



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 02:58 PM UTC

PDB ID : 5NUO / pdb_00005nuo
Title : Structural basis for maintenance of bacterial outer membrane lipid asymmetry
Authors : Abellon-Ruiz, J.; Kaptan, S.S.; Basle, A.; Claudi, B.; Bumann, D.;
Kleinekathofer, U.; van den Berg, B.
Deposited on : 2017-05-01
Resolution : 3.20 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

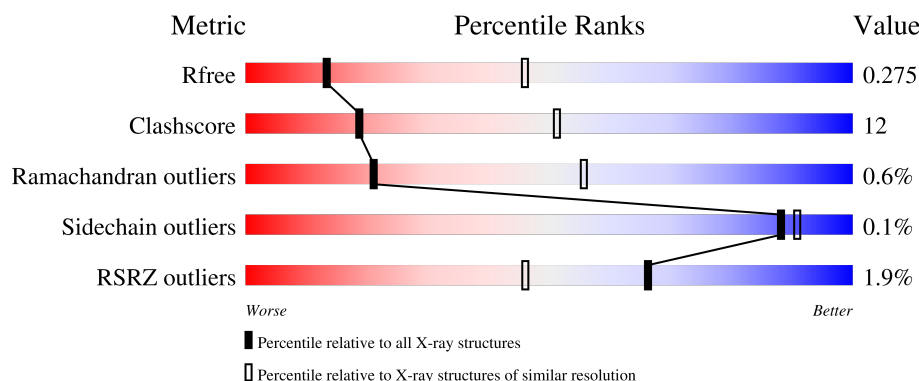
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	340	84% 16%
1	C	340	81% 19%
1	E	340	77% 23%
2	B	236	53% 31% 17%
2	D	236	56% 28% 15%

Continued on next page...

Continued from previous page...

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
4	C8E	E	403	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12971 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 Outer membrane protein F.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	340	Total	C	N	O	S	0	0	0
			2627	1654	438	532	3			
1	A	340	Total	C	N	O	S	0	0	0
			2627	1654	438	532	3			
1	E	340	Total	C	N	O	S	0	0	0
			2627	1654	438	532	3			

- Molecule 2 is a protein called ABC transporter permease.

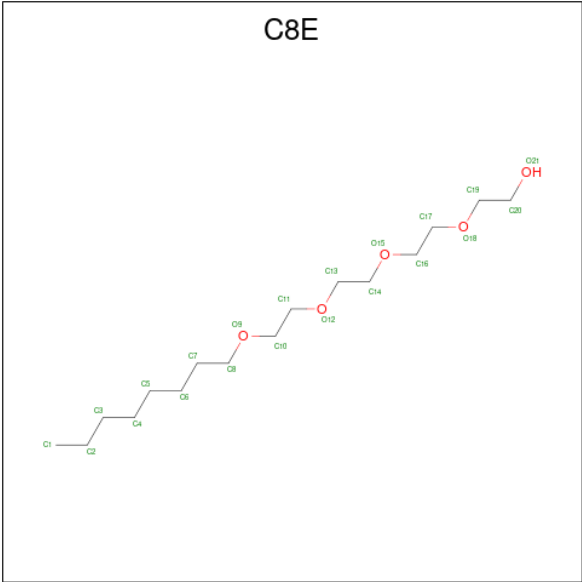
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	200	Total	C	N	O	S	0	0	0
			1601	1033	272	288	8			
2	B	197	Total	C	N	O	S	0	0	0
			1580	1022	266	284	8			
2	F	199	Total	C	N	O	S	0	0	0
			1597	1031	271	287	8			

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is (HYDROXYETHYLOXY)TRI(ETHYLOXY)OCTANE (CCD ID: C8E) (formula: C₁₆H₃₄O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			15	12	3		
4	C	1	Total	C	O	0	0
			16	13	3		
4	C	1	Total	C	O	0	0
			10	9	1		
4	C	1	Total	C	O	0	0
			16	13	3		
4	D	1	Total	C	O	0	0
			12	8	4		
4	D	1	Total	C	O	0	0
			13	11	2		
4	D	1	Total	C	O	0	0
			14	12	2		
4	D	1	Total	C	O	0	0
			9	6	3		
4	D	1	Total	C	O	0	0
			12	8	4		
4	A	1	Total	C	O	0	0
			19	14	5		
4	A	1	Total	C	O	0	0
			21	16	5		
4	A	1	Total	C	O	0	0
			14	11	3		
4	A	1	Total	C	O	0	0
			12	8	4		
4	B	1	Total	C	O	0	0
			21	16	5		

Continued on next page...

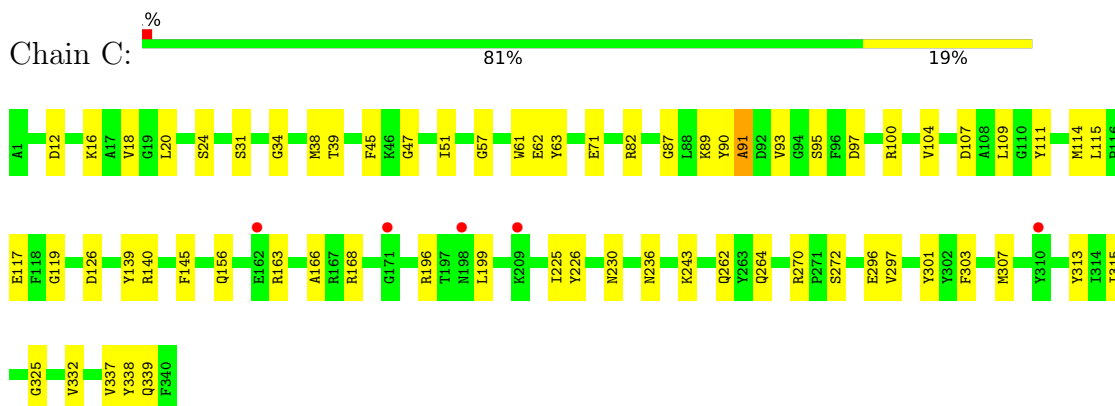
Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	E	1	Total	C	O	0	0
			13	9	4		
4	E	1	Total	C	O	0	0
			12	8	4		
4	E	1	Total	C	O	0	0
			11	10	1		
4	E	1	Total	C	O	0	0
			14	9	5		
4	F	1	Total	C	O	0	0
			12	10	2		
4	F	1	Total	C	O	0	0
			16	13	3		

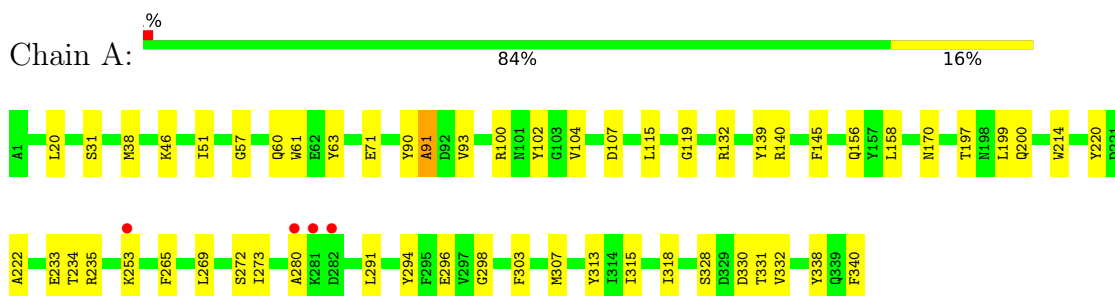
3 Residue-property plots

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.

