wwPDB X-ray Structure Validation Summary Report (i)

Aug 26, 2026 – 05:03 am BST

PDB ID	:	6T66 / pdb_00006t66
Title	:	Crystal structure of the Vibrio cholerae replicative helicase (DnaB) with GDP-AlF4
Authors	:	Legrand, P.; Quevillon-Cheruel, S.; Li de la Sierra-Gallay, I.; Walbott, H.
Deposited on	:	2019-10-17
Resolution	:	3.90 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:

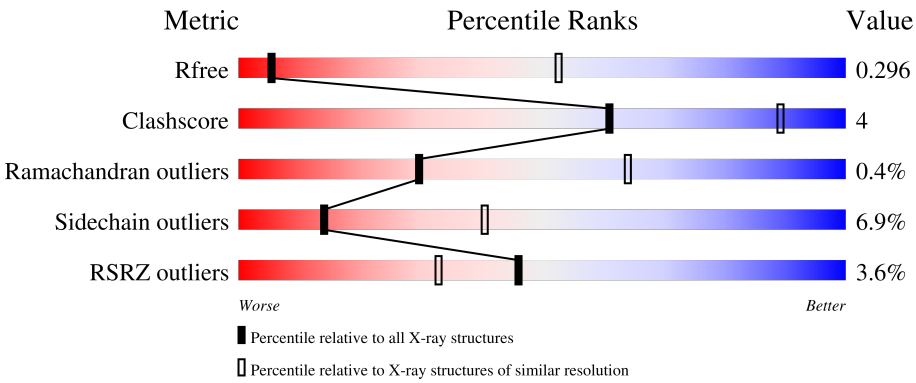
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 3.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1270 (4.10-3.70)
Clashscore	190562	1034 (4.08-3.72)
Ramachandran outliers	187476	1251 (4.10-3.70)
Sidechain outliers	187428	1243 (4.10-3.70)
RSRZ outliers	180081	1269 (4.10-3.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	474	3% 76% 16% • 7%
1	B	474	2% 76% 16% • 7%
1	C	474	5% 76% 15% • 7%
1	D	474	4% 77% 15% • 7%
1	E	474	3% 76% 16% • 7%

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Mol	Chain	Length	Quality of chain
1	F	474	2% 78% 15% 7%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 20822 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 Replicative DNA helicase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	440	3433	2139	603	676	15	0	0	0
1	B	441	3437	2141	604	677	15	0	0	0
1	C	440	3433	2139	603	676	15	0	0	0
1	D	441	3437	2141	604	677	15	0	0	0
1	E	440	3433	2139	603	676	15	0	0	0
1	F	442	3445	2147	605	678	15	0	0	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	469	HIS	-	expression tag	UNP A0A085R2T8
A	470	HIS	-	expression tag	UNP A0A085R2T8
A	471	HIS	-	expression tag	UNP A0A085R2T8
A	472	HIS	-	expression tag	UNP A0A085R2T8
A	473	HIS	-	expression tag	UNP A0A085R2T8
A	474	HIS	-	expression tag	UNP A0A085R2T8
B	469	HIS	-	expression tag	UNP A0A085R2T8
B	470	HIS	-	expression tag	UNP A0A085R2T8
B	471	HIS	-	expression tag	UNP A0A085R2T8
B	472	HIS	-	expression tag	UNP A0A085R2T8
B	473	HIS	-	expression tag	UNP A0A085R2T8
B	474	HIS	-	expression tag	UNP A0A085R2T8
C	469	HIS	-	expression tag	UNP A0A085R2T8
C	470	HIS	-	expression tag	UNP A0A085R2T8
C	471	HIS	-	expression tag	UNP A0A085R2T8
C	472	HIS	-	expression tag	UNP A0A085R2T8
C	473	HIS	-	expression tag	UNP A0A085R2T8

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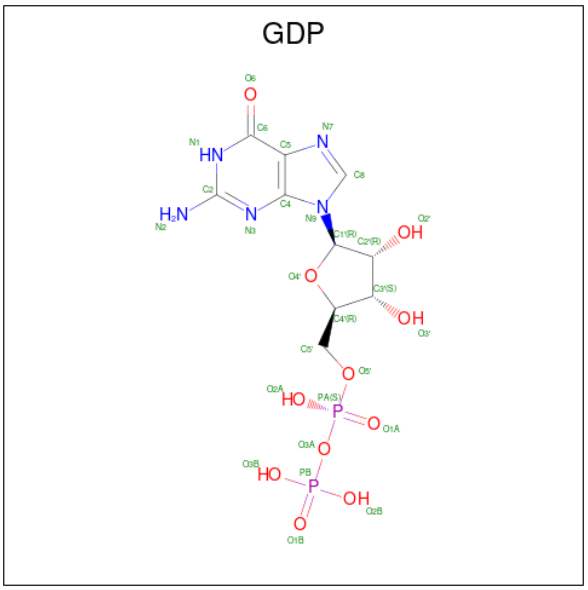
Chain	Residue	Modelled	Actual	Comment	Reference
C	474	HIS	-	expression tag	UNP A0A085R2T8
D	469	HIS	-	expression tag	UNP A0A085R2T8
D	470	HIS	-	expression tag	UNP A0A085R2T8
D	471	HIS	-	expression tag	UNP A0A085R2T8
D	472	HIS	-	expression tag	UNP A0A085R2T8
D	473	HIS	-	expression tag	UNP A0A085R2T8
D	474	HIS	-	expression tag	UNP A0A085R2T8
E	469	HIS	-	expression tag	UNP A0A085R2T8
E	470	HIS	-	expression tag	UNP A0A085R2T8
E	471	HIS	-	expression tag	UNP A0A085R2T8
E	472	HIS	-	expression tag	UNP A0A085R2T8
E	473	HIS	-	expression tag	UNP A0A085R2T8
E	474	HIS	-	expression tag	UNP A0A085R2T8
F	469	HIS	-	expression tag	UNP A0A085R2T8
F	470	HIS	-	expression tag	UNP A0A085R2T8
F	471	HIS	-	expression tag	UNP A0A085R2T8
F	472	HIS	-	expression tag	UNP A0A085R2T8
F	473	HIS	-	expression tag	UNP A0A085R2T8
F	474	HIS	-	expression tag	UNP A0A085R2T8

- Molecule 2 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	28	10	5	11	2	0	0

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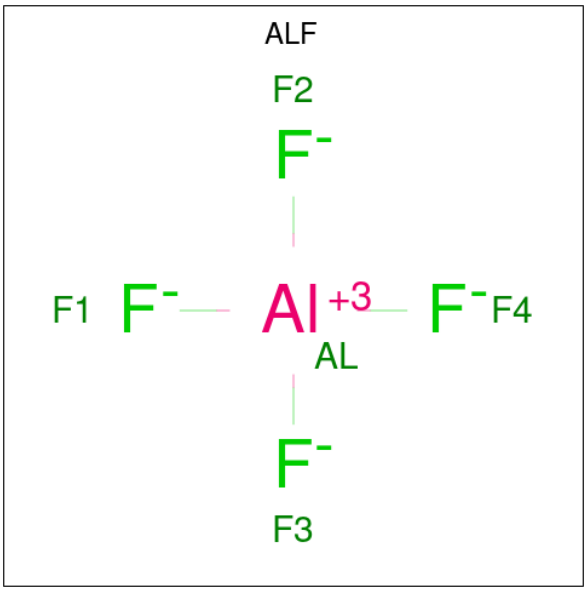
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	B	1	28	10	5	11	2	0	0
			Total	C	N	O	P		
2	C	1	28	10	5	11	2	0	0
			Total	C	N	O	P		
2	D	1	28	10	5	11	2	0	0
			Total	C	N	O	P		
2	E	1	28	10	5	11	2	0	0
			Total	C	N	O	P		
2	F	1	28	10	5	11	2	0	0

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 4 is TETRAFLUOROALUMINATE ION (CCD ID: ALF) (formula: AlF_4) (labeled as "Ligand of Interest" by depositor).



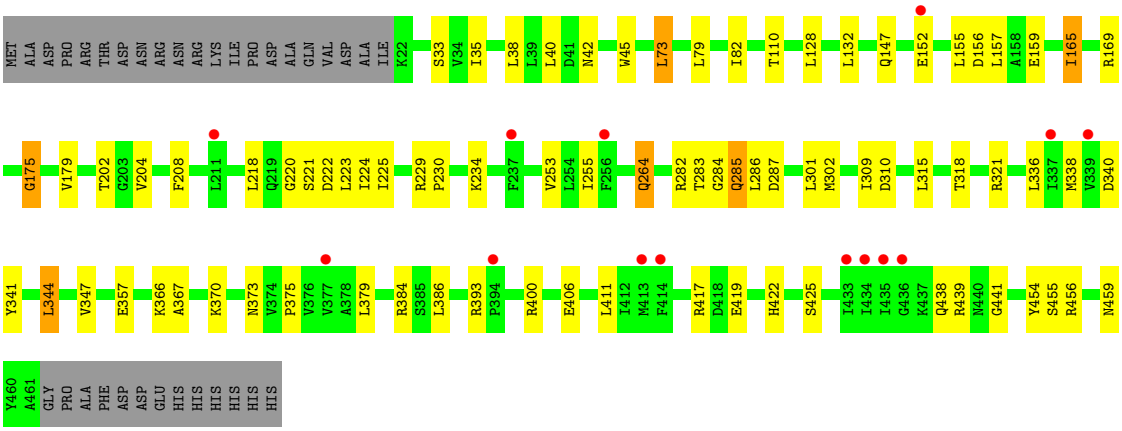
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Al	F		
4	A	1	5	1	4	0	0
4	B	1	5	1	4	0	0
4	C	1	5	1	4	0	0
4	D	1	5	1	4	0	0
4	E	1	5	1	4	0	0
4	F	1	5	1	4	0	0

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.

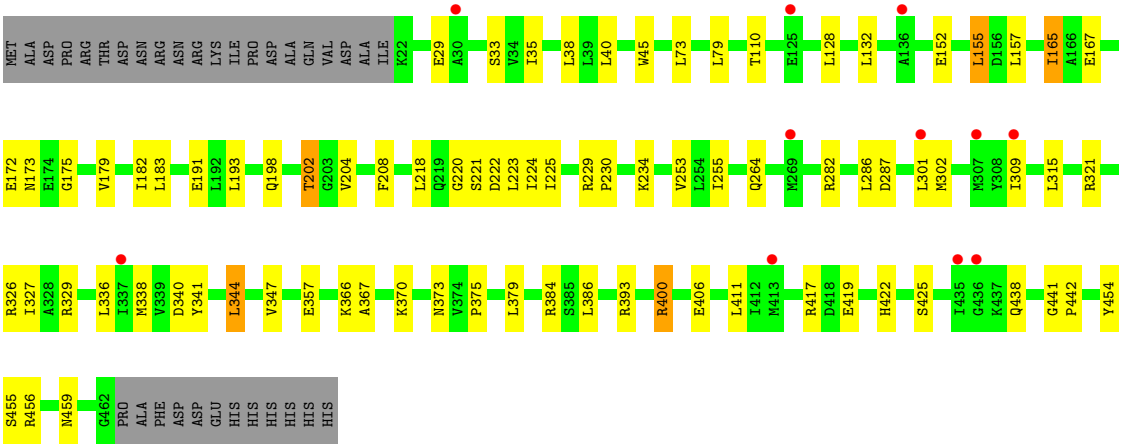
• Molecule 1: Replicative DNA helicase

Chain A:



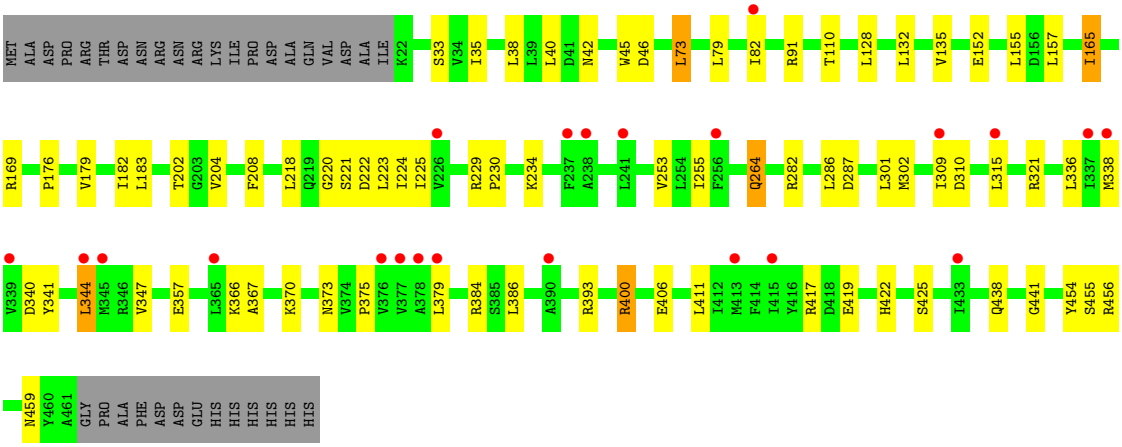
• Molecule 1: Replicative DNA helicase

Chain B:



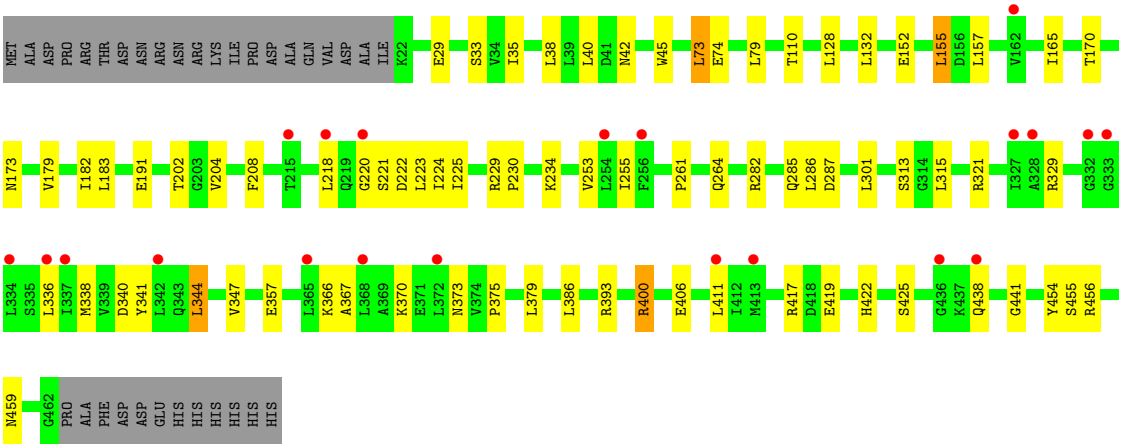
• Molecule 1: Replicative DNA helicase

Chain C:



