



wwPDB X-ray Structure Validation Summary Report ⓘ

May 14, 2020 – 09:38 pm BST

PDB ID : 5KNN
Title : Evolutionary gain of alanine mischarging to non-cognate tRNAs with a G4:U69 base pair
Authors : Sun, L.; He, W.; Yang, X.-L.
Deposited on : 2016-06-28
Resolution : 2.68 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

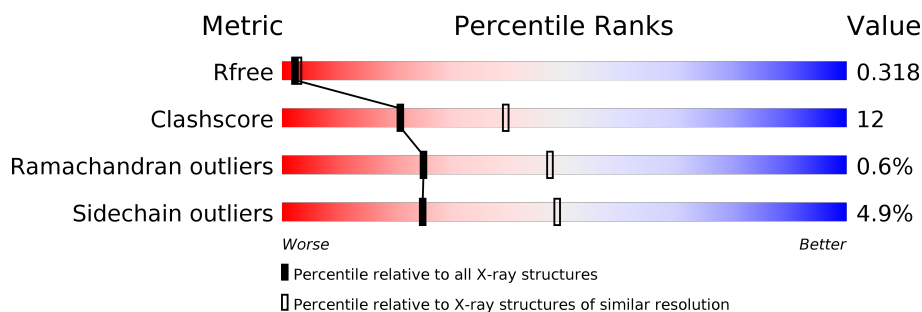
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.68 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}	130704	3863 (2.70-2.66)
Clashscore	141614	4210 (2.70-2.66)
Ramachandran outliers	138981	4141 (2.70-2.66)
Sidechain outliers	138945	4141 (2.70-2.66)

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 on 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	450	78% 19% .
1	B	450	73% 22% . .
1	C	450	66% 26% 5% . .
1	D	450	72% 23% . .
1	E	450	74% 22% . .
1	F	450	74% 23% . .
1	G	450	73% 24% . .

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Mol	Chain	Length	Quality of chain
1	H	450	 A horizontal bar chart showing the quality of the chain. The bar is divided into four segments: green (69%), yellow (25%), orange, and red. Below the green segment is the label '69%' and below the yellow segment is '25%'. To the right of the bar are two small black dots.

2 Entry composition

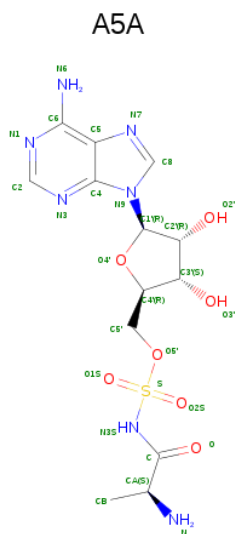
There are 2 unique types of molecules in this entry. The entry contains 28584 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Alanine-tRNA ligase, cytoplasmic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	450	Total	C	N	O	S	0	0	0
			3560	2255	613	676	16			
1	B	450	Total	C	N	O	S	0	0	0
			3560	2255	613	676	16			
1	C	444	Total	C	N	O	S	0	0	0
			3514	2227	604	667	16			
1	D	447	Total	C	N	O	S	0	0	0
			3536	2241	608	671	16			
1	E	450	Total	C	N	O	S	0	0	0
			3560	2255	613	676	16			
1	F	449	Total	C	N	O	S	0	0	0
			3551	2250	611	674	16			
1	G	449	Total	C	N	O	S	0	0	0
			3551	2250	611	674	16			
1	H	446	Total	C	N	O	S	0	0	0
			3528	2235	607	670	16			

- Molecule 2 is '5'-O-(N-(L-ALANYL)-SULFAMOYL)ADENOSINE (three-letter code: A5A) (formula: C₁₃H₁₉N₇O₇S).

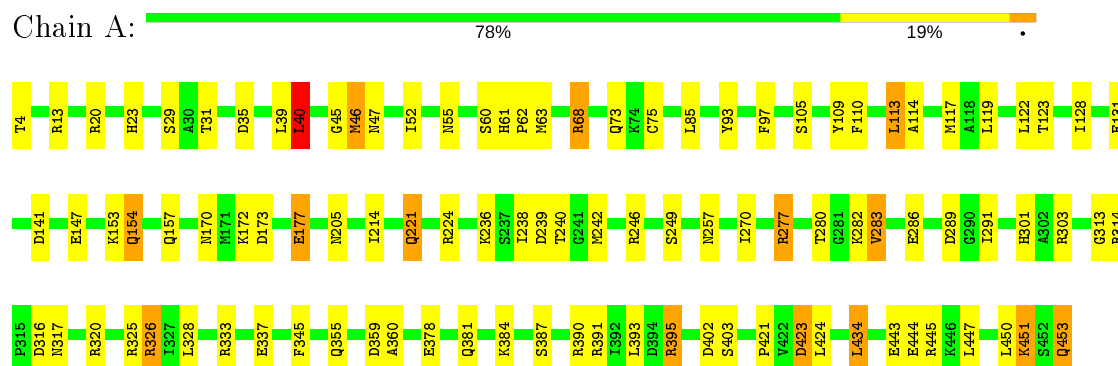


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 28	C 13	N 7	O 7	S 1	0	0
2	B	1	Total 28	C 13	N 7	O 7	S 1	0	0
2	C	1	Total 28	C 13	N 7	O 7	S 1	0	0
2	D	1	Total 28	C 13	N 7	O 7	S 1	0	0
2	E	1	Total 28	C 13	N 7	O 7	S 1	0	0
2	F	1	Total 28	C 13	N 7	O 7	S 1	0	0
2	G	1	Total 28	C 13	N 7	O 7	S 1	0	0
2	H	1	Total 28	C 13	N 7	O 7	S 1	0	0

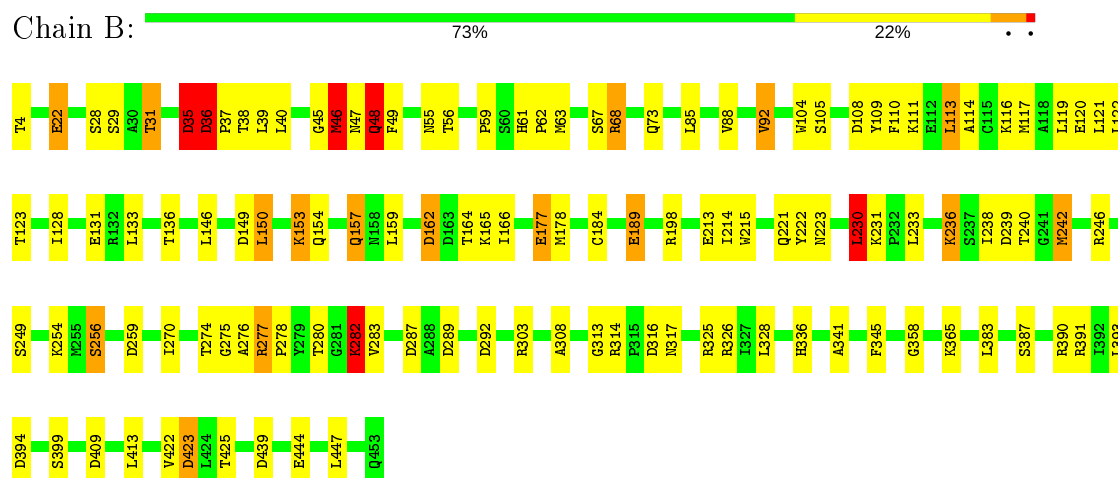
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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. 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. 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.