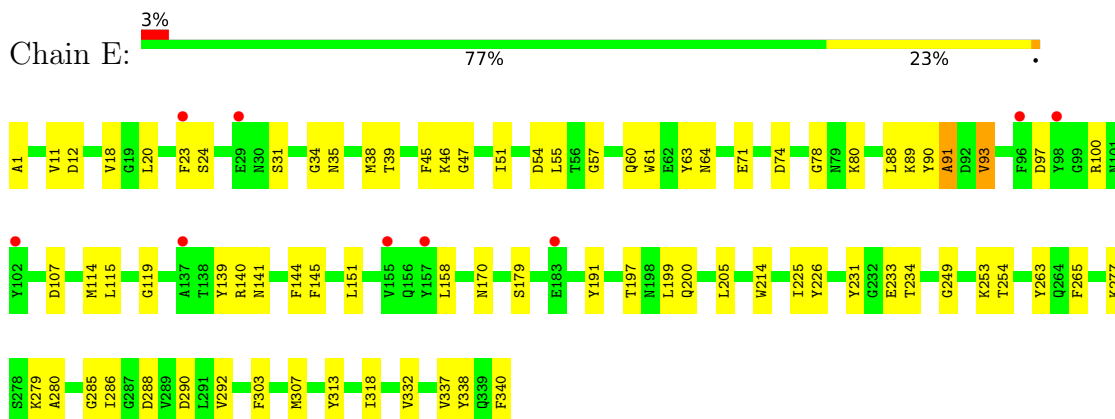
• Molecule 1: Outer membrane protein F



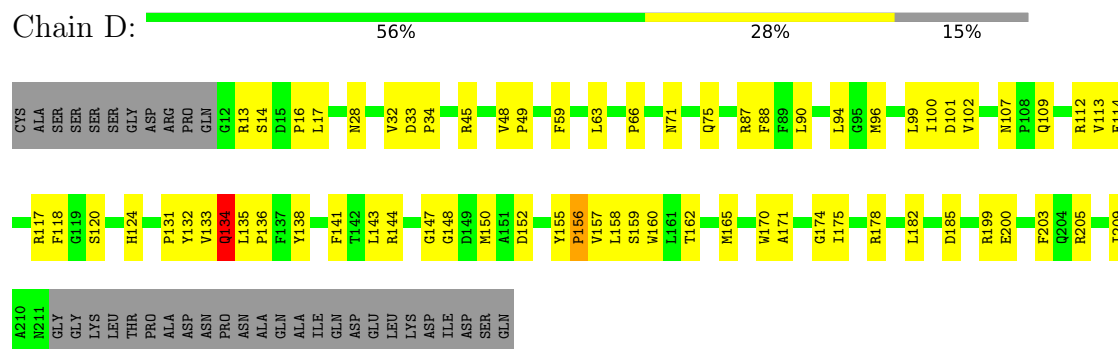
• Molecule 1: Outer membrane protein F



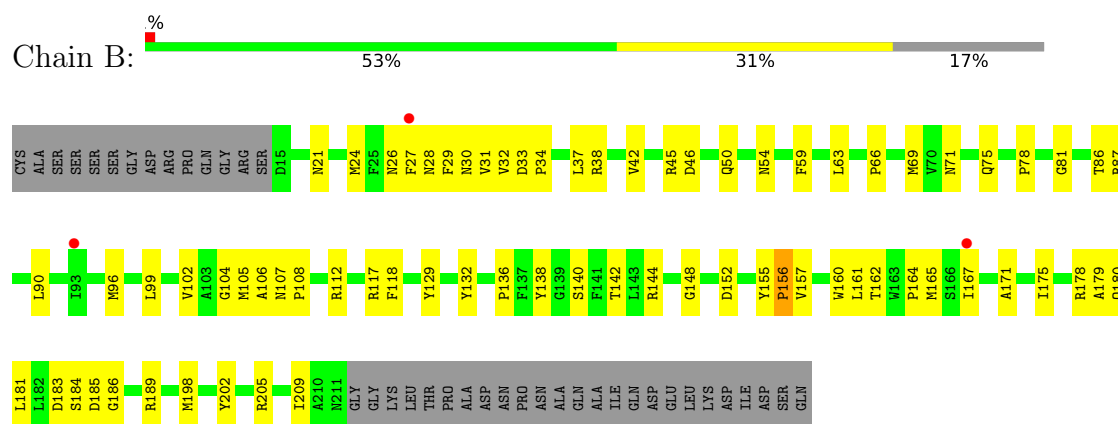
• Molecule 1: Outer membrane protein F



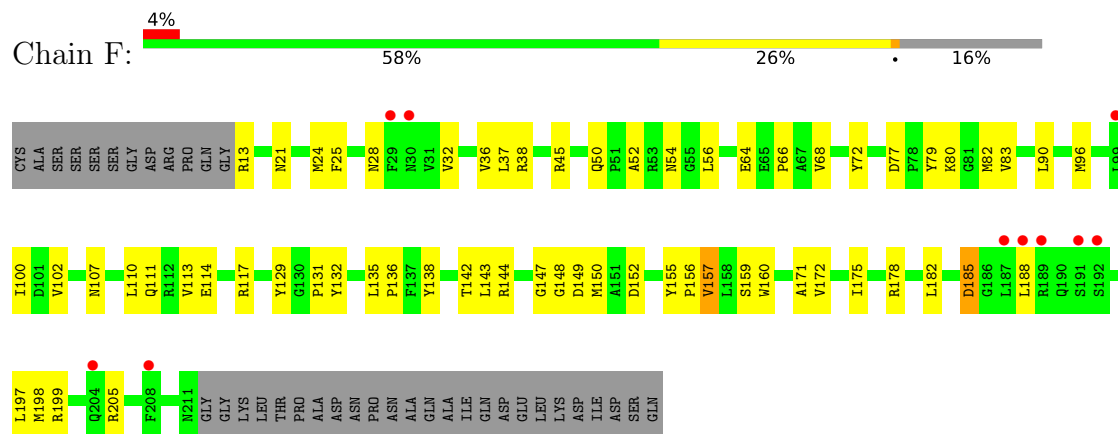
- Molecule 2: ABC transporter permease



- 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	95.60Å 146.46Å 234.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	88.55 – 3.20 88.55 – 3.20	Depositor EDS
% Data completeness (in resolution range)	91.8 (88.55-3.20) 98.7 (88.55-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.11 (at 3.07Å)	Xtriage
Refinement program	PHENIX (1.11.1 _2575: ???)	Depositor
R, R_{free}	0.223 , 0.269 0.236 , 0.275	Depositor DCC
R_{free} test set	3119 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	79.2	Xtriage
Anisotropy	0.618	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 42.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	12971	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.40% 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: C8E, SO4

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	0.42	0/2683	0.65	0/3628
1	C	0.43	0/2683	0.65	0/3628
1	E	0.38	0/2683	0.64	0/3628
2	B	0.33	0/1630	0.70	2/2219 (0.1%)
2	D	0.87	3/1651 (0.2%)	1.28	9/2246 (0.4%)
2	F	0.35	0/1647	0.65	0/2241
All	All	0.48	3/12977 (0.0%)	0.76	11/17590 (0.1%)

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
2	D	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	134	GLN	CD-NE2	20.32	1.75	1.33
2	D	134	GLN	CD-OE1	-18.39	0.88	1.23
2	D	134	GLN	CA-C	-13.19	1.37	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	134	GLN	OE1-CD-NE2	-34.10	88.50	122.60
2	D	134	GLN	CA-CB-CG	32.94	179.99	114.10
2	D	134	GLN	N-CA-C	9.09	123.23	108.41
2	D	134	GLN	CG-CD-NE2	-7.27	105.50	116.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	134	GLN	O-C-N	6.80	131.16	123.27
2	B	156	PRO	CA-C-N	6.34	133.38	121.97
2	B	156	PRO	C-N-CA	6.34	133.38	121.97
2	D	134	GLN	CB-CG-CD	-6.30	101.90	112.60
2	D	156	PRO	N-CA-C	5.80	119.62	111.33
2	D	156	PRO	CA-C-N	5.11	131.17	121.97
2	D	156	PRO	C-N-CA	5.11	131.17	121.97

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	134	GLN	Sidechain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2627	0	2444	50	0
1	C	2627	0	2444	61	0
1	E	2627	0	2442	65	0
2	B	1580	0	1507	47	0
2	D	1601	0	1528	56	0
2	F	1597	0	1525	53	0
3	A	10	0	0	0	0
3	C	10	0	0	0	0
3	E	10	0	0	0	0
4	A	66	0	93	2	0
4	B	21	0	34	2	0
4	C	57	0	92	5	0
4	D	60	0	84	8	0
4	E	50	0	65	3	0
4	F	28	0	46	2	0
All	All	12971	0	12304	301	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 12.

