wwPDB X-ray Structure Validation Summary Report (i)

Nov 29, 2023 – 03:30 pm GMT

PDB ID	:	8ORU
Title	:	cyclic 2,3-diphosphoglycerate synthetase from the hyperthermophilic archaeon Methanothermus fervidus bound to 2,3-diphosphoglycerate and ADP.
Authors	:	De Rose, S.A.; Isupov, M.
Deposited on	:	2023-04-17
Resolution	:	2.23 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 (i) 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 (i)) were used in the production of this report:

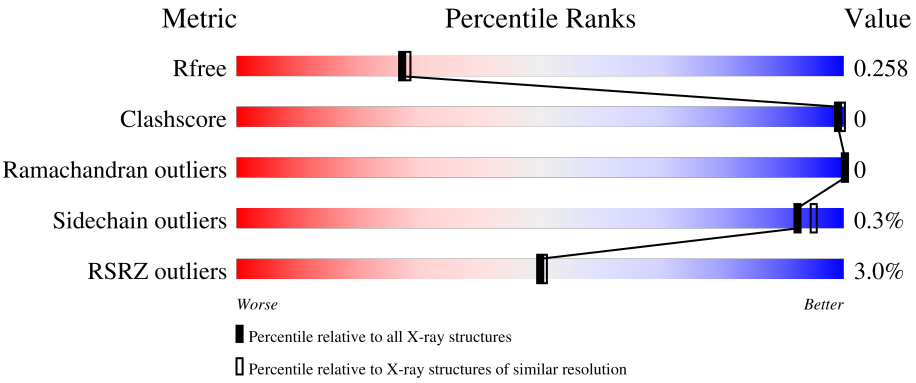
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.23 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	2391 (2.26-2.22)
Clashscore	141614	2539 (2.26-2.22)
Ramachandran outliers	138981	2489 (2.26-2.22)
Sidechain outliers	138945	2490 (2.26-2.22)
RSRZ outliers	127900	2353 (2.26-2.22)

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 <=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	AAA	459	1% 99%
1	BBB	459	2% 98%
1	CCC	459	5% 99%
1	DDD	459	4% 99%

2 Entry composition

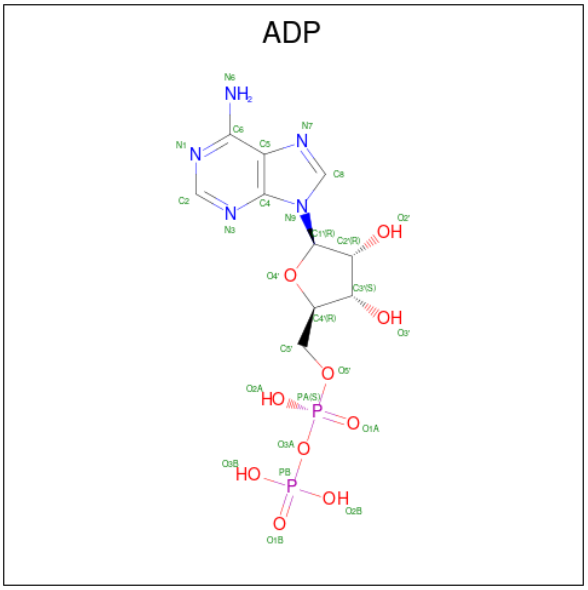
There are 7 unique types of molecules in this entry. The entry contains 29322 atoms, of which 14785 are hydrogens and 0 are deuteriums.

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 Cyclic 2,3-diphosphoglycerate synthetase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	AAA	459	Total	C	H	N	O	S	70	0	0
			7222	2276	3664	596	667	19			
1	BBB	459	Total	C	H	N	O	S	71	0	0
			7222	2276	3664	596	667	19			
1	CCC	459	Total	C	H	N	O	S	71	0	0
			7222	2276	3664	596	667	19			
1	DDD	459	Total	C	H	N	O	S	71	0	0
			7222	2276	3664	596	667	19			

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	AAA	1	Total	C	H	N	O	P	2	0
			39	10	12	5	10	2		
2	BBB	1	Total	C	H	N	O	P	2	0
			39	10	12	5	10	2		

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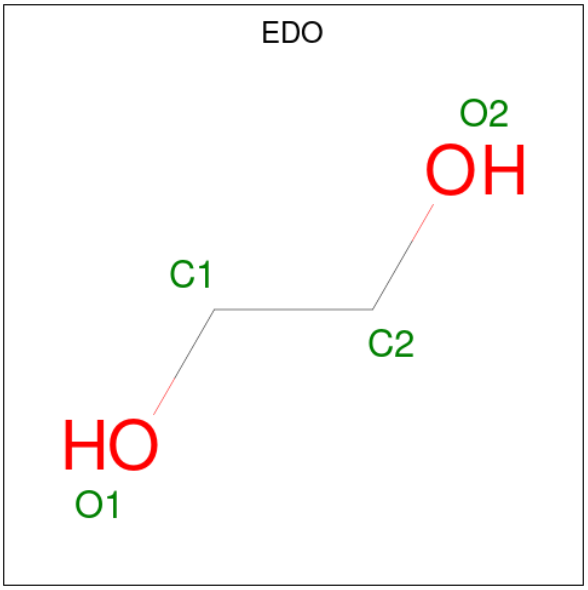
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	CCC	1	Total	C	H	N	O	P	2	0
			39	10	12	5	10	2		
2	DDD	1	Total	C	H	N	O	P	2	0
			39	10	12	5	10	2		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	AAA	1	Total	C	H	O	1	0
			10	2	6	2		
3	AAA	1	Total	C	H	O	1	0
			10	2	6	2		
3	BBB	1	Total	C	H	O	1	0
			10	2	6	2		
3	BBB	1	Total	C	H	O	1	0
			10	2	6	2		
3	BBB	1	Total	C	H	O	1	0
			10	2	6	2		
3	BBB	1	Total	C	H	O	1	0
			10	2	6	2		
3	CCC	1	Total	C	H	O	1	0
			10	2	6	2		
3	CCC	1	Total	C	H	O	1	0
			10	2	6	2		
3	CCC	1	Total	C	H	O	1	0
			10	2	6	2		

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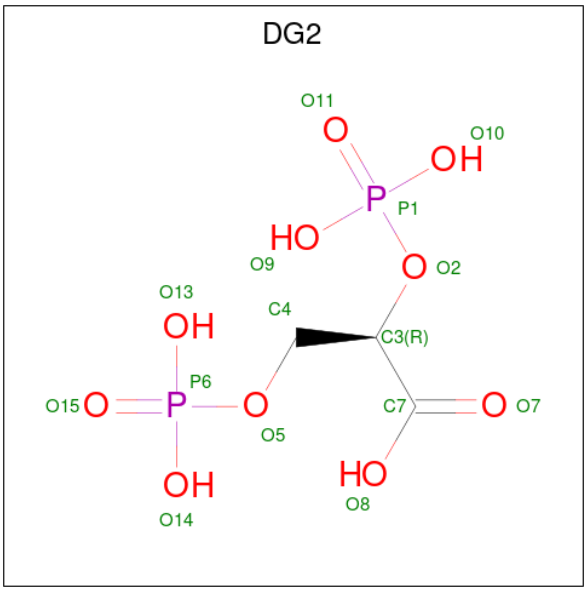
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	DDD	1	Total C H O 10 2 6 2	1	0
3	DDD	1	Total C H O 10 2 6 2	1	0

- Molecule 4 is (2R)-2,3-diphosphoglyceric acid (three-letter code: DG2) (formula: $C_3H_8O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).

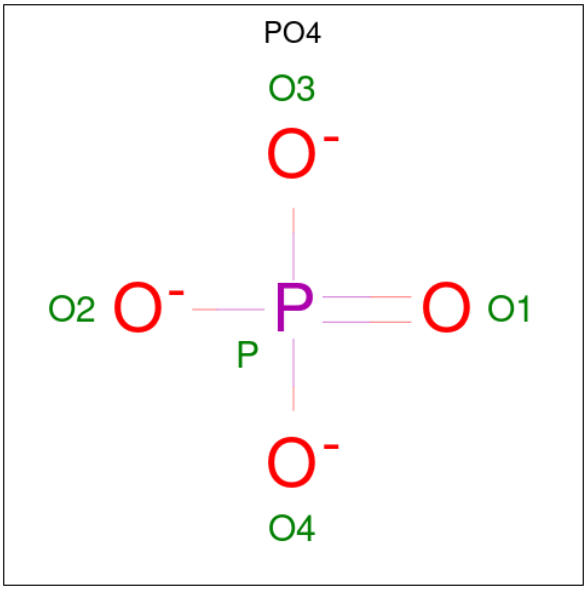


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	AAA	1	Total C H O P 18 3 3 10 2	0	0
4	AAA	1	Total C H O P 18 3 3 10 2	0	0
4	BBB	1	Total C H O P 18 3 3 10 2	0	0
4	CCC	1	Total C H O P 18 3 3 10 2	0	0
4	DDD	1	Total C H O P 18 3 3 10 2	0	0
4	DDD	1	Total C O P 15 3 10 2	0	0

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	AAA	2	Total Mg 2 2	0	0
5	BBB	2	Total Mg 2 2	0	0
5	CCC	2	Total Mg 2 2	0	0
5	DDD	2	Total Mg 2 2	0	0

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	BBB	1	Total O P 5 4 1	0	0

- Molecule 7 is water.

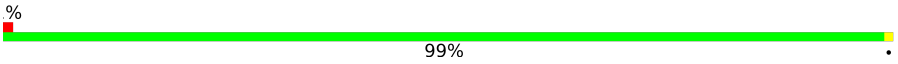
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	AAA	20	Total O 20 20	0	0
7	BBB	13	Total O 13 13	0	0
7	CCC	12	Total O 12 12	0	0
7	DDD	5	Total O 5 5	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

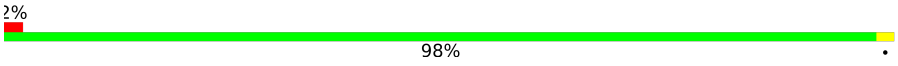
• Molecule 1: Cyclic 2,3-diphosphoglycerate synthetase

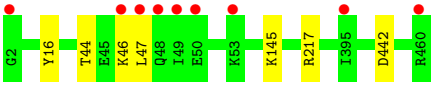
Chain AAA:



• Molecule 1: Cyclic 2,3-diphosphoglycerate synthetase

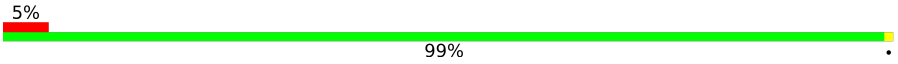
Chain BBB:

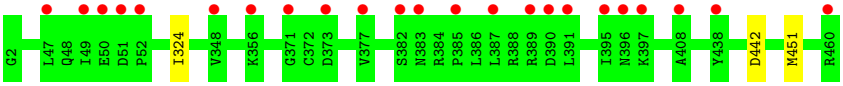




• Molecule 1: Cyclic 2,3-diphosphoglycerate synthetase

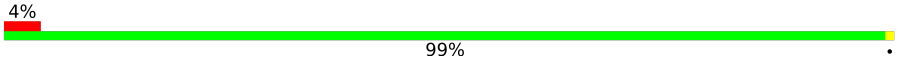
Chain CCC:

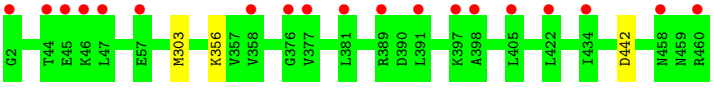




• Molecule 1: Cyclic 2,3-diphosphoglycerate synthetase

Chain DDD:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	71.23Å 71.48Å 103.54Å 97.02° 103.42° 99.05°	Depositor
Resolution (Å)	69.92 – 2.23 69.62 – 2.23	Depositor EDS
% Data completeness (in resolution range)	85.3 (69.92-2.23) 85.3 (69.62-2.23)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.04 (at 2.22Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.216 , 0.256 0.221 , 0.258	Depositor DCC
R_{free} test set	4008 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	58.1	Xtriage
Anisotropy	0.099	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 43.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	29322	wwPDB-VP
Average B, all atoms (Å^2)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.03% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: PO4, EDO, ADP, DG2, MG

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	AAA	0.67	0/3622	0.79	1/4900 (0.0%)
1	BBB	0.66	0/3622	0.78	0/4900
1	CCC	0.66	0/3622	0.78	0/4900
1	DDD	0.65	0/3622	0.77	0/4900
All	All	0.66	0/14488	0.78	1/19600 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AAA	174	ARG	NE-CZ-NH1	-6.28	117.16	120.30

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	AAA	3558	3664	3653	2	2
1	BBB	3558	3664	3653	3	2
1	CCC	3558	3664	3653	2	0
1	DDD	3558	3664	3653	4	0
2	AAA	27	12	12	0	0
2	BBB	27	12	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	CCC	27	12	12	0	0
2	DDD	27	12	12	1	0
3	AAA	8	12	12	0	0
3	BBB	16	24	24	0	0
3	CCC	12	18	18	1	0
3	DDD	8	12	12	0	0
4	AAA	30	6	8	0	0
4	BBB	15	3	4	0	0
4	CCC	15	3	4	0	0
4	DDD	30	3	8	3	0
5	AAA	2	0	0	0	0
5	BBB	2	0	0	0	0
5	CCC	2	0	0	0	0
5	DDD	2	0	0	0	0
6	BBB	5	0	0	0	0
7	AAA	20	0	0	0	0
7	BBB	13	0	0	0	0
7	CCC	12	0	0	0	0
7	DDD	5	0	0	0	0
All	All	14537	14785	14750	9	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 0.

