wwPDB X-ray Structure Validation Summary Report (i)

Nov 20, 2023 – 03:17 PM JST

PDB ID	:	7CS5
Title	:	IiPLR1 with NADP+ and (-)pinoresinol
Authors	:	Shao, K.; Zhang, P.
Deposited on	:	2020-08-14
Resolution	:	2.19 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:

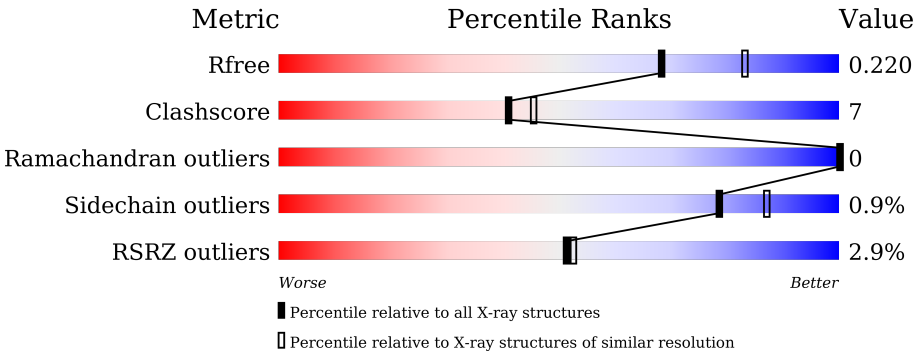
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.19 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	6864 (2.20-2.16)
Clashscore	141614	7689 (2.20-2.16)
Ramachandran outliers	138981	7564 (2.20-2.16)
Sidechain outliers	138945	7564 (2.20-2.16)
RSRZ outliers	127900	6738 (2.20-2.16)

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	A	317	5% 78% 12% 10%
1	B	317	2% 83% 8% 9%
1	C	317	2% 81% 9% 10%
1	D	317	3% 78% 11% 10%
1	E	317	% 82% 8% 10%
1	F	317	3% 83% 6% 10%

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	GEF	B	401	-	X	-	-
2	GEF	C	401	-	X	X	-
2	GEF	E	401	-	X	X	-
2	GEF	F	401	-	X	-	-

2 Entry composition (i)

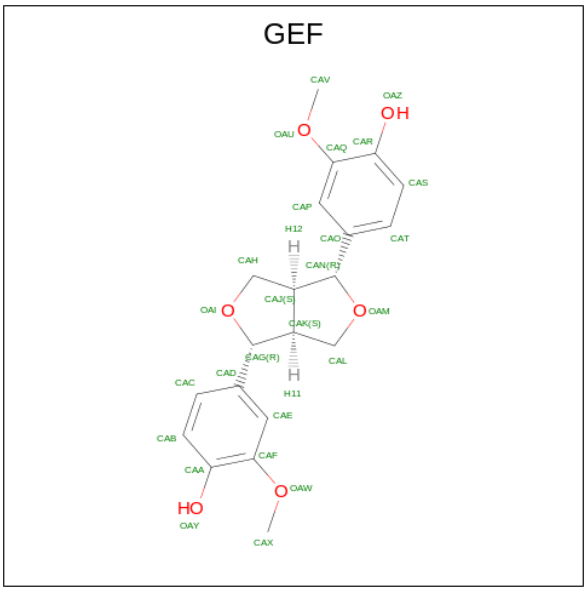
There are 4 unique types of molecules in this entry. The entry contains 15191 atoms, of which 156 are hydrogens and 0 are deuteriums.

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 Pinoresinol-lariciresinol reductase.

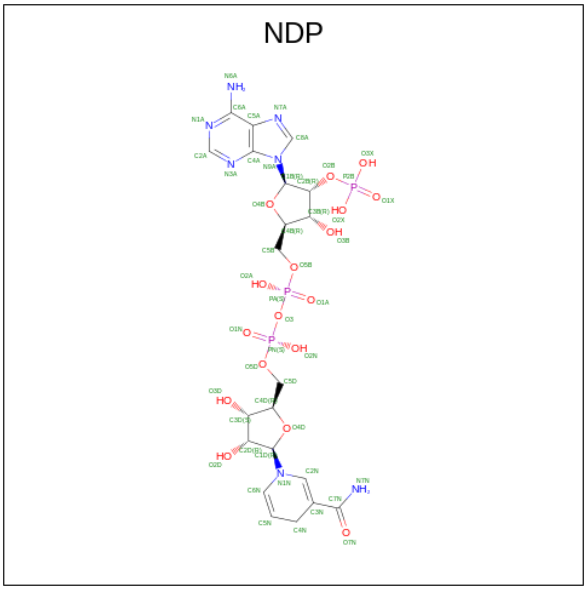
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	285	Total	C	N	O	S	0	0	0
			2243	1426	379	429	9			
1	A	284	Total	C	N	O	S	0	0	0
			2234	1421	377	427	9			
1	F	285	Total	C	N	O	S	0	0	0
			2237	1422	377	429	9			
1	D	285	Total	C	N	O	S	0	0	0
			2243	1426	379	429	9			
1	C	285	Total	C	N	O	S	0	0	0
			2243	1426	379	429	9			
1	B	290	Total	C	N	O	S	0	0	0
			2286	1454	387	436	9			

- Molecule 2 is 4-[(3R,3aS,6R,6aS)-6-(3-methoxy-4-oxidanyl-phenyl)-1,3,3a,4,6,6a-hexahydrofuro[3,4-c]furan-3-yl]-2-methoxy-phenol (three-letter code: GEF) (formula: $C_{20}H_{22}O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	E	1	Total C O 26 20 6	0	0
2	A	1	Total C O 26 20 6	0	0
2	F	1	Total C O 26 20 6	0	0
2	D	1	Total C O 26 20 6	0	0
2	C	1	Total C O 26 20 6	0	0
2	B	1	Total C O 26 20 6	0	0

- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	1	Total C H N O P 74 21 26 7 17 3	0	0
3	A	1	Total C H N O P 74 21 26 7 17 3	0	0
3	F	1	Total C H N O P 74 21 26 7 17 3	0	0
3	D	1	Total C H N O P 74 21 26 7 17 3	0	0
3	C	1	Total C H N O P 74 21 26 7 17 3	0	0

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	B	1	Total	C	H	N	O	P	0	0
			74	21	26	7	17	3		

- Molecule 4 is water.

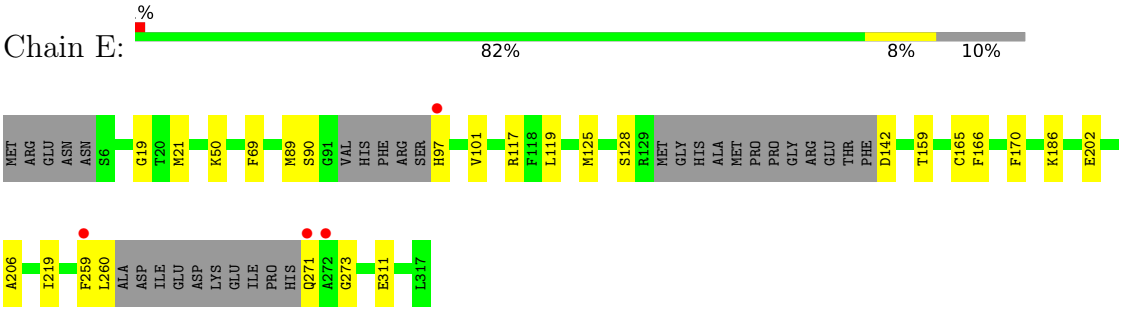
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	193	Total	O	0	0
			193	193		
4	A	156	Total	O	0	0
			156	156		
4	F	175	Total	O	0	0
			175	175		
4	D	178	Total	O	0	0
			178	178		
4	C	202	Total	O	0	0
			202	202		
4	B	201	Total	O	0	0
			201	201		

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.

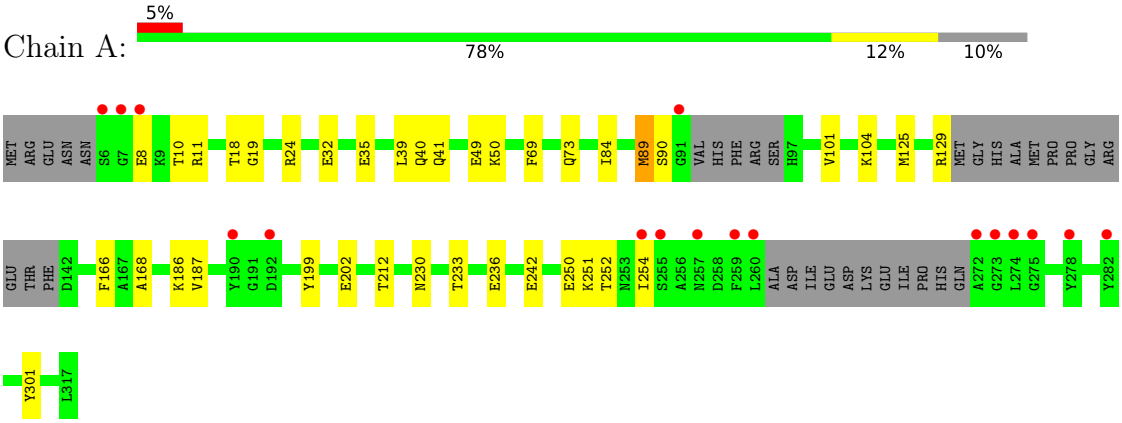
• Molecule 1: Pinoresinol-lariciresinol reductase

Chain E:



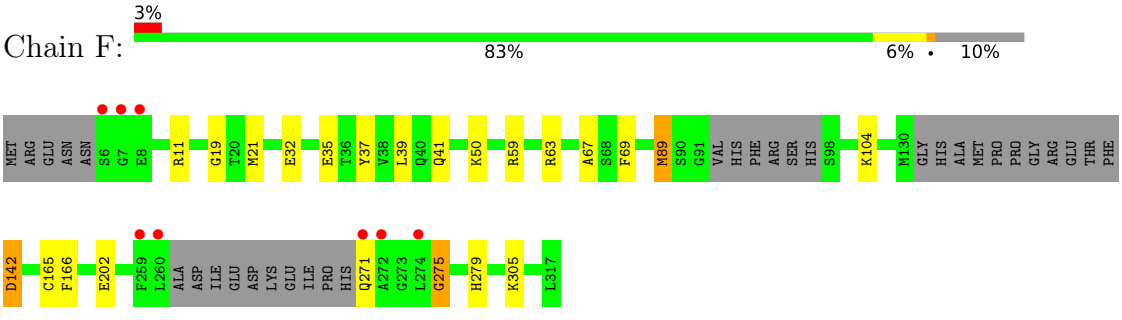
• Molecule 1: Pinoresinol-lariciresinol reductase

Chain A:



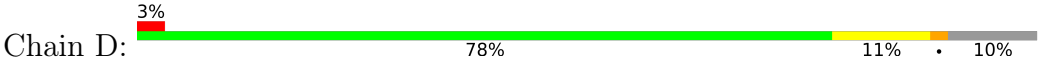
• Molecule 1: Pinoresinol-lariciresinol reductase

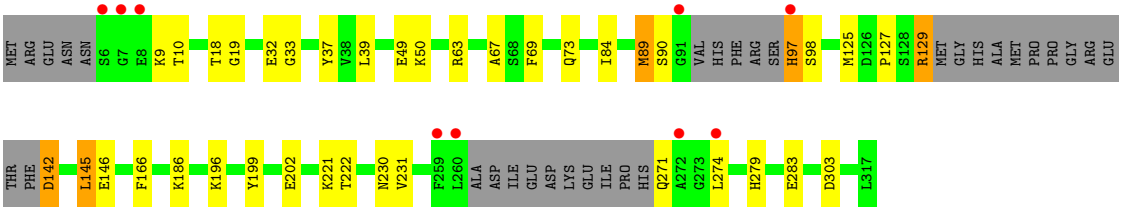
Chain F:



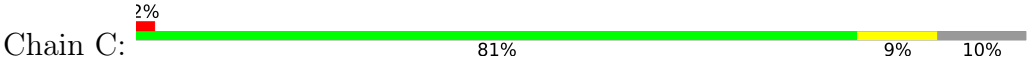
• Molecule 1: Pinoresinol-lariciresinol reductase

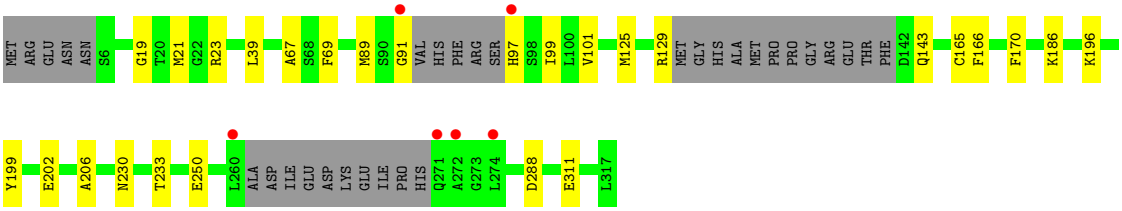
Chain D:



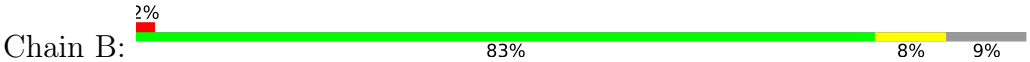


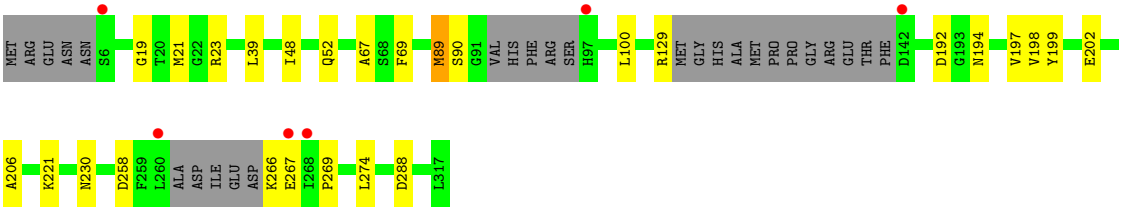
• Molecule 1: Pinoresinol-lariciresinol reductase





• Molecule 1: Pinoresinol-lariciresinol reductase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α, β, γ	244.95Å 244.95Å 75.74Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.50 – 2.19 39.50 – 2.19	Depositor EDS
% Data completeness (in resolution range)	99.7 (39.50-2.19) 96.1 (39.50-2.19)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.03 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.10_2155, PHENIX 1.10_2155	Depositor
R, R_{free}	0.183 , 0.220 0.184 , 0.220	Depositor DCC
R_{free} test set	2007 reflections (1.51%)	wwPDB-VP
Wilson B-factor (Å^2)	28.3	Xtriage
Anisotropy	0.007	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 43.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.025 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	15191	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 32.19 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.7928e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: NDP, GEF

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	0.40	0/2271	0.56	0/3067
1	B	0.42	0/2325	0.59	1/3140 (0.0%)
1	C	0.40	0/2280	0.56	0/3079
1	D	0.38	0/2280	0.56	0/3079
1	E	0.41	0/2280	0.56	0/3079
1	F	0.39	0/2273	0.56	0/3069
All	All	0.40	0/13709	0.57	1/18513 (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	E	0	1
1	F	0	1
All	All	0	2

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	B	274	LEU	C-N-CA	-5.82	110.07	122.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	128	SER	Peptide

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Mol	Chain	Res	Type	Group
1	F	275	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	2234	0	2240	41	0
1	B	2286	0	2292	24	0
1	C	2243	0	2248	25	0
1	D	2243	0	2248	45	0
1	E	2243	0	2248	22	0
1	F	2237	0	2242	21	0
2	A	26	0	0	3	0
2	B	26	0	0	5	0
2	C	26	0	0	9	0
2	D	26	0	0	3	0
2	E	26	0	0	9	0
2	F	26	0	0	5	0
3	A	48	26	26	11	0
3	B	48	26	26	6	0
3	C	48	26	26	3	0
3	D	48	26	26	9	0
3	E	48	26	26	7	0
3	F	48	26	26	10	0
4	A	156	0	0	4	0
4	B	201	0	0	3	0
4	C	202	0	0	4	0
4	D	178	0	0	12	0
4	E	193	0	0	5	0
4	F	175	0	0	4	0
All	All	15035	156	13674	197	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 197 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)
2:E:401:GEF:OAM	2:E:401:GEF:CAN	1.89	1.18
2:F:401:GEF:OAM	2:F:401:GEF:CAN	1.87	1.14
2:B:401:GEF:OAM	2:B:401:GEF:CAN	1.92	1.07
2:C:401:GEF:CAN	2:C:401:GEF:OAM	1.83	1.06
2:C:401:GEF:OAM	2:C:401:GEF:CAO	2.09	1.00

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	276/317 (87%)	267 (97%)	9 (3%)	0	100	100
1	B	282/317 (89%)	275 (98%)	7 (2%)	0	100	100
1	C	277/317 (87%)	270 (98%)	7 (2%)	0	100	100
1	D	277/317 (87%)	272 (98%)	5 (2%)	0	100	100
1	E	277/317 (87%)	274 (99%)	3 (1%)	0	100	100
1	F	277/317 (87%)	271 (98%)	6 (2%)	0	100	100
All	All	1666/1902 (88%)	1629 (98%)	37 (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	A	242/271 (89%)	240 (99%)	2 (1%)	81 89
1	B	248/271 (92%)	247 (100%)	1 (0%)	91 95
1	C	243/271 (90%)	242 (100%)	1 (0%)	91 95
1	D	243/271 (90%)	238 (98%)	5 (2%)	53 64
1	E	243/271 (90%)	242 (100%)	1 (0%)	91 95
1	F	242/271 (89%)	239 (99%)	3 (1%)	71 81
All	All	1461/1626 (90%)	1448 (99%)	13 (1%)	78 87

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	97	HIS
1	D	129	ARG
1	B	89	MET
1	D	145	LEU
1	C	89	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	81	GLN
1	A	41	GLN
1	D	73	GLN

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)

12 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	$\#\|Z\| > 2$
3	NDP	E	402	-	45,52,52	3.80	17 (37%)	53,80,80	2.34	11 (20%)
2	GEF	E	401	-	29,29,29	7.84	11 (37%)	42,42,42	9.51	30 (71%)
2	GEF	D	401	-	29,29,29	3.29	9 (31%)	42,42,42	8.24	26 (61%)
2	GEF	C	401	-	29,29,29	7.31	11 (37%)	42,42,42	9.30	28 (66%)
3	NDP	A	402	-	45,52,52	3.93	16 (35%)	53,80,80	2.34	11 (20%)
2	GEF	F	401	-	29,29,29	7.54	12 (41%)	42,42,42	9.47	31 (73%)
2	GEF	A	401	-	29,29,29	3.46	9 (31%)	42,42,42	8.07	20 (47%)
3	NDP	B	402	-	45,52,52	3.65	15 (33%)	53,80,80	2.32	10 (18%)
3	NDP	D	402	-	45,52,52	3.98	18 (40%)	53,80,80	2.39	11 (20%)
3	NDP	C	402	-	45,52,52	3.91	18 (40%)	53,80,80	2.19	9 (16%)
2	GEF	B	401	-	29,29,29	8.30	12 (41%)	42,42,42	9.61	31 (73%)
3	NDP	F	402	-	45,52,52	3.80	15 (33%)	53,80,80	2.14	8 (15%)

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
3	NDP	E	402	-	-	5/30/77/77	0/5/5/5
2	GEF	E	401	-	-	8/12/34/34	0/4/4/4
2	GEF	D	401	-	-	8/12/34/34	0/4/4/4
2	GEF	C	401	-	-	8/12/34/34	0/4/4/4
3	NDP	A	402	-	-	7/30/77/77	0/5/5/5
2	GEF	F	401	-	-	5/12/34/34	0/4/4/4
2	GEF	A	401	-	-	8/12/34/34	0/4/4/4
3	NDP	B	402	-	-	4/30/77/77	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NDP	D	402	-	-	6/30/77/77	0/5/5/5
3	NDP	C	402	-	-	4/30/77/77	0/5/5/5
2	GEF	B	401	-	-	6/12/34/34	0/4/4/4
3	NDP	F	402	-	-	4/30/77/77	0/5/5/5

The worst 5 of 163 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	GEF	OAM-CAN	33.83	1.92	1.43
2	E	401	GEF	OAM-CAN	31.55	1.89	1.43
2	F	401	GEF	OAM-CAN	30.45	1.87	1.43
2	C	401	GEF	OAM-CAN	27.76	1.83	1.43
3	D	402	NDP	O4B-C1B	15.52	1.62	1.41

The worst 5 of 226 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	401	GEF	OAM-CAN-CAJ	-30.18	72.23	104.77
2	D	401	GEF	OAI-CAG-CAK	-29.37	73.11	104.77
2	A	401	GEF	OAI-CAG-CAK	-28.89	73.63	104.77
2	B	401	GEF	OAM-CAL-CAK	-28.77	65.44	105.58
2	F	401	GEF	OAM-CAN-CAJ	-27.65	74.96	104.77

There are no chirality outliers.

5 of 73 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	402	NDP	C5B-O5B-PA-O3
3	A	402	NDP	C5B-O5B-PA-O3
3	D	402	NDP	C5B-O5B-PA-O3
2	E	401	GEF	CAR-CAQ-OAU-CAV
2	A	401	GEF	CAR-CAQ-OAU-CAV

There are no ring outliers.

12 monomers are involved in 76 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	402	NDP	7	0
2	E	401	GEF	9	0
2	D	401	GEF	3	0

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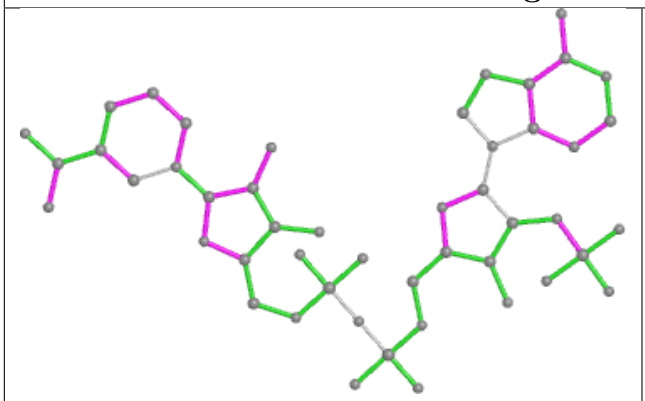
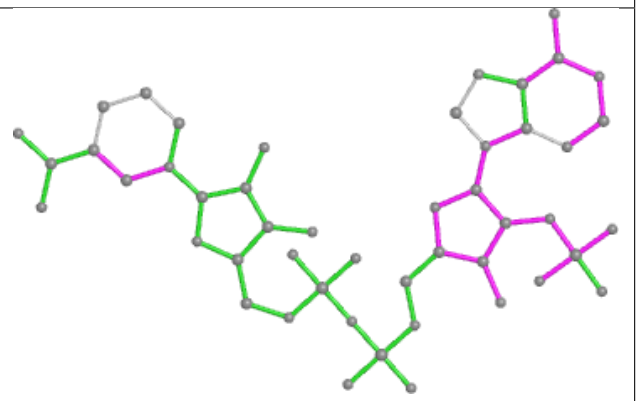
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	401	GEF	9	0
3	A	402	NDP	11	0
2	F	401	GEF	5	0
2	A	401	GEF	3	0
3	B	402	NDP	6	0
3	D	402	NDP	9	0
3	C	402	NDP	3	0
2	B	401	GEF	5	0
3	F	402	NDP	10	0

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.

