



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 11, 2025 – 06:10 PM EDT

PDB ID : 8VC0
Title : HIV-1 CA crosslinked pentamer in complex with GS-CA1
Authors : Piacentini, J.; Ganser-Pornillos, B.K.; Pornillos, O.
Deposited on : 2023-12-13
Resolution : 3.46 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 1.21
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.004 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.41.4

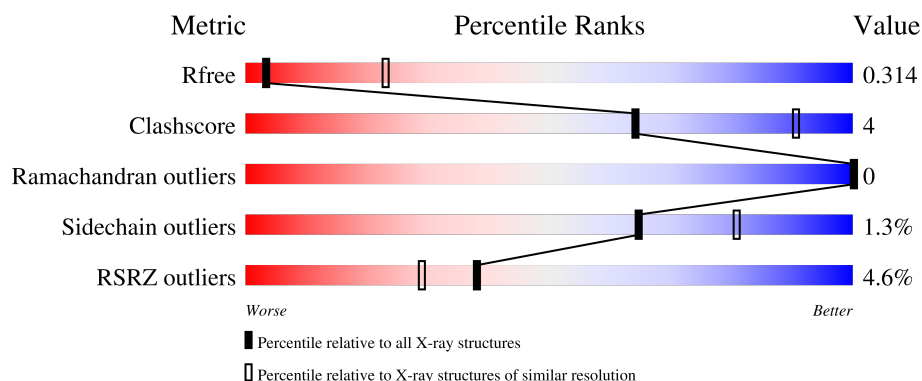
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.46 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.



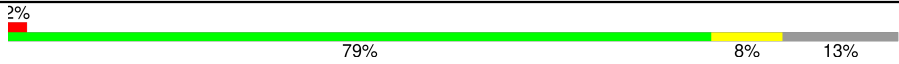
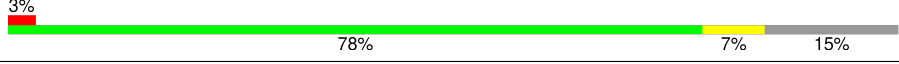
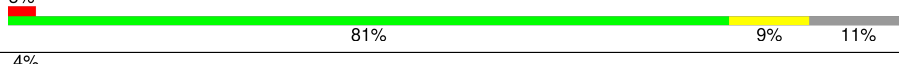


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	1597 (3.52-3.40)
Clashscore	180529	1041 (3.50-3.42)
Ramachandran outliers	177936	1026 (3.50-3.42)
Sidechain outliers	177891	1027 (3.50-3.42)
RSRZ outliers	164620	1596 (3.52-3.40)

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	231	 4% 78% 9% 13%
1	B	231	 3% 76% 9% 15%
1	C	231	 2% 75% 8% 16%
1	D	231	 3% 79% 7% 13%
1	E	231	 8% 75% 12% 13%

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Mol	Chain	Length	Quality of chain
1	F	231	 2% 79% 8% 13%
1	G	231	 3% 78% 7% 15%
1	H	231	 3% 81% 9% 11%
1	I	231	 4% 77% 8% 14%
1	J	231	 7% 77% 11% 12%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 28350 atoms, of which 13387 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 Capsid protein p24.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	201	Total	C	H	N	O	S	0	0	0
			2805	919	1344	254	276	12			
1	B	196	Total	C	H	N	O	S	0	0	0
			2637	877	1249	244	255	12			
1	C	193	Total	C	H	N	O	S	0	0	0
			2416	822	1101	231	253	9			
1	D	200	Total	C	H	N	O	S	0	0	0
			2653	885	1245	243	269	11			
1	E	202	Total	C	H	N	O	S	0	0	0
			2934	948	1433	261	280	12			
1	F	201	Total	C	H	N	O	S	0	0	0
			2822	924	1365	251	271	11			
1	G	197	Total	C	H	N	O	S	0	0	0
			2657	880	1265	239	260	13			
1	H	206	Total	C	H	N	O	S	0	0	0
			2796	930	1321	257	277	11			
1	I	198	Total	C	H	N	O	S	0	0	0
			2665	889	1256	249	261	10			
1	J	203	Total	C	H	N	O	S	0	0	0
			2965	956	1448	265	284	12			

There are 40 discrepancies between the modelled and reference sequences:

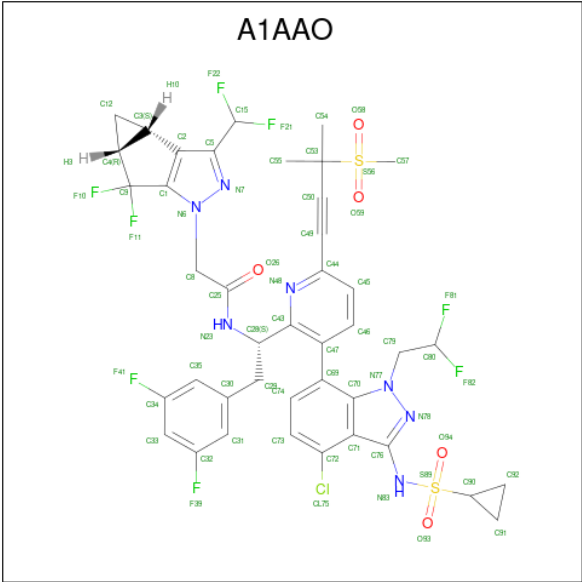
Chain	Residue	Modelled	Actual	Comment	Reference
A	21	CYS	ASN	engineered mutation	UNP P12497
A	22	CYS	ALA	engineered mutation	UNP P12497
A	184	ALA	TRP	engineered mutation	UNP P12497
A	185	ALA	MET	engineered mutation	UNP P12497
B	21	CYS	ASN	engineered mutation	UNP P12497
B	22	CYS	ALA	engineered mutation	UNP P12497
B	184	ALA	TRP	engineered mutation	UNP P12497
B	185	ALA	MET	engineered mutation	UNP P12497
C	21	CYS	ASN	engineered mutation	UNP P12497

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Chain	Residue	Modelled	Actual	Comment	Reference
C	22	CYS	ALA	engineered mutation	UNP P12497
C	184	ALA	TRP	engineered mutation	UNP P12497
C	185	ALA	MET	engineered mutation	UNP P12497
D	21	CYS	ASN	engineered mutation	UNP P12497
D	22	CYS	ALA	engineered mutation	UNP P12497
D	184	ALA	TRP	engineered mutation	UNP P12497
D	185	ALA	MET	engineered mutation	UNP P12497
E	21	CYS	ASN	engineered mutation	UNP P12497
E	22	CYS	ALA	engineered mutation	UNP P12497
E	184	ALA	TRP	engineered mutation	UNP P12497
E	185	ALA	MET	engineered mutation	UNP P12497
F	21	CYS	ASN	engineered mutation	UNP P12497
F	22	CYS	ALA	engineered mutation	UNP P12497
F	184	ALA	TRP	engineered mutation	UNP P12497
F	185	ALA	MET	engineered mutation	UNP P12497
G	21	CYS	ASN	engineered mutation	UNP P12497
G	22	CYS	ALA	engineered mutation	UNP P12497
G	184	ALA	TRP	engineered mutation	UNP P12497
G	185	ALA	MET	engineered mutation	UNP P12497
H	21	CYS	ASN	engineered mutation	UNP P12497
H	22	CYS	ALA	engineered mutation	UNP P12497
H	184	ALA	TRP	engineered mutation	UNP P12497
H	185	ALA	MET	engineered mutation	UNP P12497
I	21	CYS	ASN	engineered mutation	UNP P12497
I	22	CYS	ALA	engineered mutation	UNP P12497
I	184	ALA	TRP	engineered mutation	UNP P12497
I	185	ALA	MET	engineered mutation	UNP P12497
J	21	CYS	ASN	engineered mutation	UNP P12497
J	22	CYS	ALA	engineered mutation	UNP P12497
J	184	ALA	TRP	engineered mutation	UNP P12497
J	185	ALA	MET	engineered mutation	UNP P12497

- Molecule 2 is N-[(1S)-1-{(3M)-3-{4-chloro-3-[(cyclopropanesulfonyl)amino]-1-(2,2-difluoroethyl)-1H-indazol-7-yl}-6-[3-(methanesulfonyl)-3-methylbut-1-yn-1-yl]pyridin-2-yl}-2-(3,5-difluorophenyl)ethyl]-2-[(3bS,4aR)-3-(difluoromethyl)-5,5-difluoro-3b,4,4a,5-tetrahydro-1H-cyclopropa[3,4]cyclopenta[1,2-c]pyrazol-1-yl]acetamide (three-letter code: A1AAO) (formula: C₄₁H₃₆ClF₈N₇O₅S₂) (labeled as "Ligand of Interest" by depositor).

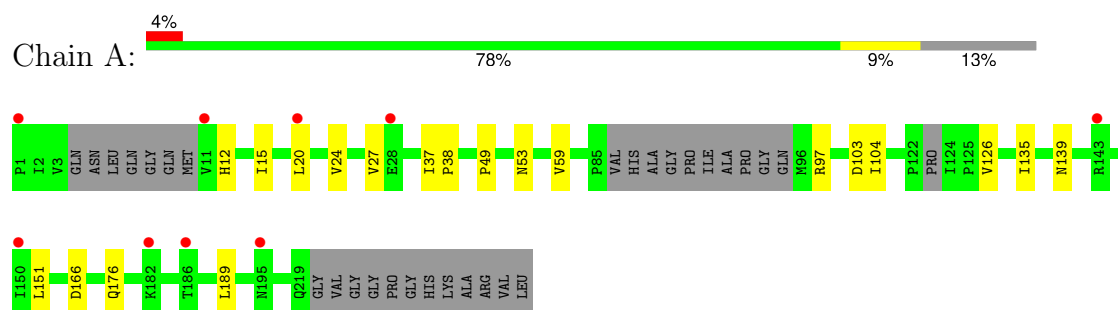


Mol	Chain	Residues	Atoms								ZeroOcc	AltConf
2	A	1	Total	C	Cl	F	H	N	O	S	0	0
			100	41	1	8	36	7	5	2		
2	B	1	Total	C	Cl	F	H	N	O	S	0	0
			100	41	1	8	36	7	5	2		
2	C	1	Total	C	Cl	F	H	N	O	S	0	0
			100	41	1	8	36	7	5	2		
2	D	1	Total	C	Cl	F	H	N	O	S	0	0
			100	41	1	8	36	7	5	2		
2	E	1	Total	C	Cl	F	H	N	O	S	0	0
			100	41	1	8	36	7	5	2		
2	F	1	Total	C	Cl	F	H	N	O	S	0	0
			100	41	1	8	36	7	5	2		
2	G	1	Total	C	Cl	F	H	N	O	S	0	0
			100	41	1	8	36	7	5	2		
2	H	1	Total	C	Cl	F	H	N	O	S	0	0
			100	41	1	8	36	7	5	2		
2	I	1	Total	C	Cl	F	H	N	O	S	0	0
			100	41	1	8	36	7	5	2		
2	J	1	Total	C	Cl	F	H	N	O	S	0	0
			100	41	1	8	36	7	5	2		