The worst 5 of 9 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:DDD:356:LYS:NZ	4:DDD:504:DG2:H3	2.15	0.62
1:AAA:14:GLU:OE1	1:BBB:145:LYS:NZ	2.44	0.48
1:AAA:84:TYR:CE2	1:CCC:451:MET:CE	2.98	0.47
1:CCC:324:ILE:HG22	3:CCC:505:EDO:H11	1.98	0.46
1:BBB:16:TYR:CD2	1:BBB:46:LYS:HE3	2.51	0.46

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:AAA:184:GLU:OE1	1:BBB:217:ARG:NH1[1_445]	2.00	0.20
1:AAA:184:GLU:OE1	1:BBB:217:ARG:HH12[1_445]	1.50	0.10

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	AAA	457/459 (100%)	446 (98%)	11 (2%)	0	100	100
1	BBB	457/459 (100%)	448 (98%)	9 (2%)	0	100	100
1	CCC	457/459 (100%)	447 (98%)	10 (2%)	0	100	100
1	DDD	457/459 (100%)	447 (98%)	10 (2%)	0	100	100
All	All	1828/1836 (100%)	1788 (98%)	40 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	AAA	391/391 (100%)	390 (100%)	1 (0%)	92	95
1	BBB	391/391 (100%)	390 (100%)	1 (0%)	92	95
1	CCC	391/391 (100%)	390 (100%)	1 (0%)	92	95
1	DDD	391/391 (100%)	390 (100%)	1 (0%)	92	95
All	All	1564/1564 (100%)	1560 (100%)	4 (0%)	92	95

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	442	ASP
1	BBB	442	ASP

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Mol	Chain	Res	Type
1	CCC	442	ASP
1	DDD	442	ASP

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

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 (i)

Of 30 ligands modelled in this entry, 8 are monoatomic - leaving 22 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	$\#\|Z\| > 2$
4	DG2	AAA	503	-	13,14,14	0.89	0	18,21,21	1.08	2 (11%)
4	DG2	DDD	503	5	13,14,14	1.40	2 (15%)	18,21,21	0.83	0
3	EDO	BBB	606	-	3,3,3	0.15	0	2,2,2	0.10	0
3	EDO	BBB	601	-	3,3,3	0.27	0	2,2,2	0.71	0
3	EDO	AAA	502	-	3,3,3	0.25	0	2,2,2	0.45	0
4	DG2	DDD	504	-	13,14,14	0.89	0	18,21,21	1.13	2 (11%)
3	EDO	CCC	505	-	3,3,3	0.25	0	2,2,2	0.31	0
3	EDO	BBB	604	-	3,3,3	0.06	0	2,2,2	0.16	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	DG2	BBB	602	-	13,14,14	0.98	0	18,21,21	1.02	1 (5%)
3	EDO	CCC	504	-	3,3,3	0.13	0	2,2,2	0.23	0
3	EDO	DDD	505	-	3,3,3	0.14	0	2,2,2	0.09	0
2	ADP	DDD	501	5	24,29,29	0.69	0	29,45,45	1.00	3 (10%)
4	DG2	CCC	503	5	13,14,14	1.03	1 (7%)	18,21,21	0.94	1 (5%)
6	PO4	BBB	609	5	4,4,4	0.58	0	6,6,6	0.67	0
4	DG2	AAA	504	5	13,14,14	1.17	1 (7%)	18,21,21	1.03	1 (5%)
3	EDO	CCC	502	-	3,3,3	0.15	0	2,2,2	0.50	0
2	ADP	AAA	501	5	24,29,29	0.69	0	29,45,45	0.93	2 (6%)
3	EDO	DDD	502	-	3,3,3	0.21	0	2,2,2	0.38	0
2	ADP	BBB	603	5	24,29,29	0.70	0	29,45,45	0.96	2 (6%)
3	EDO	AAA	505	-	3,3,3	0.04	0	2,2,2	0.05	0
2	ADP	CCC	501	5	24,29,29	0.65	0	29,45,45	0.92	2 (6%)
3	EDO	BBB	605	-	3,3,3	0.13	0	2,2,2	0.28	0

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
4	DG2	AAA	503	-	-	4/15/15/15	-
4	DG2	DDD	503	5	-	7/15/15/15	-
3	EDO	BBB	606	-	-	0/1/1/1	-
3	EDO	BBB	601	-	-	0/1/1/1	-
3	EDO	AAA	502	-	-	0/1/1/1	-
4	DG2	DDD	504	-	-	8/15/15/15	-
3	EDO	CCC	505	-	-	0/1/1/1	-
3	EDO	BBB	604	-	-	0/1/1/1	-
4	DG2	BBB	602	-	-	7/15/15/15	-
3	EDO	CCC	504	-	-	0/1/1/1	-
3	EDO	DDD	505	-	-	0/1/1/1	-
2	ADP	DDD	501	5	-	2/12/32/32	0/3/3/3
4	DG2	CCC	503	5	-	4/15/15/15	-
4	DG2	AAA	504	5	-	2/15/15/15	-
3	EDO	CCC	502	-	-	1/1/1/1	-
2	ADP	AAA	501	5	-	3/12/32/32	0/3/3/3
3	EDO	DDD	502	-	-	0/1/1/1	-
2	ADP	BBB	603	5	-	3/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	AAA	505	-	-	0/1/1/1	-
2	ADP	CCC	501	5	-	2/12/32/32	0/3/3/3
3	EDO	BBB	605	-	-	0/1/1/1	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	DDD	503	DG2	P1-O2	3.23	1.65	1.59
4	AAA	504	DG2	P1-O2	2.84	1.64	1.59
4	DDD	503	DG2	C3-C7	2.63	1.54	1.52
4	CCC	503	DG2	P1-O2	2.03	1.63	1.59

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	DDD	501	ADP	PA-O3A-PB	-2.65	123.72	132.83
4	DDD	504	DG2	O2-C3-C4	2.65	110.91	106.56
4	AAA	504	DG2	O7-C7-C3	-2.49	116.68	122.57
2	DDD	501	ADP	O4'-C1'-C2'	-2.48	103.30	106.93
4	AAA	503	DG2	O7-C7-C3	-2.48	116.72	122.57

There are no chirality outliers.

5 of 43 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	AAA	503	DG2	O2-C3-C7-O7
4	AAA	503	DG2	O2-C3-C7-O8
4	AAA	504	DG2	C3-O2-P1-O9
4	BBB	602	DG2	C7-C3-C4-O5
4	BBB	602	DG2	O2-C3-C7-O7

There are no ring outliers.

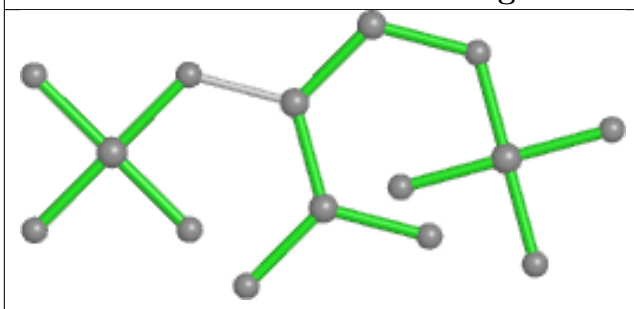
3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	DDD	504	DG2	3	0
3	CCC	505	EDO	1	0
2	DDD	501	ADP	1	0

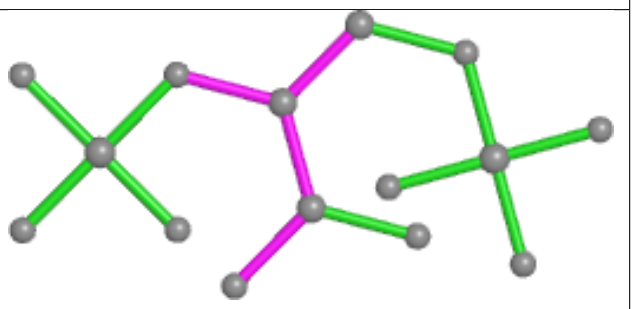
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

