



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:28 AM UTC

PDB ID : 2G0B / pdb_00002g0b
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

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:

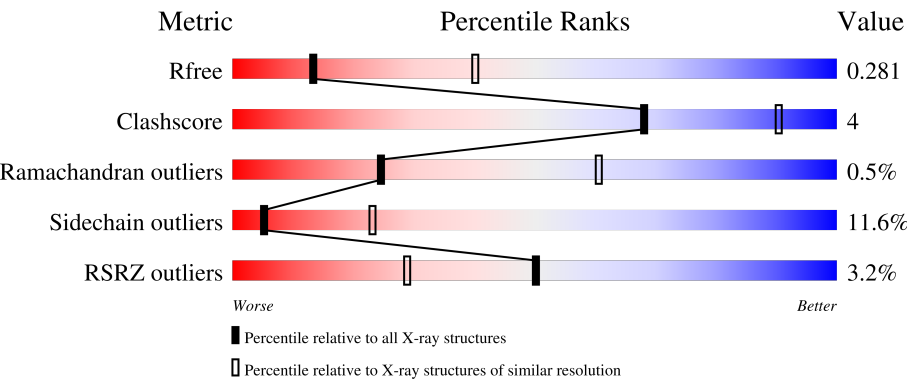
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 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}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (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 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	198	2% 76% 18% • 5%
1	B	198	2% 77% 16% • 5%
1	C	198	2% 77% 14% • 7%
1	D	198	2% 79% 10% • 9%
1	E	198	75% 16% • 9%

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Mol	Chain	Length	Quality of chain
1	F	198	77% 14% • 7%
1	G	198	5% 71% 14% • 12%
1	H	198	14% 70% 15% • 14%

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:

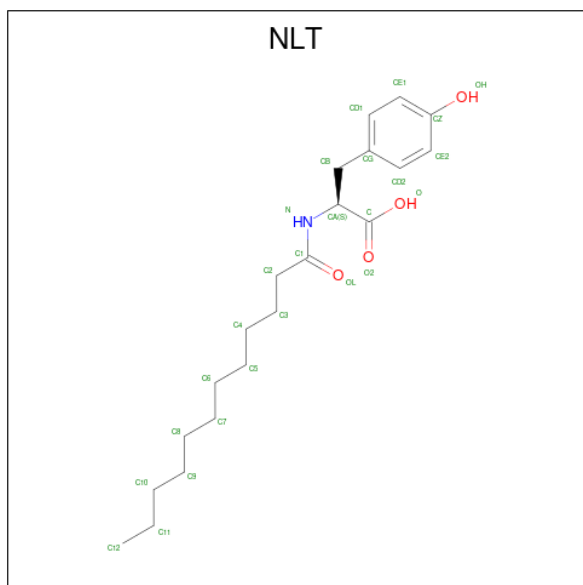
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	cloning artifact	UNP Q8KNZ7
A	0	SER	-	cloning artifact	UNP Q8KNZ7
B	-1	GLY	-	cloning artifact	UNP Q8KNZ7
B	0	SER	-	cloning artifact	UNP Q8KNZ7
C	-1	GLY	-	cloning artifact	UNP Q8KNZ7
C	0	SER	-	cloning artifact	UNP Q8KNZ7
D	-1	GLY	-	cloning artifact	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 (CCD ID: NLT) (formula: $C_{21}H_{33}NO_4$).



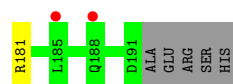
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			26	21	1	4		
2	B	1	Total	C	N	O	0	0
			26	21	1	4		
2	C	1	Total	C	N	O	0	0
			26	21	1	4		
2	D	1	Total	C	N	O	0	0
			26	21	1	4		
2	E	1	Total	C	N	O	0	0
			26	21	1	4		
2	F	1	Total	C	N	O	0	0
			26	21	1	4		
2	G	1	Total	C	N	O	0	0
			26	21	1	4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

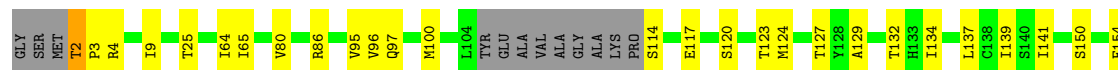
- Molecule 1: FeeM





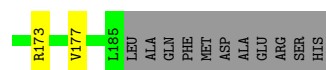
• Molecule 1: FeeM

Chain E: 75% 16% 9%



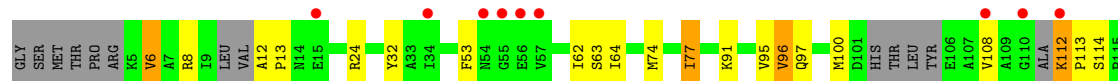
• Molecule 1: FeeM

Chain F: 77% 14% 7%



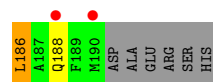
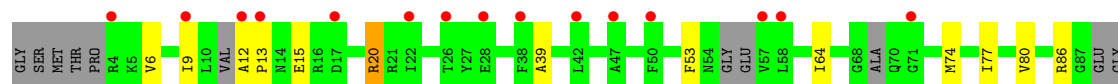
• Molecule 1: FeeM

Chain G: 5% 71% 14% 12%



• Molecule 1: FeeM

Chain H: 14% 70% 15% 14%



4 Data and refinement statistics

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	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) 99.9 (29.75-3.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.73 (at 3.00Å)	Xtriage
Refinement program	REFMAC refmac_5.1.24	Depositor
R, R_{free}	0.255 , 0.292 0.245 , 0.281	Depositor DCC
R_{free} test set	2458 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	82.3	Xtriage
Anisotropy	0.011	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 56.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	11507	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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: 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	0.73	1/1495 (0.1%)	0.86	0/2033
1	B	0.72	3/1504 (0.2%)	0.87	0/2048
1	C	0.61	1/1462 (0.1%)	0.85	0/1992
1	D	0.65	2/1446 (0.1%)	0.82	0/1967
1	E	0.67	2/1446 (0.1%)	0.83	0/1967
1	F	0.69	1/1462 (0.1%)	0.86	0/1992
1	G	0.58	1/1374 (0.1%)	0.82	0/1865
1	H	0.60	2/1364 (0.1%)	0.81	0/1849
All	All	0.66	13/11553 (0.1%)	0.84	0/15713

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	124	MET	SD-CE	-9.85	1.54	1.79
1	E	177	VAL	CA-CB	8.31	1.58	1.54
1	B	124	MET	SD-CE	-7.75	1.60	1.79
1	D	177	VAL	CA-CB	7.58	1.57	1.54
1	D	124	MET	SD-CE	-6.69	1.62	1.79
1	H	177	VAL	CA-C	6.40	1.58	1.52
1	B	190	MET	SD-CE	6.28	1.95	1.79
1	B	177	VAL	CA-CB	6.12	1.57	1.54
1	H	177	VAL	CA-CB	6.07	1.58	1.53
1	A	177	VAL	CA-CB	6.06	1.57	1.54
1	C	177	VAL	CA-CB	5.92	1.57	1.54
1	F	177	VAL	CA-CB	5.79	1.57	1.54
1	G	177	VAL	CA-CB	5.42	1.57	1.54

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	1461	0	1443	12	0
1	B	1468	0	1452	18	0
1	C	1427	0	1410	10	0
1	D	1413	0	1393	7	0
1	E	1413	0	1393	10	0
1	F	1427	0	1410	14	1
1	G	1345	0	1321	10	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	83	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 4.

