



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 28, 2023 – 03:45 AM EDT

PDB ID : 3KFK
Title : Crystal structures of a group II chaperonin from *Methanococcus maripaludis*
Authors : Pereira, J.H.; Ralston, C.Y.; Douglas, N.; Meyer, D.; Knee, K.M.; Goulet, D.R.; King, J.A.; Frydman, J.; Adams, P.D.
Deposited on : 2009-10-27
Resolution : 6.00 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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35
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) : 2.35

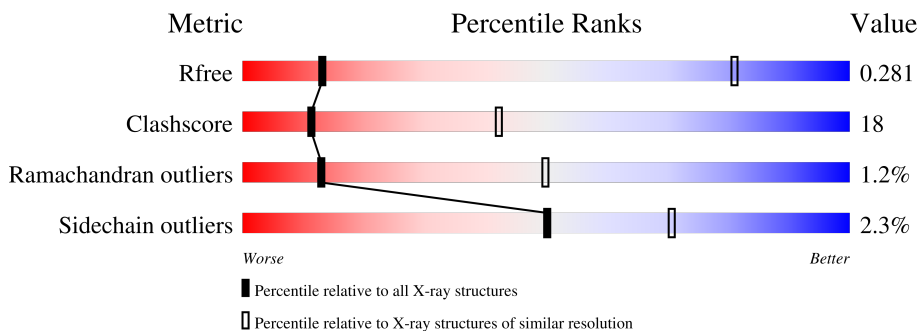
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 6.00 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	1000 (8.00-3.88)
Clashscore	141614	1049 (8.00-3.90)
Ramachandran outliers	138981	1016 (8.00-3.86)
Sidechain outliers	138945	1017 (8.00-3.82)

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	521	75% (green), 17% (yellow), 7% (orange), 7% (grey)
1	B	521	69% (green), 23% (yellow), 7% (orange), 7% (grey)
1	C	521	72% (green), 20% (yellow), 7% (orange), 7% (grey)
1	D	521	75% (green), 15% (yellow), 7% (orange), 7% (grey)

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
2	AGS	D	544	-	-	X	-

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 14619 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 Chaperonin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	487	3629	2249	631	725	24	0	0	0
1	B	487	3629	2249	631	725	24	0	0	0
1	C	487	3629	2249	631	725	24	0	0	0
1	D	484	3608	2235	627	722	24	0	0	0

