



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 09:03 PM UTC

PDB ID : 8JUQ / pdb_00008juq
Title : Crystal structure of Chitoporin from *Vibrio harveyi* in complex with gentamicin c1a
Authors : Sanram, S.; Suginta, W.; Robinson, R.
Deposited on : 2023-06-27
Resolution : 2.21 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

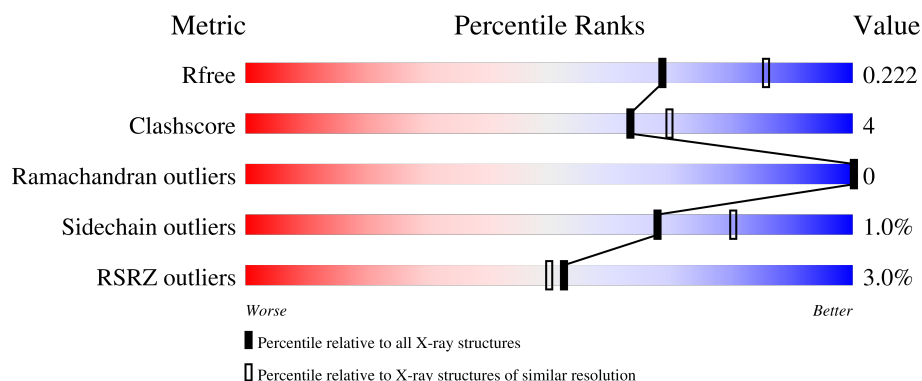
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.21 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	7682 (2.24-2.20)
Clashscore	190562	8402 (2.24-2.20)
Ramachandran outliers	187476	8303 (2.24-2.20)
Sidechain outliers	187428	8304 (2.24-2.20)
RSRZ outliers	180081	7683 (2.24-2.20)

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	350	2% 91% 8%
1	B	350	0% 91% 9%
1	C	350	2% 90% 10%
1	G	350	3% 92% 7%
1	H	350	3% 91% 9%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	I	350	6% 86% 14%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 17092 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.

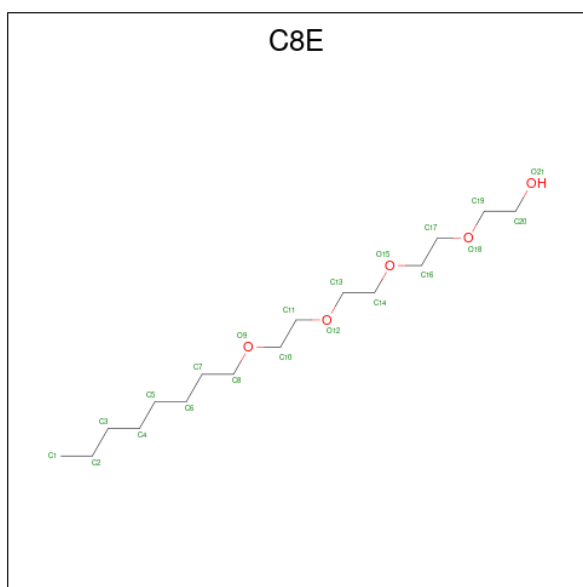
- Molecule 1 is a protein called Chitoporin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	350	Total	C	N	O	S	0	0	0
			2715	1707	448	551	9			
1	B	350	Total	C	N	O	S	0	0	0
			2711	1705	448	549	9			
1	C	350	Total	C	N	O	S	0	0	0
			2692	1691	447	545	9			
1	G	350	Total	C	N	O	S	0	0	0
			2685	1688	445	544	8			
1	H	350	Total	C	N	O	S	0	0	0
			2699	1697	447	546	9			
1	I	350	Total	C	N	O	S	0	0	0
			2665	1672	443	542	8			

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

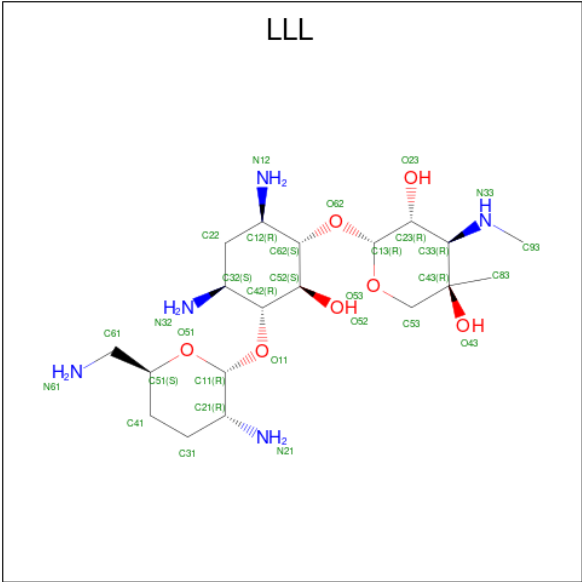
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Na	0	0
			3	3		
2	B	3	Total	Na	0	0
			3	3		
2	C	3	Total	Na	0	0
			3	3		
2	G	3	Total	Na	0	0
			3	3		
2	H	3	Total	Na	0	0
			3	3		
2	I	3	Total	Na	0	0
			3	3		

- Molecule 3 is (HYDROXYETHYLOXY)TRI(ETHYLOXY)OCTANE (CCD ID: C8E) (formula: C₁₆H₃₄O₅) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 4 is (2R,3R,4R,5R)-2-((1S,2S,3R,4S,6R)-4,6-DIAMINO-3-((2R,3R,6S)-3-AMINO-6-(AMINOMETHYL)-TETRAHYDRO-2H-PYRAN-2-YLOXY)-2-HYDROXYCYCLOHEXYLOXY)-5-METHYL-4-(METHYLAMINO)-TETRAHYDRO-2H-PYRAN-3,5-DIOL (CCD ID: LLL) (formula: C₁₉H₃₉N₅O₇).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	C	N	O	0	0
			31	19	5	7		

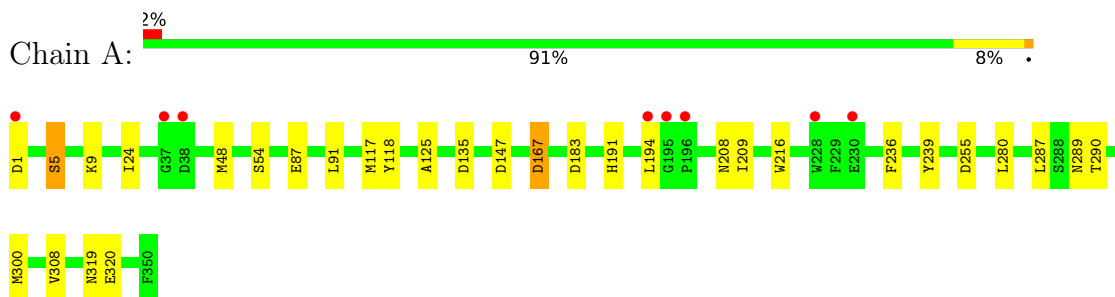
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	143	Total	O	0	0
			143	143		
5	B	151	Total	O	0	0
			151	151		
5	C	147	Total	O	0	0
			147	147		
5	G	100	Total	O	0	0
			100	100		
5	H	103	Total	O	0	0
			103	103		
5	I	81	Total	O	0	0
			81	81		

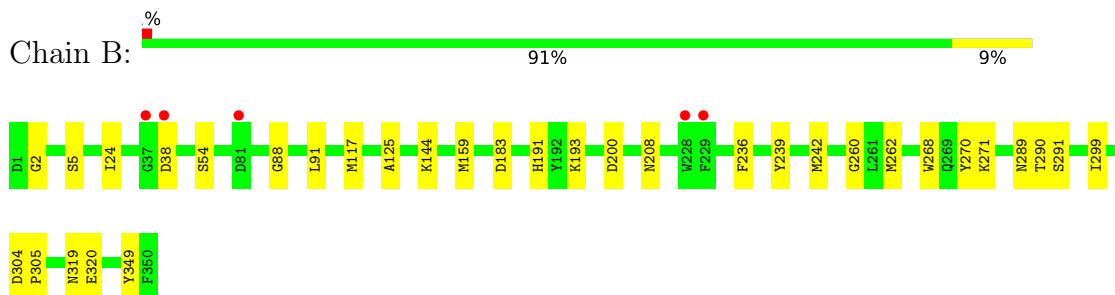
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

