



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:53 PM UTC

PDB ID : 3ZIX / pdb_00003zix
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 ⓘ 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:

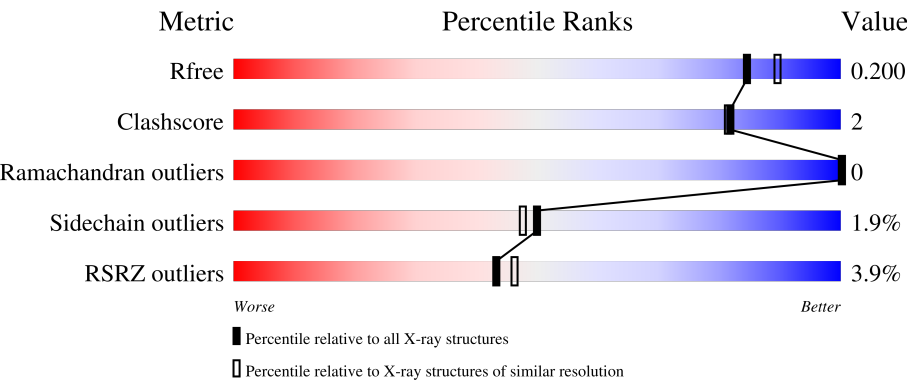
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal 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 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}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (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 $\leq 5\%$. 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	286	3% 95% 5%
1	B	286	3% 91% 6% .
1	C	286	3% 92% 8% .
1	D	286	7% 95% .
1	E	286	6% 94% 6%

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Mol	Chain	Length	Quality of chain
1	F	286	% 92% 7% •

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 15272 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	277	Total	C	N	O	S	0	4	0
			2139	1358	342	435	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:

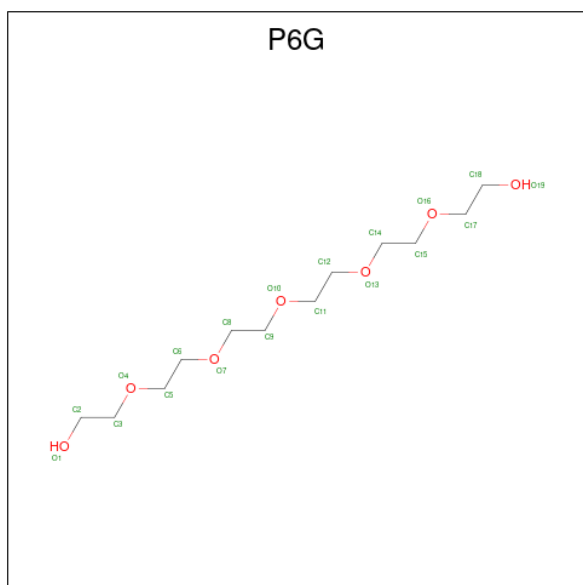
Chain	Residue	Modelled	Actual	Comment	Reference
A	34	GLY	-	expression tag	UNP P01558
A	35	ALA	-	expression tag	UNP P01558
A	36	MET	-	expression tag	UNP P01558
A	37	GLY	-	expression tag	UNP P01558
B	34	GLY	-	expression tag	UNP P01558
B	35	ALA	-	expression tag	UNP P01558
B	36	MET	-	expression tag	UNP P01558
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 (CCD ID: P6G) (formula: $C_{12}H_{26}O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			19	12	7		
2	A	1	Total	C	O	0	0
			14	9	5		
2	A	1	Total	C	O	0	0
			10	6	4		
2	B	1	Total	C	O	0	0
			17	11	6		
2	B	1	Total	C	O	0	0
			11	7	4		
2	C	1	Total	C	O	0	0
			16	10	6		
2	C	1	Total	C	O	0	0
			8	5	3		
2	D	1	Total	C	O	0	0
			16	10	6		

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

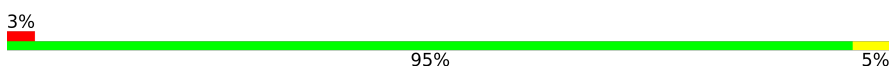
- Molecule 3 is water.

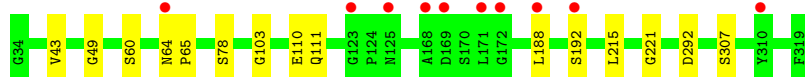
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	305	Total	O	0	0
			305	305		
3	B	314	Total	O	0	0
			314	314		
3	C	266	Total	O	0	0
			266	266		
3	D	272	Total	O	0	0
			272	272		
3	E	268	Total	O	0	0
			268	268		
3	F	336	Total	O	0	0
			336	336		

3 Residue-property plots [i](#)

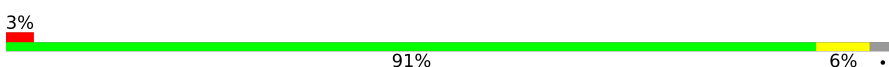
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

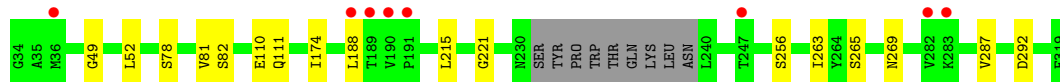
- Molecule 1: HEAT-LABILE ENTEROTOXIN B CHAIN

Chain A: 

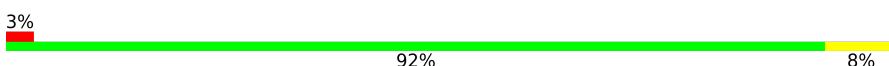


- Molecule 1: HEAT-LABILE ENTEROTOXIN B CHAIN

Chain B: 



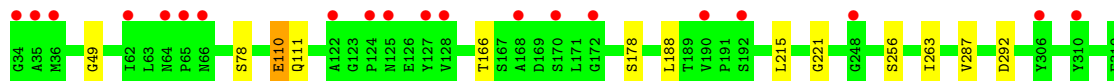
- Molecule 1: HEAT-LABILE ENTEROTOXIN B CHAIN

Chain C: 

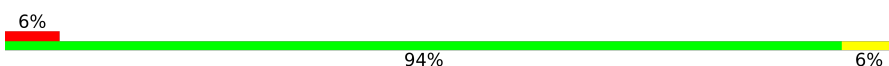


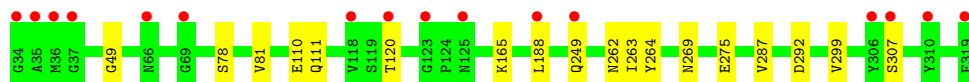
- Molecule 1: HEAT-LABILE ENTEROTOXIN B CHAIN

Chain D: 

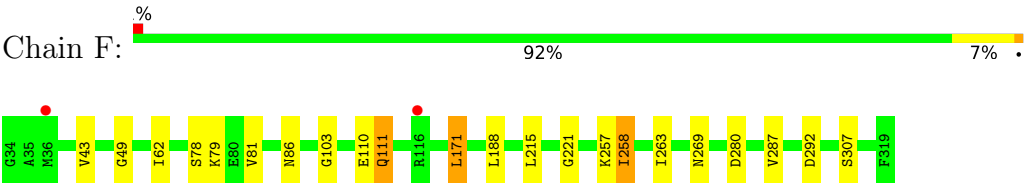


- Molecule 1: HEAT-LABILE ENTEROTOXIN B CHAIN

Chain E: 



- Molecule 1: HEAT-LABILE ENTEROTOXIN B CHAIN



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	2.08 (at 1.90Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.176 , 0.197 (Not available) , 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)	0.32 , 67.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.005 for h+2*k,-h-l 0.012 for h,-k,-h-l 0.038 for -h-2*k,-k,l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	15272	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.*

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: 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	0.79	0/2315	1.02	0/3141
1	B	0.82	0/2200	1.02	1/2989 (0.0%)
1	C	0.79	0/2292	1.02	2/3112 (0.1%)
1	D	0.79	0/2301	1.02	2/3129 (0.1%)
1	E	0.82	0/2278	1.02	0/3099
1	F	0.83	0/2299	0.99	1/3121 (0.0%)
All	All	0.81	0/13685	1.02	6/18591 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	86	ASN	CA-CB-CG	5.97	118.57	112.60
1	B	265	SER	N-CA-C	-5.18	102.09	110.32
1	C	280	ASP	CA-CB-CG	5.12	117.72	112.60
1	D	256	SER	CA-C-N	5.12	127.65	120.28
1	D	256	SER	C-N-CA	5.12	127.65	120.28
1	C	128	VAL	N-CA-C	5.05	115.39	108.12

