Full wwPDB X-ray Structure Validation Report (i)

Dec 17, 2023 – 02:43 pm GMT

PDB ID	:	3ZIX
Title	:	Clostridium perfringens Enterotoxin with the 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 (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:

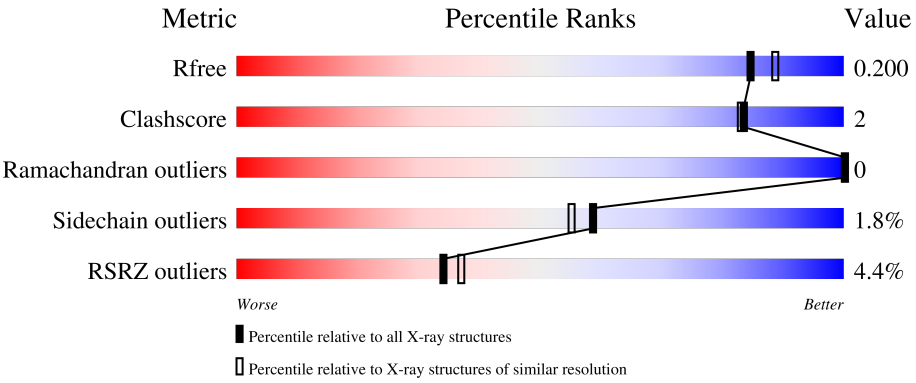
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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% 95% 5%
1	B	286	2% 95% 5%
1	C	286	7% 92% 7%
1	D	286	6% 96%
1	E	286	8% 94% 6%

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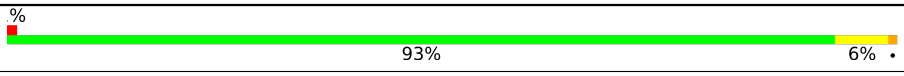
Mol	Chain	Length	Quality of chain
1	F	286	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 15361 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
			2251	1427	363	458	3			
1	B	286	Total	C	N	O	S	0	4	0
			2228	1415	357	452	4			
1	C	286	Total	C	N	O	S	0	4	0
			2237	1419	363	452	3			
1	D	286	Total	C	N	O	S	0	7	0
			2236	1419	358	456	3			
1	E	286	Total	C	N	O	S	0	5	0
			2220	1412	357	448	3			
1	F	286	Total	C	N	O	S	0	4	0
			2243	1420	365	455	3			

There are 24 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
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
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
D	34	GLY	-	expression tag	UNP P01558
D	35	ALA	-	expression tag	UNP P01558
D	36	MET	-	expression tag	UNP P01558
D	37	GLY	-	expression tag	UNP P01558
E	34	GLY	-	expression tag	UNP P01558

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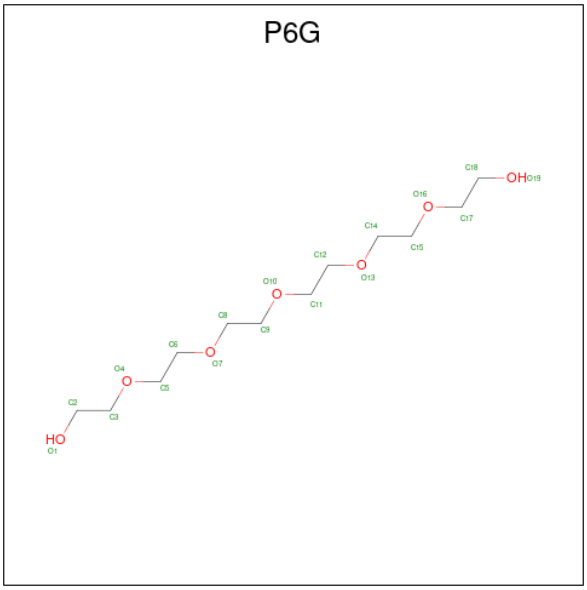
Chain	Residue	Modelled	Actual	Comment	Reference
E	35	ALA	-	expression tag	UNP P01558
E	36	MET	-	expression tag	UNP P01558
E	37	GLY	-	expression tag	UNP P01558
F	34	GLY	-	expression tag	UNP P01558
F	35	ALA	-	expression tag	UNP P01558
F	36	MET	-	expression tag	UNP P01558
F	37	GLY	-	expression tag	UNP P01558

- 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
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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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	305	Total O 305 305	0	0
3	B	314	Total O 314 314	0	0
3	C	266	Total O 266 266	0	0
3	D	272	Total O 272 272	0	0
3	E	268	Total O 268 268	0	0
3	F	336	Total O 336 336	0	0

3 Residue-property plots (i)

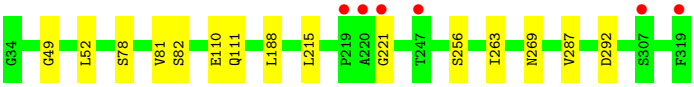
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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:

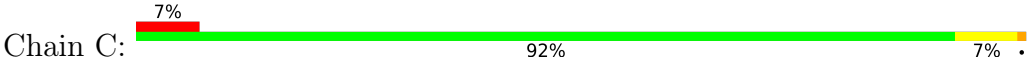
• Molecule 1: HEAT-LABILE ENTEROTOXIN B CHAIN

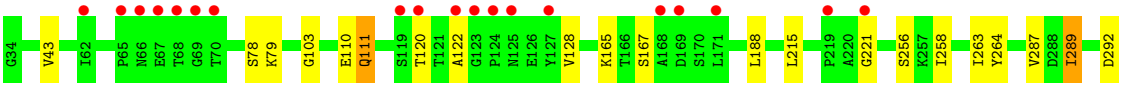
Chain B:

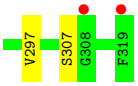


• Molecule 1: HEAT-LABILE ENTEROTOXIN B CHAIN

Chain C:

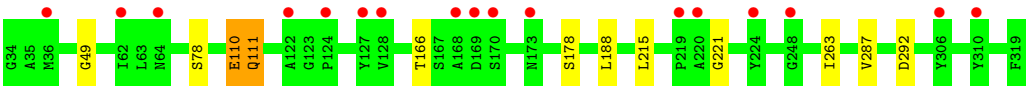






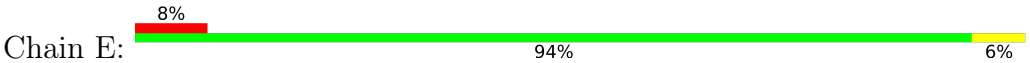
• Molecule 1: HEAT-LABILE ENTEROTOXIN B CHAIN

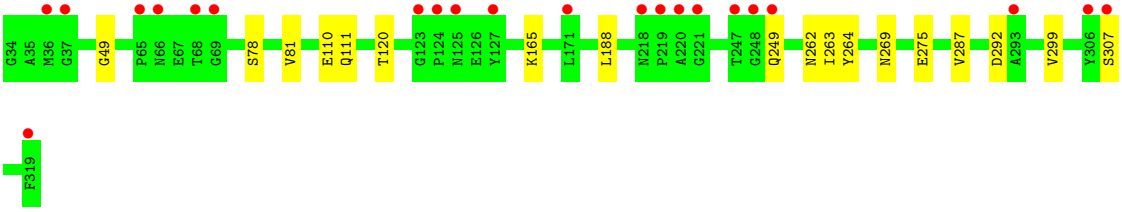
Chain D:



• Molecule 1: HEAT-LABILE ENTEROTOXIN B CHAIN

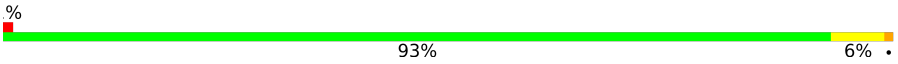
Chain E:

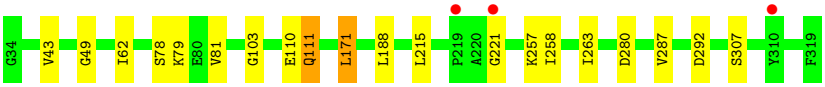




• Molecule 1: HEAT-LABILE ENTEROTOXIN B CHAIN

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	191.68Å 128.29Å 137.20Å 90.00° 133.81° 90.00°	Depositor
Resolution (Å)	47.03 – 1.90 47.03 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.8 (47.03-1.90) 98.8 (47.03-1.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.08 (at 1.90Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.176 , 0.197 0.180 , 0.200	Depositor DCC
R_{free} test set	9299 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	32.8	Xtriage
Anisotropy	0.105	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 62.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.005 for h+2*l,k,-h-l 0.012 for h,-k,-h-l 0.038 for -h-2*l,-k,l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	15361	wwPDB-VP
Average B, all atoms (Å^2)	45.0	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	0/2315	0.66	0/3141
1	B	0.54	0/2284	0.64	0/3105
1	C	0.51	0/2292	0.65	0/3112
1	D	0.51	0/2301	0.66	0/3129
1	E	0.52	0/2278	0.66	0/3099
1	F	0.55	0/2299	0.64	0/3121
All	All	0.52	0/13769	0.65	0/18707

