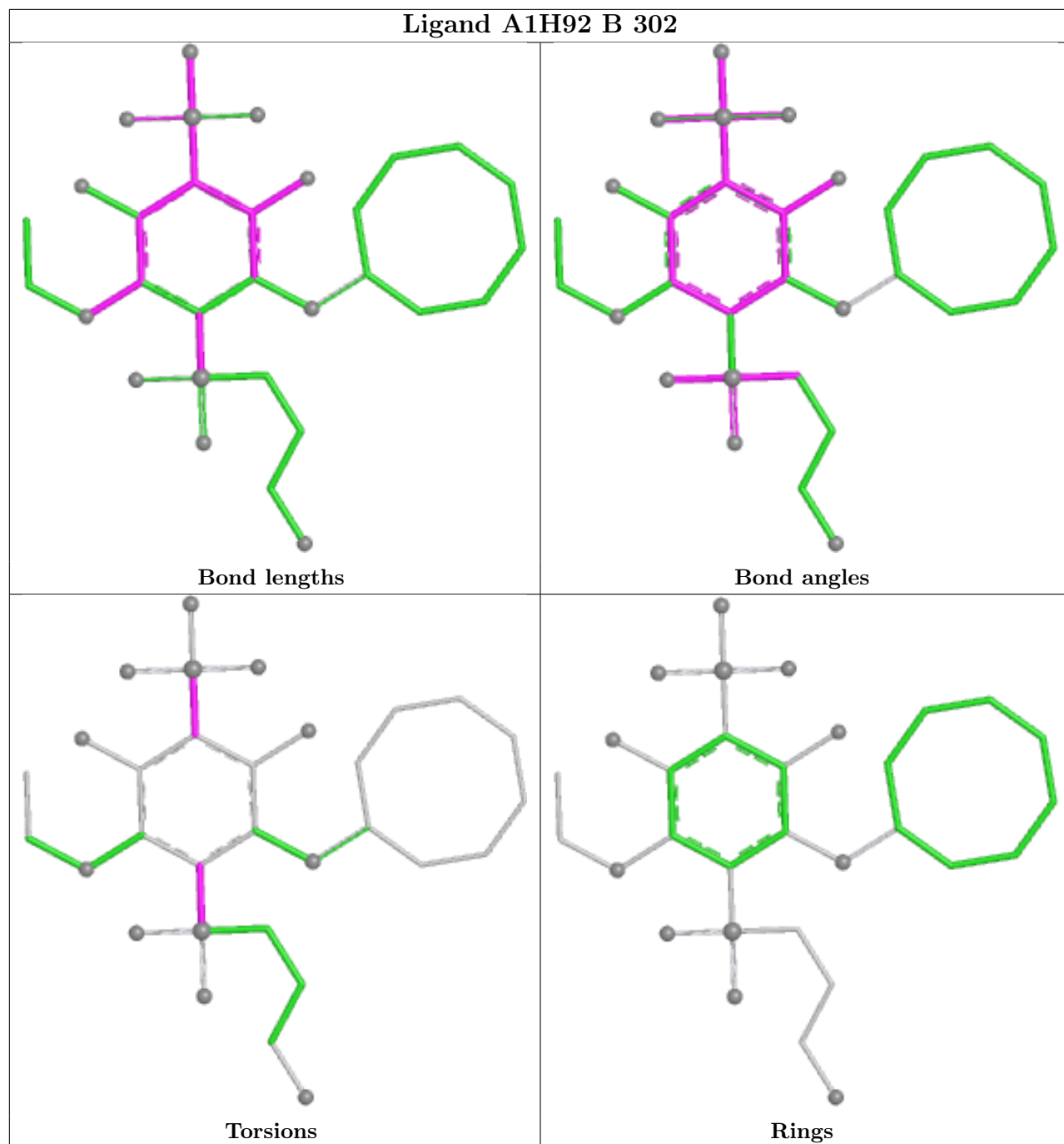


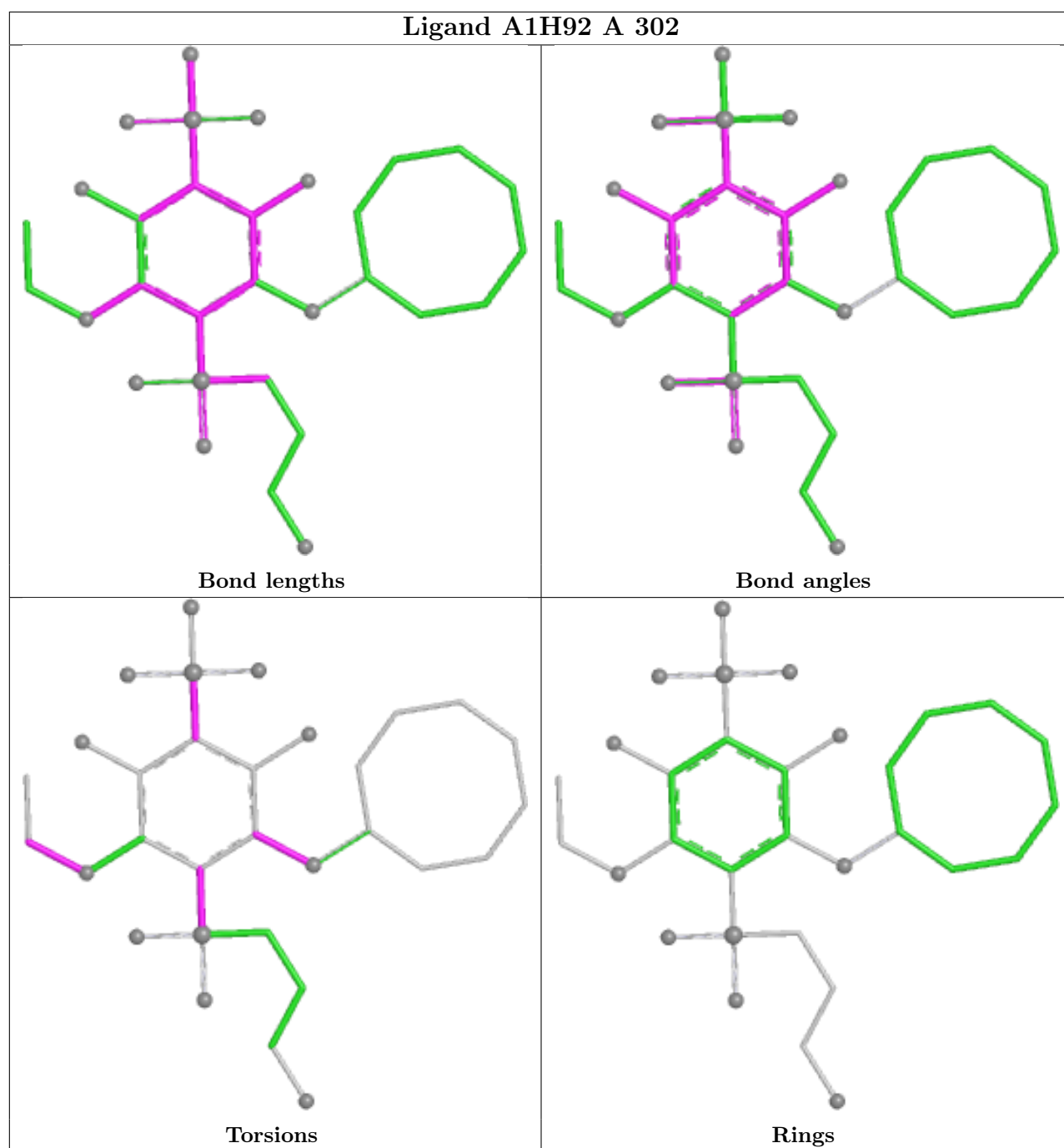
Rings

Ligand A1H92 C 302



Ligand A1H92 B 302





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%)	0.78	36 (13%)	6 7	6, 13, 54, 164	0
1	B	260/263 (98%)	2.58	81 (31%)	1 1	6, 15, 180, 358	0
1	C	260/263 (98%)	0.22	15 (5%)	29 31	6, 11, 30, 147	0
1	D	260/263 (98%)	0.54	31 (11%)	9 10	6, 12, 38, 94	1 (0%)
All	All	1040/1052 (98%)	1.03	163 (15%)	5 6	6, 13, 63, 358	1 (0%)

