



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 10:30 AM UTC

PDB ID : 8QEH / pdb_00008qeh
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 wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

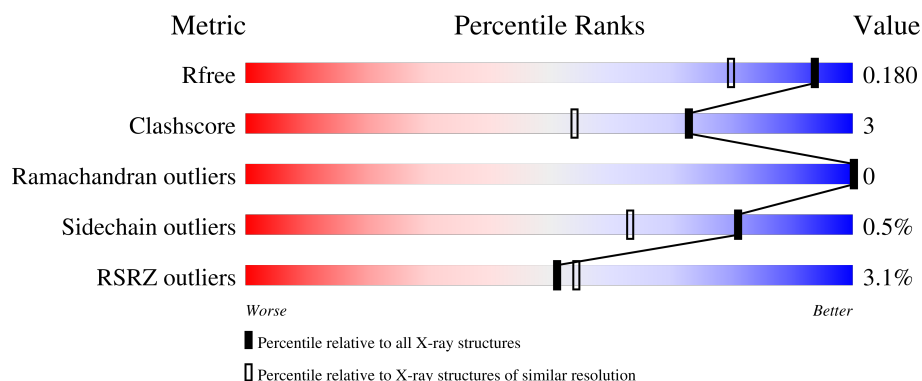
1 Overall quality at a glance

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}	180053	3234 (1.46-1.42)
Clashscore	190562	3289 (1.46-1.42)
Ramachandran outliers	187476	3248 (1.46-1.42)
Sidechain outliers	187428	3248 (1.46-1.42)
RSRZ outliers	180081	3234 (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 $\leq 5\%$. 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	4% 87% 8% .
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

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
1	A	337	Total	C	N	O	S	0	25	0
			2955	1879	509	551	16			

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

Continued on next page...

Continued from previous page...

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

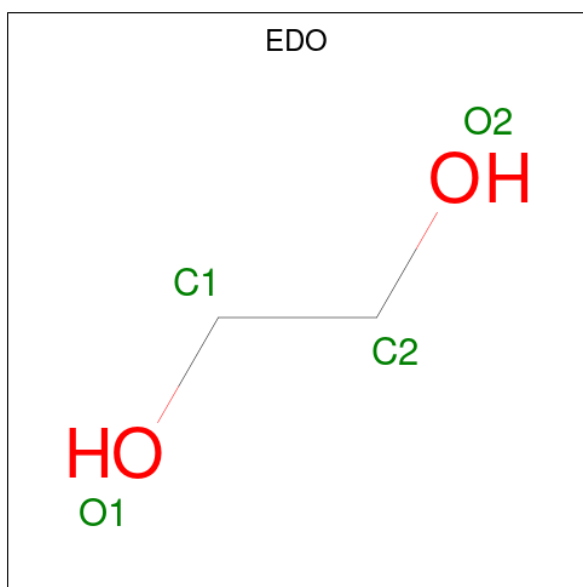
- Molecule 3 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2.

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:

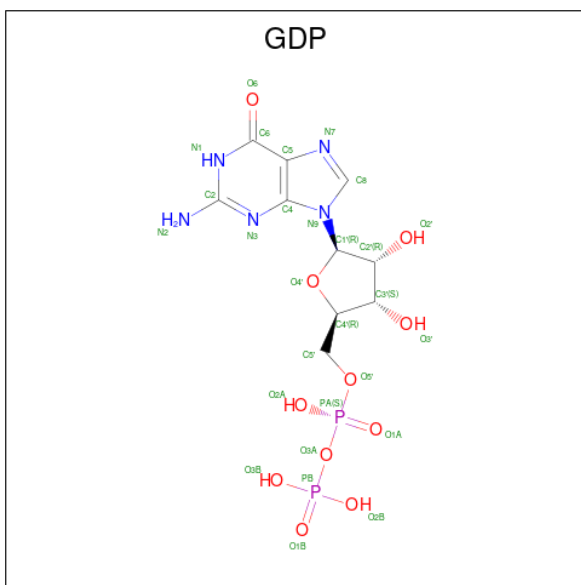
Chain	Residue	Modelled	Actual	Comment	Reference
G	69	SER	CYS	engineered mutation	UNP P59768

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

- Molecule 5 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂) (labeled as "Ligand of Interest" by depositor).



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

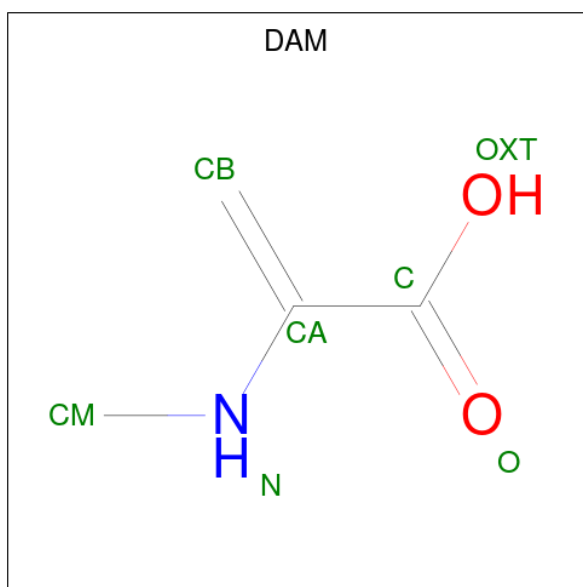
- Molecule 6 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

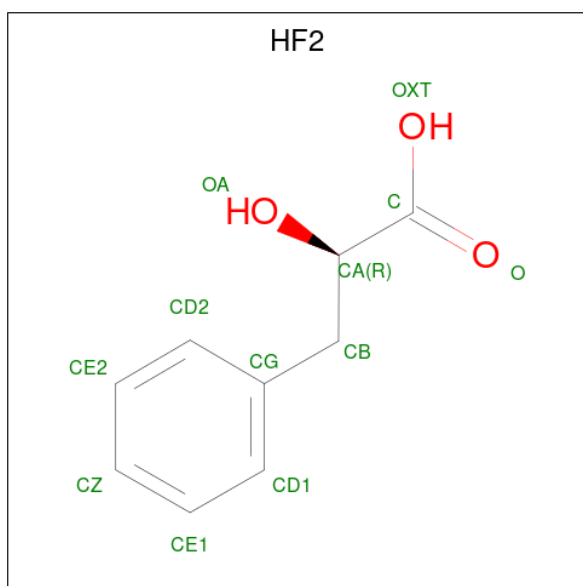
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Cl 1 1	0	0

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



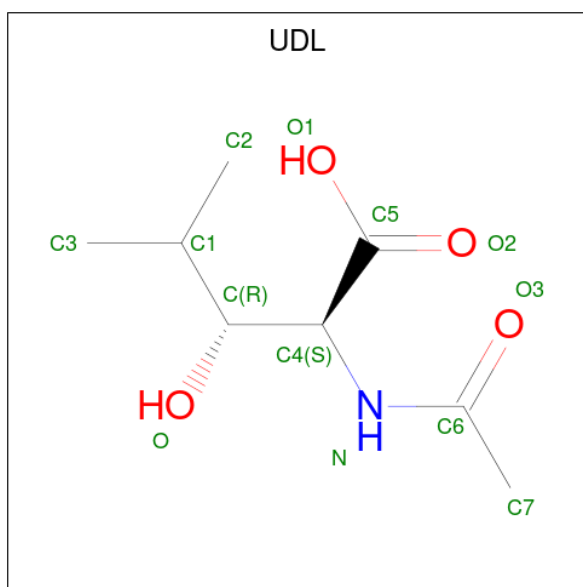
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			6	4	1	1		

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



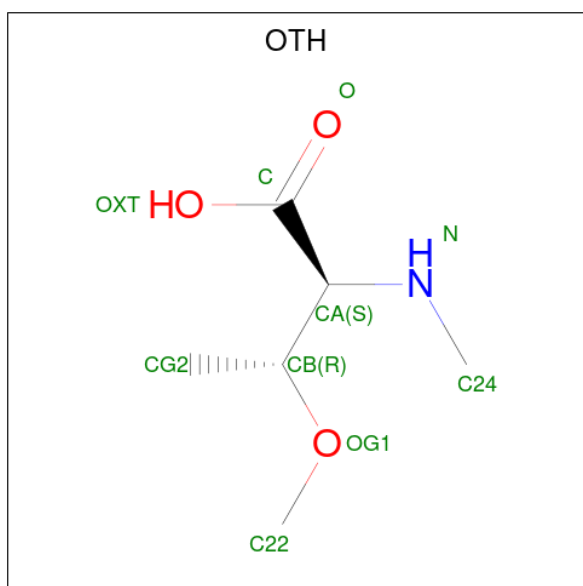
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			11	9	2		

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



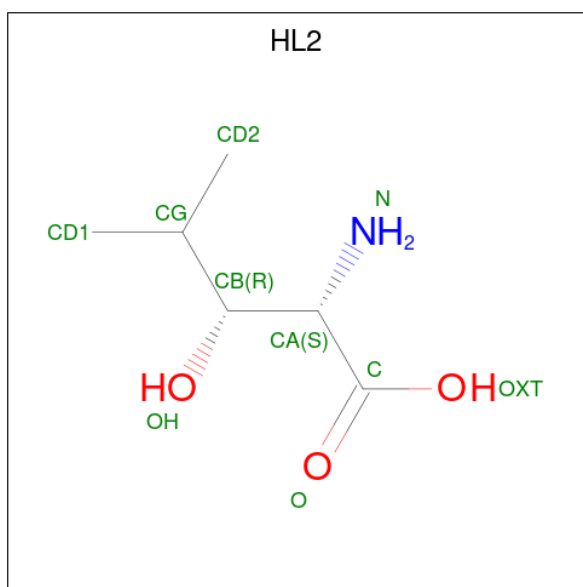
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	A	1	Total	C	N	O	0	0
			12	8	1	3		