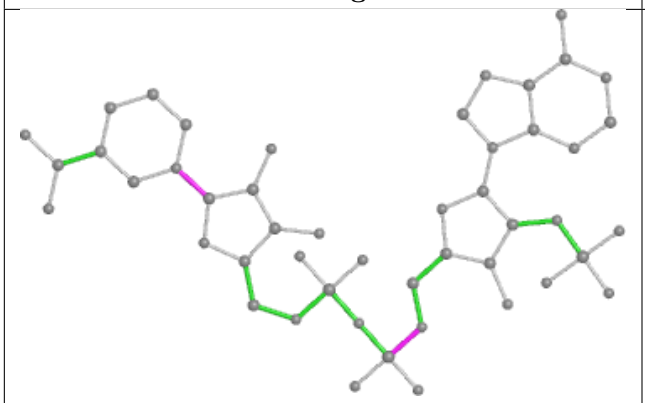
Ligand NDP E 402



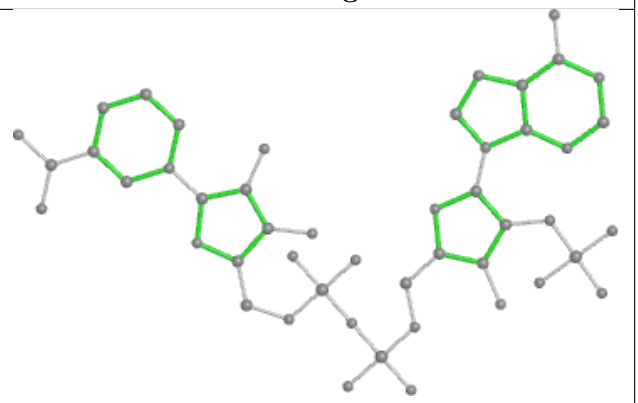
Bond lengths



Bond angles

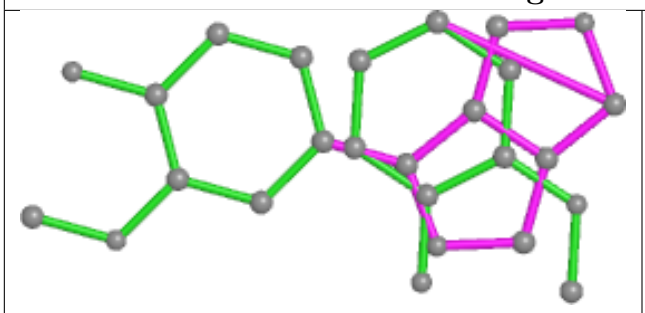


Torsions

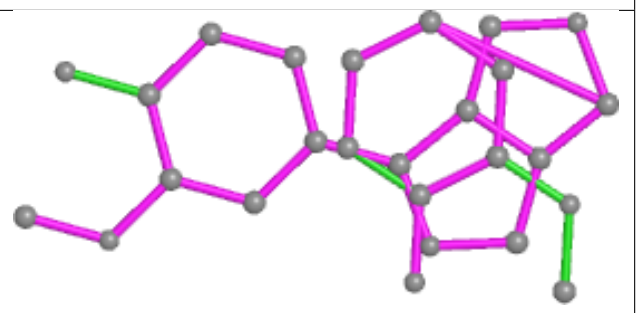


Rings

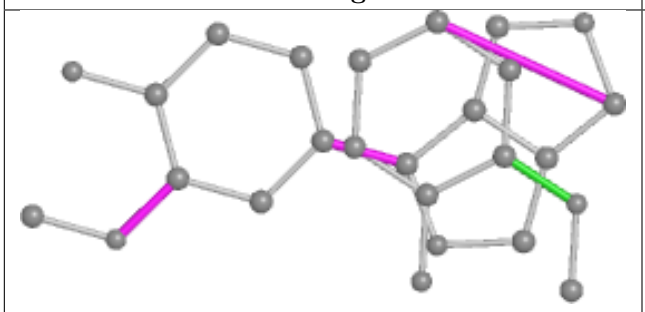
Ligand GEF E 401



Bond lengths



Bond angles



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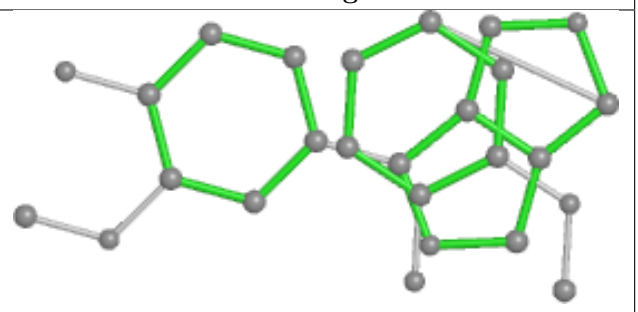
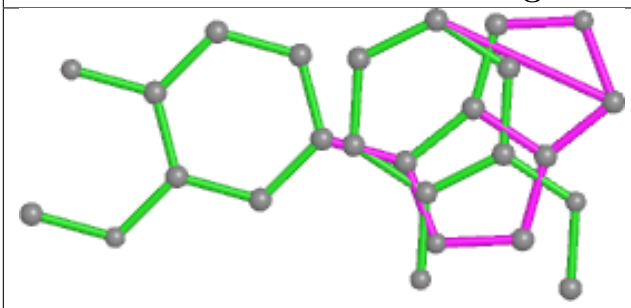
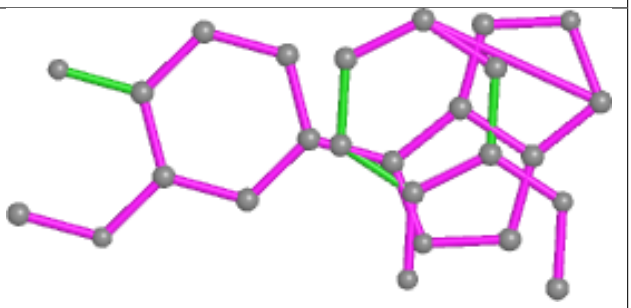


Rings

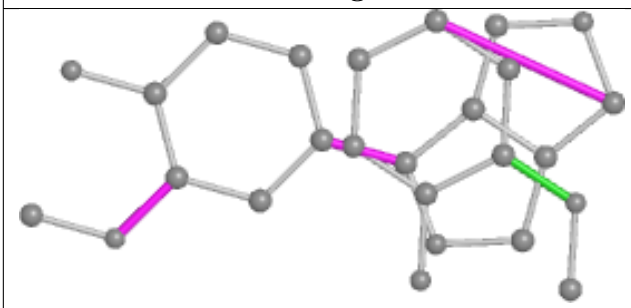
Ligand GEF D 401



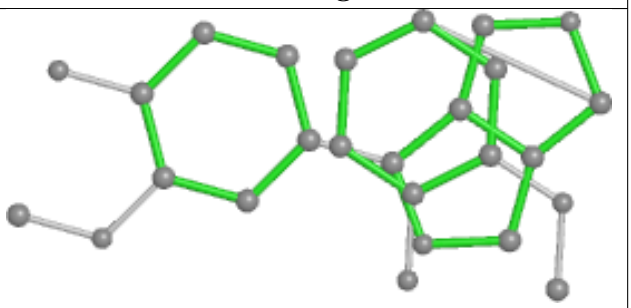
Bond lengths



Bond angles

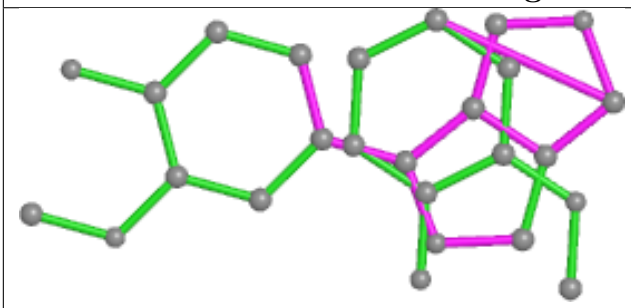


Torsions

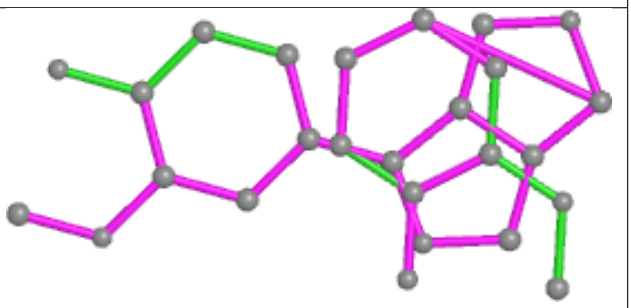


Rings

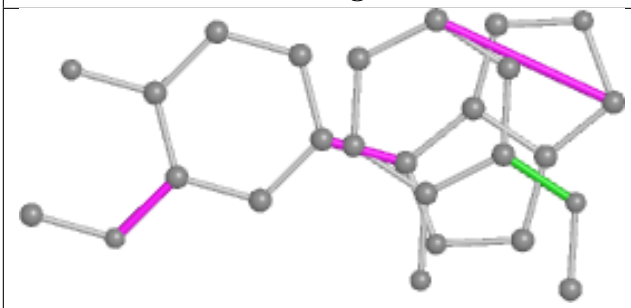
Ligand GEF C 401



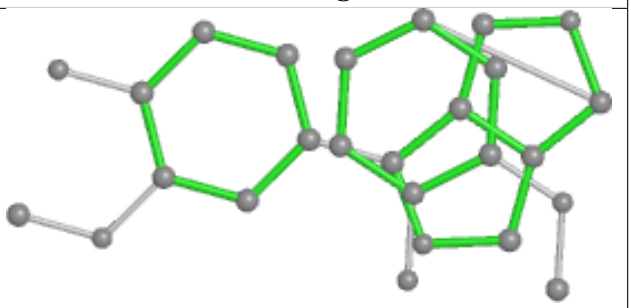
Bond lengths



Bond angles

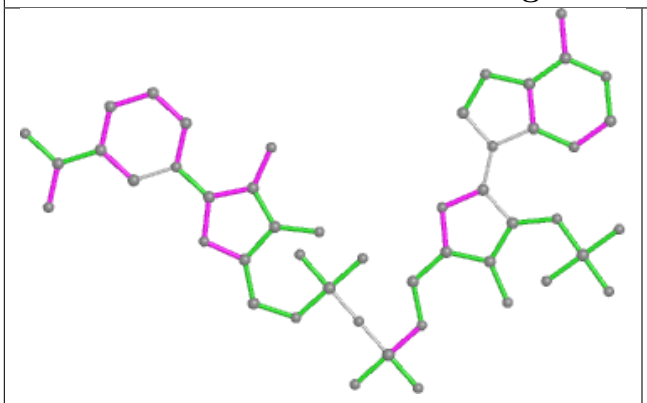


Torsions



Rings

Ligand NDP A 402



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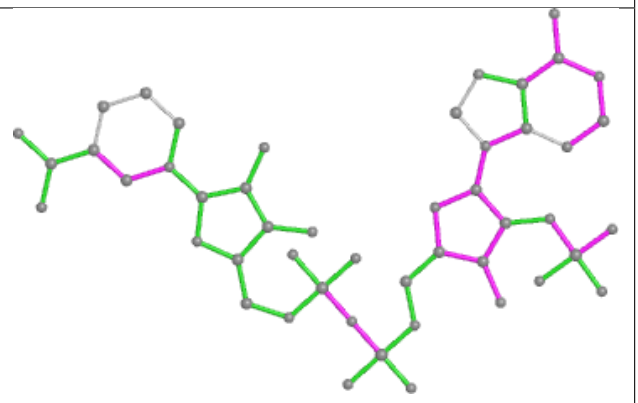
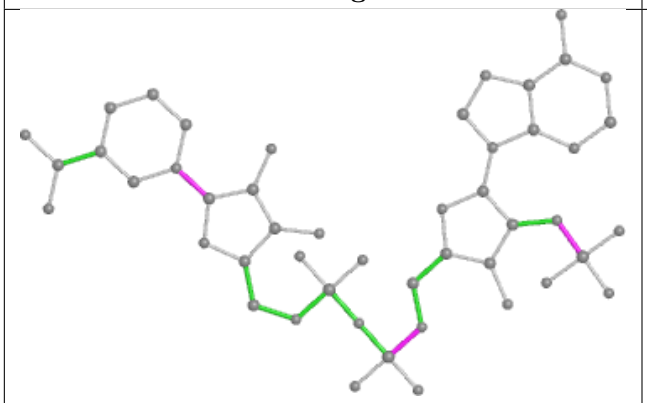


Bond angles



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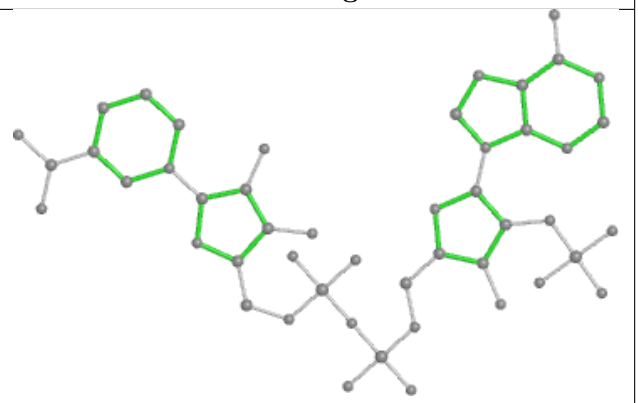
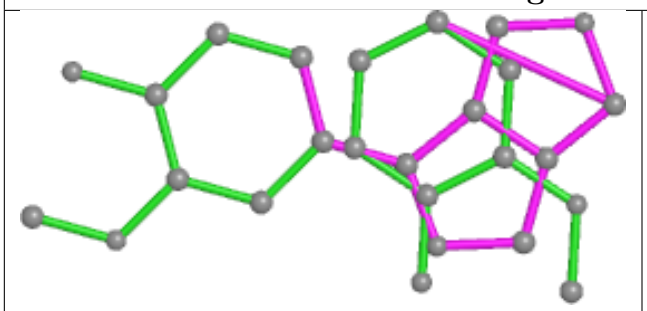


