Full wwPDB X-ray Structure Validation Report

Apr 19, 2021 – 08:21 am BST

PDB ID	:	6T66
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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ⓘ) were used in the production of this report:

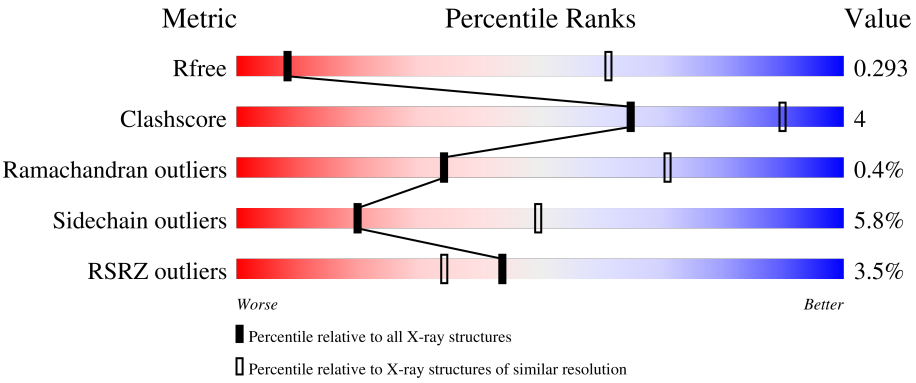
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.18
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.18

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}	130704	1002 (4.14-3.66)
Clashscore	141614	1004 (4.12-3.68)
Ramachandran outliers	138981	1021 (4.14-3.66)
Sidechain outliers	138945	1014 (4.14-3.66)
RSRZ outliers	127900	1275 (4.20-3.60)

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	2% 77% 15% • 7%
1	B	474	% 77% 15% • 7%
1	C	474	2% 78% 14% • 7%
1	D	474	3% 78% 14% • 7%
1	E	474	7% 77% 15% 7%

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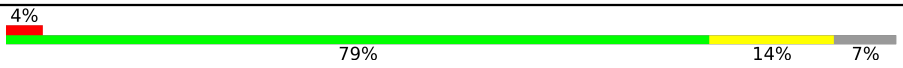
Mol	Chain	Length	Quality of chain
1	F	474	

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
4	ALF	D	503	-	-	-	X
4	ALF	F	503	-	-	-	X

2 Entry composition

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

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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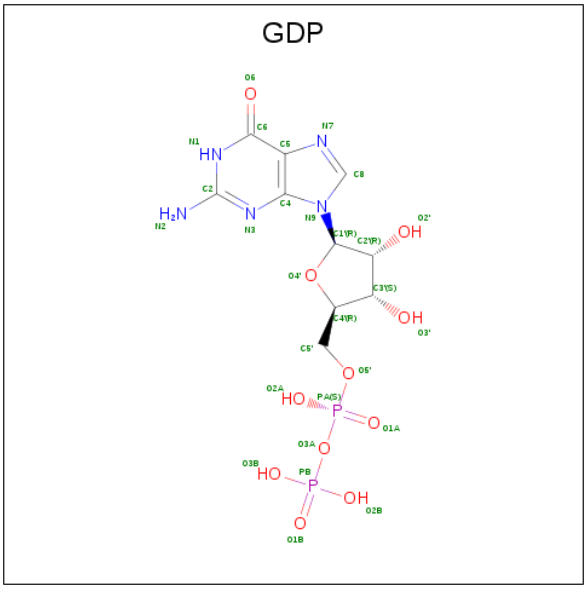
Chain	Residue	Modelled	Actual	Comment	Reference
C	474	HIS	-	expression tag	UNP A0A085R2T8
D	469	HIS	-	expression tag	UNP A0A085R2T8
D	470	HIS	-	expression tag	UNP A0A085R2T8
D	471	HIS	-	expression tag	UNP A0A085R2T8
D	472	HIS	-	expression tag	UNP A0A085R2T8
D	473	HIS	-	expression tag	UNP A0A085R2T8
D	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 (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$) (labeled as "Ligand of Interest" by depositor).



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

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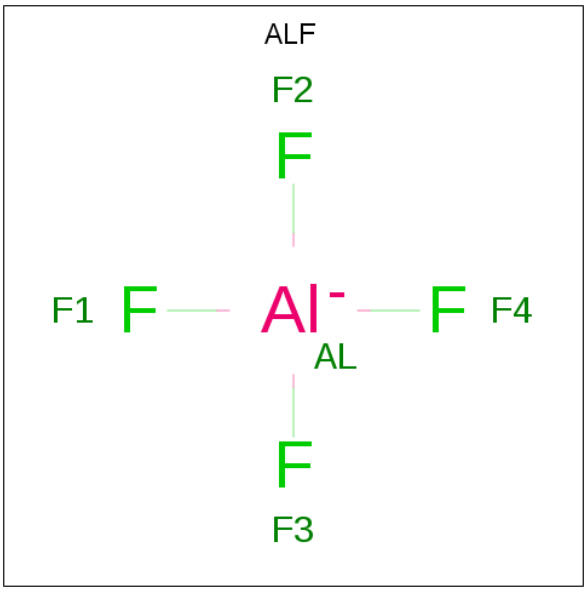
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
2	C	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
2	D	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
2	E	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
2	F	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

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

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

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



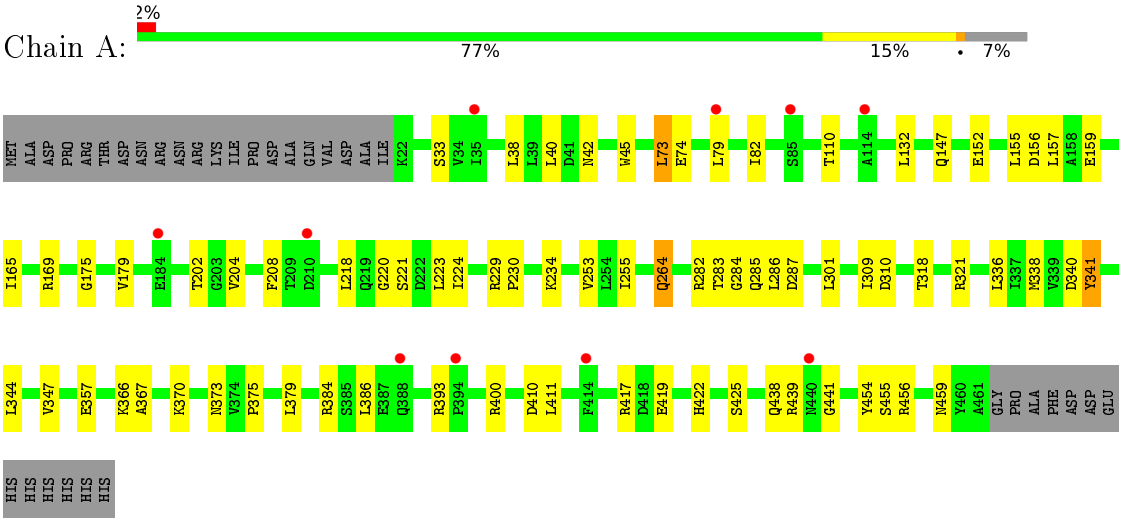
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Al F 5 1 4	0	0
4	B	1	Total Al F 5 1 4	0	0
4	C	1	Total Al F 5 1 4	0	0
4	D	1	Total Al F 5 1 4	0	0
4	E	1	Total Al F 5 1 4	0	0
4	F	1	Total Al F 5 1 4	0	0

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.

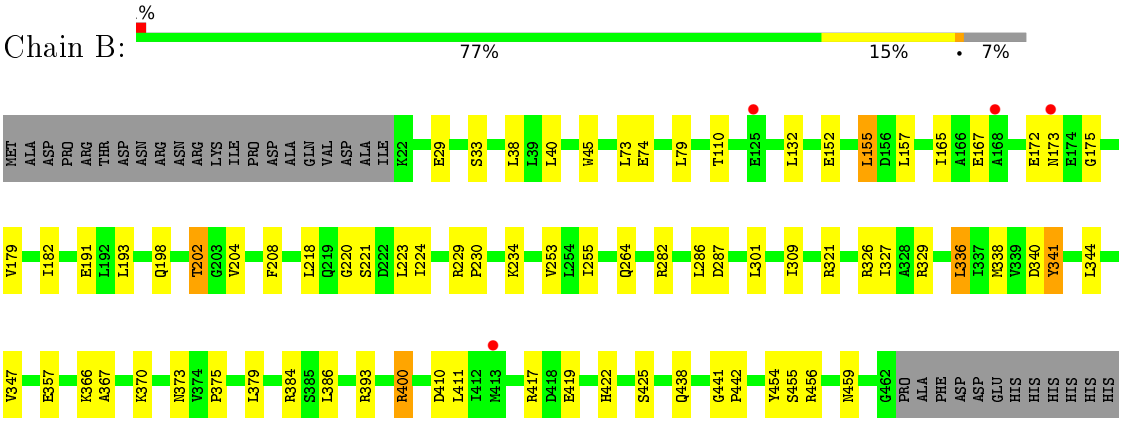
- Molecule 1: Replicative DNA helicase

Chain A:



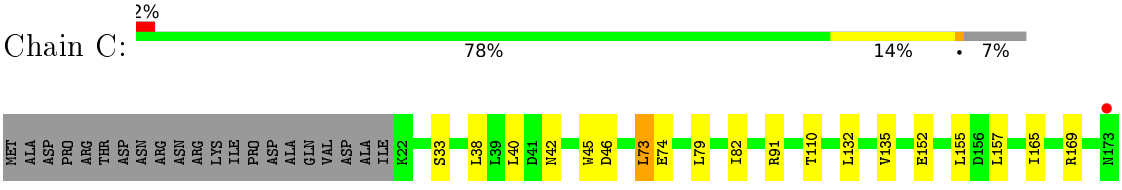
- Molecule 1: Replicative DNA helicase

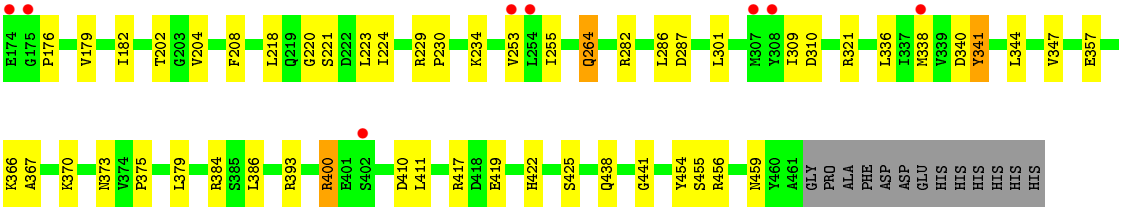
Chain B:



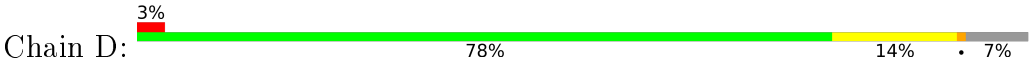
- Molecule 1: Replicative DNA helicase

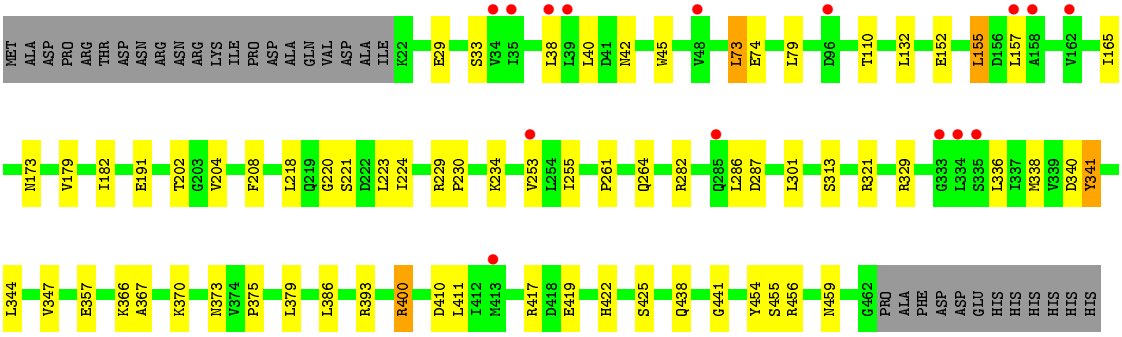
Chain C:



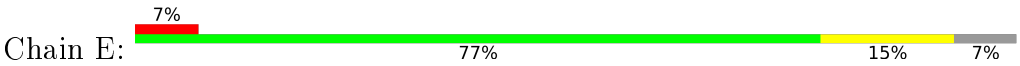


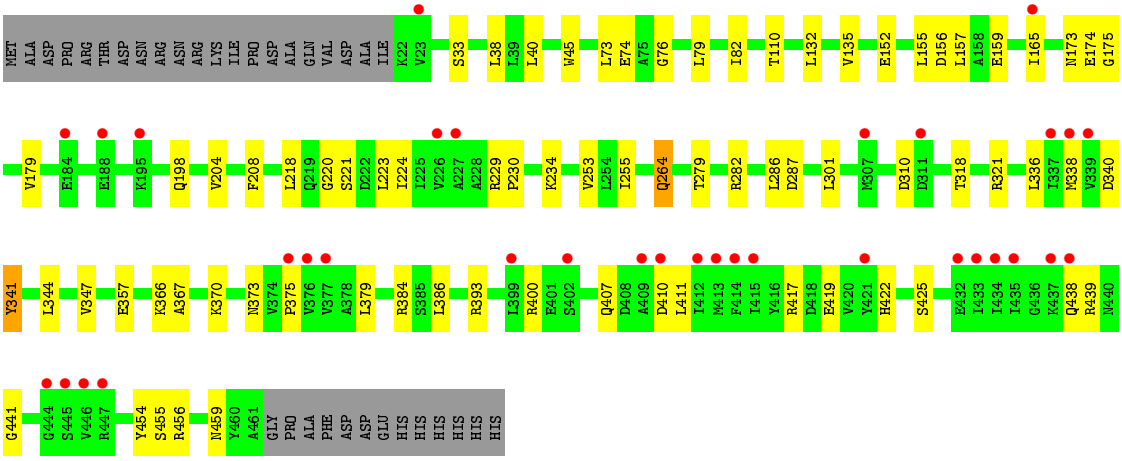
• Molecule 1: Replicative DNA helicase



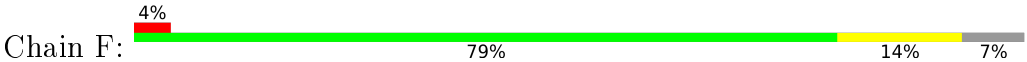


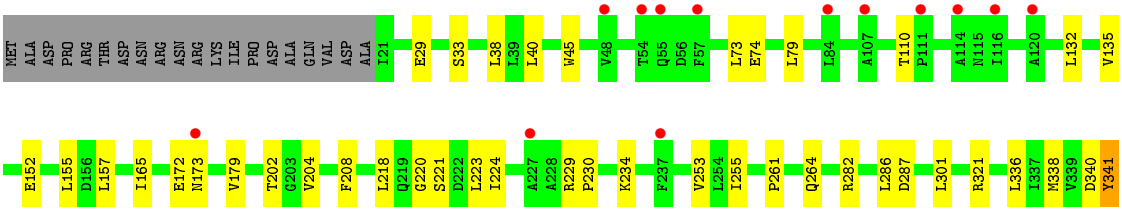
• Molecule 1: Replicative DNA helicase

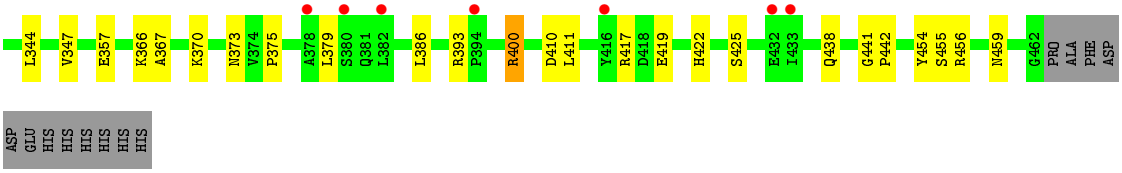




• Molecule 1: Replicative DNA helicase






L344
V347
E357
K366
A367
K370
N373
V374
P375
A378
L379
S380
Q381
L382
L386
R393
P394
R400
D410
L411
Y416
R417
D418
E419
H422
S425
E432
I433
Q438
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 0.270 , 0.293	Depositor DCC
R_{free} test set	1373 reflections (5.07%)	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)	0.21 , 82.9	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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ALF, GDP, 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	A	0.38	0/3482	0.57	0/4708
1	B	0.38	0/3486	0.57	0/4713
1	C	0.38	0/3482	0.56	0/4708
1	D	0.38	0/3486	0.57	0/4713
1	E	0.39	0/3482	0.58	0/4708
1	F	0.38	0/3494	0.57	0/4724
All	All	0.38	0/20912	0.57	0/28274

There are no bond length outliers.

There are no bond angle outliers.

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	A	3433	0	3440	35	0
1	B	3437	0	3443	36	0
1	C	3433	0	3440	34	0
1	D	3437	0	3443	30	0
1	E	3433	0	3440	33	0
1	F	3445	0	3454	29	0
2	A	28	0	12	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	172	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.

