



# Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 11:24 am BST

PDB ID : 2G0B  
Title : The structure of FeeM, an N-acyl amino acid synthase from uncultured soil microbes  
Authors : Van Wagoner, R.M.; Clardy, J.  
Deposited on : 2006-02-11  
Resolution : 3.00 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

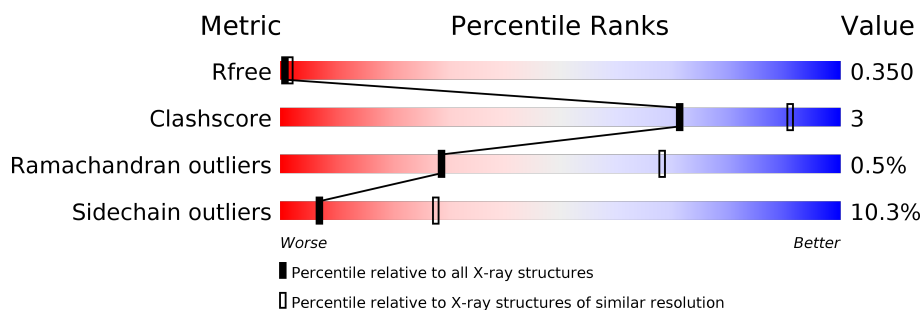
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	198	76% 18% • 5%
1	B	198	78% 15% • 5%
1	C	198	77% 14% • 7%
1	D	198	79% 10% • 9%
1	E	198	75% 16% • 9%
1	F	198	77% 12% • 7%
1	G	198	73% 13% • 12%

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Mol	Chain	Length	Quality of chain
1	H	198	 A horizontal bar chart showing the quality of the chain. The bar is divided into three segments: a green segment representing 70%, a yellow segment representing 15%, and a small orange segment representing 14%. The segments are labeled with their respective percentages below the bar.

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11507 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 FeeM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	188	Total	C	N	O	S	0	0	0
			1461	942	241	272	6			
1	B	189	Total	C	N	O	S	0	0	0
			1468	948	243	272	5			
1	C	184	Total	C	N	O	S	0	0	0
			1427	920	237	266	4			
1	D	181	Total	C	N	O	S	0	0	0
			1413	911	234	263	5			
1	E	181	Total	C	N	O	S	0	0	0
			1413	911	234	263	5			
1	F	184	Total	C	N	O	S	0	0	0
			1427	920	237	266	4			
1	G	174	Total	C	N	O	S	0	0	0
			1345	866	222	253	4			
1	H	170	Total	C	N	O	S	0	0	0
			1336	864	222	245	5			

There are 16 discrepancies between the modelled and reference sequences:

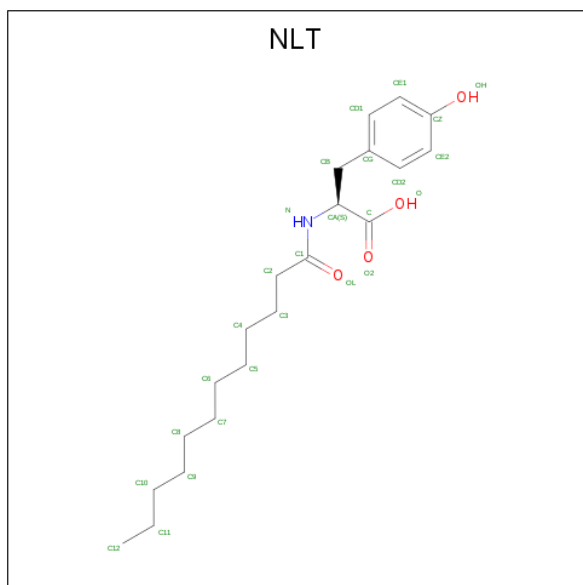
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	CLONING ARTIFACT	UNP Q8KNZ7
A	0	SER	-	CLONING ARTIFACT	UNP Q8KNZ7
B	-1	GLY	-	CLONING ARTIFACT	UNP Q8KNZ7
B	0	SER	-	CLONING ARTIFACT	UNP Q8KNZ7
C	-1	GLY	-	CLONING ARTIFACT	UNP Q8KNZ7
C	0	SER	-	CLONING ARTIFACT	UNP Q8KNZ7
D	-1	GLY	-	CLONING ARTIFACT	UNP Q8KNZ7
D	0	SER	-	CLONING ARTIFACT	UNP Q8KNZ7
E	-1	GLY	-	CLONING ARTIFACT	UNP Q8KNZ7
E	0	SER	-	CLONING ARTIFACT	UNP Q8KNZ7
F	-1	GLY	-	CLONING ARTIFACT	UNP Q8KNZ7
F	0	SER	-	CLONING ARTIFACT	UNP Q8KNZ7
G	-1	GLY	-	CLONING ARTIFACT	UNP Q8KNZ7

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Chain	Residue	Modelled	Actual	Comment	Reference
G	0	SER	-	CLONING ARTIFACT	UNP Q8KNZ7
H	-1	GLY	-	CLONING ARTIFACT	UNP Q8KNZ7
H	0	SER	-	CLONING ARTIFACT	UNP Q8KNZ7

- Molecule 2 is N-DODECANOYL-L-TYROSINE (three-letter code: NLT) (formula:  $C_{21}H_{33}NO_4$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			26	21	1	4		
2	B	1	Total	C	N	O	0	0
			26	21	1	4		
2	C	1	Total	C	N	O	0	0
			26	21	1	4		
2	D	1	Total	C	N	O	0	0
			26	21	1	4		
2	E	1	Total	C	N	O	0	0
			26	21	1	4		
2	F	1	Total	C	N	O	0	0
			26	21	1	4		
2	G	1	Total	C	N	O	0	0
			26	21	1	4		
2	H	1	Total	C	N	O	0	0
			26	21	1	4		

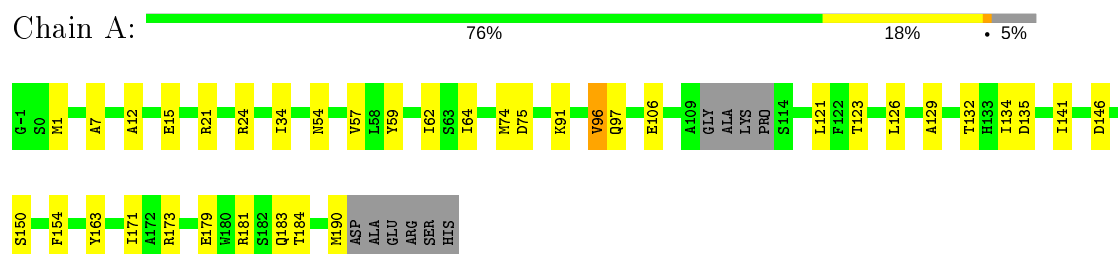
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	9	Total	O	0	0
			9	9		

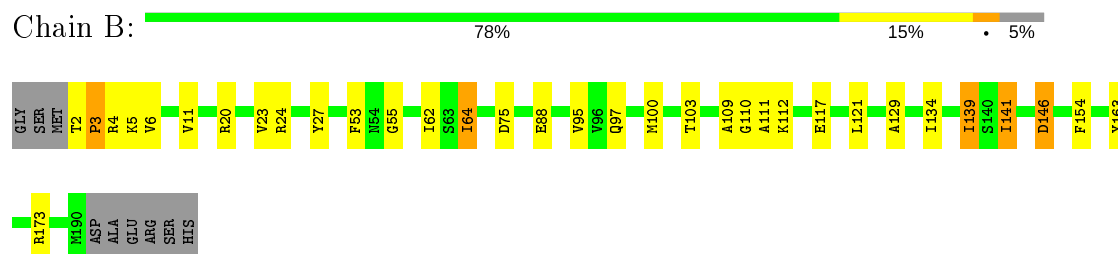
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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. 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. 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.