All (83) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:100:MET:HE3	1:C:100:MET:HB3	1.67	0.47
1:F:50:PHE:CD2	1:F:124:MET:HG2	2.49	0.47
1:B:100:MET:HE3	1:B:100:MET:HB3	1.75	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
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:G:100:MET:HB3	1:G:100:MET:HE2	1.79	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:124:MET:HE2	1:D:124:MET:HB2	1.79	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:HD23	1:G:152:LEU:HA	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:E:100:MET:HE3	1:E:100:MET:HB3	1.95	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:54:ASN:HB2	1:A:59:TYR:CD2	2.55	0.41
1:A:154:PHE:HB3	1:A:173:ARG:HB3	2.02	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:B:2:THR:CB	1:B:3:PRO:CD	2.93	0.41
1:E:65:ILE:HD12	1:E:96:VAL:HG11	2.02	0.41
1:C:139:ILE:HA	1:C:139:ILE:HD13	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

5.3.1 Protein backbone

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%)	24	60
1	B	187/198 (94%)	182 (97%)	2 (1%)	3 (2%)	7	34
1	C	182/198 (92%)	177 (97%)	4 (2%)	1 (0%)	24	60
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%)	11	43
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%)	24	60

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

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%)	133 (89%)	17 (11%)	5	24
1	B	150/157 (96%)	138 (92%)	12 (8%)	11	38
1	C	146/157 (93%)	126 (86%)	20 (14%)	3	17
1	D	146/157 (93%)	128 (88%)	18 (12%)	4	21
1	E	146/157 (93%)	128 (88%)	18 (12%)	4	21
1	F	146/157 (93%)	133 (91%)	13 (9%)	9	34
1	G	137/157 (87%)	117 (85%)	20 (15%)	3	15
1	H	138/157 (88%)	121 (88%)	17 (12%)	4	21
All	All	1159/1256 (92%)	1024 (88%)	135 (12%)	5	23

All (135) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	21	ARG
1	A	26	THR
1	A	34	ILE
1	A	57	VAL
1	A	64	ILE
1	A	74	MET
1	A	96	VAL
1	A	108	VAL
1	A	141	ILE
1	A	150	SER
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	8	ARG
1	B	11	VAL
1	B	20	ARG
1	B	24	ARG
1	B	64	ILE
1	B	86	ARG
1	B	88	GLU
1	B	100	MET
1	B	103	THR
1	B	112	LYS

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Mol	Chain	Res	Type
1	B	139	ILE
1	B	141	ILE
1	C	4	ARG
1	C	9	ILE
1	C	14	ASN
1	C	21	ARG
1	C	24	ARG
1	C	26	THR
1	C	63	SER
1	C	64	ILE
1	C	77	ILE
1	C	86	ARG
1	C	100	MET
1	C	112	LYS
1	C	120	SER
1	C	124	MET
1	C	127	THR
1	C	139	ILE
1	C	140	SER
1	C	150	SER
1	C	166	VAL
1	C	181	ARG
1	D	4	ARG
1	D	9	ILE
1	D	77	ILE
1	D	80	VAL
1	D	94	GLU
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

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Mol	Chain	Res	Type
1	E	25	THR
1	E	64	ILE
1	E	80	VAL
1	E	86	ARG
1	E	95	VAL
1	E	114	SER
1	E	120	SER
1	E	127	THR
1	E	132	THR
1	E	137	LEU
1	E	139	ILE
1	E	141	ILE
1	E	150	SER
1	E	171	ILE
1	E	179	GLU
1	E	181	ARG
1	F	2	THR
1	F	5	LYS
1	F	11	VAL
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	G	6	VAL
1	G	8	ARG
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	95	VAL
1	G	96	VAL
1	G	108	VAL
1	G	112	LYS
1	G	114	SER

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Mol	Chain	Res	Type
1	G	127	THR
1	G	139	ILE
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
1	H	64	ILE
1	H	74	MET
1	H	80	VAL
1	H	86	ARG
1	H	95	VAL
1	H	100	MET
1	H	120	SER
1	H	127	THR
1	H	139	ILE
1	H	140	SER
1	H	141	ILE
1	H	179	GLU
1	H	181	ARG
1	H	186	LEU
1	H	188	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	97	GLN
1	B	66	ASN
1	B	97	GLN
1	C	54	ASN
1	C	66	ASN
1	D	66	ASN
1	D	97	GLN
1	D	162	HIS
1	E	162	HIS
1	F	70	GLN
1	F	133	HIS
1	F	145	HIS
1	G	30	GLN
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 oligosaccharides 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	C	402	-	26,26,26	0.67	0	31,31,31	0.71	0
2	NLT	G	406	-	26,26,26	0.72	1 (3%)	31,31,31	0.94	1 (3%)
2	NLT	H	407	-	26,26,26	0.65	0	31,31,31	0.69	0
2	NLT	F	405	-	26,26,26	0.72	0	31,31,31	0.76	0
2	NLT	A	400	-	26,26,26	0.65	0	31,31,31	0.71	0
2	NLT	E	404	-	26,26,26	0.72	0	31,31,31	0.70	0
2	NLT	B	401	-	26,26,26	0.68	0	31,31,31	0.88	0
2	NLT	D	403	-	26,26,26	0.70	0	31,31,31	0.81	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	C	402	-	-	11/23/23/23	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NLT	G	406	-	-	9/23/23/23	0/1/1/1
2	NLT	H	407	-	-	4/23/23/23	0/1/1/1
2	NLT	F	405	-	-	6/23/23/23	0/1/1/1
2	NLT	A	400	-	-	3/23/23/23	0/1/1/1
2	NLT	E	404	-	-	7/23/23/23	0/1/1/1
2	NLT	B	401	-	-	9/23/23/23	0/1/1/1
2	NLT	D	403	-	-	9/23/23/23	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	406	NLT	OH-CZ	-2.04	1.32	1.37

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	406	NLT	CB-CA-C	-2.30	104.97	110.45
2	D	403	NLT	CB-CA-C	-2.07	105.53	110.45

There are no chirality outliers.