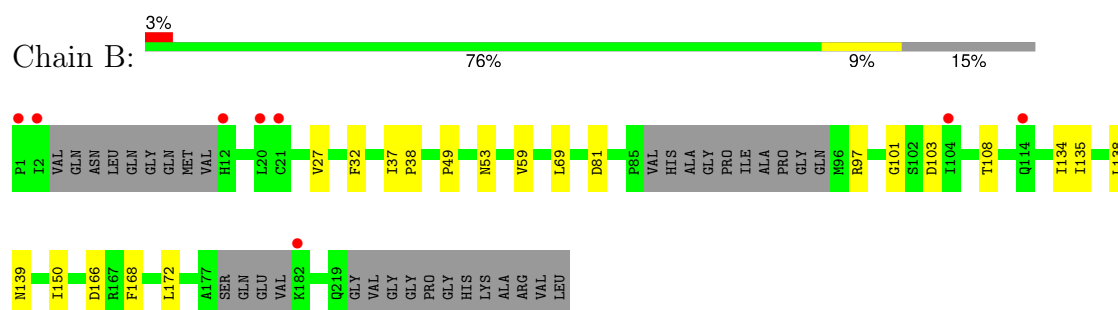
3 Residue-property plots [i](#)

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.

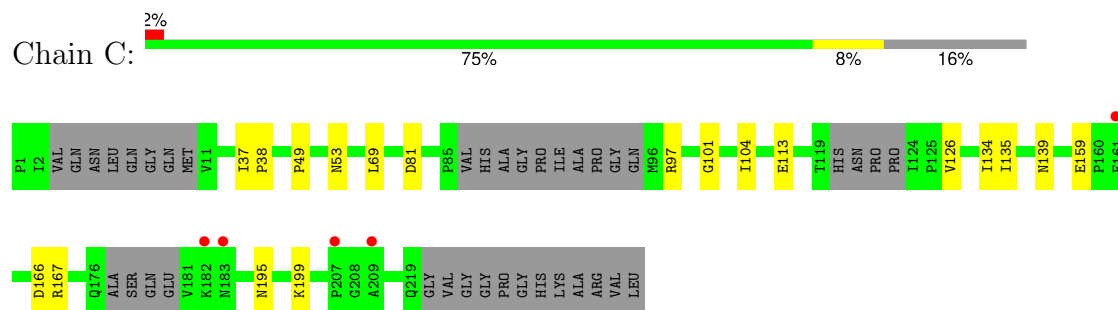
- Molecule 1: Capsid protein p24



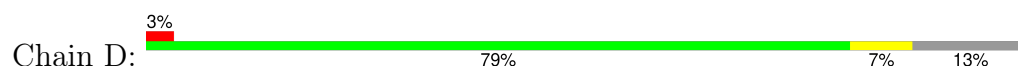
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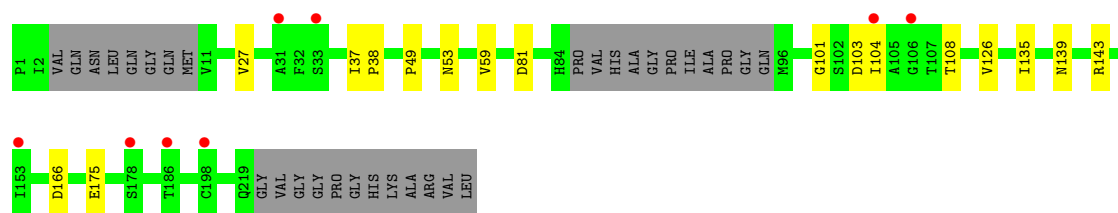


- Molecule 1: Capsid protein p24

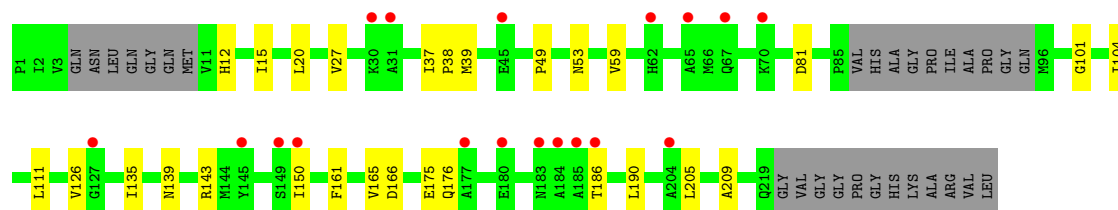
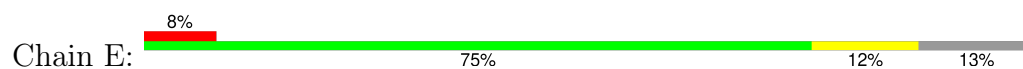


- Molecule 1: Capsid protein p24

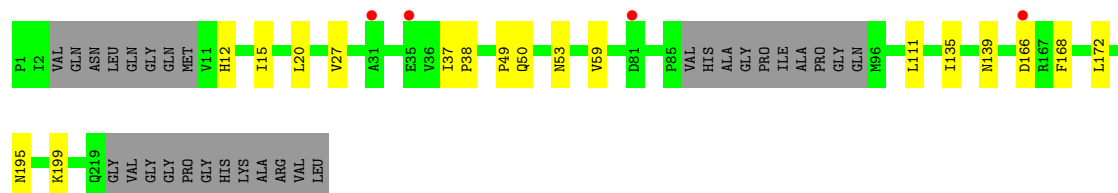
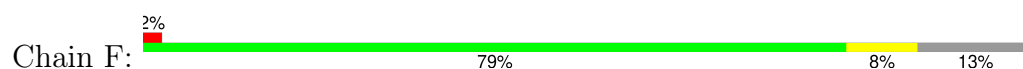




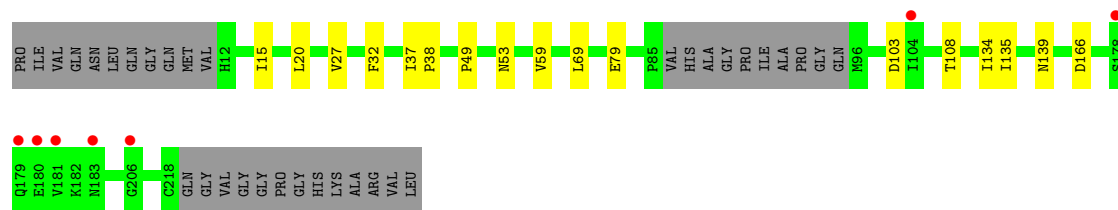
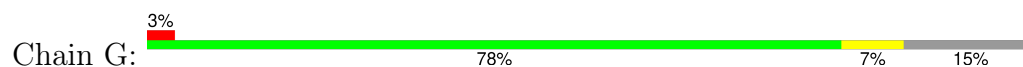
• Molecule 1: Capsid protein p24



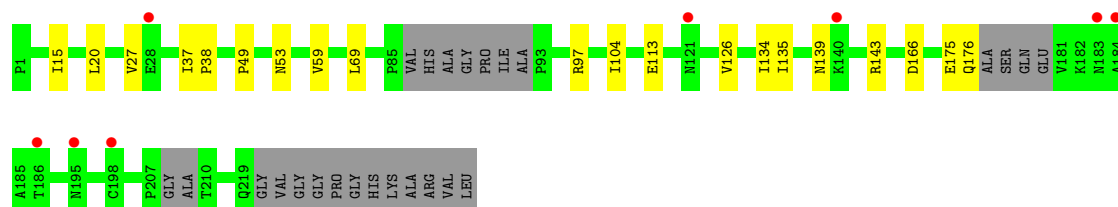
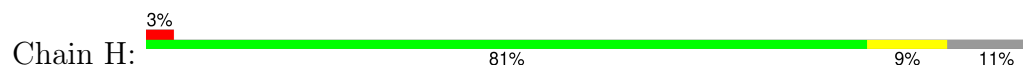
• Molecule 1: Capsid protein p24



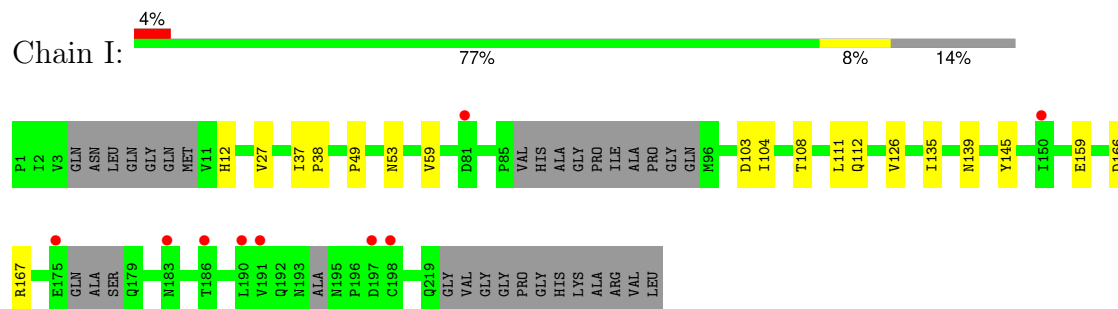
• Molecule 1: Capsid protein p24



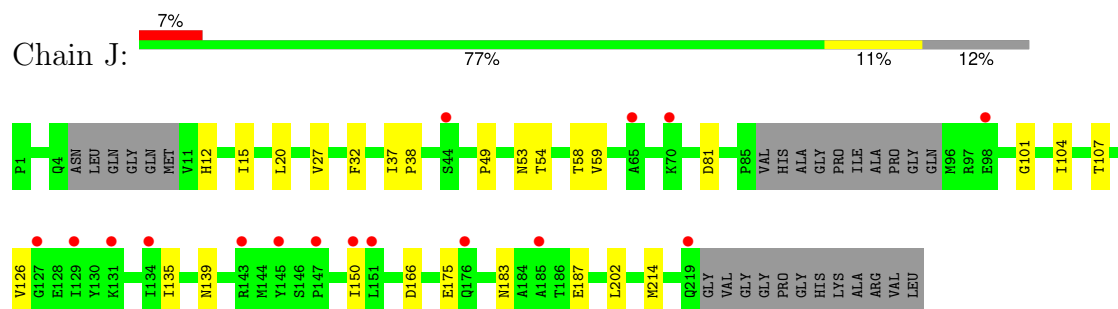
• Molecule 1: Capsid protein p24



● Molecule 1: Capsid protein p24



● Molecule 1: Capsid protein p24



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	137.40Å 149.46Å 157.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.18 – 3.46 42.18 – 3.46	Depositor EDS
% Data completeness (in resolution range)	57.8 (42.18-3.46) 58.0 (42.18-3.46)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.56 (at 3.48Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.257 , 0.315 0.257 , 0.314	Depositor DCC
R_{free} test set	2162 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å ²)	45.2	Xtriage
Anisotropy	1.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 20.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.029 for -h,l,k	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	28350	wwPDB-VP
Average B, all atoms (Å ²)	44.0	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 38.61 % 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 3.5912e-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: A1AAO

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	0.25	0/1491	0.45	0/2035
1	B	0.24	0/1418	0.44	0/1937
1	C	0.24	0/1340	0.42	0/1835
1	D	0.24	0/1437	0.43	0/1969
1	E	0.25	0/1533	0.45	0/2089
1	F	0.24	0/1488	0.44	0/2036
1	G	0.25	0/1421	0.44	0/1947
1	H	0.24	0/1507	0.44	0/2061
1	I	0.25	0/1439	0.44	0/1966
1	J	0.25	0/1549	0.46	0/2110
All	All	0.25	0/14623	0.44	0/19985

There are no bond length outliers.