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ILE	deletion	UNP Q877G8
A	?	-	LYS	deletion	UNP Q877G8
A	?	-	GLU	deletion	UNP Q877G8
A	?	-	THR	deletion	UNP Q877G8
A	?	-	ASP	deletion	UNP Q877G8
A	?	-	ALA	deletion	UNP Q877G8
A	?	-	GLU	deletion	UNP Q877G8
A	?	-	ILE	deletion	UNP Q877G8
A	?	-	ARG	deletion	UNP Q877G8
A	?	-	ILE	deletion	UNP Q877G8
A	?	-	THR	deletion	UNP Q877G8
A	?	-	ASP	deletion	UNP Q877G8
A	?	-	PRO	deletion	UNP Q877G8
A	?	-	LYS	deletion	UNP Q877G8
A	?	-	LEU	deletion	UNP Q877G8
A	?	-	MET	deletion	UNP Q877G8
A	?	-	GLU	deletion	UNP Q877G8
A	?	-	PHE	deletion	UNP Q877G8
A	?	-	ILE	deletion	UNP Q877G8
A	264	THR	GLN	engineered mutation	UNP Q877G8
A	265	ALA	GLU	engineered mutation	UNP Q877G8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	266	SER	GLU	engineered mutation	UNP Q877G8
A	267	GLU	LYS	engineered mutation	UNP Q877G8
B	?	-	ILE	deletion	UNP Q877G8
B	?	-	LYS	deletion	UNP Q877G8
B	?	-	GLU	deletion	UNP Q877G8
B	?	-	THR	deletion	UNP Q877G8
B	?	-	ASP	deletion	UNP Q877G8
B	?	-	ALA	deletion	UNP Q877G8
B	?	-	GLU	deletion	UNP Q877G8
B	?	-	ILE	deletion	UNP Q877G8
B	?	-	ARG	deletion	UNP Q877G8
B	?	-	ILE	deletion	UNP Q877G8
B	?	-	THR	deletion	UNP Q877G8
B	?	-	ASP	deletion	UNP Q877G8
B	?	-	PRO	deletion	UNP Q877G8
B	?	-	LYS	deletion	UNP Q877G8
B	?	-	LEU	deletion	UNP Q877G8
B	?	-	MET	deletion	UNP Q877G8
B	?	-	GLU	deletion	UNP Q877G8
B	?	-	PHE	deletion	UNP Q877G8
B	?	-	ILE	deletion	UNP Q877G8
B	264	THR	GLN	engineered mutation	UNP Q877G8
B	265	ALA	GLU	engineered mutation	UNP Q877G8
B	266	SER	GLU	engineered mutation	UNP Q877G8
B	267	GLU	LYS	engineered mutation	UNP Q877G8
C	?	-	ILE	deletion	UNP Q877G8
C	?	-	LYS	deletion	UNP Q877G8
C	?	-	GLU	deletion	UNP Q877G8
C	?	-	THR	deletion	UNP Q877G8
C	?	-	ASP	deletion	UNP Q877G8
C	?	-	ALA	deletion	UNP Q877G8
C	?	-	GLU	deletion	UNP Q877G8
C	?	-	ILE	deletion	UNP Q877G8
C	?	-	ARG	deletion	UNP Q877G8
C	?	-	ILE	deletion	UNP Q877G8
C	?	-	THR	deletion	UNP Q877G8
C	?	-	ASP	deletion	UNP Q877G8
C	?	-	PRO	deletion	UNP Q877G8
C	?	-	LYS	deletion	UNP Q877G8
C	?	-	LEU	deletion	UNP Q877G8
C	?	-	MET	deletion	UNP Q877G8
C	?	-	GLU	deletion	UNP Q877G8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	PHE	deletion	UNP Q877G8
C	?	-	ILE	deletion	UNP Q877G8
C	264	THR	GLN	engineered mutation	UNP Q877G8
C	265	ALA	GLU	engineered mutation	UNP Q877G8
C	266	SER	GLU	engineered mutation	UNP Q877G8
C	267	GLU	LYS	engineered mutation	UNP Q877G8
D	?	-	ILE	deletion	UNP Q877G8
D	?	-	LYS	deletion	UNP Q877G8
D	?	-	GLU	deletion	UNP Q877G8
D	?	-	THR	deletion	UNP Q877G8
D	?	-	ASP	deletion	UNP Q877G8
D	?	-	ALA	deletion	UNP Q877G8
D	?	-	GLU	deletion	UNP Q877G8
D	?	-	ILE	deletion	UNP Q877G8
D	?	-	ARG	deletion	UNP Q877G8
D	?	-	ILE	deletion	UNP Q877G8
D	?	-	THR	deletion	UNP Q877G8
D	?	-	ASP	deletion	UNP Q877G8
D	?	-	PRO	deletion	UNP Q877G8
D	?	-	LYS	deletion	UNP Q877G8
D	?	-	LEU	deletion	UNP Q877G8
D	?	-	MET	deletion	UNP Q877G8
D	?	-	GLU	deletion	UNP Q877G8
D	?	-	PHE	deletion	UNP Q877G8
D	?	-	ILE	deletion	UNP Q877G8
D	264	THR	GLN	engineered mutation	UNP Q877G8
D	265	ALA	GLU	engineered mutation	UNP Q877G8
D	266	SER	GLU	engineered mutation	UNP Q877G8
D	267	GLU	LYS	engineered mutation	UNP Q877G8

- Molecule 2 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: $C_{10}H_{16}N_5O_{12}P_3S$).

4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	150.53Å 209.53Å 266.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	58.56 – 6.00 58.56 – 6.00	Depositor EDS
% Data completeness (in resolution range)	95.1 (58.56-6.00) 95.6 (58.56-6.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.31 (at 6.17Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.4_162)	Depositor
R, R_{free}	0.241 , 0.270 0.247 , 0.281	Depositor DCC
R_{free} test set	496 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å ²)	342.4	Xtrriage
Anisotropy	0.400	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 386.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	14619	wwPDB-VP
Average B, all atoms (Å ²)	555.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.39% 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: AGS

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	0.31	0/3649	0.46	2/4911 (0.0%)
1	B	0.31	0/3649	0.46	2/4911 (0.0%)
1	C	0.32	0/3649	0.47	2/4911 (0.0%)
1	D	0.31	0/3627	0.46	2/4881 (0.0%)
All	All	0.31	0/14574	0.46	8/19614 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	3
1	C	0	4
1	D	0	4
All	All	0	13

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	263	GLU	N-CA-C	6.25	127.89	111.00
1	C	263	GLU	N-CA-C	6.17	127.64	111.00
1	D	263	GLU	N-CA-C	6.12	127.51	111.00
1	B	263	GLU	N-CA-C	6.10	127.48	111.00
1	A	240	GLU	N-CA-C	5.84	126.77	111.00

There are no chirality outliers.

5 of 13 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	355	PHE	Peptide
1	A	398	GLY	Peptide
1	B	211	GLY	Peptide
1	B	358	GLU	Peptide
1	B	398	GLY	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3629	0	3764	131	2
1	B	3629	0	3762	204	0
1	C	3629	0	3762	151	1
1	D	3608	0	3736	99	1
2	A	31	0	12	5	0
2	B	31	0	12	5	0
2	C	31	0	12	6	0
2	D	31	0	12	11	0
All	All	14619	0	15072	525	2

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 18.