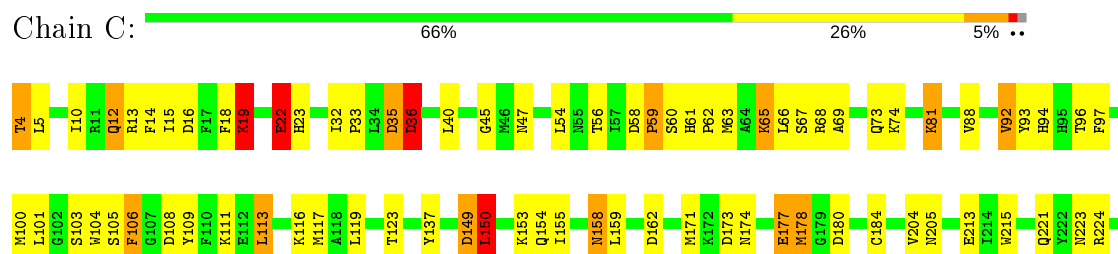
- Molecule 1: Alanine-tRNA ligase, cytoplasmic

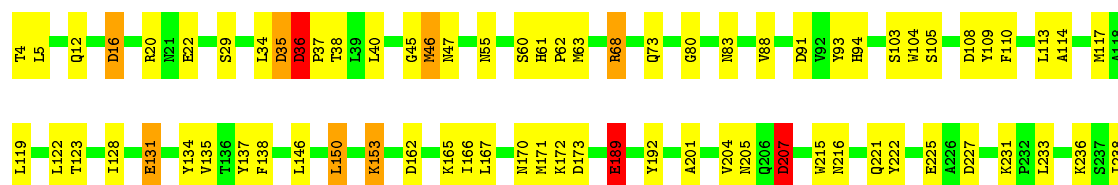


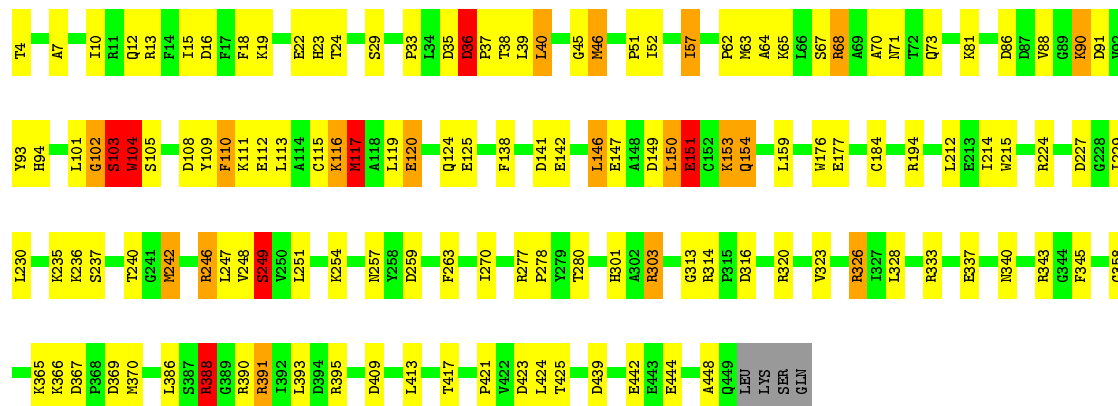
- Molecule 1: Alanine-tRNA ligase, cytoplasmic



- Molecule 1: Alanine-tRNA ligase, cytoplasmic







4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	52.17Å 98.26Å 201.38Å 90.07° 89.95° 90.11°	Depositor
Resolution (Å)	49.13 – 2.68 49.13 – 2.68	Depositor EDS
% Data completeness (in resolution range)	93.4 (49.13-2.68) 99.4 (49.13-2.68)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.31 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0107	Depositor
R, R_{free}	0.216 , 0.254 0.282 , 0.318	Depositor DCC
R_{free} test set	5439 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	47.6	Xtriage
Anisotropy	0.130	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 22.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.066 for h,-k,-l 0.079 for -h,k,-l 0.146 for -h,-k,l	Xtriage
Reported twinning fraction	0.441 for H, K, L 0.076 for -h,-k,l 0.275 for h,-k,-l 0.209 for -H, K, -L	Depositor
Outliers	0 of 112184 reflections	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	28584	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.34% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: A5A

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	0.77	1/3635 (0.0%)	1.01	22/4915 (0.4%)
1	B	0.78	4/3635 (0.1%)	1.01	26/4915 (0.5%)
1	C	0.86	6/3589 (0.2%)	1.16	39/4854 (0.8%)
1	D	0.81	2/3611 (0.1%)	1.11	29/4884 (0.6%)
1	E	0.79	2/3635 (0.1%)	1.04	26/4915 (0.5%)
1	F	0.80	1/3626 (0.0%)	0.99	22/4903 (0.4%)
1	G	0.81	0/3626	1.08	28/4903 (0.6%)
1	H	0.87	5/3603 (0.1%)	1.16	36/4873 (0.7%)
All	All	0.81	21/28960 (0.1%)	1.07	228/39162 (0.6%)

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	1
1	B	0	2
1	C	0	2
1	E	0	1
1	F	0	1
1	G	0	1
1	H	0	4
All	All	0	12

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	151	GLU	C-O	-7.96	1.08	1.23
1	C	149	ASP	CG-OD2	-7.35	1.08	1.25
1	C	442	GLU	CD-OE1	7.21	1.33	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	177	GLU	CD-OE1	6.73	1.33	1.25
1	B	177	GLU	CD-OE1	-6.72	1.18	1.25

The worst 5 of 228 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	149	ASP	CB-CG-OD1	13.34	130.31	118.30
1	E	402	ASP	CB-CG-OD2	-12.89	106.70	118.30
1	H	303	ARG	NE-CZ-NH1	11.53	126.07	120.30
1	D	367	ASP	CB-CG-OD1	11.23	128.41	118.30
1	D	367	ASP	CB-CG-OD2	-10.24	109.09	118.30

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	451	LYS	Peptide
1	B	277	ARG	Peptide
1	B	36	ASP	Peptide
1	C	22	GLU	Peptide
1	C	36	ASP	Peptide

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	3560	0	3499	56	1
1	B	3560	0	3499	90	0
1	C	3514	0	3449	127	0
1	D	3536	0	3473	79	1
1	E	3560	0	3499	79	2
1	F	3551	0	3491	79	2
1	G	3551	0	3491	86	1
1	H	3528	0	3462	119	1
2	A	28	0	19	1	0
2	B	28	0	19	0	0
2	C	28	0	19	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	28	0	19	1	0
2	E	28	0	19	2	0
2	F	28	0	19	0	0
2	G	28	0	19	0	0
2	H	28	0	19	0	0
All	All	28584	0	28015	692	4

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 12.

