Full wwPDB X-ray Structure Validation Report (i)

Mar 8, 2025 – 12:23 pm GMT

PDB ID	:	8QEH
Title	:	Crystal structure of the G11 protein heterotrimer bound to FR900359 inhibitor
Authors	:	Muehle, J.; Rodrigues, M.J.; Guixa-Gonzalez, R.; Deupi, X.; Schertler, G.F.X.
Deposited on	:	2023-08-31
Resolution	:	1.43 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

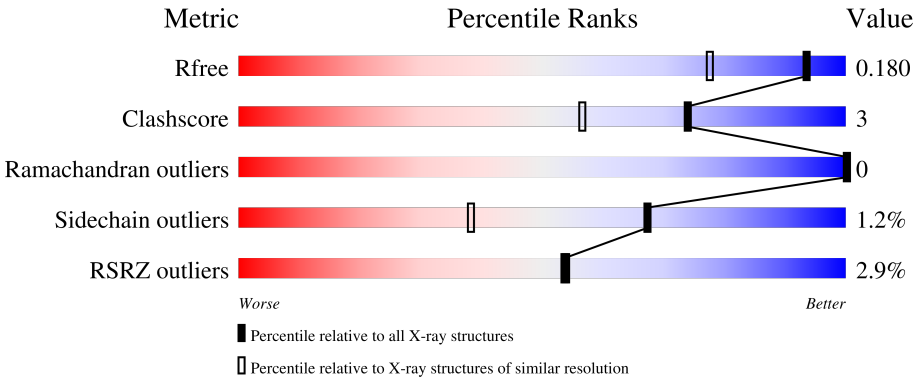
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41

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 1.43 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}	164625	2809 (1.46-1.42)
Clashscore	180529	3008 (1.46-1.42)
Ramachandran outliers	177936	2971 (1.46-1.42)
Sidechain outliers	177891	2971 (1.46-1.42)
RSRZ outliers	164620	2809 (1.46-1.42)

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	352	3% 88% 7%
2	B	344	% 92% 6%
3	G	71	7% 82% 15%

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
16	DMS	G	102	-	-	X	-

2 Entry composition (i)

There are 17 unique types of molecules in this entry. The entry contains 6966 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 Guanine nucleotide-binding protein subunit alpha-11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	337	2955	1879	509	551	16	0	25	0

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	8	GLY	-	expression tag	UNP P29992
A	9	CYS	-	expression tag	UNP P29992
A	10	THR	-	expression tag	UNP P29992
A	11	LEU	-	expression tag	UNP P29992
A	12	SER	-	expression tag	UNP P29992
A	13	ALA	-	expression tag	UNP P29992
A	14	GLU	-	expression tag	UNP P29992
A	15	ASP	-	expression tag	UNP P29992
A	16	LYS	-	expression tag	UNP P29992
A	17	ALA	-	expression tag	UNP P29992
A	18	ALA	-	expression tag	UNP P29992
A	19	VAL	-	expression tag	UNP P29992
A	20	GLU	-	expression tag	UNP P29992
A	21	ARG	-	expression tag	UNP P29992
A	22	SER	-	expression tag	UNP P29992
A	23	LYS	-	expression tag	UNP P29992
A	24	MET	-	expression tag	UNP P29992
A	25	ILE	-	expression tag	UNP P29992
A	26	ASP	-	expression tag	UNP P29992
A	27	ARG	-	expression tag	UNP P29992
A	28	ASN	-	expression tag	UNP P29992
A	29	LEU	-	expression tag	UNP P29992
A	30	ARG	-	expression tag	UNP P29992
A	31	GLU	-	expression tag	UNP P29992
A	32	ASP	-	expression tag	UNP P29992
A	33	GLY	-	expression tag	UNP P29992
A	34	GLU	-	expression tag	UNP P29992

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Chain	Residue	Modelled	Actual	Comment	Reference
A	35	LYS	-	expression tag	UNP P29992

- Molecule 2 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	335	Total	C	N	O	S	0	16	0
			2651	1639	470	514	28			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	PRO	-	expression tag	UNP P62873
B	-2	GLY	-	expression tag	UNP P62873
B	-1	SER	-	expression tag	UNP P62873
B	0	SER	-	expression tag	UNP P62873
B	1	GLY	-	expression tag	UNP P62873

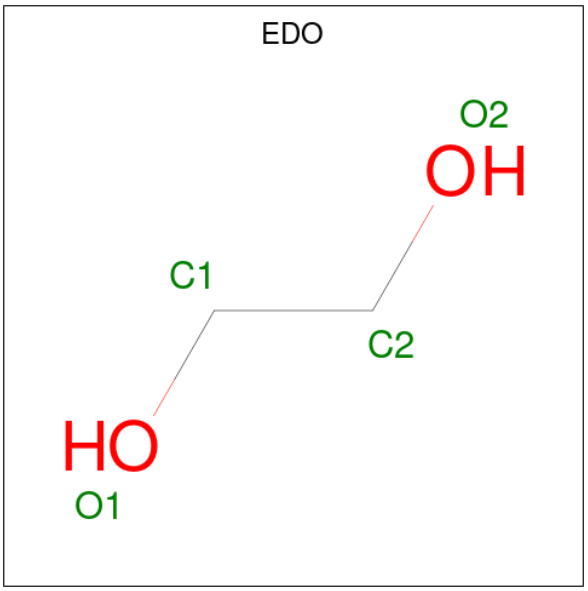
- Molecule 3 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	60	Total	C	N	O	S	0	1	0
			459	290	79	87	3			

There is a discrepancy between the modelled and reference sequences:

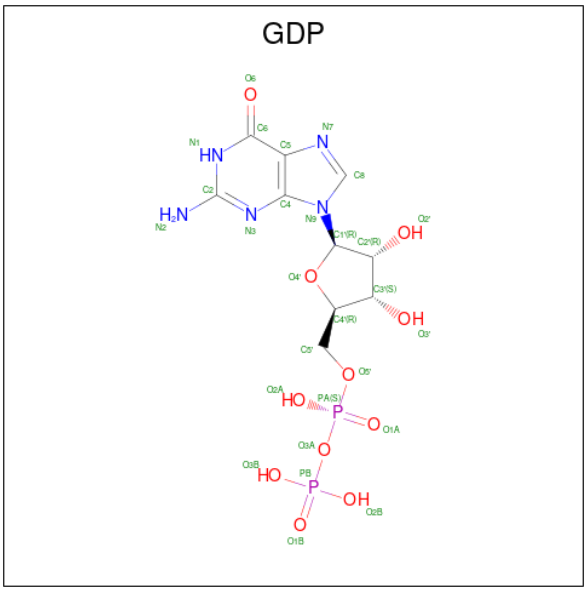
Chain	Residue	Modelled	Actual	Comment	Reference
G	69	SER	CYS	engineered mutation	UNP P59768

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0

- Molecule 5 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
5	A	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

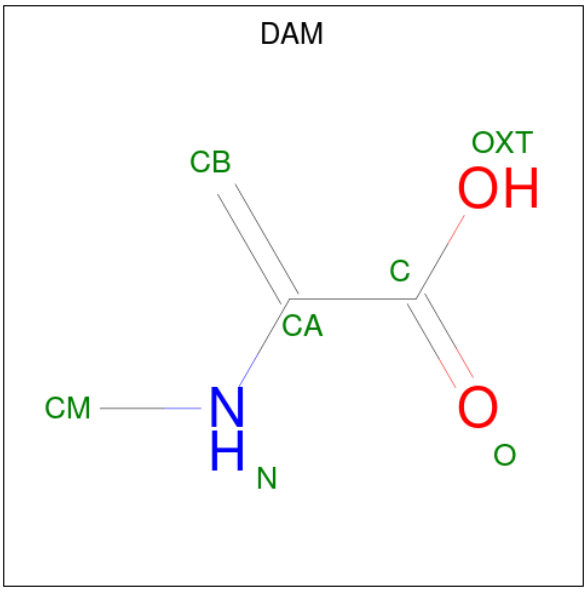
- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Zn	0	0
			1	1		

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

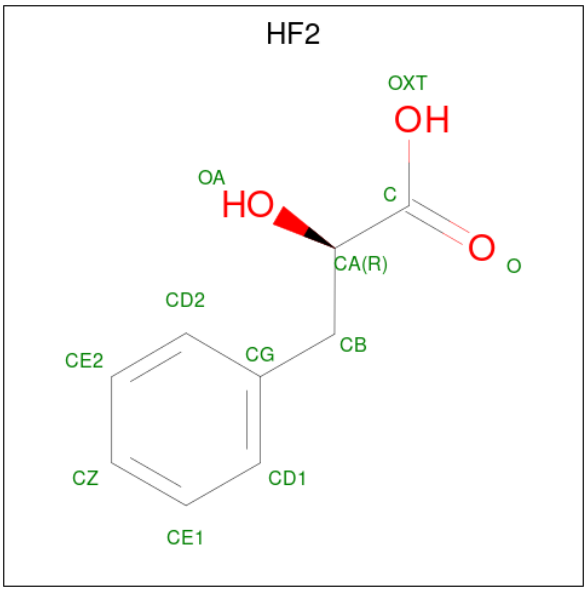
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Cl	0	0
			1	1		

- Molecule 8 is N-METHYL-ALPHA-BETA-DEHYDROALANINE (three-letter code: DAM) (formula: $C_4H_7NO_2$) (labeled as "Ligand of Interest" by depositor).



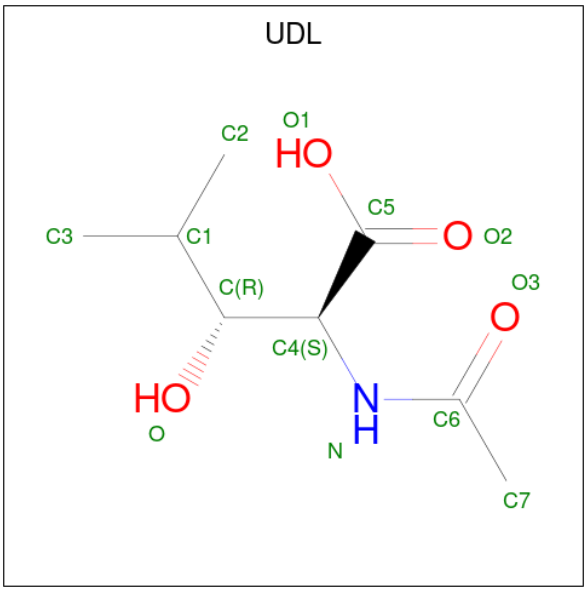
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C N O 6 4 1 1	0	0

- Molecule 9 is (2R)-2-hydroxy-3-phenylpropanoic acid (three-letter code: HF2) (formula: $C_9H_{10}O_3$) (labeled as "Ligand of Interest" by depositor).



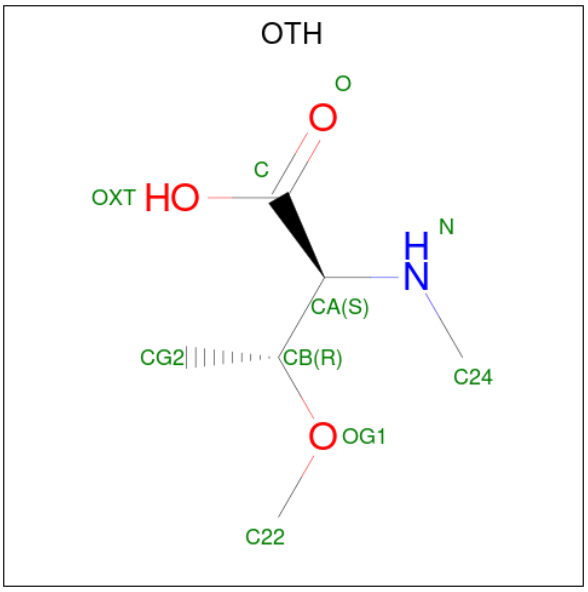
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C O 11 9 2	0	0

- Molecule 10 is (2 {S},3 {R})-2-acetamido-4-methyl-3-oxidanyl-pentanoic acid (three-letter code: UDL) (formula: $C_8H_{15}NO_4$) (labeled as "Ligand of Interest" by depositor).



