



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:25 AM UTC

PDB ID : 3RBH / pdb_00003rbh
Title : Structure of alginate export protein AlgE from *Pseudomonas aeruginosa*
Authors : Whitney, J.C.; Hay, I.D.; Li, C.; Eckford, P.D.; Robinson, H.; Amaya, M.F.;
Wood, L.F.; Ohman, D.E.; Bear, C.E.; Rehm, B.H.; Howell, P.L.
Deposited on : 2011-03-29
Resolution : 2.30 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

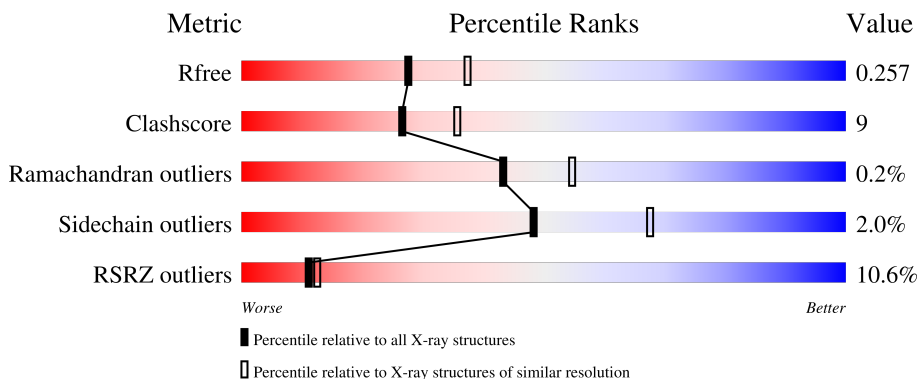
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	479	10% 75% 15% 11%
1	B	479	7% 71% 18% 10%
1	C	479	10% 70% 16% 15%
1	D	479	9% 71% 14% 14%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14038 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 Alginate production protein AlgE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	428	Total	C	N	O	Se	0	2	0
			3305	2073	585	643	4			
1	B	429	Total	C	N	O	Se	0	5	0
			3328	2084	588	652	4			
1	C	409	Total	C	N	O	Se	0	1	0
			3165	1987	564	610	4			
1	D	410	Total	C	N	O	Se	0	1	0
			3165	1992	560	609	4			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	12	MSE	-	expression tag	UNP P18895
A	13	GLY	-	expression tag	UNP P18895
A	14	SER	-	expression tag	UNP P18895
A	15	SER	-	expression tag	UNP P18895
A	16	HIS	-	expression tag	UNP P18895
A	17	HIS	-	expression tag	UNP P18895
A	18	HIS	-	expression tag	UNP P18895
A	19	HIS	-	expression tag	UNP P18895
A	20	HIS	-	expression tag	UNP P18895
A	21	HIS	-	expression tag	UNP P18895
A	22	SER	-	expression tag	UNP P18895
A	23	SER	-	expression tag	UNP P18895
A	24	GLY	-	expression tag	UNP P18895
A	25	LEU	-	expression tag	UNP P18895
A	26	VAL	-	expression tag	UNP P18895
A	27	PRO	-	expression tag	UNP P18895
A	28	ARG	-	expression tag	UNP P18895
A	29	GLY	-	expression tag	UNP P18895
A	30	SER	-	expression tag	UNP P18895
A	31	HIS	-	expression tag	UNP P18895
A	32	MSE	-	expression tag	UNP P18895

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	12	MSE	-	expression tag	UNP P18895
B	13	GLY	-	expression tag	UNP P18895
B	14	SER	-	expression tag	UNP P18895
B	15	SER	-	expression tag	UNP P18895
B	16	HIS	-	expression tag	UNP P18895
B	17	HIS	-	expression tag	UNP P18895
B	18	HIS	-	expression tag	UNP P18895
B	19	HIS	-	expression tag	UNP P18895
B	20	HIS	-	expression tag	UNP P18895
B	21	HIS	-	expression tag	UNP P18895
B	22	SER	-	expression tag	UNP P18895
B	23	SER	-	expression tag	UNP P18895
B	24	GLY	-	expression tag	UNP P18895
B	25	LEU	-	expression tag	UNP P18895
B	26	VAL	-	expression tag	UNP P18895
B	27	PRO	-	expression tag	UNP P18895
B	28	ARG	-	expression tag	UNP P18895
B	29	GLY	-	expression tag	UNP P18895
B	30	SER	-	expression tag	UNP P18895
B	31	HIS	-	expression tag	UNP P18895
B	32	MSE	-	expression tag	UNP P18895
C	12	MSE	-	expression tag	UNP P18895
C	13	GLY	-	expression tag	UNP P18895
C	14	SER	-	expression tag	UNP P18895
C	15	SER	-	expression tag	UNP P18895
C	16	HIS	-	expression tag	UNP P18895
C	17	HIS	-	expression tag	UNP P18895
C	18	HIS	-	expression tag	UNP P18895
C	19	HIS	-	expression tag	UNP P18895
C	20	HIS	-	expression tag	UNP P18895
C	21	HIS	-	expression tag	UNP P18895
C	22	SER	-	expression tag	UNP P18895
C	23	SER	-	expression tag	UNP P18895
C	24	GLY	-	expression tag	UNP P18895
C	25	LEU	-	expression tag	UNP P18895
C	26	VAL	-	expression tag	UNP P18895
C	27	PRO	-	expression tag	UNP P18895
C	28	ARG	-	expression tag	UNP P18895
C	29	GLY	-	expression tag	UNP P18895
C	30	SER	-	expression tag	UNP P18895
C	31	HIS	-	expression tag	UNP P18895
C	32	MSE	-	expression tag	UNP P18895

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	12	MSE	-	expression tag	UNP P18895
D	13	GLY	-	expression tag	UNP P18895
D	14	SER	-	expression tag	UNP P18895
D	15	SER	-	expression tag	UNP P18895
D	16	HIS	-	expression tag	UNP P18895
D	17	HIS	-	expression tag	UNP P18895
D	18	HIS	-	expression tag	UNP P18895
D	19	HIS	-	expression tag	UNP P18895
D	20	HIS	-	expression tag	UNP P18895
D	21	HIS	-	expression tag	UNP P18895
D	22	SER	-	expression tag	UNP P18895
D	23	SER	-	expression tag	UNP P18895
D	24	GLY	-	expression tag	UNP P18895
D	25	LEU	-	expression tag	UNP P18895
D	26	VAL	-	expression tag	UNP P18895
D	27	PRO	-	expression tag	UNP P18895
D	28	ARG	-	expression tag	UNP P18895
D	29	GLY	-	expression tag	UNP P18895
D	30	SER	-	expression tag	UNP P18895
D	31	HIS	-	expression tag	UNP P18895
D	32	MSE	-	expression tag	UNP P18895

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Ca 1 1	0	0
2	B	1	Total Ca 1 1	0	0
2	C	1	Total Ca 1 1	0	0
2	D	1	Total Ca 1 1	0	0