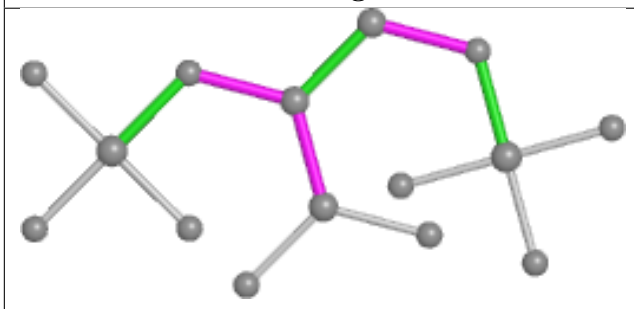
Ligand DG2 AAA 503



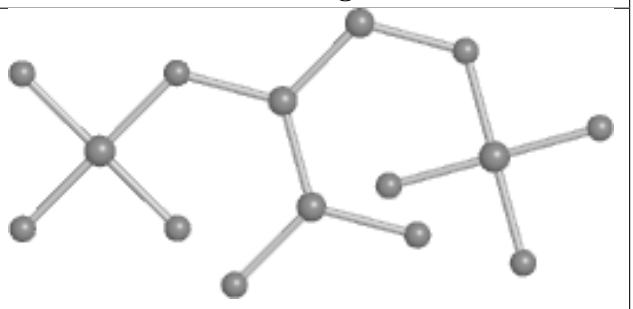
Bond lengths



Bond angles

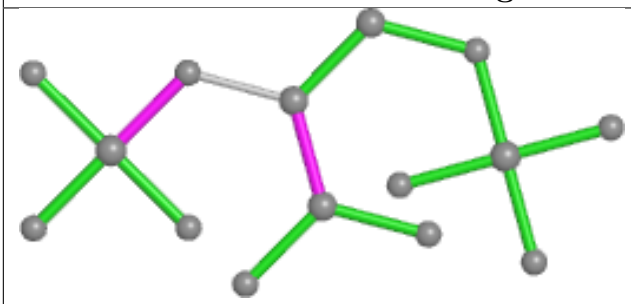


Torsions

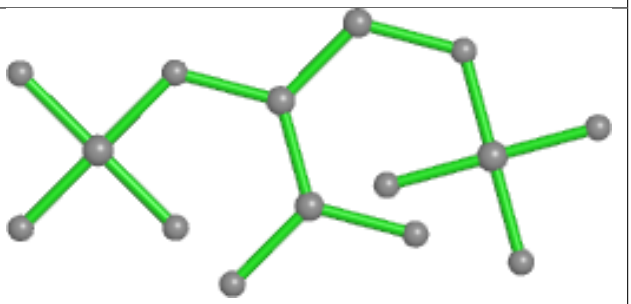


Rings

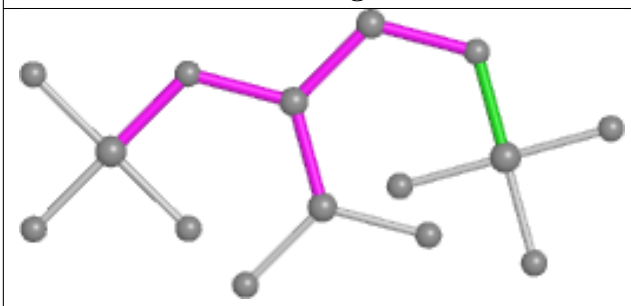
Ligand DG2 DDD 503



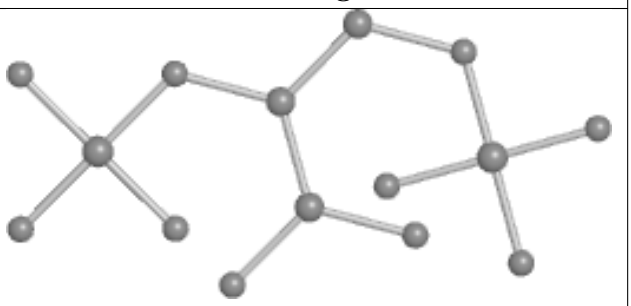
Bond lengths



Bond angles

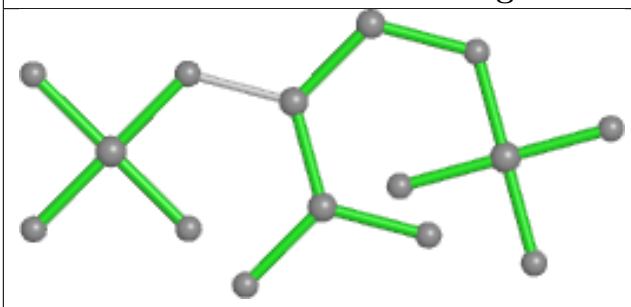


Torsions

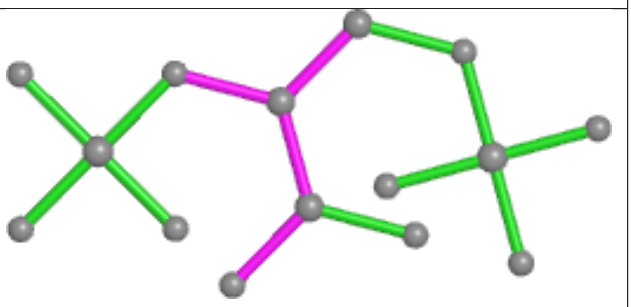


Rings

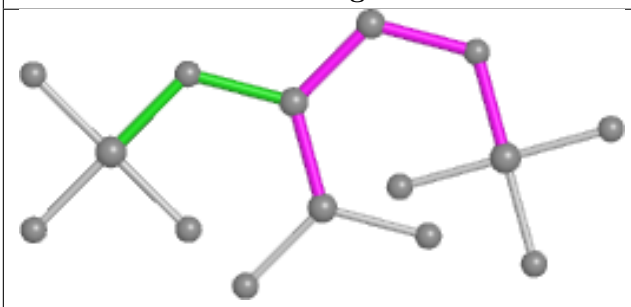
Ligand DG2 DDD 504



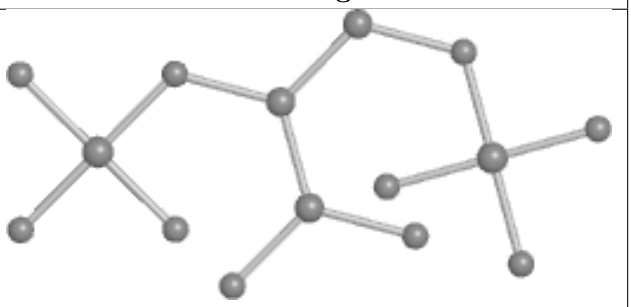
Bond lengths



Bond angles

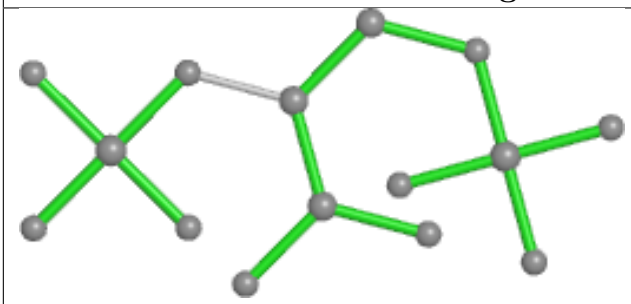


Torsions

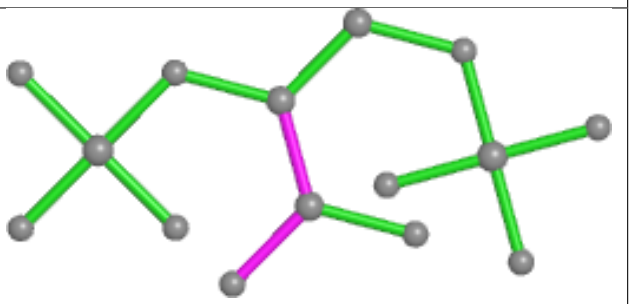


Rings

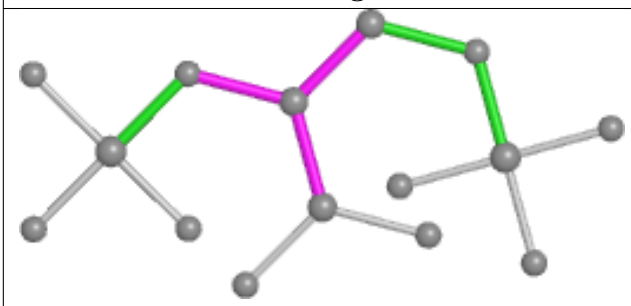
Ligand DG2 BBB 602



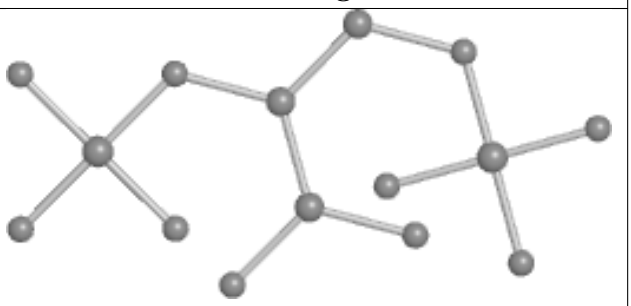
Bond lengths



Bond angles

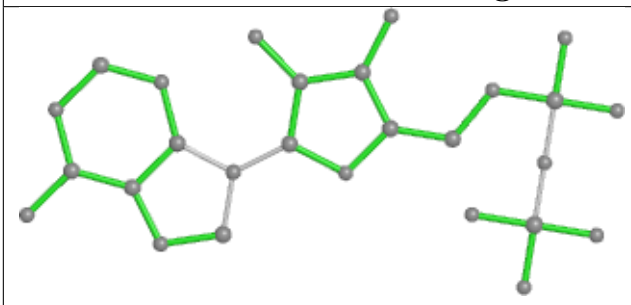


Torsions

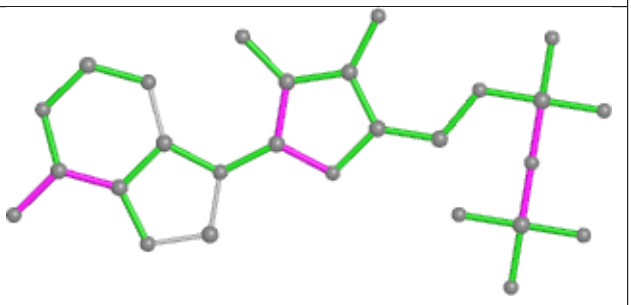


Rings

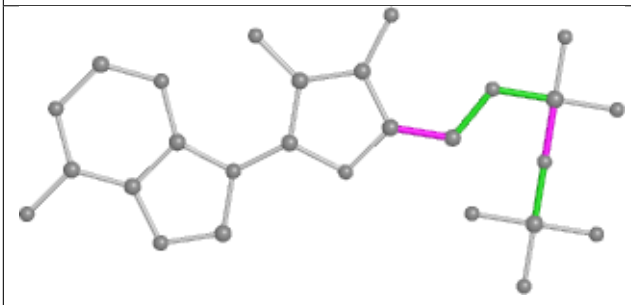
Ligand ADP DDD 501



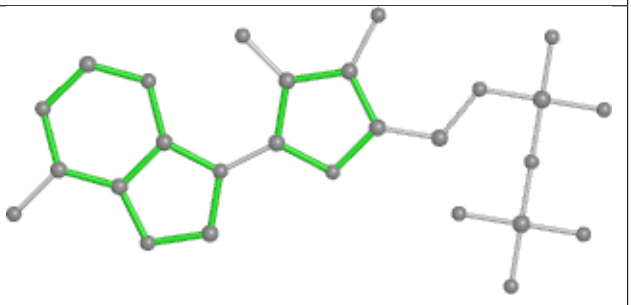
Bond lengths



Bond angles

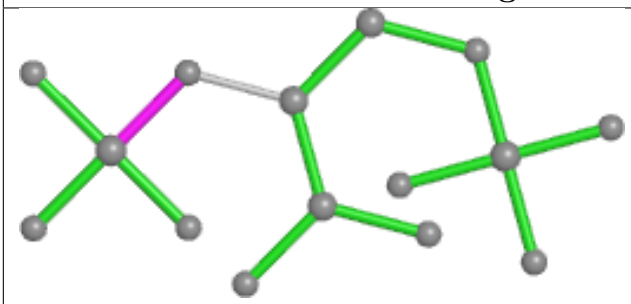


Torsions

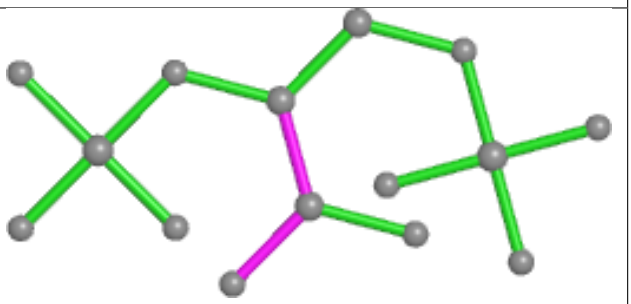


Rings

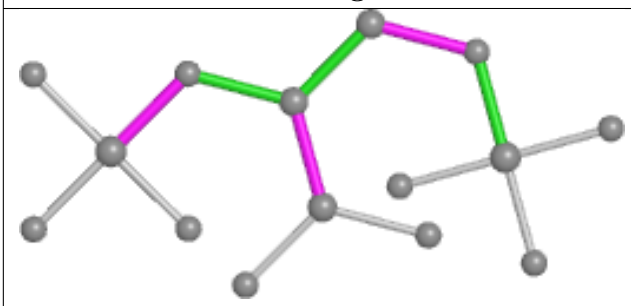
Ligand DG2 CCC 503



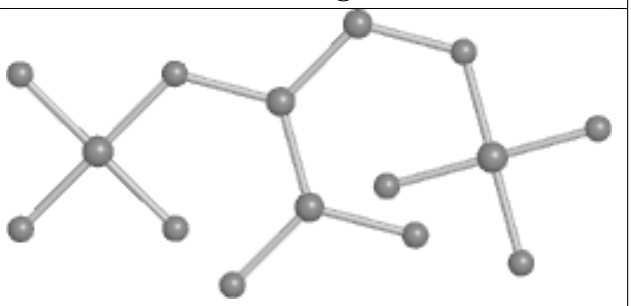
Bond lengths



Bond angles

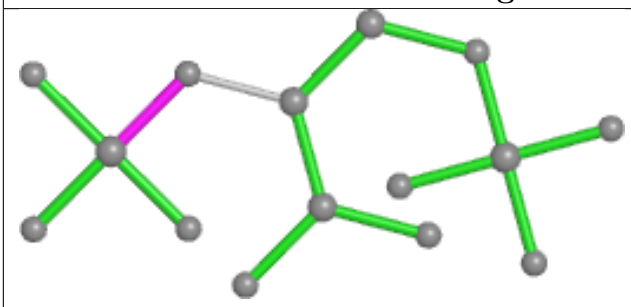


Torsions

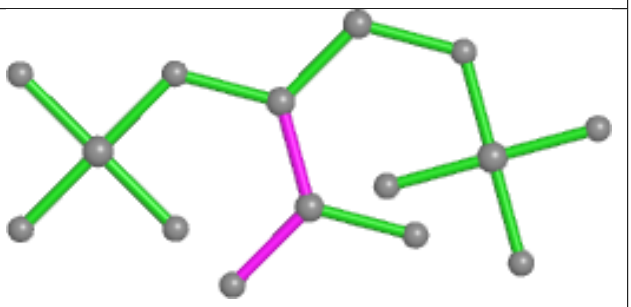


Rings

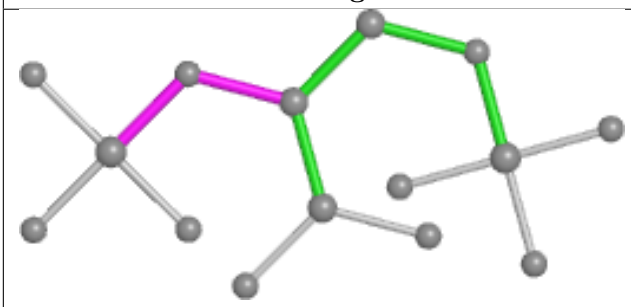
Ligand DG2 AAA 504



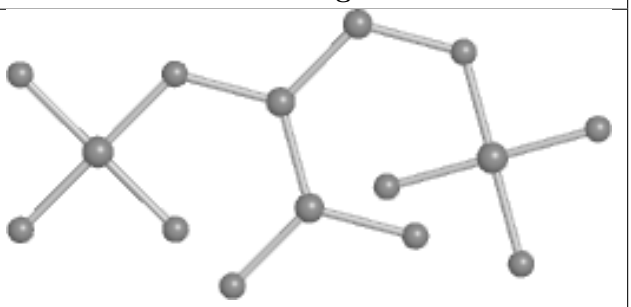
Bond lengths



Bond angles

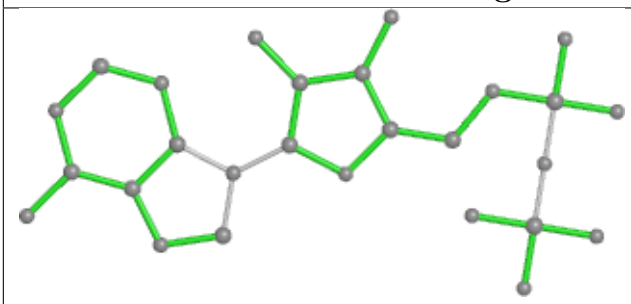


Torsions

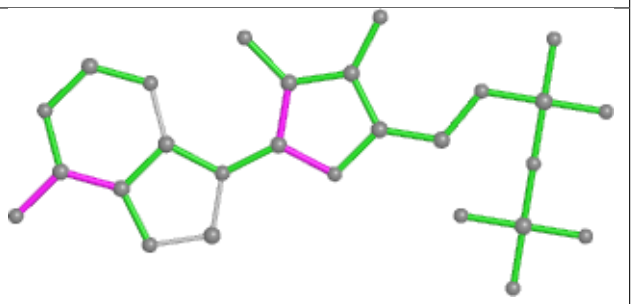


Rings

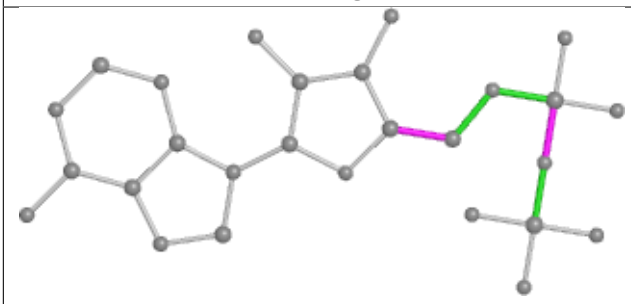
Ligand ADP AAA 501



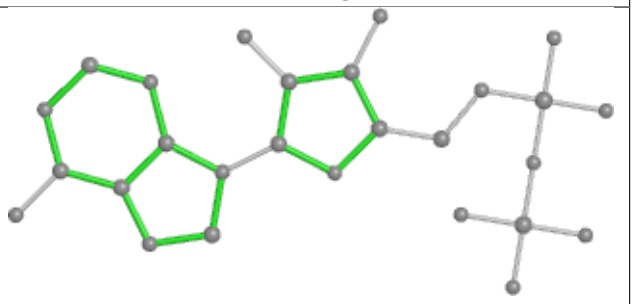
Bond lengths



Bond angles

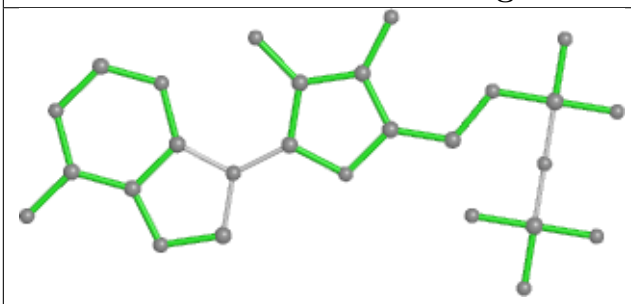


Torsions

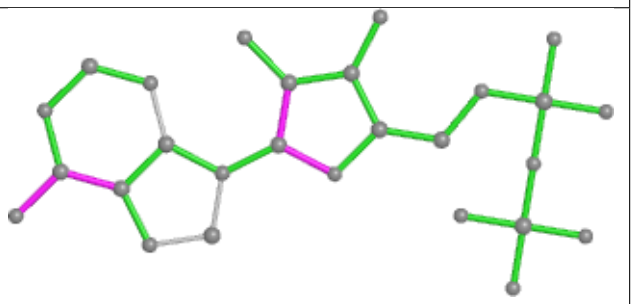


Rings

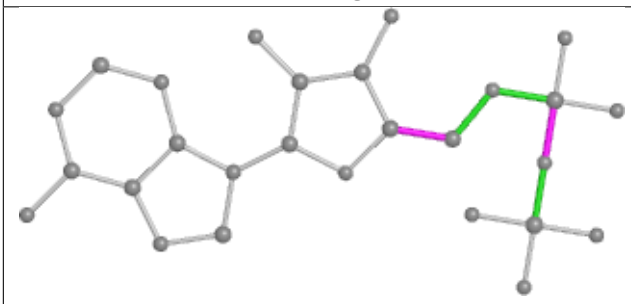
Ligand ADP BBB 603



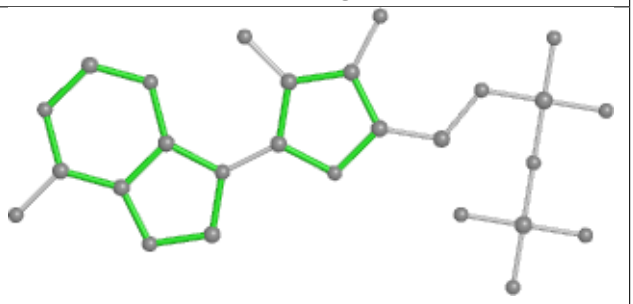
Bond lengths



Bond angles

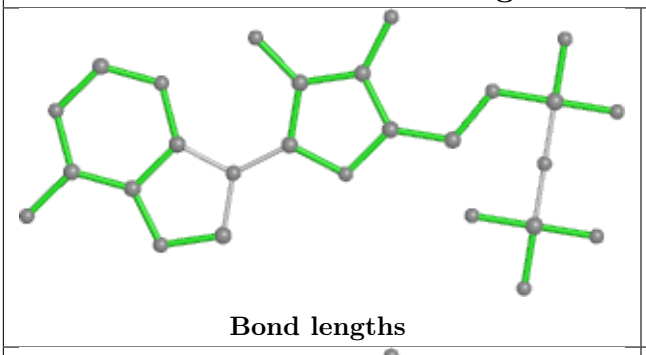


Torsions

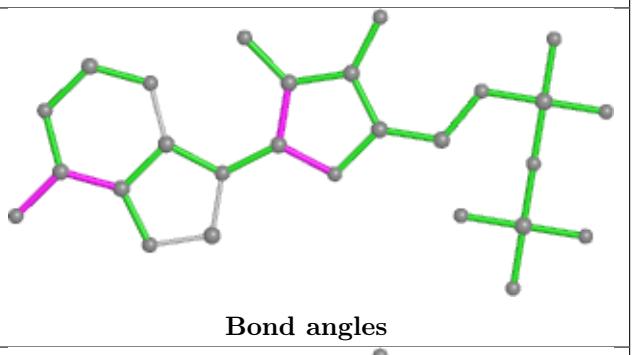


Rings

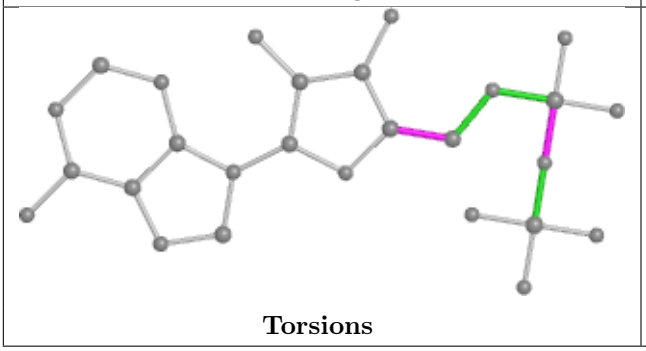
Ligand ADP CCC 501



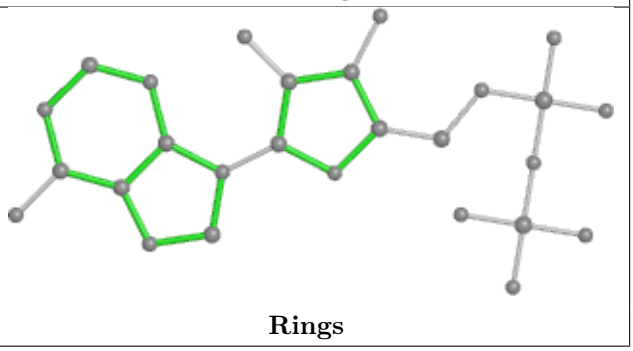