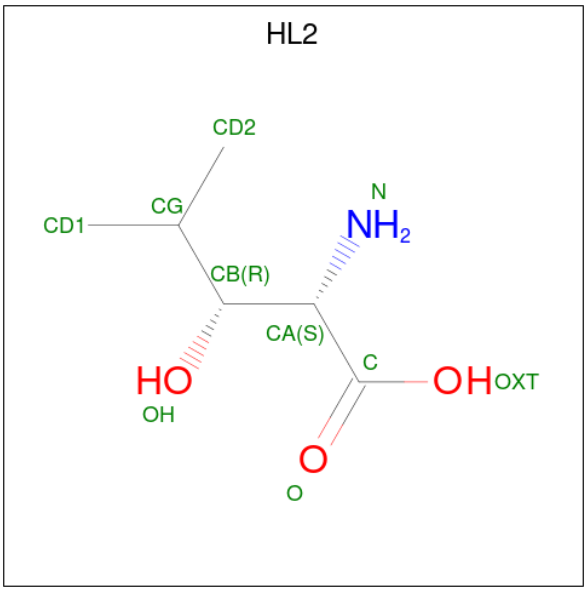
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
10	A	1	12	8	1	3	0	0

- Molecule 11 is N,O-dimethyl-L-threonine (three-letter code: OTH) (formula: $C_6H_{13}NO_3$) (labeled as "Ligand of Interest" by depositor).



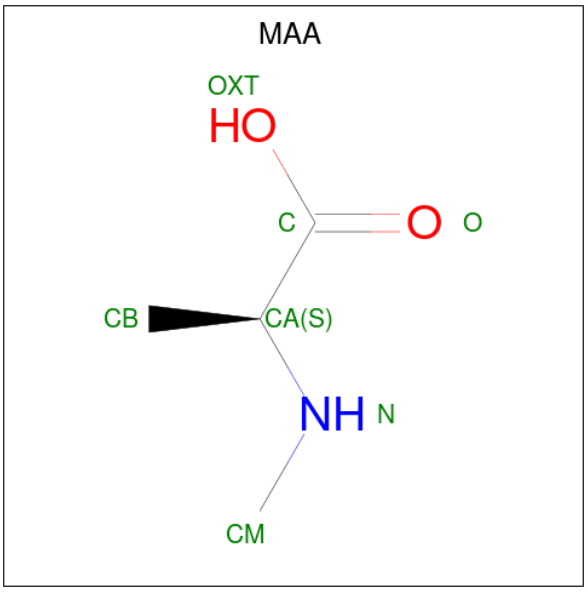
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
11	A	1	9	6	1	2	0	0

- Molecule 12 is (2S,3R)-2-amino-3-hydroxy-4-methylpentanoic acid (three-letter code: HL2) (formula: $C_6H_{13}NO_3$) (labeled as "Ligand of Interest" by depositor).



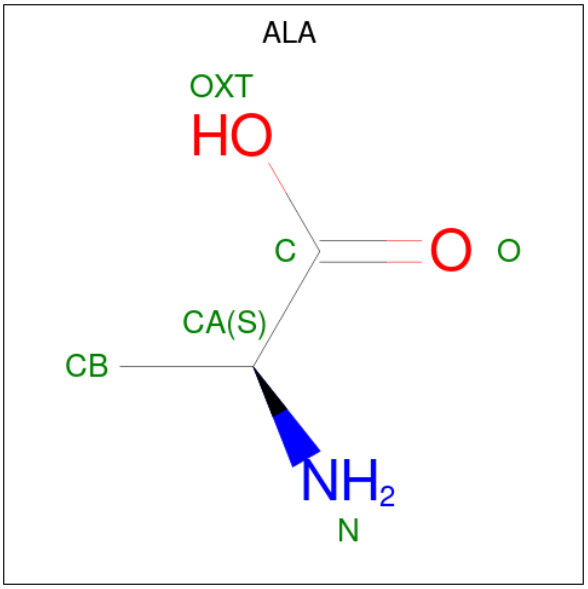
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	1	Total C N O 9 6 1 2	0	0
12	A	1	Total C N O 9 6 1 2	0	0

- Molecule 13 is N-methyl-L-alanine (three-letter code: MAA) (formula: $C_4H_9NO_2$) (labeled as "Ligand of Interest" by depositor).



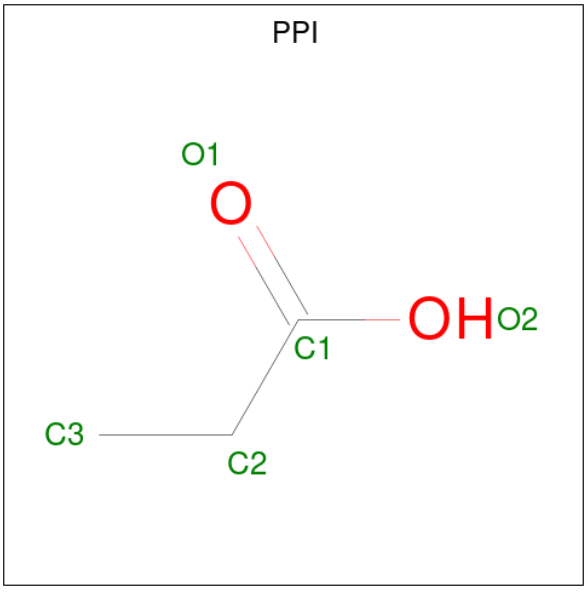
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	B	1	Total C N O 6 4 1 1	0	0

- Molecule 14 is ALANINE (three-letter code: ALA) (formula: $C_3H_7NO_2$) (labeled as "Ligand of Interest" by depositor).



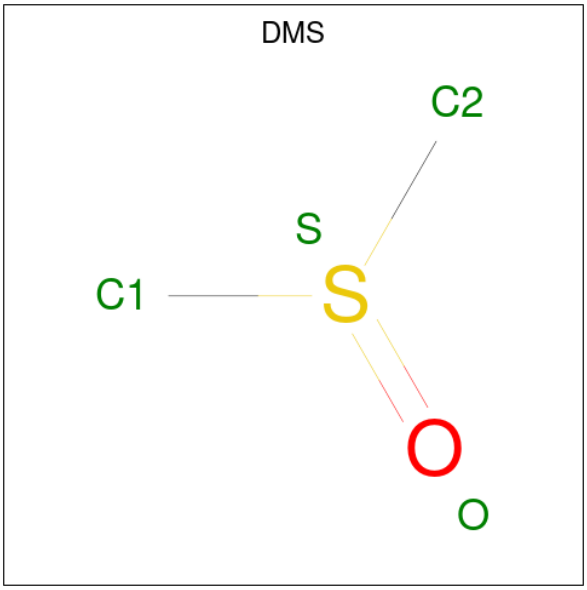
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	B	1	Total	C	N	O	0	0
			5	3	1	1		

- Molecule 15 is PROPANOIC ACID (three-letter code: PPI) (formula: $C_3H_6O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	B	1	Total	C	O	0	0
			4	3	1		

- Molecule 16 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	G	1	Total C O S 4 2 1 1	0	0
16	G	1	Total C O S 4 2 1 1	0	0
16	G	1	Total C O S 4 2 1 1	0	0

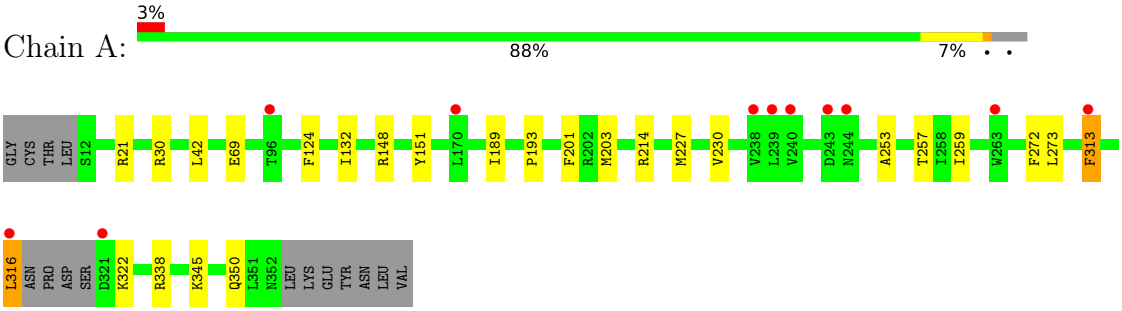
- Molecule 17 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	358	Total O 358 358	0	2
17	B	361	Total O 361 361	0	2
17	G	41	Total O 41 41	0	0

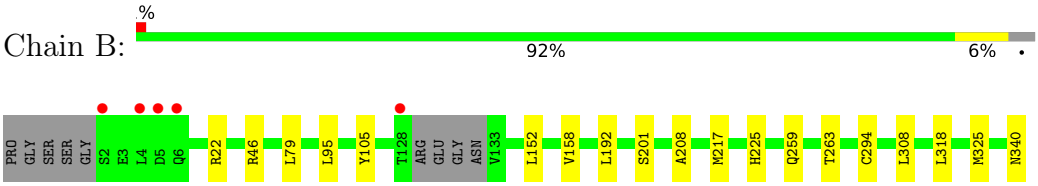
3 Residue-property plots (i)

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.

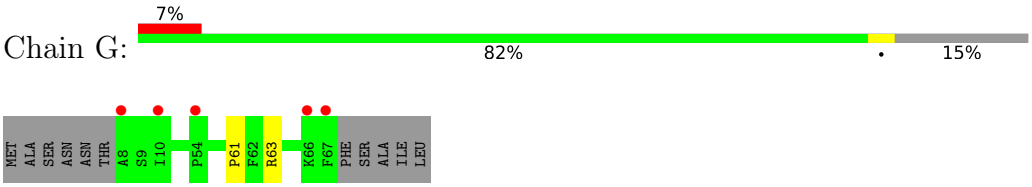
• Molecule 1: Guanine nucleotide-binding protein subunit alpha-11



• Molecule 2: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1



• Molecule 3: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	72.64Å 95.81Å 126.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	63.11 – 1.43 63.11 – 1.43	Depositor EDS
% Data completeness (in resolution range)	100.0 (63.11-1.43) 100.0 (63.11-1.43)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.25 (at 1.43Å)	Xtriage
Refinement program	REFMAC 5.8.0352	Depositor
R, R_{free}	0.140 , 0.180 0.137 , 0.180	Depositor DCC
R_{free} test set	7963 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å^2)	15.1	Xtriage
Anisotropy	1.283	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 49.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	6966	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.83% 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: DMS, GDP, DAM, HL2, ZN, PPI, CL, EDO, UDL, HF2, MAA, OTH

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.40	0/3006	0.69	1/4047 (0.0%)
2	B	0.40	0/2697	0.77	0/3657
3	G	0.38	0/466	0.59	0/630
All	All	0.40	0/6169	0.72	1/8334 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	B	0	2
All	All	0	3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	30	ARG	NE-CZ-NH2	-5.59	117.51	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	214[A]	ARG	Sidechain
2	B	22	ARG	Sidechain
2	B	46	ARG	Sidechain

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	2955	0	2907	18	0
2	B	2651	0	2528	13	0
3	G	459	0	447	8	0
4	A	16	0	24	0	0
4	B	12	0	18	3	0
5	A	28	0	12	0	0
6	A	1	0	0	0	0
7	A	1	0	0	0	0
8	A	6	0	5	0	0
9	A	11	0	8	0	0
10	A	12	0	0	0	0
11	A	9	0	11	0	0
12	A	18	0	19	1	0
13	B	6	0	7	0	0
14	B	5	0	4	0	0
15	B	4	0	5	0	0
16	G	12	0	18	8	0
17	A	358	0	0	3	0
17	B	361	0	0	0	0
17	G	41	0	0	0	0
All	All	6966	0	6013	37	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 3.