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	9	0
1	B	2139	0	2082	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
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	15272	0	13205	66	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 (66) 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:C:110[B]:GLU:H	1:C:110[B]:GLU:CD	1.96	0.72
1:B:263:ILE:HD11	1:B:287:VAL:HG21	1.73	0.70
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:F:79:LYS:NZ	1:F:110[A]:GLU:OE2	2.39	0.48
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:64:ASN:C	1:A:65:PRO:N	2.80	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	279/286 (98%)	274 (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	1724/1716 (100%)	1701 (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	185/247 (75%)	181 (98%)	4 (2%)	45	42
1	B	237/247 (96%)	233 (98%)	4 (2%)	53	52
1	C	249/247 (101%)	243 (98%)	6 (2%)	43	38
1	D	249/247 (101%)	246 (99%)	3 (1%)	63	63
1	E	247/247 (100%)	242 (98%)	5 (2%)	48	46
1	F	251/247 (102%)	244 (97%)	7 (3%)	38	32
All	All	1418/1482 (96%)	1389 (98%)	29 (2%)	50	46

All (29) 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	292	ASP
1	A	307	SER
1	B	174	ILE
1	B	256	SER
1	B	269	ASN
1	B	292	ASP
1	C	66	ASN
1	C	188	LEU
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	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	258	ILE
1	F	269	ASN
1	F	292	ASP

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Mol	Chain	Res	Type
1	F	307	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	ASN
1	A	218	ASN
1	A	309	ASN
1	A	317	GLN
1	B	66	ASN
1	B	295	GLN
1	B	309	ASN
1	C	61	GLN
1	C	249	GLN
1	C	309	ASN
1	D	218	ASN
1	D	249	GLN
1	D	295	GLN
1	D	309	ASN
1	E	241	HIS
1	E	295	GLN
1	E	309	ASN
1	F	61	GLN
1	F	66	ASN
1	F	218	ASN
1	F	295	GLN
1	F	309	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	403	-	9,9,18	0.45	0	8,8,17	0.29	0
2	P6G	C	401	-	7,7,18	0.49	0	6,6,17	0.17	0
2	P6G	D	401	-	9,9,18	0.48	0	8,8,17	0.29	0
2	P6G	B	400	-	16,16,18	0.53	0	15,15,17	0.66	0
2	P6G	A	401	-	13,13,18	0.48	0	12,12,17	0.24	0
2	P6G	F	400	-	18,18,18	0.42	0	17,17,17	0.52	0
2	P6G	F	401	-	7,7,18	0.48	0	6,6,17	0.20	0
2	P6G	A	402	-	9,9,18	0.48	0	8,8,17	0.25	0
2	P6G	E	400	-	13,13,18	0.55	0	12,12,17	0.22	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
2	P6G	E	401	-	12,12,18	0.50	0	11,11,17	0.24	0
2	P6G	D	400	-	15,15,18	0.49	0	14,14,17	0.53	0
2	P6G	C	400	-	15,15,18	0.52	0	14,14,17	0.43	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	403	-	-	4/7/7/16	-
2	P6G	C	401	-	-	4/5/5/16	-
2	P6G	D	401	-	-	1/7/7/16	-
2	P6G	B	400	-	-	5/14/14/16	-
2	P6G	A	401	-	-	6/11/11/16	-
2	P6G	F	400	-	-	7/16/16/16	-
2	P6G	F	401	-	-	2/5/5/16	-
2	P6G	A	402	-	-	2/7/7/16	-
2	P6G	E	400	-	-	5/11/11/16	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	P6G	A	400	-	-	3/16/16/16	-
2	P6G	B	401	-	-	2/8/8/16	-
2	P6G	E	401	-	-	4/10/10/16	-
2	P6G	D	400	-	-	2/13/13/16	-
2	P6G	C	400	-	-	12/13/13/16	-

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	O16-C17-C18-O19
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	401	P6G	O1-C2-C3-O4
2	B	400	P6G	O4-C5-C6-O7
2	E	401	P6G	O7-C8-C9-O10
2	C	401	P6G	O4-C5-C6-O7
2	B	400	P6G	O10-C11-C12-O13
2	B	400	P6G	O13-C14-C15-O16
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	A	402	P6G	C5-C6-O7-C8
2	E	401	P6G	C12-C11-O10-C9
2	E	403	P6G	C9-C8-O7-C6
2	C	400	P6G	C12-C11-O10-C9
2	B	400	P6G	C15-C14-O13-C12

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Mol	Chain	Res	Type	Atoms
2	D	400	P6G	O4-C5-C6-O7
2	E	403	P6G	O4-C5-C6-O7
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	F	400	P6G	O1-C2-C3-O4
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
2	E	401	P6G	O4-C5-C6-O7

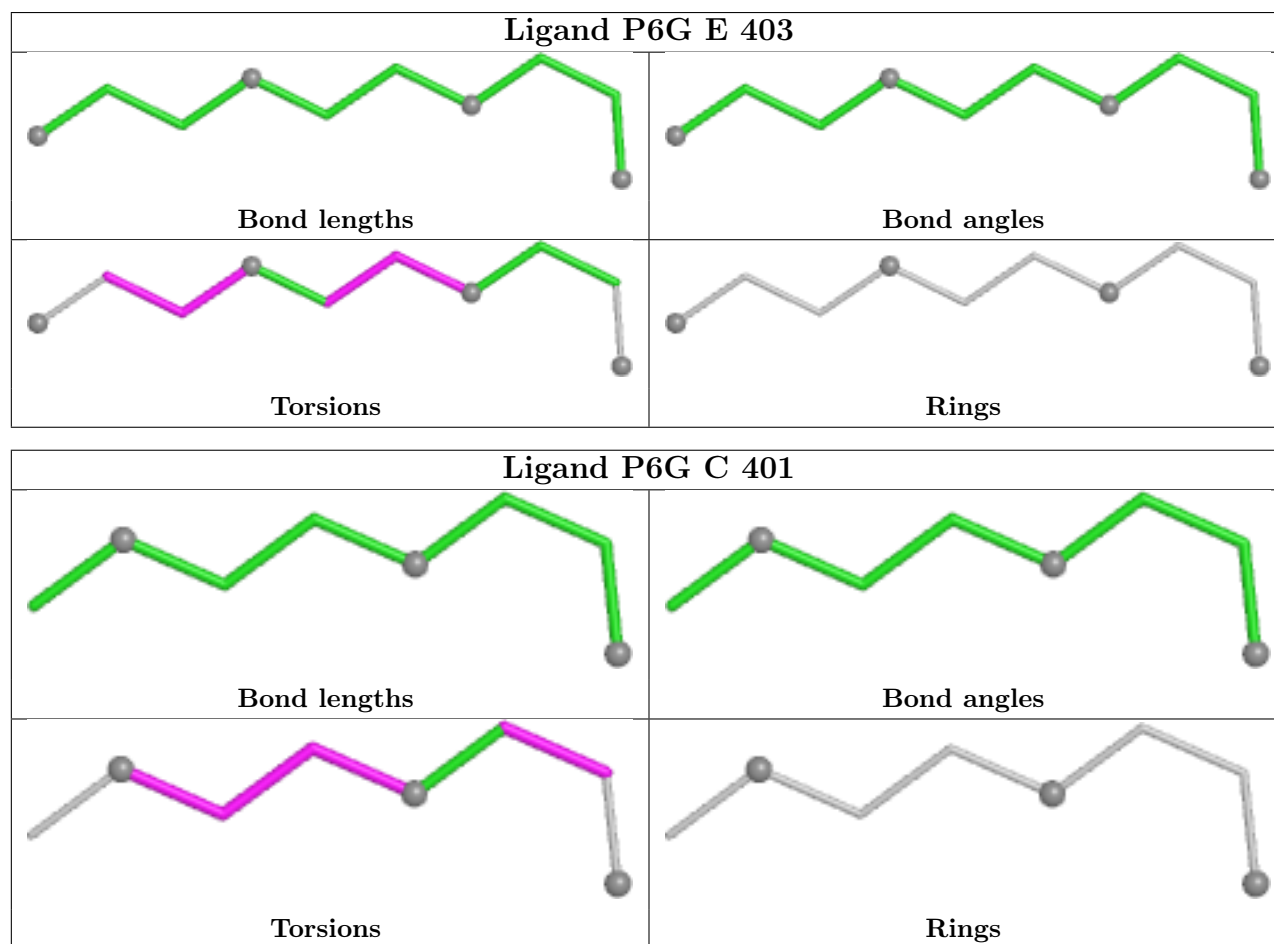
There are no ring outliers.