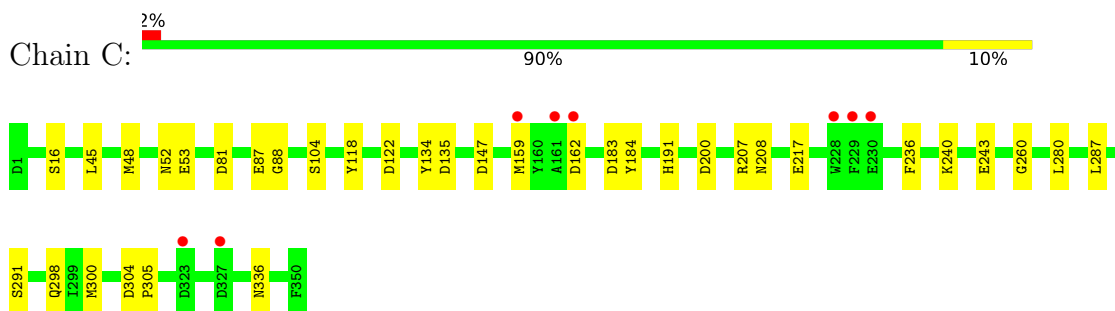
• Molecule 1: Chitoporin



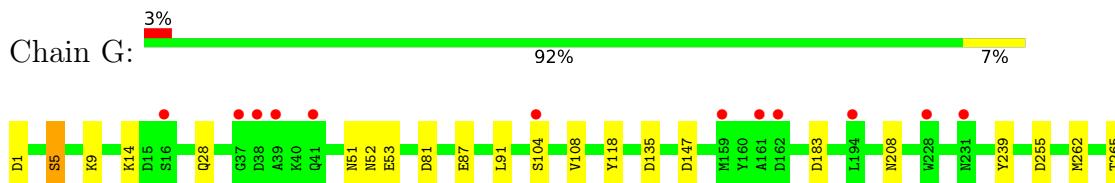
• Molecule 1: Chitoporin



• Molecule 1: Chitoporin

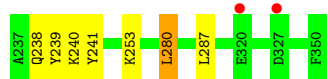
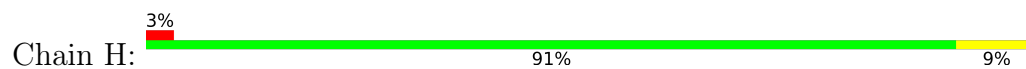


• Molecule 1: Chitoporin

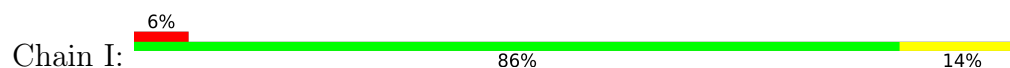




● Molecule 1: Chitoporin



● Molecule 1: Chitoporin



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	99.33Å 102.92Å 172.58Å 90.00° 95.29° 90.00°	Depositor
Resolution (Å)	31.38 – 2.21 31.38 – 2.21	Depositor EDS
% Data completeness (in resolution range)	98.2 (31.38-2.21) 98.1 (31.38-2.21)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.43 (at 2.22Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.189 , 0.222 0.189 , 0.222	Depositor DCC
R_{free} test set	8486 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	30.2	Xtriage
Anisotropy	0.249	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 39.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	17092	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.06% 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: NA, LLL, 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	0.44	0/2784	0.62	0/3773
1	B	0.46	0/2780	0.62	0/3768
1	C	0.43	0/2759	0.61	0/3739
1	G	0.37	0/2752	0.57	0/3732
1	H	0.36	0/2766	0.55	0/3747
1	I	0.32	0/2730	0.50	0/3703
All	All	0.40	0/16571	0.58	0/22462

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [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	2715	0	2458	20	0
1	B	2711	0	2454	25	0
1	C	2692	0	2431	22	0
1	G	2685	0	2418	22	0
1	H	2699	0	2449	20	0
1	I	2665	0	2386	29	0
2	A	3	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	3	0	0	0	0
2	C	3	0	0	0	0
2	G	3	0	0	0	0
2	H	3	0	0	0	0
2	I	3	0	0	0	0
3	A	31	0	47	2	0
3	B	24	0	30	2	0
3	C	65	0	90	3	0
3	G	16	0	21	2	0
3	H	15	0	19	1	0
4	C	31	0	39	2	0
5	A	143	0	0	0	0
5	B	151	0	0	0	0
5	C	147	0	0	1	0
5	G	100	0	0	1	0
5	H	103	0	0	0	0
5	I	81	0	0	0	0
All	All	17092	0	14842	124	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 4.