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



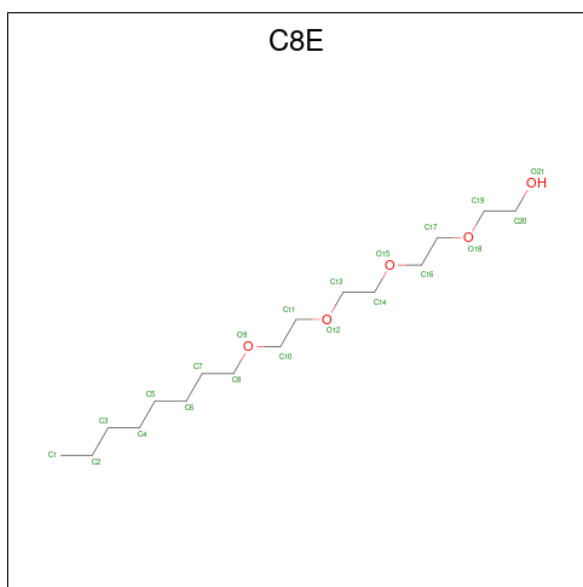
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		

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



Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			11	10	1		
4	A	1	Total	C	O	0	0
			10	9	1		
4	A	1	Total	C	O	0	0
			10	9	1		
4	B	1	Total	C	O	0	0
			9	8	1		
4	B	1	Total	C	O	0	0
			12	10	2		
4	B	1	Total	C	O	0	0
			21	16	5		
4	B	1	Total	C	O	0	0
			9	8	1		
4	B	1	Total	C	O	0	0
			9	8	1		
4	B	1	Total	C	O	0	0
			13	11	2		
4	B	1	Total	C	O	0	0
			10	9	1		
4	B	1	Total	C	O	0	0
			8	6	2		
4	C	1	Total	C	O	0	0
			21	16	5		
4	C	1	Total	C	O	0	0
			12	10	2		
4	C	1	Total	C	O	0	0
			12	10	2		
4	C	1	Total	C	O	0	0
			10	8	2		
4	C	1	Total	C	O	0	0
			9	8	1		
4	C	1	Total	C	O	0	0
			18	14	4		
4	D	1	Total	C	O	0	0
			11	10	1		
4	D	1	Total	C	O	0	0
			21	16	5		
4	D	1	Total	C	O	0	0
			19	15	4		
4	D	1	Total	C	O	0	0
			16	13	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	Total C O 9 8 1	0	0
4	D	1	Total C 8 8	0	0
4	D	1	Total C O 12 10 2	0	0
4	D	1	Total C O 13 11 2	0	0
4	D	1	Total C O 15 12 3	0	0
4	D	1	Total C O 13 11 2	0	0
4	D	1	Total C O 9 8 1	0	0

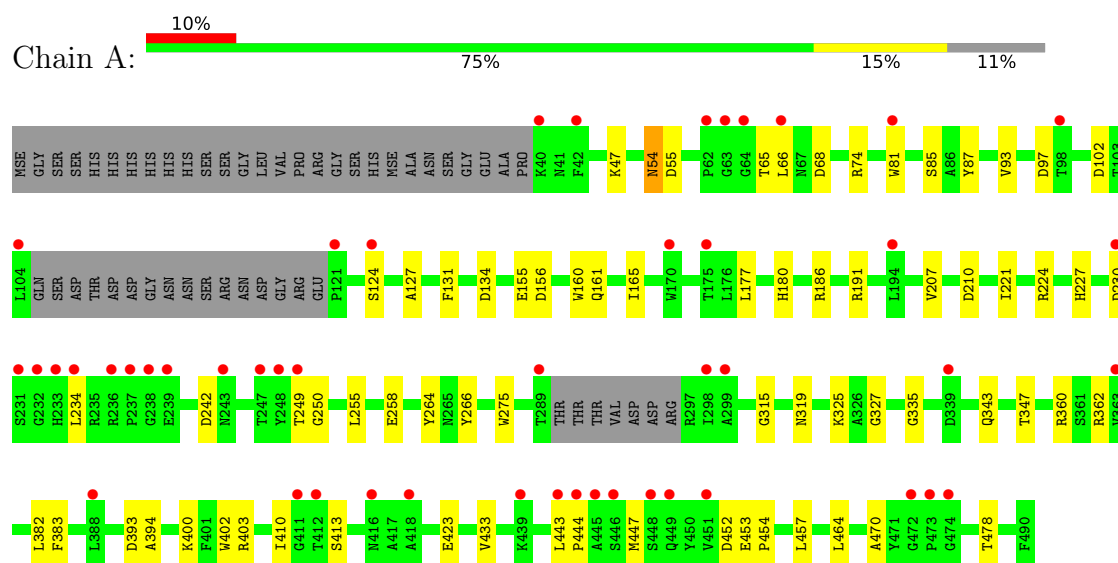
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	166	Total O 166 166	0	0
5	B	155	Total O 155 155	0	0
5	C	142	Total O 142 142	0	0
5	D	149	Total O 149 149	0	0

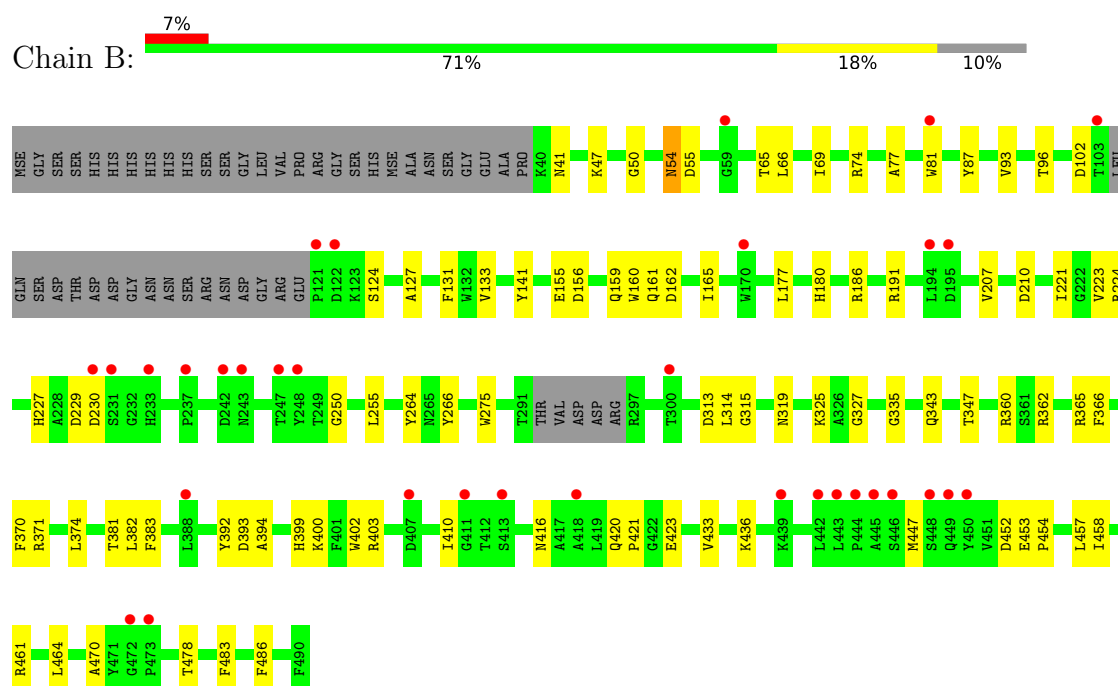
3 Residue-property plots [i](#)

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.