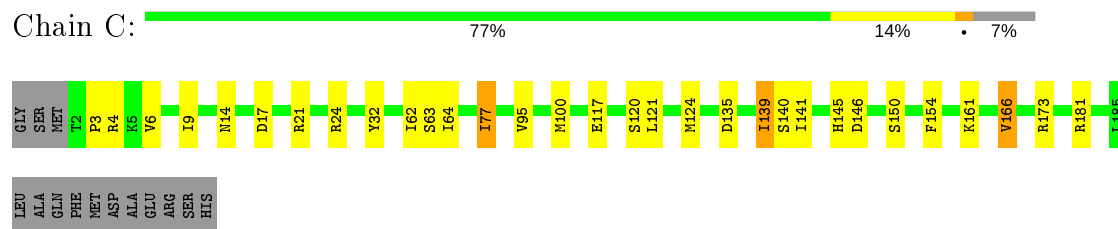
#### • Molecule 1: FeeM



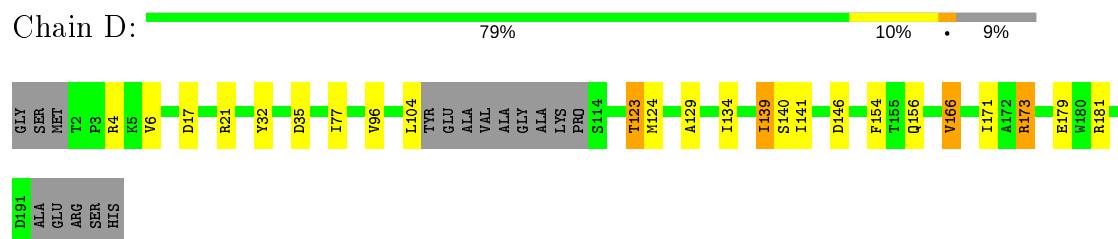
#### • Molecule 1: FeeM



#### • Molecule 1: FeeM

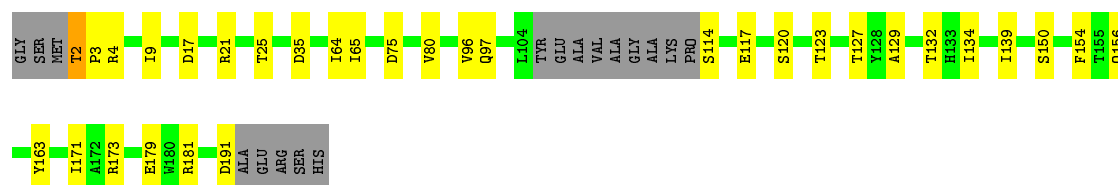


#### • Molecule 1: FeeM




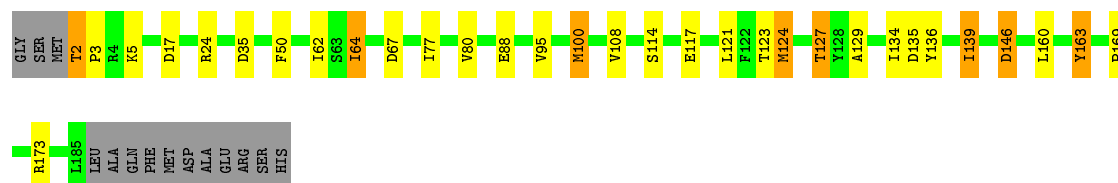
#### • Molecule 1: FeeM

Chain E:  75% 16% 9%



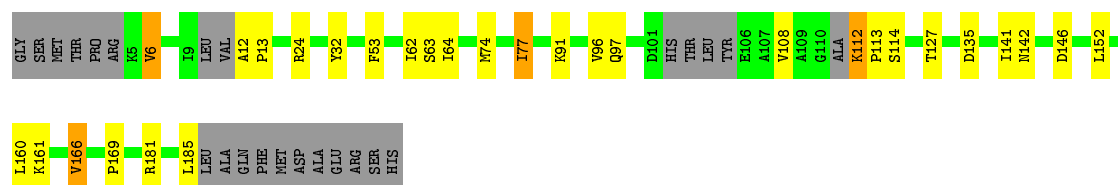
• Molecule 1: FeeM

Chain F:  77% 12% 7%



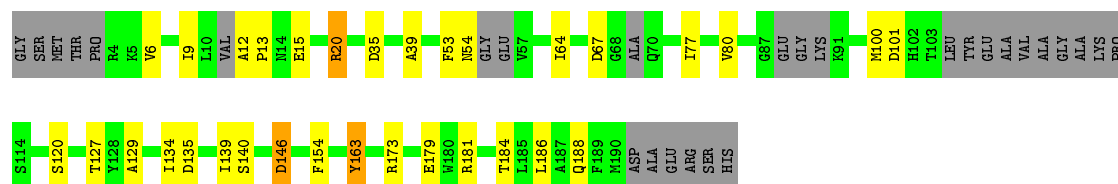
• Molecule 1: FeeM

Chain G:  73% 13% 12%



• Molecule 1: FeeM

Chain H:  70% 15% 14%





## 4 Data and refinement statistics

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	182.83Å 182.83Å 287.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.75 – 3.00 29.75 – 3.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.75-3.00) 100.0 (29.75-3.00)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.73 (at 3.00Å)	Xtriage
Refinement program	REFMAC refmac_5.1.24	Depositor
R, $R_{free}$	0.255 , 0.292 0.322 , 0.350	Depositor DCC
$R_{free}$ test set	2458 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	82.3	Xtriage
Anisotropy	0.011	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 49.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.79	EDS
Total number of atoms	11507	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.45% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: NLT

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	0.55	0/1495	0.66	2/2033 (0.1%)
1	B	0.53	0/1504	0.65	2/2048 (0.1%)
1	C	0.45	0/1462	0.64	3/1992 (0.2%)
1	D	0.46	0/1446	0.64	3/1967 (0.2%)
1	E	0.47	0/1446	0.64	4/1967 (0.2%)
1	F	0.52	0/1462	0.65	3/1992 (0.2%)
1	G	0.43	0/1374	0.62	2/1865 (0.1%)
1	H	0.43	0/1364	0.62	5/1849 (0.3%)
All	All	0.48	0/11553	0.64	24/15713 (0.2%)

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	35	ASP	CB-CG-OD2	5.89	123.60	118.30
1	G	146	ASP	CB-CG-OD2	5.64	123.37	118.30
1	E	191	ASP	CB-CG-OD2	5.62	123.36	118.30
1	D	35	ASP	CB-CG-OD2	5.55	123.29	118.30
1	E	75	ASP	CB-CG-OD2	5.40	123.16	118.30
1	H	146	ASP	CB-CG-OD2	5.39	123.15	118.30
1	E	35	ASP	CB-CG-OD2	5.35	123.11	118.30
1	F	135	ASP	CB-CG-OD2	5.29	123.06	118.30
1	H	67	ASP	CB-CG-OD2	5.29	123.06	118.30
1	B	75	ASP	CB-CG-OD2	5.28	123.05	118.30
1	F	17	ASP	CB-CG-OD2	5.28	123.05	118.30
1	E	17	ASP	CB-CG-OD2	5.26	123.03	118.30
1	G	135	ASP	CB-CG-OD2	5.23	123.00	118.30
1	D	146	ASP	CB-CG-OD2	5.17	122.95	118.30
1	C	135	ASP	CB-CG-OD2	5.16	122.95	118.30
1	D	17	ASP	CB-CG-OD2	5.15	122.93	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	146	ASP	CB-CG-OD2	5.13	122.92	118.30
1	F	146	ASP	CB-CG-OD2	5.11	122.90	118.30
1	C	17	ASP	CB-CG-OD2	5.08	122.87	118.30
1	H	135	ASP	CB-CG-OD2	5.04	122.84	118.30
1	C	146	ASP	CB-CG-OD2	5.03	122.83	118.30
1	A	135	ASP	CB-CG-OD2	5.02	122.82	118.30
1	H	101	ASP	CB-CG-OD2	5.01	122.81	118.30
1	A	75	ASP	CB-CG-OD2	5.00	122.80	118.30