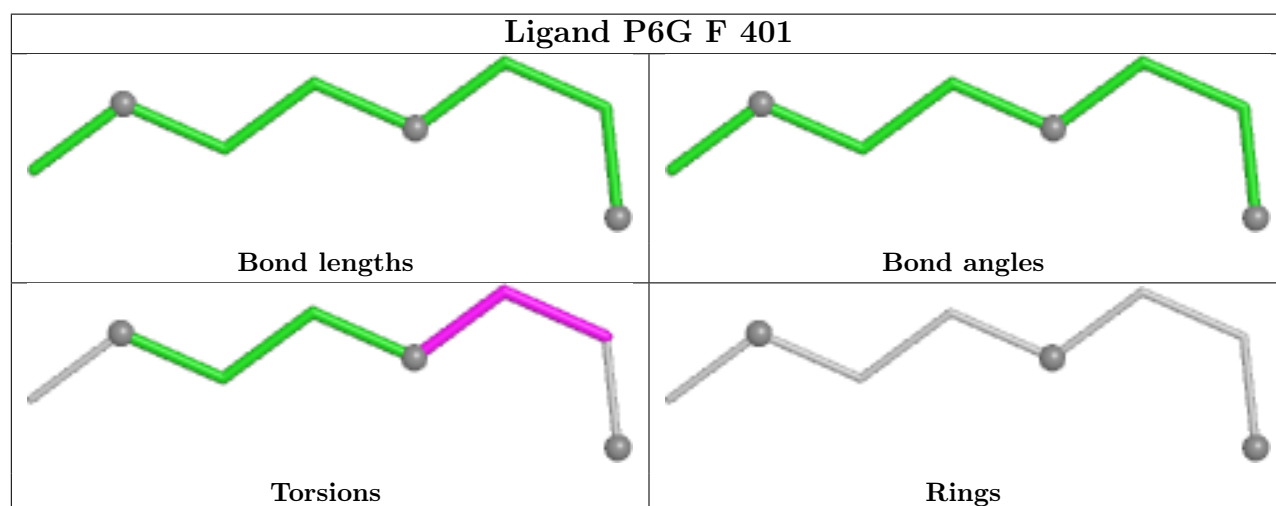
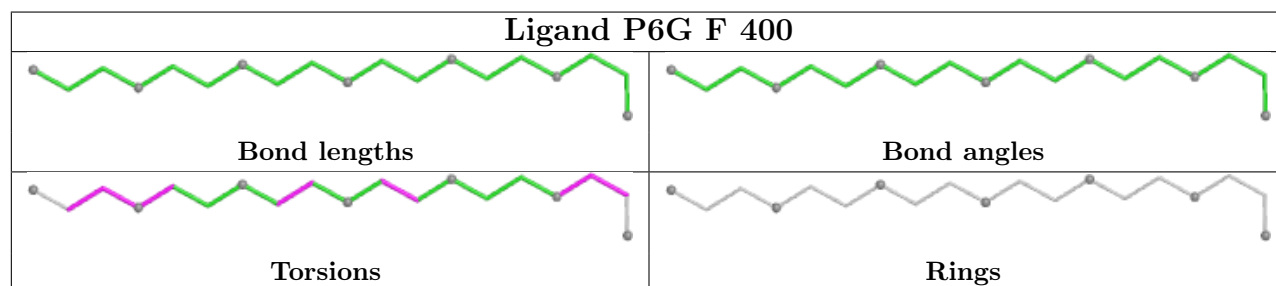
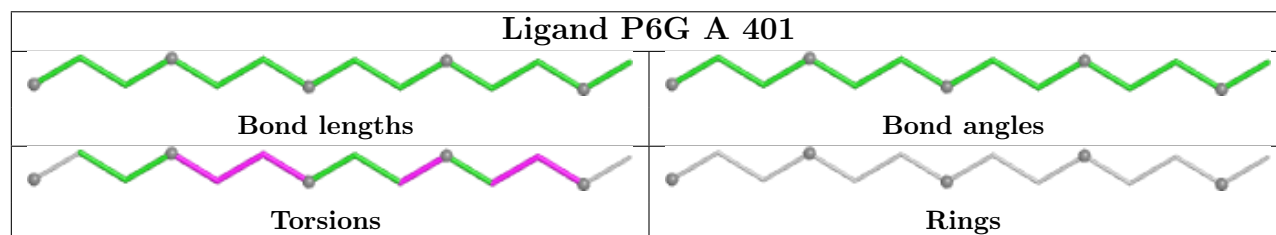
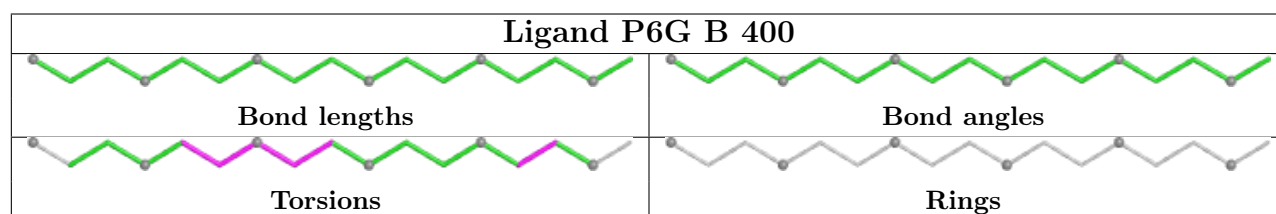
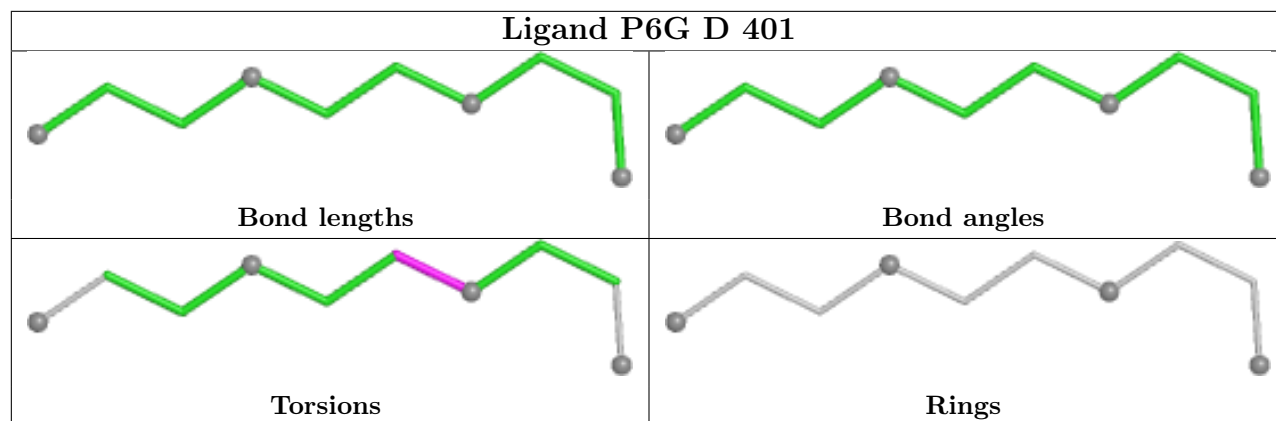
4 monomers are involved in 7 short contacts:

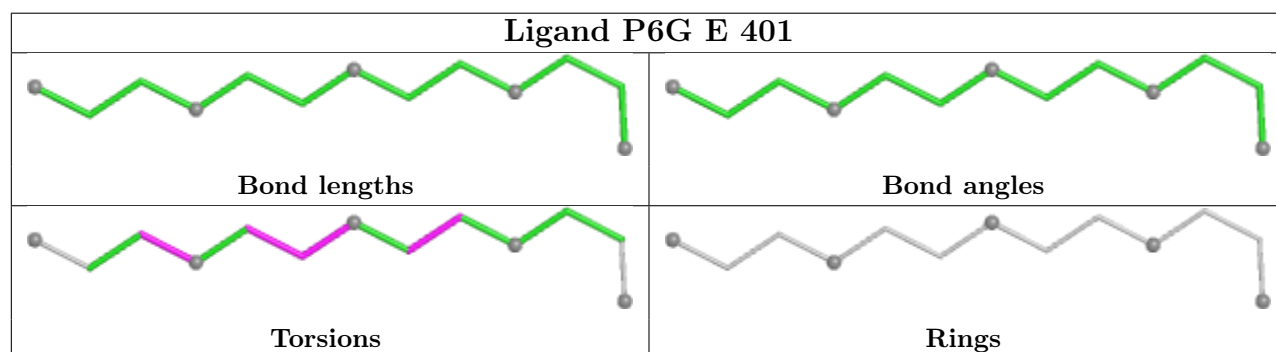
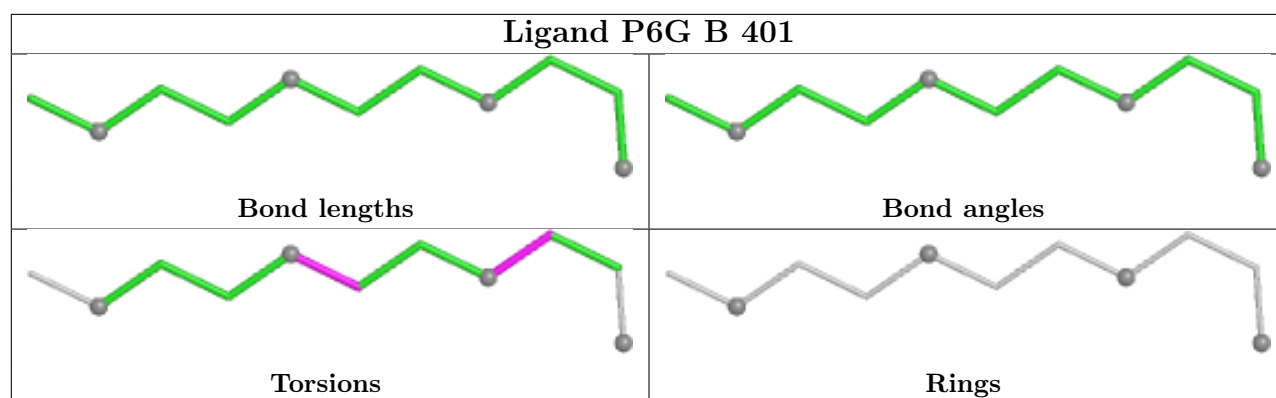
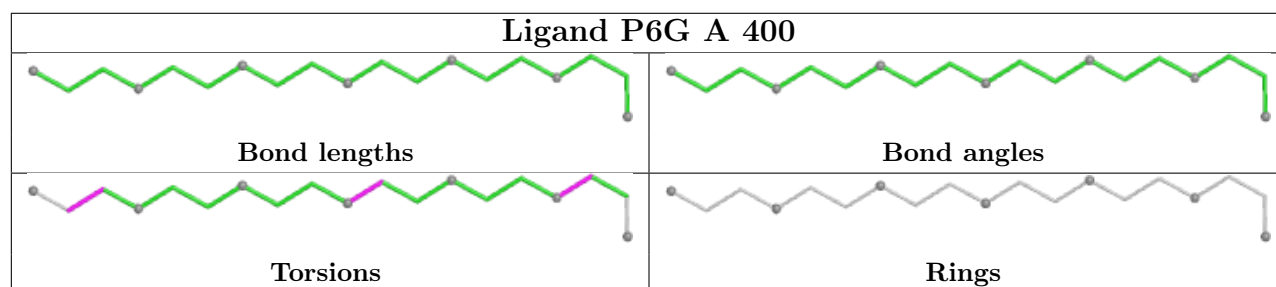
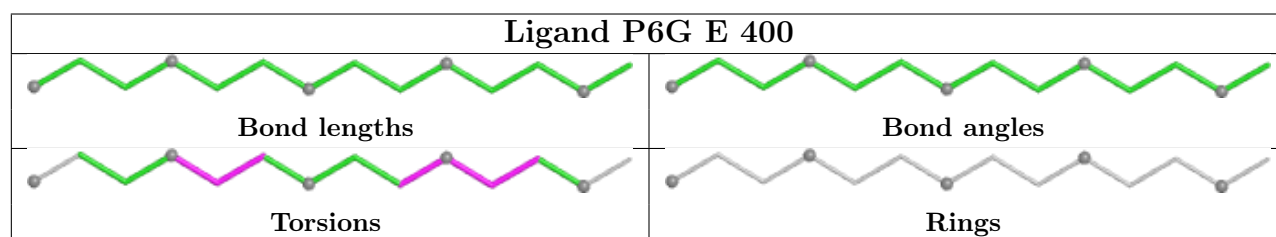
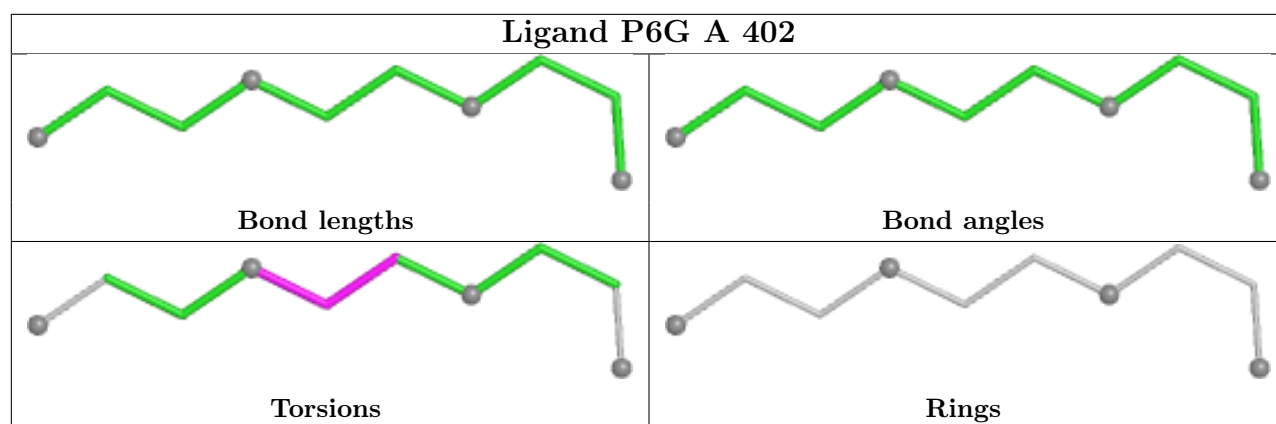
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	400	P6G	4	0
2	F	400	P6G	1	0
2	F	401	P6G	1	0
2	E	400	P6G	1	0

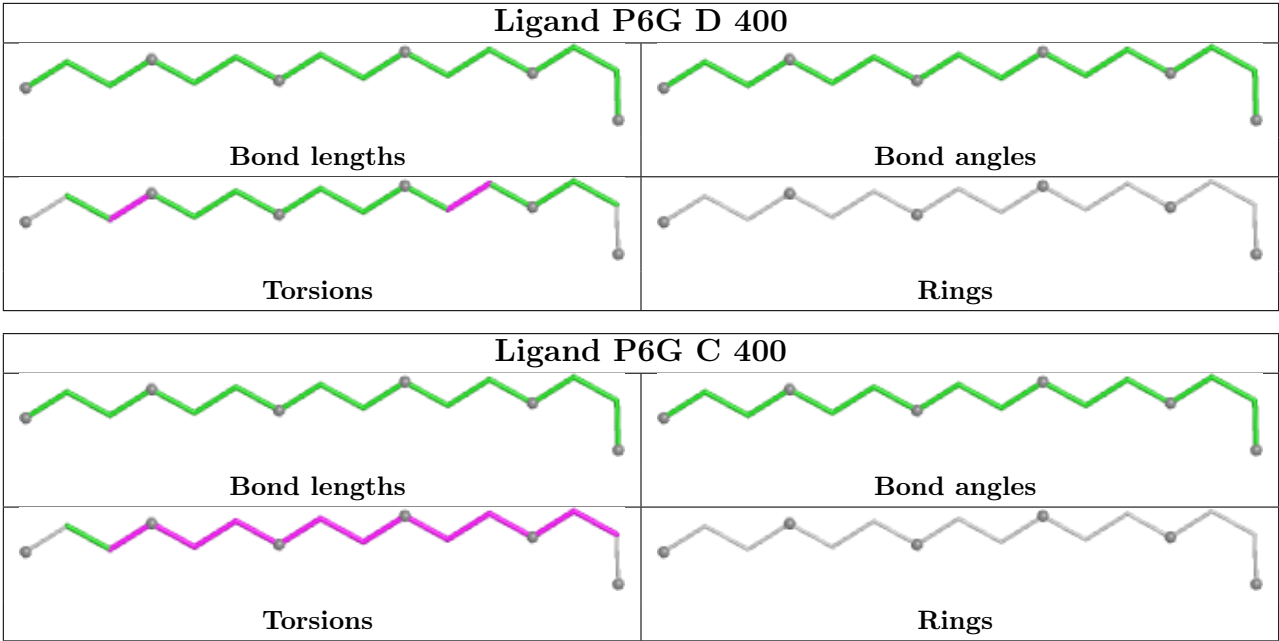
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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 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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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, 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	286/286 (100%)	0.14	10 (3%) 47 50	14, 45, 68, 81	6 (2%)
1	B	277/286 (96%)	0.00	8 (2%) 53 57	18, 40, 67, 90	4 (1%)
1	C	286/286 (100%)	0.10	10 (3%) 47 50	20, 43, 79, 101	4 (1%)
1	D	286/286 (100%)	0.24	20 (6%) 22 24	17, 45, 76, 96	7 (2%)
1	E	286/286 (100%)	0.22	16 (5%) 30 32	19, 43, 74, 103	5 (1%)
1	F	286/286 (100%)	-0.17	2 (0%) 84 86	19, 36, 58, 83	4 (1%)
All	All	1707/1716 (99%)	0.09	66 (3%) 43 46	14, 42, 72, 103	30 (1%)