The worst 5 of 525 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:210:LYS:CB	1:A:358:GLU:H	1.13	1.53
2:D:544:AGS:PG	2:D:544:AGS:S1G	1.49	1.49
2:B:544:AGS:PG	2:B:544:AGS:S1G	1.49	1.48
2:A:544:AGS:PG	2:A:544:AGS:S1G	1.49	1.47
2:C:544:AGS:PG	2:C:544:AGS:S1G	1.49	1.47

All (2) 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:A:225:LYS:CB	1:C:335:GLN:CG[8_444]	2.14	0.06
1:A:518:ALA:N	1:D:49:VAL:O[2_545]	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	485/521 (93%)	454 (94%)	26 (5%)	5 (1%)	15	54
1	B	485/521 (93%)	449 (93%)	30 (6%)	6 (1%)	13	50
1	C	485/521 (93%)	446 (92%)	34 (7%)	5 (1%)	15	54
1	D	480/521 (92%)	442 (92%)	31 (6%)	7 (2%)	10	45
All	All	1935/2084 (93%)	1791 (93%)	121 (6%)	23 (1%)	13	50

5 of 23 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	358	GLU
1	C	328	ASN
1	C	329	ILE
1	D	358	GLU
1	D	361	HIS

5.3.2 Protein sidechains [i](#)

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	388/413 (94%)	376 (97%)	12 (3%)	40	62
1	B	388/413 (94%)	379 (98%)	9 (2%)	50	71
1	C	388/413 (94%)	383 (99%)	5 (1%)	69	82
1	D	386/413 (94%)	377 (98%)	9 (2%)	50	71
All	All	1550/1652 (94%)	1515 (98%)	35 (2%)	50	71

5 of 35 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	196	GLU
1	D	198	LYS
1	D	327	THR
1	B	45	ASP
1	A	386	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	11	ASN
1	B	129	GLN
1	C	11	ASN
1	C	129	GLN
1	D	11	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 monosaccharides in this entry.

5.6 Ligand geometry

4 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	AGS	C	544	-	26,33,33	3.90	4 (15%)	26,52,52	1.19	3 (11%)
2	AGS	B	544	-	26,33,33	3.89	4 (15%)	26,52,52	1.18	3 (11%)
2	AGS	D	544	-	26,33,33	3.90	4 (15%)	26,52,52	1.18	3 (11%)
2	AGS	A	544	-	26,33,33	3.90	4 (15%)	26,52,52	1.19	3 (11%)

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	AGS	C	544	-	-	3/17/38/38	0/3/3/3
2	AGS	B	544	-	-	3/17/38/38	0/3/3/3
2	AGS	D	544	-	-	3/17/38/38	0/3/3/3
2	AGS	A	544	-	-	3/17/38/38	0/3/3/3

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	544	AGS	PG-S1G	-18.89	1.49	1.90
2	A	544	AGS	PG-S1G	-18.88	1.49	1.90
2	D	544	AGS	PG-S1G	-18.88	1.49	1.90
2	B	544	AGS	PG-S1G	-18.85	1.49	1.90
2	A	544	AGS	O4'-C1'	2.66	1.44	1.41

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	544	AGS	C5-C6-N6	2.75	124.53	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	544	AGS	C5-C6-N6	2.71	124.47	120.35
2	C	544	AGS	C5-C6-N6	2.69	124.44	120.35
2	B	544	AGS	C5-C6-N6	2.67	124.42	120.35
2	C	544	AGS	O4'-C1'-C2'	-2.39	103.44	106.93

