



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:28 PM UTC

PDB ID : 5NUP / pdb_00005nup
Title : Structural basis for maintenance of bacterial outer membrane lipid asymmetry
Authors : Abellon-Ruiz, J.; Kaptan, S.S.; Basle, A.; Claudi, B.; Bumann, D.;
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Deposited on : 2017-05-01
Resolution : 2.90 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

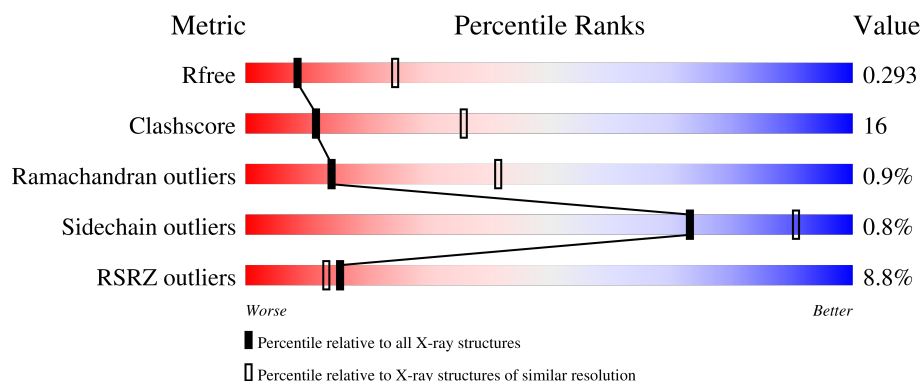
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	344	5% 73% 27%
1	B	344	8% 71% 29%
1	C	344	9% 73% 26%
2	D	236	6% 53% 29% 16%
2	E	236	11% 57% 26% 16%

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Mol	Chain	Length	Quality of chain
2	F	236	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	C8E	E	301	-	-	-	X
3	C8E	F	301	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13238 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 OmpK36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	344	Total	C	N	O	S	0	0	0
			2693	1687	453	551	2			
1	B	344	Total	C	N	O	S	0	0	0
			2693	1687	453	551	2			
1	C	344	Total	C	N	O	S	0	0	0
			2693	1687	453	551	2			

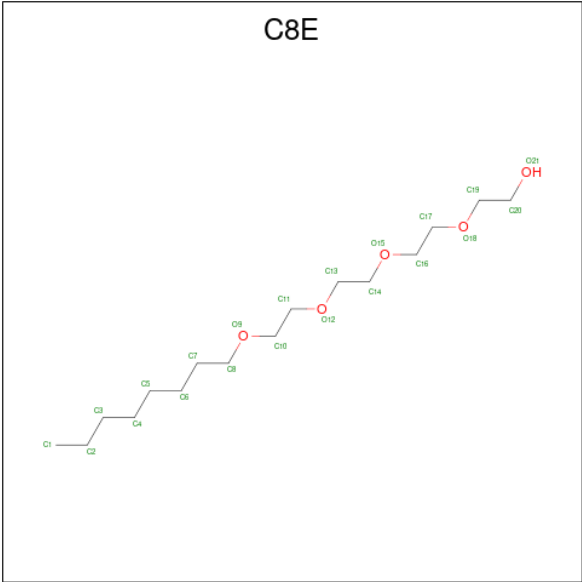
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	231	ARG	GLN	conflict	UNP D6QLY0
B	231	ARG	GLN	conflict	UNP D6QLY0
C	231	ARG	GLN	conflict	UNP D6QLY0

- Molecule 2 is a protein called ABC transporter permease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	199	Total	C	N	O	S	0	0	0
			1597	1031	271	287	8			
2	E	199	Total	C	N	O	S	0	0	0
			1597	1031	271	287	8			
2	F	204	Total	C	N	O	S	0	0	0
			1620	1044	276	292	8			

- Molecule 3 is (HYDROXYETHYLOXY)TRI(ETHYLOXY)OCTANE (CCD ID: C8E) (formula: C₁₆H₃₄O₅).



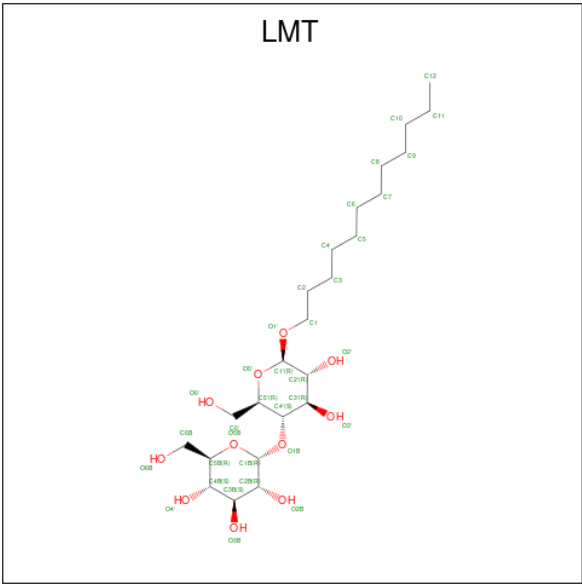
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			16	13	3		
3	A	1	Total	C	O	0	0
			10	9	1		
3	A	1	Total	C	O	0	0
			13	11	2		
3	A	1	Total	C	O	0	0
			9	6	3		
3	A	1	Total	C	O	0	0
			16	13	3		
3	A	1	Total	C	O	0	0
			11	10	1		
3	B	1	Total	C	O	0	0
			11	10	1		
3	B	1	Total	C	O	0	0
			18	14	4		
3	B	1	Total	C	O	0	0
			16	13	3		
3	B	1	Total	C	O	0	0
			15	12	3		
3	C	1	Total	C	O	0	0
			16	13	3		
3	C	1	Total	C	O	0	0
			21	16	5		
3	C	1	Total	C	O	0	0
			13	11	2		
3	C	1	Total	C	O	0	0
			16	13	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	C	O	0	0
			13	11	2		
3	D	1	Total	C	O	0	0
			12	10	2		
3	E	1	Total	C		0	0
			8	8			
3	E	1	Total	C	O	0	0
			20	16	4		
3	F	1	Total	C	O	0	0
			7	6	1		

- Molecule 4 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).

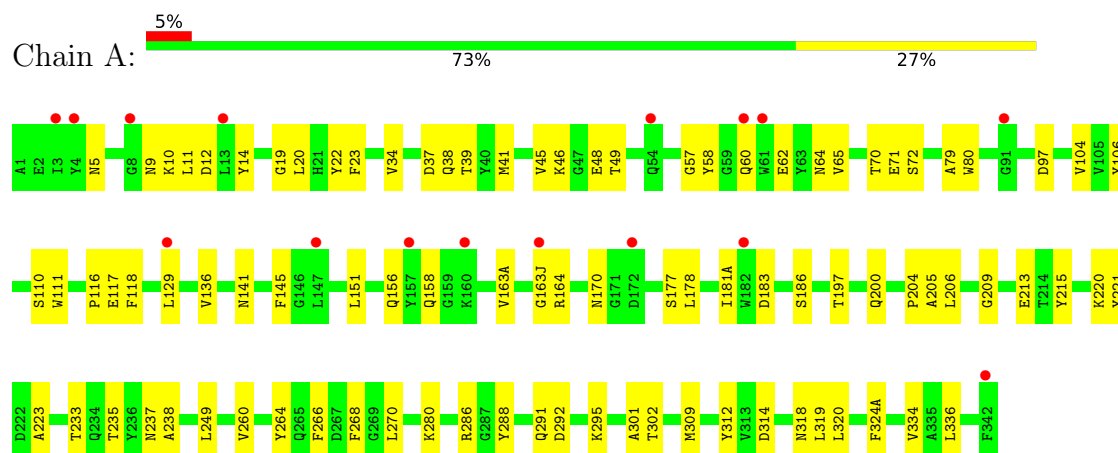


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			35	24	11		
4	B	1	Total	C	O	0	0
			25	14	11		
4	F	1	Total	C	O	0	0
			24	13	11		

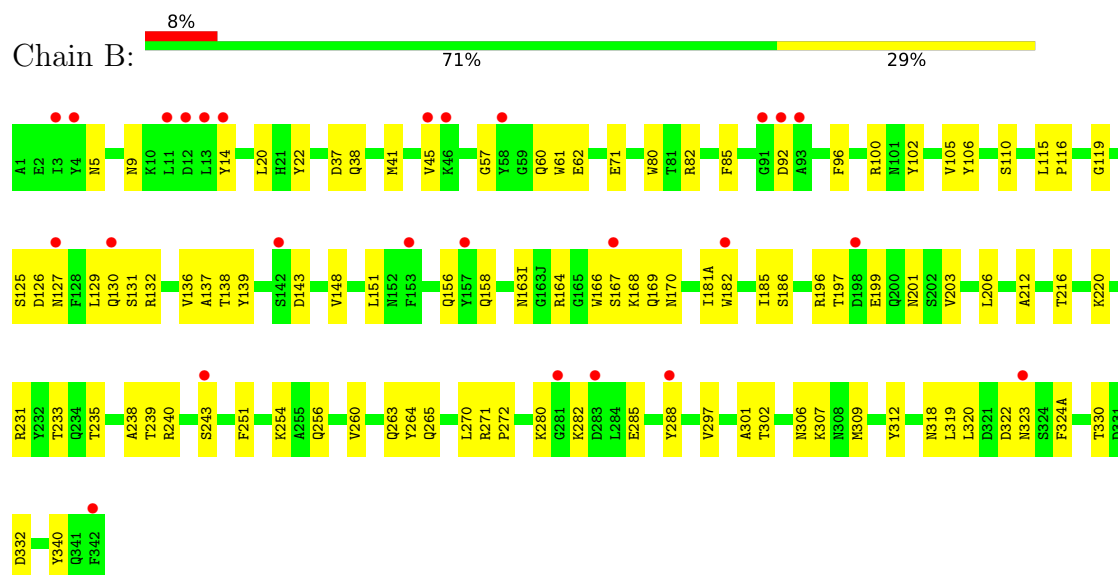
3 Residue-property plots

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: OmpK36

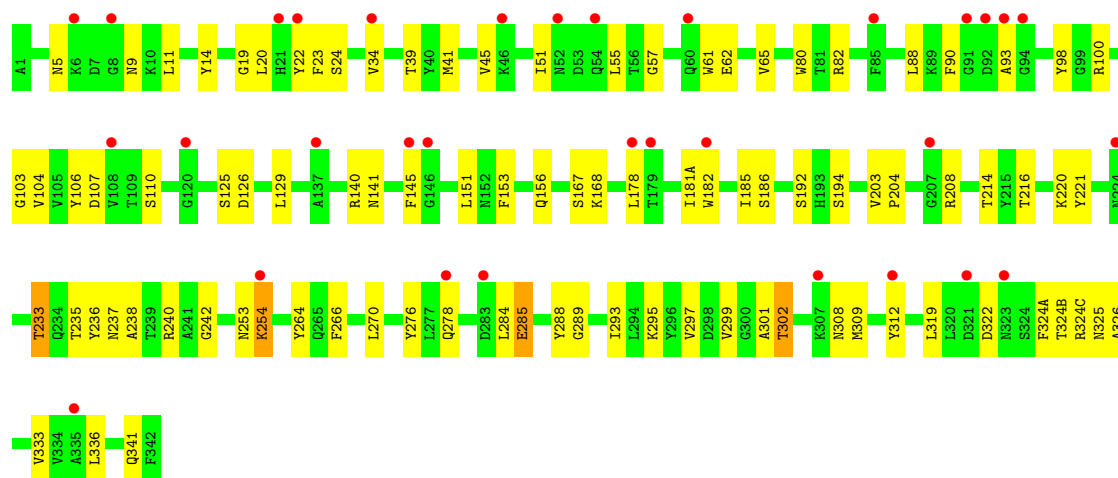


• Molecule 1: OmpK36

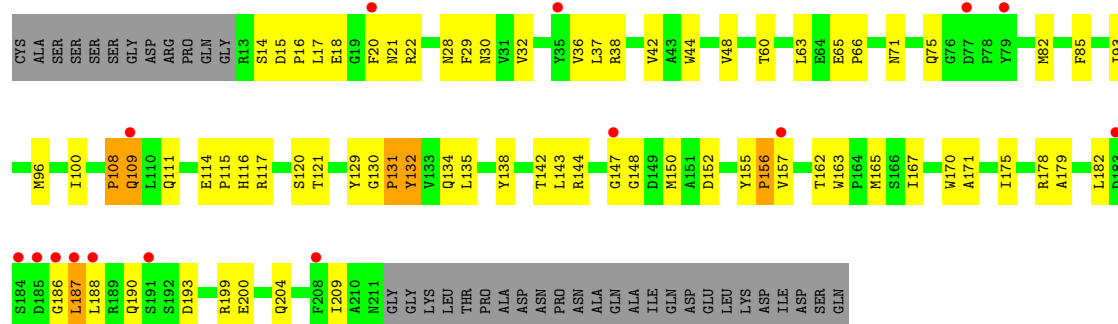


• Molecule 1: OmpK36

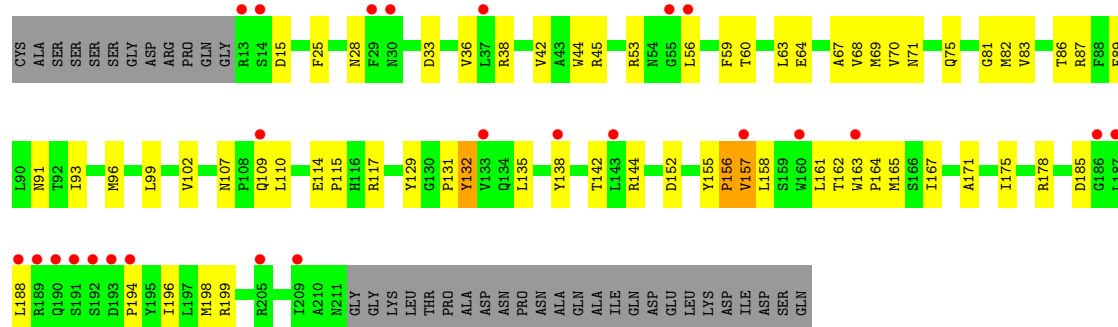




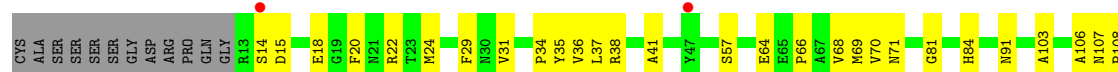
• Molecule 2: ABC transporter permease

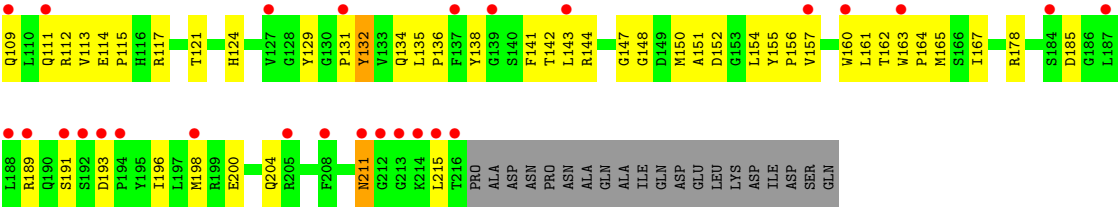


• Molecule 2: ABC transporter permease



• Molecule 2: ABC transporter permease





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	92.38Å 145.24Å 232.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	68.38 – 2.90 68.38 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (68.38-2.90) 100.0 (68.38-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.09 (at 2.91Å)	Xtriage
Refinement program	PHENIX (1.11.1 _2575: ???)	Depositor
R, R_{free}	0.241 , 0.290 0.244 , 0.293	Depositor DCC
R_{free} test set	3409 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	60.2	Xtriage
Anisotropy	0.931	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 43.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	13238	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: LMT, C8E

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	0.46	0/2753	0.79	0/3727
1	B	0.45	0/2753	0.76	0/3727
1	C	0.44	1/2753 (0.0%)	0.74	0/3727
2	D	0.43	0/1647	0.85	5/2241 (0.2%)
2	E	0.41	0/1647	0.79	3/2241 (0.1%)
2	F	0.40	0/1670	0.75	0/2272
All	All	0.44	1/13223 (0.0%)	0.78	8/17935 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	254	LYS	CE-NZ	5.03	1.64	1.49

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	156	PRO	CA-C-N	8.35	137.00	121.97
2	D	156	PRO	C-N-CA	8.35	137.00	121.97
2	E	109	GLN	CA-CB-CG	-7.68	98.74	114.10
2	D	108	PRO	CA-C-N	-6.75	108.84	122.55
2	D	108	PRO	C-N-CA	-6.75	108.84	122.55
2	D	109	GLN	CA-CB-CG	6.64	127.38	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	156	PRO	CA-C-N	6.40	133.50	121.97
2	E	156	PRO	C-N-CA	6.40	133.50	121.97

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	92	ASP	Peptide

5.2 Too-close contacts [i](#)

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	2693	0	2479	75	0
1	B	2693	0	2479	94	0
1	C	2693	0	2479	73	0
2	D	1597	0	1525	66	0
2	E	1597	0	1525	57	0
2	F	1620	0	1537	63	0
3	A	75	0	114	5	0
3	B	60	0	98	2	0
3	C	66	0	105	5	0
3	D	25	0	37	0	0
3	E	28	0	46	3	0
3	F	7	0	10	0	0
4	B	60	0	64	5	0
4	F	24	0	20	0	0
All	All	13238	0	12518	411	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 16.