The worst 5 of 692 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:277:ARG:NH2	1:A:289:ASP:OD2	1.76	1.18
1:H:40:LEU:O	1:H:320:ARG:NH1	1.84	1.10
1:H:10:ILE:HD11	1:H:251:LEU:HD12	1.16	1.09
1:F:153:LYS:CE	1:F:166:ILE:HG23	1.86	1.04
1:B:222:TYR:HB3	1:B:230:LEU:HD22	1.39	1.01

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:377:GLU:OE1	1:F:395:ARG:NH1[1_546]	1.89	0.31
1:A:154:GLN:NE2	1:F:55:ASN:O[1_545]	2.10	0.10
1:E:445:ARG:NE	1:G:405:THR:OG1[1_655]	2.12	0.08
1:D:388:ARG:NH2	1:H:366:LYS:O[1_645]	2.15	0.05

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	448/450 (100%)	436 (97%)	11 (2%)	1 (0%)	47	71
1	B	448/450 (100%)	431 (96%)	12 (3%)	5 (1%)	14	31
1	C	442/450 (98%)	426 (96%)	12 (3%)	4 (1%)	17	37
1	D	445/450 (99%)	431 (97%)	14 (3%)	0	100	100
1	E	448/450 (100%)	436 (97%)	11 (2%)	1 (0%)	47	71
1	F	447/450 (99%)	434 (97%)	11 (2%)	2 (0%)	34	58
1	G	447/450 (99%)	429 (96%)	15 (3%)	3 (1%)	22	44
1	H	444/450 (99%)	421 (95%)	18 (4%)	5 (1%)	14	31
All	All	3569/3600 (99%)	3444 (96%)	104 (3%)	21 (1%)	25	47

5 of 21 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	35	ASP
1	B	37	PRO
1	C	22	GLU
1	F	37	PRO
1	H	37	PRO

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	379/379 (100%)	360 (95%)	19 (5%)	24	47
1	B	379/379 (100%)	358 (94%)	21 (6%)	21	43
1	C	374/379 (99%)	355 (95%)	19 (5%)	24	46
1	D	376/379 (99%)	357 (95%)	19 (5%)	24	46
1	E	379/379 (100%)	363 (96%)	16 (4%)	30	55
1	F	378/379 (100%)	362 (96%)	16 (4%)	30	55
1	G	378/379 (100%)	361 (96%)	17 (4%)	27	52
1	H	375/379 (99%)	353 (94%)	22 (6%)	19	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3018/3032 (100%)	2869 (95%)	149 (5%)	25 49

5 of 149 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	92	VAL
1	E	155	ILE
1	H	230	LEU
1	D	150	LEU
1	D	390	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	340	ASN
1	E	154	GLN
1	H	257	ASN
1	E	94	HIS
1	E	205	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

8 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	A5A	H	500	-	26,30,30	1.40	5 (19%)	30,45,45	1.67	3 (10%)
2	A5A	B	500	-	26,30,30	1.72	5 (19%)	30,45,45	2.38	8 (26%)
2	A5A	C	500	-	26,30,30	1.83	7 (26%)	30,45,45	2.34	10 (33%)
2	A5A	A	500	-	26,30,30	1.59	3 (11%)	30,45,45	3.02	11 (36%)
2	A5A	F	500	-	26,30,30	2.04	6 (23%)	30,45,45	2.09	7 (23%)
2	A5A	G	500	-	26,30,30	1.40	4 (15%)	30,45,45	1.99	7 (23%)
2	A5A	D	500	-	26,30,30	1.35	5 (19%)	30,45,45	2.51	10 (33%)
2	A5A	E	500	-	26,30,30	1.48	5 (19%)	30,45,45	2.28	6 (20%)

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	A5A	H	500	-	-	0/14/35/35	0/3/3/3
2	A5A	B	500	-	-	5/14/35/35	0/3/3/3
2	A5A	C	500	-	-	4/14/35/35	0/3/3/3
2	A5A	A	500	-	-	4/14/35/35	0/3/3/3
2	A5A	F	500	-	-	5/14/35/35	0/3/3/3
2	A5A	G	500	-	-	2/14/35/35	0/3/3/3
2	A5A	D	500	-	-	3/14/35/35	0/3/3/3
2	A5A	E	500	-	-	4/14/35/35	0/3/3/3

The worst 5 of 40 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	500	A5A	O1S-S	5.99	1.47	1.42
2	F	500	A5A	O2S-S	4.80	1.46	1.42
2	B	500	A5A	O2S-S	4.74	1.46	1.42
2	A	500	A5A	O2S-S	4.72	1.46	1.42
2	C	500	A5A	O5'-S	-4.45	1.50	1.59

The worst 5 of 62 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	A5A	O2S-S-O1S	-13.49	99.75	120.76
2	E	500	A5A	O2S-S-O1S	-9.56	105.87	120.76
2	B	500	A5A	O2S-S-O1S	-9.00	106.74	120.76
2	D	500	A5A	O2S-S-O1S	-8.75	107.13	120.76
2	G	500	A5A	O2S-S-O1S	-7.88	108.48	120.76

There are no chirality outliers.

5 of 27 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	500	A5A	C5'-O5'-S-N3S
2	C	500	A5A	C5'-O5'-S-N3S
2	C	500	A5A	C5'-O5'-S-O2S
2	C	500	A5A	C3'-C4'-C5'-O5'
2	A	500	A5A	C5'-O5'-S-N3S

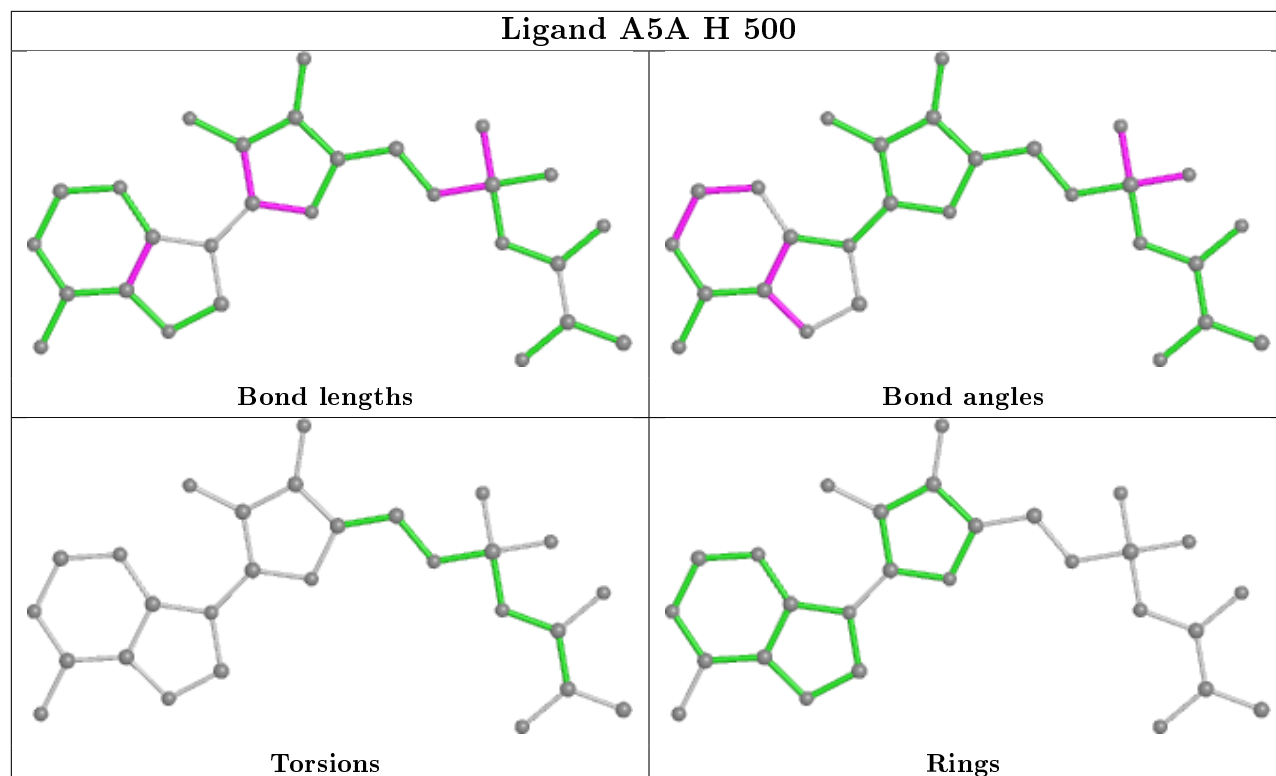
There are no ring outliers.