All (124) 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:159:MET:HE3	1:B:193:LYS:HE3	1.31	1.09
1:H:239:TYR:HB2	3:H:404:C8E:H161	1.62	0.81
1:G:1:ASP:N	5:G:501:HOH:O	2.23	0.72
1:B:159:MET:CE	1:B:193:LYS:HE3	2.16	0.70
1:H:280:LEU:HD23	1:H:287:LEU:HD12	1.75	0.68
1:G:239:TYR:HB2	3:G:404:C8E:H162	1.77	0.66
1:G:268:TRP:HE3	1:G:299:ILE:HD11	1.61	0.66
1:A:289:ASN:HB3	1:A:320:GLU:HG3	1.78	0.64
1:B:239:TYR:HB2	3:B:405:C8E:H132	1.79	0.64
1:G:1:ASP:OD2	1:H:148:ARG:NH2	2.29	0.63
1:G:9:LYS:NZ	1:H:76:GLU:OE1	2.31	0.63
1:A:1:ASP:O	1:A:5:SER:HA	1.98	0.63
1:G:1:ASP:OD2	1:H:148:ARG:NH1	2.31	0.63
1:A:280:LEU:HD23	1:A:287:LEU:HD12	1.79	0.63
1:I:167:ASP:O	1:I:188:ILE:HD12	2.00	0.62
1:G:53:GLU:OE2	1:I:2:GLY:HA2	2.03	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:LYS:HD2	1:B:242:MET:SD	2.43	0.58
1:C:280:LEU:HD23	1:C:287:LEU:HD12	1.85	0.58
1:B:268:TRP:HE3	1:B:299:ILE:HD11	1.70	0.56
1:G:268:TRP:CE3	1:G:299:ILE:HD11	2.41	0.55
1:A:255:ASP:OD2	3:A:405:C8E:H161	2.07	0.55
1:I:32:ARG:HG2	1:I:341:GLU:HG3	1.88	0.55
1:G:28:GLN:HB3	1:G:51:ASN:HB3	1.89	0.54
1:I:262:MET:HG3	1:I:271:LYS:HG3	1.91	0.52
1:C:87:GLU:CD	1:C:87:GLU:H	2.18	0.51
1:I:61:LYS:HD3	1:I:72:ILE:HG22	1.93	0.50
1:B:5:SER:HB3	1:C:122:ASP:OD2	2.12	0.50
1:A:48:MET:HB3	3:C:409:C8E:H161	1.93	0.50
1:C:134:TYR:O	1:C:240:LYS:NZ	2.46	0.49
1:I:144:LYS:HE2	1:I:145:TYR:CZ	2.47	0.49
1:I:147:ASP:OD1	1:I:148:ARG:N	2.45	0.49
1:C:191:HIS:CD2	1:C:200:ASP:OD1	2.66	0.48
1:H:19:TYR:CZ	1:I:21:VAL:HB	2.48	0.48
1:I:290:THR:HA	1:I:319:ASN:HB2	1.95	0.48
1:A:118:TYR:HE1	1:A:135:ASP:OD1	1.96	0.48
1:H:241:TYR:OH	1:H:253:LYS:HD3	2.13	0.48
1:G:118:TYR:CG	1:G:147:ASP:HA	2.49	0.48
1:A:183:ASP:HA	1:A:208:ASN:HB2	1.96	0.48
1:C:207:ARG:HD3	1:C:217:GLU:HG3	1.94	0.47
1:C:291:SER:OG	3:C:407:C8E:H192	2.14	0.47
1:G:183:ASP:HA	1:G:208:ASN:HB2	1.97	0.47
1:H:118:TYR:CG	1:H:147:ASP:HA	2.50	0.47
1:H:125:ALA:HA	1:H:236:PHE:CE1	2.50	0.47
1:B:290:THR:HA	1:B:319:ASN:HB2	1.98	0.46
1:I:236:PHE:CE2	1:I:260:GLY:HA3	2.51	0.46
1:C:159:MET:HE3	1:C:159:MET:HB2	1.69	0.46
1:A:9:LYS:HG3	1:B:24:ILE:HD11	1.98	0.45
1:B:262:MET:HG3	1:B:271:LYS:HG3	1.98	0.45
1:I:24:ILE:O	1:I:54:SER:HA	2.16	0.45
1:A:239:TYR:HB2	3:A:405:C8E:H71	1.98	0.45
1:B:291:SER:OG	3:B:404:C8E:H142	2.16	0.45
1:C:118:TYR:CG	1:C:147:ASP:HA	2.52	0.45
1:H:5:SER:HB3	1:I:122:ASP:OD2	2.17	0.45
1:G:14:LYS:HE2	1:H:59:ARG:NH2	2.32	0.45
1:I:92:GLY:HA2	1:I:96:THR:OG1	2.16	0.45
1:A:87:GLU:OE1	1:A:87:GLU:N	2.36	0.45
1:B:270:TYR:CD2	1:B:299:ILE:HD13	2.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:87:GLU:OE1	1:G:87:GLU:N	2.35	0.45
1:C:48:MET:HB2	1:C:48:MET:HE2	1.72	0.45
1:I:168:ALA:HB2	1:I:188:ILE:HD13	1.98	0.45
1:A:300:MET:HE2	1:A:308:VAL:HG21	1.99	0.45
1:B:38:ASP:OD1	1:B:38:ASP:C	2.59	0.45
1:H:15:ASP:OD2	1:H:62:LYS:HD3	2.17	0.44
1:H:24:ILE:O	1:H:54:SER:HA	2.17	0.44
1:I:144:LYS:HD2	1:I:242:MET:HE3	1.98	0.44
1:I:166:ILE:HG23	1:I:188:ILE:HD11	1.98	0.44
1:I:241:TYR:OH	1:I:253:LYS:HD3	2.17	0.44
1:G:52:ASN:HB3	1:G:81:ASP:HB3	1.99	0.44
1:A:24:ILE:O	1:A:54:SER:HA	2.17	0.44
1:B:289:ASN:HB3	1:B:320:GLU:HG2	1.99	0.44
1:C:243:GLU:HG3	5:C:505:HOH:O	2.18	0.44
1:I:304:ASP:CG	1:I:305:PRO:HD2	2.43	0.44
1:G:255:ASP:OD2	3:G:404:C8E:H82	2.18	0.44
1:A:167:ASP:OD1	1:A:191:HIS:NE2	2.48	0.43
1:B:117:MET:HE2	1:B:117:MET:HB2	1.82	0.43
4:C:401:LLL:O23	4:C:401:LLL:H62	2.19	0.43
1:G:1:ASP:OD2	1:H:148:ARG:CZ	2.66	0.43
1:B:24:ILE:O	1:B:54:SER:HA	2.18	0.43
1:G:1:ASP:O	1:G:5:SER:HA	2.17	0.43
1:B:304:ASP:CG	1:B:305:PRO:HD2	2.44	0.43
1:I:53:GLU:HG2	1:I:79:TYR:CD2	2.53	0.43
1:B:2:GLY:HA2	1:C:53:GLU:OE2	2.19	0.43
1:C:236:PHE:CE2	1:C:260:GLY:HA3	2.53	0.43
1:G:91:LEU:O	1:H:88:GLY:HA2	2.18	0.43
1:C:183:ASP:HA	1:C:208:ASN:HB2	2.01	0.43
1:B:236:PHE:CE2	1:B:260:GLY:HA3	2.54	0.42
1:I:315:MET:HG3	1:I:340:ASN:OD1	2.20	0.42
1:B:125:ALA:HA	1:B:236:PHE:CE1	2.55	0.42
1:I:296:SER:HB2	1:I:314:ARG:HB3	2.01	0.42
1:G:347:GLU:OE1	1:I:4:ASN:HB2	2.19	0.42
1:C:52:ASN:HB3	1:C:81:ASP:HB3	2.01	0.42
1:G:135:ASP:OD1	1:G:135:ASP:C	2.63	0.42
1:A:118:TYR:CG	1:A:147:ASP:HA	2.55	0.42
1:I:91:LEU:HD23	1:I:91:LEU:HA	1.89	0.42
1:B:91:LEU:O	1:C:88:GLY:HA2	2.19	0.42
1:B:191:HIS:ND1	1:B:200:ASP:OD1	2.50	0.42
1:A:9:LYS:HG2	1:B:349:TYR:CZ	2.54	0.42
1:C:304:ASP:CG	1:C:305:PRO:HD2	2.45	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:262:MET:HE3	1:G:262:MET:HB2	1.92	0.41
1:I:277:ASN:O	1:I:291:SER:HB2	2.19	0.41
1:H:61:LYS:HG2	1:H:72:ILE:HG22	2.01	0.41
1:C:184:TYR:CD1	3:C:409:C8E:H201	2.55	0.41
1:A:117:MET:HE2	1:A:117:MET:HB2	1.86	0.41
1:A:209:ILE:HB	1:A:216:TRP:HB2	2.02	0.41
1:A:290:THR:HA	1:A:319:ASN:HB2	2.02	0.41
1:H:134:TYR:O	1:H:240:LYS:NZ	2.53	0.41
1:I:127:ASN:OD1	1:I:271:LYS:NZ	2.36	0.41
1:I:289:ASN:HD22	1:I:289:ASN:HA	1.75	0.41
1:C:159:MET:HG2	1:C:162:ASP:HA	2.03	0.41
1:B:183:ASP:HA	1:B:208:ASN:HB2	2.03	0.41
1:G:290:THR:HA	1:G:319:ASN:HB2	2.03	0.41
1:H:14:LYS:HB3	1:H:14:LYS:HE2	1.85	0.41
1:I:270:TYR:N	1:I:270:TYR:CD1	2.89	0.41
1:A:125:ALA:HA	1:A:236:PHE:CE1	2.56	0.41
1:C:135:ASP:OD1	1:C:135:ASP:C	2.63	0.41
1:I:45:LEU:HD13	1:I:336:ASN:HB3	2.02	0.41
1:H:222:LEU:HD11	1:H:238:GLN:OE1	2.21	0.41
1:I:29:ALA:HB1	1:I:48:MET:HE2	2.03	0.41
4:C:401:LLL:H1	4:C:401:LLL:H122	1.86	0.40
1:H:67:PHE:CD2	1:H:69:PRO:HD2	2.56	0.40
1:B:268:TRP:CE3	1:B:299:ILE:HD11	2.54	0.40
1:A:91:LEU:O	1:B:88:GLY:HA2	2.21	0.40
1:C:45:LEU:HD13	1:C:336:ASN:HB3	2.04	0.40
1:C:298:GLN:NE2	1:C:300:MET:HE3	2.36	0.40

There are no symmetry-related clashes.