All (411) 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:216:THR:HB	1:B:233:THR:HG22	1.26	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:256:GLN:HE21	1:B:282:LYS:HE3	0.95	1.09
1:A:22:TYR:OH	1:A:117:GLU:OE1	1.76	1.02
1:B:256:GLN:NE2	1:B:282:LYS:HE3	1.78	0.97
2:F:29:PHE:O	2:F:189:ARG:NH1	2.02	0.92
1:B:256:GLN:HE21	1:B:282:LYS:CE	1.83	0.88
1:B:216:THR:CB	1:B:233:THR:HG22	2.06	0.84
2:F:114:GLU:HG3	2:F:115:PRO:HD2	1.59	0.84
1:A:41:MET:CE	1:A:65:VAL:HG22	2.08	0.84
2:E:178:ARG:NH2	2:E:185:ASP:OD1	2.13	0.82
1:A:20:LEU:HD23	1:A:38:GLN:HB2	1.62	0.81
1:C:103:GLY:HA2	1:C:156:GLN:HE22	1.47	0.80
1:B:105:VAL:HG11	1:B:130:GLN:OE1	1.81	0.80
1:C:270:LEU:HD11	1:C:301:ALA:HB1	1.65	0.79
1:C:55:LEU:HD12	2:F:106:ALA:HA	1.65	0.79
2:D:117:ARG:HH11	2:D:152:ASP:HB2	1.47	0.78
1:B:263:GLN:NE2	1:B:271:ARG:HE	1.81	0.78
1:C:299:VAL:HG12	3:C:401:C8E:H22	1.66	0.76
1:A:268:PHE:HB3	2:D:109:GLN:HG2	1.67	0.75
2:D:75:GLN:HE21	2:D:121:THR:HG22	1.50	0.75
2:E:33:ASP:OD1	2:E:178:ARG:NH1	2.19	0.75
1:C:302:THR:HB	1:C:312:TYR:HB3	1.68	0.75
1:B:235:THR:HG23	1:B:238:ALA:HB3	1.67	0.74
1:A:197:THR:H	1:A:200:GLN:HG3	1.52	0.73
2:D:15:ASP:HB3	2:D:18:GLU:HB2	1.70	0.72
1:A:129:LEU:O	1:A:129:LEU:HD23	1.90	0.72
2:E:188:LEU:O	2:E:188:LEU:HD23	1.90	0.72
1:B:216:THR:HG22	1:B:233:THR:HB	1.73	0.71
2:F:91:ASN:HD21	2:F:103:ALA:H	1.37	0.71
1:C:276:TYR:OH	1:C:278:GLN:NE2	2.23	0.71
2:E:42:VAL:HG13	2:E:45:ARG:HH12	1.55	0.70
1:B:309:MET:HE3	1:C:57:GLY:HA3	1.72	0.70
1:B:136:VAL:HG12	1:B:158:GLN:HB2	1.74	0.70
1:C:216:THR:HG23	1:C:233:THR:HG22	1.73	0.69
1:C:236:TYR:HE2	1:C:254:LYS:HE3	1.57	0.69
1:B:20:LEU:HD23	1:B:38:GLN:HB2	1.73	0.69
1:A:41:MET:HE3	1:A:65:VAL:HG22	1.75	0.69
1:C:23:PHE:HE1	1:C:336:LEU:HD12	1.58	0.68
2:D:179:ALA:HA	2:D:182:LEU:HD13	1.76	0.68
1:C:19:GLY:HA2	1:C:39:THR:HG23	1.76	0.68
2:F:178:ARG:HH12	2:F:185:ASP:HB3	1.59	0.68
1:A:19:GLY:HA2	1:A:39:THR:HG23	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:91:ASN:ND2	2:F:103:ALA:H	1.93	0.67
1:B:168:LYS:HG2	1:B:240:ARG:HH12	1.60	0.67
2:D:156:PRO:O	2:D:157:VAL:HG22	1.94	0.67
1:A:70:THR:HG22	1:A:72:SER:N	2.10	0.67
2:D:28:ASN:HA	2:D:32:VAL:HG22	1.77	0.67
2:E:129:TYR:HD1	2:E:142:THR:HG21	1.58	0.66
1:B:265:GLN:NE2	1:B:271:ARG:HB2	2.10	0.66
2:E:15:ASP:OD2	2:E:199:ARG:NH1	2.29	0.66
2:D:66:PRO:HG2	2:D:157:VAL:HG11	1.79	0.66
2:D:129:TYR:HB3	2:D:142:THR:HG21	1.78	0.66
1:A:70:THR:HG22	1:A:72:SER:H	1.62	0.65
2:D:167:ILE:HA	2:D:170:TRP:HB3	1.77	0.65
1:C:168:LYS:HG2	1:C:240:ARG:HH12	1.61	0.65
1:C:182:TRP:HB2	1:C:185:ILE:HD13	1.79	0.64
1:C:295:LYS:HG2	1:C:319:LEU:HB2	1.79	0.64
2:D:130:GLY:H	2:D:142:THR:HG22	1.62	0.64
2:E:188:LEU:HD21	2:E:194:PRO:HB3	1.80	0.64
1:B:167:SER:O	1:B:240:ARG:NH1	2.29	0.64
1:C:242:GLY:HA3	1:C:326:ALA:HB1	1.80	0.64
2:E:82:MET:O	2:E:86:THR:HG23	1.98	0.64
1:A:57:GLY:HA3	1:C:309:MET:SD	2.37	0.64
2:E:114:GLU:HG3	2:E:115:PRO:CD	2.28	0.64
2:E:142:THR:HG22	2:E:144:ARG:H	1.62	0.63
1:A:49:THR:CG2	1:C:309:MET:HG3	2.29	0.63
1:A:23:PHE:HE1	1:A:336:LEU:HD12	1.63	0.63
1:C:270:LEU:HD22	2:E:86:THR:HG22	1.80	0.63
1:A:280:LYS:HE3	1:A:292:ASP:OD2	1.98	0.62
1:A:49:THR:HG21	1:C:309:MET:HG3	1.80	0.62
1:C:336:LEU:HD22	2:E:93:ILE:HG21	1.79	0.62
2:E:157:VAL:HG13	2:E:158:LEU:HG	1.81	0.62
1:B:309:MET:HE1	1:B:340:TYR:HD1	1.64	0.62
2:E:83:VAL:HG13	2:E:110:LEU:HD23	1.81	0.61
1:C:23:PHE:HB3	3:E:302:C8E:H131	1.82	0.61
2:E:114:GLU:HG3	2:E:115:PRO:HD2	1.82	0.61
2:F:36:VAL:HG22	2:F:37:LEU:H	1.65	0.61
2:E:38:ARG:O	2:E:42:VAL:HG23	2.00	0.61
1:C:55:LEU:HD22	1:C:88:LEU:HD23	1.82	0.61
2:E:117:ARG:HB3	2:E:152:ASP:OD2	2.01	0.61
2:D:178:ARG:O	2:D:182:LEU:HD13	2.01	0.61
1:B:280:LYS:NZ	4:B:406:LMT:H4B	2.14	0.60
2:F:34:PRO:HG3	2:F:189:ARG:HH11	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:167:SER:HB2	1:B:240:ARG:HD3	1.82	0.60
2:E:25:PHE:CD1	2:E:198:MET:HE2	2.36	0.60
2:D:147:GLY:HA2	2:D:150:MET:SD	2.42	0.60
2:D:187:LEU:HD22	2:D:190:GLN:HB2	1.84	0.60
2:F:117:ARG:HB3	2:F:152:ASP:OD1	2.00	0.60
2:E:129:TYR:CD1	2:E:142:THR:HG21	2.37	0.60
1:B:169:GLN:NE2	1:B:197:THR:OG1	2.34	0.60
2:F:24:MET:HE2	2:F:136:PRO:HB3	1.84	0.59
1:B:127:ASN:HB2	1:B:240:ARG:NH2	2.16	0.59
2:E:69:MET:HG3	2:E:81:GLY:O	2.03	0.59
2:E:188:LEU:CD2	2:E:194:PRO:HB3	2.34	0.58
2:F:24:MET:HG3	2:F:136:PRO:HD3	1.86	0.58
2:F:200:GLU:O	2:F:204:GLN:HG3	2.03	0.58
1:B:41:MET:HE3	1:C:61:TRP:CG	2.39	0.57
1:B:306:ASN:HB2	1:B:307:LYS:NZ	2.18	0.57
2:D:129:TYR:HB3	2:D:142:THR:CG2	2.34	0.57
2:E:71:ASN:O	2:E:75:GLN:HG3	2.05	0.57
2:F:71:ASN:HB3	2:F:121:THR:HG21	1.85	0.57
1:C:125:SER:O	1:C:240:ARG:NH2	2.38	0.57
2:F:142:THR:HG22	2:F:144:ARG:H	1.69	0.57
1:B:158:GLN:NE2	1:B:170:ASN:OD1	2.38	0.56
2:E:87:ARG:HD2	2:E:110:LEU:O	2.05	0.56
1:A:20:LEU:HD21	1:A:22:TYR:CE1	2.40	0.56
2:F:129:TYR:HB3	2:F:142:THR:HG21	1.87	0.56
2:F:163:TRP:O	2:F:167:ILE:HG12	2.05	0.56
2:D:22:ARG:NH1	2:D:193:ASP:OD2	2.38	0.56
2:F:124:HIS:ND1	2:F:211:ASN:OD1	2.39	0.56
2:F:135:LEU:HB2	2:F:138:TYR:HB3	1.87	0.56
1:A:334:VAL:HG21	3:A:406:C8E:H102	1.88	0.56
1:B:129:LEU:HD22	1:B:156:GLN:OE1	2.06	0.56
2:E:64:GLU:O	2:E:68:VAL:HG23	2.06	0.56
1:A:309:MET:SD	1:B:57:GLY:HA3	2.46	0.56
1:A:336:LEU:HD22	2:D:93:ILE:HG21	1.88	0.56
1:C:141:ASN:OD1	1:C:145:PHE:N	2.24	0.56
1:B:280:LYS:HZ1	4:B:406:LMT:C3B	2.19	0.55
2:D:14:SER:OG	2:D:15:ASP:N	2.40	0.55
1:C:264:TYR:HB2	3:C:403:C8E:H31	1.88	0.55
1:A:41:MET:HE2	1:A:65:VAL:HG22	1.86	0.55
2:E:135:LEU:HB2	2:E:138:TYR:HB3	1.89	0.55
1:A:58:TYR:OH	1:A:97:ASP:HB3	2.07	0.55
1:A:266:PHE:HZ	3:A:401:C8E:H102	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:71:ASN:ND2	2:E:117:ARG:HA	2.22	0.54
2:D:163:TRP:NE1	2:D:167:ILE:HD11	2.22	0.54
2:F:69:MET:HB2	2:F:81:GLY:O	2.08	0.54
1:B:270:LEU:HD11	1:B:301:ALA:HB1	1.89	0.54
2:E:196:ILE:HD12	2:E:199:ARG:NH2	2.22	0.54
1:C:107:ASP:OD2	1:C:140:ARG:NH2	2.41	0.54
1:C:236:TYR:CE2	1:C:254:LYS:HE3	2.42	0.54
2:F:134:GLN:OE1	2:F:198:MET:HE1	2.08	0.54
2:F:151:ALA:HA	2:F:154:LEU:HD13	1.89	0.54
2:F:66:PRO:HG2	2:F:157:VAL:HG22	1.88	0.54
2:D:29:PHE:HB3	2:D:30:ASN:OD1	2.07	0.54
2:D:38:ARG:O	2:D:42:VAL:HG23	2.07	0.54
2:F:36:VAL:O	2:F:38:ARG:N	2.41	0.54
1:C:5:ASN:HA	1:C:9:ASN:O	2.06	0.53
2:D:36:VAL:O	2:D:38:ARG:N	2.40	0.53
2:F:112:ARG:HG2	2:F:113:VAL:N	2.22	0.53
2:F:29:PHE:CE2	2:F:189:ARG:NH2	2.76	0.53
1:B:82:ARG:O	1:B:100:ARG:HD3	2.08	0.53
2:D:117:ARG:HB3	2:D:152:ASP:OD1	2.08	0.53
1:A:5:ASN:HA	1:A:9:ASN:O	2.08	0.53
1:B:280:LYS:HZ1	4:B:406:LMT:H4B	1.72	0.53
1:C:129:LEU:HD22	1:C:156:GLN:NE2	2.23	0.53
1:A:104:VAL:HG22	1:A:156:GLN:HE21	1.74	0.53
2:D:60:THR:HA	2:D:63:LEU:HD12	1.91	0.53
2:E:156:PRO:O	2:E:157:VAL:HG12	2.09	0.53
1:A:46:LYS:HG2	1:A:60:GLN:HG3	1.91	0.53
1:B:260:VAL:HG13	4:B:405:LMT:H122	1.91	0.53
2:E:60:THR:HA	2:E:63:LEU:CD1	2.39	0.53
2:F:162:THR:HB	2:F:164:PRO:HD2	1.90	0.52
2:E:45:ARG:HH11	2:E:45:ARG:HB3	1.75	0.52
2:E:67:ALA:HA	2:E:70:VAL:HG12	1.89	0.52
1:C:297:VAL:HG23	1:C:319:LEU:HD11	1.90	0.52
1:A:136:VAL:HG12	1:A:158:GLN:HB2	1.91	0.52
1:A:264:TYR:HB2	3:A:404:C8E:H191	1.92	0.52
1:B:288:TYR:CD1	1:B:324(A):PHE:HB2	2.44	0.52
2:D:71:ASN:O	2:D:75:GLN:HG3	2.09	0.52
1:C:24:SER:HB2	1:C:333:VAL:HG22	1.92	0.52
1:C:167:SER:O	1:C:240:ARG:NH1	2.42	0.52
1:B:307:LYS:HE2	1:B:307:LYS:H	1.75	0.52
1:A:104:VAL:HG22	1:A:129:LEU:HD21	1.91	0.52
3:A:406:C8E:H22	2:D:85:PHE:CZ	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:196:ARG:NH1	1:B:201:ASN:OD1	2.36	0.51
2:D:171:ALA:O	2:D:175:ILE:HG13	2.09	0.51
2:D:44:TRP:O	2:D:48:VAL:HG22	2.10	0.51
1:B:96:PHE:CE1	1:B:137:ALA:HB1	2.46	0.51
1:C:14:TYR:OH	1:C:62:GLU:HB2	2.10	0.51
1:B:265:GLN:HE22	1:B:271:ARG:HB2	1.74	0.51
1:A:318:ASN:ND2	1:A:320:LEU:H	2.09	0.51
1:C:324(C):ARG:HG3	1:C:325:ASN:N	2.26	0.51
1:A:163(A):VAL:HA	1:A:163(J):GLY:HA3	1.93	0.50
2:F:71:ASN:HB3	2:F:121:THR:CG2	2.41	0.50
2:F:129:TYR:HB3	2:F:142:THR:CG2	2.42	0.50
1:A:270:LEU:HD11	1:A:301:ALA:HB1	1.92	0.50
1:C:90:PHE:HB2	1:C:93:ALA:HB3	1.92	0.50
2:D:186:GLY:C	2:D:188:LEU:H	2.18	0.50
2:F:29:PHE:CD2	2:F:189:ARG:NH2	2.79	0.50
1:C:266:PHE:HZ	3:C:402:C8E:H51	1.77	0.50
1:C:141:ASN:HB3	1:C:153:PHE:CE1	2.47	0.50
2:F:161:LEU:HD12	2:F:165:MET:HB3	1.92	0.50
2:E:45:ARG:HB3	2:E:45:ARG:NH1	2.26	0.50
1:B:116:PRO:HB3	1:B:302:THR:HG22	1.93	0.50
1:A:37:ASP:HB3	1:B:163(I):ASN:ND2	2.27	0.50
1:A:104:VAL:H	1:A:156:GLN:NE2	2.10	0.50
1:A:14:TYR:OH	1:A:62:GLU:HB2	2.12	0.50
1:A:71:GLU:HB3	1:B:80:TRP:CD1	2.47	0.50
1:B:216:THR:HB	1:B:233:THR:CG2	2.18	0.50
2:F:135:LEU:HD23	2:F:141:PHE:HB3	1.93	0.50
1:A:295:LYS:HG2	1:A:319:LEU:HB2	1.94	0.49
1:B:127:ASN:HB2	1:B:240:ARG:HH21	1.75	0.49
2:E:107:ASN:HB3	2:E:110:LEU:HD12	1.94	0.49
2:D:132:TYR:CE2	2:D:199:ARG:HG3	2.47	0.49
2:D:167:ILE:HG23	2:D:170:TRP:HD1	1.77	0.49
2:E:178:ARG:HH22	2:E:185:ASP:CG	2.20	0.49
1:A:104:VAL:N	1:A:156:GLN:HE22	2.10	0.49
1:A:205:ALA:HB1	1:A:286:ARG:NH1	2.27	0.49
1:B:167:SER:HA	1:B:251:PHE:CZ	2.48	0.49
1:C:192:SER:HB3	1:C:214:THR:OG1	2.12	0.49
2:F:114:GLU:HG3	2:F:115:PRO:CD	2.38	0.49
1:A:235:THR:HB	1:A:238:ALA:HB3	1.94	0.49
1:C:288:TYR:CD1	1:C:324(A):PHE:HB2	2.46	0.49
2:E:132:TYR:CE1	2:E:199:ARG:HG3	2.48	0.49
1:B:100:ARG:NH2	1:B:126:ASP:OD1	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:SER:HA	1:B:131:SER:HB3	1.94	0.49
2:F:152:ASP:HA	2:F:155:TYR:CE1	2.48	0.49