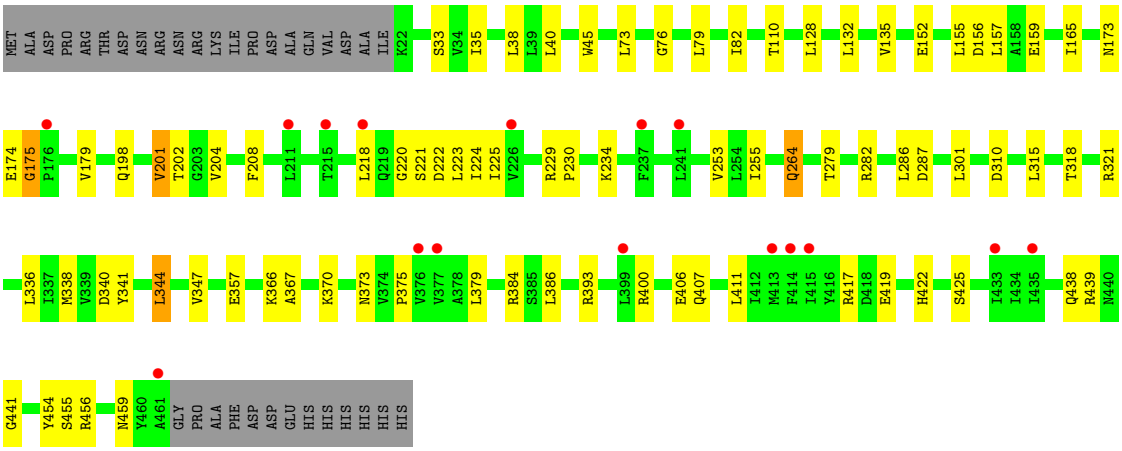
• Molecule 1: Replicative DNA helicase

Chain D:



• Molecule 1: Replicative DNA helicase

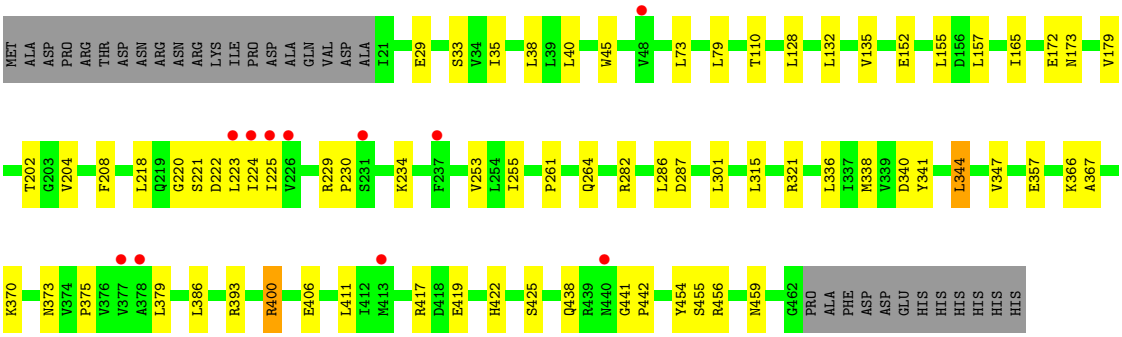
Chain E:



• Molecule 1: Replicative DNA helicase

Chain F:

2%
78%
15%
7%


MET ALA ASP PRO ARG THR ASP ASN ARG ASN ARG LYS ILE PRO ASP ALA GLN VAL ASP ALA I21 E29 S33 V34 I35 L38 L39 L40 W45 V48 L73 L79 T110 L128 L132 V135 E152 L155 D156 L157 I165 E172 N173 V179
T202 G203 V204 F208 L218 Q219 G220 S221 D222 L223 I224 I225 V226 R229 P230 S231 K234 F237 V253 L254 I255 P261 Q264 R282 L286 D287 L301 L315 R321 L336 I337 M338 V339 D340 Y341 L344 V347 E357 K366 A367
K370 N373 V374 P375 V376 V377 A378 L379 L386 R393 R400 E406 L411 I412 M413 R417 D418 E419 H422 S425 Q438 R439 N440 G441 P442 Y454 S455 R456 N459 G462 PRO ALA PHE ASP ASP GLU HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	118.98Å 123.29Å 263.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.63 – 3.90 49.63 – 3.90	Depositor EDS
% Data completeness (in resolution range)	75.2 (49.63-3.90) 75.1 (49.63-3.90)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.45 (at 3.88Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.255 , 0.276 0.269 , 0.296	Depositor DCC
R_{free} test set	1373 reflections (3.55%)	wwPDB-VP
Wilson B-factor (Å^2)	159.9	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.22 , 99.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.22$	Xtriage
Estimated twinning fraction	0.066 for k,h,-l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	20822	wwPDB-VP
Average B, all atoms (Å^2)	198.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.26% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ALF, GDP

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	0.73	0/3482	1.34	2/4708 (0.0%)
1	B	0.73	0/3486	1.34	1/4713 (0.0%)
1	C	0.73	0/3482	1.34	1/4708 (0.0%)
1	D	0.72	0/3486	1.35	3/4713 (0.1%)
1	E	0.74	0/3482	1.35	4/4708 (0.1%)
1	F	0.73	0/3494	1.34	1/4724 (0.0%)
All	All	0.73	0/20912	1.35	12/28274 (0.0%)

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	222	ASP	CA-CB-CG	6.43	119.03	112.60
1	E	222	ASP	CA-CB-CG	6.35	118.95	112.60
1	A	222	ASP	CA-CB-CG	6.33	118.93	112.60
1	D	222	ASP	CA-CB-CG	6.30	118.91	112.60
1	B	222	ASP	CA-CB-CG	6.30	118.90	112.60

There are no chirality outliers.

There are no planarity outliers.

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	3433	0	3440	36	0
1	B	3437	0	3443	38	0
1	C	3433	0	3440	36	0
1	D	3437	0	3443	31	0
1	E	3433	0	3440	33	0
1	F	3445	0	3454	29	0
2	A	28	0	12	2	0
2	B	28	0	12	0	0
2	C	28	0	12	0	0
2	D	28	0	12	0	0
2	E	28	0	12	1	0
2	F	28	0	12	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
4	C	5	0	0	0	0
4	D	5	0	0	0	0
4	E	5	0	0	0	0
4	F	5	0	0	0	0
All	All	20822	0	20732	175	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 4.

The worst 5 of 175 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:82:ILE:HD13	1:F:29:GLU:HB2	1.58	0.83
1:E:33:SER:HA	1:E:110:THR:HG21	1.71	0.73
1:A:33:SER:HA	1:A:110:THR:HG21	1.71	0.73
1:C:33:SER:HA	1:C:110:THR:HG21	1.72	0.72
1:F:33:SER:HA	1:F:110:THR:HG21	1.71	0.72

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	438/474 (92%)	414 (94%)	23 (5%)	1 (0%)	43	74
1	B	439/474 (93%)	415 (94%)	21 (5%)	3 (1%)	18	53
1	C	438/474 (92%)	417 (95%)	21 (5%)	0	100	100
1	D	439/474 (93%)	417 (95%)	21 (5%)	1 (0%)	43	74
1	E	438/474 (92%)	414 (94%)	20 (5%)	4 (1%)	14	47
1	F	440/474 (93%)	417 (95%)	21 (5%)	2 (0%)	24	59
All	All	2632/2844 (92%)	2494 (95%)	127 (5%)	11 (0%)	30	64

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	172	GLU
1	F	172	GLU
1	B	173	ASN
1	E	173	ASN
1	E	174	GLU

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	374/403 (93%)	347 (93%)	27 (7%)	13	39
1	B	374/403 (93%)	347 (93%)	27 (7%)	13	39
1	C	374/403 (93%)	348 (93%)	26 (7%)	14	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	374/403 (93%)	348 (93%)	26 (7%)	14	40
1	E	374/403 (93%)	348 (93%)	26 (7%)	14	40
1	F	375/403 (93%)	352 (94%)	23 (6%)	17	43
All	All	2245/2418 (93%)	2090 (93%)	155 (7%)	14	40

5 of 155 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	201	VAL
1	F	286	LEU
1	E	286	LEU
1	E	455	SER
1	F	400	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 56 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	115	ASN
1	F	459	ASN
1	D	440	ASN
1	F	306	ASN
1	F	205	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 18 ligands modelled in this entry, 6 are monoatomic - leaving 12 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	GDP	D	501	4,3	28,30,30	0.39	0	44,47,47	0.53	0
4	ALF	E	503	2	0,4,4	-	-	-		
4	ALF	F	503	2	0,4,4	-	-	-		
2	GDP	F	501	4,3	28,30,30	0.48	0	44,47,47	0.53	0
2	GDP	E	501	4,3	28,30,30	0.40	0	44,47,47	0.53	0
4	ALF	D	503	2	0,4,4	-	-	-		
2	GDP	B	501	4,3	28,30,30	0.49	0	44,47,47	0.53	0
4	ALF	C	503	2	0,4,4	-	-	-		
4	ALF	A	503	2	0,4,4	-	-	-		
2	GDP	A	501	4,3	28,30,30	0.51	0	44,47,47	0.52	0
2	GDP	C	501	4,3	28,30,30	0.42	0	44,47,47	0.52	0
4	ALF	B	503	2	0,4,4	-	-	-		

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	GDP	D	501	4,3	-	6/16/32/32	0/3/3/3
2	GDP	F	501	4,3	-	4/16/32/32	0/3/3/3
2	GDP	E	501	4,3	-	6/16/32/32	0/3/3/3
2	GDP	B	501	4,3	-	4/16/32/32	0/3/3/3
2	GDP	A	501	4,3	-	4/16/32/32	0/3/3/3
2	GDP	C	501	4,3	-	6/16/32/32	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 30 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	GDP	C5'-O5'-PA-O3A
2	A	501	GDP	C5'-O5'-PA-O2A
2	B	501	GDP	C5'-O5'-PA-O3A
2	C	501	GDP	C5'-O5'-PA-O3A
2	C	501	GDP	C5'-O5'-PA-O1A

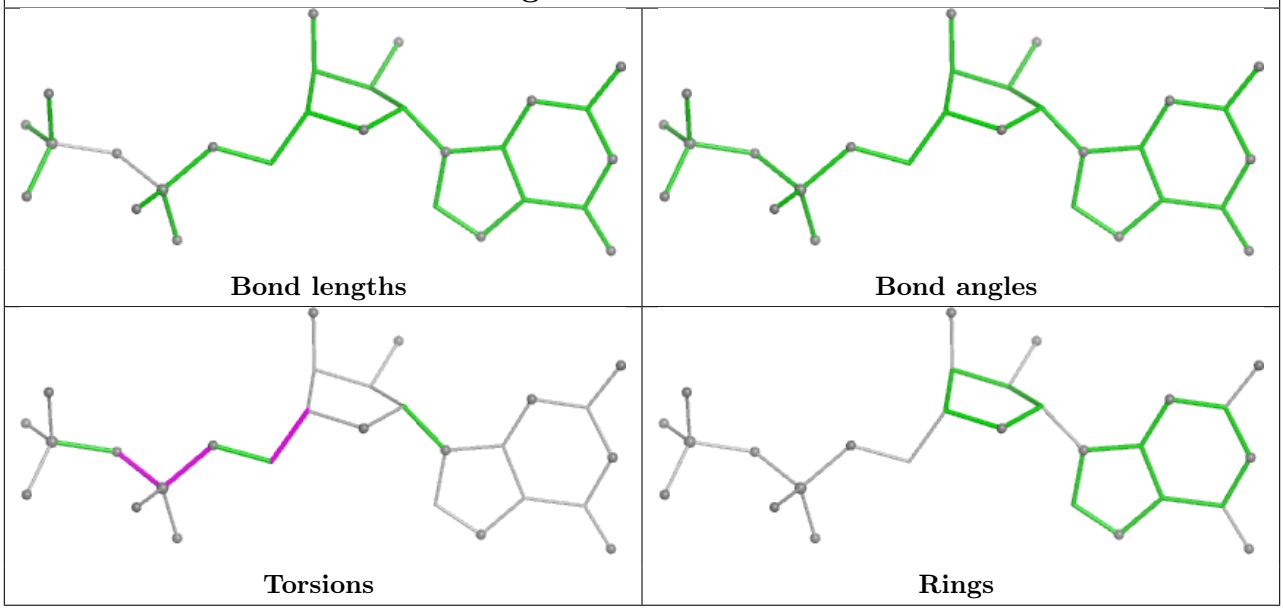
There are no ring outliers.