4 monomers are involved in 7 short contacts:

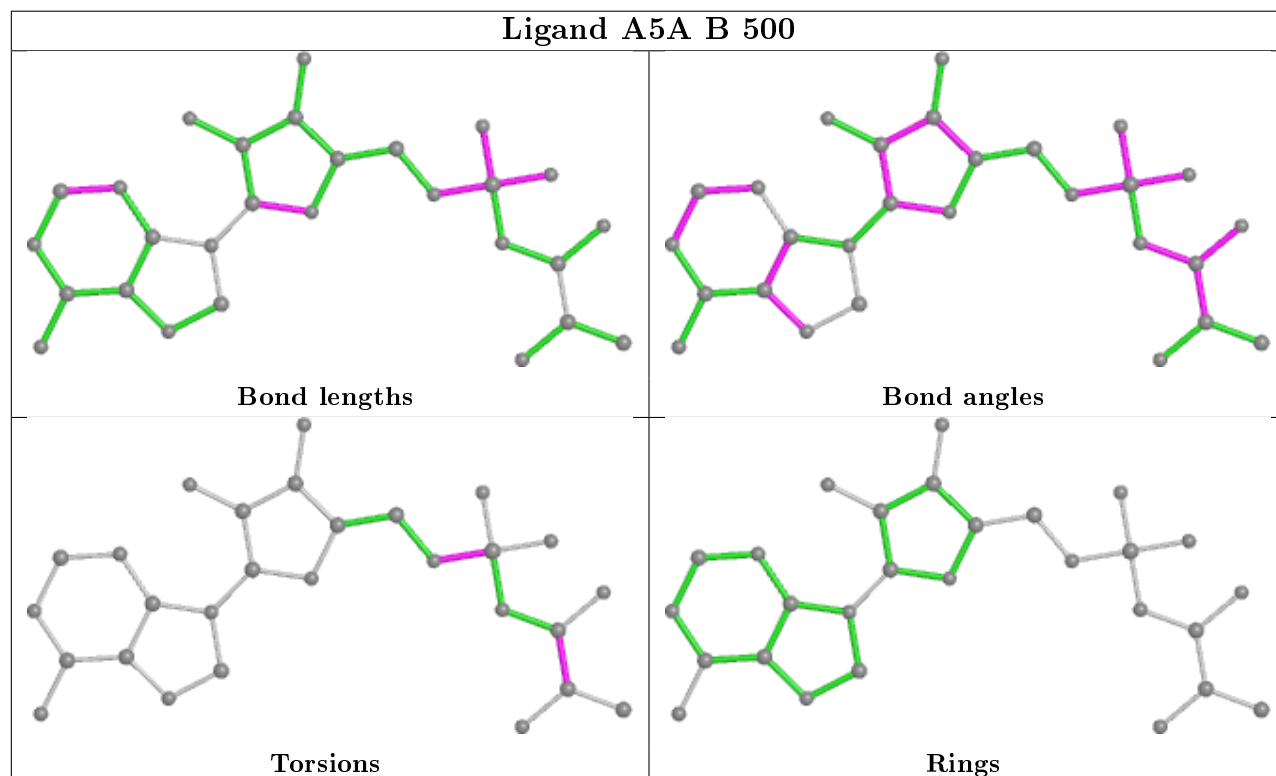
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	500	A5A	3	0
2	A	500	A5A	1	0
2	D	500	A5A	1	0
2	E	500	A5A	2	0

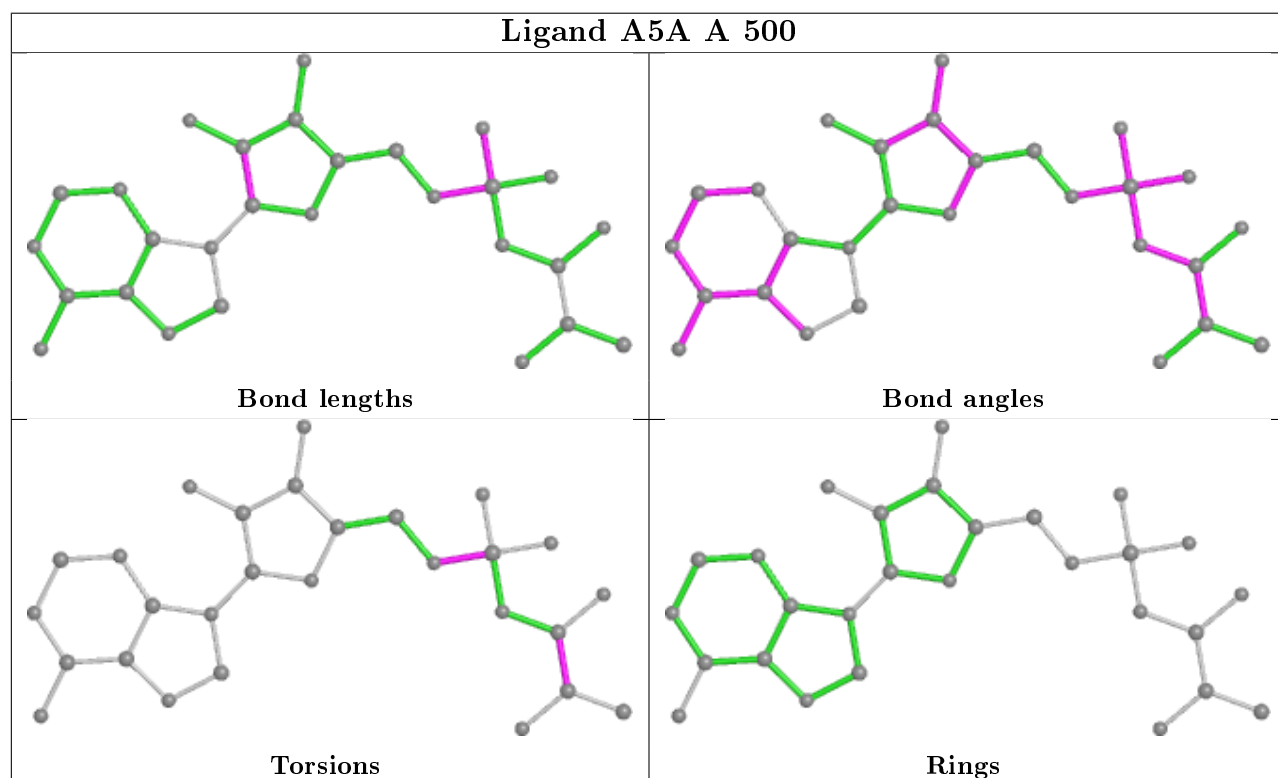
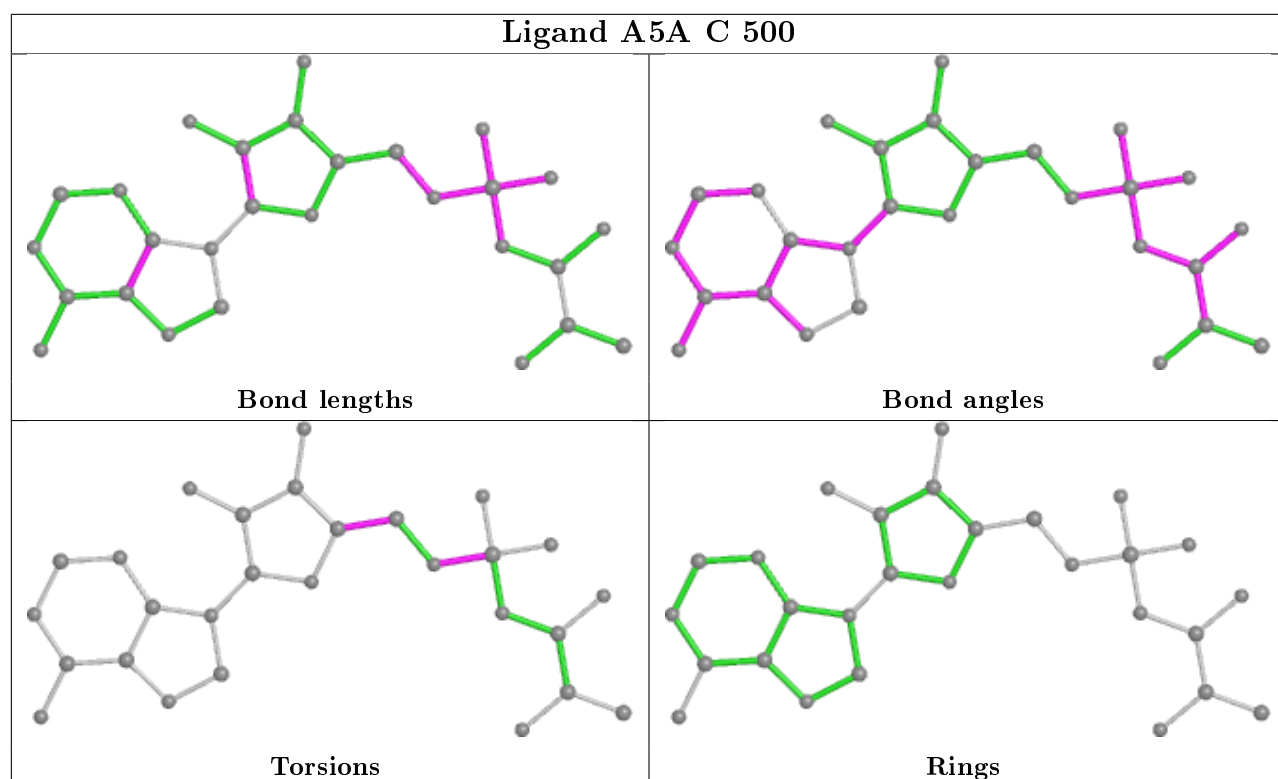
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 A5A H 500