All (172) 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
1:D:33:SER:HA	1:D:110:THR:HG21	1.71	0.72
1:B:33:SER:HA	1:B:110:THR:HG21	1.71	0.71
1:D:261:PRO:HG3	1:E:439:ARG:O	1.91	0.69
1:A:347:VAL:HG12	1:A:357:GLU:HG3	1.78	0.66
1:B:326:ARG:HG2	1:C:46:ASP:HB3	1.76	0.66
1:C:347:VAL:HG12	1:C:357:GLU:HG3	1.78	0.65
1:E:384:ARG:HB3	1:F:400:ARG:HG2	1.78	0.65
1:E:347:VAL:HG12	1:E:357:GLU:HG3	1.78	0.65
1:B:347:VAL:HG12	1:B:357:GLU:HG3	1.78	0.64
1:C:384:ARG:HB3	1:D:400:ARG:HG2	1.79	0.64
1:A:439:ARG:HG2	1:F:261:PRO:HD3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:347:VAL:HG12	1:D:357:GLU:HG3	1.78	0.64
1:F:347:VAL:HG12	1:F:357:GLU:HG3	1.78	0.63
1:D:329:ARG:HH12	1:E:76:GLY:HA2	1.63	0.63
1:E:229:ARG:HH22	1:F:400:ARG:HD3	1.67	0.59
1:E:159:GLU:HB3	1:E:318:THR:HG23	1.86	0.56
1:A:229:ARG:HG3	1:A:230:PRO:HD2	1.89	0.55
1:A:283:THR:HA	1:B:202:THR:HG21	1.89	0.55
1:F:229:ARG:HG3	1:F:230:PRO:HD2	1.89	0.55
1:B:309:ILE:HD12	1:C:182:ILE:HD13	1.90	0.54
1:D:229:ARG:HG3	1:D:230:PRO:HD2	1.90	0.54
1:C:229:ARG:HG3	1:C:230:PRO:HD2	1.89	0.54
1:E:341:TYR:HB3	1:E:344:LEU:HB2	1.90	0.53
1:C:341:TYR:HB3	1:C:344:LEU:HB2	1.91	0.53
1:E:229:ARG:HG3	1:E:230:PRO:HD2	1.89	0.53
1:F:132:LEU:HD12	1:F:165:ILE:HD13	1.89	0.53
1:D:341:TYR:HB3	1:D:344:LEU:HB2	1.91	0.53
1:A:156:ASP:HA	1:A:318:THR:HG21	1.91	0.53
1:A:341:TYR:HB3	1:A:344:LEU:HB2	1.90	0.52
1:B:341:TYR:HB3	1:B:344:LEU:HB2	1.90	0.52
1:B:229:ARG:HG3	1:B:230:PRO:HD2	1.91	0.52
1:D:29:GLU:HB2	1:E:82:ILE:HD13	1.90	0.52
1:A:159:GLU:HB3	1:A:318:THR:HG23	1.91	0.52
1:D:264:GLN:HE22	1:D:282:ARG:HH22	1.57	0.52
1:E:159:GLU:HB3	1:E:318:THR:CG2	2.40	0.52
1:A:438:GLN:HG2	1:A:441:GLY:H	1.75	0.52
1:D:132:LEU:HD12	1:D:165:ILE:HD13	1.92	0.52
1:E:132:LEU:HD12	1:E:165:ILE:HD13	1.92	0.52
1:F:438:GLN:HG2	1:F:441:GLY:H	1.76	0.52
1:A:384:ARG:HB3	1:B:400:ARG:HG2	1.92	0.51
1:F:341:TYR:HB3	1:F:344:LEU:HB2	1.90	0.51
1:C:169:ARG:HD3	1:D:155:LEU:HD22	1.92	0.51
1:B:438:GLN:HG2	1:B:441:GLY:H	1.75	0.51
1:C:438:GLN:HG2	1:C:441:GLY:H	1.76	0.51
1:B:264:GLN:HE22	1:B:282:ARG:HH22	1.58	0.51
1:B:132:LEU:HD12	1:B:165:ILE:HD13	1.92	0.50
1:E:156:ASP:HA	1:E:318:THR:HG21	1.93	0.50
1:D:438:GLN:HG2	1:D:441:GLY:H	1.75	0.50
1:C:132:LEU:HD12	1:C:165:ILE:HD13	1.93	0.50
1:E:438:GLN:HG2	1:E:441:GLY:H	1.75	0.50
1:A:132:LEU:HD12	1:A:165:ILE:HD13	1.93	0.50
1:F:264:GLN:HE22	1:F:282:ARG:HH22	1.59	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:38:LEU:HD21	1:F:45:TRP:HD1	1.78	0.49
1:E:264:GLN:HE22	1:E:282:ARG:HH22	1.59	0.49
1:F:224:ILE:HG12	1:F:411:LEU:HD23	1.94	0.49
1:A:284:GLY:HA3	1:B:193:LEU:HB3	1.95	0.49
1:A:321:ARG:HH22	1:A:367:ALA:HB3	1.78	0.49
1:D:313:SER:HB2	1:E:407:GLN:HA	1.96	0.48
1:E:38:LEU:HD21	1:E:45:TRP:HD1	1.78	0.48
1:A:159:GLU:HB3	1:A:318:THR:CG2	2.43	0.48
1:C:264:GLN:HE22	1:C:282:ARG:HH22	1.61	0.48
1:A:224:ILE:HG12	1:A:411:LEU:HD23	1.95	0.48
1:B:224:ILE:HG12	1:B:411:LEU:HD23	1.95	0.48
1:E:224:ILE:HG12	1:E:411:LEU:HD23	1.95	0.47
1:F:321:ARG:HH22	1:F:367:ALA:HB3	1.79	0.47
1:D:38:LEU:HD21	1:D:45:TRP:HD1	1.80	0.47
1:A:38:LEU:HD21	1:A:45:TRP:HD1	1.80	0.47
1:C:224:ILE:HG12	1:C:411:LEU:HD23	1.95	0.47
1:C:321:ARG:HH22	1:C:367:ALA:HB3	1.79	0.47
1:C:38:LEU:HD21	1:C:45:TRP:HD1	1.80	0.47
1:D:255:ILE:HG13	1:D:338:MET:HB3	1.97	0.47
1:B:255:ILE:HG13	1:B:338:MET:HB3	1.98	0.46
1:B:38:LEU:HD21	1:B:45:TRP:HD1	1.80	0.46
1:D:224:ILE:HG12	1:D:411:LEU:HD23	1.96	0.46
1:E:255:ILE:HG13	1:E:338:MET:HB3	1.97	0.46
1:A:147:GLN:HA	1:C:91:ARG:HA	1.97	0.46
1:A:264:GLN:HE22	1:A:282:ARG:HH22	1.62	0.46
1:E:279:THR:CG2	1:F:442:PRO:HD3	2.46	0.46
1:B:321:ARG:HH22	1:B:367:ALA:HB3	1.79	0.46
1:C:255:ILE:HG13	1:C:338:MET:HB3	1.97	0.46
1:B:223:LEU:HD22	1:B:366:LYS:HB2	1.98	0.46
1:A:285:GLN:HB3	1:B:198:GLN:OE1	2.16	0.45
1:B:384:ARG:HB3	1:C:400:ARG:HG2	1.97	0.45
1:B:204:VAL:HB	1:B:218:LEU:HB2	1.98	0.45
1:D:321:ARG:HH22	1:D:367:ALA:HB3	1.79	0.45
1:A:340:ASP:HA	1:A:379:LEU:HD12	1.99	0.45
1:E:221:SER:HB3	1:E:373:ASN:HA	1.98	0.45
1:E:223:LEU:HD22	1:E:366:LYS:HB2	1.99	0.45
1:E:253:VAL:HG12	1:E:336:LEU:HB3	1.98	0.45
1:A:223:LEU:HD22	1:A:366:LYS:HB2	1.99	0.45
1:E:321:ARG:HH22	1:E:367:ALA:HB3	1.80	0.45
1:A:253:VAL:HG12	1:A:336:LEU:HB3	1.99	0.45
1:A:255:ILE:HG13	1:A:338:MET:HB3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:253:VAL:HG12	1:C:336:LEU:HB3	1.99	0.45
1:C:340:ASP:HA	1:C:379:LEU:HD12	1.99	0.45
1:D:221:SER:HB3	1:D:373:ASN:HA	1.98	0.45
1:F:340:ASP:HA	1:F:379:LEU:HD12	1.99	0.45
1:A:204:VAL:HB	1:A:218:LEU:HB2	1.99	0.45
1:A:422:HIS:HB2	1:A:425:SER:HB3	1.99	0.45
1:B:340:ASP:HA	1:B:379:LEU:HD12	1.98	0.45
1:F:253:VAL:HG12	1:F:336:LEU:HB3	1.99	0.45
1:B:253:VAL:HG12	1:B:336:LEU:HB3	1.98	0.45
1:B:327:ILE:HD11	1:C:176:PRO:CG	2.47	0.45
1:E:340:ASP:HA	1:E:379:LEU:HD12	1.99	0.45
1:F:204:VAL:HB	1:F:218:LEU:HB2	1.98	0.45
1:F:221:SER:HB3	1:F:373:ASN:HA	1.98	0.45
1:A:221:SER:HB3	1:A:373:ASN:HA	1.98	0.44
1:C:223:LEU:HD22	1:C:366:LYS:HB2	1.99	0.44
1:D:204:VAL:HB	1:D:218:LEU:HB2	1.98	0.44
1:D:253:VAL:HG12	1:D:336:LEU:HB3	1.98	0.44
1:F:223:LEU:HD22	1:F:366:LYS:HB2	1.98	0.44
1:C:204:VAL:HB	1:C:218:LEU:HB2	1.98	0.44
1:F:422:HIS:HB2	1:F:425:SER:HB3	1.99	0.44
1:D:422:HIS:HB2	1:D:425:SER:HB3	1.99	0.44
1:D:223:LEU:HD22	1:D:366:LYS:HB2	1.99	0.44
1:F:255:ILE:HG13	1:F:338:MET:HB3	1.97	0.44
1:B:221:SER:HB3	1:B:373:ASN:HA	1.98	0.44
1:B:422:HIS:HB2	1:B:425:SER:HB3	1.99	0.44
1:C:221:SER:HB3	1:C:373:ASN:HA	1.98	0.44
1:D:417:ARG:HG2	1:D:419:GLU:HG2	2.00	0.44
1:F:417:ARG:HG2	1:F:419:GLU:HG2	2.00	0.44
1:D:340:ASP:HA	1:D:379:LEU:HD12	1.99	0.44
1:E:417:ARG:HG2	1:E:419:GLU:HG2	2.00	0.44
1:B:29:GLU:HB2	1:C:82:ILE:HD13	1.98	0.44
1:E:422:HIS:HB2	1:E:425:SER:HB3	1.99	0.43
1:B:326:ARG:CG	1:C:46:ASP:HB3	2.45	0.43
1:C:234:LYS:HB3	1:C:379:LEU:HD22	2.01	0.43
1:C:417:ARG:HG2	1:C:419:GLU:HG2	2.01	0.43
1:C:309:ILE:HD12	1:D:182:ILE:HD13	1.99	0.43
1:E:204:VAL:HB	1:E:218:LEU:HB2	1.99	0.43
1:A:220:GLY:HA2	1:A:375:PRO:HD3	2.00	0.43
1:D:220:GLY:HA2	1:D:375:PRO:HD3	2.01	0.43
1:A:234:LYS:HB3	1:A:379:LEU:HD22	2.01	0.43
2:A:501:GDP:N2	1:B:442:PRO:HB3	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:220:GLY:HA2	1:F:375:PRO:HD3	2.01	0.43
1:E:208:PHE:HA	1:E:459:ASN:HD21	1.84	0.43
1:A:221:SER:HB2	1:A:370:LYS:HA	2.01	0.42
1:B:417:ARG:HG2	1:B:419:GLU:HG2	2.00	0.42
1:C:220:GLY:HA2	1:C:375:PRO:HD3	2.01	0.42
1:C:221:SER:HB2	1:C:370:LYS:HA	2.00	0.42
1:A:417:ARG:HG2	1:A:419:GLU:HG2	2.01	0.42
1:B:234:LYS:HB3	1:B:379:LEU:HD22	2.01	0.42
1:E:234:LYS:HB3	1:E:379:LEU:HD22	2.01	0.42
1:F:208:PHE:HA	1:F:459:ASN:HD21	1.84	0.42
1:A:309:ILE:HD12	1:B:182:ILE:HD13	2.00	0.42
1:C:422:HIS:HB2	1:C:425:SER:HB3	2.00	0.42
2:E:501:GDP:C2	1:F:442:PRO:HB3	2.55	0.42
1:F:234:LYS:HB3	1:F:379:LEU:HD22	2.01	0.42
1:D:208:PHE:HA	1:D:459:ASN:HD21	1.85	0.42
1:E:220:GLY:HA2	1:E:375:PRO:HD3	2.01	0.42
1:E:135:VAL:HG21	1:E:165:ILE:HD11	2.02	0.41
1:F:135:VAL:HG21	1:F:165:ILE:HD11	2.02	0.41
1:B:220:GLY:HA2	1:B:375:PRO:HD3	2.01	0.41
1:D:221:SER:HB2	1:D:370:LYS:HA	2.01	0.41
1:F:221:SER:HB2	1:F:370:LYS:HA	2.01	0.41
1:B:221:SER:HB2	1:B:370:LYS:HA	2.01	0.41
1:C:208:PHE:HA	1:C:459:ASN:HD21	1.85	0.41
1:A:208:PHE:HA	1:A:459:ASN:HD21	1.85	0.41
1:E:221:SER:HB2	1:E:370:LYS:HA	2.01	0.41
1:B:208:PHE:HA	1:B:459:ASN:HD21	1.85	0.41
1:D:234:LYS:HB3	1:D:379:LEU:HD22	2.02	0.41
2:A:501:GDP:H2'	1:B:438:GLN:O	2.21	0.41
1:D:42:ASN:HB3	1:D:73:LEU:HD21	2.03	0.41
1:A:169:ARG:HD3	1:B:155:LEU:HD22	2.03	0.40
1:A:42:ASN:HB3	1:A:73:LEU:HD21	2.03	0.40
1:C:42:ASN:HB3	1:C:73:LEU:HD21	2.03	0.40
1:C:135:VAL:HG21	1:C:165:ILE:HD11	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	47 79
1	B	439/474 (93%)	415 (94%)	21 (5%)	3 (1%)	22 60
1	C	438/474 (92%)	417 (95%)	21 (5%)	0	100 100
1	D	439/474 (93%)	417 (95%)	21 (5%)	1 (0%)	47 79
1	E	438/474 (92%)	414 (94%)	20 (5%)	4 (1%)	17 54
1	F	440/474 (93%)	417 (95%)	21 (5%)	2 (0%)	29 67
All	All	2632/2844 (92%)	2494 (95%)	127 (5%)	11 (0%)	34 71

All (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
1	A	175	GLY
1	D	173	ASN
1	E	175	GLY
1	F	173	ASN
1	B	175	GLY
1	E	198	GLN

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	374/403 (93%)	352 (94%)	22 (6%)	19	49
1	B	374/403 (93%)	350 (94%)	24 (6%)	17	47
1	C	374/403 (93%)	352 (94%)	22 (6%)	19	49
1	D	374/403 (93%)	353 (94%)	21 (6%)	21	51
1	E	374/403 (93%)	353 (94%)	21 (6%)	21	51
1	F	375/403 (93%)	355 (95%)	20 (5%)	22	52
All	All	2245/2418 (93%)	2115 (94%)	130 (6%)	20	50

All (130) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	LEU
1	A	73	LEU
1	A	74	GLU
1	A	79	LEU
1	A	152	GLU
1	A	155	LEU
1	A	157	LEU
1	A	179	VAL
1	A	202	THR
1	A	264	GLN
1	A	286	LEU
1	A	287	ASP
1	A	301	LEU
1	A	310	ASP
1	A	341	TYR
1	A	386	LEU
1	A	393	ARG
1	A	400	ARG
1	A	410	ASP
1	A	454	TYR
1	A	455	SER
1	A	456	ARG
1	B	40	LEU
1	B	73	LEU
1	B	74	GLU
1	B	79	LEU
1	B	152	GLU
1	B	155	LEU
1	B	157	LEU
1	B	167	GLU

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Mol	Chain	Res	Type
1	B	179	VAL
1	B	191	GLU
1	B	202	THR
1	B	286	LEU
1	B	287	ASP
1	B	301	LEU
1	B	329	ARG
1	B	336	LEU
1	B	341	TYR
1	B	386	LEU
1	B	393	ARG
1	B	400	ARG
1	B	410	ASP
1	B	454	TYR
1	B	455	SER
1	B	456	ARG
1	C	40	LEU
1	C	73	LEU
1	C	74	GLU
1	C	79	LEU
1	C	152	GLU
1	C	155	LEU
1	C	157	LEU
1	C	179	VAL
1	C	202	THR
1	C	264	GLN
1	C	286	LEU
1	C	287	ASP
1	C	301	LEU
1	C	310	ASP
1	C	341	TYR
1	C	386	LEU
1	C	393	ARG
1	C	400	ARG
1	C	410	ASP
1	C	454	TYR
1	C	455	SER
1	C	456	ARG
1	D	40	LEU
1	D	73	LEU
1	D	74	GLU
1	D	79	LEU

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Mol	Chain	Res	Type
1	D	152	GLU
1	D	155	LEU
1	D	157	LEU
1	D	179	VAL
1	D	191	GLU
1	D	202	THR
1	D	286	LEU
1	D	287	ASP
1	D	301	LEU
1	D	341	TYR
1	D	386	LEU
1	D	393	ARG
1	D	400	ARG
1	D	410	ASP
1	D	454	TYR
1	D	455	SER
1	D	456	ARG
1	E	40	LEU
1	E	73	LEU
1	E	74	GLU
1	E	79	LEU
1	E	152	GLU
1	E	155	LEU
1	E	157	LEU
1	E	179	VAL
1	E	264	GLN
1	E	286	LEU
1	E	287	ASP
1	E	301	LEU
1	E	310	ASP
1	E	341	TYR
1	E	386	LEU
1	E	393	ARG
1	E	400	ARG
1	E	410	ASP
1	E	454	TYR
1	E	455	SER
1	E	456	ARG
1	F	40	LEU
1	F	73	LEU
1	F	74	GLU
1	F	79	LEU

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Mol	Chain	Res	Type
1	F	152	GLU
1	F	155	LEU
1	F	157	LEU
1	F	179	VAL
1	F	202	THR
1	F	286	LEU
1	F	287	ASP
1	F	301	LEU
1	F	341	TYR
1	F	386	LEU
1	F	393	ARG
1	F	400	ARG
1	F	410	ASP
1	F	454	TYR
1	F	455	SER
1	F	456	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	115	ASN
1	A	205	ASN
1	A	240	ASN
1	A	264	GLN
1	A	278	GLN
1	A	285	GLN
1	B	115	ASN
1	B	205	ASN
1	B	240	ASN
1	B	264	GLN
1	B	278	GLN
1	B	285	GLN
1	B	440	ASN
1	C	115	ASN
1	C	205	ASN
1	C	240	ASN
1	C	264	GLN
1	C	278	GLN
1	C	285	GLN
1	C	440	ASN
1	D	115	ASN
1	D	205	ASN