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

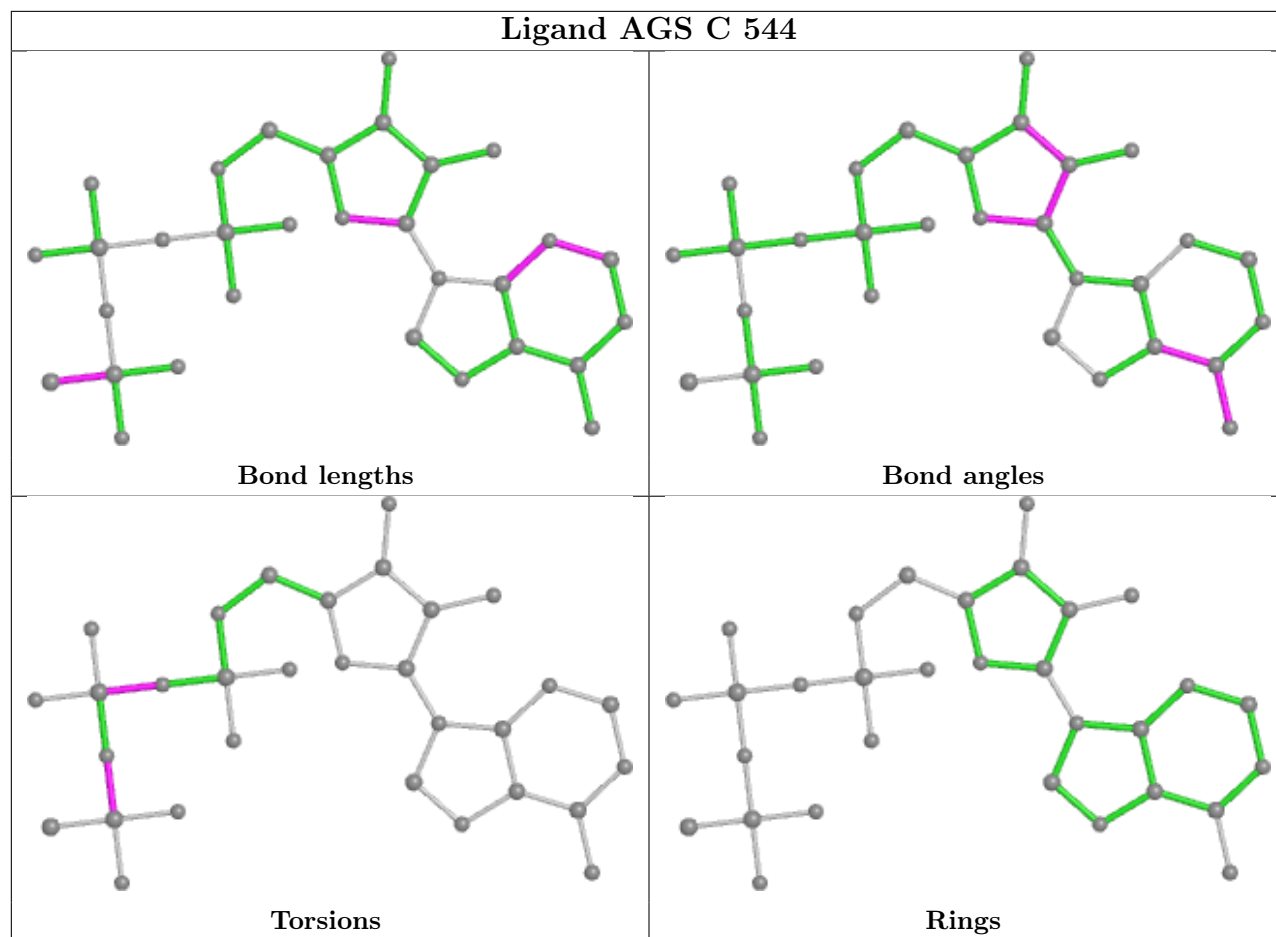
Mol	Chain	Res	Type	Atoms
2	A	544	AGS	PB-O3B-PG-O2G
2	A	544	AGS	PB-O3B-PG-O3G
2	B	544	AGS	PB-O3B-PG-O2G
2	B	544	AGS	PB-O3B-PG-O3G
2	C	544	AGS	PB-O3B-PG-O2G

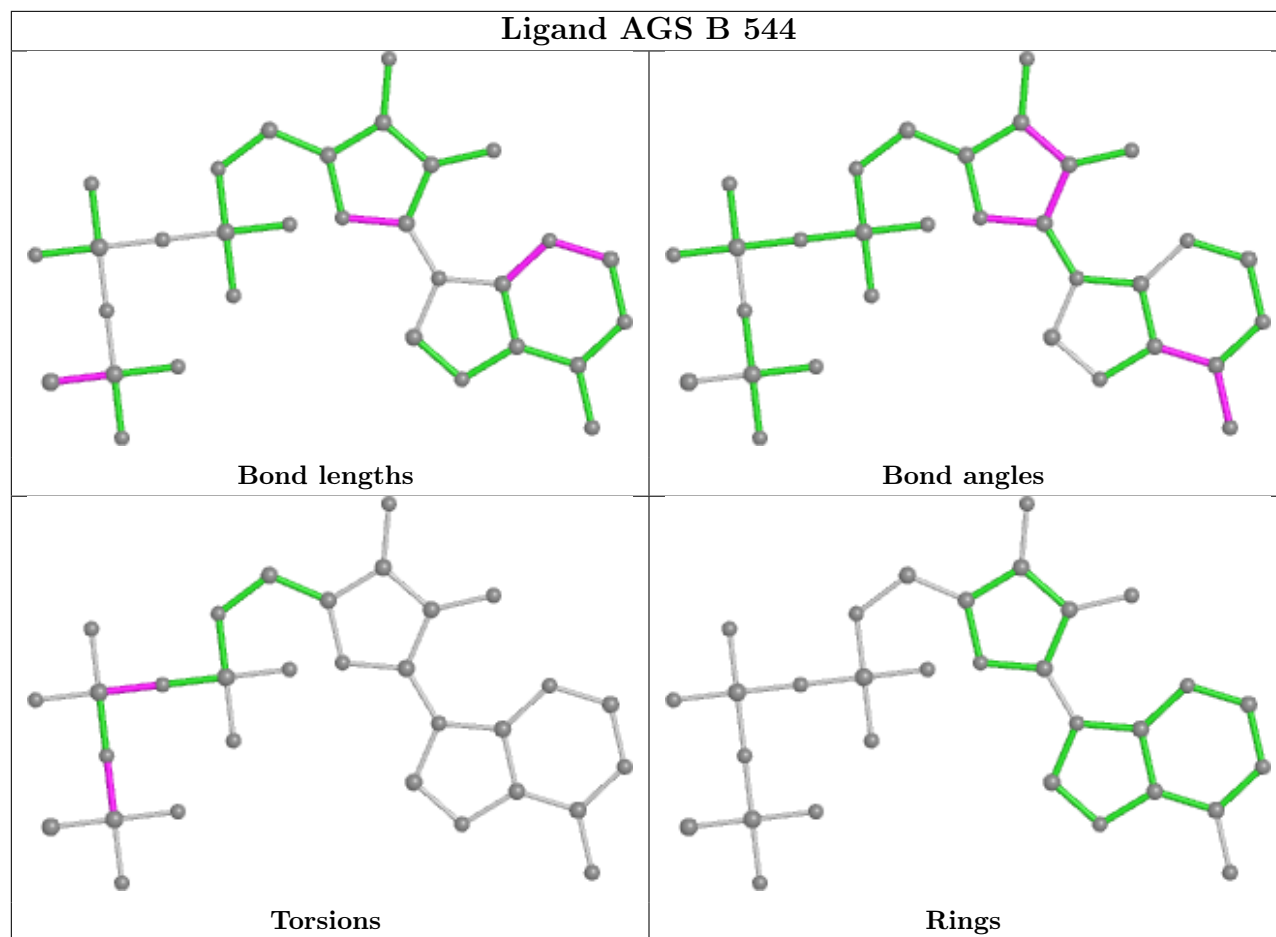
There are no ring outliers.