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	2251	0	2191	8	0
1	B	2228	0	2158	10	0
1	C	2237	0	2181	15	0
1	D	2236	0	2168	10	0
1	E	2220	0	2160	11	0
1	F	2243	0	2189	17	0
2	A	43	0	55	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	28	0	34	4	0
2	C	24	0	30	0	0
2	D	26	0	34	0	0
2	E	37	0	46	1	0
2	F	27	0	35	2	0
3	A	305	0	0	2	0
3	B	314	0	0	1	0
3	C	266	0	0	0	0
3	D	272	0	0	0	0
3	E	268	0	0	2	0
3	F	336	0	0	0	0
All	All	15361	0	13281	65	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 (65) 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:D:110[A]:GLU:HG3	1:F:110[A]:GLU:HG3	1.46	0.96
1:A:110[A]:GLU:HG2	1:C:110[A]:GLU:HG3	1.47	0.92
1:F:62:ILE:HG21	1:F:171:LEU:HD21	1.63	0.81
1:E:263[B]:ILE:HD11	1:E:287:VAL:HG21	1.63	0.80
1:B:263:ILE:HD11	1:B:287:VAL:HG21	1.73	0.70
1:C:110[B]:GLU:H	1:C:110[B]:GLU:CD	1.96	0.67
1:F:78:SER:HA	1:F:111[B]:GLN:HG3	1.81	0.63
1:E:49:GLY:HA3	1:E:188:LEU:HG	1.80	0.62
1:E:264:TYR:HE1	1:E:299[B]:VAL:CG1	2.13	0.62
1:C:263:ILE:HD11	1:C:287:VAL:HG21	1.80	0.62
1:D:263:ILE:HD11	1:D:287:VAL:HG21	1.83	0.60
1:D:110[A]:GLU:CG	1:F:110[A]:GLU:HG3	2.27	0.60
1:C:120:THR:HG21	1:C:165:LYS:HD3	1.85	0.58
1:A:49:GLY:HA3	1:A:188:LEU:HG	1.86	0.57
1:E:110:GLU:HG2	3:E:2125:HOH:O	2.05	0.57
1:E:110:GLU:CG	3:E:2125:HOH:O	2.54	0.56
1:E:264:TYR:HE1	1:E:299[B]:VAL:HG11	1.71	0.56
1:B:49:GLY:HA3	1:B:188:LEU:HG	1.88	0.54
1:D:49:GLY:HA3	1:D:188:LEU:HG	1.90	0.54
1:B:82:SER:HA	2:B:400:P6G:H172	1.89	0.53
1:A:78:SER:HA	1:A:111[A]:GLN:HG3	1.92	0.52
1:B:263:ILE:CD1	1:B:287:VAL:HG21	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:120:THR:HG21	1:E:165:LYS:HD3	1.92	0.51
1:B:81:VAL:O	2:B:400:P6G:H172	2.11	0.50
1:F:280:ASP:HA	2:F:401:P6G:H62	1.93	0.50
1:F:49:GLY:HA3	1:F:188:LEU:HG	1.93	0.49
1:F:79:LYS:NZ	1:F:110[A]:GLU:OE2	2.39	0.49
1:D:78:SER:HA	1:D:111[A]:GLN:HG3	1.93	0.49
1:B:82:SER:HB2	2:B:400:P6G:H122	1.94	0.49
1:C:122:ALA:HB2	1:C:128:VAL:HG22	1.94	0.49
1:C:79:LYS:HE3	1:C:110[A]:GLU:OE2	2.13	0.48
1:B:78:SER:HA	1:B:111:GLN:HG3	1.94	0.48
1:D:166[A]:THR:HG21	1:D:178:SER:OG	2.13	0.47
1:E:81:VAL:O	2:E:400:P6G:H152	2.14	0.47
1:C:263:ILE:CD1	1:C:287:VAL:HG21	2.45	0.47
1:C:287:VAL:HG23	1:C:289:ILE:HD12	1.97	0.47
1:D:110[A]:GLU:HG3	1:F:110[A]:GLU:CG	2.32	0.46
1:F:215:LEU:O	1:F:221:GLY:HA2	2.15	0.46
1:A:192:SER:HB2	3:A:2018:HOH:O	2.16	0.46
1:D:215:LEU:O	1:D:221:GLY:HA2	2.17	0.45
1:A:110[B]:GLU:HG2	3:A:2139:HOH:O	2.17	0.45
1:C:78:SER:HA	1:C:111[A]:GLN:HG3	1.99	0.45
1:D:263:ILE:CD1	1:D:287:VAL:HG21	2.46	0.45
1:B:110:GLU:HG2	3:B:2144:HOH:O	2.16	0.44
1:E:78:SER:HA	1:E:111:GLN:HG3	1.99	0.44
1:A:215:LEU:O	1:A:221:GLY:HA2	2.18	0.44
1:B:215:LEU:O	1:B:221:GLY:HA2	2.17	0.44
1:C:128:VAL:HG12	1:C:167:SER:HB3	1.99	0.44
1:C:215:LEU:O	1:C:221:GLY:HA2	2.17	0.44
1:A:43:VAL:HG21	1:A:103:GLY:HA3	2.01	0.43
1:E:262:ASN:HB2	1:E:299[B]:VAL:CG1	2.49	0.43
1:E:264:TYR:HE1	1:E:299[B]:VAL:HG12	1.82	0.43
1:A:110[A]:GLU:HG2	1:C:110[A]:GLU:CG	2.34	0.42
1:C:43:VAL:HG21	1:C:103:GLY:HA3	2.02	0.42
1:F:263:ILE:HD11	1:F:287:VAL:HG21	2.02	0.42
1:B:52:LEU:HD22	2:B:400:P6G:H121	2.01	0.42
1:F:62:ILE:CG2	1:F:171:LEU:HD21	2.40	0.41
1:F:263:ILE:CD1	1:F:287:VAL:HG21	2.51	0.41
1:C:264:TYR:HB2	1:C:297[B]:VAL:HG13	2.01	0.41
1:D:110[B]:GLU:OE1	1:F:110[B]:GLU:HG2	2.21	0.41
1:F:81:VAL:O	2:F:400:P6G:H51	2.20	0.41
1:F:257:LYS:HG3	1:F:258:ILE:HG23	2.02	0.40
1:F:43:VAL:HG21	1:F:103:GLY:HA3	2.03	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%)	285 (99%)	4 (1%)	0	100	100
1	B	288/286 (101%)	283 (98%)	5 (2%)	0	100	100
1	C	288/286 (101%)	285 (99%)	3 (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%)	1710 (99%)	23 (1%)	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	251/247 (102%)	246 (98%)	5 (2%)	55	51
1	B	246/247 (100%)	243 (99%)	3 (1%)	71	70
1	C	249/247 (101%)	241 (97%)	8 (3%)	39	30
1	D	249/247 (101%)	244 (98%)	5 (2%)	55	51
1	E	247/247 (100%)	242 (98%)	5 (2%)	55	51
1	F	251/247 (102%)	246 (98%)	5 (2%)	55	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1493/1482 (101%)	1462 (98%)	31 (2%)	59 48

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60[A]	SER
1	A	60[B]	SER
1	A	171	LEU
1	A	292	ASP
1	A	307	SER
1	B	256	SER
1	B	269	ASN
1	B	292	ASP
1	C	111[A]	GLN
1	C	111[B]	GLN
1	C	188	LEU
1	C	256	SER
1	C	258	ILE
1	C	289	ILE
1	C	292	ASP
1	C	307	SER
1	D	110[A]	GLU
1	D	110[B]	GLU
1	D	111[A]	GLN
1	D	111[B]	GLN
1	D	292	ASP
1	E	249	GLN
1	E	269	ASN
1	E	275	GLU
1	E	292	ASP
1	E	307	SER
1	F	111[A]	GLN
1	F	111[B]	GLN
1	F	171	LEU
1	F	292	ASP
1	F	307	SER

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

Mol	Chain	Res	Type
1	B	269	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 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	E	401	-	12,12,18	0.50	0	11,11,17	0.25	0
2	P6G	F	401	-	7,7,18	0.48	0	6,6,17	0.21	0
2	P6G	D	400	-	15,15,18	0.48	0	14,14,17	0.54	0
2	P6G	B	400	-	16,16,18	0.53	0	15,15,17	0.66	0
2	P6G	C	400	-	15,15,18	0.51	0	14,14,17	0.43	0
2	P6G	D	401	-	9,9,18	0.47	0	8,8,17	0.29	0
2	P6G	E	403	-	9,9,18	0.45	0	8,8,17	0.29	0
2	P6G	A	402	-	9,9,18	0.48	0	8,8,17	0.26	0
2	P6G	A	401	-	13,13,18	0.47	0	12,12,17	0.25	0
2	P6G	E	400	-	13,13,18	0.54	0	12,12,17	0.22	0
2	P6G	F	400	-	18,18,18	0.42	0	17,17,17	0.53	0
2	P6G	C	401	-	7,7,18	0.49	0	6,6,17	0.17	0
2	P6G	A	400	-	18,18,18	0.50	0	17,17,17	0.46	0
2	P6G	B	401	-	10,10,18	0.45	0	9,9,17	0.26	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	E	401	-	-	4/10/10/16	-
2	P6G	F	401	-	-	2/5/5/16	-
2	P6G	D	400	-	-	2/13/13/16	-
2	P6G	B	400	-	-	5/14/14/16	-
2	P6G	C	400	-	-	12/13/13/16	-
2	P6G	D	401	-	-	1/7/7/16	-
2	P6G	E	403	-	-	4/7/7/16	-
2	P6G	A	402	-	-	2/7/7/16	-
2	P6G	A	401	-	-	6/11/11/16	-
2	P6G	E	400	-	-	5/11/11/16	-
2	P6G	F	400	-	-	7/16/16/16	-
2	P6G	C	401	-	-	4/5/5/16	-
2	P6G	A	400	-	-	3/16/16/16	-
2	P6G	B	401	-	-	2/8/8/16	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (59) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	400	P6G	O4-C5-C6-O7
2	C	400	P6G	O10-C11-C12-O13
2	C	400	P6G	O7-C8-C9-O10
2	A	401	P6G	O4-C5-C6-O7
2	A	402	P6G	O4-C5-C6-O7
2	F	400	P6G	O7-C8-C9-O10
2	E	400	P6G	O4-C5-C6-O7
2	E	403	P6G	O7-C8-C9-O10
2	A	401	P6G	O10-C11-C12-O13
2	F	400	P6G	O10-C11-C12-O13
2	A	400	P6G	O16-C17-C18-O19
2	C	400	P6G	O1-C2-C3-O4
2	C	401	P6G	O1-C2-C3-O4
2	F	400	P6G	O16-C17-C18-O19
2	B	400	P6G	O4-C5-C6-O7

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Mol	Chain	Res	Type	Atoms
2	F	401	P6G	O1-C2-C3-O4
2	E	401	P6G	O7-C8-C9-O10
2	C	401	P6G	O4-C5-C6-O7
2	B	400	P6G	O13-C14-C15-O16
2	B	400	P6G	O10-C11-C12-O13
2	C	401	P6G	C5-C6-O7-C8
2	F	400	P6G	C14-C15-O16-C17
2	A	400	P6G	C2-C3-O4-C5
2	D	400	P6G	O4-C5-C6-O7
2	A	402	P6G	C5-C6-O7-C8
2	C	400	P6G	C12-C11-O10-C9
2	E	403	P6G	O4-C5-C6-O7
2	B	400	P6G	C15-C14-O13-C12
2	E	401	P6G	C12-C11-O10-C9
2	E	403	P6G	C9-C8-O7-C6
2	B	400	P6G	C11-C12-O13-C14
2	A	401	P6G	C12-C11-O10-C9
2	D	400	P6G	C15-C14-O13-C12
2	E	403	P6G	C6-C5-O4-C3
2	A	401	P6G	C6-C5-O4-C3
2	A	401	P6G	C9-C8-O7-C6
2	C	401	P6G	C6-C5-O4-C3
2	F	400	P6G	C18-C17-O16-C15
2	F	401	P6G	C2-C3-O4-C5
2	C	400	P6G	C15-C14-O13-C12
2	E	401	P6G	C9-C8-O7-C6
2	C	400	P6G	C11-C12-O13-C14
2	E	400	P6G	C11-C12-O13-C14
2	B	401	P6G	C2-C3-O4-C5
2	A	400	P6G	C8-C9-O10-C11
2	C	400	P6G	C6-C5-O4-C3
2	C	400	P6G	C5-C6-O7-C8
2	E	400	P6G	C5-C6-O7-C8
2	A	401	P6G	C11-C12-O13-C14
2	B	401	P6G	C5-C6-O7-C8
2	E	400	P6G	O10-C11-C12-O13
2	F	400	P6G	C2-C3-O4-C5
2	C	400	P6G	C9-C8-O7-C6
2	C	400	P6G	C2-C3-O4-C5
2	E	400	P6G	C9-C8-O7-C6
2	C	400	P6G	C8-C9-O10-C11
2	D	401	P6G	C6-C5-O4-C3

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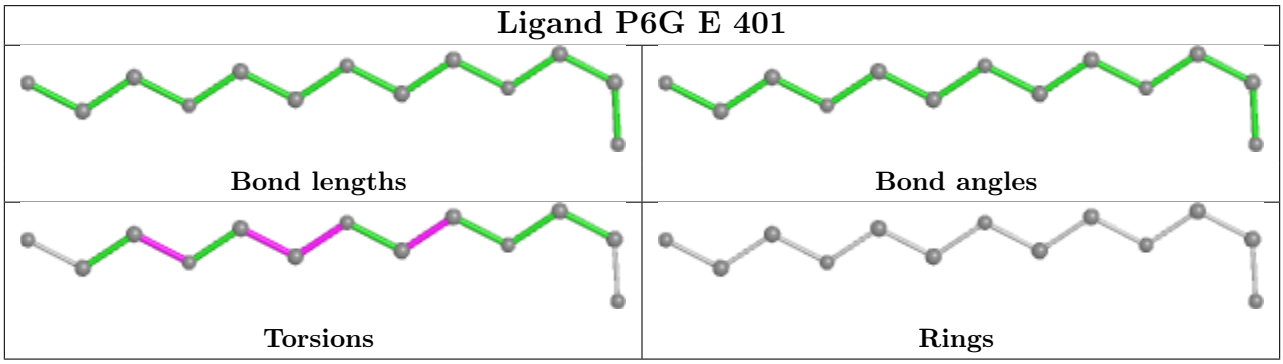
Mol	Chain	Res	Type	Atoms
2	F	400	P6G	O1-C2-C3-O4
2	E	401	P6G	O4-C5-C6-O7

There are no ring outliers.