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Mol	Chain	Res	Type
1	D	240	ASN
1	D	264	GLN
1	D	278	GLN
1	D	285	GLN
1	D	440	ASN
1	E	115	ASN
1	E	205	ASN
1	E	240	ASN
1	E	264	GLN
1	E	278	GLN
1	E	285	GLN
1	E	381	GLN
1	F	115	ASN
1	F	205	ASN
1	F	240	ASN
1	F	264	GLN
1	F	278	GLN
1	F	285	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

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	B	501	3	24,30,30	1.08	2 (8%)	31,47,47	2.07	5 (16%)
4	ALF	D	503	-	0,4,4	0.00	-	-		
2	GDP	E	501	3	24,30,30	1.09	2 (8%)	31,47,47	2.10	5 (16%)
4	ALF	B	503	-	0,4,4	0.00	-	-		
4	ALF	F	503	-	0,4,4	0.00	-	-		
2	GDP	D	501	3	24,30,30	1.03	2 (8%)	31,47,47	2.09	5 (16%)
2	GDP	C	501	3	24,30,30	1.05	2 (8%)	31,47,47	2.07	5 (16%)
2	GDP	F	501	3	24,30,30	1.10	2 (8%)	31,47,47	2.10	5 (16%)
4	ALF	E	503	-	0,4,4	0.00	-	-		
2	GDP	A	501	3	24,30,30	1.11	2 (8%)	31,47,47	2.09	5 (16%)
4	ALF	C	503	-	0,4,4	0.00	-	-		
4	ALF	A	503	-	0,4,4	0.00	-	-		

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	B	501	3	-	4/12/32/32	0/3/3/3
2	GDP	E	501	3	-	6/12/32/32	0/3/3/3
2	GDP	D	501	3	-	6/12/32/32	0/3/3/3
2	GDP	C	501	3	-	6/12/32/32	0/3/3/3
2	GDP	F	501	3	-	4/12/32/32	0/3/3/3
2	GDP	A	501	3	-	4/12/32/32	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	GDP	C6-N1	3.44	1.39	1.33
2	C	501	GDP	C6-N1	3.40	1.39	1.33
2	F	501	GDP	C6-N1	3.39	1.38	1.33
2	E	501	GDP	C6-N1	3.38	1.38	1.33
2	B	501	GDP	C6-N1	3.33	1.38	1.33
2	D	501	GDP	C6-N1	3.32	1.38	1.33
2	E	501	GDP	C6-C5	2.72	1.46	1.41
2	F	501	GDP	C6-C5	2.41	1.45	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	GDP	C6-C5	2.26	1.45	1.41
2	D	501	GDP	C6-C5	2.21	1.45	1.41
2	B	501	GDP	C6-C5	2.17	1.45	1.41
2	C	501	GDP	C6-C5	2.14	1.45	1.41

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	501	GDP	C5-C6-N1	-8.36	111.99	123.43
2	F	501	GDP	C5-C6-N1	-8.28	112.11	123.43
2	A	501	GDP	C5-C6-N1	-8.24	112.16	123.43
2	D	501	GDP	C5-C6-N1	-8.19	112.22	123.43
2	C	501	GDP	C5-C6-N1	-8.15	112.28	123.43
2	B	501	GDP	C5-C6-N1	-8.07	112.39	123.43
2	F	501	GDP	C6-N1-C2	5.90	125.30	115.93
2	E	501	GDP	C6-N1-C2	5.85	125.23	115.93
2	A	501	GDP	C6-N1-C2	5.85	125.22	115.93
2	D	501	GDP	C6-N1-C2	5.84	125.22	115.93
2	C	501	GDP	C6-N1-C2	5.80	125.14	115.93
2	B	501	GDP	C6-N1-C2	5.78	125.12	115.93
2	B	501	GDP	C6-C5-C4	-2.94	117.99	120.80
2	F	501	GDP	C6-C5-C4	-2.89	118.04	120.80
2	D	501	GDP	C6-C5-C4	-2.88	118.05	120.80
2	C	501	GDP	C6-C5-C4	-2.87	118.06	120.80
2	A	501	GDP	C6-C5-C4	-2.86	118.07	120.80
2	E	501	GDP	C6-C5-C4	-2.85	118.08	120.80
2	B	501	GDP	N3-C2-N1	-2.82	123.47	127.22
2	F	501	GDP	N3-C2-N1	-2.79	123.50	127.22
2	D	501	GDP	N3-C2-N1	-2.77	123.52	127.22
2	A	501	GDP	N3-C2-N1	-2.75	123.56	127.22
2	C	501	GDP	N3-C2-N1	-2.74	123.57	127.22
2	E	501	GDP	N3-C2-N1	-2.64	123.70	127.22
2	A	501	GDP	C2-N3-C4	-2.11	112.95	115.36
2	D	501	GDP	C2-N3-C4	-2.09	112.97	115.36
2	C	501	GDP	C2-N3-C4	-2.07	112.99	115.36
2	E	501	GDP	C2-N3-C4	-2.05	113.01	115.36
2	B	501	GDP	C2-N3-C4	-2.03	113.04	115.36
2	F	501	GDP	C2-N3-C4	-2.00	113.07	115.36

There are no chirality outliers.

All (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
2	C	501	GDP	C5'-O5'-PA-O2A
2	D	501	GDP	C5'-O5'-PA-O3A
2	D	501	GDP	C5'-O5'-PA-O1A
2	D	501	GDP	C5'-O5'-PA-O2A
2	E	501	GDP	C5'-O5'-PA-O3A
2	E	501	GDP	C5'-O5'-PA-O1A
2	E	501	GDP	C5'-O5'-PA-O2A
2	F	501	GDP	C5'-O5'-PA-O3A
2	A	501	GDP	O4'-C4'-C5'-O5'
2	B	501	GDP	O4'-C4'-C5'-O5'
2	C	501	GDP	O4'-C4'-C5'-O5'
2	D	501	GDP	O4'-C4'-C5'-O5'
2	E	501	GDP	O4'-C4'-C5'-O5'
2	F	501	GDP	O4'-C4'-C5'-O5'
2	A	501	GDP	C5'-O5'-PA-O1A
2	B	501	GDP	C5'-O5'-PA-O1A
2	B	501	GDP	C5'-O5'-PA-O2A
2	F	501	GDP	C5'-O5'-PA-O1A
2	F	501	GDP	C5'-O5'-PA-O2A
2	C	501	GDP	PB-O3A-PA-O2A
2	D	501	GDP	PB-O3A-PA-O2A
2	E	501	GDP	PB-O3A-PA-O2A
2	C	501	GDP	PB-O3A-PA-O1A
2	D	501	GDP	PB-O3A-PA-O1A
2	E	501	GDP	PB-O3A-PA-O1A

There are no ring outliers.

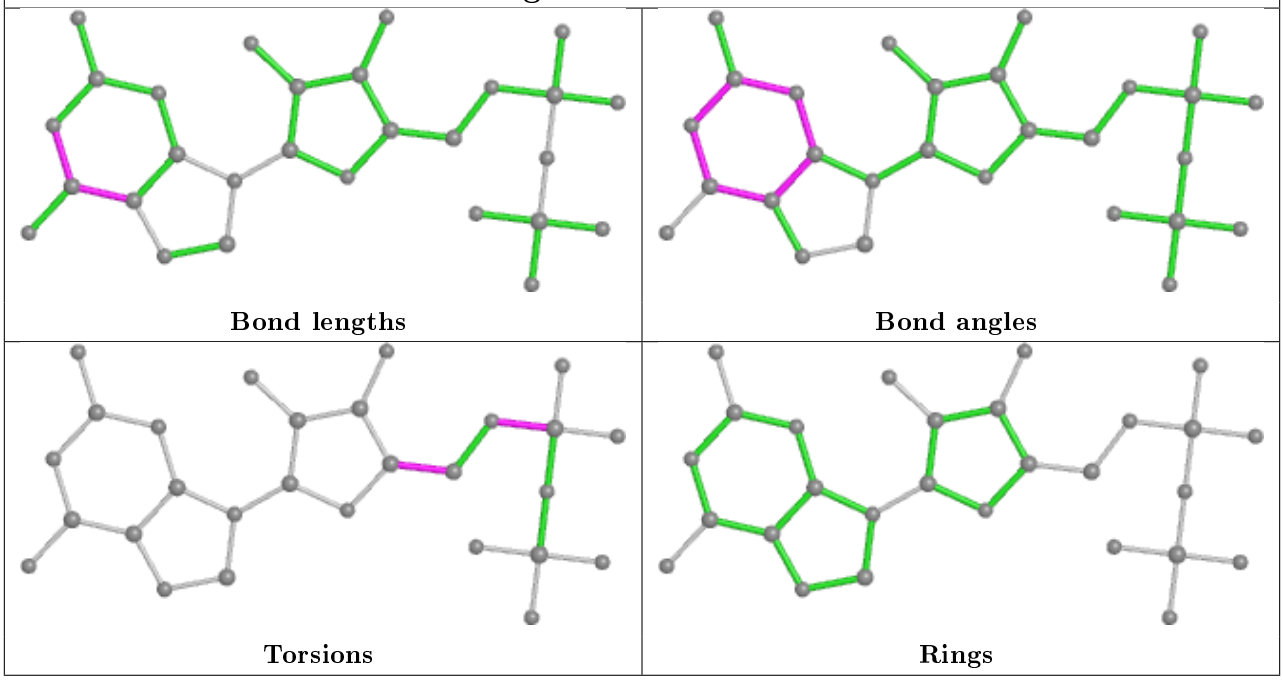
2 monomers are involved in 3 short contacts:

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

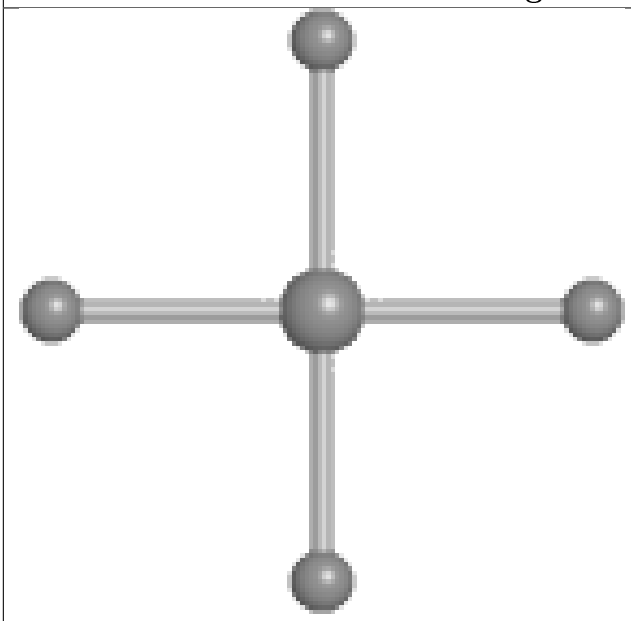
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 B 501



Ligand ALF D 503



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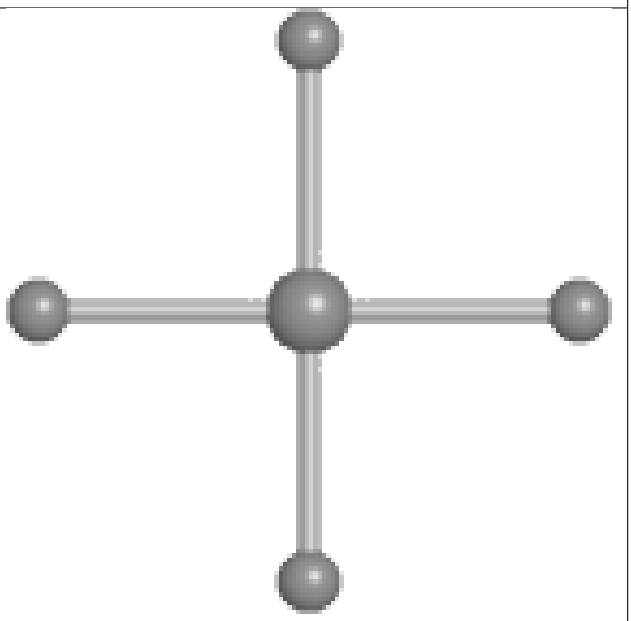
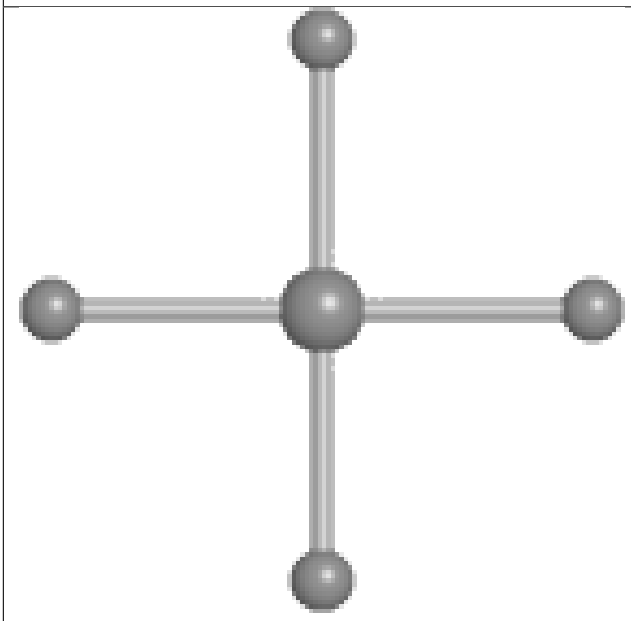
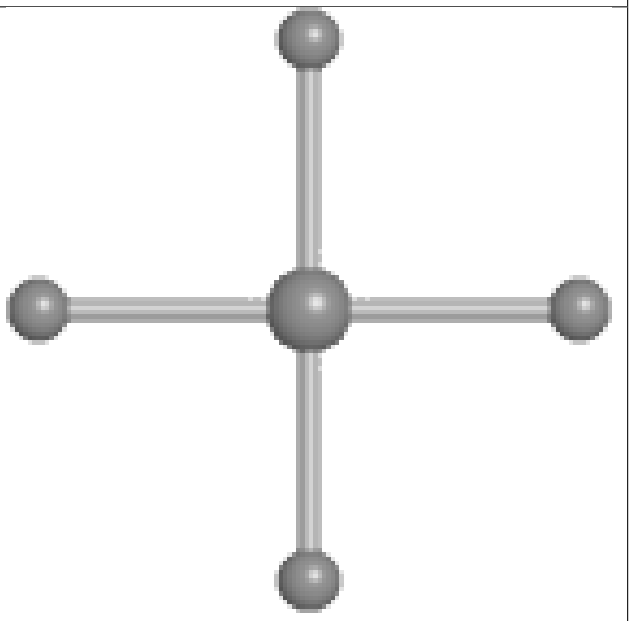


Bond angles

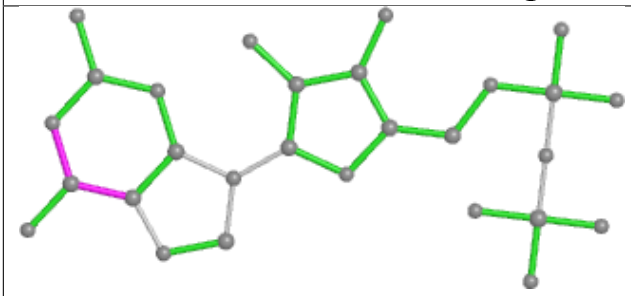


Torsions



Rings

Ligand GDP E 501



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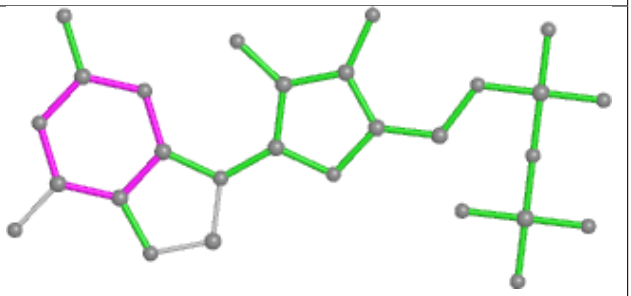

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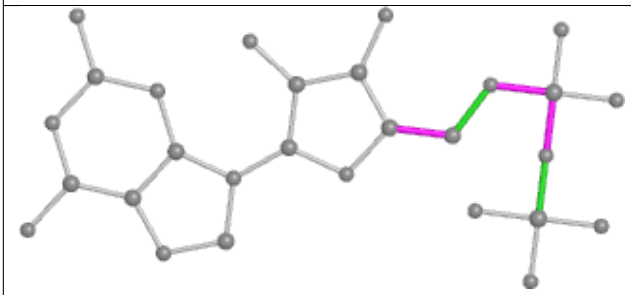

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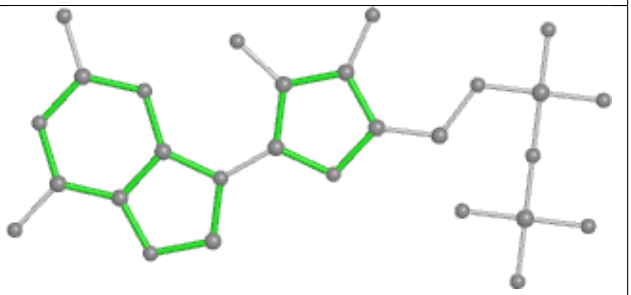
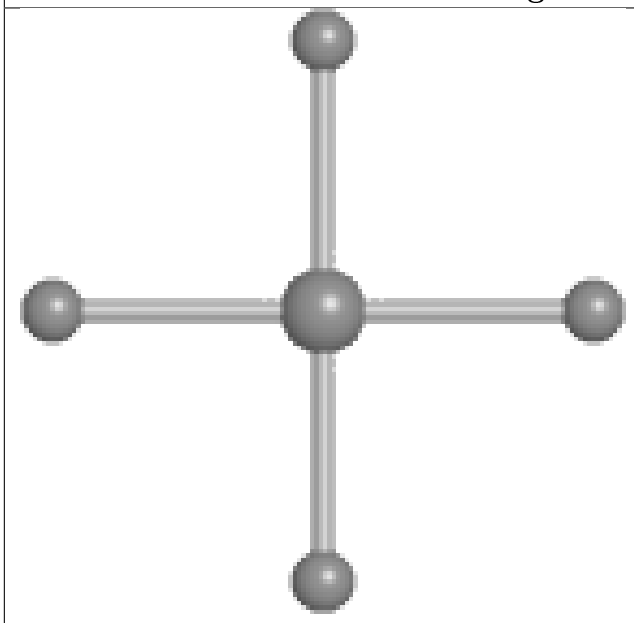