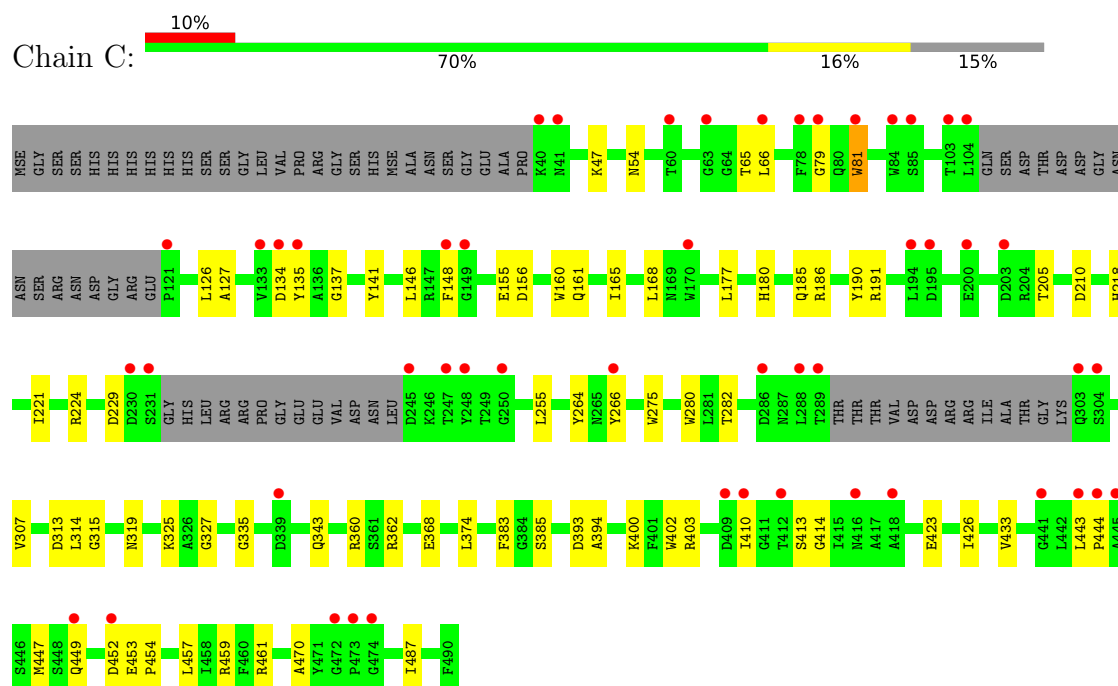
• Molecule 1: Alginate production protein AlgE



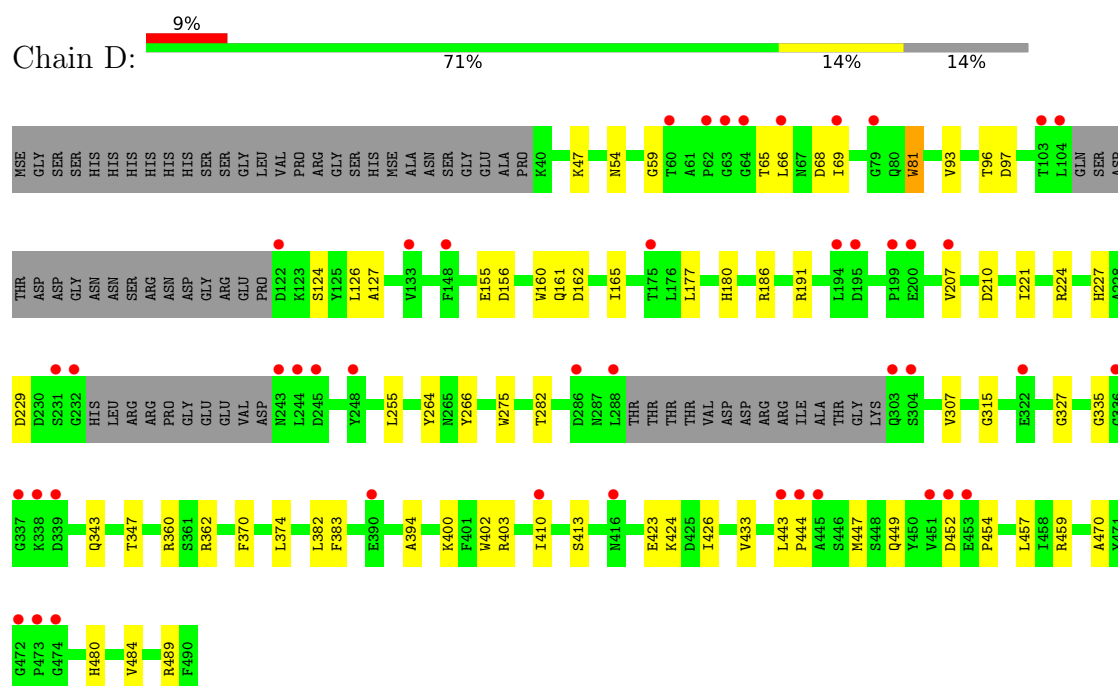
• Molecule 1: Alginate production protein AlgE



• Molecule 1: Alginate production protein AlgE



• Molecule 1: Alginate production protein AlgE



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	162.02Å 90.70Å 160.28Å 90.00° 107.65° 90.00°	Depositor
Resolution (Å)	44.76 – 2.30 44.76 – 2.30	Depositor EDS
% Data completeness (in resolution range)	94.0 (44.76-2.30) 99.6 (44.76-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.49 (at 2.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, R_{free}	0.221 , 0.259 0.220 , 0.257	Depositor DCC
R_{free} test set	4891 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	34.7	Xtriage
Anisotropy	0.481	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 67.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for 1/2*h-3/2*k,-1/2*h-1/2*k,-1/2*h +1/2*k-l 0.000 for 1/2*h+3/2*k,1/2*h-1/2*k,-1/2*h- 1/2*k-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	14038	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 25.60 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.0790e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: CA, C8E, EDO

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	0.48	0/3387	0.75	2/4598 (0.0%)
1	B	0.48	0/3410	0.74	2/4633 (0.0%)
1	C	0.49	0/3244	0.74	0/4401
1	D	0.49	0/3244	0.74	0/4403
All	All	0.49	0/13285	0.75	4/18035 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	453	GLU	CA-C-N	5.42	125.04	119.56
1	B	453	GLU	C-N-CA	5.42	125.04	119.56
1	A	453	GLU	CA-C-N	5.33	124.94	119.56
1	A	453	GLU	C-N-CA	5.33	124.94	119.56

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	3305	0	2965	50	0
1	B	3328	0	2978	71	0
1	C	3165	0	2842	65	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3165	0	2842	52	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	24	0	36	1	0
3	B	32	0	48	4	0
3	C	28	0	42	2	0
3	D	12	0	18	2	0
4	A	44	0	74	3	0
4	B	91	0	142	14	0
4	C	82	0	129	8	0
4	D	146	0	244	8	0
5	A	166	0	0	2	0
5	B	155	0	0	11	0
5	C	142	0	0	11	0
5	D	149	0	0	6	0
All	All	14038	0	12360	240	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 9.