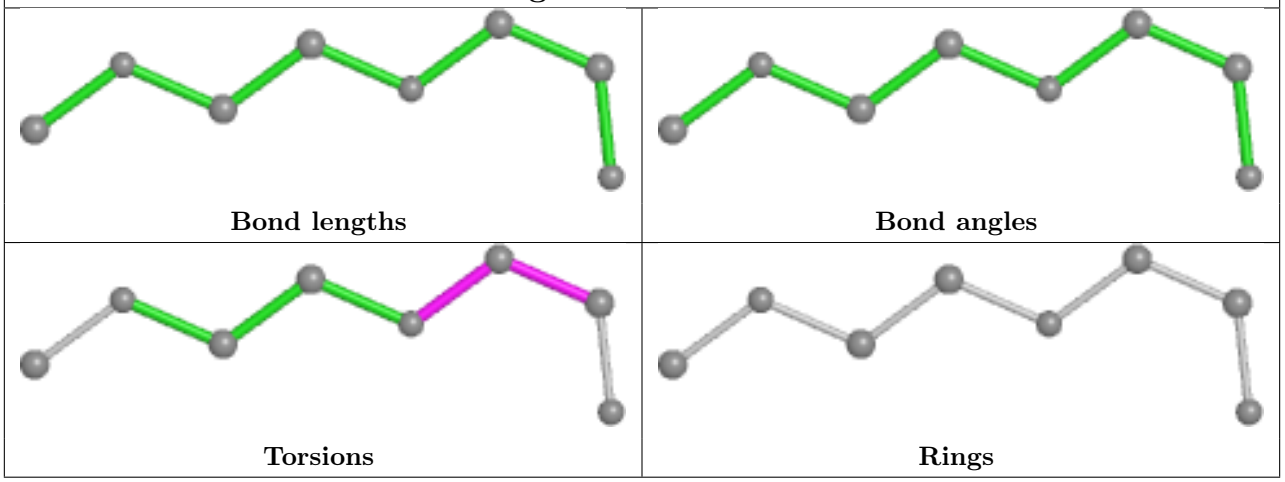
4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	401	P6G	1	0
2	B	400	P6G	4	0
2	E	400	P6G	1	0
2	F	400	P6G	1	0

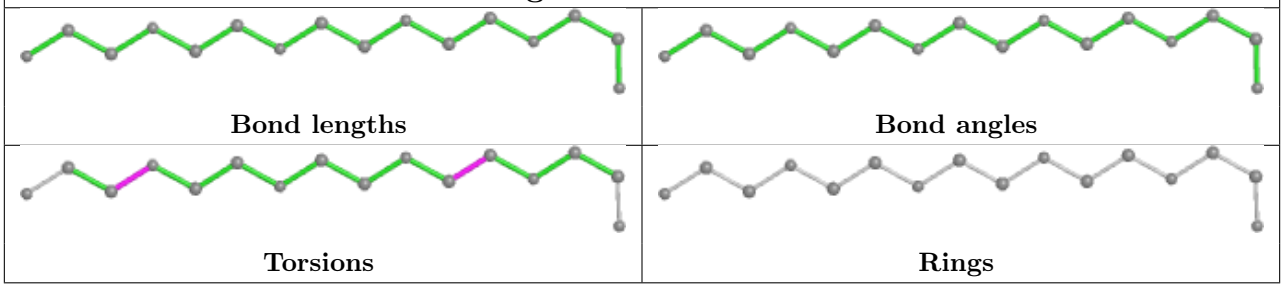
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 F 401



Ligand P6G D 400



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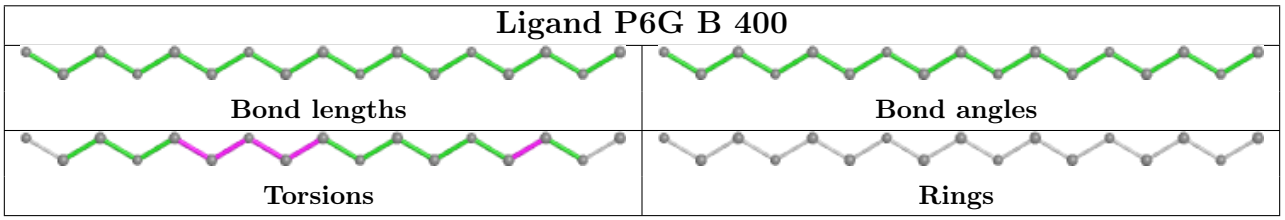

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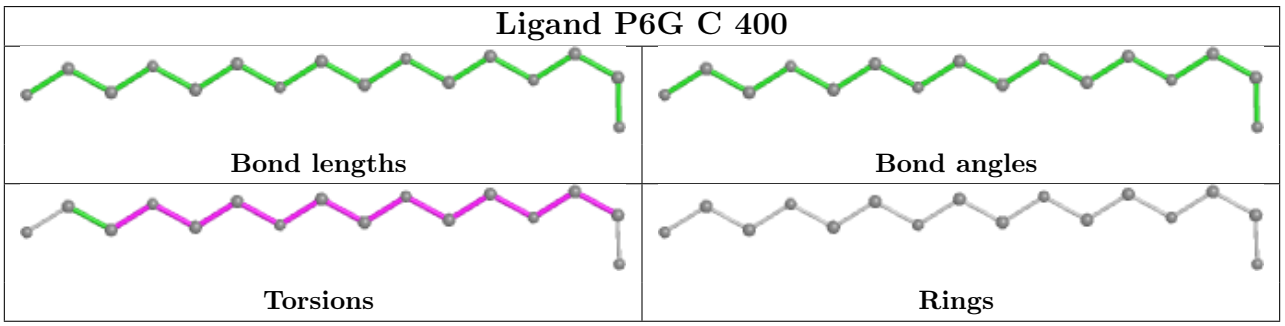
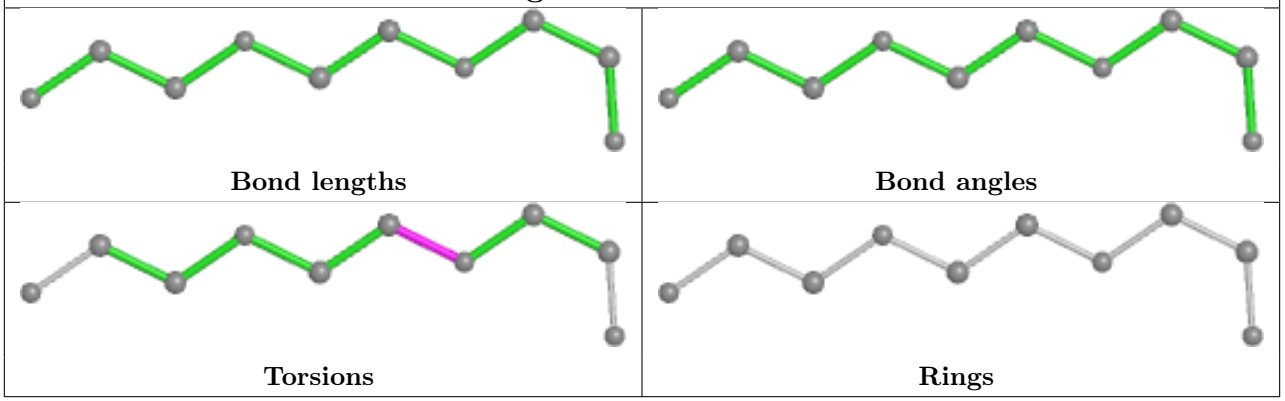
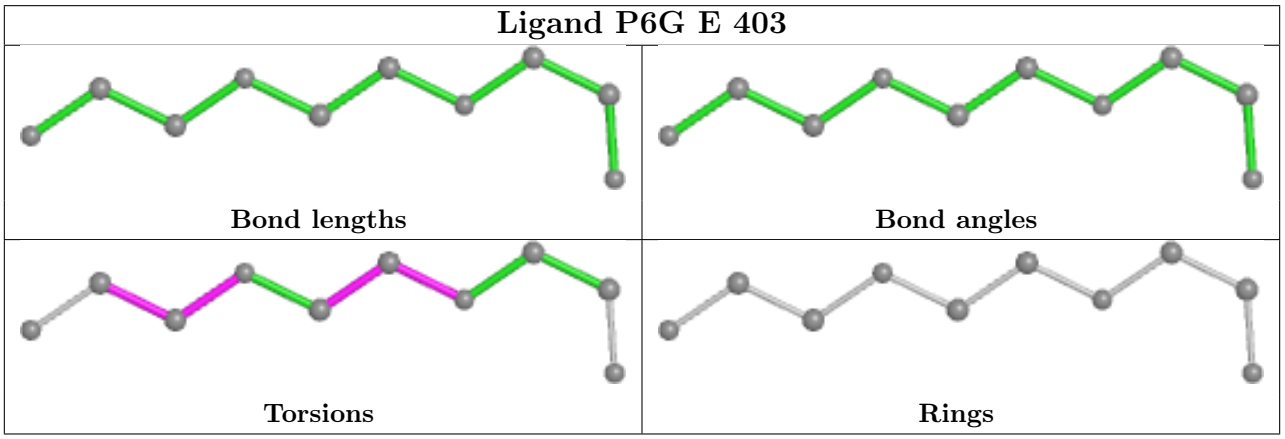