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	171	LEU	4.8
1	D	125	ASN	3.7
1	A	125	ASN	3.7
1	E	249	GLN	3.7
1	A	168	ALA	3.6
1	E	37	GLY	3.4
1	E	34	GLY	3.3
1	E	36	MET	3.2
1	E	125	ASN	3.2
1	D	168	ALA	3.1
1	D	64	ASN	3.0
1	D	170	SER	3.0
1	C	125	ASN	3.0
1	D	128	VAL	2.9
1	F	116	ARG	2.9
1	C	289	ILE	2.8
1	C	34	GLY	2.8
1	E	120	THR	2.7
1	B	282	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	36[A]	MET	2.7
1	C	66	ASN	2.7
1	B	189	THR	2.7
1	D	65	PRO	2.6
1	E	319	PHE	2.6
1	D	127	TYR	2.6
1	D	310	TYR	2.6
1	D	34	GLY	2.6
1	D	35	ALA	2.6
1	C	120	THR	2.6
1	B	247	THR	2.5
1	B	188	LEU	2.5
1	A	64	ASN	2.5
1	E	306	TYR	2.5
1	D	62	ILE	2.5
1	D	36	MET	2.5
1	D	66	ASN	2.4
1	E	35	ALA	2.4
1	D	190	VAL	2.4
1	E	123	GLY	2.4
1	E	66	ASN	2.4
1	D	192	SER	2.4
1	A	310	TYR	2.3
1	B	190	VAL	2.3
1	E	307	SER	2.3
1	E	188	LEU	2.3
1	B	191	PRO	2.3
1	C	194	ASP	2.3
1	C	123	GLY	2.2
1	D	122	ALA	2.2
1	A	188	LEU	2.2
1	C	119	SER	2.2
1	D	172	GLY	2.2
1	E	310	TYR	2.2
1	C	218	ASN	2.2
1	E	69	GLY	2.2
1	B	283	LYS	2.2
1	C	62	ILE	2.1
1	A	169	ASP	2.1
1	A	172	GLY	2.1
1	D	306	TYR	2.1
1	D	248	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	118	VAL	2.1
1	F	36	MET	2.0
1	A	192	SER	2.0
1	A	123	GLY	2.0
1	D	124	PRO	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

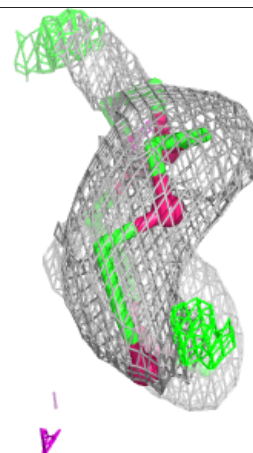
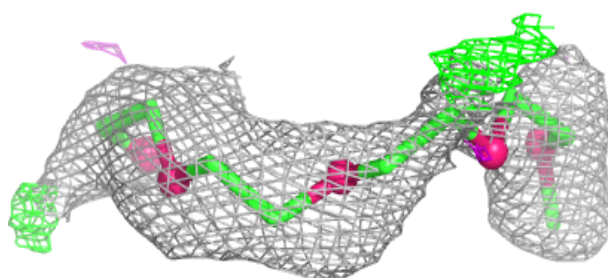
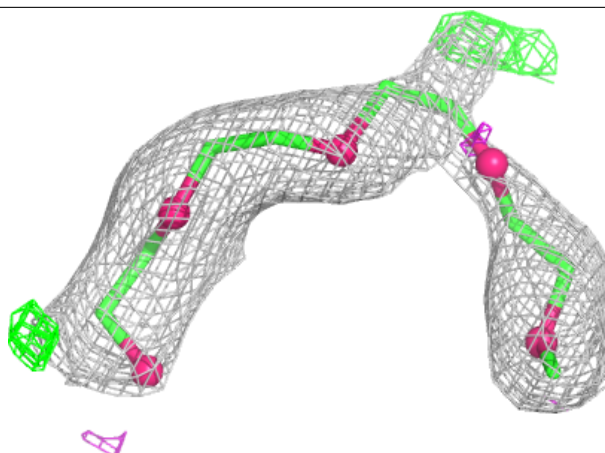
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
2	P6G	A	401	14/19	0.79	0.18	74,77,80,81	0
2	P6G	F	401	8/19	0.79	0.20	61,64,72,73	0
2	P6G	B	401	11/19	0.81	0.16	60,62,65,65	0
2	P6G	B	400	17/19	0.82	0.17	45,52,61,61	0
2	P6G	A	402	10/19	0.83	0.15	69,74,84,85	0
2	P6G	D	401	10/19	0.84	0.17	74,75,76,77	0
2	P6G	C	401	8/19	0.86	0.15	57,59,62,63	0
2	P6G	E	403	10/19	0.88	0.11	53,59,62,63	0
2	P6G	E	401	13/19	0.89	0.12	57,62,65,66	0
2	P6G	A	400	19/19	0.89	0.14	45,59,68,71	0
2	P6G	F	400	19/19	0.89	0.24	27,36,43,48	19
2	P6G	E	400	14/19	0.89	0.12	49,53,63,65	0
2	P6G	C	400	16/19	0.90	0.13	57,61,67,67	0
2	P6G	D	400	16/19	0.90	0.12	45,53,70,72	0

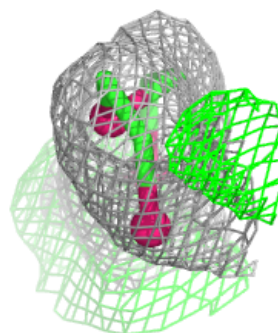
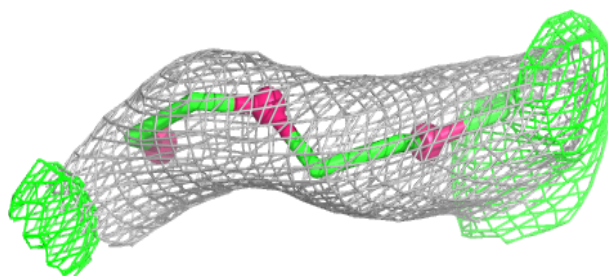
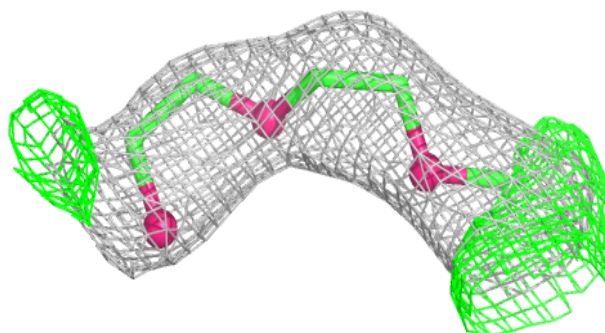
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around P6G 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)