Bond lengths



Bond angles



Torsions



Rings

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

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, 95^{th} 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	AAA	459/459 (100%)	0.24	4 (0%)	84	84	35, 60, 100, 185	0
1	BBB	459/459 (100%)	0.29	9 (1%)	65	66	35, 66, 110, 175	0
1	CCC	459/459 (100%)	0.42	23 (5%)	28	28	40, 70, 133, 184	0
1	DDD	459/459 (100%)	0.41	19 (4%)	37	37	44, 76, 130, 168	0
All	All	1836/1836 (100%)	0.34	55 (2%)	50	50	35, 68, 123, 185	0

The worst 5 of 55 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	460	ARG	9.7
1	AAA	460	ARG	9.6
1	DDD	47	LEU	8.1
1	DDD	460	ARG	5.8
1	BBB	47	LEU	5.5

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

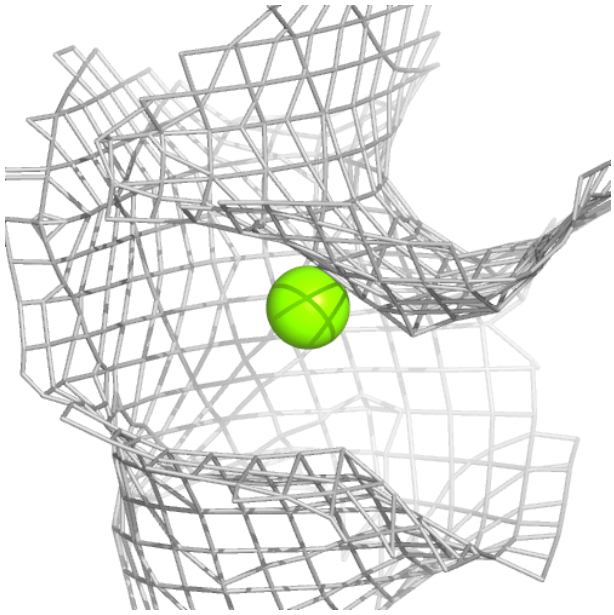
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

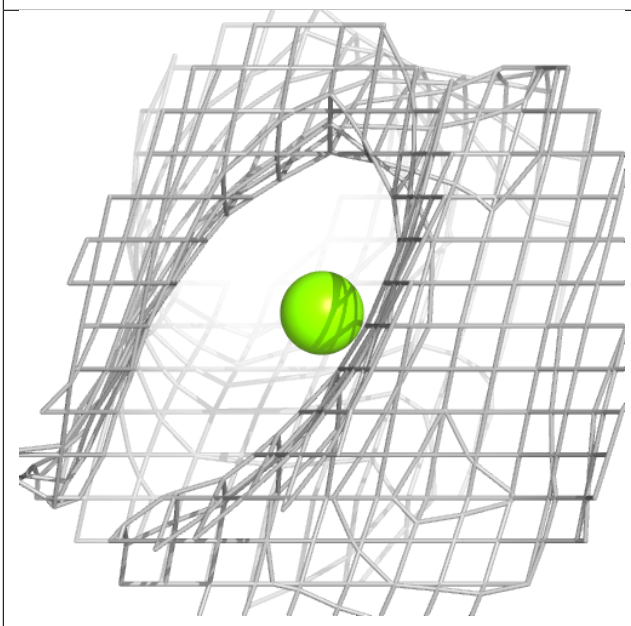
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	MG	DDD	507	1/1	0.60	0.09	101,101,101,101	0
5	MG	BBB	608	1/1	0.61	0.09	73,73,73,73	0
3	EDO	DDD	502	4/4	0.73	0.19	69,80,80,81	1
4	DG2	DDD	504	15/15	0.73	0.15	124,148,186,196	0
3	EDO	BBB	605	4/4	0.77	0.14	57,78,81,86	1
3	EDO	CCC	505	4/4	0.79	0.16	67,76,79,83	1
3	EDO	BBB	601	4/4	0.80	0.17	53,70,71,78	1
3	EDO	CCC	502	4/4	0.81	0.16	67,77,80,85	1
4	DG2	AAA	503	15/15	0.85	0.10	106,126,162,166	0
3	EDO	CCC	504	4/4	0.87	0.15	66,70,93,98	1
3	EDO	BBB	604	4/4	0.87	0.19	55,59,67,67	1
4	DG2	BBB	602	15/15	0.87	0.13	98,116,146,166	0
5	MG	CCC	506	1/1	0.88	0.09	58,58,58,58	0
3	EDO	AAA	505	4/4	0.90	0.16	53,68,85,92	1
5	MG	DDD	506	1/1	0.91	0.14	55,55,55,55	0
5	MG	BBB	607	1/1	0.91	0.18	51,51,51,51	0
3	EDO	DDD	505	4/4	0.92	0.15	66,68,70,73	1
5	MG	AAA	506	1/1	0.93	0.11	50,50,50,50	0
5	MG	AAA	507	1/1	0.94	0.08	79,79,79,79	0
3	EDO	BBB	606	4/4	0.94	0.12	63,78,88,91	1
4	DG2	AAA	504	15/15	0.96	0.14	48,73,91,93	0
3	EDO	AAA	502	4/4	0.96	0.11	50,54,61,62	1
4	DG2	CCC	503	15/15	0.96	0.15	58,84,112,112	0
4	DG2	DDD	503	15/15	0.96	0.17	59,138,187,196	0
2	ADP	BBB	603	27/27	0.98	0.14	43,56,71,85	2
2	ADP	CCC	501	27/27	0.98	0.13	41,65,83,89	2
6	PO4	BBB	609	5/5	0.98	0.12	57,59,62,71	0
2	ADP	AAA	501	27/27	0.99	0.15	34,54,79,88	2
2	ADP	DDD	501	27/27	0.99	0.14	45,66,78,82	2
5	MG	CCC	507	1/1	0.99	0.10	80,80,80,80	0