1:A:23:PHE:CE1	1:A:336:LEU:HD12	2.46	0.49
1:B:20:LEU:CD1	1:B:312:TYR:OH	2.61	0.49
1:C:23:PHE:CE1	1:C:336:LEU:HD12	2.44	0.49
1:A:65:VAL:HG12	1:A:79:ALA:CB	2.43	0.49
2:D:144:ARG:O	2:D:148:GLY:HA3	2.13	0.49
2:F:18:GLU:OE1	2:F:22:ARG:NH2	2.45	0.49
1:C:308:ASN:ND2	1:C:341:GLN:O	2.37	0.49
2:D:96:MET:HB2	2:D:100:ILE:HD12	1.94	0.49
1:A:116:PRO:HB3	1:A:302:THR:HG22	1.95	0.48
1:B:158:GLN:HE21	1:B:170:ASN:CG	2.21	0.48
2:D:28:ASN:HA	2:D:32:VAL:CG2	2.42	0.48
1:A:104:VAL:HG13	1:A:156:GLN:NE2	2.28	0.48
1:B:307:LYS:H	1:B:307:LYS:CE	2.26	0.48
1:C:22:TYR:HD2	1:C:34:VAL:HG12	1.77	0.48
2:D:108:PRO:O	2:D:111:GLN:HG3	2.14	0.48
1:A:209:GLY:HA3	1:A:237:ASN:ND2	2.28	0.48
1:C:41:MET:HG3	1:C:65:VAL:HB	1.95	0.48
2:D:18:GLU:OE1	2:D:22:ARG:NH2	2.47	0.48
3:E:302:C8E:H41	3:E:302:C8E:H13	1.61	0.48
1:B:169:GLN:HB3	1:B:197:THR:HG21	1.95	0.48
2:E:91:ASN:OD1	2:E:102:VAL:N	2.47	0.48
1:A:10:LYS:NZ	1:A:48:GLU:OE1	2.25	0.47
1:B:323:ASN:HB2	1:B:324(A):PHE:H	1.78	0.47
1:C:100:ARG:HH12	1:C:126:ASP:CG	2.22	0.47
1:C:151:LEU:HD11	1:C:178:LEU:HD11	1.96	0.47
1:C:106:TYR:O	1:C:110:SER:HB3	2.14	0.47
1:C:126:ASP:HB3	1:C:168:LYS:HB3	1.96	0.47
2:D:200:GLU:O	2:D:204:GLN:HG3	2.13	0.47
2:E:44:TRP:CD1	2:E:53:ARG:HD3	2.48	0.47
1:B:306:ASN:HB2	1:B:307:LYS:HZ1	1.78	0.47
1:C:203:VAL:HG12	1:C:204:PRO:HD3	1.97	0.47
1:A:206:LEU:HD22	1:A:249:LEU:HB3	1.97	0.47
1:A:11:LEU:HD11	1:A:45:VAL:CG2	2.44	0.47
1:A:186:SER:HB2	1:A:220:LYS:HG2	1.96	0.47
1:C:100:ARG:NH1	1:C:126:ASP:OD2	2.47	0.47
1:A:22:TYR:OH	1:A:117:GLU:CD	2.56	0.47
1:A:41:MET:HE2	1:A:65:VAL:CG2	2.45	0.47
1:A:197:THR:N	1:A:200:GLN:HG3	2.23	0.47
1:C:186:SER:HB2	1:C:220:LYS:HG2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:TYR:O	1:A:110:SER:HB3	2.13	0.47
2:E:171:ALA:O	2:E:175:ILE:HG13	2.15	0.47
2:F:64:GLU:O	2:F:68:VAL:HG23	2.14	0.47
1:A:116:PRO:HB2	1:A:314:ASP:HB2	1.97	0.47
1:A:141:ASN:OD1	1:A:145:PHE:N	2.45	0.46
1:B:143:ASP:N	1:B:143:ASP:OD1	2.48	0.46
2:D:147:GLY:HA2	2:D:150:MET:HG3	1.97	0.46
2:E:70:VAL:HG11	2:E:155:TYR:CE2	2.50	0.46
2:E:28:ASN:ND2	2:E:135:LEU:O	2.46	0.46
1:B:235:THR:HG21	1:B:239:THR:H	1.80	0.46
1:B:264:TYR:O	1:B:272:PRO:HD2	2.16	0.46
1:C:270:LEU:HD22	2:E:86:THR:CG2	2.45	0.46
2:F:147:GLY:HA2	2:F:150:MET:HG3	1.96	0.46
1:A:270:LEU:HD21	2:D:82:MET:HE3	1.97	0.46
1:C:284:LEU:HB2	1:C:288:TYR:O	2.15	0.46
2:F:144:ARG:O	2:F:148:GLY:HA3	2.16	0.46
1:C:293:ILE:HD13	1:C:324(A):PHE:CZ	2.51	0.46
2:D:152:ASP:HA	2:D:155:TYR:CE1	2.50	0.46
1:B:20:LEU:HD21	1:B:22:TYR:CE1	2.49	0.46
1:B:280:LYS:HZ1	4:B:406:LMT:C4B	2.29	0.46
2:F:24:MET:HE3	2:F:24:MET:HA	1.97	0.46
1:A:318:ASN:HD21	1:A:320:LEU:HD13	1.81	0.46
1:B:186:SER:HB2	1:B:220:LYS:HG2	1.98	0.46
2:D:162:THR:OG1	2:D:165:MET:HE3	2.15	0.46
1:B:318:ASN:OD1	1:B:320:LEU:CD2	2.64	0.46
2:D:116:HIS:CE1	2:D:209:ILE:HG23	2.51	0.46
1:A:104:VAL:HB	1:A:177:SER:HB3	1.98	0.45
2:E:96:MET:O	2:E:99:LEU:HD23	2.16	0.45
2:E:163:TRP:O	2:E:167:ILE:HG13	2.15	0.45
2:F:84:HIS:HE1	2:F:113:VAL:HG12	1.81	0.45
2:D:30:ASN:OD1	2:D:30:ASN:N	2.50	0.45
2:F:114:GLU:H	2:F:215:LEU:CB	2.29	0.45
2:D:188:LEU:HD12	2:D:188:LEU:HA	1.80	0.45
2:F:193:ASP:OD2	2:F:196:ILE:HG12	2.17	0.45
1:A:158:GLN:HE21	1:A:170:ASN:CG	2.23	0.45
1:B:148:VAL:HG13	1:B:151:LEU:HB3	1.98	0.45
1:C:299:VAL:CG1	3:C:401:C8E:H22	2.42	0.45
2:F:141:PHE:CZ	2:F:143:LEU:HD12	2.51	0.45
2:D:28:ASN:HD22	2:D:134:GLN:HE21	1.65	0.45
1:B:14:TYR:OH	1:B:62:GLU:HB3	2.17	0.45
1:B:196:ARG:HD2	1:B:212:ALA:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:231:ARG:HE	1:B:233:THR:CG2	2.30	0.45
2:F:14:SER:HB2	2:F:15:ASP:H	1.58	0.45
2:F:38:ARG:HH11	2:F:185:ASP:CG	2.24	0.45
1:A:288:TYR:CD1	1:A:324(A):PHE:HB2	2.51	0.45
2:E:161:LEU:HD23	2:E:165:MET:HB3	1.98	0.45
1:B:100:ARG:HH22	1:B:126:ASP:CG	2.25	0.45
1:B:309:MET:CE	1:B:340:TYR:HD1	2.29	0.45
1:C:322:ASP:HA	1:C:324(B):THR:HG21	1.99	0.45
2:F:64:GLU:OE1	2:F:115:PRO:HG3	2.17	0.45
2:F:134:GLN:HE22	2:F:198:MET:CE	2.30	0.45
1:B:235:THR:HG21	1:B:239:THR:OG1	2.17	0.45
2:D:36:VAL:HG22	2:D:37:LEU:H	1.82	0.45
2:F:132:TYR:OH	2:F:198:MET:SD	2.74	0.45
2:D:15:ASP:OD1	2:D:199:ARG:NH1	2.46	0.44
2:E:158:LEU:HA	2:E:161:LEU:CD1	2.47	0.44
1:A:266:PHE:CZ	3:A:401:C8E:H102	2.52	0.44
2:D:114:GLU:HG3	2:D:115:PRO:HD2	1.99	0.44
1:A:151:LEU:HD11	1:A:178:LEU:HD11	1.98	0.44
1:B:199:GLU:O	1:B:203:VAL:HG12	2.17	0.44
2:D:179:ALA:CA	2:D:182:LEU:HD13	2.46	0.44
1:A:12:ASP:HB3	1:A:46:LYS:HB2	1.98	0.44
1:A:111:TRP:CD2	1:A:220:LYS:HD3	2.53	0.44
2:F:57:SER:C	2:F:112:ARG:HH22	2.26	0.44
2:F:156:PRO:HB3	2:F:160:TRP:NE1	2.33	0.44
1:A:64:ASN:ND2	1:A:80:TRP:CZ2	2.86	0.44
1:B:254:LYS:HD3	1:B:282:LYS:HD2	1.99	0.44
2:F:31:VAL:O	2:F:35:TYR:HB2	2.18	0.44
2:F:57:SER:O	2:F:112:ARG:NH2	2.51	0.44
1:C:185:ILE:HG13	1:C:221:TYR:HD2	1.82	0.44
1:B:139:TYR:HB2	2:D:96:MET:HE3	1.99	0.44
1:B:264:TYR:HE2	3:B:404:C8E:H51	1.83	0.44
1:A:22:TYR:HD2	1:A:34:VAL:HG12	1.82	0.43
1:A:221:TYR:CZ	1:A:223:ALA:HB3	2.53	0.43
1:B:102:TYR:CE1	1:B:132:ARG:HG3	2.53	0.43
1:B:182:TRP:HB2	1:B:185:ILE:HD13	2.00	0.43
2:D:187:LEU:HD13	2:D:187:LEU:HA	1.61	0.43
1:B:41:MET:HE3	1:C:61:TRP:CD2	2.54	0.43
1:B:185:ILE:HA	1:B:220:LYS:O	2.18	0.43
1:C:266:PHE:CZ	3:C:402:C8E:H51	2.53	0.43
2:F:108:PRO:HA	2:F:111:GLN:HE21	1.83	0.43
1:B:166:TRP:CD1	1:B:166:TRP:H	2.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:167:SER:HA	1:B:251:PHE:HZ	1.82	0.43
2:F:22:ARG:NH1	2:F:193:ASP:OD2	2.51	0.43
1:A:11:LEU:HA	1:A:11:LEU:HD12	1.73	0.43
1:C:285:GLU:H	1:C:285:GLU:HG2	1.58	0.43
2:D:16:PRO:C	2:D:17:LEU:HD23	2.43	0.43
2:D:20:PHE:C	2:D:20:PHE:CD2	2.97	0.43
2:D:186:GLY:C	2:D:188:LEU:N	2.76	0.43
1:A:118:PHE:CD2	1:A:314:ASP:OD2	2.72	0.42
1:B:231:ARG:HE	1:B:233:THR:HG23	1.84	0.42
2:E:89:PHE:HB2	3:E:302:C8E:H11	2.01	0.42
1:B:60:GLN:HG2	1:B:85:PHE:CZ	2.55	0.42
1:B:216:THR:HG22	1:B:233:THR:CB	2.46	0.42
2:D:21:ASN:ND2	2:D:132:TYR:O	2.50	0.42
2:D:60:THR:HA	2:D:63:LEU:CD1	2.49	0.42
2:F:132:TYR:CD2	2:F:132:TYR:C	2.96	0.42
1:B:126:ASP:HB3	1:B:168:LYS:HB3	2.01	0.42
1:B:332:ASP:OD1	1:B:332:ASP:N	2.52	0.42
2:E:161:LEU:HB3	2:E:165:MET:HB2	2.01	0.42
1:A:302:THR:HB	1:A:312:TYR:HB3	2.02	0.42
1:B:71:GLU:HB3	1:C:80:TRP:CD1	2.55	0.42
1:B:138:THR:OG1	1:B:156:GLN:NE2	2.50	0.42
1:C:20:LEU:HD13	1:C:312:TYR:OH	2.19	0.42
2:E:152:ASP:HA	2:E:155:TYR:CE1	2.54	0.42
1:C:11:LEU:HD12	1:C:11:LEU:HA	1.87	0.42
2:D:163:TRP:CE2	2:D:167:ILE:HD11	2.54	0.42
2:F:20:PHE:C	2:F:20:PHE:CD2	2.98	0.42
1:A:65:VAL:HG12	1:A:79:ALA:HB1	2.01	0.42
2:D:178:ARG:O	2:D:182:LEU:CD1	2.67	0.42
2:E:36:VAL:O	2:E:38:ARG:N	2.51	0.42
2:F:24:MET:CE	2:F:136:PRO:HB3	2.48	0.42
1:B:20:LEU:HD13	1:B:312:TYR:OH	2.19	0.42
1:B:182:TRP:HE3	1:B:185:ILE:HD13	1.85	0.42
1:B:309:MET:HE1	1:B:340:TYR:CD1	2.50	0.42
2:D:129:TYR:CD1	2:D:142:THR:HG21	2.55	0.42
1:B:37:ASP:OD1	1:C:98:TYR:OH	2.30	0.42
1:B:297:VAL:HG23	1:B:319:LEU:HD11	2.01	0.42
1:C:276:TYR:CE2	1:C:278:GLN:NE2	2.88	0.42
2:D:147:GLY:HA2	2:D:150:MET:CG	2.50	0.42
2:E:38:ARG:NE	2:E:185:ASP:OD2	2.38	0.42
2:E:157:VAL:HG13	2:E:158:LEU:N	2.35	0.42
2:F:107:ASN:ND2	2:F:109:GLN:OE1	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:5:ASN:HA	1:B:9:ASN:O	2.20	0.41
1:B:45:VAL:HG22	1:B:61:TRP:HE3	1.84	0.41
1:B:322:ASP:HA	1:B:330:THR:HG21	2.02	0.41
1:C:55:LEU:HA	1:C:55:LEU:HD23	1.82	0.41
2:D:135:LEU:HB2	2:D:138:TYR:HB3	2.01	0.41
2:D:143:LEU:HA	2:D:143:LEU:HD23	1.78	0.41
1:A:215:TYR:O	1:A:233:THR:HA	2.20	0.41
1:C:11:LEU:HD11	1:C:45:VAL:CG1	2.50	0.41
1:C:208:ARG:HG2	1:C:208:ARG:HH11	1.84	0.41
1:C:235:THR:HB	1:C:238:ALA:HB3	2.01	0.41
2:F:37:LEU:O	2:F:41:ALA:N	2.52	0.41
1:A:117:GLU:HB2	1:A:312:TYR:CE1	2.55	0.41
1:B:100:ARG:NH1	1:B:132:ARG:HB3	2.34	0.41
1:C:51:ILE:HB	1:C:55:LEU:HB3	2.02	0.41
2:D:132:TYR:CD1	2:D:132:TYR:C	2.97	0.41
2:F:24:MET:HE2	2:F:136:PRO:CB	2.51	0.41
1:B:158:GLN:NE2	1:B:170:ASN:CG	2.79	0.41
3:B:402:C8E:H172	3:B:402:C8E:H141	1.80	0.41
1:A:204:PRO:O	1:A:205:ALA:HB3	2.20	0.41
1:A:280:LYS:HE3	1:A:292:ASP:CG	2.46	0.41
1:B:206:LEU:HD22	1:B:285:GLU:H	1.86	0.41
2:E:132:TYR:CD2	2:E:132:TYR:C	2.97	0.41
1:B:115:LEU:HD22	1:B:119:GLY:HA3	2.03	0.41
2:D:131:PRO:HB2	2:D:132:TYR:H	1.61	0.41
2:E:56:LEU:HD12	2:E:56:LEU:HA	1.68	0.41
2:E:161:LEU:HD12	2:E:161:LEU:N	2.36	0.41
2:F:69:MET:CG	2:F:70:VAL:N	2.83	0.41
2:F:129:TYR:HD1	2:F:142:THR:HG21	1.85	0.41
1:B:216:THR:CG2	1:B:233:THR:CG2	2.99	0.41
2:E:59:PHE:O	2:E:63:LEU:HD12	2.21	0.41
2:E:162:THR:HB	2:E:164:PRO:HD2	2.02	0.41
2:D:37:LEU:HD13	2:D:178:ARG:HG2	2.02	0.40
2:D:120:SER:OG	2:D:209:ILE:HG22	2.21	0.40
1:C:237:ASN:ND2	1:C:253:ASN:HA	2.36	0.40
1:B:106:TYR:O	1:B:110:SER:HB3	2.22	0.40
1:C:62:GLU:OE1	1:C:82:ARG:NE	2.51	0.40
1:C:104:VAL:H	1:C:156:GLN:NE2	2.19	0.40
2:F:147:GLY:HA2	2:F:150:MET:SD	2.61	0.40
1:A:288:TYR:HB3	1:A:291:GLN:HG3	2.03	0.40
2:E:188:LEU:HD23	2:E:188:LEU:C	2.43	0.40
2:F:129:TYR:CD1	2:F:142:THR:HG21	2.57	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	342/344 (99%)	313 (92%)	27 (8%)	2 (1%)	21	51
1	B	342/344 (99%)	316 (92%)	25 (7%)	1 (0%)	36	65
1	C	342/344 (99%)	317 (93%)	23 (7%)	2 (1%)	21	51
2	D	197/236 (84%)	179 (91%)	15 (8%)	3 (2%)	8	28
2	E	197/236 (84%)	175 (89%)	19 (10%)	3 (2%)	8	28
2	F	202/236 (86%)	182 (90%)	16 (8%)	4 (2%)	6	22
All	All	1622/1740 (93%)	1482 (91%)	125 (8%)	15 (1%)	14	41