All (240) 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:370:PHE:HB3	5:B:603:HOH:O	1.53	1.09
1:B:366:PHE:O	5:B:603:HOH:O	1.84	0.95
1:B:381[B]:THR:HG22	1:B:399:HIS:ND1	1.86	0.90
1:D:443:LEU:HD12	1:D:444:PRO:HD2	1.60	0.83
1:D:480:HIS:ND1	4:D:498:C8E:H102	1.97	0.79
1:A:81:TRP:CH2	1:C:148:PHE:HZ	2.01	0.79
1:B:370:PHE:CD2	5:B:603:HOH:O	2.37	0.77
1:B:370:PHE:HD2	5:B:603:HOH:O	1.69	0.75
1:B:223:VAL:HG11	3:B:495:EDO:H22	1.67	0.74
1:D:65:THR:O	1:D:66:LEU:HD23	1.90	0.70
1:B:141:TYR:OH	4:B:500:C8E:H102	1.93	0.69
1:C:160:TRP:CD1	5:C:552:HOH:O	2.48	0.67
1:C:335:GLY:HA2	1:C:343:GLN:HA	1.77	0.67
1:C:134:ASP:O	5:C:592:HOH:O	2.12	0.67
1:B:141:TYR:CZ	4:B:500:C8E:H102	2.30	0.66
1:D:186:ARG:HD3	5:D:608:HOH:O	1.94	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:343:GLN:O	5:D:624:HOH:O	2.14	0.65
1:A:266:TYR:CZ	1:A:360:ARG:HG2	2.31	0.65
1:B:483:PHE:CE2	5:B:609:HOH:O	2.49	0.65
1:A:65:THR:O	1:A:66:LEU:HD12	1.96	0.65
1:B:365:ARG:HH12	1:B:381[B]:THR:HG21	1.60	0.65
1:D:335:GLY:HA2	1:D:343:GLN:HA	1.79	0.65
1:C:443:LEU:HD12	1:C:444:PRO:HD2	1.78	0.64
1:A:335:GLY:HA2	1:A:343:GLN:HA	1.80	0.64
1:C:65:THR:O	1:C:66:LEU:HD12	1.99	0.63
1:C:79:GLY:HA3	1:C:81:TRP:CH2	2.33	0.63
1:B:266:TYR:CZ	1:B:360:ARG:HG2	2.33	0.63
1:C:266:TYR:CZ	1:C:360:ARG:HG2	2.34	0.62
1:A:81:TRP:CH2	1:C:148:PHE:CZ	2.85	0.62
1:C:453:GLU:HG2	1:C:487:ILE:HD13	1.83	0.60
1:B:69:ILE:CD1	4:B:8:C8E:H72	2.32	0.60
1:C:368:GLU:HB2	5:C:601:HOH:O	2.01	0.59
1:B:335:GLY:HA2	1:B:343:GLN:HA	1.82	0.59
1:C:126:LEU:HG	4:C:497:C8E:H71	1.85	0.59
1:C:135:TYR:HA	5:C:546:HOH:O	2.02	0.59
1:A:81:TRP:CE3	1:A:81:TRP:N	2.70	0.59
1:C:180:HIS:HB2	1:C:210:ASP:OD2	2.03	0.59
1:D:126:LEU:HG	4:D:495:C8E:H82	1.84	0.59
1:D:156:ASP:HB3	1:D:264:TYR:CD2	2.38	0.58
1:A:394:ALA:HA	1:A:433:VAL:O	2.03	0.58
1:A:275:TRP:CE2	1:A:315:GLY:HA3	2.38	0.58
1:B:371:ARG:NH2	5:B:609:HOH:O	2.36	0.58
1:C:79:GLY:HA3	1:C:81:TRP:CZ2	2.39	0.58
1:D:370:PHE:O	1:D:413:SER:HB2	2.04	0.58
1:C:280:TRP:CE3	4:C:498:C8E:H32	2.39	0.58
1:A:234:LEU:HG	1:A:249:THR:HG23	1.85	0.58
1:B:65:THR:O	1:B:66:LEU:HD12	2.04	0.58
1:C:205:THR:HG23	5:C:579:HOH:O	2.03	0.58
1:B:275:TRP:CE2	1:B:315:GLY:HA3	2.39	0.57
1:B:458:ILE:HD12	4:B:8:C8E:H141	1.85	0.57
1:B:394:ALA:HA	1:B:433:VAL:O	2.05	0.57
1:A:275:TRP:CZ2	1:A:315:GLY:HA3	2.40	0.57
1:D:403:ARG:O	1:D:424:LYS:HG3	2.05	0.56
1:C:452:ASP:C	1:C:453:GLU:HG3	2.30	0.56
1:B:223:VAL:CG1	3:B:495:EDO:H22	2.34	0.56
1:B:81:TRP:HZ2	4:B:497:C8E:H72	1.71	0.55
1:C:137:GLY:HA3	5:C:558:HOH:O	2.06	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:394:ALA:HA	1:C:433:VAL:O	2.07	0.55
1:D:81:TRP:HZ2	4:D:5:C8E:H171	1.70	0.55
1:D:266:TYR:CZ	1:D:360:ARG:HG2	2.42	0.55
1:B:461:ARG:NH1	5:B:609:HOH:O	2.26	0.55
1:C:156:ASP:HB3	1:C:264:TYR:CD2	2.41	0.55
1:D:96:THR:HA	4:D:494:C8E:H102	1.89	0.55
1:D:443:LEU:HD21	1:D:449:GLN:NE2	2.21	0.54
1:B:275:TRP:CZ2	1:B:315:GLY:HA3	2.42	0.54
1:D:394:ALA:HA	1:D:433:VAL:O	2.08	0.54
1:A:180:HIS:HB2	1:A:210:ASP:OD2	2.07	0.54
1:A:400:LYS:HD2	1:A:402:TRP:CZ2	2.43	0.53
1:A:81:TRP:N	1:A:81:TRP:HE3	2.07	0.53
1:B:370:PHE:CB	5:B:603:HOH:O	2.31	0.53
1:D:180:HIS:HB2	1:D:210:ASP:OD2	2.09	0.53
1:B:381[B]:THR:CG2	1:B:399:HIS:ND1	2.69	0.53
1:D:400:LYS:HD2	1:D:402:TRP:CZ2	2.44	0.53
1:B:180:HIS:HB2	1:B:210:ASP:OD2	2.09	0.52
1:A:347:THR:HG23	3:A:3:EDO:O2	2.09	0.52
1:B:458:ILE:HD12	4:B:8:C8E:H171	1.90	0.52
1:C:400:LYS:HD2	1:C:402:TRP:CZ2	2.45	0.52
1:B:156:ASP:HB3	1:B:264:TYR:CD2	2.44	0.52
1:A:81:TRP:CZ2	1:C:148:PHE:CZ	2.98	0.52
1:C:275:TRP:CZ2	1:C:315:GLY:HA3	2.45	0.52
1:D:443:LEU:HD22	1:D:489:ARG:CZ	2.39	0.52
1:C:280:TRP:NE1	4:C:498:C8E:H112	2.24	0.52