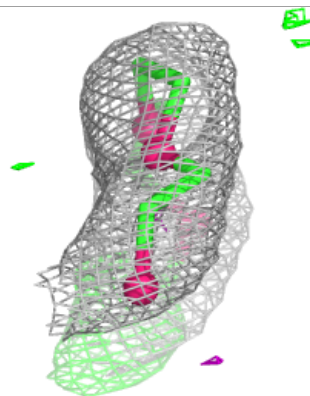
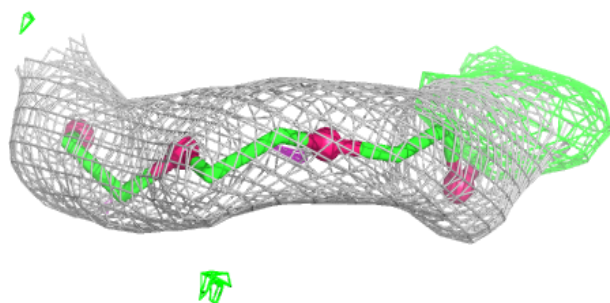
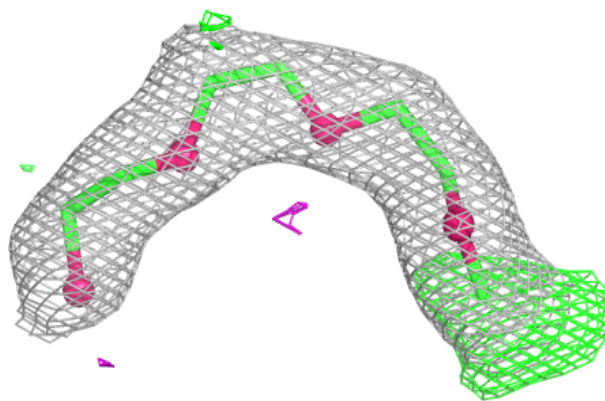
**Electron density around P6G F 401:**

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



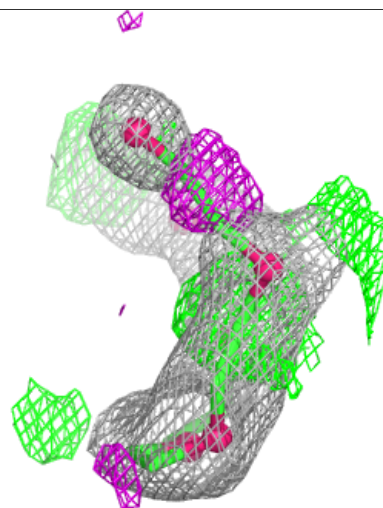
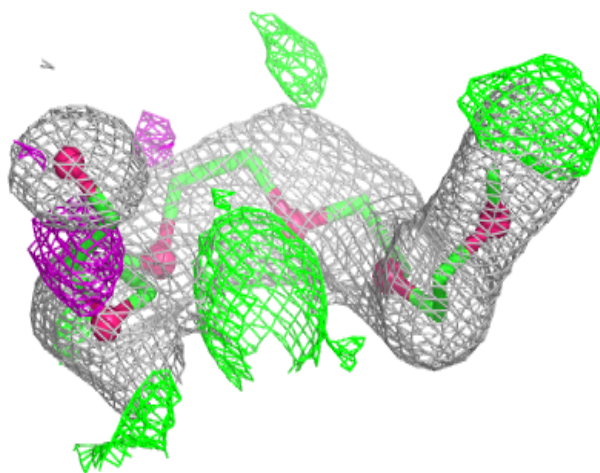
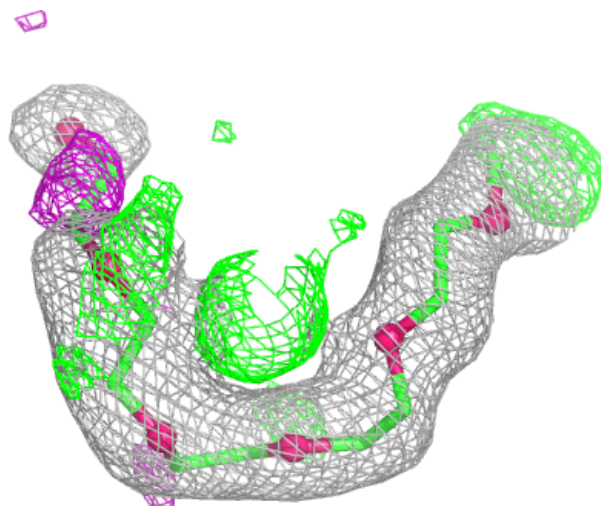
Electron density around P6G B 401:

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



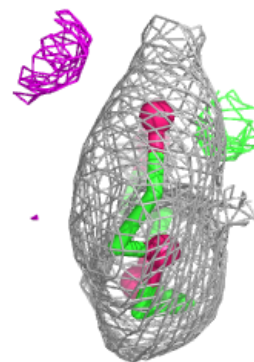
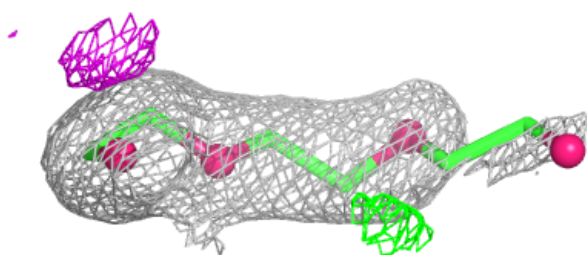
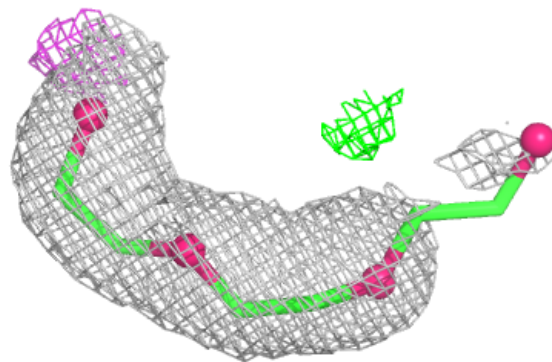
Electron density around P6G B 400:

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

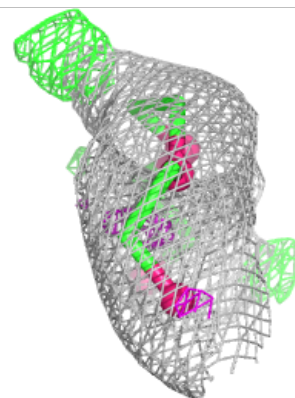
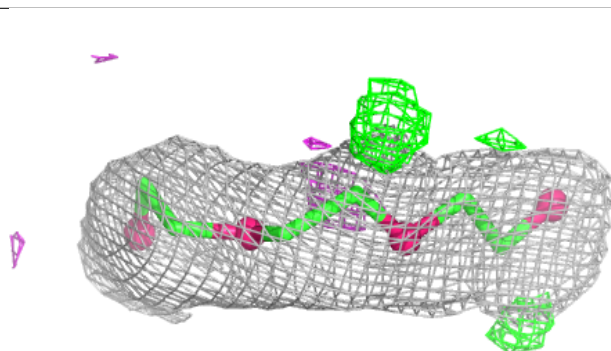
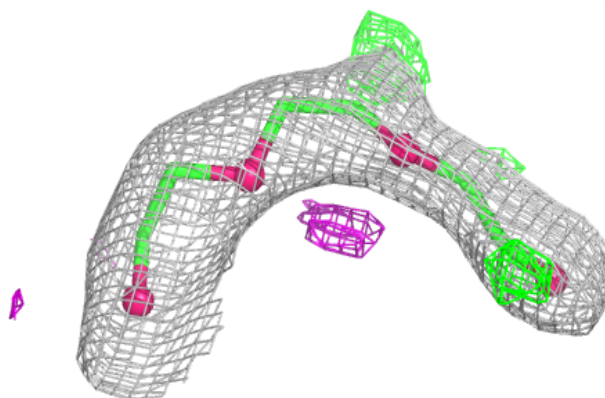


Electron density around P6G A 402:

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

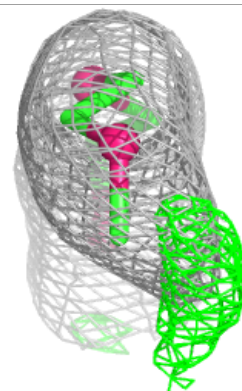
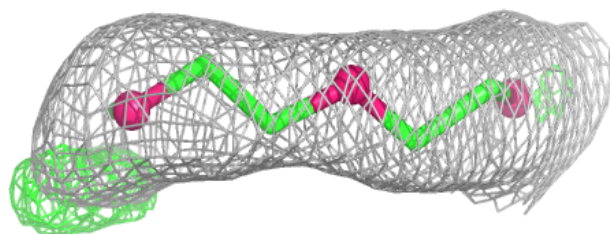
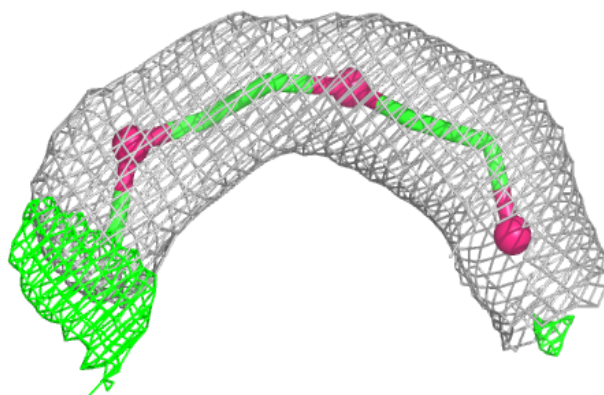
**Electron density around P6G D 401:**

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

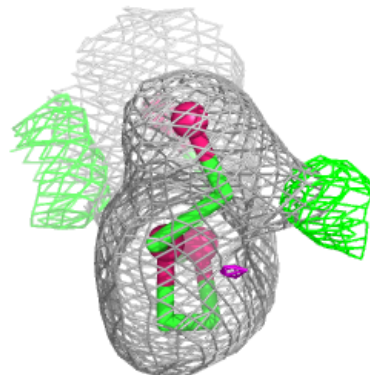
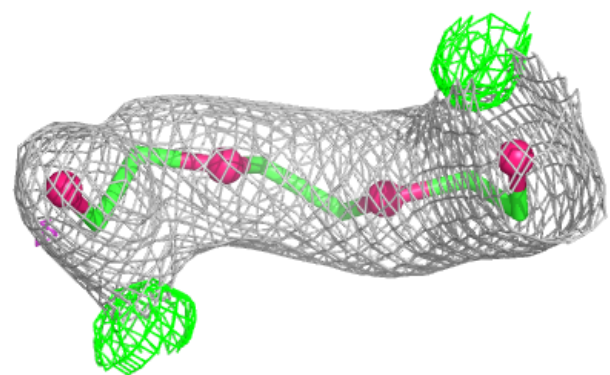
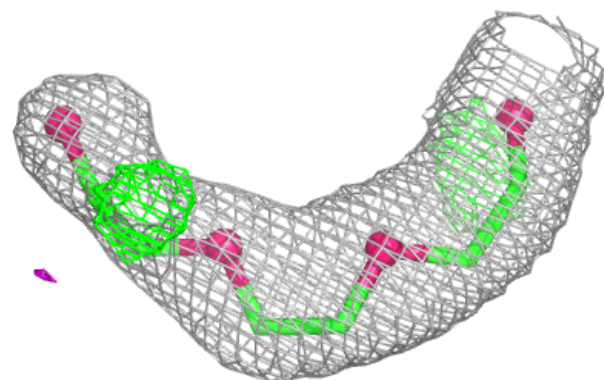


Electron density around P6G C 401:

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

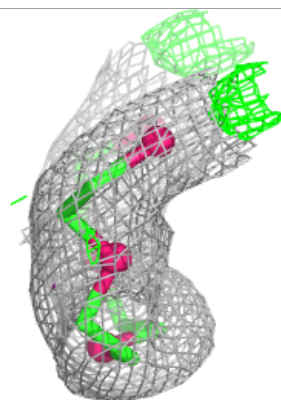
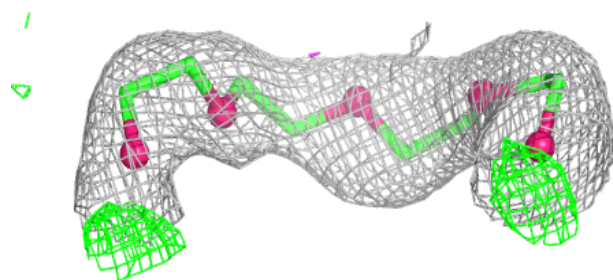
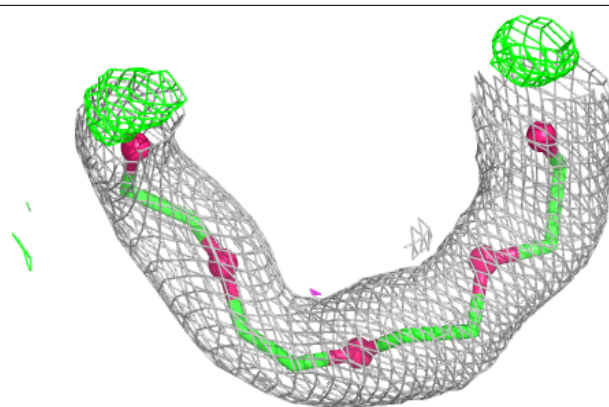
**Electron density around P6G E 403:**

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

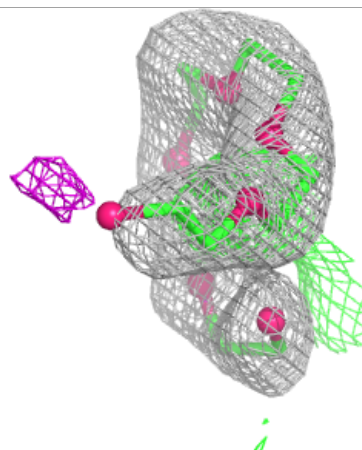
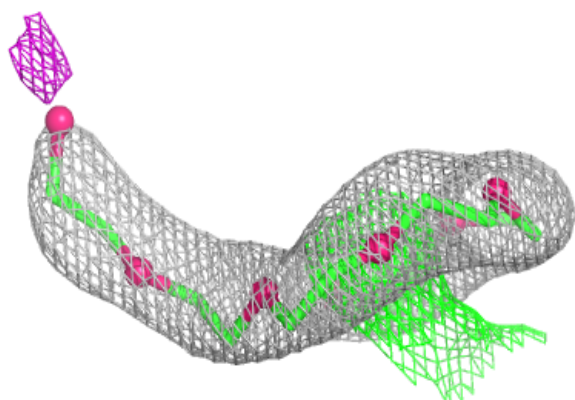
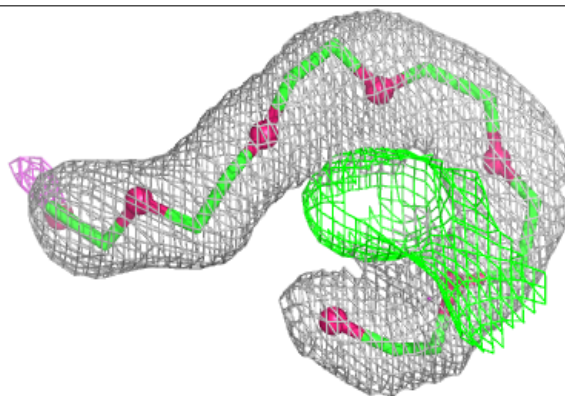


Electron density around P6G E 401:

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

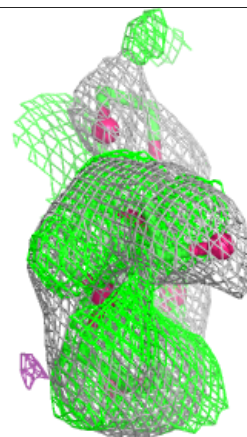
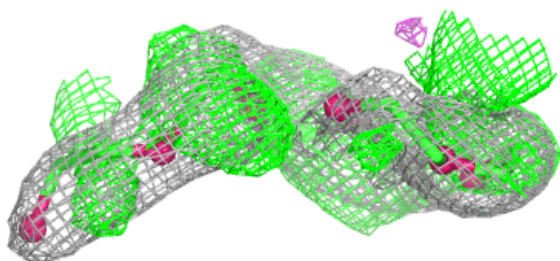
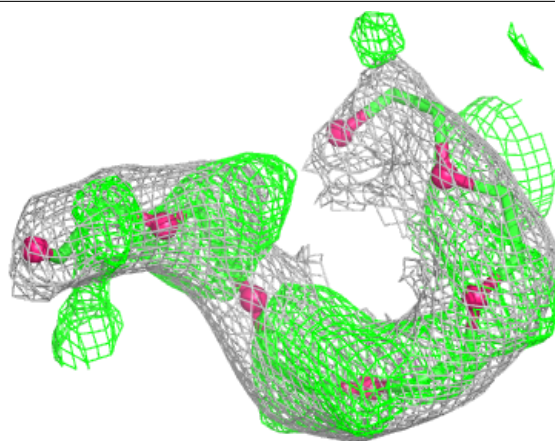
**Electron density around P6G A 400:**