Rings

Ligand GEF F 401



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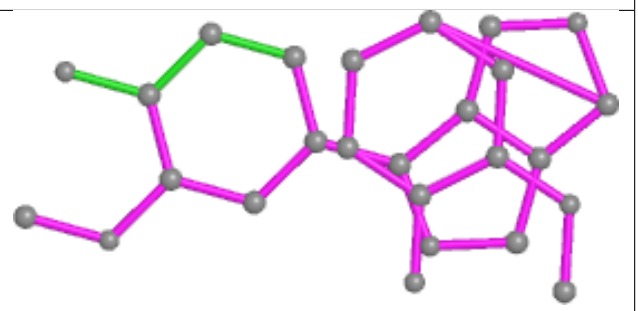
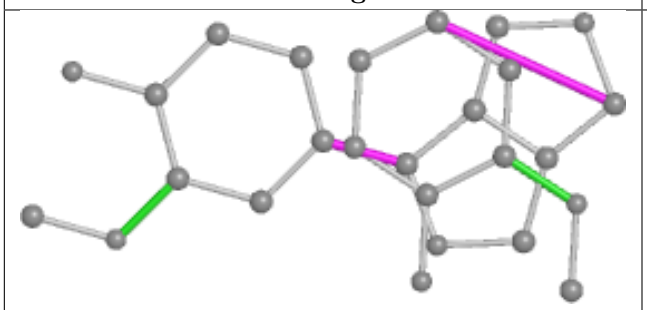


Bond angles



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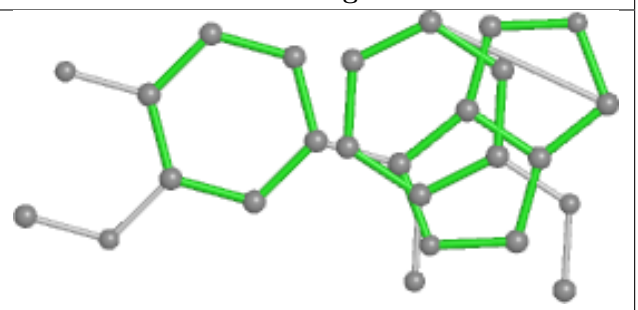
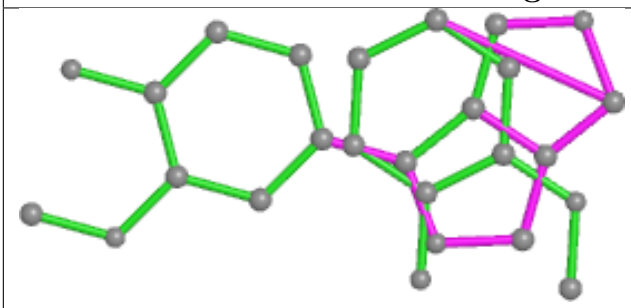


Rings

Ligand GEF A 401



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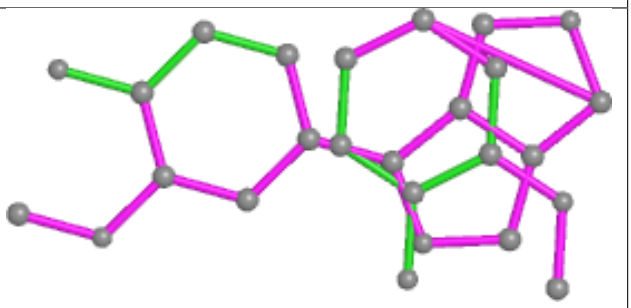
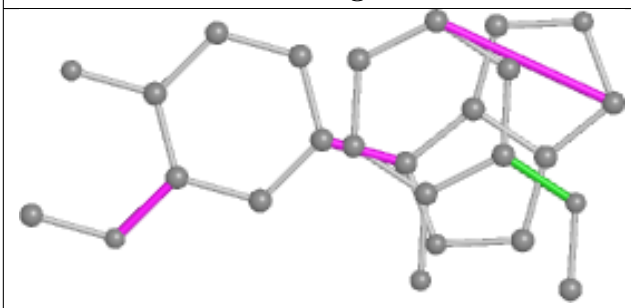


Bond angles



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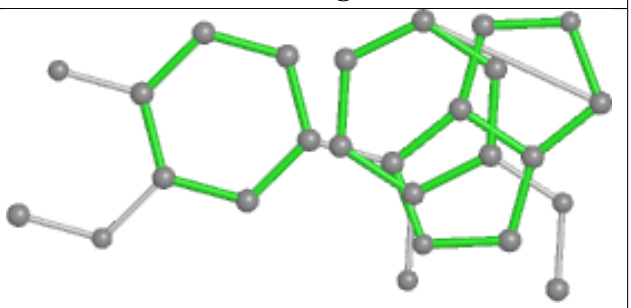
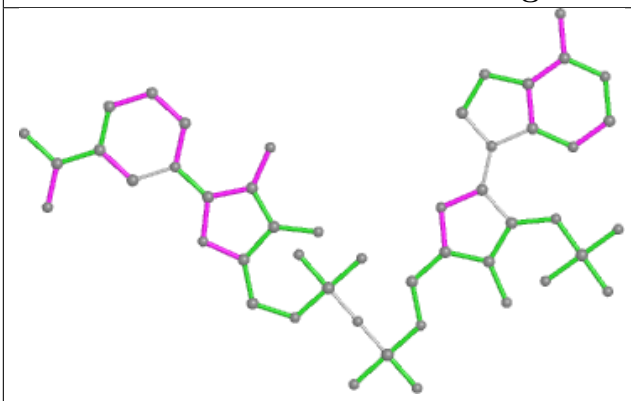


Rings

Ligand NDP B 402



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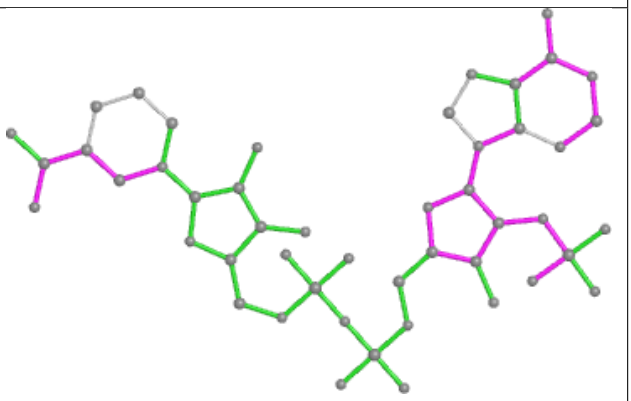
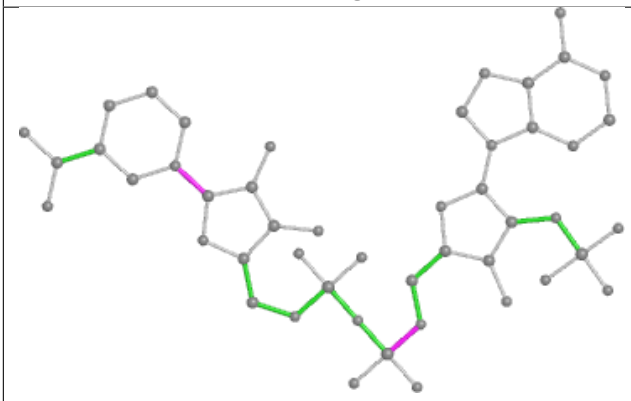
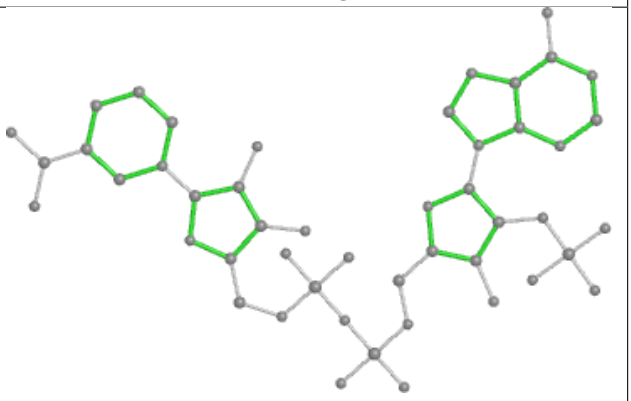


Bond angles

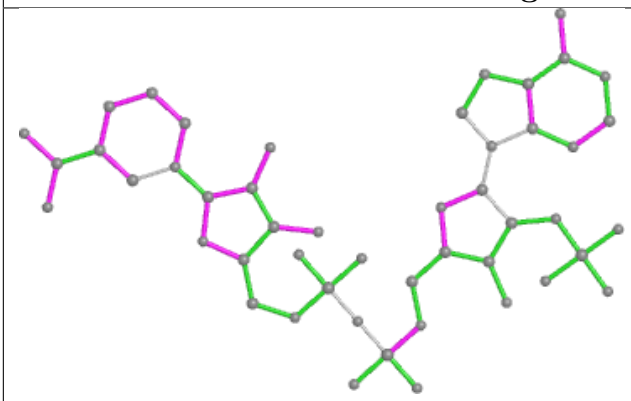


Torsions

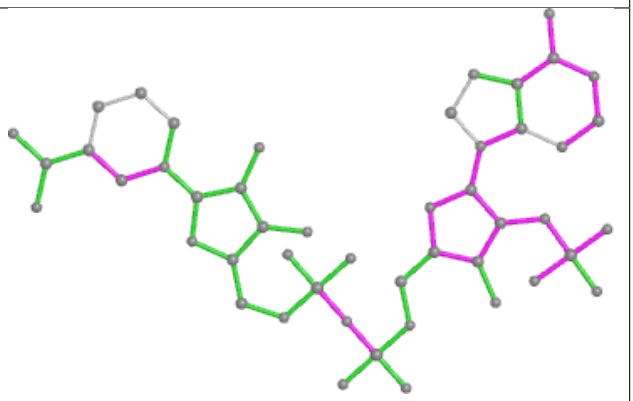


Rings

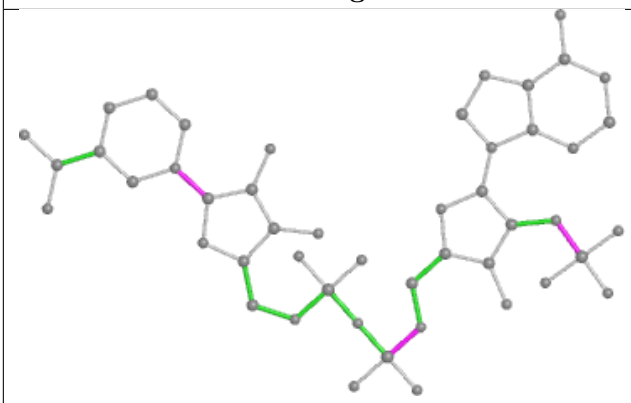
Ligand NDP D 402



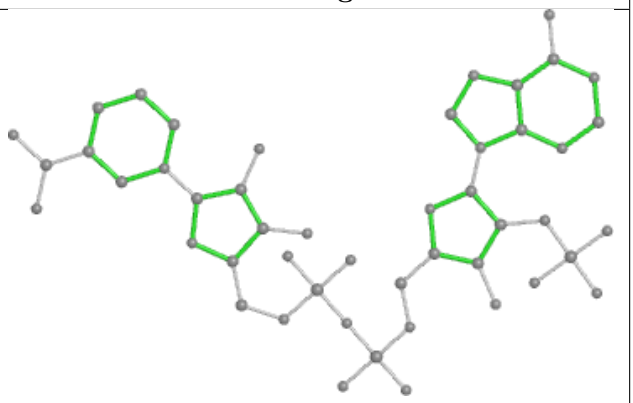
Bond lengths



Bond angles

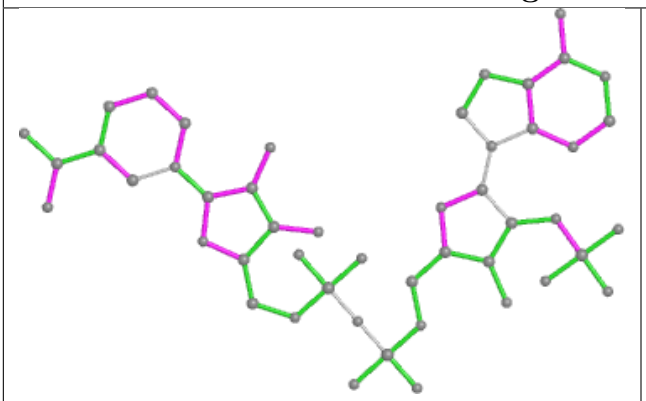


Torsions



Rings

Ligand NDP C 402



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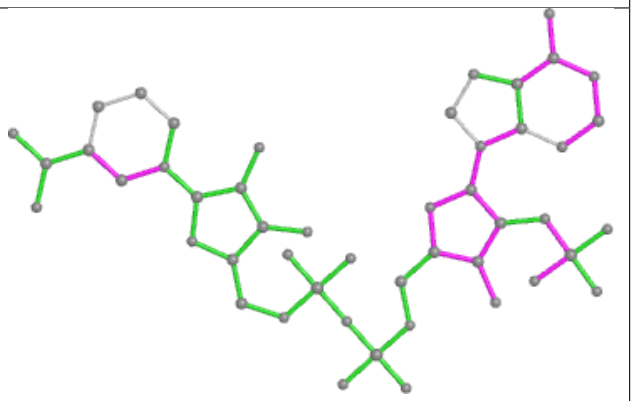
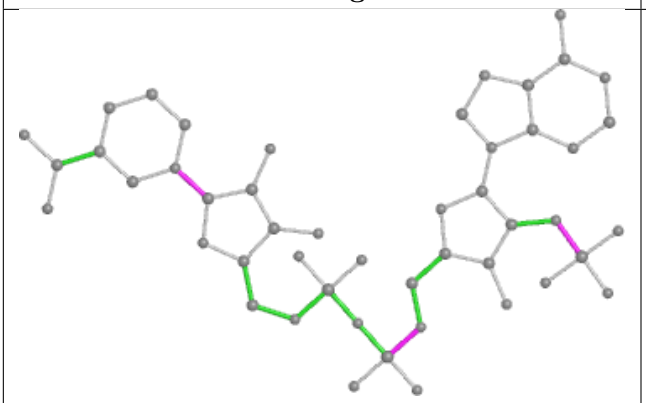