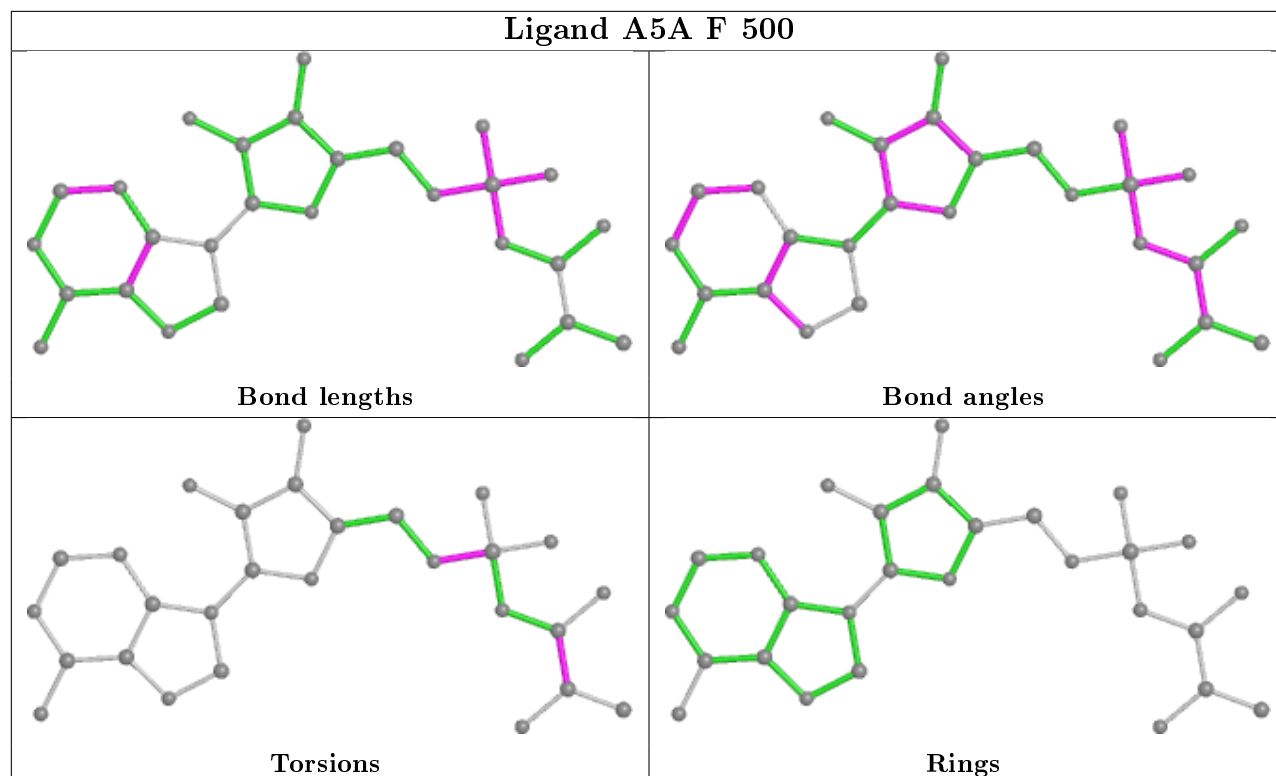


Ligand A5A B 500

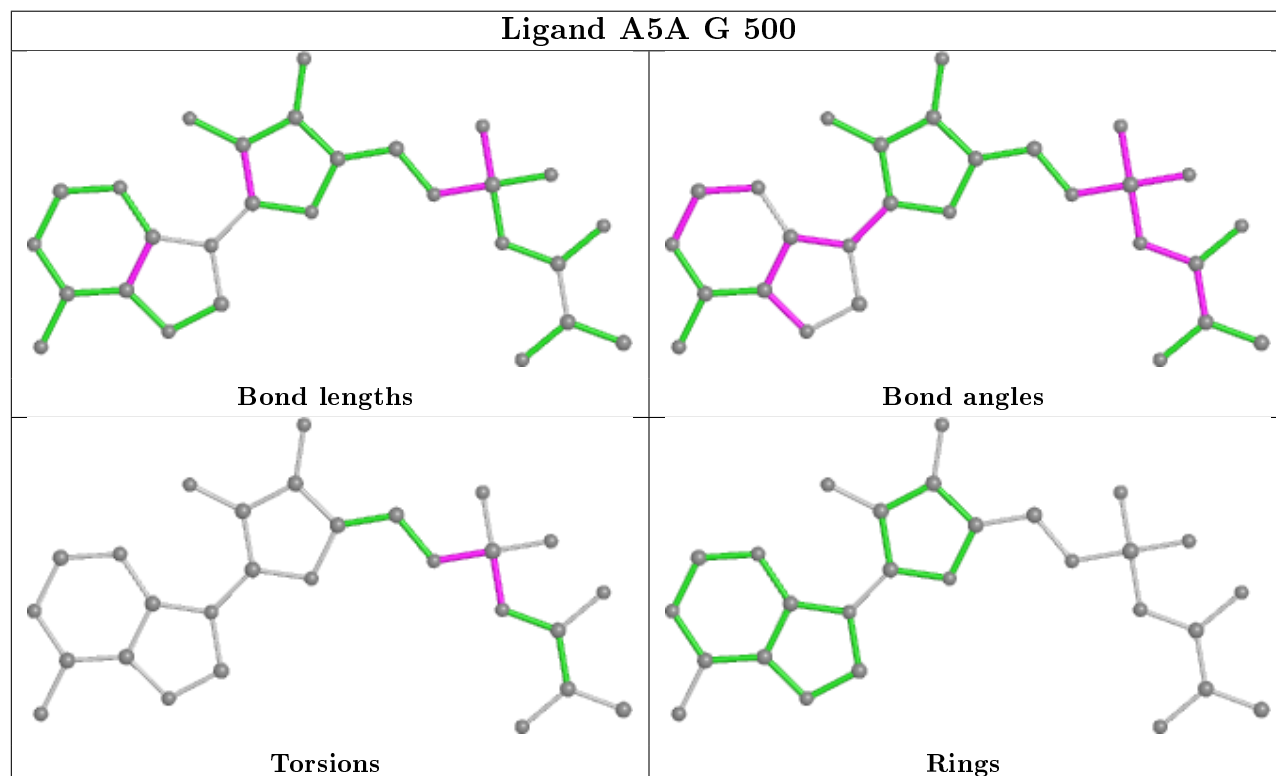


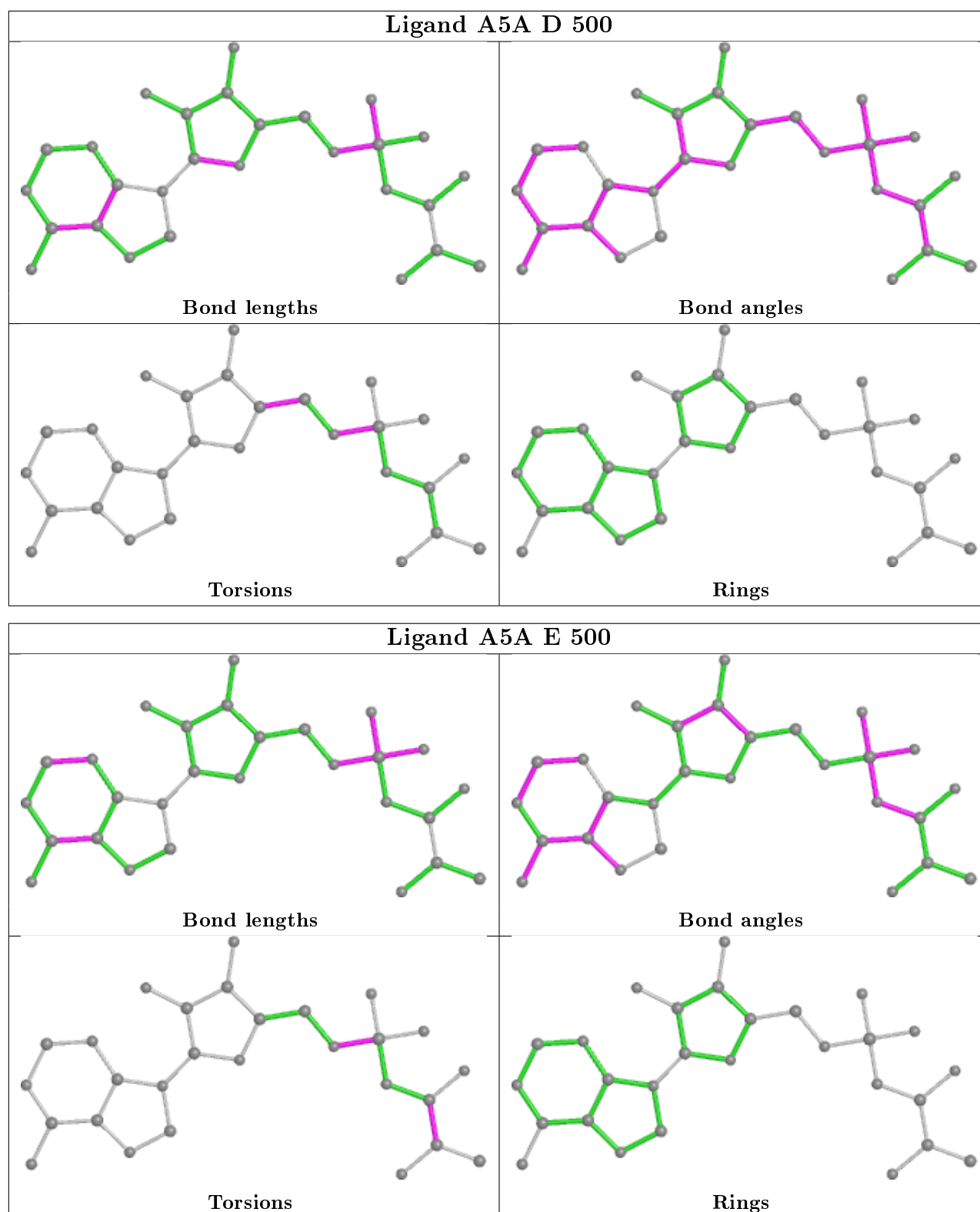


Ligand A5A F 500



Ligand A5A G 500