All (58) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	401	NLT	C-CA-N-C1
2	G	406	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	D	403	NLT	C11-C10-C9-C8
2	G	406	NLT	C5-C6-C7-C8
2	D	403	NLT	C7-C8-C9-C10
2	D	403	NLT	C4-C5-C6-C7
2	F	405	NLT	C4-C5-C6-C7
2	B	401	NLT	C7-C8-C9-C10

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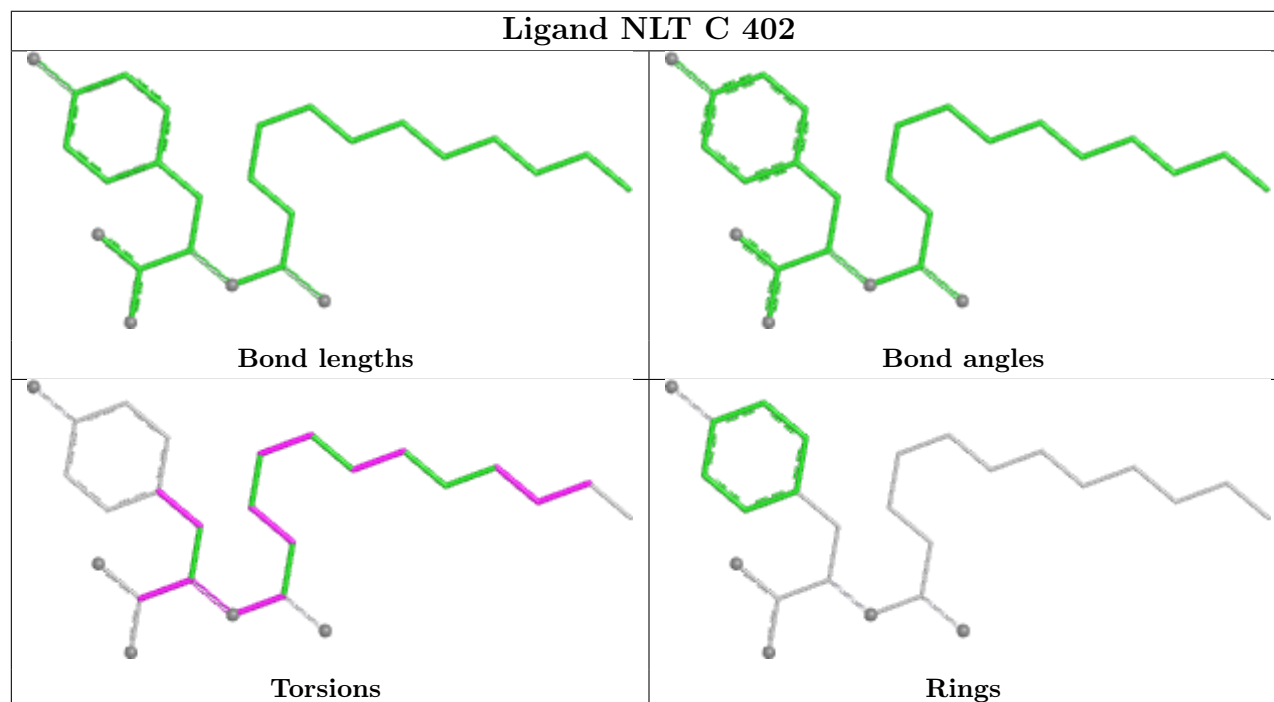
Mol	Chain	Res	Type	Atoms
2	D	403	NLT	CA-CB-CG-CD1
2	A	400	NLT	C7-C8-C9-C10
2	D	403	NLT	CA-CB-CG-CD2
2	F	405	NLT	C1-C2-C3-C4
2	G	406	NLT	C7-C8-C9-C10
2	E	404	NLT	C6-C7-C8-C9
2	C	402	NLT	C11-C10-C9-C8
2	H	407	NLT	C4-C5-C6-C7
2	E	404	NLT	CA-CB-CG-CD2
2	H	407	NLT	CA-CB-CG-CD2
2	E	404	NLT	CA-CB-CG-CD1
2	H	407	NLT	CA-CB-CG-CD1
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	D	403	NLT	O-C-CA-N
2	A	400	NLT	N-CA-CB-CG
2	G	406	NLT	C4-C5-C6-C7
2	D	403	NLT	C6-C7-C8-C9
2	C	402	NLT	C3-C4-C5-C6
2	C	402	NLT	C-CA-N-C1
2	D	403	NLT	O2-C-CA-N
2	E	404	NLT	C9-C10-C11-C12
2	C	402	NLT	CA-CB-CG-CD1
2	C	402	NLT	C5-C6-C7-C8
2	B	401	NLT	CA-CB-CG-CD1
2	C	402	NLT	CA-CB-CG-CD2
2	G	406	NLT	C6-C7-C8-C9
2	B	401	NLT	O2-C-CA-N
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	B	401	NLT	O-C-CA-N
2	C	402	NLT	C9-C10-C11-C12
2	A	400	NLT	C-CA-CB-CG
2	C	402	NLT	O2-C-CA-N
2	D	403	NLT	C9-C10-C11-C12
2	G	406	NLT	O2-C-CA-N
2	F	405	NLT	CA-CB-CG-CD1
2	E	404	NLT	C4-C5-C6-C7

There are no ring outliers.