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



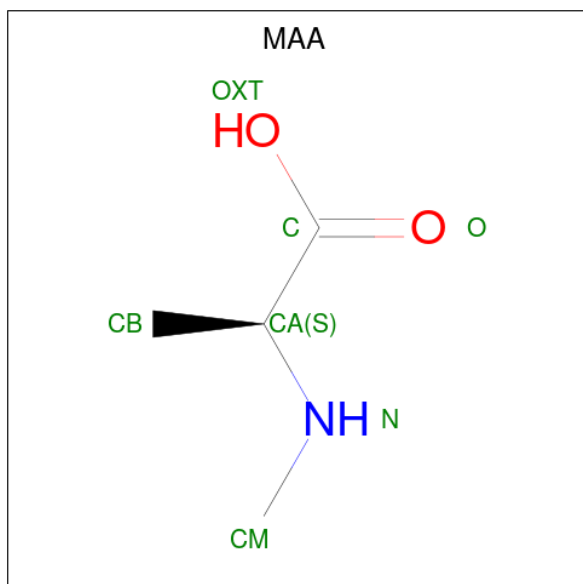
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	A	1	Total	C	N	O	0	0
			9	6	1	2		

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



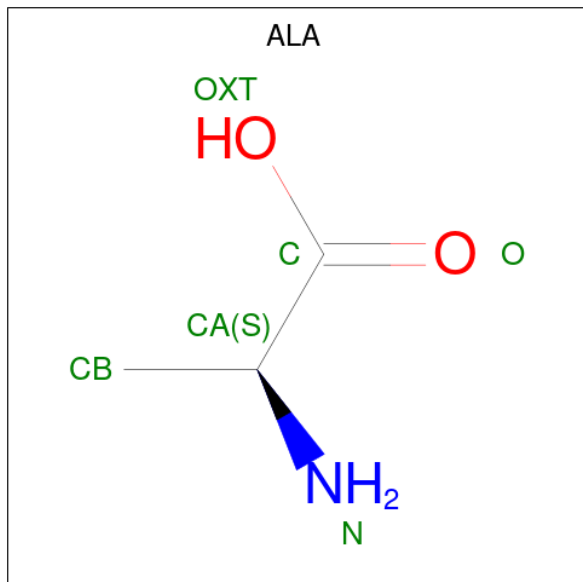
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	A	1	Total	C	N	O	0	0
			9	6	1	2		
12	A	1	Total	C	N	O	0	0
			9	6	1	2		

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



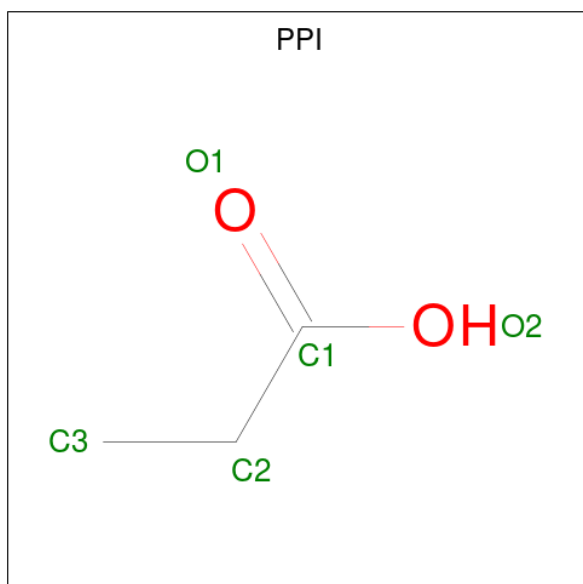
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	B	1	Total	C	N	O	0	0
			6	4	1	1		

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



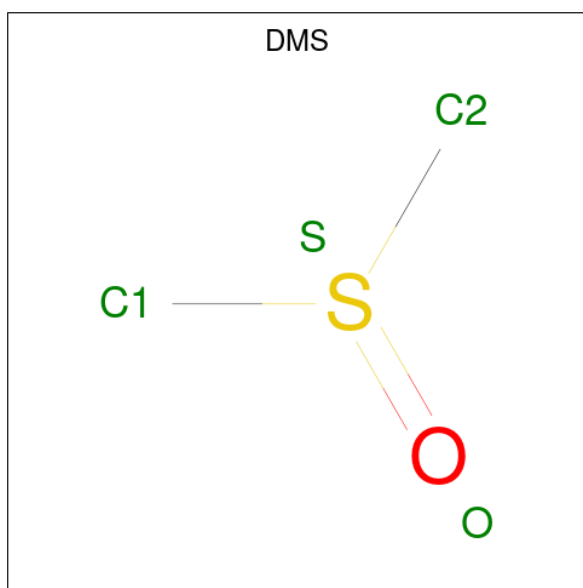
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
14	B	1	5	3	1	1	0	0

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



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

- Molecule 16 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C_2H_6OS).



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

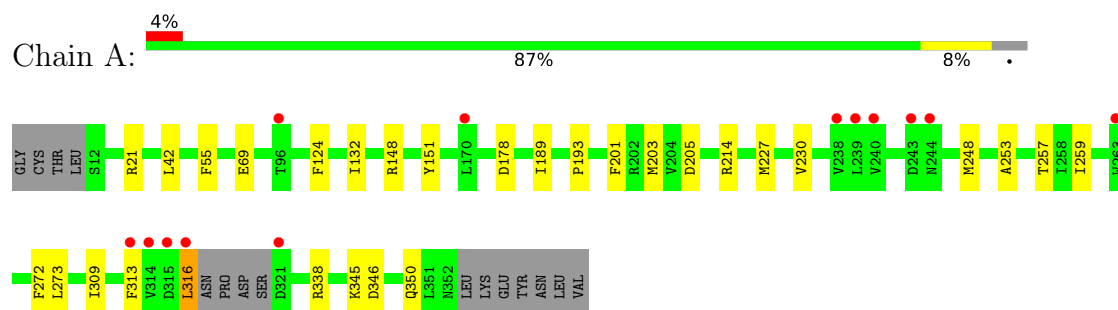
- Molecule 17 is water.

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

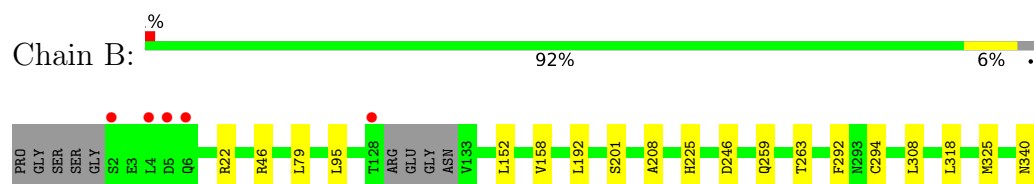
3 Residue-property plots [i](#)

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.

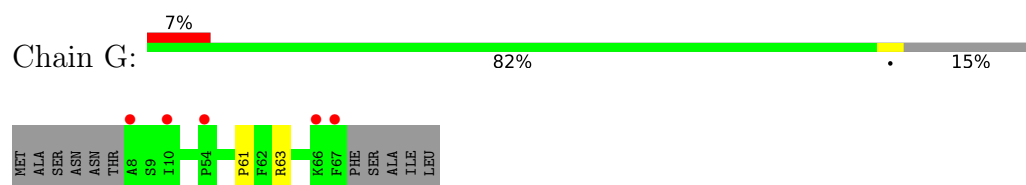
- Molecule 1: Guanine nucleotide-binding protein subunit alpha-11



- 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

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
$\langle I/\sigma(I) \rangle$ 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	7962 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	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: MAA, HF2, OTH, UDL, PPI, HL2, CL, ZN, DMS, DAM, GDP, EDO

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	0.52	0/3006	0.87	3/4047 (0.1%)
2	B	0.56	0/2697	0.88	2/3657 (0.1%)
3	G	0.55	0/466	0.88	0/630
All	All	0.54	0/6169	0.87	5/8334 (0.1%)

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 (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	205	ASP	CA-CB-CG	7.68	120.28	112.60
2	B	246	ASP	CA-CB-CG	5.81	118.41	112.60
1	A	178	ASP	CA-CB-CG	5.23	117.83	112.60
1	A	346	ASP	CA-CB-CG	5.18	117.78	112.60
2	B	292	PHE	CA-CB-CG	5.04	118.84	113.80

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	20	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	39	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.

The worst 5 of 39 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:227:MET:HE3	1:A:272:PHE:CE2	2.11	0.84

Continued on next page...

Continued from previous page...

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
1:A:227:MET:HE3	1:A:272:PHE:HE2	1.47	0.79
3:G:63:ARG:HH21	16:G:102:DMS:H13	1.51	0.74
1:A:230[B]:VAL:HG13	1:A:273[B]:LEU:HD23	1.70	0.72

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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%)	313 (99%)	3 (1%)	70	44
2	B	285/285 (100%)	285 (100%)	0	100	100
3	G	44/58 (76%)	44 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	645/660 (98%)	642 (100%)	3 (0%)	81	63

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	316	LEU
1	A	345	LYS
1	A	350	GLN