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	181(A)	ILE
1	A	183	ASP
2	D	131	PRO
2	E	132	TYR
2	F	131	PRO
1	B	181(A)	ILE
2	D	132	TYR
2	E	131	PRO
2	F	191	SER
2	F	211	ASN
1	C	181(A)	ILE
1	C	289	GLY
2	D	187	LEU
2	F	132	TYR
2	E	157	VAL

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	276/276 (100%)	273 (99%)	3 (1%)	65	88
1	B	276/276 (100%)	274 (99%)	2 (1%)	76	92
1	C	276/276 (100%)	272 (99%)	4 (1%)	59	85
2	D	168/197 (85%)	167 (99%)	1 (1%)	78	93
2	E	168/197 (85%)	168 (100%)	0	100	100
2	F	168/197 (85%)	168 (100%)	0	100	100
All	All	1332/1419 (94%)	1322 (99%)	10 (1%)	73	90

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	164	ARG
1	A	213	GLU
1	A	260	VAL
1	B	164	ARG
1	B	243	SER
1	C	194	SER
1	C	233	THR
1	C	285	GLU
1	C	302	THR
2	D	65	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	GLN
1	A	78	GLN
1	A	156	GLN
1	A	158	GLN
1	A	200	GLN
1	A	224	ASN
1	A	257	ASN

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Mol	Chain	Res	Type
1	A	291	GLN
1	A	308	ASN
1	A	318	ASN
1	A	341	GLN
1	B	52	ASN
1	B	78	GLN
1	B	158	GLN
1	B	169	GLN
1	B	211	ASN
1	B	256	GLN
1	B	263	GLN
1	B	265	GLN
1	B	291	GLN
1	C	78	GLN
1	C	156	GLN
1	C	224	ASN
1	C	237	ASN
1	C	253	ASN
1	C	278	GLN
2	D	75	GLN
2	D	116	HIS
2	E	30	ASN
2	E	62	ASN
2	F	58	ASN
2	F	75	GLN
2	F	91	ASN
2	F	111	GLN
2	F	180	GLN

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

22 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$
3	C8E	C	401	-	15,15,20	0.39	0	14,14,19	0.60	0
4	LMT	F	302	-	25,25,36	1.21	3 (12%)	36,36,47	1.26	3 (8%)
3	C8E	C	404	-	15,15,20	0.47	0	14,14,19	0.57	0
3	C8E	C	403	-	12,12,20	0.47	0	11,11,19	0.33	0
3	C8E	A	404	-	8,8,20	0.55	0	7,7,19	0.31	0
3	C8E	C	402	-	20,20,20	0.46	0	19,19,19	0.52	0
3	C8E	D	301	-	12,12,20	0.34	0	11,11,19	0.57	0
4	LMT	B	406	-	25,25,36	1.28	3 (12%)	36,36,47	1.41	6 (16%)
3	C8E	D	302	-	11,11,20	0.48	0	10,10,19	0.50	0
3	C8E	A	406	-	10,10,20	0.47	0	9,9,19	0.69	0
3	C8E	E	301	-	7,7,20	0.41	0	6,6,19	0.28	0
3	C8E	F	301	-	6,6,20	0.36	0	5,5,19	0.28	0
3	C8E	E	302	-	19,19,20	0.43	0	18,18,19	0.32	0
3	C8E	A	401	-	15,15,20	0.35	0	14,14,19	0.46	0
3	C8E	A	403	-	11,11,20	0.44	0	9,9,19	0.34	0
3	C8E	B	401	-	10,10,20	0.37	0	9,9,19	0.65	0
3	C8E	A	402	-	9,9,20	0.31	0	8,8,19	0.49	0
3	C8E	B	404	-	14,14,20	0.40	0	13,13,19	0.35	0
3	C8E	A	405	-	15,15,20	0.51	0	14,14,19	0.49	0
4	LMT	B	405	-	36,36,36	1.08	2 (5%)	47,47,47	1.07	4 (8%)
3	C8E	B	403	-	15,15,20	0.48	0	14,14,19	0.61	0
3	C8E	B	402	-	17,17,20	0.44	0	16,16,19	0.34	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
3	C8E	C	401	-	-	4/13/13/18	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	LMT	F	302	-	-	8/10/50/61	0/2/2/2
3	C8E	C	404	-	-	7/13/13/18	-
3	C8E	C	403	-	-	5/10/10/18	-
3	C8E	A	404	-	-	3/6/6/18	-
3	C8E	C	402	-	-	7/18/18/18	-
3	C8E	D	301	-	-	6/10/10/18	-
4	LMT	B	406	-	-	2/10/50/61	0/2/2/2
3	C8E	D	302	-	-	5/9/9/18	-
3	C8E	A	406	-	-	2/8/8/18	-
3	C8E	E	301	-	-	3/5/5/18	-
3	C8E	F	301	-	-	2/4/4/18	-
3	C8E	E	302	-	-	11/17/17/18	-
3	C8E	A	401	-	-	10/13/13/18	-
3	C8E	A	403	-	-	3/7/7/18	-
3	C8E	B	401	-	-	5/8/8/18	-
3	C8E	A	402	-	-	4/7/7/18	-
3	C8E	B	404	-	-	5/12/12/18	-
3	C8E	A	405	-	-	8/13/13/18	-
4	LMT	B	405	-	-	10/21/61/61	0/2/2/2
3	C8E	B	403	-	-	7/13/13/18	-
3	C8E	B	402	-	-	10/15/15/18	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	406	LMT	O2'-C2'	-2.74	1.36	1.43
4	F	302	LMT	O2'-C2'	-2.63	1.36	1.43
4	B	405	LMT	O3B-C3B	-2.38	1.37	1.43
4	B	406	LMT	O3B-C3B	-2.31	1.37	1.43
4	F	302	LMT	O3'-C3'	-2.29	1.37	1.43
4	F	302	LMT	O2B-C2B	-2.25	1.37	1.43
4	B	405	LMT	O3'-C3'	-2.24	1.37	1.43
4	B	406	LMT	O3'-C3'	-2.20	1.37	1.43

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	406	LMT	O5'-C5'-C4'	3.87	117.72	109.72
4	F	302	LMT	O5'-C5'-C4'	3.01	115.94	109.72
4	F	302	LMT	O1'-C1'-C2'	2.98	111.58	108.14
4	B	406	LMT	O5B-C5B-C4B	2.82	114.79	109.70
4	B	405	LMT	O1'-C1'-C2'	2.61	112.24	108.27
4	B	406	LMT	O1B-C4'-C5'	-2.45	103.04	109.48
4	B	405	LMT	C3B-C4B-C5B	-2.40	105.88	110.23
4	B	406	LMT	O5B-C5B-C6B	2.34	112.24	106.44
4	B	405	LMT	C1'-O5'-C5'	-2.29	109.25	113.72
4	B	406	LMT	O1'-C1'-C2'	2.27	110.76	108.14
4	B	405	LMT	C3'-C4'-C5'	-2.24	105.95	110.93
4	F	302	LMT	O5'-C5'-C6'	2.20	111.89	106.44
4	B	406	LMT	O5'-C1'-C2'	-2.09	106.08	110.37

There are no chirality outliers.

All (127) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	405	LMT	O5'-C1'-O1'-C1
4	F	302	LMT	O5'-C1'-O1'-C1
4	F	302	LMT	O5'-C5'-C6'-O6'
4	B	405	LMT	O5B-C5B-C6B-O6B
4	F	302	LMT	O5B-C5B-C6B-O6B
4	F	302	LMT	C2'-C1'-O1'-C1
4	B	406	LMT	O5B-C5B-C6B-O6B
4	B	405	LMT	C4B-C5B-C6B-O6B
3	D	301	C8E	O9-C10-C11-O12
4	F	302	LMT	C4B-C5B-C6B-O6B
3	B	403	C8E	O12-C13-C14-O15
3	E	302	C8E	O12-C13-C14-O15
3	A	401	C8E	O9-C10-C11-O12
3	C	401	C8E	O12-C13-C14-O15
3	A	405	C8E	O12-C13-C14-O15
4	B	406	LMT	C4B-C5B-C6B-O6B
3	D	302	C8E	O9-C10-C11-O12
4	F	302	LMT	C4'-C5'-C6'-O6'
3	A	401	C8E	O12-C13-C14-O15
3	C	403	C8E	C6-C7-C8-O9
3	A	401	C8E	C6-C7-C8-O9
3	B	403	C8E	O9-C10-C11-O12
3	B	402	C8E	O12-C13-C14-O15
3	A	402	C8E	C6-C7-C8-O9
4	B	405	LMT	O1'-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
3	A	405	C8E	C6-C7-C8-O9
3	B	402	C8E	C6-C7-C8-O9
3	B	404	C8E	C4-C5-C6-C7
3	C	403	C8E	C2-C3-C4-C5
3	B	402	C8E	C5-C6-C7-C8
3	F	301	C8E	C4-C5-C6-C7
3	C	404	C8E	C4-C5-C6-C7
3	A	401	C8E	C2-C3-C4-C5
3	A	402	C8E	C2-C3-C4-C5
3	B	402	C8E	C1-C2-C3-C4
3	A	402	C8E	C5-C6-C7-C8
3	E	302	C8E	C1-C2-C3-C4
3	B	404	C8E	O9-C10-C11-O12
3	C	402	C8E	C16-C17-O18-C19
3	B	403	C8E	C1-C2-C3-C4
3	B	404	C8E	C3-C4-C5-C6
3	D	301	C8E	C5-C6-C7-C8
3	B	401	C8E	C4-C5-C6-C7
3	A	404	C8E	O18-C19-C20-O21
4	B	405	LMT	C7-C8-C9-C10
3	D	301	C8E	C2-C3-C4-C5
3	E	302	C8E	O15-C16-C17-O18
4	B	405	LMT	C4-C5-C6-C7
3	B	403	C8E	C3-C4-C5-C6
4	F	302	LMT	C5'-C4'-O1B-C1B
3	E	302	C8E	C2-C3-C4-C5
3	E	301	C8E	C4-C5-C6-C7
3	A	405	C8E	C3-C4-C5-C6
3	E	301	C8E	C3-C4-C5-C6
4	B	405	LMT	C5-C6-C7-C8
3	D	301	C8E	C1-C2-C3-C4
3	B	401	C8E	C2-C3-C4-C5
3	E	302	C8E	C20-C19-O18-C17
4	B	405	LMT	C9-C10-C11-C12
3	F	301	C8E	C3-C4-C5-C6
3	A	401	C8E	C1-C2-C3-C4
3	D	302	C8E	C2-C3-C4-C5
3	A	403	C8E	C14-C13-O12-C11
3	C	403	C8E	C4-C5-C6-C7
4	F	302	LMT	C3'-C4'-O1B-C1B
3	C	404	C8E	O12-C13-C14-O15
3	D	302	C8E	C10-C11-O12-C13