1:C:443:LEU:HD21	1:C:449:GLN:NE2	2.25	0.52
1:B:141:TYR:CE1	4:B:500:C8E:H102	2.45	0.51
1:B:400:LYS:HD2	1:B:402:TRP:CZ2	2.46	0.51
1:C:453:GLU:HG2	1:C:487:ILE:CD1	2.40	0.51
1:C:127:ALA:HB2	1:C:191:ARG:HG2	1.93	0.51
1:C:190:TYR:HA	4:C:7:C8E:H101	1.93	0.51
1:D:93:VAL:O	1:D:124:SER:HA	2.11	0.51
4:C:498:C8E:H52	4:C:498:C8E:O9	2.11	0.50
1:C:185:GLN:NE2	5:C:579:HOH:O	2.44	0.50
1:D:155:GLU:HG3	1:D:161:GLN:HG2	1.93	0.50
1:B:347:THR:HG23	3:B:6:EDO:O2	2.12	0.50
1:C:362:ARG:HD3	1:C:452:ASP:OD1	2.12	0.50
1:A:230:ASP:HB2	1:A:250:GLY:H	1.77	0.50
1:D:165:ILE:HG13	1:D:186:ARG:HG2	1.94	0.50
1:D:347:THR:HG23	3:D:7:EDO:O1	2.12	0.50
1:B:161:GLN:NE2	5:B:632:HOH:O	2.45	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:165:ILE:HG13	1:C:186:ARG:HG2	1.93	0.49
1:D:275:TRP:CZ2	1:D:315:GLY:HA3	2.47	0.49
1:A:360:ARG:HH21	1:A:454:PRO:CG	2.26	0.49
1:D:443:LEU:CD1	1:D:444:PRO:HD2	2.36	0.49
1:B:360:ARG:NH2	1:B:454:PRO:CG	2.76	0.48
1:D:127:ALA:HB2	1:D:191:ARG:HG2	1.95	0.48
1:A:207:VAL:HG13	1:A:227:HIS:HB3	1.95	0.48
1:A:360:ARG:NH2	1:A:454:PRO:CG	2.76	0.48
1:A:255:LEU:HD12	1:A:255:LEU:N	2.28	0.48
1:A:165:ILE:HG13	1:A:186:ARG:HG2	1.95	0.48
1:A:443:LEU:HD12	1:A:444:PRO:HD2	1.94	0.48
1:D:275:TRP:CE2	1:D:315:GLY:HA3	2.48	0.48
1:C:275:TRP:CE2	1:C:315:GLY:HA3	2.49	0.48
1:D:459:ARG:HD2	5:D:563:HOH:O	2.12	0.48
1:B:207:VAL:HG13	1:B:227:HIS:HB3	1.96	0.48
1:B:360:ARG:HH21	1:B:454:PRO:CG	2.26	0.47
1:D:457:LEU:C	1:D:457:LEU:HD12	2.39	0.47
1:B:69:ILE:HD11	4:B:8:C8E:H72	1.96	0.47
1:D:360:ARG:NH2	1:D:454:PRO:CG	2.77	0.47
1:D:255:LEU:N	1:D:255:LEU:HD12	2.29	0.47
1:D:360:ARG:HH21	1:D:454:PRO:CG	2.27	0.47
1:A:156:ASP:HB3	1:A:264:TYR:CD2	2.49	0.47
1:C:457:LEU:HD12	1:C:457:LEU:C	2.40	0.47
1:D:362:ARG:HD3	1:D:452:ASP:OD1	2.15	0.47
1:B:207:VAL:CG1	1:B:227:HIS:HB3	2.45	0.47
1:C:447:MSE:HA	1:C:447:MSE:HE2	1.97	0.47
1:D:447:MSE:HE2	1:D:447:MSE:HA	1.97	0.47
1:C:360:ARG:NH2	1:C:454:PRO:CG	2.77	0.47
1:C:155:GLU:HG3	1:C:161:GLN:HG2	1.96	0.47
1:C:255:LEU:HD12	1:C:255:LEU:N	2.30	0.46
1:B:160:TRP:CE2	1:B:224:ARG:HD2	2.50	0.46
1:C:134:ASP:C	5:C:592:HOH:O	2.56	0.46
1:C:443:LEU:HD21	1:C:449:GLN:HE21	1.79	0.46
1:B:486:PHE:CD1	4:B:8:C8E:H142	2.51	0.46
1:A:207:VAL:CG1	1:A:227:HIS:HB3	2.45	0.46
1:B:127:ALA:HB2	1:B:191:ARG:HG2	1.98	0.46
1:C:190:TYR:HA	4:C:7:C8E:C10	2.45	0.46
4:D:5:C8E:H201	5:D:643:HOH:O	2.15	0.46
1:B:255:LEU:N	1:B:255:LEU:HD12	2.31	0.46
1:B:447:MSE:HE2	1:B:447:MSE:HA	1.96	0.46
1:D:402:TRP:HB3	1:D:424:LYS:HG2	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:165:ILE:HG13	1:B:186:ARG:HG2	1.97	0.46
1:A:81:TRP:HE1	4:A:494:C8E:C11	2.29	0.46
1:A:447:MSE:HA	1:A:447:MSE:HE2	1.96	0.46
1:C:360:ARG:HH21	1:C:454:PRO:CG	2.28	0.46
1:C:141:TYR:HE1	4:C:496:C8E:H101	1.81	0.46
4:A:495:C8E:H12	4:A:495:C8E:H42	1.65	0.46
1:A:87:TYR:O	1:A:131:PHE:HA	2.16	0.45
1:C:327:GLY:HA3	1:C:383:PHE:CZ	2.51	0.45
1:A:266:TYR:CE2	1:A:360:ARG:HG2	2.50	0.45
1:D:207:VAL:CG1	1:D:227:HIS:HB3	2.46	0.45
1:B:403:ARG:HG2	1:B:410:ILE:CG2	2.46	0.45
1:B:457:LEU:HD12	1:B:457:LEU:C	2.40	0.45
1:C:160:TRP:NE1	5:C:552:HOH:O	2.50	0.45
1:B:87:TYR:O	1:B:131:PHE:HA	2.15	0.45
1:D:69:ILE:HD11	4:D:9:C8E:H22	1.97	0.45
1:A:54:ASN:HA	1:A:55:ASP:HA	1.71	0.45
1:B:319:ASN:OD1	1:B:325:LYS:HE2	2.17	0.45
1:A:155:GLU:HG3	1:A:161:GLN:HG2	1.98	0.45
1:D:374:LEU:HD12	1:D:374:LEU:HA	1.73	0.45
1:A:457:LEU:C	1:A:457:LEU:HD12	2.42	0.44
1:D:160:TRP:CE2	1:D:224:ARG:HD2	2.52	0.44
4:B:8:C8E:H141	4:B:8:C8E:H171	1.59	0.44
1:A:319:ASN:OD1	1:A:325:LYS:HE2	2.17	0.44
1:C:423:GLU:HB2	1:C:470:ALA:HA	2.00	0.44
1:A:127:ALA:HB2	1:A:191:ARG:HG2	1.99	0.44