Rings

Ligand ALF B 503



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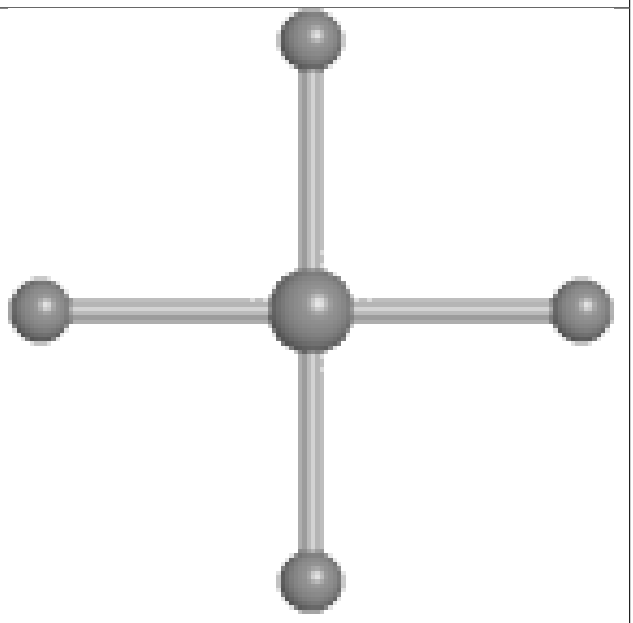

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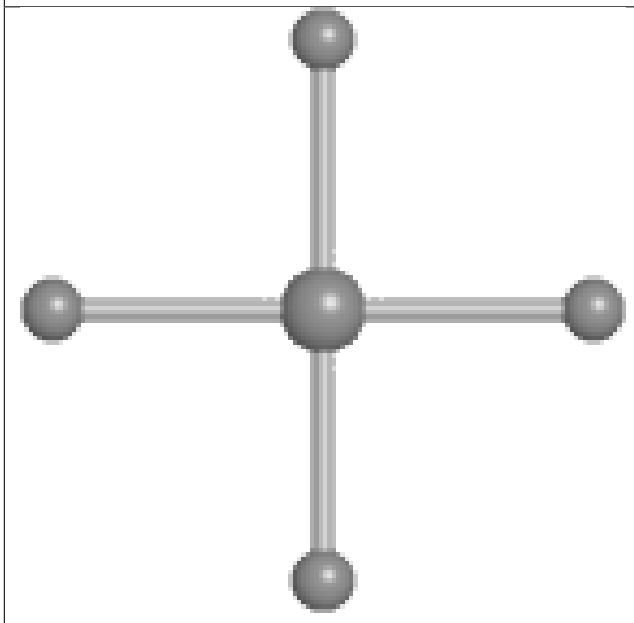

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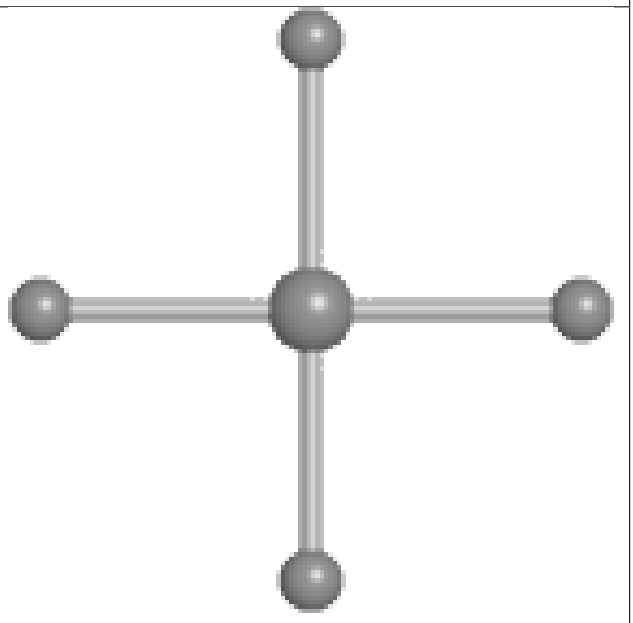
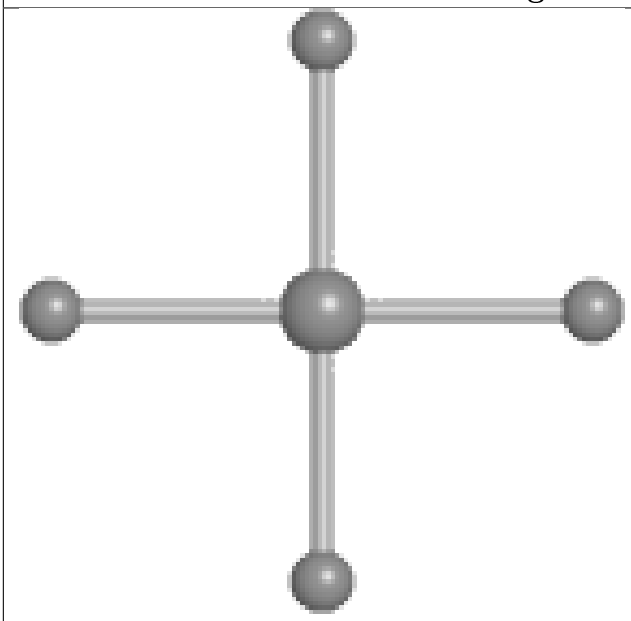


Rings

Ligand ALF F 503



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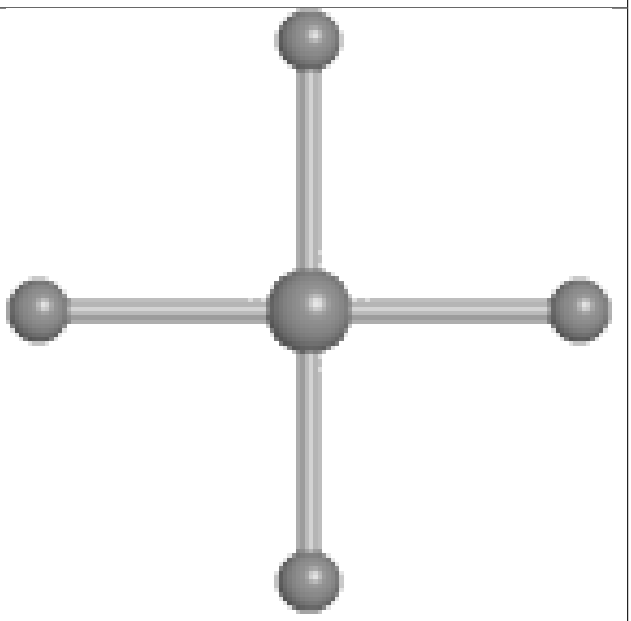

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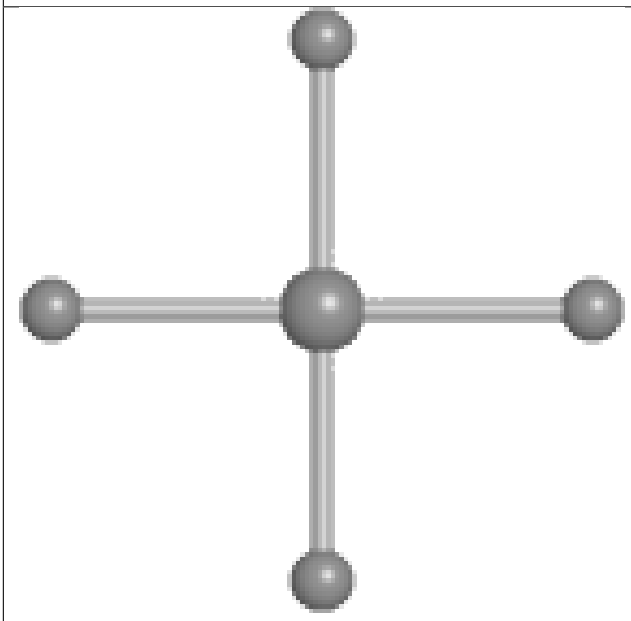

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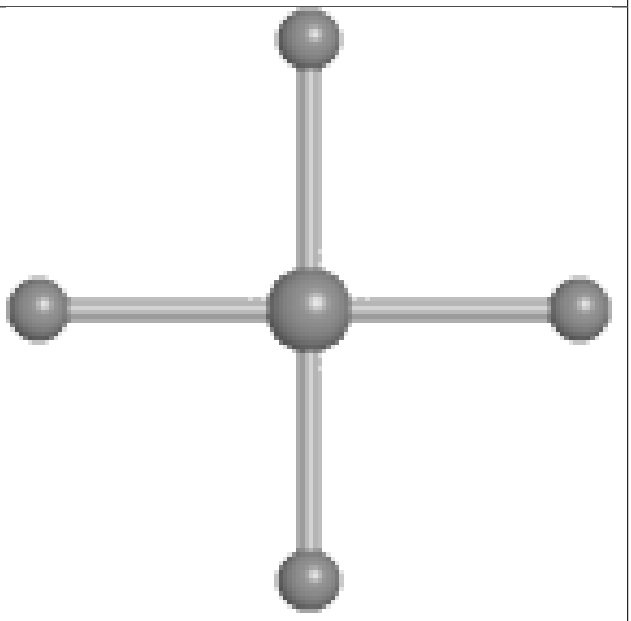
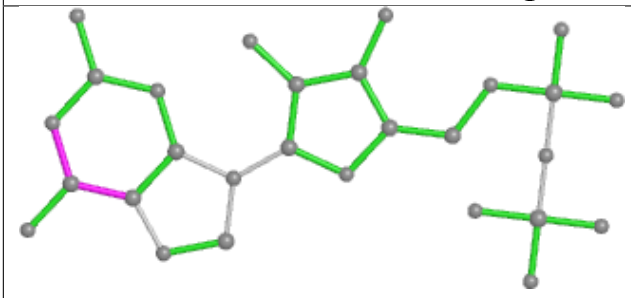
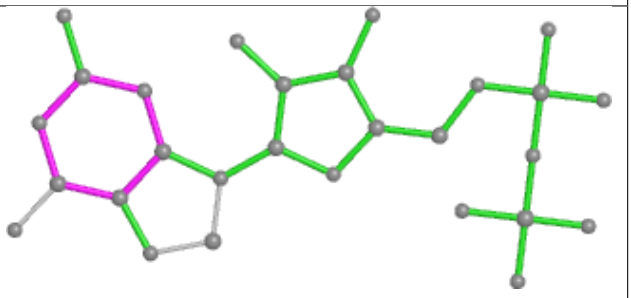
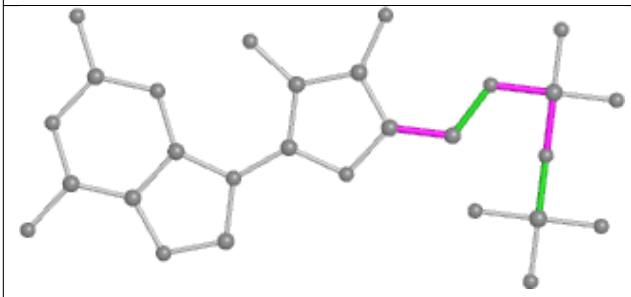
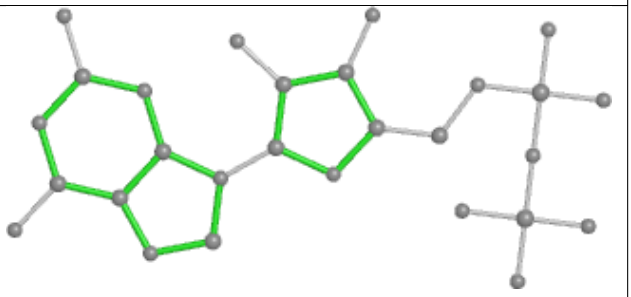


Rings

Ligand GDP D 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

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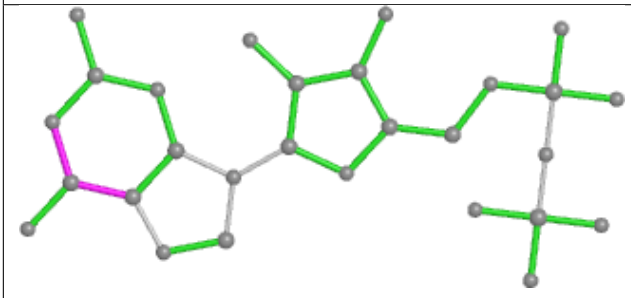
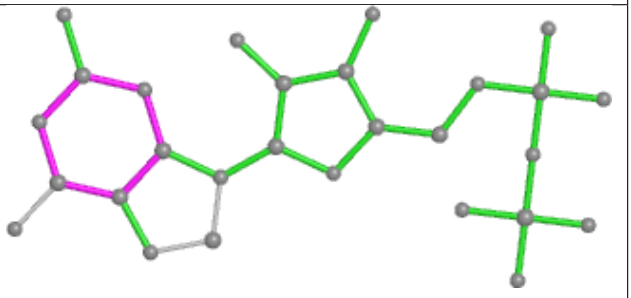
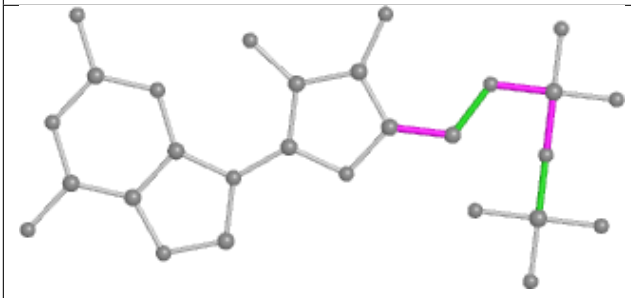
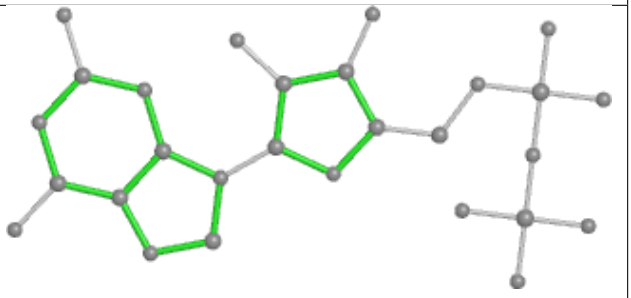
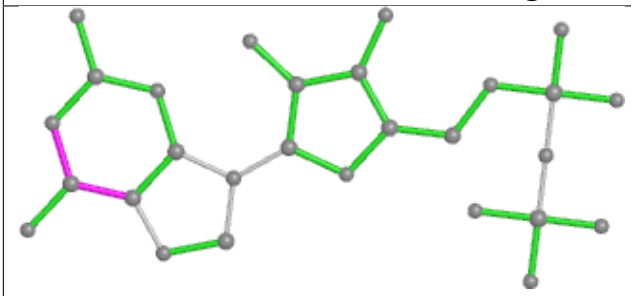
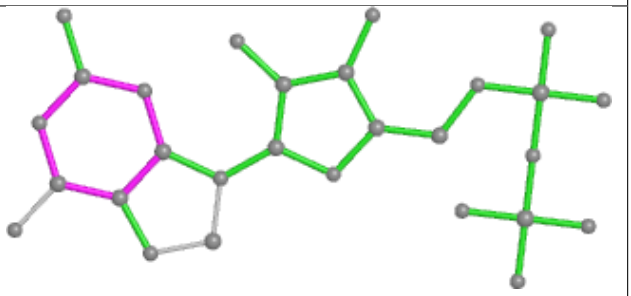
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GDP F 501



Bond lengths



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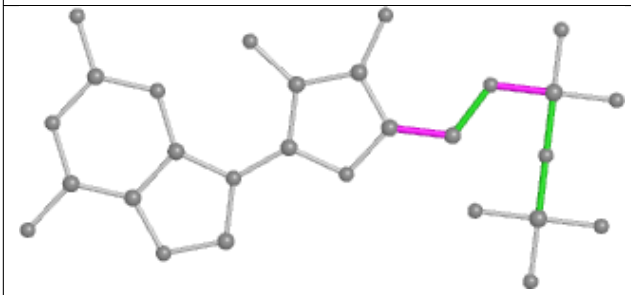

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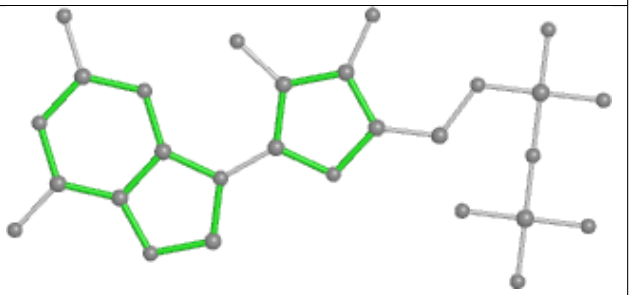
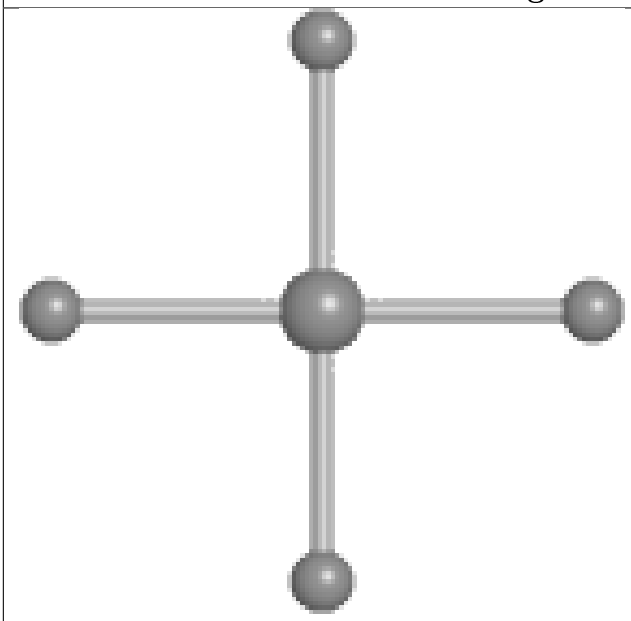