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	348/350 (99%)	337 (97%)	11 (3%)	0	100	100
1	B	348/350 (99%)	339 (97%)	9 (3%)	0	100	100
1	C	348/350 (99%)	339 (97%)	9 (3%)	0	100	100
1	G	348/350 (99%)	338 (97%)	10 (3%)	0	100	100
1	H	348/350 (99%)	338 (97%)	10 (3%)	0	100	100
1	I	348/350 (99%)	339 (97%)	9 (3%)	0	100	100
All	All	2088/2100 (99%)	2030 (97%)	58 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	265/267 (99%)	262 (99%)	3 (1%)	65	78
1	B	264/267 (99%)	264 (100%)	0	100	100
1	C	260/267 (97%)	258 (99%)	2 (1%)	73	84
1	G	258/267 (97%)	254 (98%)	4 (2%)	55	70
1	H	262/267 (98%)	257 (98%)	5 (2%)	50	64
1	I	254/267 (95%)	253 (100%)	1 (0%)	84	91
All	All	1563/1602 (98%)	1548 (99%)	15 (1%)	68	80

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	SER
1	A	167	ASP
1	A	194	LEU
1	C	16	SER
1	C	104	SER
1	G	5	SER
1	G	104	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	108	VAL
1	G	265	THR
1	H	98	VAL
1	H	102	SER
1	H	104	SER
1	H	234	SER
1	H	280	LEU
1	I	226	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	GLN
1	A	226	GLN
1	B	41	GLN
1	B	63	GLN
1	B	198	GLN
1	C	41	GLN
1	C	198	GLN
1	G	63	GLN
1	H	63	GLN
1	H	198	GLN
1	H	251	ASN
1	H	269	GLN
1	I	289	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

Of 30 ligands modelled in this entry, 18 are monoatomic - leaving 12 for Mogul analysis.

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	B	405	-	13,13,20	0.50	0	12,12,19	0.41	0
3	C8E	H	404	-	14,14,20	0.49	0	13,13,19	0.20	0
3	C8E	C	408	-	9,9,20	0.43	0	8,8,19	0.22	0
3	C8E	A	405	-	20,20,20	0.42	0	19,19,19	0.51	0
3	C8E	C	405	-	13,13,20	0.46	0	12,12,19	0.27	0
3	C8E	C	406	-	9,9,20	0.46	0	8,8,19	0.38	0
3	C8E	A	404	-	9,9,20	0.49	0	8,8,19	0.24	0
3	C8E	G	404	-	15,15,20	0.41	0	14,14,19	0.26	0
3	C8E	B	404	-	9,9,20	0.39	0	8,8,19	0.48	0
3	C8E	C	407	-	20,20,20	0.42	0	19,19,19	0.41	0
3	C8E	C	409	-	9,9,20	0.41	0	8,8,19	0.44	0
4	LLL	C	401	-	31,33,33	0.58	0	33,49,49	0.78	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	B	405	-	-	8/11/11/18	-
3	C8E	H	404	-	-	8/12/12/18	-
3	C8E	C	408	-	-	6/7/7/18	-
3	C8E	A	405	-	-	5/18/18/18	-
3	C8E	C	405	-	-	5/11/11/18	-
3	C8E	C	406	-	-	5/7/7/18	-
3	C8E	A	404	-	-	5/7/7/18	-
3	C8E	G	404	-	-	12/13/13/18	-
3	C8E	B	404	-	-	5/7/7/18	-
3	C8E	C	407	-	-	12/18/18/18	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	C8E	C	409	-	-	5/7/7/18	-
4	LLL	C	401	-	-	4/11/65/65	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (80) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	401	LLL	C23-C33-N33-C93
4	C	401	LLL	O53-C13-O62-C62
4	C	401	LLL	C23-C13-O62-C62
3	H	404	C8E	O12-C13-C14-O15
3	C	408	C8E	O15-C16-C17-O18
3	C	409	C8E	O15-C16-C17-O18
3	B	405	C8E	O12-C13-C14-O15
3	G	404	C8E	O9-C10-C11-O12
3	A	404	C8E	O18-C19-C20-O21
3	C	409	C8E	C20-C19-O18-C17
3	A	405	C8E	O18-C19-C20-O21
3	B	404	C8E	O12-C13-C14-O15
3	C	406	C8E	O18-C19-C20-O21
3	B	405	C8E	O9-C10-C11-O12
3	H	404	C8E	C7-C8-O9-C10
3	C	406	C8E	O12-C13-C14-O15
3	C	408	C8E	O18-C19-C20-O21
3	C	407	C8E	C6-C7-C8-O9
3	G	404	C8E	O12-C13-C14-O15
3	C	407	C8E	C5-C6-C7-C8
3	G	404	C8E	C6-C7-C8-O9
3	C	407	C8E	C4-C5-C6-C7
3	H	404	C8E	O9-C10-C11-O12
3	A	404	C8E	O12-C13-C14-O15
3	B	404	C8E	O18-C19-C20-O21
3	G	404	C8E	O18-C19-C20-O21
3	C	407	C8E	O12-C13-C14-O15
3	C	407	C8E	C3-C4-C5-C6
3	C	407	C8E	C2-C3-C4-C5
3	A	405	C8E	O15-C16-C17-O18
3	A	405	C8E	C4-C5-C6-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	C	406	C8E	C13-C14-O15-C16
3	C	408	C8E	O12-C13-C14-O15
3	B	405	C8E	C20-C19-O18-C17
3	C	408	C8E	C16-C17-O18-C19
3	G	404	C8E	C11-C10-O9-C8
3	A	405	C8E	C10-C11-O12-C13
3	B	405	C8E	C10-C11-O12-C13
3	C	407	C8E	C16-C17-O18-C19
3	A	405	C8E	C1-C2-C3-C4
3	C	407	C8E	C20-C19-O18-C17
3	G	404	C8E	C13-C14-O15-C16
3	G	404	C8E	C17-C16-O15-C14
3	B	405	C8E	C16-C17-O18-C19
3	C	405	C8E	C16-C17-O18-C19
3	B	404	C8E	C17-C16-O15-C14
3	H	404	C8E	C20-C19-O18-C17
3	H	404	C8E	C10-C11-O12-C13
3	A	404	C8E	C17-C16-O15-C14
3	B	404	C8E	C20-C19-O18-C17
3	C	406	C8E	C20-C19-O18-C17
3	C	409	C8E	C13-C14-O15-C16
3	C	408	C8E	C17-C16-O15-C14
3	C	407	C8E	C7-C8-O9-C10
3	A	404	C8E	C13-C14-O15-C16
3	B	405	C8E	O18-C19-C20-O21
3	C	407	C8E	C13-C14-O15-C16
3	H	404	C8E	C17-C16-O15-C14
3	H	404	C8E	O15-C16-C17-O18
3	C	409	C8E	C16-C17-O18-C19
3	C	408	C8E	C13-C14-O15-C16
3	G	404	C8E	C16-C17-O18-C19
3	C	405	C8E	O18-C19-C20-O21
3	B	405	C8E	C17-C16-O15-C14
3	G	404	C8E	C7-C8-O9-C10
3	C	405	C8E	O12-C13-C14-O15
3	G	404	C8E	C20-C19-O18-C17
4	C	401	LLL	O51-C11-O11-C42
3	B	404	C8E	C16-C17-O18-C19
3	C	407	C8E	C17-C16-O15-C14
3	C	406	C8E	O15-C16-C17-O18
3	H	404	C8E	C11-C10-O9-C8
3	A	404	C8E	O15-C16-C17-O18

Continued on next page...

Continued from previous page...