All (301) 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)
2:D:134:GLN:NE2	2:D:134:GLN:CD	1.75	1.42
2:D:132:TYR:OH	2:D:134:GLN:NE2	1.83	1.10
2:D:134:GLN:NE2	2:D:134:GLN:OE1	1.94	0.99
2:D:28:ASN:HA	2:D:32:VAL:HG12	1.51	0.92
1:C:196:ARG:HH11	1:C:236:ASN:HB3	1.37	0.89
2:B:50:GLN:OE1	2:B:54:ASN:ND2	2.08	0.86
1:C:57:GLY:HA3	1:E:307:MET:HE3	1.57	0.84
2:F:24:MET:HE2	2:F:136:PRO:HB3	1.59	0.82
2:F:28:ASN:HA	2:F:32:VAL:HG22	1.65	0.78
1:E:197:THR:HG22	1:E:199:LEU:H	1.47	0.77
2:D:174:GLY:HA3	4:D:305:C8E:H101	1.66	0.77
2:B:45:ARG:NH1	2:B:46:ASP:OD1	2.19	0.76
2:D:178:ARG:NH2	2:D:185:ASP:OD1	2.19	0.76
2:D:114:GLU:OE1	2:D:205:ARG:NH2	2.17	0.74
2:B:26:ASN:OD1	2:B:30:ASN:ND2	2.18	0.74
2:F:132:TYR:HE2	2:F:199:ARG:HB2	1.51	0.74
2:F:129:TYR:HD2	2:F:142:THR:HG21	1.51	0.74
1:C:20:LEU:HB3	1:C:38:MET:HB2	1.71	0.72
2:D:66:PRO:HG2	2:D:157:VAL:HG21	1.71	0.72
2:B:28:ASN:HA	2:B:32:VAL:HG22	1.71	0.72
1:E:20:LEU:HB3	1:E:38:MET:HB2	1.71	0.72
1:C:262:GLN:HG2	1:C:272:SER:HB2	1.72	0.71
2:D:117:ARG:HB3	2:D:152:ASP:OD2	1.89	0.71
1:A:197:THR:HB	1:A:200:GLN:HG3	1.71	0.71
2:D:17:LEU:HD12	2:D:133:VAL:HG12	1.71	0.70
1:C:93:VAL:O	1:C:139:TYR:OH	2.07	0.70
1:C:307:MET:HE3	1:A:57:GLY:HA3	1.74	0.69
2:F:178:ARG:NH2	2:F:185:ASP:OD1	2.23	0.67
2:F:38:ARG:HG3	2:F:178:ARG:NH2	2.09	0.67
2:B:63:LEU:HD13	2:B:161:LEU:HD11	1.77	0.67
2:D:147:GLY:HA2	2:D:150:MET:HG3	1.76	0.67
1:A:307:MET:HE3	1:E:57:GLY:HA3	1.77	0.67
1:A:313:TYR:HE2	1:A:315:ILE:HG12	1.60	0.67
1:A:318:ILE:HG22	1:A:328:SER:HA	1.78	0.66
2:B:140:SER:HB2	2:B:198:MET:HE1	1.79	0.65
1:C:115:LEU:HD22	1:C:119:GLY:HA3	1.79	0.64
1:A:280:ALA:HB2	1:A:291:LEU:HD11	1.79	0.64
2:B:21:ASN:ND2	2:B:132:TYR:O	2.30	0.64
2:F:50:GLN:O	2:F:54:ASN:ND2	2.29	0.64
2:F:24:MET:HE3	2:F:24:MET:HA	1.80	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:62:GLU:OE1	1:C:82:ARG:NH1	2.33	0.62
2:B:104:GLY:H	2:B:106:ALA:H	1.47	0.62
1:C:303:PHE:HB3	1:A:51:ILE:HD13	1.82	0.62
1:A:313:TYR:CE2	1:A:315:ILE:HG12	2.35	0.62
2:B:117:ARG:HB3	2:B:152:ASP:OD2	2.00	0.61
1:A:313:TYR:HD1	1:A:332:VAL:HB	1.66	0.61
1:E:313:TYR:HD1	1:E:332:VAL:HB	1.66	0.61
2:F:37:LEU:HG	2:F:178:ARG:HG3	1.83	0.61
4:C:403:C8E:H41	4:C:404:C8E:H22	1.83	0.60
2:D:45:ARG:HD3	2:D:182:LEU:HD12	1.82	0.60
2:F:56:LEU:HD23	2:F:172:VAL:HG11	1.82	0.60
1:C:100:ARG:NH2	1:E:71:GLU:OE2	2.35	0.60
1:E:89:LYS:HD3	4:E:406:C8E:H171	1.83	0.60
2:F:114:GLU:OE1	2:F:205:ARG:NH2	2.31	0.60
1:E:31:SER:HB2	1:E:34:GLY:H	1.66	0.60
1:C:24:SER:OG	1:C:34:GLY:O	2.18	0.59
2:D:170:TRP:CD1	4:D:304:C8E:H192	2.37	0.59
1:C:296:GLU:HG2	1:C:297:VAL:N	2.11	0.59
1:E:115:LEU:HD22	1:E:119:GLY:HA3	1.84	0.59
2:F:66:PRO:HG2	2:F:157:VAL:HG11	1.84	0.59
1:C:104:VAL:HG21	1:C:156:GLN:HB2	1.84	0.59
2:F:129:TYR:CD2	2:F:142:THR:HG21	2.36	0.58
1:C:51:ILE:HG21	1:E:303:PHE:HB3	1.83	0.58
1:A:20:LEU:HB3	1:A:38:MET:HB2	1.85	0.58
2:D:170:TRP:CZ2	4:D:305:C8E:H111	2.39	0.58
1:A:313:TYR:CD1	1:A:332:VAL:HB	2.38	0.58
2:D:71:ASN:OD1	2:D:118:PHE:HA	2.03	0.58
1:A:197:THR:HG22	1:A:199:LEU:H	1.69	0.58
2:F:77:ASP:OD2	2:F:80:LYS:HE2	2.03	0.58
1:C:51:ILE:HD13	1:E:303:PHE:HB3	1.85	0.57
2:B:156:PRO:HB3	2:B:160:TRP:CZ2	2.39	0.57
2:D:28:ASN:HA	2:D:32:VAL:CG1	2.30	0.57
1:E:1:ALA:HB1	1:E:12:ASP:OD1	2.04	0.57
1:A:220:TYR:CZ	1:A:222:ALA:HB3	2.39	0.57
1:C:57:GLY:CA	1:E:307:MET:HE3	2.31	0.56
2:F:142:THR:HG22	2:F:144:ARG:H	1.70	0.56
1:E:265:PHE:CE2	2:F:82:MET:HG2	2.41	0.56
1:C:31:SER:HB2	1:C:34:GLY:H	1.71	0.56
1:C:93:VAL:HG11	2:F:100:ILE:HG23	1.88	0.56
1:C:307:MET:HE1	1:C:338:TYR:HB2	1.88	0.56
1:C:313:TYR:HD1	1:C:332:VAL:HB	1.71	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:133:VAL:HG22	2:D:141:PHE:O	2.06	0.55
2:F:117:ARG:HB3	2:F:152:ASP:OD2	2.07	0.55
1:C:90:TYR:HB2	1:C:93:VAL:HB	1.89	0.54
2:B:171:ALA:O	2:B:175:ILE:HG13	2.07	0.54
1:E:307:MET:HE1	1:E:338:TYR:HB2	1.89	0.54
2:D:170:TRP:HD1	4:D:304:C8E:H192	1.73	0.54
1:E:231:TYR:OH	1:E:233:GLU:OE2	2.24	0.54
1:E:225:ILE:HD11	4:E:405:C8E:H82	1.89	0.54
1:C:115:LEU:HD22	1:C:119:GLY:CA	2.36	0.54
1:C:166:ALA:HB2	1:C:199:LEU:HD22	1.90	0.54
1:A:61:TRP:CZ2	1:A:63:TYR:HB2	2.43	0.54
2:B:37:LEU:HD22	2:B:178:ARG:HG3	1.90	0.54
4:D:302:C8E:H62	1:A:145:PHE:HE2	1.73	0.53
2:B:164:PRO:O	2:B:167:ILE:HG13	2.08	0.53
1:E:24:SER:HB2	1:E:35:ASN:HB2	1.89	0.53
2:F:13:ARG:HD2	2:F:199:ARG:NH1	2.23	0.53
1:E:141:ASN:OD1	1:E:144:PHE:HA	2.08	0.53
1:C:262:GLN:OE1	1:C:270:ARG:NH1	2.42	0.53
2:D:90:LEU:HB3	2:D:102:VAL:HG23	1.91	0.53
1:E:18:VAL:HG13	1:E:337:VAL:HG22	1.90	0.53
1:E:277:LYS:HA	1:E:292:VAL:O	2.09	0.53
2:D:134:GLN:NE2	2:D:134:GLN:CG	2.66	0.53
2:B:59:PHE:HB2	2:B:99:LEU:HD12	1.91	0.52
1:C:20:LEU:HD11	1:C:117:GLU:OE1	2.10	0.52
1:E:114:MET:HE2	1:E:226:TYR:CZ	2.44	0.52
1:E:205:LEU:HB2	1:E:249:GLY:HA3	1.90	0.52
1:C:87:GLY:HA3	1:C:97:ASP:HB3	1.92	0.52
2:B:96:MET:SD	1:E:139:TYR:HB2	2.49	0.51
2:D:152:ASP:HA	2:D:155:TYR:CE2	2.46	0.51
1:E:93:VAL:O	1:E:139:TYR:OH	2.23	0.51
1:E:263:TYR:CD1	4:E:405:C8E:H71	2.46	0.51
1:A:303:PHE:HB3	1:E:51:ILE:HD13	1.92	0.51
1:C:71:GLU:OE2	1:A:100:ARG:NH2	2.41	0.51
2:D:87:ARG:NH1	2:D:101:ASP:OD1	2.44	0.51
1:C:313:TYR:CD1	1:C:332:VAL:HB	2.45	0.51
2:B:66:PRO:HG2	2:B:157:VAL:HG11	1.93	0.51
2:F:21:ASN:O	2:F:25:PHE:N	2.42	0.50
2:D:171:ALA:O	2:D:175:ILE:HG13	2.11	0.50
1:E:197:THR:HB	1:E:200:GLN:HG3	1.93	0.50
1:C:114:MET:HE2	1:C:226:TYR:CZ	2.46	0.50
1:E:107:ASP:OD2	1:E:140:ARG:NH2	2.45	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:50:GLN:OE1	2:F:54:ASN:ND2	2.37	0.50
2:B:107:ASN:OD1	2:B:108:PRO:HD2	2.11	0.50
2:B:183:ASP:C	2:B:185:ASP:H	2.20	0.49
2:F:147:GLY:HA2	2:F:150:MET:HG3	1.93	0.49
1:E:191:TYR:HD2	1:E:214:TRP:HB3	1.77	0.49
2:F:135:LEU:HB2	2:F:138:TYR:HB3	1.95	0.49
2:D:99:LEU:HD23	4:D:302:C8E:H21	1.95	0.49
1:A:235:ARG:HG2	1:A:253:LYS:HE2	1.95	0.49
1:C:104:VAL:HG23	1:C:156:GLN:CD	2.37	0.49
1:C:93:VAL:HG11	2:F:100:ILE:HG12	1.95	0.49
2:F:155:TYR:HB2	2:F:156:PRO:HD2	1.94	0.49
2:F:156:PRO:O	2:F:157:VAL:HG22	2.13	0.49
1:C:93:VAL:CG1	2:F:100:ILE:HG12	2.43	0.48
1:A:307:MET:HE3	1:E:57:GLY:CA	2.42	0.48
1:C:89:LYS:NZ	1:C:95:SER:HB3	2.29	0.48
2:B:102:VAL:HG12	1:E:90:TYR:CE1	2.48	0.48
1:E:18:VAL:O	1:E:39:THR:HG23	2.13	0.48
1:C:47:GLY:HA3	1:E:338:TYR:CE2	2.49	0.48
2:D:94:LEU:O	1:A:90:TYR:OH	2.28	0.48
1:A:158:LEU:HD22	1:A:170:ASN:OD1	2.13	0.48
2:F:79:TYR:CD2	4:F:302:C8E:H131	2.49	0.48
1:C:104:VAL:CG2	1:C:156:GLN:HB2	2.43	0.48
1:C:126:ASP:HB2	1:C:168:ARG:HH11	1.78	0.48
2:D:117:ARG:NH1	2:D:158:LEU:HD11	2.29	0.48
2:D:144:ARG:O	2:D:148:GLY:HA3	2.13	0.48
2:D:162:THR:OG1	2:D:165:MET:HG3	2.13	0.48
2:B:179:ALA:C	2:B:181:LEU:H	2.22	0.48
1:E:1:ALA:HB2	1:E:340:PHE:O	2.13	0.48
2:F:24:MET:CG	2:F:136:PRO:HD3	2.43	0.48
1:E:141:ASN:HD21	1:E:145:PHE:H	1.60	0.48
4:C:403:C8E:H21	4:C:404:C8E:H11	1.96	0.48
1:A:107:ASP:OD1	1:A:140:ARG:NH2	2.47	0.47
1:A:340:PHE:CD2	1:E:11:VAL:HG21	2.48	0.47
2:D:59:PHE:HB2	2:D:99:LEU:HD12	1.97	0.47
2:B:138:TYR:O	2:B:138:TYR:HD1	1.97	0.47
1:A:265:PHE:HZ	4:B:301:C8E:H81	1.79	0.47
2:F:90:LEU:HB3	2:F:102:VAL:CG2	2.45	0.47
2:B:78:PRO:HB2	4:B:301:C8E:H82	1.95	0.47
4:D:302:C8E:H62	1:A:145:PHE:CE2	2.49	0.47
4:C:406:C8E:H21	2:F:52:ALA:HA	1.97	0.47
2:D:13:ARG:HG2	2:D:14:SER:H	1.80	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:TYR:O	1:A:91:ALA:C	2.57	0.47
2:F:188:LEU:HD13	2:F:198:MET:HE3	1.96	0.47
1:C:90:TYR:O	1:C:91:ALA:C	2.57	0.47
1:C:225:ILE:HD11	4:C:404:C8E:H101	1.96	0.47
2:D:107:ASN:OD1	2:D:109:GLN:NE2	2.48	0.47
1:A:119:GLY:HA2	1:A:294:TYR:OH	2.14	0.47
2:B:156:PRO:O	2:B:157:VAL:HG22	2.15	0.47
2:F:144:ARG:O	2:F:148:GLY:HA3	2.14	0.47
1:C:18:VAL:O	1:C:39:THR:HG23	2.14	0.47
2:D:96:MET:SD	1:A:139:TYR:HB2	2.55	0.47
2:D:63:LEU:HA	2:D:157:VAL:HG11	1.96	0.46
1:A:158:LEU:CD2	1:A:170:ASN:OD1	2.63	0.46
1:A:338:TYR:CE2	1:E:47:GLY:HA3	2.50	0.46
2:B:71:ASN:OD1	2:B:118:PHE:HA	2.15	0.46
2:B:205:ARG:O	2:B:209:ILE:HD13	2.14	0.46
1:C:115:LEU:HG	1:C:296:GLU:OE1	2.16	0.46
2:D:100:ILE:HG23	1:A:93:VAL:HG11	1.97	0.46
1:A:115:LEU:HD22	1:A:119:GLY:HA3	1.98	0.46
1:C:20:LEU:HA	1:C:20:LEU:HD23	1.72	0.46
2:B:186:GLY:HA2	2:B:189:ARG:HB2	1.97	0.46
2:F:37:LEU:CG	2:F:178:ARG:HG3	2.45	0.46
1:C:18:VAL:HG13	1:C:337:VAL:HG22	1.97	0.46
2:D:143:LEU:HA	2:D:143:LEU:HD23	1.65	0.46
2:F:54:ASN:ND2	2:F:54:ASN:H	2.13	0.46
2:F:83:VAL:HG13	2:F:110:LEU:HD23	1.98	0.46
1:E:279:LYS:HE3	1:E:288:ASP:HB3	1.98	0.46
2:F:107:ASN:HB3	2:F:110:LEU:HG	1.98	0.46
1:C:145:PHE:CE1	4:C:406:C8E:H51	2.51	0.46
1:E:46:LYS:HG2	1:E:60:GLN:CD	2.41	0.46
1:A:234:THR:O	1:A:253:LYS:HA	2.16	0.45
2:F:117:ARG:HH21	2:F:149:ASP:HB3	1.81	0.45
2:D:87:ARG:NH1	2:D:112:ARG:HB2	2.31	0.45
1:A:273:ILE:HA	1:A:296:GLU:O	2.17	0.45
2:B:140:SER:HB2	2:B:198:MET:CE	2.44	0.45
2:D:136:PRO:C	2:D:138:TYR:H	2.24	0.45
2:D:156:PRO:HB3	2:D:160:TRP:CZ2	2.52	0.45
1:E:54:ASP:HA	1:E:91:ALA:HB2	1.99	0.45
1:E:61:TRP:CZ2	1:E:63:TYR:HB2	2.51	0.45
2:D:71:ASN:O	2:D:75:GLN:HG3	2.17	0.45
2:B:27:PHE:O	2:B:31:VAL:HG12	2.17	0.45
2:F:197:LEU:HD23	2:F:197:LEU:HA	1.71	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:71:GLU:HG3	1:A:100:ARG:NH2	2.32	0.45
2:D:88:PHE:HE2	4:D:301:C8E:H202	1.82	0.45
2:F:171:ALA:O	2:F:175:ILE:HG13	2.17	0.45
2:D:147:GLY:HA2	2:D:150:MET:CG	2.44	0.44
1:A:31:SER:OG	1:A:331:THR:OG1	2.35	0.44
2:D:96:MET:HE3	4:A:403:C8E:H172	2.00	0.44
2:B:33:ASP:OD1	2:B:38:ARG:HB2	2.18	0.44
2:B:142:THR:OG1	2:B:202:TYR:OH	2.23	0.44
2:F:132:TYR:HE2	2:F:199:ARG:CB	2.26	0.44
2:D:156:PRO:HA	2:D:159:SER:HB3	1.98	0.44
1:E:90:TYR:HB2	1:E:93:VAL:HB	2.00	0.44
2:F:136:PRO:C	2:F:138:TYR:H	2.24	0.44
2:B:87:ARG:NH2	2:B:112:ARG:HD3	2.33	0.44
2:D:33:ASP:HB3	2:D:34:PRO:HD3	1.98	0.44
2:D:132:TYR:HB2	2:D:203:PHE:HZ	1.82	0.44
1:E:23:PHE:HB2	1:E:332:VAL:HG13	1.99	0.44
2:D:133:VAL:HG23	2:D:135:LEU:HD13	2.00	0.44
1:A:315:ILE:HA	1:A:330:ASP:OD2	2.18	0.44
1:E:254:THR:HA	1:E:279:LYS:O	2.17	0.44
1:C:47:GLY:HA3	1:E:338:TYR:CZ	2.53	0.44
1:C:307:MET:HE2	1:C:307:MET:HB2	1.79	0.44
2:B:144:ARG:O	2:B:148:GLY:HA3	2.18	0.44
2:F:72:TYR:CZ	2:F:80:LYS:HG2	2.53	0.44
1:C:111:TYR:HB2	1:C:230:ASN:HD21	1.82	0.43
2:B:24:MET:HG3	2:B:136:PRO:HD3	1.99	0.43
1:C:20:LEU:HD11	1:C:117:GLU:CD	2.44	0.43
1:C:163:ARG:HD2	1:C:168:ARG:CB	2.47	0.43
1:E:191:TYR:CD2	1:E:214:TRP:HB3	2.53	0.43
1:C:230:ASN:HD22	1:C:230:ASN:HA	1.66	0.43
1:A:115:LEU:HD22	1:A:119:GLY:CA	2.48	0.43
2:F:147:GLY:HA2	2:F:150:MET:SD	2.59	0.43
2:B:38:ARG:O	2:B:42:VAL:HG23	2.19	0.43
2:D:100:ILE:HG12	1:A:93:VAL:CG1	2.48	0.43
1:E:64:ASN:ND2	1:E:78:GLY:O	2.52	0.43
2:D:16:PRO:HG2	2:D:131:PRO:HB3	2.00	0.43
2:B:90:LEU:HB3	2:B:102:VAL:CG2	2.48	0.43
1:A:71:GLU:HB3	1:E:80:LYS:HD2	2.01	0.43
1:E:88:LEU:HD23	1:E:88:LEU:HA	1.84	0.43
1:C:109:LEU:HA	1:C:230:ASN:OD1	2.19	0.43
1:C:307:MET:HE3	1:A:57:GLY:CA	2.45	0.43
2:D:120:SER:O	2:D:124:HIS:N	2.46	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:69:MET:HE2	2:B:69:MET:HB3	1.95	0.42
2:B:152:ASP:HA	2:B:155:TYR:CE1	2.53	0.42
1:A:272:SER:N	1:A:298:GLY:O	2.50	0.42
1:E:12:ASP:O	1:E:45:PHE:HA	2.18	0.42
1:E:97:ASP:OD1	1:E:97:ASP:N	2.52	0.42
2:D:100:ILE:HD13	1:A:90:TYR:CE2	2.54	0.42
2:B:29:PHE:O	2:B:34:PRO:HD3	2.19	0.42
1:C:12:ASP:O	1:C:45:PHE:HA	2.19	0.42
1:A:102:TYR:CE1	1:A:132:ARG:HG3	2.54	0.42
2:F:96:MET:HE3	4:F:301:C8E:H81	2.02	0.42
1:C:313:TYR:HE2	1:C:315:ILE:HG12	1.84	0.42
1:E:254:THR:HG22	1:E:280:ALA:HA	2.01	0.42
1:E:279:LYS:HD2	1:E:290:ASP:OD1	2.20	0.42
1:C:109:LEU:HA	1:C:109:LEU:HD23	1.88	0.42
2:B:69:MET:HG3	2:B:81:GLY:O	2.20	0.42
1:E:234:THR:O	1:E:253:LYS:HA	2.20	0.42
2:F:132:TYR:CD1	2:F:132:TYR:C	2.95	0.42
1:C:107:ASP:OD2	1:C:140:ARG:NH2	2.53	0.41
1:E:115:LEU:HD22	1:E:119:GLY:CA	2.50	0.41
1:C:243:LYS:HD2	1:C:325:GLY:O	2.20	0.41
1:C:301:TYR:CD2	2:D:90:LEU:HD11	2.55	0.41
1:A:269:LEU:HD22	2:B:86:THR:OG1	2.20	0.41
1:A:214:TRP:NE1	1:A:233:GLU:HB2	2.34	0.41
2:B:162:THR:OG1	2:B:165:MET:HG3	2.20	0.41
1:E:151:LEU:HD12	1:E:179:SER:O	2.20	0.41
2:F:142:THR:HG22	2:F:143:LEU:N	2.35	0.41
1:A:104:VAL:HG23	1:A:156:GLN:CD	2.45	0.41
2:D:48:VAL:HA	2:D:49:PRO:HD3	1.96	0.41
2:B:136:PRO:C	2:B:138:TYR:H	2.28	0.41
1:E:285:GLY:C	1:E:286:ILE:HD12	2.46	0.41
1:E:318:ILE:HD13	1:E:318:ILE:HA	1.95	0.41
4:A:404:C8E:H162	4:A:404:C8E:H192	1.78	0.41
2:F:159:SER:HG	2:F:160:TRP:CD1	2.39	0.41
1:C:16:LYS:HB3	1:C:339:GLN:HB3	2.03	0.41
2:D:120:SER:HB3	2:D:209:ILE:HG22	2.03	0.41
1:E:55:LEU:HD23	1:E:55:LEU:HA	1.90	0.41
1:E:74:ASP:OD1	1:E:74:ASP:N	2.52	0.41
1:E:158:LEU:HD22	1:E:170:ASN:OD1	2.21	0.41
1:C:264:GLN:OE1	1:C:270:ARG:HB2	2.20	0.41
2:B:45:ARG:HD2	2:B:46:ASP:OD1	2.21	0.41
1:A:307:MET:HE3	1:E:57:GLY:C	2.47	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:32:VAL:O	2:F:36:VAL:HB	2.21	0.40
2:F:111:GLN:O	2:F:113:VAL:HG13	2.21	0.40
2:D:112:ARG:HG3	2:D:113:VAL:N	2.34	0.40
1:C:61:TRP:CZ2	1:C:63:TYR:HB2	2.57	0.40
2:D:199:ARG:HG3	2:D:200:GLU:N	2.37	0.40
1:A:46:LYS:HG3	1:A:60:GLN:CD	2.46	0.40
2:B:24:MET:HE2	2:B:136:PRO:HG3	2.02	0.40
2:F:152:ASP:HA	2:F:155:TYR:CE2	2.57	0.40
2:D:162:THR:HG23	2:D:165:MET:SD	2.61	0.40
1:A:71:GLU:HG3	1:E:100:ARG:NH2	2.35	0.40
2:B:71:ASN:O	2:B:75:GLN:HG3	2.20	0.40
2:B:105:MET:SD	1:E:90:TYR:HB3	2.61	0.40
2:F:45:ARG:HE	2:F:182:LEU:HD12	1.86	0.40
2:B:66:PRO:HG2	2:B:157:VAL:HG21	2.02	0.40
2:F:64:GLU:O	2:F:68:VAL:HG23	2.22	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	338/340 (99%)	316 (94%)	21 (6%)	1 (0%)	36	68
1	C	338/340 (99%)	319 (94%)	18 (5%)	1 (0%)	36	68
1	E	338/340 (99%)	316 (94%)	20 (6%)	2 (1%)	21	56
2	B	195/236 (83%)	176 (90%)	16 (8%)	3 (2%)	8	37
2	D	198/236 (84%)	180 (91%)	18 (9%)	0	100	100
2	F	197/236 (84%)	177 (90%)	17 (9%)	3 (2%)	8	37
All	All	1604/1728 (93%)	1484 (92%)	110 (7%)	10 (1%)	21	56