5.7 Other polymers ⓘ

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

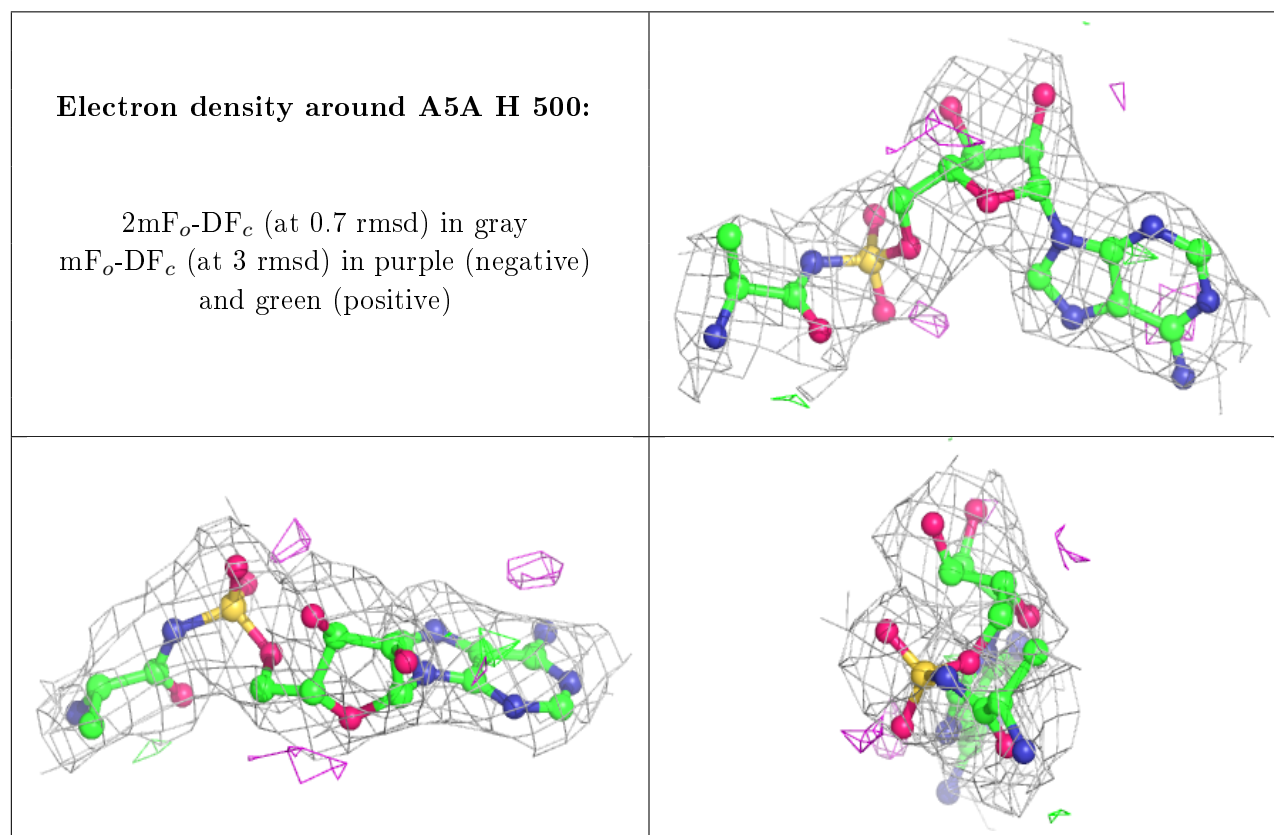
6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands ⓘ

