



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 20, 2026 – 07:34 PM UTC

PDB ID : 3JSK / pdb_00003jsk
Title : Thiazole synthase from Neurospora crassa
Authors : Kang, Y.N.; Bale, S.; Ealick, S.E.
Deposited on : 2009-09-10
Resolution : 2.70 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 : 4-5-2 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

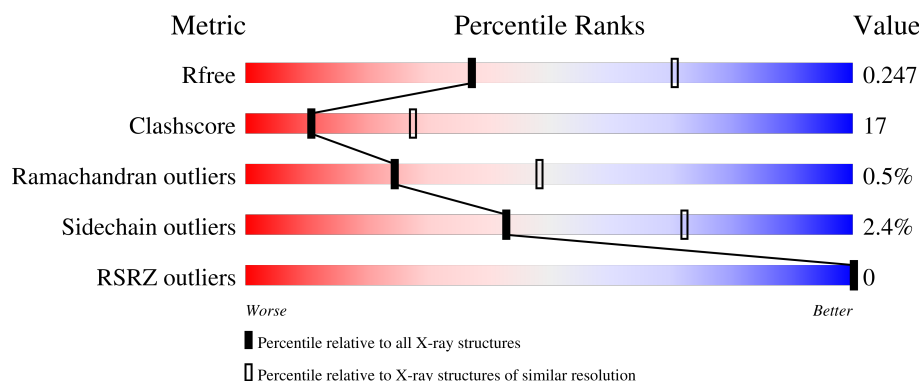
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	344	56% 25% • 15%
1	B	344	56% 26% • 15%
1	C	344	58% 24% • 15%
1	D	344	57% 25% • 15%
1	E	344	60% 22% • 15%

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Mol	Chain	Length	Quality of chain
1	F	344	
1	G	344	
1	H	344	
1	I	344	
1	J	344	
1	K	344	
1	L	344	
1	M	344	
1	N	344	
1	O	344	
1	P	344	

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
1	DHA	A	232	-	X	-	-
1	DHA	B	232	-	X	-	-
1	DHA	D	232	-	X	-	-
1	DHA	E	232	-	X	-	-
1	DHA	F	232	-	X	-	-
1	DHA	K	232	-	X	-	-
1	DHA	N	232	-	X	-	-
1	DHA	P	232	-	X	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 36053 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.

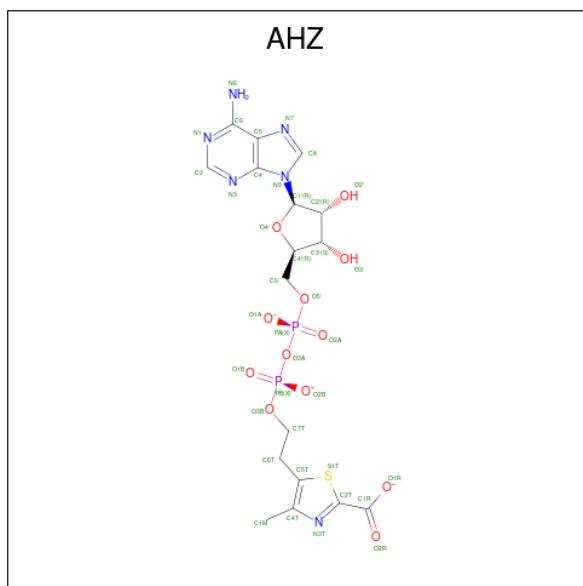
- Molecule 1 is a protein called CyPBP37 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	292	Total	C	N	O	S	0	0	0
			2193	1377	386	416	14			
1	B	291	Total	C	N	O	S	0	0	0
			2188	1374	385	415	14			
1	C	292	Total	C	N	O	S	0	0	0
			2193	1377	386	416	14			
1	D	292	Total	C	N	O	S	0	0	0
			2193	1377	386	416	14			
1	E	291	Total	C	N	O	S	0	0	0
			2188	1374	385	415	14			
1	F	292	Total	C	N	O	S	0	0	0
			2193	1377	386	416	14			
1	G	291	Total	C	N	O	S	0	0	0
			2188	1374	385	415	14			
1	H	291	Total	C	N	O	S	0	0	0
			2188	1374	385	415	14			
1	I	291	Total	C	N	O	S	0	0	0
			2188	1374	385	415	14			
1	J	291	Total	C	N	O	S	0	0	0
			2188	1374	385	415	14			
1	K	291	Total	C	N	O	S	0	0	0
			2188	1374	385	415	14			
1	L	291	Total	C	N	O	S	0	0	0
			2188	1374	385	415	14			
1	M	291	Total	C	N	O	S	0	0	0
			2188	1374	385	415	14			
1	N	292	Total	C	N	O	S	0	0	0
			2193	1377	386	416	14			
1	O	292	Total	C	N	O	S	0	0	0
			2193	1377	386	416	14			
1	P	291	Total	C	N	O	S	0	0	0
			2188	1374	385	415	14			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	232	DHA	CYS	engineered mutation	UNP Q9HGR2
B	232	DHA	CYS	engineered mutation	UNP Q9HGR2
C	232	DHA	CYS	engineered mutation	UNP Q9HGR2
D	232	DHA	CYS	engineered mutation	UNP Q9HGR2
E	232	DHA	CYS	engineered mutation	UNP Q9HGR2
F	232	DHA	CYS	engineered mutation	UNP Q9HGR2
G	232	DHA	CYS	engineered mutation	UNP Q9HGR2
H	232	DHA	CYS	engineered mutation	UNP Q9HGR2
I	232	DHA	CYS	engineered mutation	UNP Q9HGR2
J	232	DHA	CYS	engineered mutation	UNP Q9HGR2
K	232	DHA	CYS	engineered mutation	UNP Q9HGR2
L	232	DHA	CYS	engineered mutation	UNP Q9HGR2
M	232	DHA	CYS	engineered mutation	UNP Q9HGR2
N	232	DHA	CYS	engineered mutation	UNP Q9HGR2
O	232	DHA	CYS	engineered mutation	UNP Q9HGR2
P	232	DHA	CYS	engineered mutation	UNP Q9HGR2

- Molecule 2 is ADENOSINE DIPHOSPHATE 5-(BETA-ETHYL)-4-METHYL-THIAZOLE-2-CARBOXYLIC ACID (CCD ID: AHZ) (formula: C₁₇H₁₉N₆O₁₂P₂S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			38	17	6	12	2	1		
2	B	1	Total	C	N	O	P	S	0	0
			38	17	6	12	2	1		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	S	0	0
			38	17	6	12	2	1		
2	D	1	Total	C	N	O	P	S	0	0
			38	17	6	12	2	1		
2	E	1	Total	C	N	O	P	S	0	0
			38	17	6	12	2	1		
2	F	1	Total	C	N	O	P	S	0	0
			38	17	6	12	2	1		
2	G	1	Total	C	N	O	P	S	0	0
			38	17	6	12	2	1		
2	H	1	Total	C	N	O	P	S	0	0
			38	17	6	12	2	1		
2	I	1	Total	C	N	O	P	S	0	0
			38	17	6	12	2	1		
2	J	1	Total	C	N	O	P	S	0	0
			38	17	6	12	2	1		
2	K	1	Total	C	N	O	P	S	0	0
			38	17	6	12	2	1		
2	L	1	Total	C	N	O	P	S	0	0
			38	17	6	12	2	1		
2	M	1	Total	C	N	O	P	S	0	0
			38	17	6	12	2	1		
2	N	1	Total	C	N	O	P	S	0	0
			38	17	6	12	2	1		
2	O	1	Total	C	N	O	P	S	0	0
			38	17	6	12	2	1		
2	P	1	Total	C	N	O	P	S	0	0
			38	17	6	12	2	1		

- Molecule 3 is FE (II) ION (CCD ID: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Fe	0	0
			1	1		
3	B	1	Total	Fe	0	0
			1	1		
3	C	1	Total	Fe	0	0
			1	1		
3	D	1	Total	Fe	0	0
			1	1		
3	E	1	Total	Fe	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	F	1	Total 1	Fe 1	0	0
3	G	1	Total 1	Fe 1	0	0
3	H	1	Total 1	Fe 1	0	0
3	I	1	Total 1	Fe 1	0	0
3	J	1	Total 1	Fe 1	0	0
3	K	2	Total 2	Fe 2	0	0
3	L	1	Total 1	Fe 1	0	0
3	M	2	Total 2	Fe 2	0	0
3	N	1	Total 1	Fe 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	30	Total 30	O 30	0	0
4	B	16	Total 16	O 16	0	0
4	C	32	Total 32	O 32	0	0
4	D	21	Total 21	O 21	0	0
4	E	29	Total 29	O 29	0	0
4	F	24	Total 24	O 24	0	0
4	G	21	Total 21	O 21	0	0
4	H	23	Total 23	O 23	0	0
4	I	44	Total 44	O 44	0	0
4	J	20	Total 20	O 20	0	0

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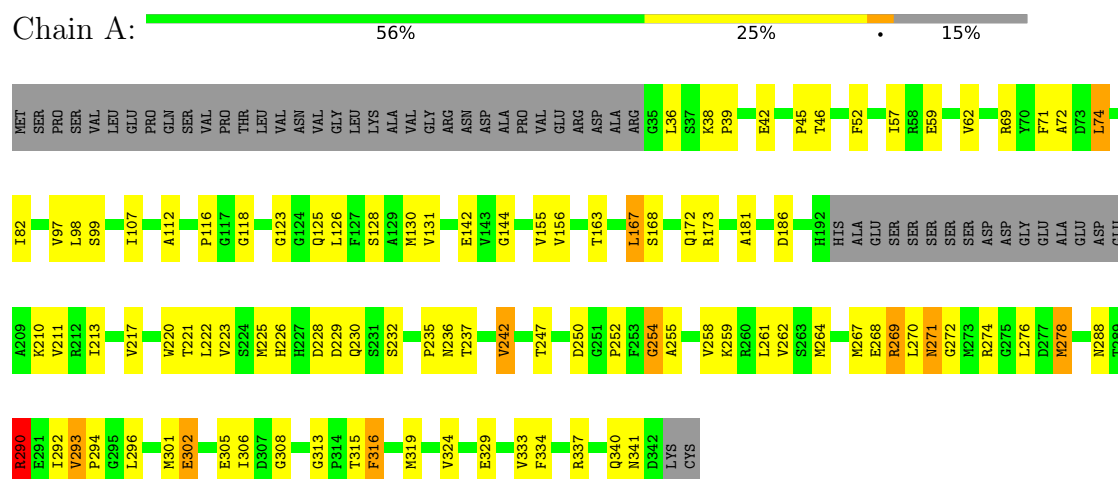
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	K	25	Total 25	O 25	0	0
4	L	21	Total 21	O 21	0	0
4	M	19	Total 19	O 19	0	0
4	N	17	Total 17	O 17	0	0
4	O	25	Total 25	O 25	0	0
4	P	24	Total 24	O 24	0	0