There are no bond angle outliers.

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	1461	1344	1344	13	0
1	B	1388	1249	1249	12	0
1	C	1315	1101	1101	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1408	1245	1245	8	0
1	E	1501	1433	1433	14	0
1	F	1457	1365	1365	10	0
1	G	1392	1265	1265	7	0
1	H	1475	1321	1321	10	0
1	I	1409	1256	1256	11	0
1	J	1517	1448	1448	12	0
2	A	64	36	0	0	0
2	B	64	36	0	0	0
2	C	64	36	0	0	0
2	D	64	36	0	0	0
2	E	64	36	0	0	0
2	F	64	36	0	0	0
2	G	64	36	0	0	0
2	H	64	36	0	0	0
2	I	64	36	0	0	0
2	J	64	36	0	1	0
All	All	14963	13387	13027	107	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.

The worst 5 of 107 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:D:27:VAL:HG11	1:D:59:VAL:HG13	1.55	0.88
1:I:27:VAL:HG11	1:I:59:VAL:HG13	1.59	0.83
1:B:150:ILE:HG21	1:B:172:LEU:HD23	1.62	0.81
1:D:81:ASP:OD1	1:D:101:GLY:N	2.15	0.79
1:F:12:HIS:NE2	1:F:111:LEU:HD21	1.98	0.78

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	193/231 (84%)	186 (96%)	7 (4%)	0	100	100
1	B	188/231 (81%)	181 (96%)	7 (4%)	0	100	100
1	C	183/231 (79%)	175 (96%)	8 (4%)	0	100	100
1	D	194/231 (84%)	186 (96%)	8 (4%)	0	100	100
1	E	196/231 (85%)	187 (95%)	9 (5%)	0	100	100
1	F	195/231 (84%)	186 (95%)	9 (5%)	0	100	100
1	G	193/231 (84%)	181 (94%)	12 (6%)	0	100	100
1	H	198/231 (86%)	187 (94%)	11 (6%)	0	100	100
1	I	188/231 (81%)	181 (96%)	7 (4%)	0	100	100
1	J	197/231 (85%)	187 (95%)	10 (5%)	0	100	100
All	All	1925/2310 (83%)	1837 (95%)	88 (5%)	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	141/193 (73%)	140 (99%)	1 (1%)	81	89
1	B	125/193 (65%)	124 (99%)	1 (1%)	79	87
1	C	108/193 (56%)	107 (99%)	1 (1%)	75	86
1	D	127/193 (66%)	126 (99%)	1 (1%)	79	87
1	E	152/193 (79%)	150 (99%)	2 (1%)	65	81
1	F	142/193 (74%)	141 (99%)	1 (1%)	81	89
1	G	128/193 (66%)	125 (98%)	3 (2%)	45	71
1	H	136/193 (70%)	134 (98%)	2 (2%)	60	78
1	I	127/193 (66%)	125 (98%)	2 (2%)	58	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	J	154/193 (80%)	150 (97%)	4 (3%)	41 68
All	All	1340/1930 (69%)	1322 (99%)	18 (1%)	65 81

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	32	PHE
1	J	187	GLU
1	J	183	ASN
1	G	79	GLU
1	I	166	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

10 ligands are modelled in this entry.

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
2	A1AAO	I	301	-	56,71,71	0.96	1 (1%)	61,113,113	1.25	7 (11%)
2	A1AAO	C	301	-	56,71,71	0.99	2 (3%)	61,113,113	1.21	7 (11%)
2	A1AAO	H	301	-	56,71,71	1.00	2 (3%)	61,113,113	1.21	7 (11%)
2	A1AAO	E	301	-	56,71,71	0.98	2 (3%)	61,113,113	1.26	6 (9%)
2	A1AAO	J	301	-	56,71,71	0.97	1 (1%)	61,113,113	1.24	7 (11%)
2	A1AAO	G	301	-	56,71,71	0.98	2 (3%)	61,113,113	1.20	6 (9%)
2	A1AAO	D	301	-	56,71,71	0.97	1 (1%)	61,113,113	1.25	8 (13%)
2	A1AAO	A	301	-	56,71,71	0.97	2 (3%)	61,113,113	1.22	7 (11%)
2	A1AAO	B	301	-	56,71,71	0.97	2 (3%)	61,113,113	1.23	7 (11%)
2	A1AAO	F	301	-	56,71,71	0.97	2 (3%)	61,113,113	1.23	6 (9%)

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
2	A1AAO	I	301	-	-	3/38/77/77	0/8/8/8
2	A1AAO	C	301	-	-	4/38/77/77	0/8/8/8
2	A1AAO	H	301	-	-	4/38/77/77	0/8/8/8
2	A1AAO	E	301	-	-	3/38/77/77	0/8/8/8
2	A1AAO	J	301	-	-	6/38/77/77	0/8/8/8
2	A1AAO	G	301	-	-	4/38/77/77	0/8/8/8
2	A1AAO	D	301	-	-	4/38/77/77	0/8/8/8
2	A1AAO	A	301	-	-	4/38/77/77	0/8/8/8
2	A1AAO	B	301	-	-	4/38/77/77	0/8/8/8
2	A1AAO	F	301	-	-	5/38/77/77	0/8/8/8

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	301	A1AAO	C72-C71	-2.29	1.39	1.43
2	A	301	A1AAO	C72-C71	-2.24	1.39	1.43
2	F	301	A1AAO	C72-C71	-2.20	1.40	1.43
2	G	301	A1AAO	C72-C71	-2.17	1.40	1.43
2	E	301	A1AAO	C79-N77	-2.15	1.43	1.47

The worst 5 of 68 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	301	A1AAO	C5-N7-N6	4.43	108.30	104.48
2	I	301	A1AAO	C5-N7-N6	4.35	108.23	104.48
2	E	301	A1AAO	C5-N7-N6	4.35	108.23	104.48
2	J	301	A1AAO	C5-N7-N6	4.32	108.21	104.48
2	B	301	A1AAO	C5-N7-N6	4.23	108.13	104.48

There are no chirality outliers.

5 of 41 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	A1AAO	C50-C53-S56-O58
2	A	301	A1AAO	C76-N83-S89-O93
2	B	301	A1AAO	C50-C53-S56-O58
2	B	301	A1AAO	C76-N83-S89-O93
2	C	301	A1AAO	C50-C53-S56-O58

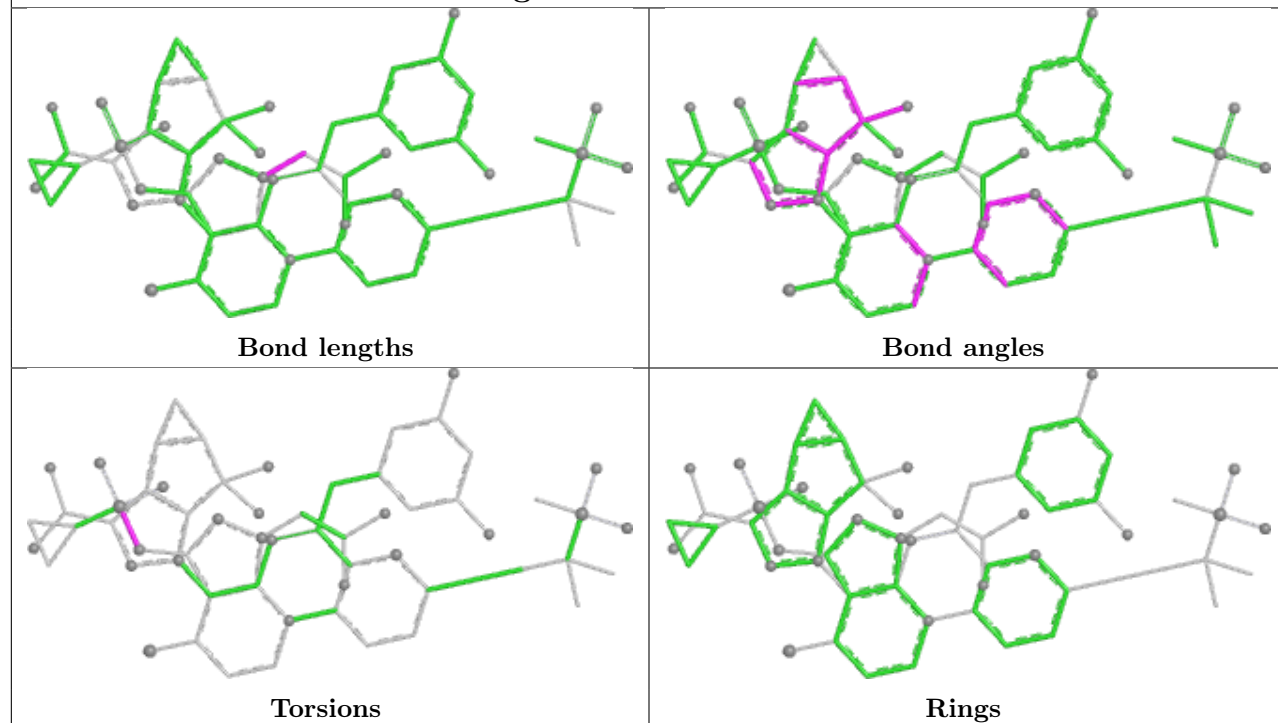
There are no ring outliers.