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	91	ALA
1	A	91	ALA
2	F	131	PRO
2	F	185	ASP
2	B	180	GLN
1	E	91	ALA
2	B	129	TYR
2	B	184	SER
2	F	157	VAL
1	E	93	VAL

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	263/263 (100%)	263 (100%)	0	100	100
1	C	263/263 (100%)	263 (100%)	0	100	100
1	E	263/263 (100%)	263 (100%)	0	100	100
2	B	166/197 (84%)	166 (100%)	0	100	100
2	D	168/197 (85%)	167 (99%)	1 (1%)	78	84
2	F	168/197 (85%)	168 (100%)	0	100	100
All	All	1291/1380 (94%)	1290 (100%)	1 (0%)	88	91

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	134	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	223	ASN
1	C	230	ASN
1	C	252	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	62	ASN
2	D	109	GLN
2	D	134	GLN
1	A	9	ASN
1	A	30	ASN
1	A	60	GLN
1	A	252	ASN
1	E	35	ASN
1	E	322	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

26 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	$\# Z > 2$
4	C8E	D	301	-	11,11,20	0.46	0	10,10,19	0.60	0
3	SO4	C	402	-	4,4,4	0.24	0	6,6,6	0.33	0
3	SO4	A	401	-	4,4,4	0.25	0	6,6,6	0.16	0
4	C8E	E	403	-	12,12,20	0.49	0	11,11,19	0.40	0
4	C8E	C	405	-	9,9,20	0.32	0	8,8,19	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	C8E	D	304	-	8,8,20	0.55	0	7,7,19	0.47	0
4	C8E	B	301	-	20,20,20	0.44	0	19,19,19	0.44	0
4	C8E	F	302	-	15,15,20	0.39	0	14,14,19	0.31	0
4	C8E	E	405	-	10,10,20	0.47	0	9,9,19	0.40	0
4	C8E	C	404	-	15,15,20	0.42	0	14,14,19	0.38	0
4	C8E	A	405	-	13,13,20	0.38	0	12,12,19	0.45	0
4	C8E	A	403	-	18,18,20	0.44	0	17,17,19	0.34	0
3	SO4	E	401	-	4,4,4	0.25	0	6,6,6	0.43	0
4	C8E	D	302	-	12,12,20	0.42	0	11,11,19	0.57	0
4	C8E	A	406	-	11,11,20	0.46	0	10,10,19	0.39	0
4	C8E	E	406	-	13,13,20	0.50	0	12,12,19	0.47	0
4	C8E	C	406	-	15,15,20	0.44	0	14,14,19	0.30	0
3	SO4	E	402	-	4,4,4	0.23	0	6,6,6	0.25	0
4	C8E	C	403	-	14,14,20	0.41	0	13,13,19	0.35	0
3	SO4	A	402	-	4,4,4	0.29	0	6,6,6	0.35	0
4	C8E	D	305	-	11,11,20	0.53	0	10,10,19	0.66	0
4	C8E	A	404	-	20,20,20	0.49	0	19,19,19	0.35	0
4	C8E	E	404	-	11,11,20	0.57	0	10,10,19	0.56	0
4	C8E	D	303	-	13,13,20	0.42	0	12,12,19	0.54	0
3	SO4	C	401	-	4,4,4	0.25	0	6,6,6	0.48	0
4	C8E	F	301	-	11,11,20	0.36	0	10,10,19	0.50	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
4	C8E	D	301	-	-	3/9/9/18	-
4	C8E	E	403	-	-	6/10/10/18	-
4	C8E	C	405	-	-	4/7/7/18	-
4	C8E	D	304	-	-	2/6/6/18	-
4	C8E	B	301	-	-	9/18/18/18	-
4	C8E	F	302	-	-	8/13/13/18	-
4	C8E	E	405	-	-	3/8/8/18	-
4	C8E	C	404	-	-	8/13/13/18	-
4	C8E	A	405	-	-	7/11/11/18	-
4	C8E	A	403	-	-	12/16/16/18	-
4	C8E	D	302	-	-	5/10/10/18	-
4	C8E	A	406	-	-	3/9/9/18	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	C8E	E	406	-	-	10/11/11/18	-
4	C8E	C	406	-	-	7/13/13/18	-
4	C8E	C	403	-	-	5/12/12/18	-
4	C8E	D	305	-	-	4/9/9/18	-
4	C8E	A	404	-	-	10/18/18/18	-
4	C8E	E	404	-	-	5/9/9/18	-
4	C8E	D	303	-	-	7/11/11/18	-
4	C8E	F	301	-	-	6/9/9/18	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (124) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	406	C8E	C17-C16-O15-C14
4	C	404	C8E	O12-C13-C14-O15
4	A	404	C8E	O12-C13-C14-O15
4	E	406	C8E	O15-C16-C17-O18
4	E	404	C8E	O15-C16-C17-O18
4	A	406	C8E	O12-C13-C14-O15
4	A	406	C8E	O15-C16-C17-O18
4	A	404	C8E	O15-C16-C17-O18
4	B	301	C8E	O12-C13-C14-O15
4	E	404	C8E	O12-C13-C14-O15
4	D	303	C8E	O9-C10-C11-O12
4	E	403	C8E	O15-C16-C17-O18
4	A	404	C8E	C6-C7-C8-O9
4	E	406	C8E	O18-C19-C20-O21
4	F	302	C8E	C6-C7-C8-O9
4	A	405	C8E	C6-C7-C8-O9
4	C	405	C8E	C7-C8-O9-C10
4	A	403	C8E	O15-C16-C17-O18
4	D	302	C8E	O9-C10-C11-O12
4	D	301	C8E	O15-C16-C17-O18
4	E	406	C8E	O12-C13-C14-O15
4	A	403	C8E	C5-C6-C7-C8
4	D	301	C8E	O18-C19-C20-O21
4	B	301	C8E	O18-C19-C20-O21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	E	405	C8E	C2-C3-C4-C5
4	C	406	C8E	C2-C3-C4-C5
4	F	301	C8E	C4-C5-C6-C7
4	E	403	C8E	O12-C13-C14-O15
4	D	302	C8E	C5-C6-C7-C8
4	F	302	C8E	C5-C6-C7-C8
4	D	305	C8E	O9-C10-C11-O12
4	A	403	C8E	O18-C19-C20-O21
4	C	405	C8E	C3-C4-C5-C6
4	A	405	C8E	O9-C10-C11-O12
4	D	302	C8E	C6-C7-C8-O9
4	A	404	C8E	C16-C17-O18-C19
4	F	301	C8E	C3-C4-C5-C6
4	E	403	C8E	O9-C10-C11-O12
4	A	405	C8E	C4-C5-C6-C7
4	D	303	C8E	C3-C4-C5-C6
4	D	303	C8E	C4-C5-C6-C7
4	A	404	C8E	C2-C3-C4-C5
4	A	404	C8E	O9-C10-C11-O12
4	F	302	C8E	C2-C3-C4-C5
4	B	301	C8E	C3-C4-C5-C6
4	A	403	C8E	O9-C10-C11-O12
4	B	301	C8E	C2-C3-C4-C5
4	F	301	C8E	C6-C7-C8-O9
4	A	403	C8E	O12-C13-C14-O15
4	E	403	C8E	C7-C8-O9-C10
4	D	302	C8E	C3-C4-C5-C6
4	E	404	C8E	C10-C11-O12-C13
4	C	406	C8E	C1-C2-C3-C4
4	C	403	C8E	O9-C10-C11-O12
4	D	305	C8E	O12-C13-C14-O15
4	A	404	C8E	C1-C2-C3-C4
4	C	403	C8E	C2-C3-C4-C5
4	E	405	C8E	C4-C5-C6-C7
4	A	403	C8E	C3-C4-C5-C6
4	C	405	C8E	C6-C7-C8-O9
4	D	303	C8E	C11-C10-O9-C8
4	C	403	C8E	C14-C13-O12-C11
4	D	304	C8E	C17-C16-O15-C14
4	C	406	C8E	O9-C10-C11-O12
4	B	301	C8E	C13-C14-O15-C16
4	F	301	C8E	C1-C2-C3-C4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	A	405	C8E	C11-C10-O9-C8
4	A	405	C8E	C7-C8-O9-C10
4	D	302	C8E	C10-C11-O12-C13
4	E	404	C8E	C16-C17-O18-C19
4	E	406	C8E	C10-C11-O12-C13
4	E	404	C8E	C17-C16-O15-C14
4	A	403	C8E	C11-C10-O9-C8
4	A	404	C8E	C10-C11-O12-C13
4	A	403	C8E	C6-C7-C8-O9
4	C	404	C8E	C11-C10-O9-C8
4	A	406	C8E	C16-C17-O18-C19
4	C	405	C8E	C2-C3-C4-C5
4	C	406	C8E	C11-C10-O9-C8
4	B	301	C8E	C16-C17-O18-C19
4	E	406	C8E	O9-C10-C11-O12
4	E	403	C8E	C14-C13-O12-C11
4	E	406	C8E	C13-C14-O15-C16
4	C	404	C8E	O9-C10-C11-O12
4	E	406	C8E	C20-C19-O18-C17
4	C	404	C8E	C1-C2-C3-C4
4	E	403	C8E	C13-C14-O15-C16
4	D	303	C8E	C7-C8-O9-C10
4	F	302	C8E	C3-C4-C5-C6
4	A	405	C8E	C2-C3-C4-C5
4	D	303	C8E	C6-C7-C8-O9
4	C	404	C8E	C7-C8-O9-C10
4	C	404	C8E	C13-C14-O15-C16
4	C	406	C8E	C5-C6-C7-C8
4	A	403	C8E	C4-C5-C6-C7
4	C	406	C8E	C7-C8-O9-C10
4	E	405	C8E	C7-C8-O9-C10
4	A	403	C8E	C17-C16-O15-C14
4	C	404	C8E	C10-C11-O12-C13
4	E	406	C8E	C14-C13-O12-C11
4	D	305	C8E	C17-C16-O15-C14
4	D	304	C8E	O15-C16-C17-O18
4	A	405	C8E	C10-C11-O12-C13
4	A	404	C8E	C14-C13-O12-C11
4	D	305	C8E	C16-C17-O18-C19
4	C	406	C8E	C13-C14-O15-C16
4	C	403	C8E	C3-C4-C5-C6
4	A	403	C8E	C20-C19-O18-C17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	C	404	C8E	C4-C5-C6-C7
4	A	403	C8E	C10-C11-O12-C13
4	C	403	C8E	C7-C8-O9-C10
4	B	301	C8E	C10-C11-O12-C13
4	F	301	C8E	C7-C8-O9-C10
4	F	301	C8E	C5-C6-C7-C8
4	D	303	C8E	C2-C3-C4-C5
4	B	301	C8E	C20-C19-O18-C17
4	F	302	C8E	O9-C10-C11-O12
4	A	404	C8E	C17-C16-O15-C14
4	B	301	C8E	O9-C10-C11-O12
4	F	302	C8E	C7-C8-O9-C10
4	E	406	C8E	C16-C17-O18-C19
4	F	302	C8E	O12-C13-C14-O15
4	F	302	C8E	C10-C11-O12-C13
4	D	301	C8E	O12-C13-C14-O15