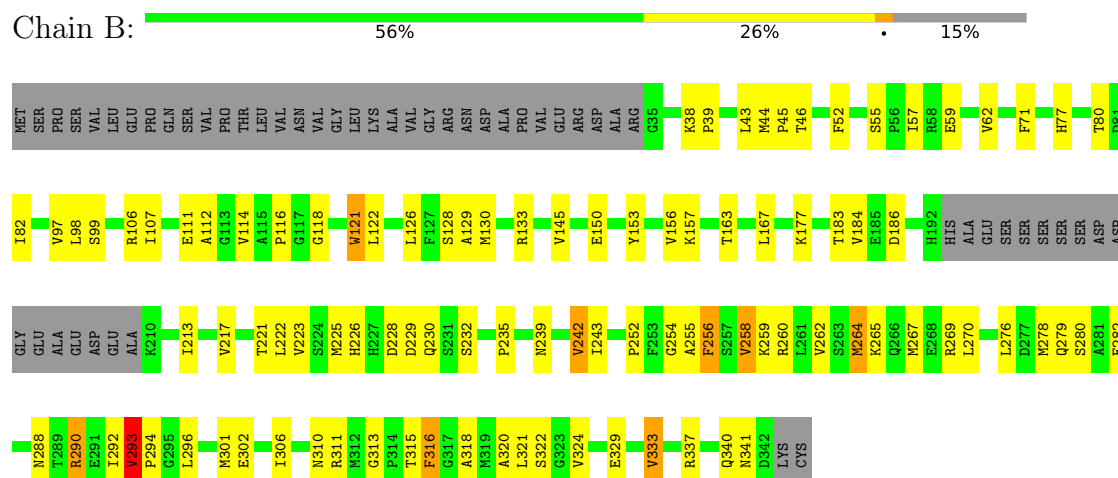
3 Residue-property plots

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: CyPBP37 protein



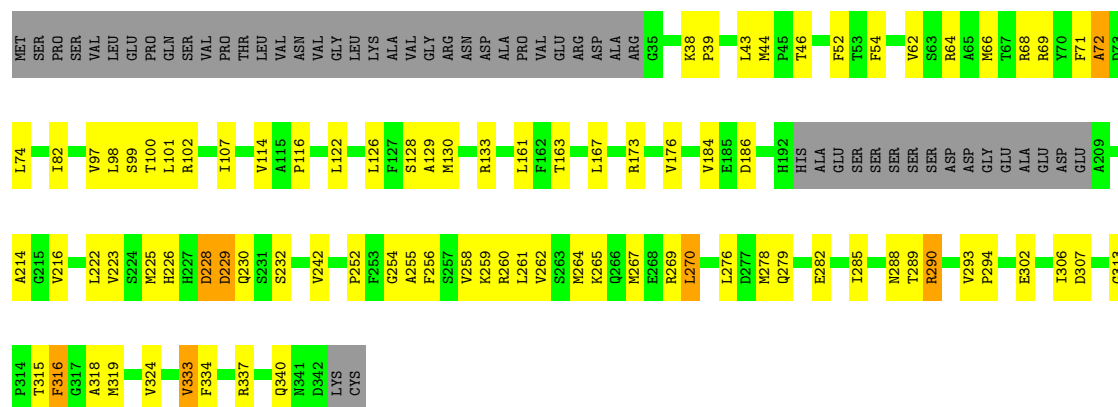
• Molecule 1: CyPBP37 protein



• Molecule 1: CyPBP37 protein

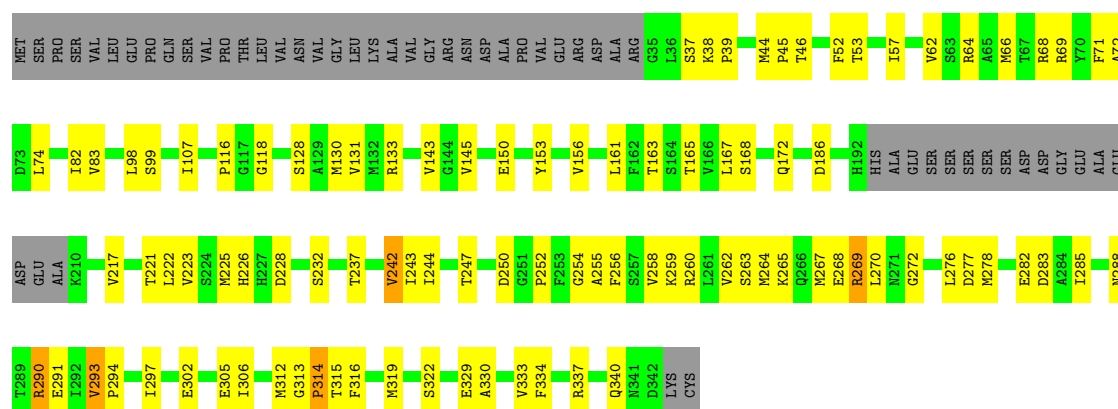






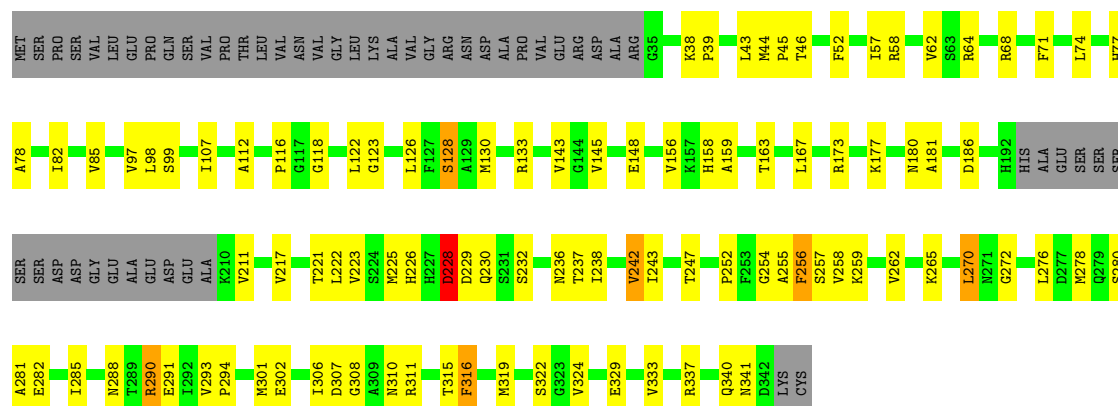
• Molecule 1: CyPBP37 protein

Chain G: 56% 27% 15%



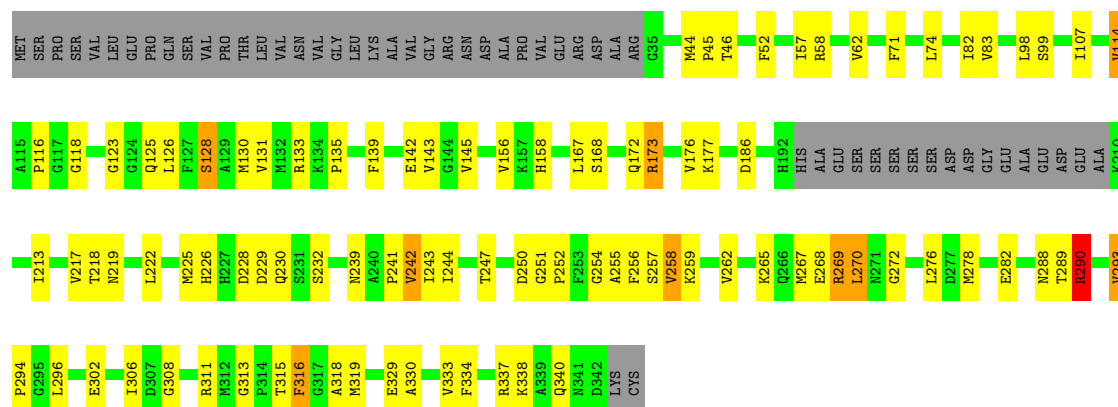
• Molecule 1: CyPBP37 protein

Chain H: 56% 27% 15%



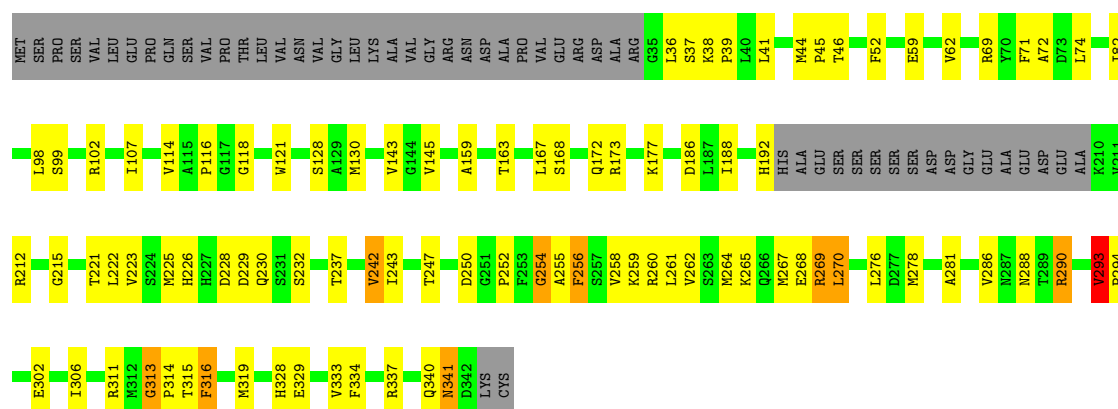
• Molecule 1: CyPBP37 protein

Chain I: 57% 25% 15%



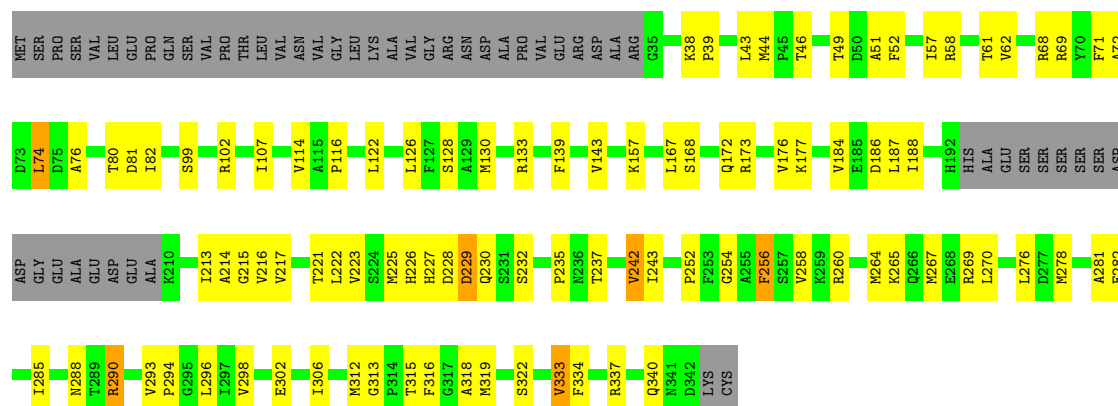
• Molecule 1: CyPBP37 protein

Chain J: 58% 24% 15%



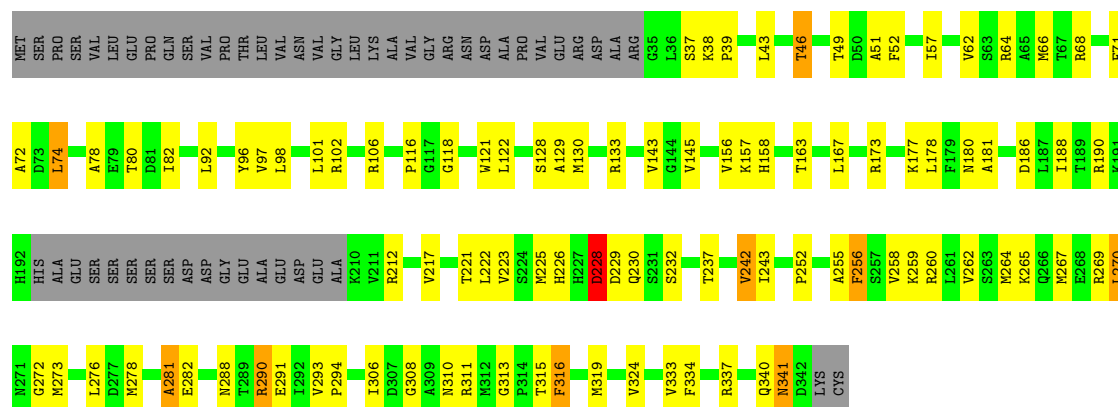
• Molecule 1: CyPBP37 protein

Chain K: 56% 26% 15%



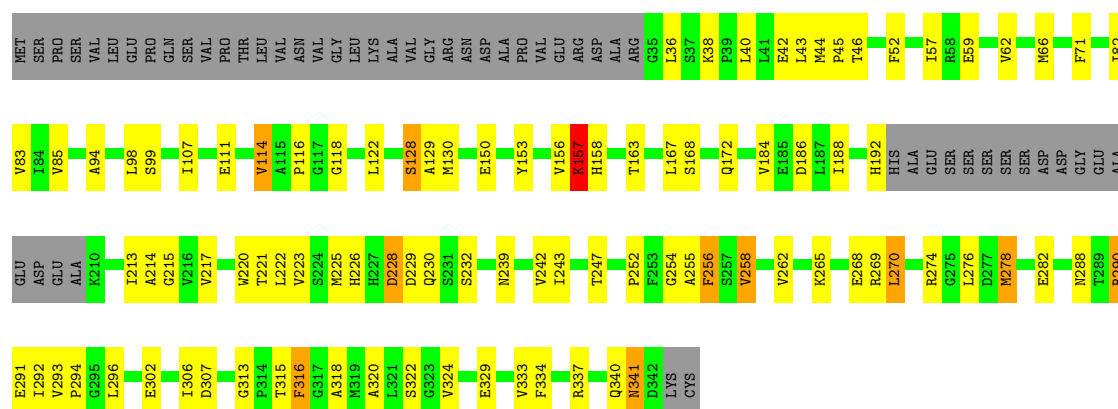
• Molecule 1: CyPBP37 protein

Chain L: 56% 26% 15%



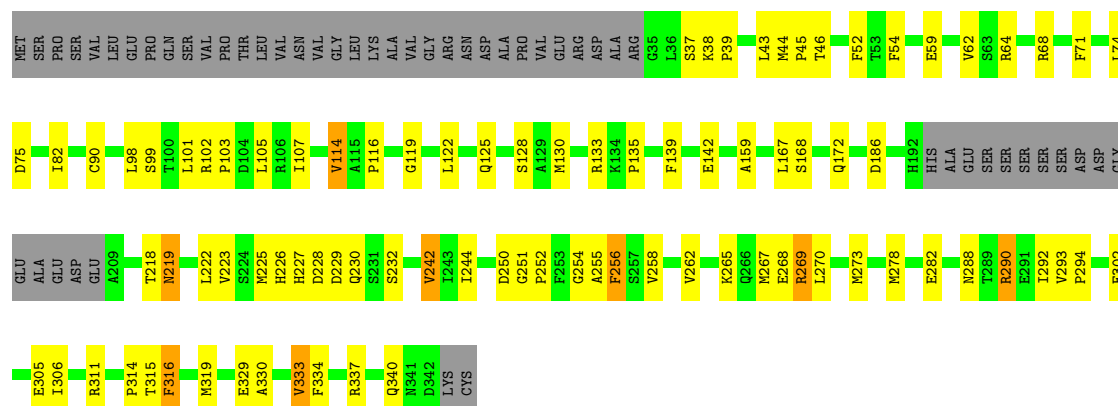
• Molecule 1: CyPBP37 protein

Chain M: 56% 25% 15%



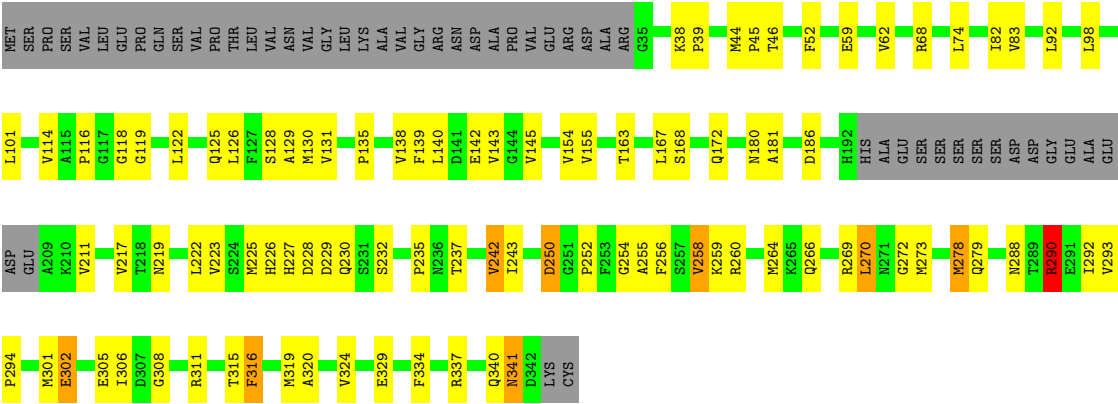
• Molecule 1: CyPBP37 protein

Chain N: 59% 24% 15%

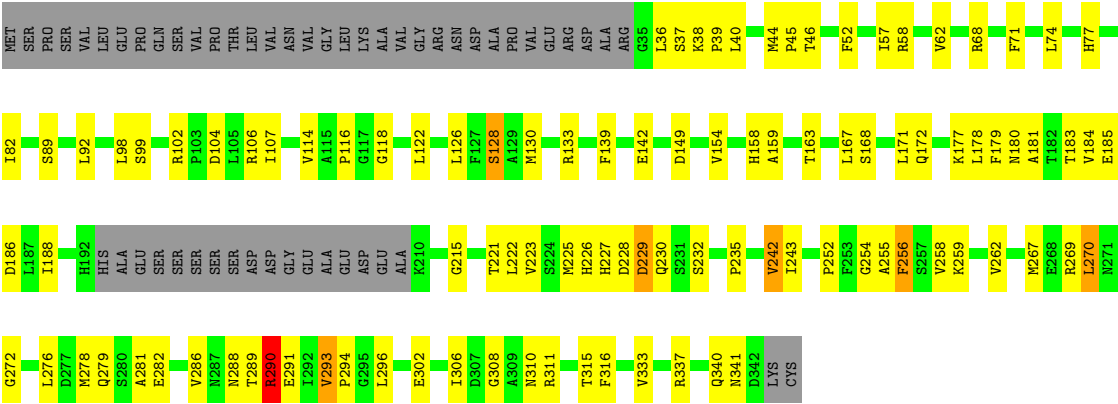


• Molecule 1: CyPBP37 protein

Chain O: 57% 25% 15%



● Molecule 1: CyPBP37 protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	158.24Å 125.91Å 158.21Å 90.00° 90.22° 90.00°	Depositor
Resolution (Å)	49.98 – 2.70 49.98 – 2.70	Depositor EDS
% Data completeness (in resolution range)	92.2 (49.98-2.70) 92.0 (49.98-2.70)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.02 (at 2.69Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.202 , 0.246 0.203 , 0.247	Depositor DCC
R_{free} test set	16493 reflections (9.96%)	wwPDB-VP
Wilson B-factor (Å ²)	34.2	Xtriage
Anisotropy	0.280	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 14.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.024 for -l,k,h 0.417 for -h,-k,l 0.024 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	36053	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% of the height of the origin peak. No significant pseudotranslation is detected.*

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: FE2, DHA, AHZ

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	0.53	0/2223	1.02	18/3011 (0.6%)
1	B	0.50	0/2218	1.02	14/3004 (0.5%)
1	C	0.51	0/2223	1.01	11/3011 (0.4%)
1	D	0.51	0/2223	0.99	10/3011 (0.3%)
1	E	0.51	0/2218	1.00	10/3004 (0.3%)
1	F	0.51	0/2223	1.00	10/3011 (0.3%)
1	G	0.52	0/2218	0.98	9/3004 (0.3%)
1	H	0.52	0/2218	1.00	11/3004 (0.4%)
1	I	0.51	0/2218	0.98	11/3004 (0.4%)
1	J	0.52	0/2218	0.99	15/3004 (0.5%)
1	K	0.52	0/2218	0.98	9/3004 (0.3%)
1	L	0.51	0/2218	0.95	8/3004 (0.3%)
1	M	0.50	0/2218	1.02	9/3004 (0.3%)
1	N	0.51	0/2223	1.01	6/3011 (0.2%)
1	O	0.52	0/2223	0.99	13/3011 (0.4%)
1	P	0.49	0/2218	0.96	6/3004 (0.2%)
All	All	0.51	0/35518	0.99	170/48106 (0.4%)

There are no bond length outliers.