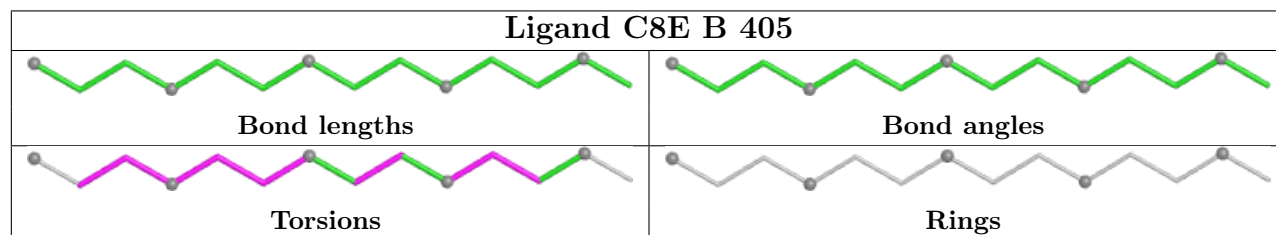
Mol	Chain	Res	Type	Atoms
3	C	405	C8E	C13-C14-O15-C16
3	G	404	C8E	C14-C13-O12-C11
3	C	409	C8E	O18-C19-C20-O21
3	G	404	C8E	O15-C16-C17-O18
3	C	407	C8E	O9-C10-C11-O12
3	B	405	C8E	O15-C16-C17-O18
3	C	405	C8E	O15-C16-C17-O18

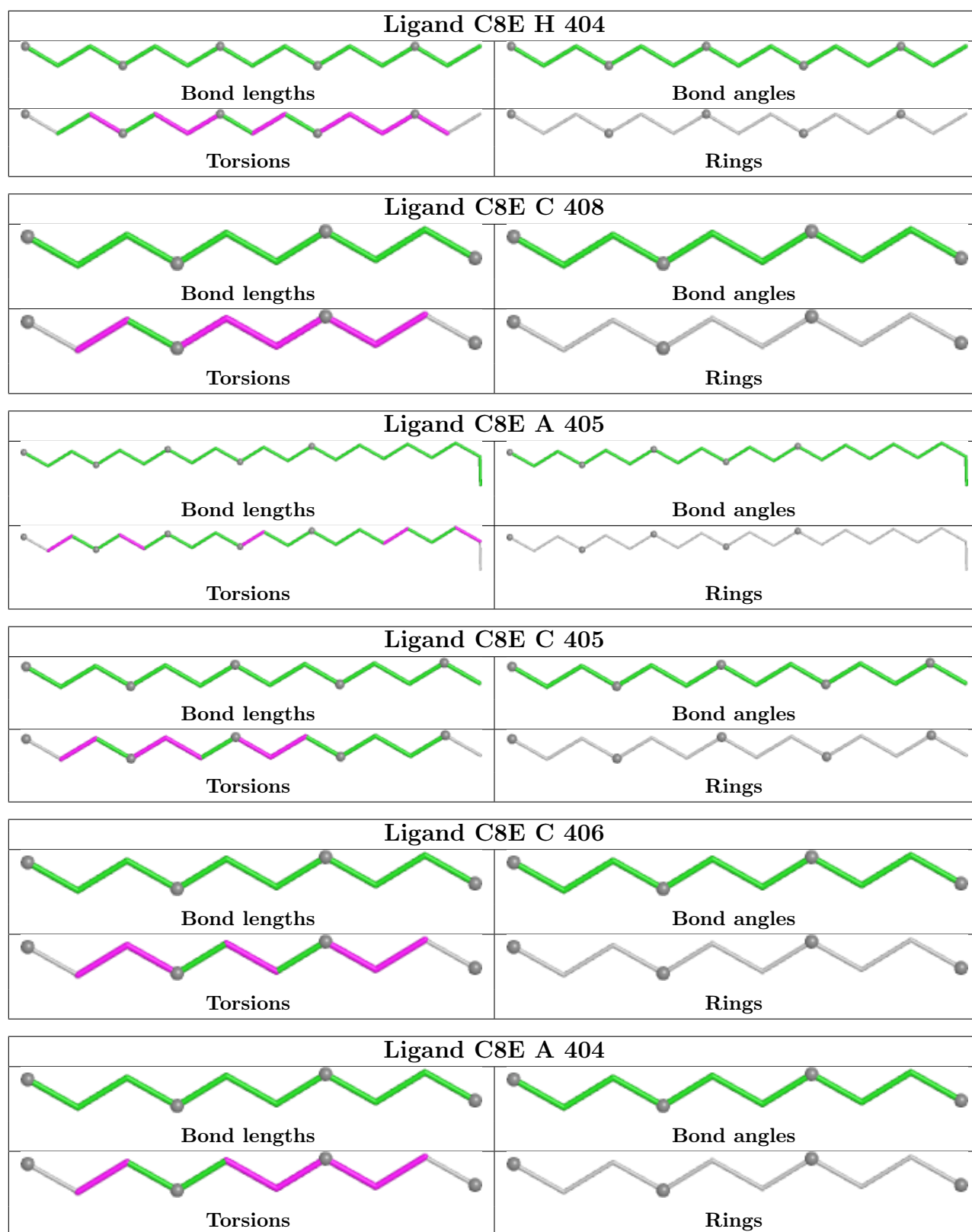
There are no ring outliers.

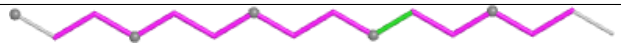
8 monomers are involved in 12 short contacts:

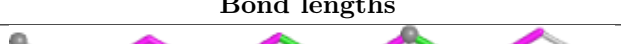
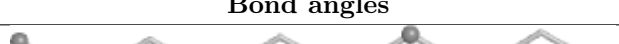
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	405	C8E	1	0
3	H	404	C8E	1	0
3	A	405	C8E	2	0
3	G	404	C8E	2	0
3	B	404	C8E	1	0
3	C	407	C8E	1	0
3	C	409	C8E	2	0
4	C	401	LLL	2	0

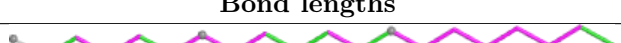
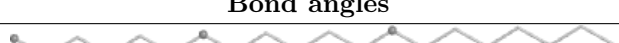
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

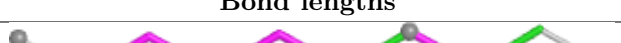
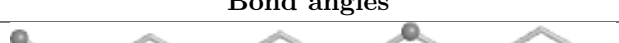