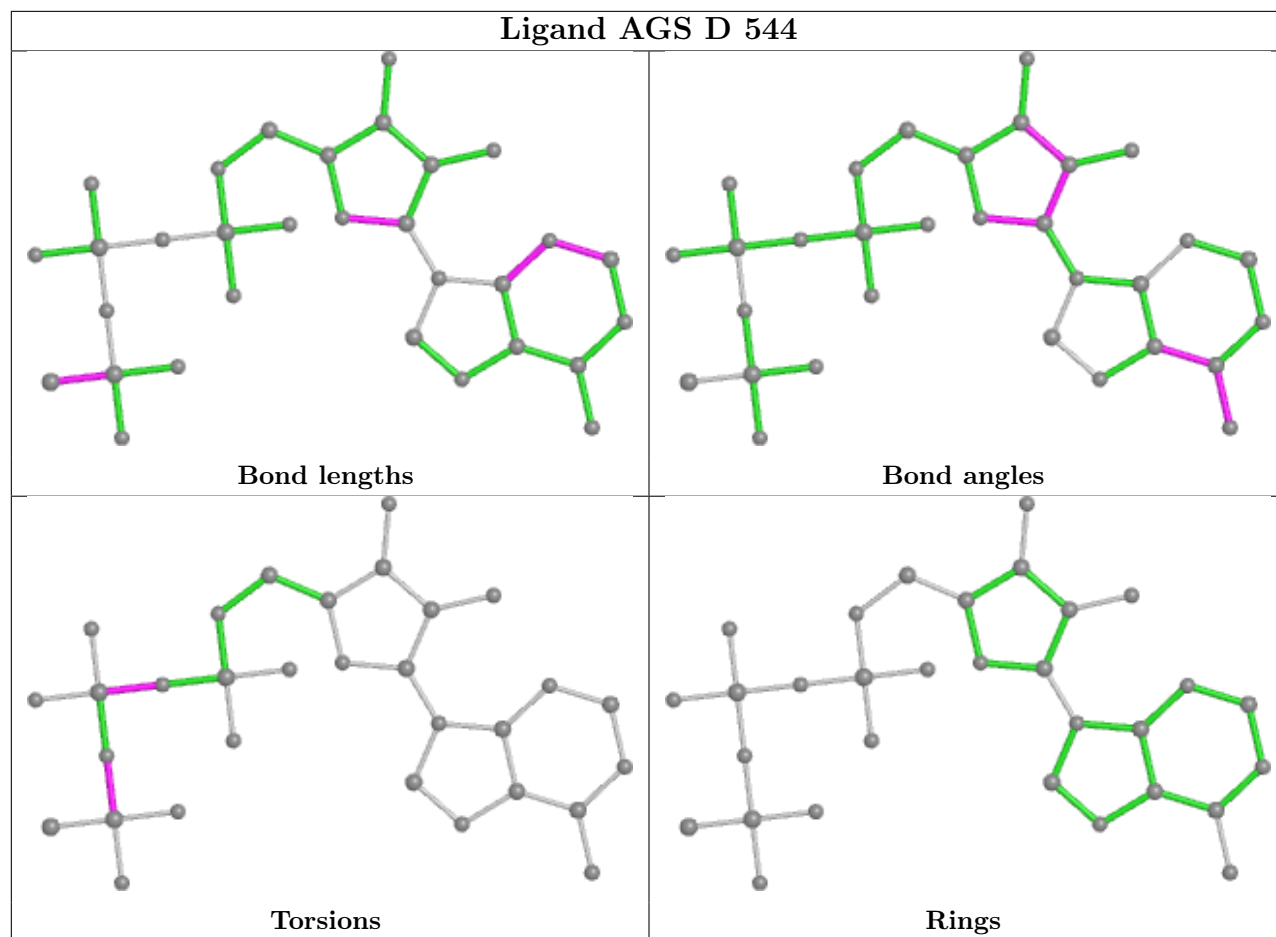
4 monomers are involved in 27 short contacts:

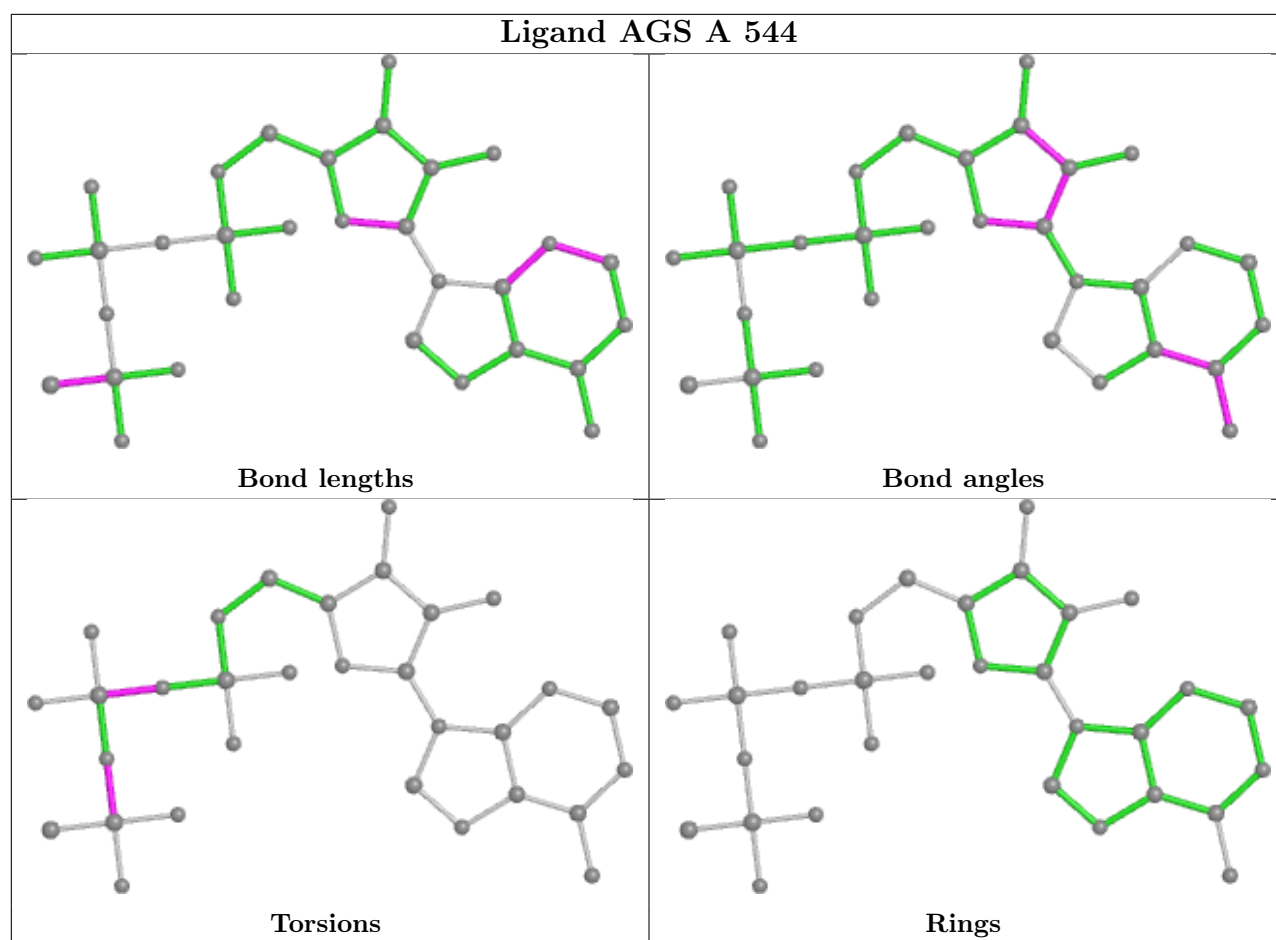
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	544	AGS	6	0
2	B	544	AGS	5	0
2	D	544	AGS	11	0
2	A	544	AGS	5	0

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](#)