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

Mol	Chain	Res	Type
1	A	126	HIS
1	A	222	ASN
3	G	25	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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
16	DMS	G	101	-	3,3,3	0.30	0	3,3,3	0.09	0
4	EDO	A	401	-	3,3,3	0.33	0	2,2,2	0.43	0
14	ALA	B	405	13,8	3,4,5	0.71	0	2,4,6	1.10	0
9	HF2	A	409	10,8	10,11,12	0.74	0	11,13,15	0.46	0
4	EDO	A	402	-	3,3,3	0.19	0	2,2,2	0.05	0
15	PPI	B	406	12	3,3,4	0.73	0	1,2,4	0.95	0
4	EDO	B	402	-	3,3,3	0.07	0	2,2,2	0.48	0
8	DAM	A	408	9,14	4,5,6	1.68	1 (25%)	3,5,7	3.74	2 (66%)
16	DMS	G	102	-	3,3,3	0.09	0	3,3,3	0.21	0
4	EDO	A	403	-	3,3,3	0.38	0	2,2,2	0.62	0
5	GDP	A	405	-	29,30,30	0.45	0	45,47,47	0.58	0
10	UDL	A	410	9,11	10,11,12	0.56	0	11,14,16	0.57	0
4	EDO	B	403	-	3,3,3	0.55	0	2,2,2	0.21	0
12	HL2	A	412	13,12,11	7,8,9	0.48	0	7,10,12	1.30	1 (14%)
4	EDO	A	404	-	3,3,3	0.46	0	2,2,2	0.44	0
4	EDO	B	401	-	3,3,3	0.08	0	2,2,2	0.12	0
11	OTH	A	411	10,12	7,8,9	0.82	0	5,9,11	0.95	0
13	MAA	B	404	14,12	4,5,6	0.58	0	2,5,7	1.01	0
12	HL2	A	413	15,12	7,8,9	0.44	0	7,10,12	1.03	1 (14%)
16	DMS	G	103	-	3,3,3	0.41	0	3,3,3	0.25	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
9	HF2	A	409	10,8	-	0/5/6/8	0/1/1/1
4	EDO	A	402	-	-	0/1/1/1	-
15	PPI	B	406	12	-	0/0/1/2	-
4	EDO	B	401	-	-	1/1/1/1	-
11	OTH	A	411	10,12	-	5/8/10/12	-
13	MAA	B	404	14,12	-	1/2/4/6	-
5	GDP	A	405	-	-	1/16/32/32	0/3/3/3
12	HL2	A	413	15,12	-	1/9/10/12	-
4	EDO	B	402	-	-	1/1/1/1	-
8	DAM	A	408	9,14	-	0/0/4/6	-
10	UDL	A	410	9,11	-	0/13/14/16	-
4	EDO	A	403	-	-	0/1/1/1	-
4	EDO	A	401	-	-	0/1/1/1	-
4	EDO	B	403	-	-	1/1/1/1	-
12	HL2	A	412	13,12,11	-	0/9/10/12	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	A	404	-	-	1/1/1/1	-
14	ALA	B	405	13,8	-	1/1/2/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	408	DAM	C-CA	-2.72	1.40	1.45

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	408	DAM	CB-CA-N	-5.54	112.18	125.84
12	A	412	HL2	O-C-CA	-3.09	116.81	124.77
8	A	408	DAM	O-C-CA	-3.05	121.36	125.33
12	A	413	HL2	O-C-CA	-2.30	118.86	124.77

There are no chirality outliers.

5 of 13 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
14	B	405	ALA	O-C-CA-CB
4	B	401	EDO	O1-C1-C2-O2
11	A	411	OTH	N-CA-CB-CG2

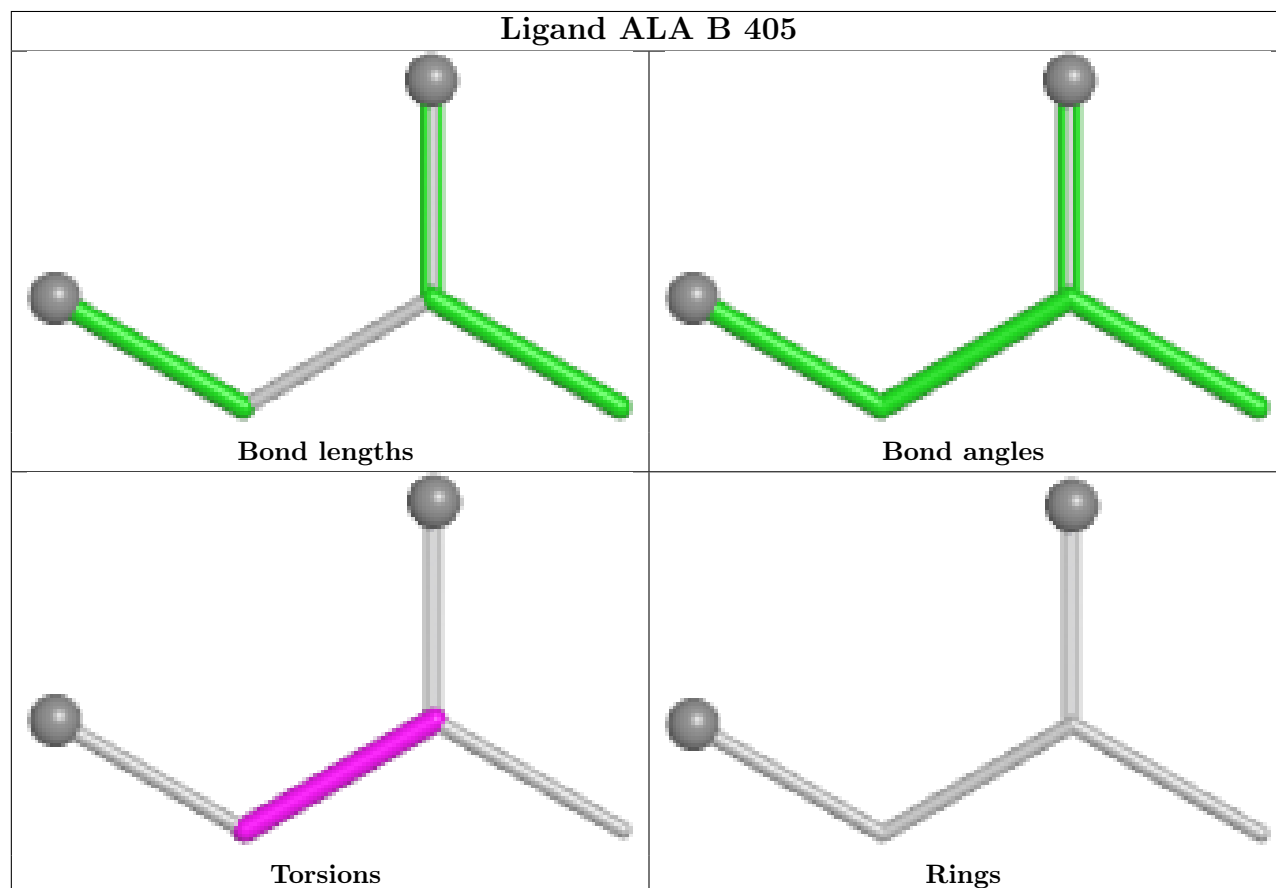
There are no ring outliers.

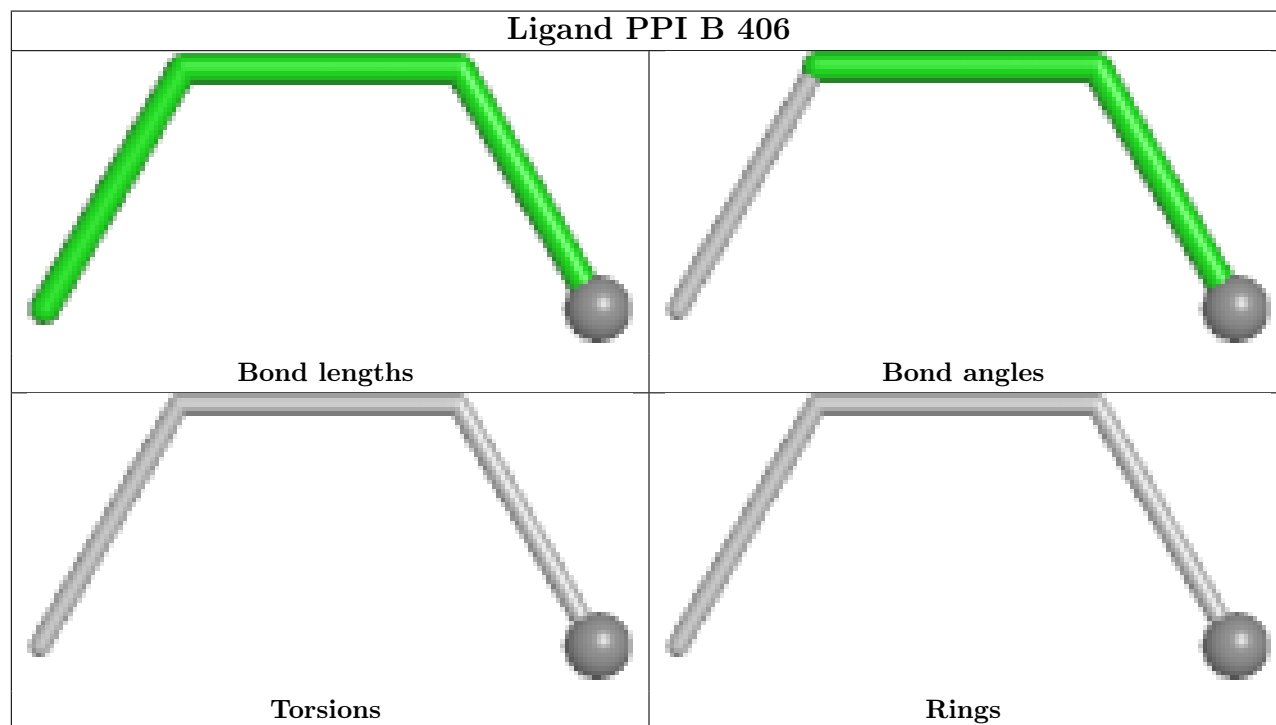
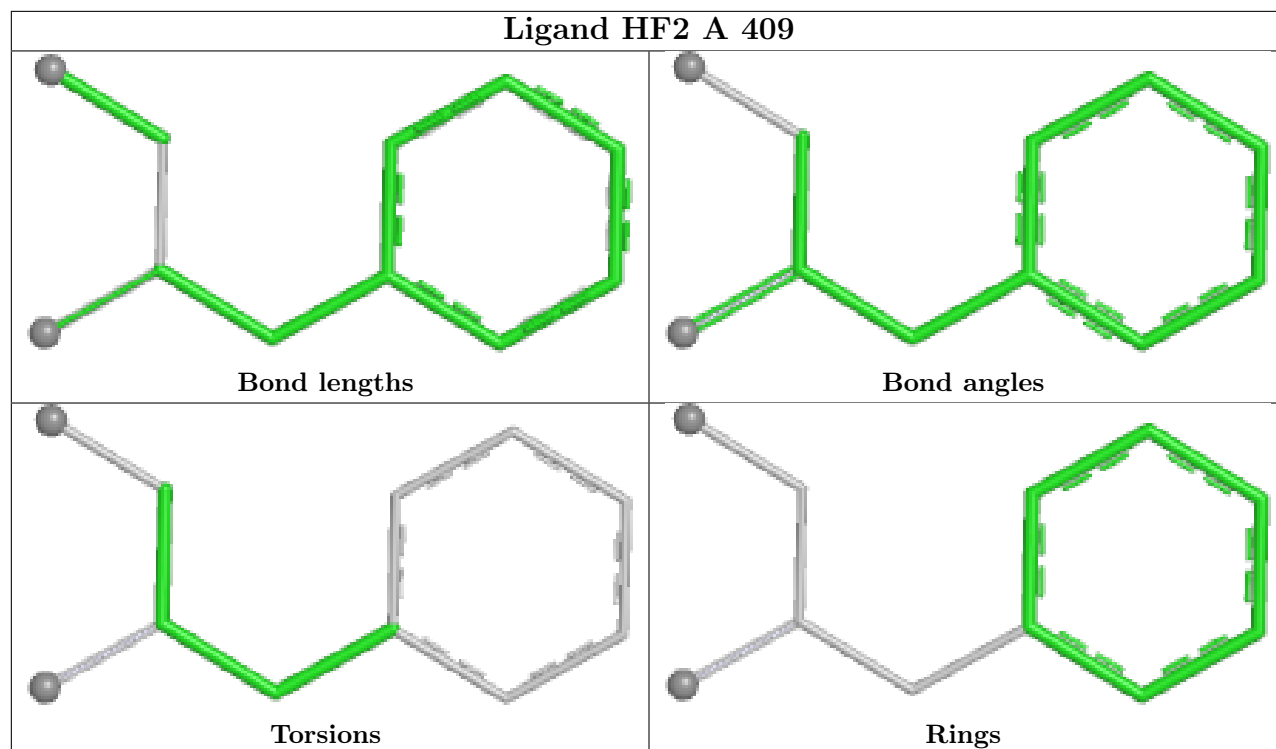
5 monomers are involved in 12 short contacts:

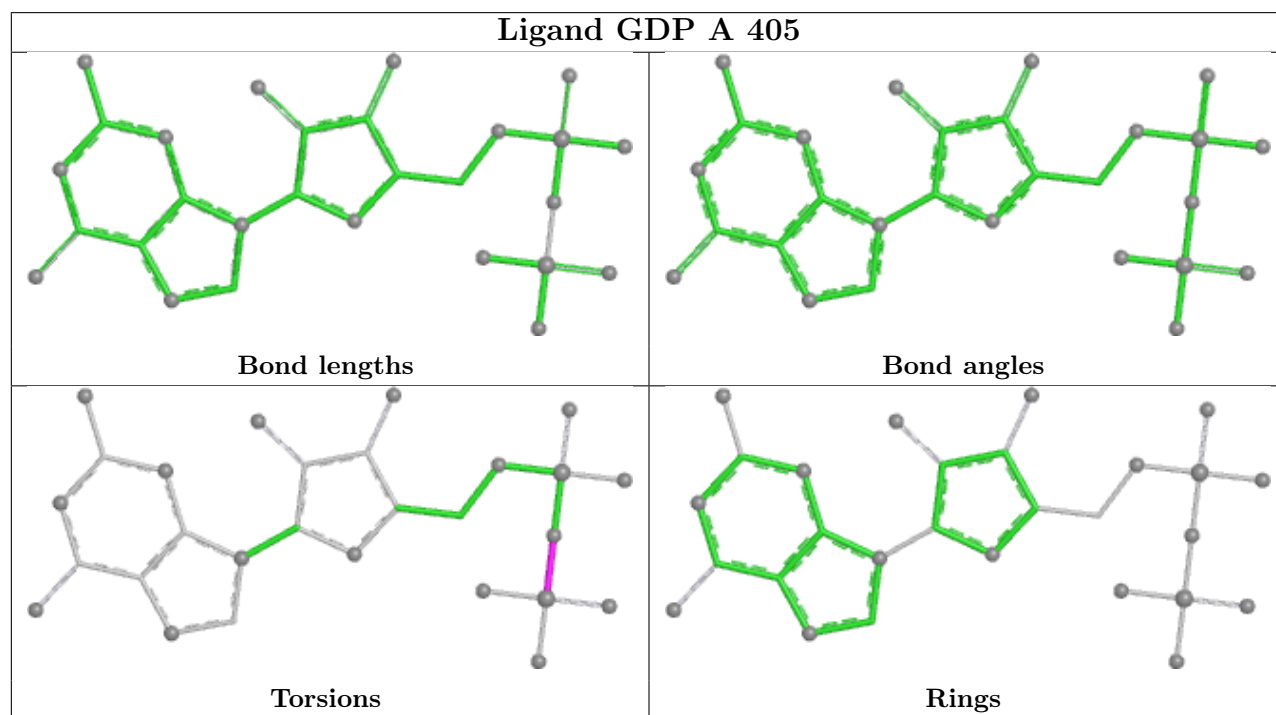
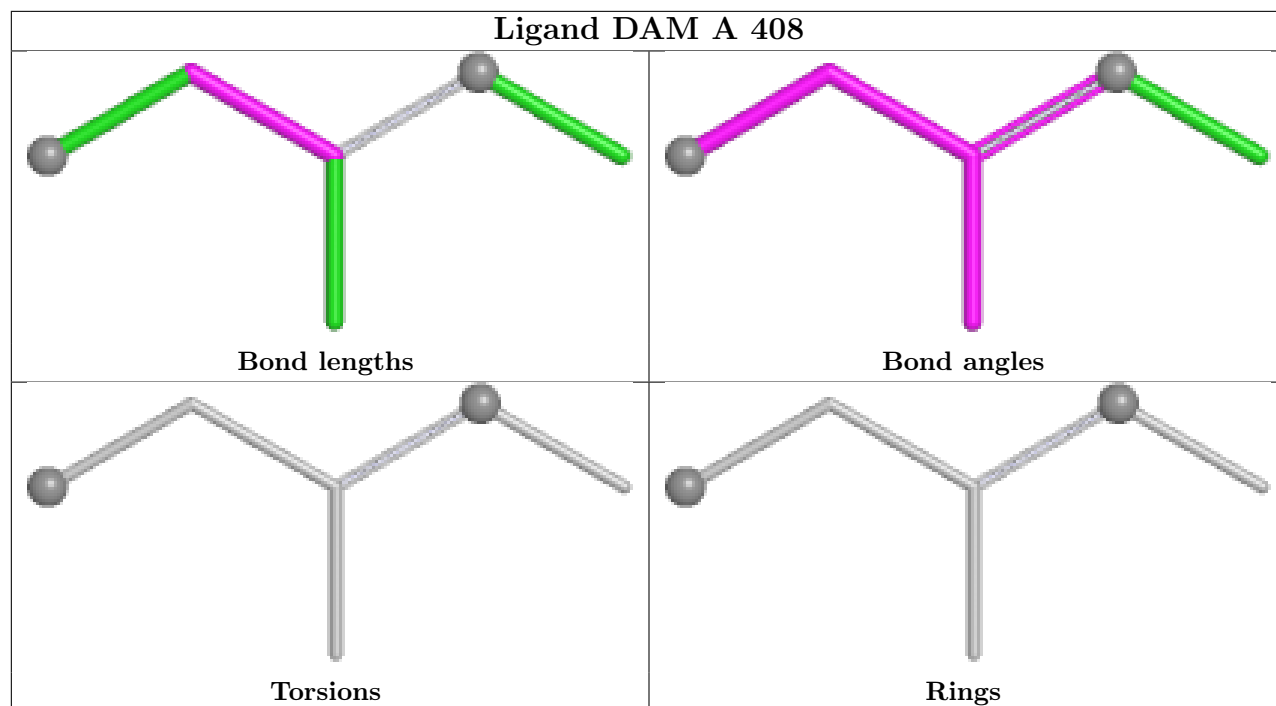
Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	G	102	DMS	6	0
4	B	403	EDO	2	0
4	B	401	EDO	1	0
12	A	413	HL2	1	0
16	G	103	DMS	2	0

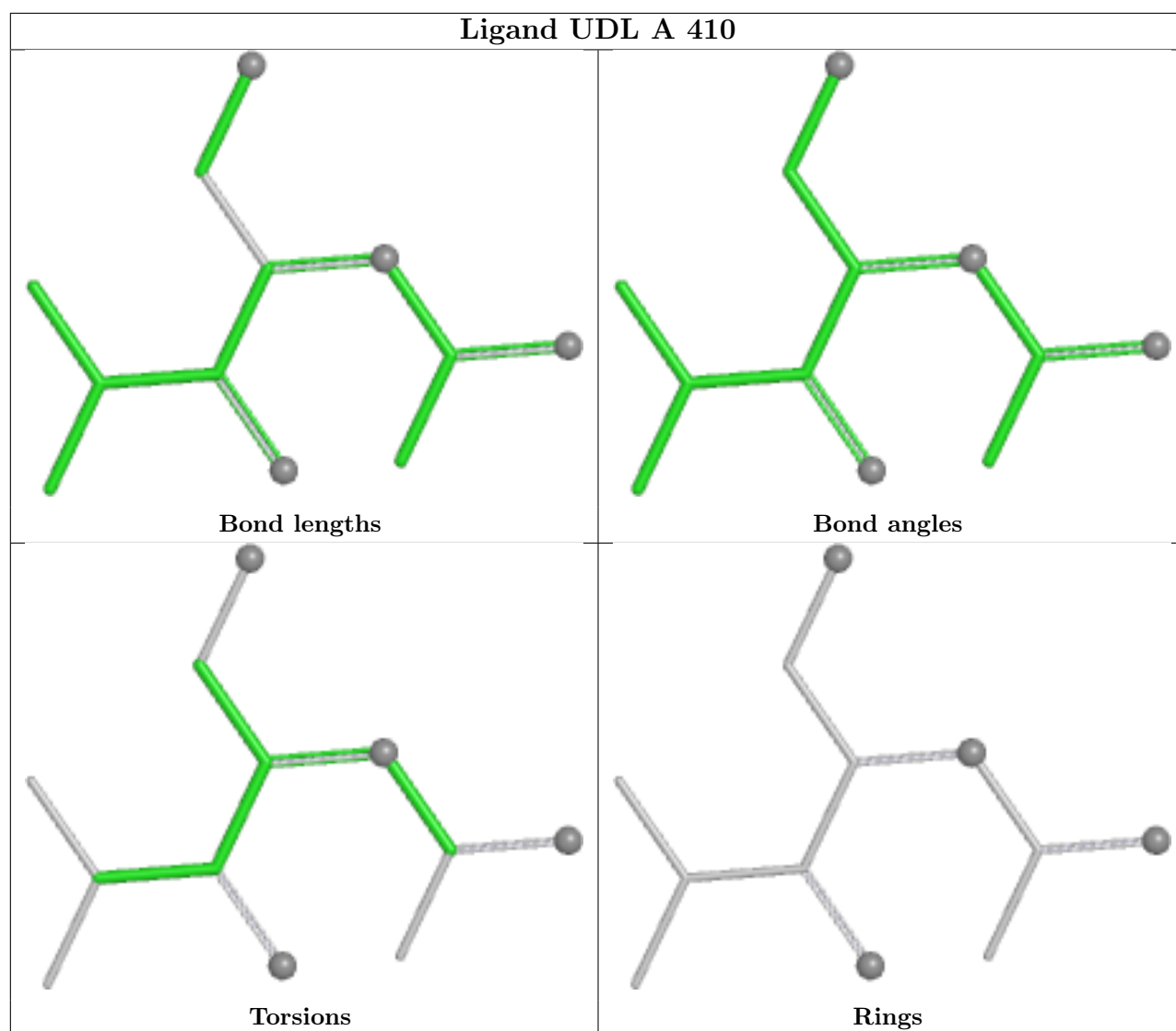
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