All (163) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	79	ILE	24.2
1	B	140	LEU	22.8
1	B	88	ALA	20.7
1	B	82	LEU	18.8
1	B	207	VAL	18.5
1	B	21	PRO	18.1
1	B	51	GLY	16.8
1	B	86	TYR	16.3
1	B	52	TYR	15.8
1	B	87	SER	15.7
1	B	81	GLY	14.4
1	A	128	PRO	14.4
1	B	46	PRO	14.0
1	B	121	HIS	13.7
1	B	53	ASN	13.1
1	B	84	SER	12.0
1	B	89	THR	11.9
1	D	240	PRO	11.7
1	A	240	PRO	11.5
1	B	240	PRO	11.5
1	B	85	ARG	11.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	124	SER	11.3
1	B	141	ALA	11.0
1	B	78	HIS	10.9
1	B	45	THR	10.6
1	B	49	PHE	10.1
1	B	50	GLN	10.0
1	B	22	SER	9.9
1	B	20	TYR	9.8
1	B	80	GLN	9.4
1	B	48	GLU	9.4
1	B	142	VAL	9.3
1	B	143	LEU	9.3
1	B	76	ASP	9.2
1	B	83	GLN	9.2
1	A	15	SER	8.7
1	A	127	TYR	8.6
1	B	122	TYR	8.6
1	C	254	ASP	8.4
1	B	77	MET	8.2
1	B	239	SER	8.1
1	D	57	ASN	7.8
1	A	238	PRO	7.7
1	D	238	PRO	7.5
1	B	47	LEU	7.5
1	A	76	ASP	7.4
1	A	239	SER	7.4
1	A	125	ASP	7.3
1	A	132	THR	7.1
1	B	19	LYS	7.0
1	B	59	GLN	6.9
1	B	186	GLU	6.8
1	D	239	SER	6.6
1	B	127	TYR	6.4
1	B	8	PHE	6.3
1	B	187	ARG	6.1
1	B	73	LEU	6.1
1	B	123	ASN	6.1
1	A	133	ALA	6.0
1	C	238	PRO	5.9
1	B	189	ALA	5.8
1	B	44	LEU	5.5
1	B	120	VAL	5.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	8	PHE	5.4
1	B	139	GLY	5.2
1	D	59	GLN	5.0
1	C	255	GLU	5.0
1	B	195	ARG	4.8
1	A	122	TYR	4.8
1	C	8	PHE	4.7
1	B	133	ALA	4.6
1	C	256	ARG	4.6
1	B	119	ILE	4.4
1	C	240	PRO	4.4
1	B	238	PRO	4.4
1	A	237	ASP	4.3
1	D	125	ASP	4.3
1	C	239	SER	4.2
1	D	254	ASP	4.2
1	D	220	GLN	4.1
1	A	236	ASP	4.1
1	B	206	THR	4.0
1	B	181	GLU	4.0
1	C	76	ASP	4.0
1	A	126	LEU	4.0
1	A	254	ASP	3.9
1	A	75	SER	3.9
1	A	129	ASP	3.8
1	D	241	ARG	3.8
1	A	55	SER	3.7
1	B	126	LEU	3.6
1	B	74	PRO	3.5
1	A	79	ILE	3.5
1	B	185	PRO	3.4
1	A	8	PHE	3.3
1	D	58	LYS	3.2
1	C	4	LYS	3.2
1	A	48	GLU	3.2
1	A	255	GLU	3.2
1	B	180	ILE	3.2
1	B	188	THR	3.1
1	A	165	HIS	3.1
1	D	85	ARG	3.1
1	D	257	LEU	3.1
1	D	149	MET	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	254	ASP	3.0
1	A	4	LYS	3.0
1	B	149	MET	2.9
1	A	124	SER	2.9
1	A	135	ASN	2.9
1	D	236	ASP	2.9
1	C	36	ASP	2.8
1	C	58	LYS	2.8
1	D	56	ALA	2.8
1	B	182	GLU	2.8
1	B	154	PRO	2.8
1	D	53	ASN	2.8
1	A	50	GLN	2.8
1	A	51	GLY	2.8
1	D	255	GLU	2.7
1	B	135	ASN	2.7
1	B	125	ASP	2.7
1	D	4	LYS	2.7
1	B	184	LEU	2.7
1	D	256	ARG	2.7
1	A	241	ARG	2.6
1	B	134	SER	2.6
1	B	130	ALA	2.6
1	B	137	SER	2.6
1	D	99	ASN	2.6
1	C	257	LEU	2.5
1	D	187	ARG	2.5
1	D	138	GLU	2.5
1	A	131	SER	2.4
1	B	263	SER	2.4
1	A	85	ARG	2.4
1	B	234	HIS	2.3
1	C	237	ASP	2.3
1	D	48	GLU	2.3
1	A	256	ARG	2.3
1	D	37	ILE	2.3
1	A	26	LEU	2.3
1	D	76	ASP	2.3
1	A	19	LYS	2.3
1	A	137	SER	2.2
1	D	137	SER	2.2
1	A	257	LEU	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	99	ASN	2.2
1	B	144	ALA	2.2
1	D	45	THR	2.2
1	D	168	TYR	2.2
1	B	257	LEU	2.1
1	D	154	PRO	2.1
1	C	220	GLN	2.1
1	B	208	LEU	2.1
1	B	175	VAL	2.1
1	C	236	ASP	2.1
1	B	136	LYS	2.1
1	B	138	GLU	2.1
1	B	260	THR	2.1
1	B	4	LYS	2.0
1	B	236	ASP	2.0
1	D	174	PHE	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
3	A1H92	B	302	31/31	0.98	0.07	8,12,26,28	0
3	A1H92	A	302	31/31	0.99	0.07	7,14,22,23	0
3	A1H92	C	302	31/31	0.99	0.05	6,10,16,19	0
3	A1H92	D	302	31/31	0.99	0.06	6,10,16,18	0
2	ZN	A	301	1/1	1.00	0.02	6,6,6,6	0
2	ZN	B	301	1/1	1.00	0.03	9,9,9,9	0
2	ZN	C	301	1/1	1.00	0.02	6,6,6,6	0