All (37) 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:230[B]:VAL:CG1	1:A:273[B]:LEU:HD23	2.10	0.81
3:G:63:ARG:HH21	16:G:102:DMS:H12	1.52	0.73
1:A:230[B]:VAL:HG13	1:A:273[B]:LEU:HD23	1.70	0.72
2:B:325[B]:MET:HE2	3:G:61:PRO:HD2	1.79	0.65
2:B:259:GLN:HA	4:B:401:EDO:H12	1.80	0.64
2:B:225:HIS:CD2	4:B:403:EDO:H21	2.37	0.59
1:A:259:ILE:HD11	1:A:316:LEU:HD13	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:63:ARG:HH21	16:G:102:DMS:C1	2.19	0.54
3:G:63:ARG:HE	16:G:102:DMS:C2	2.21	0.53
1:A:338[A]:ARG:NH1	17:A:502:HOH:O	2.30	0.52
2:B:325[A]:MET:HG2	3:G:61:PRO:HD2	1.91	0.52
3:G:63:ARG:HG2	16:G:102:DMS:H23	1.92	0.52
1:A:230[B]:VAL:CG1	1:A:273[B]:LEU:CD2	2.85	0.51
1:A:259:ILE:CD1	1:A:316:LEU:HD13	2.40	0.51
1:A:148:ARG:HA	1:A:151:TYR:CE1	2.46	0.49
2:B:152[B]:LEU:CD1	2:B:158:VAL:HG23	2.42	0.49
2:B:263:THR:HG21	4:B:403:EDO:H22	1.96	0.48
1:A:227:MET:CE	1:A:272:PHE:HE2	2.26	0.48
1:A:230[A]:VAL:HG21	1:A:313:PHE:CZ	2.49	0.48
1:A:42:LEU:HD12	1:A:203[A]:MET:SD	2.53	0.48
2:B:318:LEU:C	2:B:318:LEU:HD12	2.34	0.47
1:A:69[B]:GLU:HG2	17:A:709:HOH:O	2.14	0.47
3:G:63:ARG:HE	16:G:102:DMS:H21	1.80	0.47
1:A:253:ALA:O	1:A:257[A]:THR:HG23	2.16	0.46
1:A:227:MET:CE	1:A:272:PHE:CE2	3.00	0.44
3:G:63:ARG:NH2	16:G:102:DMS:C1	2.80	0.44
2:B:152[A]:LEU:HD23	2:B:192:LEU:HD13	2.00	0.43
1:A:193:PRO:HA	1:A:201:PHE:O	2.18	0.43
1:A:230[B]:VAL:HG13	1:A:273[B]:LEU:CD2	2.44	0.42
1:A:189:ILE:HG23	12:A:413:HL2:HD1B	2.01	0.42
2:B:294[B]:CYS:HB2	2:B:308:LEU:HB2	2.02	0.42
2:B:340:ASN:HB2	16:G:103:DMS:H21	2.02	0.42
2:B:79:LEU:HG	2:B:95:LEU:HD21	2.01	0.42
1:A:21:ARG:HD3	17:A:805:HOH:O	2.19	0.41
1:A:124:PHE:HE1	1:A:132[A]:ILE:HD12	1.86	0.41
2:B:201:SER:O	2:B:208:ALA:HA	2.21	0.41
2:B:340:ASN:HB2	16:G:103:DMS:C2	2.51	0.41

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	360/352 (102%)	357 (99%)	3 (1%)	0	100	100
2	B	347/344 (101%)	332 (96%)	15 (4%)	0	100	100
3	G	59/71 (83%)	59 (100%)	0	0	100	100
All	All	766/767 (100%)	748 (98%)	18 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	316/317 (100%)	311 (98%)	5 (2%)	58	26
2	B	285/285 (100%)	283 (99%)	2 (1%)	81	61
3	G	44/58 (76%)	44 (100%)	0	100	100
All	All	645/660 (98%)	638 (99%)	7 (1%)	67	42

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	313	PHE
1	A	316	LEU
1	A	322	LYS
1	A	345	LYS
1	A	350	GLN
2	B	105	TYR
2	B	217	MET

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

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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 22 ligands modelled in this entry, 2 are monoatomic - leaving 20 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	$\#\|Z\| > 2$
12	HL2	A	413	15,12	7,8,9	0.43	0	7,10,12	1.02	1 (14%)
16	DMS	G	101	-	3,3,3	0.31	0	3,3,3	0.10	0
4	EDO	A	402	-	3,3,3	0.19	0	2,2,2	0.04	0
5	GDP	A	405	-	24,30,30	0.89	1 (4%)	30,47,47	0.85	1 (3%)
14	ALA	B	405	8,13	3,4,5	0.75	0	2,4,6	1.13	0
8	DAM	A	408	9,14	4,5,6	1.67	1 (25%)	3,5,7	3.75	2 (66%)
15	PPI	B	406	12	3,3,4	0.72	0	2,2,4	0.99	0
12	HL2	A	412	13,12,11	7,8,9	0.47	0	7,10,12	1.27	1 (14%)
16	DMS	G	102	-	3,3,3	0.10	0	3,3,3	0.21	0
16	DMS	G	103	-	3,3,3	0.41	0	3,3,3	0.24	0
13	MAA	B	404	14,12	4,5,6	0.56	0	1,5,7	1.14	0
9	HF2	A	409	8,10	10,11,12	0.70	0	12,13,15	0.49	0
10	UDL	A	410	9,11	10,11,12	0.55	0	11,14,16	1.02	1 (9%)
4	EDO	A	401	-	3,3,3	0.36	0	2,2,2	0.52	0
11	OTH	A	411	10,12	7,8,9	0.78	0	6,9,11	0.81	0
4	EDO	A	403	-	3,3,3	0.38	0	2,2,2	0.72	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	EDO	B	402	-	3,3,3	0.07	0	2,2,2	0.58	0
4	EDO	A	404	-	3,3,3	0.47	0	2,2,2	0.53	0
4	EDO	B	401	-	3,3,3	0.08	0	2,2,2	0.18	0
4	EDO	B	403	-	3,3,3	0.54	0	2,2,2	0.16	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	HL2	A	413	15,12	-	1/9/10/12	-
15	PPI	B	406	12	-	0/0/1/2	-
12	HL2	A	412	13,12,11	-	0/9/10/12	-
4	EDO	B	402	-	-	1/1/1/1	-
9	HF2	A	409	8,10	-	0/5/6/8	0/1/1/1
13	MAA	B	404	14,12	-	1/1/4/6	-
4	EDO	A	402	-	-	0/1/1/1	-
4	EDO	A	404	-	-	1/1/1/1	-
4	EDO	B	401	-	-	1/1/1/1	-
10	UDL	A	410	9,11	-	0/12/14/16	-
5	GDP	A	405	-	-	1/12/32/32	0/3/3/3
4	EDO	B	403	-	-	1/1/1/1	-
4	EDO	A	401	-	-	0/1/1/1	-
11	OTH	A	411	10,12	-	4/7/10/12	-
14	ALA	B	405	8,13	-	0/0/2/4	-
4	EDO	A	403	-	-	0/1/1/1	-
8	DAM	A	408	9,14	-	0/0/4/6	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	408	DAM	C-CA	-2.78	1.40	1.45
5	A	405	GDP	C5-C6	-2.04	1.43	1.47

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	408	DAM	CB-CA-N	-5.66	112.18	125.91
12	A	412	HL2	O-C-CA	-3.04	116.81	124.78
8	A	408	DAM	O-C-CA	-3.01	121.36	125.22
10	A	410	UDL	C4-N-C6	-2.85	120.00	123.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	A	413	HL2	O-C-CA	-2.26	118.86	124.78
5	A	405	GDP	PA-O3A-PB	-2.04	125.84	132.83

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	A	411	OTH	N-CA-CB-OG1
11	A	411	OTH	C-CA-CB-CG2
4	B	401	EDO	O1-C1-C2-O2
11	A	411	OTH	N-CA-CB-CG2
5	A	405	GDP	PA-O3A-PB-O1B
4	B	402	EDO	O1-C1-C2-O2
11	A	411	OTH	CB-CA-N-C24
4	B	403	EDO	O1-C1-C2-O2
13	B	404	MAA	CB-CA-N-CM
4	A	404	EDO	O1-C1-C2-O2
12	A	413	HL2	O-C-CA-CB

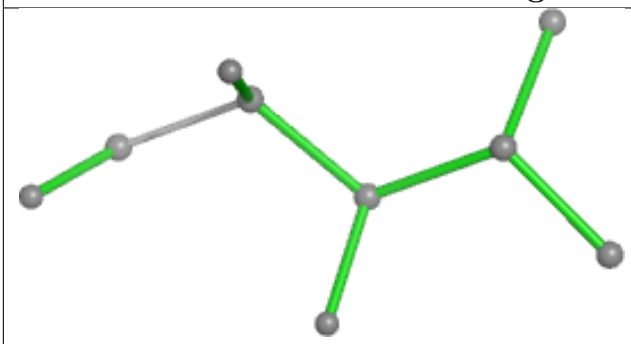
There are no ring outliers.

5 monomers are involved in 12 short contacts:

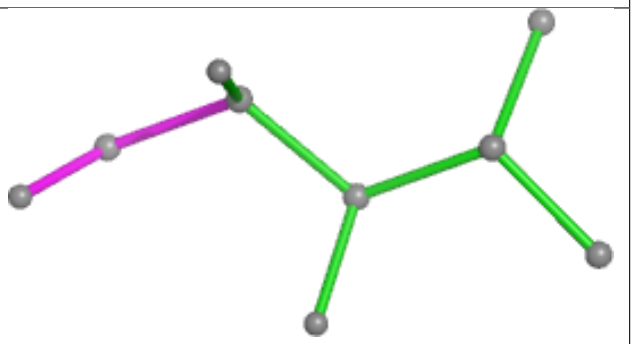
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	A	413	HL2	1	0
16	G	102	DMS	6	0
16	G	103	DMS	2	0
4	B	401	EDO	1	0
4	B	403	EDO	2	0

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.

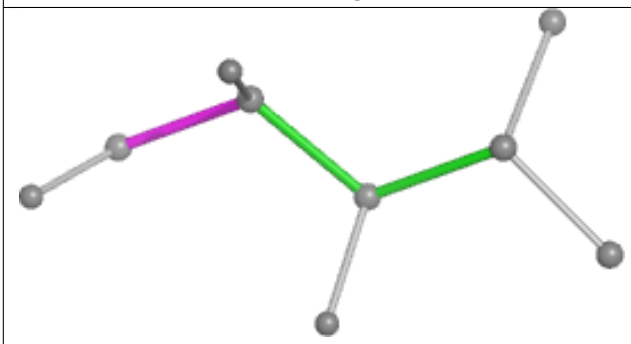
Ligand HL2 A 413



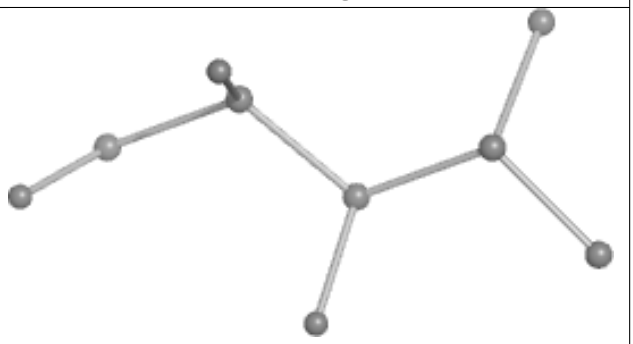
Bond lengths



Bond angles

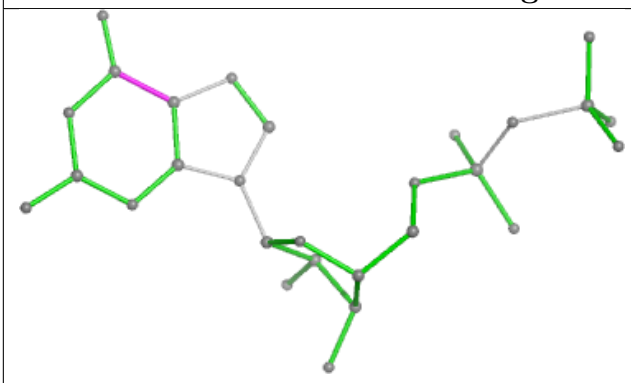


Torsions



Rings

Ligand GDP A 405



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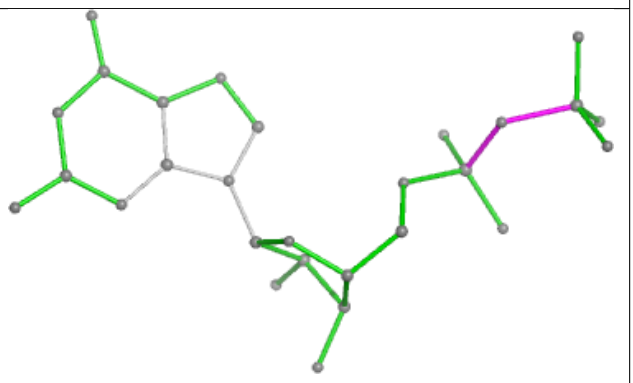

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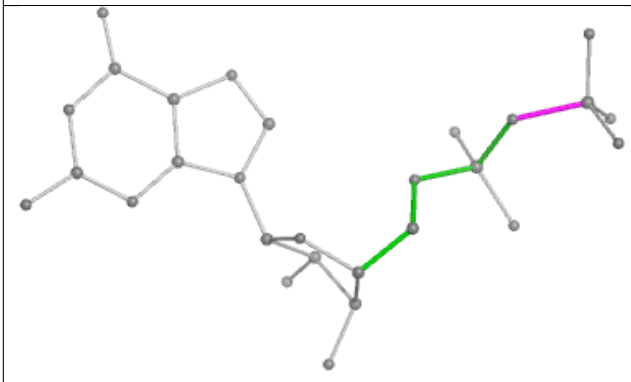