Rings

Ligand ALF E 503



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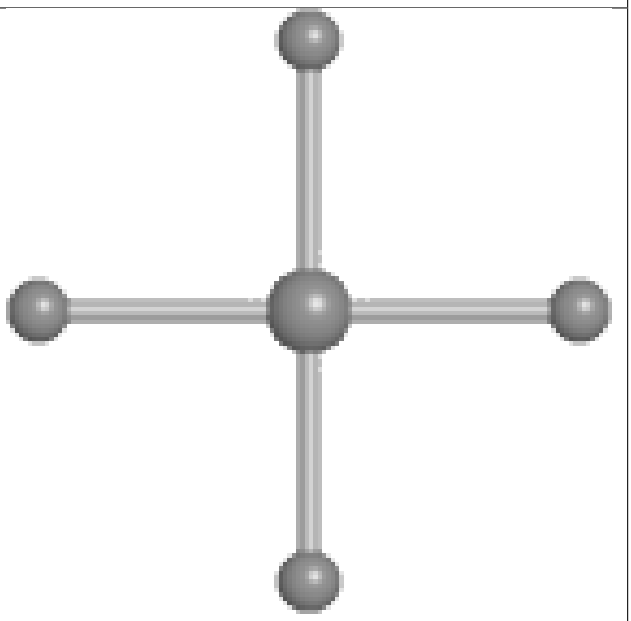

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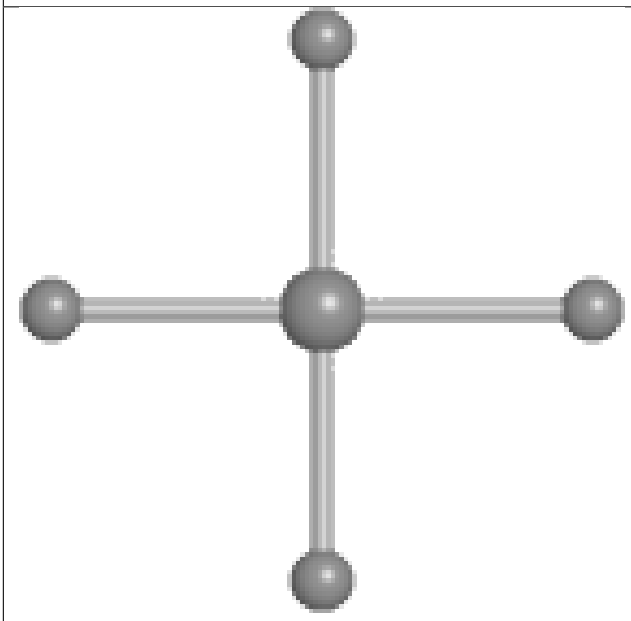

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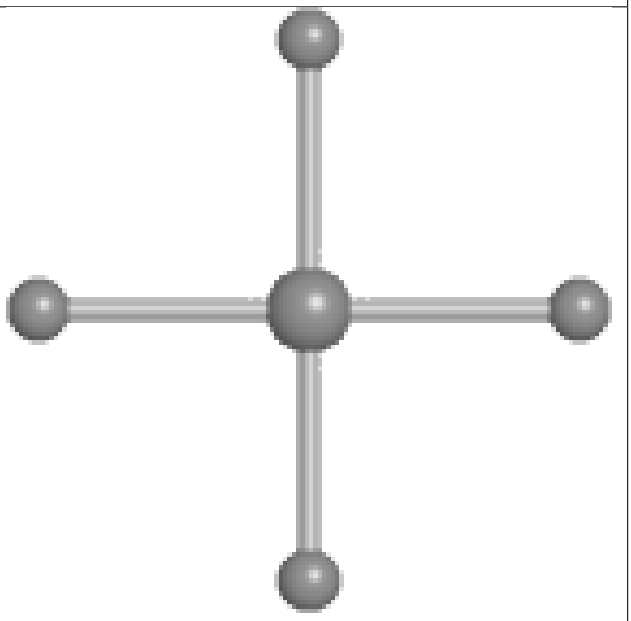
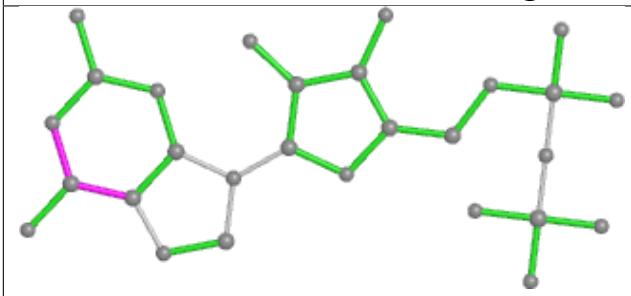


Rings

Ligand GDP A 501



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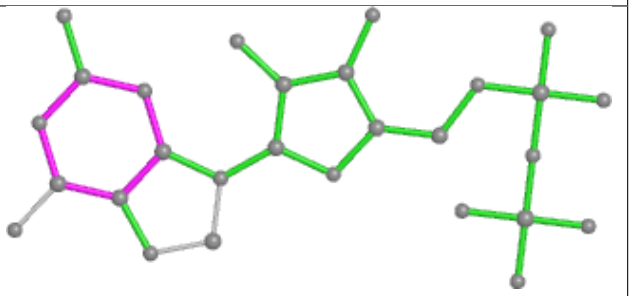

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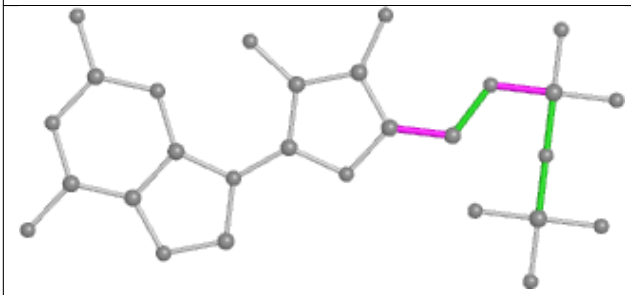

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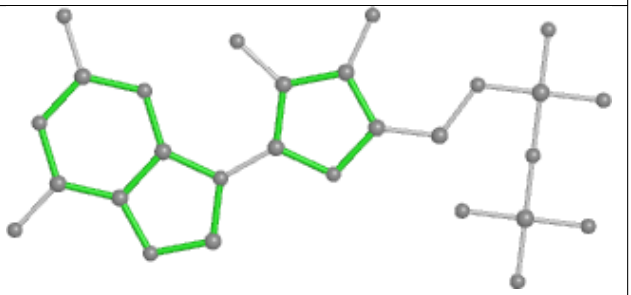
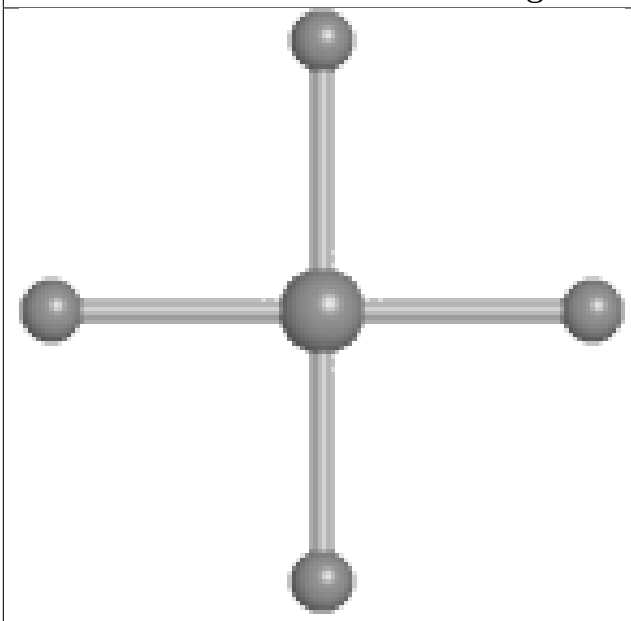


Rings

Ligand ALF C 503



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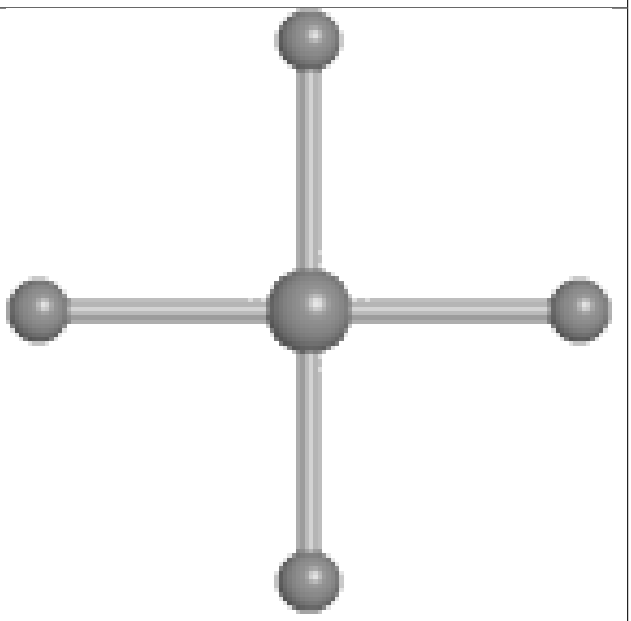

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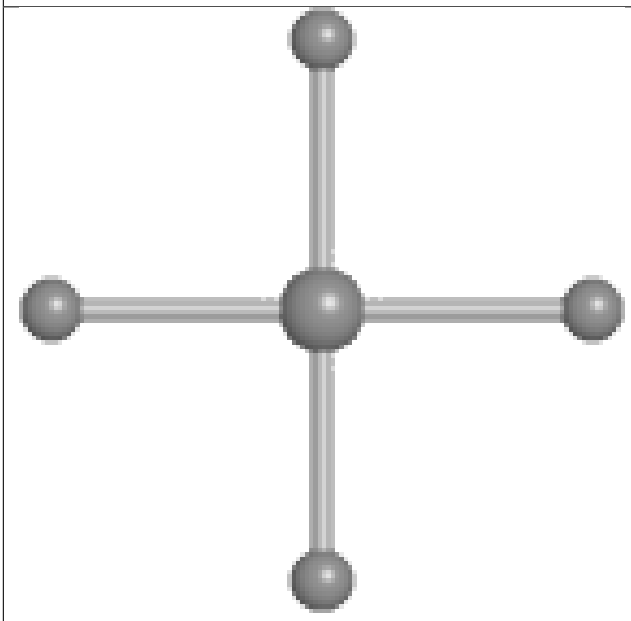

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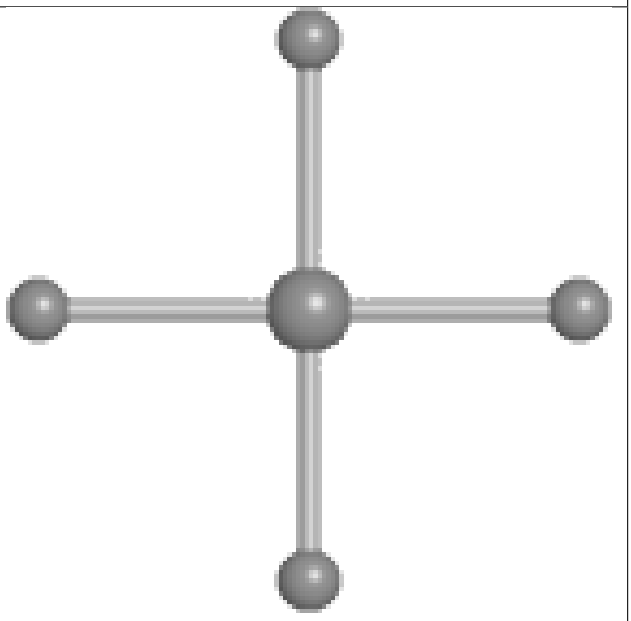
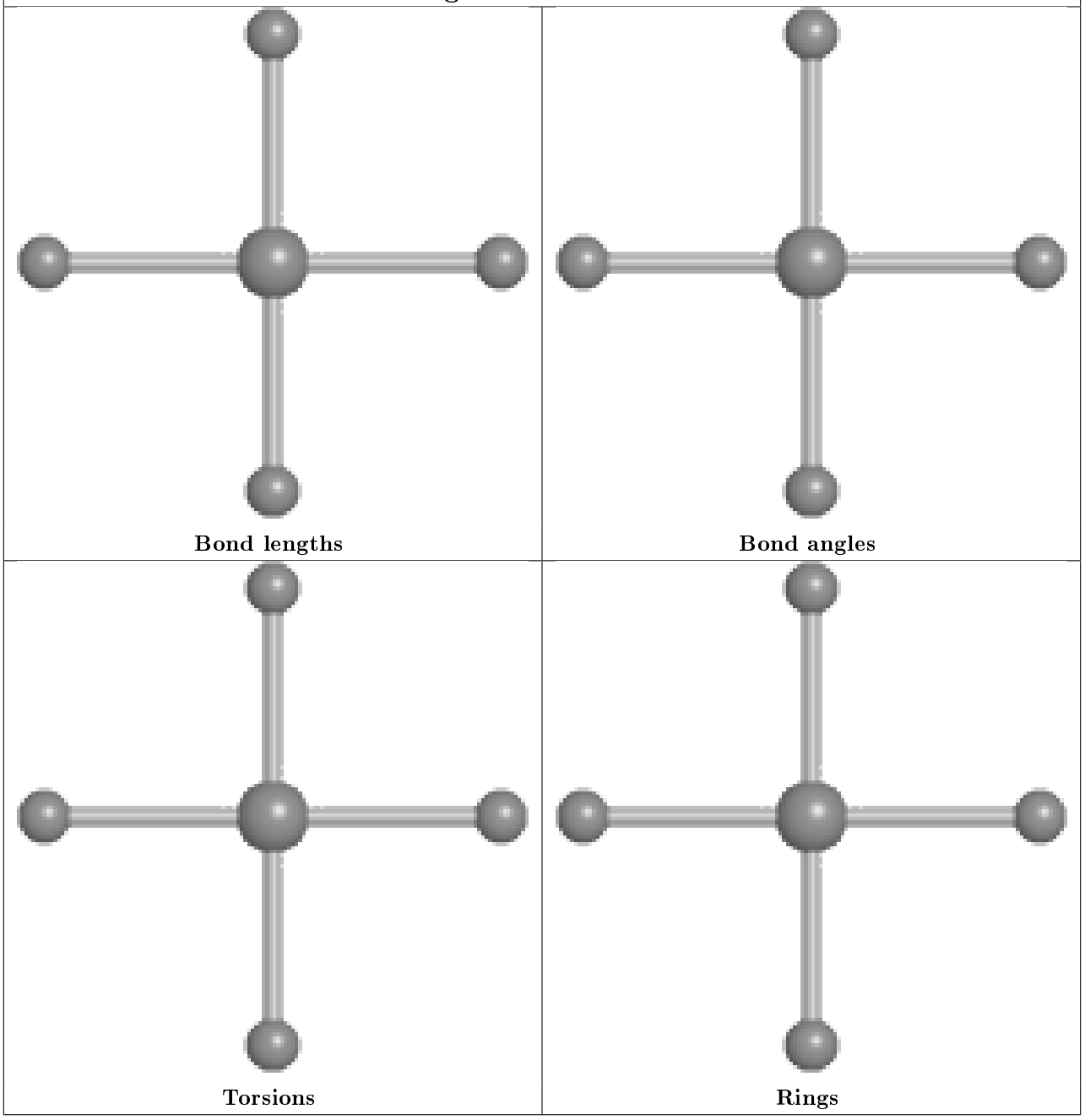


Rings

Ligand ALF A 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

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	440/474 (92%)	-0.03	10 (2%)	60	50	145, 180, 227, 250	0
1	B	441/474 (93%)	-0.21	4 (0%)	84	77	129, 170, 225, 244	0
1	C	440/474 (92%)	-0.04	9 (2%)	65	55	131, 185, 215, 229	0
1	D	441/474 (93%)	-0.01	15 (3%)	45	35	153, 204, 265, 276	0
1	E	440/474 (92%)	0.15	34 (7%)	13	10	186, 223, 251, 264	0
1	F	442/474 (93%)	0.03	20 (4%)	33	27	183, 215, 249, 269	0
All	All	2644/2844 (92%)	-0.02	92 (3%)	44	34	129, 195, 248, 276	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	416	TYR	6.9
1	E	438	GLN	6.1
1	E	414	PHE	5.0
1	E	446	VAL	4.9
1	E	402	SER	4.8
1	E	409	ALA	4.6
1	C	174	GLU	4.5
1	E	415	ILE	4.4
1	E	399	LEU	3.9
1	E	433	ILE	3.9
1	F	378	ALA	3.8
1	D	335	SER	3.7
1	B	168	ALA	3.6
1	B	173	ASN	3.6
1	E	413	MET	3.5
1	E	445	SER	3.5
1	E	447	ARG	3.4
1	D	34	VAL	3.3
1	E	376	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	333	GLY	3.3
1	D	253	VAL	3.2
1	E	375	PRO	3.2
1	E	410	ASP	3.2
1	A	440	ASN	3.1
1	B	413	MET	3.1
1	A	35	ILE	3.1
1	E	227	ALA	3.0
1	D	334	LEU	3.0
1	E	434	ILE	2.9
1	E	444	GLY	2.8
1	E	311	ASP	2.8
1	D	38	LEU	2.7
1	F	433	ILE	2.7
1	C	173	ASN	2.7
1	D	35	ILE	2.7
1	D	157	LEU	2.7
1	F	120	ALA	2.6
1	C	338	MET	2.6
1	F	237	PHE	2.6
1	E	337	ILE	2.6
1	E	188	GLU	2.6
1	F	114	ALA	2.6
1	F	227	ALA	2.5
1	A	388	GLN	2.5
1	F	380	SER	2.5
1	D	413	MET	2.5
1	D	96	ASP	2.4
1	E	339	VAL	2.4
1	F	394	PRO	2.4
1	F	382	LEU	2.4
1	E	377	VAL	2.4
1	A	414	PHE	2.4
1	F	84	LEU	2.4
1	E	184	GLU	2.3
1	C	254	LEU	2.3
1	F	57	PHE	2.3
1	C	307	MET	2.3
1	C	402	SER	2.3
1	C	253	VAL	2.3
1	A	184	GLU	2.3
1	A	210	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	23	VAL	2.3
1	A	79	LEU	2.2
1	F	48	VAL	2.2
1	F	107	ALA	2.2
1	E	165	ILE	2.2
1	A	85	SER	2.2
1	A	394	PRO	2.2
1	D	48	VAL	2.2
1	E	421	TYR	2.2
1	E	307	MET	2.2
1	E	195	LYS	2.2
1	E	435	ILE	2.2
1	D	158	ALA	2.2
1	E	338	MET	2.2
1	E	432	GLU	2.2
1	D	39	LEU	2.1
1	E	437	LYS	2.1
1	C	175	GLY	2.1
1	F	55	GLN	2.1
1	F	54	THR	2.1
1	A	114	ALA	2.1
1	C	308	TYR	2.1
1	F	116	ILE	2.1
1	D	162	VAL	2.1
1	F	111	PRO	2.0
1	F	173	ASN	2.0
1	B	125	GLU	2.0
1	F	432	GLU	2.0
1	D	285	GLN	2.0
1	E	412	ILE	2.0
1	E	226	VAL	2.0

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 monosaccharides in this entry.