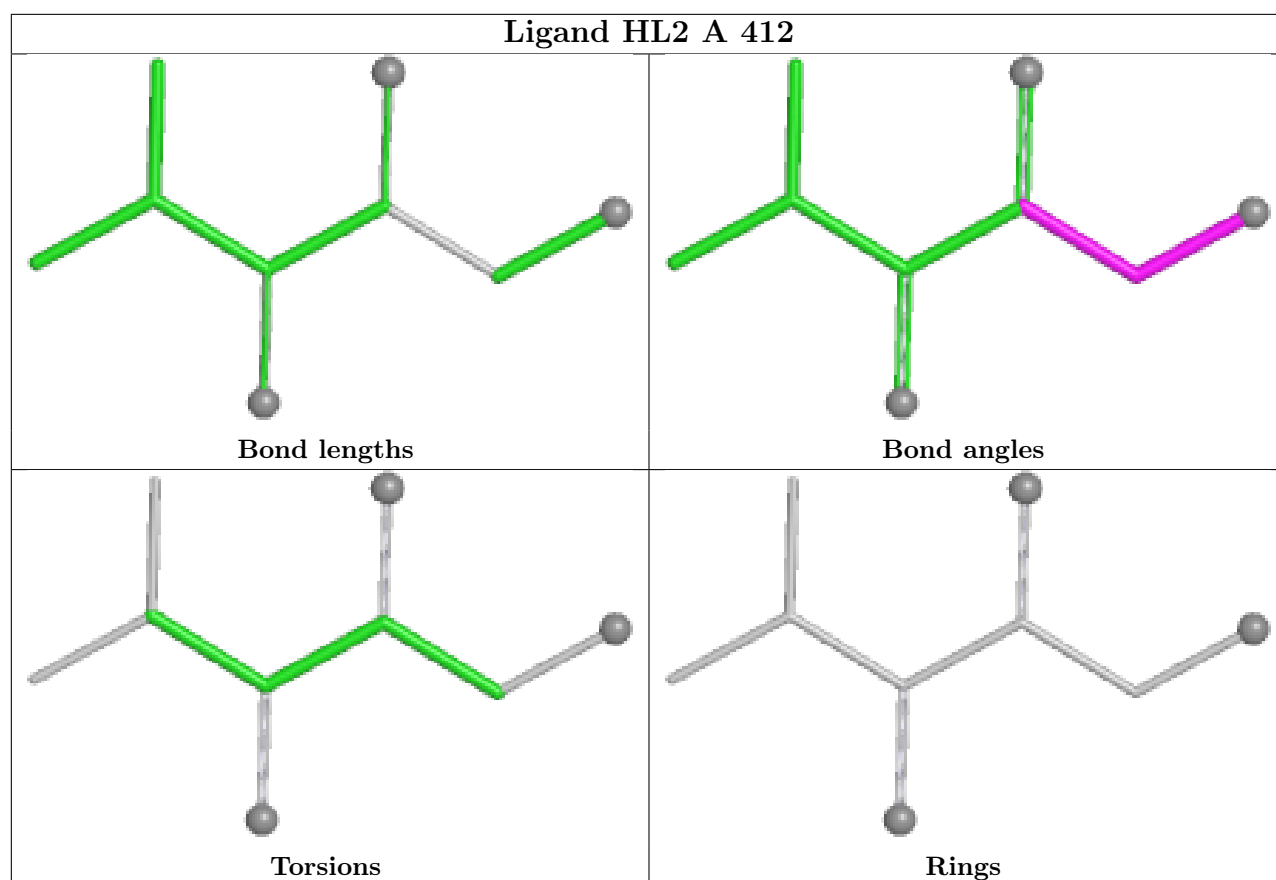
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD 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.