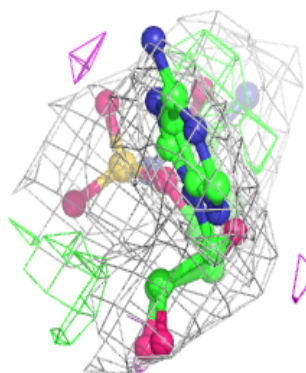
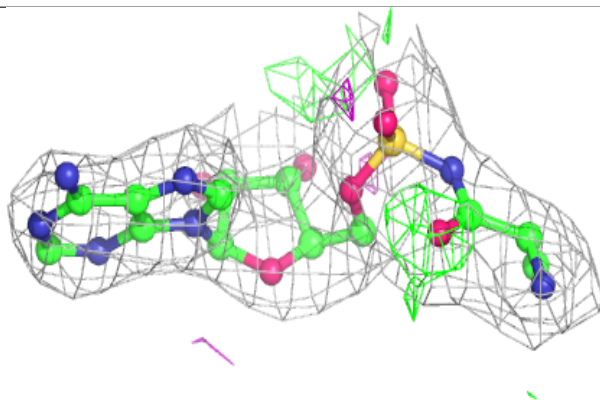
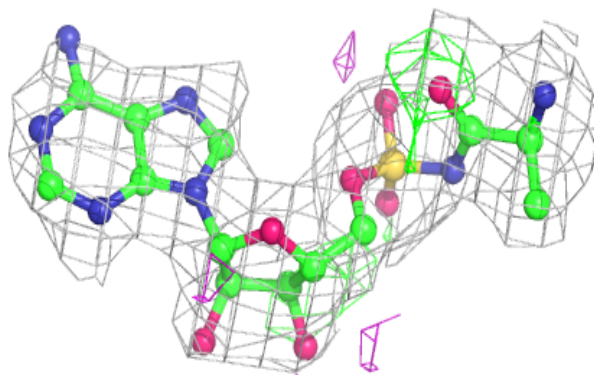
Unable to reproduce the depositors R factor - this section is therefore empty.

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.

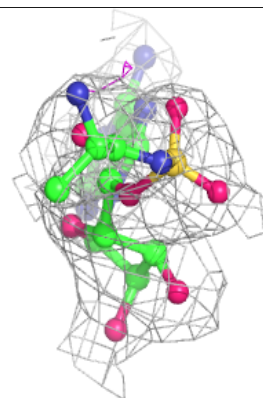
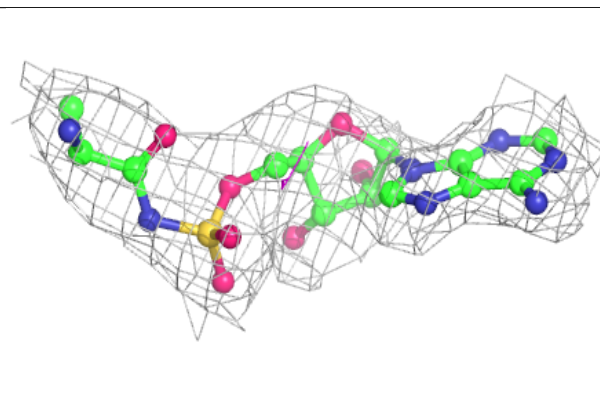
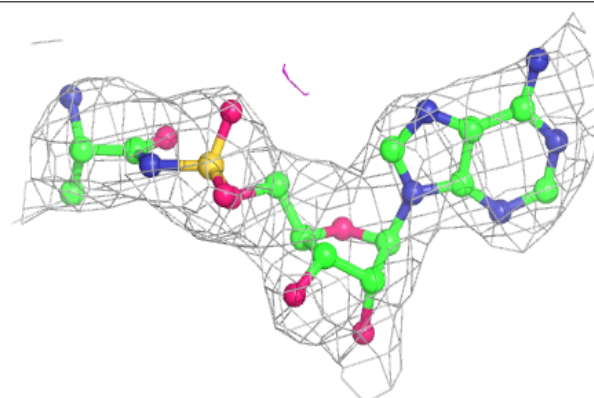


Electron density around A5A B 500:

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

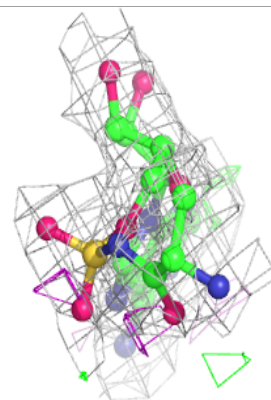
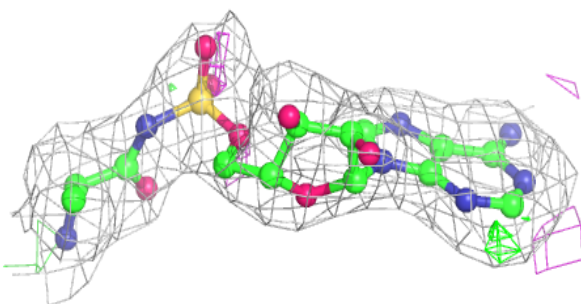
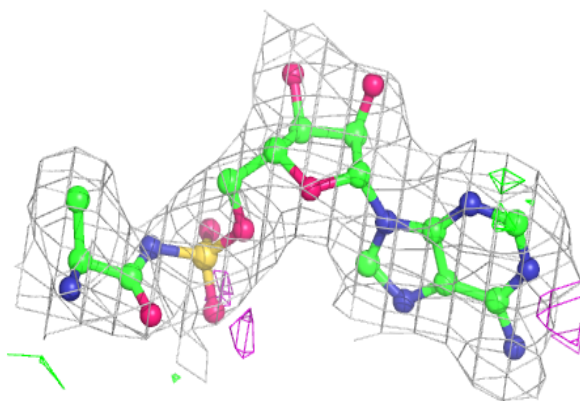
**Electron density around A5A C 500:**