1 monomer is involved in 1 short contact:

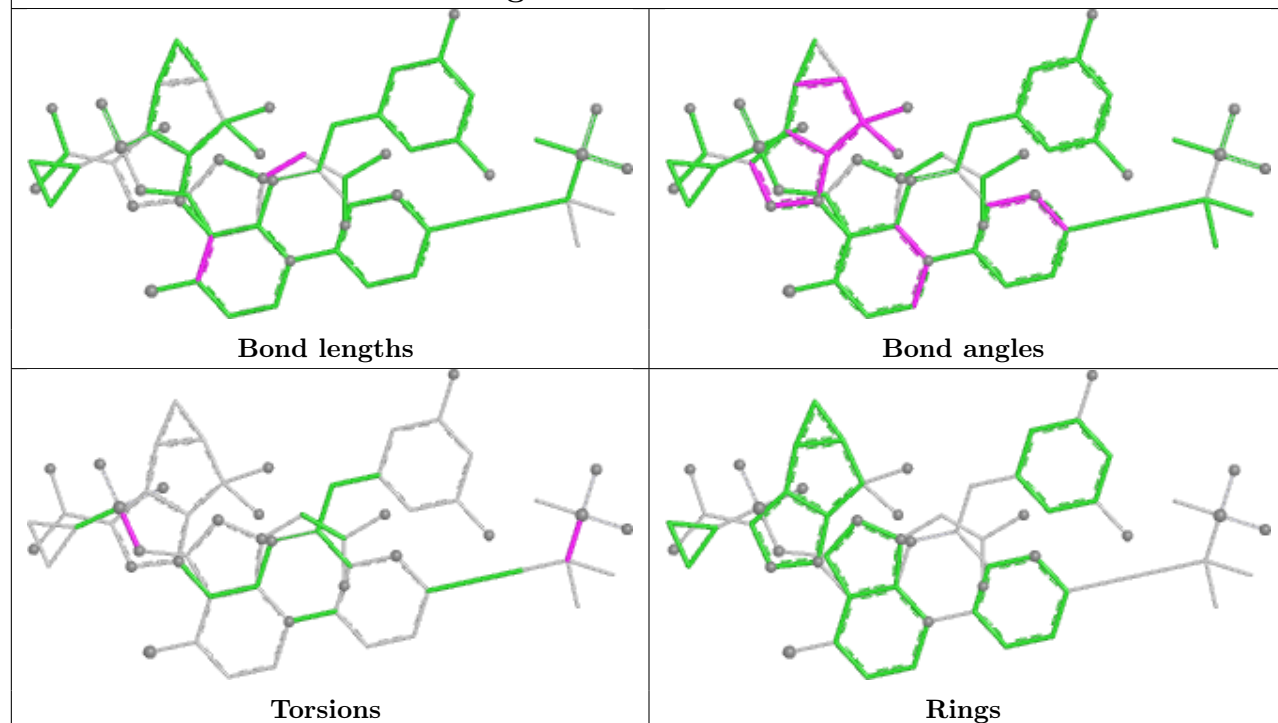
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	301	A1AAO	1	0

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.