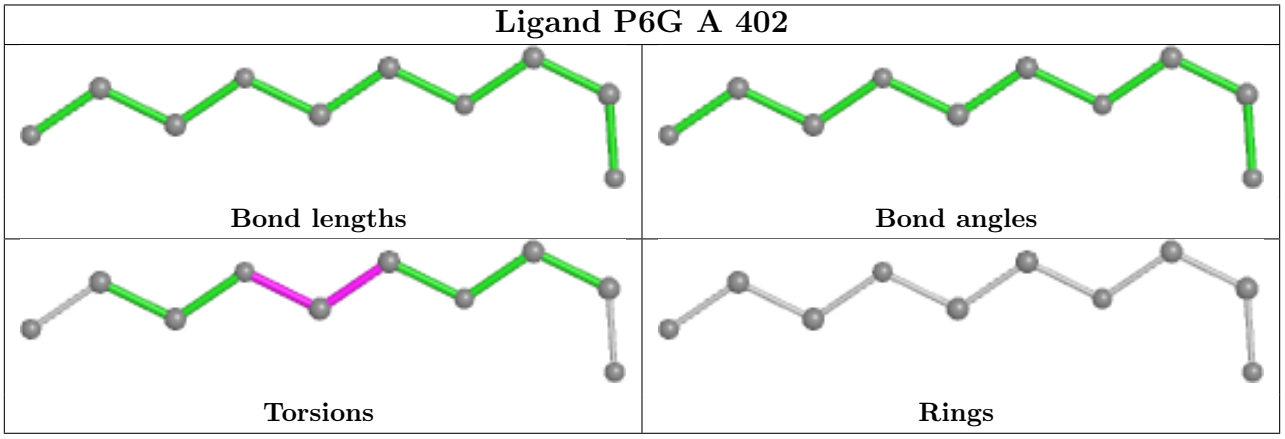
Ligand P6G D 401



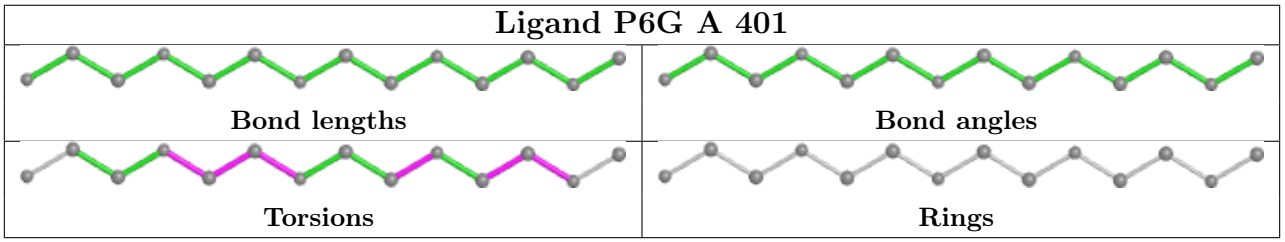
Ligand P6G E 403



Ligand P6G A 402



Ligand P6G A 401



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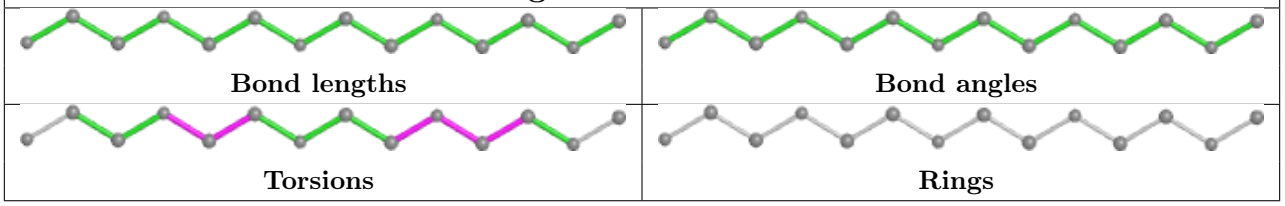
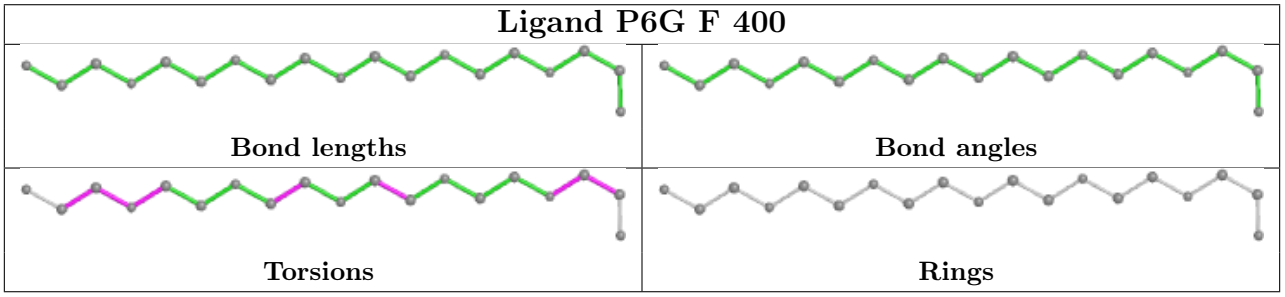
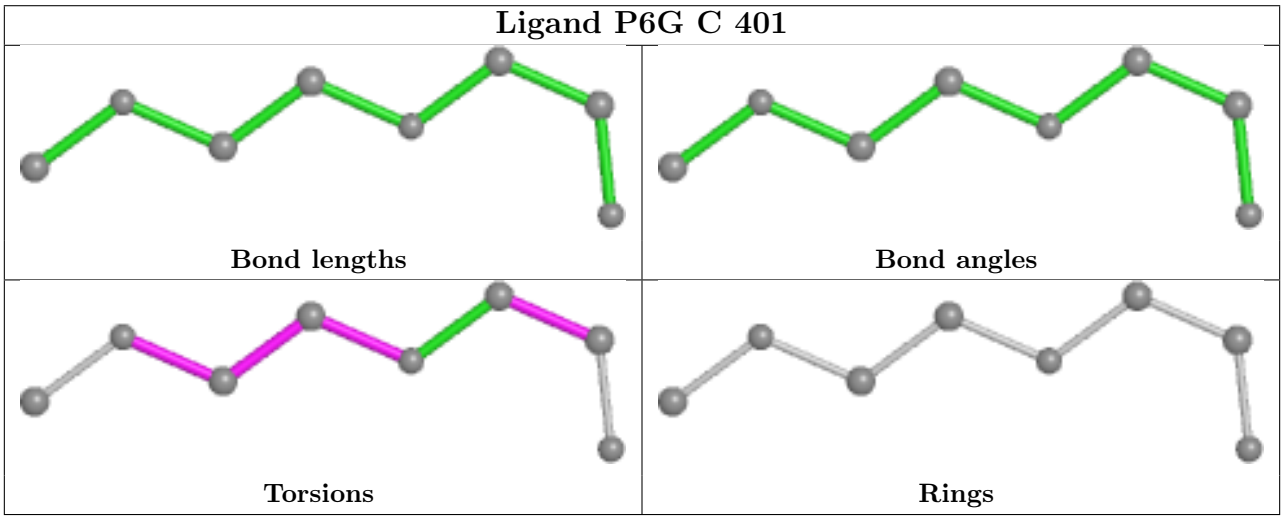


Ligand P6G F 400



Ligand P6G C 401



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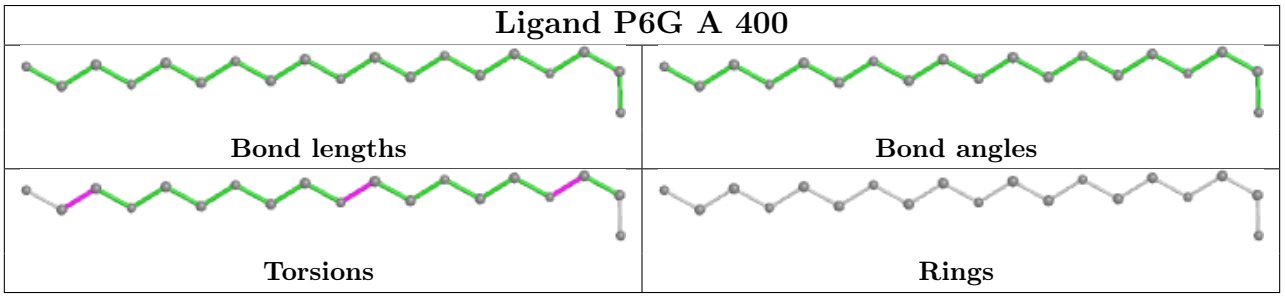
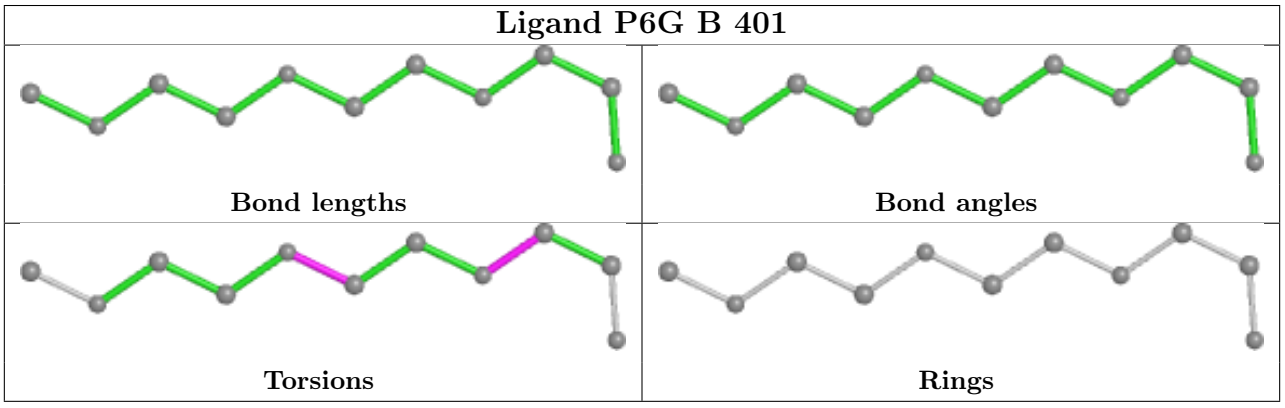


Ligand P6G B 401



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	2.80

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%)	-0.10	6 (2%)	63	66	25, 45, 68, 81	0
1	B	286/286 (100%)	-0.10	6 (2%)	63	66	23, 40, 66, 90	0
1	C	286/286 (100%)	0.21	21 (7%)	15	16	24, 43, 79, 101	0
1	D	286/286 (100%)	0.03	17 (5%)	22	25	26, 45, 76, 96	0
1	E	286/286 (100%)	0.12	22 (7%)	13	15	23, 44, 74, 103	0
1	F	286/286 (100%)	-0.10	3 (1%)	82	84	22, 36, 58, 83	0
All	All	1716/1716 (100%)	0.01	75 (4%)	34	37	22, 42, 72, 103	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	171	LEU	5.5
1	C	66	ASN	4.8
1	E	249	GLN	4.7
1	C	319	PHE	4.6
1	C	219	PRO	4.5
1	B	219	PRO	4.4
1	E	127	TYR	4.3
1	C	62	ILE	4.2
1	C	127	TYR	4.2
1	C	65	PRO	4.1
1	C	124	PRO	3.9
1	C	68	THR	3.8
1	D	168	ALA	3.6
1	C	69	GLY	3.6
1	B	319	PHE	3.6
1	D	219	PRO	3.6
1	C	122	ALA	3.5
1	C	120	THR	3.5
1	E	221	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	123	GLY	3.4
1	D	169	ASP	3.4
1	D	122	ALA	3.3
1	D	310	TYR	3.3
1	D	128	VAL	3.3
1	C	168	ALA	3.3
1	C	125	ASN	3.2
1	E	69	GLY	3.2
1	D	173	ASN	3.1
1	E	68	THR	3.1
1	E	247	THR	3.1
1	D	124	PRO	3.1
1	E	319	PHE	3.1
1	F	219	PRO	3.0
1	E	220	ALA	3.0
1	E	307	SER	3.0
1	E	306	TYR	3.0
1	E	66	ASN	2.9
1	B	247	THR	2.9
1	E	248	GLY	2.9
1	D	64	ASN	2.8
1	F	310	TYR	2.8
1	D	170	SER	2.7
1	B	307	SER	2.7
1	C	70	THR	2.7
1	D	306	TYR	2.6
1	E	123	GLY	2.6
1	B	220	ALA	2.5
1	E	218	ASN	2.5
1	C	119	SER	2.5
1	C	308	GLY	2.4
1	D	127	TYR	2.4
1	E	36	MET	2.4
1	E	125	ASN	2.4
1	A	310	TYR	2.3
1	A	220	ALA	2.3
1	E	293	ALA	2.3
1	A	125	ASN	2.3
1	C	67	GLU	2.3
1	E	37	GLY	2.2
1	E	124	PRO	2.2
1	C	169	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	62	ILE	2.2
1	B	221	GLY	2.2
1	D	220	ALA	2.2
1	E	171	LEU	2.2
1	D	224	TYR	2.2
1	E	219	PRO	2.2
1	F	221	GLY	2.2
1	C	171	LEU	2.1
1	C	221	GLY	2.1
1	D	36	MET	2.0
1	A	307	SER	2.0
1	D	248	GLY	2.0
1	E	65	PRO	2.0
1	A	169	ASP	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	F	401	8/19	0.75	0.16	61,64,72,73	0
2	P6G	A	401	14/19	0.77	0.18	74,77,80,81	0
2	P6G	D	401	10/19	0.78	0.12	74,75,76,77	0
2	P6G	C	401	8/19	0.84	0.14	57,59,62,63	0
2	P6G	B	400	17/19	0.84	0.16	45,52,61,61	0
2	P6G	B	401	11/19	0.84	0.10	60,62,65,65	0
2	P6G	F	400	19/19	0.85	0.52	27,36,43,48	19
2	P6G	E	401	13/19	0.86	0.11	57,62,65,66	0
2	P6G	A	402	10/19	0.88	0.17	69,74,84,85	0