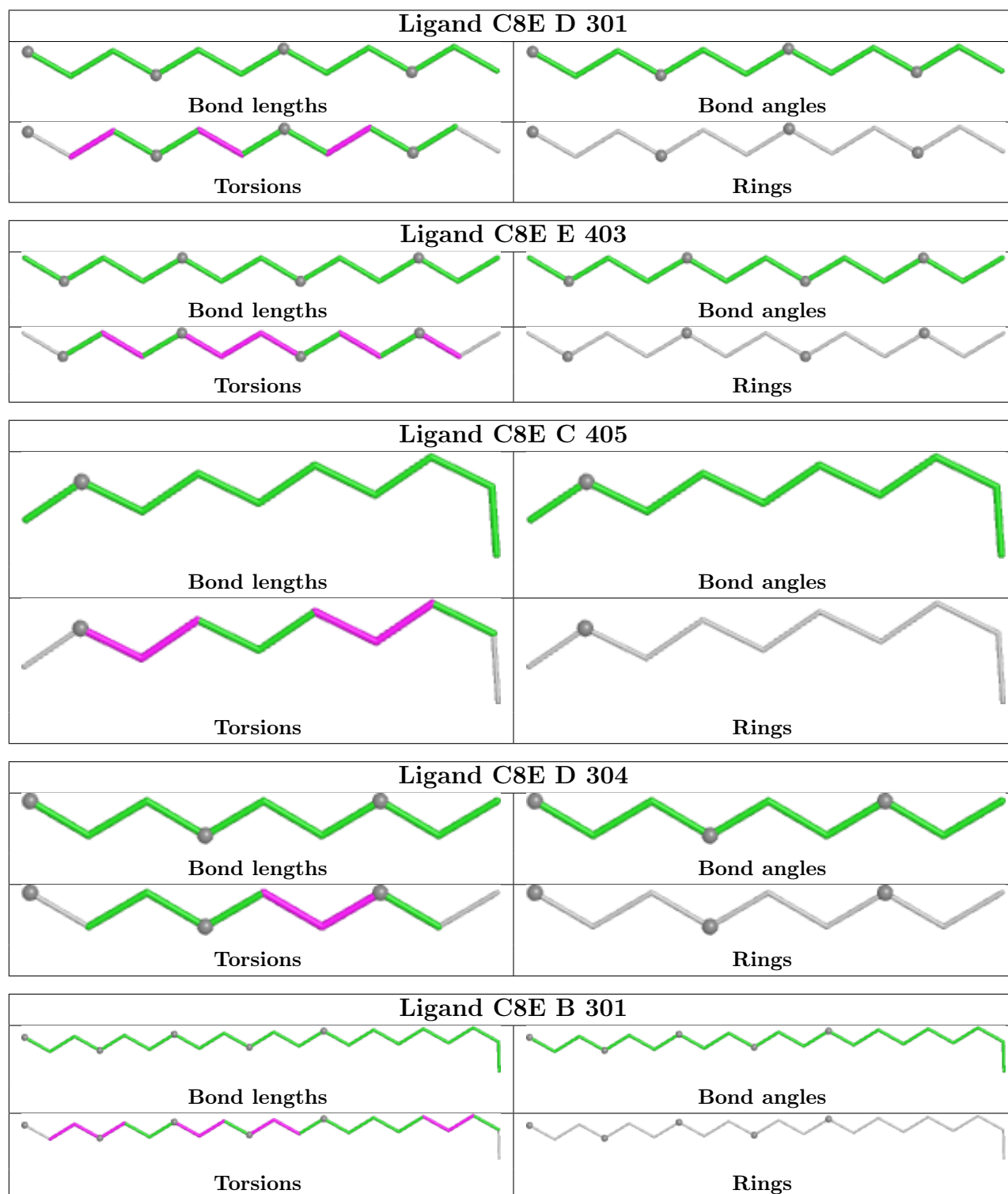
There are no ring outliers.

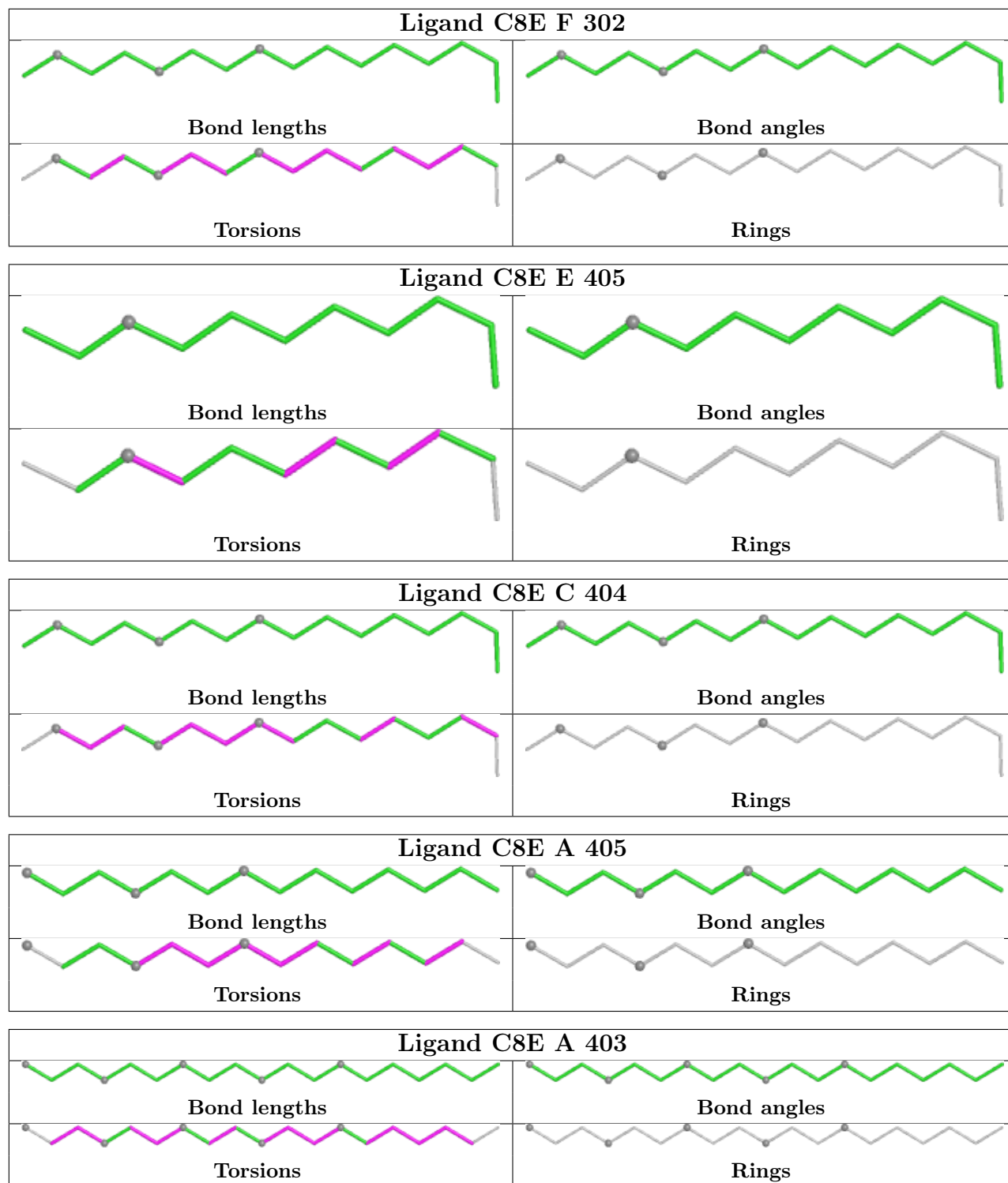
14 monomers are involved in 22 short contacts:

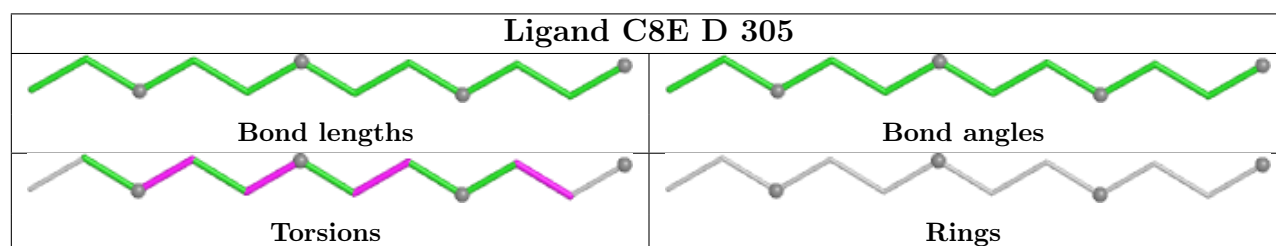
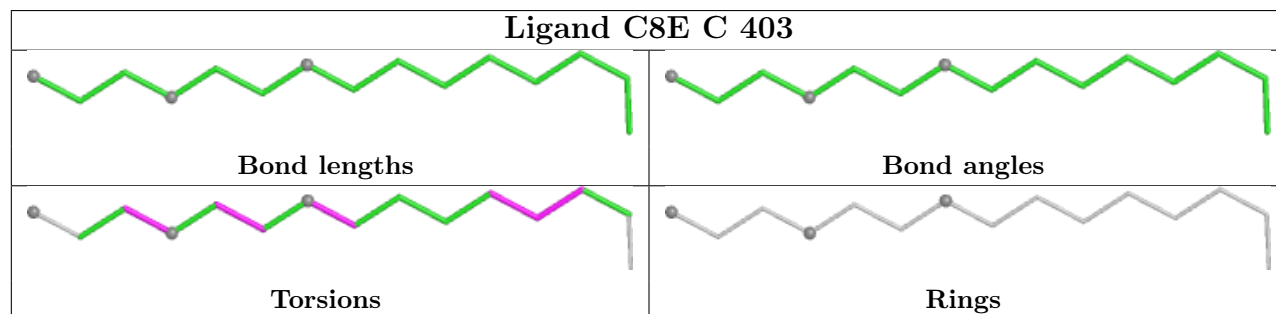
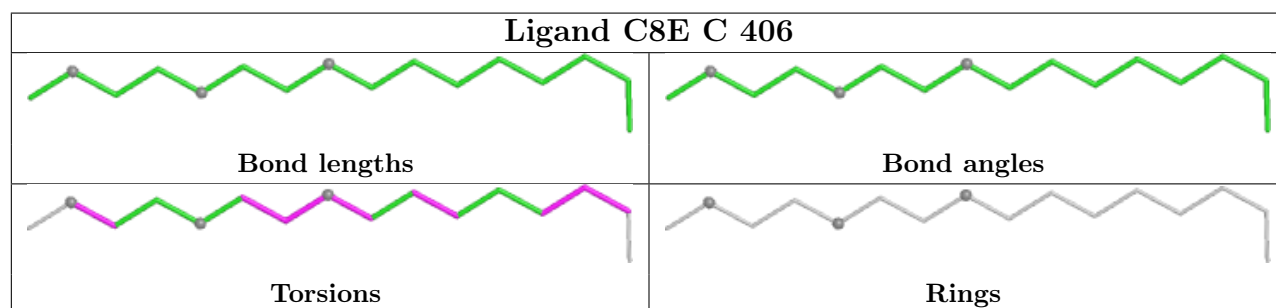
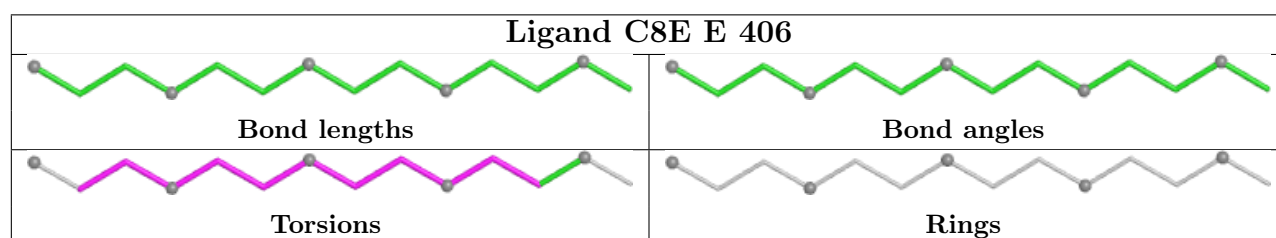
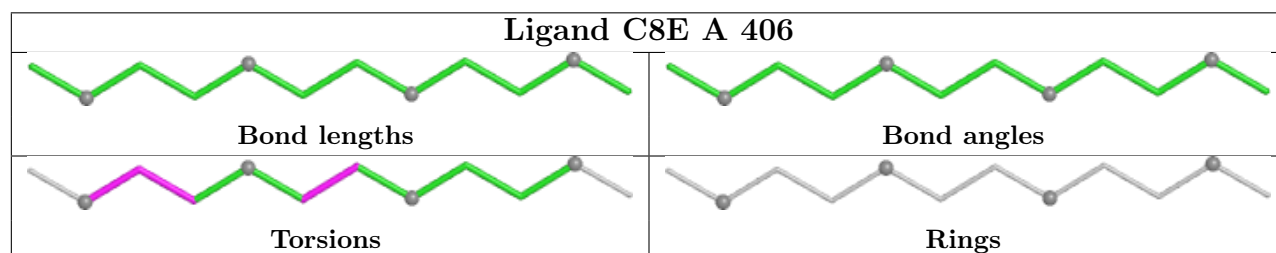
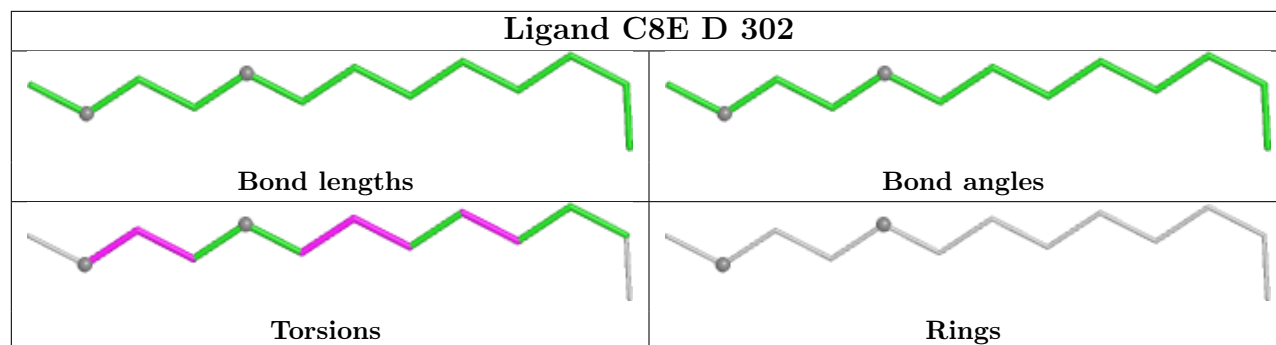
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	301	C8E	1	0
4	D	304	C8E	2	0
4	B	301	C8E	2	0
4	F	302	C8E	1	0
4	E	405	C8E	2	0
4	C	404	C8E	3	0
4	A	403	C8E	1	0
4	D	302	C8E	3	0
4	E	406	C8E	1	0
4	C	406	C8E	2	0
4	C	403	C8E	2	0
4	D	305	C8E	2	0
4	A	404	C8E	1	0
4	F	301	C8E	1	0

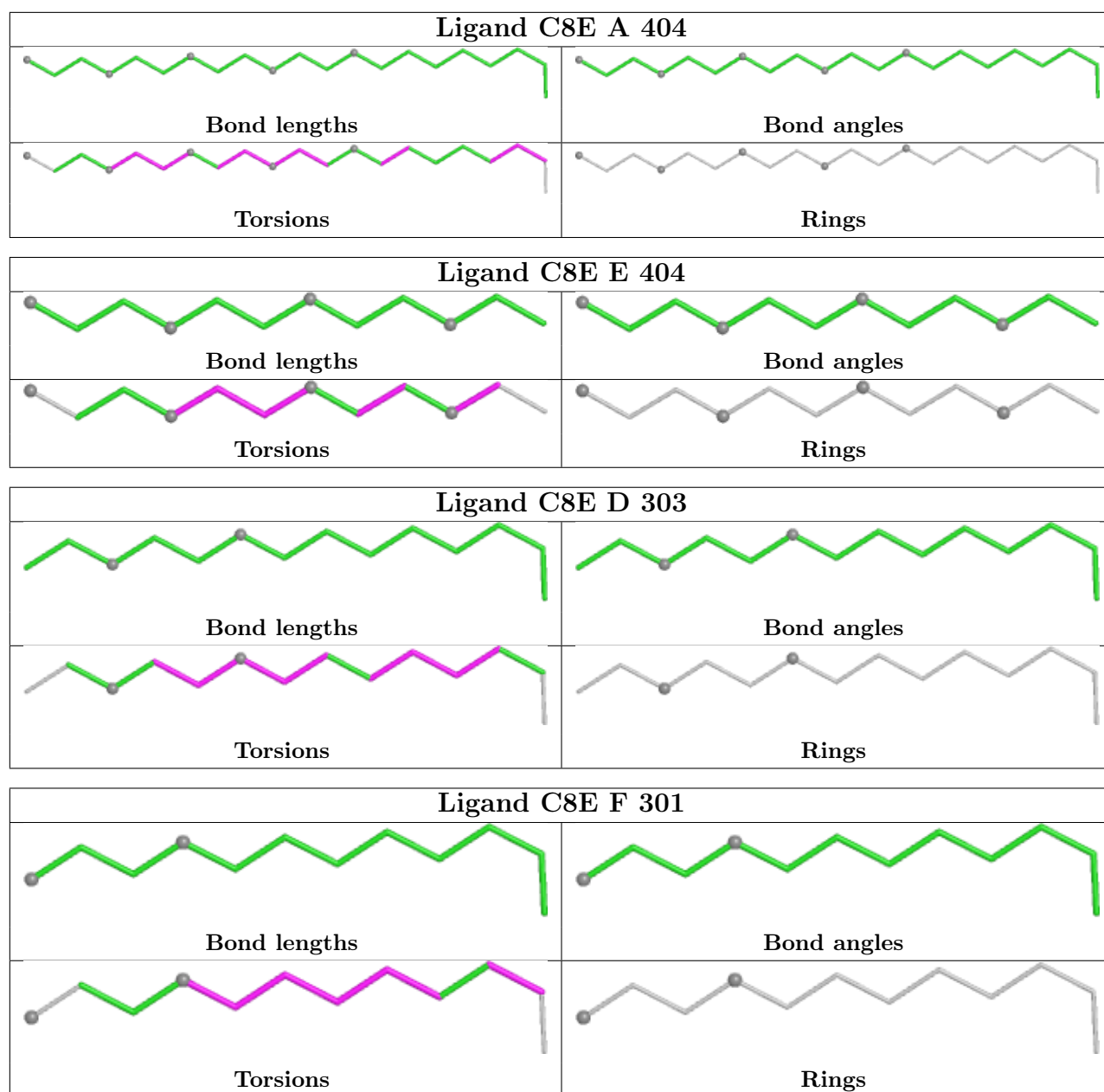
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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