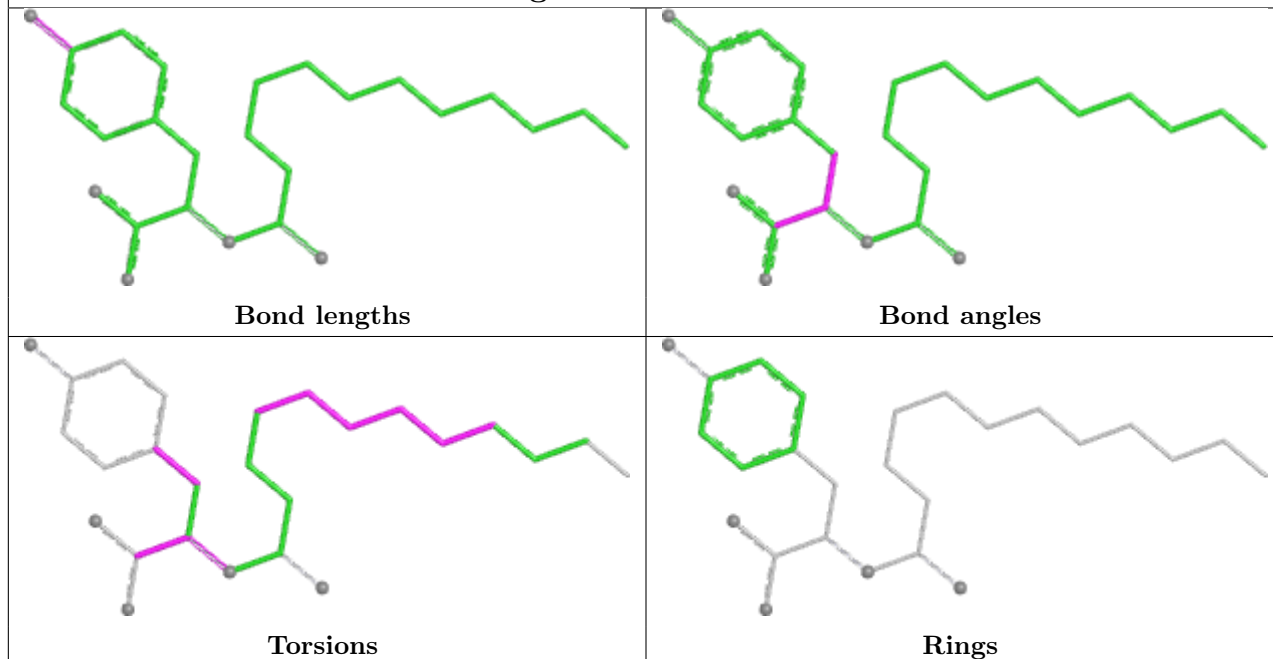
5 monomers are involved in 5 short contacts:

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

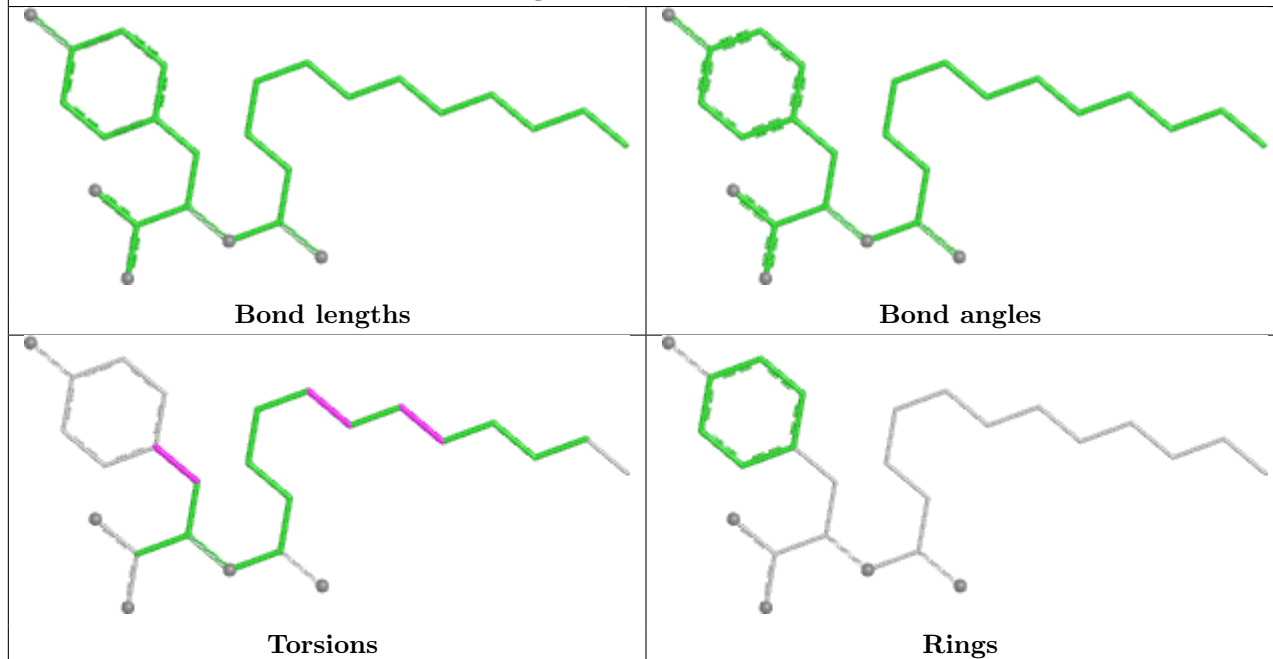
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