The worst 5 of 170 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	254	GLY	N-CA-C	10.38	126.15	112.25
1	H	254	GLY	N-CA-C	9.92	125.54	112.25
1	F	254	GLY	N-CA-C	9.38	124.83	112.25
1	N	254	GLY	N-CA-C	9.26	124.66	112.25
1	M	114	VAL	N-CA-C	-9.11	101.97	110.53

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	2193	0	2207	89	0
1	B	2188	0	2202	92	0
1	C	2193	0	2207	89	0
1	D	2193	0	2207	85	0
1	E	2188	0	2202	68	0
1	F	2193	0	2207	80	0
1	G	2188	0	2202	81	0
1	H	2188	0	2202	88	0
1	I	2188	0	2202	82	0
1	J	2188	0	2202	80	0
1	K	2188	0	2202	92	0
1	L	2188	0	2202	94	0
1	M	2188	0	2202	94	0
1	N	2193	0	2207	82	0
1	O	2193	0	2207	79	0
1	P	2188	0	2202	98	0
2	A	38	0	19	3	0
2	B	38	0	19	2	0
2	C	38	0	19	3	0
2	D	38	0	19	0	0
2	E	38	0	19	1	0
2	F	38	0	19	1	0
2	G	38	0	19	3	0
2	H	38	0	19	3	0
2	I	38	0	19	4	0
2	J	38	0	19	2	0
2	K	38	0	19	0	0
2	L	38	0	19	3	0
2	M	38	0	19	3	0
2	N	38	0	19	0	0
2	O	38	0	19	3	0
2	P	38	0	19	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
3	K	2	0	0	0	0
3	L	1	0	0	0	0
3	M	2	0	0	0	0
3	N	1	0	0	0	0
4	A	30	0	0	4	0
4	B	16	0	0	1	0
4	C	32	0	0	2	0
4	D	21	0	0	0	0
4	E	29	0	0	0	0
4	F	24	0	0	1	0
4	G	21	0	0	0	0
4	H	23	0	0	0	0
4	I	44	0	0	0	0
4	J	20	0	0	3	0
4	K	25	0	0	3	0
4	L	21	0	0	1	0
4	M	19	0	0	1	0
4	N	17	0	0	2	0
4	O	25	0	0	0	0
4	P	24	0	0	0	0
All	All	36053	0	35566	1185	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 17.

The worst 5 of 1185 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:G:278:MET:HE1	1:H:62:VAL:HG21	1.31	1.11
1:J:278:MET:HE1	1:K:62:VAL:HG21	1.18	1.10
1:H:258:VAL:HG12	1:H:270:LEU:HD11	1.31	1.10
1:J:62:VAL:HG21	1:K:278:MET:HE1	1.36	1.04
1:B:278:MET:HE1	1:C:62:VAL:HG21	1.41	1.01

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	287/344 (83%)	270 (94%)	16 (6%)	1 (0%)	36	60
1	B	286/344 (83%)	268 (94%)	18 (6%)	0	100	100
1	C	287/344 (83%)	266 (93%)	20 (7%)	1 (0%)	36	60
1	D	287/344 (83%)	266 (93%)	20 (7%)	1 (0%)	36	60
1	E	286/344 (83%)	266 (93%)	17 (6%)	3 (1%)	12	32
1	F	287/344 (83%)	268 (93%)	18 (6%)	1 (0%)	36	60
1	G	286/344 (83%)	266 (93%)	17 (6%)	3 (1%)	12	32
1	H	286/344 (83%)	266 (93%)	20 (7%)	0	100	100
1	I	286/344 (83%)	268 (94%)	17 (6%)	1 (0%)	36	60
1	J	286/344 (83%)	269 (94%)	15 (5%)	2 (1%)	18	41
1	K	286/344 (83%)	264 (92%)	20 (7%)	2 (1%)	18	41
1	L	286/344 (83%)	266 (93%)	19 (7%)	1 (0%)	36	60
1	M	286/344 (83%)	267 (93%)	17 (6%)	2 (1%)	18	41
1	N	287/344 (83%)	264 (92%)	20 (7%)	3 (1%)	12	32
1	O	287/344 (83%)	269 (94%)	17 (6%)	1 (0%)	36	60
1	P	286/344 (83%)	268 (94%)	17 (6%)	1 (0%)	36	60
All	All	4582/5504 (83%)	4271 (93%)	288 (6%)	23 (0%)	24	48

5 of 23 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	269	ARG
1	E	250	ASP
1	E	229	ASP
1	F	229	ASP
1	G	269	ARG

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	235/280 (84%)	230 (98%)	5 (2%)	47	75
1	B	235/280 (84%)	228 (97%)	7 (3%)	36	66
1	C	235/280 (84%)	230 (98%)	5 (2%)	47	75
1	D	235/280 (84%)	229 (97%)	6 (3%)	40	70
1	E	235/280 (84%)	233 (99%)	2 (1%)	70	87
1	F	235/280 (84%)	229 (97%)	6 (3%)	40	70
1	G	235/280 (84%)	231 (98%)	4 (2%)	53	79
1	H	235/280 (84%)	230 (98%)	5 (2%)	47	75
1	I	235/280 (84%)	228 (97%)	7 (3%)	36	66
1	J	235/280 (84%)	228 (97%)	7 (3%)	36	66
1	K	235/280 (84%)	231 (98%)	4 (2%)	53	79
1	L	235/280 (84%)	228 (97%)	7 (3%)	36	66
1	M	235/280 (84%)	228 (97%)	7 (3%)	36	66
1	N	235/280 (84%)	230 (98%)	5 (2%)	47	75
1	O	235/280 (84%)	228 (97%)	7 (3%)	36	66
1	P	235/280 (84%)	228 (97%)	7 (3%)	36	66
All	All	3760/4480 (84%)	3669 (98%)	91 (2%)	43	72

5 of 91 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	333	VAL
1	M	341	ASN
1	L	74	LEU
1	M	157	LYS
1	N	290	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 60 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	310	ASN
1	P	172	GLN
1	K	310	ASN
1	O	341	ASN
1	P	341	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

16 non-standard protein/DNA/RNA residues 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$
1	DHA	P	232	1	3,4,5	2.08	2 (66%)	2,4,6	4.27	2 (100%)
1	DHA	K	232	1	3,4,5	1.94	2 (66%)	2,4,6	3.95	2 (100%)
1	DHA	L	232	1	3,4,5	1.75	1 (33%)	2,4,6	3.90	2 (100%)
1	DHA	E	232	1	3,4,5	2.16	2 (66%)	2,4,6	4.17	2 (100%)
1	DHA	M	232	1	3,4,5	1.89	1 (33%)	2,4,6	4.04	2 (100%)
1	DHA	H	232	1	3,4,5	1.94	1 (33%)	2,4,6	3.82	2 (100%)
1	DHA	F	232	1	3,4,5	2.17	2 (66%)	2,4,6	4.06	2 (100%)
1	DHA	D	232	1	3,4,5	2.10	2 (66%)	2,4,6	4.17	2 (100%)
1	DHA	I	232	1	3,4,5	1.92	1 (33%)	2,4,6	3.95	2 (100%)
1	DHA	B	232	1	3,4,5	1.95	2 (66%)	2,4,6	4.05	2 (100%)
1	DHA	G	232	1	3,4,5	1.76	1 (33%)	2,4,6	4.08	2 (100%)
1	DHA	N	232	1	3,4,5	1.89	2 (66%)	2,4,6	3.98	2 (100%)
1	DHA	C	232	1	3,4,5	1.85	1 (33%)	2,4,6	4.10	2 (100%)
1	DHA	O	232	1	3,4,5	1.79	1 (33%)	2,4,6	4.00	2 (100%)
1	DHA	A	232	1	3,4,5	1.81	2 (66%)	2,4,6	3.89	2 (100%)
1	DHA	J	232	1	3,4,5	1.83	1 (33%)	2,4,6	4.10	2 (100%)

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
1	DHA	P	232	1	-	0/0/2/4	-
1	DHA	K	232	1	-	0/0/2/4	-
1	DHA	L	232	1	-	0/0/2/4	-
1	DHA	E	232	1	-	0/0/2/4	-
1	DHA	M	232	1	-	0/0/2/4	-
1	DHA	H	232	1	-	0/0/2/4	-
1	DHA	F	232	1	-	0/0/2/4	-
1	DHA	D	232	1	-	0/0/2/4	-
1	DHA	I	232	1	-	0/0/2/4	-
1	DHA	B	232	1	-	0/0/2/4	-
1	DHA	G	232	1	-	0/0/2/4	-
1	DHA	N	232	1	-	0/0/2/4	-
1	DHA	C	232	1	-	0/0/2/4	-
1	DHA	O	232	1	-	0/0/2/4	-
1	DHA	A	232	1	-	0/0/2/4	-
1	DHA	J	232	1	-	0/0/2/4	-

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	232	DHA	O-C	2.78	1.28	1.22
1	H	232	DHA	O-C	2.71	1.28	1.22
1	E	232	DHA	C-CA	2.71	1.49	1.45
1	I	232	DHA	C-CA	2.71	1.49	1.45
1	M	232	DHA	C-CA	2.67	1.49	1.45

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	232	DHA	O-C-CA	-5.14	115.89	125.53
1	D	232	DHA	O-C-CA	-4.99	116.17	125.53
1	E	232	DHA	O-C-CA	-4.94	116.27	125.53
1	B	232	DHA	O-C-CA	-4.84	116.45	125.53
1	J	232	DHA	O-C-CA	-4.84	116.46	125.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 32 ligands modelled in this entry, 16 are monoatomic - leaving 16 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
2	AHZ	J	500	3	40,41,41	1.52	7 (17%)	55,62,62	2.13	12 (21%)
2	AHZ	K	500	3	40,41,41	1.57	8 (20%)	55,62,62	2.10	14 (25%)
2	AHZ	N	500	3	40,41,41	1.64	7 (17%)	55,62,62	2.10	11 (20%)
2	AHZ	M	500	3	40,41,41	1.65	7 (17%)	55,62,62	2.17	12 (21%)
2	AHZ	A	500	3	40,41,41	1.54	7 (17%)	55,62,62	2.13	12 (21%)
2	AHZ	F	500	3	40,41,41	1.60	7 (17%)	55,62,62	2.06	12 (21%)
2	AHZ	D	500	3	40,41,41	1.62	7 (17%)	55,62,62	2.10	14 (25%)
2	AHZ	L	500	3	40,41,41	1.72	7 (17%)	55,62,62	2.15	11 (20%)
2	AHZ	C	500	3	40,41,41	1.43	7 (17%)	55,62,62	2.05	11 (20%)
2	AHZ	E	500	3	40,41,41	1.44	7 (17%)	55,62,62	2.12	12 (21%)
2	AHZ	H	500	3	40,41,41	1.71	7 (17%)	55,62,62	2.19	12 (21%)
2	AHZ	P	500	3	40,41,41	1.56	8 (20%)	55,62,62	2.10	14 (25%)
2	AHZ	G	500	3	40,41,41	1.57	7 (17%)	55,62,62	2.18	14 (25%)
2	AHZ	I	500	3	40,41,41	1.54	7 (17%)	55,62,62	2.11	12 (21%)
2	AHZ	B	500	3	40,41,41	1.56	7 (17%)	55,62,62	2.13	11 (20%)
2	AHZ	O	500	3	40,41,41	1.66	7 (17%)	55,62,62	2.19	13 (23%)

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	AHZ	J	500	3	-	8/26/43/43	0/4/4/4
2	AHZ	K	500	3	-	9/26/43/43	0/4/4/4
2	AHZ	N	500	3	-	9/26/43/43	0/4/4/4
2	AHZ	M	500	3	-	7/26/43/43	0/4/4/4
2	AHZ	A	500	3	-	8/26/43/43	0/4/4/4
2	AHZ	F	500	3	-	9/26/43/43	0/4/4/4
2	AHZ	D	500	3	-	10/26/43/43	0/4/4/4
2	AHZ	L	500	3	-	10/26/43/43	0/4/4/4
2	AHZ	C	500	3	-	8/26/43/43	0/4/4/4
2	AHZ	E	500	3	-	7/26/43/43	0/4/4/4
2	AHZ	H	500	3	-	10/26/43/43	0/4/4/4
2	AHZ	P	500	3	-	11/26/43/43	0/4/4/4
2	AHZ	G	500	3	-	9/26/43/43	0/4/4/4
2	AHZ	I	500	3	-	12/26/43/43	0/4/4/4
2	AHZ	B	500	3	-	10/26/43/43	0/4/4/4
2	AHZ	O	500	3	-	8/26/43/43	0/4/4/4

The worst 5 of 114 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	500	AHZ	PB-O3A	5.30	1.65	1.59
2	F	500	AHZ	PB-O3A	5.00	1.64	1.59
2	H	500	AHZ	PB-O3A	4.88	1.64	1.59
2	M	500	AHZ	PB-O3A	4.72	1.64	1.59
2	O	500	AHZ	PB-O3A	4.41	1.64	1.59

The worst 5 of 197 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	500	AHZ	C5T-S1T-C2T	7.91	95.43	91.34
2	M	500	AHZ	C5T-S1T-C2T	7.36	95.15	91.34
2	O	500	AHZ	C5T-S1T-C2T	7.35	95.14	91.34
2	G	500	AHZ	C5T-S1T-C2T	7.20	95.07	91.34
2	L	500	AHZ	C5T-S1T-C2T	7.11	95.02	91.34

There are no chirality outliers.

5 of 145 torsion outliers are listed below:

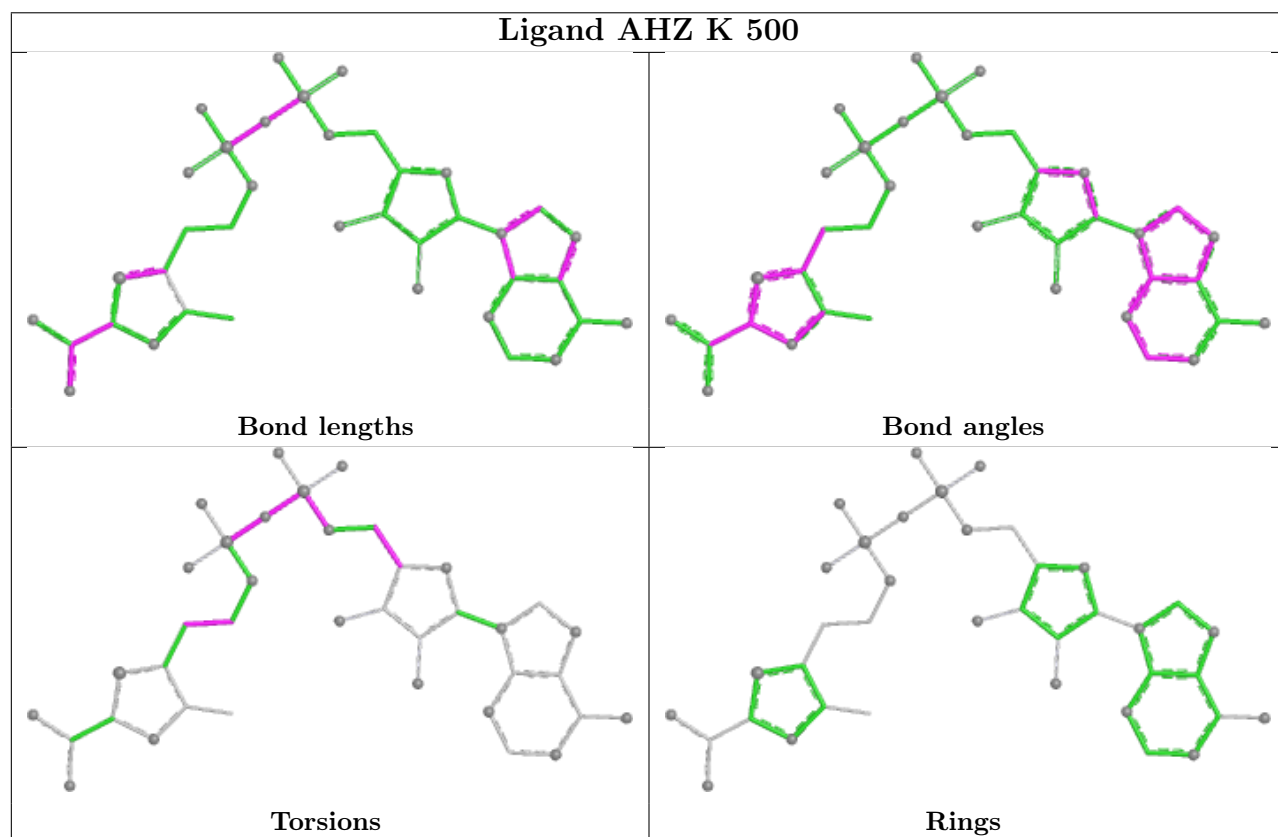
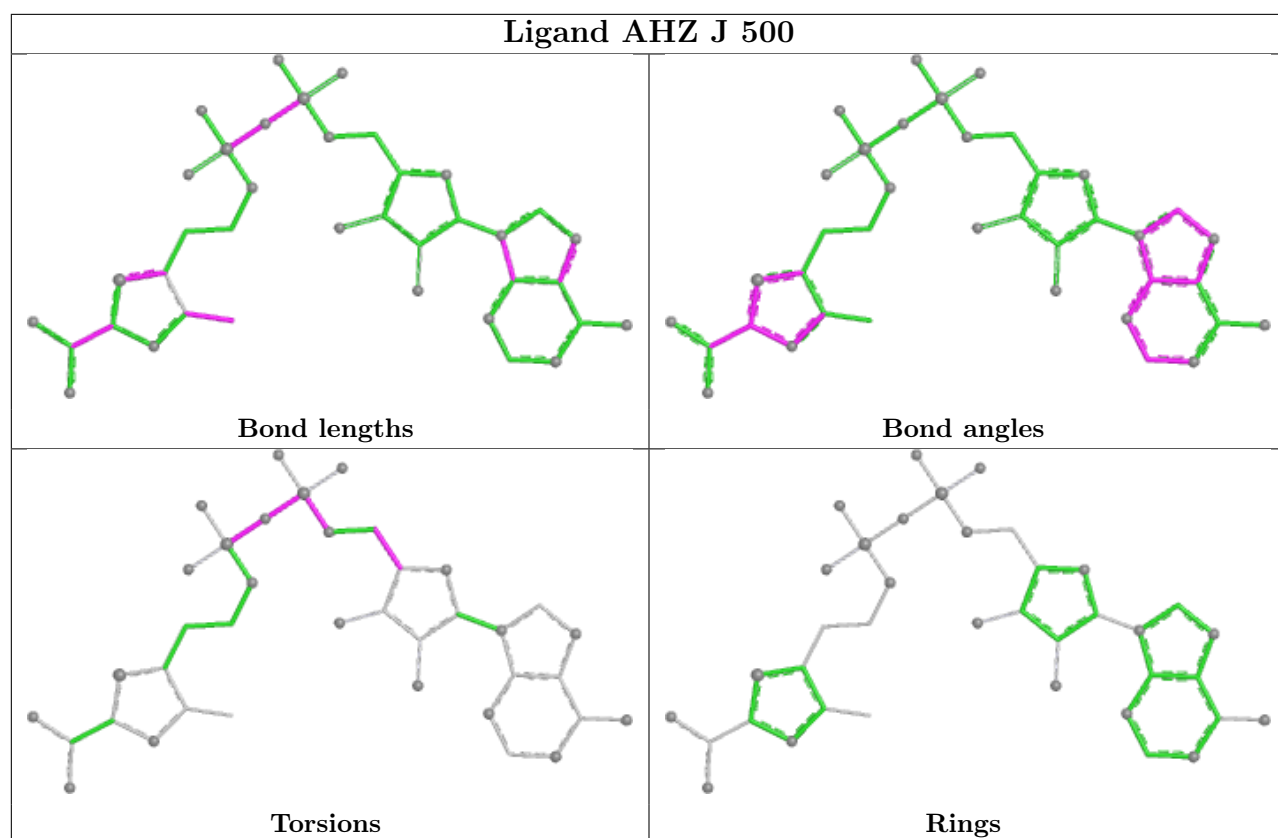
Mol	Chain	Res	Type	Atoms
2	A	500	AHZ	C5'-O5'-PA-O2A
2	A	500	AHZ	C5'-O5'-PA-O1A
2	A	500	AHZ	C5'-O5'-PA-O3A
2	A	500	AHZ	C5T-C6T-C7T-O3B
2	B	500	AHZ	C5'-O5'-PA-O2A