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	1461	0	1443	12	0
1	B	1468	0	1452	17	0
1	C	1427	0	1410	9	0
1	D	1413	0	1393	6	0
1	E	1413	0	1393	9	0
1	F	1427	0	1410	15	1
1	G	1345	0	1321	9	0
1	H	1336	0	1315	9	0
2	A	26	0	31	1	0
2	B	26	0	31	1	0
2	C	26	0	31	0	0
2	D	26	0	31	1	0
2	E	26	0	31	0	0
2	F	26	0	31	1	0
2	G	26	0	31	1	0
2	H	26	0	31	0	0
3	A	9	0	0	0	0
All	All	11507	0	11385	79	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (79) 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:B:2:THR:HB	1:B:3:PRO:HD2	1.39	1.03
1:B:23:VAL:HG21	1:B:97:GLN:HG3	1.69	0.74
1:G:6:VAL:HG23	1:G:53:PHE:HB2	1.73	0.71
1:B:2:THR:CB	1:B:3:PRO:HD2	2.19	0.71
1:G:96:VAL:HG22	1:G:97:GLN:HG2	1.73	0.71
1:A:146:ASP:OD2	1:A:173:ARG:NH1	2.27	0.68
1:H:77:ILE:HD11	1:H:163:TYR:HA	1.78	0.66
1:B:27:TYR:OH	2:B:401:NLT:O2	2.18	0.62
1:A:91:LYS:HE2	1:A:132:THR:HG22	1.82	0.61
1:D:154:PHE:HB3	1:D:173:ARG:HB3	1.83	0.61
1:F:146:ASP:OD2	1:F:173:ARG:NH1	2.37	0.58
1:E:156:GLN:HB2	1:E:173:ARG:HH21	1.69	0.58
1:H:184:THR:HG22	1:H:186:LEU:H	1.71	0.56
1:B:109:ALA:O	1:B:111:ALA:N	2.37	0.56
1:A:123:THR:HG21	1:B:117:GLU:OE2	2.05	0.56
1:A:7:ALA:HB3	1:B:5:LYS:HB2	1.88	0.55
1:F:62:ILE:HG22	1:F:121:LEU:HD22	1.90	0.53
1:E:96:VAL:HG22	1:E:97:GLN:HG2	1.90	0.53
1:C:32:TYR:HB3	1:C:166:VAL:HG22	1.90	0.53
1:C:117:GLU:OE2	1:D:123:THR:HG21	2.07	0.53
1:G:77:ILE:HG23	1:G:161:LYS:HD2	1.90	0.52
1:H:146:ASP:OD1	1:H:173:ARG:NH1	2.41	0.52
1:A:129:ALA:HA	1:A:134:ILE:HD12	1.92	0.52
1:C:77:ILE:HG23	1:C:161:LYS:HD2	1.90	0.51
1:F:77:ILE:CD1	1:F:163:TYR:HA	2.40	0.51
1:B:154:PHE:HB3	1:B:173:ARG:HB3	1.93	0.50
1:G:32:TYR:HB3	1:G:166:VAL:HG22	1.92	0.50
1:E:9:ILE:HD11	1:F:2:THR:HG23	1.93	0.50
1:F:64:ILE:HG22	1:F:95:VAL:HG13	1.93	0.49
1:B:62:ILE:HG22	1:B:121:LEU:HD22	1.95	0.49
1:A:12:ALA:HB3	1:A:15:GLU:HG3	1.96	0.48
1:E:154:PHE:HB3	1:E:173:ARG:HB3	1.94	0.48
1:D:139:ILE:HD11	2:D:403:NLT:H62	1.96	0.48
1:B:2:THR:HB	1:B:3:PRO:CD	2.28	0.48
1:G:62:ILE:HD11	2:G:406:NLT:H52	1.95	0.47
1:E:123:THR:HG21	1:F:117:GLU:OE2	2.15	0.47
1:F:100:MET:HE3	1:F:100:MET:HB3	1.73	0.47
1:F:50:PHE:CD2	1:F:124:MET:HG2	2.49	0.47
1:H:154:PHE:HB3	1:H:173:ARG:HB3	1.95	0.47
1:A:96:VAL:HG13	1:A:97:GLN:HG2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:139:ILE:HG23	1:B:141:ILE:HG23	1.97	0.47
1:G:112:LYS:HE2	1:G:113:PRO:HD2	1.96	0.46
1:F:139:ILE:HD11	2:F:405:NLT:H71	1.96	0.46
1:C:6:VAL:HG13	1:D:6:VAL:HG22	1.97	0.46
1:B:129:ALA:HA	1:B:134:ILE:HD12	1.97	0.46
1:B:95:VAL:HB	1:B:139:ILE:HD11	1.97	0.45
1:G:160:LEU:HD11	1:G:169:PRO:HB3	1.97	0.45
1:C:95:VAL:HB	1:C:139:ILE:HD11	1.97	0.45
1:H:6:VAL:HB	1:H:53:PHE:HB2	1.98	0.45
1:B:146:ASP:OD2	1:B:173:ARG:NH1	2.49	0.45
1:D:129:ALA:HA	1:D:134:ILE:HD12	1.98	0.45
1:B:6:VAL:HB	1:B:53:PHE:HB2	1.99	0.44
1:A:62:ILE:HG22	1:A:121:LEU:HD22	2.00	0.44
1:D:32:TYR:HB3	1:D:166:VAL:HG22	1.99	0.44
1:B:64:ILE:HG22	1:B:95:VAL:HG13	2.01	0.43
1:A:24:ARG:HG3	1:A:34:ILE:HD13	2.01	0.42
1:H:129:ALA:HA	1:H:134:ILE:HD12	2.01	0.42
1:C:154:PHE:HB3	1:C:173:ARG:HB3	2.02	0.42
1:G:152:LEU:HA	1:G:152:LEU:HD23	1.89	0.42
1:C:62:ILE:HG22	1:C:121:LEU:HD22	2.01	0.42
1:E:2:THR:HA	1:E:3:PRO:HD3	1.91	0.42
1:A:126:LEU:HD13	2:A:400:NLT:H121	2.01	0.42
1:H:12:ALA:HA	1:H:13:PRO:HD3	1.91	0.42
1:F:160:LEU:HD11	1:F:169:PRO:HB3	2.02	0.42
1:F:123:THR:O	1:F:127:THR:OG1	2.36	0.42
1:A:154:PHE:HB3	1:A:173:ARG:HB3	2.02	0.41
1:A:54:ASN:HB2	1:A:59:TYR:CD2	2.55	0.41
1:E:129:ALA:HA	1:E:134:ILE:HD12	2.03	0.41
1:C:139:ILE:HG23	1:C:141:ILE:HG23	2.01	0.41
1:F:129:ALA:HA	1:F:134:ILE:HD12	2.02	0.41
1:F:77:ILE:HD12	1:F:163:TYR:HA	2.03	0.41
1:H:12:ALA:HB3	1:H:15:GLU:HB2	2.02	0.41
1:H:20:ARG:HH21	1:H:39:ALA:HB1	1.85	0.41
1:E:65:ILE:HD12	1:E:96:VAL:HG11	2.02	0.41
1:B:2:THR:CB	1:B:3:PRO:CD	2.93	0.41
1:C:139:ILE:HD13	1:C:139:ILE:HA	1.78	0.40
1:F:77:ILE:HG21	1:F:77:ILE:HD13	1.82	0.40
1:E:117:GLU:HG3	1:F:123:THR:HG21	2.04	0.40
1:G:12:ALA:HA	1:G:13:PRO:HD3	1.92	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:88:GLU:OE2	1:F:136:TYR:OH[6_565]	2.05	0.15

## 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	184/198 (93%)	176 (96%)	7 (4%)	1 (0%)	29	68
1	B	187/198 (94%)	182 (97%)	2 (1%)	3 (2%)	9	40
1	C	182/198 (92%)	177 (97%)	4 (2%)	1 (0%)	29	68
1	D	177/198 (89%)	169 (96%)	8 (4%)	0	100	100
1	E	177/198 (89%)	174 (98%)	3 (2%)	0	100	100
1	F	182/198 (92%)	174 (96%)	6 (3%)	2 (1%)	14	50
1	G	166/198 (84%)	157 (95%)	9 (5%)	0	100	100
1	H	158/198 (80%)	153 (97%)	5 (3%)	0	100	100
All	All	1413/1584 (89%)	1362 (96%)	44 (3%)	7 (0%)	29	68

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	110	GLY
1	B	3	PRO
1	C	3	PRO
1	A	106	GLU
1	F	67	ASP
1	B	55	GLY
1	F	3	PRO

### 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	150/157 (96%)	135 (90%)	15 (10%)	7	29
1	B	150/157 (96%)	138 (92%)	12 (8%)	12	40
1	C	146/157 (93%)	129 (88%)	17 (12%)	5	23
1	D	146/157 (93%)	130 (89%)	16 (11%)	6	25
1	E	146/157 (93%)	130 (89%)	16 (11%)	6	25
1	F	146/157 (93%)	133 (91%)	13 (9%)	9	35
1	G	137/157 (87%)	121 (88%)	16 (12%)	5	22
1	H	138/157 (88%)	124 (90%)	14 (10%)	7	29
All	All	1159/1256 (92%)	1040 (90%)	119 (10%)	7	28

All (119) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	21	ARG
1	A	57	VAL
1	A	64	ILE
1	A	74	MET
1	A	96	VAL
1	A	141	ILE
1	A	150	SER
1	A	163	TYR
1	A	171	ILE
1	A	179	GLU
1	A	181	ARG
1	A	183	GLN
1	A	184	THR
1	A	190	MET
1	B	4	ARG
1	B	11	VAL
1	B	20	ARG
1	B	24	ARG
1	B	64	ILE
1	B	88	GLU
1	B	100	MET
1	B	103	THR