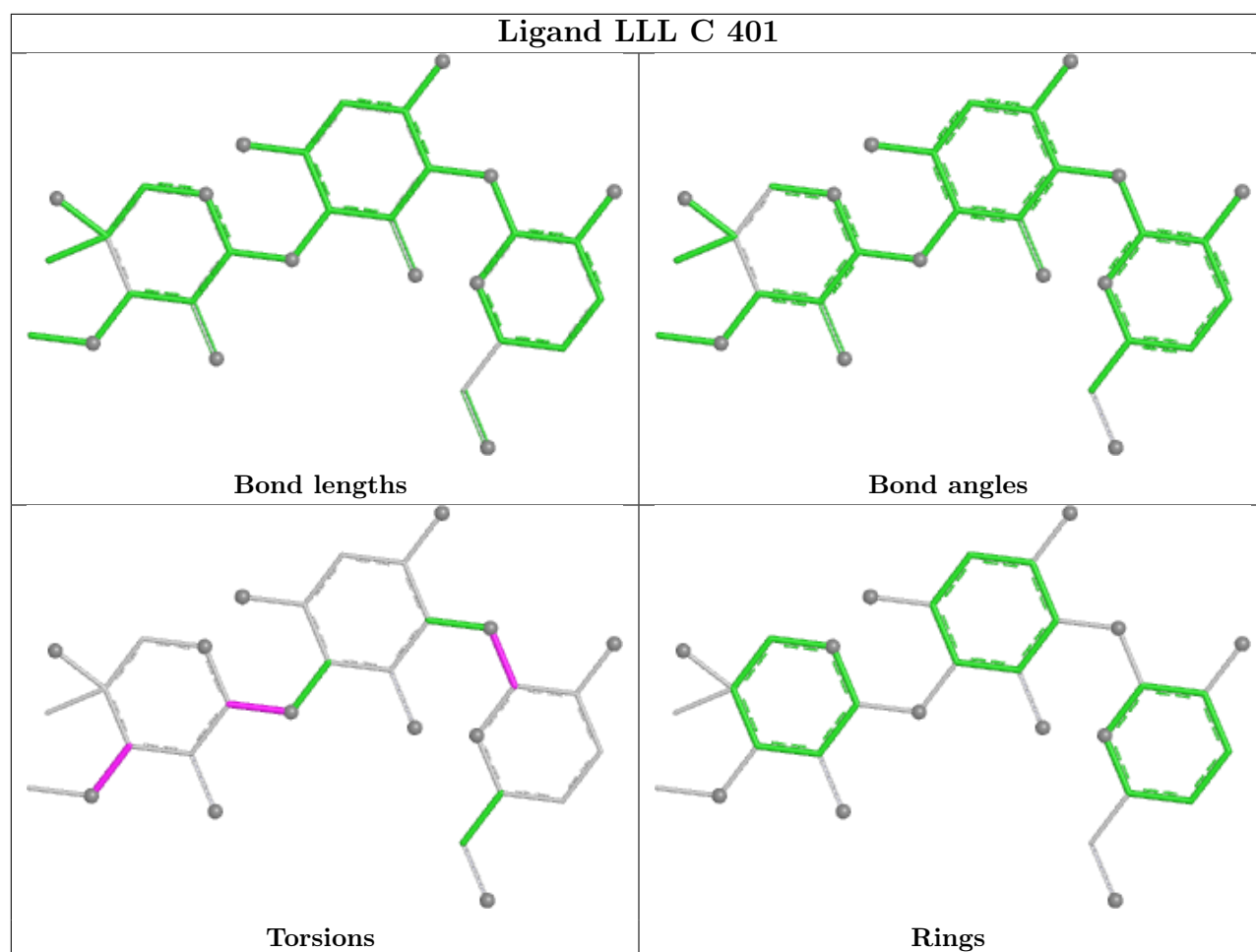


Ligand C8E G 404	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand C8E B 404	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand C8E C 407	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand C8E C 409	
 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	350/350 (100%)	0.02	8 (2%) 61 59	16, 27, 43, 57	0
1	B	350/350 (100%)	-0.07	5 (1%) 73 72	14, 25, 40, 56	0
1	C	350/350 (100%)	-0.02	8 (2%) 61 59	16, 26, 46, 65	0
1	G	350/350 (100%)	0.33	12 (3%) 48 45	22, 35, 53, 67	0
1	H	350/350 (100%)	0.29	11 (3%) 51 49	23, 34, 50, 69	0
1	I	350/350 (100%)	0.57	20 (5%) 29 26	25, 40, 62, 74	0
All	All	2100/2100 (100%)	0.18	64 (3%) 52 50	14, 31, 53, 74	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	228	TRP	5.3
1	I	228	TRP	5.0
1	I	162	ASP	4.8
1	C	228	TRP	4.3
1	C	162	ASP	4.0
1	A	1	ASP	3.7
1	A	228	TRP	3.6
1	I	161	ALA	3.4
1	B	228	TRP	3.4
1	H	229	PHE	3.3
1	A	38	ASP	3.2
1	I	231	ASN	3.0
1	C	161	ALA	2.9
1	H	231	ASN	2.9
1	I	200	ASP	2.9
1	I	103	ALA	2.9
1	G	161	ALA	2.9
1	I	105	TRP	2.8
1	H	68	GLU	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	195	GLY	2.8
1	B	229	PHE	2.8
1	I	37	GLY	2.7
1	A	196	PRO	2.7
1	G	37	GLY	2.7
1	I	320	GLU	2.7
1	G	228	TRP	2.7
1	I	68	GLU	2.6
1	C	323	ASP	2.6
1	C	229	PHE	2.6
1	G	16	SER	2.6
1	I	329	ALA	2.5
1	H	327	ASP	2.5
1	A	194	LEU	2.5
1	I	11	TYR	2.5
1	A	37	GLY	2.4
1	I	159	MET	2.4
1	I	160	TYR	2.4
1	B	37	GLY	2.4
1	G	39	ALA	2.4
1	H	200	ASP	2.3
1	B	81	ASP	2.3
1	A	230	GLU	2.3
1	G	231	ASN	2.3
1	I	38	ASP	2.3
1	H	230	GLU	2.3
1	B	38	ASP	2.2
1	G	38	ASP	2.2
1	I	104	SER	2.2
1	I	288	SER	2.2
1	H	38	ASP	2.2
1	H	182	ASP	2.2
1	I	245	ASP	2.2
1	C	159	MET	2.2
1	G	159	MET	2.2
1	G	162	ASP	2.2
1	C	230	GLU	2.2
1	H	6	ASP	2.1
1	I	283	ASP	2.1
1	I	36	SER	2.1
1	C	327	ASP	2.1
1	H	320	GLU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	194	LEU	2.1
1	G	104	SER	2.0
1	G	41	GLN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	LLL	C	401	31/31	0.43	0.24	53,68,75,79	0
3	C8E	C	406	10/21	0.83	0.16	48,52,54,55	0
3	C8E	A	405	21/21	0.83	0.15	32,48,58,64	0
3	C8E	H	404	15/21	0.84	0.15	43,51,58,58	0
3	C8E	C	407	21/21	0.84	0.17	37,51,58,62	0
3	C8E	C	409	10/21	0.86	0.13	29,39,48,49	0
3	C8E	B	405	14/21	0.86	0.13	30,43,52,54	0
3	C8E	C	405	14/21	0.86	0.14	35,46,54,55	0
3	C8E	G	404	16/21	0.87	0.13	40,47,54,55	0
2	NA	A	401	1/1	0.88	0.13	30,30,30,30	0
3	C8E	C	408	10/21	0.88	0.13	38,53,54,54	0
3	C8E	B	404	10/21	0.89	0.12	35,37,48,49	0
3	C8E	A	404	10/21	0.90	0.12	39,43,51,51	0
2	NA	B	403	1/1	0.91	0.12	30,30,30,30	0
2	NA	H	403	1/1	0.92	0.17	38,38,38,38	0
2	NA	I	402	1/1	0.92	0.08	41,41,41,41	0
2	NA	I	403	1/1	0.93	0.12	38,38,38,38	0
2	NA	C	404	1/1	0.94	0.05	22,22,22,22	1
2	NA	G	403	1/1	0.95	0.10	42,42,42,42	0
2	NA	B	402	1/1	0.95	0.04	24,24,24,24	0

Continued on next page...

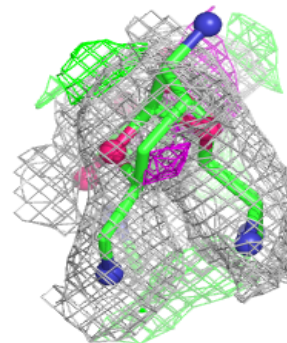
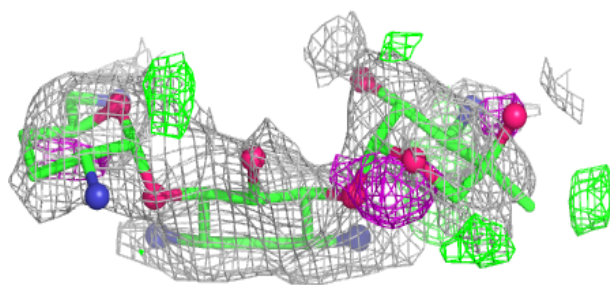
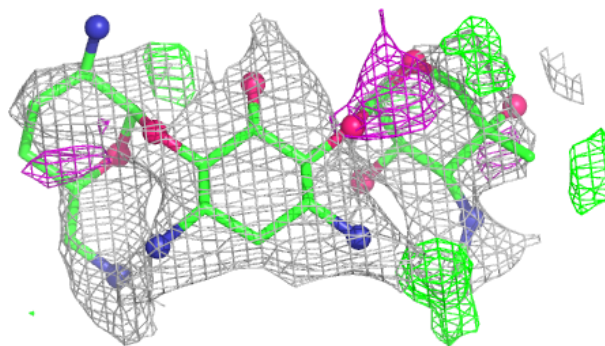
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NA	G	401	1/1	0.96	0.11	21,21,21,21	0
2	NA	C	402	1/1	0.97	0.06	25,25,25,25	0
2	NA	H	401	1/1	0.97	0.12	22,22,22,22	0
2	NA	H	402	1/1	0.97	0.04	34,34,34,34	0
2	NA	A	402	1/1	0.98	0.10	12,12,12,12	0
2	NA	G	402	1/1	0.98	0.05	37,37,37,37	0
2	NA	B	401	1/1	0.99	0.06	12,12,12,12	0
2	NA	A	403	1/1	0.99	0.04	25,25,25,25	0
2	NA	C	403	1/1	0.99	0.12	12,12,12,12	0
2	NA	I	401	1/1	1.00	0.03	25,25,25,25	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.