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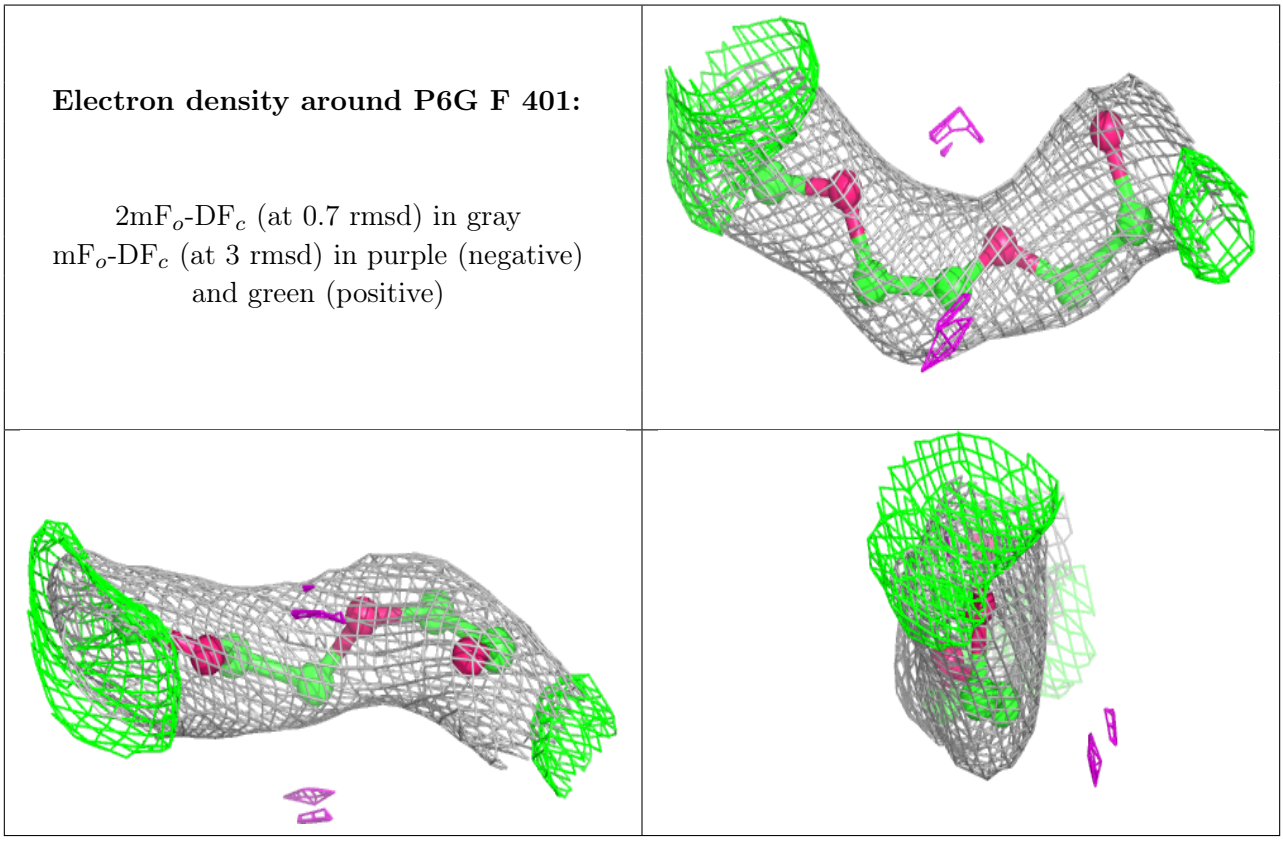
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	P6G	E	403	10/19	0.88	0.18	53,59,62,63	0
2	P6G	C	400	16/19	0.90	0.16	57,61,67,67	0
2	P6G	A	400	19/19	0.91	0.14	45,59,68,71	0
2	P6G	D	400	16/19	0.92	0.09	45,53,70,72	0
2	P6G	E	400	14/19	0.92	0.11	49,53,63,65	0

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.

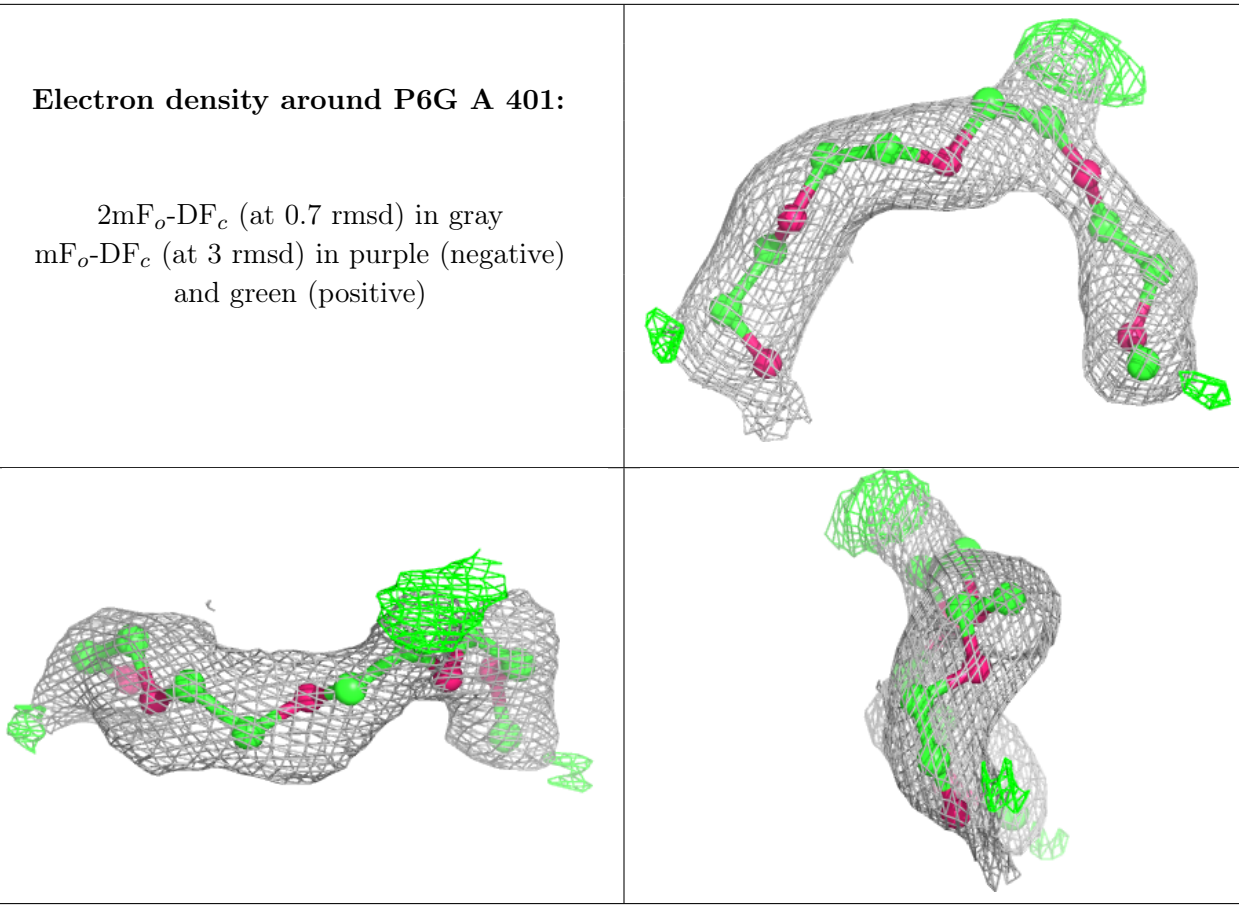
Electron density around P6G F 401:

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



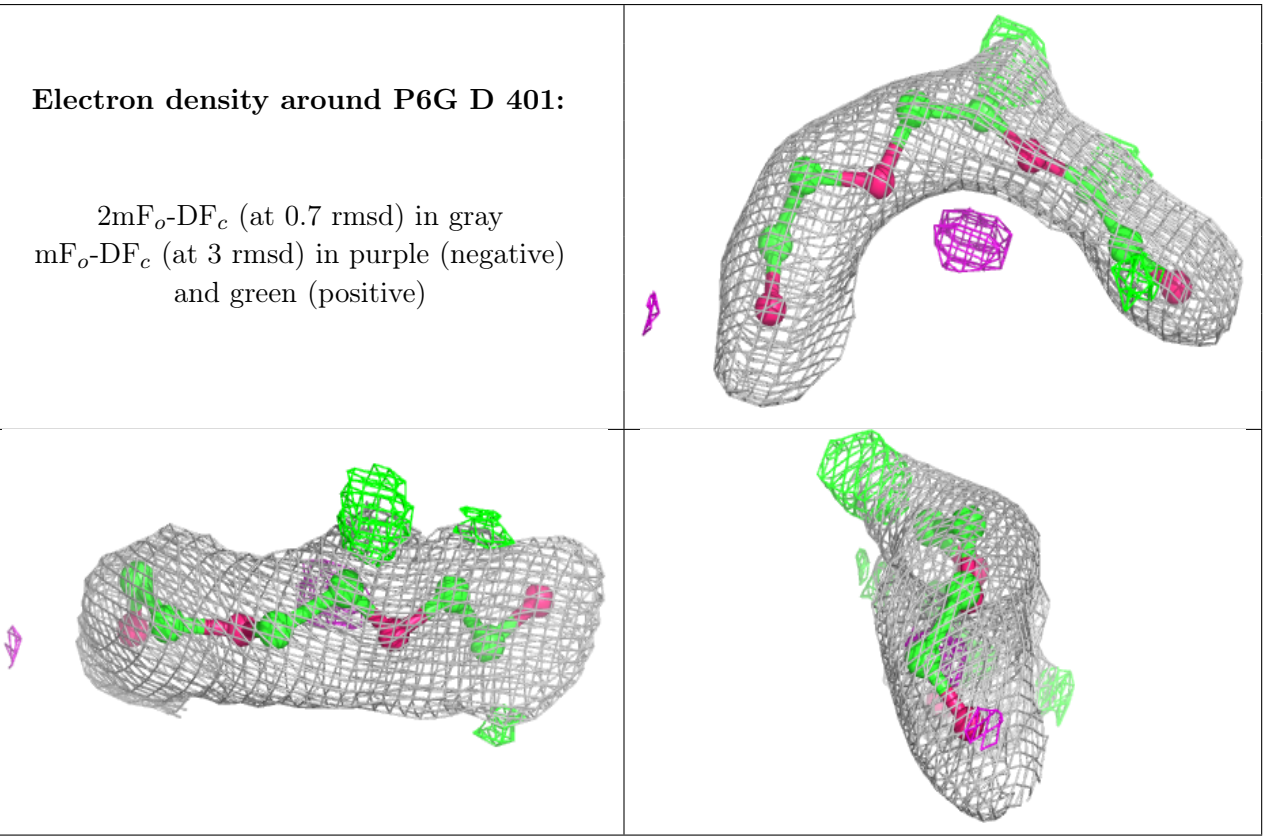
Electron density around P6G A 401:

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



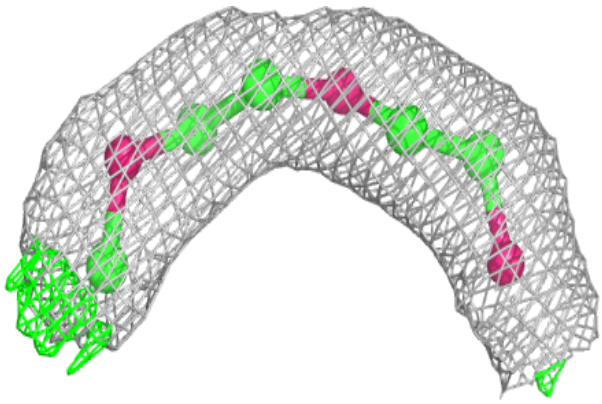
Electron density around P6G D 401:

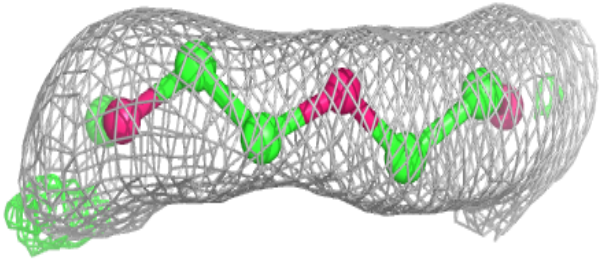
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

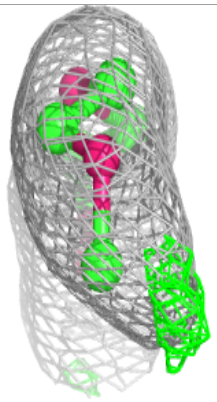


Electron density around P6G C 401:

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

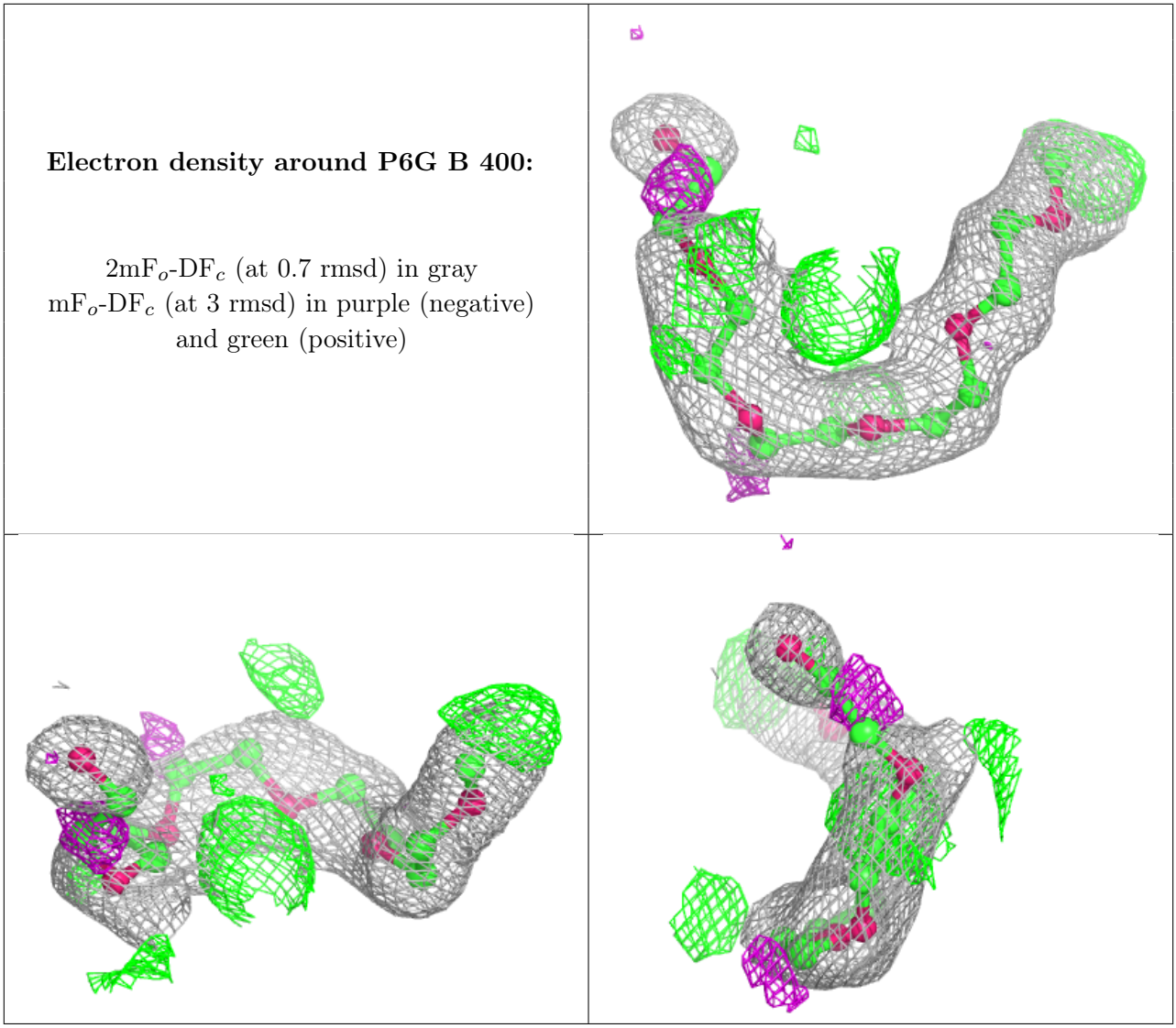






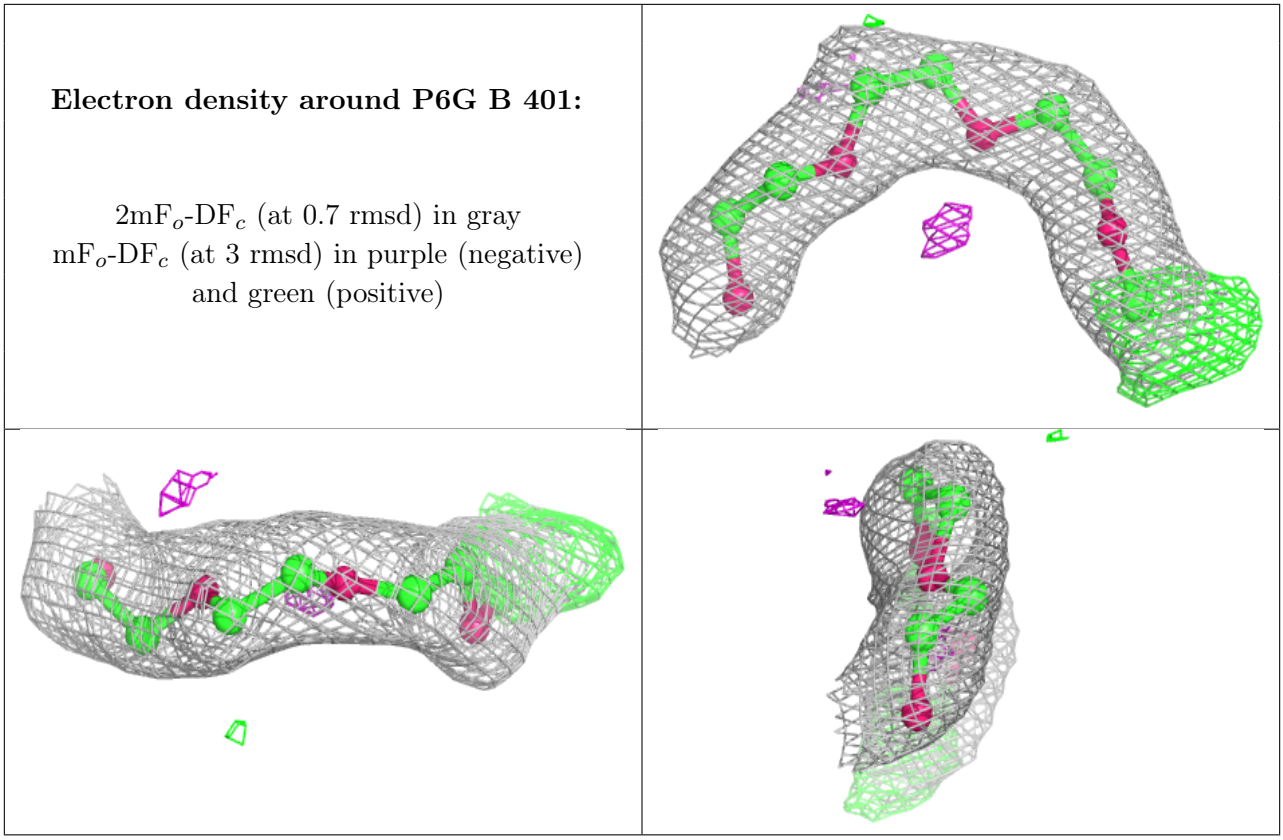
Electron density around P6G B 400:

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



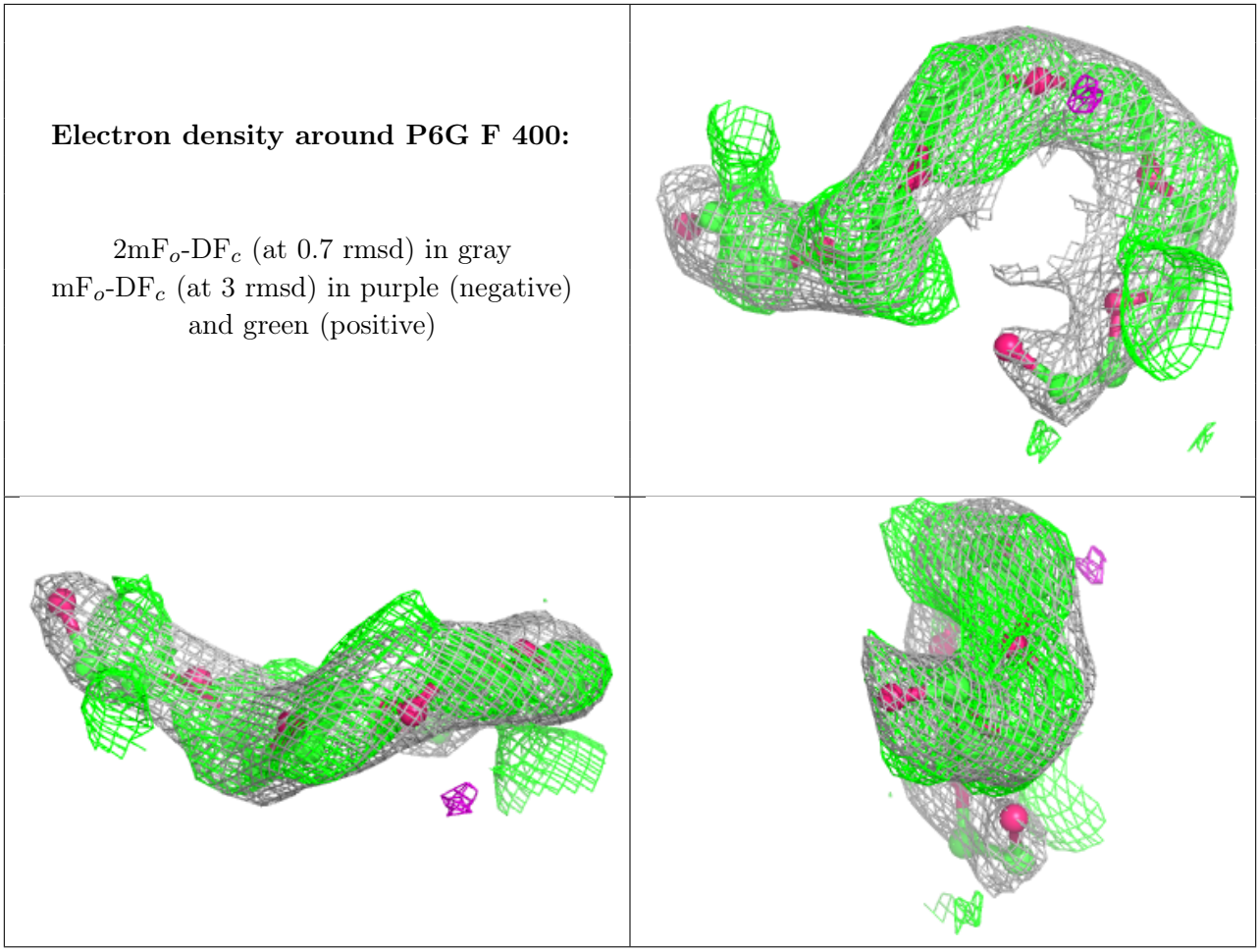
Electron density around P6G B 401:

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



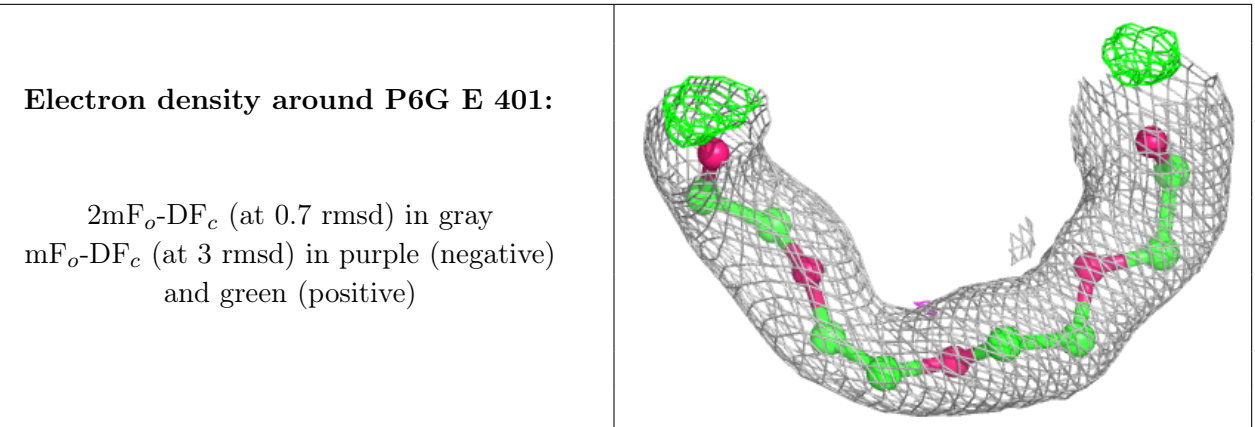
Electron density around P6G F 400:

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



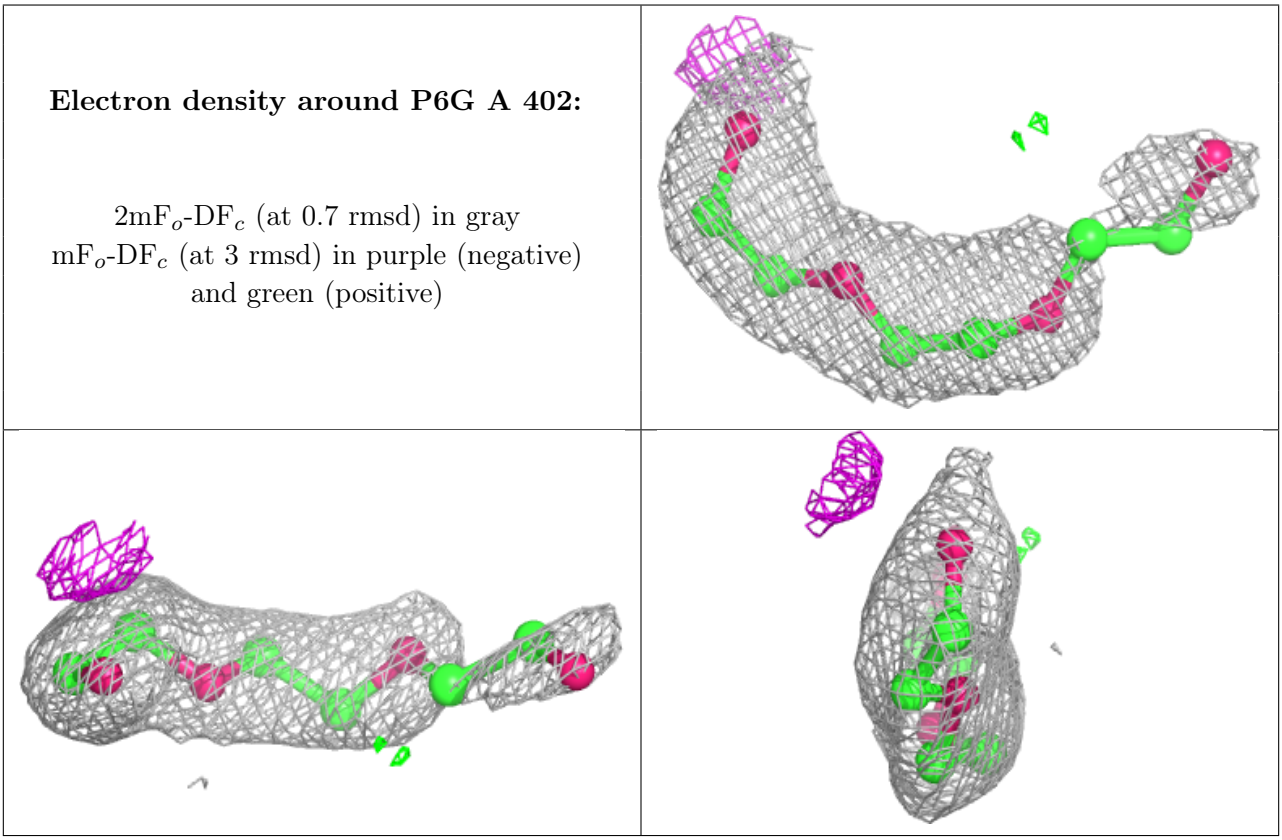
Electron density around P6G E 401:

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



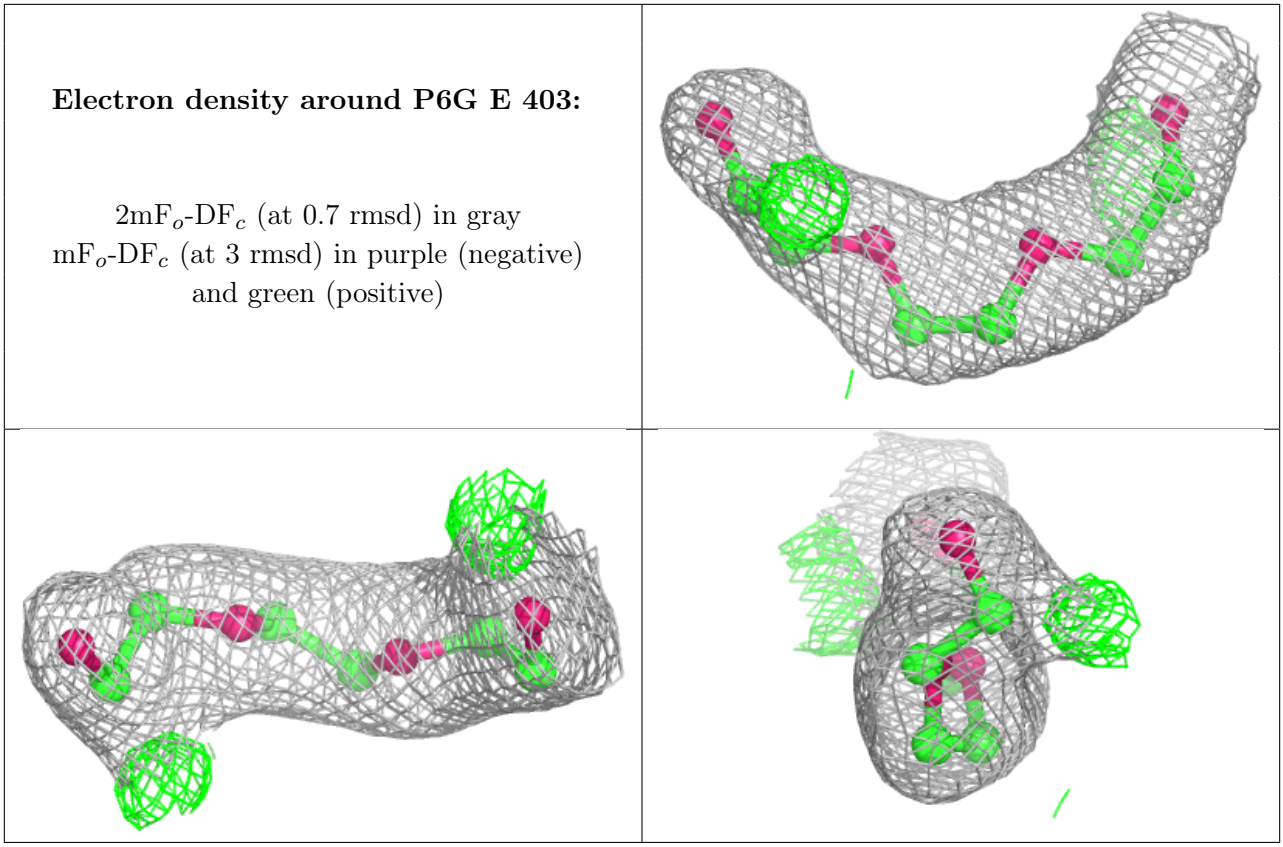
Electron density around P6G A 402:

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



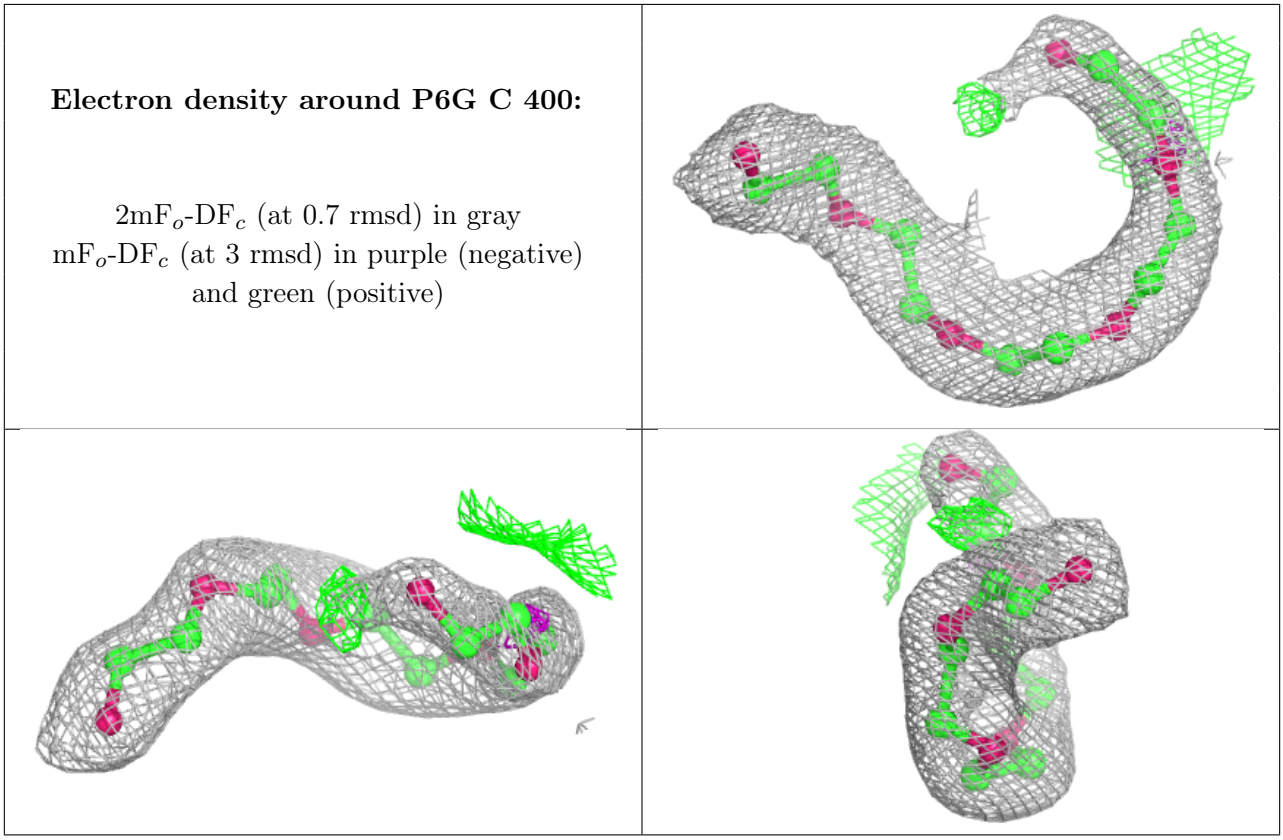
Electron density around P6G E 403:

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



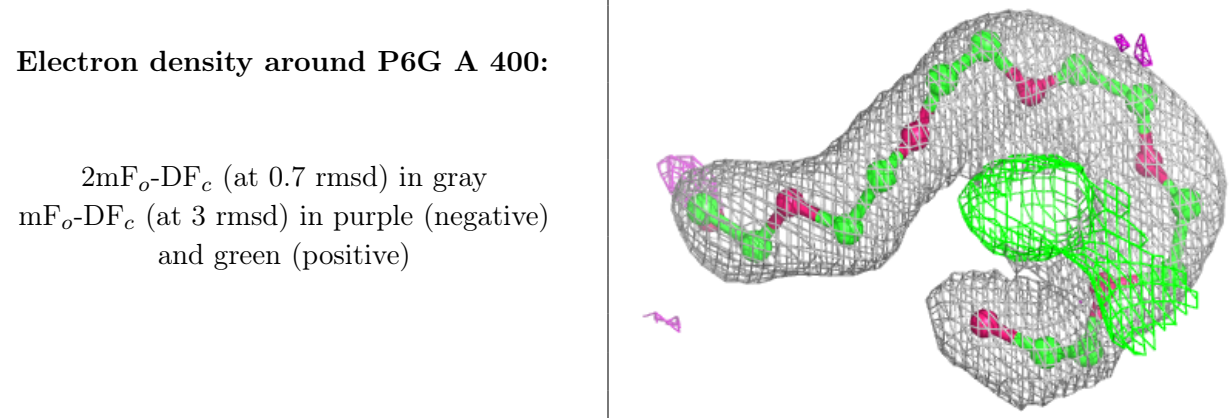
Electron density around P6G C 400:

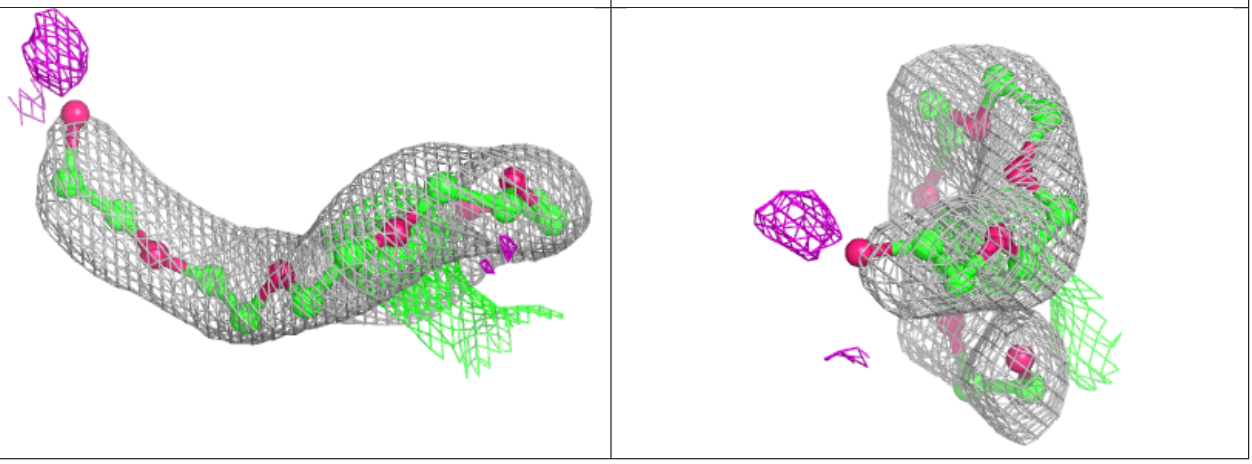
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around P6G A 400:

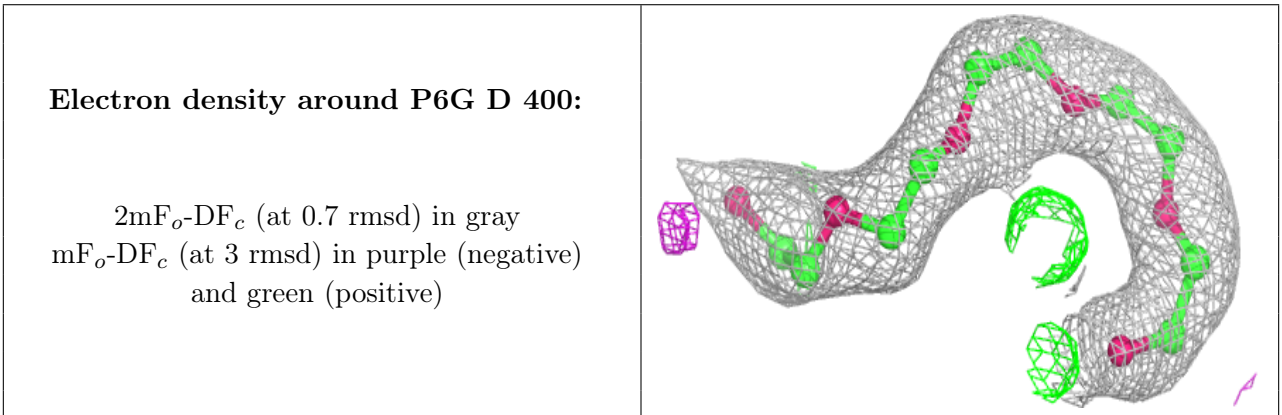
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

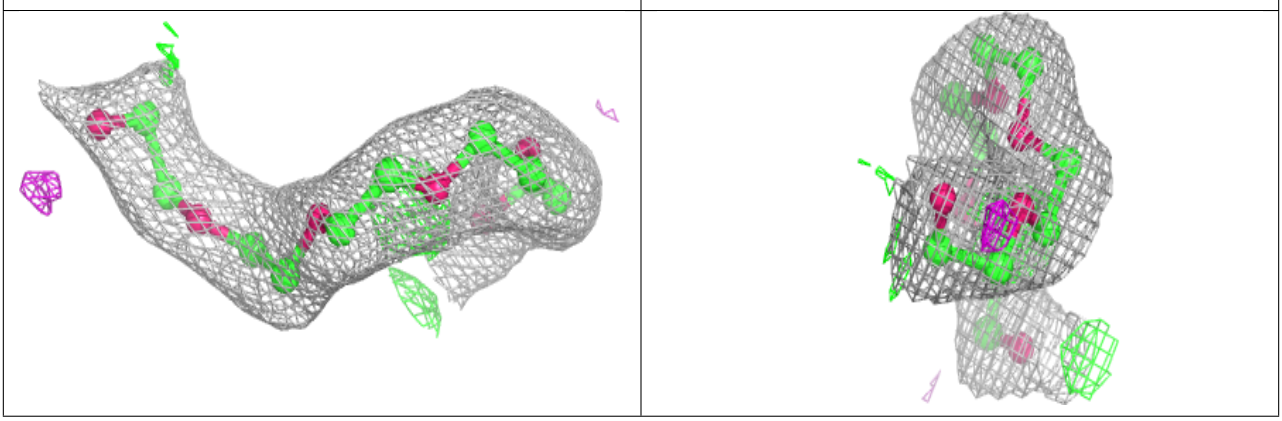




Electron density around P6G D 400:

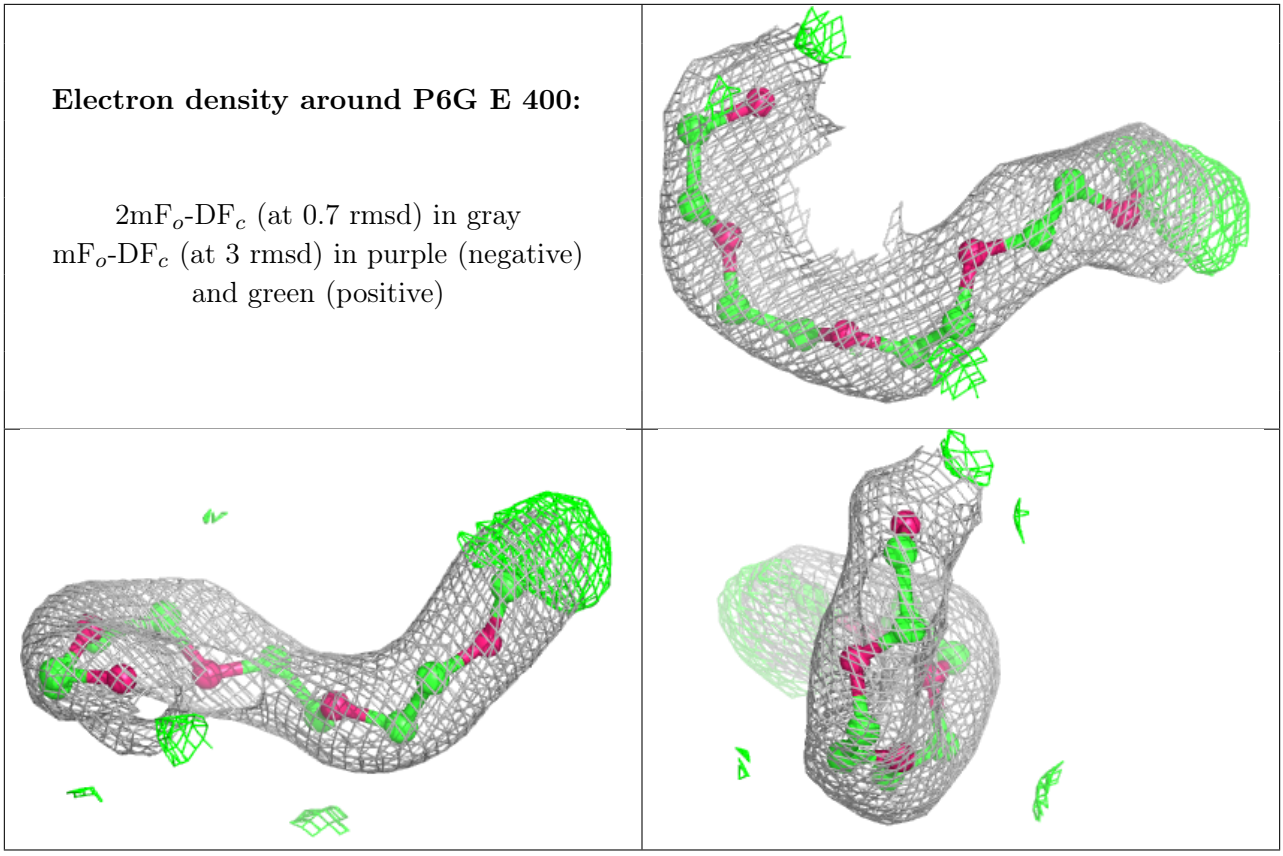
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





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)



6.5 Other polymers (i)

There are no such residues in this entry.