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Mol	Chain	Res	Type
1	B	112	LYS
1	B	139	ILE
1	B	141	ILE
1	B	163	TYR
1	C	4	ARG
1	C	9	ILE
1	C	14	ASN
1	C	21	ARG
1	C	24	ARG
1	C	63	SER
1	C	64	ILE
1	C	77	ILE
1	C	100	MET
1	C	120	SER
1	C	124	MET
1	C	139	ILE
1	C	140	SER
1	C	145	HIS
1	C	150	SER
1	C	166	VAL
1	C	181	ARG
1	D	4	ARG
1	D	21	ARG
1	D	77	ILE
1	D	96	VAL
1	D	104	LEU
1	D	123	THR
1	D	124	MET
1	D	139	ILE
1	D	140	SER
1	D	141	ILE
1	D	156	GLN
1	D	166	VAL
1	D	171	ILE
1	D	173	ARG
1	D	179	GLU
1	D	181	ARG
1	E	2	THR
1	E	4	ARG
1	E	21	ARG
1	E	25	THR
1	E	64	ILE

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Mol	Chain	Res	Type
1	E	80	VAL
1	E	114	SER
1	E	120	SER
1	E	127	THR
1	E	132	THR
1	E	139	ILE
1	E	150	SER
1	E	163	TYR
1	E	171	ILE
1	E	179	GLU
1	E	181	ARG
1	F	2	THR
1	F	5	LYS
1	F	24	ARG
1	F	35	ASP
1	F	64	ILE
1	F	80	VAL
1	F	100	MET
1	F	108	VAL
1	F	114	SER
1	F	124	MET
1	F	127	THR
1	F	139	ILE
1	F	163	TYR
1	G	6	VAL
1	G	24	ARG
1	G	63	SER
1	G	64	ILE
1	G	74	MET
1	G	77	ILE
1	G	91	LYS
1	G	108	VAL
1	G	112	LYS
1	G	114	SER
1	G	127	THR
1	G	141	ILE
1	G	142	ASN
1	G	166	VAL
1	G	181	ARG
1	G	185	LEU
1	H	9	ILE
1	H	20	ARG

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Mol	Chain	Res	Type
1	H	54	ASN
1	H	64	ILE
1	H	80	VAL
1	H	100	MET
1	H	120	SER
1	H	127	THR
1	H	139	ILE
1	H	140	SER
1	H	163	TYR
1	H	179	GLU
1	H	181	ARG
1	H	188	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	54	ASN
1	G	142	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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

8 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	NLT	G	406	-	23,26,26	0.60	0	26,31,31	0.82	0
2	NLT	E	404	-	23,26,26	0.57	0	26,31,31	0.64	0
2	NLT	A	400	-	23,26,26	0.49	0	26,31,31	0.58	0
2	NLT	B	401	-	23,26,26	0.59	0	26,31,31	0.73	0
2	NLT	F	405	-	23,26,26	0.64	0	26,31,31	0.56	0
2	NLT	D	403	-	23,26,26	0.58	0	26,31,31	0.81	1 (3%)
2	NLT	C	402	-	23,26,26	0.57	0	26,31,31	0.69	0
2	NLT	H	407	-	23,26,26	0.50	0	26,31,31	0.77	1 (3%)

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	NLT	G	406	-	-	8/19/23/23	0/1/1/1
2	NLT	E	404	-	-	9/19/23/23	0/1/1/1
2	NLT	A	400	-	-	4/19/23/23	0/1/1/1
2	NLT	B	401	-	-	7/19/23/23	0/1/1/1
2	NLT	F	405	-	-	7/19/23/23	0/1/1/1
2	NLT	D	403	-	-	9/19/23/23	0/1/1/1
2	NLT	C	402	-	-	10/19/23/23	0/1/1/1
2	NLT	H	407	-	-	6/19/23/23	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	407	NLT	CB-CA-N	2.34	113.26	109.01
2	D	403	NLT	CB-CA-N	2.04	112.72	109.01

There are no chirality outliers.

All (60) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	406	NLT	C-CA-N-C1
2	C	402	NLT	C-CA-N-C1
2	A	400	NLT	CB-CA-N-C1
2	A	400	NLT	C-CA-CB-CG
2	B	401	NLT	C-CA-N-C1
2	F	405	NLT	C-CA-N-C1
2	C	402	NLT	C1-C2-C3-C4
2	C	402	NLT	OL-C1-N-CA
2	C	402	NLT	C2-C1-N-CA
2	E	404	NLT	C7-C8-C9-C10
2	E	404	NLT	C11-C10-C9-C8
2	F	405	NLT	C11-C10-C9-C8
2	F	405	NLT	C7-C8-C9-C10
2	B	401	NLT	C11-C10-C9-C8
2	H	407	NLT	C6-C7-C8-C9
2	G	406	NLT	C5-C6-C7-C8
2	D	403	NLT	C11-C10-C9-C8
2	D	403	NLT	C4-C5-C6-C7
2	D	403	NLT	C7-C8-C9-C10
2	F	405	NLT	C4-C5-C6-C7
2	B	401	NLT	C7-C8-C9-C10
2	A	400	NLT	C7-C8-C9-C10
2	D	403	NLT	CA-CB-CG-CD1
2	E	404	NLT	CB-CA-N-C1
2	D	403	NLT	CB-CA-N-C1
2	H	407	NLT	CB-CA-N-C1
2	D	403	NLT	CA-CB-CG-CD2
2	E	404	NLT	C-CA-N-C1
2	G	406	NLT	C7-C8-C9-C10
2	F	405	NLT	C1-C2-C3-C4
2	E	404	NLT	C6-C7-C8-C9
2	C	402	NLT	C11-C10-C9-C8
2	H	407	NLT	C4-C5-C6-C7
2	E	404	NLT	CA-CB-CG-CD2
2	E	404	NLT	CA-CB-CG-CD1
2	H	407	NLT	CA-CB-CG-CD1
2	H	407	NLT	CA-CB-CG-CD2
2	G	406	NLT	CA-CB-CG-CD2
2	G	406	NLT	CA-CB-CG-CD1
2	G	406	NLT	C3-C4-C5-C6
2	G	406	NLT	C4-C5-C6-C7
2	D	403	NLT	C6-C7-C8-C9
2	C	402	NLT	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
2	C	402	NLT	CA-CB-CG-CD1
2	A	400	NLT	C-CA-N-C1
2	E	404	NLT	C9-C10-C11-C12
2	C	402	NLT	C5-C6-C7-C8
2	C	402	NLT	CA-CB-CG-CD2
2	B	401	NLT	CA-CB-CG-CD1
2	G	406	NLT	C6-C7-C8-C9
2	F	405	NLT	C5-C6-C7-C8
2	B	401	NLT	C5-C6-C7-C8
2	B	401	NLT	CA-CB-CG-CD2
2	B	401	NLT	C9-C10-C11-C12
2	D	403	NLT	C-CA-N-C1
2	C	402	NLT	C9-C10-C11-C12
2	D	403	NLT	C9-C10-C11-C12
2	F	405	NLT	CA-CB-CG-CD1
2	H	407	NLT	C-CA-N-C1
2	E	404	NLT	C4-C5-C6-C7

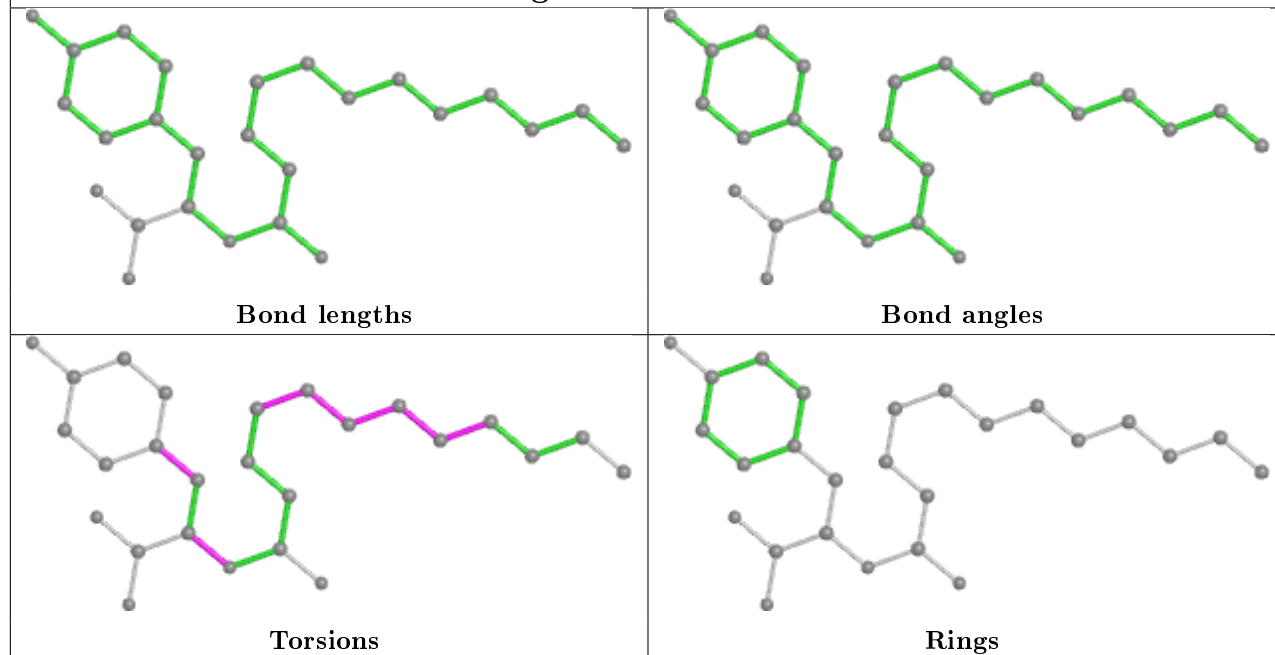
There are no ring outliers.