4:B:497:C8E:H112	3:D:492:EDO:H11	1.98	0.44
1:C:374:LEU:HD12	1:C:374:LEU:HA	1.73	0.44
1:A:362:ARG:HD3	1:A:452:ASP:OD1	2.18	0.44
1:C:160:TRP:CE2	1:C:224:ARG:HD2	2.53	0.44
1:C:319:ASN:OD1	1:C:325:LYS:HE2	2.18	0.44
1:C:413[A]:SER:OG	1:C:414:GLY:N	2.50	0.44
1:B:313:ASP:O	1:B:314:LEU:HD23	2.18	0.44
1:B:381[B]:THR:HG22	1:B:399:HIS:CE1	2.51	0.44
1:D:327:GLY:HA3	1:D:383:PHE:CZ	2.53	0.44
1:A:74:ARG:HH22	1:A:102:ASP:HB2	1.83	0.44
1:A:81:TRP:CD1	5:A:577:HOH:O	2.70	0.43
1:C:282:THR:HA	1:C:307:VAL:O	2.18	0.43
1:D:59:GLY:HA2	5:D:621:HOH:O	2.17	0.43
1:B:74:ARG:HH22	1:B:102:ASP:HB2	1.82	0.43
1:B:50:GLY:HA3	4:B:8:C8E:H51	2.01	0.43
1:B:362:ARG:HD3	1:B:452:ASP:OD1	2.17	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:464:LEU:HD11	1:B:478:THR:OG1	2.18	0.43
1:C:402:TRP:C	1:C:426:ILE:HD12	2.44	0.43
1:C:403:ARG:HG2	1:C:410:ILE:CG2	2.49	0.43
1:C:461:ARG:NH2	5:C:638:HOH:O	2.41	0.43
4:A:494:C8E:H82	1:C:168:LEU:HD22	2.00	0.43
4:B:501:C8E:H41	4:B:501:C8E:H13	1.78	0.43
1:C:190:TYR:C	4:C:7:C8E:H72	2.44	0.43
1:D:68:ASP:OD1	1:D:97:ASP:HB2	2.19	0.43
1:D:403:ARG:HG2	1:D:410:ILE:CG2	2.48	0.43
1:B:159:GLN:OE1	3:B:4:EDO:H21	2.19	0.43
1:D:423:GLU:HB2	1:D:470:ALA:HA	2.01	0.43
1:B:54:ASN:HA	1:B:55:ASP:HA	1.71	0.43
1:D:207:VAL:HG13	1:D:227:HIS:HB3	2.01	0.42
1:C:400:LYS:CD	1:C:402:TRP:CZ2	3.03	0.42
1:A:400:LYS:CD	1:A:402:TRP:CZ2	3.02	0.42
1:B:392:TYR:CE1	1:B:436:LYS:HG3	2.53	0.42
1:B:381[B]:THR:HG23	5:B:551:HOH:O	2.19	0.42
1:A:81:TRP:HD1	5:A:577:HOH:O	2.02	0.42
1:A:160:TRP:CE2	1:A:224:ARG:HD2	2.54	0.42
1:A:423:GLU:HB2	1:A:470:ALA:HA	2.01	0.42
1:A:85:SER:OG	1:A:134:ASP:HB3	2.19	0.42
1:A:327:GLY:HA3	1:A:383:PHE:CZ	2.54	0.42
1:A:464:LEU:HD11	1:A:478:THR:OG1	2.20	0.42
1:B:93:VAL:O	1:B:124:SER:HA	2.20	0.42
1:D:65:THR:C	1:D:66:LEU:HD23	2.44	0.42
1:D:162:ASP:CG	1:D:362:ARG:HH22	2.21	0.42
1:B:155:GLU:HG3	1:B:161:GLN:HG2	2.01	0.42
1:B:400:LYS:CD	1:B:402:TRP:CZ2	3.03	0.42
1:B:374:LEU:HD12	1:B:374:LEU:HA	1.73	0.41
1:A:93:VAL:O	1:A:124:SER:HA	2.20	0.41
1:A:81:TRP:CZ2	1:C:148:PHE:CE1	3.08	0.41
1:B:327:GLY:HA3	1:B:383:PHE:CZ	2.55	0.41
1:B:416:ASN:ND2	5:B:578:HOH:O	2.53	0.41
1:B:423:GLU:HB2	1:B:470:ALA:HA	2.02	0.41
1:D:81:TRP:CZ2	4:D:5:C8E:H171	2.51	0.41
1:D:402:TRP:C	1:D:426:ILE:HD12	2.45	0.41
1:A:393:ASP:OD1	1:A:393:ASP:C	2.63	0.41
1:B:393:ASP:OD1	1:B:393:ASP:C	2.61	0.41
1:B:486:PHE:HB2	4:B:8:C8E:H112	2.01	0.41
1:D:400:LYS:CD	1:D:402:TRP:CZ2	3.04	0.41
1:A:266:TYR:CZ	1:A:360:ARG:CG	3.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:41:ASN:O	1:B:77:ALA:HA	2.21	0.41
1:B:266:TYR:CE2	1:B:360:ARG:HG2	2.56	0.41
1:C:146:LEU:HD11	1:C:168:LEU:HD11	2.02	0.41
1:A:403:ARG:HG2	1:A:410:ILE:CG2	2.50	0.41
1:B:162:ASP:CG	1:B:362:ARG:HH22	2.28	0.41
1:C:313:ASP:O	1:C:314:LEU:HD23	2.21	0.41
1:C:218:HIS:O	3:C:493:EDO:H12	2.21	0.41
1:C:385:SER:HA	3:C:11:EDO:H21	2.03	0.41
1:C:443:LEU:CD1	1:C:444:PRO:HD2	2.50	0.41
1:B:230:ASP:HB2	1:B:250:GLY:H	1.85	0.41
1:C:393:ASP:OD1	1:C:393:ASP:C	2.63	0.41
1:C:459:ARG:HD2	5:C:607:HOH:O	2.20	0.40
1:D:484:VAL:HB	4:D:9:C8E:H12	2.02	0.40
1:B:69:ILE:HG22	1:B:96:THR:HG23	2.03	0.40
1:A:68:ASP:OD1	1:A:97:ASP:HB2	2.21	0.40
1:D:282:THR:HA	1:D:307:VAL:O	2.21	0.40
1:A:81:TRP:O	1:A:81:TRP:CG	2.74	0.40
1:B:420:GLN:HA	1:B:421:PRO:HD3	1.98	0.40
1:D:186:ARG:HB3	5:D:608:HOH:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	424/479 (88%)	404 (95%)	19 (4%)	1 (0%)	43	55
1	B	428/479 (89%)	411 (96%)	16 (4%)	1 (0%)	43	55
1	C	402/479 (84%)	387 (96%)	14 (4%)	1 (0%)	43	55
1	D	403/479 (84%)	386 (96%)	16 (4%)	1 (0%)	43	55
All	All	1657/1916 (86%)	1588 (96%)	65 (4%)	4 (0%)	43	55

