Full wwPDB X-ray Structure Validation Report ⓘ

Apr 28, 2024 – 12:07 am BST

PDB ID	:	3ZIW
Title	:	Clostridium perfringens enterotoxin, D48A mutation and N-terminal 37 residues deleted
Authors	:	Yelland, T.; Naylor, C.E.; Savva, C.G.; Basak, A.K.
Deposited on	:	2013-01-14
Resolution	:	1.90 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 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:

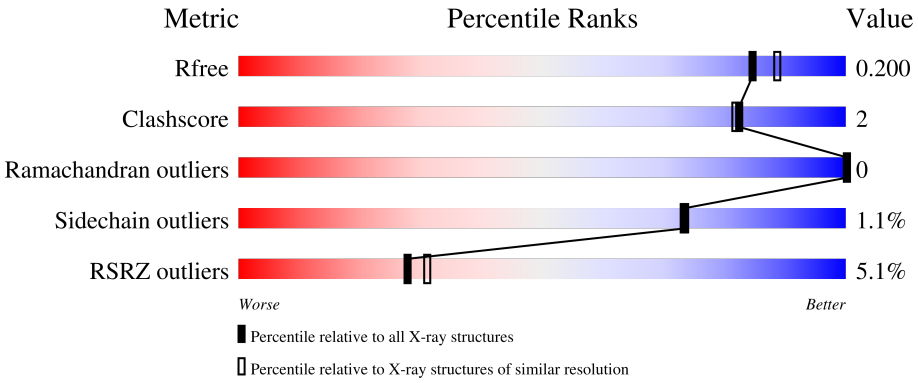
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 1.90 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.



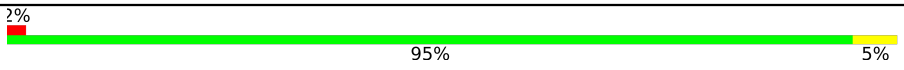
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	286	2% 96% .
1	B	286	2% 95% 5%
1	C	286	9% 93% 6% .
1	D	286	7% 95% .
1	E	286	7% 94% 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	286	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 15261 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 HEAT-LABILE ENTEROTOXIN B CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	286	Total	C	N	O	S	0	6	0
			2248	1426	363	456	3			
1	B	286	Total	C	N	O	S	0	4	0
			2225	1414	357	450	4			
1	C	286	Total	C	N	O	S	0	4	0
			2234	1418	363	450	3			
1	D	286	Total	C	N	O	S	0	7	0
			2233	1418	358	454	3			
1	E	286	Total	C	N	O	S	0	5	0
			2217	1411	357	446	3			
1	F	286	Total	C	N	O	S	0	4	0
			2240	1419	365	453	3			

There are 30 discrepancies between the modelled and reference sequences:

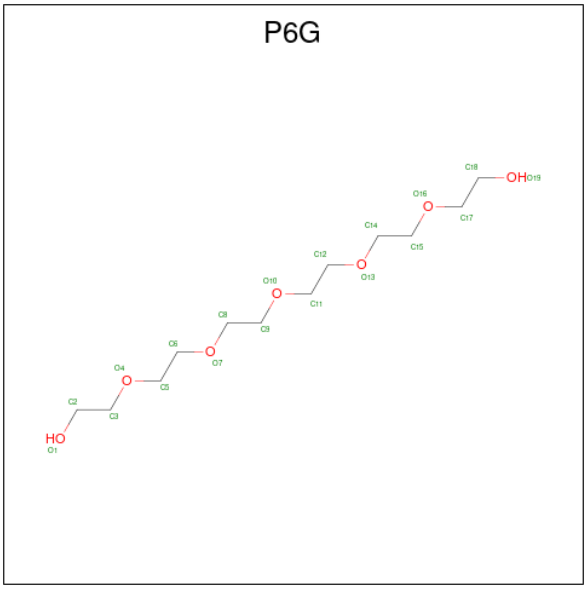
Chain	Residue	Modelled	Actual	Comment	Reference
A	34	GLY	-	expression tag	UNP P01558
A	35	ALA	-	expression tag	UNP P01558
A	36	MET	-	expression tag	UNP P01558
A	37	GLY	-	expression tag	UNP P01558
A	48	ALA	ASP	engineered mutation	UNP P01558
B	34	GLY	-	expression tag	UNP P01558
B	35	ALA	-	expression tag	UNP P01558
B	36	MET	-	expression tag	UNP P01558
B	37	GLY	-	expression tag	UNP P01558
B	48	ALA	ASP	engineered mutation	UNP P01558
C	34	GLY	-	expression tag	UNP P01558
C	35	ALA	-	expression tag	UNP P01558
C	36	MET	-	expression tag	UNP P01558
C	37	GLY	-	expression tag	UNP P01558
C	48	ALA	ASP	engineered mutation	UNP P01558
D	34	GLY	-	expression tag	UNP P01558
D	35	ALA	-	expression tag	UNP P01558

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	36	MET	-	expression tag	UNP P01558
D	37	GLY	-	expression tag	UNP P01558
D	48	ALA	ASP	engineered mutation	UNP P01558
E	34	GLY	-	expression tag	UNP P01558
E	35	ALA	-	expression tag	UNP P01558
E	36	MET	-	expression tag	UNP P01558
E	37	GLY	-	expression tag	UNP P01558
E	48	ALA	ASP	engineered mutation	UNP P01558
F	34	GLY	-	expression tag	UNP P01558
F	35	ALA	-	expression tag	UNP P01558
F	36	MET	-	expression tag	UNP P01558
F	37	GLY	-	expression tag	UNP P01558
F	48	ALA	ASP	engineered mutation	UNP P01558

- Molecule 2 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula: $C_{12}H_{26}O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 19 12 7	0	0
2	A	1	Total C O 14 9 5	0	0
2	A	1	Total C O 10 6 4	0	0
2	B	1	Total C O 17 11 6	0	0
2	B	1	Total C O 11 7 4	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total C O 16 10 6	0	0
2	C	1	Total C O 8 5 3	0	0
2	D	1	Total C O 16 10 6	0	0
2	D	1	Total C O 10 6 4	0	0
2	E	1	Total C O 14 9 5	0	0
2	E	1	Total C O 13 8 5	0	0
2	E	1	Total C O 10 6 4	0	0
2	F	1	Total C O 19 12 7	0	0
2	F	1	Total C O 8 5 3	0	0

- Molecule 3 is water.

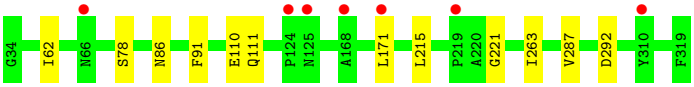
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	307	Total O 307 307	0	0
3	B	306	Total O 306 306	0	0
3	C	249	Total O 249 249	0	0
3	D	259	Total O 259 259	0	0
3	E	251	Total O 251 251	0	0
3	F	307	Total O 307 307	0	0

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.

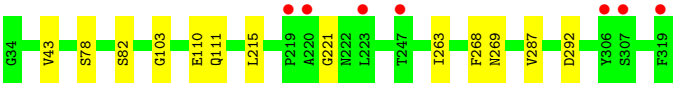
• Molecule 1: HEAT-LABILE ENTEROTOXIN B CHAIN

Chain A:



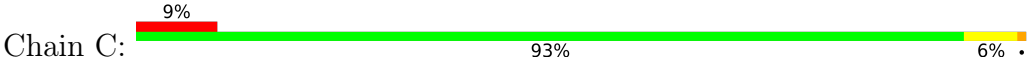
• Molecule 1: HEAT-LABILE ENTEROTOXIN B CHAIN

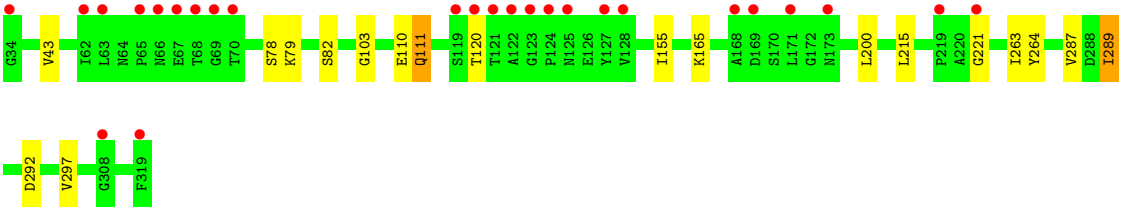
Chain B:



• Molecule 1: HEAT-LABILE ENTEROTOXIN B CHAIN

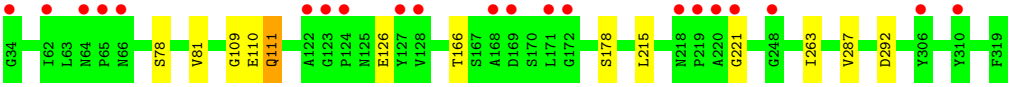
Chain C:





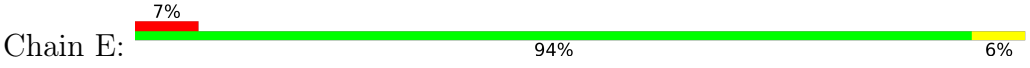
• Molecule 1: HEAT-LABILE ENTEROTOXIN B CHAIN

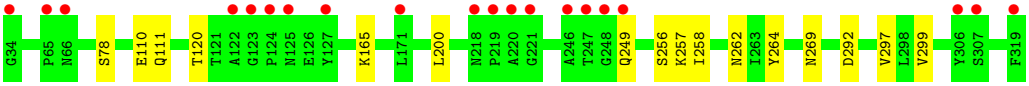
Chain D:



• Molecule 1: HEAT-LABILE ENTEROTOXIN B CHAIN

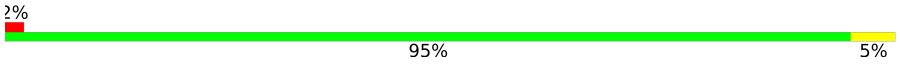
Chain E:

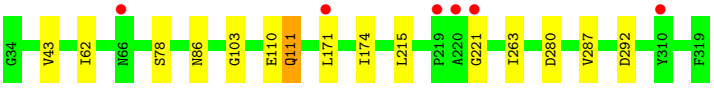




• Molecule 1: HEAT-LABILE ENTEROTOXIN B CHAIN

Chain F:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	190.66Å 128.02Å 136.43Å 90.00° 133.81° 90.00°	Depositor
Resolution (Å)	49.23 – 1.90 49.23 – 1.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.23-1.90) 100.0 (49.23-1.90)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.48 (at 1.90Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.175 , 0.196 0.180 , 0.200	Depositor DCC
R_{free} test set	9298 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	36.5	Xtriage
Anisotropy	0.143	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 56.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.002 for h+2*l,k,-h-l 0.014 for h,-k,-h-l 0.035 for -h-2*l,-k,l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	15261	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% 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: P6G

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	0.50	0/2312	0.67	0/3137
1	B	0.50	0/2281	0.65	0/3101
1	C	0.48	0/2289	0.65	0/3108
1	D	0.50	0/2298	0.66	0/3125
1	E	0.48	0/2275	0.66	0/3095
1	F	0.52	0/2296	0.65	0/3117
All	All	0.50	0/13751	0.66	0/18683

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	2248	0	2192	11	0
1	B	2225	0	2159	11	0
1	C	2234	0	2182	20	0
1	D	2233	0	2169	12	0
1	E	2217	0	2161	13	0
1	F	2240	0	2190	15	0
2	A	43	0	55	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	28	0	34	1	0
2	C	24	0	30	1	0
2	D	26	0	34	1	0
2	E	37	0	46	0	0
2	F	27	0	35	1	0
3	A	307	0	0	2	0
3	B	306	0	0	0	0
3	C	249	0	0	0	0
3	D	259	0	0	0	0
3	E	251	0	0	0	0
3	F	307	0	0	1	0
All	All	15261	0	13287	67	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 2.