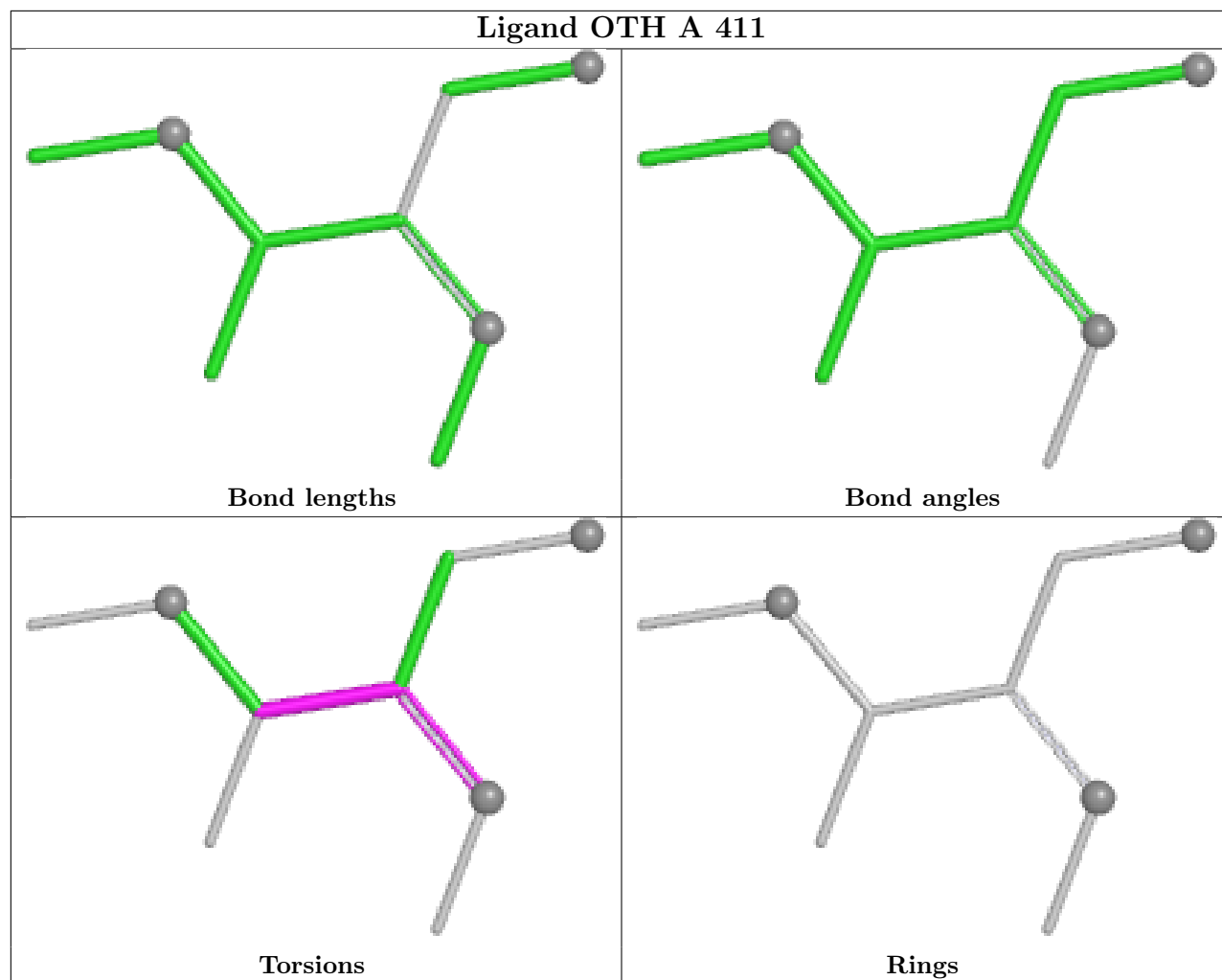


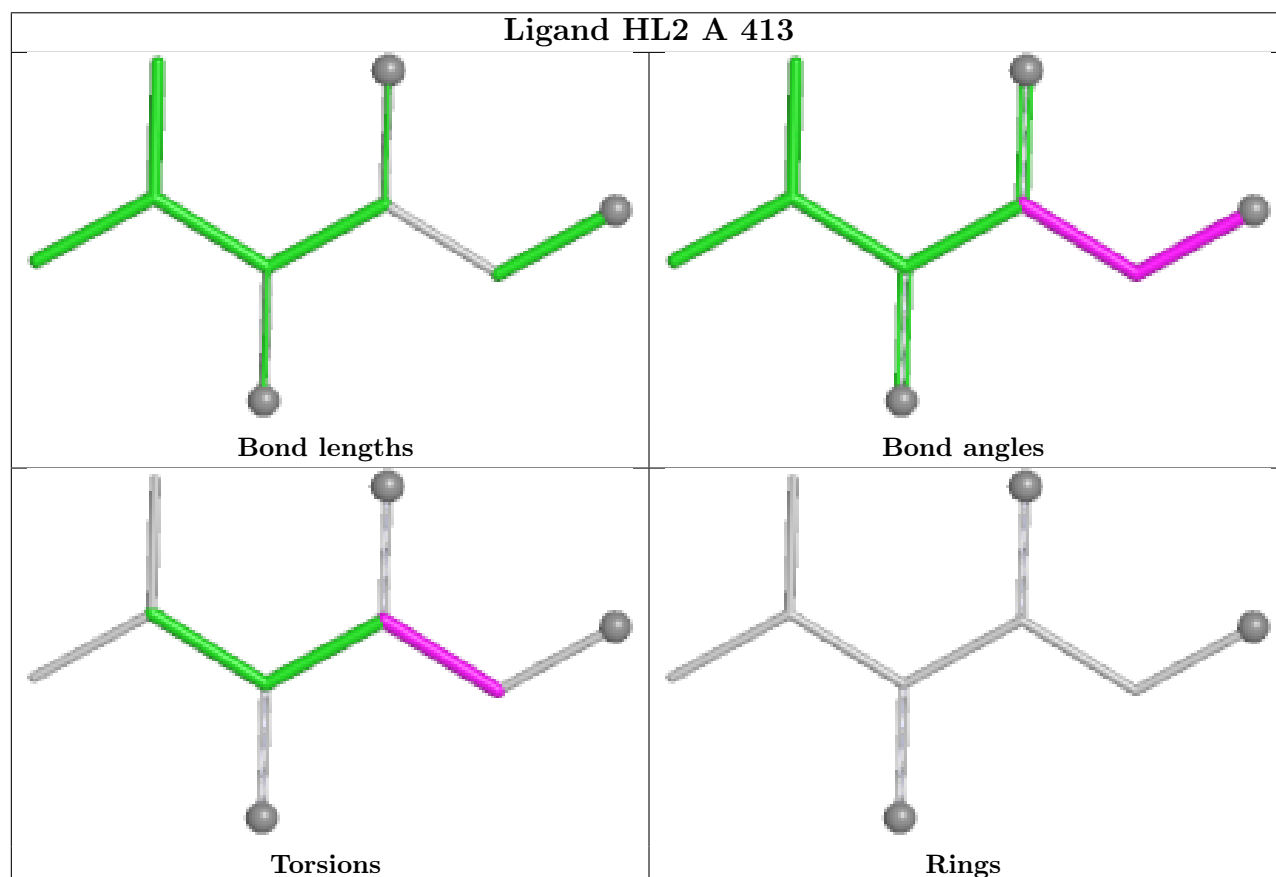
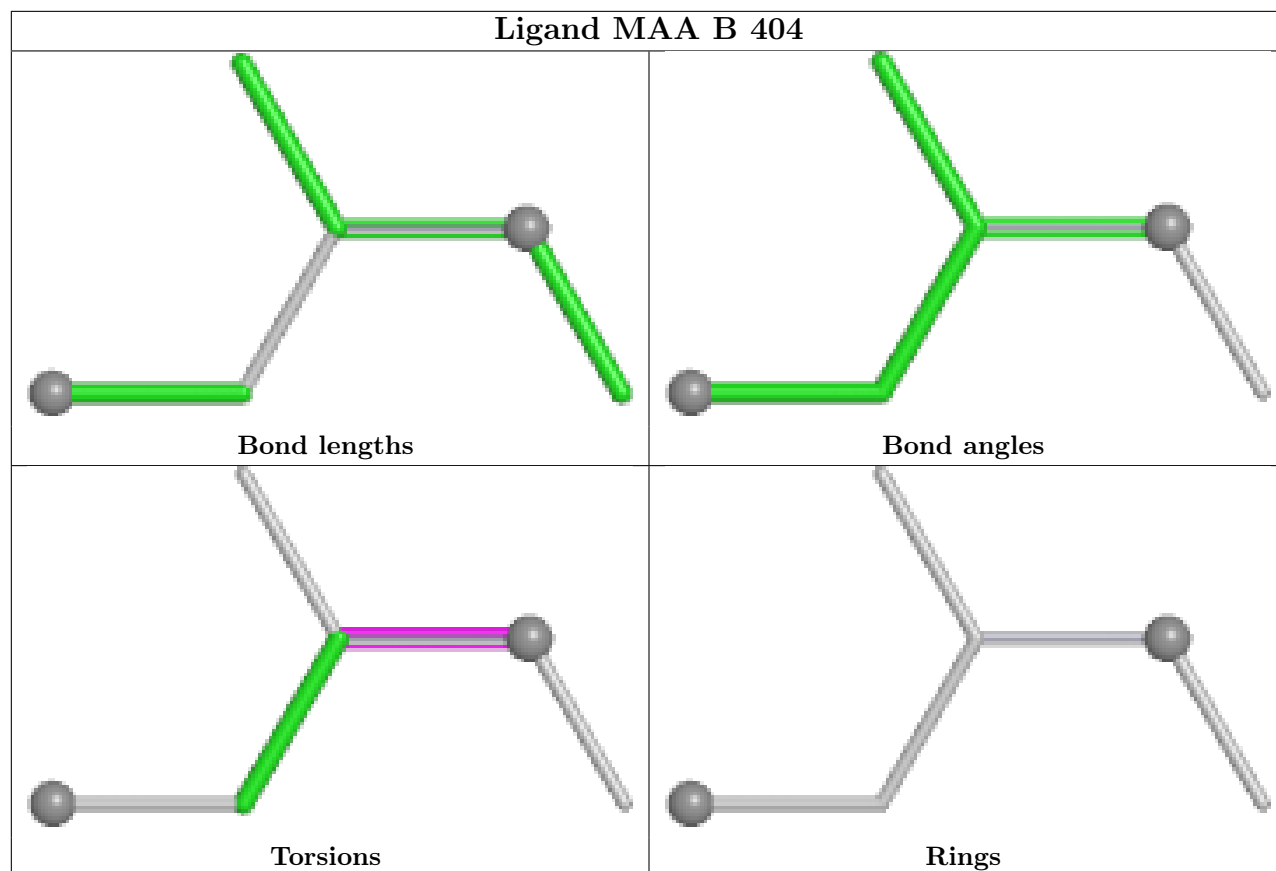












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	337/352 (95%)	-0.00	13 (3%)	43 46	6, 25, 53, 72	25 (7%)
2	B	335/344 (97%)	-0.31	5 (1%)	72 76	7, 19, 45, 77	16 (4%)
3	G	60/71 (84%)	0.51	5 (8%)	17 19	17, 36, 69, 83	1 (1%)
All	All	732/767 (95%)	-0.10	23 (3%)	51 54	6, 23, 53, 83	42 (5%)

The worst 5 of 23 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	G	8	ALA	6.9
2	B	4	LEU	4.2
1	A	239	LEU	3.7
1	A	321	ASP	3.5
1	A	240	VAL	3.5

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

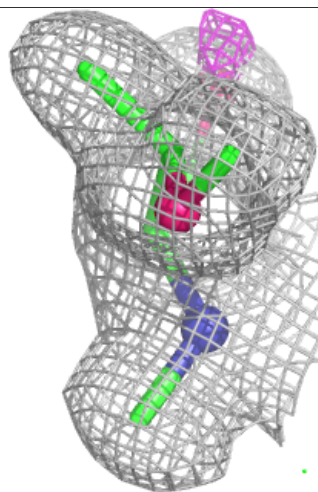
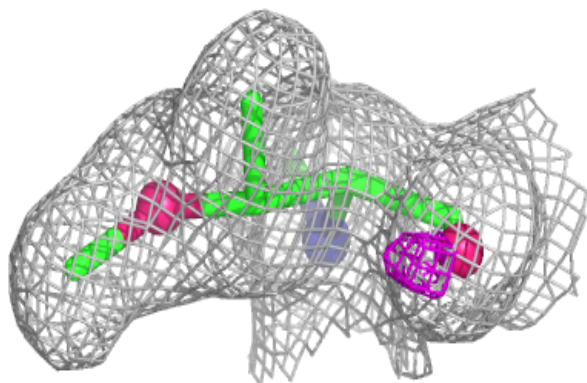
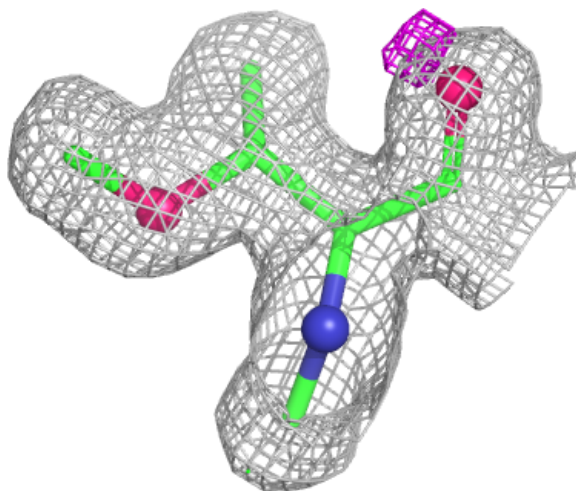
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	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.