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Mol	Chain	Res	Type	Atoms
3	A	401	C8E	C3-C4-C5-C6
3	A	401	C8E	C11-C10-O9-C8
3	C	402	C8E	C17-C16-O15-C14
3	E	302	C8E	C14-C13-O12-C11
3	A	404	C8E	C16-C17-O18-C19
3	A	405	C8E	C10-C11-O12-C13
3	A	404	C8E	C17-C16-O15-C14
3	A	401	C8E	C14-C13-O12-C11
3	B	404	C8E	C5-C6-C7-C8
3	D	301	C8E	C11-C10-O9-C8
3	B	403	C8E	C14-C13-O12-C11
3	B	402	C8E	C17-C16-O15-C14
3	B	404	C8E	C14-C13-O12-C11
4	B	405	LMT	C11-C10-C9-C8
3	C	402	C8E	C2-C3-C4-C5
3	A	405	C8E	C4-C5-C6-C7
3	C	401	C8E	C14-C13-O12-C11
3	C	404	C8E	C14-C13-O12-C11
3	E	302	C8E	C10-C11-O12-C13
3	B	401	C8E	C6-C7-C8-O9
3	C	402	C8E	O15-C16-C17-O18
3	C	402	C8E	O18-C19-C20-O21
3	A	405	C8E	C14-C13-O12-C11
3	A	403	C8E	C10-C11-O12-C13
3	A	406	C8E	C6-C7-C8-O9
3	D	302	C8E	C7-C8-O9-C10
3	B	402	C8E	C13-C14-O15-C16
3	E	302	C8E	C13-C14-O15-C16
3	C	403	C8E	C7-C8-O9-C10
3	A	401	C8E	C4-C5-C6-C7
3	C	404	C8E	C3-C4-C5-C6
3	A	406	C8E	C7-C8-O9-C10
3	C	404	C8E	C13-C14-O15-C16
3	B	403	C8E	C2-C3-C4-C5
3	E	302	C8E	C17-C16-O15-C14
3	B	402	C8E	C3-C4-C5-C6
3	A	401	C8E	C7-C8-O9-C10
3	E	302	C8E	C7-C8-O9-C10
3	E	301	C8E	C2-C3-C4-C5
3	B	403	C8E	C10-C11-O12-C13
3	B	401	C8E	C1-C2-C3-C4
3	B	402	C8E	C7-C8-O9-C10

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Mol	Chain	Res	Type	Atoms
3	D	302	C8E	C3-C4-C5-C6
3	B	401	C8E	C3-C4-C5-C6
3	B	402	C8E	C14-C13-O12-C11
3	C	403	C8E	C3-C4-C5-C6
3	C	404	C8E	O9-C10-C11-O12
3	D	301	C8E	C7-C8-O9-C10
3	C	401	C8E	C13-C14-O15-C16
3	A	405	C8E	O9-C10-C11-O12
3	B	402	C8E	C4-C5-C6-C7
3	C	402	C8E	O12-C13-C14-O15
4	B	405	LMT	C1-C2-C3-C4
3	A	403	C8E	C7-C8-O9-C10
3	C	404	C8E	C7-C8-O9-C10
3	A	402	C8E	C7-C8-O9-C10
3	A	405	C8E	C13-C14-O15-C16
3	E	302	C8E	O9-C10-C11-O12
3	C	401	C8E	O9-C10-C11-O12
3	C	402	C8E	O9-C10-C11-O12

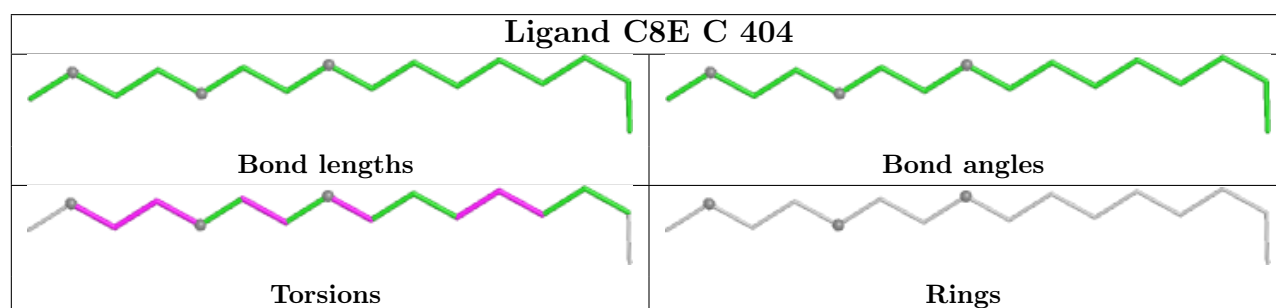
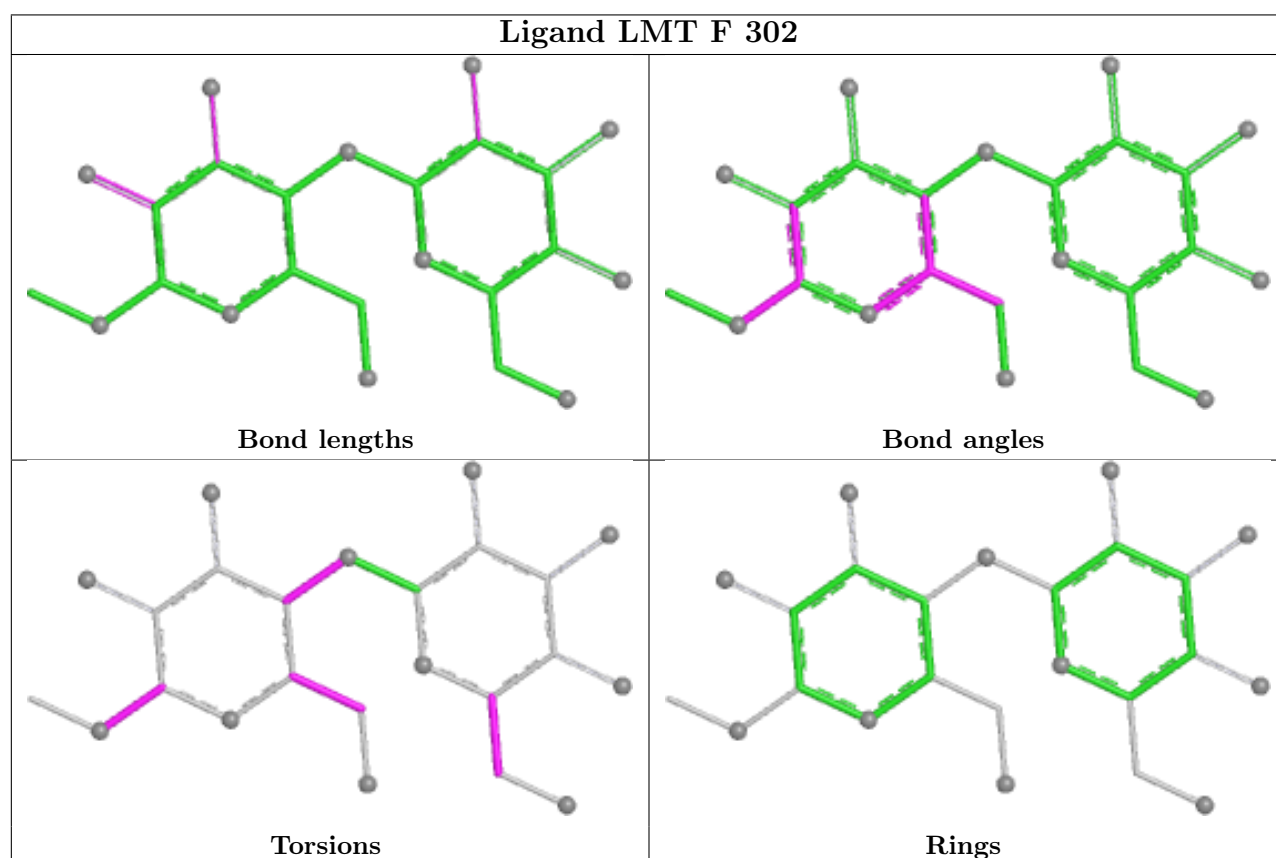
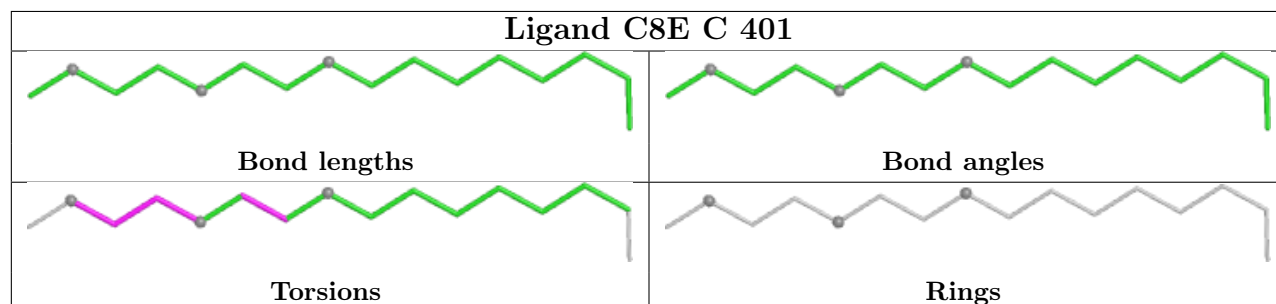
There are no ring outliers.

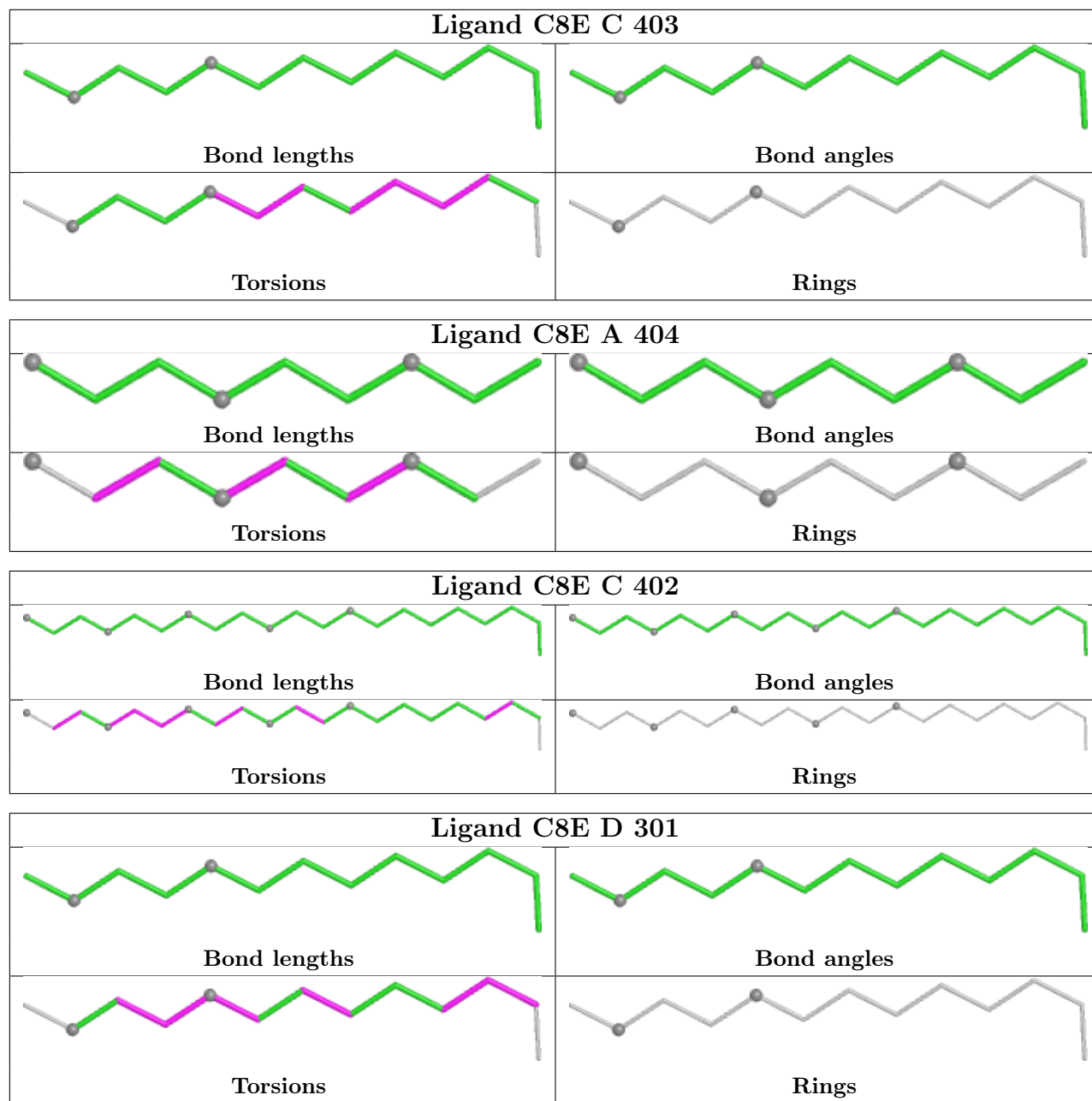
11 monomers are involved in 20 short contacts:

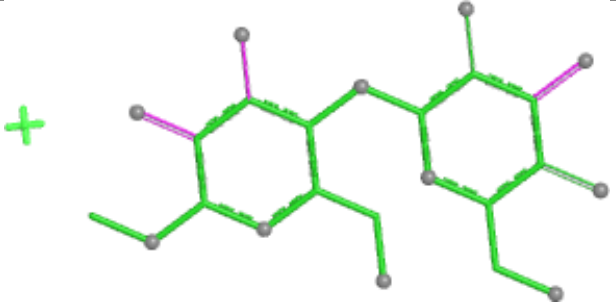
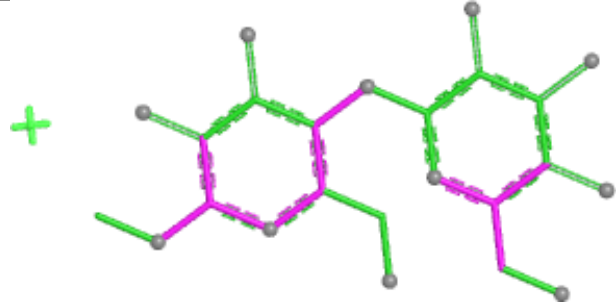
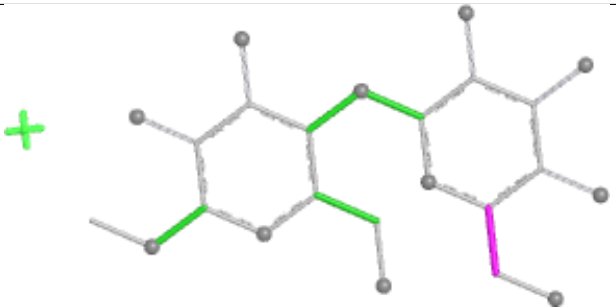
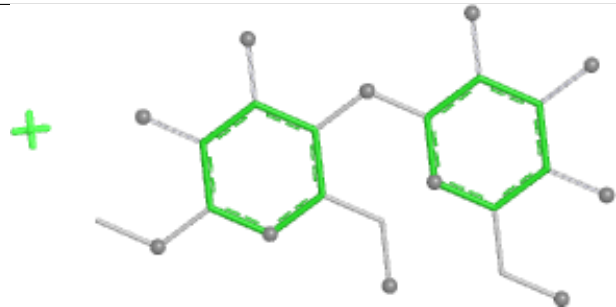
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	401	C8E	2	0
3	C	403	C8E	1	0
3	A	404	C8E	1	0
3	C	402	C8E	2	0
4	B	406	LMT	4	0
3	A	406	C8E	2	0
3	E	302	C8E	3	0
3	A	401	C8E	2	0
3	B	404	C8E	1	0
4	B	405	LMT	1	0
3	B	402	C8E	1	0