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	B	54	ASN
1	C	54	ASN
1	D	54	ASN

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	316/382 (83%)	309 (98%)	7 (2%)	45	65
1	B	320/382 (84%)	313 (98%)	7 (2%)	45	65
1	C	302/382 (79%)	297 (98%)	5 (2%)	53	72
1	D	301/382 (79%)	295 (98%)	6 (2%)	48	67
All	All	1239/1528 (81%)	1214 (98%)	25 (2%)	48	67

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	LYS
1	A	177	LEU
1	A	221	ILE
1	A	242	ASP
1	A	258	GLU
1	A	382	LEU
1	A	413	SER
1	B	47	LYS
1	B	133[A]	VAL
1	B	133[B]	VAL
1	B	177	LEU
1	B	221	ILE
1	B	229	ASP
1	B	382	LEU
1	C	47	LYS
1	C	81	TRP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	177	LEU
1	C	221	ILE
1	C	229	ASP
1	D	47	LYS
1	D	81	TRP
1	D	177	LEU
1	D	221	ILE
1	D	229	ASP
1	D	382	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	178	ASN
1	A	387	GLN
1	B	161	GLN
1	B	178	ASN
1	B	416	ASN
1	C	308	ASN
1	C	387	GLN
1	C	420	GLN
1	D	178	ASN
1	D	387	GLN

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](#)