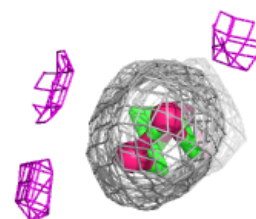
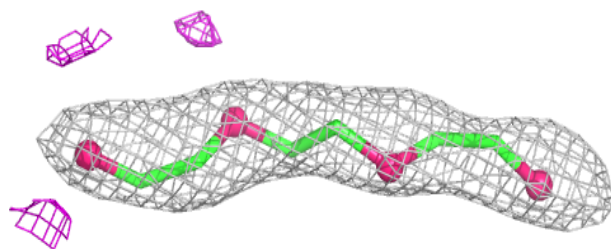
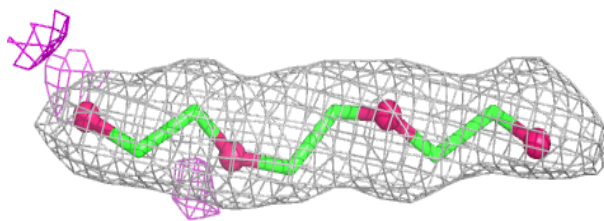
Electron density around LLL C 401:

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

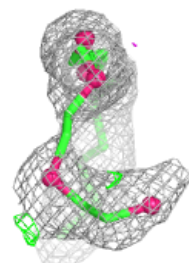
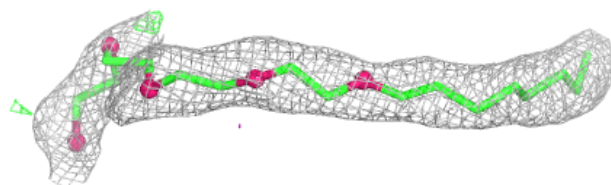
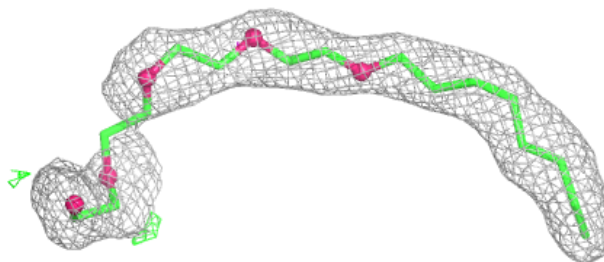


Electron density around C8E C 406:

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

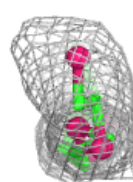
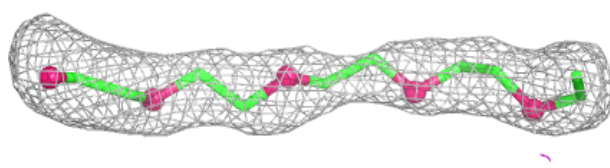
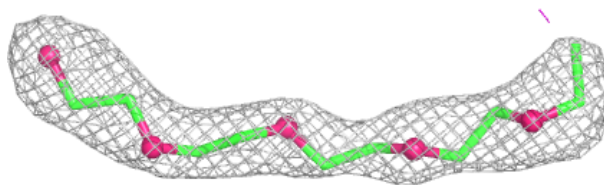
**Electron density around C8E A 405:**

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

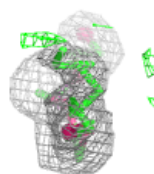
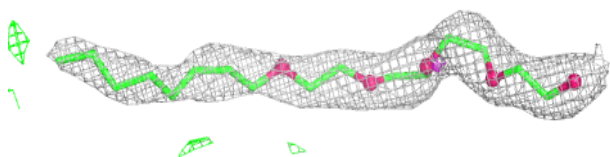
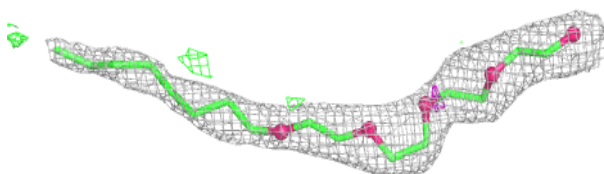


Electron density around C8E H 404:

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

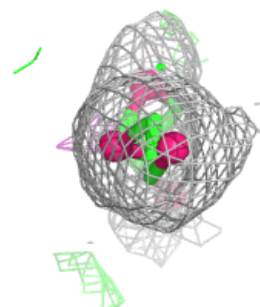
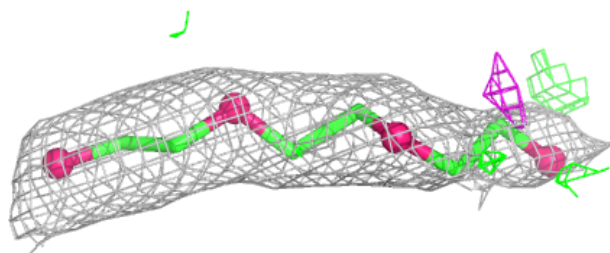
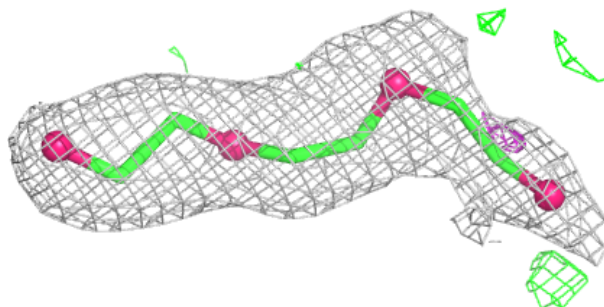
**Electron density around C8E C 407:**

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

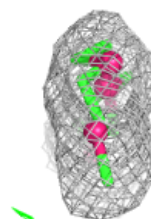
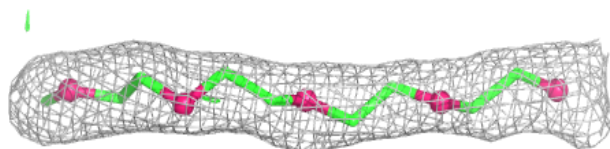
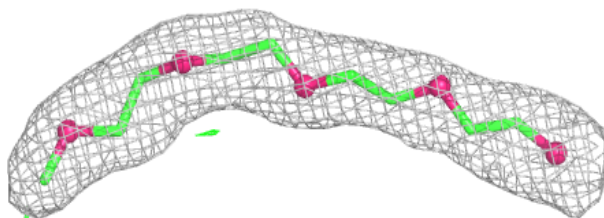


Electron density around C8E C 409:

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

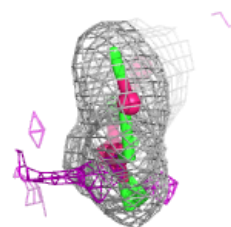
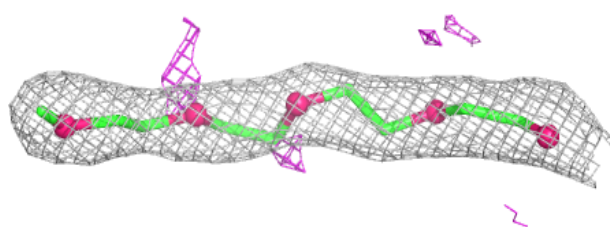
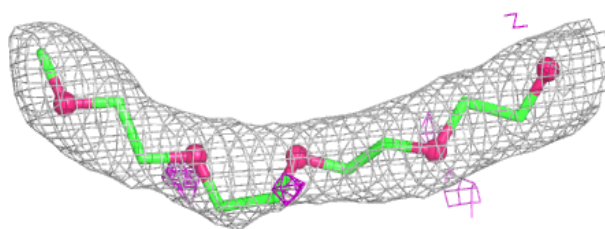
**Electron density around C8E B 405:**