Continued on next page...

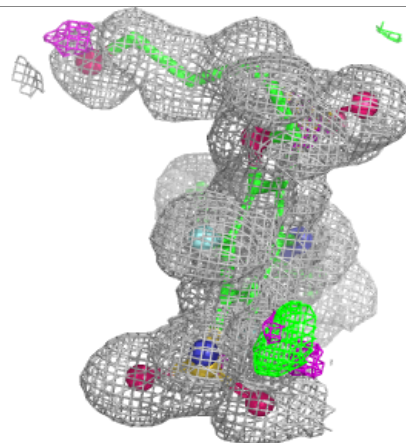
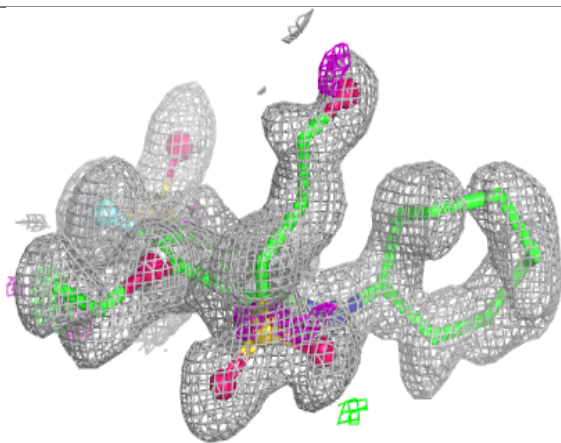
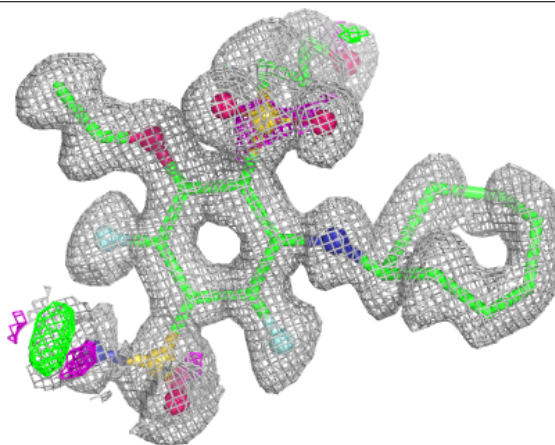
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	D	301	1/1	1.00	0.02	6,6,6,6	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.