5 monomers are involved in 5 short contacts:

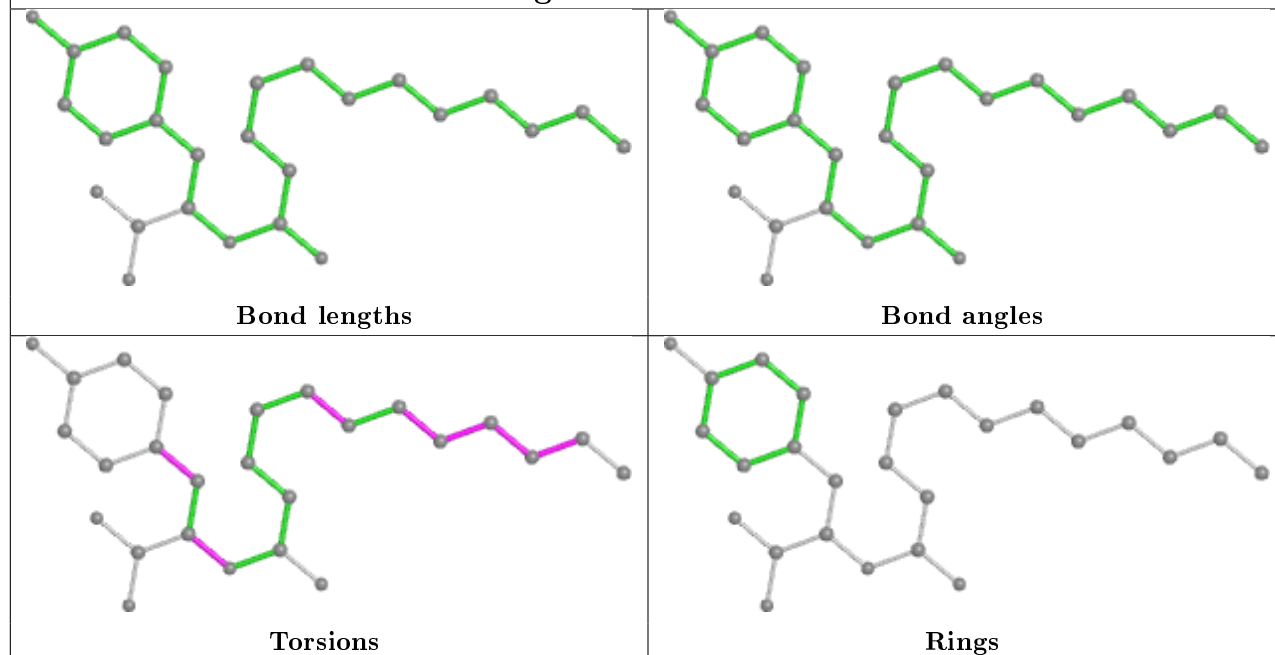
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	406	NLT	1	0
2	A	400	NLT	1	0
2	B	401	NLT	1	0
2	F	405	NLT	1	0
2	D	403	NLT	1	0

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.