2 monomers are involved in 3 short contacts:

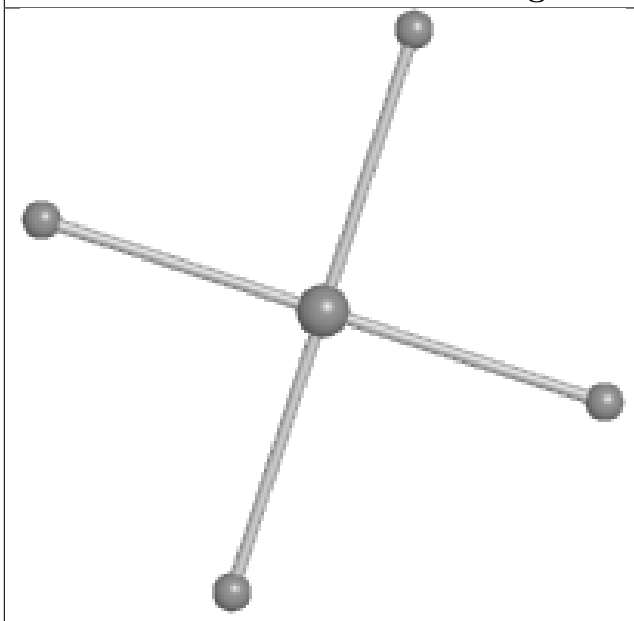
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	501	GDP	1	0
2	A	501	GDP	2	0