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

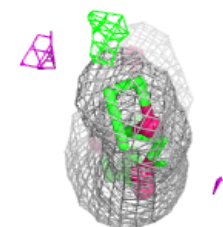
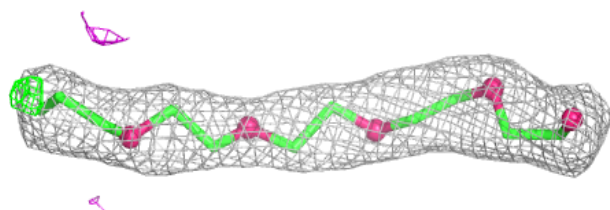
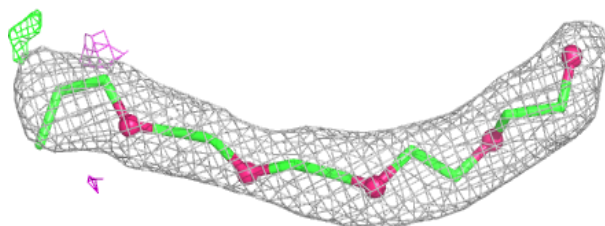


Electron density around C8E C 405:

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

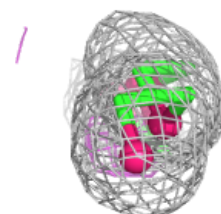
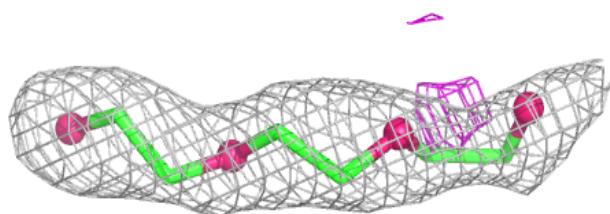
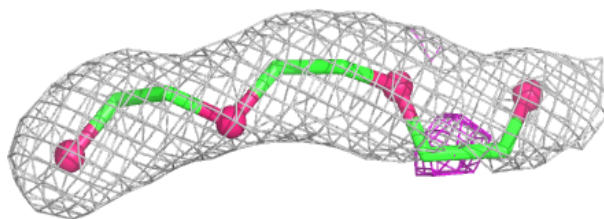
**Electron density around C8E G 404:**

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

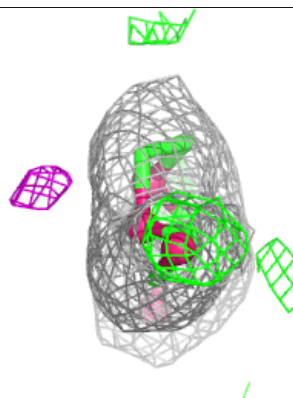
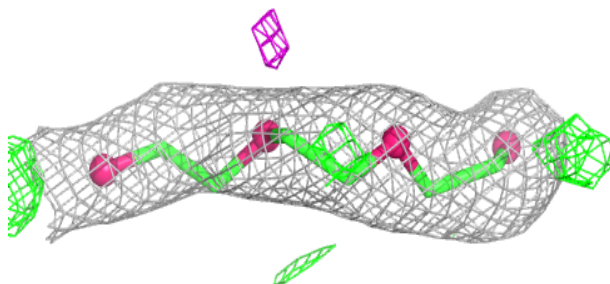
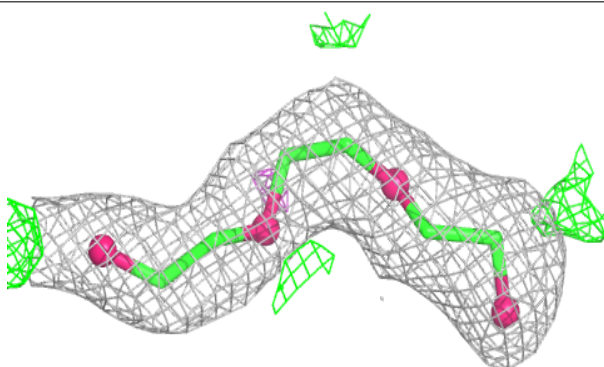


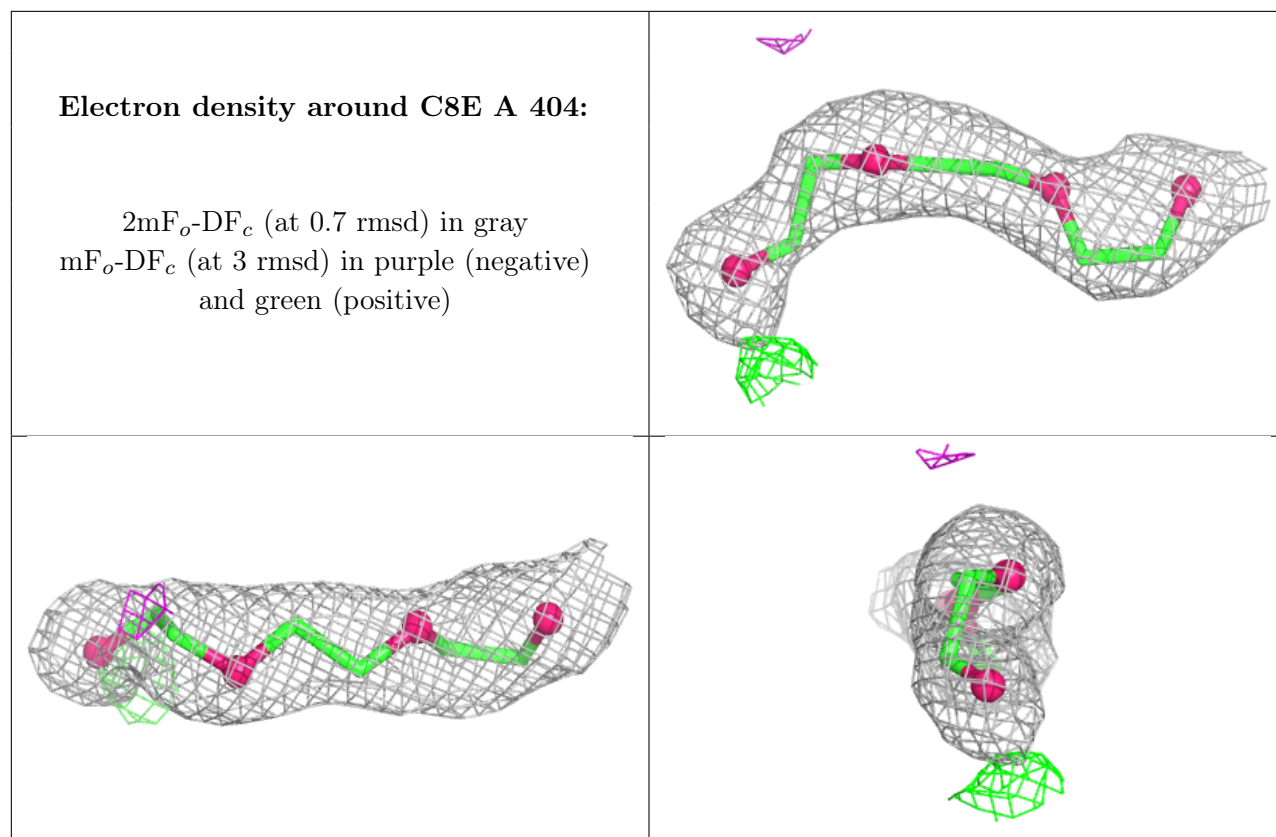
Electron density around C8E C 408:

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

**Electron density around C8E B 404:**

$2mF_o-DF_c$ (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.