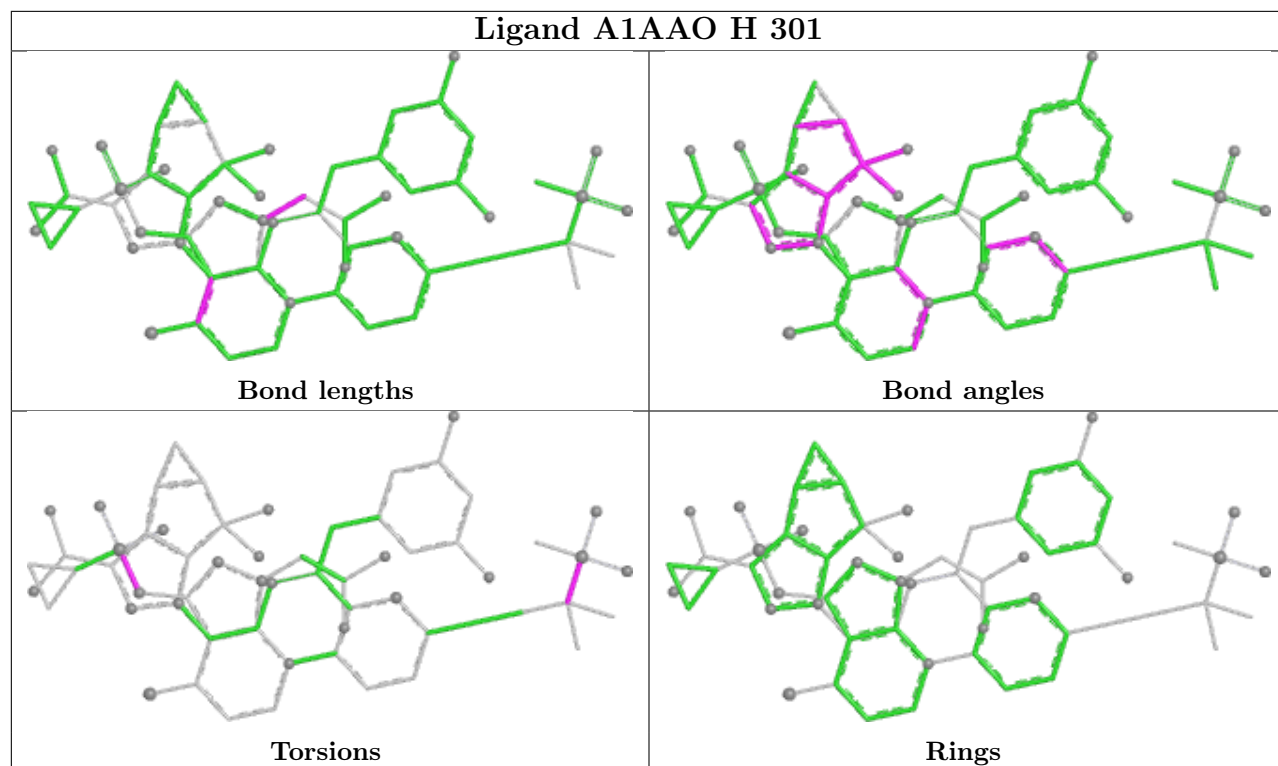
Ligand A1AAO I 301



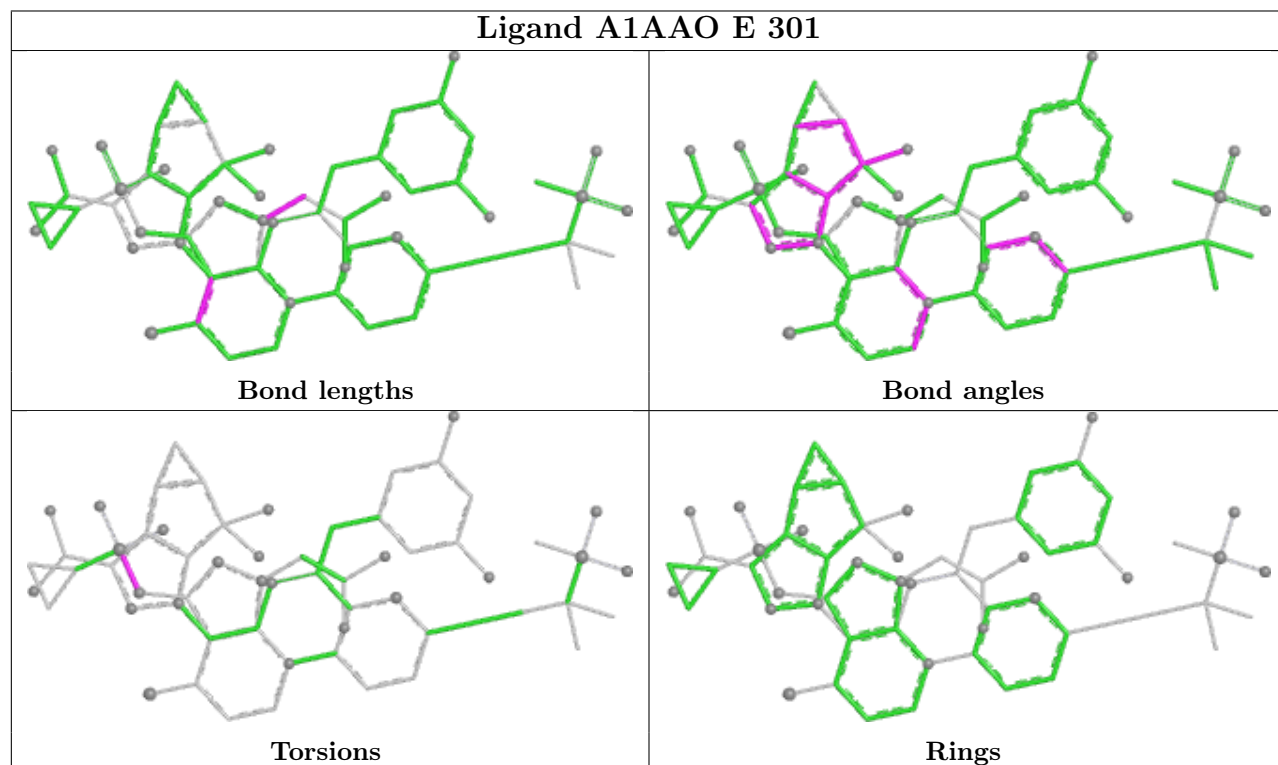
Ligand A1AAO C 301



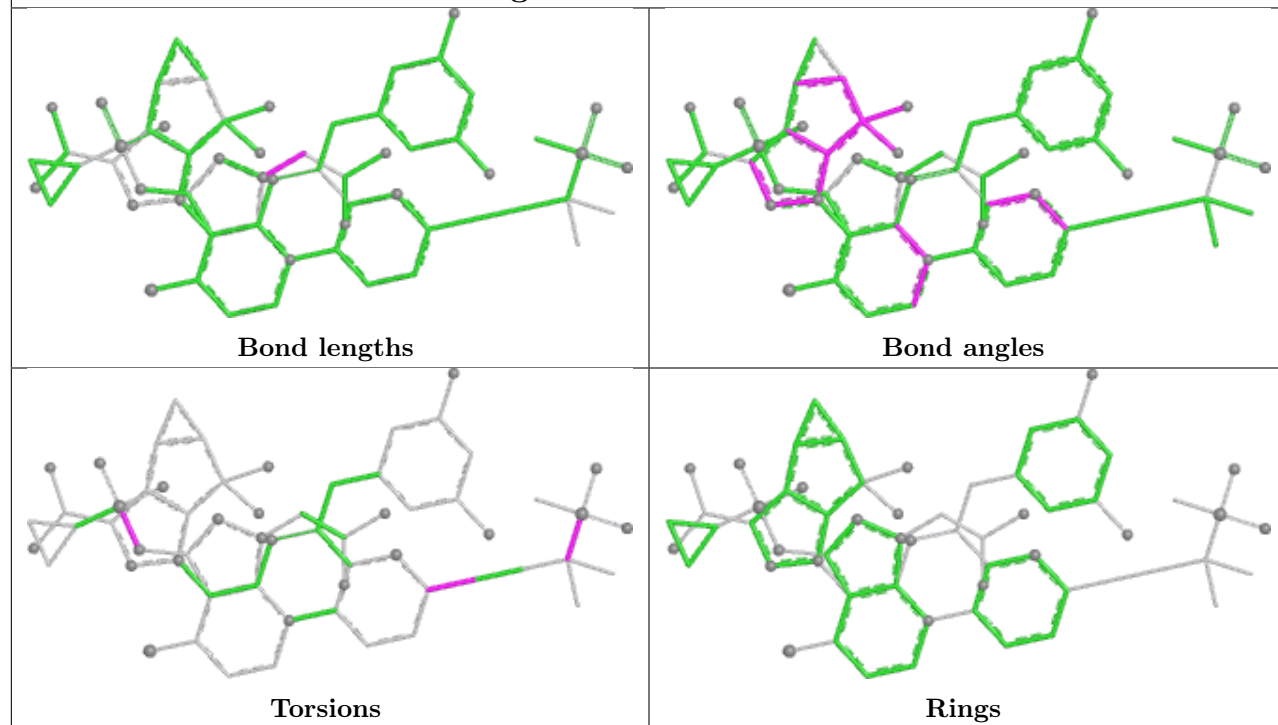
Ligand A1AAO H 301



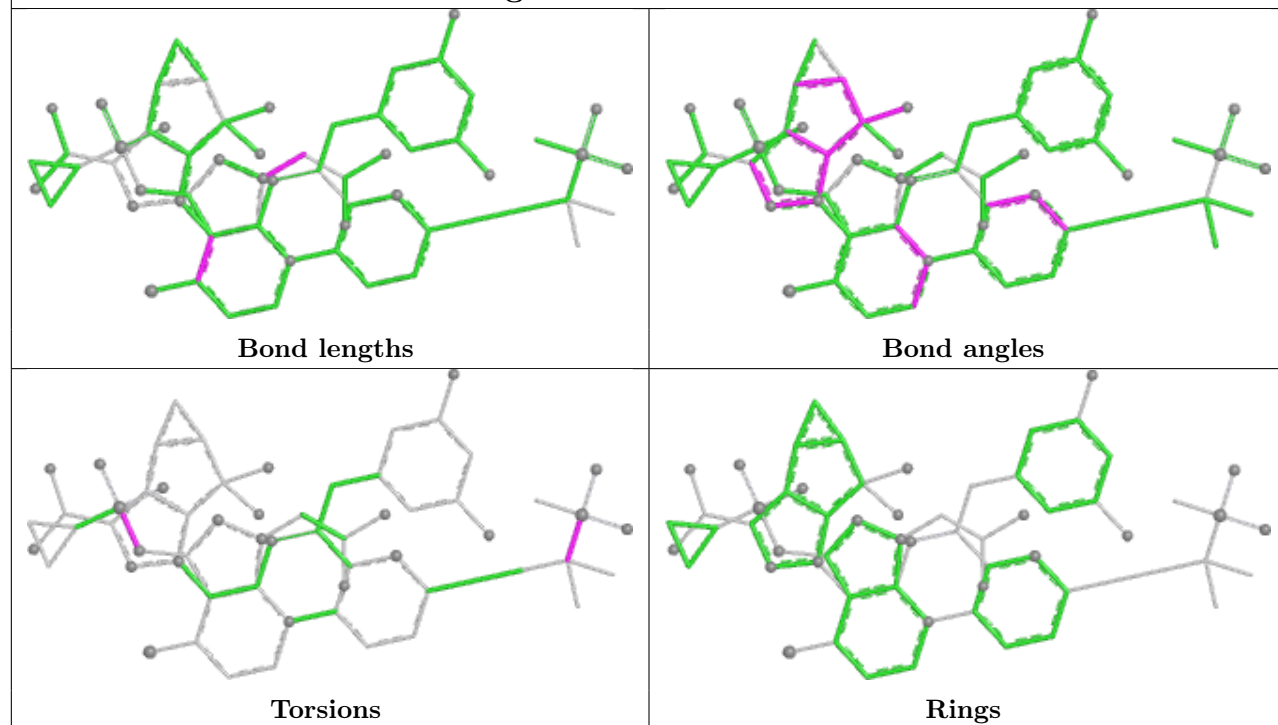
Ligand A1AAO E 301



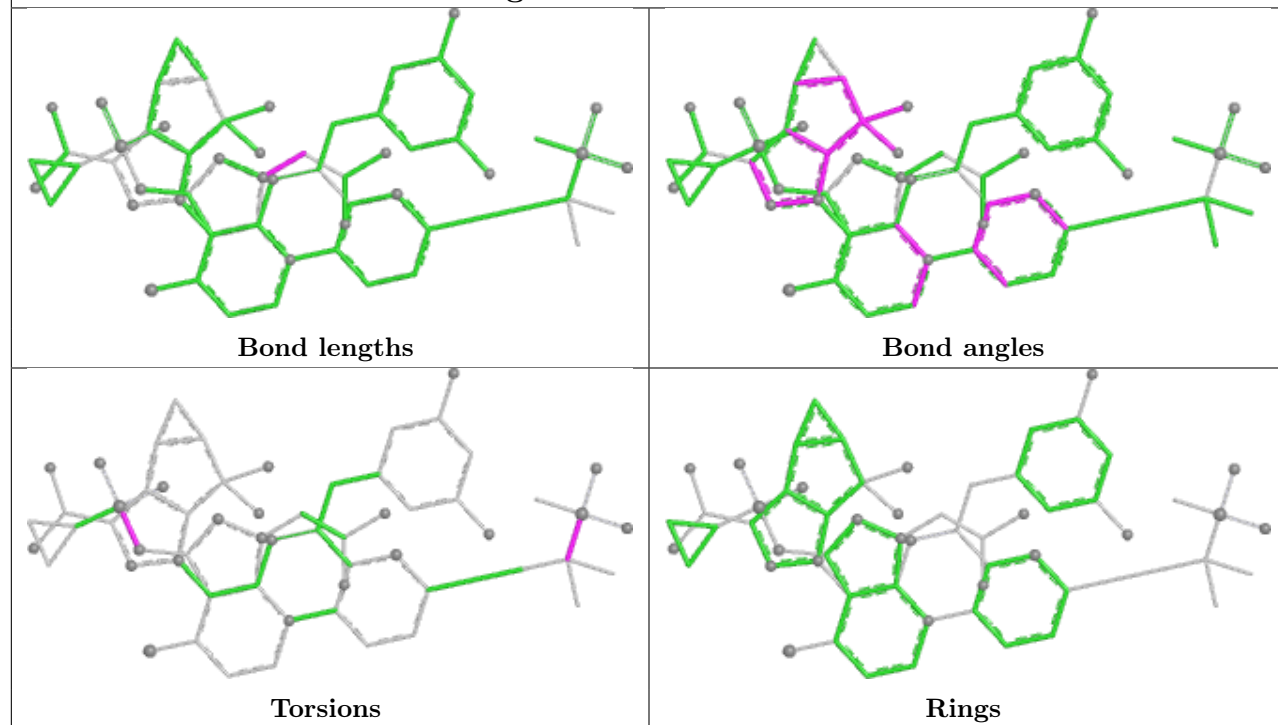
Ligand A1AAO J 301



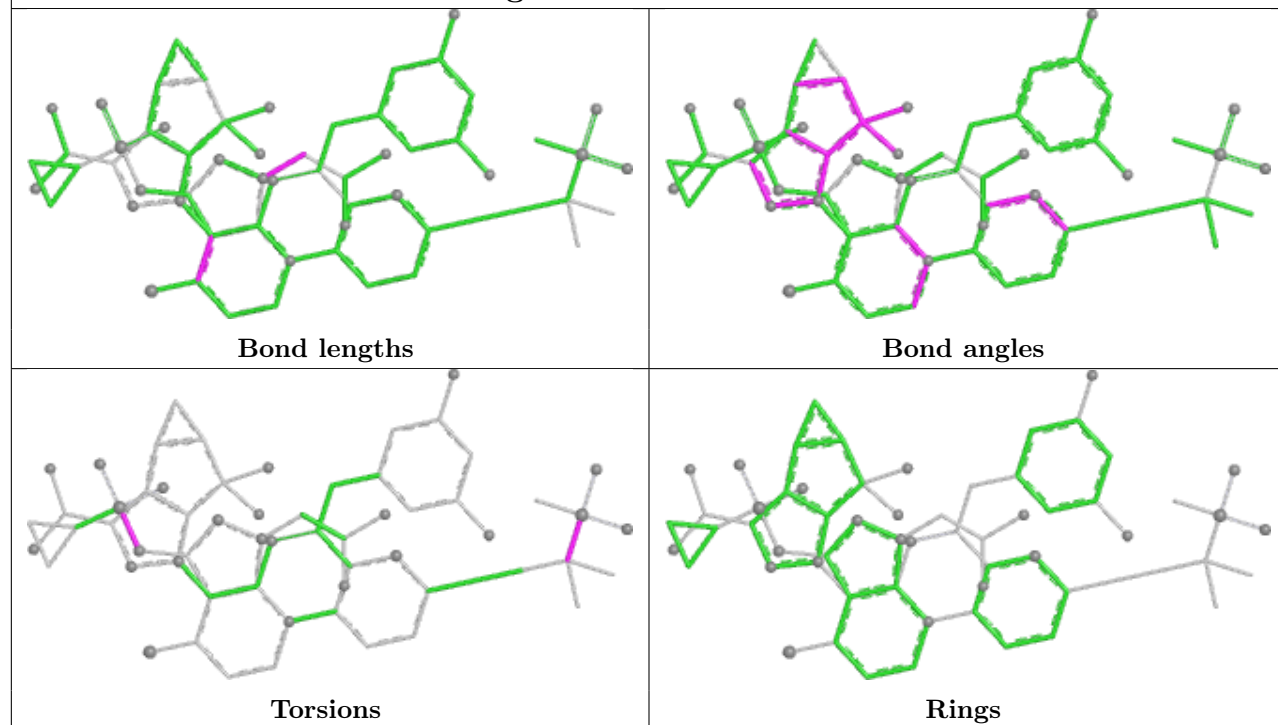
Ligand A1AAO G 301

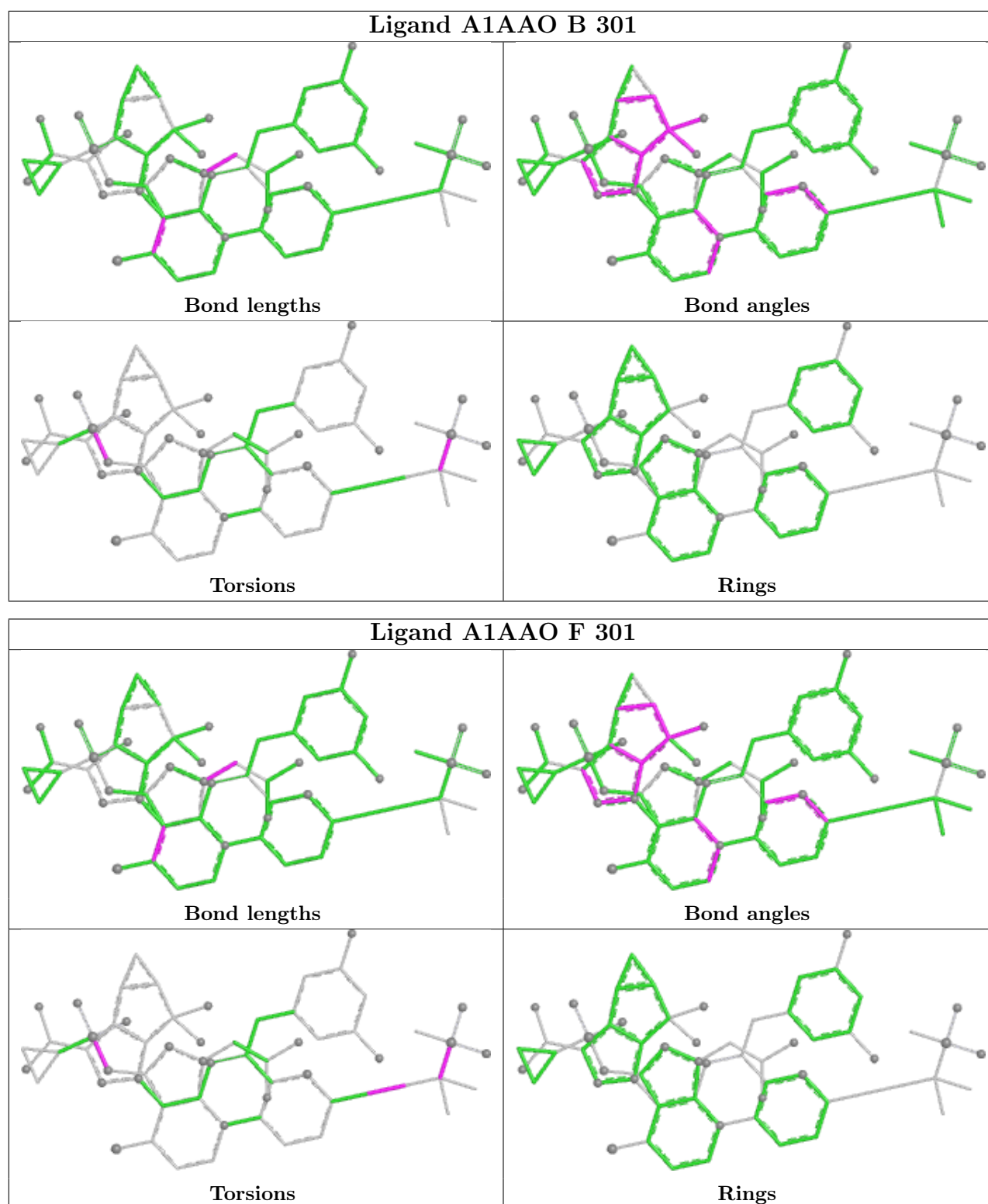


Ligand A1AAO D 301



Ligand A1AAO A 301





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	201/231 (87%)	0.29	9 (4%)	39	29	24, 44, 63, 79	0
1	B	196/231 (84%)	0.27	8 (4%)	42	31	28, 48, 68, 74	0
1	C	193/231 (83%)	0.24	5 (2%)	57	42	27, 49, 67, 75	0
1	D	200/231 (86%)	0.34	8 (4%)	43	32	27, 49, 62, 71	0
1	E	202/231 (87%)	0.46	18 (8%)	17	14	24, 40, 56, 67	0
1	F	201/231 (87%)	0.22	4 (1%)	64	48	25, 45, 65, 74	0
1	G	197/231 (85%)	0.28	7 (3%)	46	34	28, 48, 66, 78	0
1	H	206/231 (89%)	0.15	8 (3%)	44	33	26, 42, 65, 75	0
1	I	198/231 (85%)	0.27	9 (4%)	39	29	26, 44, 65, 73	0
1	J	203/231 (87%)	0.45	16 (7%)	20	17	25, 37, 55, 65	0
All	All	1997/2310 (86%)	0.30	92 (4%)	38	29	24, 44, 65, 79	0