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

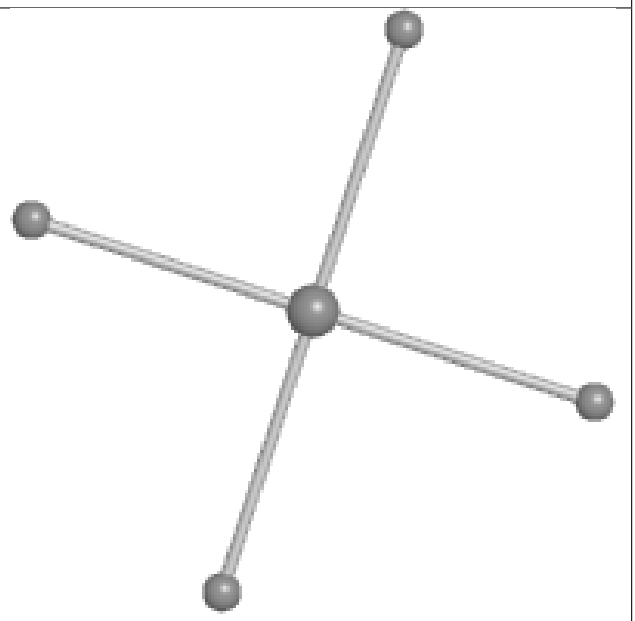
Ligand GDP D 501



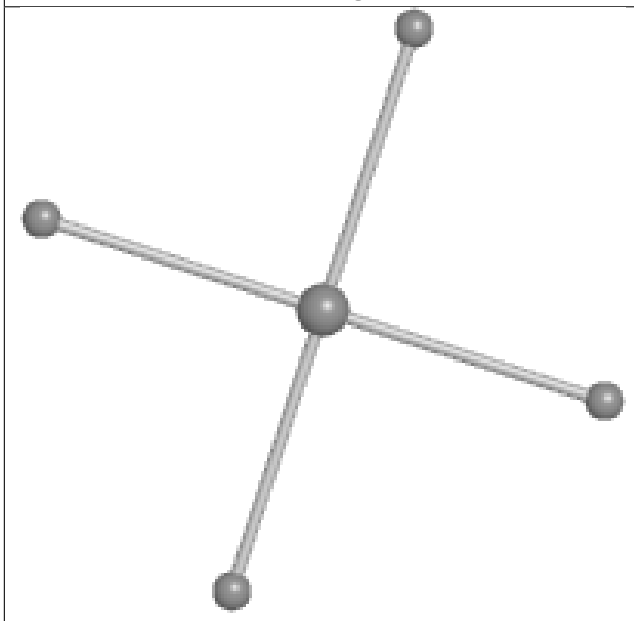
Ligand ALF E 503



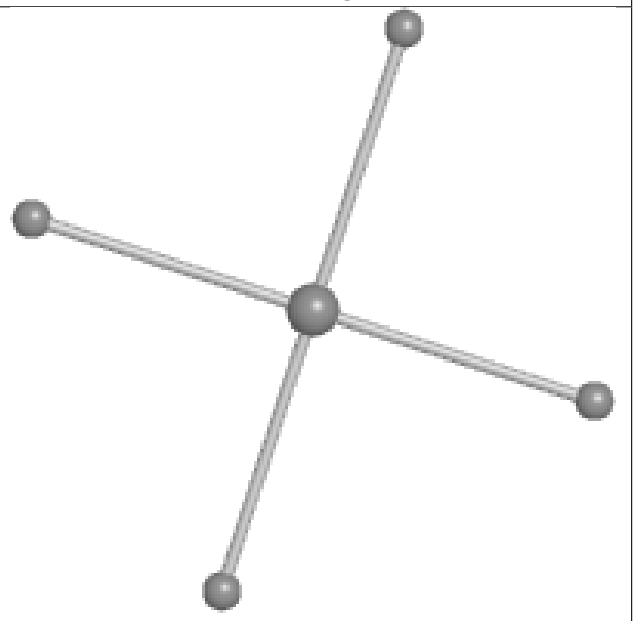
Bond lengths



Bond angles

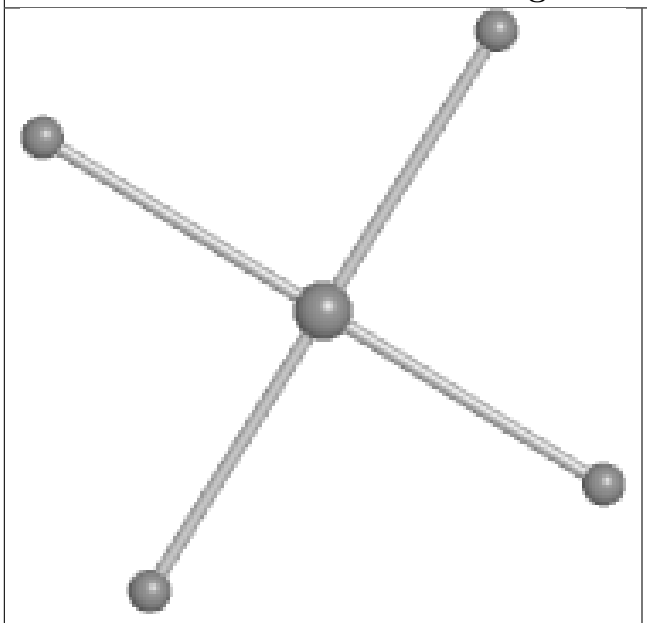


Torsions

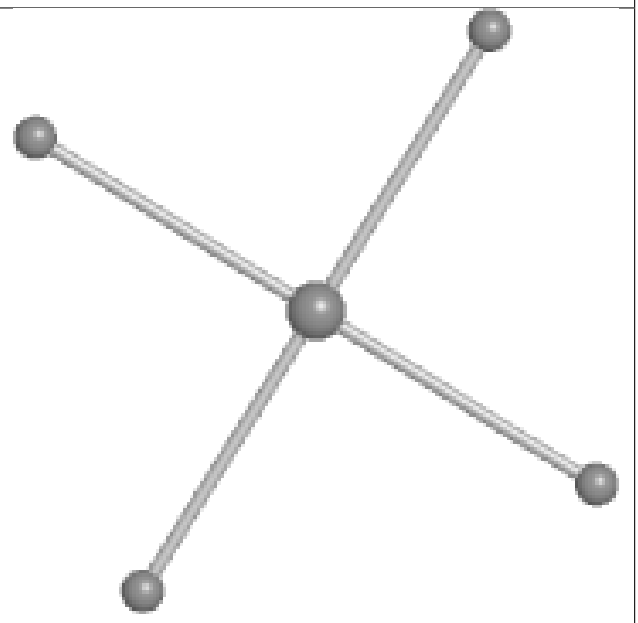


Rings

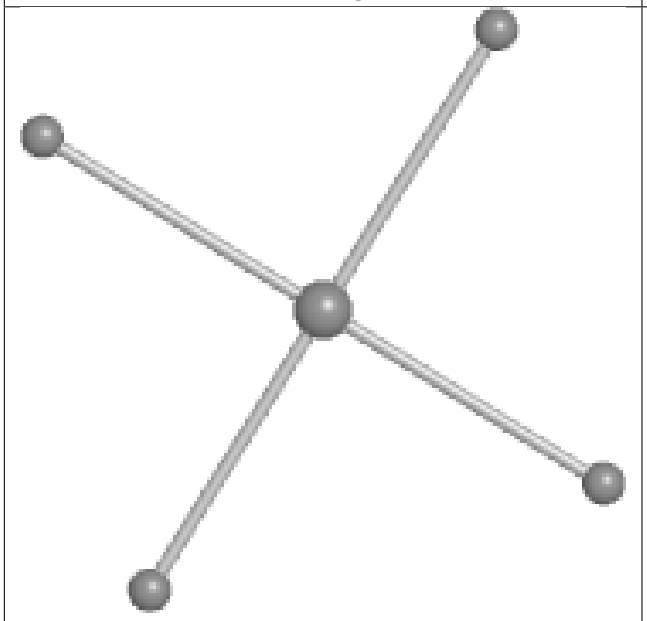
Ligand ALF F 503



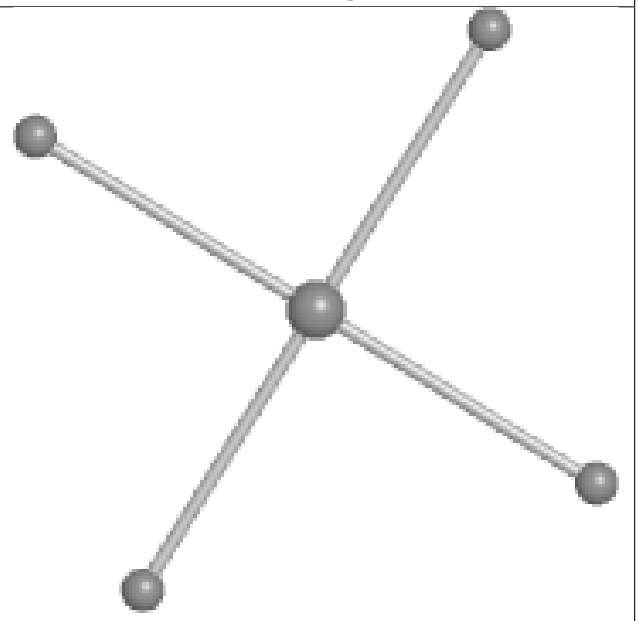
Bond lengths



Bond angles

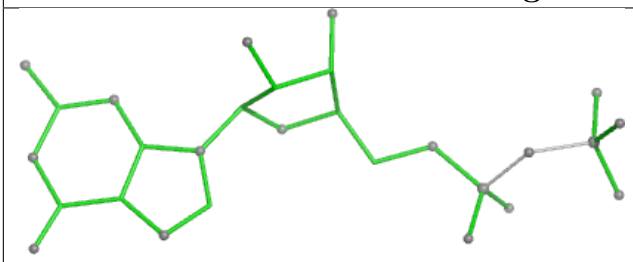


Torsions

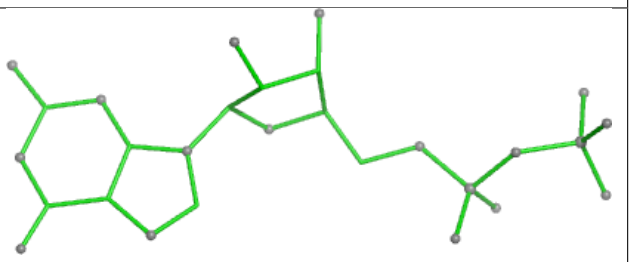


Rings

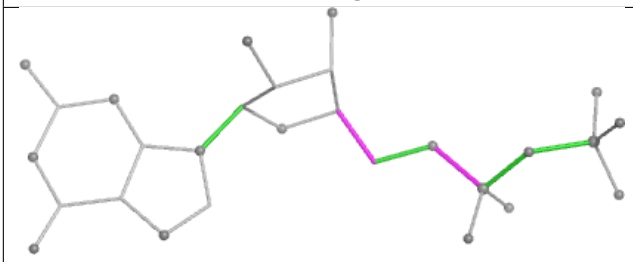
Ligand GDP F 501



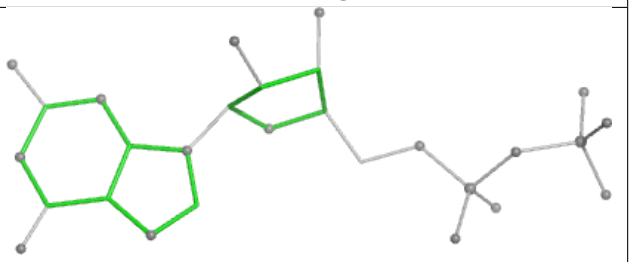
Bond lengths



Bond angles

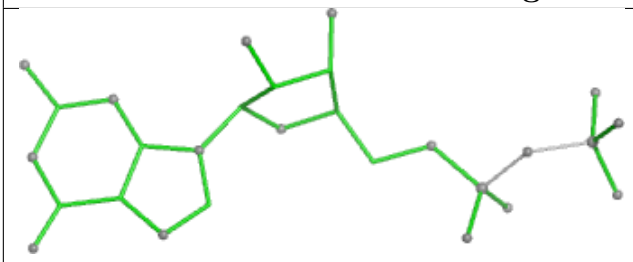


Torsions

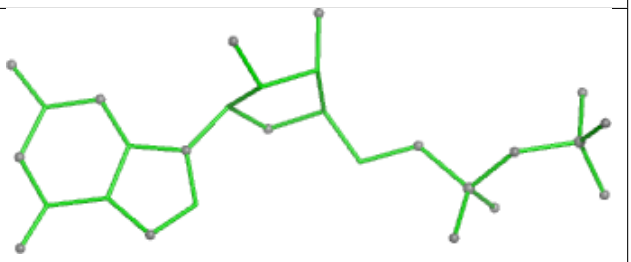


Rings

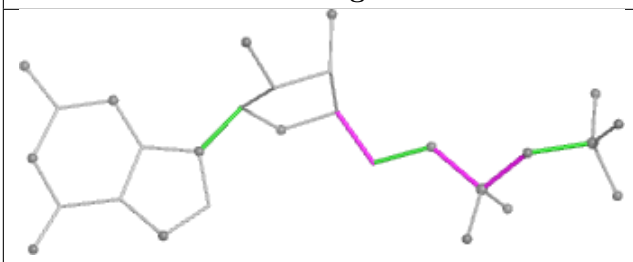
Ligand GDP E 501



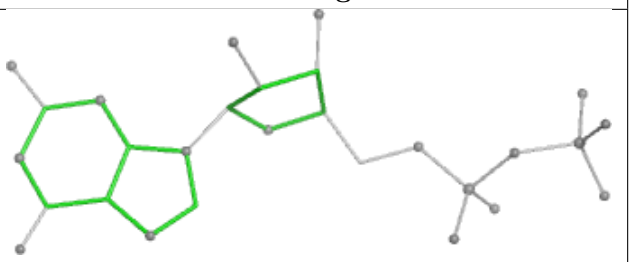
Bond lengths



Bond angles

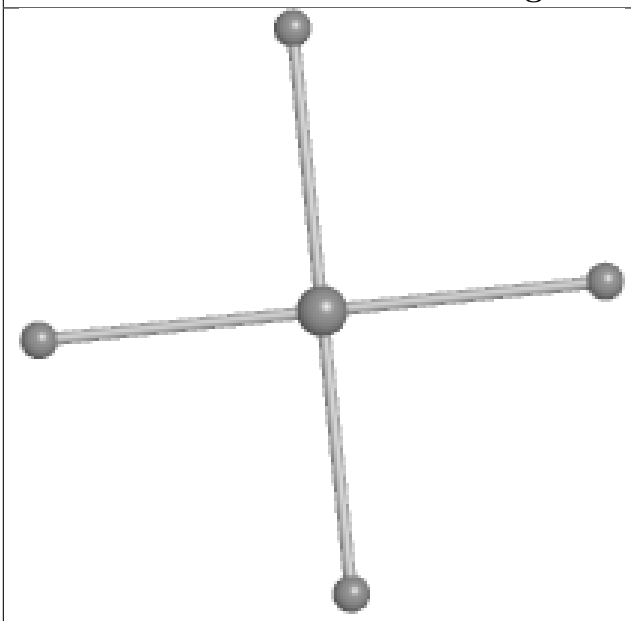


Torsions



Rings

Ligand ALF D 503



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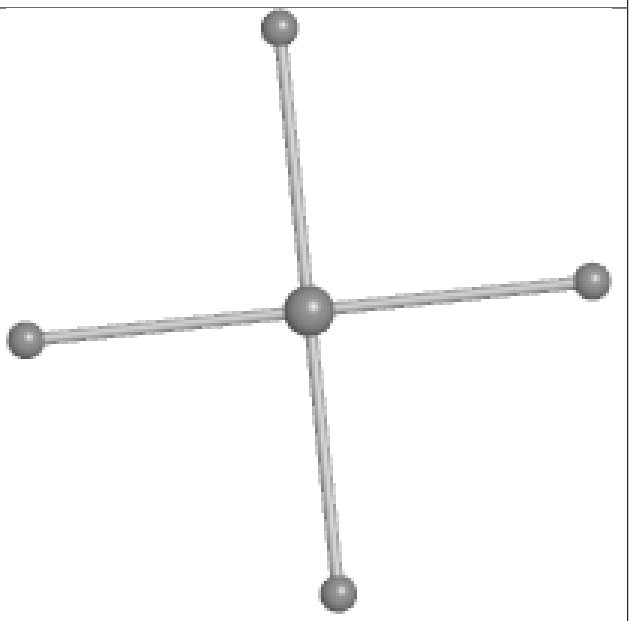
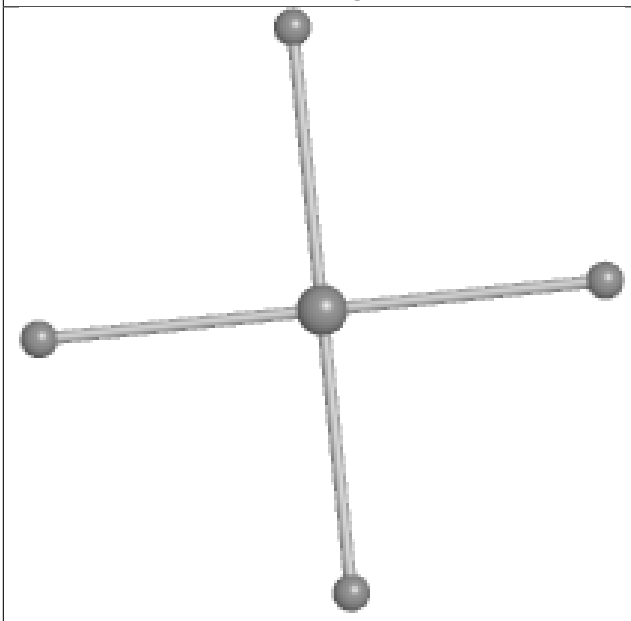
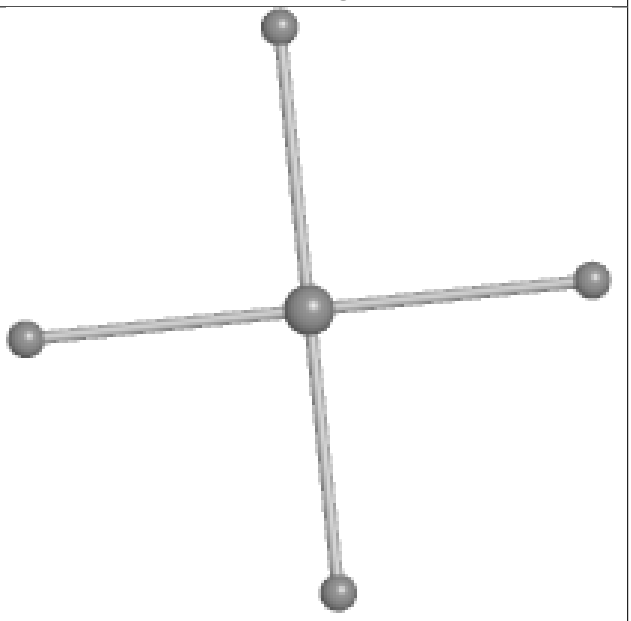


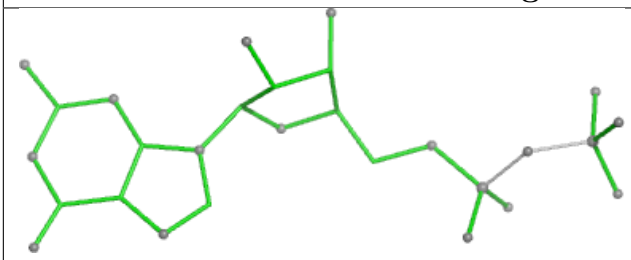
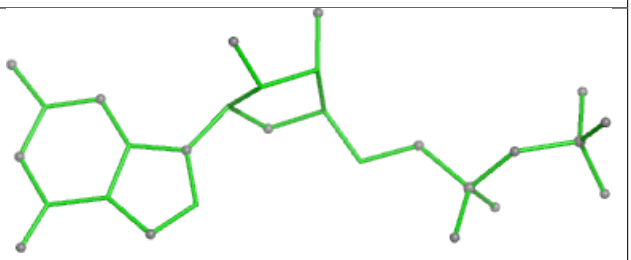
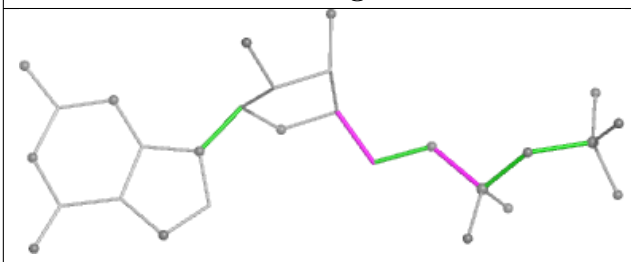
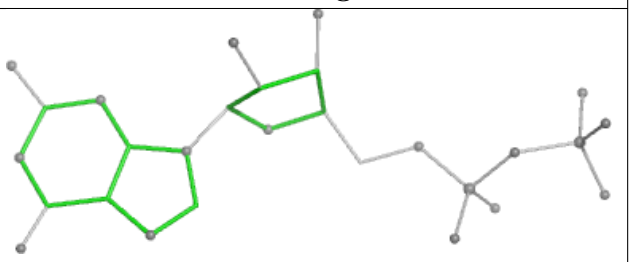
Bond angles