All (67) 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:E:110:GLU:HG3	1:F:110[A]:GLU:HG2	1.39	1.03
1:A:110[A]:GLU:HG3	1:B:110:GLU:HG2	1.44	0.97
1:B:82:SER:HA	2:B:400:P6G:H172	1.64	0.79
1:A:110[A]:GLU:HG2	1:C:110[A]:GLU:HG3	1.67	0.77
1:B:110:GLU:HG3	1:C:110[A]:GLU:HG2	1.67	0.76
1:D:110[A]:GLU:HG3	1:F:110[A]:GLU:HG3	1.69	0.75
1:A:110[A]:GLU:CG	1:B:110:GLU:HG2	2.18	0.72
1:D:110[A]:GLU:HG2	1:E:110:GLU:HG2	1.73	0.71
1:E:110:GLU:HG3	1:F:110[A]:GLU:CG	2.20	0.70
3:A:2134:HOH:O	1:C:110[B]:GLU:HG3	1.91	0.70
1:C:110[B]:GLU:H	1:C:110[B]:GLU:CD	1.95	0.68
1:E:264:TYR:HE1	1:E:299[B]:VAL:CG1	2.11	0.64
1:D:263:ILE:HD11	1:D:287:VAL:HG21	1.80	0.63
1:F:78:SER:HA	1:F:111[B]:GLN:HG3	1.81	0.63
1:C:120:THR:HG21	1:C:165:LYS:HD3	1.81	0.62
1:D:109:GLY:HA2	1:F:110[B]:GLU:OE1	2.03	0.59
1:F:280:ASP:HA	2:F:401:P6G:H62	1.85	0.59
1:A:110[B]:GLU:HG2	3:A:2135:HOH:O	2.03	0.57
1:B:263:ILE:HD11	1:B:287:VAL:HG21	1.85	0.57
1:B:110:GLU:HG3	1:C:110[A]:GLU:CG	2.37	0.55
1:D:110[B]:GLU:OE2	1:F:110[B]:GLU:HG2	2.07	0.54
1:E:120:THR:HG21	1:E:165:LYS:HD3	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:263:ILE:HD11	1:F:287:VAL:HG21	1.90	0.54
1:E:264:TYR:HE1	1:E:299[B]:VAL:HG11	1.73	0.54
1:F:62:ILE:HG21	1:F:171:LEU:CD2	2.39	0.52
1:B:263:ILE:CD1	1:B:287:VAL:HG21	2.40	0.52
1:C:263:ILE:HD11	1:C:287:VAL:HG21	1.92	0.51
1:A:78:SER:HA	1:A:111[A]:GLN:HG3	1.93	0.51
1:E:200:LEU:HD21	1:E:297[B]:VAL:HG11	1.93	0.51
1:D:110[A]:GLU:HG2	1:E:110:GLU:CG	2.41	0.51
1:E:262:ASN:HB2	1:E:299[B]:VAL:CG1	2.41	0.51
1:A:263:ILE:HD11	1:A:287:VAL:HG21	1.93	0.50
1:F:263:ILE:CD1	1:F:287:VAL:HG21	2.42	0.49
1:D:78:SER:HA	1:D:111[A]:GLN:HG3	1.94	0.49
1:C:78:SER:HA	1:C:111[A]:GLN:HG3	1.95	0.48
1:E:264:TYR:HE1	1:E:299[B]:VAL:HG12	1.79	0.47
1:D:81:VAL:O	2:D:400:P6G:H21	2.14	0.47
1:E:257:LYS:HG3	1:E:258:ILE:HG23	1.97	0.47
1:D:215:LEU:O	1:D:221:GLY:HA2	2.16	0.46
1:C:264:TYR:HB2	1:C:297[B]:VAL:HG12	1.96	0.46
1:B:78:SER:HA	1:B:111:GLN:HG3	1.97	0.46
1:C:82:SER:HB2	2:C:400:P6G:H61	1.97	0.46
1:F:215:LEU:O	1:F:221:GLY:HA2	2.16	0.46
1:D:110[A]:GLU:HG3	1:F:110[A]:GLU:CG	2.44	0.45
1:D:263:ILE:CD1	1:D:287:VAL:HG21	2.47	0.45
1:C:200:LEU:HD21	1:C:297[B]:VAL:HG11	1.98	0.45
1:C:43:VAL:HG21	1:C:103:GLY:HA3	1.99	0.44
1:C:287:VAL:HG23	1:C:289:ILE:HD12	2.00	0.44
1:B:215:LEU:O	1:B:221:GLY:HA2	2.18	0.44
1:C:79:LYS:HE3	1:C:110[A]:GLU:OE2	2.18	0.43
1:A:215:LEU:O	1:A:221:GLY:HA2	2.18	0.43
1:F:86:ASN:ND2	3:F:2082:HOH:O	2.51	0.43
1:C:215:LEU:O	1:C:221:GLY:HA2	2.18	0.43
1:C:263:ILE:CD1	1:C:287:VAL:HG21	2.49	0.43
1:E:262:ASN:HB2	1:E:299[B]:VAL:HG13	2.00	0.43
1:C:79:LYS:HD2	1:C:155:ILE:HD11	2.01	0.42
1:A:62:ILE:HD12	1:B:268:PHE:CZ	2.54	0.42
1:A:110[A]:GLU:HG2	1:C:110[A]:GLU:CG	2.44	0.42
1:A:86[B]:ASN:ND2	1:A:91:PHE:HB3	2.35	0.41
1:E:78:SER:HA	1:E:111:GLN:HG3	2.02	0.41
1:F:43:VAL:HG21	1:F:103:GLY:HA3	2.02	0.41
1:F:171:LEU:HA	1:F:174:ILE:HD12	2.01	0.41
1:A:263:ILE:CD1	1:A:287:VAL:HG21	2.51	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:166[A]:THR:HG21	1:D:178:SER:OG	2.20	0.41
1:B:43:VAL:HG21	1:B:103:GLY:HA3	2.02	0.40
1:C:264:TYR:HB2	1:C:297[B]:VAL:CG1	2.51	0.40

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	289/286 (101%)	284 (98%)	5 (2%)	0	100	100
1	B	288/286 (101%)	282 (98%)	6 (2%)	0	100	100
1	C	288/286 (101%)	284 (99%)	4 (1%)	0	100	100
1	D	291/286 (102%)	288 (99%)	3 (1%)	0	100	100
1	E	289/286 (101%)	285 (99%)	4 (1%)	0	100	100
1	F	288/286 (101%)	284 (99%)	4 (1%)	0	100	100
All	All	1733/1716 (101%)	1707 (98%)	26 (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	250/246 (102%)	248 (99%)	2 (1%)	81 82
1	B	245/246 (100%)	243 (99%)	2 (1%)	81 82
1	C	248/246 (101%)	244 (98%)	4 (2%)	62 60
1	D	248/246 (101%)	244 (98%)	4 (2%)	62 60
1	E	246/246 (100%)	242 (98%)	4 (2%)	62 60
1	F	250/246 (102%)	247 (99%)	3 (1%)	71 70
All	All	1487/1476 (101%)	1468 (99%)	19 (1%)	73 68

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	171	LEU
1	A	292	ASP
1	B	269	ASN
1	B	292	ASP
1	C	111[A]	GLN
1	C	111[B]	GLN
1	C	289	ILE
1	C	292	ASP
1	D	111[A]	GLN
1	D	111[B]	GLN
1	D	126	GLU
1	D	292	ASP
1	E	249	GLN
1	E	256	SER
1	E	269	ASN
1	E	292	ASP
1	F	111[A]	GLN
1	F	111[B]	GLN
1	F	292	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	241	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

14 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	P6G	B	400	-	16,16,18	0.57	0	15,15,17	0.80	0
2	P6G	F	401	-	7,7,18	0.45	0	6,6,17	0.24	0
2	P6G	A	401	-	13,13,18	0.50	0	12,12,17	0.19	0
2	P6G	E	403	-	9,9,18	0.46	0	8,8,17	0.24	0
2	P6G	C	401	-	7,7,18	0.48	0	6,6,17	0.19	0
2	P6G	E	401	-	12,12,18	0.48	0	11,11,17	0.21	0
2	P6G	A	400	-	18,18,18	0.53	0	17,17,17	0.45	0
2	P6G	B	401	-	10,10,18	0.48	0	9,9,17	0.24	0
2	P6G	D	401	-	9,9,18	0.47	0	8,8,17	0.24	0
2	P6G	A	402	-	9,9,18	0.46	0	8,8,17	0.30	0
2	P6G	F	400	-	18,18,18	0.39	0	17,17,17	0.75	0
2	P6G	D	400	-	15,15,18	0.45	0	14,14,17	0.38	0
2	P6G	C	400	-	15,15,18	0.49	0	14,14,17	0.28	0
2	P6G	E	400	-	13,13,18	0.53	0	12,12,17	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
2	P6G	B	400	-	-	4/14/14/16	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	P6G	F	401	-	-	3/5/5/16	-
2	P6G	A	401	-	-	7/11/11/16	-
2	P6G	E	403	-	-	2/7/7/16	-
2	P6G	C	401	-	-	3/5/5/16	-
2	P6G	E	401	-	-	4/10/10/16	-
2	P6G	A	400	-	-	6/16/16/16	-
2	P6G	B	401	-	-	4/8/8/16	-
2	P6G	D	401	-	-	0/7/7/16	-
2	P6G	A	402	-	-	3/7/7/16	-
2	P6G	F	400	-	-	2/16/16/16	-
2	P6G	D	400	-	-	1/13/13/16	-
2	P6G	C	400	-	-	9/13/13/16	-
2	P6G	E	400	-	-	6/11/11/16	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (54) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	400	P6G	O7-C8-C9-O10
2	C	400	P6G	O10-C11-C12-O13
2	A	401	P6G	O4-C5-C6-O7
2	C	400	P6G	O4-C5-C6-O7
2	A	402	P6G	O4-C5-C6-O7
2	E	400	P6G	O4-C5-C6-O7
2	A	400	P6G	O13-C14-C15-O16
2	E	401	P6G	O7-C8-C9-O10
2	B	401	P6G	O1-C2-C3-O4
2	E	400	P6G	O10-C11-C12-O13
2	A	401	P6G	O10-C11-C12-O13
2	E	400	P6G	O7-C8-C9-O10
2	A	400	P6G	O16-C17-C18-O19
2	B	400	P6G	O16-C17-C18-O19
2	F	401	P6G	O1-C2-C3-O4
2	F	400	P6G	O16-C17-C18-O19
2	A	402	P6G	O7-C8-C9-O10
2	C	401	P6G	C5-C6-O7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	A	401	P6G	O13-C14-C15-O16
2	E	401	P6G	O10-C11-C12-O13
2	F	401	P6G	C6-C5-O4-C3
2	B	400	P6G	C14-C15-O16-C17
2	C	400	P6G	C15-C14-O13-C12
2	E	400	P6G	C9-C8-O7-C6
2	C	401	P6G	C6-C5-O4-C3
2	A	401	P6G	C9-C8-O7-C6
2	A	402	P6G	C5-C6-O7-C8
2	C	400	P6G	C8-C9-O10-C11
2	E	403	P6G	C6-C5-O4-C3
2	E	403	P6G	O7-C8-C9-O10
2	C	400	P6G	C2-C3-O4-C5
2	C	400	P6G	C5-C6-O7-C8
2	C	400	P6G	C12-C11-O10-C9
2	A	400	P6G	C2-C3-O4-C5
2	E	400	P6G	C8-C9-O10-C11
2	B	401	P6G	O7-C8-C9-O10
2	A	401	P6G	C12-C11-O10-C9
2	A	401	P6G	C6-C5-O4-C3
2	B	400	P6G	O13-C14-C15-O16
2	A	400	P6G	C14-C15-O16-C17
2	B	400	P6G	C18-C17-O16-C15
2	B	401	P6G	C5-C6-O7-C8
2	A	401	P6G	C11-C12-O13-C14
2	B	401	P6G	O4-C5-C6-O7
2	C	400	P6G	C11-C12-O13-C14
2	D	400	P6G	C15-C14-O13-C12
2	F	401	P6G	C2-C3-O4-C5
2	F	400	P6G	O10-C11-C12-O13
2	A	400	P6G	C6-C5-O4-C3
2	E	401	P6G	C12-C11-O10-C9
2	A	400	P6G	C8-C9-O10-C11
2	C	401	P6G	O4-C5-C6-O7
2	E	401	P6G	C9-C8-O7-C6
2	E	400	P6G	C11-C12-O13-C14

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	400	P6G	1	0

Continued on next page...

Continued from previous page...

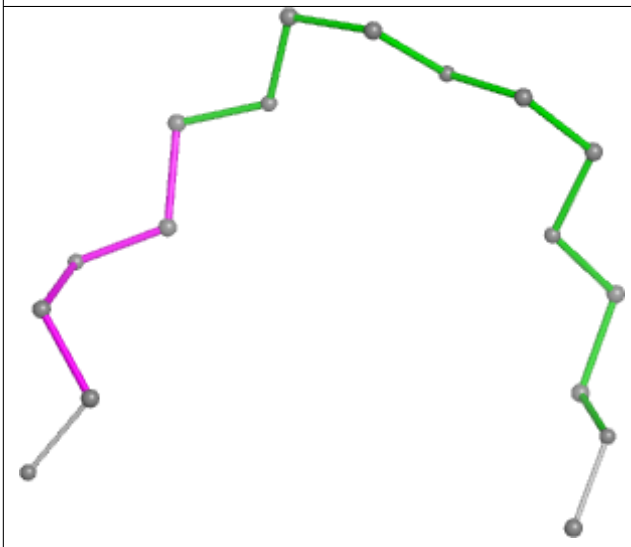
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	401	P6G	1	0
2	D	400	P6G	1	0
2	C	400	P6G	1	0

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.