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

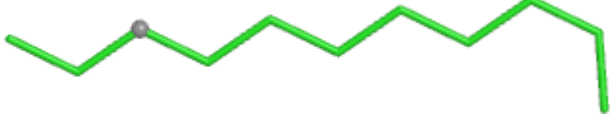
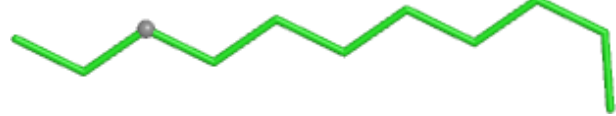
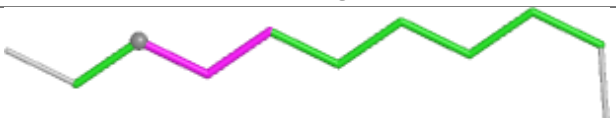
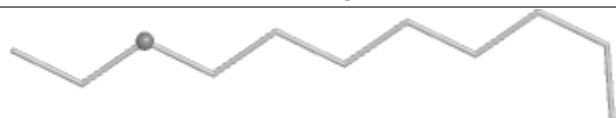
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

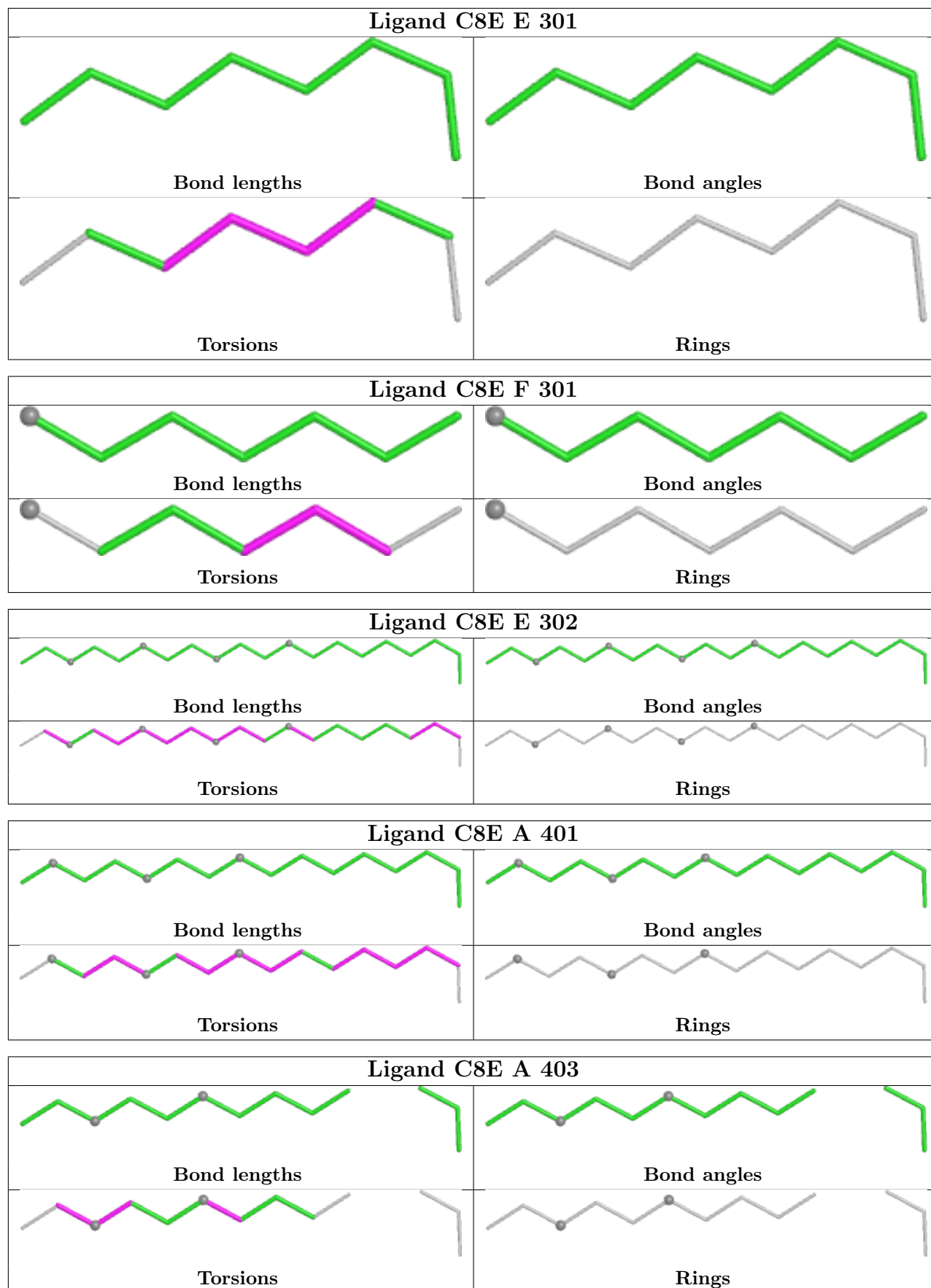


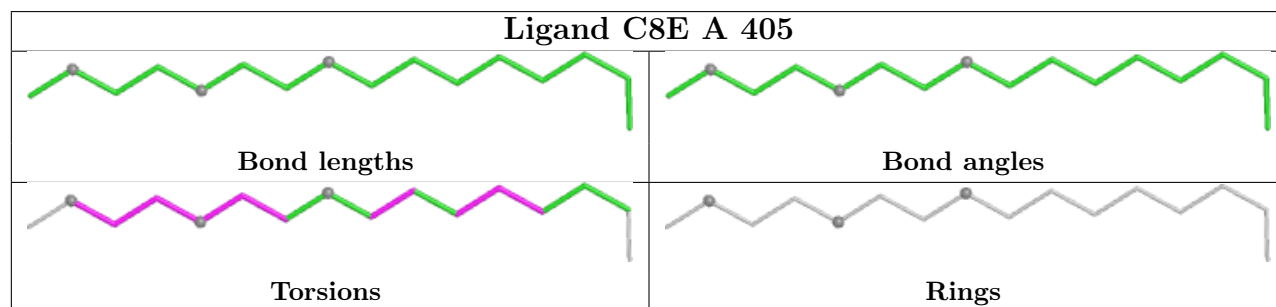
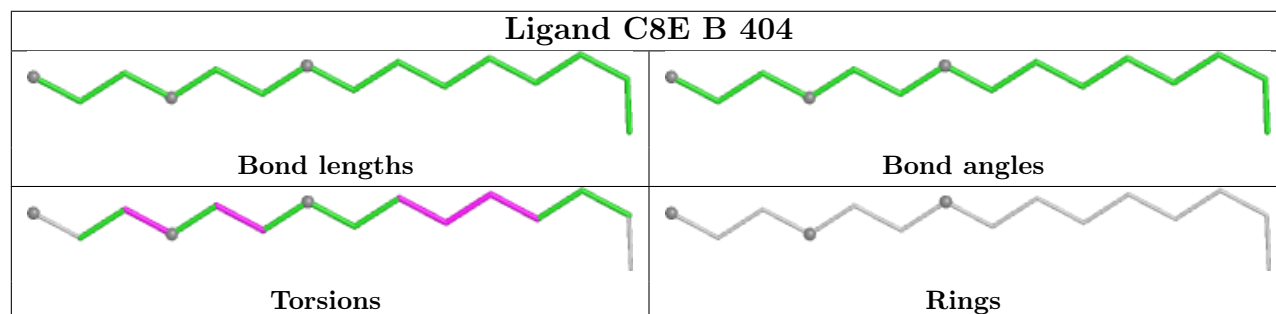
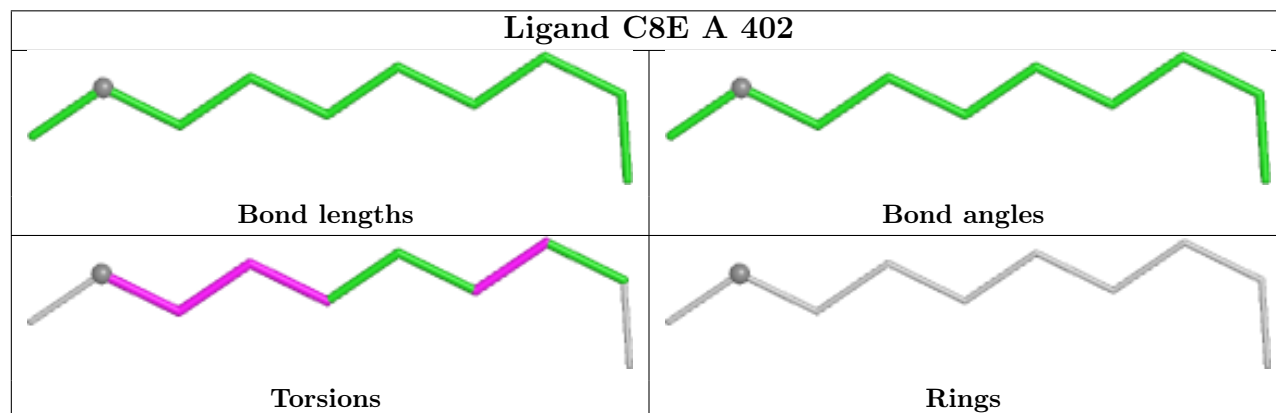
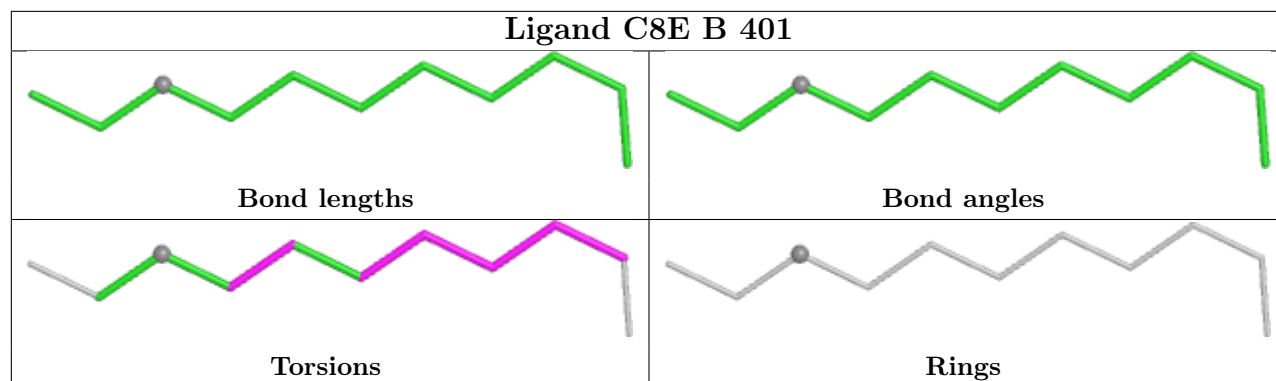


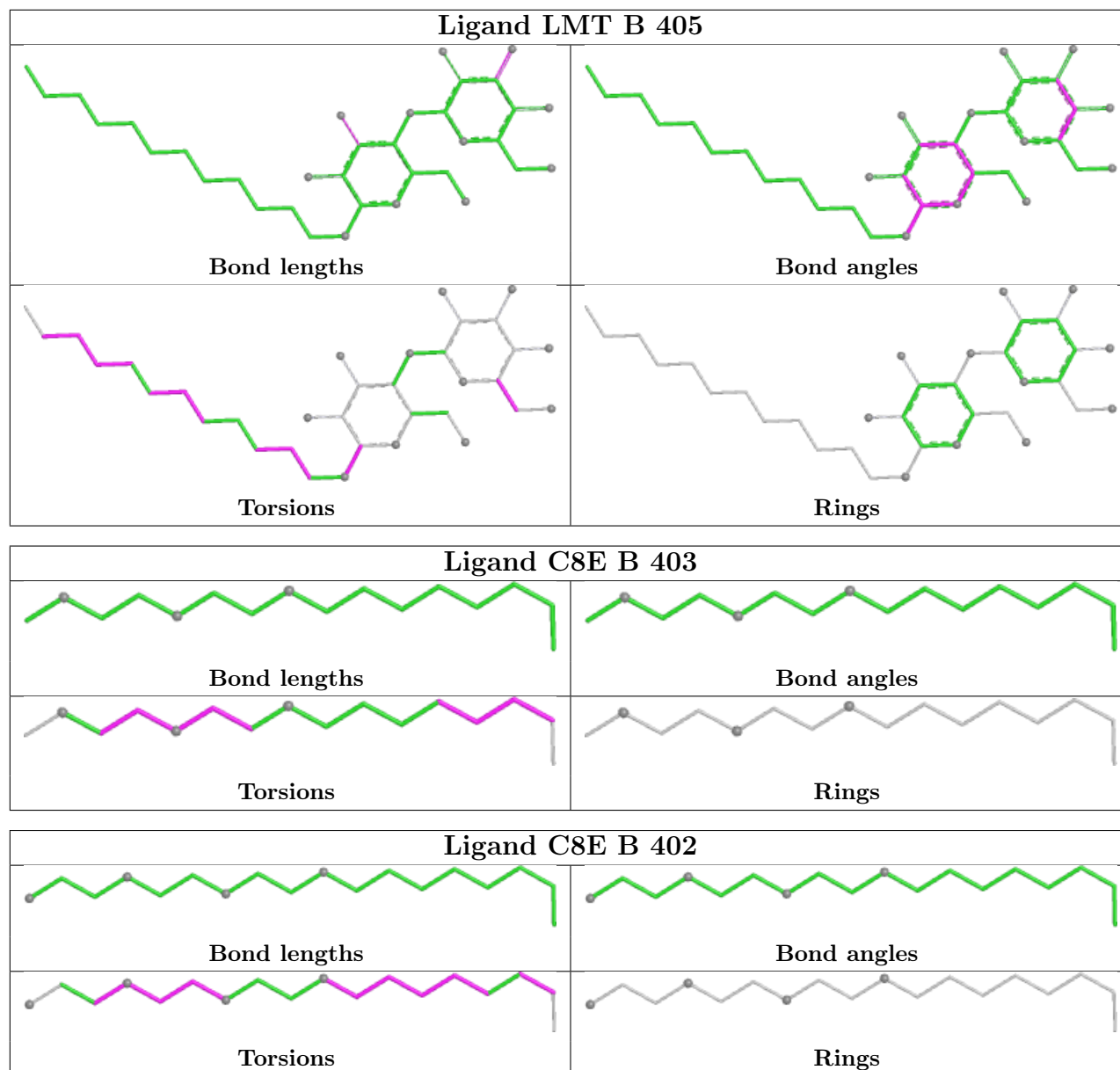
Ligand LMT B 406	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand C8E D 302	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand C8E A 406	
	