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

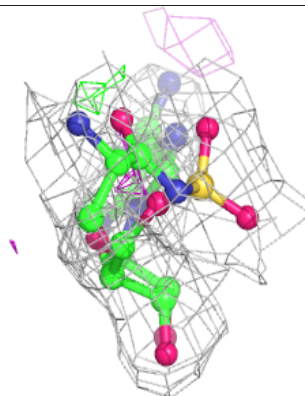
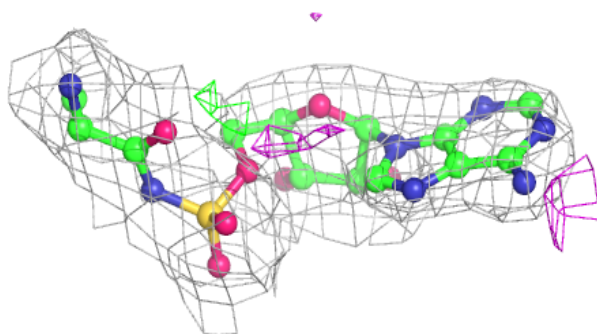
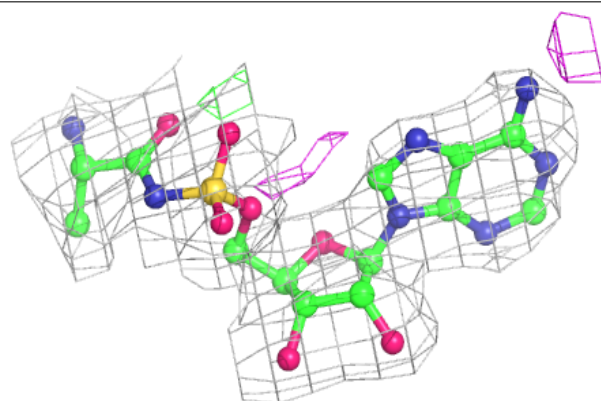


Electron density around A5A A 500:

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

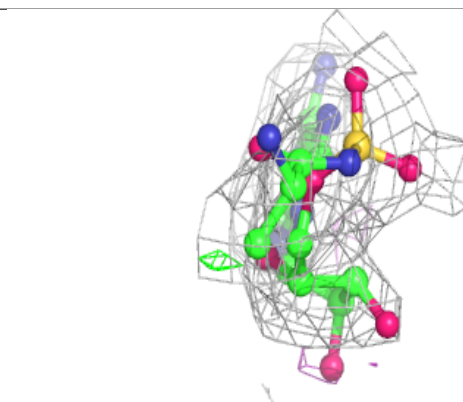
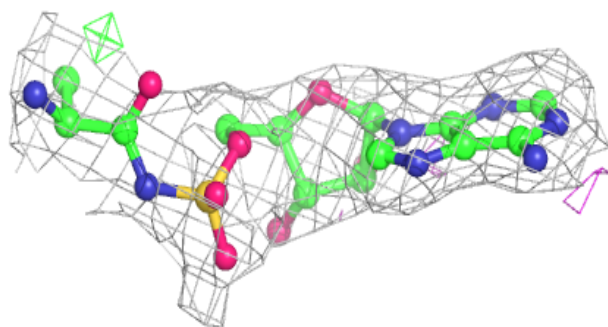
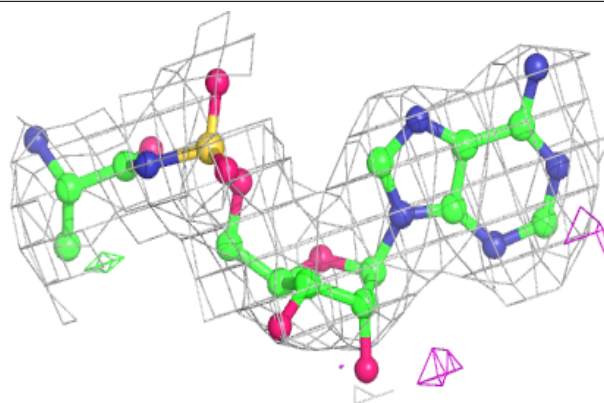
**Electron density around A5A F 500:**

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

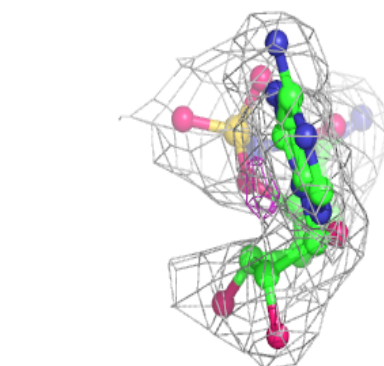
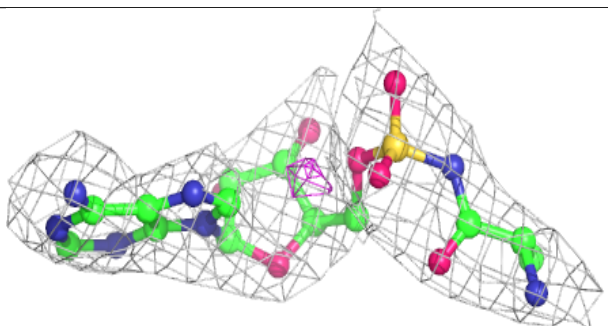
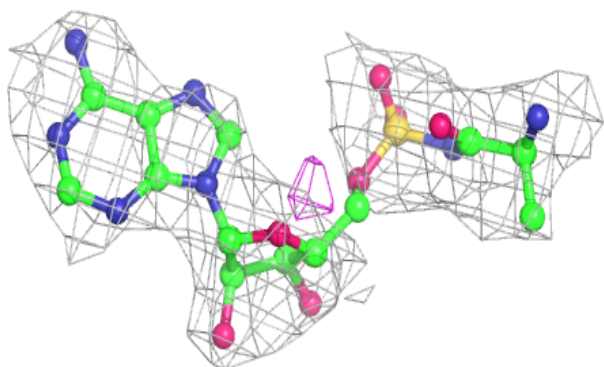


Electron density around A5A G 500:

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

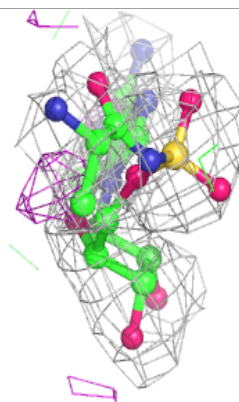
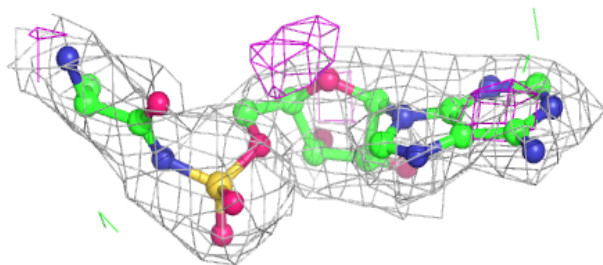
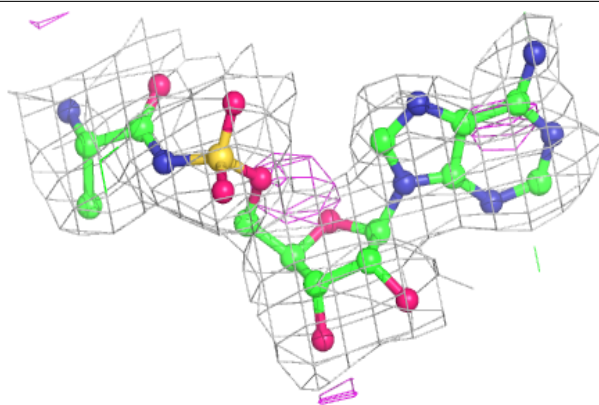
**Electron density around A5A D 500:**

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



Electron density around A5A E 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](#)

Unable to reproduce the depositors R factor - this section is therefore empty.