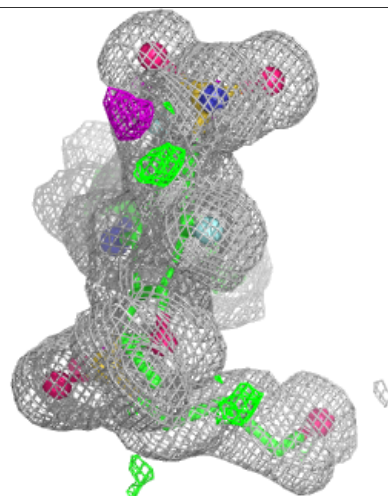
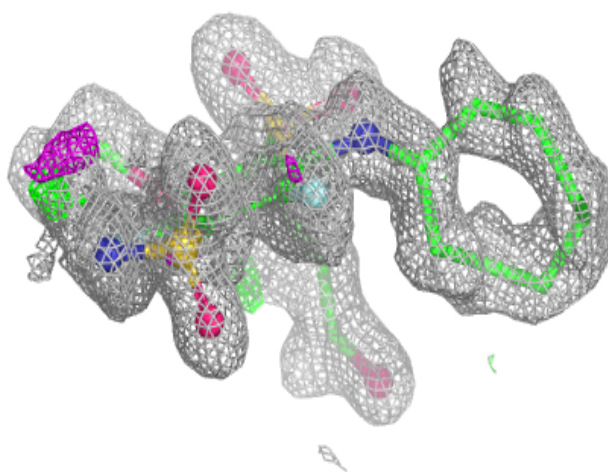
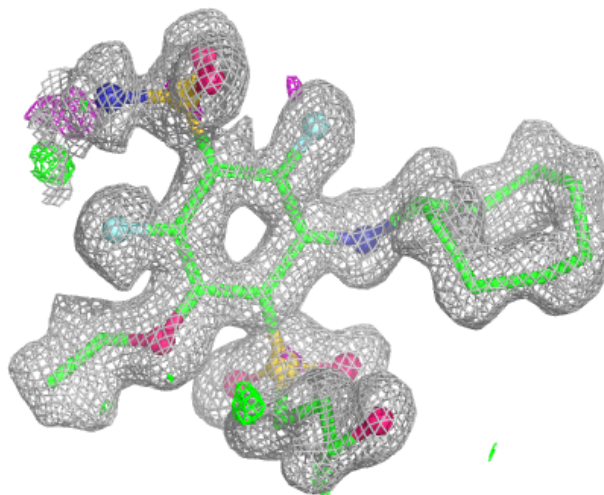
Electron density around A1H92 B 302:

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



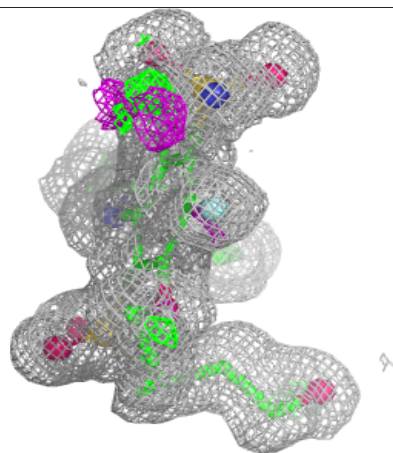
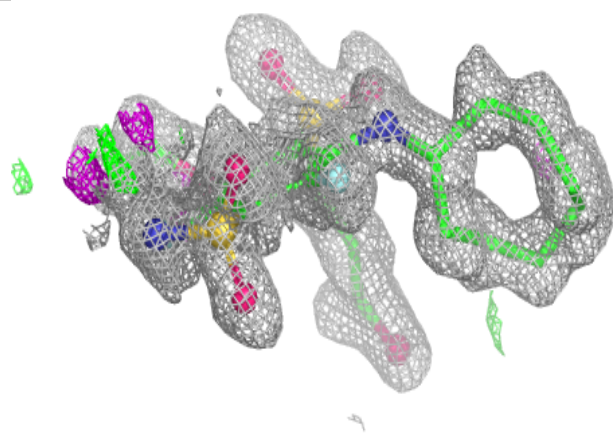
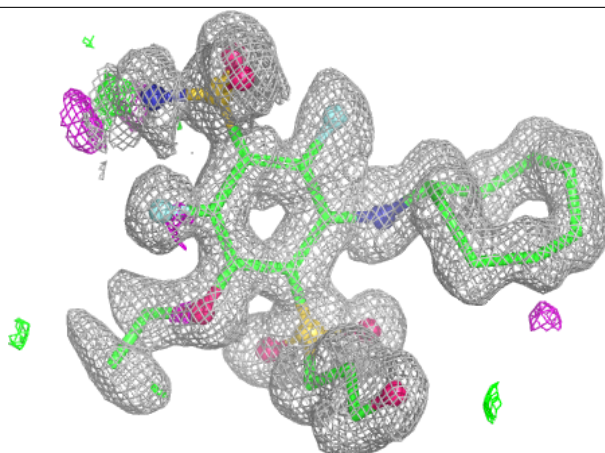
Electron density around A1H92 A 302:

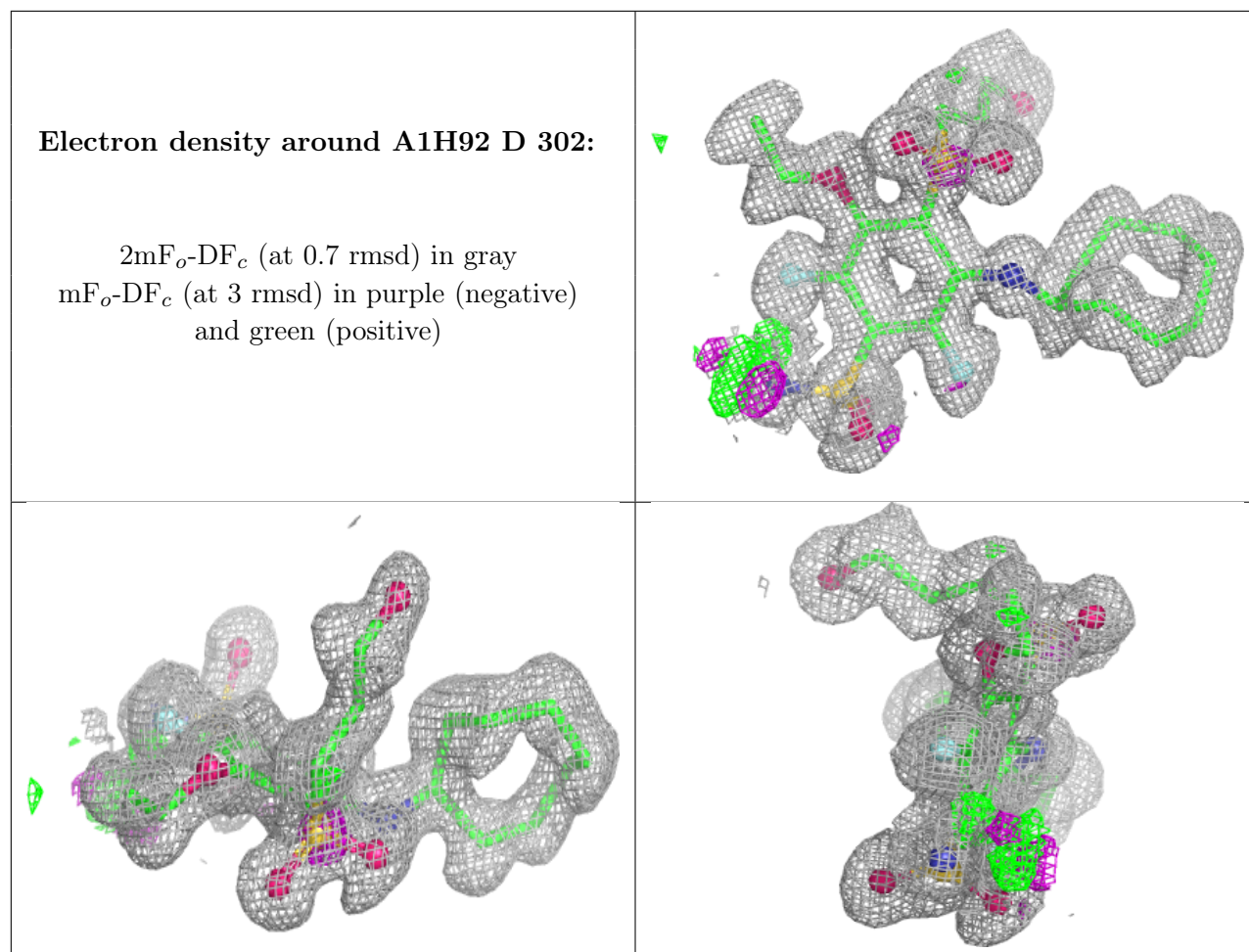
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around A1H92 C 302:

$2mF_o-DF_c$ (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.