Bond lengths	Bond angles
	
Torsions	Rings







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	344/344 (100%)	0.45	16 (4%)	36	28	48, 58, 83, 140	0
1	B	344/344 (100%)	0.62	26 (7%)	20	16	48, 61, 91, 155	0
1	C	344/344 (100%)	0.76	32 (9%)	14	12	50, 68, 103, 153	0
2	D	199/236 (84%)	0.65	15 (7%)	20	16	46, 71, 98, 165	0
2	E	199/236 (84%)	0.82	25 (12%)	8	6	56, 75, 102, 152	0
2	F	204/236 (86%)	0.84	29 (14%)	6	5	55, 80, 124, 159	0
All	All	1634/1740 (93%)	0.67	143 (8%)	15	13	46, 67, 102, 165	0

All (143) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	186	GLY	6.8
2	D	187	LEU	6.2
2	F	211	ASN	5.5
2	E	187	LEU	5.3
2	E	191	SER	5.3
2	E	163	TRP	5.3
1	A	182	TRP	4.9
2	E	192	SER	4.8
1	C	85	PHE	4.7
2	D	77	ASP	4.4
2	F	208	PHE	4.3
2	E	189	ARG	4.3
1	C	92	ASP	4.2
2	D	147	GLY	4.2
2	F	160	TRP	4.2
1	C	323	ASN	4.1
2	F	212	GLY	4.1
2	F	194	PRO	3.9
1	B	182	TRP	3.9

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Mol	Chain	Res	Type	RSRZ
1	C	91	GLY	3.8
1	B	11	LEU	3.8
2	F	187	LEU	3.7
1	C	178	LEU	3.7
2	F	189	ARG	3.7
1	B	14	TYR	3.7
2	E	157	VAL	3.6
2	F	131	PRO	3.6
2	E	190	GLN	3.6
2	F	14	SER	3.6
2	F	137	PHE	3.6
2	F	216	THR	3.6
2	D	109	GLN	3.5
1	B	46	LYS	3.5
1	B	13	LEU	3.4
2	E	193	ASP	3.4
1	C	22	TYR	3.4
2	F	213	GLY	3.3
1	A	4	TYR	3.3
1	C	21	HIS	3.3
2	D	191	SER	3.3
1	B	92	ASP	3.2
2	E	13	ARG	3.2
2	D	183	ASP	3.2
1	C	182	TRP	3.2
2	D	188	LEU	3.1
1	B	288	TYR	3.1
2	E	30	ASN	3.1
1	A	13	LEU	3.1
1	A	147	LEU	3.0
1	C	307	LYS	3.0
1	B	3	ILE	3.0
2	E	14	SER	3.0
1	C	108	VAL	3.0
1	B	157	TYR	3.0
2	F	111	GLN	3.0
2	F	127	VAL	3.0
1	A	157	TYR	2.9
1	A	172	ASP	2.9
1	B	283	ASP	2.9
1	C	283	ASP	2.9
1	B	130	GLN	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	160	LYS	2.8
1	C	312	TYR	2.8
2	F	184	SER	2.8
1	C	94	GLY	2.8
2	E	29	PHE	2.8
2	F	192	SER	2.8
1	B	91	GLY	2.8
1	B	45	VAL	2.8
2	F	188	LEU	2.7
1	C	120	GLY	2.7
1	A	91	GLY	2.7
1	B	12	ASP	2.7
2	D	157	VAL	2.7
1	C	278	GLN	2.6
2	E	37	LEU	2.6
1	B	243	SER	2.6
2	F	139	GLY	2.6
1	A	129	LEU	2.6
2	E	56	LEU	2.6
2	F	109	GLN	2.6
2	D	20	PHE	2.6
2	D	185	ASP	2.6
1	C	137	ALA	2.5
2	E	205	ARG	2.5
1	C	321	ASP	2.5
2	D	184	SER	2.5
2	E	194	PRO	2.5
2	D	186	GLY	2.5
2	E	55	GLY	2.5
2	F	47	TYR	2.5
1	C	93	ALA	2.5
2	F	198	MET	2.4
2	F	163	TRP	2.4
1	A	3	ILE	2.4
2	F	193	ASP	2.4
2	D	208	PHE	2.4
2	E	109	GLN	2.4
2	E	143	LEU	2.4
1	C	224	ASN	2.4
2	F	205	ARG	2.4
1	A	342	PHE	2.4
1	B	153	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
2	F	215	LEU	2.3
1	B	127	ASN	2.3
1	B	93	ALA	2.3
1	C	54	GLN	2.3
2	E	160	TRP	2.3
1	C	46	LYS	2.3
1	C	254	LYS	2.3
1	C	34	VAL	2.3
2	F	157	VAL	2.2
2	D	79	TYR	2.2
1	A	61	TRP	2.2
2	D	35	TYR	2.2
1	A	54	GLN	2.2
1	C	52	ASN	2.2
2	E	133	VAL	2.2
1	A	163(J)	GLY	2.2
1	C	207	GLY	2.2
1	B	4	TYR	2.2
2	E	209	ILE	2.1
2	E	138	TYR	2.1
1	C	6	LYS	2.1
2	F	214	LYS	2.1
1	B	281	GLY	2.1
1	B	58	TYR	2.1
1	B	142	SER	2.1
2	E	188	LEU	2.1
1	C	8	GLY	2.1
1	C	145	PHE	2.1
1	C	146	GLY	2.1
1	A	60	GLN	2.0
1	B	323	ASN	2.0
1	A	8	GLY	2.0
1	B	198	ASP	2.0
1	C	335	ALA	2.0
1	B	167	SER	2.0
1	C	60	GLN	2.0
2	F	191	SER	2.0
2	F	143	LEU	2.0
1	B	342	PHE	2.0
1	C	179	THR	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

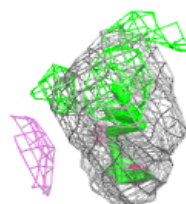
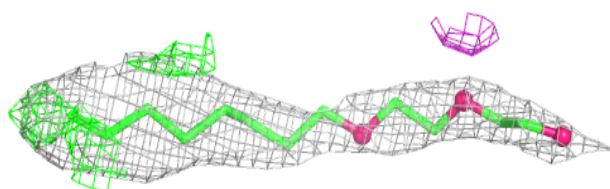
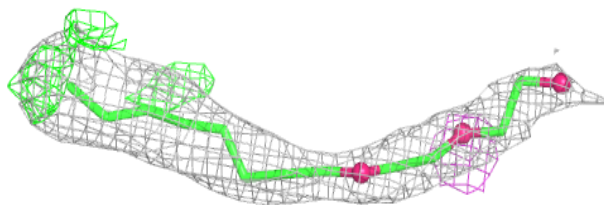
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	C8E	B	404	15/21	0.66	0.39	65,75,85,85	0
3	C8E	F	301	7/21	0.69	0.41	57,59,65,70	0
4	LMT	F	302	24/35	0.71	0.14	66,109,116,131	0
3	C8E	A	404	9/21	0.72	0.31	62,66,72,72	0
3	C8E	D	302	12/21	0.72	0.26	52,62,73,80	0
3	C8E	C	404	16/21	0.78	0.30	26,51,104,105	0
4	LMT	B	406	25/35	0.78	0.15	54,85,102,107	0
3	C8E	E	301	8/21	0.78	0.42	46,58,72,72	0
3	C8E	D	301	13/21	0.79	0.27	53,70,75,78	0
3	C8E	B	403	16/21	0.82	0.23	49,59,74,76	0
3	C8E	E	302	20/21	0.83	0.28	55,69,104,105	0
3	C8E	A	405	16/21	0.85	0.25	33,70,89,90	0
3	C8E	B	402	18/21	0.85	0.20	49,82,89,91	0
3	C8E	A	403	13/21	0.85	0.24	51,63,69,71	0
3	C8E	A	406	11/21	0.87	0.17	44,48,54,55	0
4	LMT	B	405	35/35	0.87	0.13	37,83,101,106	0
3	C8E	C	402	21/21	0.88	0.18	33,63,100,103	0
3	C8E	A	401	16/21	0.88	0.19	49,52,73,78	0
3	C8E	C	403	13/21	0.89	0.21	50,77,96,98	0
3	C8E	B	401	11/21	0.89	0.18	47,52,60,62	0
3	C8E	C	401	16/21	0.90	0.18	43,66,82,82	0
3	C8E	A	402	10/21	0.90	0.20	62,66,77,81	0

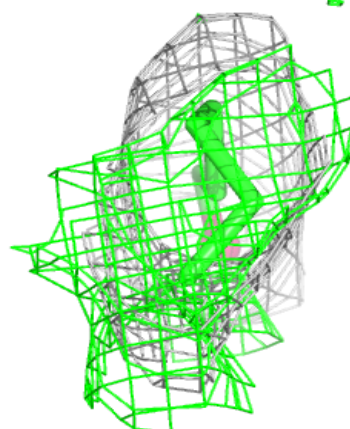
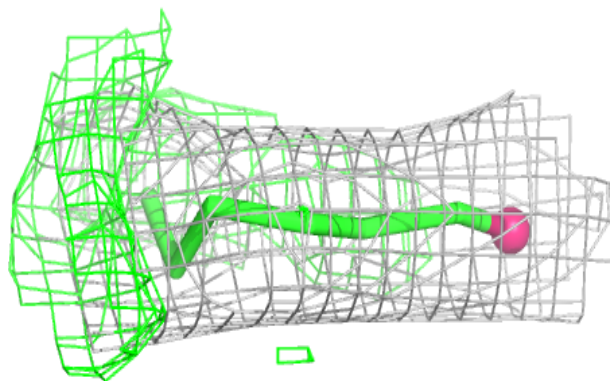
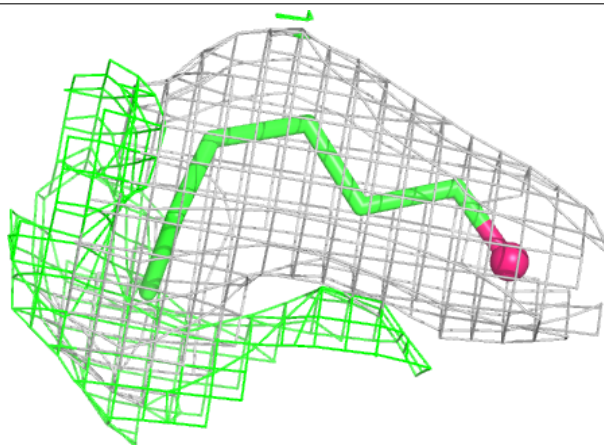
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around C8E B 404:

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

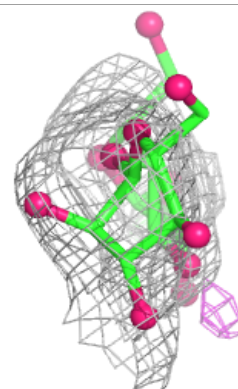
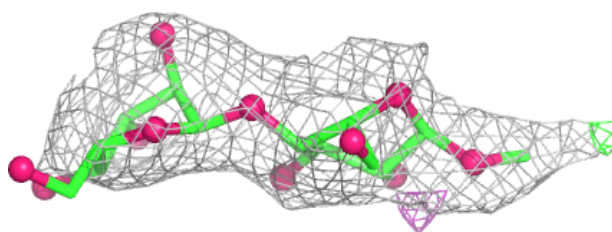
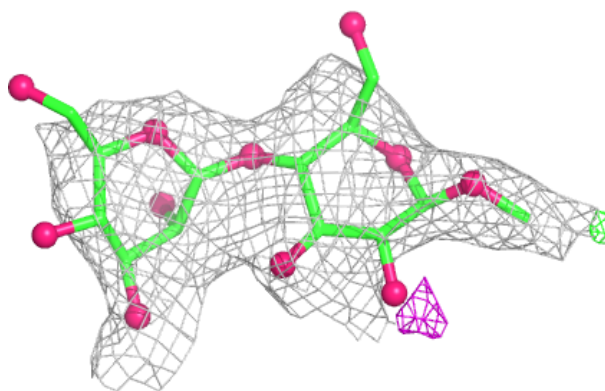
**Electron density around C8E F 301:**

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

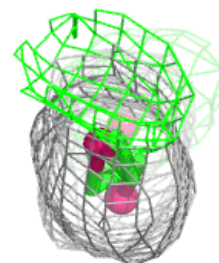
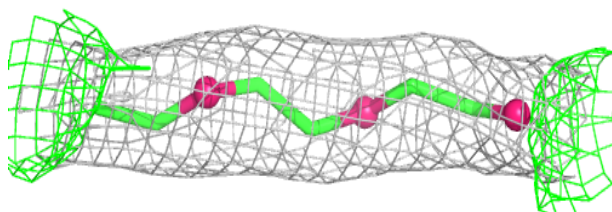
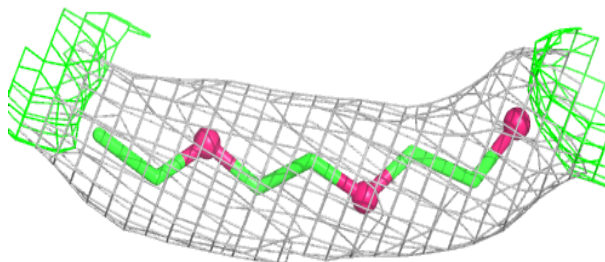


Electron density around LMT F 302:

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

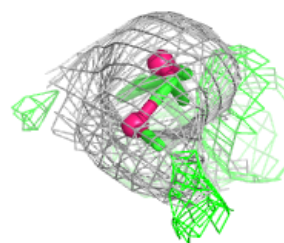
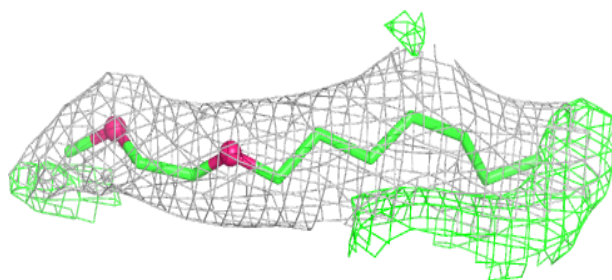
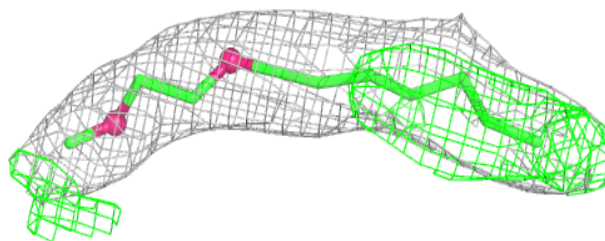
**Electron density around C8E A 404:**

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

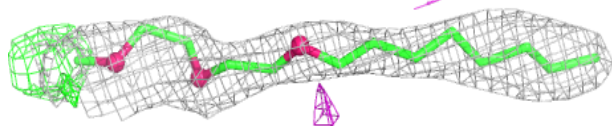
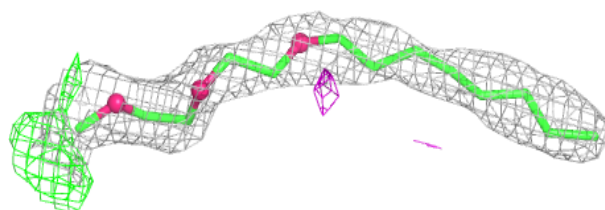


Electron density around C8E D 302:

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

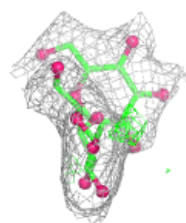
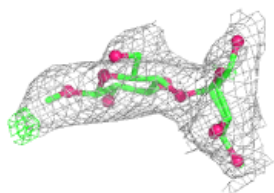
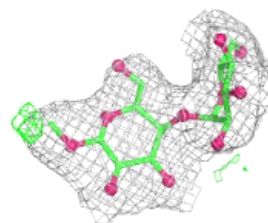
**Electron density around C8E C 404:**