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	340/340 (100%)	-0.42	4 (1%) 76 58	11, 31, 56, 75	0
1	C	340/340 (100%)	-0.25	5 (1%) 72 52	13, 27, 54, 71	0
1	E	340/340 (100%)	-0.20	9 (2%) 57 37	12, 40, 64, 78	0
2	B	197/236 (83%)	-0.03	3 (1%) 72 52	33, 58, 92, 109	0
2	D	200/236 (84%)	-0.35	0 100 100	22, 41, 58, 81	0
2	F	199/236 (84%)	0.03	10 (5%) 34 22	31, 53, 71, 106	0
All	All	1616/1728 (93%)	-0.23	31 (1%) 66 46	11, 40, 69, 109	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	192	SER	5.1
1	C	162	GLU	5.1
2	B	167	ILE	3.8
2	B	27	PHE	3.5
1	C	209	LYS	3.5
1	A	281	LYS	3.5
2	F	189	ARG	3.5
2	F	188	LEU	3.4
1	A	282	ASP	3.2
1	C	171	GLY	3.0
2	F	208	PHE	2.8
1	A	280	ALA	2.6
1	E	29	GLU	2.5
1	A	253	LYS	2.5
1	C	310	TYR	2.4
1	E	98	TYR	2.4
2	B	93	ILE	2.4
2	F	191	SER	2.3
2	F	29	PHE	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	137	ALA	2.3
1	E	155	VAL	2.3
1	E	96	PHE	2.3
1	E	157	TYR	2.2
2	F	187	LEU	2.2
2	F	30	ASN	2.2
1	E	183	GLU	2.1
2	F	99	LEU	2.1
1	E	102	TYR	2.1
1	E	23	PHE	2.1
1	C	198	ASN	2.1
2	F	204	GLN	2.1

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	C8E	A	406	12/21	0.63	0.20	39,48,53,55	0
4	C8E	C	404	16/21	0.64	0.25	17,40,57,57	0
4	C8E	A	403	19/21	0.65	0.23	37,46,53,54	0
4	C8E	D	302	13/21	0.68	0.23	8,20,49,51	0
4	C8E	C	403	15/21	0.74	0.24	23,33,50,51	0
4	C8E	D	305	12/21	0.74	0.21	26,48,55,56	0
4	C8E	D	303	14/21	0.75	0.20	22,37,57,60	0
4	C8E	E	406	14/21	0.75	0.18	32,35,53,54	0
4	C8E	C	406	16/21	0.77	0.31	40,49,60,62	0
4	C8E	E	405	11/21	0.78	0.30	35,42,57,58	0
4	C8E	A	405	14/21	0.78	0.28	30,46,50,51	0

Continued on next page...

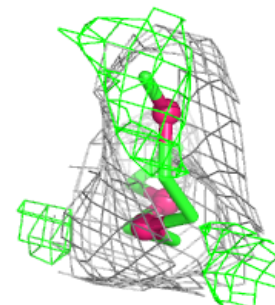
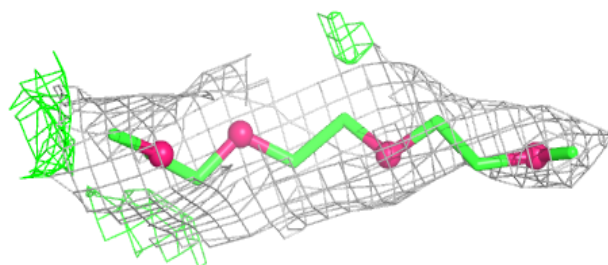
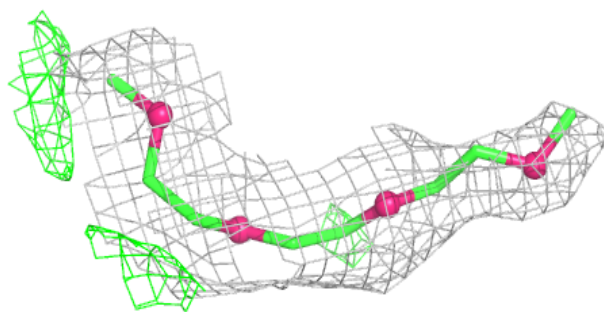
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	C8E	E	403	13/21	0.79	0.49	40,47,50,51	0
4	C8E	A	404	21/21	0.81	0.19	22,46,63,63	0
4	C8E	D	304	9/21	0.81	0.15	34,39,42,43	0
3	SO4	C	402	5/5	0.82	0.09	60,61,65,67	0
4	C8E	D	301	12/21	0.83	0.53	40,44,49,49	0
4	C8E	E	404	12/21	0.83	0.25	30,45,53,54	0
3	SO4	E	402	5/5	0.83	0.15	58,59,61,61	0
3	SO4	A	401	5/5	0.83	0.07	76,76,79,82	0
4	C8E	F	302	16/21	0.85	0.19	13,41,63,64	0
4	C8E	F	301	12/21	0.90	0.24	33,45,47,49	0
4	C8E	B	301	21/21	0.90	0.15	40,52,60,61	0
4	C8E	C	405	10/21	0.91	0.59	29,37,44,44	0
3	SO4	A	402	5/5	0.94	0.10	32,39,41,45	0
3	SO4	C	401	5/5	0.94	0.10	35,37,46,46	0
3	SO4	E	401	5/5	0.95	0.12	30,35,37,38	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.

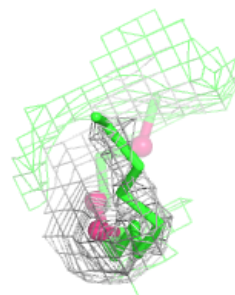
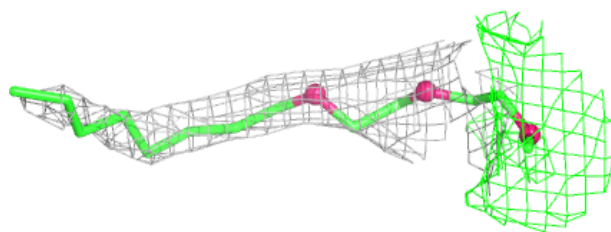
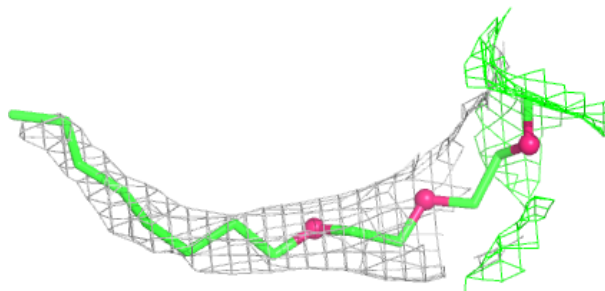
Electron density around C8E A 406:

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

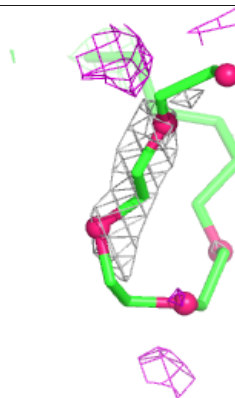
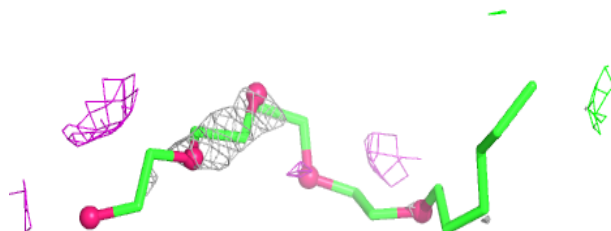
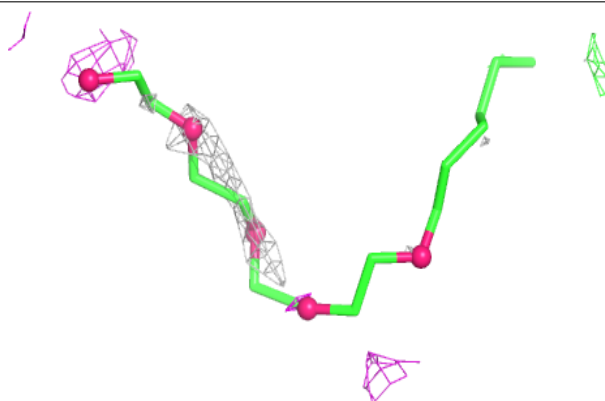


Electron density around C8E C 404:

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

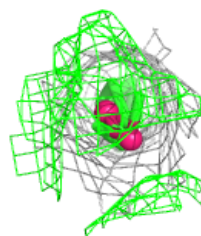
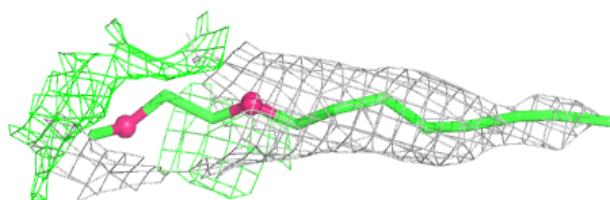
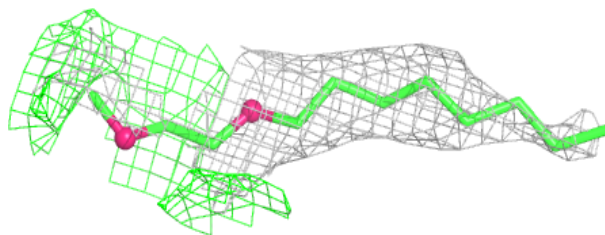
**Electron density around C8E A 403:**

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

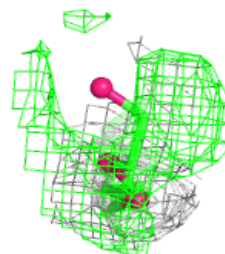
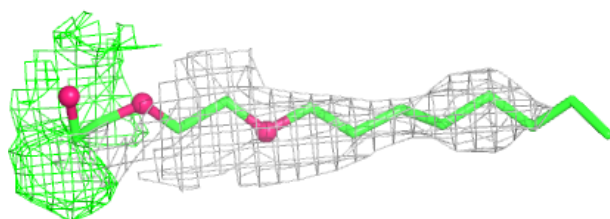
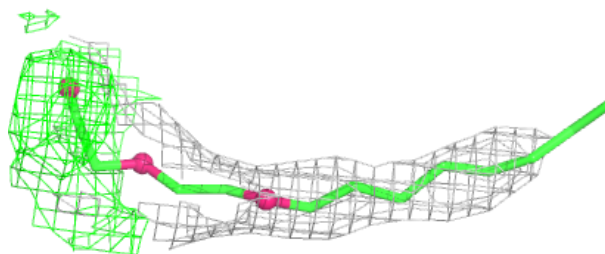


Electron density around C8E D 302:

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

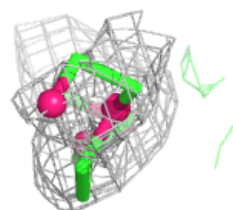
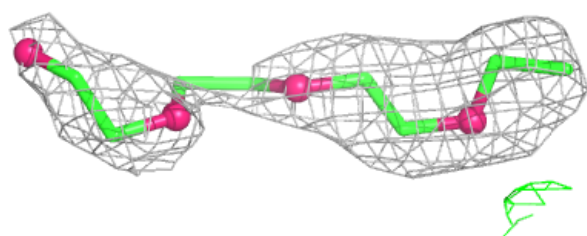
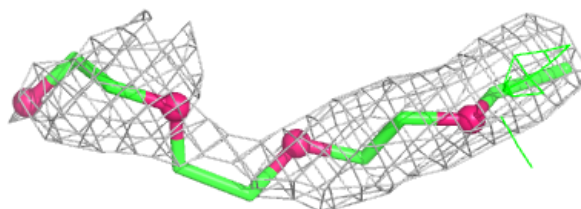
**Electron density around C8E C 403:**

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

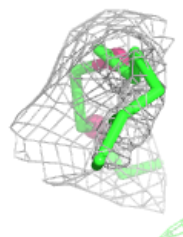
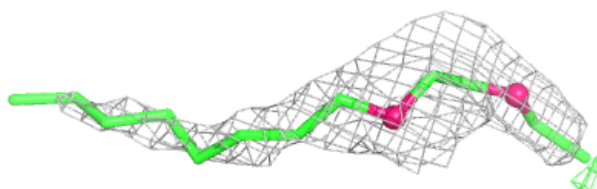
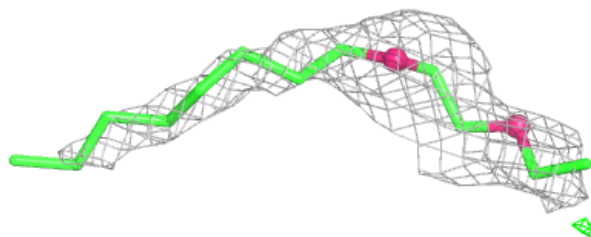