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

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

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

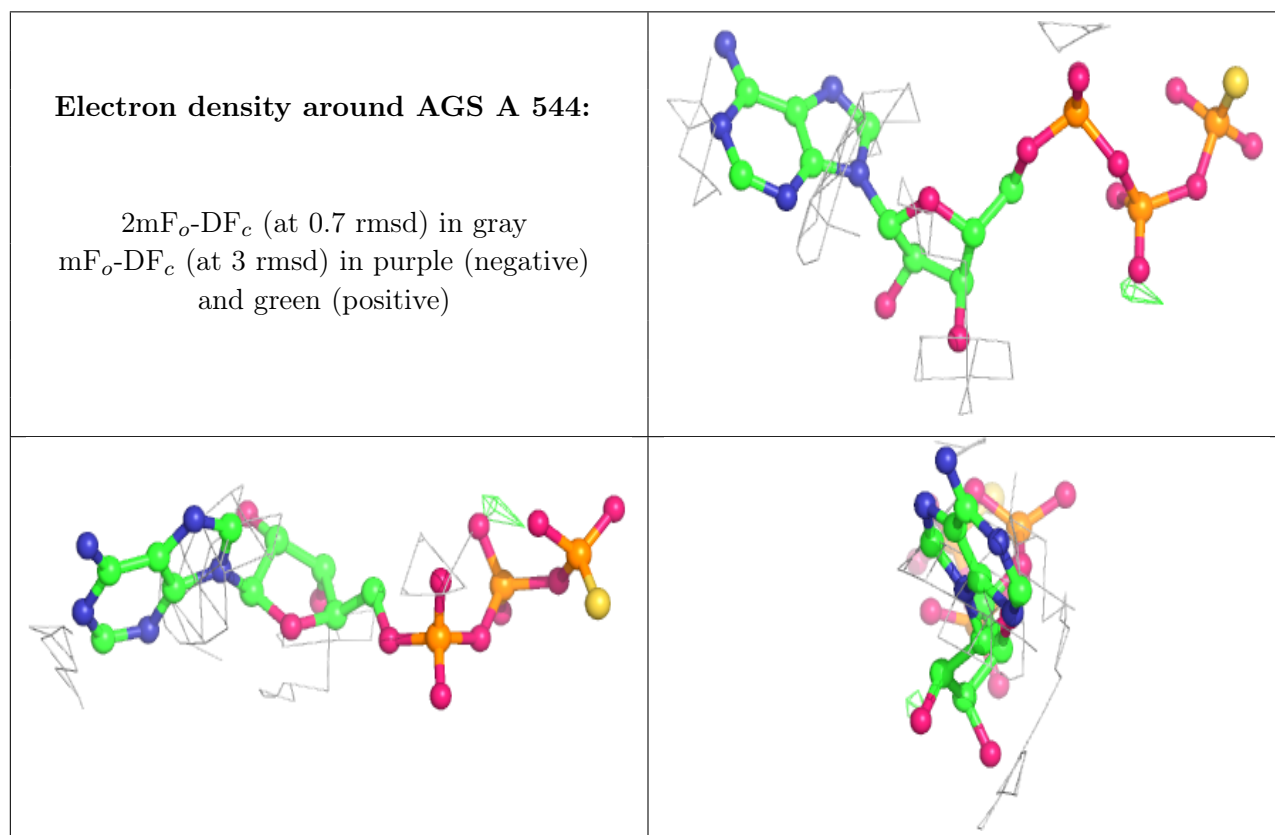
6.3 Carbohydrates [i](#)

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

6.4 Ligands [i](#)

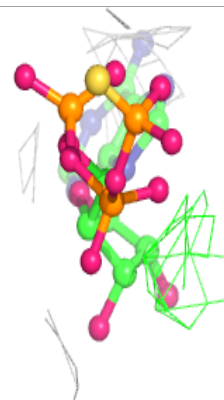
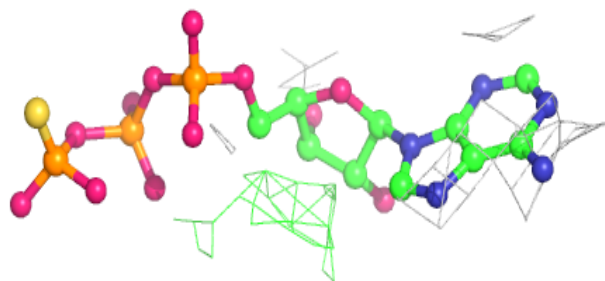
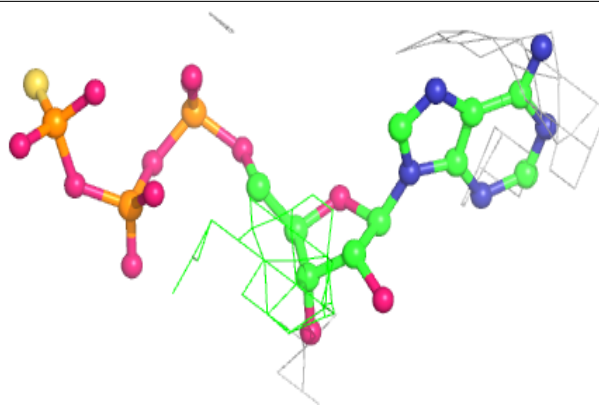
Unable to reproduce the depositors R factor - this section is therefore empty.

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.