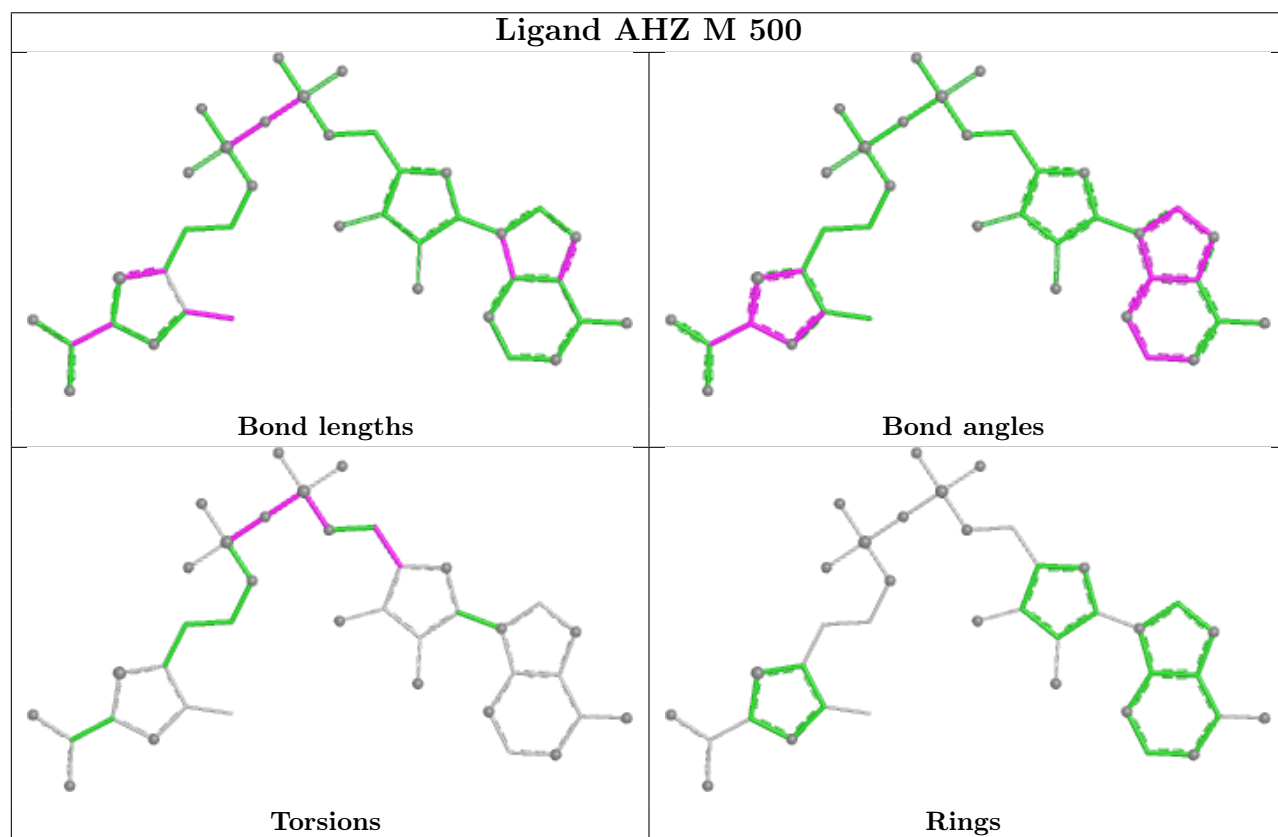
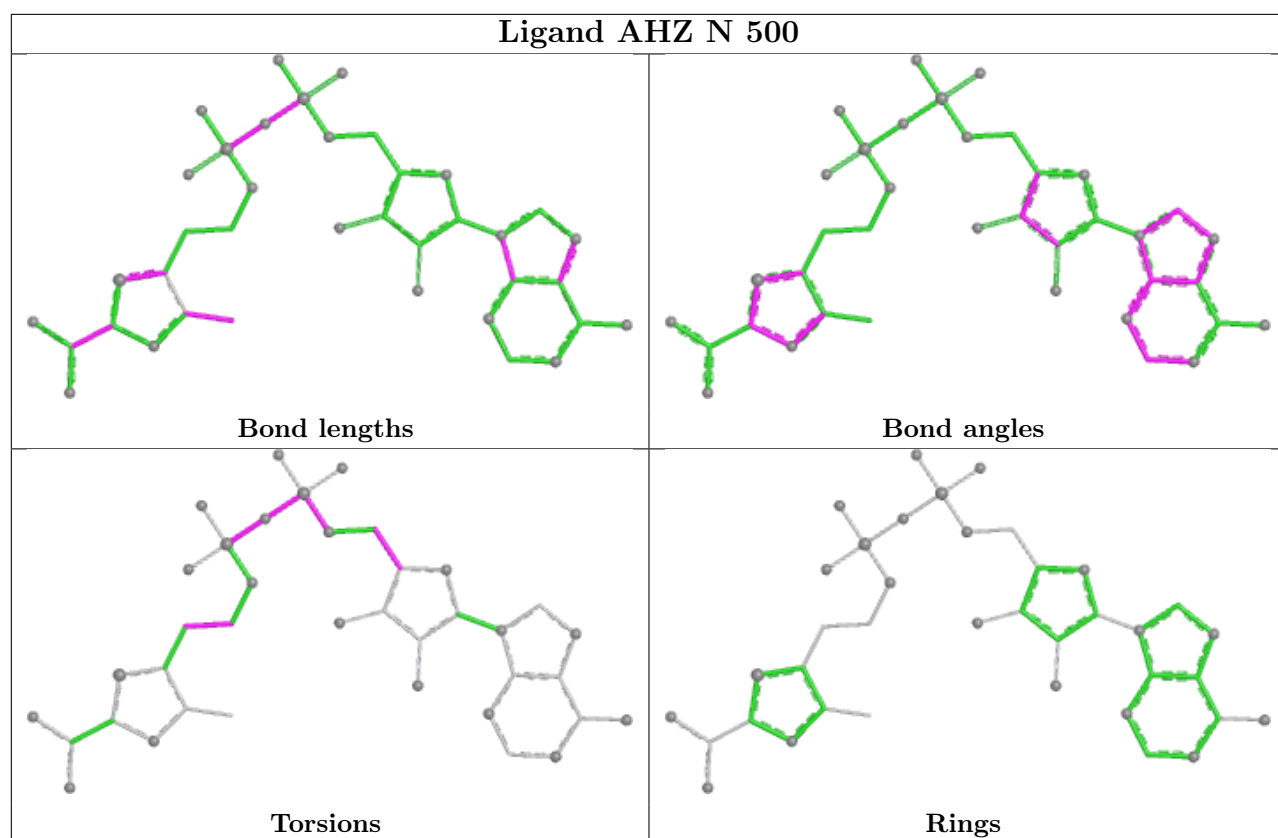
There are no ring outliers.

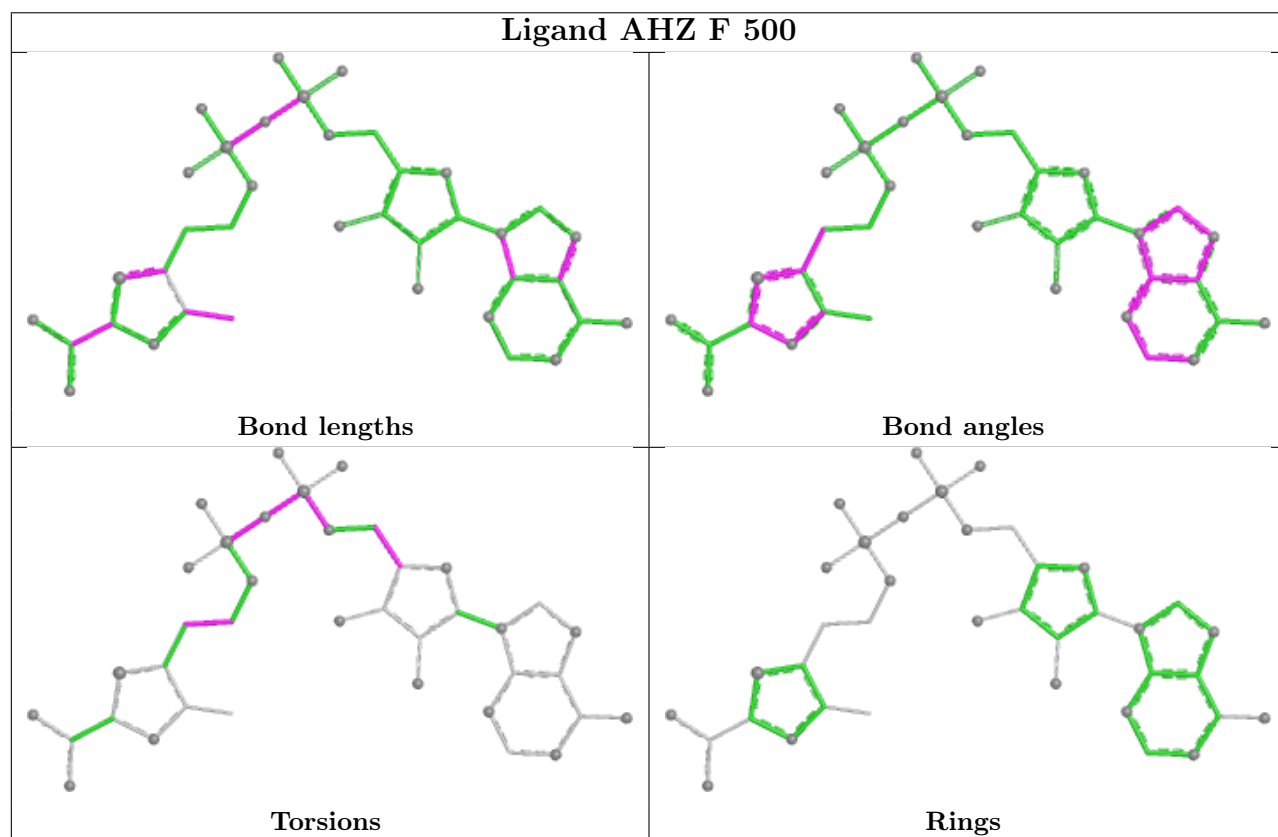
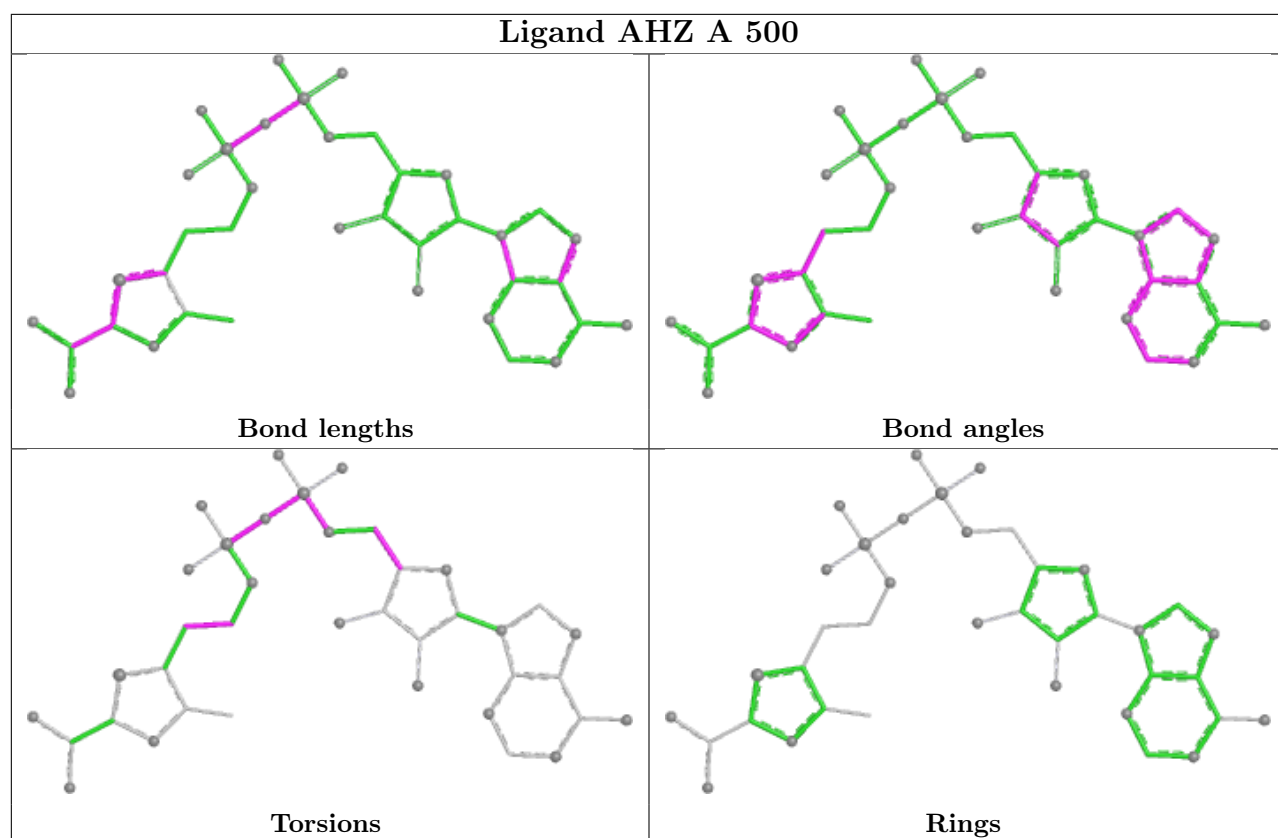
13 monomers are involved in 33 short contacts:

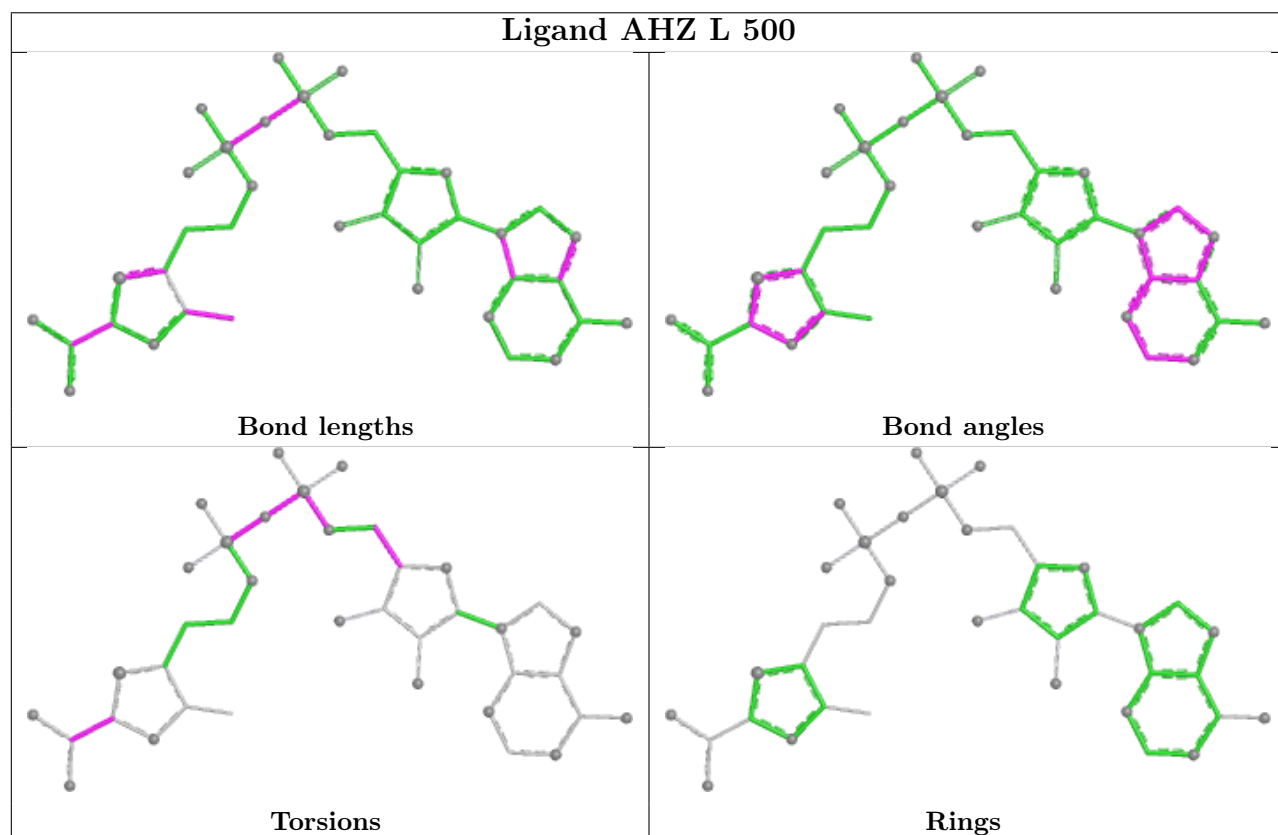
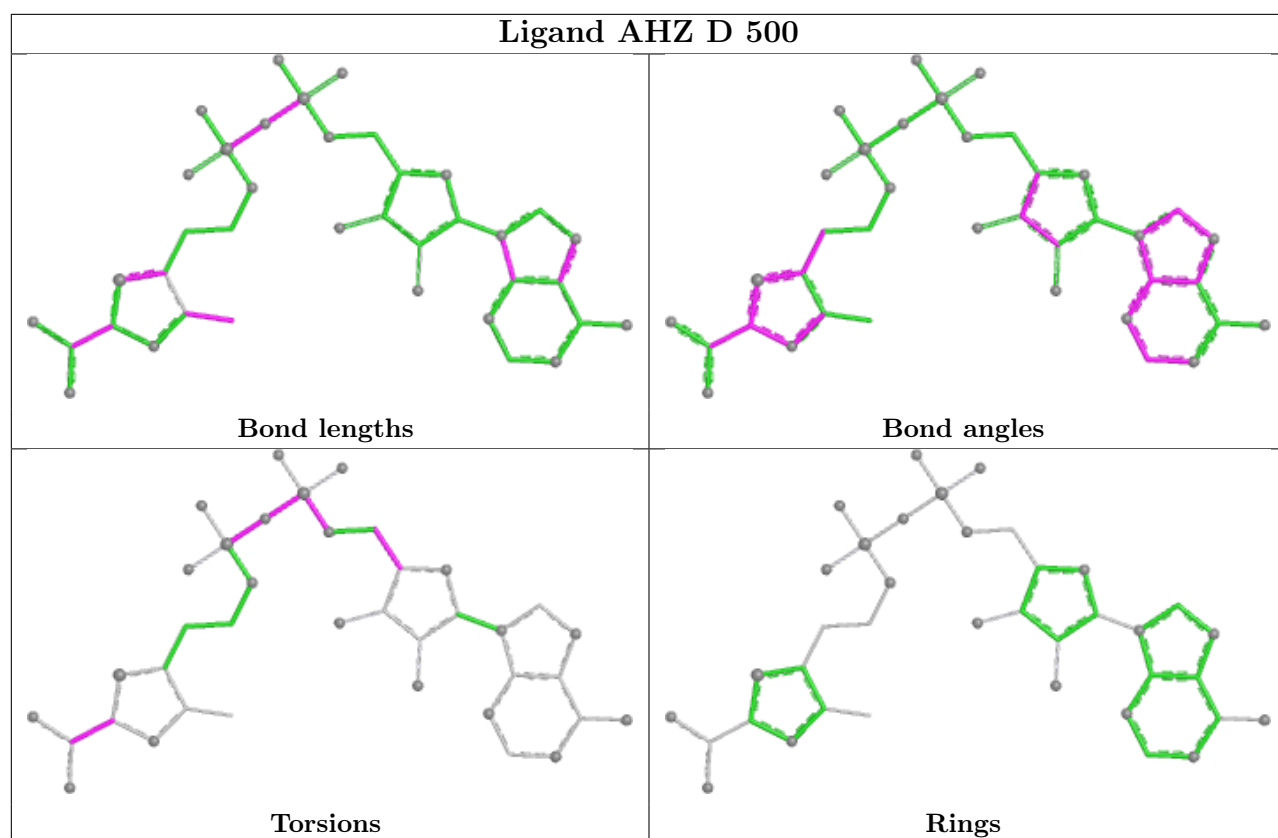
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	500	AHZ	2	0
2	M	500	AHZ	3	0
2	A	500	AHZ	3	0
2	F	500	AHZ	1	0
2	L	500	AHZ	3	0
2	C	500	AHZ	3	0
2	E	500	AHZ	1	0
2	H	500	AHZ	3	0
2	P	500	AHZ	2	0
2	G	500	AHZ	3	0
2	I	500	AHZ	4	0
2	B	500	AHZ	2	0
2	O	500	AHZ	3	0

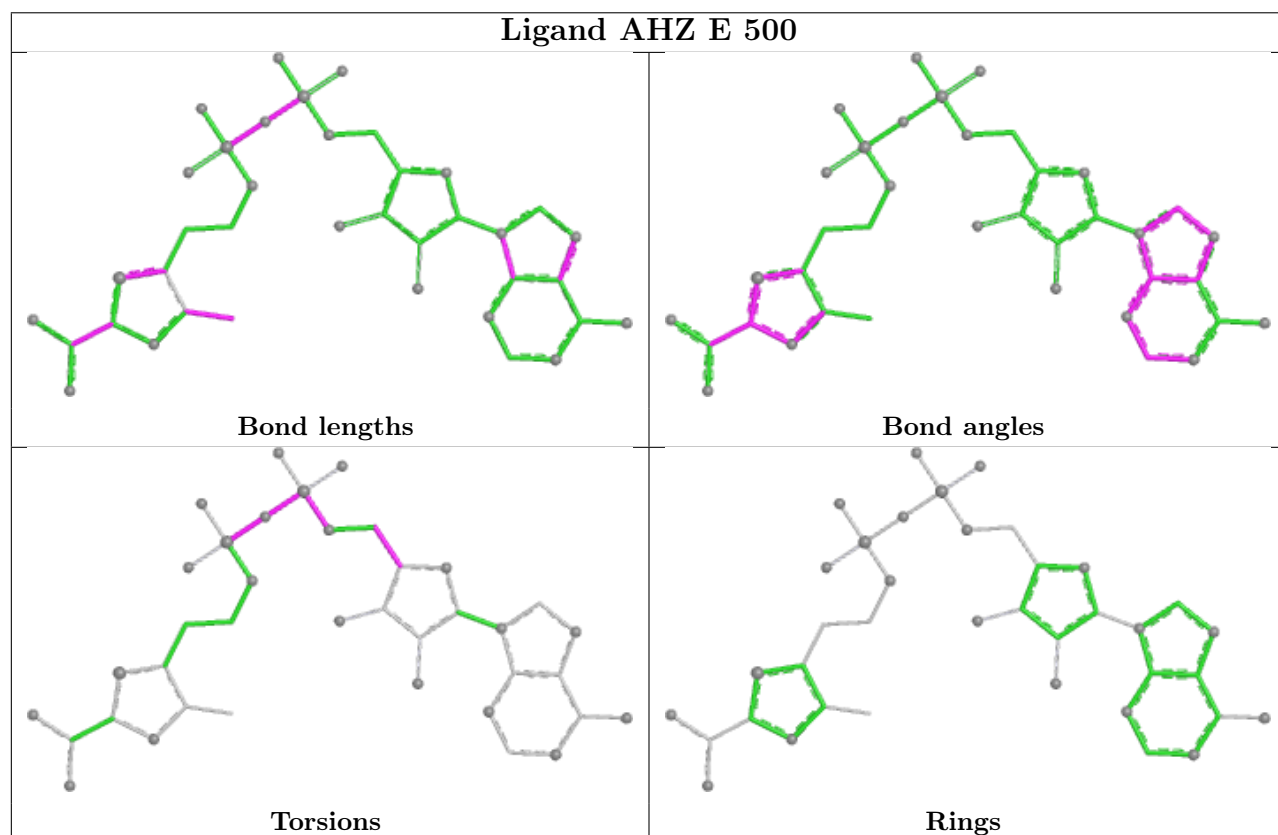
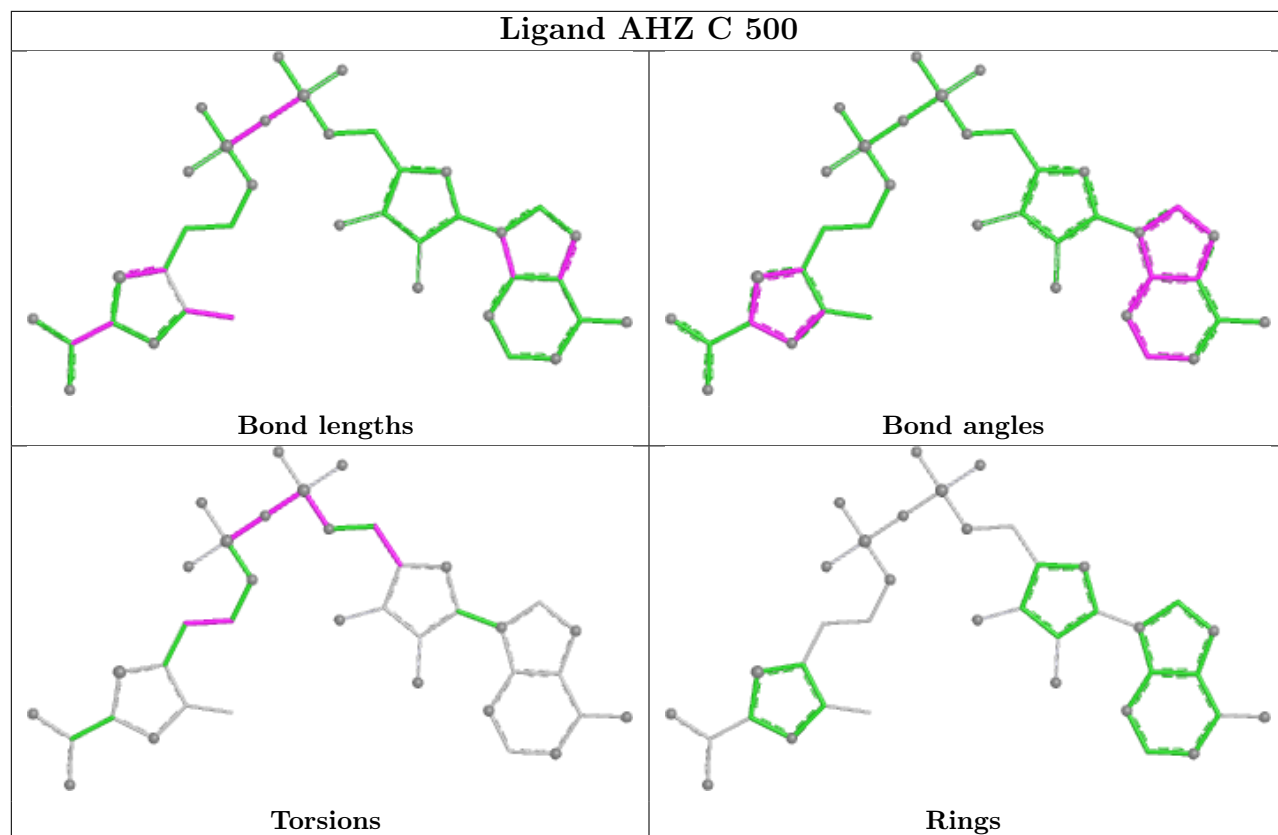
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