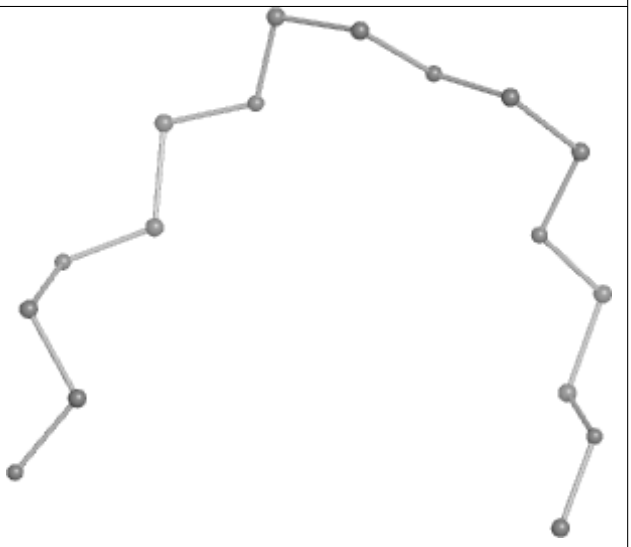
Ligand P6G B 400

Bond lengths

Bond angles

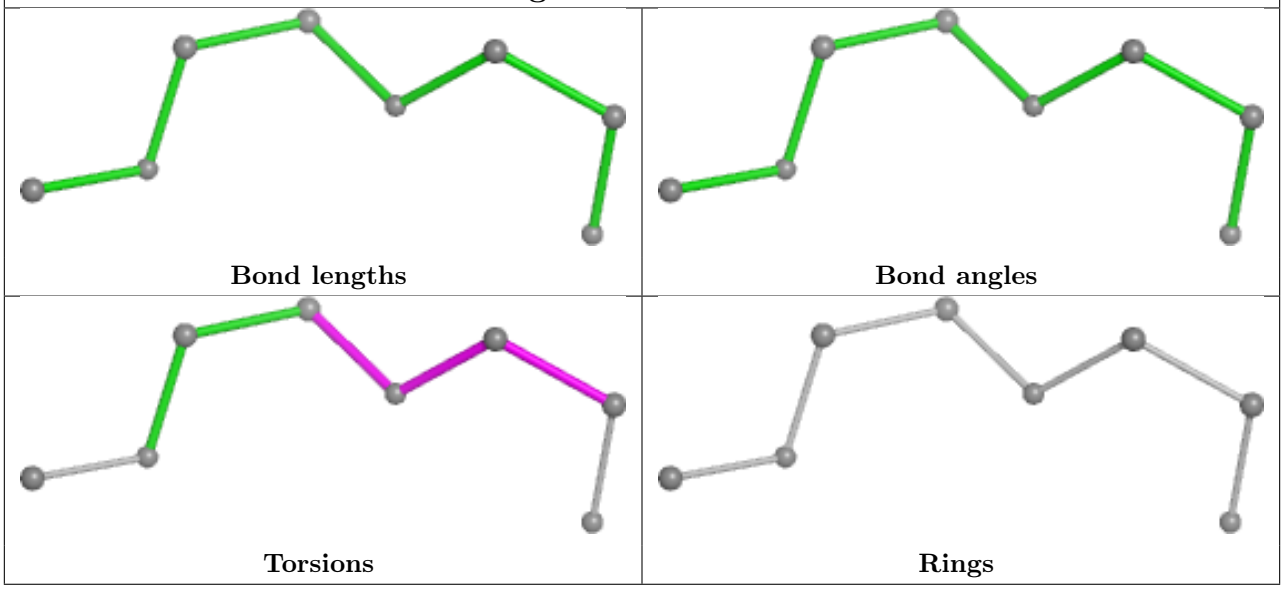


Torsions

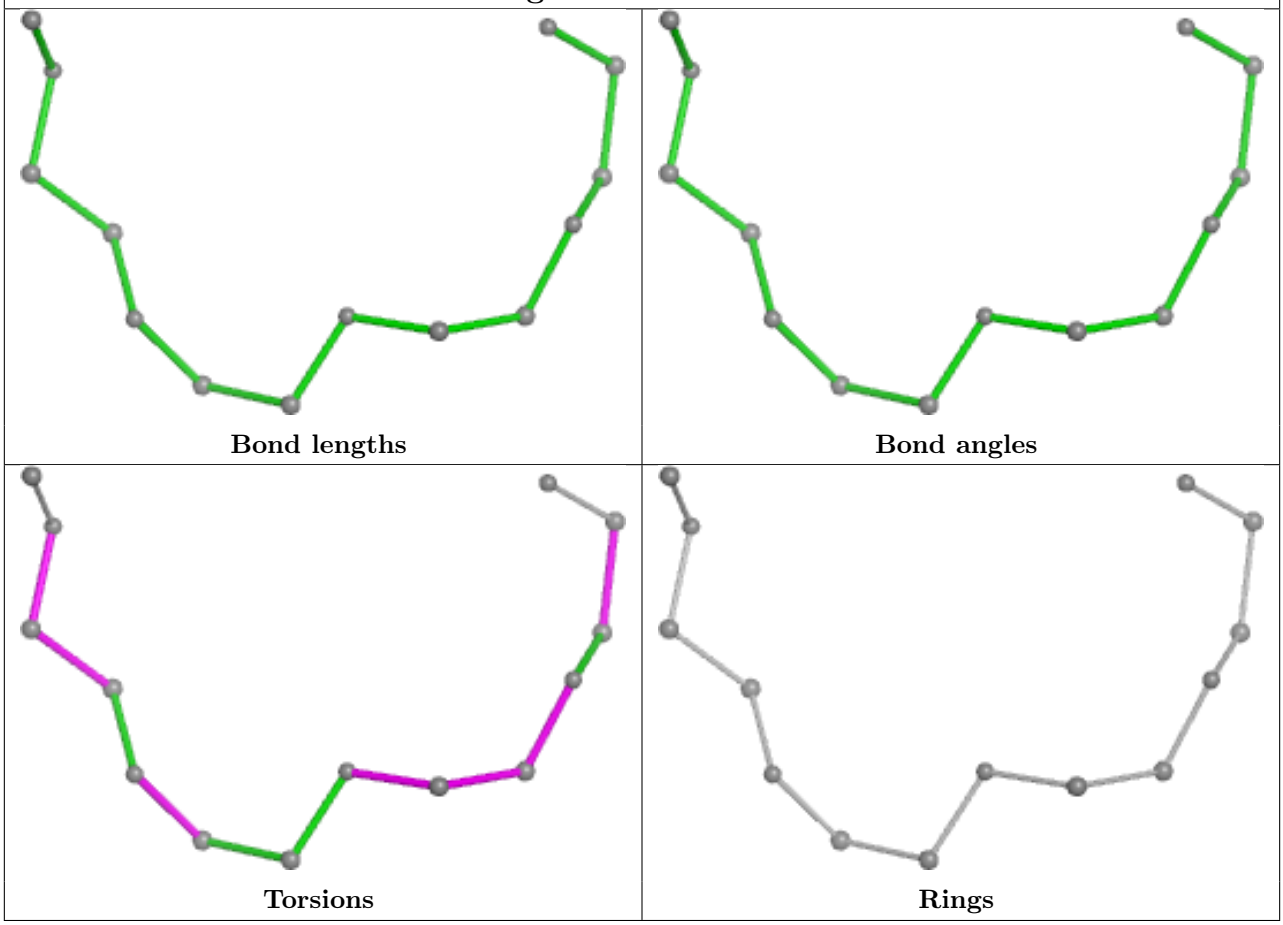


Rings

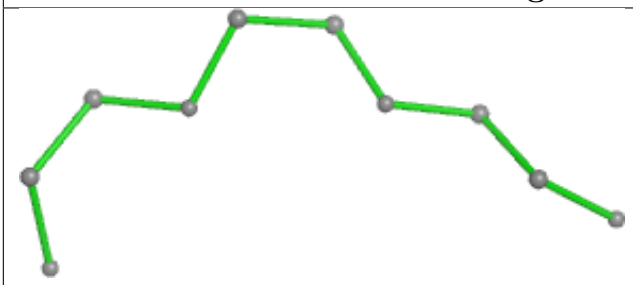
Ligand P6G F 401



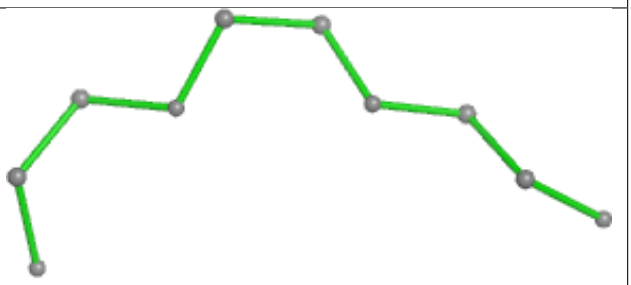
Ligand P6G A 401



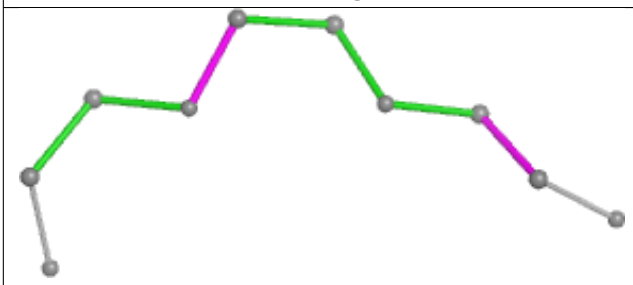
Ligand P6G E 403



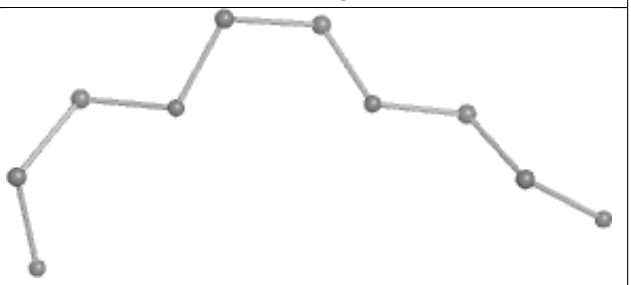
Bond lengths



Bond angles

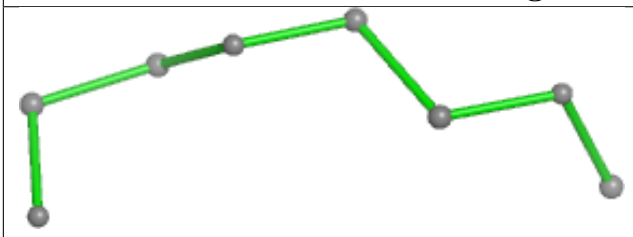


Torsions

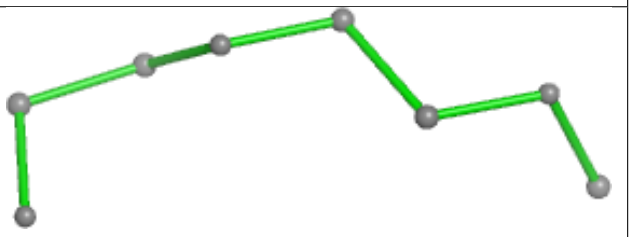


Rings

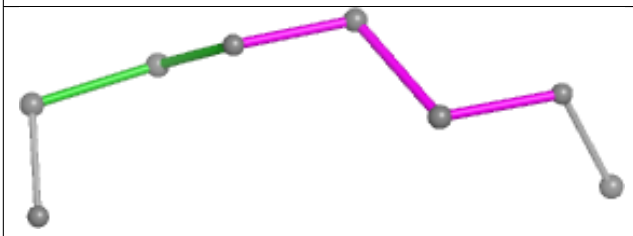
Ligand P6G C 401



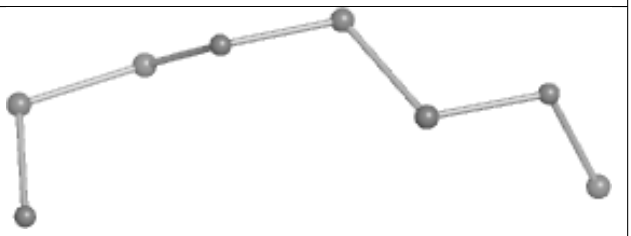
Bond lengths



Bond angles

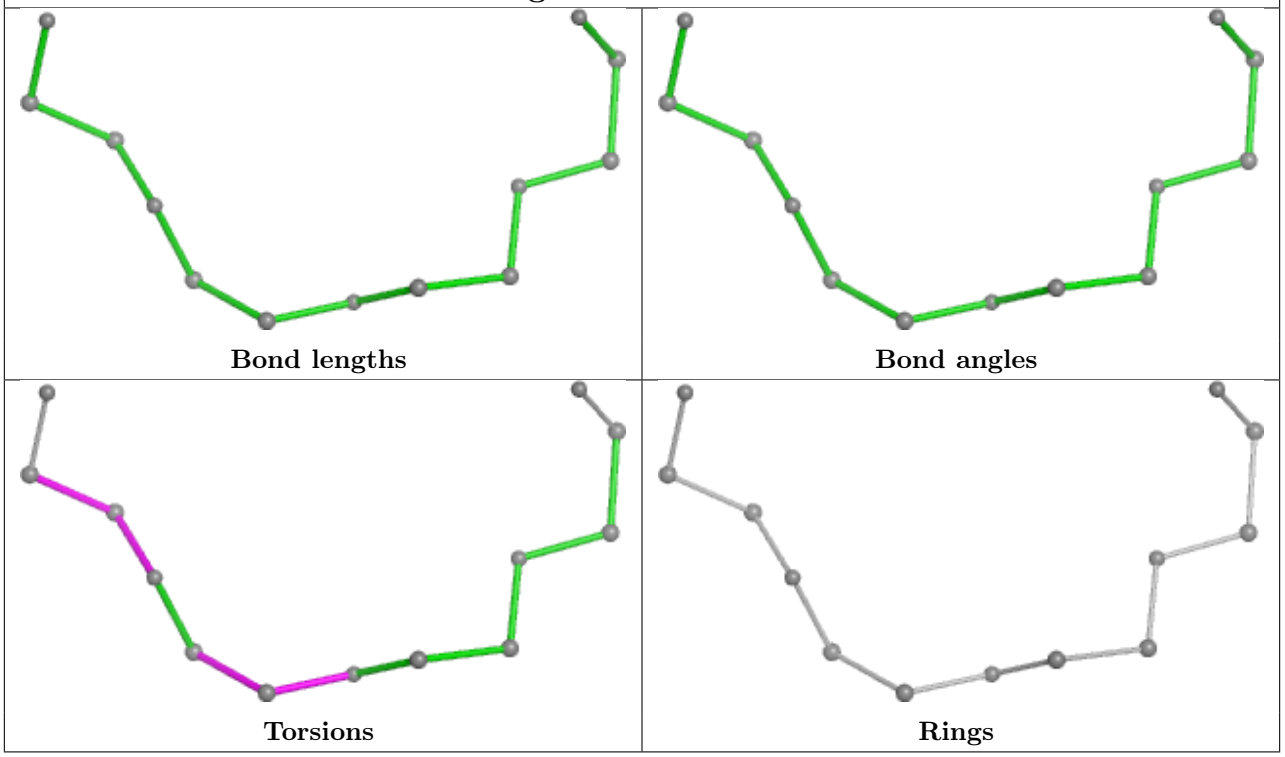


Torsions

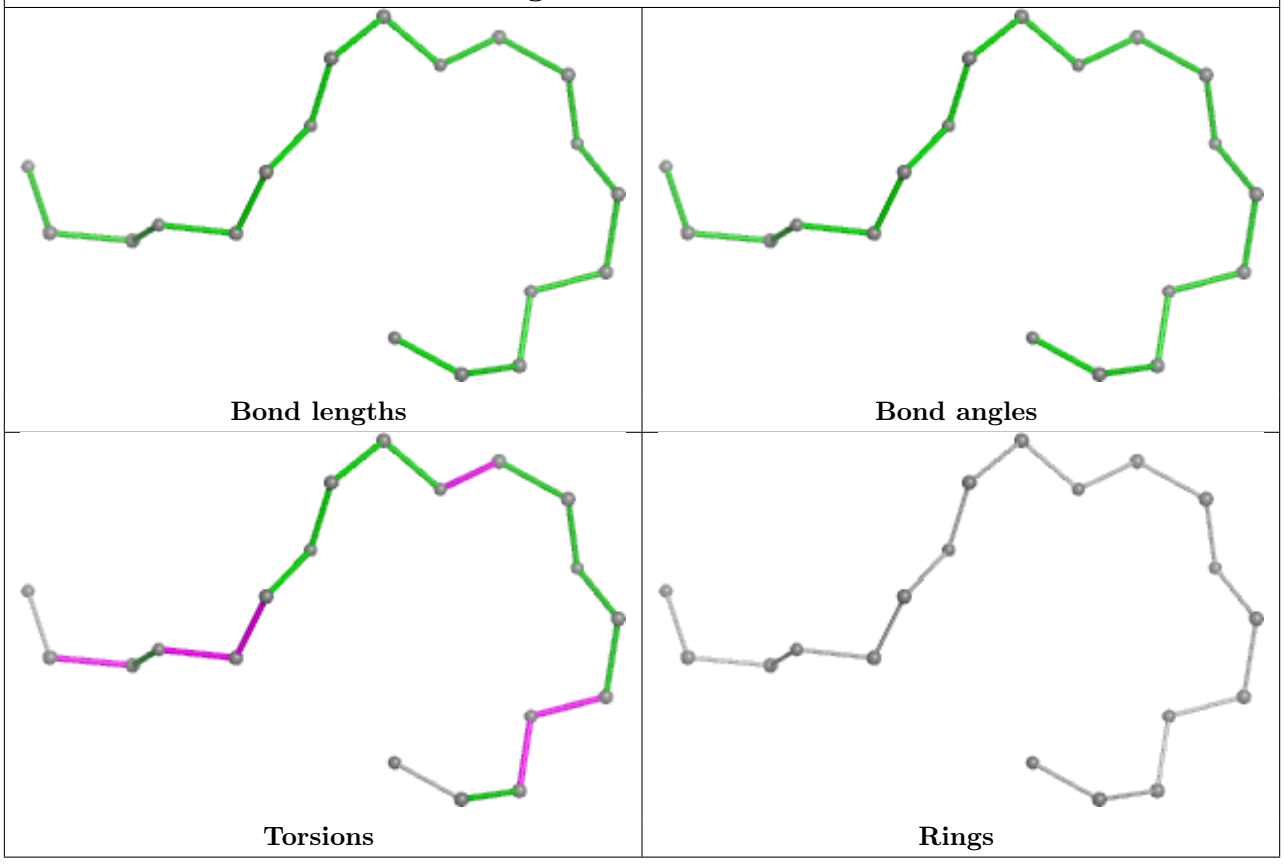


Rings

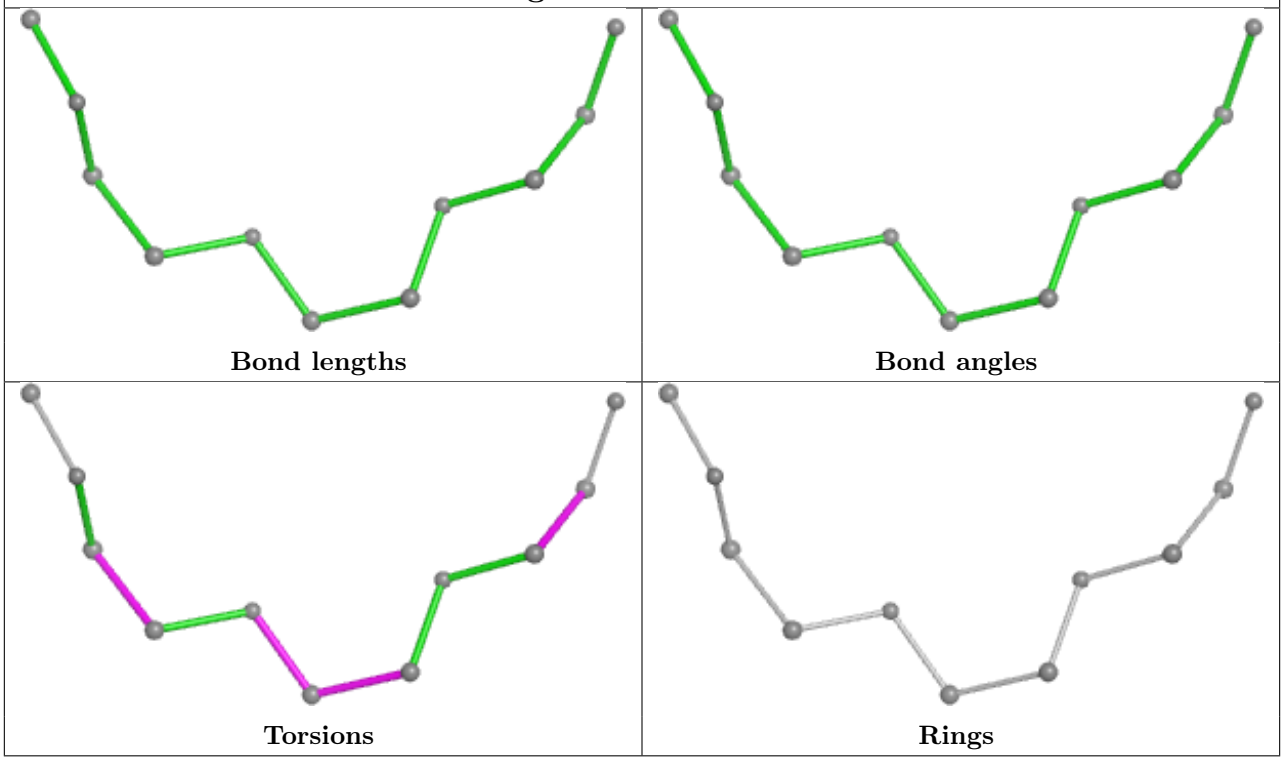
Ligand P6G E 401



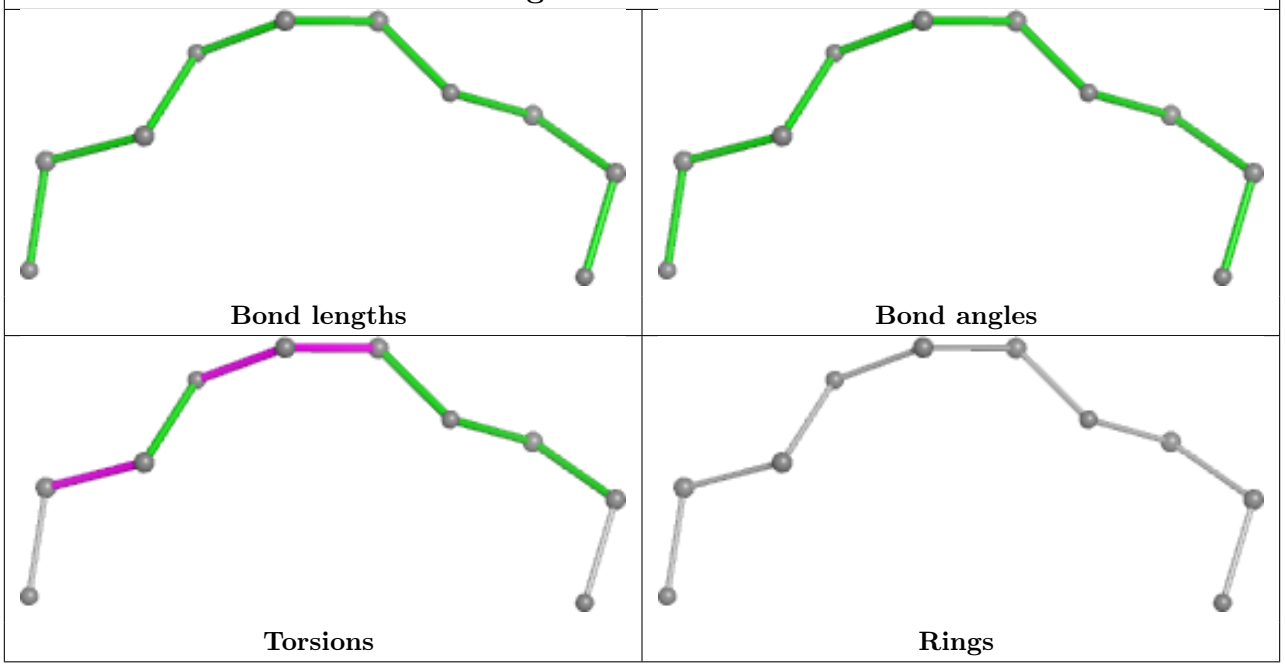
Ligand P6G A 400



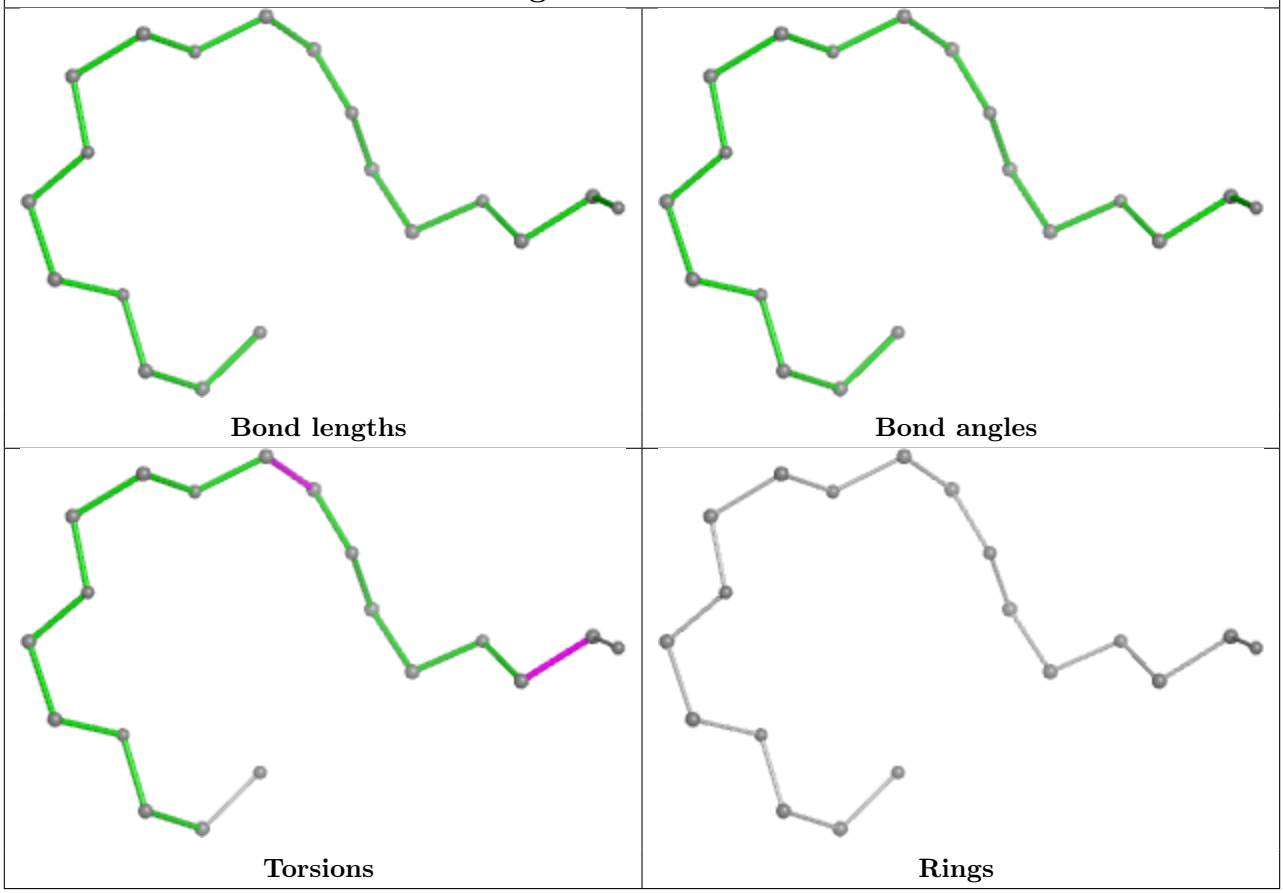
Ligand P6G B 401



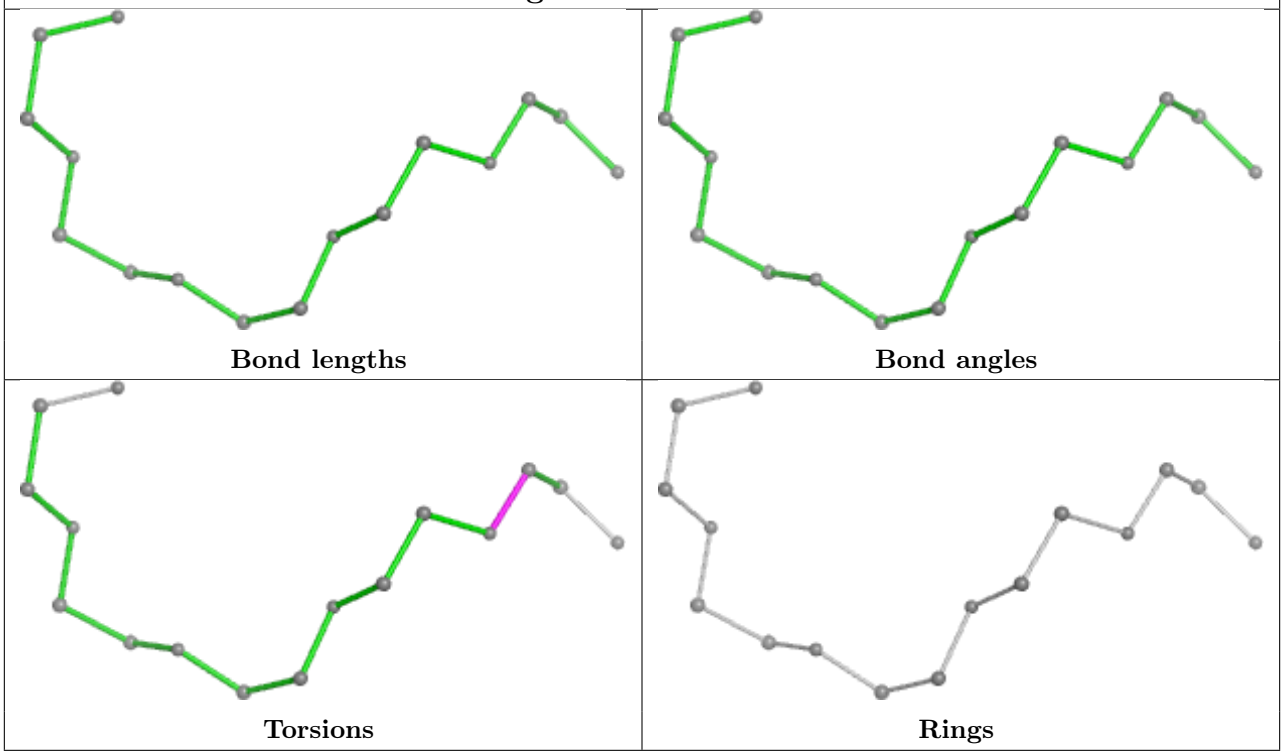
Ligand P6G A 402



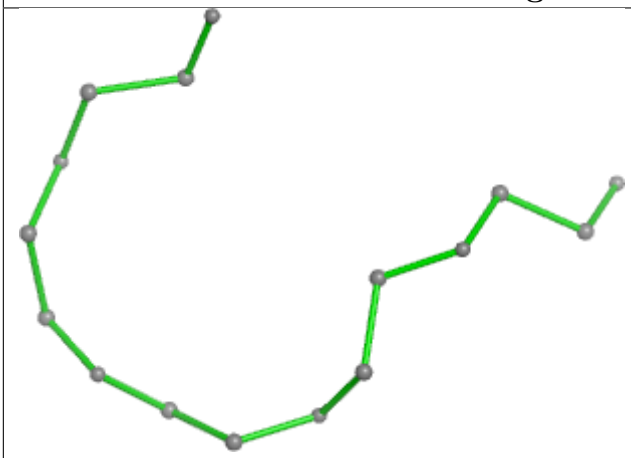
Ligand P6G F 400



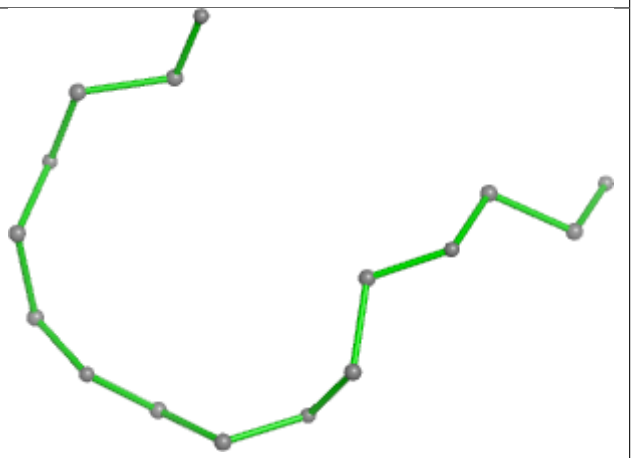
Ligand P6G D 400



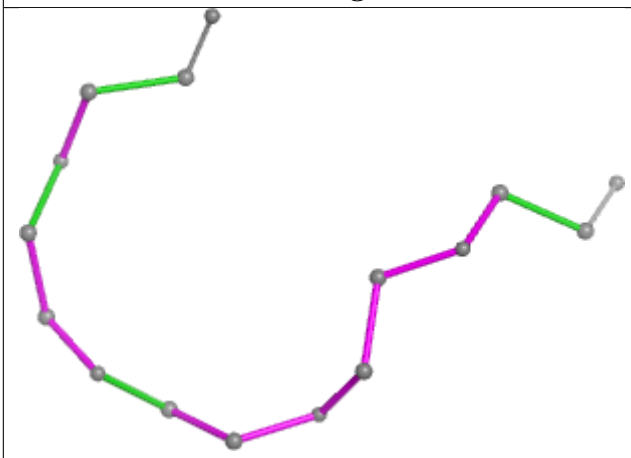
Ligand P6G C 400



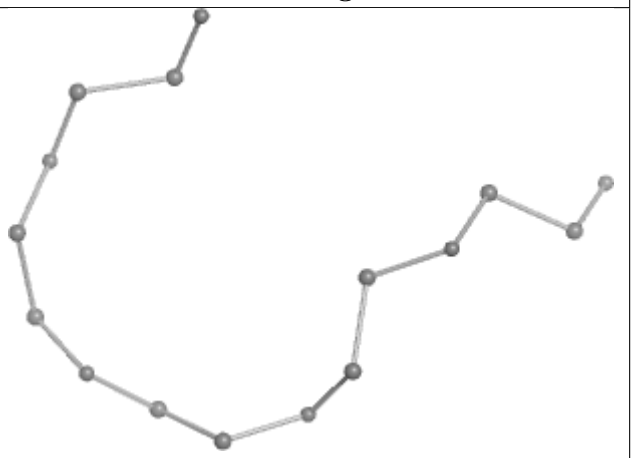
Bond lengths



Bond angles

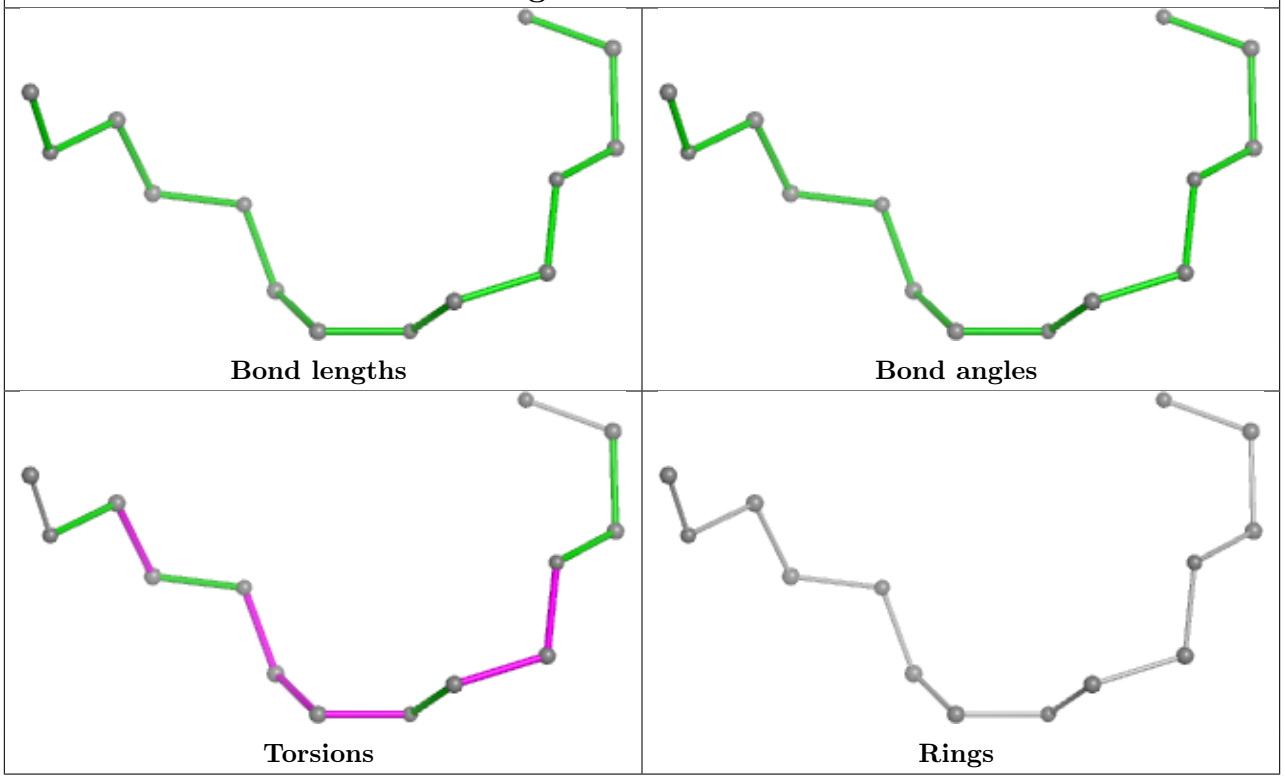


Torsions



Rings

Ligand P6G E 400