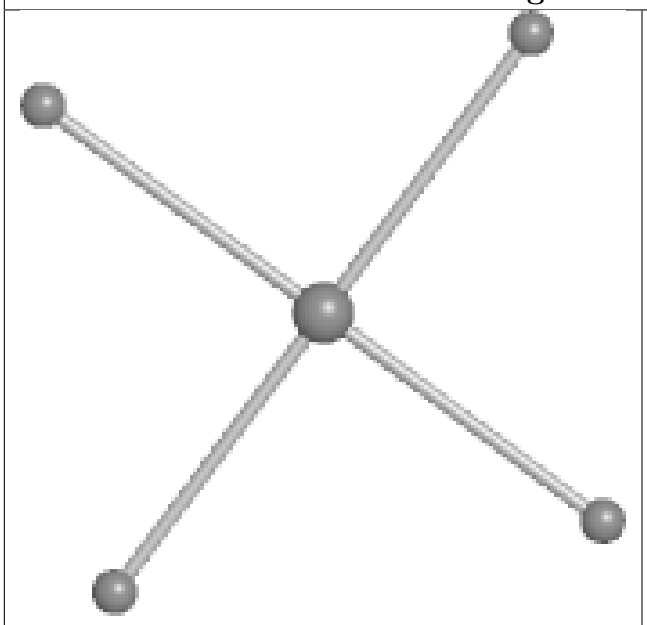
Torsions



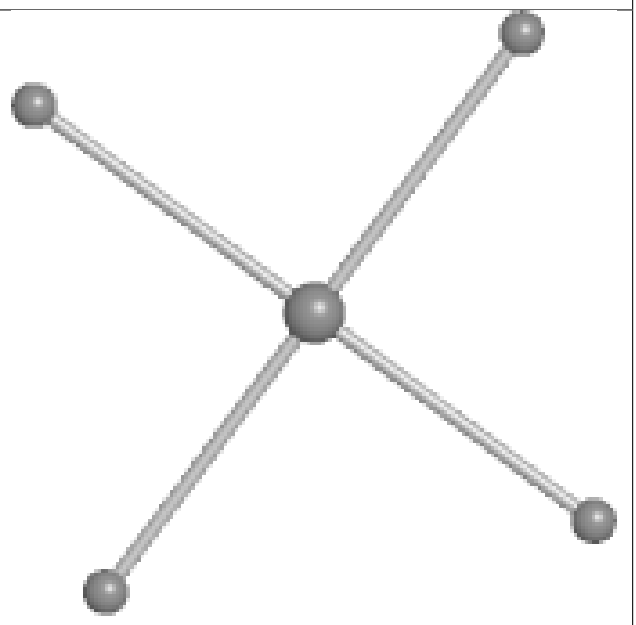
Rings

Ligand GDP B 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

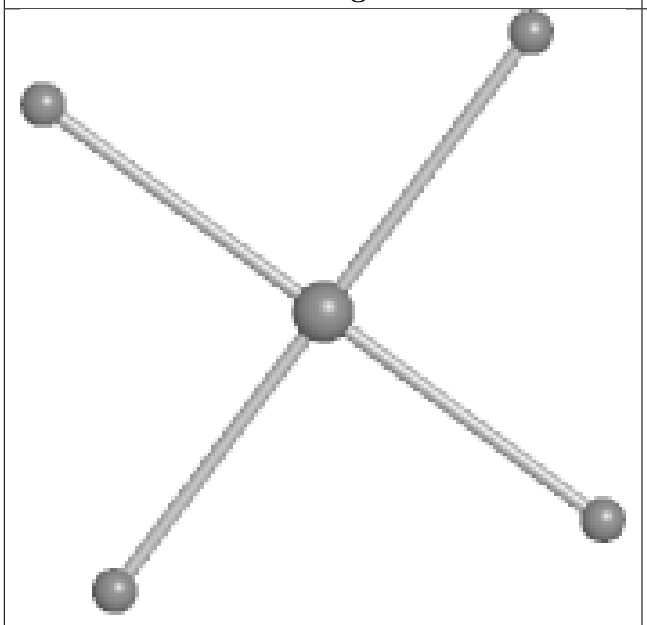
Ligand ALF C 503



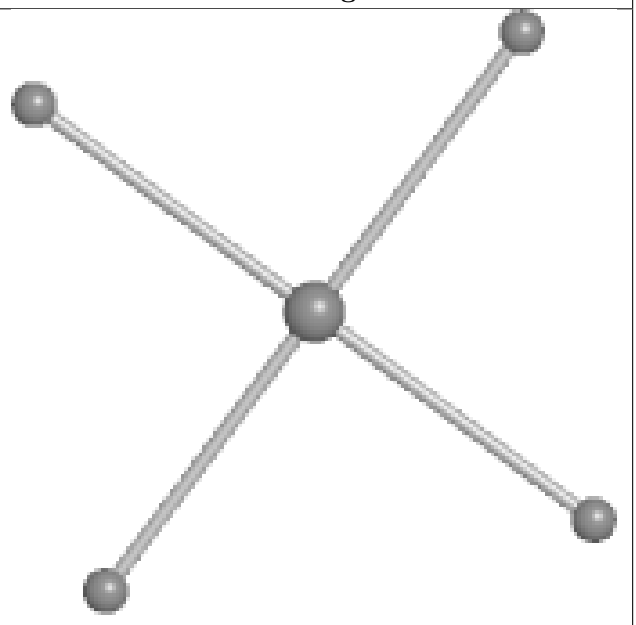
Bond lengths



Bond angles

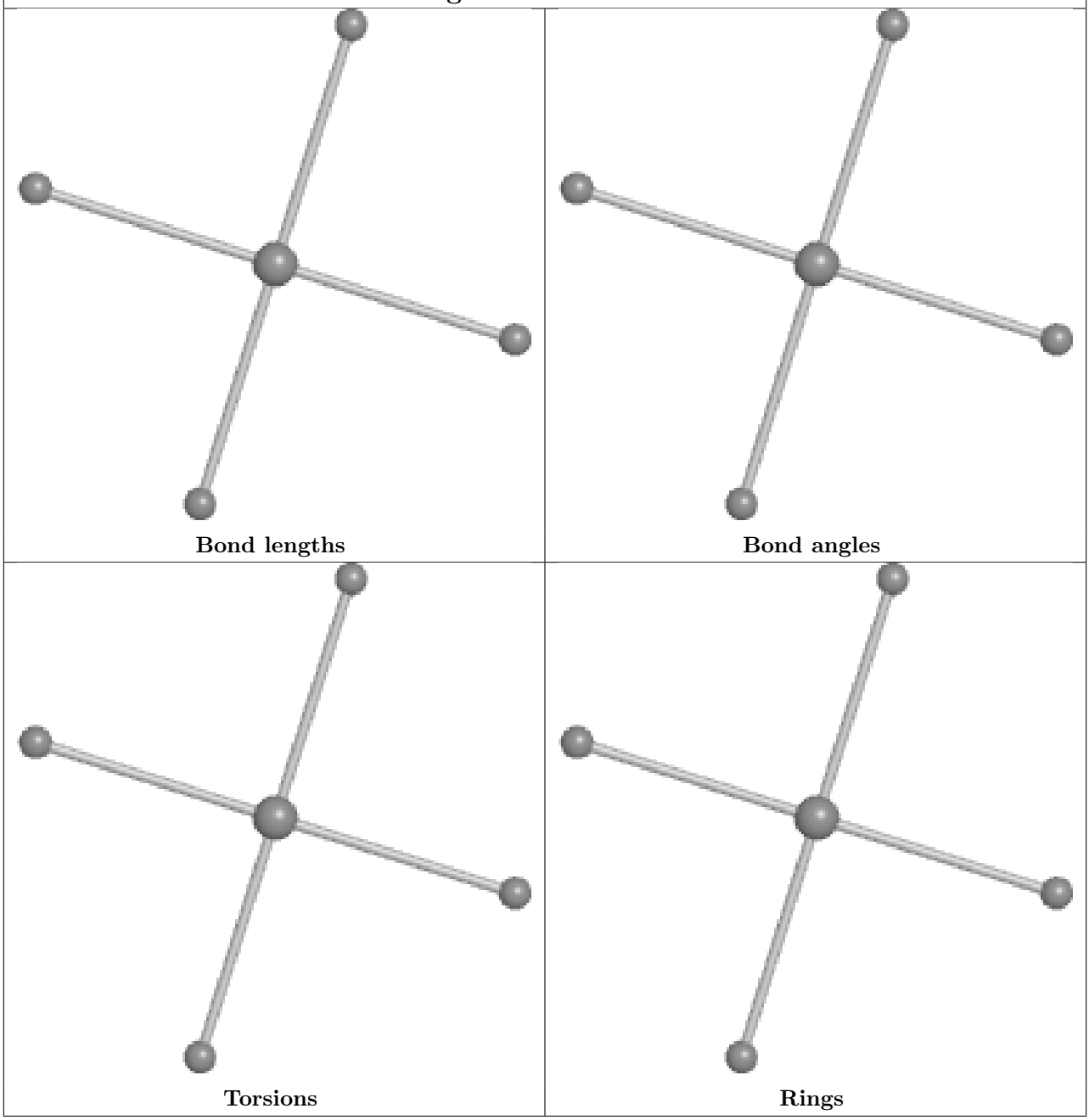


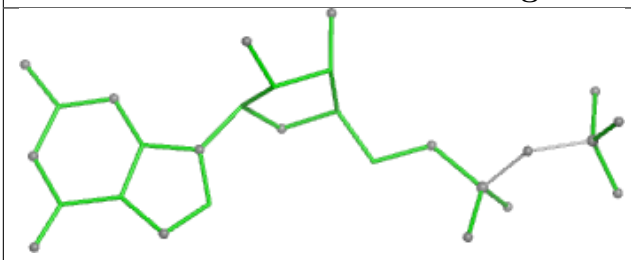
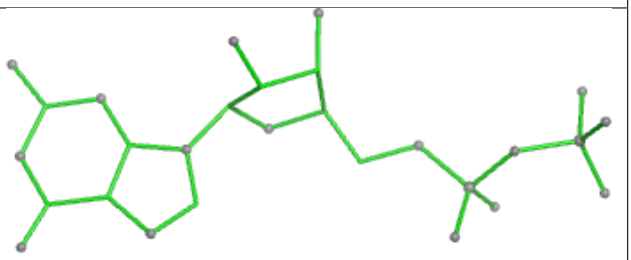
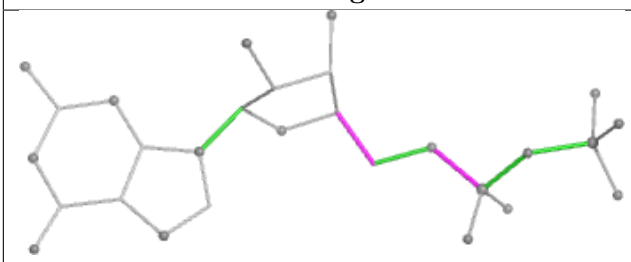
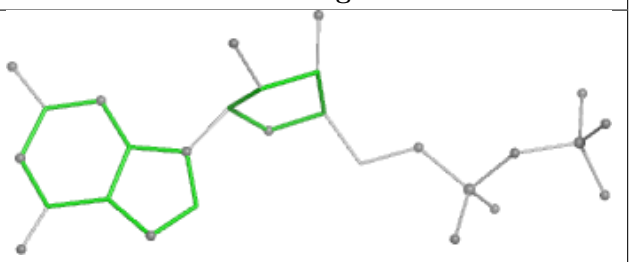
Torsions

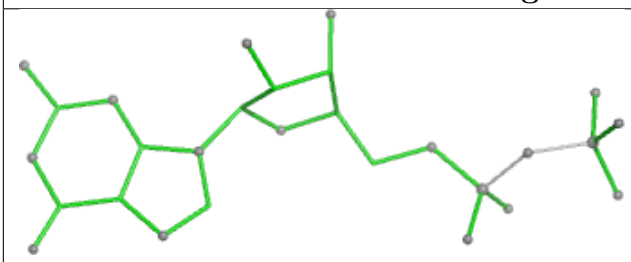
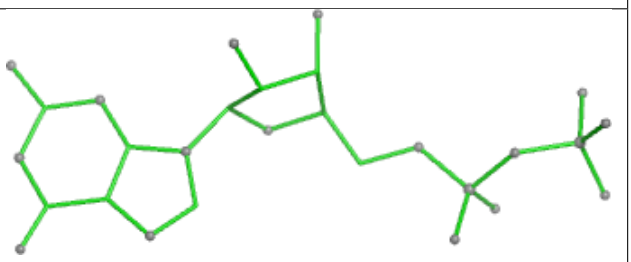
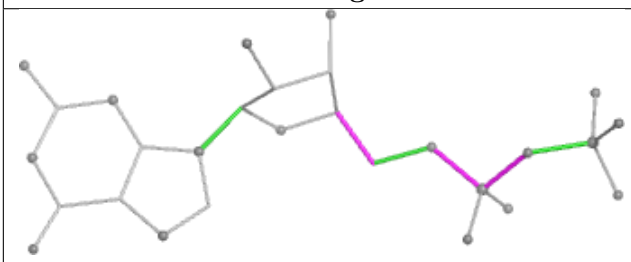
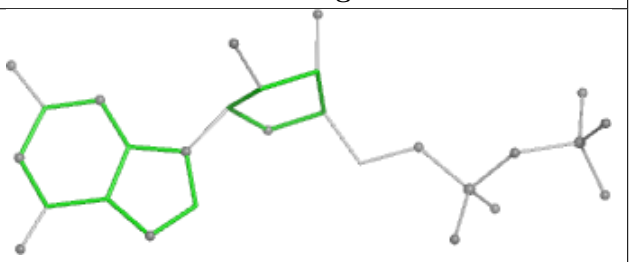


Rings

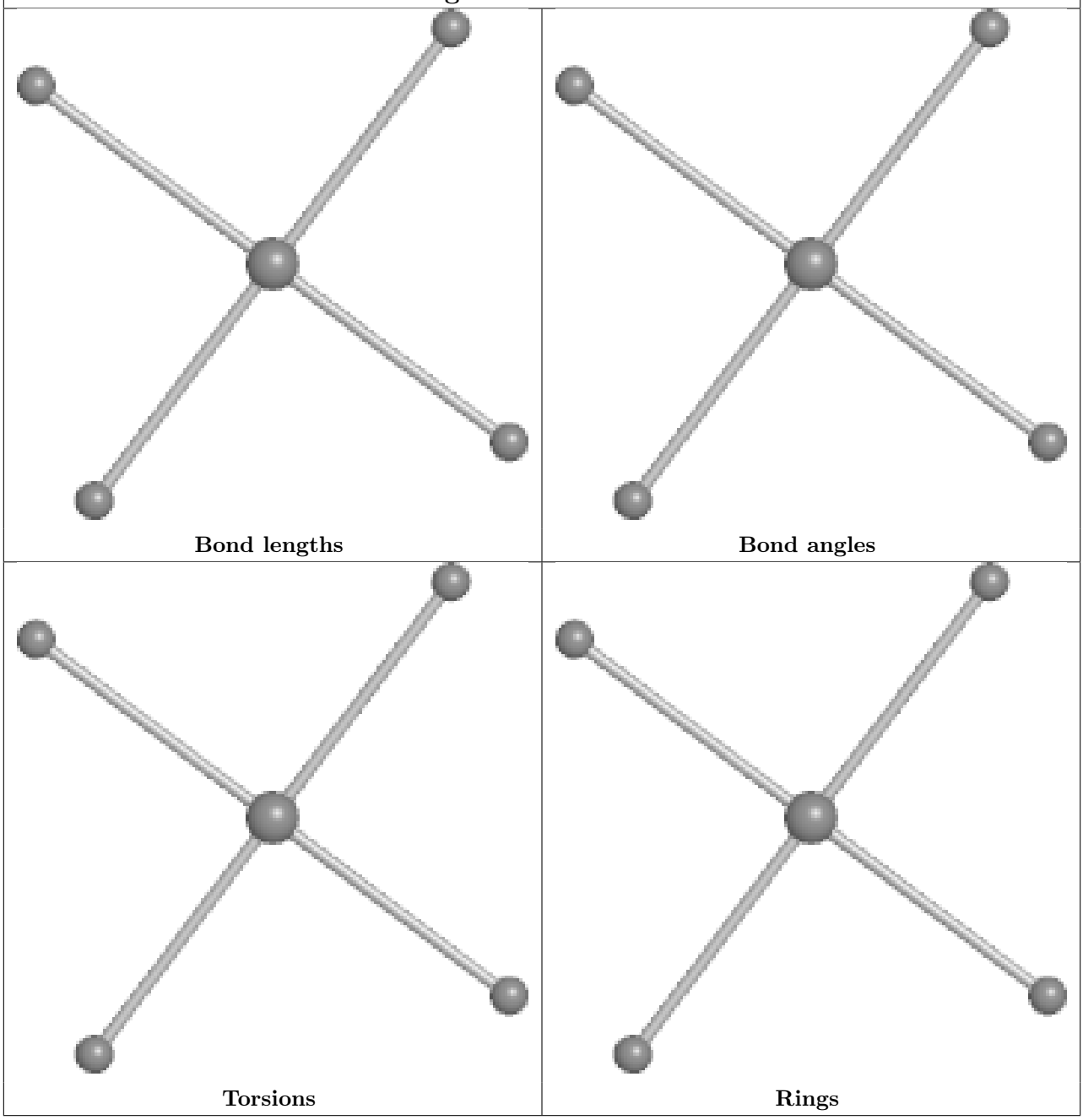
Ligand ALF A 503



Ligand GDP A 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GDP C 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ALF B 503



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	440/474 (92%)	-0.05	14 (3%)	50	35	145, 180, 227, 250	0
1	B	441/474 (93%)	-0.12	11 (2%)	58	41	130, 170, 225, 244	0
1	C	440/474 (92%)	0.02	22 (5%)	34	26	131, 185, 215, 229	0
1	D	441/474 (93%)	-0.08	21 (4%)	35	27	153, 204, 265, 276	0
1	E	440/474 (92%)	-0.11	16 (3%)	46	33	186, 223, 251, 264	0
1	F	442/474 (93%)	-0.05	11 (2%)	58	41	183, 215, 249, 269	0
All	All	2644/2844 (92%)	-0.06	95 (3%)	46	33	130, 195, 248, 276	0

The worst 5 of 95 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	413	MET	7.0
1	D	334	LEU	6.0
1	A	434	ILE	5.9
1	D	337	ILE	5.9
1	C	237	PHE	5.7

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

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

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

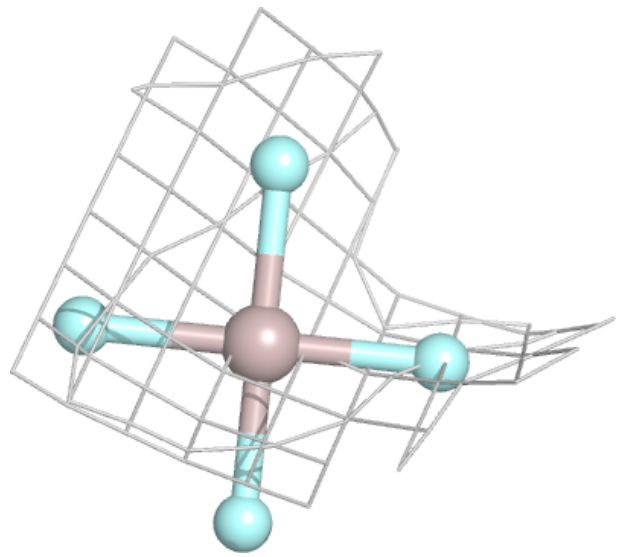
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

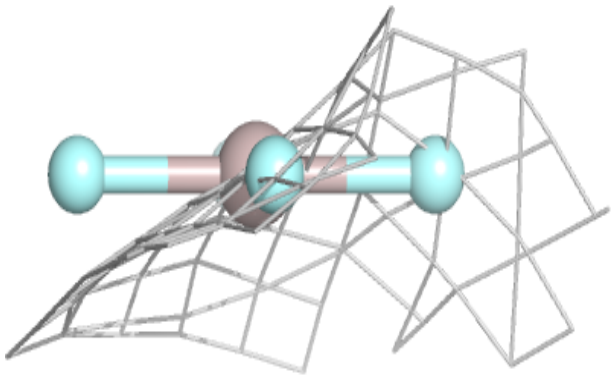
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	ALF	D	503	5/5	0.25	0.12	271,272,272,272	0
2	GDP	F	501	28/28	0.87	0.07	212,215,217,217	0
4	ALF	F	503	5/5	0.88	0.10	287,287,287,287	0
2	GDP	D	501	28/28	0.89	0.06	217,219,220,220	0
3	MG	D	502	1/1	0.90	0.12	74,74,74,74	0
4	ALF	E	503	5/5	0.91	0.07	218,218,218,218	0
4	ALF	B	503	5/5	0.94	0.12	160,160,160,161	0
2	GDP	A	501	28/28	0.94	0.08	151,159,164,165	0
2	GDP	E	501	28/28	0.94	0.07	186,187,193,193	0
3	MG	F	502	1/1	0.94	0.06	92,92,92,92	0
2	GDP	B	501	28/28	0.95	0.08	144,153,160,161	0
2	GDP	C	501	28/28	0.96	0.07	141,149,157,157	0
4	ALF	A	503	5/5	0.96	0.10	175,175,175,176	0
4	ALF	C	503	5/5	0.97	0.06	161,161,161,162	0
3	MG	A	502	1/1	0.98	0.10	63,63,63,63	0
3	MG	E	502	1/1	0.98	0.07	74,74,74,74	0
3	MG	B	502	1/1	0.98	0.13	52,52,52,52	0
3	MG	C	502	1/1	0.99	0.03	34,34,34,34	0