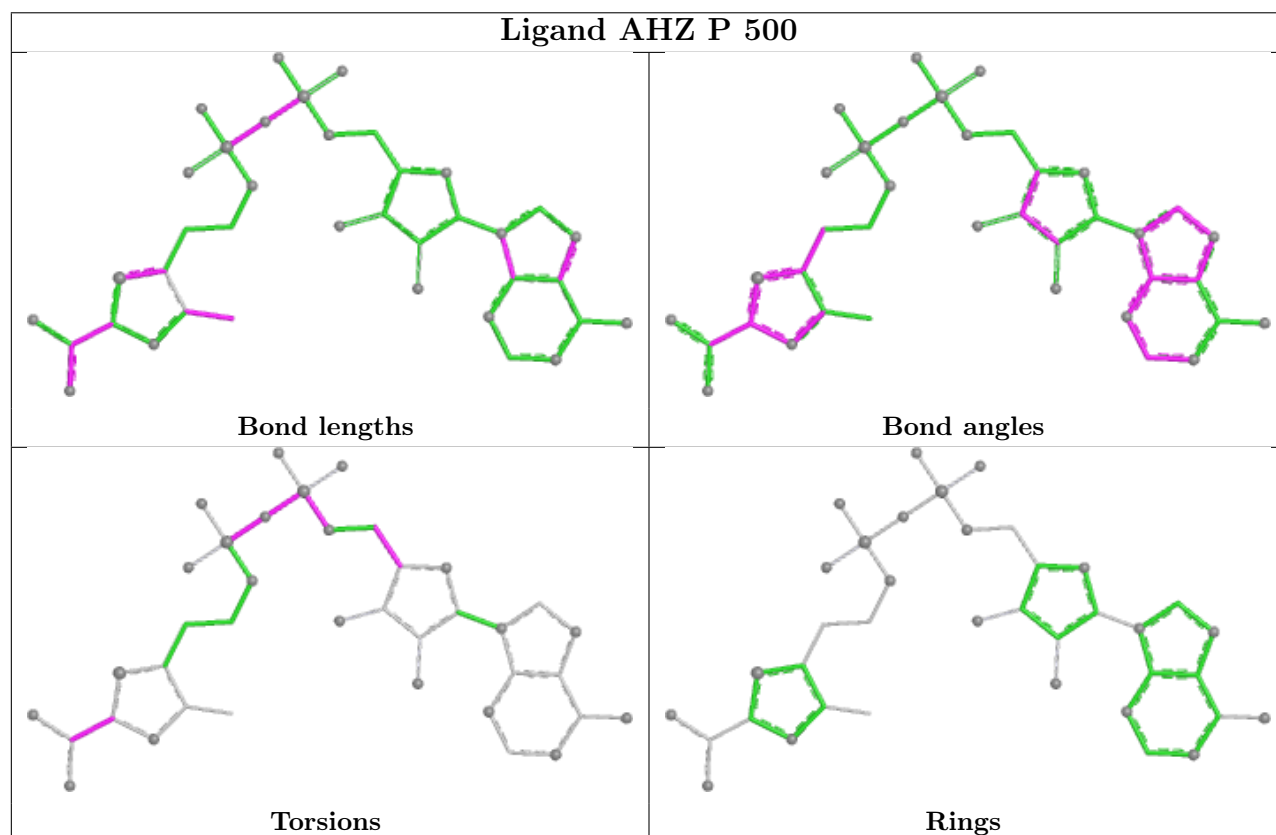
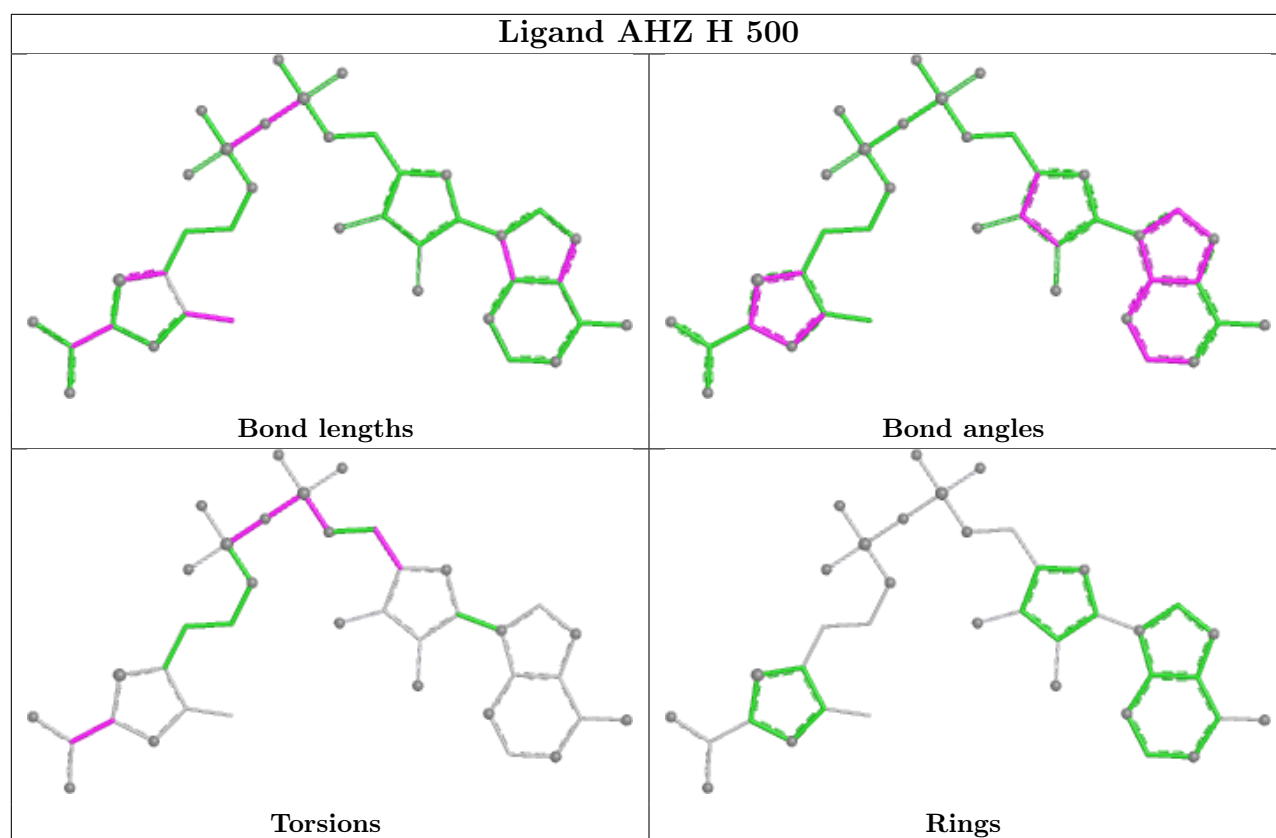


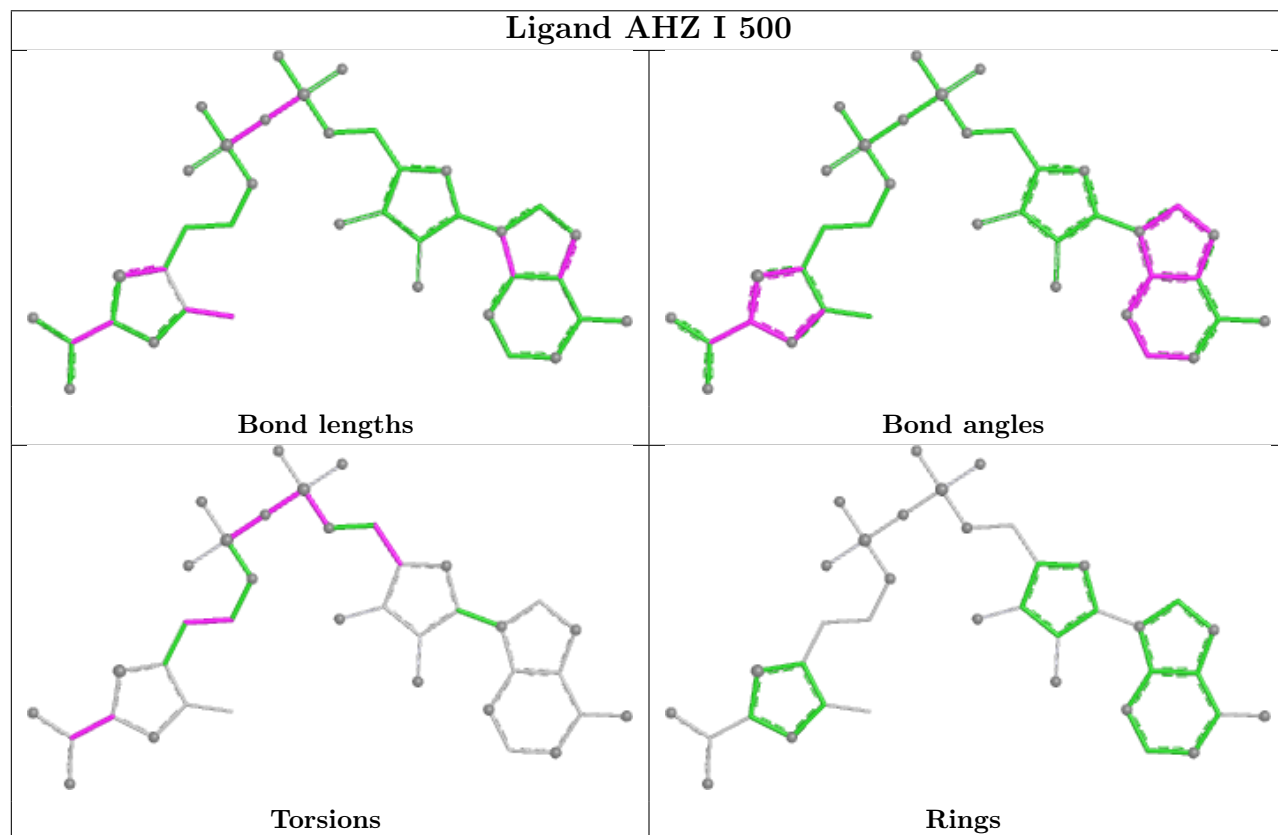
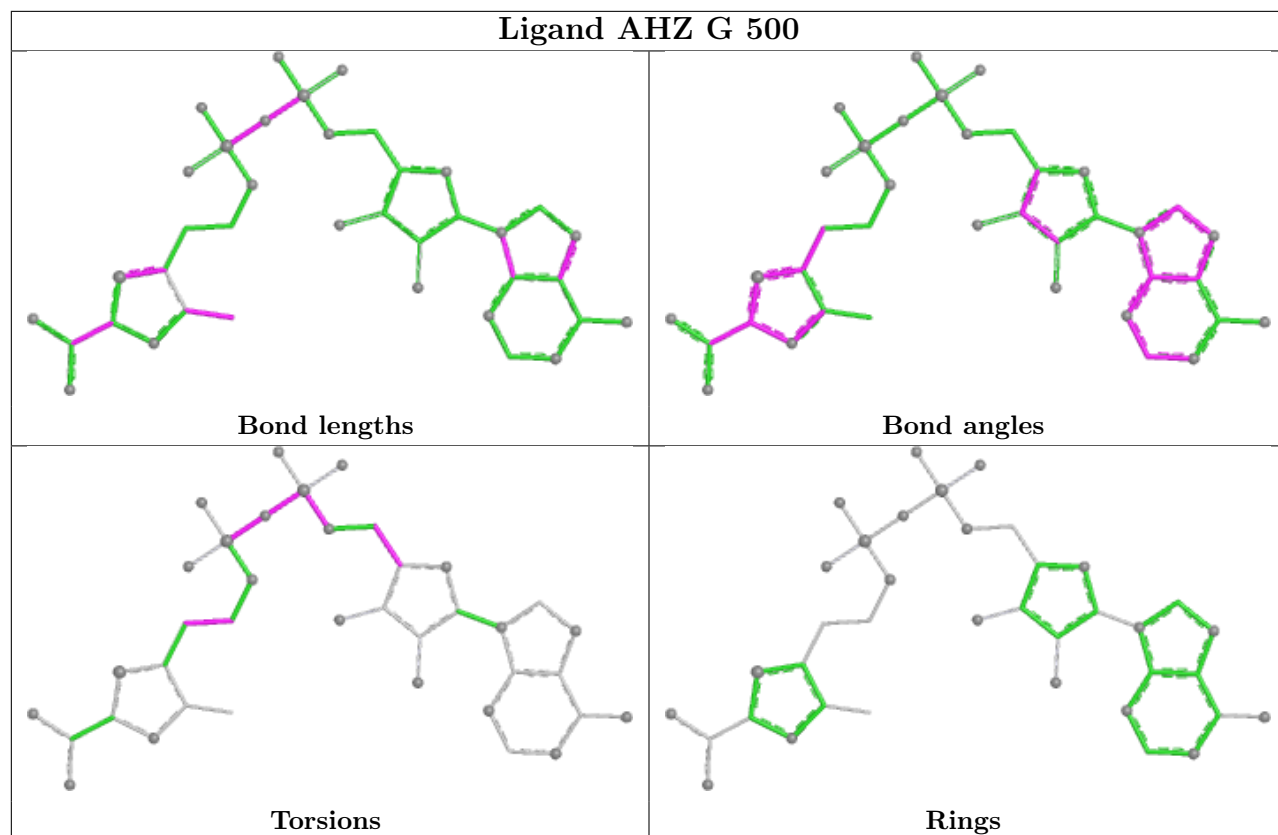


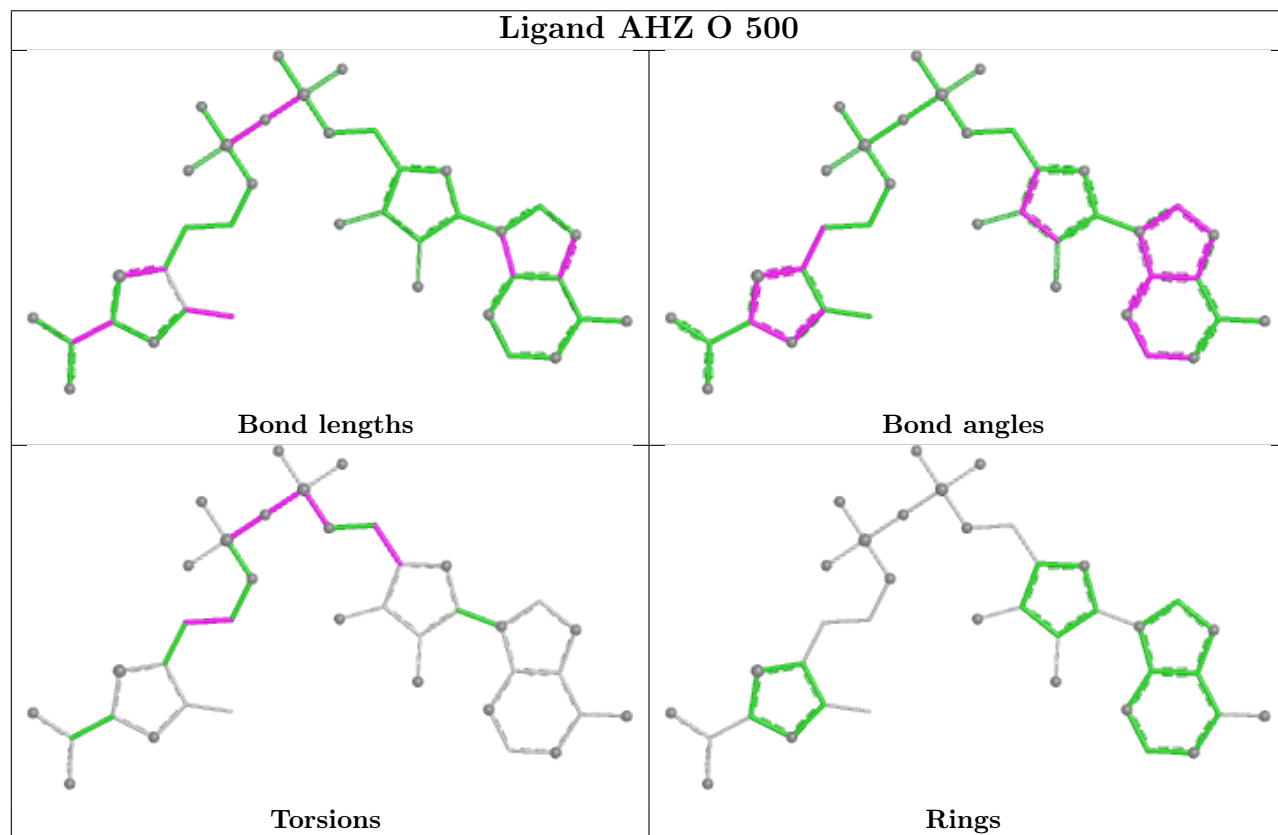
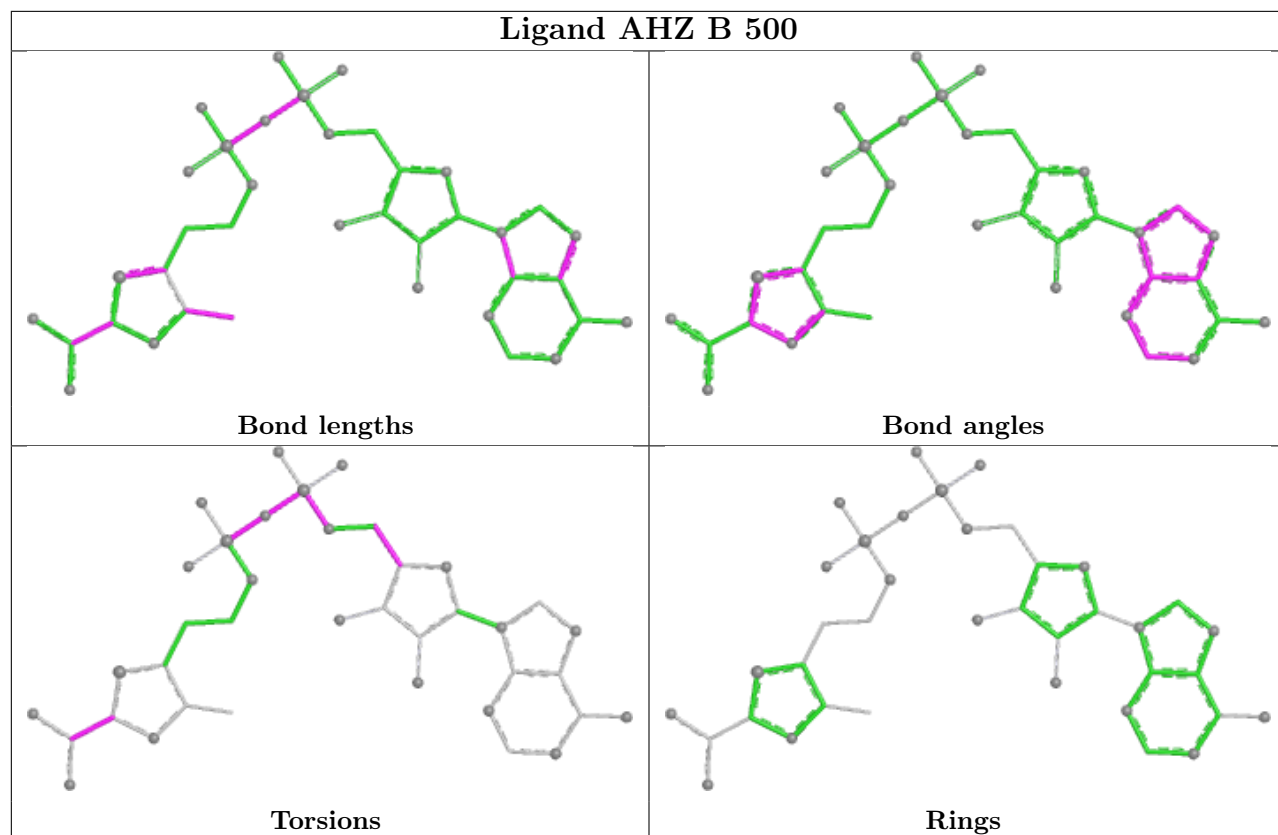