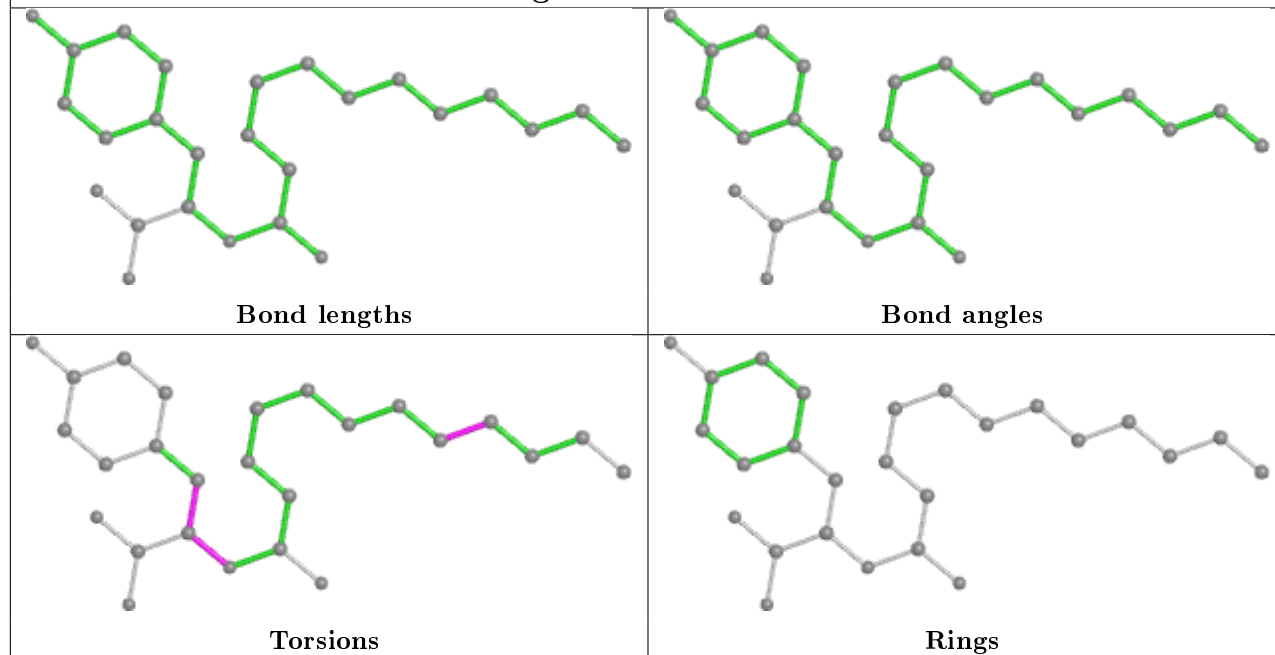
## Ligand NLT G 406



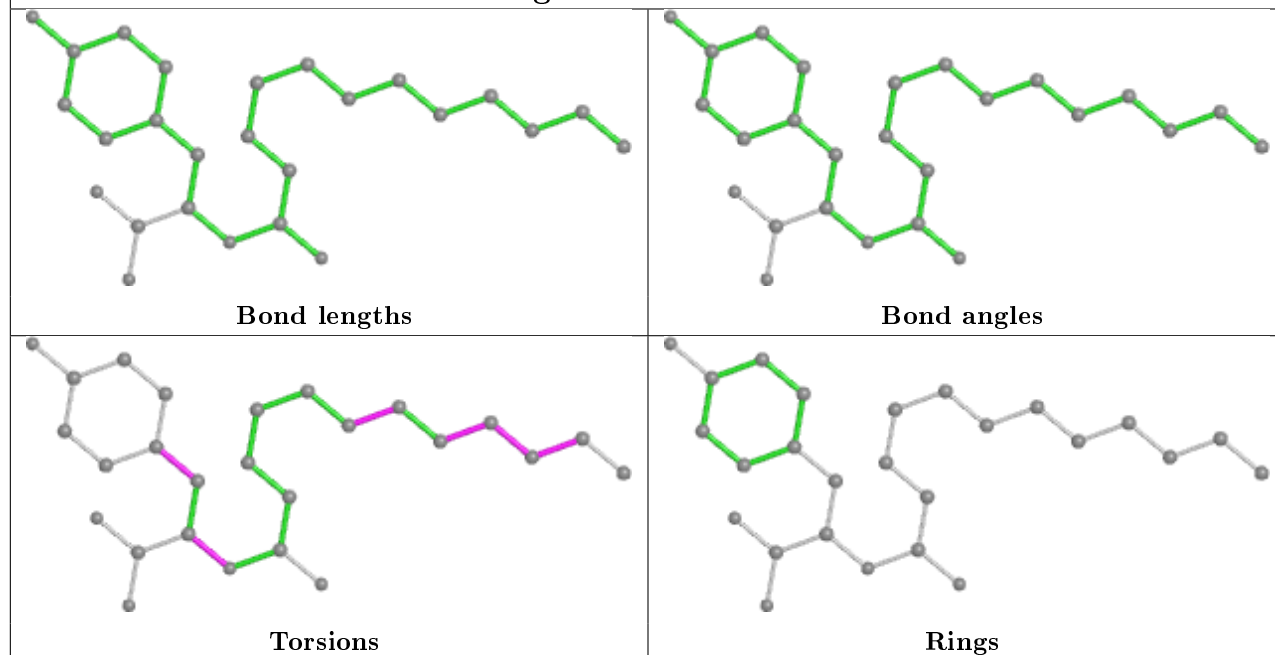
## Ligand NLT E 404



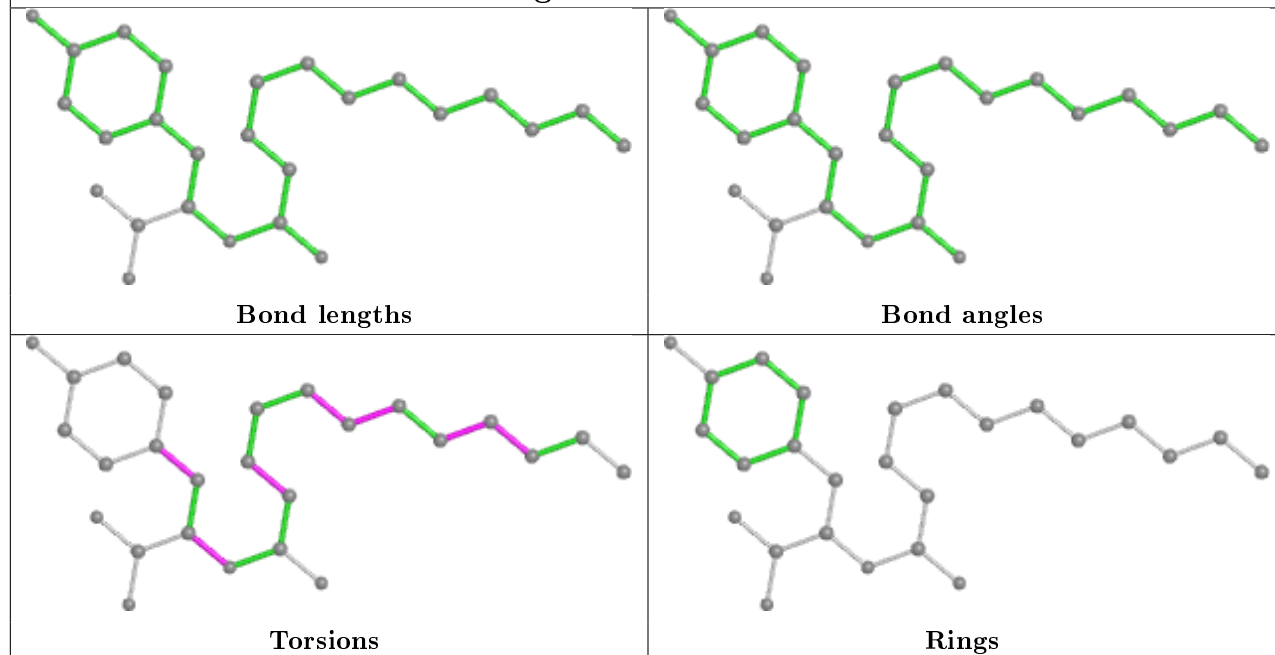
## Ligand NLT A 400



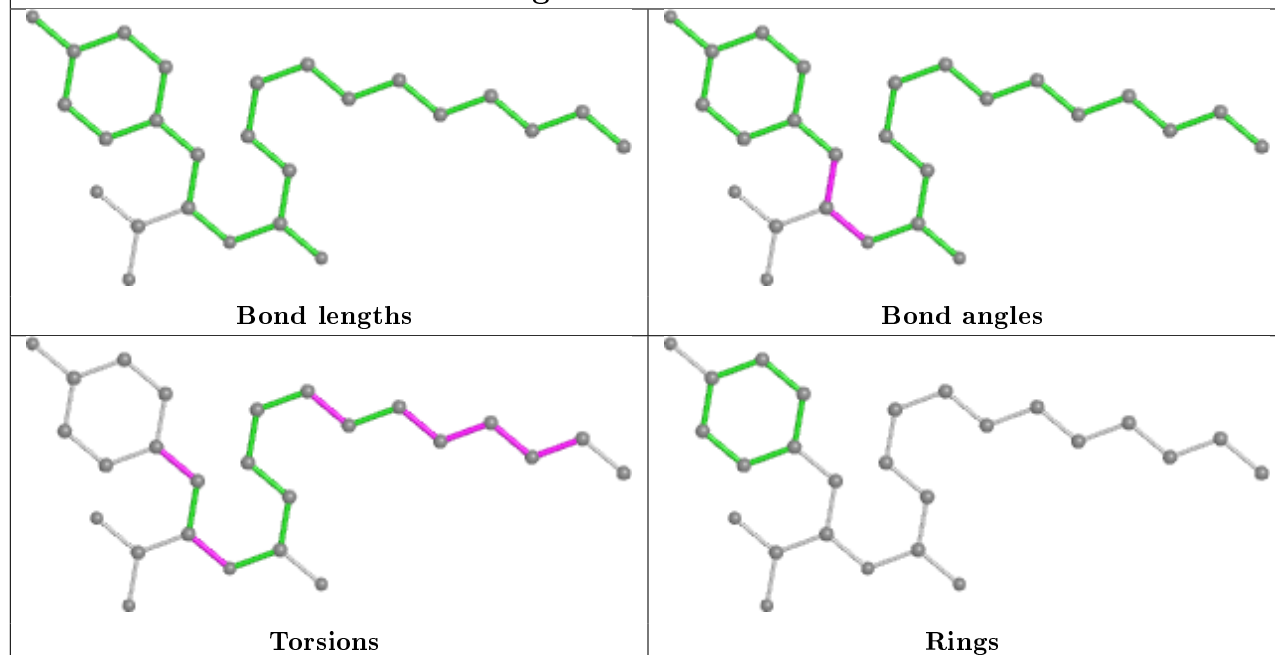
## Ligand NLT B 401



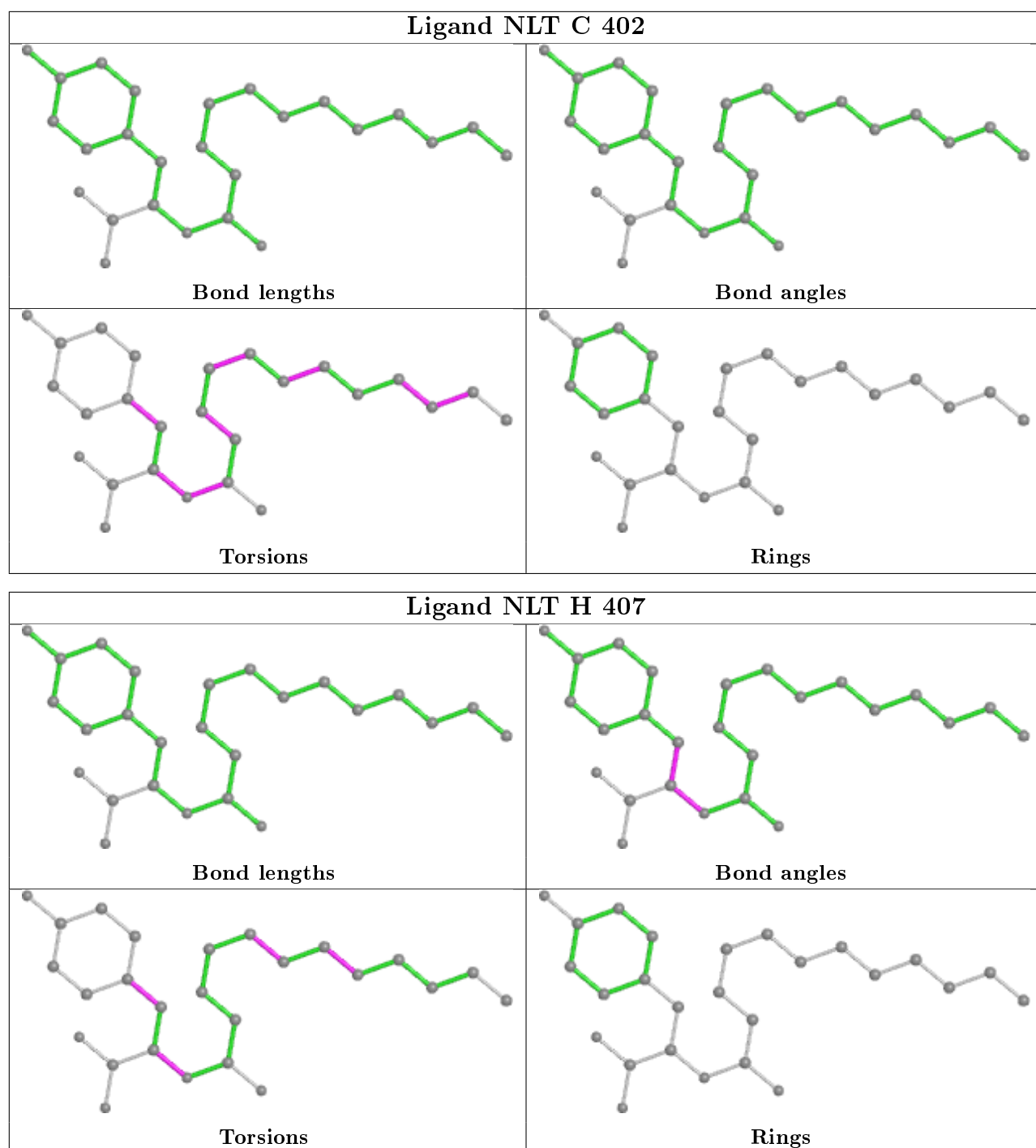
## Ligand NLT F 405



## Ligand NLT D 403







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

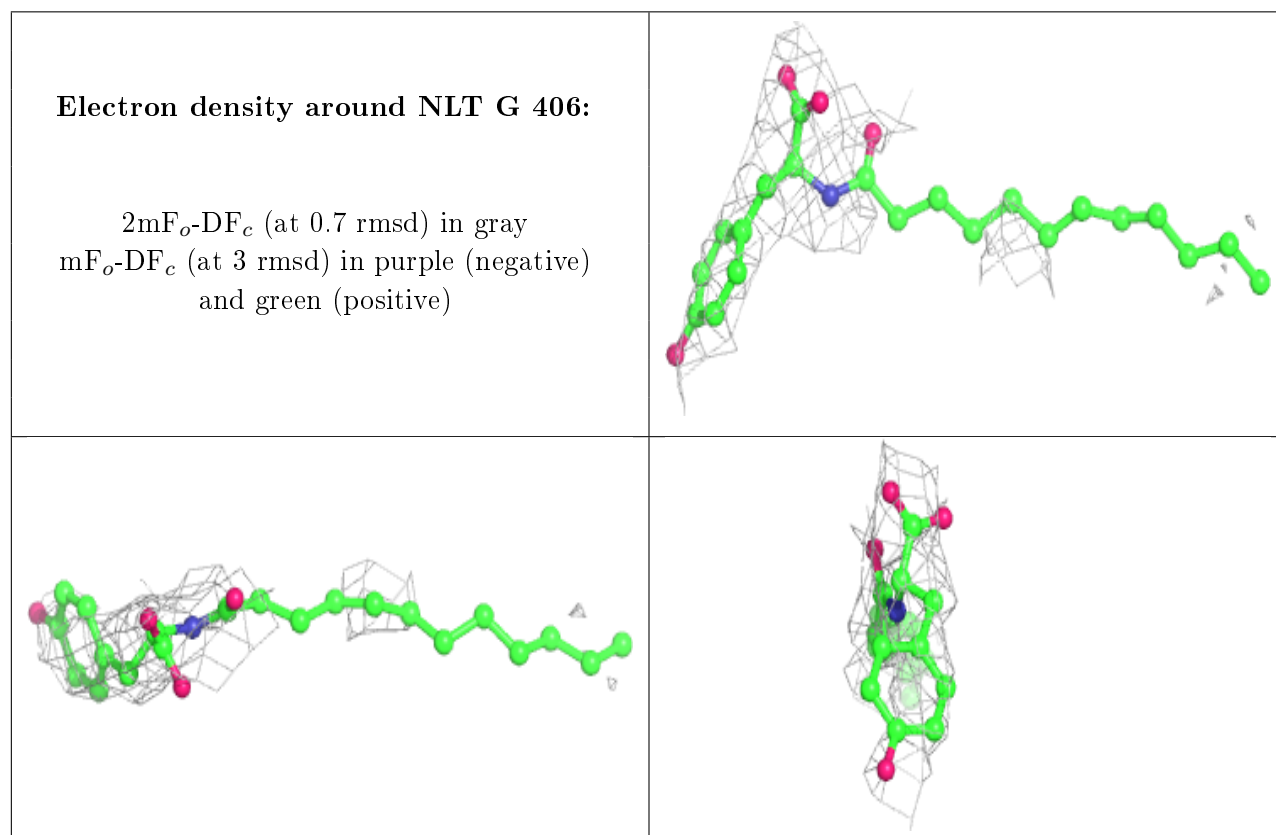
### 6.3 Carbohydrates [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands [i](#)

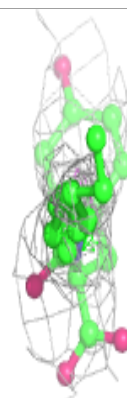