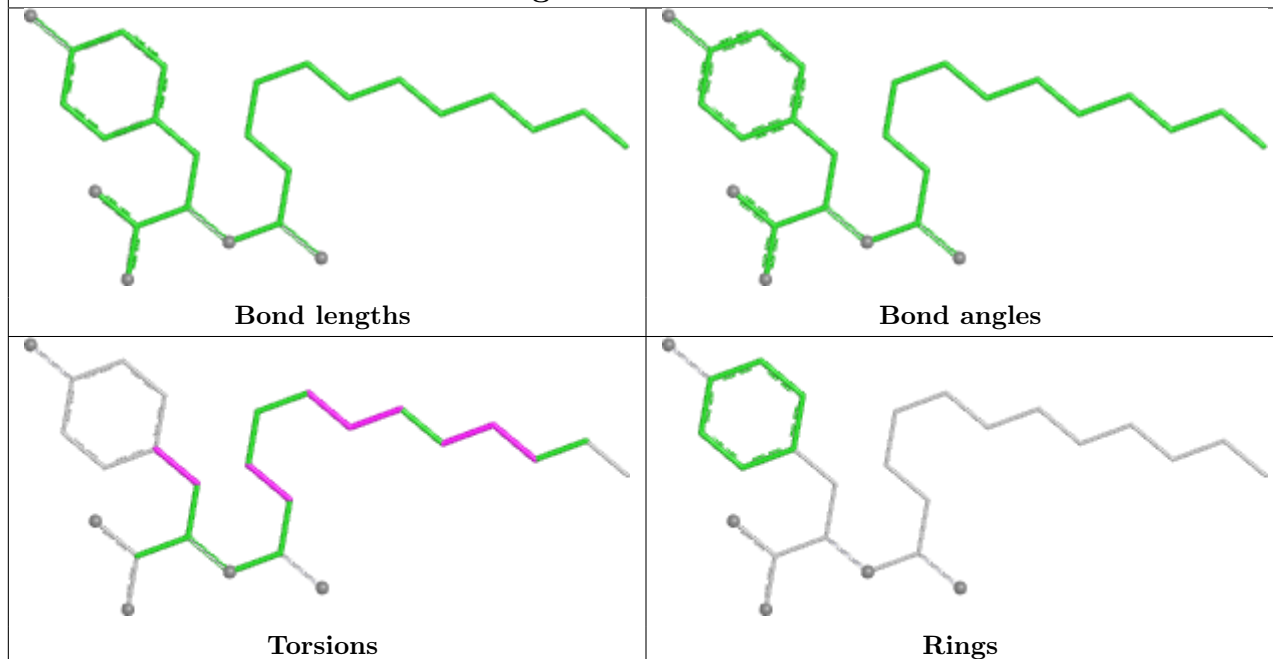
Ligand NLT G 406



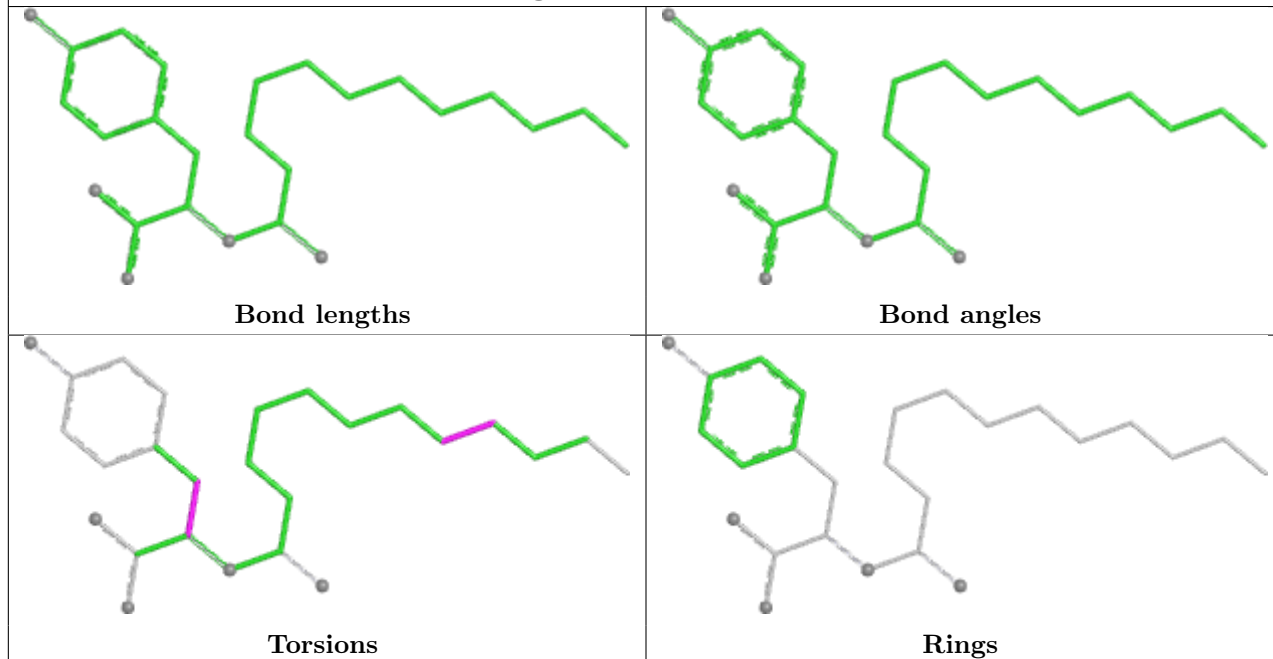
Ligand NLT H 407



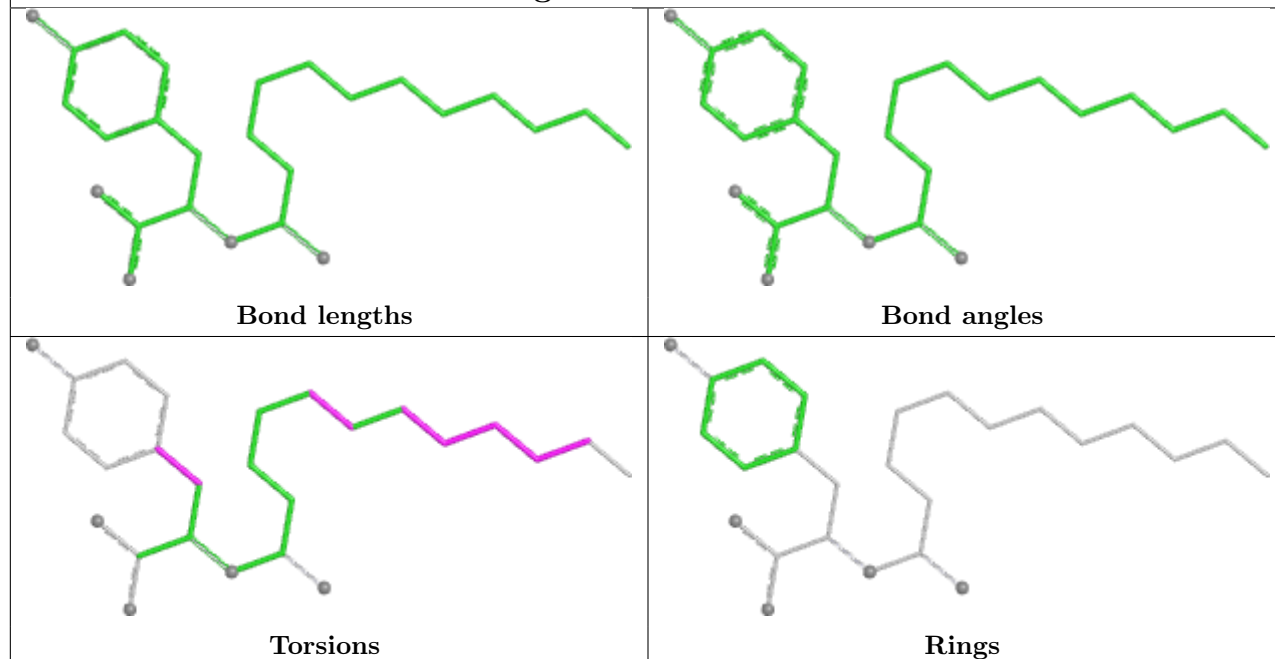
Ligand NLT F 405



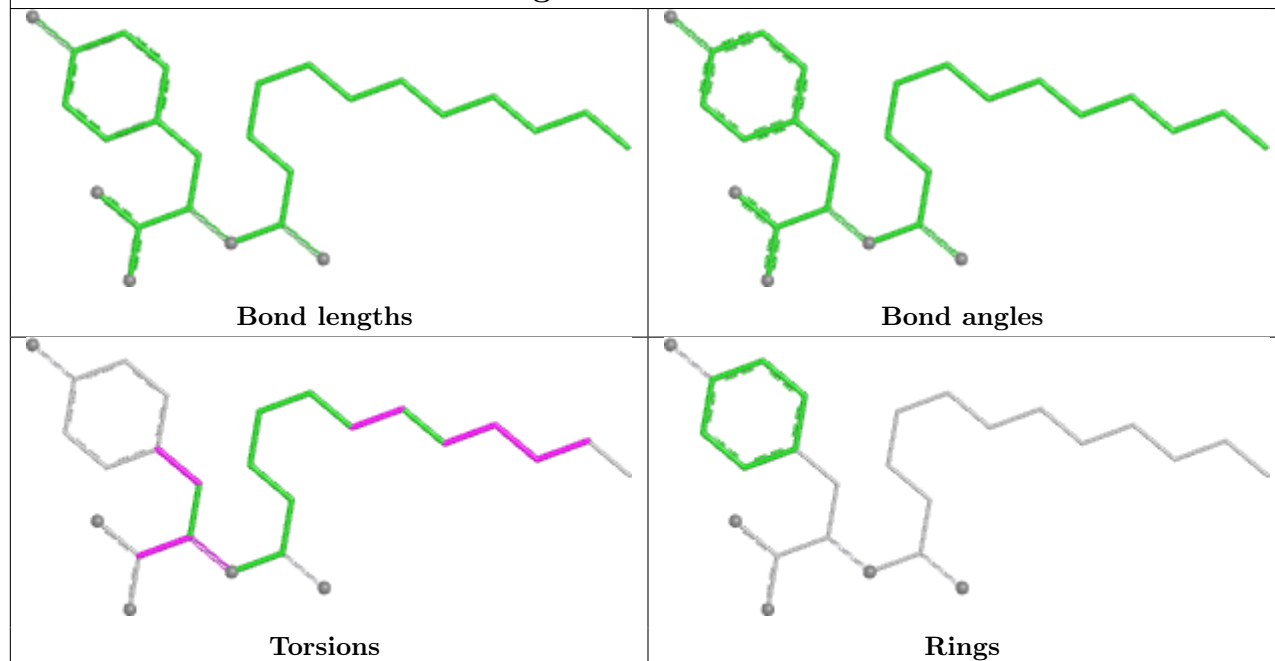
Ligand NLT A 400

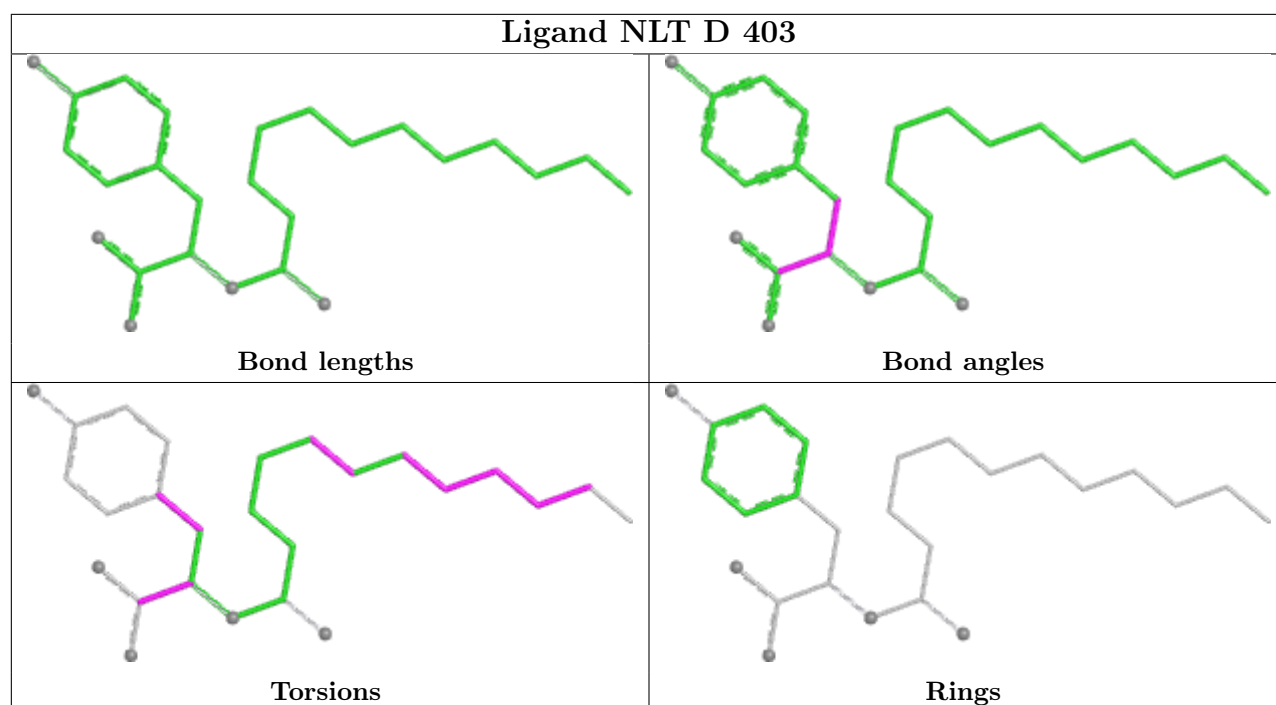


Ligand NLT E 404



Ligand NLT B 401





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 ⓘ

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	188/198 (94%)	-0.19	1 (0%) 87 72	40, 40, 42, 43	0
1	B	189/198 (95%)	-0.15	1 (0%) 87 72	40, 40, 41, 44	0
1	C	184/198 (92%)	0.06	2 (1%) 78 57	40, 40, 41, 41	0
1	D	181/198 (91%)	0.31	4 (2%) 62 39	40, 40, 41, 41	0
1	E	181/198 (91%)	-0.14	0 100 100	40, 40, 41, 42	0
1	F	184/198 (92%)	0.08	0 100 100	40, 40, 41, 42	0
1	G	174/198 (87%)	0.51	10 (5%) 29 15	40, 40, 41, 41	0
1	H	170/198 (85%)	1.14	28 (16%) 4 3	40, 40, 41, 41	0