Bond angles



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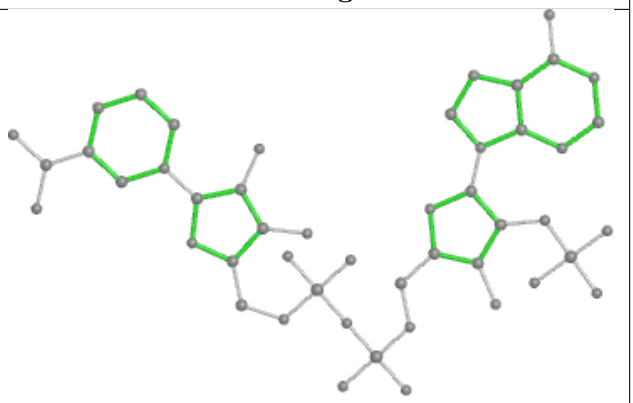
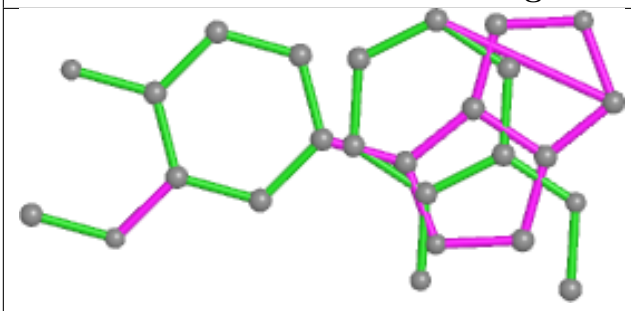
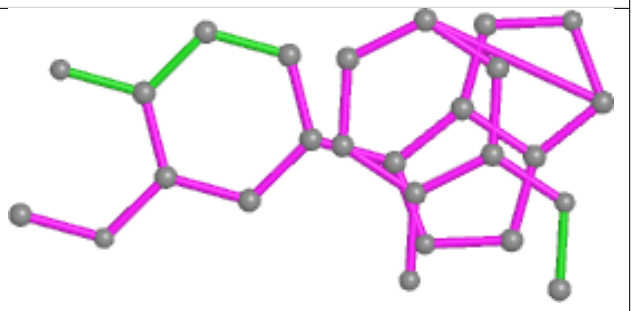


Rings

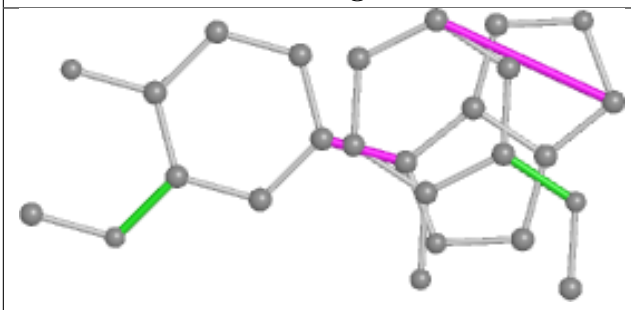
Ligand GEF B 401



Bond lengths



Bond angles



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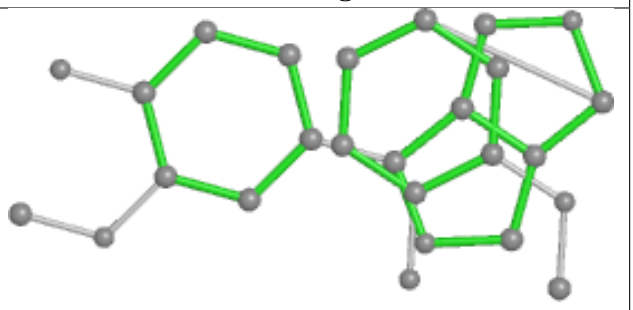
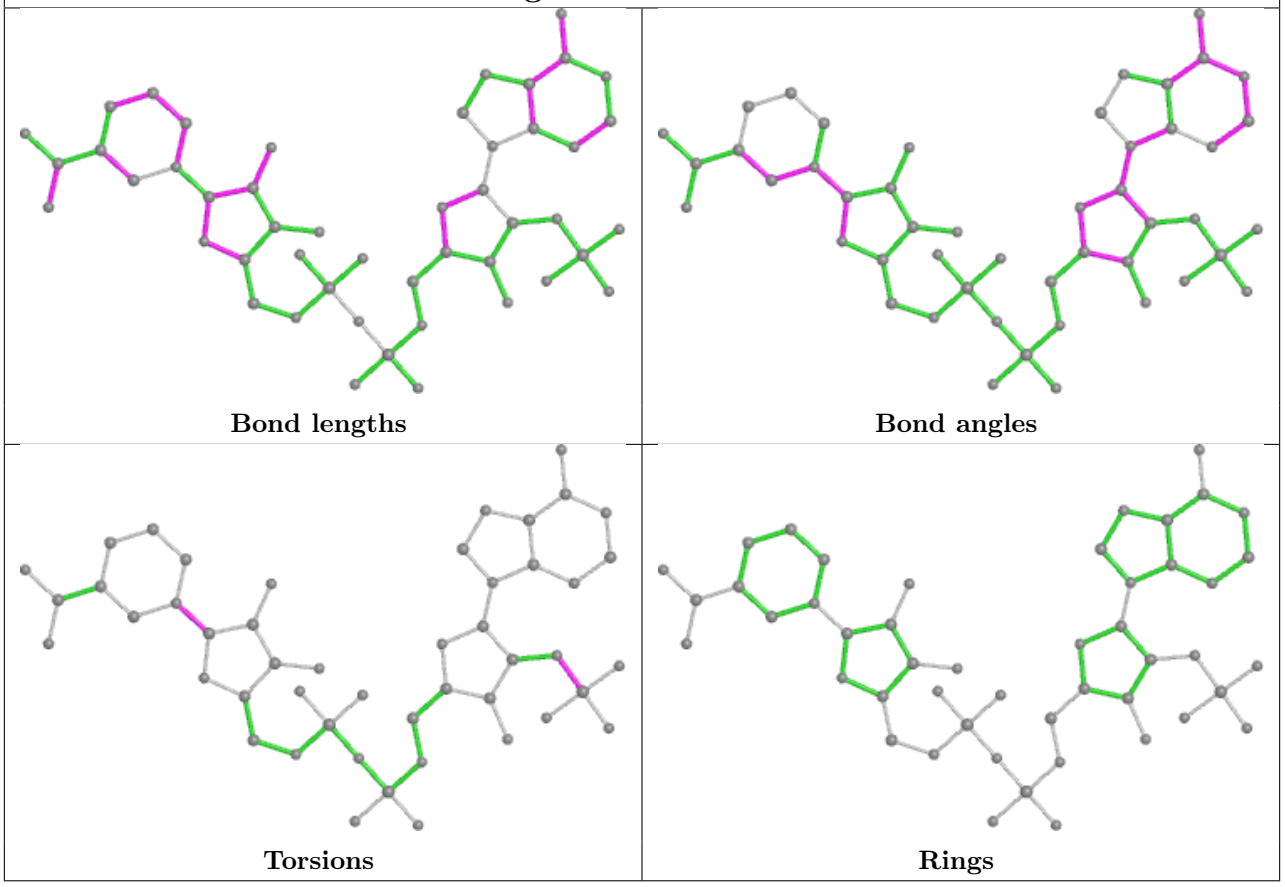


Rings

Ligand NDP F 402



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

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	A	284/317 (89%)	-0.00	17 (5%)	21	23	17, 29, 55, 83	0
1	B	290/317 (91%)	-0.29	6 (2%)	63	64	17, 25, 42, 70	0
1	C	285/317 (89%)	-0.40	6 (2%)	63	64	18, 26, 44, 63	0
1	D	285/317 (89%)	-0.09	9 (3%)	47	48	21, 30, 46, 81	0
1	E	285/317 (89%)	-0.38	4 (1%)	75	75	18, 27, 46, 76	0
1	F	285/317 (89%)	-0.10	8 (2%)	53	54	20, 31, 53, 83	0
All	All	1714/1902 (90%)	-0.21	50 (2%)	51	52	17, 28, 51, 83	0

The worst 5 of 50 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	6	SER	17.8
1	A	6	SER	14.6
1	D	6	SER	12.0
1	A	7	GLY	11.4
1	F	7	GLY	9.8

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 (i)

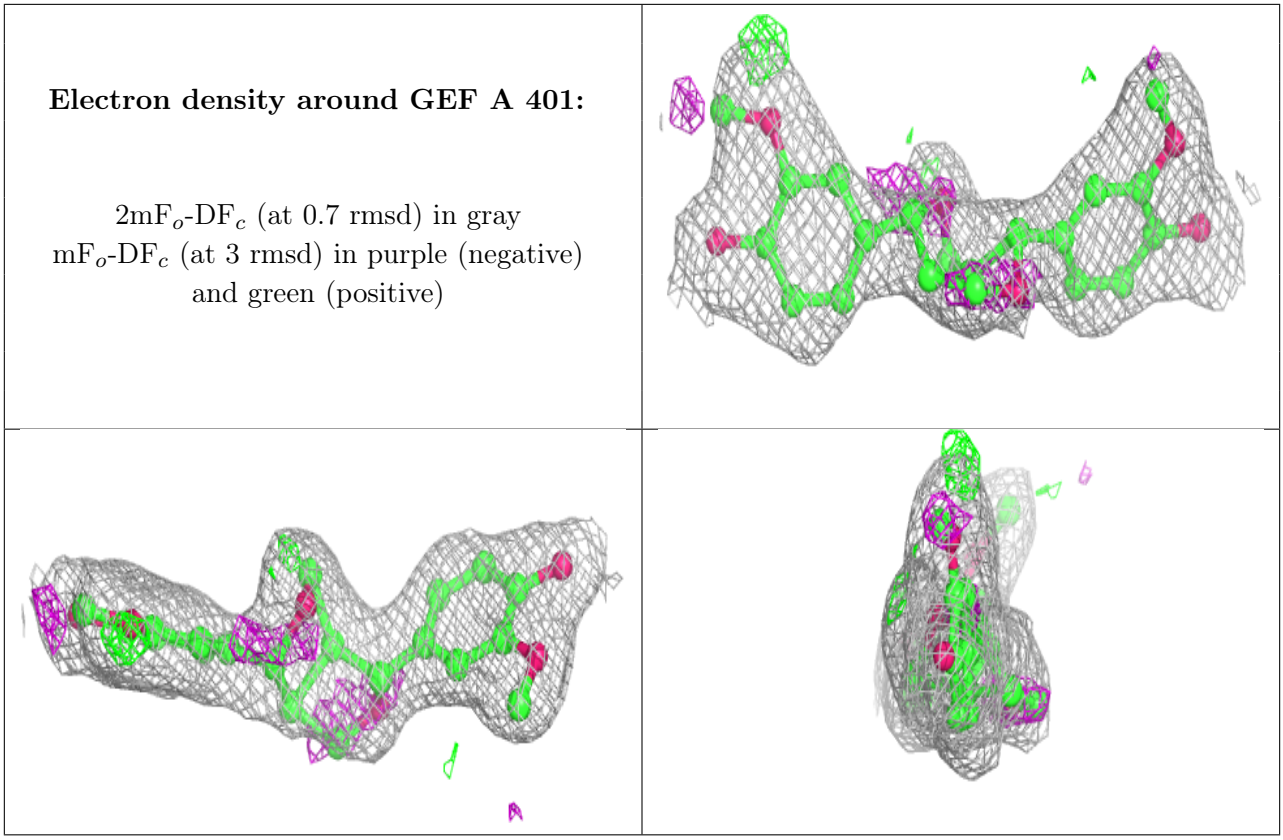
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
2	GEF	A	401	26/26	0.87	0.18	31,39,50,51	0
2	GEF	E	401	26/26	0.88	0.15	28,37,44,48	0
2	GEF	D	401	26/26	0.88	0.17	29,40,53,56	0
2	GEF	F	401	26/26	0.89	0.16	35,45,54,57	0
2	GEF	C	401	26/26	0.91	0.12	25,34,43,44	0
2	GEF	B	401	26/26	0.91	0.18	24,36,50,53	0
3	NDP	D	402	48/48	0.93	0.14	26,34,49,62	0
3	NDP	B	402	48/48	0.94	0.14	17,27,44,53	0
3	NDP	E	402	48/48	0.95	0.12	22,33,46,57	0
3	NDP	A	402	48/48	0.95	0.12	20,30,44,57	0
3	NDP	C	402	48/48	0.96	0.10	20,28,44,54	0
3	NDP	F	402	48/48	0.96	0.11	23,33,42,51	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.