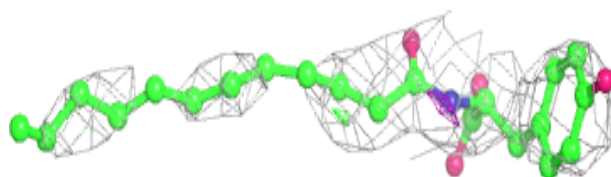
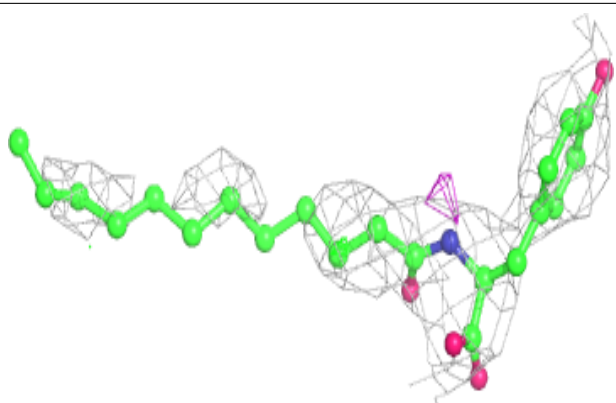
Unable to reproduce the depositors R factor - this section is therefore empty.

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.

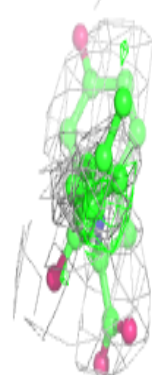
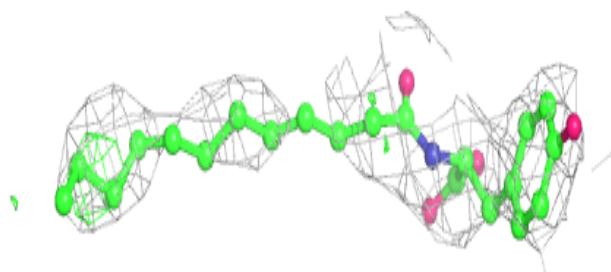
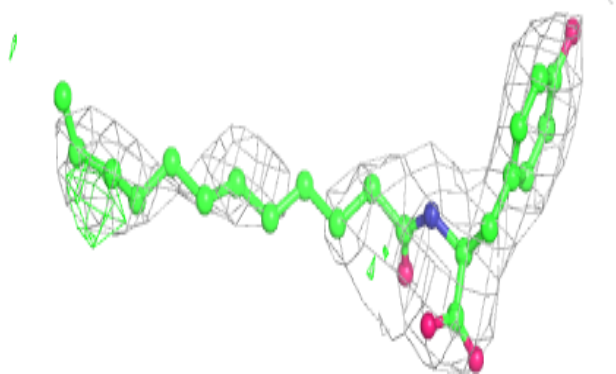


**Electron density around NLT C 402:**

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

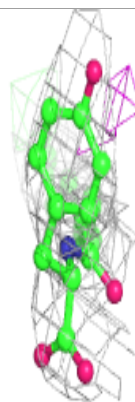
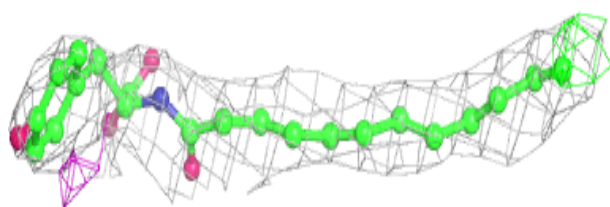
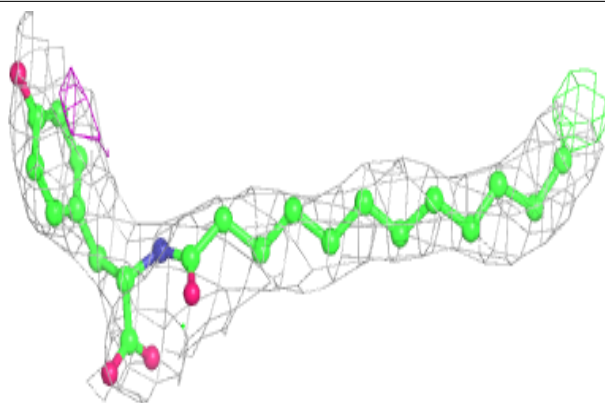
**Electron density around NLT E 404:**