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	291/344 (84%)	-1.21	0 100 100	24, 33, 52, 69	0
1	B	290/344 (84%)	-1.19	0 100 100	26, 34, 52, 68	0
1	C	291/344 (84%)	-1.19	0 100 100	25, 33, 52, 69	0
1	D	291/344 (84%)	-1.20	0 100 100	26, 33, 53, 68	0
1	E	290/344 (84%)	-1.17	0 100 100	26, 33, 52, 68	0
1	F	291/344 (84%)	-1.22	0 100 100	26, 33, 52, 68	0
1	G	290/344 (84%)	-1.17	0 100 100	26, 33, 52, 69	0
1	H	290/344 (84%)	-1.20	0 100 100	26, 33, 53, 68	0
1	I	290/344 (84%)	-1.22	0 100 100	25, 32, 51, 68	0
1	J	290/344 (84%)	-1.17	0 100 100	25, 33, 52, 68	0
1	K	290/344 (84%)	-1.22	0 100 100	25, 33, 52, 68	0
1	L	290/344 (84%)	-1.20	0 100 100	26, 33, 53, 68	0
1	M	290/344 (84%)	-1.20	0 100 100	25, 33, 52, 68	0
1	N	291/344 (84%)	-1.20	0 100 100	25, 33, 51, 69	0
1	O	291/344 (84%)	-1.22	0 100 100	25, 32, 52, 69	0
1	P	290/344 (84%)	-1.17	0 100 100	26, 33, 52, 68	0
All	All	4646/5504 (84%)	-1.20	0 100 100	24, 33, 53, 69	0

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains [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($\text{\AA}^2$)	Q<0.9
1	DHA	M	232	5/6	0.97	0.07	48,48,49,49	0
1	DHA	D	232	5/6	0.98	0.06	48,48,49,50	0
1	DHA	E	232	5/6	0.98	0.07	47,48,49,49	0
1	DHA	F	232	5/6	0.98	0.08	47,48,48,49	0
1	DHA	H	232	5/6	0.98	0.06	47,47,47,49	0
1	DHA	B	232	5/6	0.98	0.07	47,47,48,48	0
1	DHA	N	232	5/6	0.98	0.07	46,46,47,48	0
1	DHA	P	232	5/6	0.98	0.06	47,48,48,49	0
1	DHA	I	232	5/6	0.99	0.05	46,47,48,49	0
1	DHA	J	232	5/6	0.99	0.05	48,48,49,50	0
1	DHA	K	232	5/6	0.99	0.06	46,47,47,49	0
1	DHA	L	232	5/6	0.99	0.05	46,48,49,50	0
1	DHA	A	232	5/6	0.99	0.05	45,46,47,48	0
1	DHA	G	232	5/6	0.99	0.05	46,47,48,50	0
1	DHA	O	232	5/6	0.99	0.06	48,48,49,49	0
1	DHA	C	232	5/6	0.99	0.07	46,47,48,48	0

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($\text{\AA}^2$)	Q<0.9
3	FE2	L	345	1/1	0.96	0.07	100,100,100,100	0
3	FE2	E	345	1/1	0.97	0.05	100,100,100,100	0
3	FE2	G	345	1/1	0.97	0.05	87,87,87,87	0
3	FE2	K	345	1/1	0.97	0.06	99,99,99,99	0
3	FE2	C	345	1/1	0.97	0.05	100,100,100,100	0
3	FE2	M	346	1/1	0.97	0.08	100,100,100,100	0
3	FE2	N	345	1/1	0.97	0.06	100,100,100,100	0
3	FE2	J	345	1/1	0.98	0.06	100,100,100,100	0
3	FE2	D	345	1/1	0.98	0.05	97,97,97,97	0
2	AHZ	M	500	38/38	0.98	0.05	35,47,61,62	0
2	AHZ	B	500	38/38	0.98	0.06	39,48,56,58	0
3	FE2	I	345	1/1	0.98	0.04	100,100,100,100	0
2	AHZ	A	500	38/38	0.99	0.04	27,31,36,37	0

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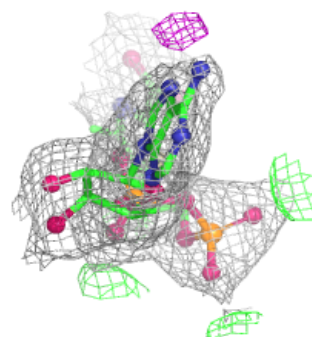
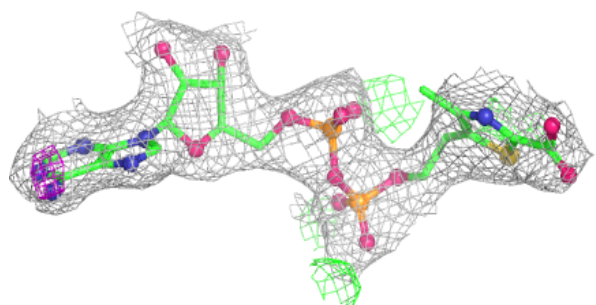
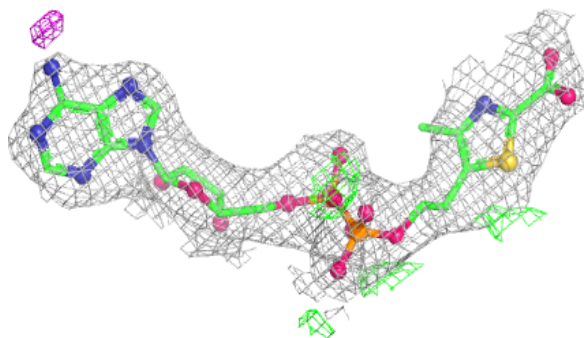
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	AHZ	N	500	38/38	0.99	0.04	26,32,47,49	0
2	AHZ	O	500	38/38	0.99	0.04	26,33,40,41	0
2	AHZ	P	500	38/38	0.99	0.05	30,42,55,57	0
3	FE2	A	345	1/1	0.99	0.05	100,100,100,100	0
3	FE2	B	345	1/1	0.99	0.05	93,93,93,93	0
2	AHZ	C	500	38/38	0.99	0.04	23,34,50,51	0
2	AHZ	D	500	38/38	0.99	0.05	33,42,56,58	0
2	AHZ	E	500	38/38	0.99	0.05	34,39,57,59	0
3	FE2	F	345	1/1	0.99	0.05	88,88,88,88	0
2	AHZ	F	500	38/38	0.99	0.04	26,32,48,50	0
3	FE2	H	345	1/1	0.99	0.04	100,100,100,100	0
2	AHZ	G	500	38/38	0.99	0.04	23,33,51,51	0
2	AHZ	H	500	38/38	0.99	0.06	33,37,59,61	0
2	AHZ	I	500	38/38	0.99	0.04	22,29,47,49	0
3	FE2	K	346	1/1	0.99	0.04	100,100,100,100	0
2	AHZ	J	500	38/38	0.99	0.05	33,38,55,57	0
3	FE2	M	345	1/1	0.99	0.04	91,91,91,91	0
2	AHZ	K	500	38/38	0.99	0.05	33,36,48,50	0
2	AHZ	L	500	38/38	0.99	0.05	34,40,63,64	0

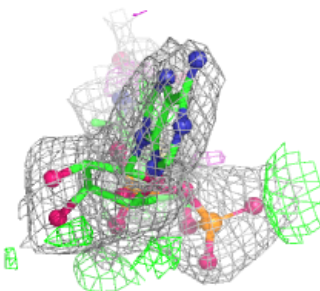
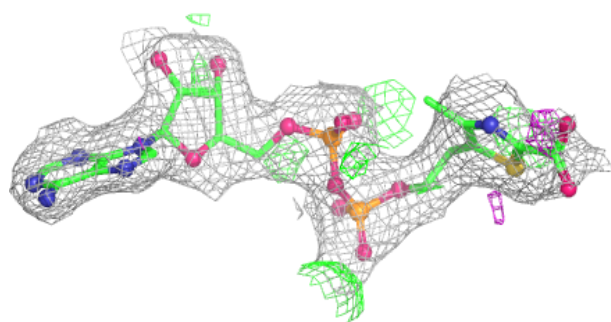
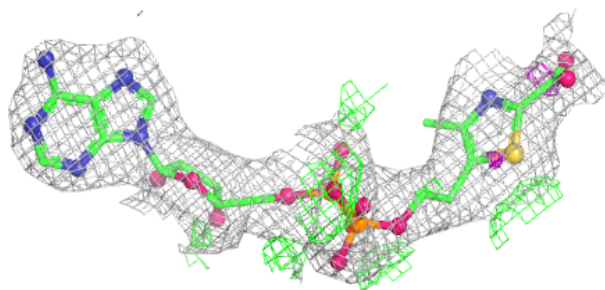
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around AHZ M 500:

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

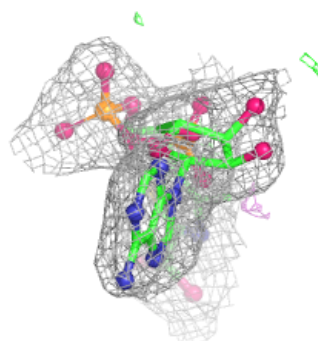
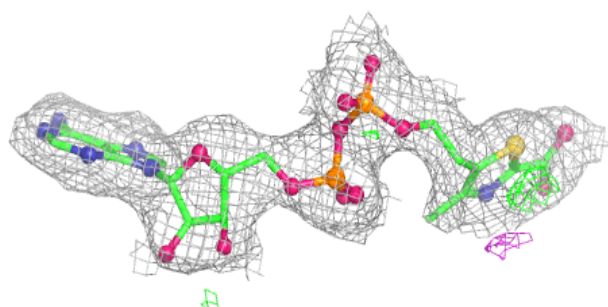
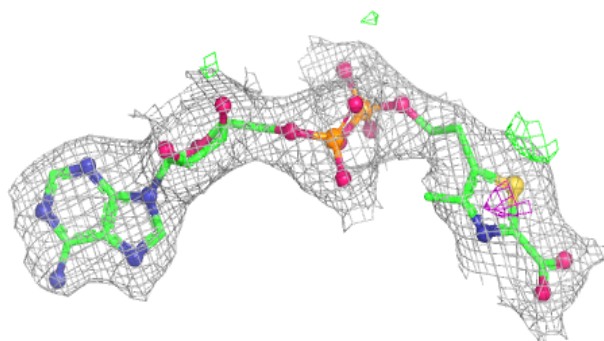
**Electron density around AHZ B 500:**

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

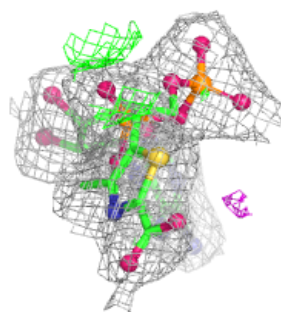
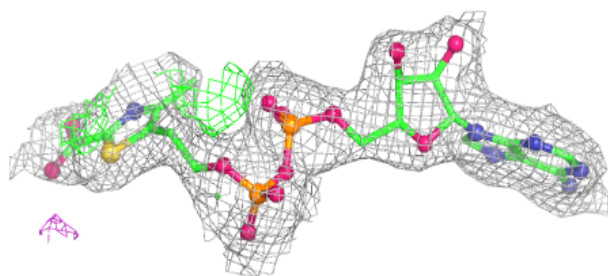
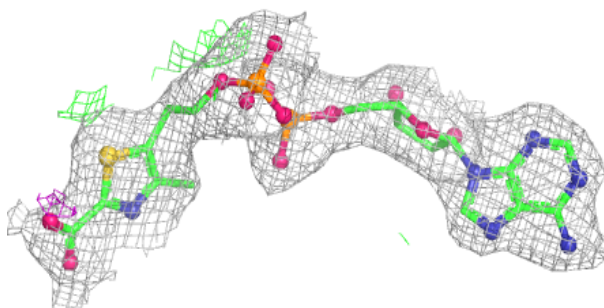


Electron density around AHZ A 500:

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

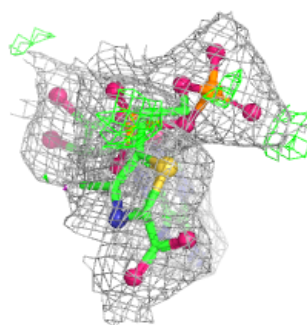
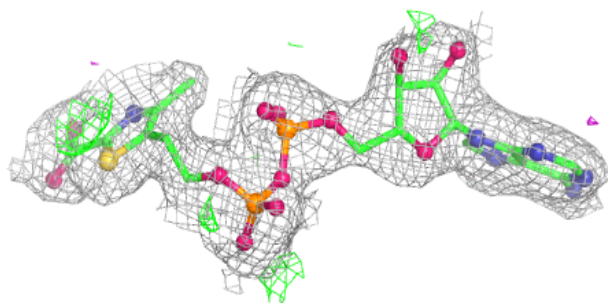
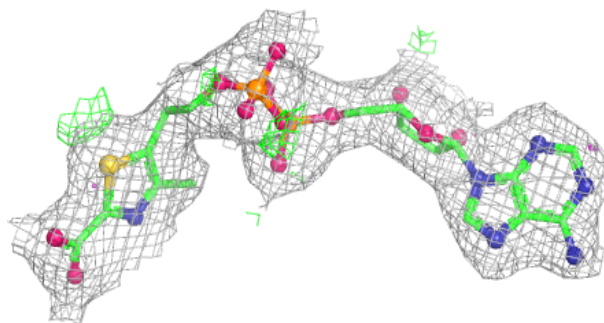
**Electron density around AHZ N 500:**

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

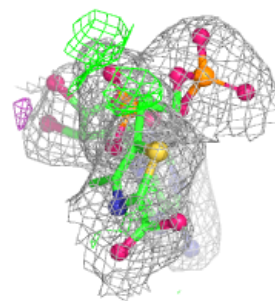
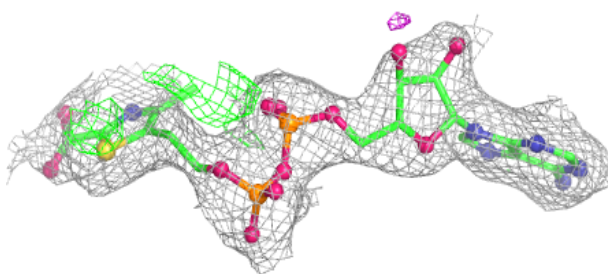
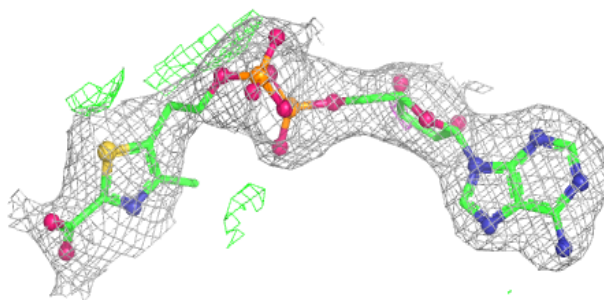