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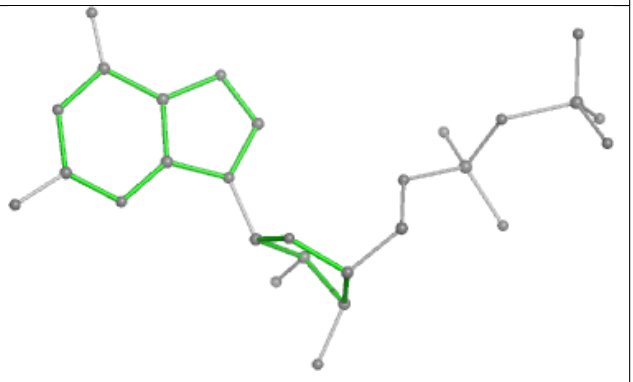
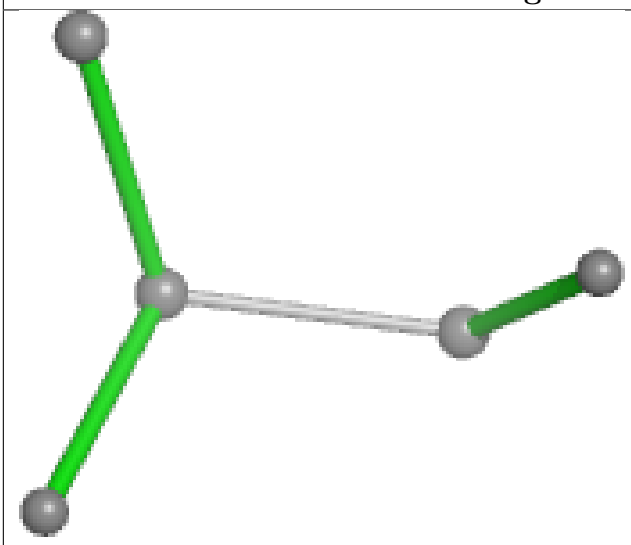


Rings

Ligand ALA B 405



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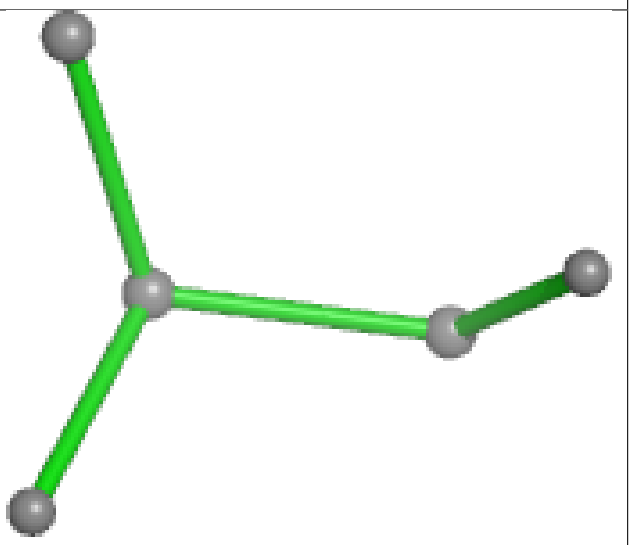

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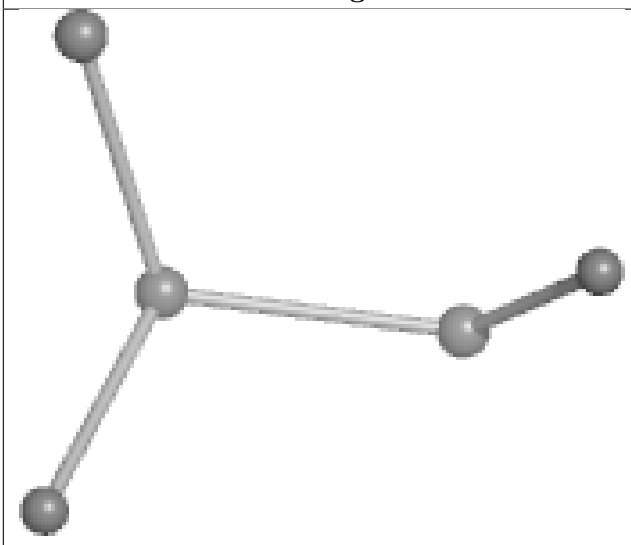

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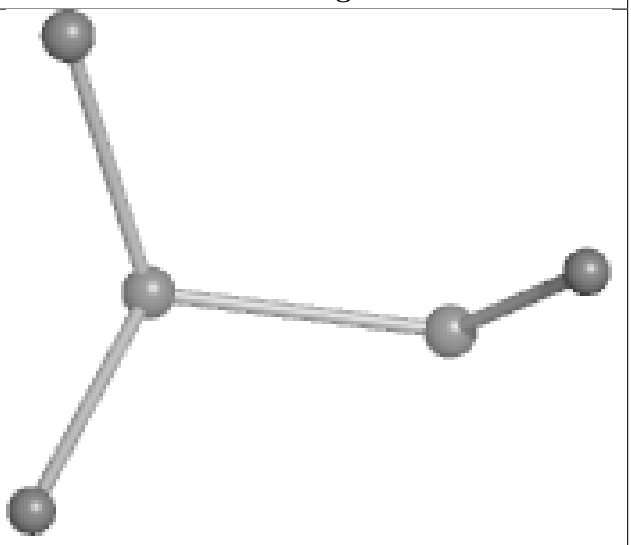
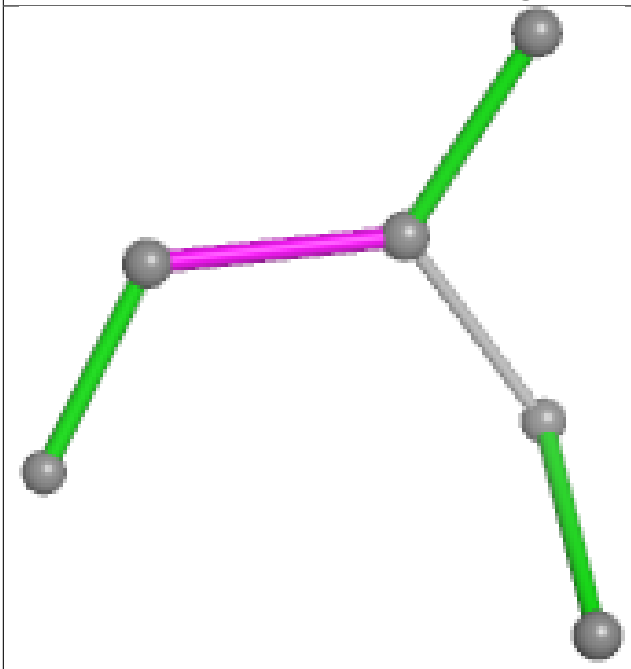
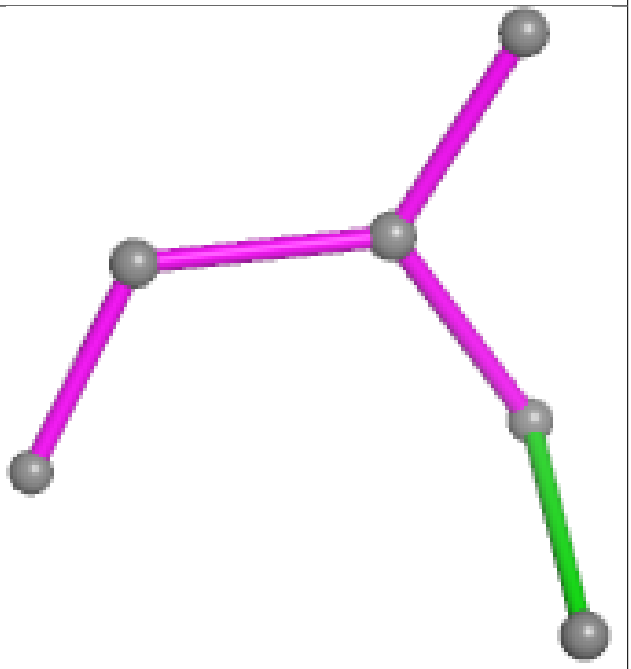


Rings

Ligand DAM A 408



Bond lengths



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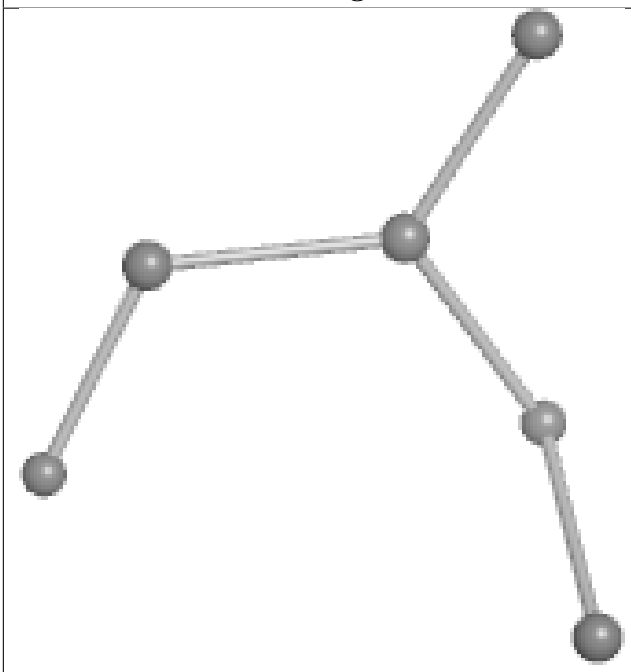
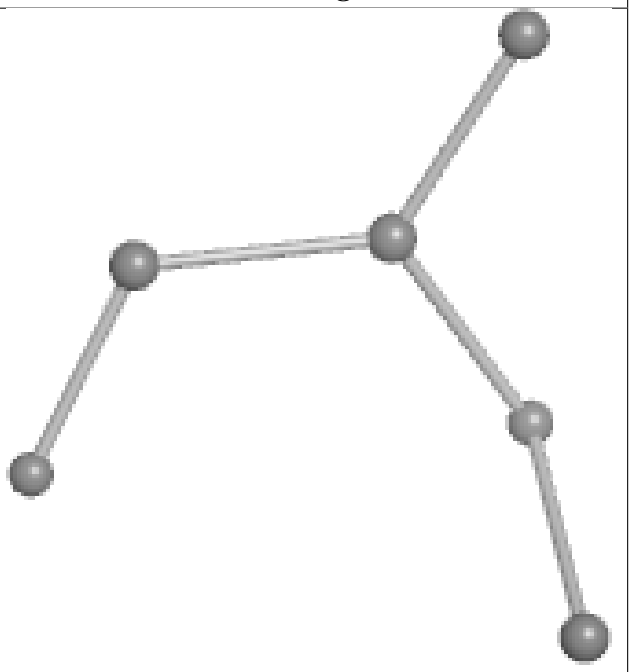
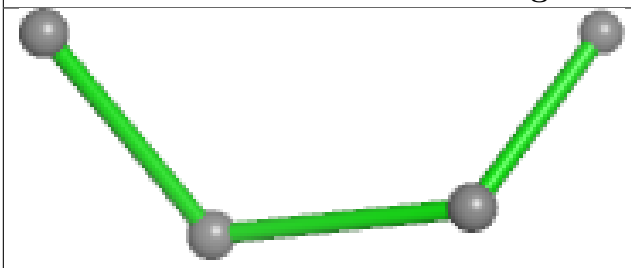


Torsions

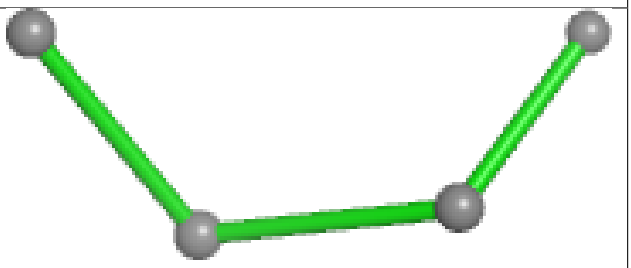


Rings

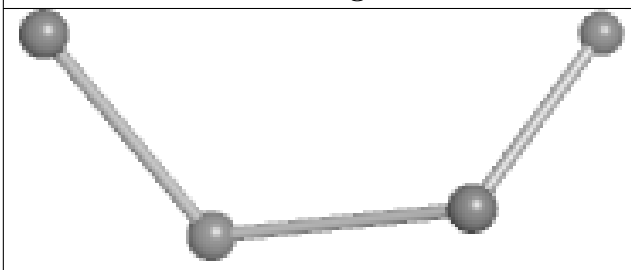
Ligand PPI B 406



Bond lengths



Bond angles



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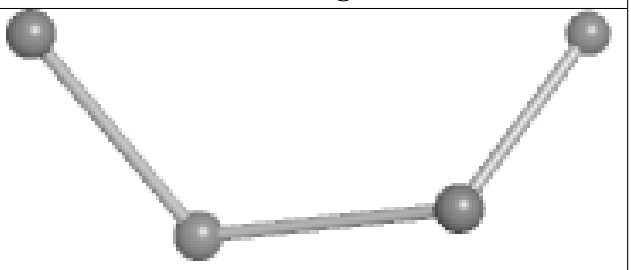
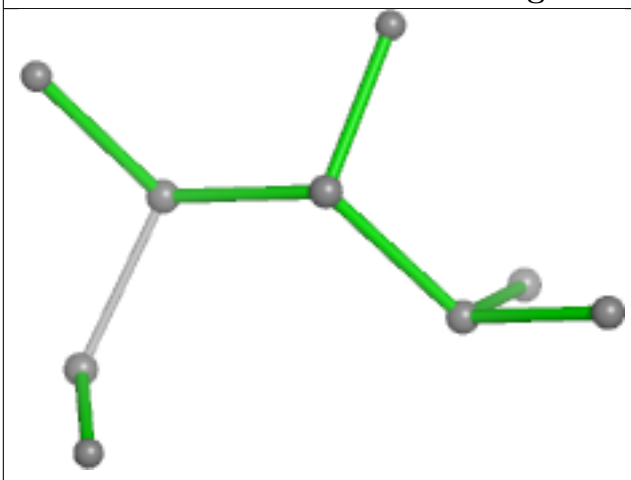