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

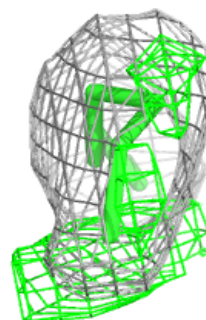
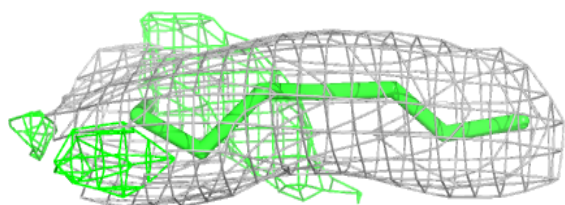
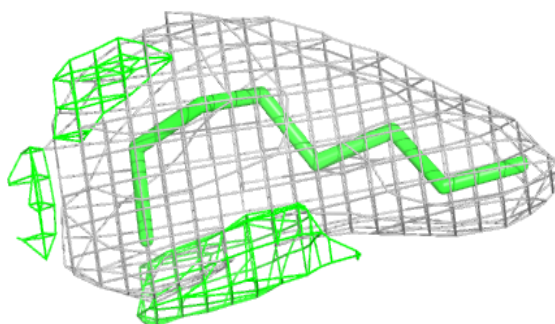


Electron density around LMT B 406:

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

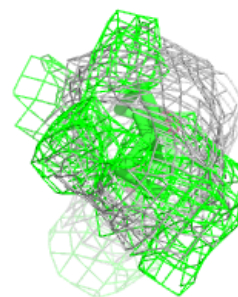
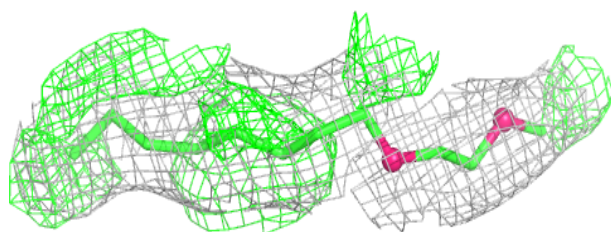
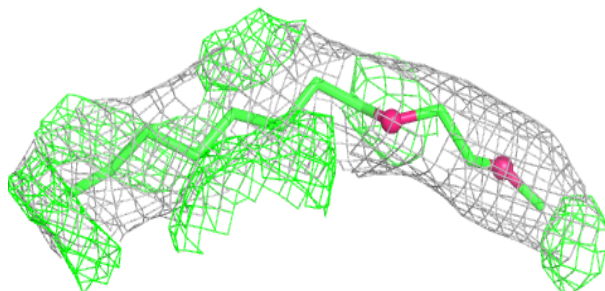
**Electron density around C8E E 301:**

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

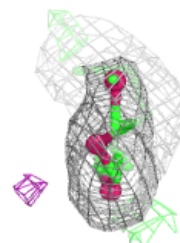
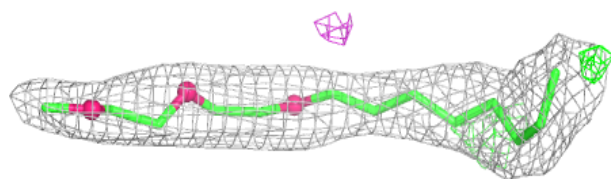
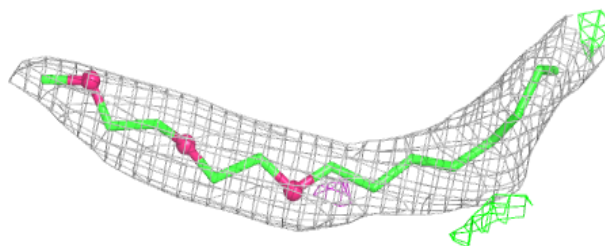


Electron density around C8E D 301:

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

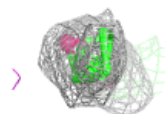
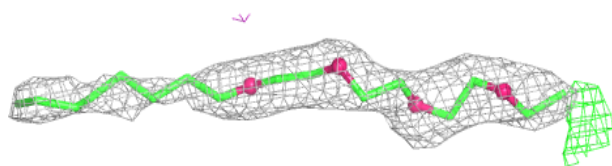
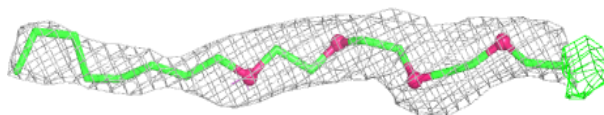
**Electron density around C8E B 403:**

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

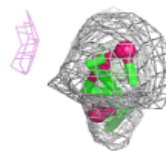
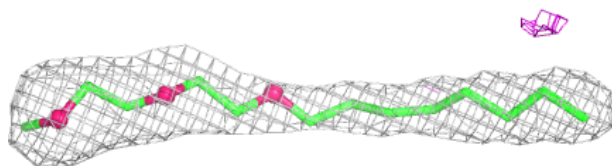
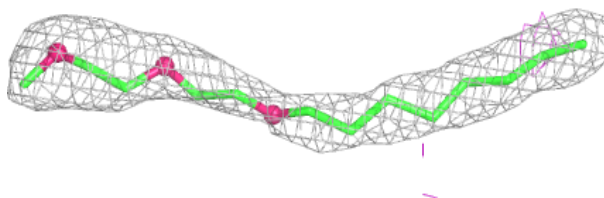


Electron density around C8E E 302:

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

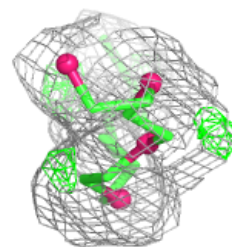
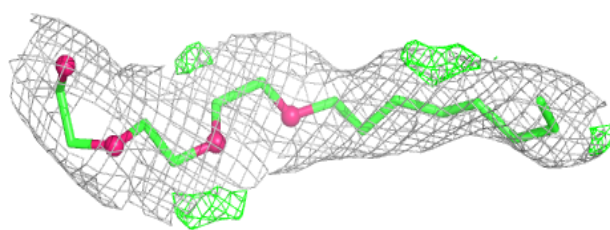
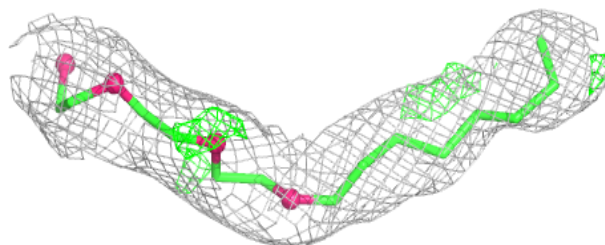
**Electron density around C8E A 405:**

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

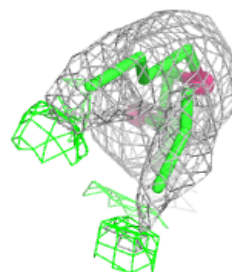
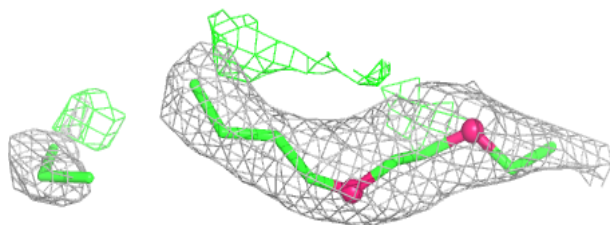
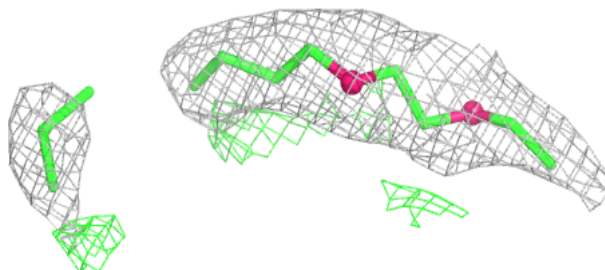


Electron density around C8E B 402:

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

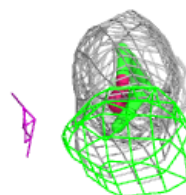
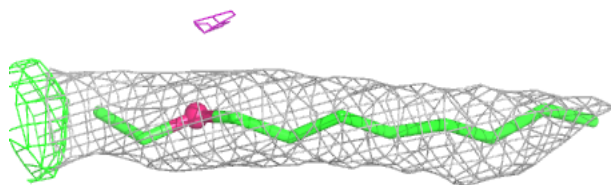
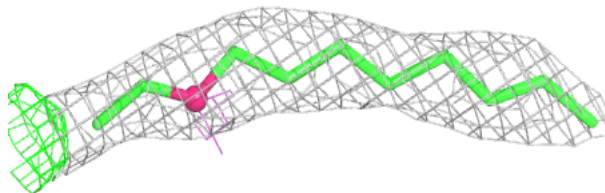
**Electron density around C8E A 403:**

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

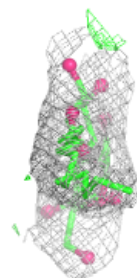
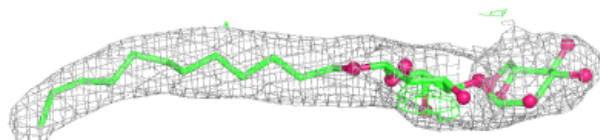
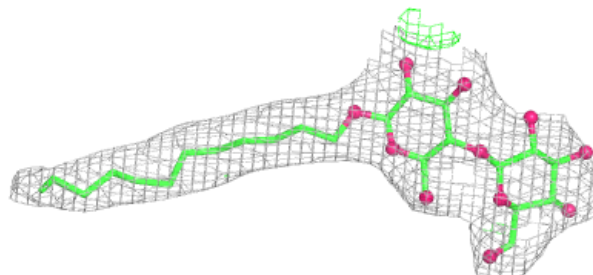


Electron density around C8E A 406:

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

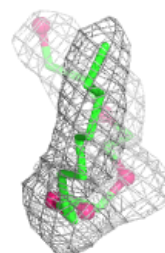
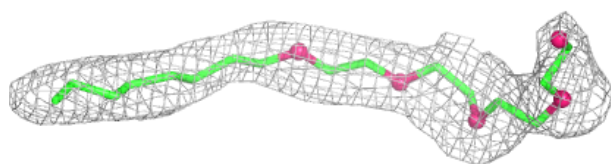
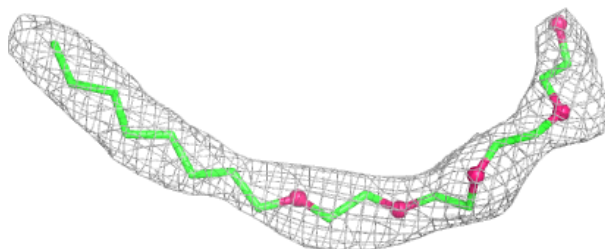
**Electron density around LMT B 405:**

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

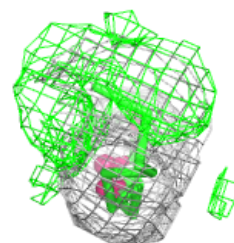
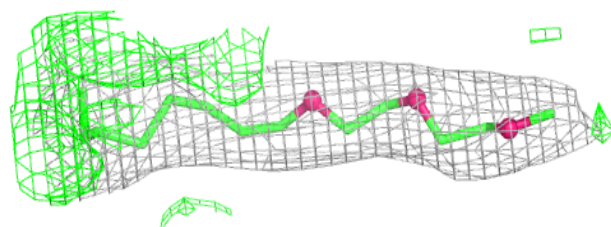
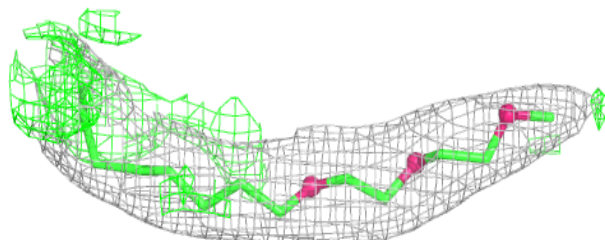


Electron density around C8E C 402:

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

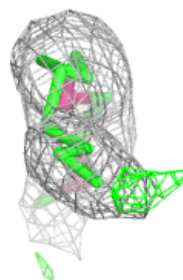
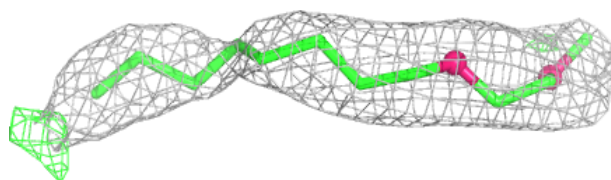
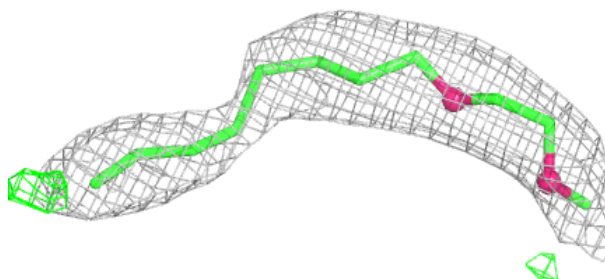
**Electron density around C8E A 401:**

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

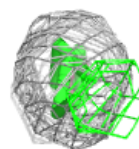
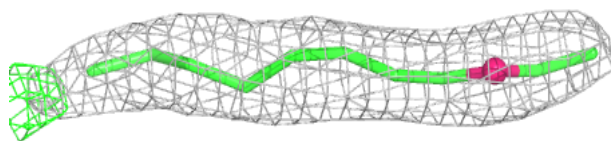
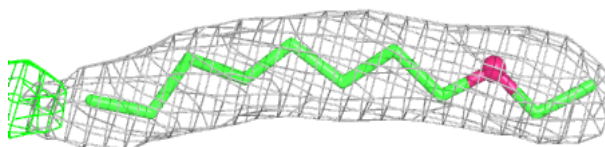


Electron density around C8E C 403:

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

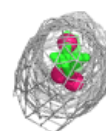
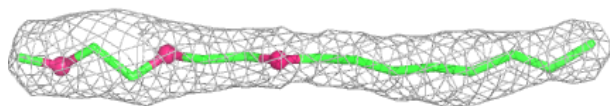
**Electron density around C8E B 401:**

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

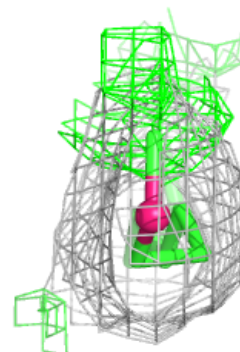
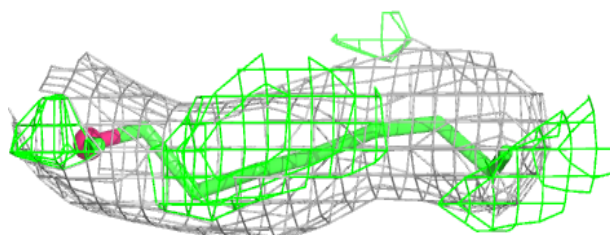
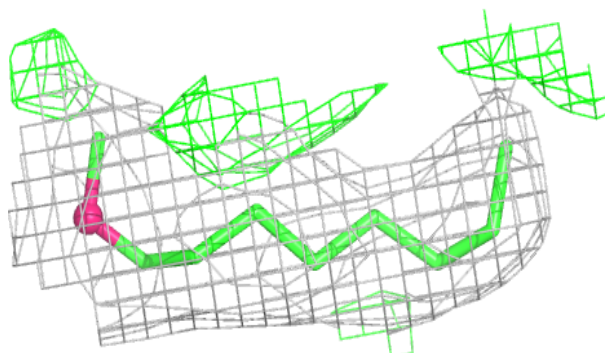


Electron density around C8E C 401:

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

**Electron density around C8E 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.