6.4 Ligands (i)

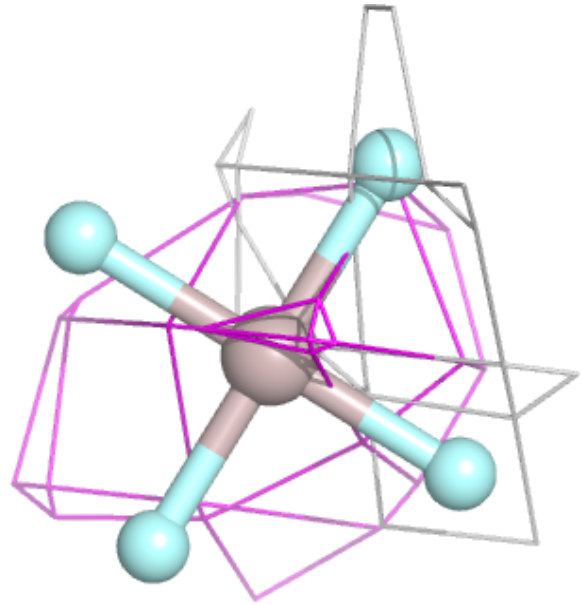
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

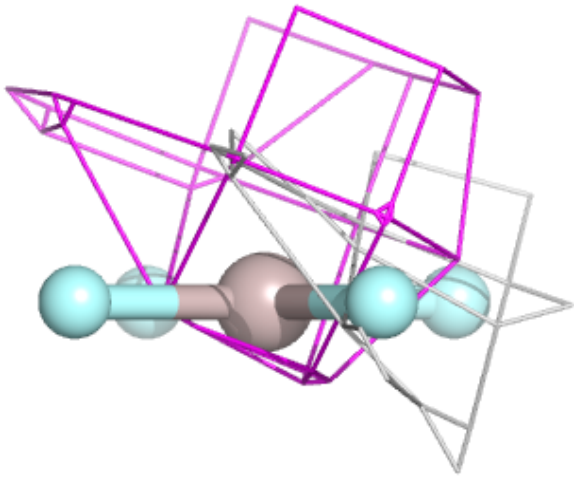
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	ALF	F	503	5/5	0.71	0.48	287,287,287,287	0
4	ALF	D	503	5/5	0.79	0.41	271,272,272,272	0
2	GDP	D	501	28/28	0.84	0.17	217,219,220,220	0
2	GDP	F	501	28/28	0.85	0.27	212,215,217,217	0
2	GDP	A	501	28/28	0.87	0.22	151,159,164,165	0
3	MG	D	502	1/1	0.88	0.16	74,74,74,74	0
2	GDP	E	501	28/28	0.89	0.28	186,187,193,193	0
2	GDP	C	501	28/28	0.90	0.28	141,149,157,157	0
2	GDP	B	501	28/28	0.92	0.35	144,153,160,161	0
3	MG	F	502	1/1	0.92	0.23	92,92,92,92	0
3	MG	E	502	1/1	0.94	0.22	74,74,74,74	0
3	MG	A	502	1/1	0.94	0.23	63,63,63,63	0
4	ALF	E	503	5/5	0.95	0.25	218,218,218,218	0
4	ALF	B	503	5/5	0.95	0.34	160,160,160,161	0
4	ALF	C	503	5/5	0.96	0.31	161,161,161,162	0
4	ALF	A	503	5/5	0.98	0.25	175,175,175,176	0
3	MG	C	502	1/1	0.99	0.17	34,34,34,34	0
3	MG	B	502	1/1	0.99	0.28	52,52,52,52	0

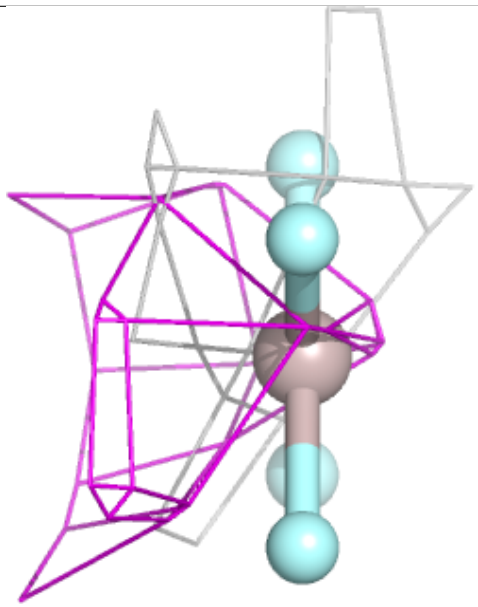
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ALF 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)

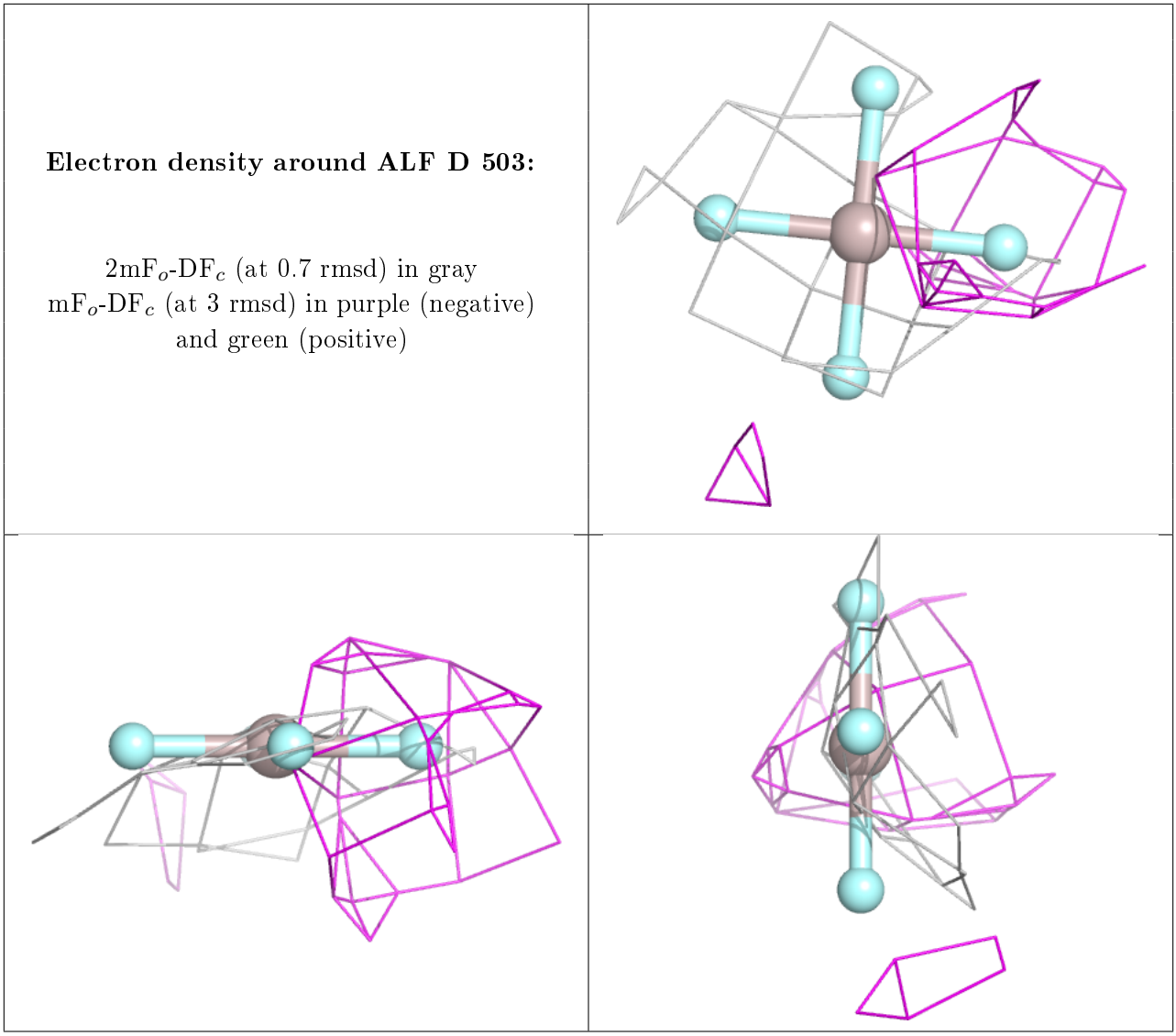






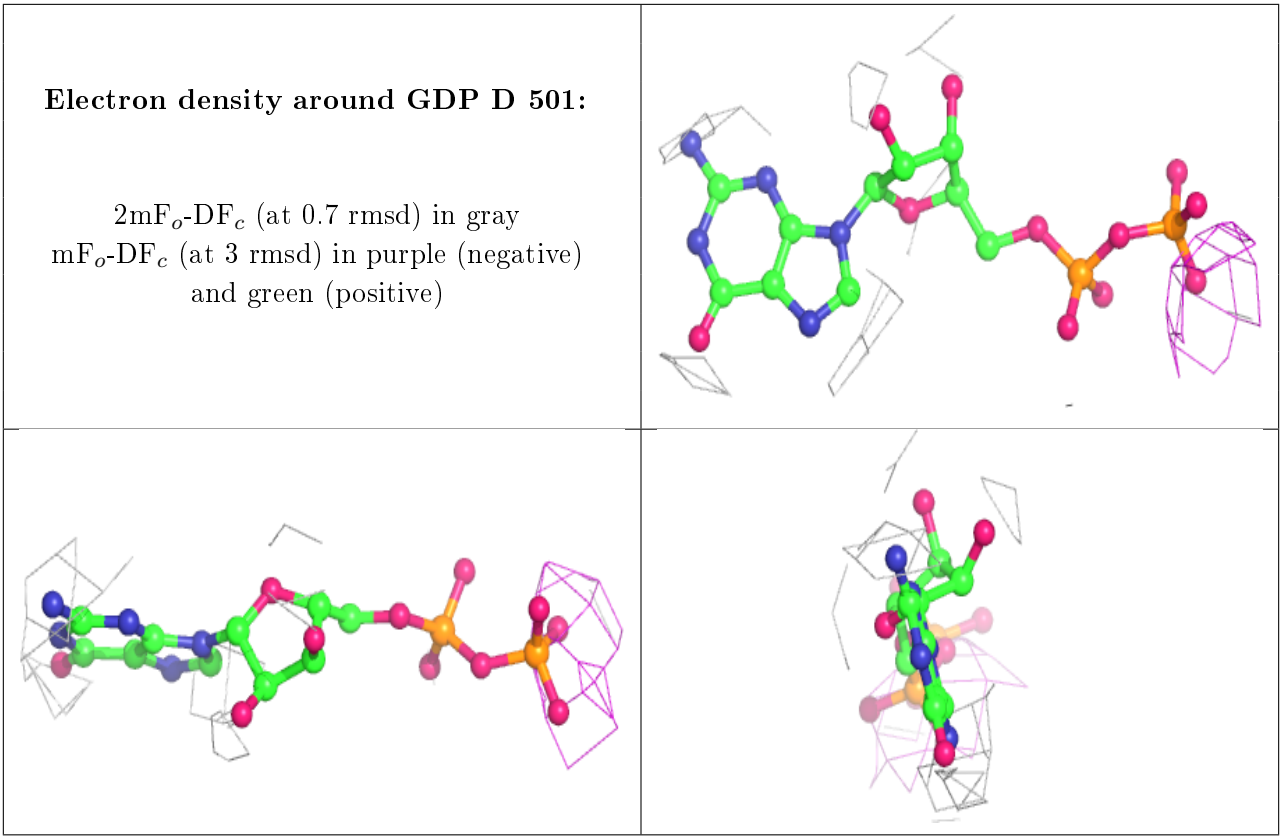
Electron density around ALF D 503:

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



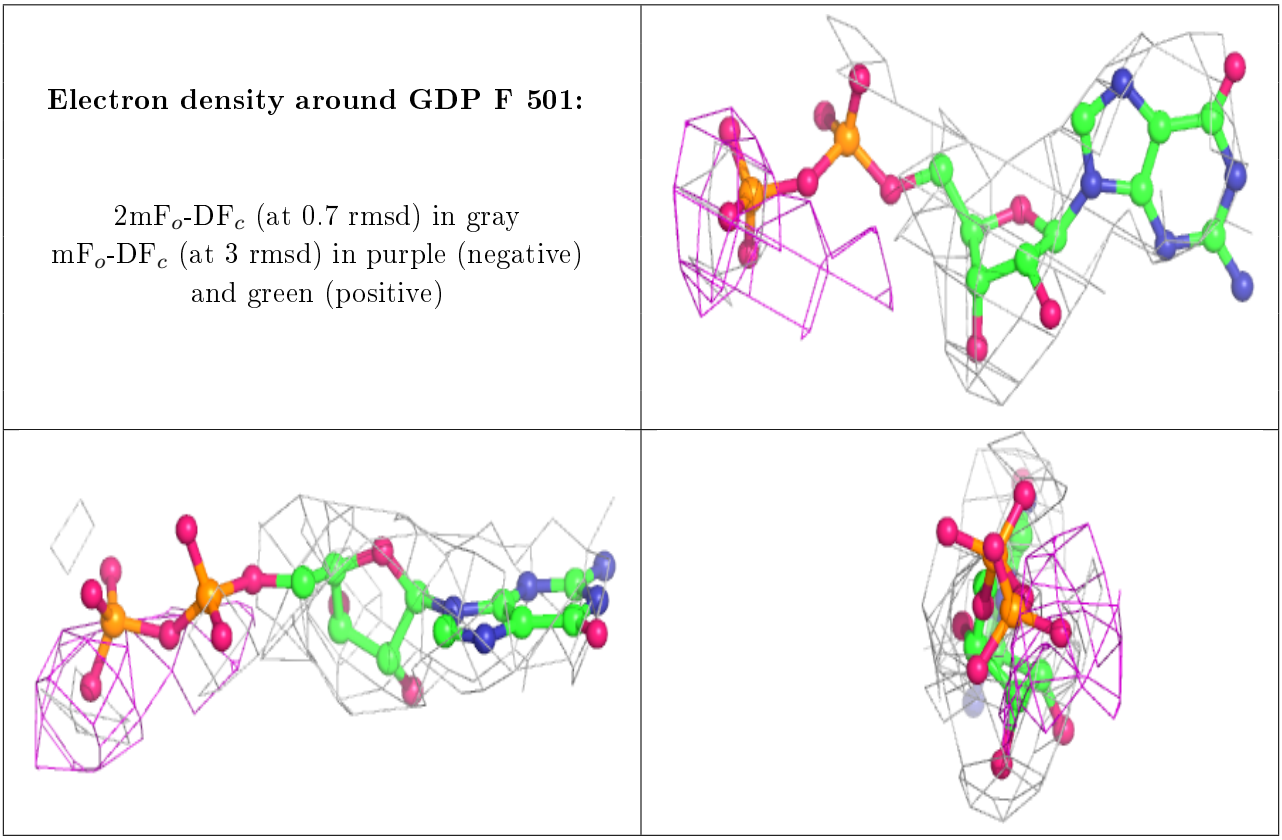
Electron density around GDP D 501:

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



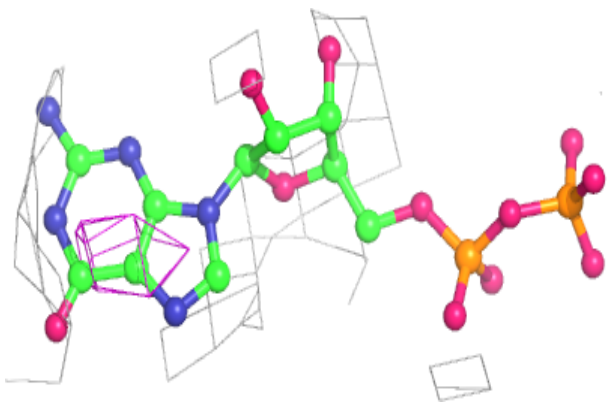
Electron density around GDP F 501:

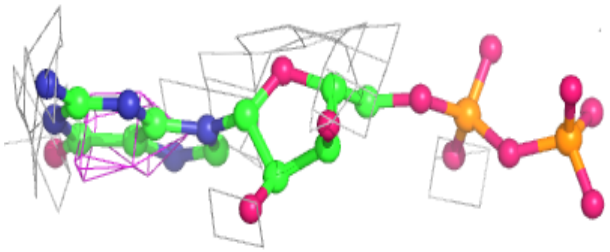
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