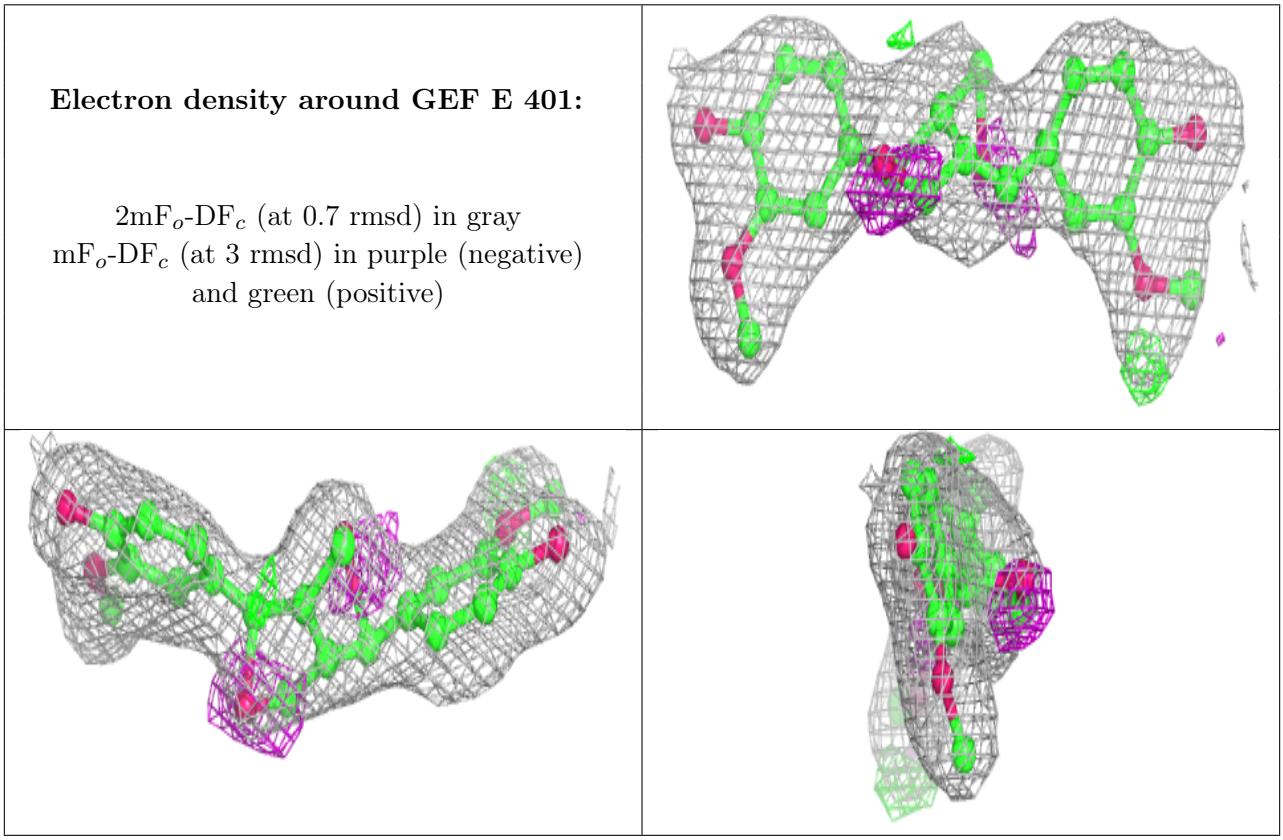
Electron density around GEF A 401:

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



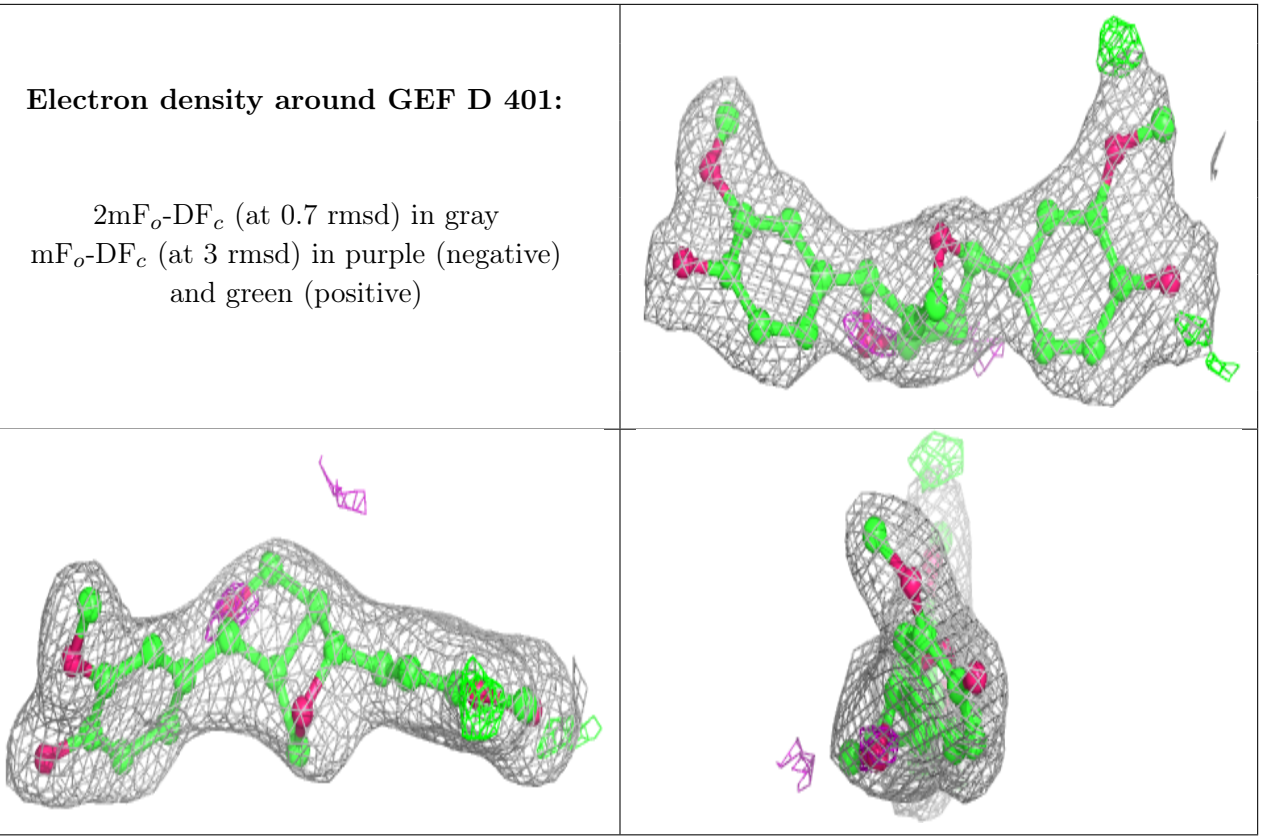
Electron density around GEF E 401:

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



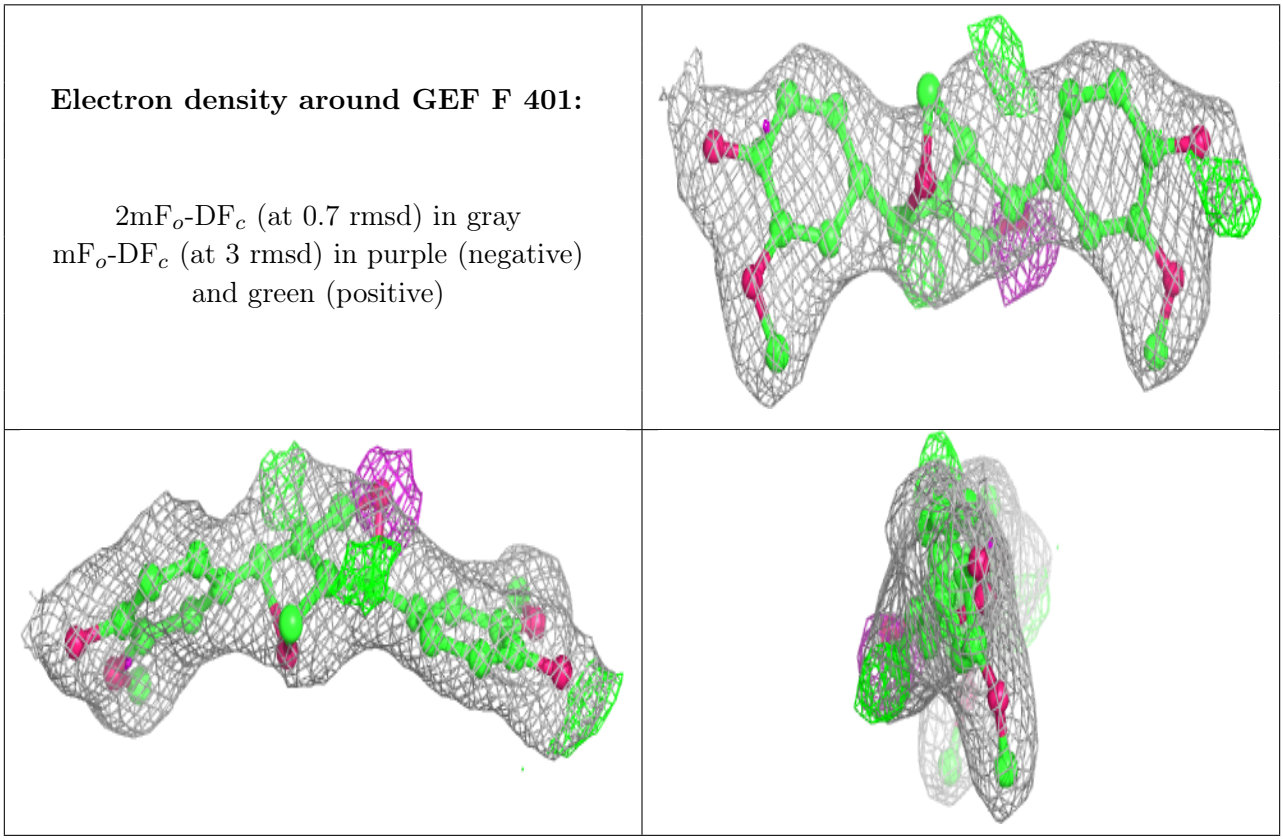
Electron density around GEF D 401:

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



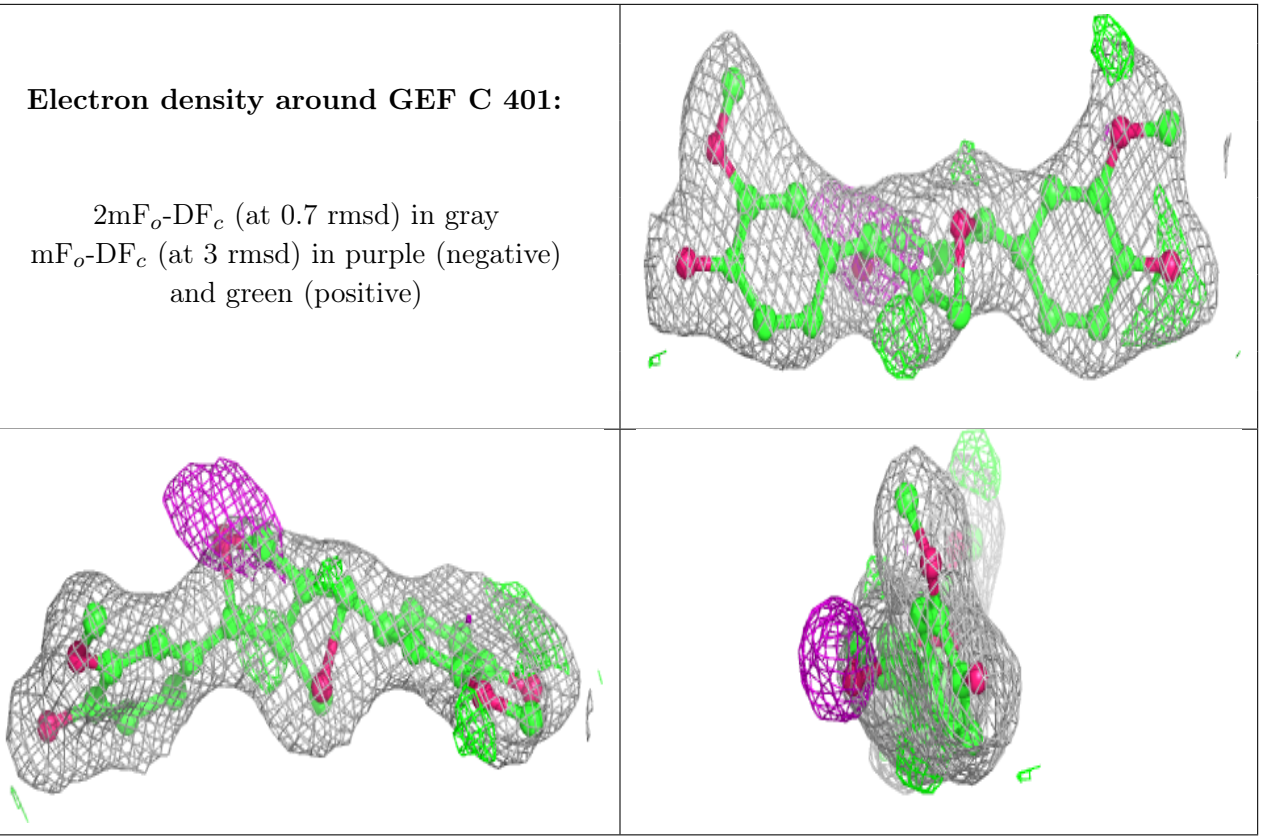
Electron density around GEF F 401:

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



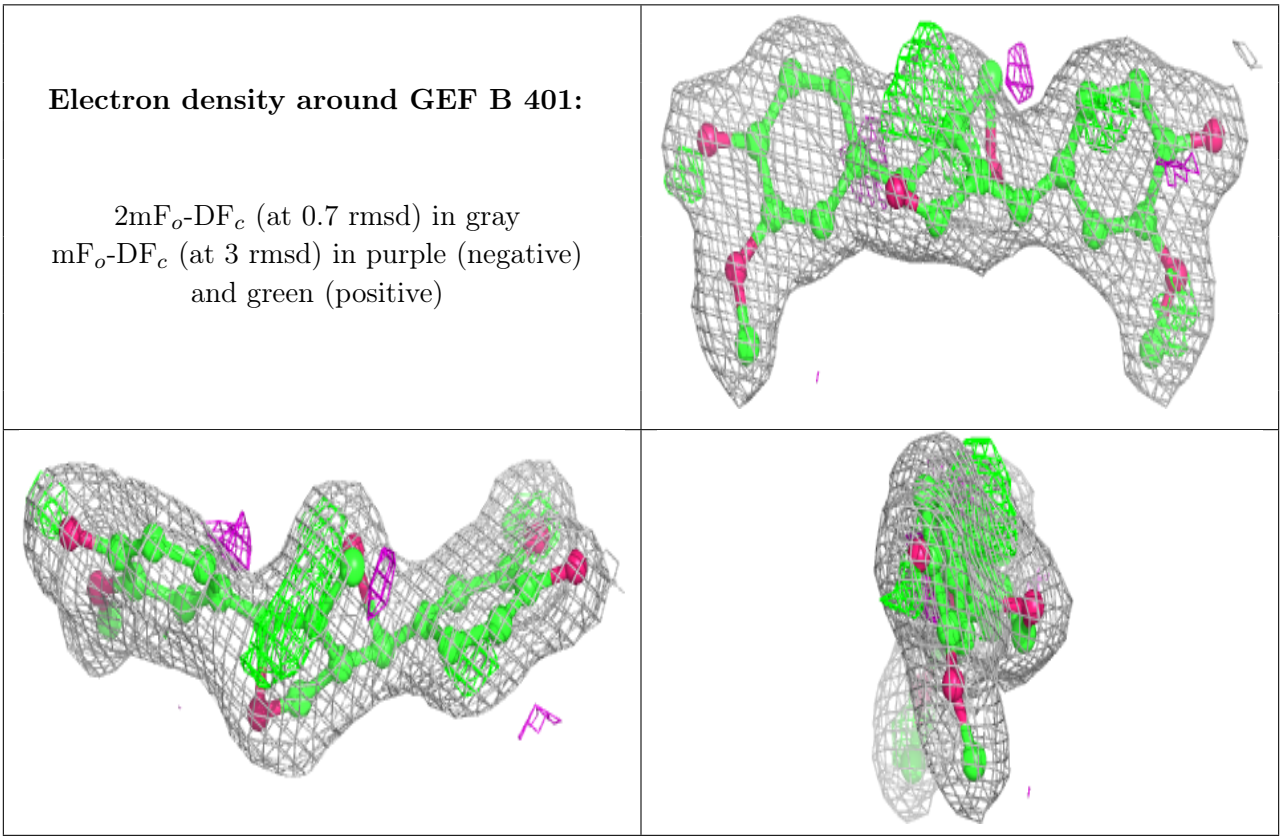
Electron density around GEF C 401:

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



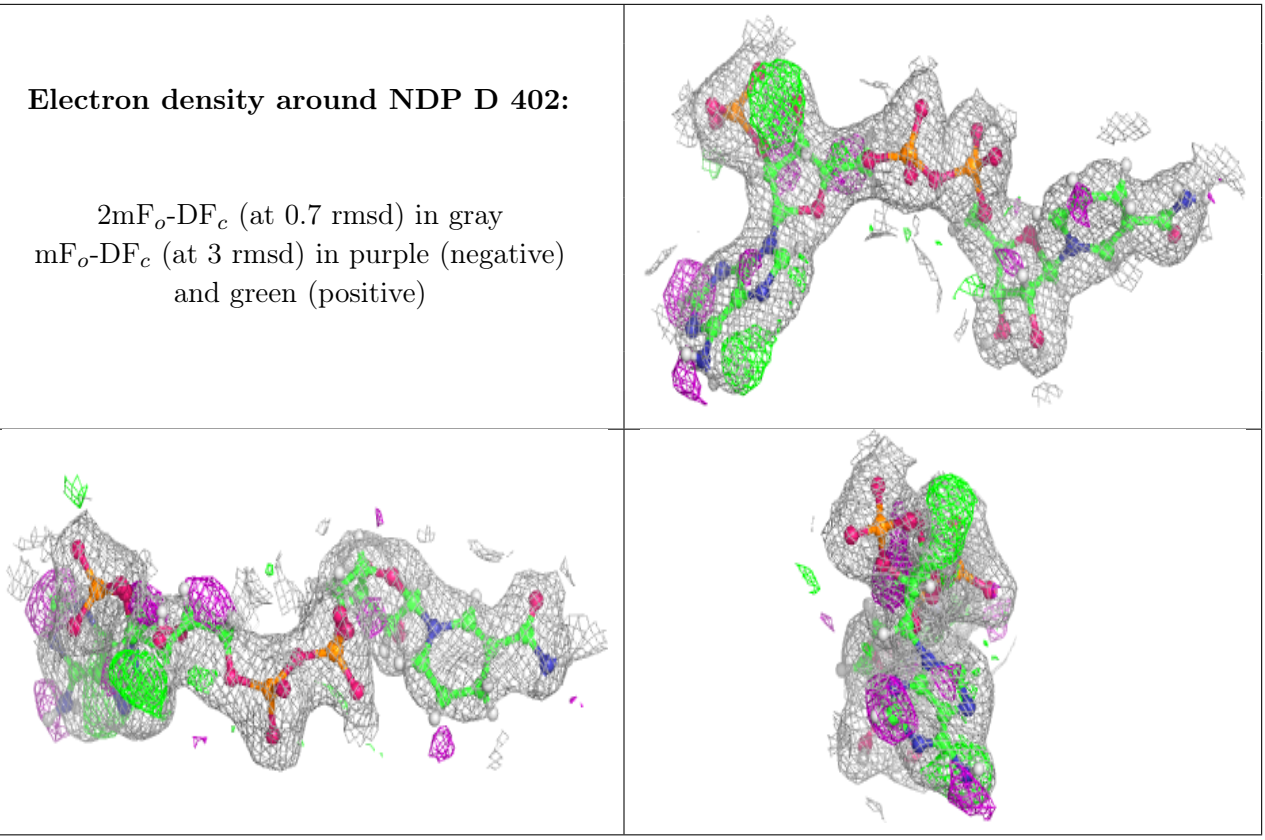
Electron density around GEF B 401:

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



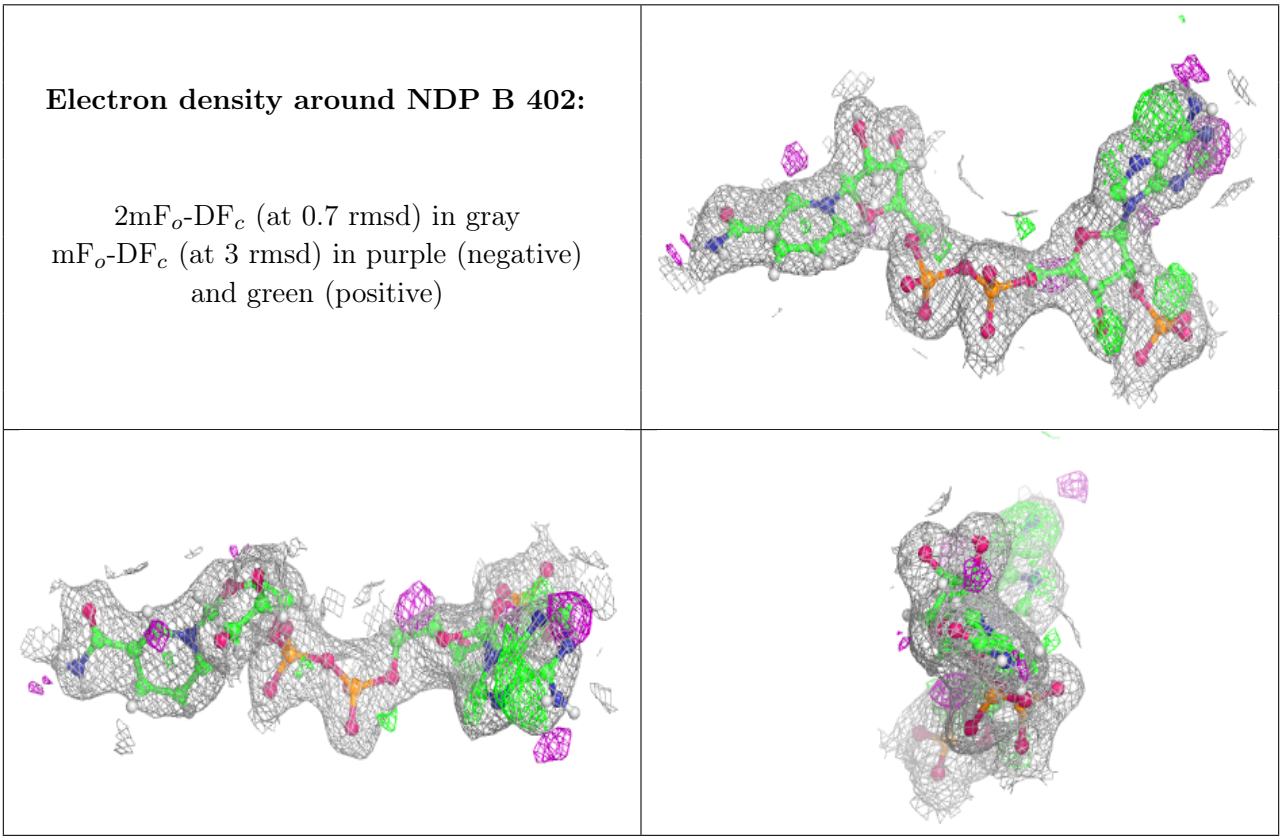
Electron density around NDP D 402:

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



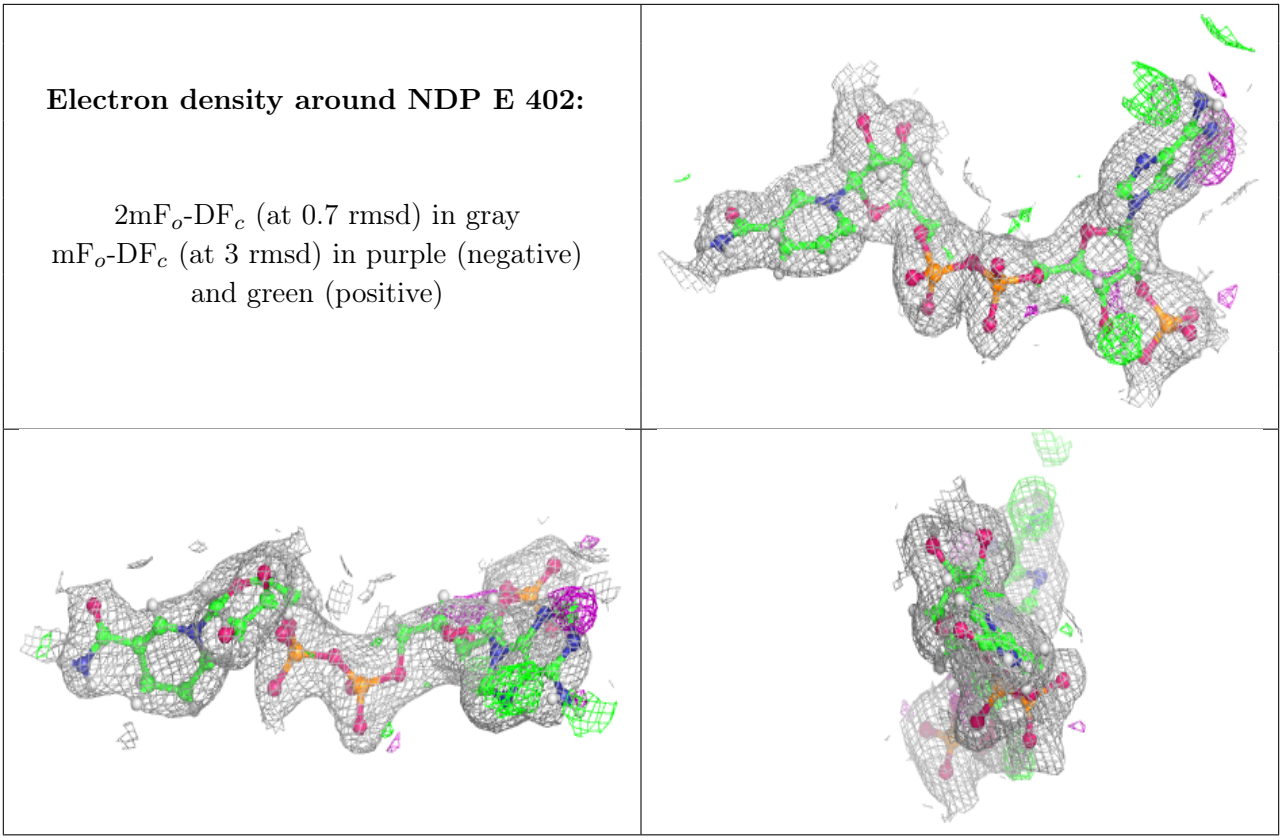
Electron density around NDP B 402:

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



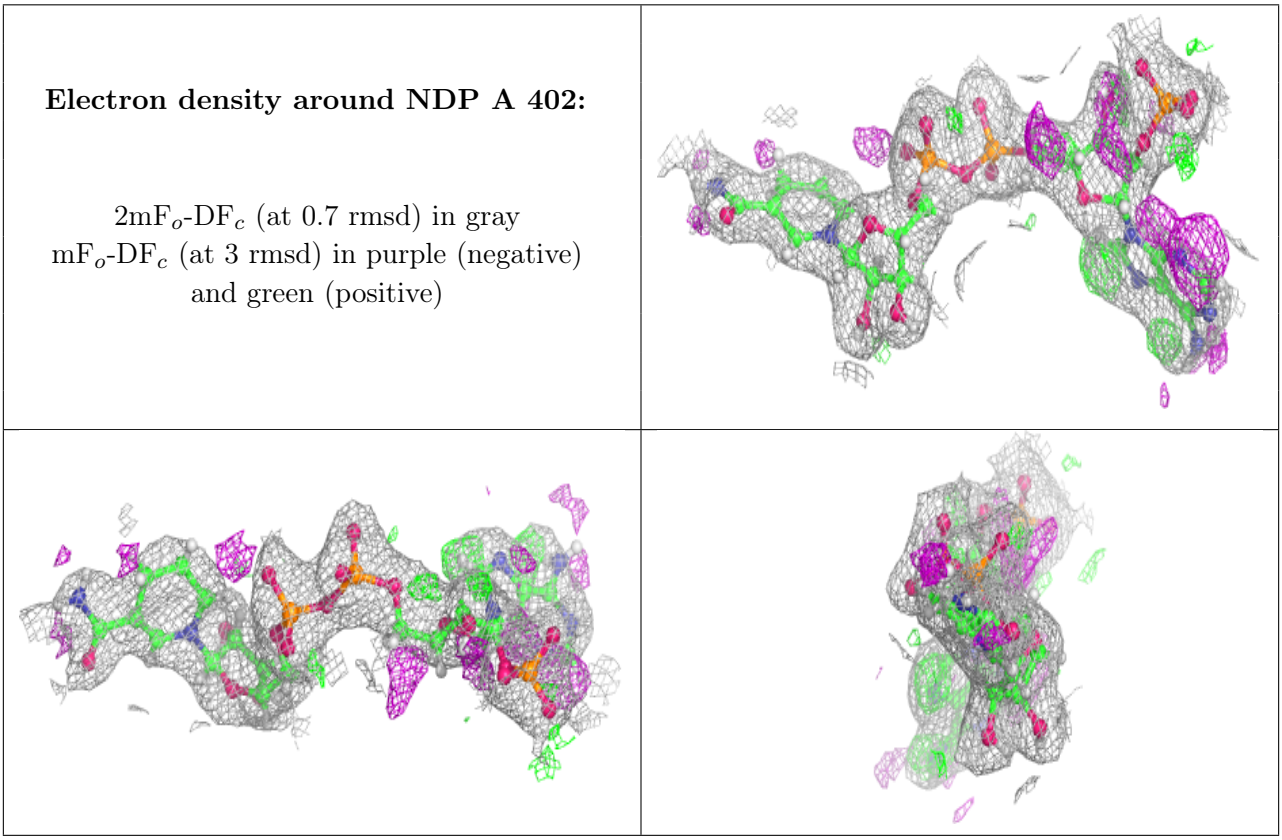
Electron density around NDP E 402:

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



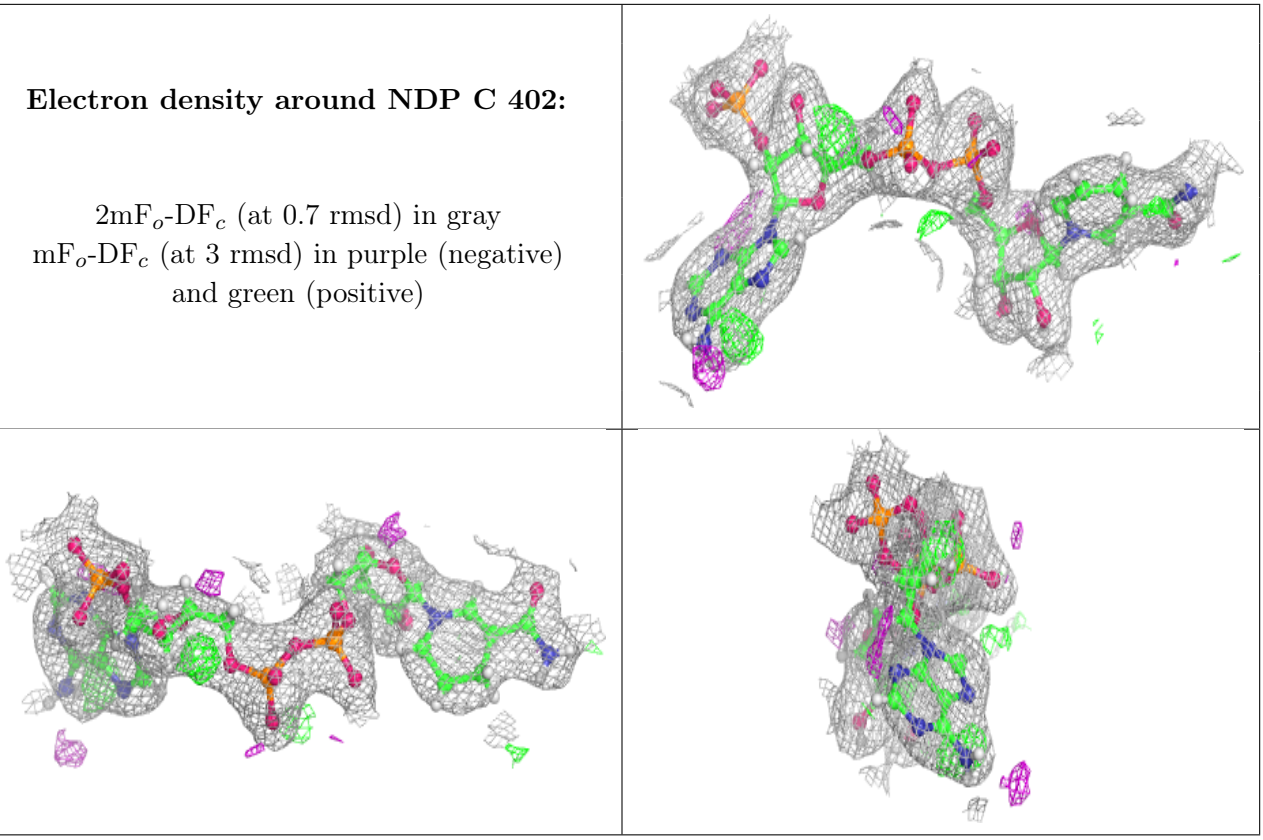
Electron density around NDP A 402:

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



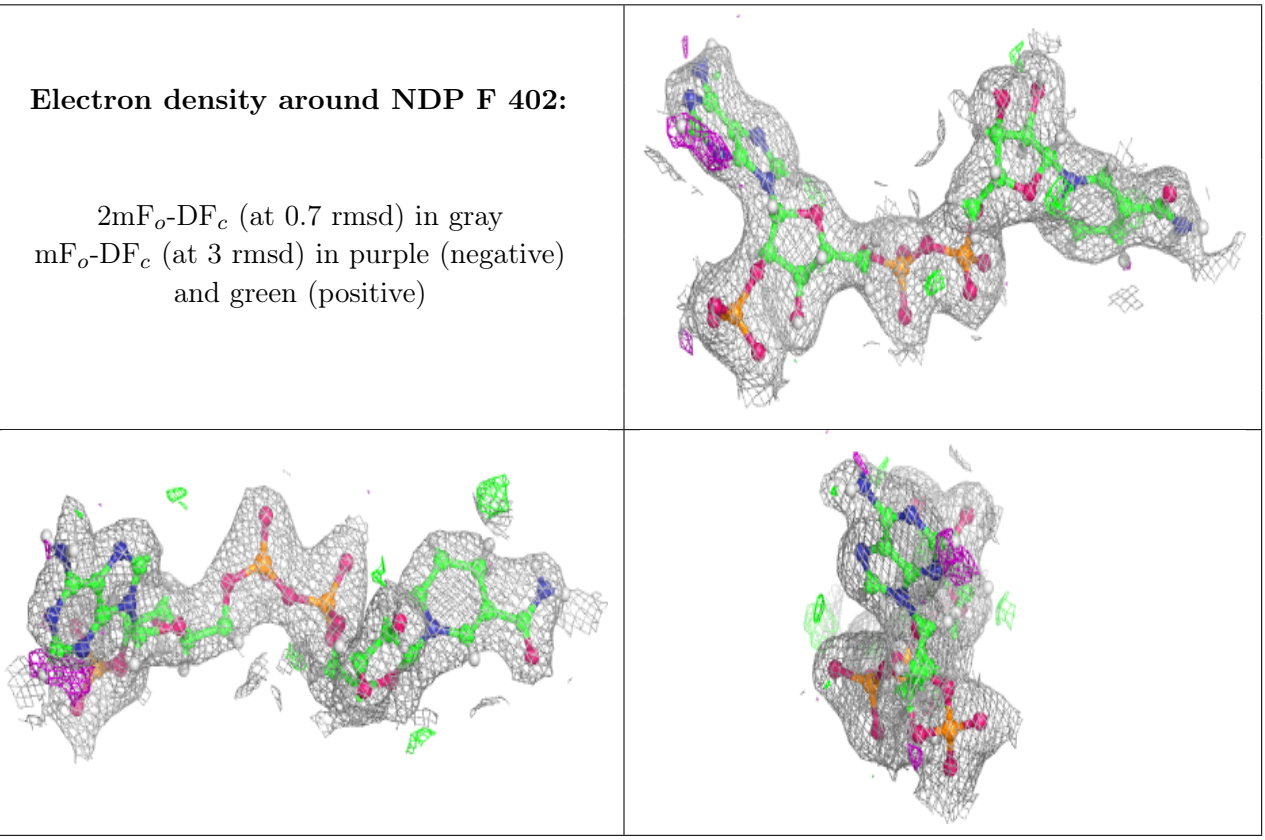
Electron density around NDP C 402:

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



Electron density around NDP F 402:

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



6.5 Other polymers (i)

There are no such residues in this entry.