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	64:ASN	C	65:PRO	N	2.76

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	286/286 (100%)	-0.09	7 (2%)	59	62	29, 47, 68, 81	0
1	B	286/286 (100%)	-0.08	7 (2%)	59	62	29, 45, 69, 94	0
1	C	286/286 (100%)	0.19	26 (9%)	9	10	31, 47, 87, 108	0
1	D	286/286 (100%)	0.04	21 (7%)	15	16	30, 47, 80, 97	0
1	E	286/286 (100%)	0.11	20 (6%)	16	18	28, 47, 77, 97	0
1	F	286/286 (100%)	-0.07	6 (2%)	63	66	27, 41, 65, 87	0
All	All	1716/1716 (100%)	0.02	87 (5%)	28	31	27, 46, 75, 108	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	171	LEU	6.1
1	D	168	ALA	5.5
1	C	127	TYR	5.3
1	B	219	PRO	4.7
1	C	122	ALA	4.5
1	C	69	GLY	4.5
1	C	124	PRO	4.4
1	C	219	PRO	4.2
1	C	123	GLY	4.2
1	E	319	PHE	4.1
1	E	249	GLN	3.9
1	C	66	ASN	3.8
1	E	220	ALA	3.8
1	C	125	ASN	3.8
1	D	122	ALA	3.7
1	C	62	ILE	3.7
1	E	221	GLY	3.6
1	E	171	LEU	3.6
1	C	68	THR	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	308	GLY	3.4
1	E	127	TYR	3.4
1	D	220	ALA	3.4
1	E	66	ASN	3.3
1	C	63	LEU	3.3
1	D	65	PRO	3.3
1	D	219	PRO	3.3
1	E	248	GLY	3.1
1	F	219	PRO	3.1
1	C	171	LEU	3.1
1	C	70	THR	3.0
1	D	123	GLY	3.0
1	F	171	LEU	3.0
1	C	319	PHE	3.0
1	C	128	VAL	3.0
1	E	218	ASN	3.0
1	D	124	PRO	3.0
1	E	307	SER	2.9
1	C	169	ASP	2.9
1	A	219	PRO	2.8
1	A	124	PRO	2.8
1	D	221	GLY	2.8
1	C	65	PRO	2.8
1	C	221	GLY	2.7
1	E	247	THR	2.7
1	D	310	TYR	2.7
1	B	319	PHE	2.6
1	D	128	VAL	2.6
1	E	65	PRO	2.6
1	A	168	ALA	2.6
1	E	123	GLY	2.6
1	C	168	ALA	2.6