The worst 5 of 92 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	179	GLN	5.5
1	G	183	ASN	4.4
1	D	186	THR	4.1
1	I	186	THR	4.0
1	A	143	ARG	3.8

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 monosaccharides in this entry.

6.4 Ligands [i](#)

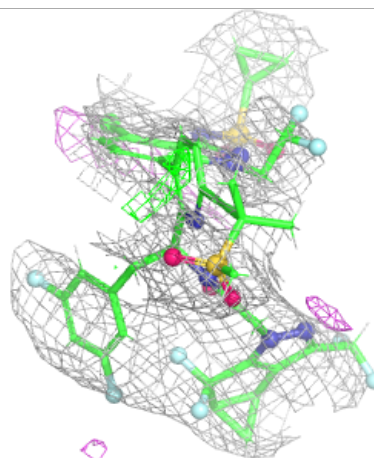
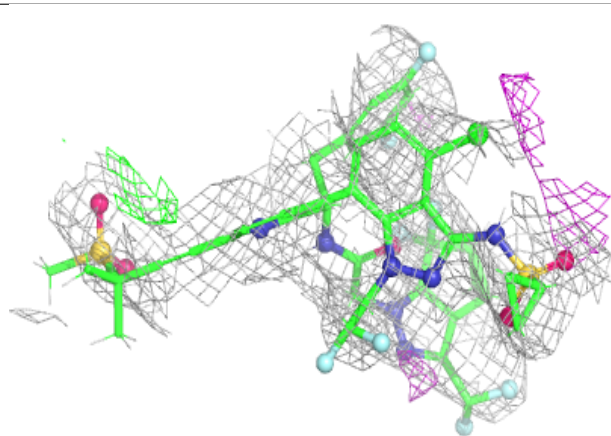
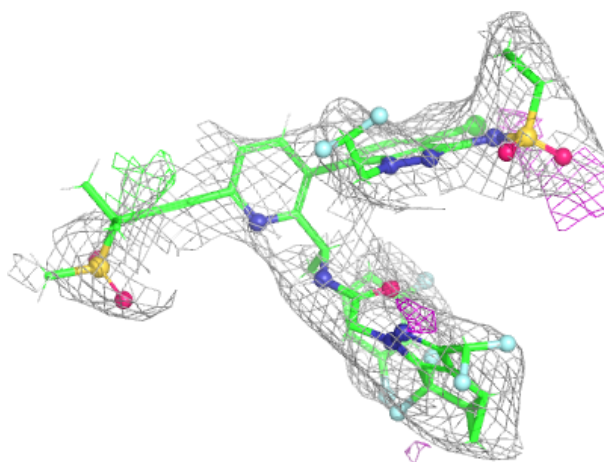
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	A1AAO	E	301	64/64	0.86	0.15	25,44,96,103	0
2	A1AAO	J	301	64/64	0.87	0.15	20,42,92,118	0
2	A1AAO	B	301	64/64	0.88	0.13	22,46,76,102	0
2	A1AAO	G	301	64/64	0.89	0.12	24,43,71,87	0
2	A1AAO	C	301	64/64	0.89	0.12	23,48,81,99	0
2	A1AAO	I	301	64/64	0.90	0.13	21,41,72,81	0
2	A1AAO	D	301	64/64	0.90	0.12	25,49,76,87	0
2	A1AAO	F	301	64/64	0.91	0.14	22,30,72,79	0
2	A1AAO	H	301	64/64	0.91	0.12	20,42,85,103	0
2	A1AAO	A	301	64/64	0.93	0.13	21,32,64,75	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.

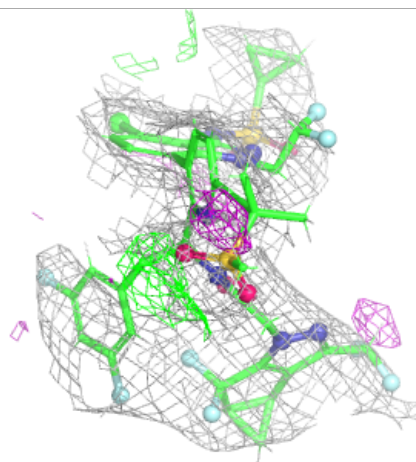
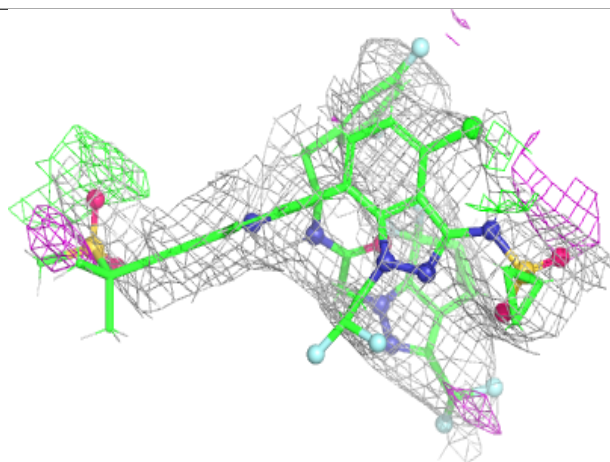
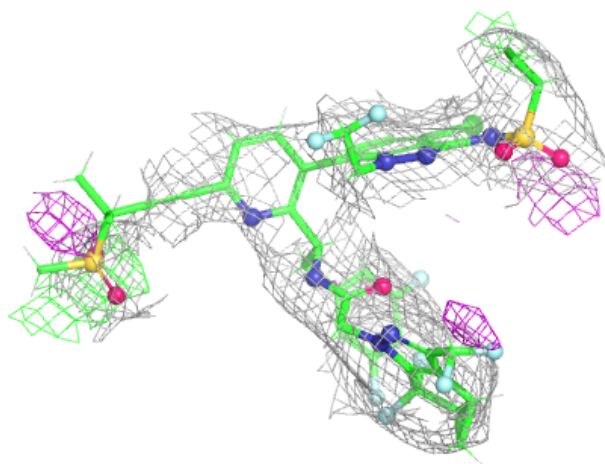
Electron density around A1AAO E 301:

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



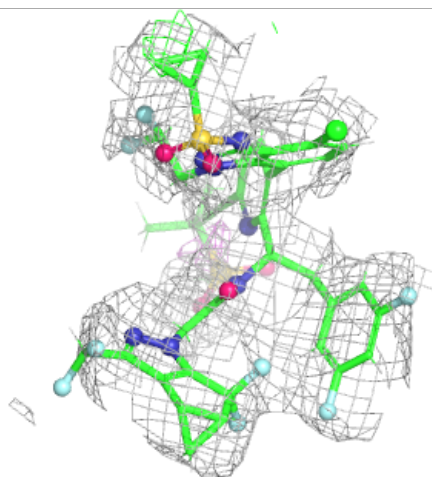
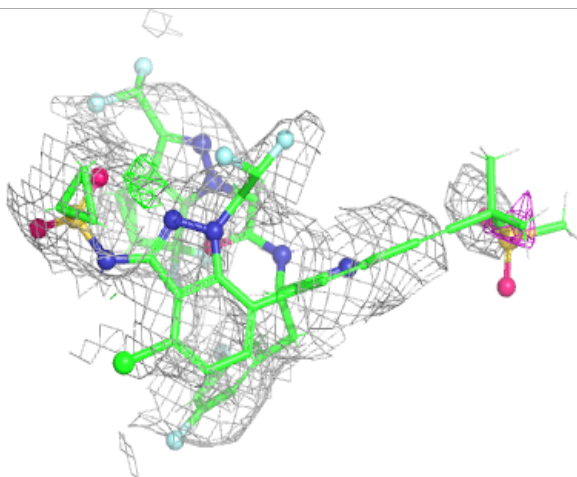
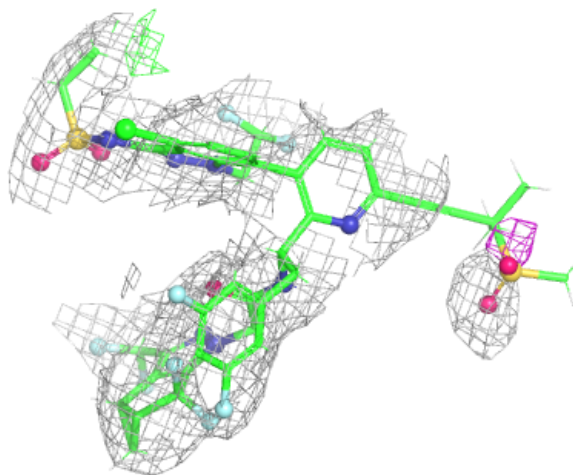
Electron density around A1AAO J 301:

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



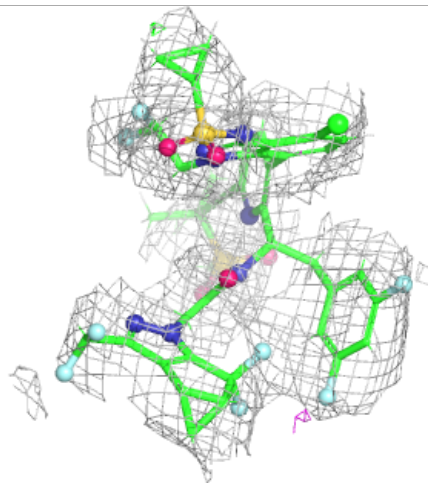
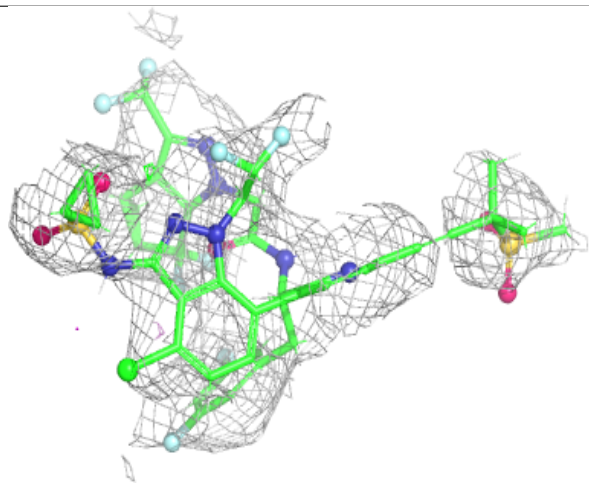
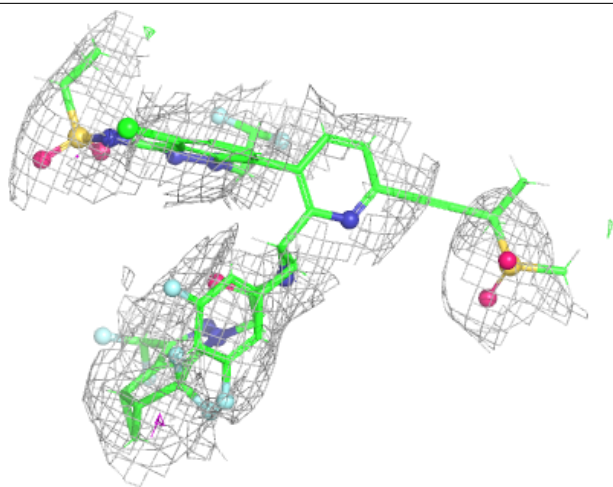
Electron density around A1AAO B 301:

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



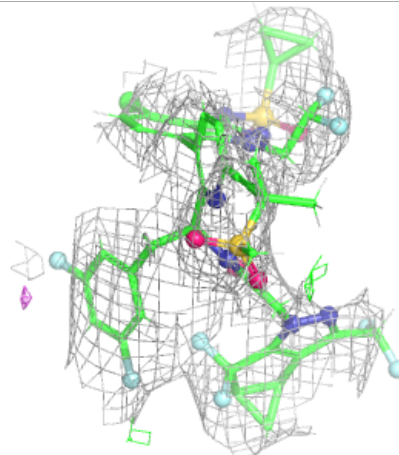
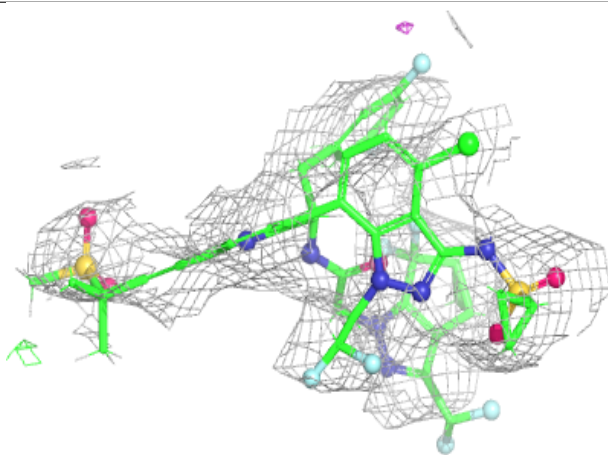
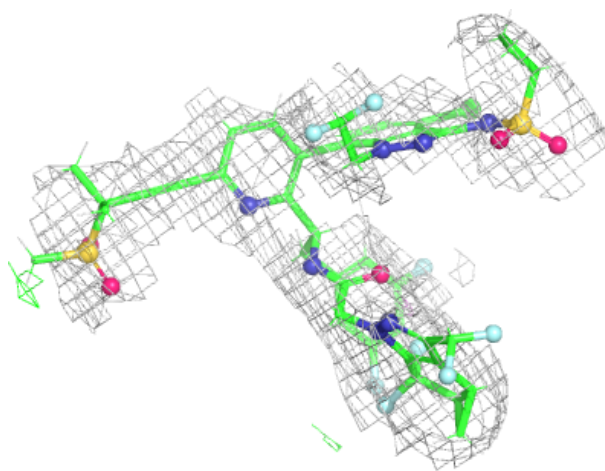
Electron density around A1AAO G 301:

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



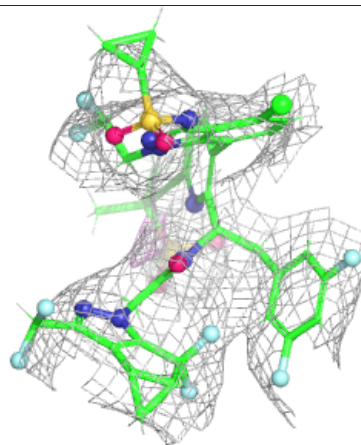
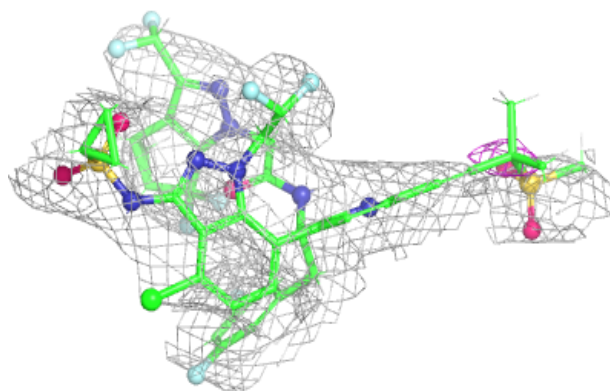
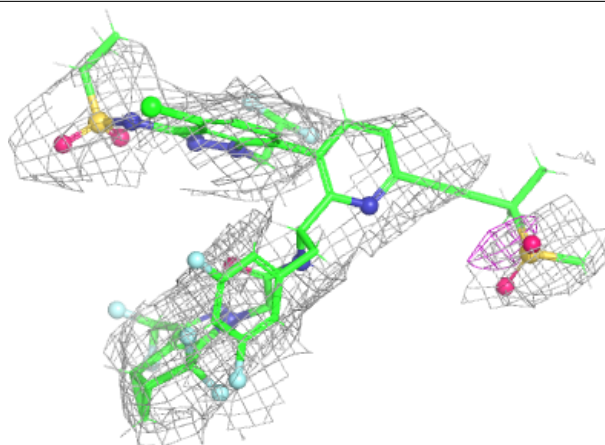
Electron density around A1AAO C 301:

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



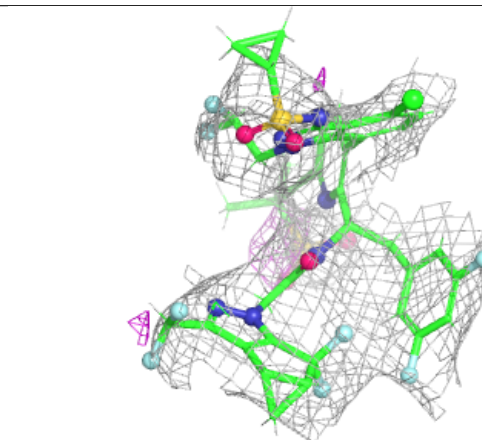
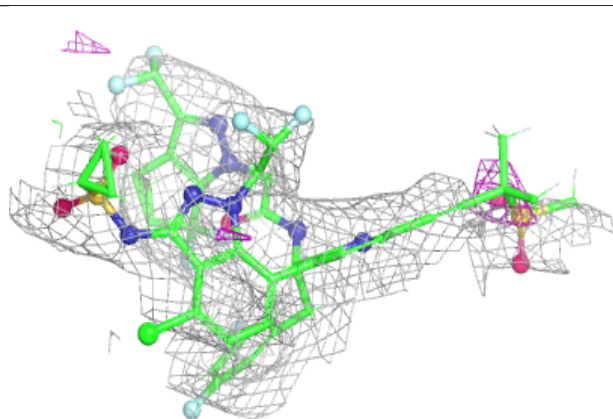
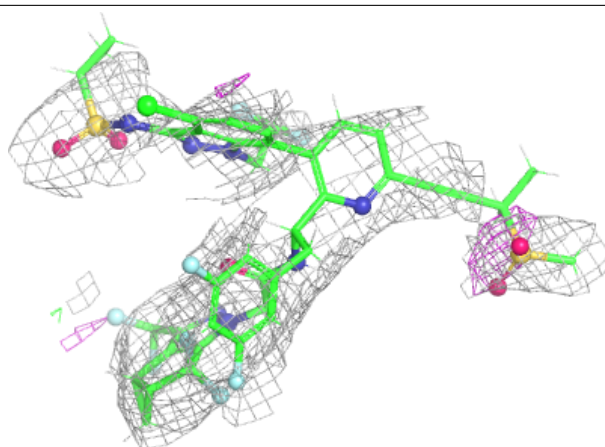
Electron density around A1AAO I 301:

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



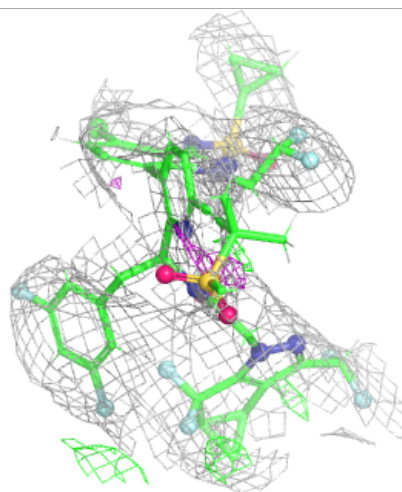
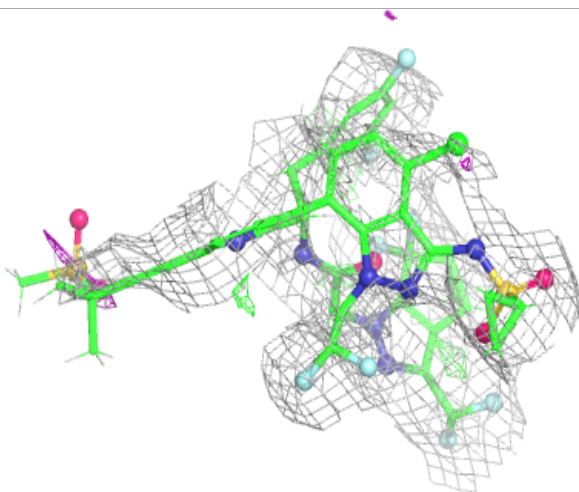
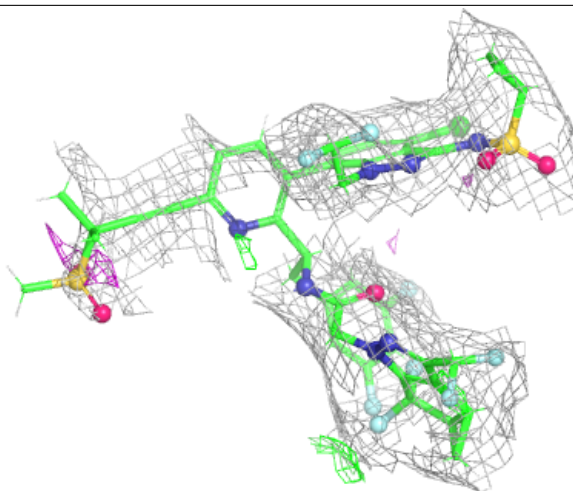
Electron density around A1AAO D 301:

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



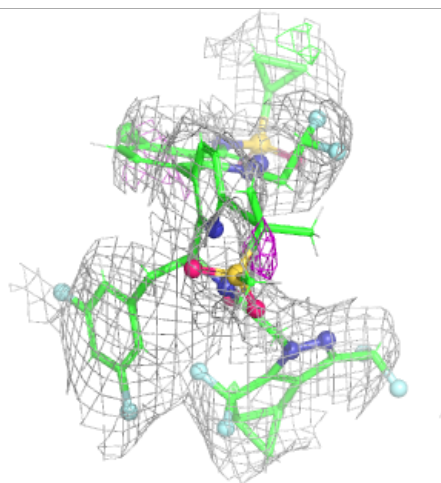
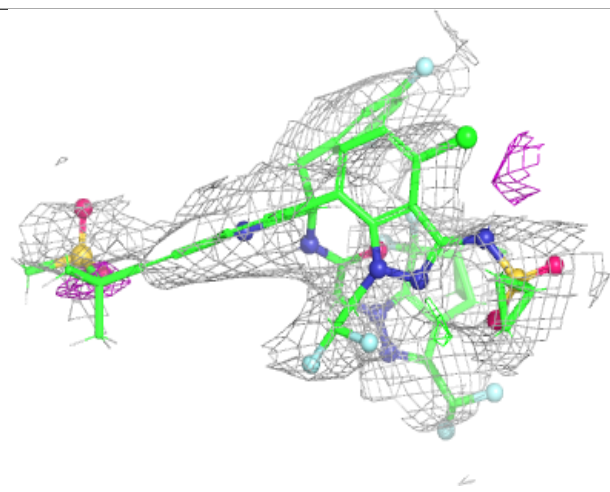
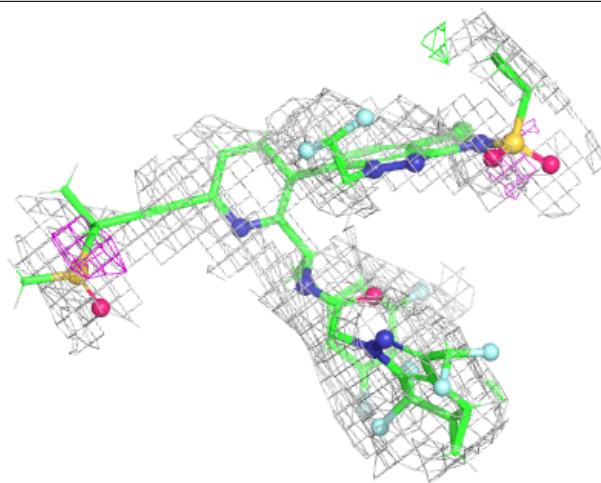
Electron density around A1AAO F 301:

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and green (positive)



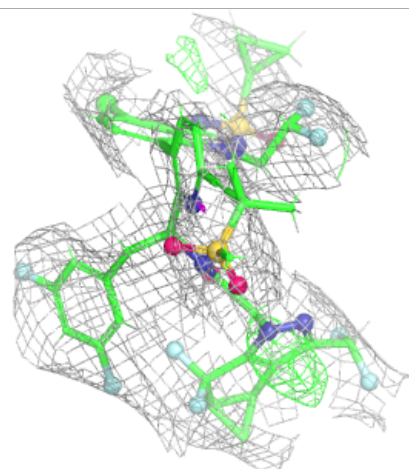
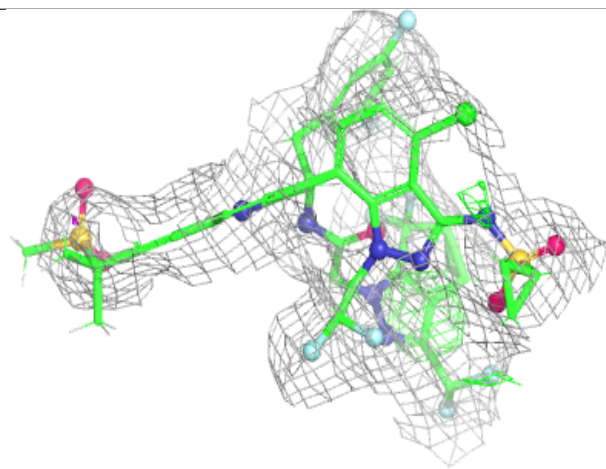
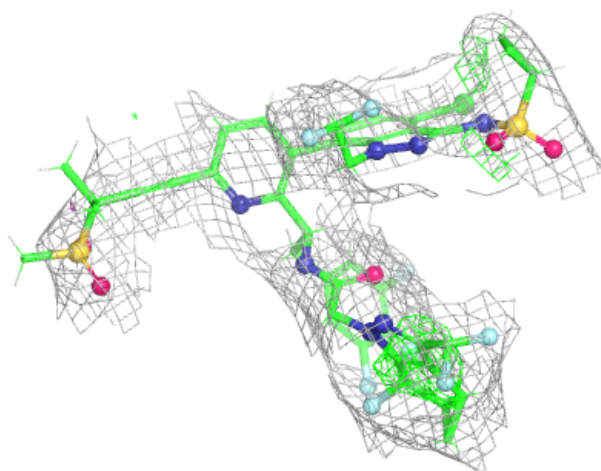
Electron density around A1AAO H 301:

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



Electron density around A1AAO A 301:

$2mF_o-DF_c$ (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.