All	All	1451/1584 (91%)	0.19	46 (3%) 50 29	40, 40, 41, 44	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	102	HIS	3.6
1	H	4	ARG	3.4
1	H	47	ALA	3.3
1	H	38	PHE	3.2
1	H	22	ILE	3.1
1	H	17	ASP	3.1
1	G	15	GLU	3.0
1	H	176	TYR	2.9
1	G	57	VAL	2.9
1	A	106	GLU	2.8
1	H	122	PHE	2.8
1	H	50	PHE	2.8
1	G	54	ASN	2.8
1	B	2	THR	2.7
1	H	130	LEU	2.7
1	H	127	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	H	190	MET	2.6
1	H	57	VAL	2.5
1	H	12	ALA	2.5
1	H	71	GLY	2.4
1	G	108	VAL	2.4
1	G	116	PHE	2.3
1	H	42	LEU	2.3
1	H	9	ILE	2.3
1	H	174	ALA	2.3
1	C	56	GLU	2.3
1	D	185	LEU	2.2
1	H	102	HIS	2.2
1	G	110	GLY	2.2
1	H	13	PRO	2.2
1	G	56	GLU	2.2
1	H	188	GLN	2.2
1	D	104	LEU	2.2
1	C	24	ARG	2.2
1	H	138	CYS	2.2
1	H	28	GLU	2.1
1	H	58	LEU	2.1
1	D	188	GLN	2.1
1	G	55	GLY	2.1
1	G	112	LYS	2.1
1	H	116	PHE	2.1
1	H	95	VAL	2.1