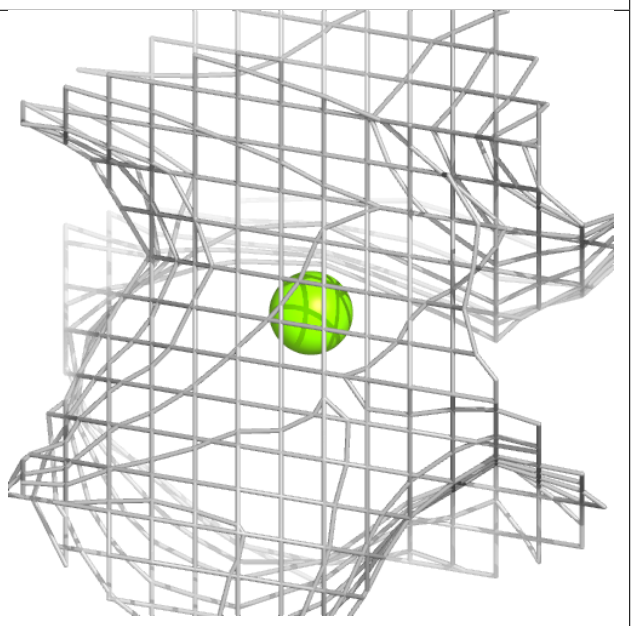
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around MG DDD 507:

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

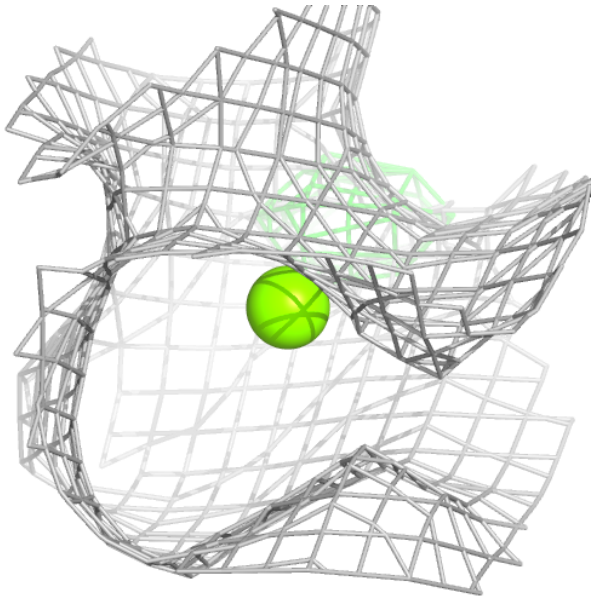


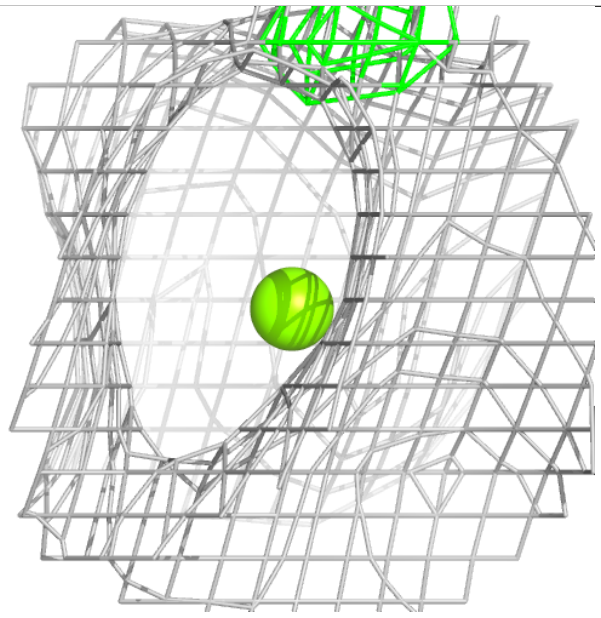


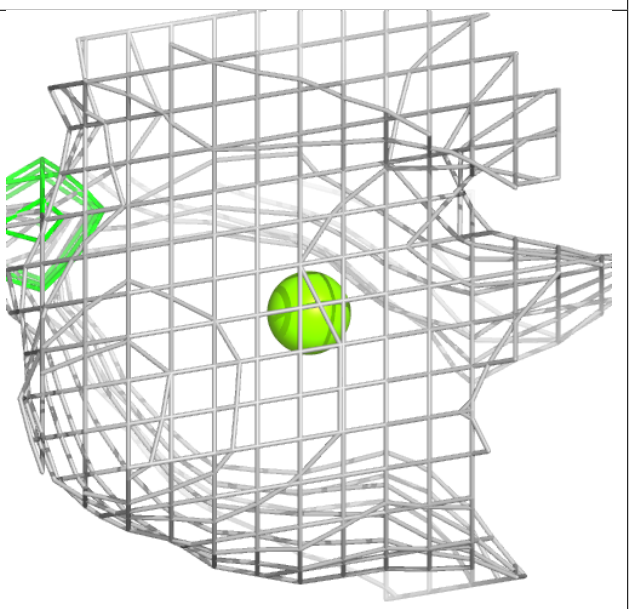


Electron density around MG BBB 608:

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

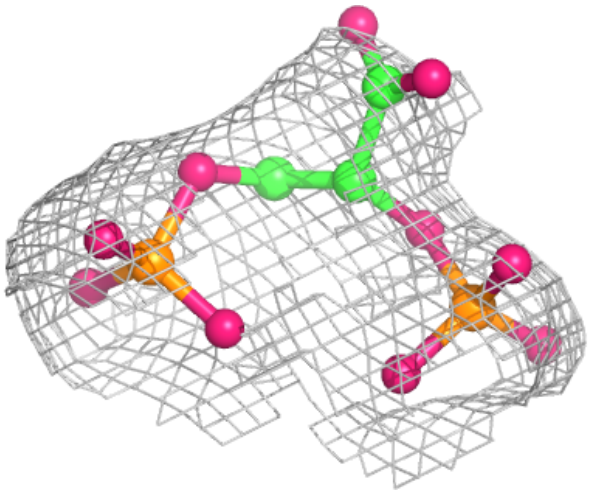


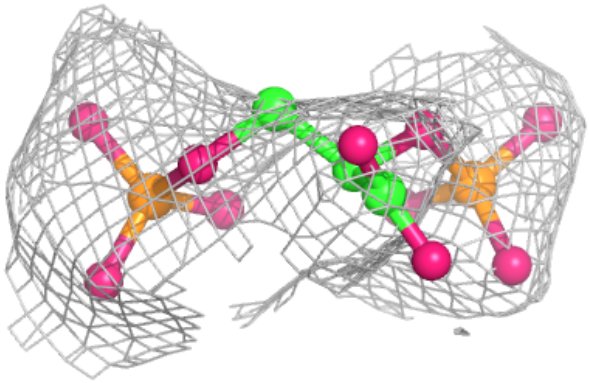


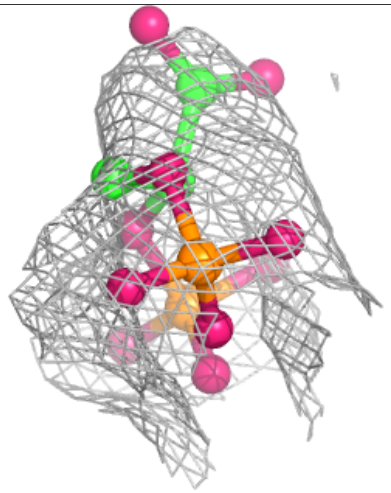


Electron density around DG2 DDD 504:

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

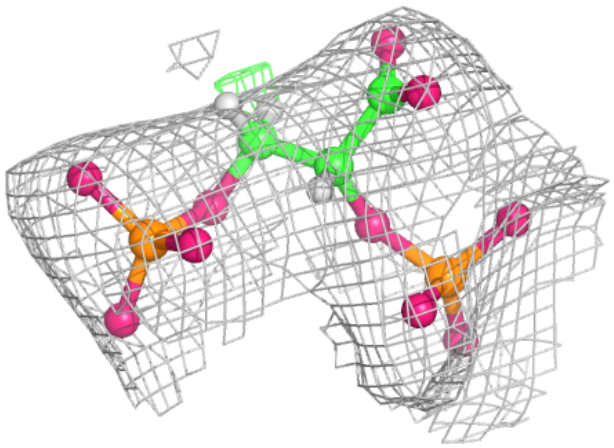


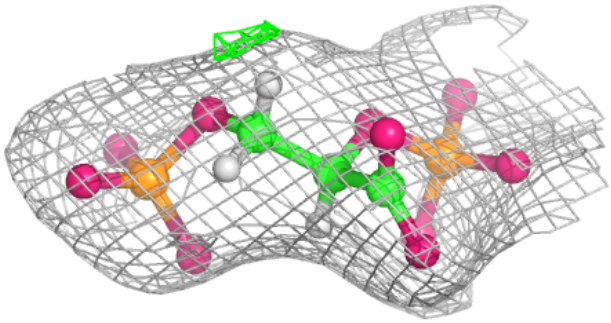


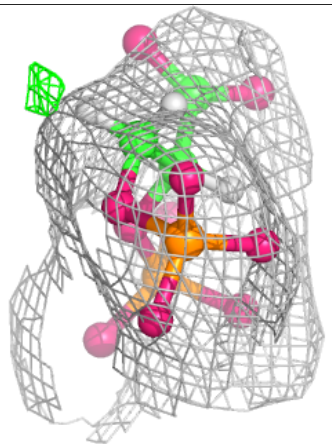


Electron density around DG2 AAA 503:

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

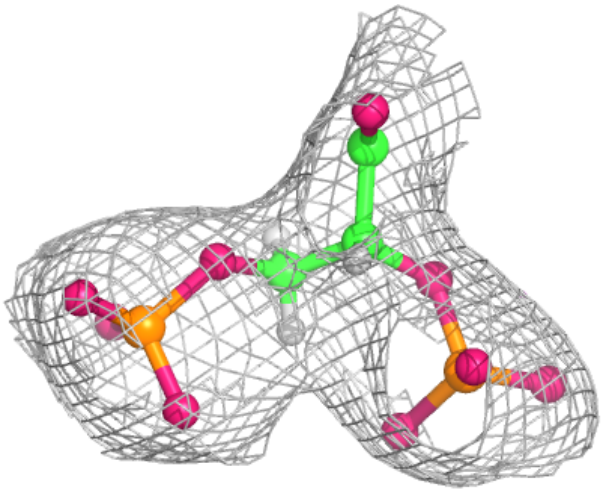


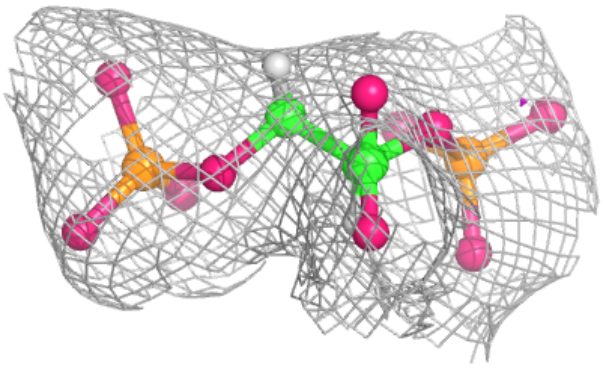


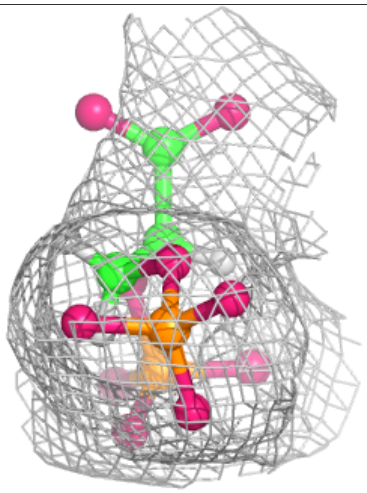


Electron density around DG2 BBB 602:

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

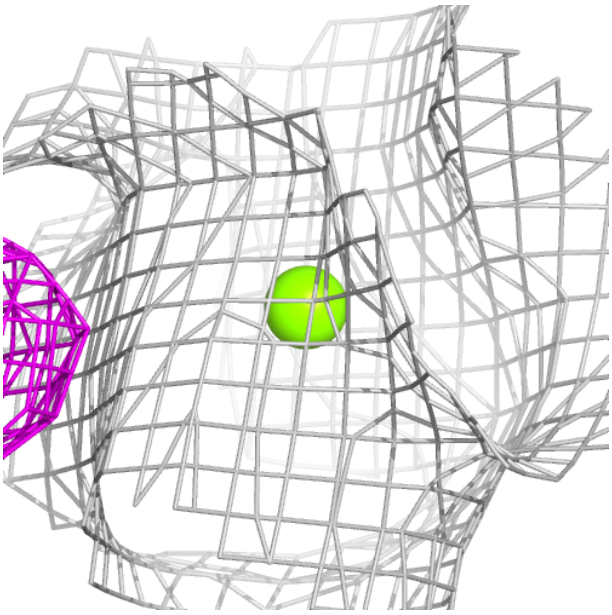


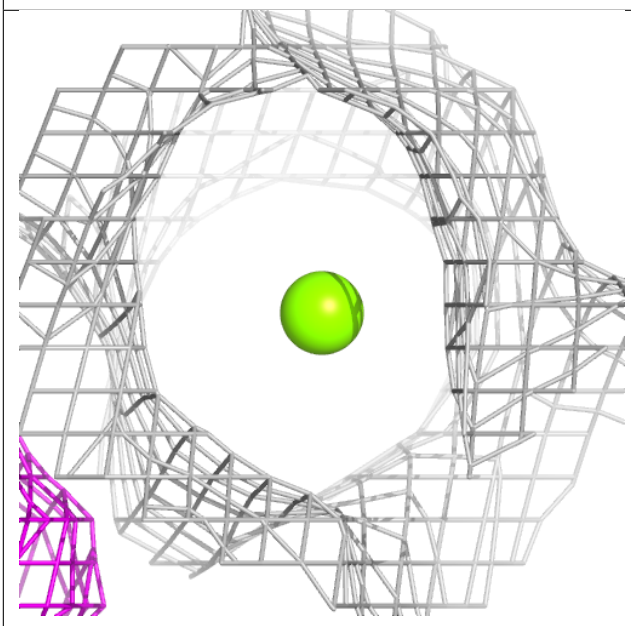


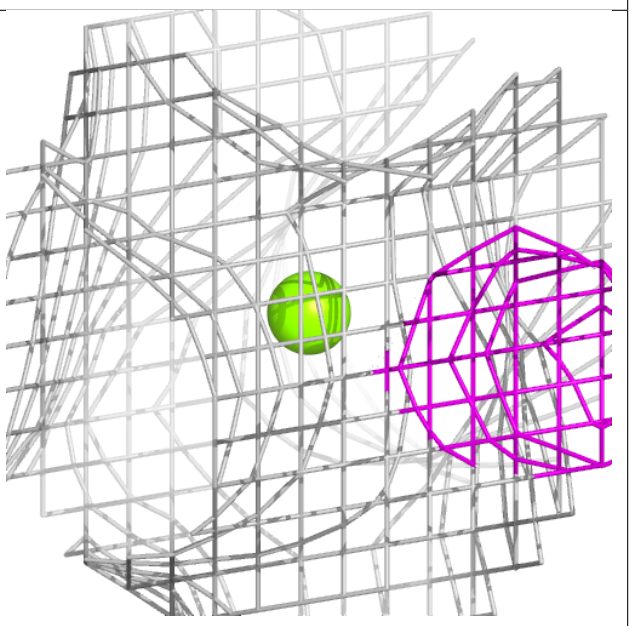


Electron density around MG CCC 506:

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

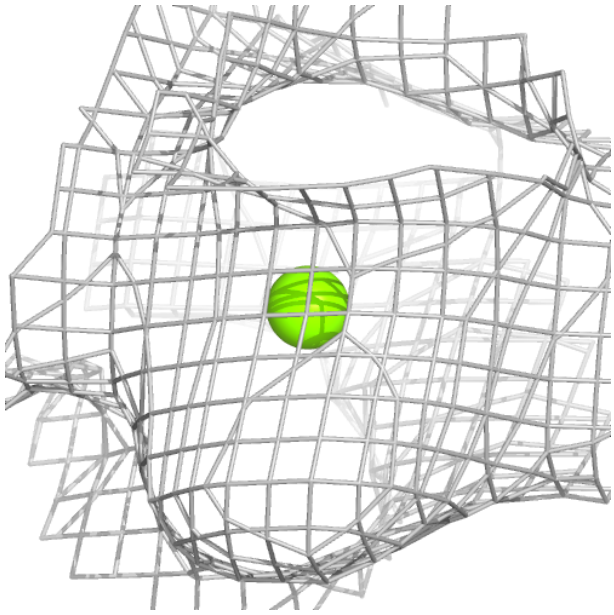


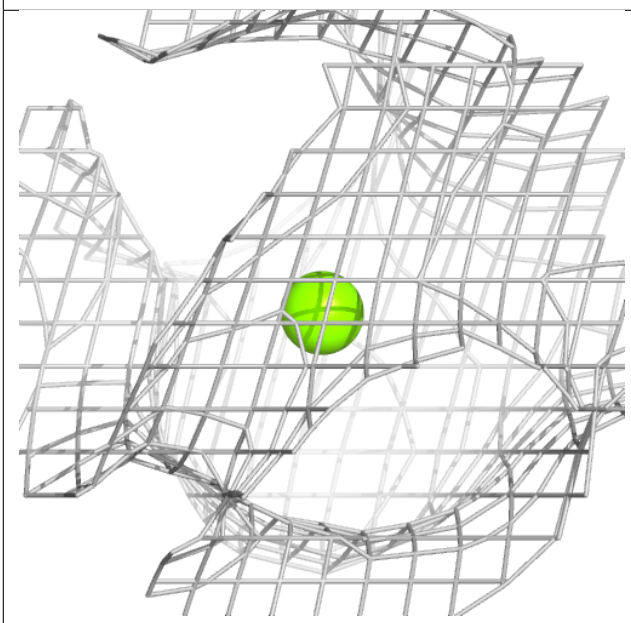


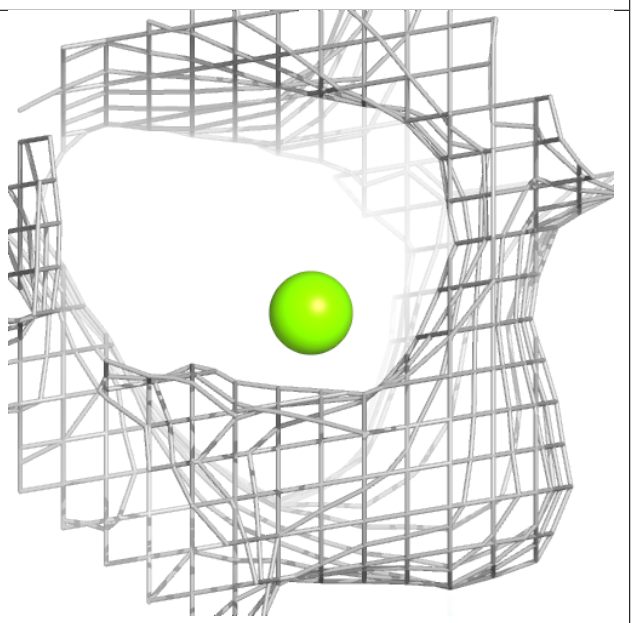


Electron density around MG DDD 506:

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

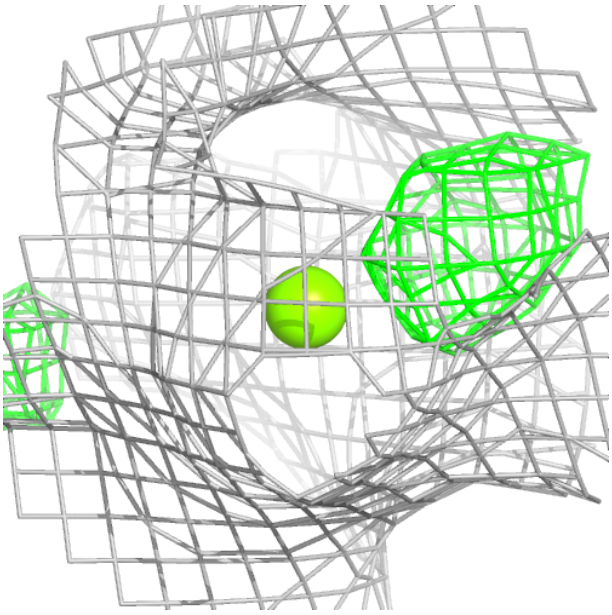


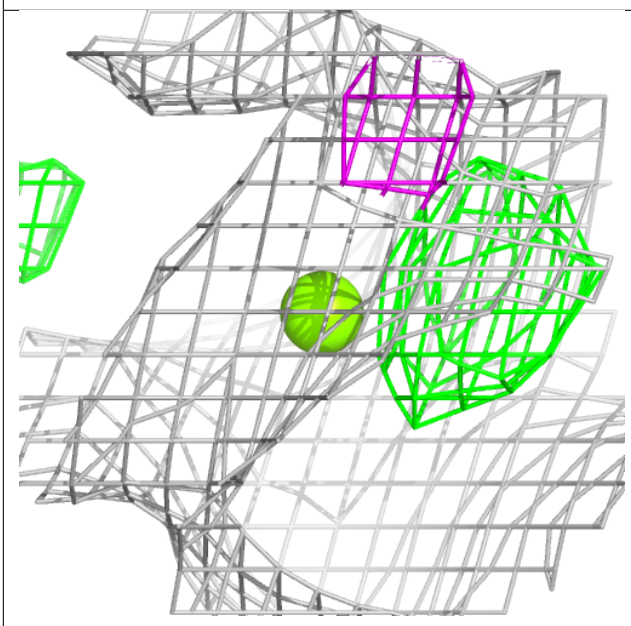


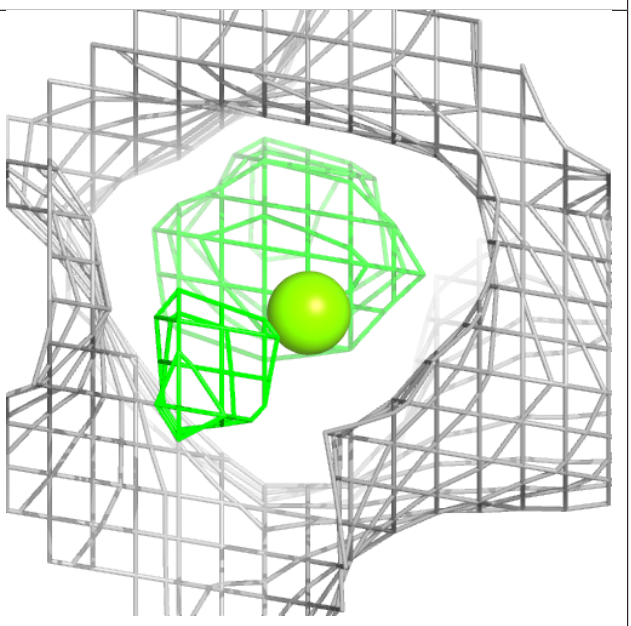


Electron density around MG BBB 607:

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

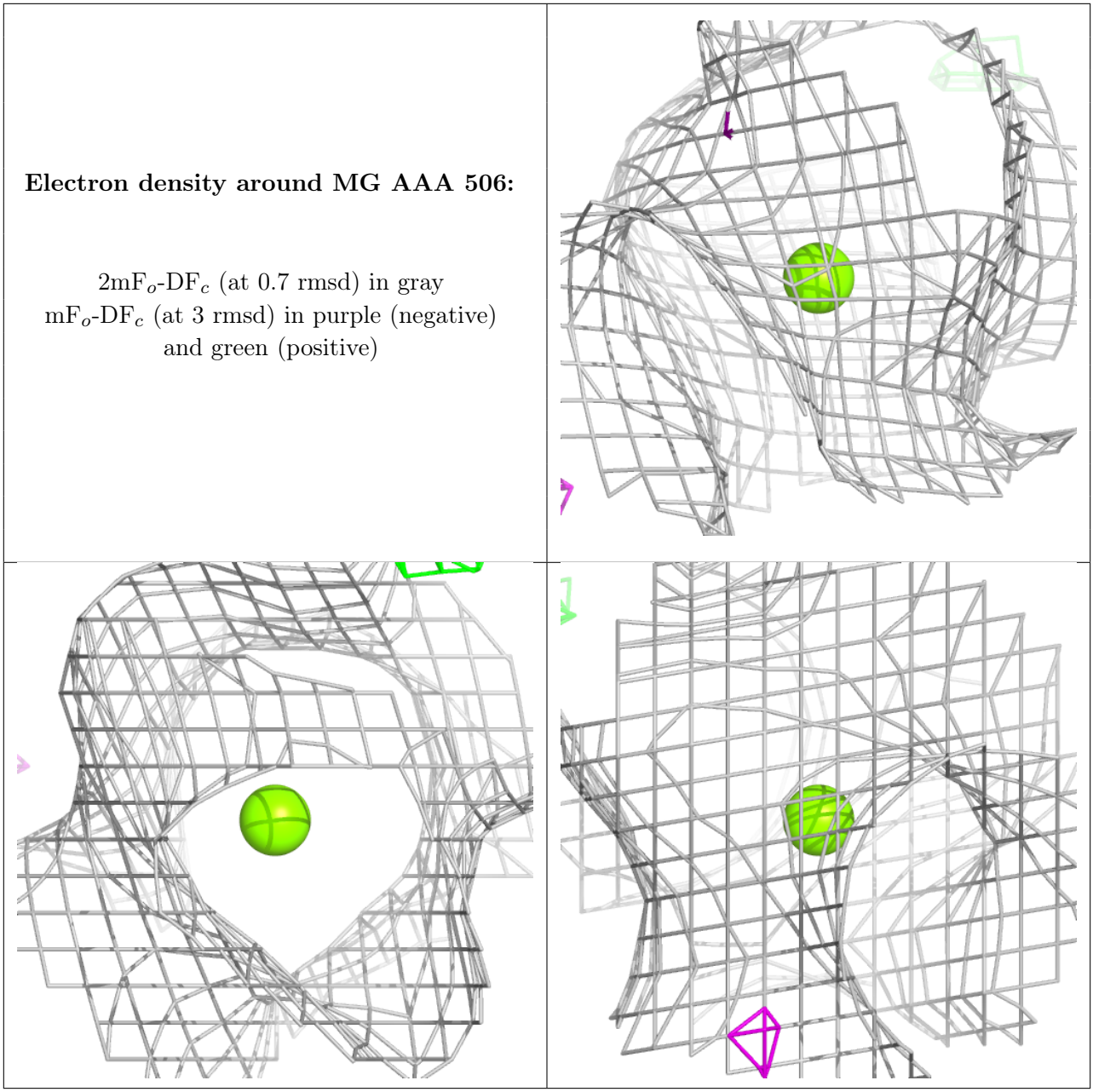






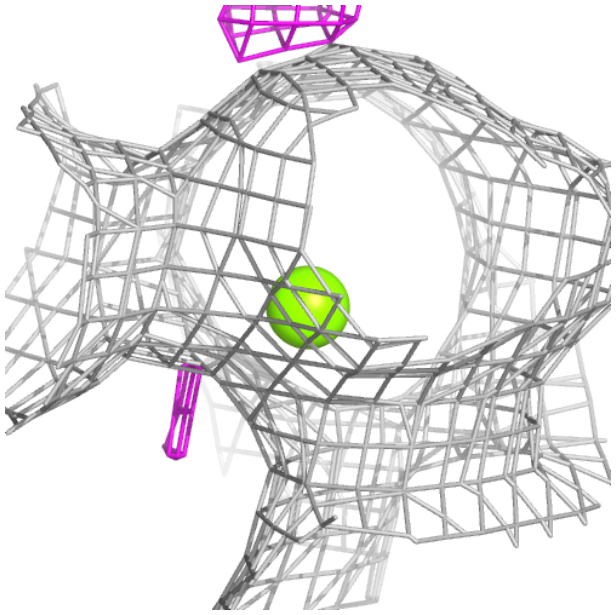
Electron density around MG AAA 506:

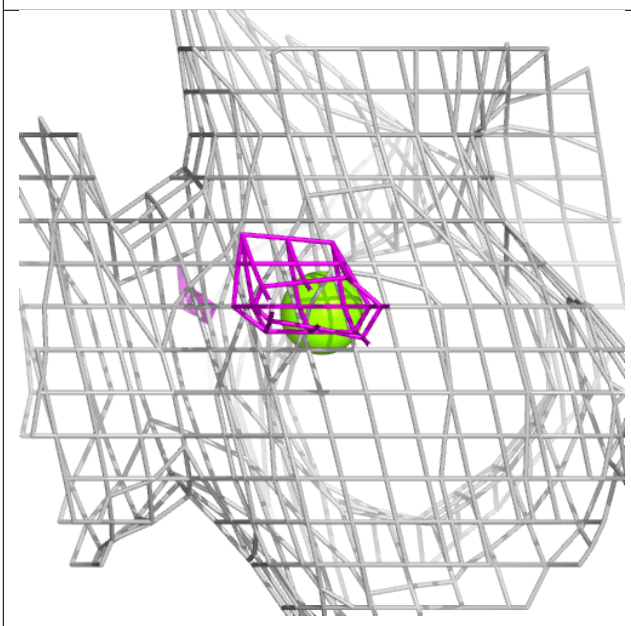
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

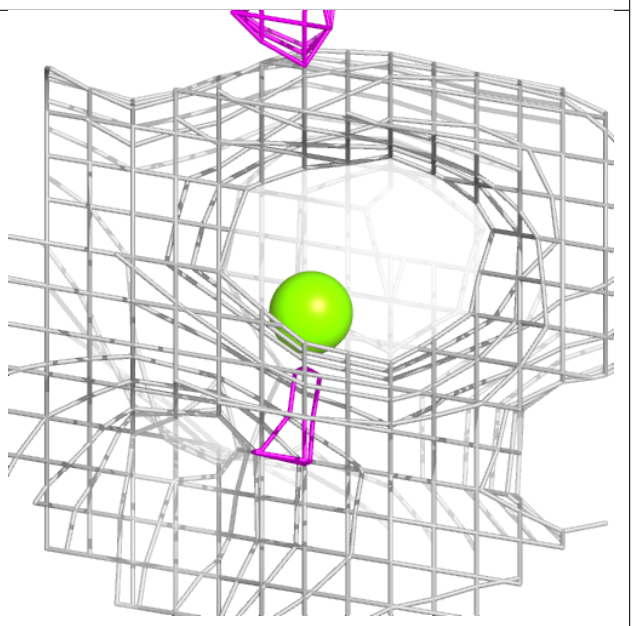


Electron density around MG AAA 507:

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

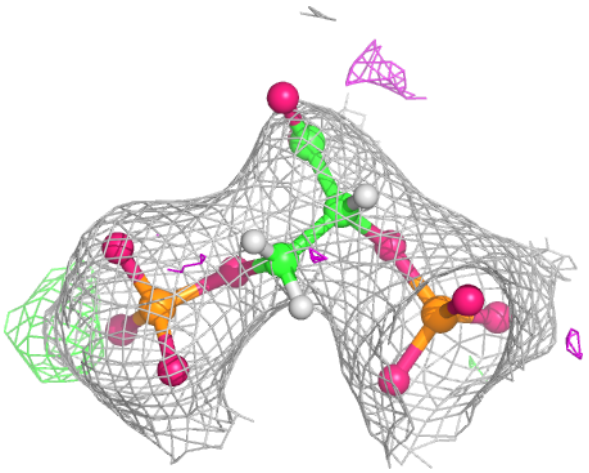


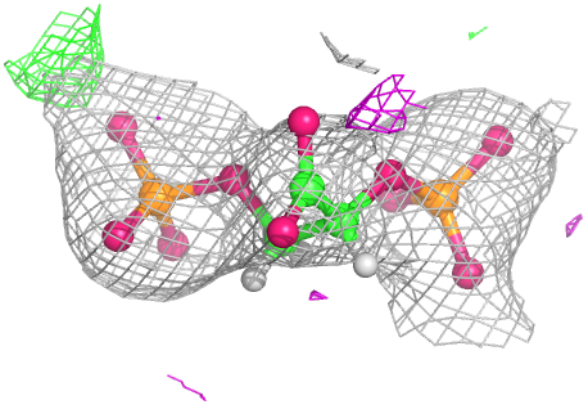


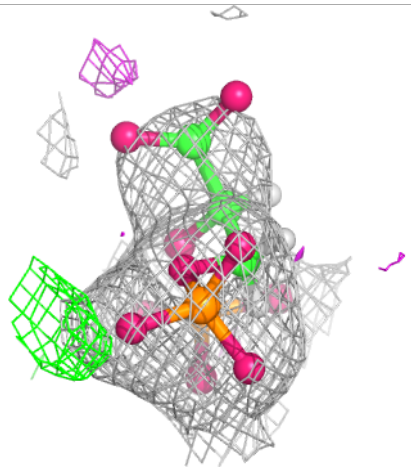


Electron density around DG2 AAA 504:

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

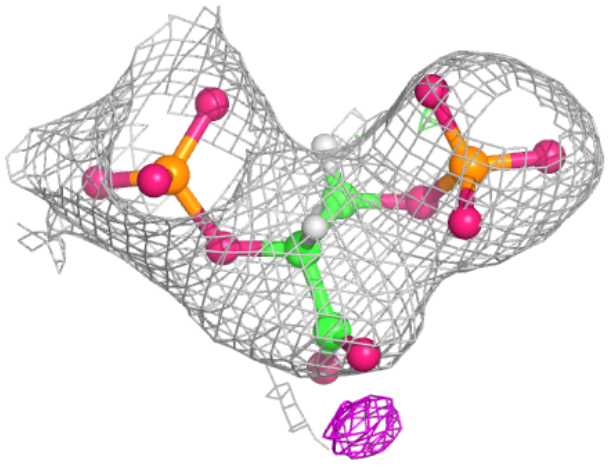


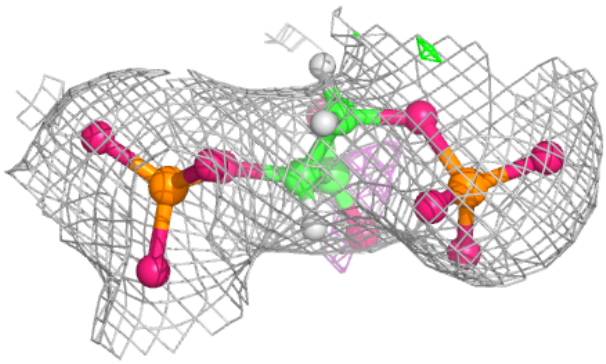


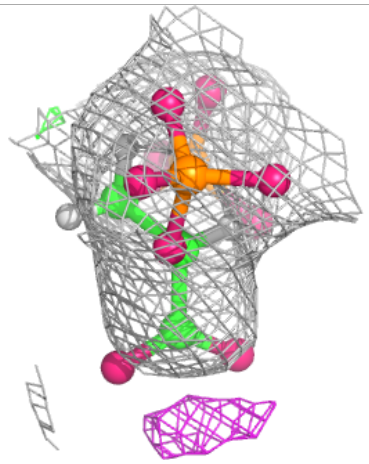


Electron density around DG2 CCC 503:

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

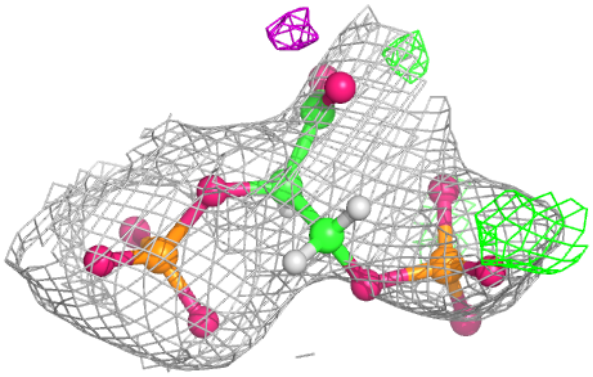


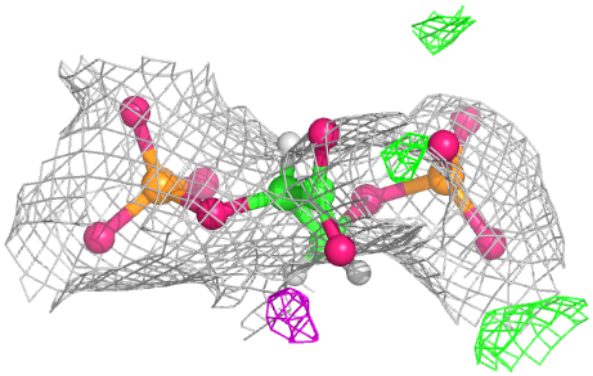


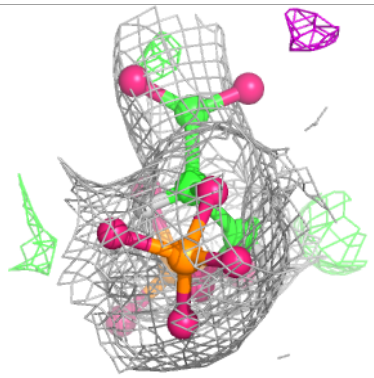


Electron density around DG2 DDD 503:

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

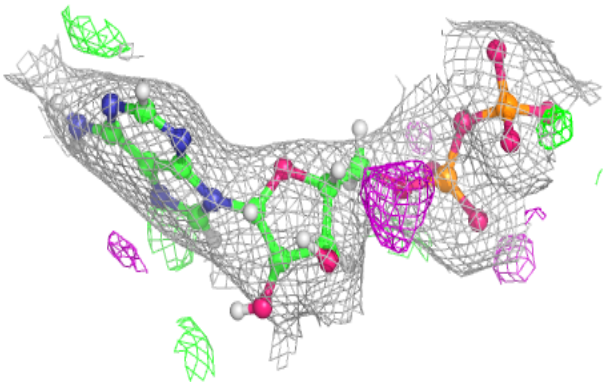


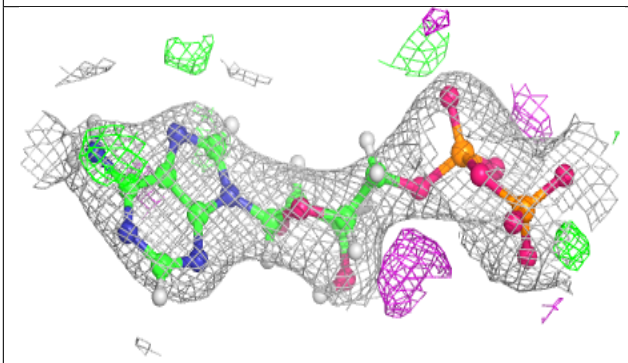


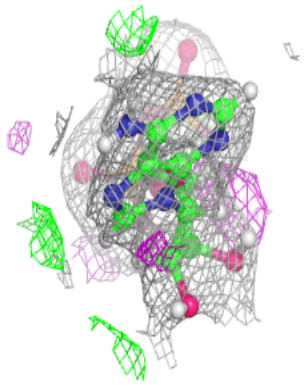


Electron density around ADP BBB 603:

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

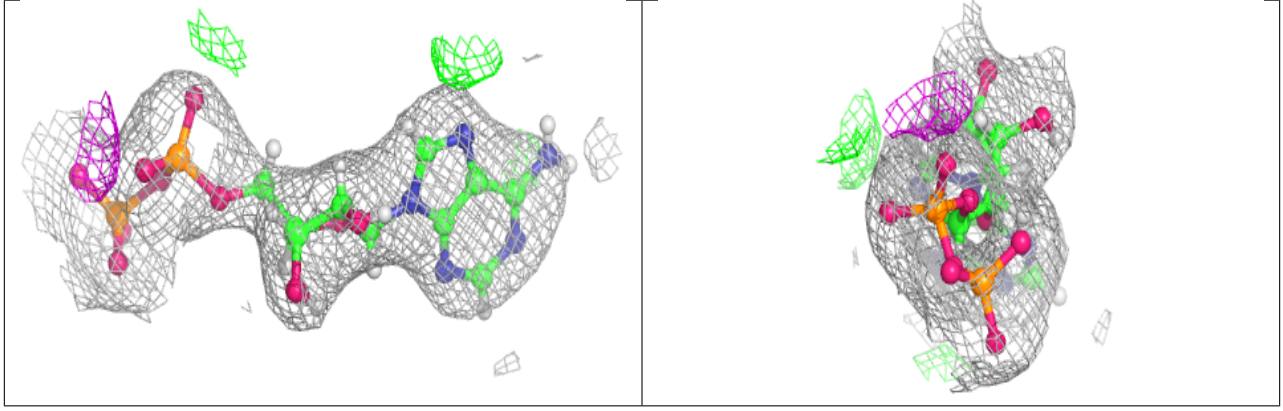






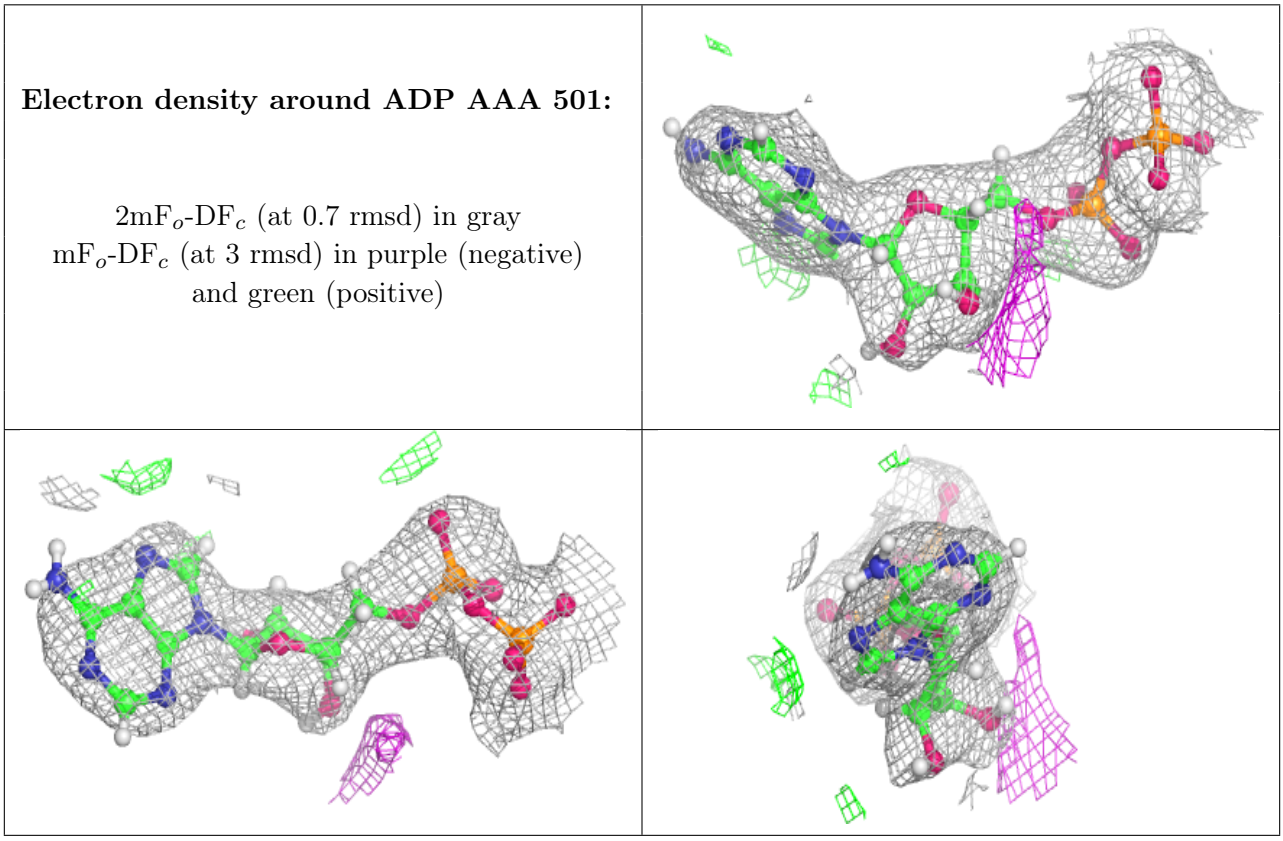
Electron density around ADP CCC 501:

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



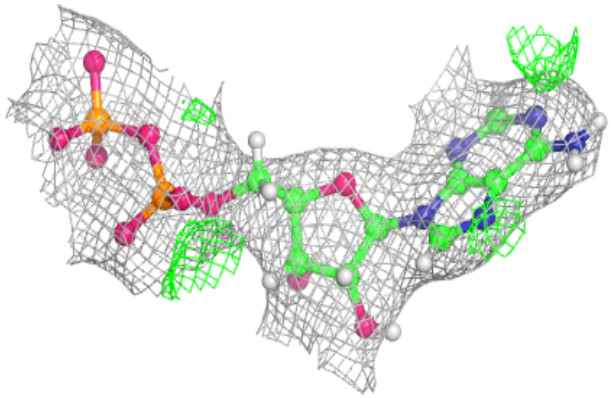
Electron density around ADP AAA 501:

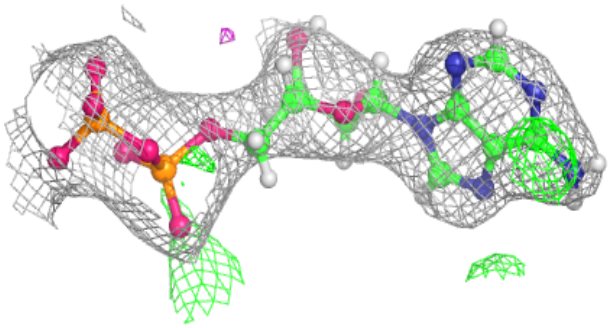
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

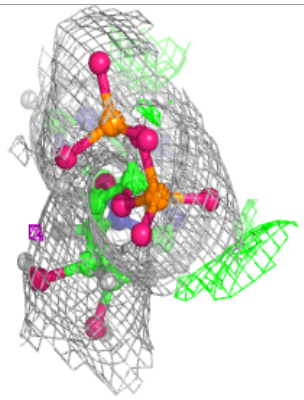


Electron density around ADP DDD 501:

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

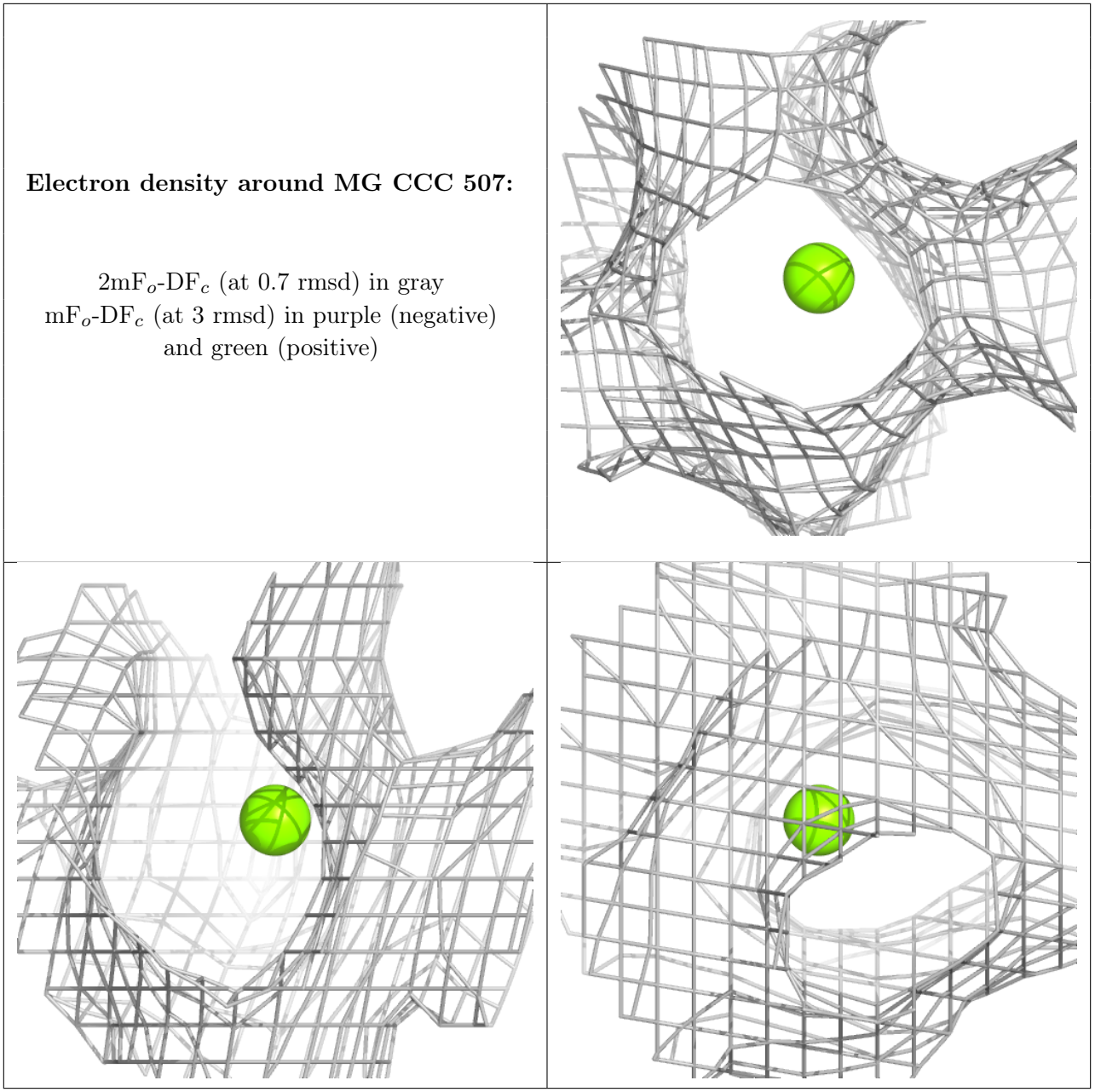






Electron density around MG CCC 507:

$2mF_o$-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

There are no such residues in this entry.