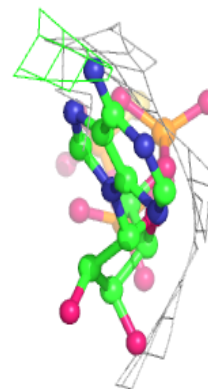
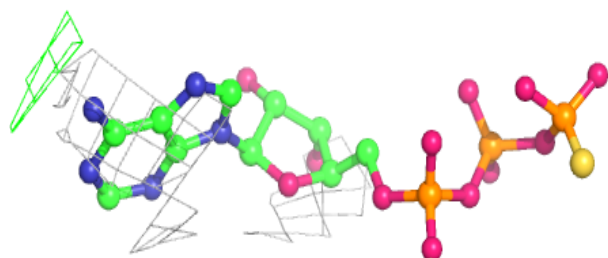
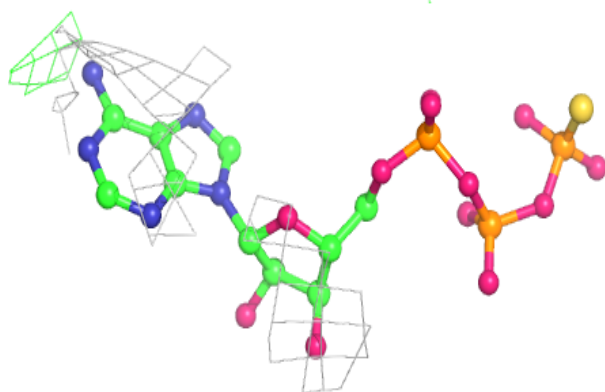


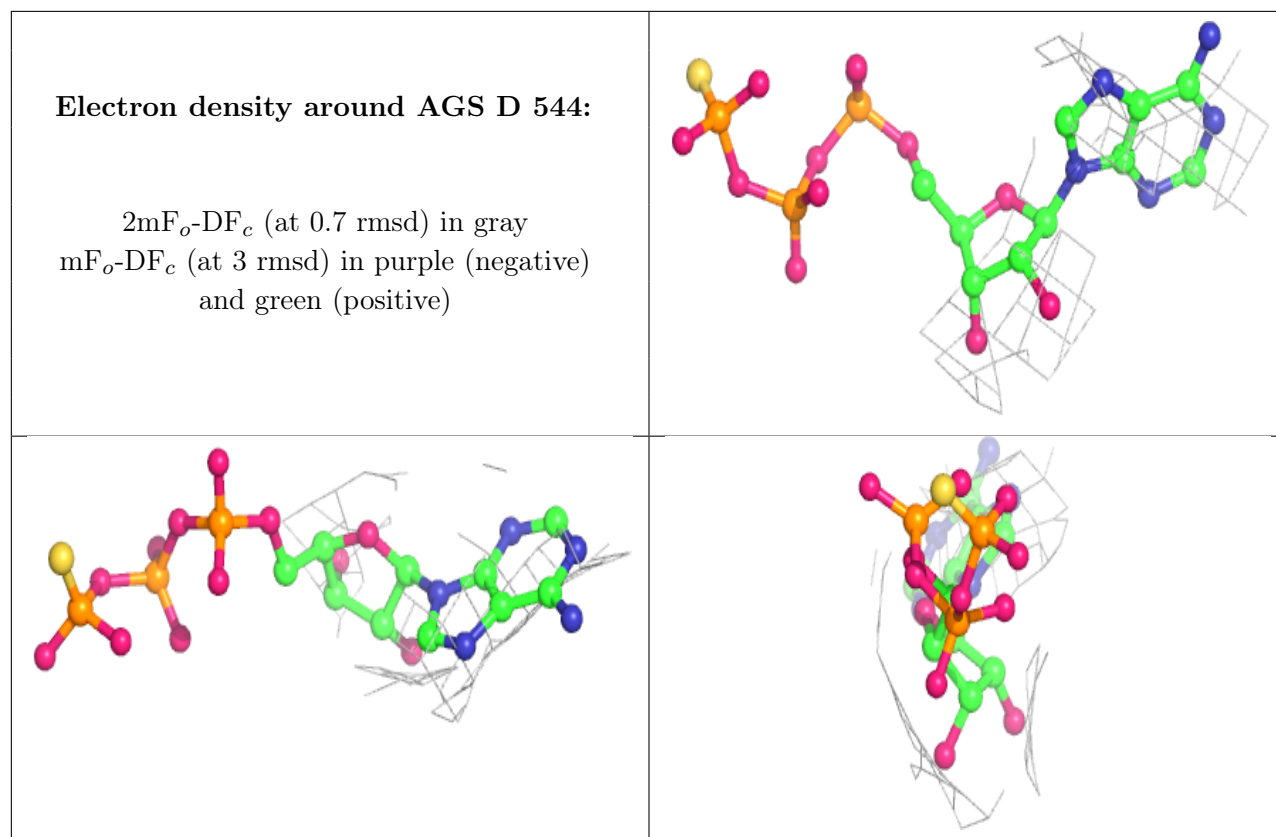
Electron density around AGS B 544:

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

**Electron density around AGS C 544:**

$2mF_o-DF_c$ (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.