Rings

Ligand HL2 A 412



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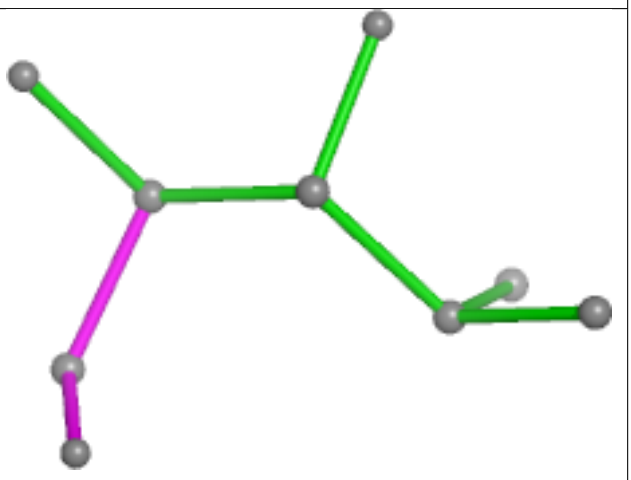
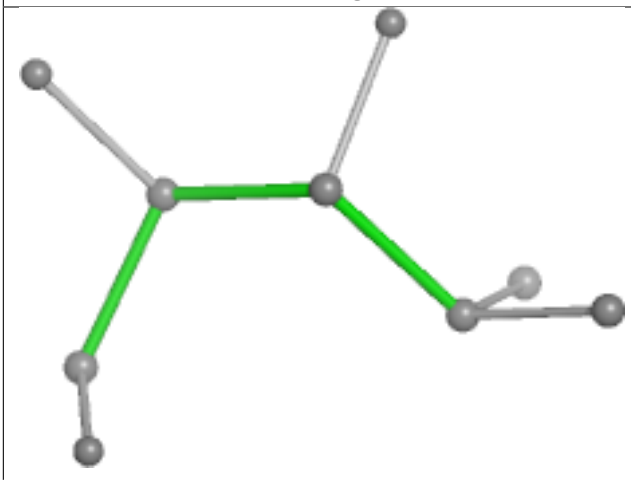
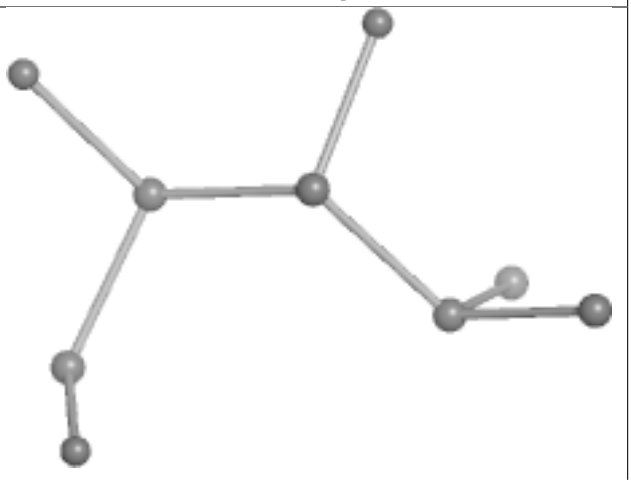


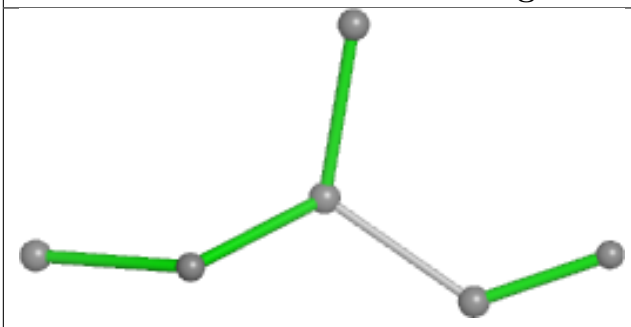
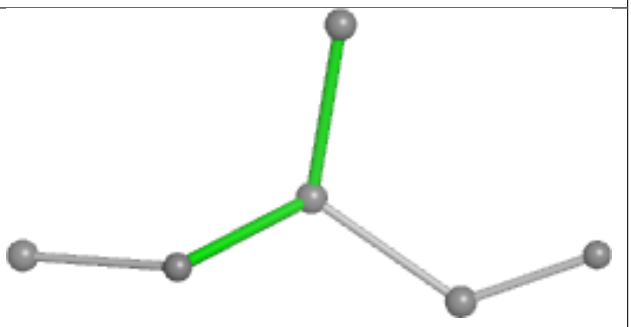
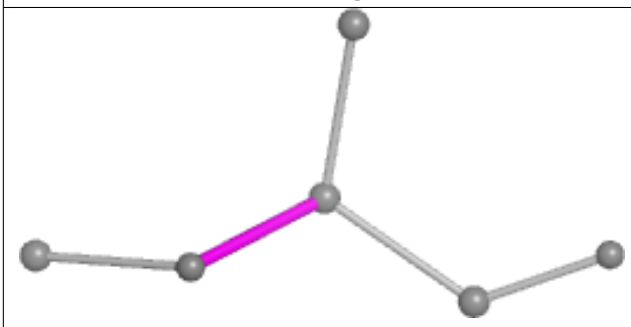
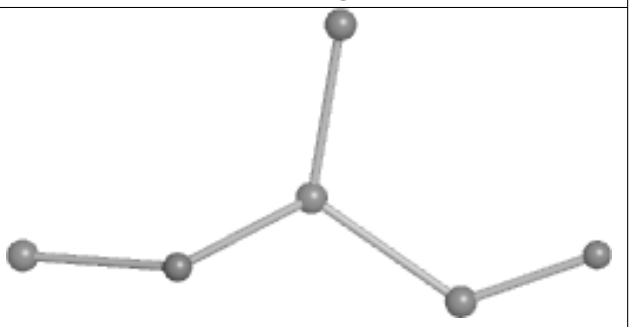
Bond angles

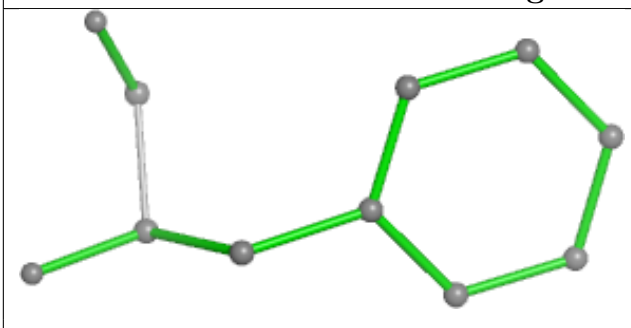
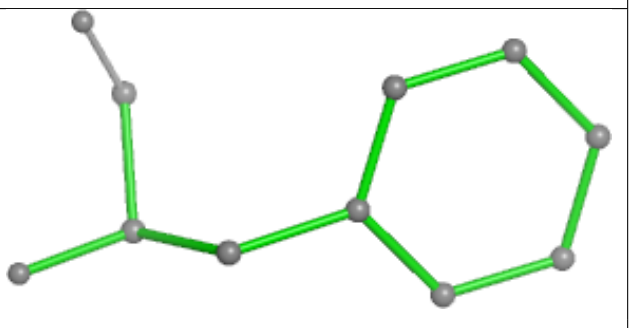
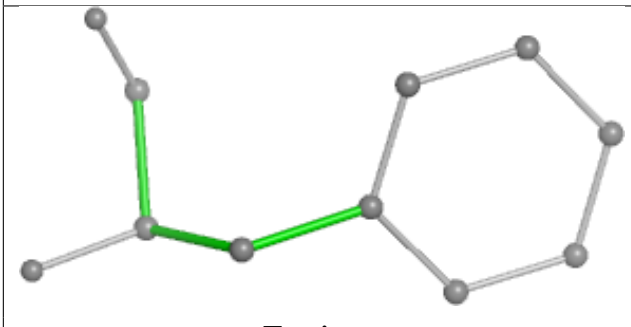
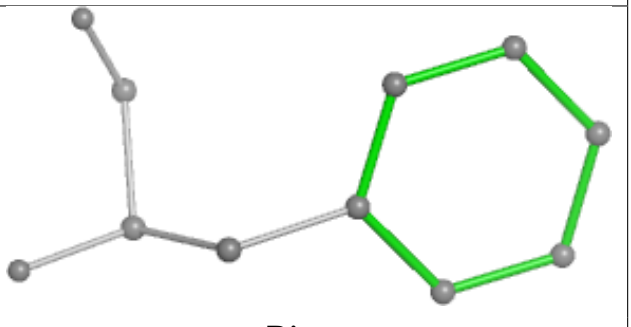


Torsions

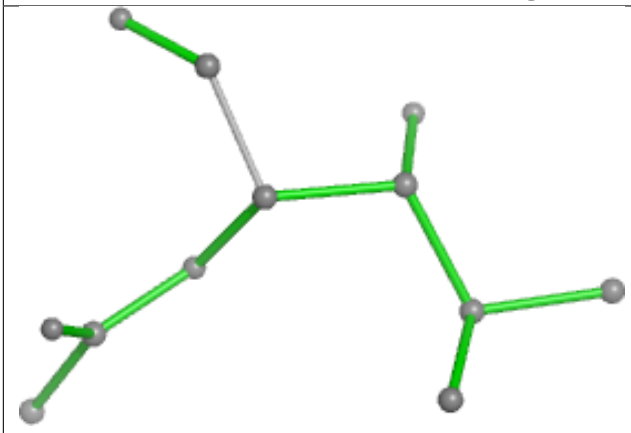


Rings

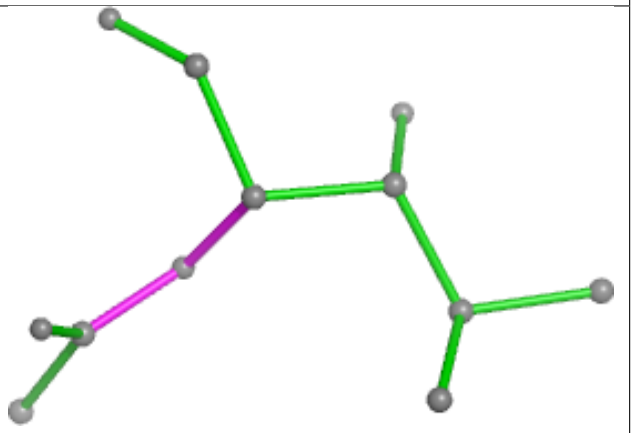
Ligand MAA B 404	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand HF2 A 409	
 Bond lengths	 Bond angles
 Torsions	 Rings