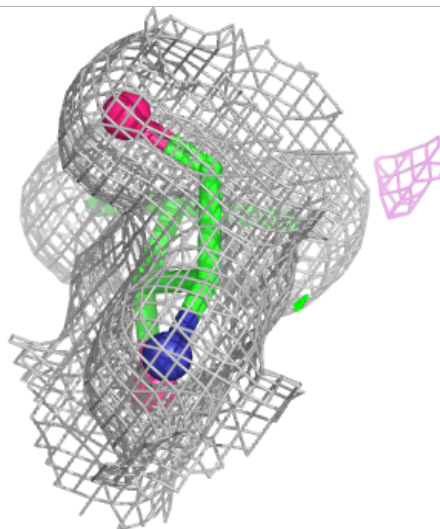
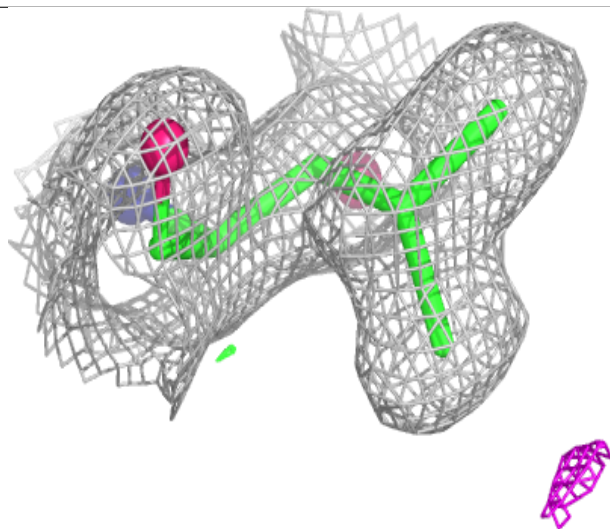
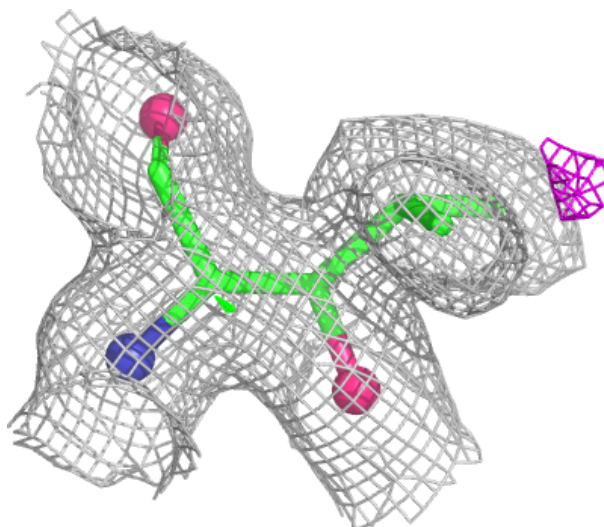
Electron density around OTH A 411:

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



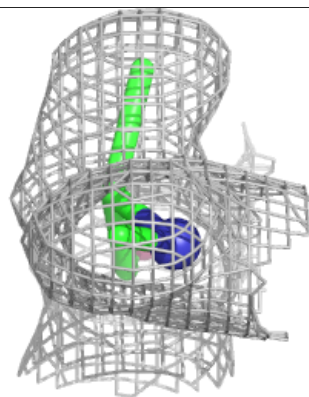
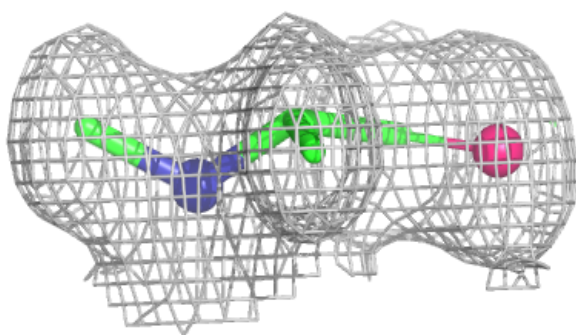
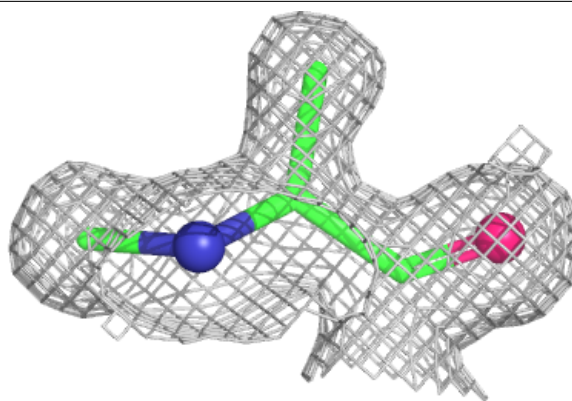
Electron density around HL2 A 412:

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



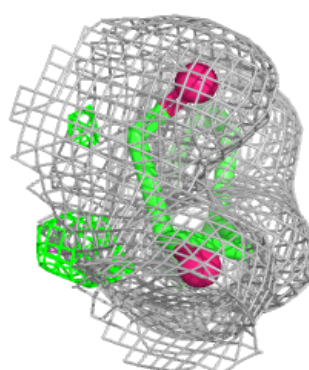
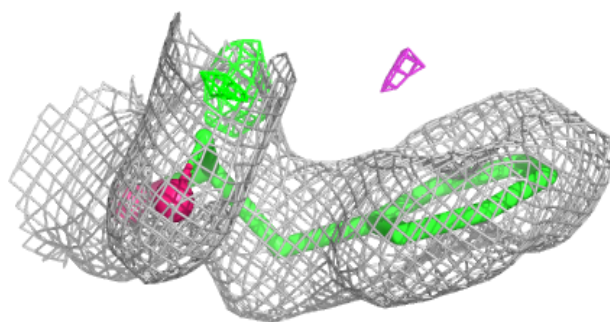
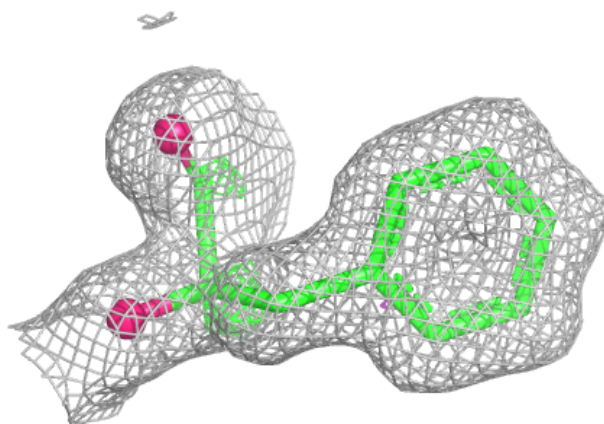
Electron density around MAA B 404:

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



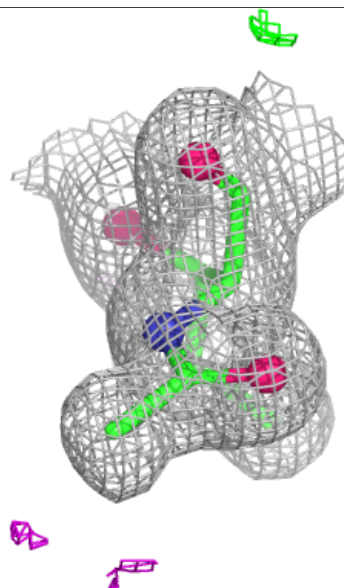
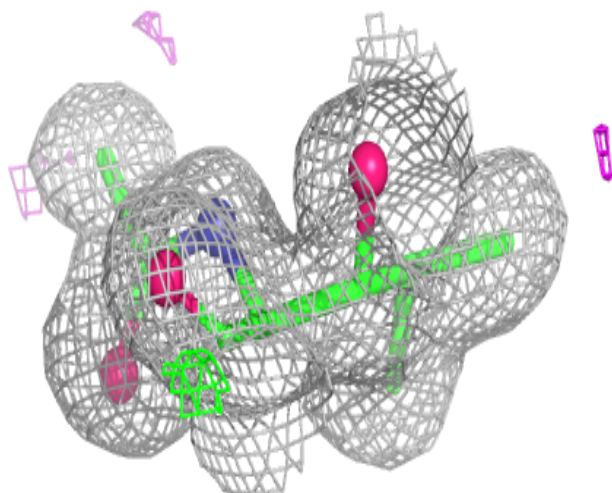
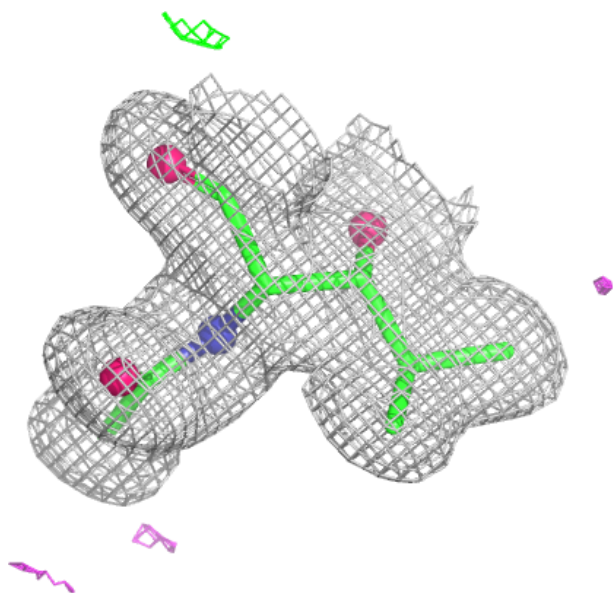
Electron density around HF2 A 409:

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



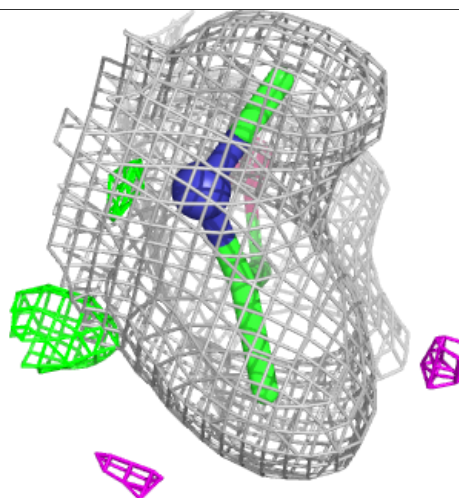
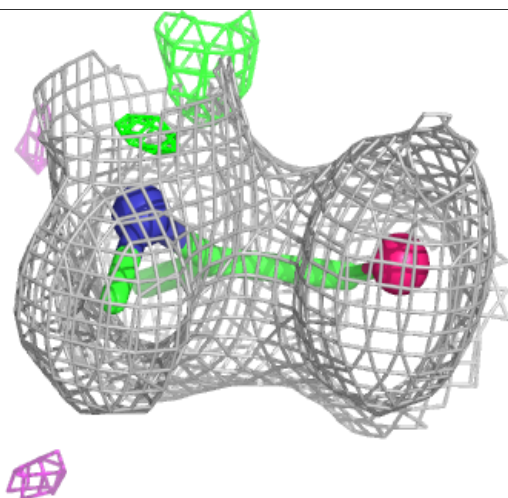
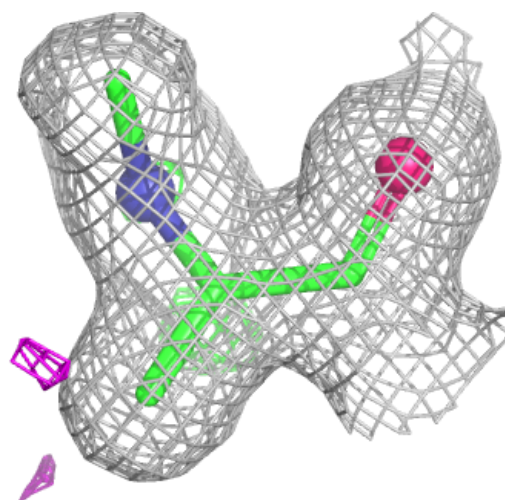
Electron density around UDL A 410:

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



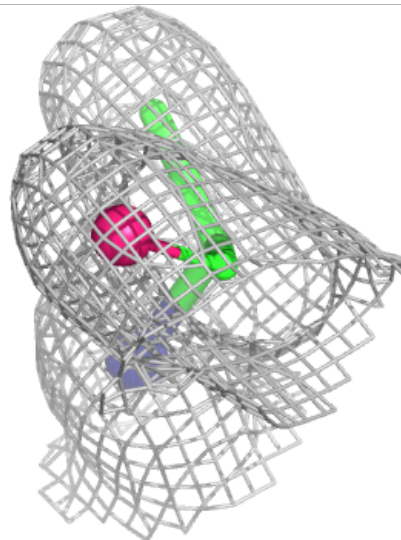
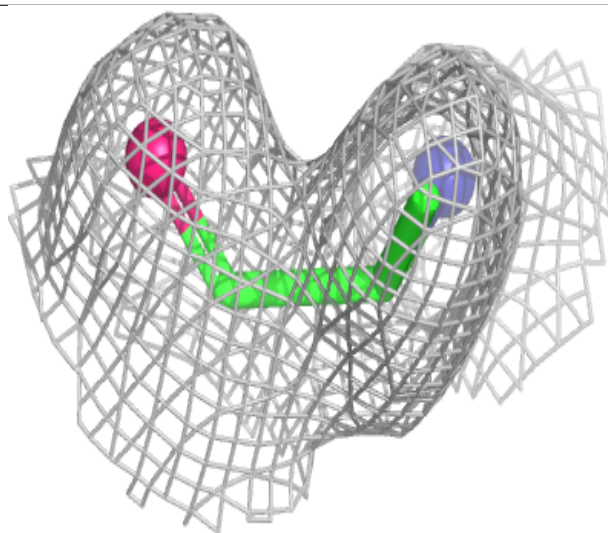
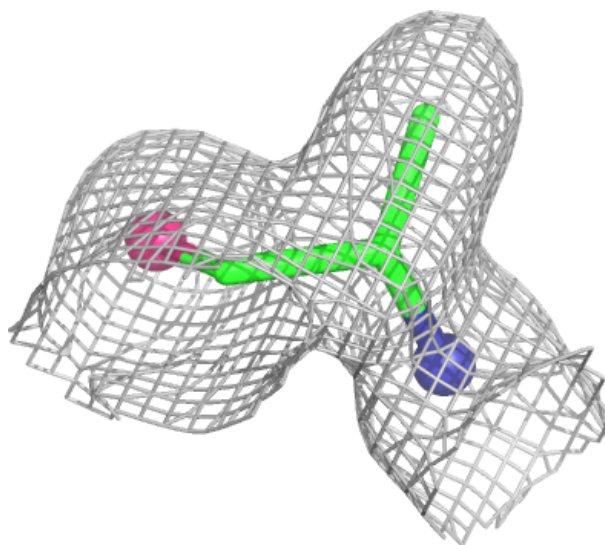
Electron density around DAM A 408:

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



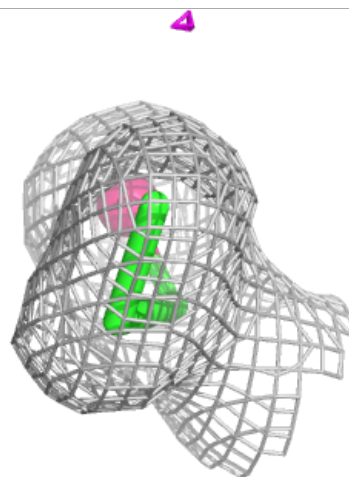
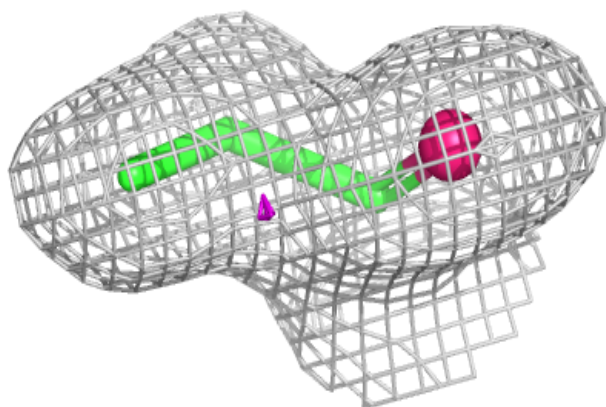
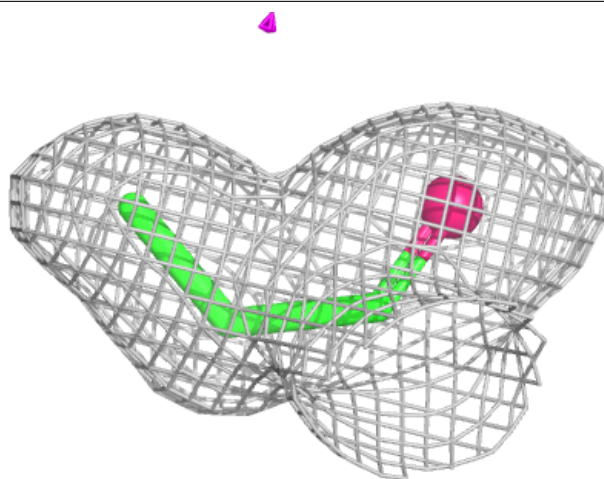
Electron density around ALA B 405:

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



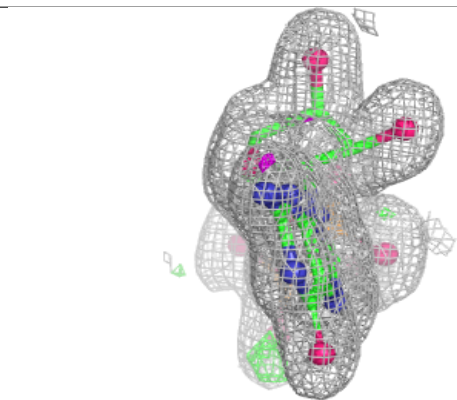
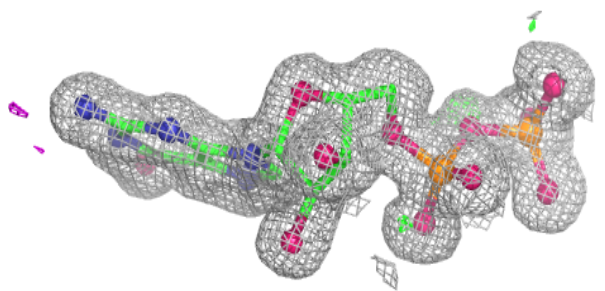
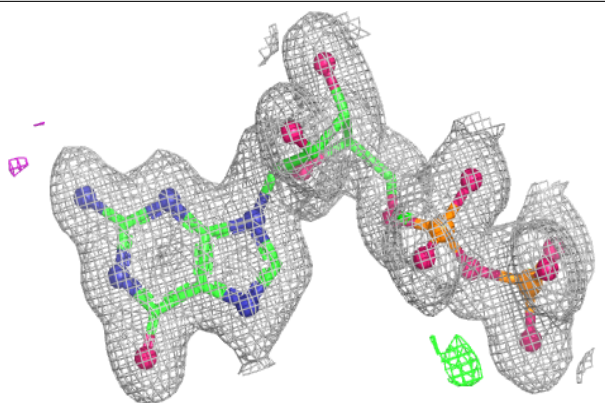
Electron density around PPI B 406:

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

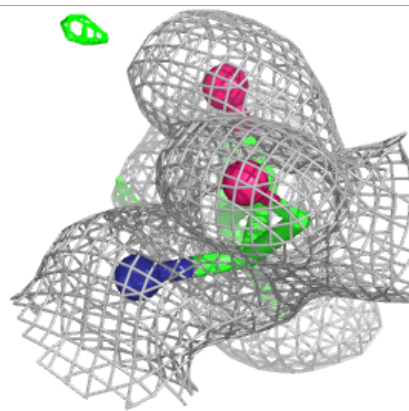
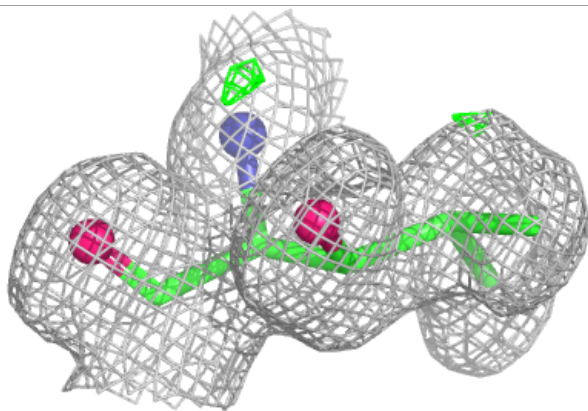
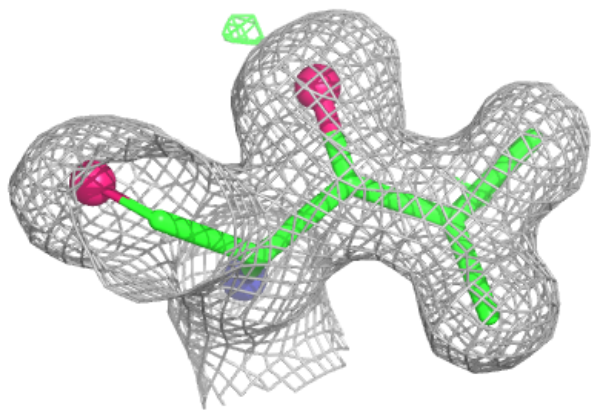


Electron density around GDP A 405:

$2mF_o-DF_c$ (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.