1	E	122	ALA	2.5
1	D	66	ASN	2.5
1	F	310	TYR	2.5
1	D	34	GLY	2.5
1	B	307	SER	2.5
1	E	34	GLY	2.5
1	D	62	ILE	2.4
1	A	310	TYR	2.4
1	D	218	ASN	2.4
1	D	172	GLY	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	219	PRO	2.4
1	E	125	ASN	2.3
1	D	248	GLY	2.3
1	C	173	ASN	2.3
1	B	220	ALA	2.3
1	A	66	ASN	2.3
1	D	127	TYR	2.3
1	E	306	TYR	2.3
1	C	67	GLU	2.2
1	F	220	ALA	2.2
1	D	169	ASP	2.2
1	D	64	ASN	2.2
1	E	246	ALA	2.2
1	A	125	ASN	2.2
1	E	124	PRO	2.1
1	B	223	LEU	2.1
1	C	34	GLY	2.1
1	C	120	THR	2.1
1	B	306	TYR	2.1
1	D	171	LEU	2.1
1	C	121	THR	2.1
1	C	119	SER	2.1
1	F	66	ASN	2.1
1	F	221	GLY	2.1
1	B	247	THR	2.0
1	D	306	TYR	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)

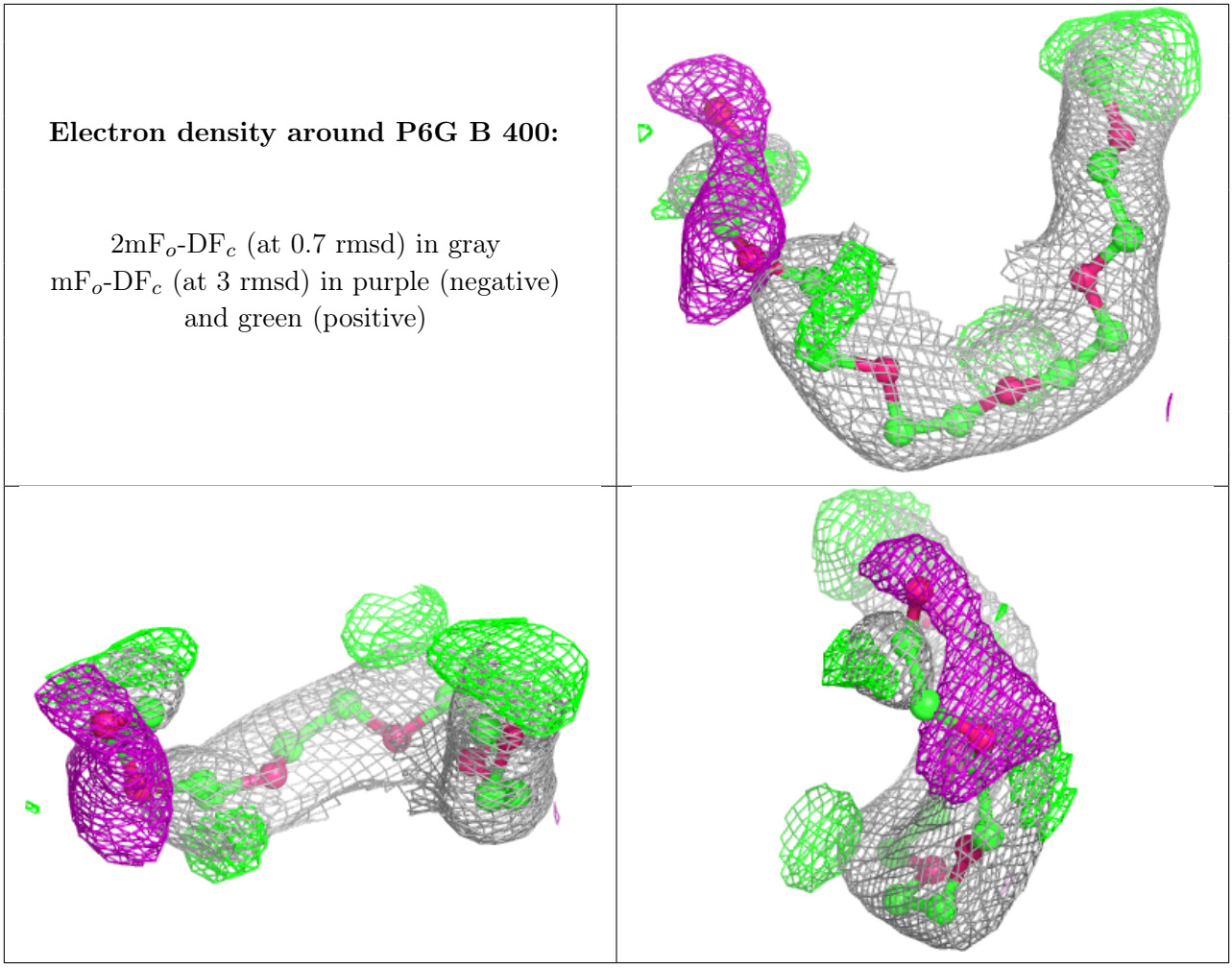
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
2	P6G	D	401	10/19	0.75	0.16	70,73,74,75	0
2	P6G	B	400	17/19	0.78	0.22	53,59,79,83	0
2	P6G	C	401	8/19	0.80	0.15	65,66,70,70	0
2	P6G	B	401	11/19	0.82	0.12	62,65,68,68	0
2	P6G	A	401	14/19	0.85	0.16	70,75,77,78	0
2	P6G	C	400	16/19	0.85	0.12	62,66,69,70	0
2	P6G	F	400	19/19	0.88	0.50	30,36,43,49	19
2	P6G	E	401	13/19	0.89	0.11	65,69,73,75	0
2	P6G	E	403	10/19	0.90	0.14	53,56,66,69	0
2	P6G	A	400	19/19	0.90	0.15	50,62,70,74	0
2	P6G	A	402	10/19	0.91	0.10	71,71,79,80	0
2	P6G	F	401	8/19	0.91	0.11	65,66,71,71	0
2	P6G	E	400	14/19	0.92	0.11	58,59,65,65	0
2	P6G	D	400	16/19	0.94	0.09	51,54,67,70	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.