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



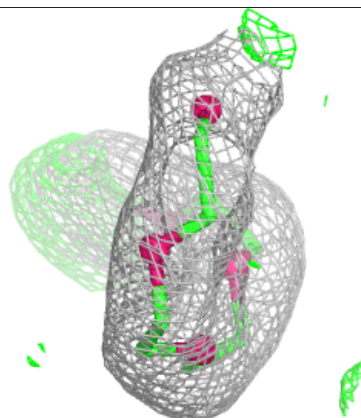
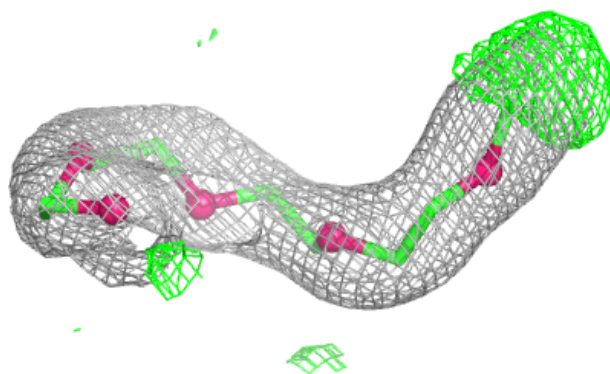
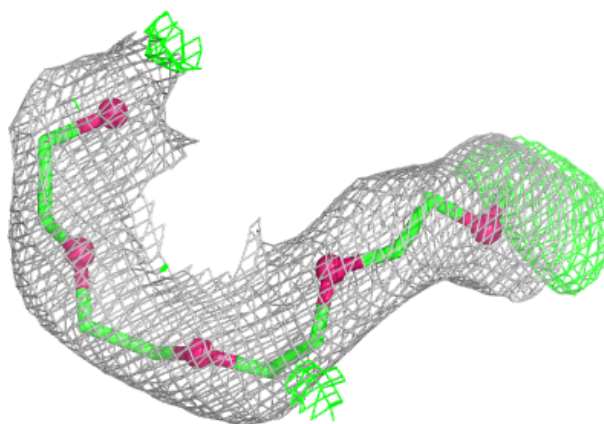
Electron density around P6G F 400:

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

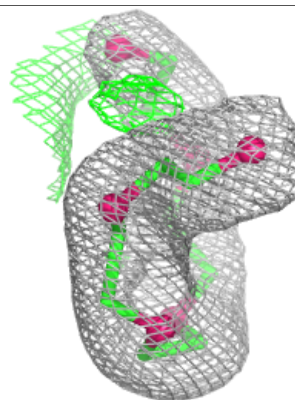
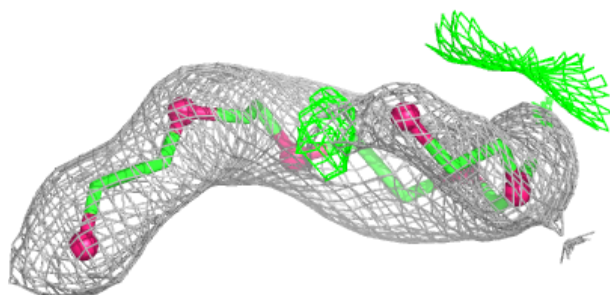
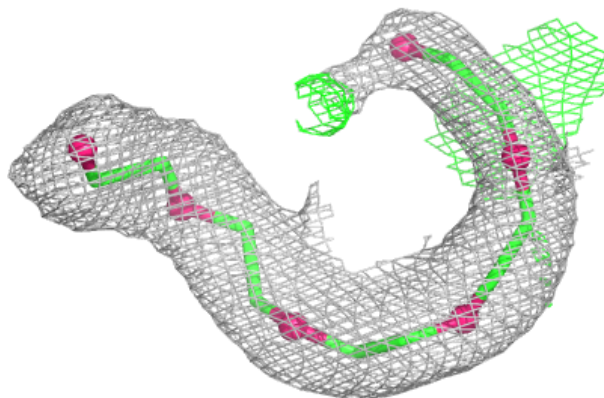


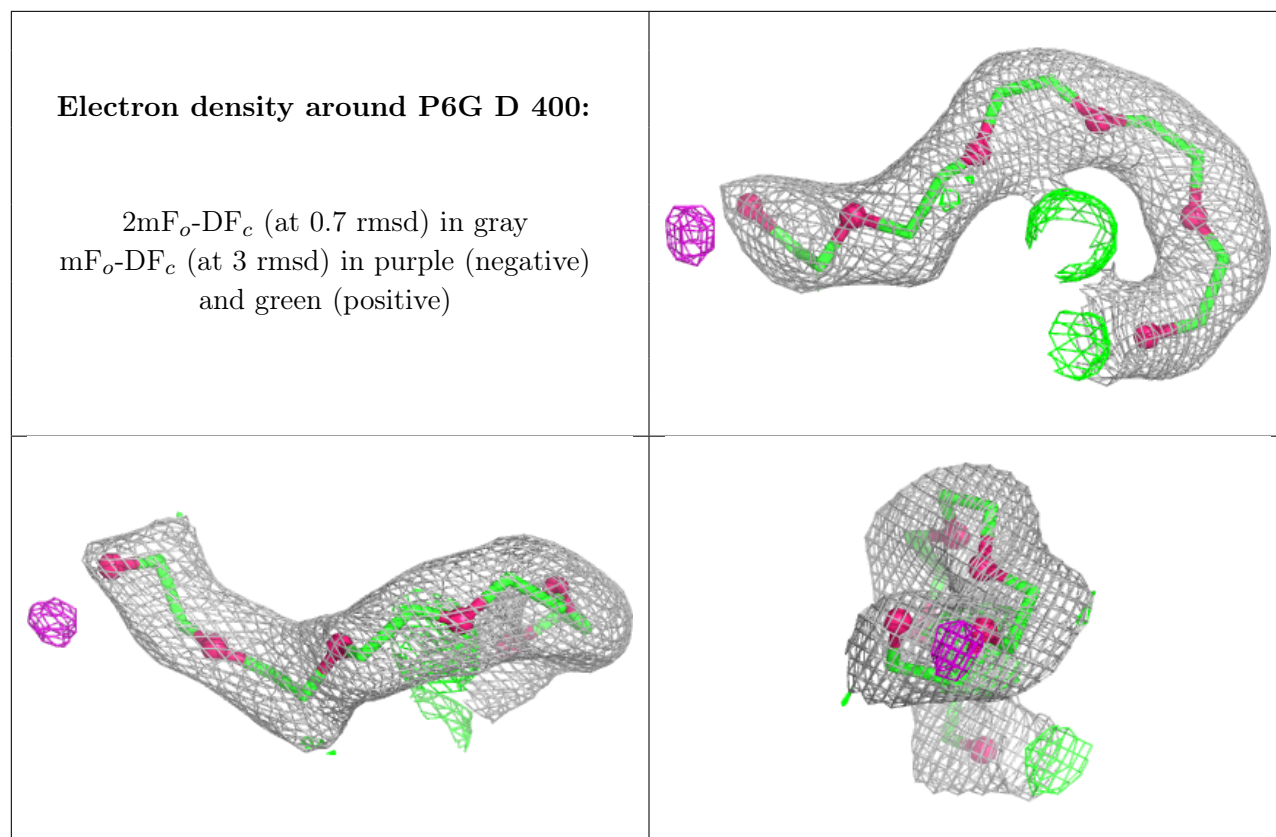
Electron density around P6G E 400:

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

**Electron density around P6G C 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 ⓘ

There are no such residues in this entry.