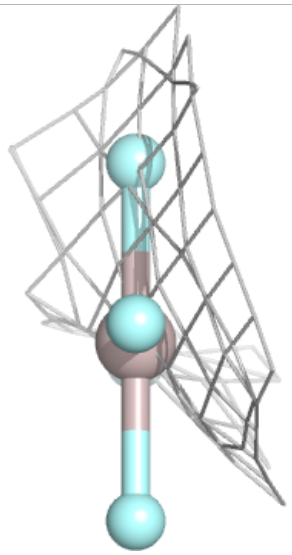
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ALF D 503:

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

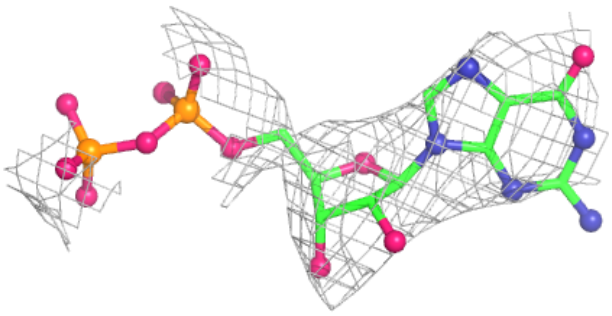


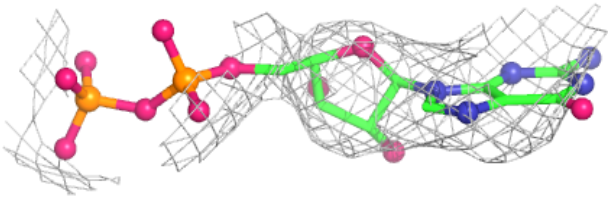


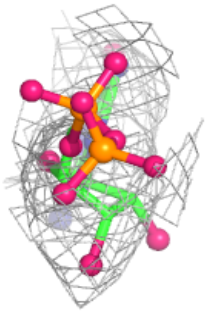


Electron density around GDP F 501:

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

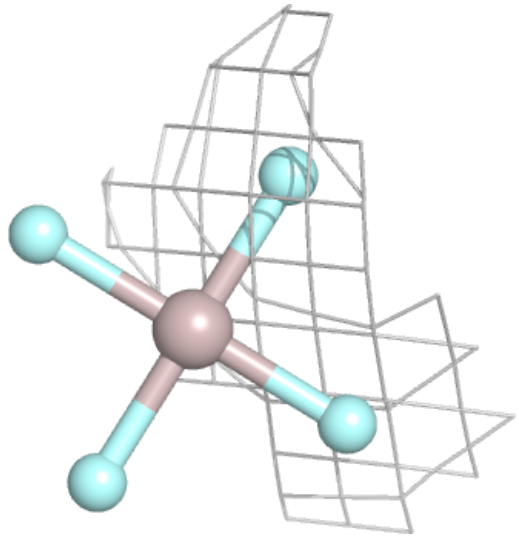


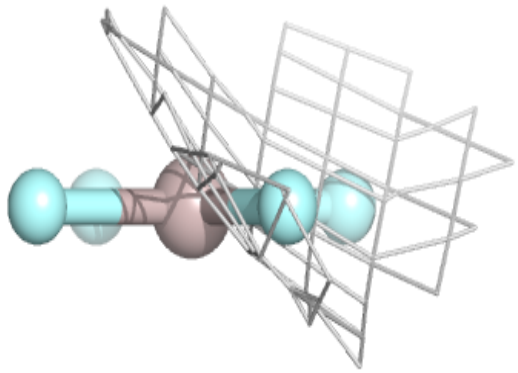


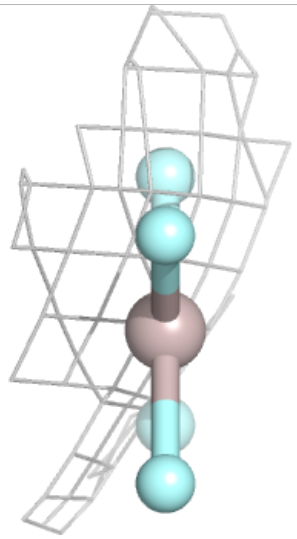


Electron density around ALF F 503:

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

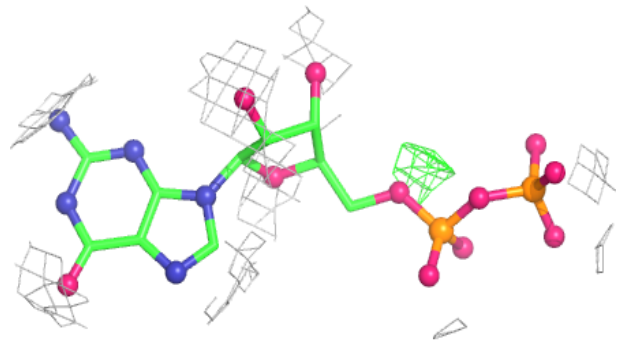


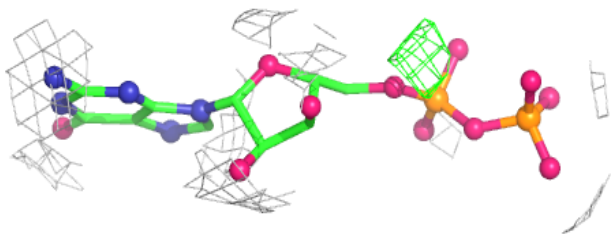


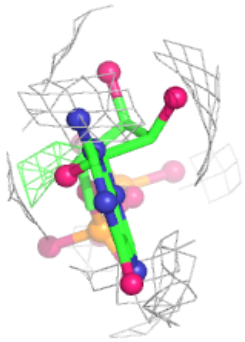


Electron density around GDP D 501:

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

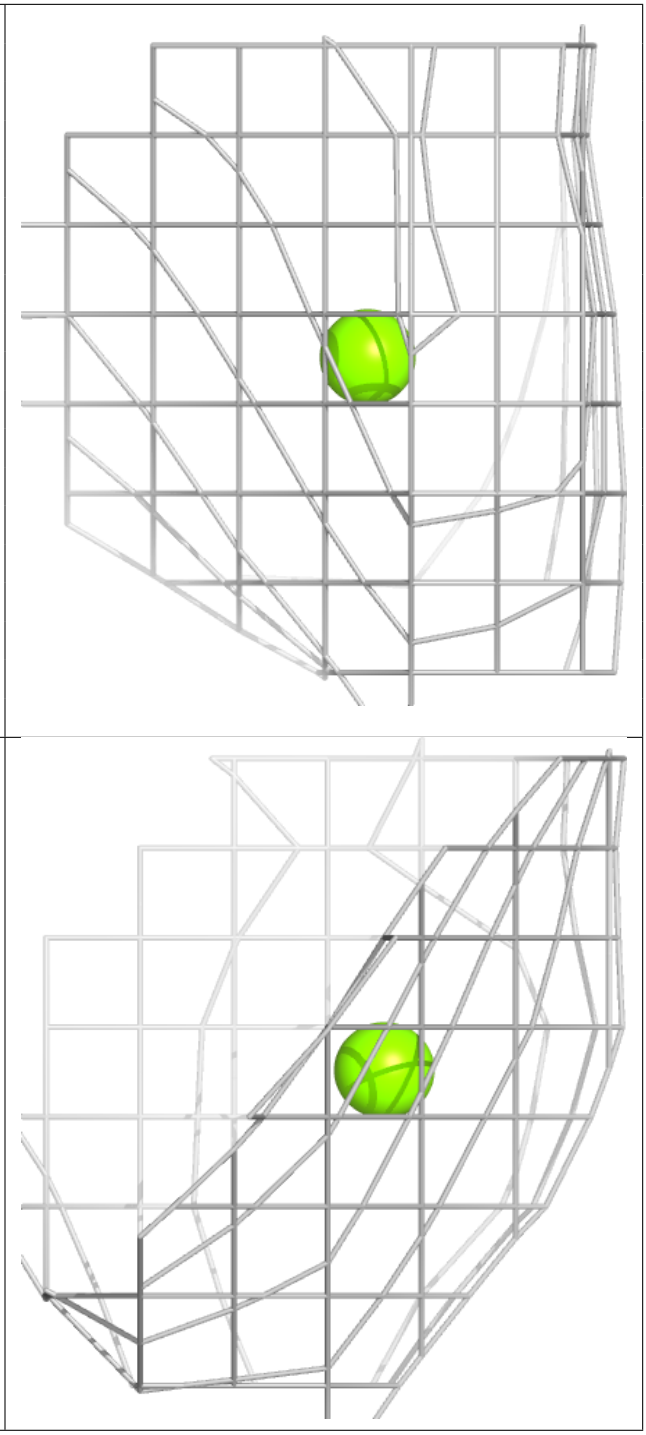






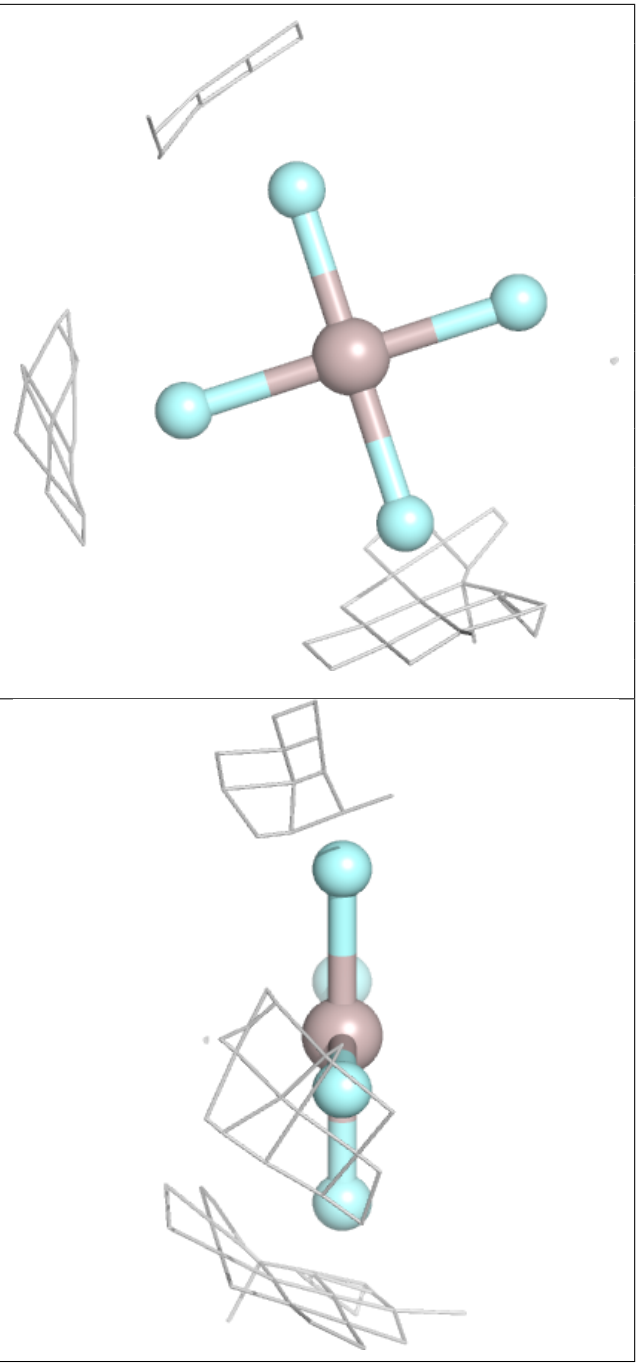
Electron density around MG D 502:

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



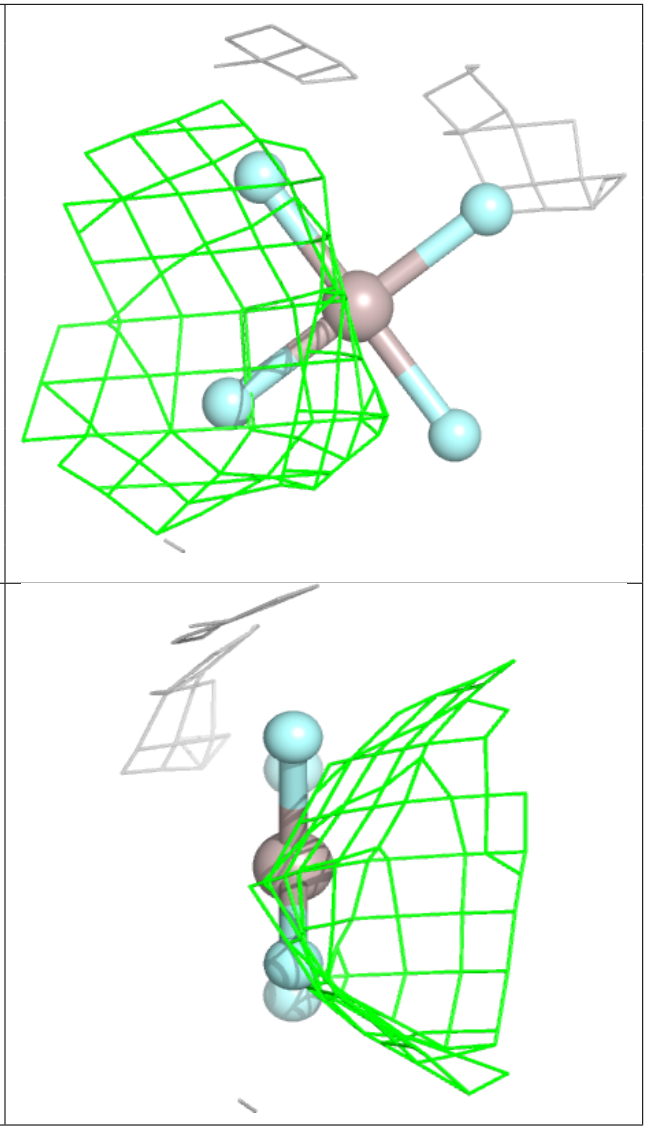
Electron density around ALF E 503:

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



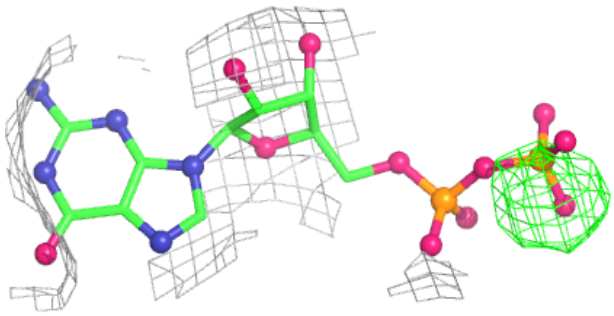
Electron density around ALF B 503:

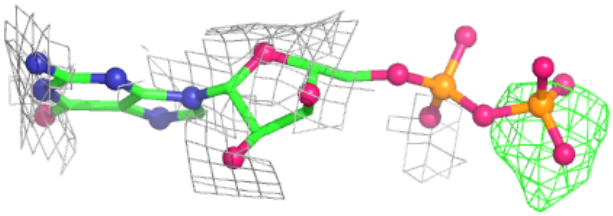
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

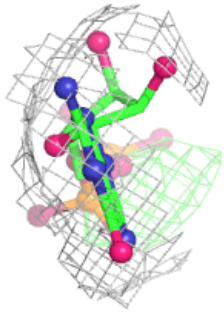


Electron density around GDP A 501:

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

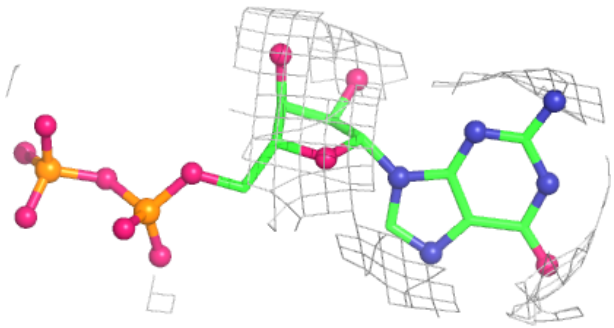


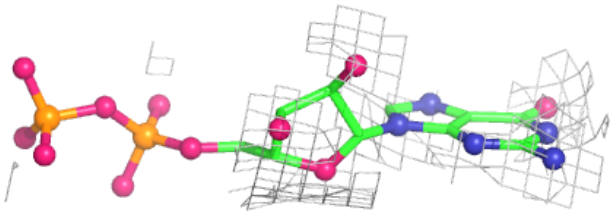


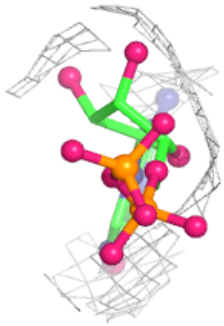


Electron density around GDP E 501:

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

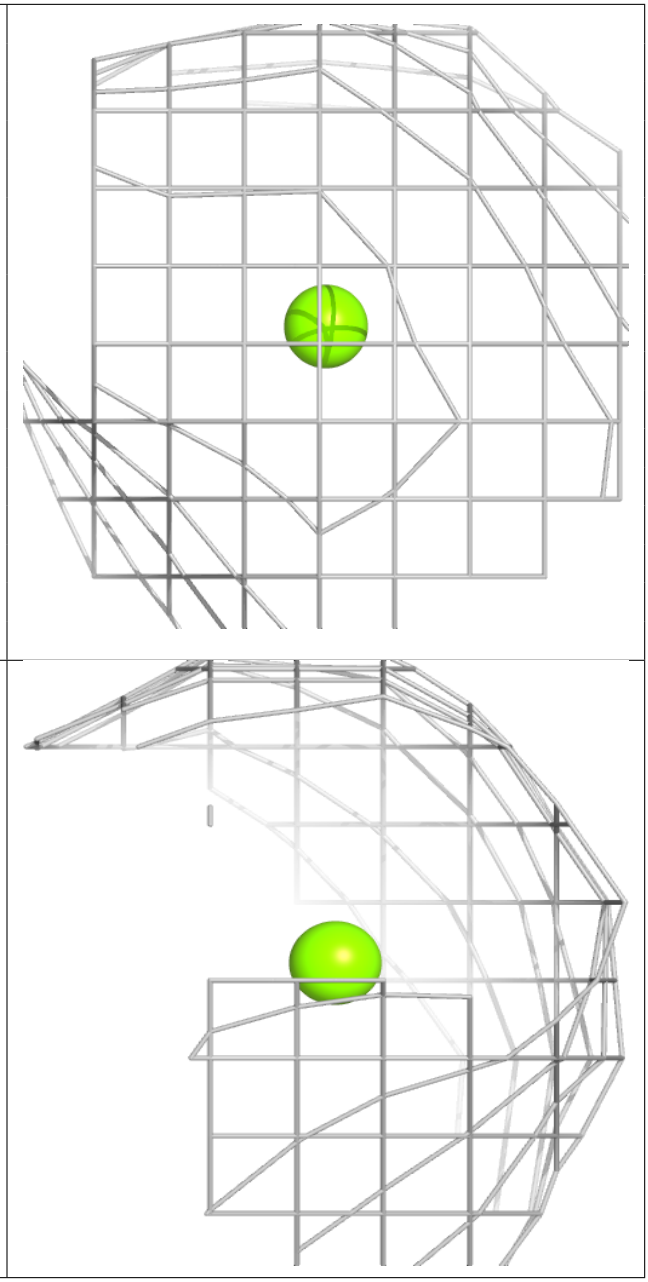






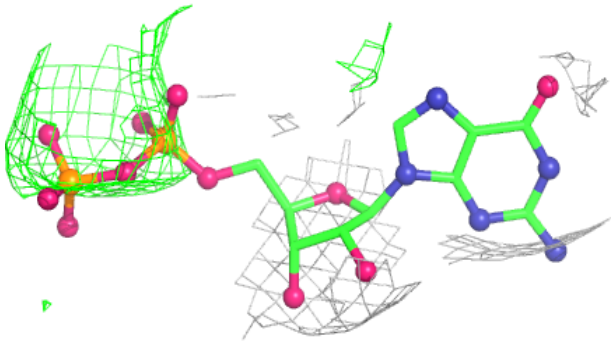
Electron density around MG F 502:

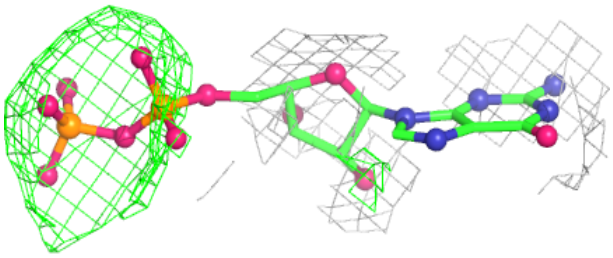
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

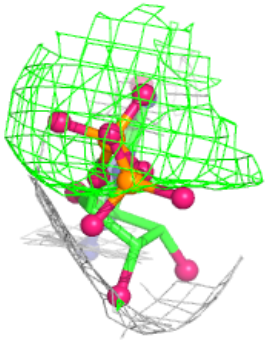


Electron density around GDP B 501:

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

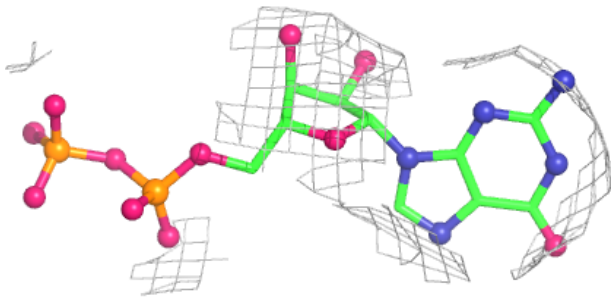


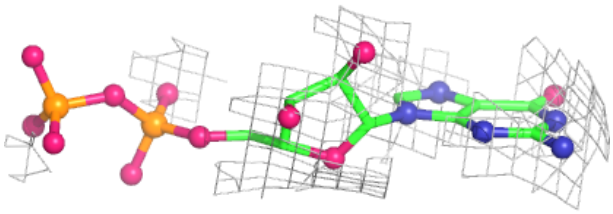


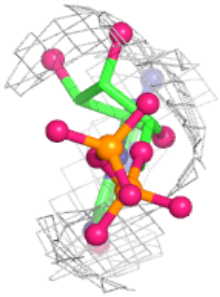


Electron density around GDP C 501:

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

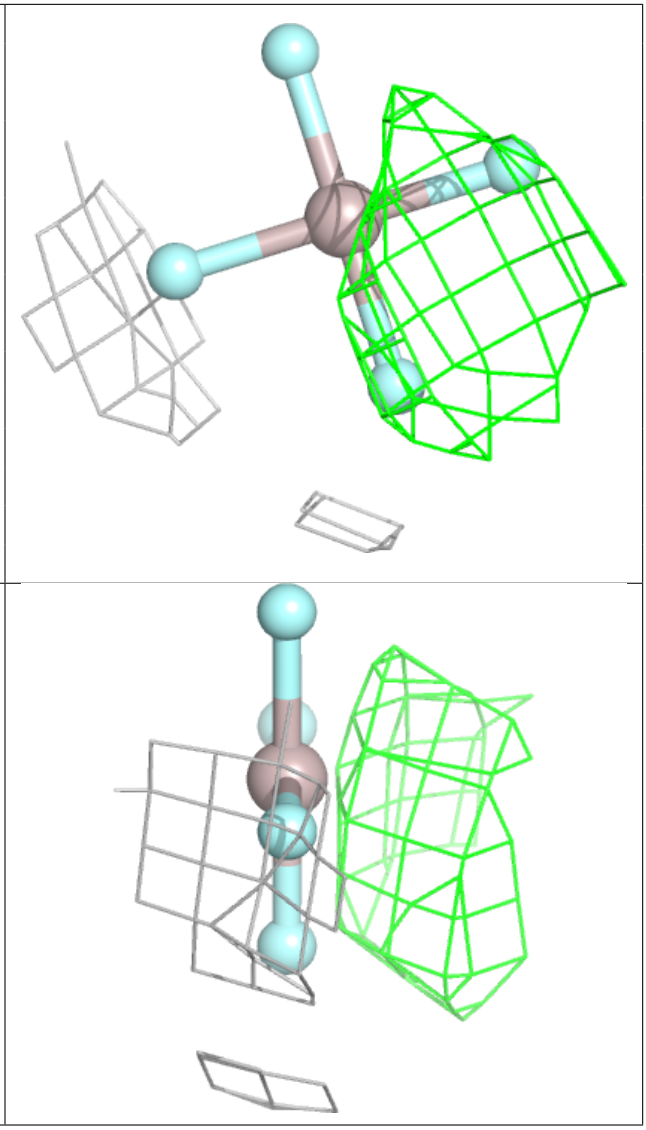


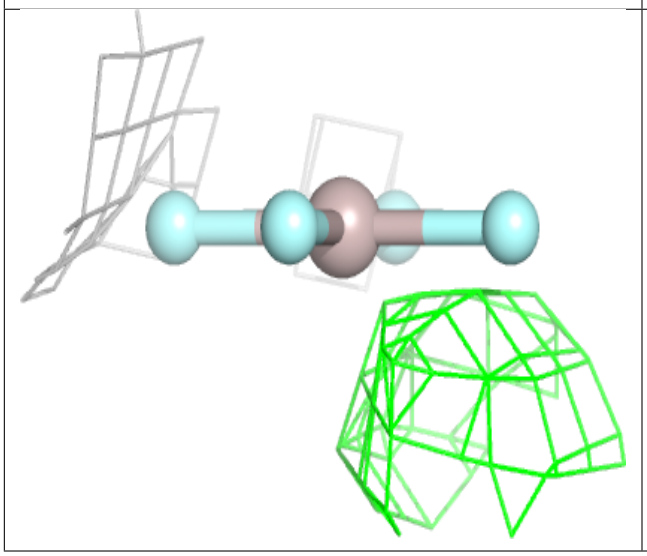




Electron density around ALF A 503:

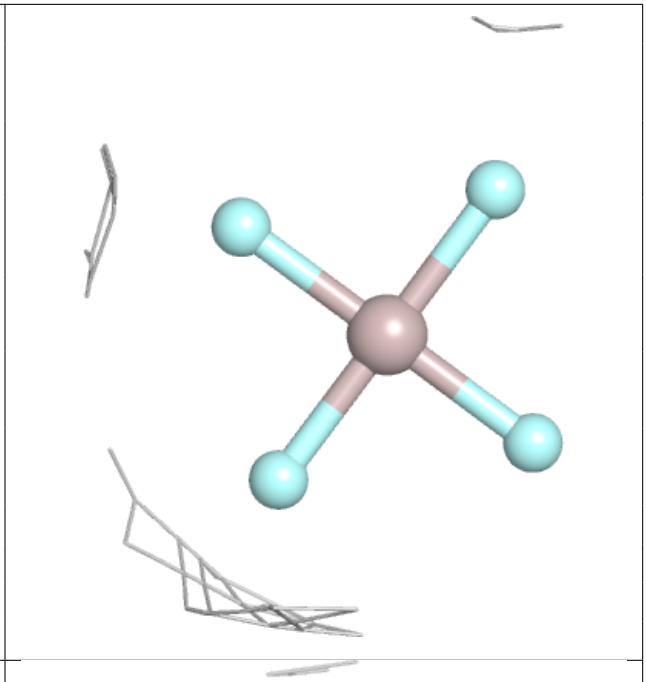
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

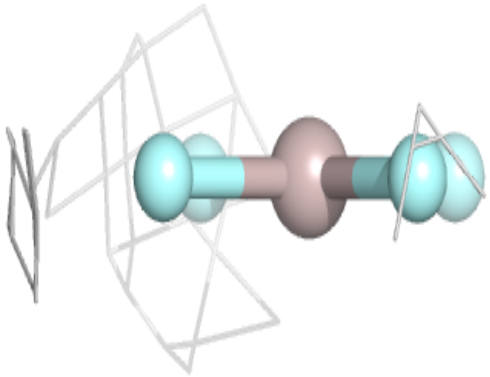


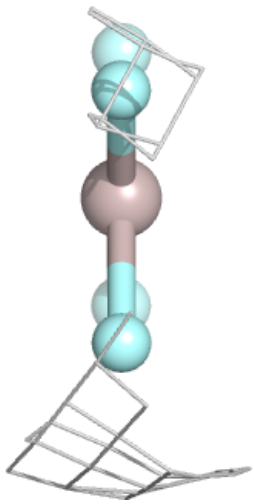


Electron density around ALF C 503:

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

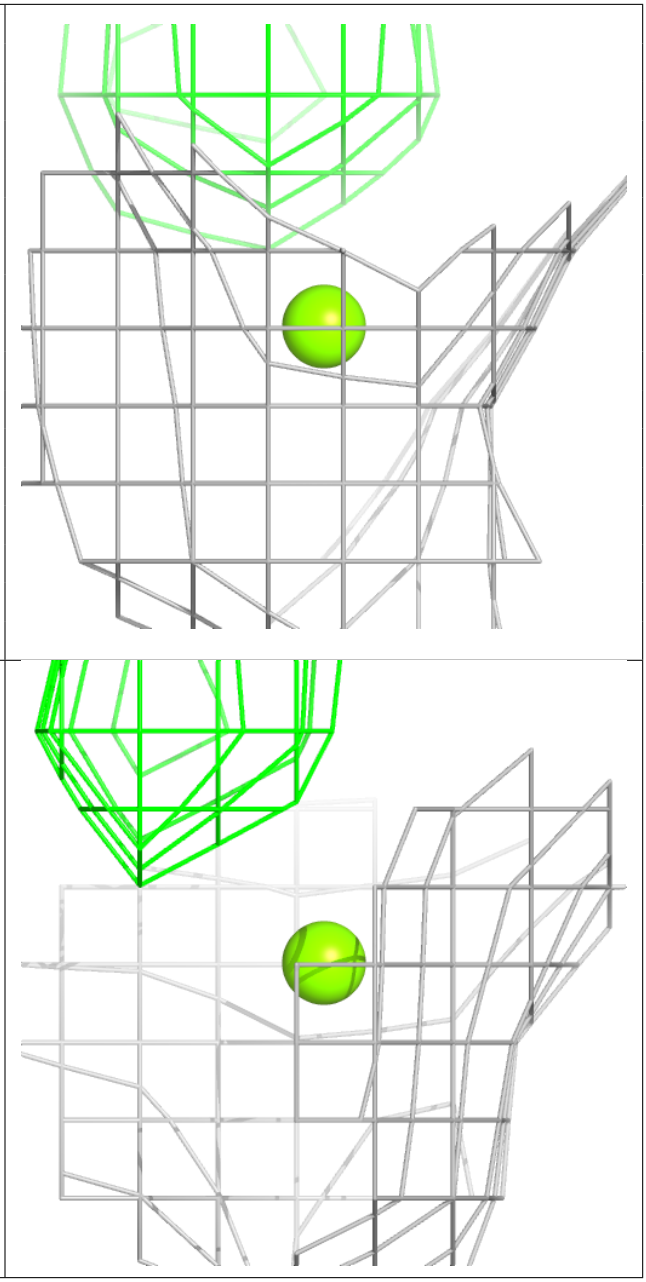






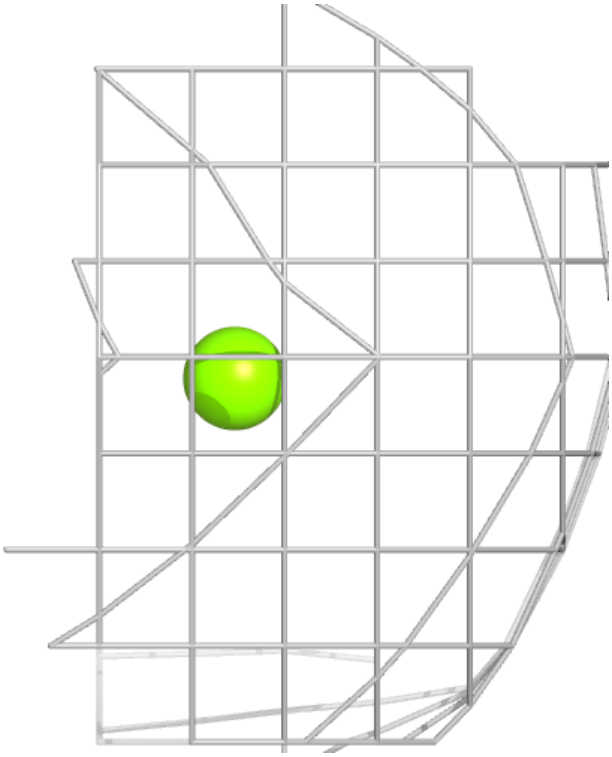
Electron density around MG A 502:

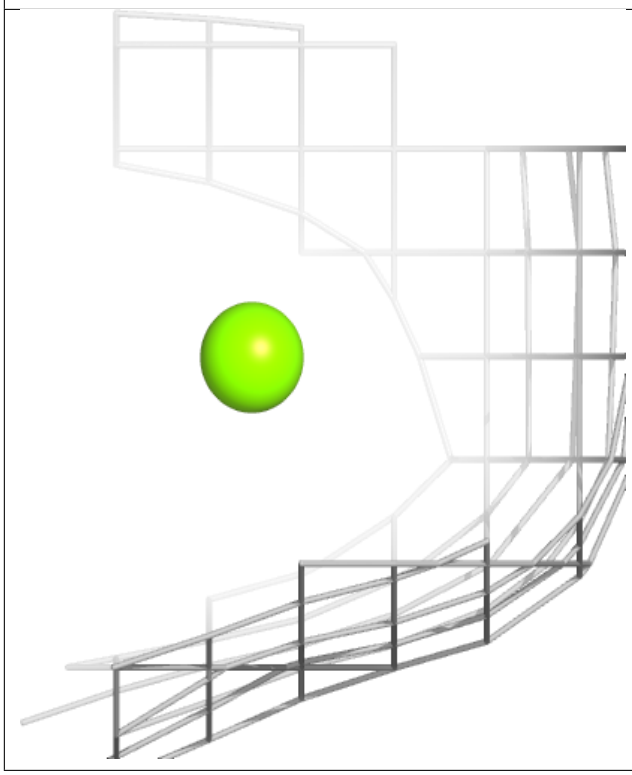
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

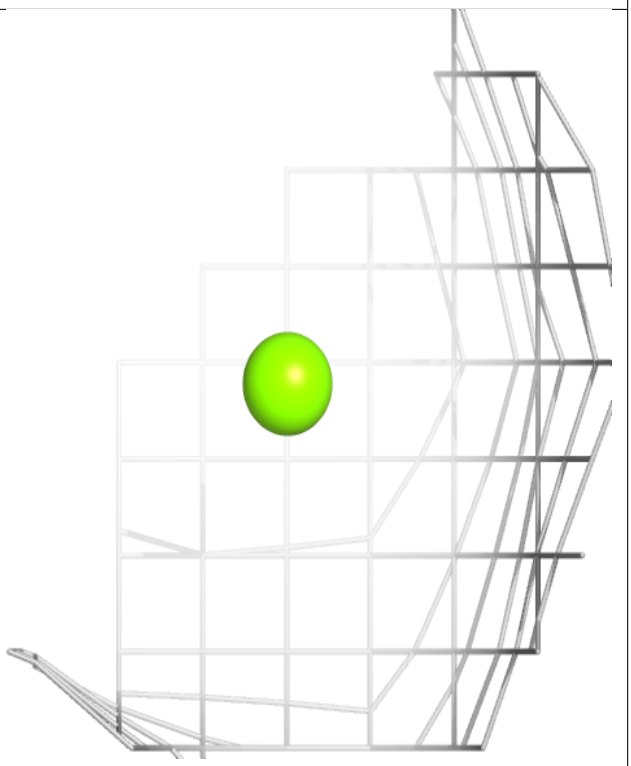


Electron density around MG E 502:

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

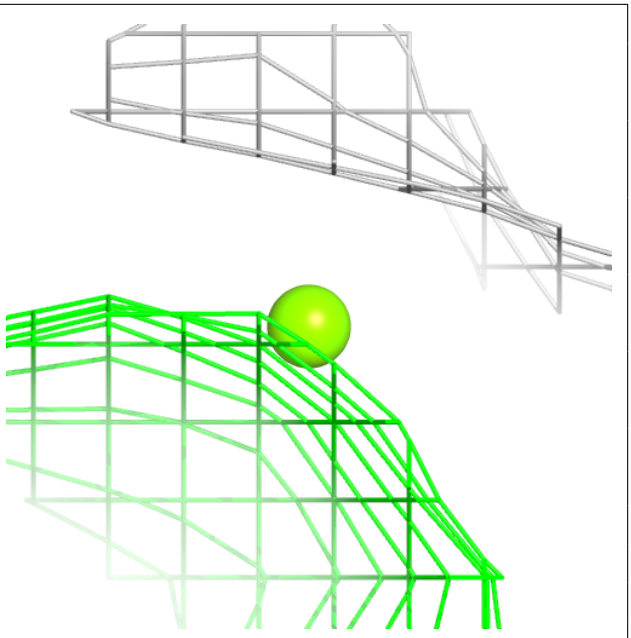


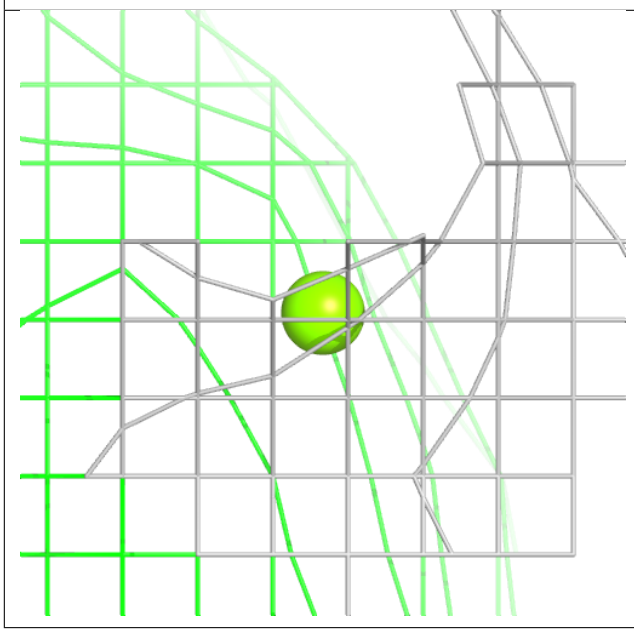


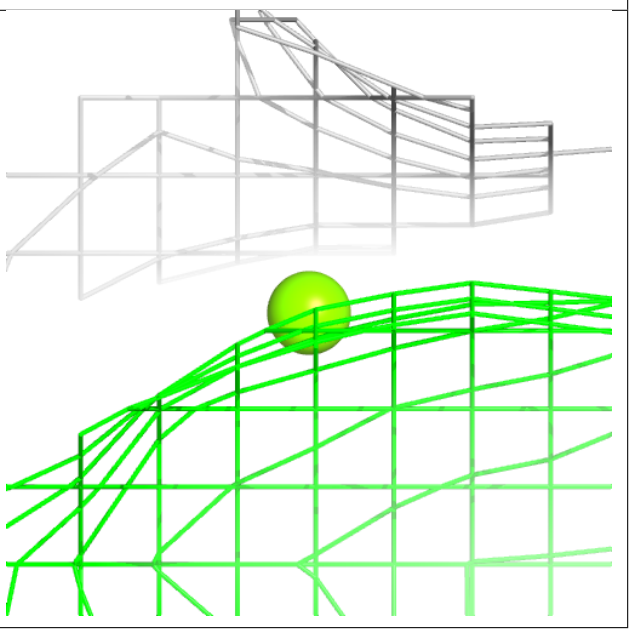


Electron density around MG B 502:

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

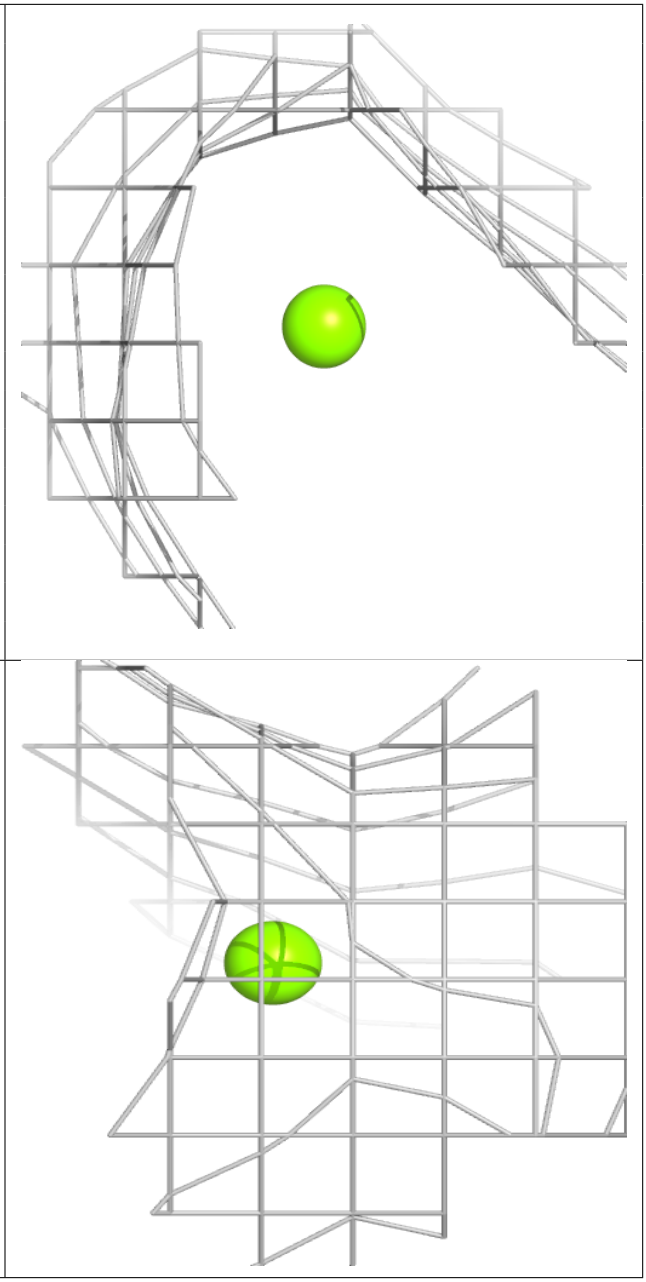






Electron density around MG C 502:

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.