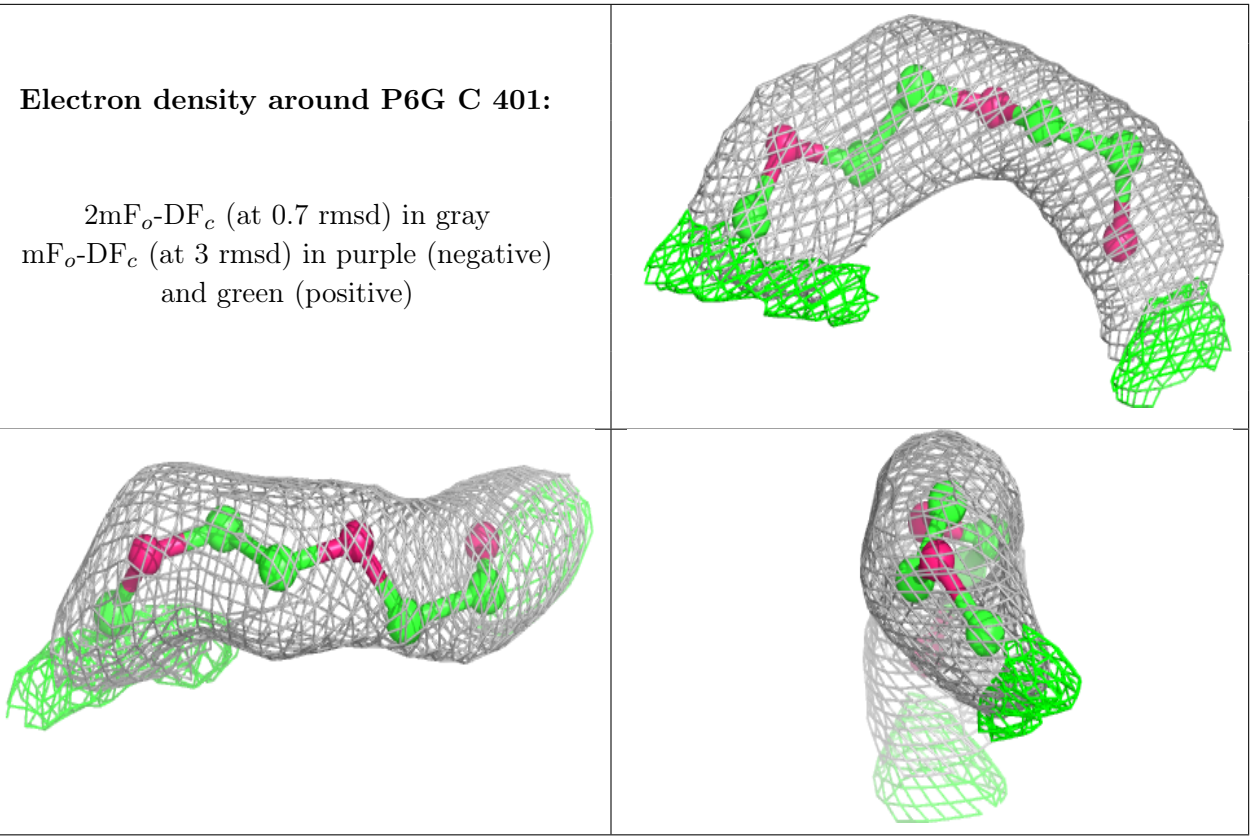
Electron density around P6G B 400:

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



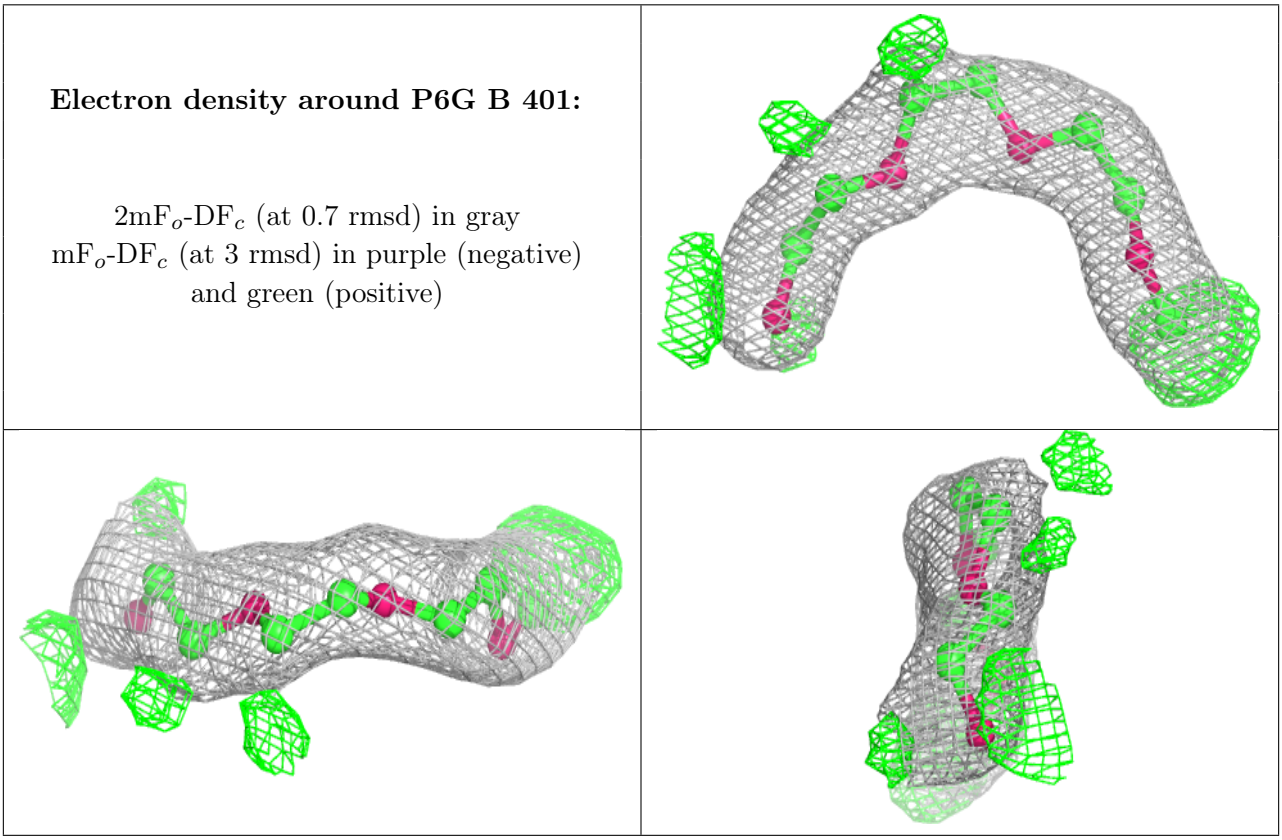
Electron density around P6G C 401:

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



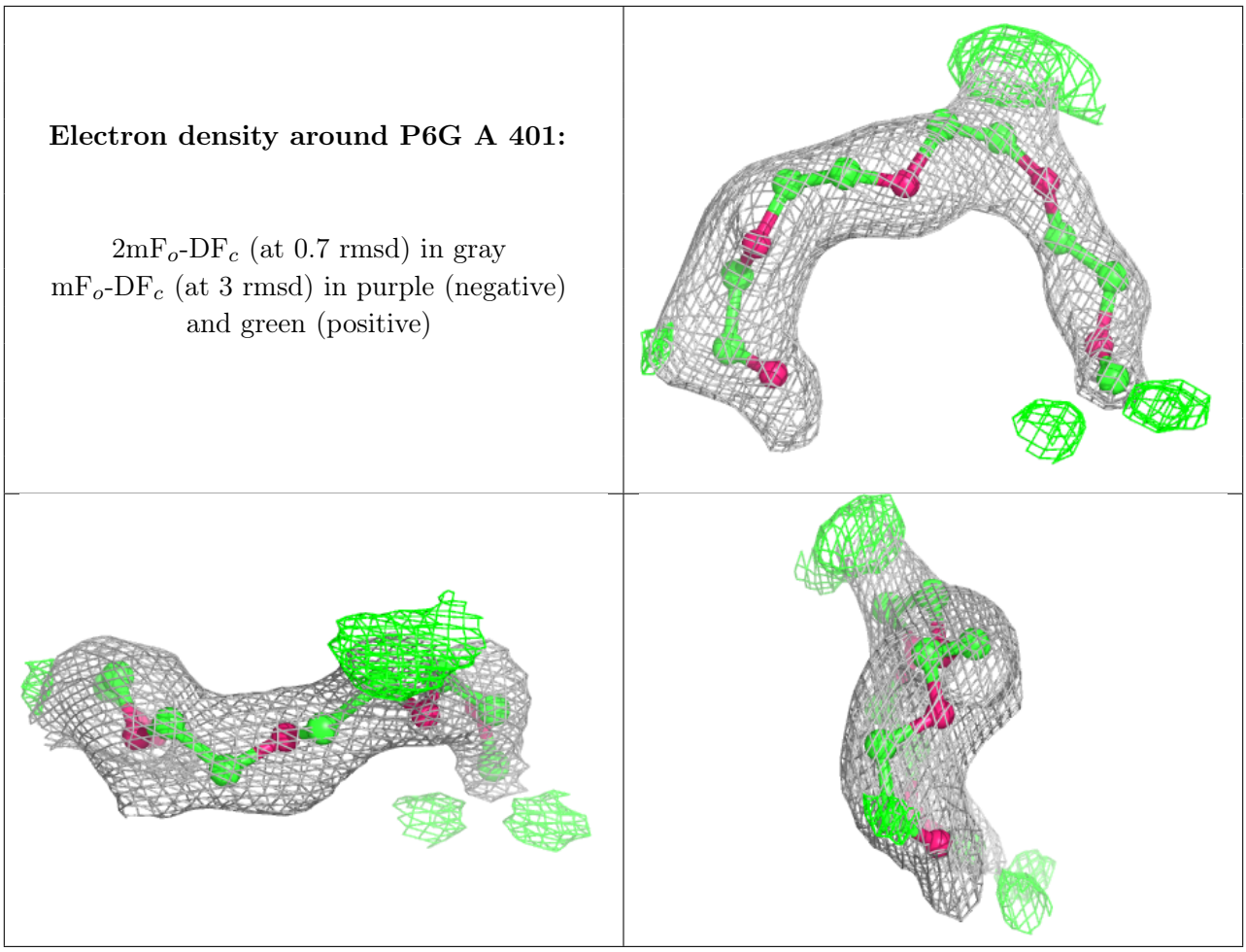
Electron density around P6G B 401:

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



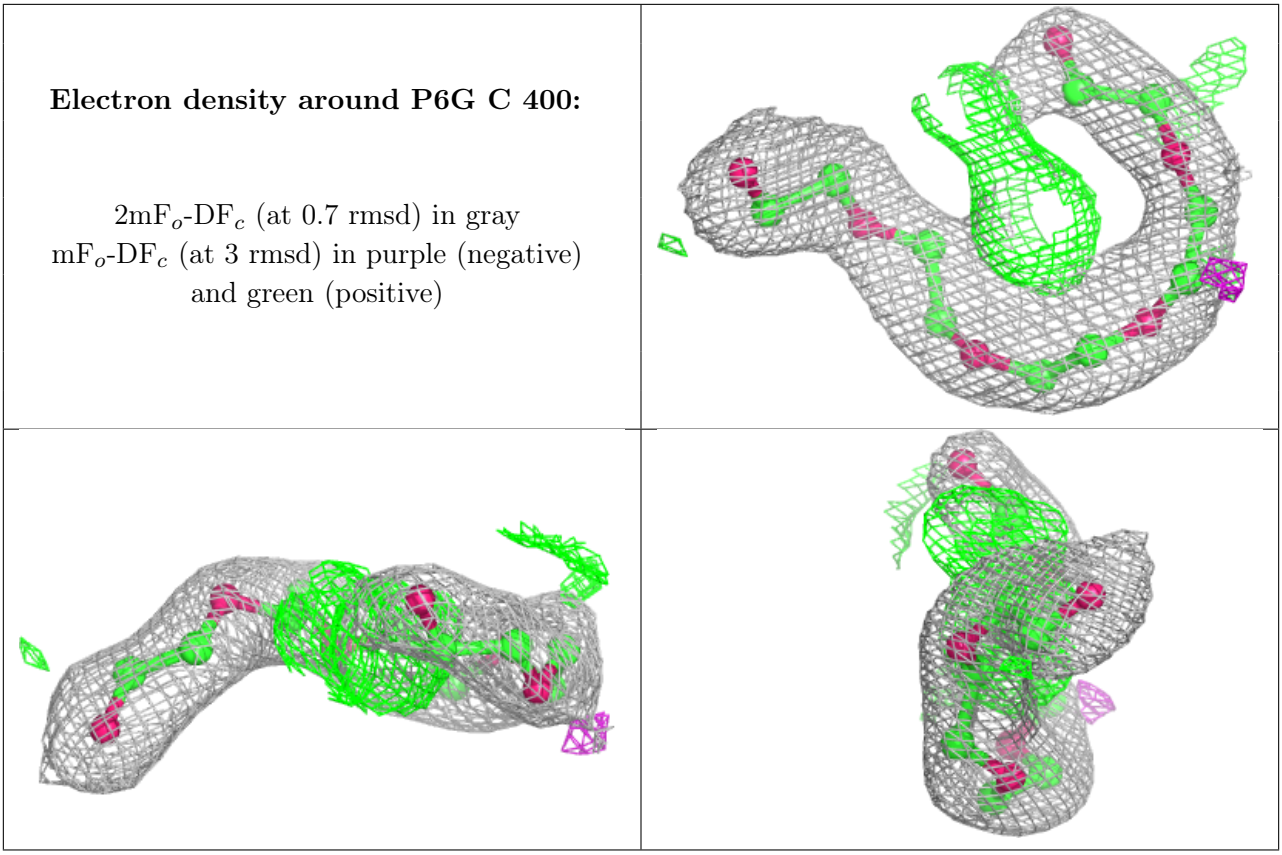
Electron density around P6G A 401:

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



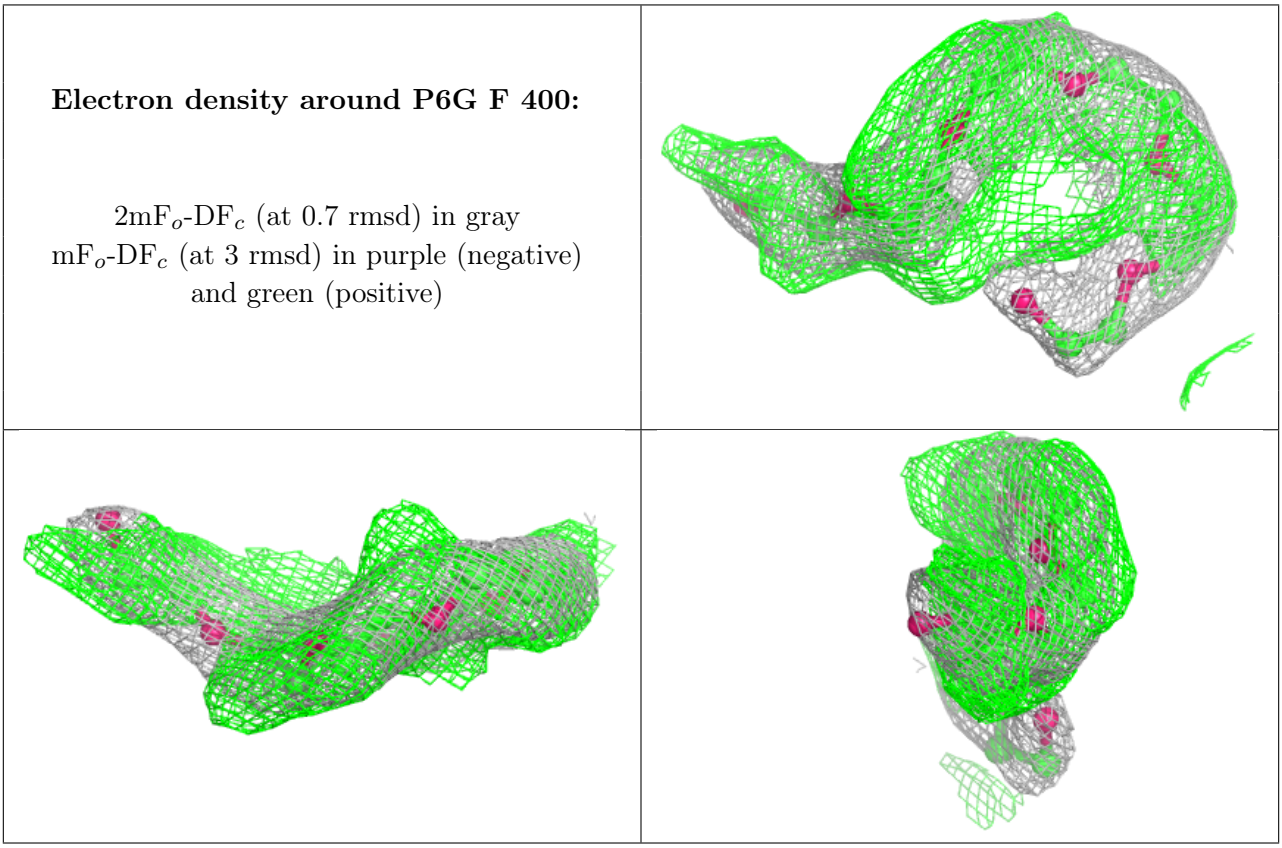
Electron density around P6G C 400:

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



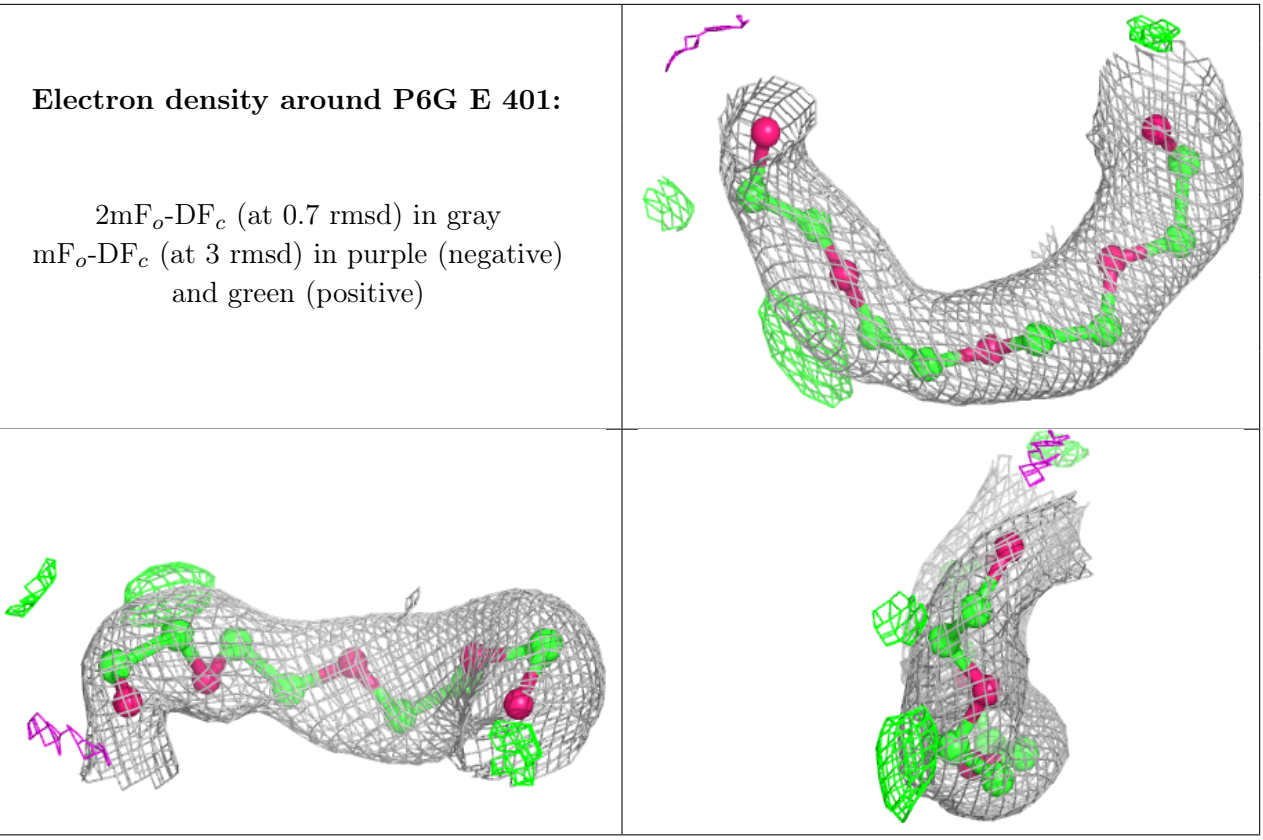
Electron density around P6G F 400:

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



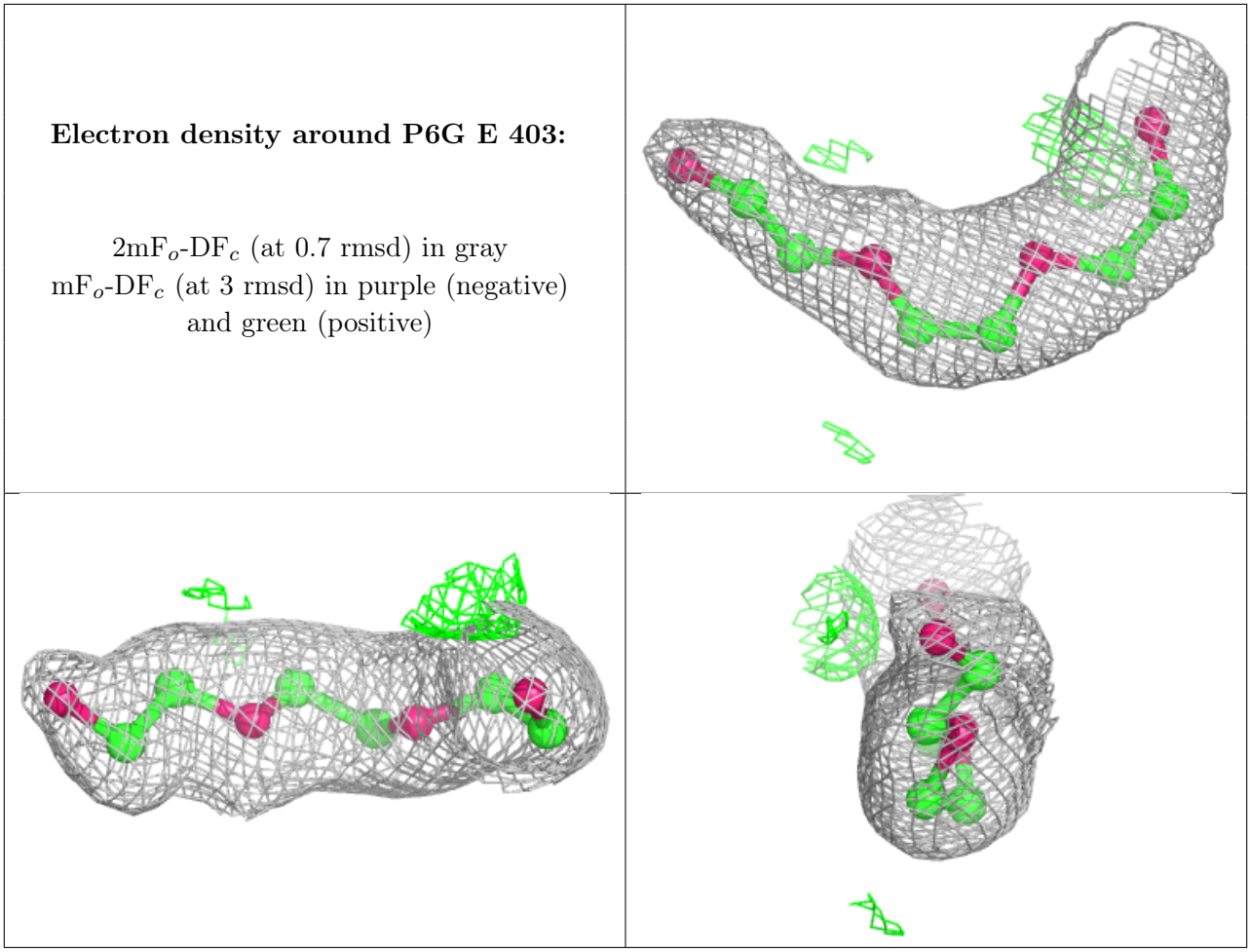
Electron density around P6G E 401:

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



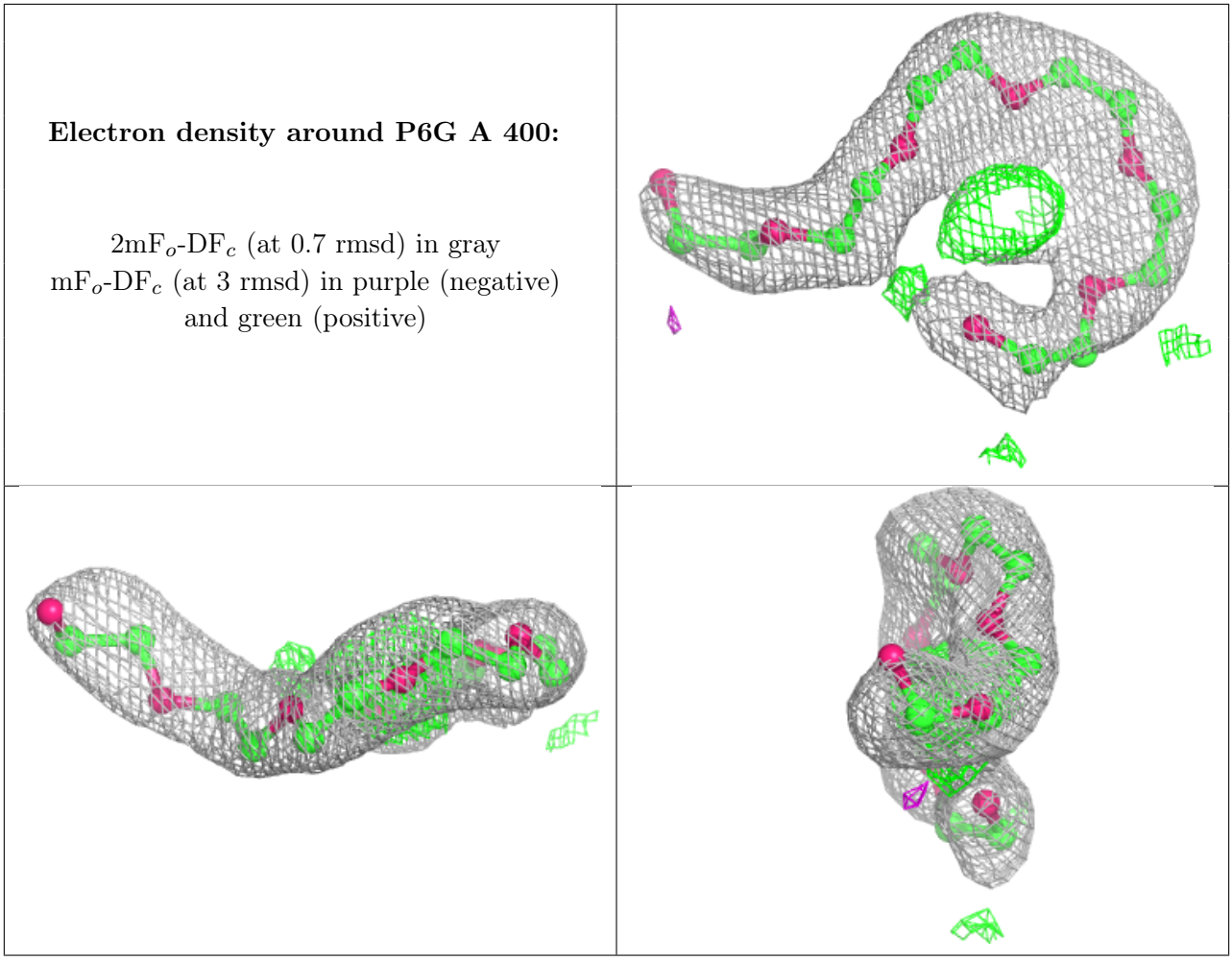
Electron density around P6G E 403:

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



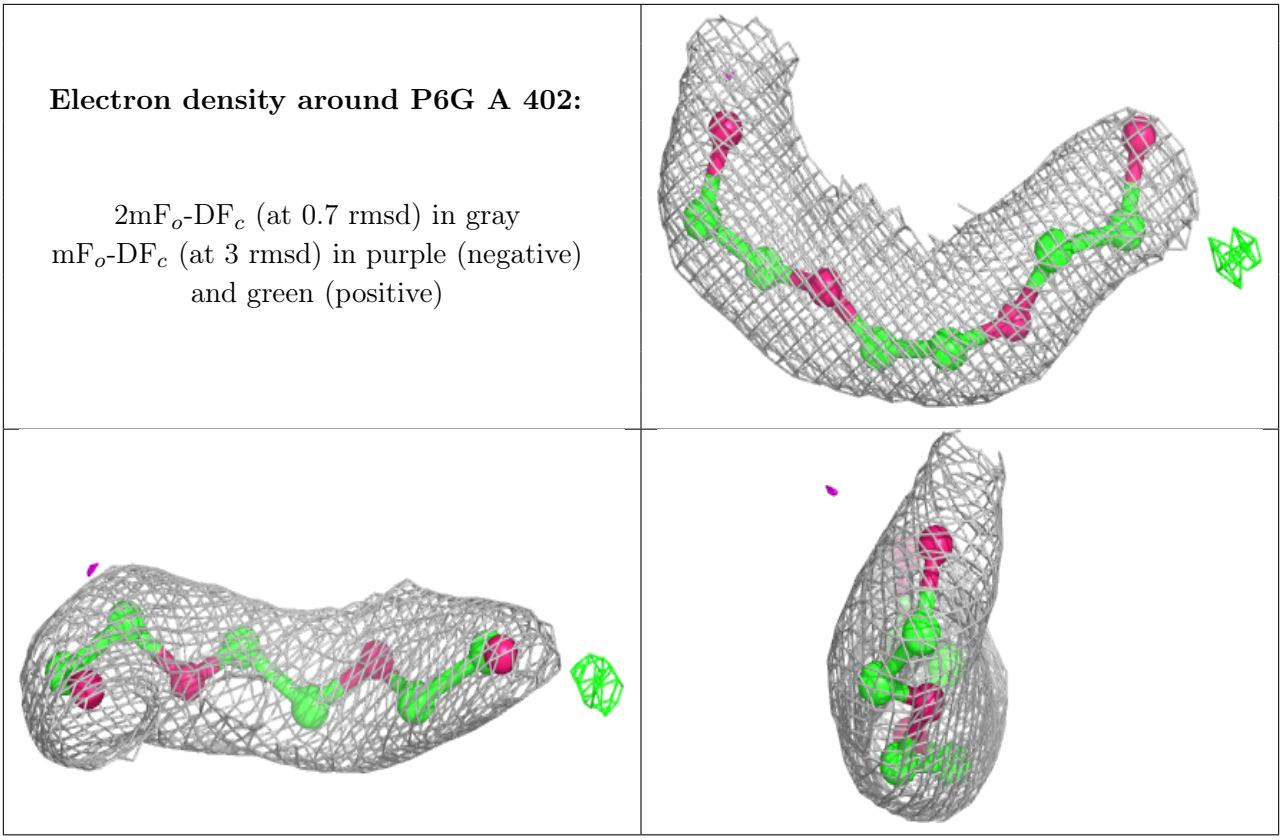
Electron density around P6G A 400:

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



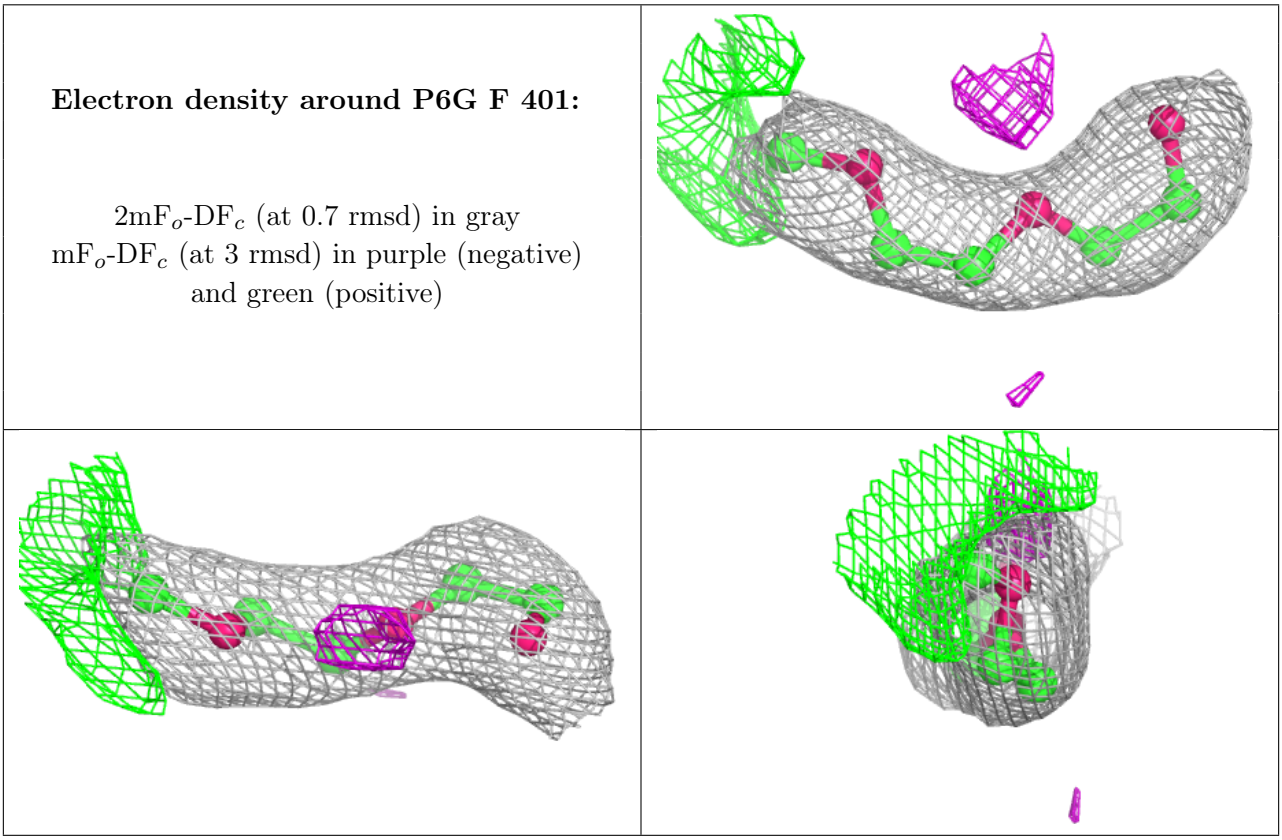
Electron density around P6G A 402:

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



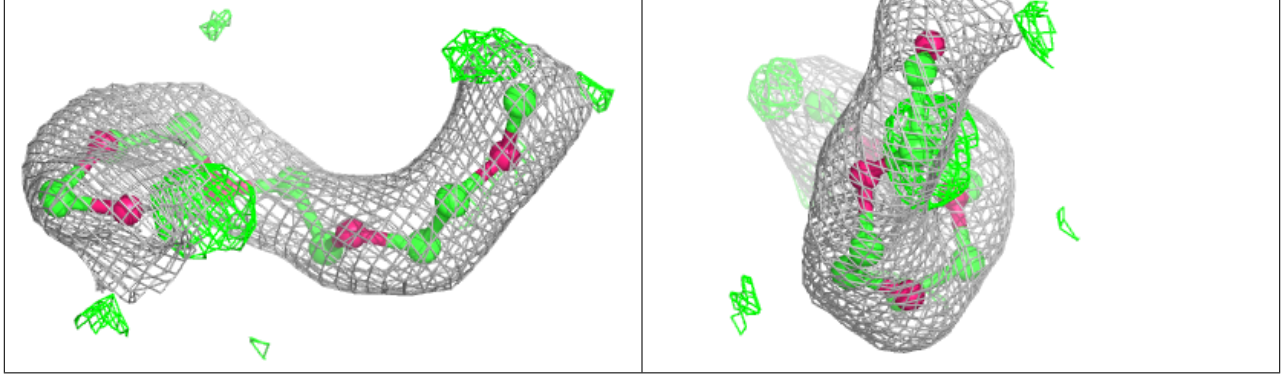
Electron density around P6G F 401:

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



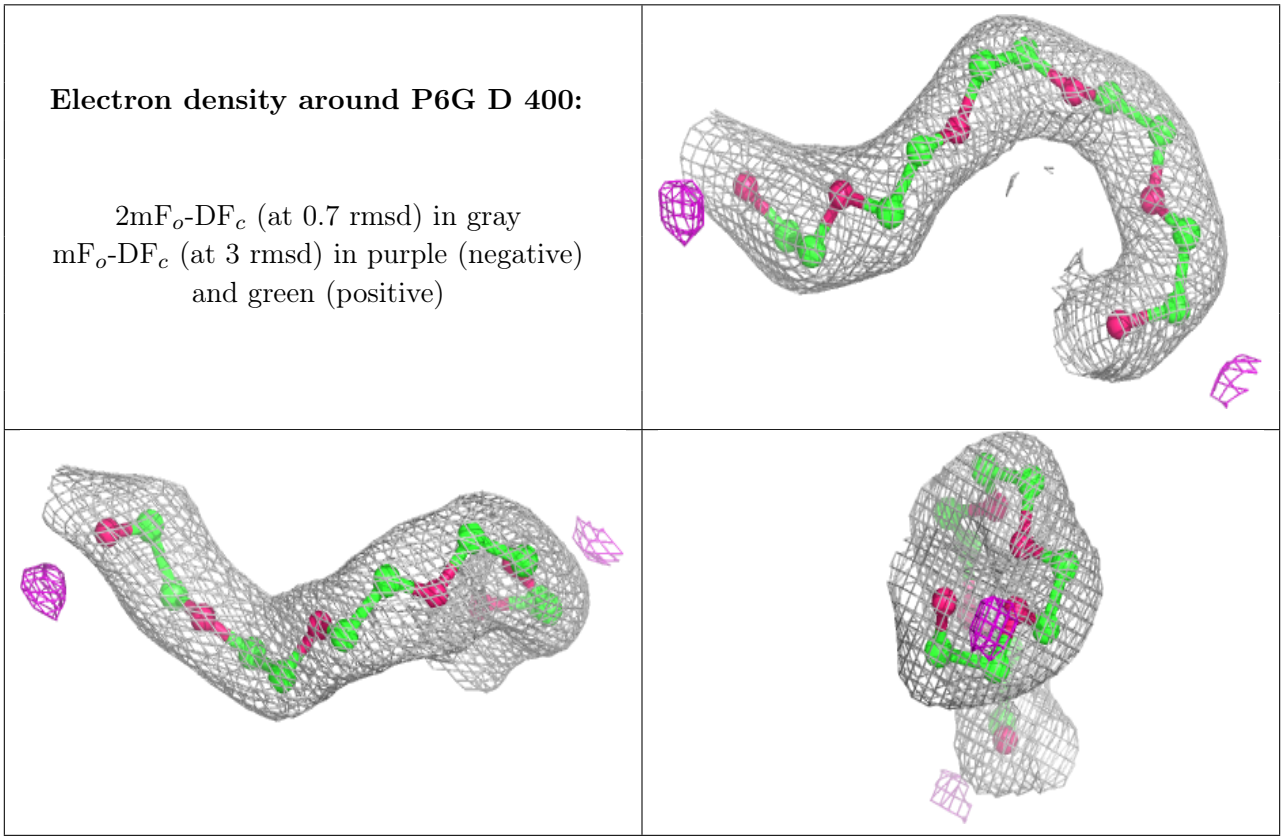
Electron density around P6G E 400:

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



Electron density around P6G D 400:

$2mF_o$-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.