1	H	98	PHE	2.1
1	H	26	THR	2.0
1	H	123	THR	2.0
1	G	34	ILE	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](#)

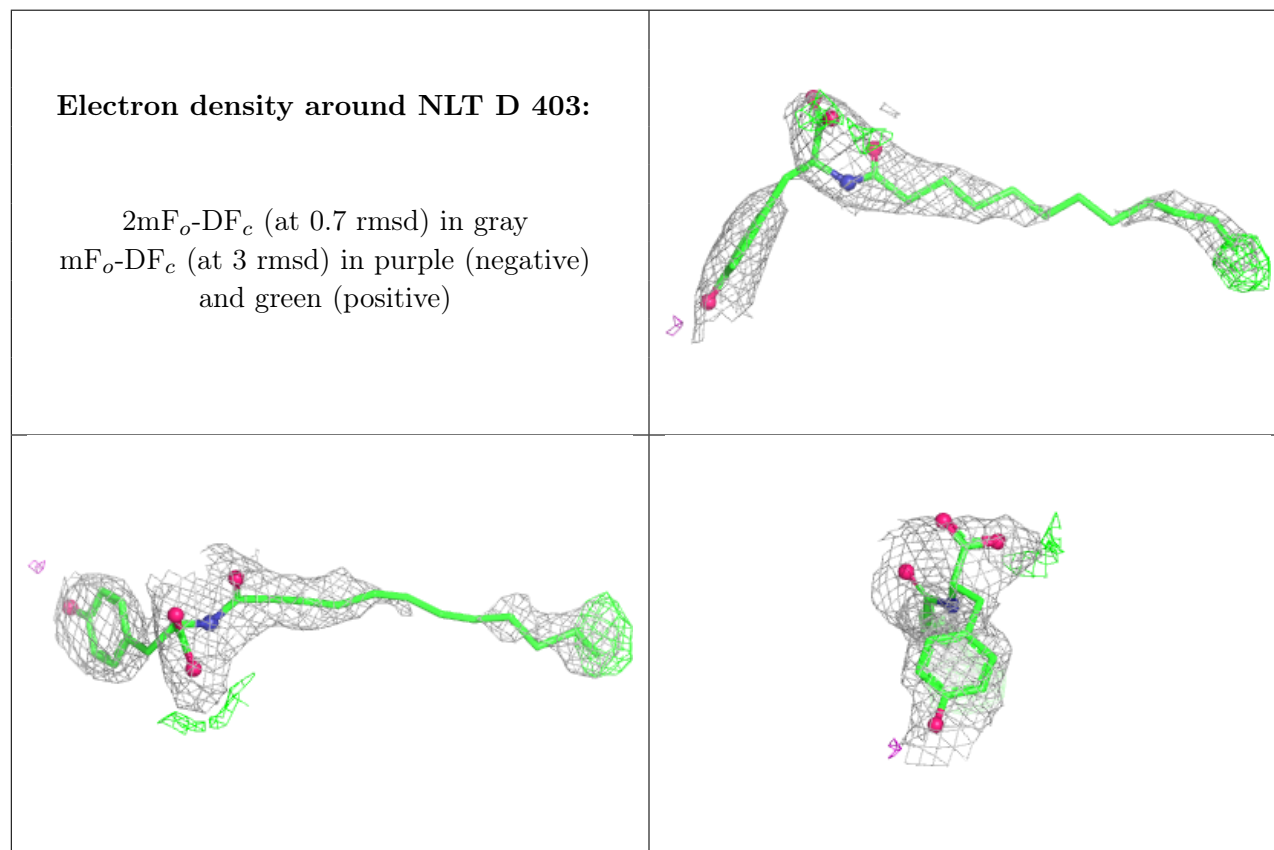
There are no oligosaccharides in this entry.

6.4 Ligands

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.

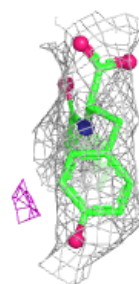
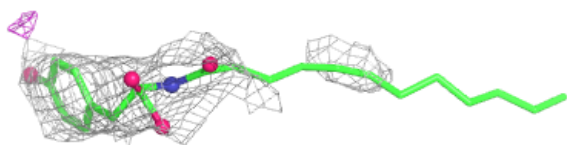
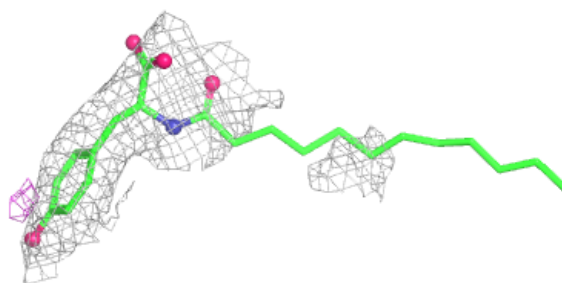
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NLT	D	403	26/26	0.81	0.16	39,41,41,41	0
2	NLT	G	406	26/26	0.83	0.15	39,40,40,40	0
2	NLT	C	402	26/26	0.84	0.15	38,40,41,41	0
2	NLT	H	407	26/26	0.84	0.18	39,40,40,40	0
2	NLT	F	405	26/26	0.86	0.17	39,40,42,42	0
2	NLT	B	401	26/26	0.86	0.13	37,40,41,42	0
2	NLT	E	404	26/26	0.86	0.13	38,40,41,41	0
2	NLT	A	400	26/26	0.88	0.14	39,40,41,42	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.