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

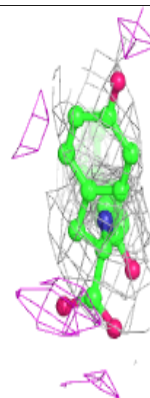
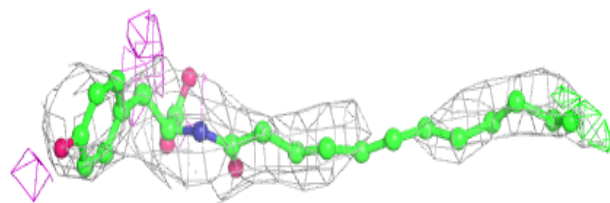
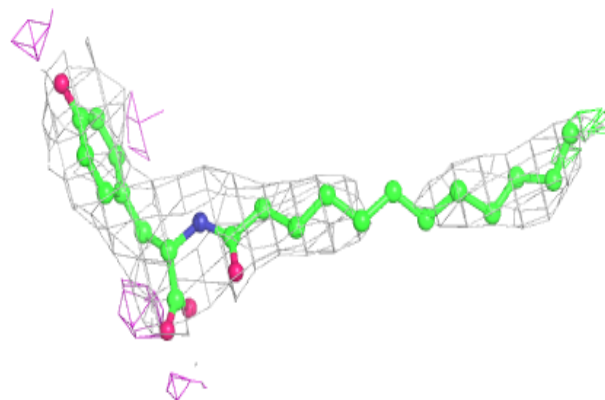


**Electron density around NLT A 400:**

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

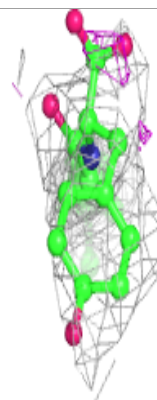
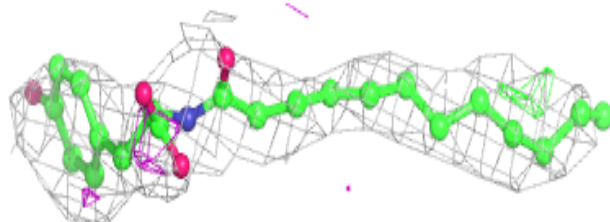
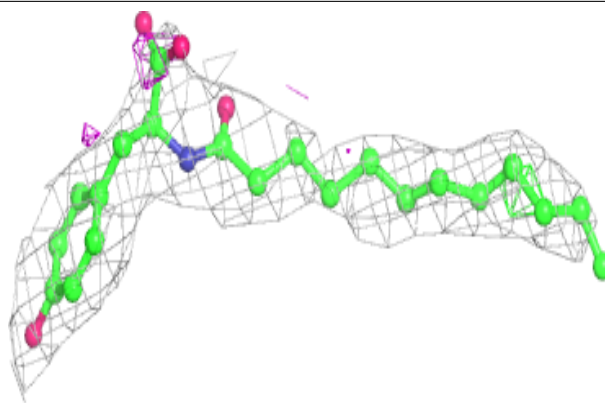
**Electron density around NLT B 401:**

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

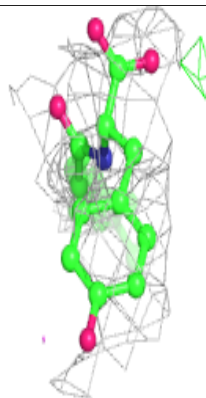
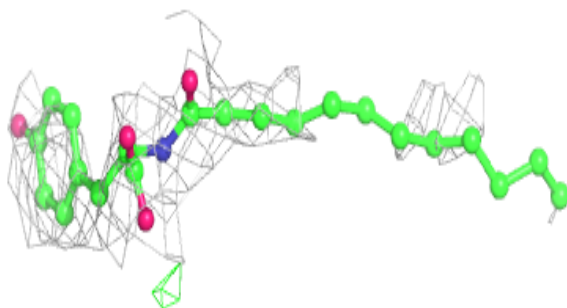
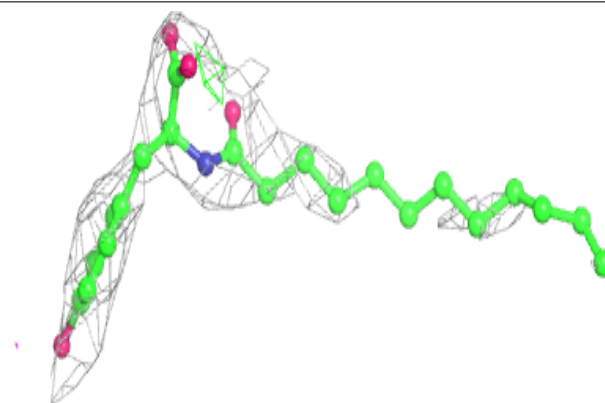


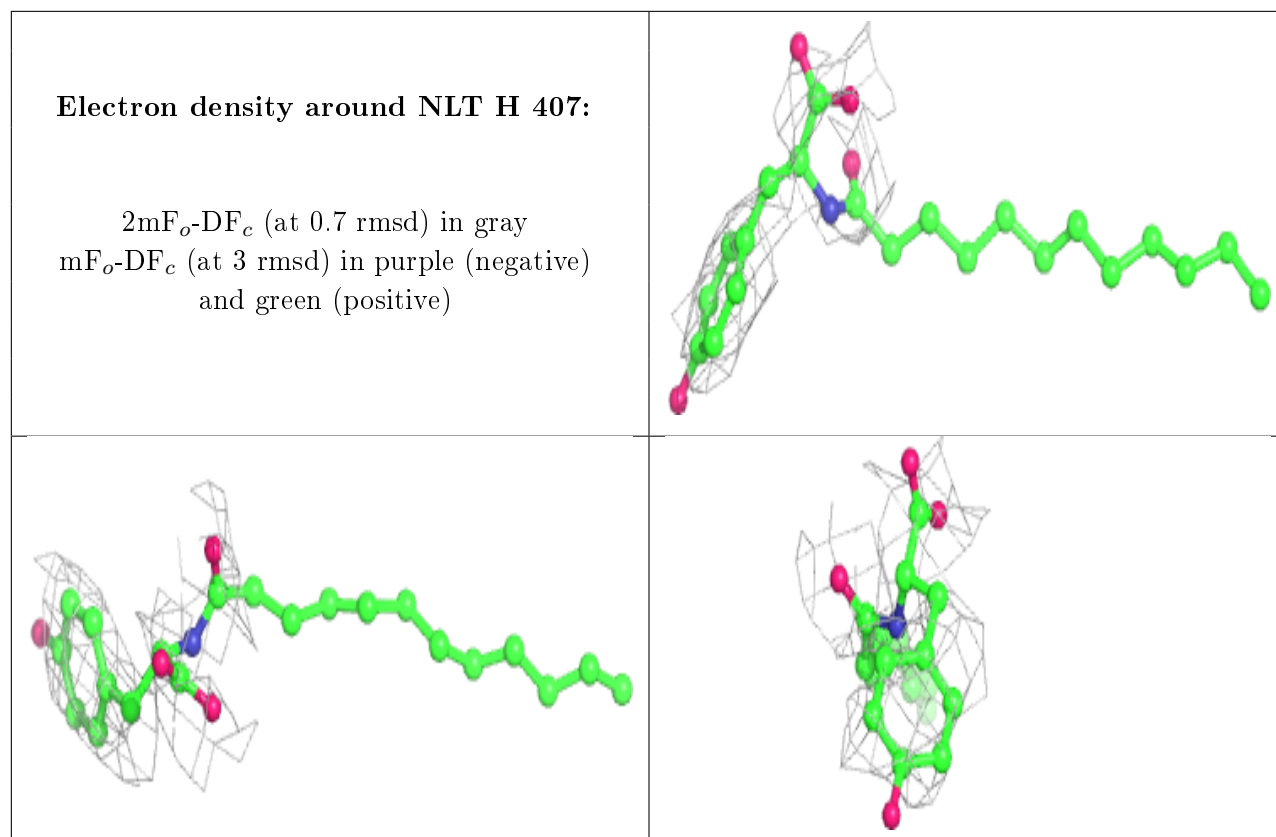
**Electron density around NLT F 405:**

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

**Electron density around NLT D 403:**

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





## 6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.