Electron density around C8E D 305:

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

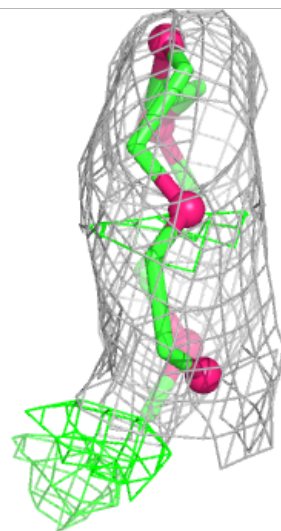
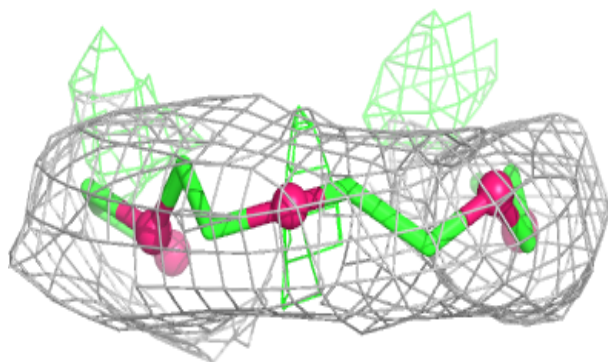
**Electron density around C8E D 303:**

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



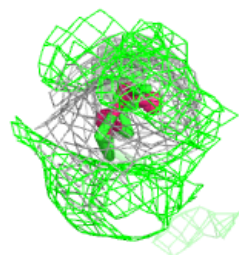
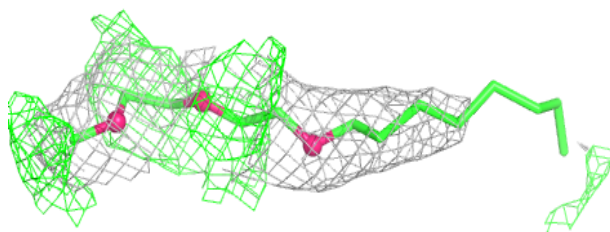
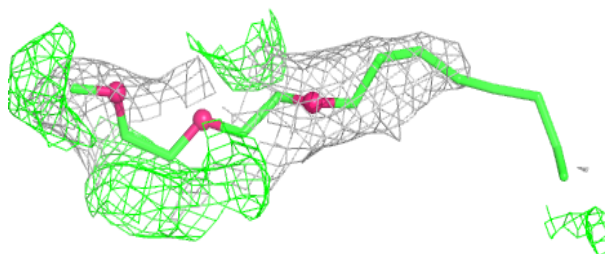
Electron density around C8E E 406:

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

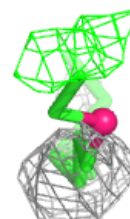
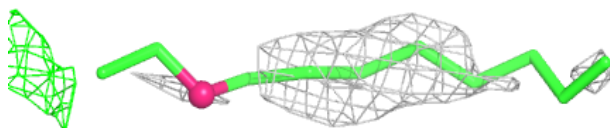
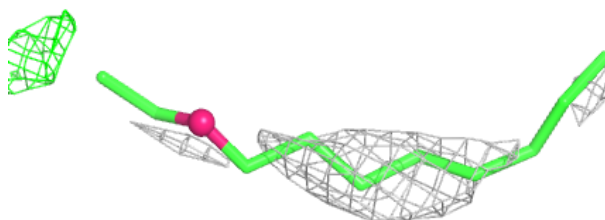


Electron density around C8E C 406:

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

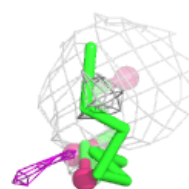
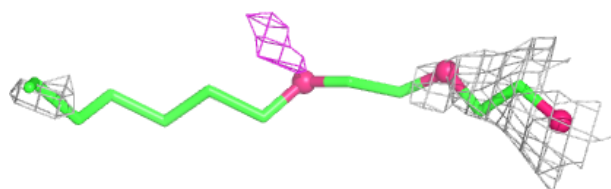
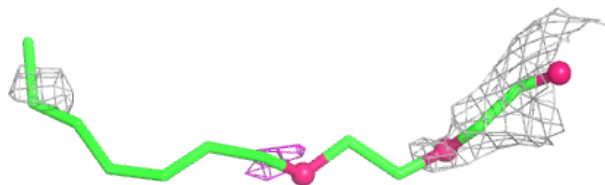
**Electron density around C8E E 405:**

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

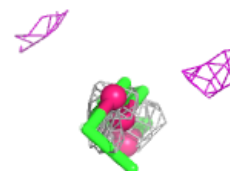
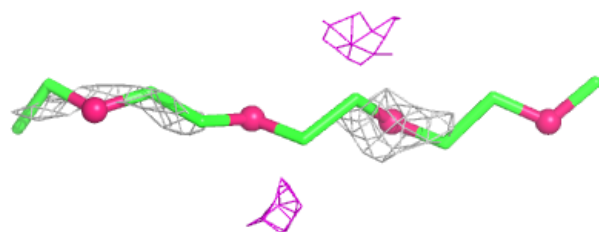
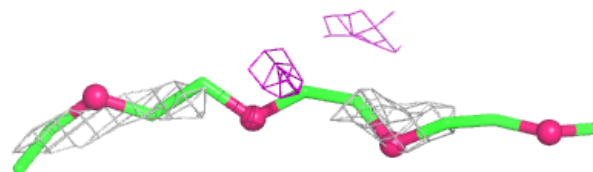


Electron density around C8E A 405:

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

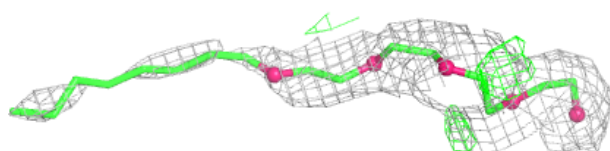
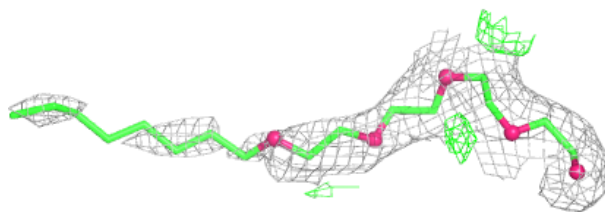
**Electron density around C8E E 403:**

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

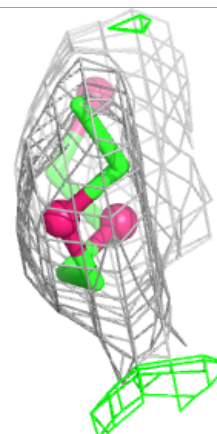
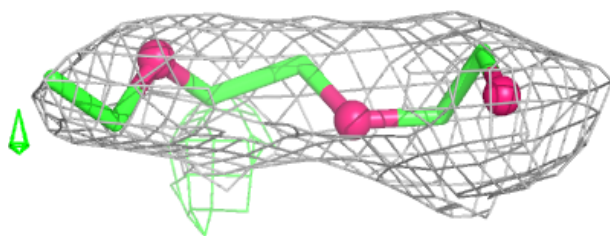
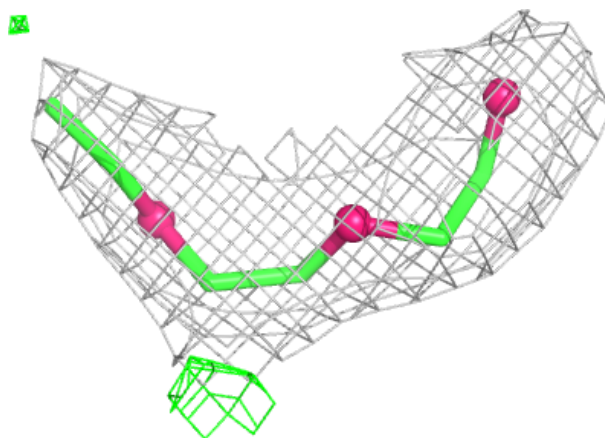


Electron density around C8E A 404:

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

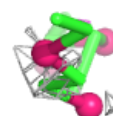
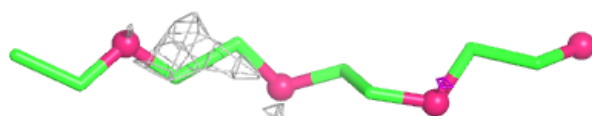
**Electron density around C8E D 304:**

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

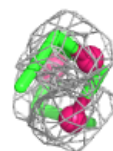
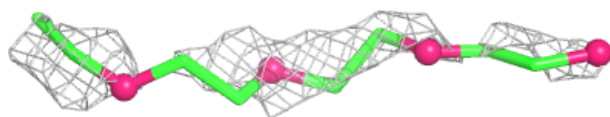
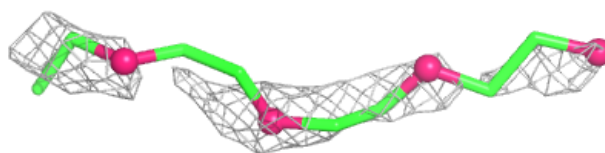


Electron density around C8E D 301:

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

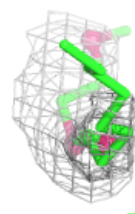
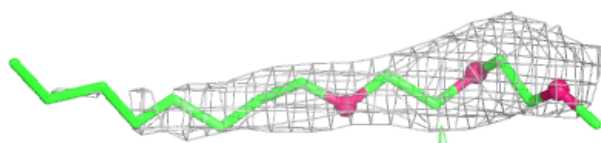
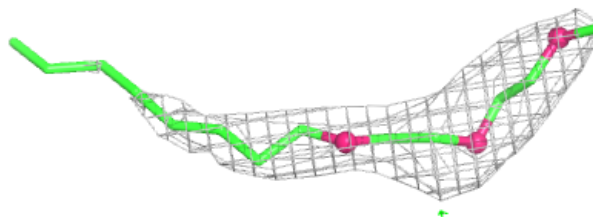
**Electron density around C8E E 404:**

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

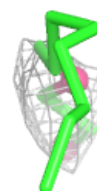
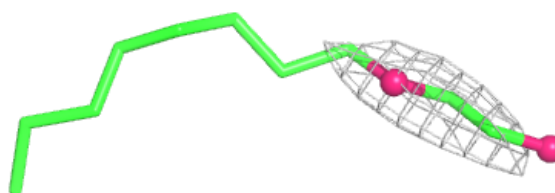


Electron density around C8E F 302:

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

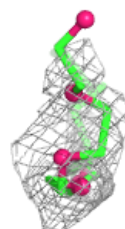
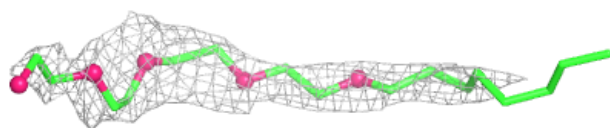
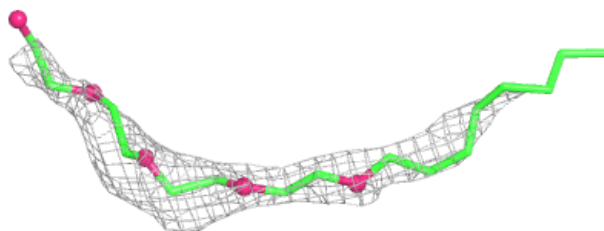
**Electron density around C8E F 301:**

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

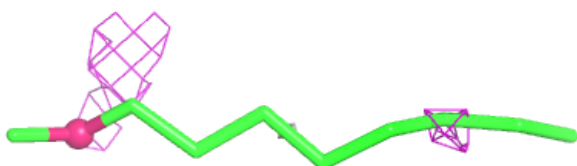
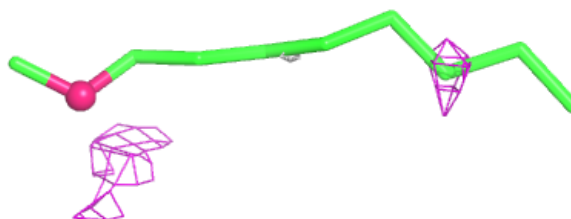


Electron density around C8E B 301:

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

**Electron density around C8E 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.