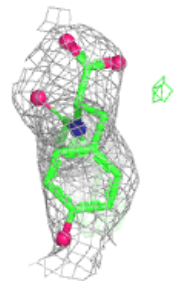
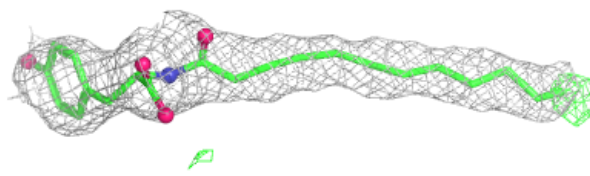
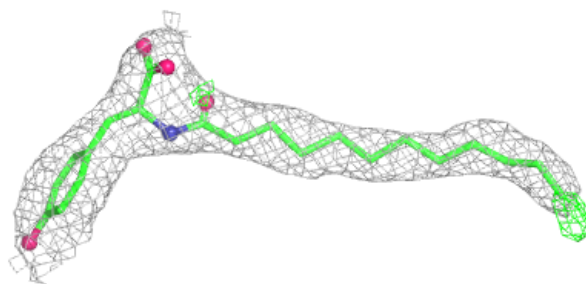


Electron density around NLT G 406:

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

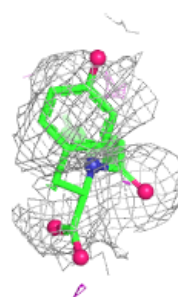
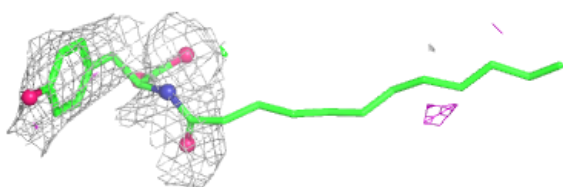
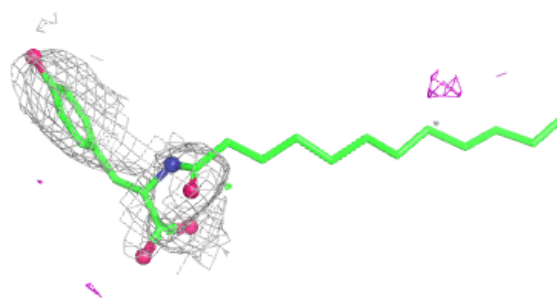
**Electron density around NLT C 402:**

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

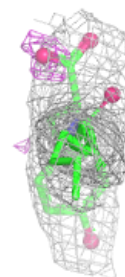
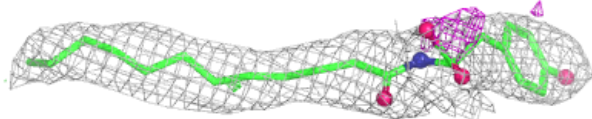
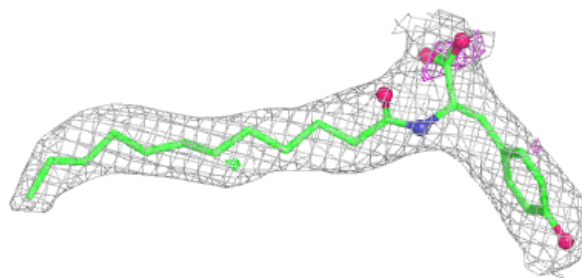


Electron density around NLT H 407:

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

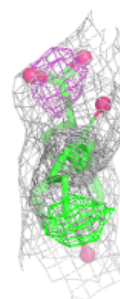
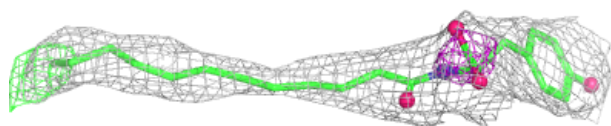
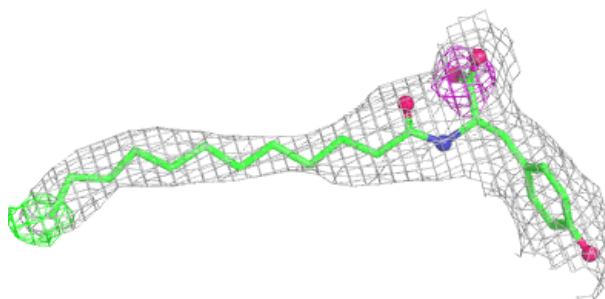
**Electron density around NLT F 405:**

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

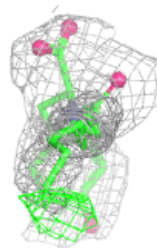
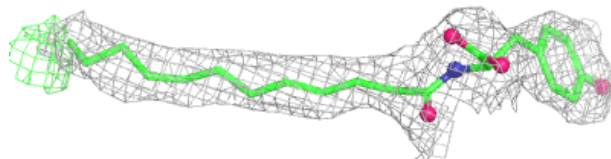
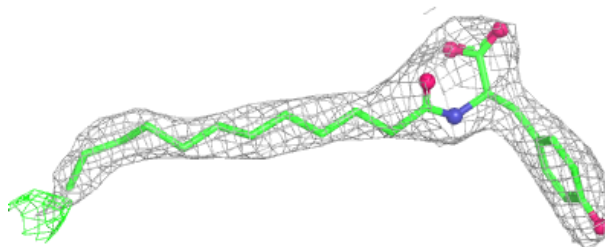


Electron density around NLT B 401:

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

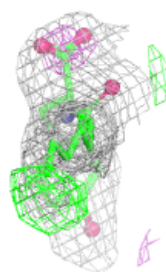
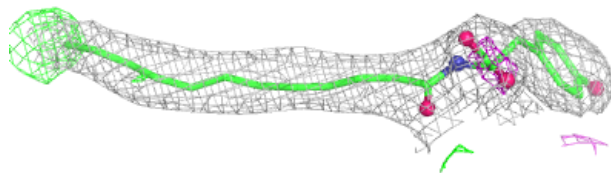
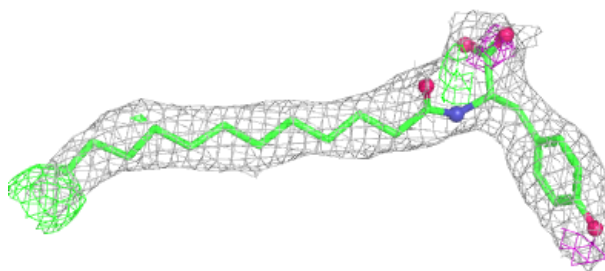
**Electron density around NLT E 404:**

$2mF_o-DF_c$ (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)



6.5 Other polymers [i](#)

There are no such residues in this entry.