Electron density around AHZ O 500:

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and green (positive)

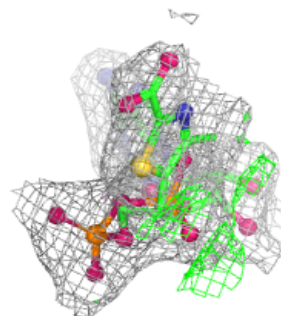
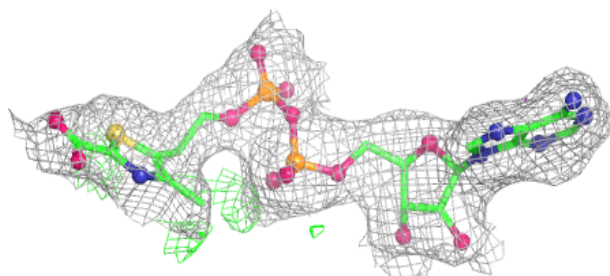
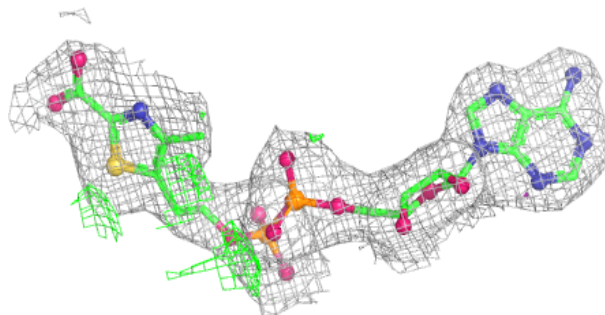
**Electron density around AHZ P 500:**

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

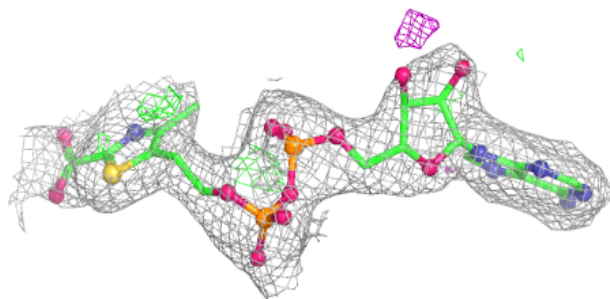
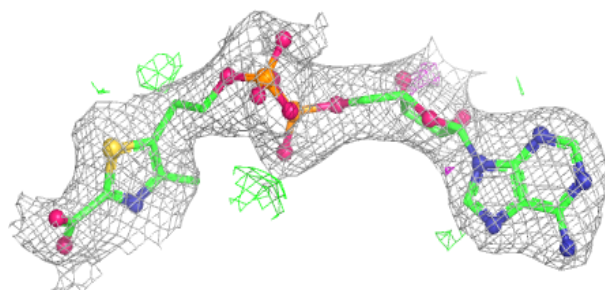


Electron density around AHZ C 500:

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

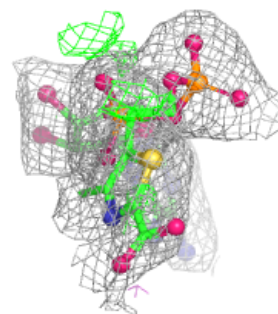
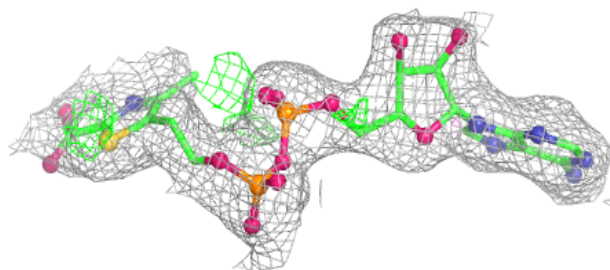
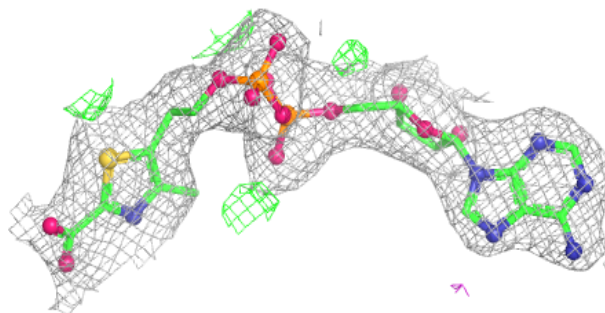
**Electron density around AHZ D 500:**

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and green (positive)

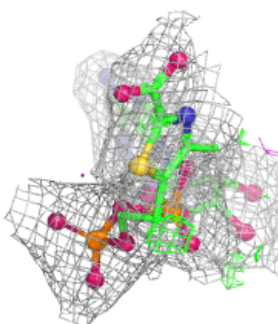
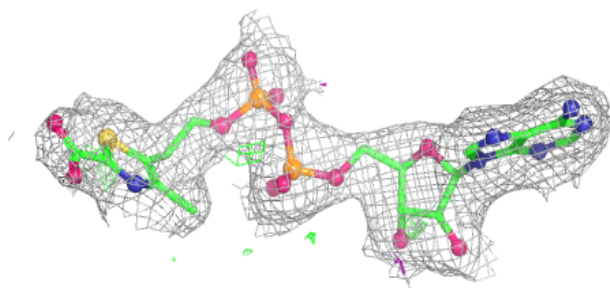
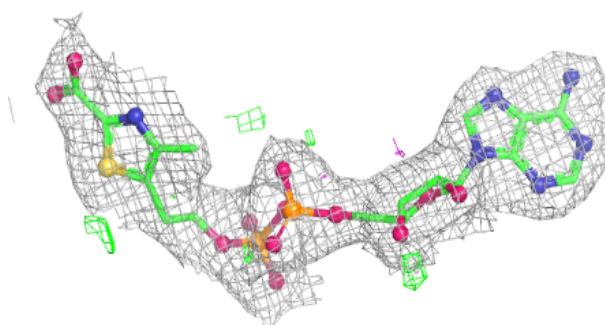


Electron density around AHZ E 500:

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and green (positive)

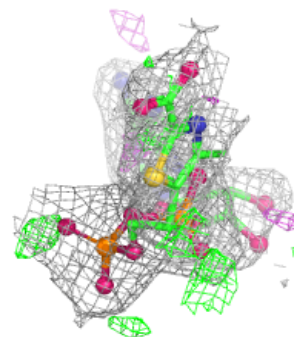
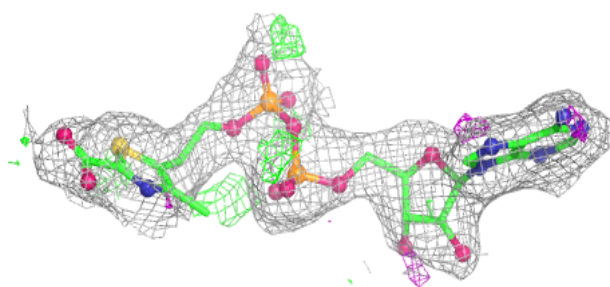
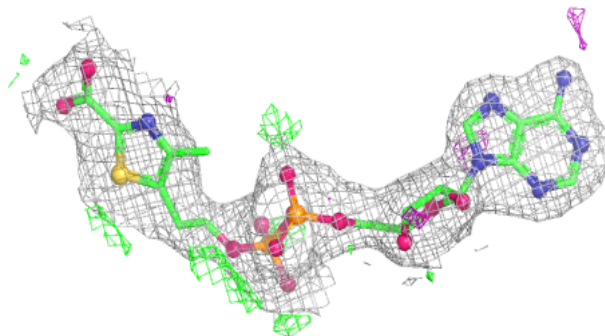
**Electron density around AHZ F 500:**

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

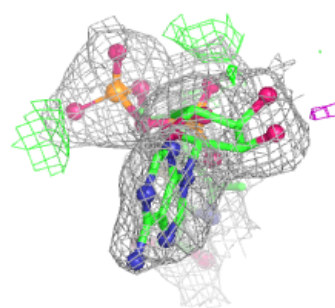
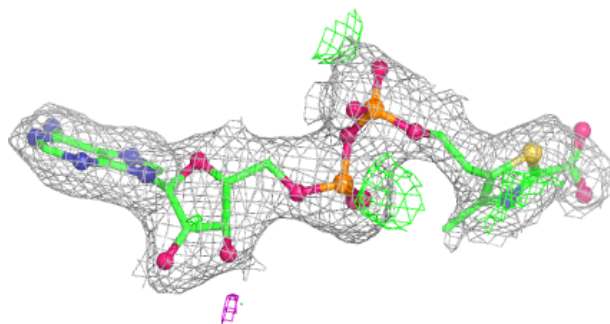
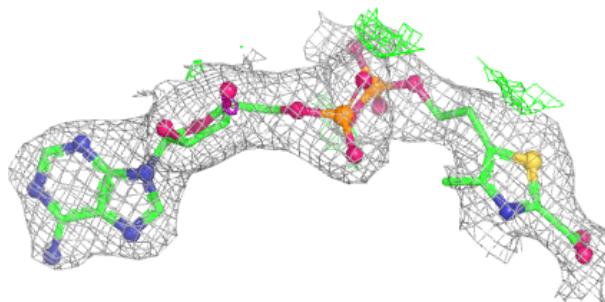


Electron density around AHZ G 500:

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and green (positive)

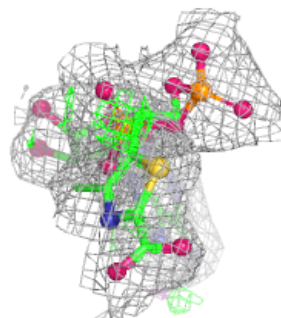
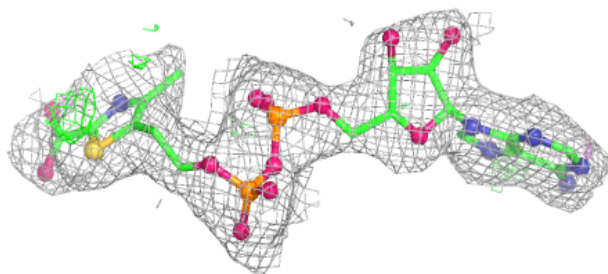
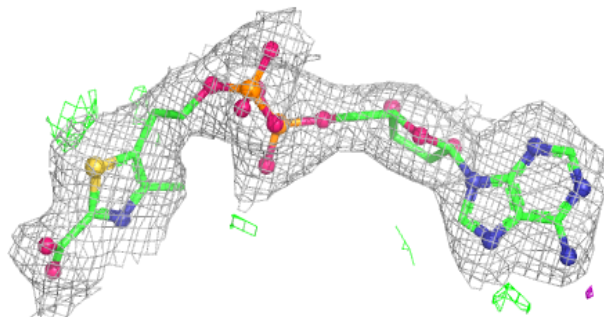
**Electron density around AHZ H 500:**

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and green (positive)

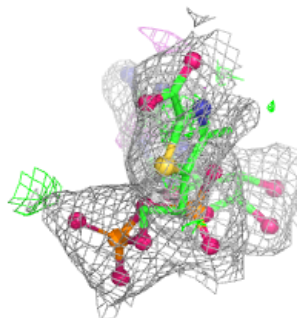
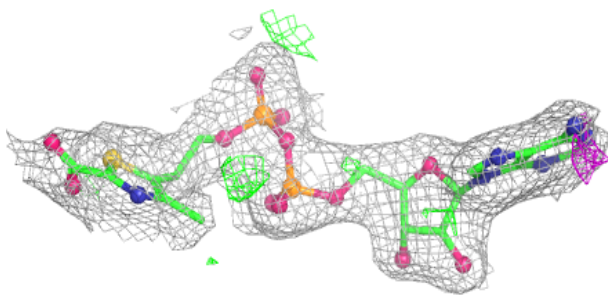
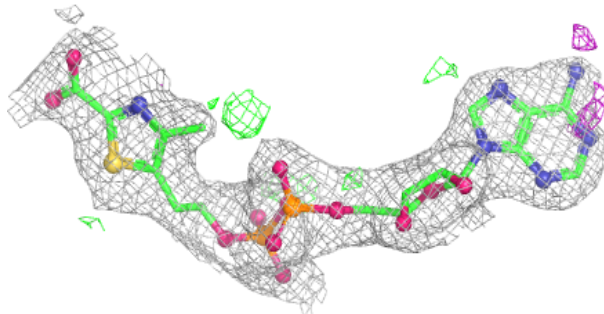


Electron density around AHZ I 500:

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

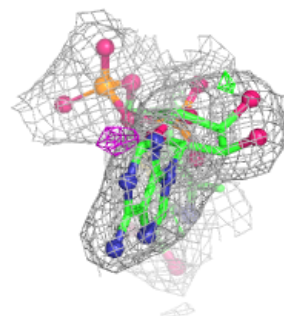
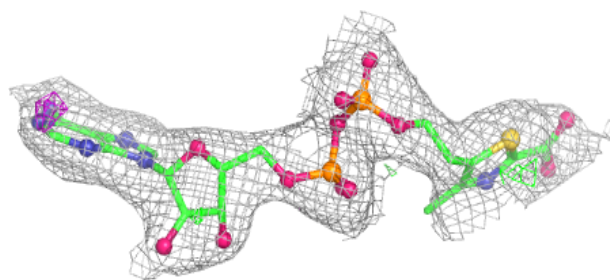
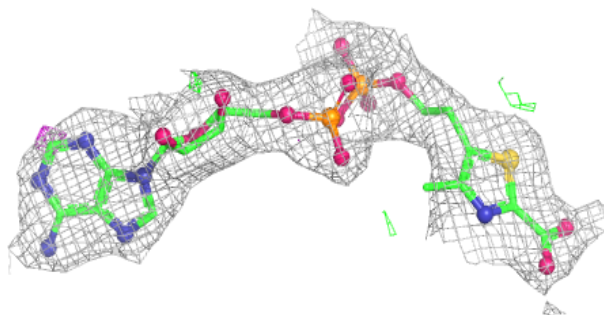
**Electron density around AHZ J 500:**

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

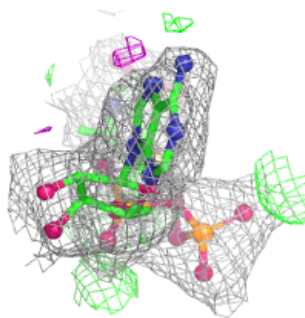
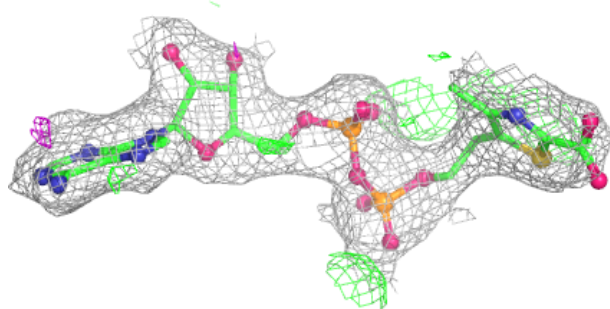
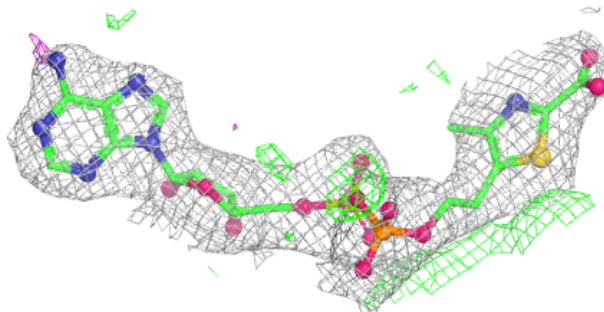


Electron density around AHZ K 500:

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

**Electron density around AHZ L 500:**

$2mF_o-DF_c$ (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.