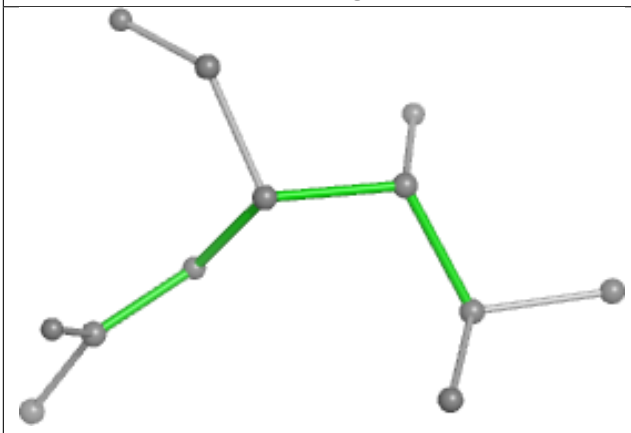
Ligand UDL A 410



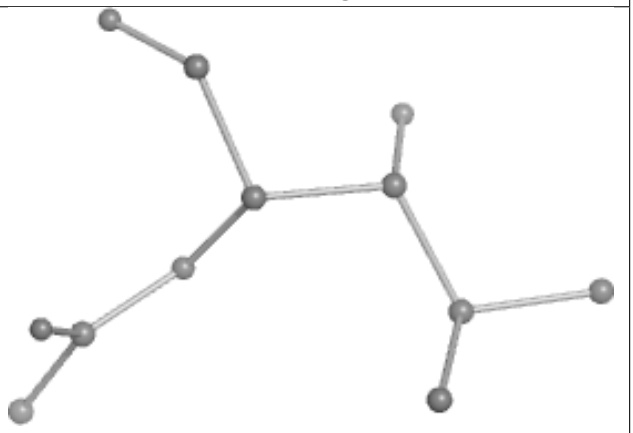
Bond lengths



Bond angles

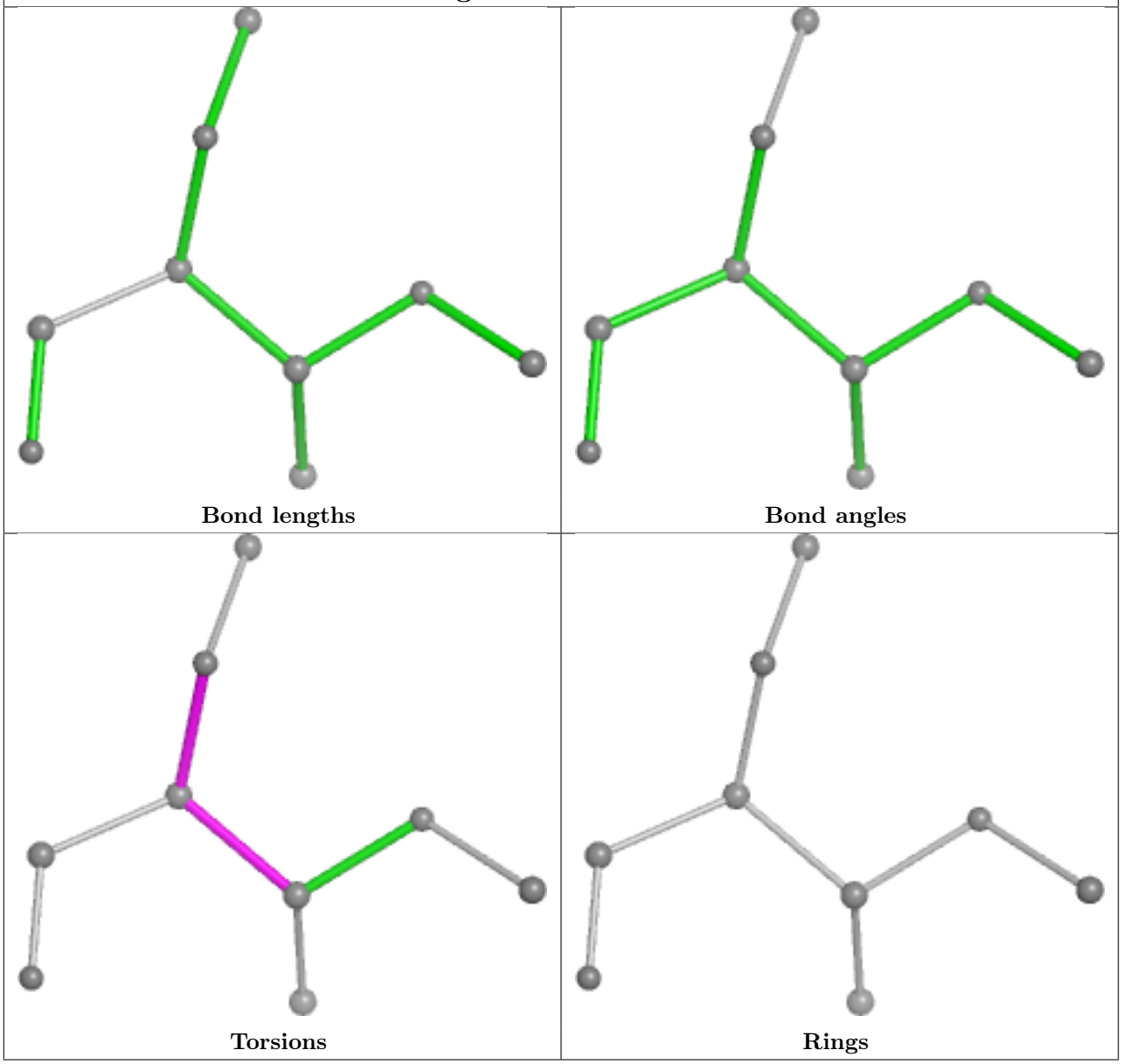


Torsions



Rings

Ligand OTH A 411



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	337/352 (95%)	-0.05	11 (3%) 49 50	6, 25, 53, 72	25 (7%)
2	B	335/344 (97%)	-0.35	5 (1%) 71 74	7, 19, 45, 77	16 (4%)
3	G	60/71 (84%)	0.45	5 (8%) 19 17	17, 36, 69, 83	1 (1%)
All	All	732/767 (95%)	-0.14	21 (2%) 54 54	6, 23, 53, 83	42 (5%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	G	8	ALA	6.7
2	B	4	LEU	4.1
1	A	239	LEU	3.6
1	A	321	ASP	3.5
1	A	240	VAL	3.4
1	A	263	TRP	3.1
3	G	10	ILE	3.0
1	A	244	ASN	3.0
2	B	128	THR	3.0
2	B	2	SER	2.8
1	A	316	LEU	2.6
3	G	54	PRO	2.5
3	G	67	PHE	2.5
2	B	6	GLN	2.3
1	A	170	LEU	2.1
1	A	243	ASP	2.1
1	A	96[A]	THR	2.1
2	B	5	ASP	2.0
1	A	313	PHE	2.0
3	G	66	LYS	2.0
1	A	238	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)

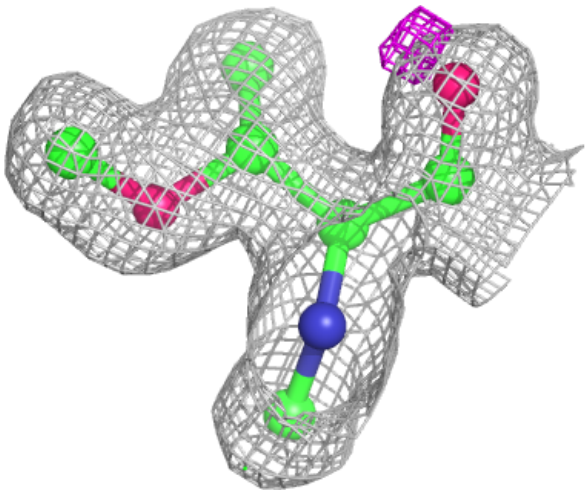
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

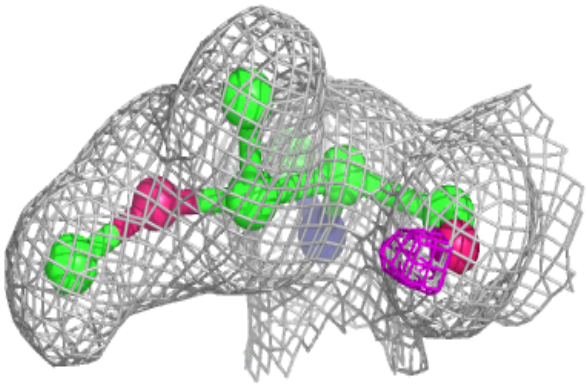
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	EDO	B	403	4/4	0.79	0.15	31,31,33,33	0
16	DMS	G	103	4/4	0.80	0.19	40,44,53,57	0
16	DMS	G	101	4/4	0.82	0.20	78,83,88,96	0
4	EDO	A	402	4/4	0.83	0.14	43,44,53,54	0
4	EDO	B	402	4/4	0.92	0.11	25,37,40,41	0
4	EDO	B	401	4/4	0.93	0.10	33,40,42,42	0
16	DMS	G	102	4/4	0.94	0.10	38,46,49,54	0
11	OTH	A	411	9/10	0.96	0.07	22,23,25,27	0
4	EDO	A	401	4/4	0.96	0.08	25,29,32,34	0
4	EDO	A	404	4/4	0.97	0.08	20,24,28,28	0
12	HL2	A	412	9/10	0.97	0.06	18,19,20,22	0
13	MAA	B	404	6/7	0.97	0.07	20,21,25,27	0
4	EDO	A	403	4/4	0.97	0.07	29,33,34,37	0
9	HF2	A	409	11/12	0.97	0.04	17,18,20,24	0
10	UDL	A	410	12/13	0.97	0.06	22,25,26,27	0
8	DAM	A	408	6/7	0.98	0.04	17,19,20,21	0
14	ALA	B	405	5/6	0.98	0.05	18,18,19,20	0
15	PPI	B	406	4/5	0.98	0.05	19,20,21,22	0
5	GDP	A	405	28/28	0.99	0.03	14,15,16,17	0
12	HL2	A	413	9/10	0.99	0.04	16,18,24,24	0
6	ZN	A	406	1/1	1.00	0.05	20,20,20,20	0
7	CL	A	407	1/1	1.00	0.07	23,23,23,23	0

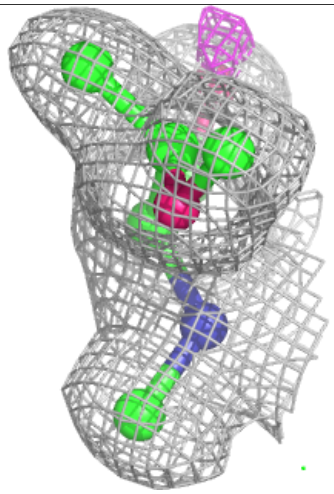
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around OTH A 411:

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

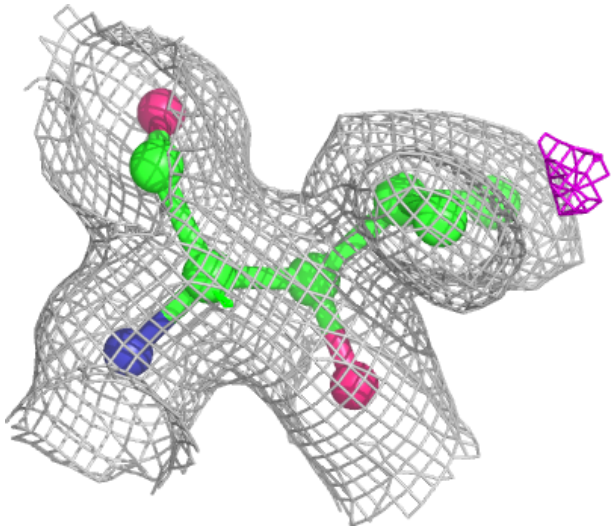


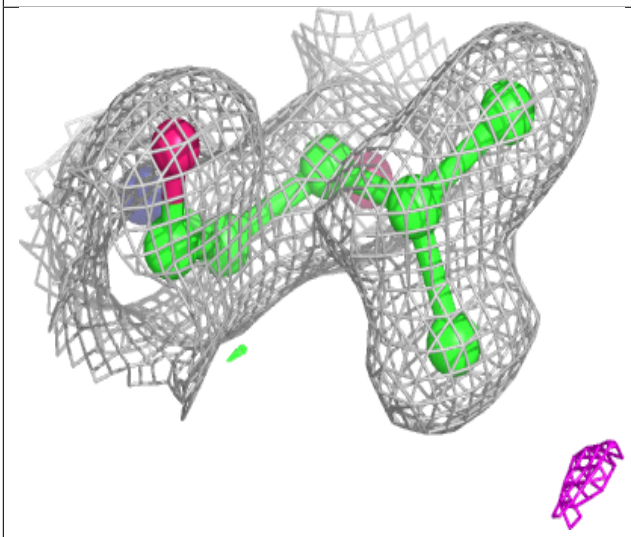


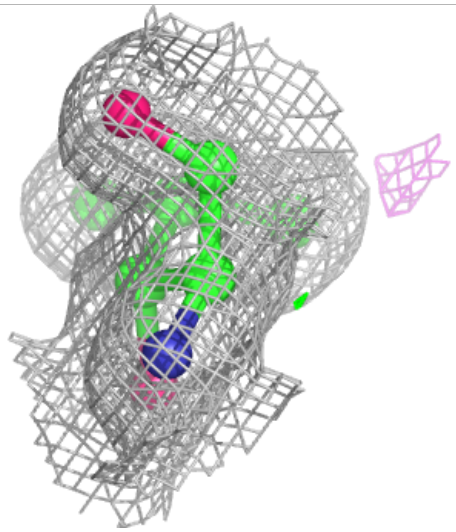


Electron density around HL2 A 412:

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

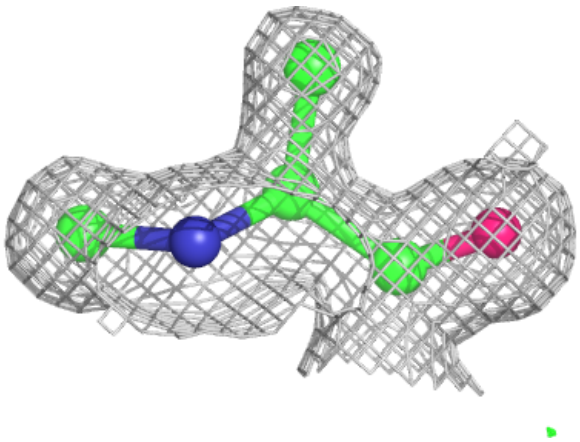


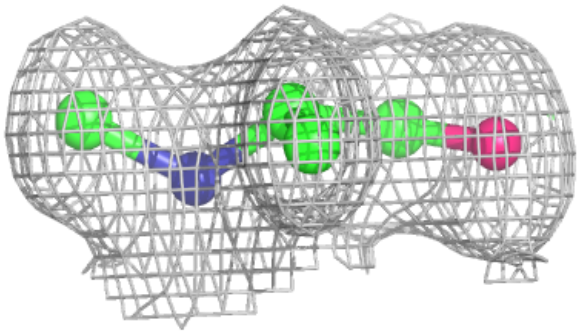


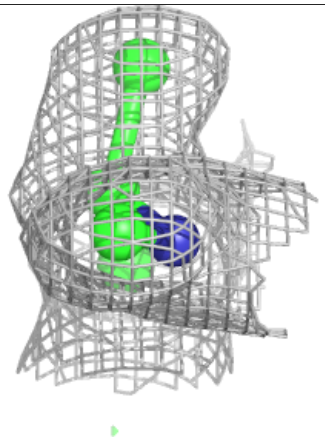


Electron density around MAA B 404:

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

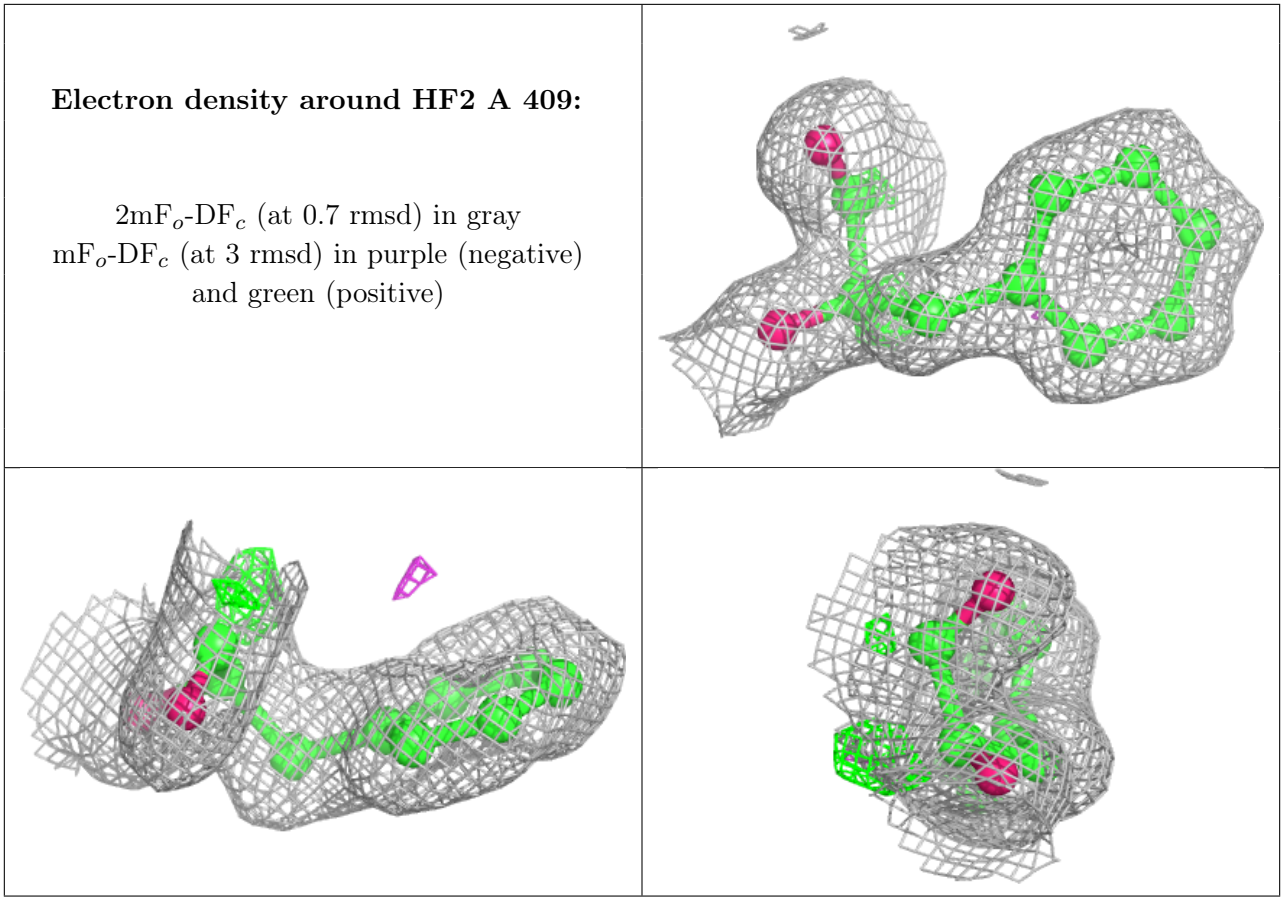






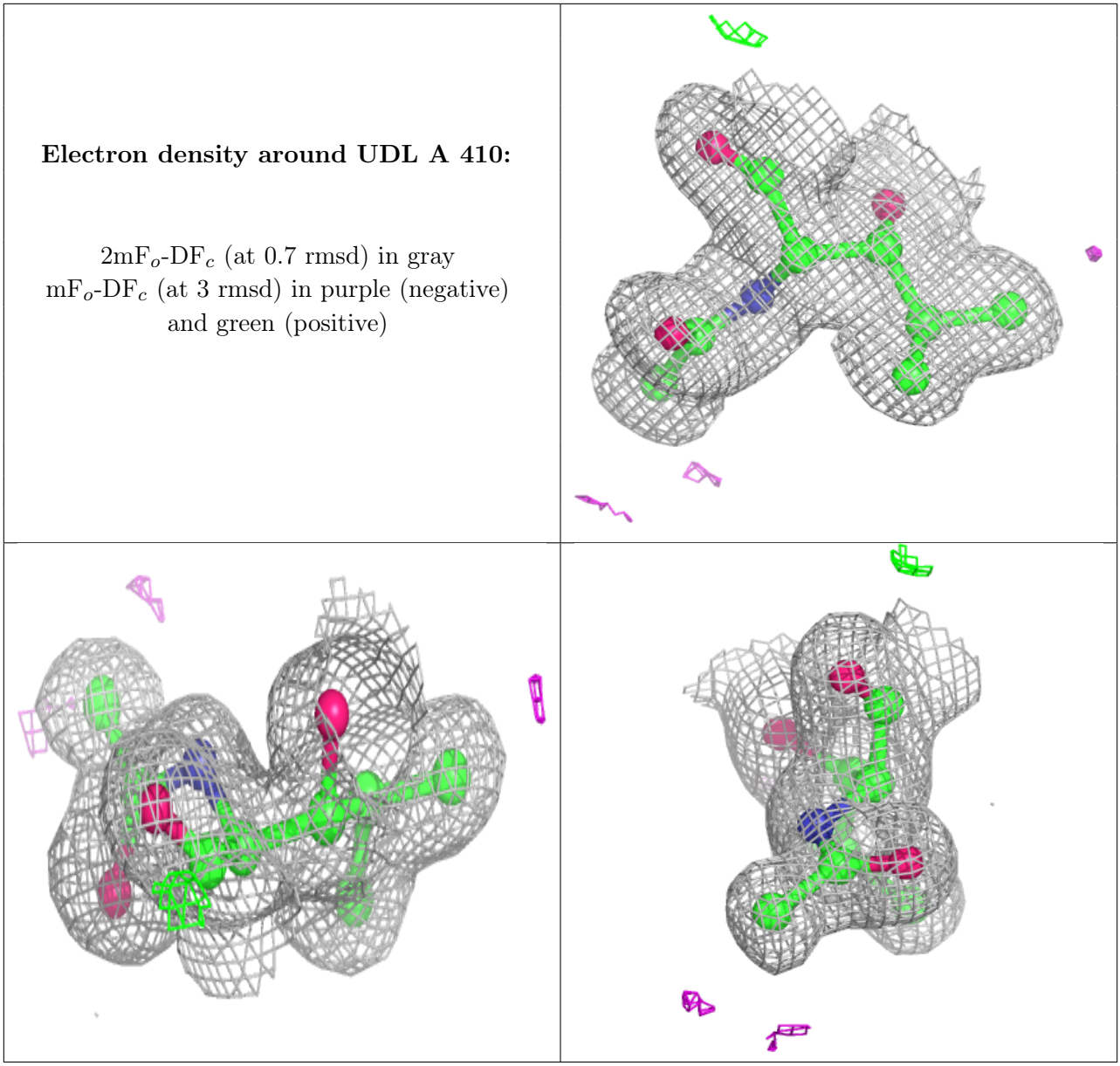
Electron density around HF2 A 409:

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



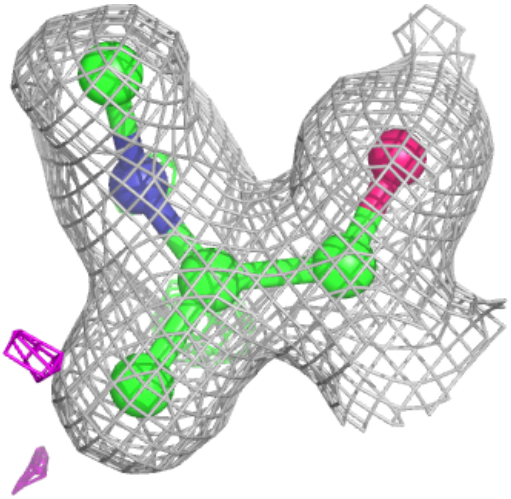
Electron density around UDL A 410:

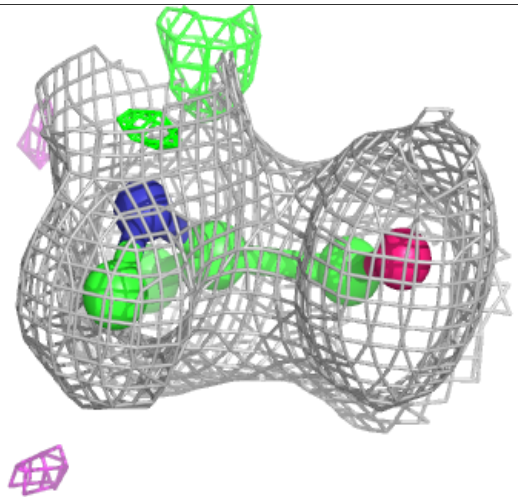
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

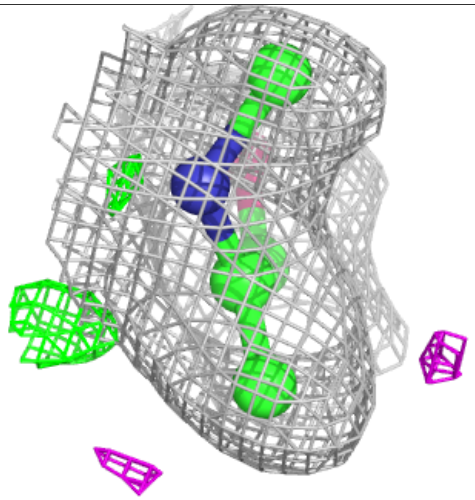


Electron density around DAM A 408:

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

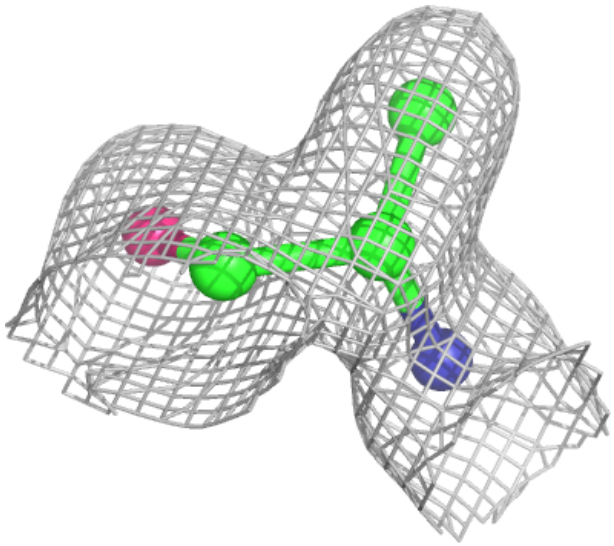


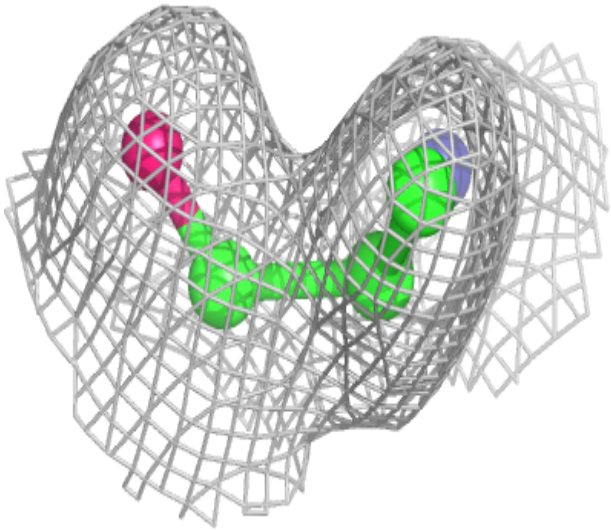


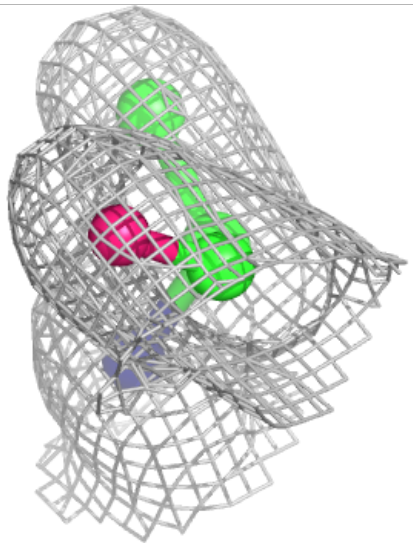


Electron density around ALA B 405:

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

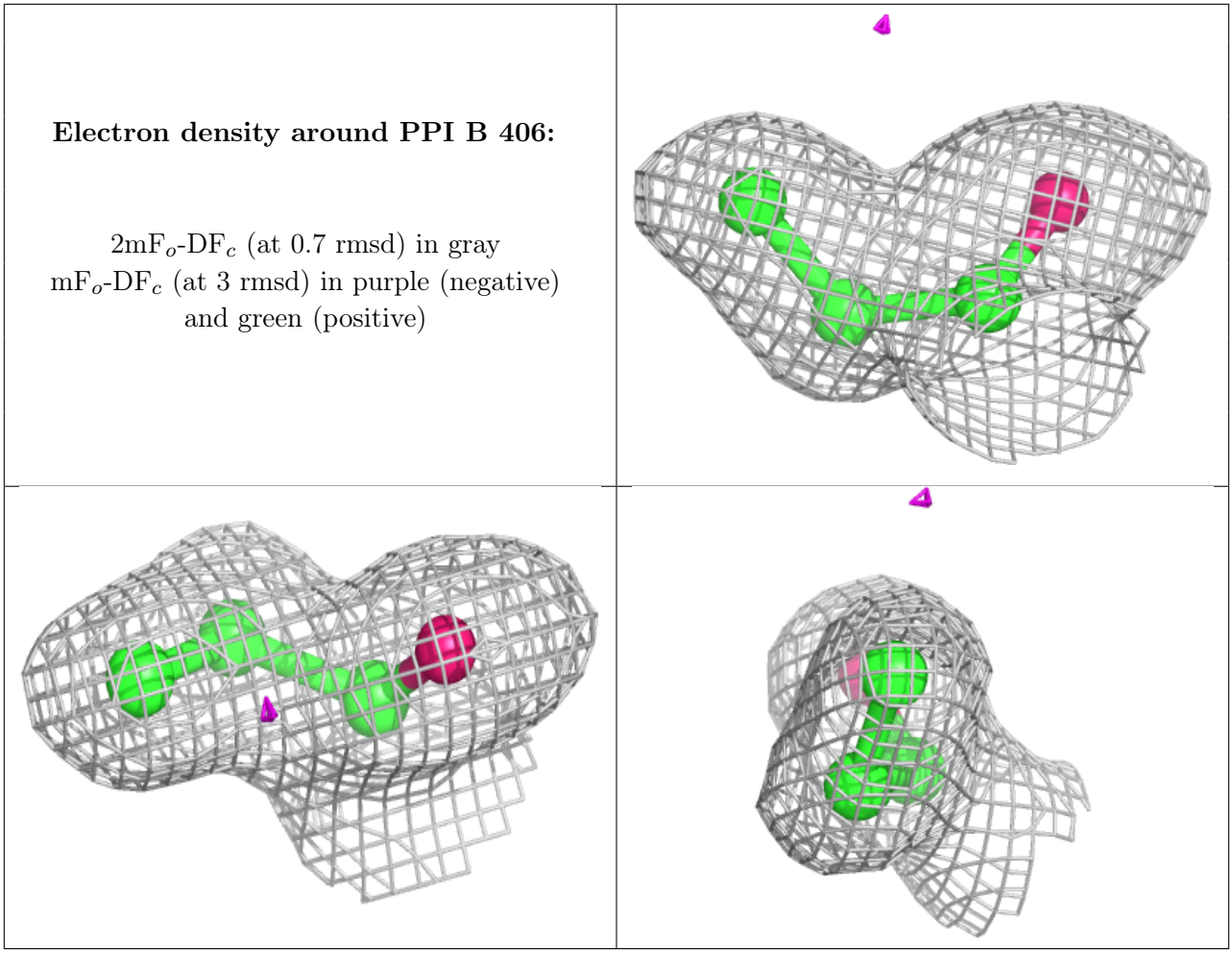






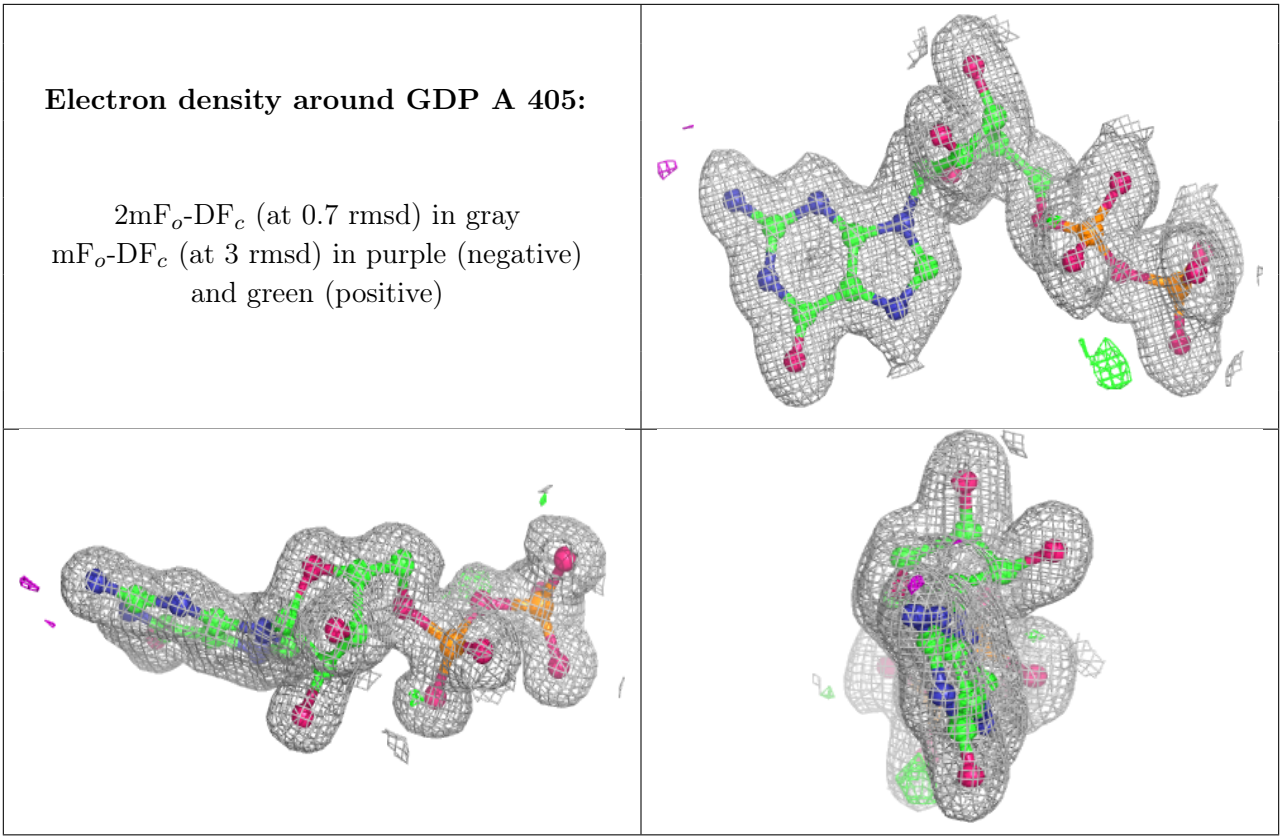
Electron density around PPI B 406:

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



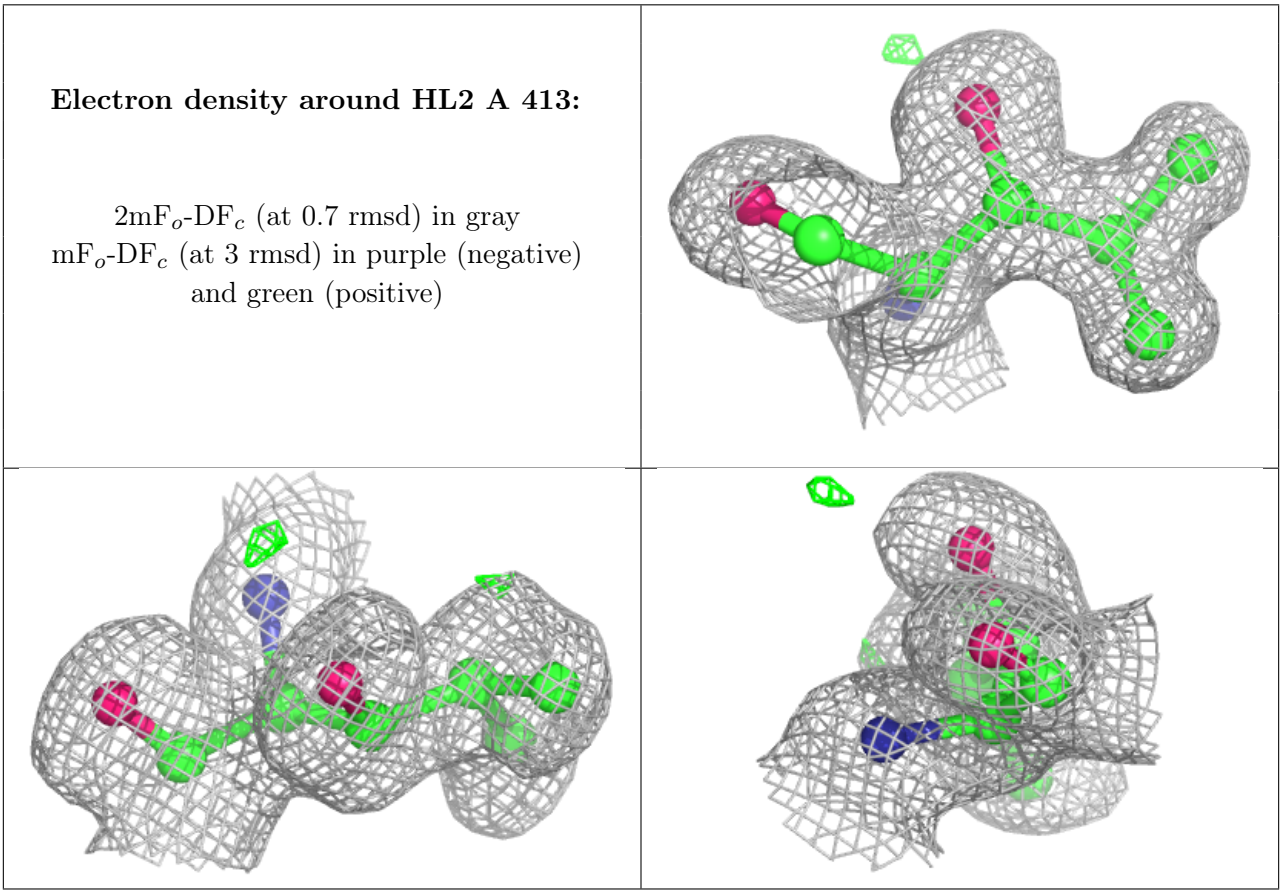
Electron density around GDP A 405:

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



Electron density around HL2 A 413:

$2mF_o$-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.