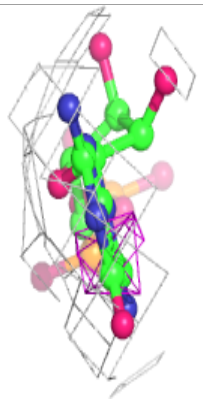


Electron density around GDP A 501:

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

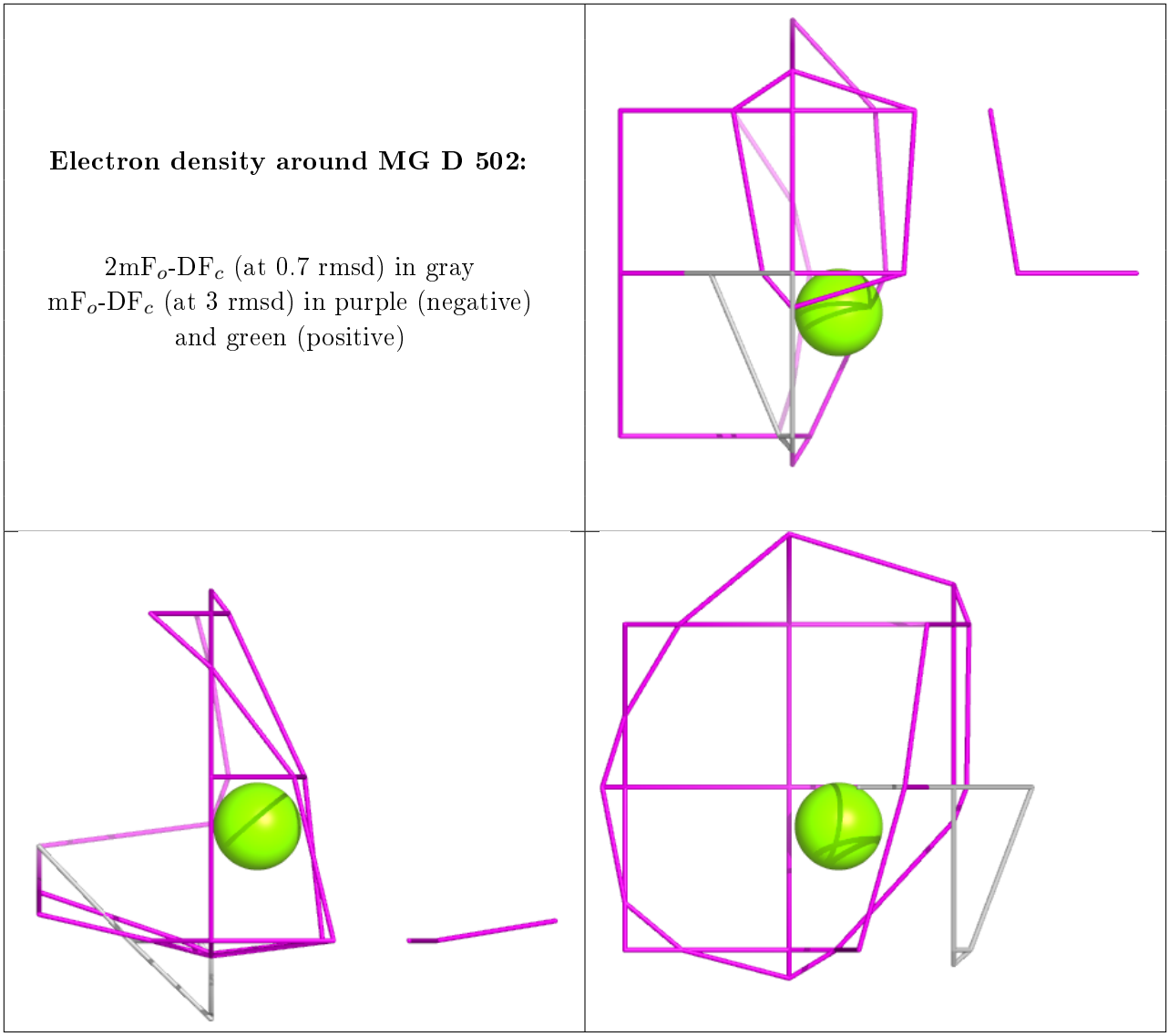






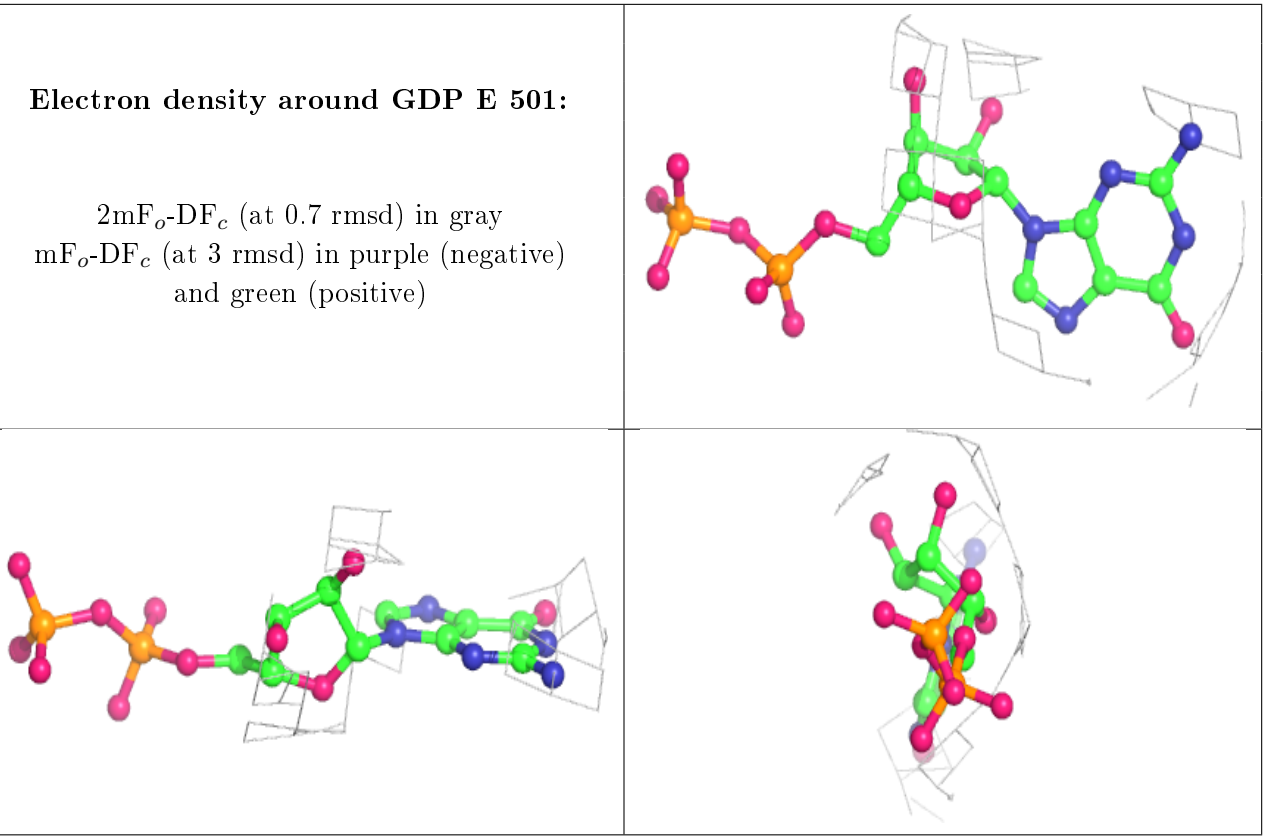
Electron density around MG D 502:

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



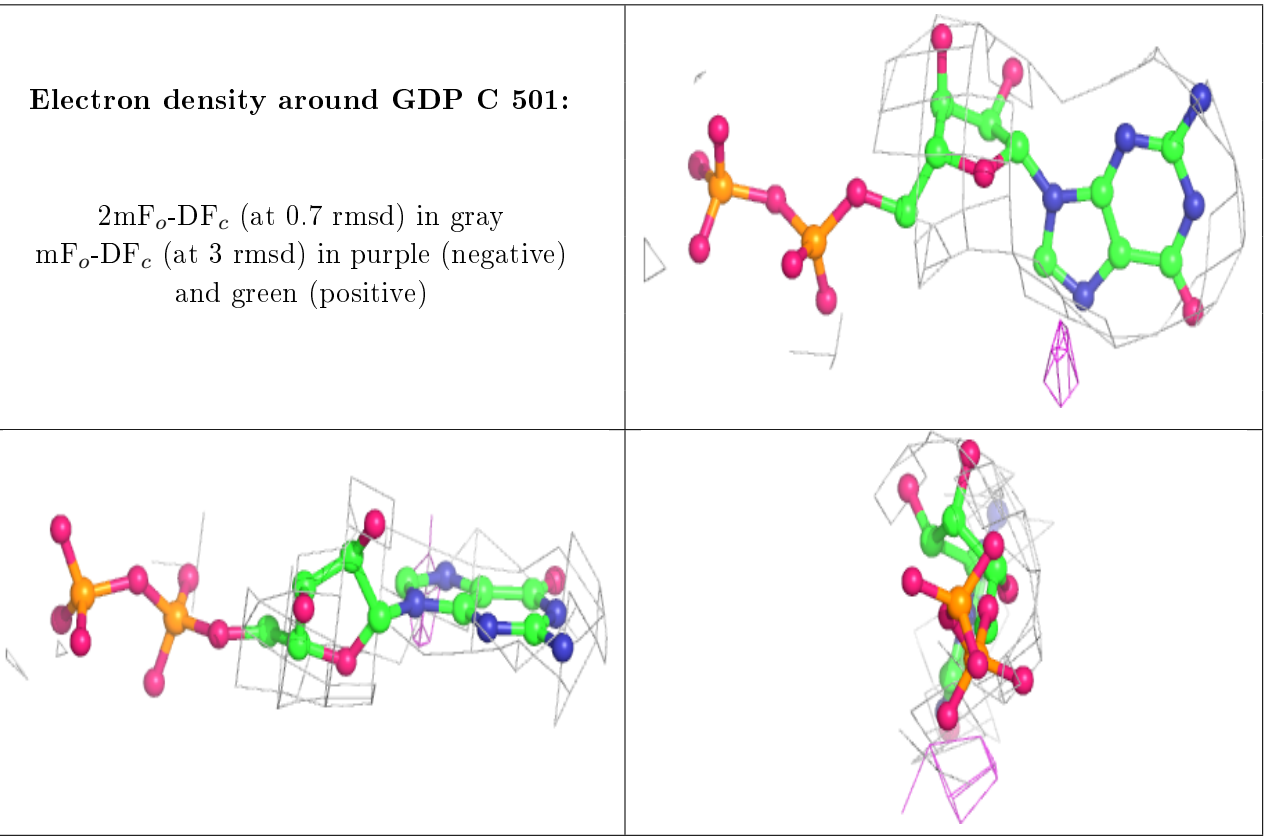
Electron density around GDP E 501:

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



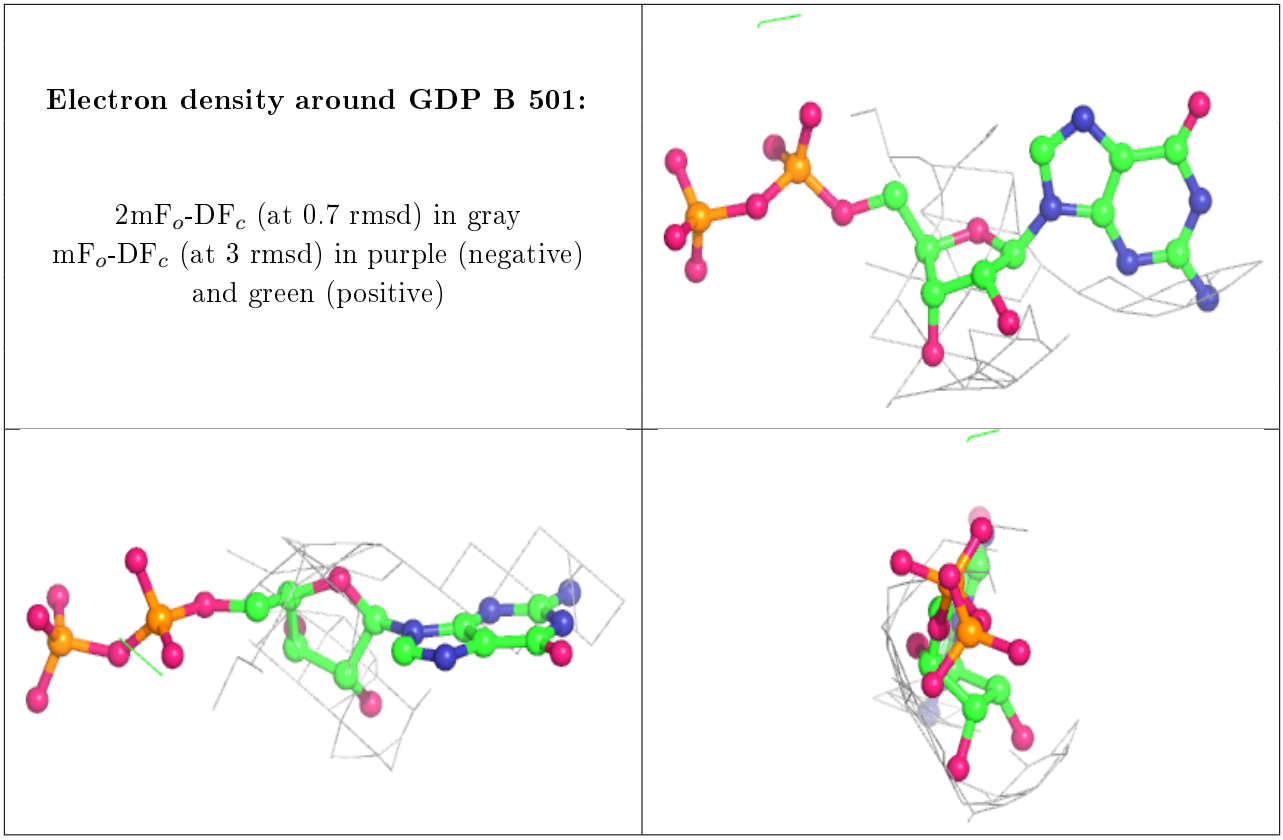
Electron density around GDP C 501:

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



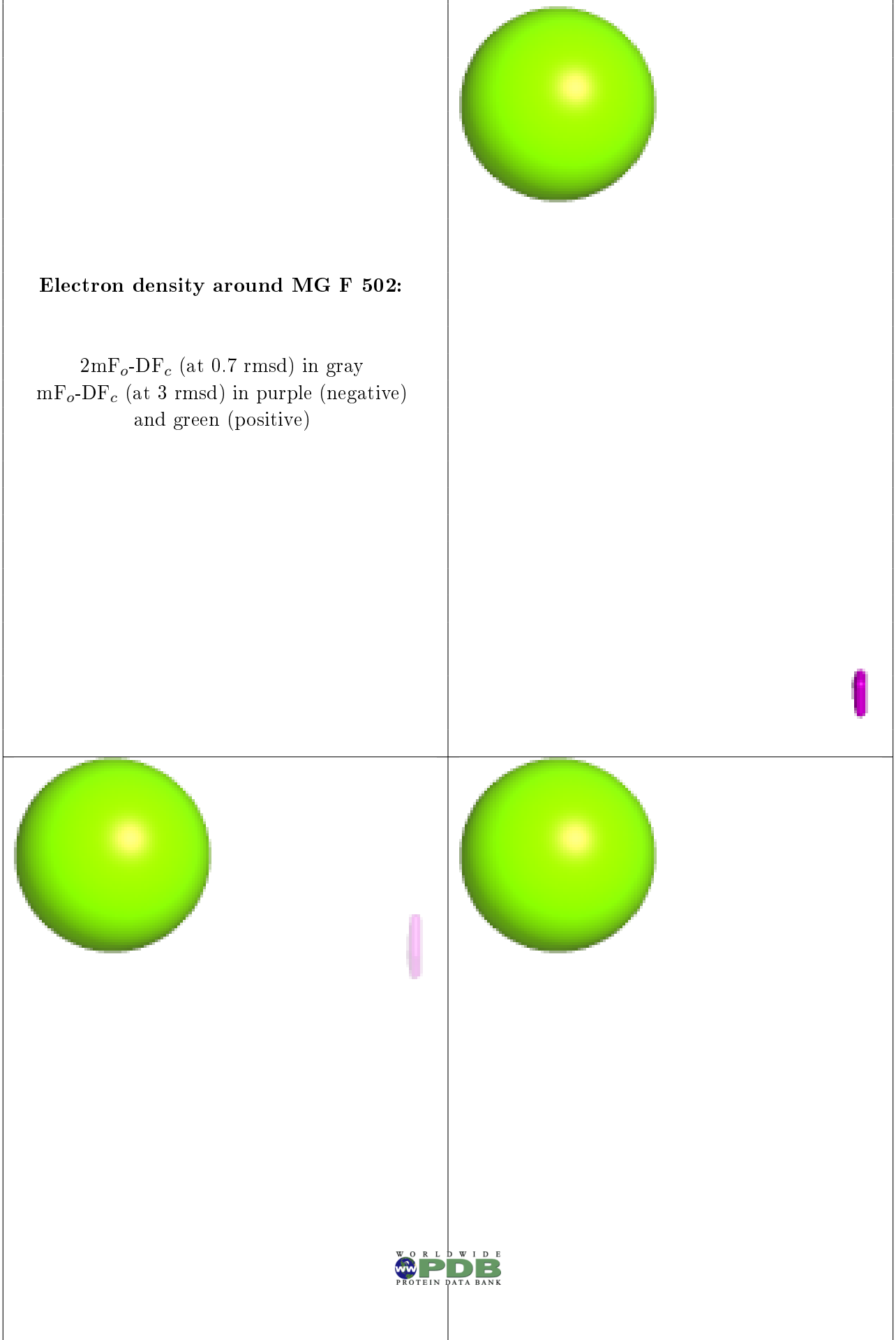
Electron density around GDP B 501:

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



Electron density around 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 MG E 502:

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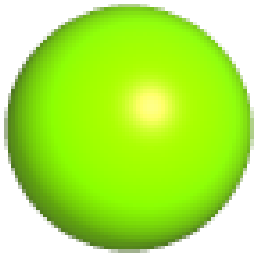
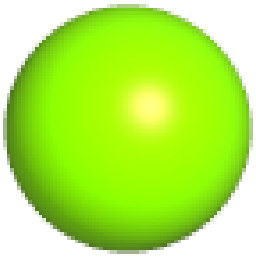
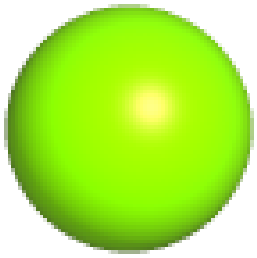
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

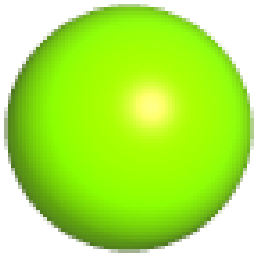


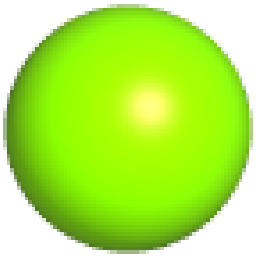


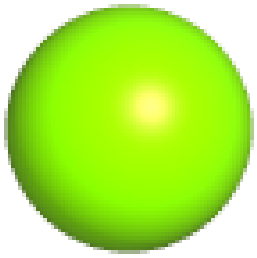


Electron density around MG A 502:

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

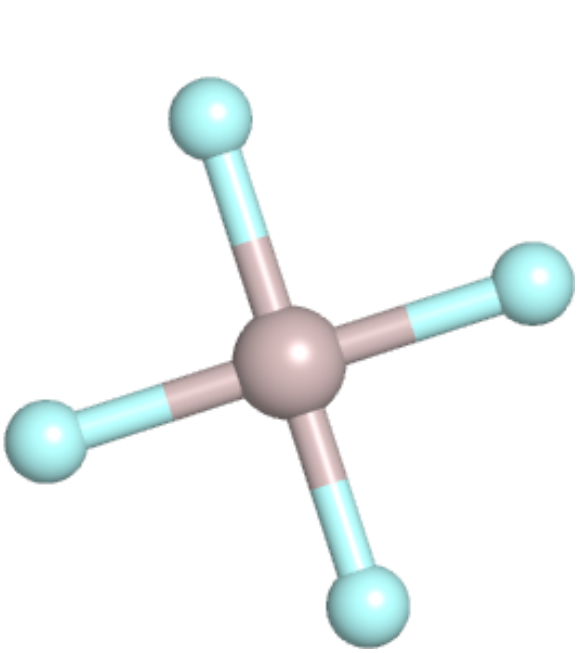


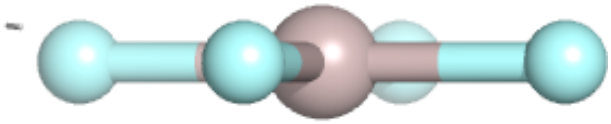


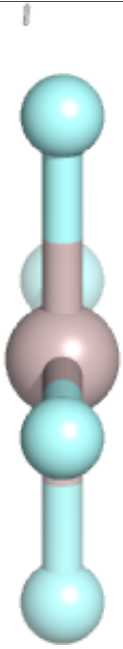


Electron density around ALF E 503:

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

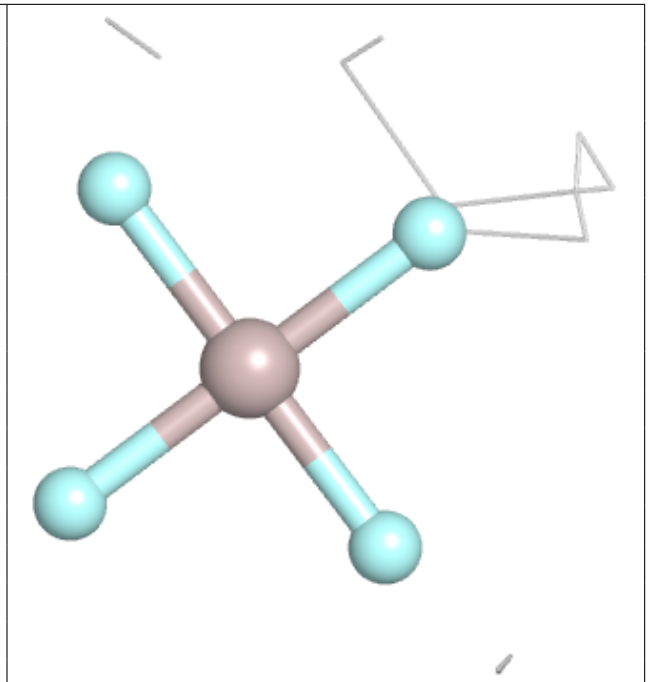


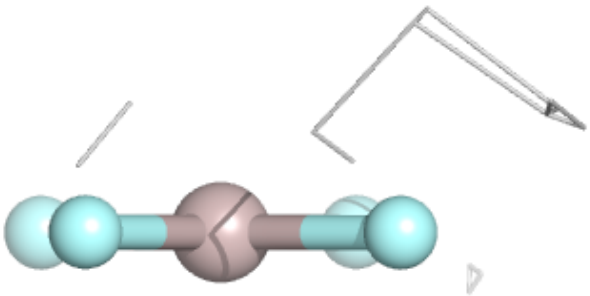


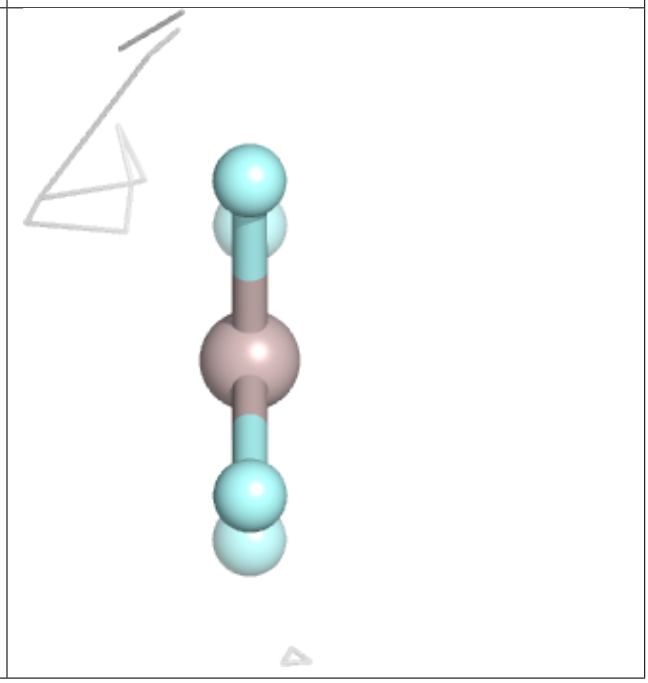


Electron density around ALF B 503:

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

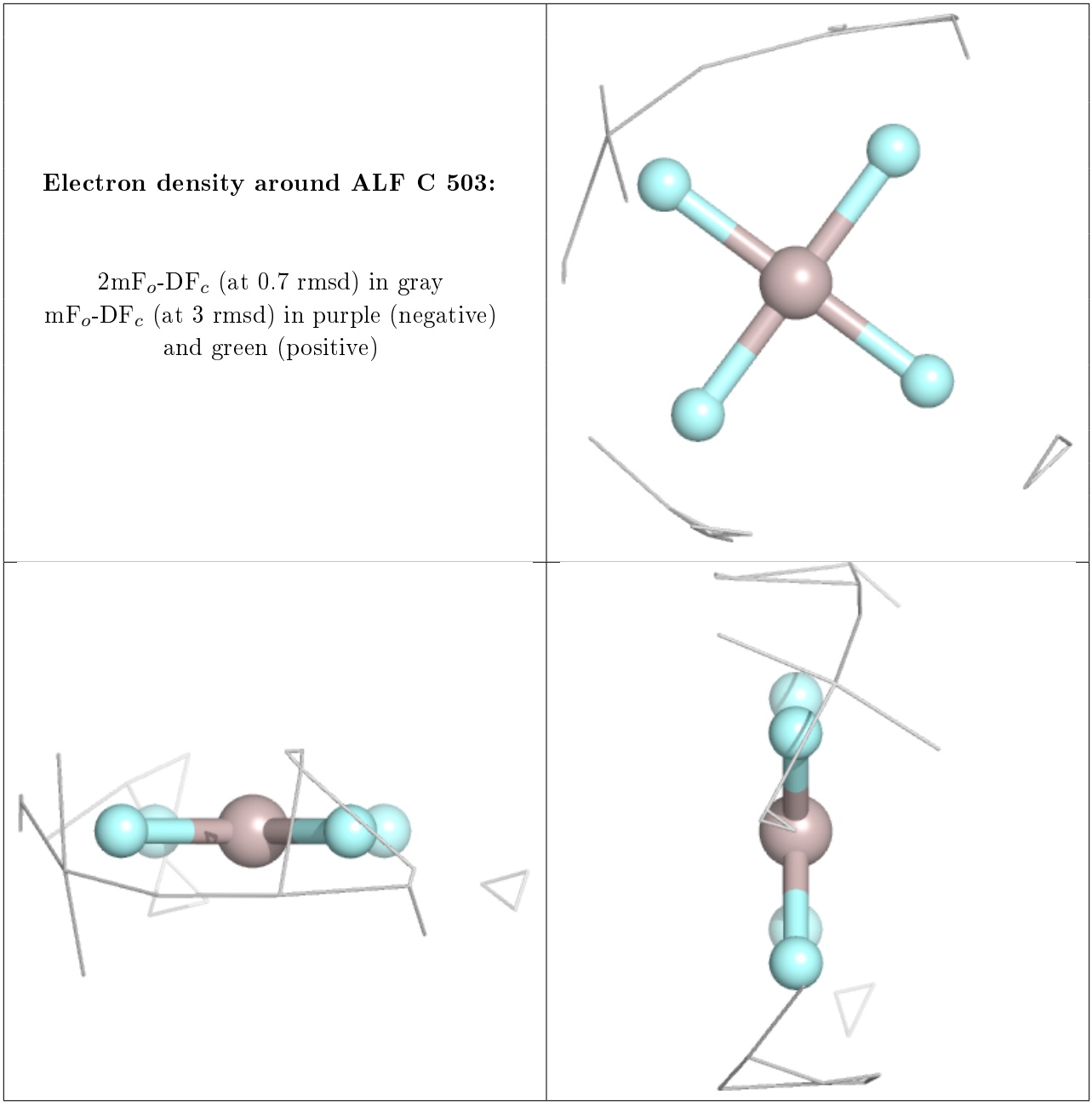






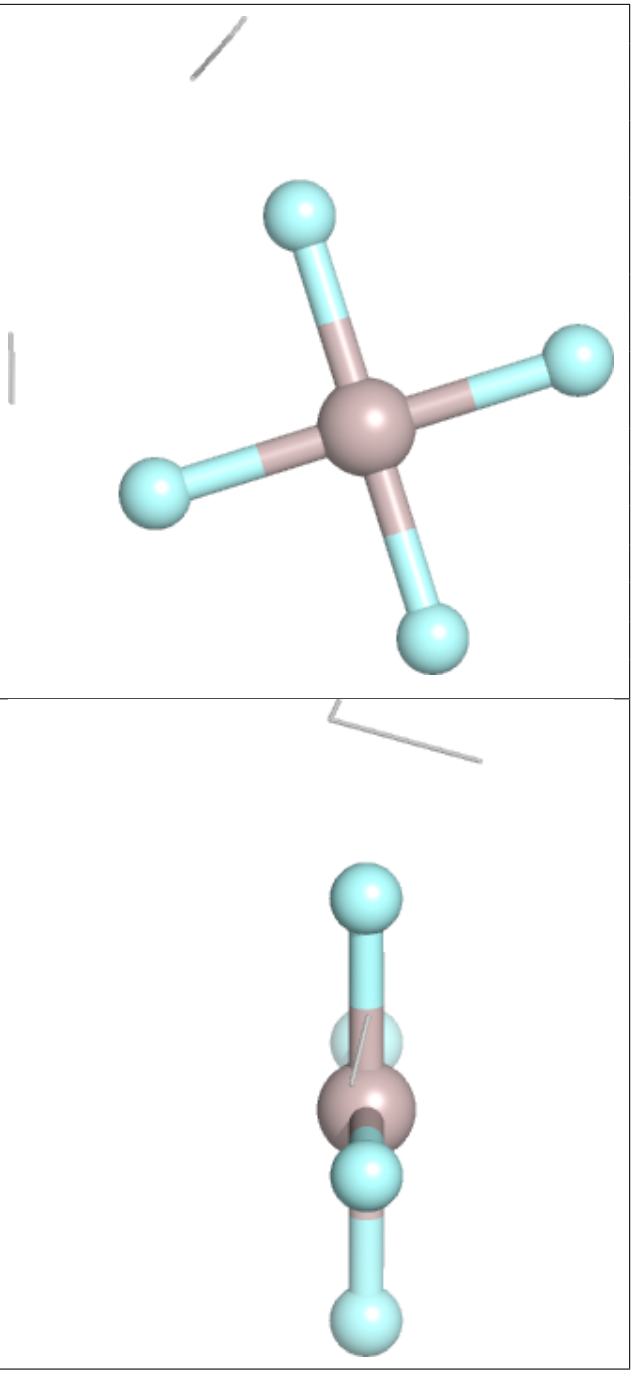
Electron density around ALF C 503:

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



Electron density around 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 MG C 502:

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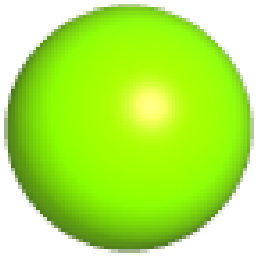
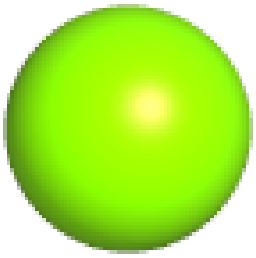
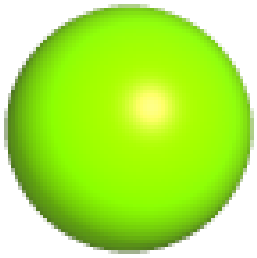
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

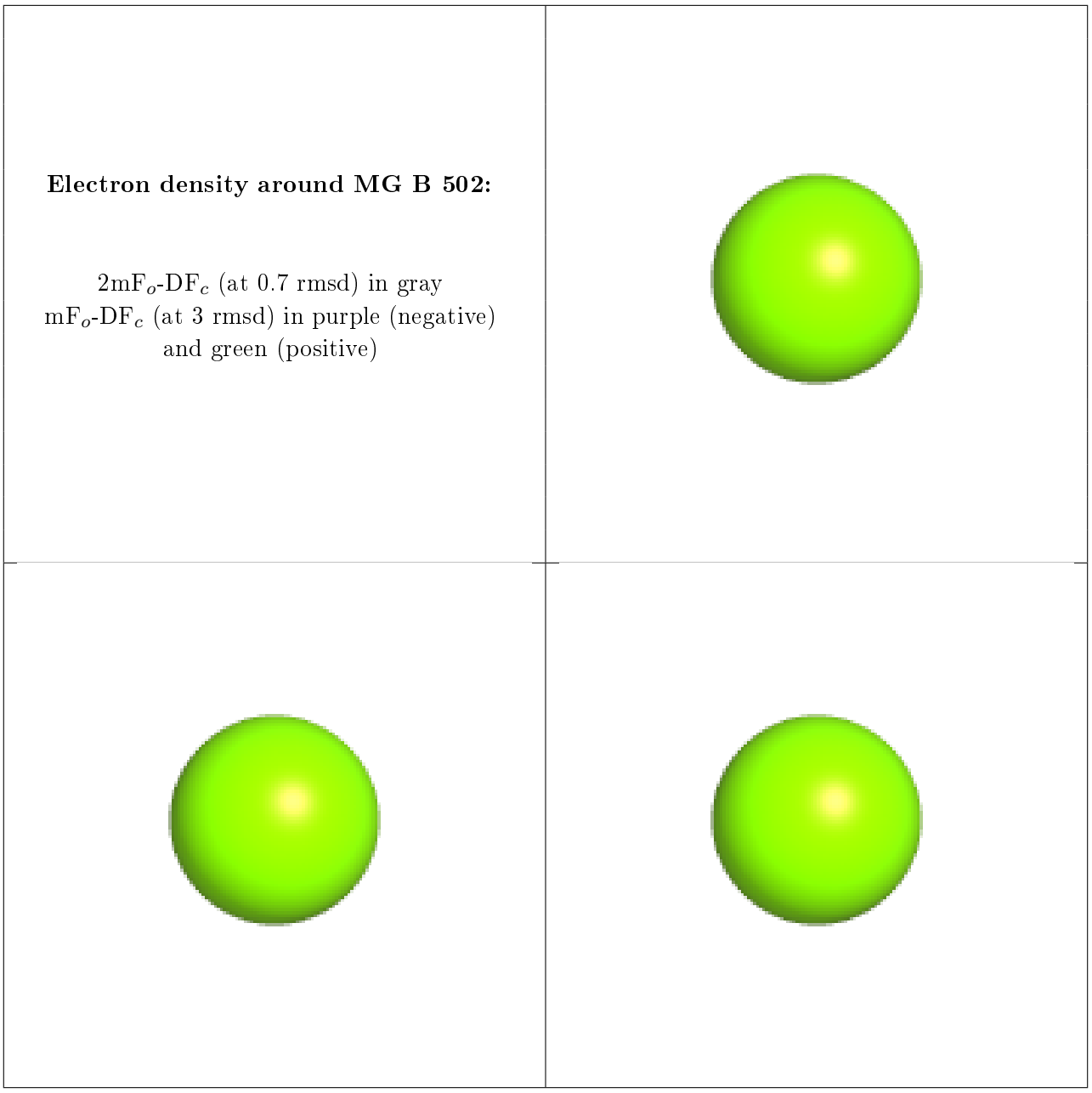






Electron density around MG B 502:

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



6.5 Other polymers

There are no such residues in this entry.