Of 57 ligands modelled in this entry, 4 are monoatomic - leaving 53 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	$\# Z > 2$
4	C8E	D	500	-	12,12,20	0.33	0	11,11,19	0.40	0
3	EDO	C	493	-	3,3,3	0.50	0	2,2,2	0.22	0
4	C8E	B	498	-	8,8,20	0.25	0	7,7,19	0.60	0
3	EDO	C	10	-	3,3,3	0.46	0	2,2,2	0.36	0
3	EDO	B	9	-	3,3,3	0.47	0	2,2,2	0.38	0
4	C8E	B	500	-	12,12,20	0.35	0	11,11,19	0.37	0
3	EDO	A	8	-	3,3,3	0.46	0	2,2,2	0.42	0
4	C8E	C	497	-	8,8,20	0.27	0	7,7,19	0.50	0
3	EDO	C	492	-	3,3,3	0.43	0	2,2,2	0.46	0
3	EDO	B	495	-	3,3,3	0.41	0	2,2,2	0.44	0
4	C8E	C	498	-	17,17,20	0.42	0	16,16,19	0.34	0
3	EDO	A	492	-	3,3,3	0.46	0	2,2,2	0.45	0
4	C8E	C	495	-	11,11,20	0.38	0	10,10,19	0.30	0
4	C8E	D	495	-	8,8,20	0.25	0	7,7,19	0.52	0
4	C8E	A	494	-	12,12,20	0.34	0	11,11,19	0.41	0
4	C8E	A	495	-	9,9,20	0.29	0	8,8,19	0.55	0
4	C8E	D	493	-	10,10,20	0.38	0	9,9,19	0.43	0
3	EDO	C	5	-	3,3,3	0.50	0	2,2,2	0.10	0
3	EDO	D	491	-	3,3,3	0.46	0	2,2,2	0.44	0
3	EDO	B	494	-	3,3,3	0.59	0	2,2,2	0.04	0
4	C8E	A	11	-	9,9,20	0.31	0	8,8,19	0.44	0
3	EDO	B	6	-	3,3,3	0.53	0	2,2,2	0.27	0
4	C8E	C	496	-	9,9,20	0.38	0	8,8,19	0.33	0
4	C8E	B	499	-	8,8,20	0.23	0	7,7,19	0.68	0
4	C8E	B	501	-	9,9,20	0.26	0	8,8,19	0.60	0
3	EDO	B	4	-	3,3,3	0.43	0	2,2,2	0.53	0
4	C8E	B	8	-	20,20,20	0.42	0	19,19,19	0.34	0
4	C8E	C	494	-	20,20,20	0.47	0	19,19,19	0.38	0
3	EDO	A	3	-	3,3,3	0.56	0	2,2,2	0.26	0
3	EDO	B	492	-	3,3,3	0.48	0	2,2,2	0.27	0
3	EDO	C	491	-	3,3,3	0.43	0	2,2,2	0.34	0
4	C8E	B	497	-	11,11,20	0.37	0	10,10,19	0.39	0
3	EDO	A	2	-	3,3,3	0.39	0	2,2,2	0.40	0
4	C8E	D	5	-	20,20,20	0.44	0	19,19,19	0.36	0
4	C8E	D	501	-	8,8,20	0.23	0	7,7,19	0.64	0
4	C8E	D	499	-	14,14,20	0.39	0	13,13,19	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	A	491	-	3,3,3	0.43	0	2,2,2	0.44	0
4	C8E	C	7	-	11,11,20	0.30	0	10,10,19	0.65	0
3	EDO	C	1	-	3,3,3	0.50	0	2,2,2	0.44	0
4	C8E	B	496	-	8,8,20	0.41	0	7,7,19	0.36	0
3	EDO	D	7	-	3,3,3	0.53	0	2,2,2	0.62	0
4	C8E	D	9	-	18,18,20	0.43	0	17,17,19	0.38	0
4	C8E	A	10	-	10,10,20	0.37	0	9,9,19	0.44	0
4	C8E	D	496	-	7,7,20	0.30	0	6,6,19	0.43	0
3	EDO	D	492	-	3,3,3	0.51	0	2,2,2	0.26	0
4	C8E	D	497	-	11,11,20	0.37	0	10,10,19	0.35	0
4	C8E	D	494	-	15,15,20	0.41	0	14,14,19	0.42	0
3	EDO	A	493	-	3,3,3	0.45	0	2,2,2	0.38	0
4	C8E	D	498	-	12,12,20	0.36	0	11,11,19	0.34	0
3	EDO	B	491	-	3,3,3	0.43	0	2,2,2	0.46	0
3	EDO	B	493	-	3,3,3	0.50	0	2,2,2	0.36	0
4	C8E	B	502	-	7,7,20	0.46	0	6,6,19	0.40	0
3	EDO	C	11	-	3,3,3	0.48	0	2,2,2	0.43	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	500	-	-	6/10/10/18	-
3	EDO	C	493	-	-	1/1/1/1	-
4	C8E	B	498	-	-	2/6/6/18	-
3	EDO	C	10	-	-	0/1/1/1	-
3	EDO	B	9	-	-	0/1/1/1	-
4	C8E	B	500	-	-	7/10/10/18	-
3	EDO	A	8	-	-	1/1/1/1	-
4	C8E	C	497	-	-	4/6/6/18	-
3	EDO	C	492	-	-	0/1/1/1	-
3	EDO	B	495	-	-	1/1/1/1	-
4	C8E	C	498	-	-	9/15/15/18	-
3	EDO	A	492	-	-	0/1/1/1	-
4	C8E	C	495	-	-	5/9/9/18	-
4	C8E	D	495	-	-	4/6/6/18	-
4	C8E	A	494	-	-	7/10/10/18	-
4	C8E	A	495	-	-	5/7/7/18	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	C8E	D	493	-	-	5/8/8/18	-
3	EDO	C	5	-	-	0/1/1/1	-
3	EDO	D	491	-	-	1/1/1/1	-
3	EDO	B	494	-	-	0/1/1/1	-
4	C8E	A	11	-	-	4/7/7/18	-
3	EDO	B	6	-	-	0/1/1/1	-
4	C8E	C	496	-	-	4/7/7/18	-
4	C8E	B	499	-	-	2/6/6/18	-
4	C8E	B	501	-	-	7/7/7/18	-
3	EDO	B	4	-	-	1/1/1/1	-
4	C8E	B	8	-	-	12/18/18/18	-
4	C8E	C	494	-	-	12/18/18/18	-
3	EDO	A	3	-	-	0/1/1/1	-
3	EDO	B	492	-	-	0/1/1/1	-
3	EDO	C	491	-	-	0/1/1/1	-
4	C8E	B	497	-	-	6/9/9/18	-
3	EDO	A	2	-	-	0/1/1/1	-
4	C8E	D	5	-	-	6/18/18/18	-
4	C8E	D	501	-	-	2/6/6/18	-
4	C8E	D	499	-	-	7/12/12/18	-
3	EDO	A	491	-	-	0/1/1/1	-
4	C8E	C	7	-	-	4/9/9/18	-
3	EDO	C	1	-	-	0/1/1/1	-
4	C8E	B	496	-	-	2/6/6/18	-
3	EDO	D	7	-	-	0/1/1/1	-
4	C8E	D	9	-	-	9/16/16/18	-
4	C8E	A	10	-	-	5/8/8/18	-
4	C8E	D	496	-	-	2/5/5/18	-
3	EDO	D	492	-	-	0/1/1/1	-
4	C8E	D	497	-	-	2/9/9/18	-
4	C8E	D	494	-	-	10/13/13/18	-
3	EDO	A	493	-	-	0/1/1/1	-
4	C8E	D	498	-	-	7/10/10/18	-
3	EDO	B	491	-	-	0/1/1/1	-
3	EDO	B	493	-	-	0/1/1/1	-
4	C8E	B	502	-	-	2/5/5/18	-
3	EDO	C	11	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (164) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	7	C8E	C7-C8-O9-C10
4	B	8	C8E	O12-C13-C14-O15
4	C	494	C8E	O9-C10-C11-O12
4	B	8	C8E	C17-C16-O15-C14
4	C	494	C8E	O12-C13-C14-O15
4	D	499	C8E	C6-C7-C8-O9
4	B	496	C8E	C6-C7-C8-O9
4	D	494	C8E	C6-C7-C8-O9
4	D	498	C8E	C6-C7-C8-O9
4	D	9	C8E	O9-C10-C11-O12
4	B	8	C8E	O18-C19-C20-O21
4	C	7	C8E	O9-C10-C11-O12
4	D	499	C8E	O12-C13-C14-O15
4	B	8	C8E	C6-C7-C8-O9
4	D	500	C8E	O9-C10-C11-O12
4	A	495	C8E	C6-C7-C8-O9
4	A	494	C8E	C6-C7-C8-O9
4	A	494	C8E	O9-C10-C11-O12
4	C	495	C8E	C6-C7-C8-O9
4	B	501	C8E	C6-C7-C8-O9
4	A	10	C8E	C6-C7-C8-O9
4	C	496	C8E	C5-C6-C7-C8
4	D	493	C8E	C4-C5-C6-C7
4	D	499	C8E	C3-C4-C5-C6
4	D	495	C8E	C4-C5-C6-C7
4	B	501	C8E	C7-C8-O9-C10
4	D	495	C8E	C3-C4-C5-C6
4	C	498	C8E	C4-C5-C6-C7
4	A	494	C8E	C3-C4-C5-C6
4	D	5	C8E	O18-C19-C20-O21
4	D	498	C8E	C3-C4-C5-C6
4	D	5	C8E	C2-C3-C4-C5
4	D	494	C8E	C3-C4-C5-C6
4	D	497	C8E	C3-C4-C5-C6
4	A	494	C8E	C5-C6-C7-C8
4	B	500	C8E	C4-C5-C6-C7
4	B	501	C8E	C4-C5-C6-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	D	499	C8E	C2-C3-C4-C5
4	B	501	C8E	C2-C3-C4-C5
4	B	501	C8E	C5-C6-C7-C8
4	D	499	C8E	C1-C2-C3-C4
4	B	497	C8E	C4-C5-C6-C7
4	D	494	C8E	C4-C5-C6-C7
4	A	495	C8E	C1-C2-C3-C4
4	C	495	C8E	C3-C4-C5-C6
4	C	494	C8E	C2-C3-C4-C5
4	D	500	C8E	C6-C7-C8-O9
4	A	495	C8E	C4-C5-C6-C7
4	B	500	C8E	C2-C3-C4-C5
4	B	498	C8E	C2-C3-C4-C5
4	A	495	C8E	C2-C3-C4-C5
4	A	11	C8E	C7-C8-O9-C10
4	D	9	C8E	O15-C16-C17-O18
4	C	497	C8E	C3-C4-C5-C6
4	D	493	C8E	C5-C6-C7-C8
4	B	501	C8E	C3-C4-C5-C6
4	B	8	C8E	C4-C5-C6-C7
4	C	494	C8E	C3-C4-C5-C6
4	D	9	C8E	C3-C4-C5-C6
4	B	496	C8E	C5-C6-C7-C8
4	C	7	C8E	C2-C3-C4-C5
4	A	494	C8E	C2-C3-C4-C5
4	C	498	C8E	C1-C2-C3-C4
4	B	500	C8E	C3-C4-C5-C6
4	C	497	C8E	C6-C7-C8-O9
4	D	494	C8E	C2-C3-C4-C5
4	A	11	C8E	C6-C7-C8-O9
4	D	493	C8E	C3-C4-C5-C6
4	D	498	C8E	C5-C6-C7-C8
4	B	499	C8E	C2-C3-C4-C5
4	C	495	C8E	C2-C3-C4-C5
4	A	11	C8E	C1-C2-C3-C4
4	A	494	C8E	C10-C11-O12-C13
4	C	496	C8E	O9-C10-C11-O12
4	D	500	C8E	C1-C2-C3-C4
4	C	498	C8E	C2-C3-C4-C5
4	D	500	C8E	C2-C3-C4-C5
4	B	498	C8E	C4-C5-C6-C7
4	D	494	C8E	O12-C13-C14-O15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	B	501	C8E	C1-C2-C3-C4
4	C	496	C8E	C11-C10-O9-C8
4	C	498	C8E	C17-C16-O15-C14
4	B	497	C8E	C3-C4-C5-C6
4	A	10	C8E	C2-C3-C4-C5
4	A	10	C8E	C4-C5-C6-C7
4	D	9	C8E	C10-C11-O12-C13
4	B	8	C8E	C11-C10-O9-C8
4	D	496	C8E	C4-C5-C6-C7
4	D	5	C8E	C13-C14-O15-C16
4	A	495	C8E	C7-C8-O9-C10
4	C	494	C8E	C10-C11-O12-C13
4	B	500	C8E	C11-C10-O9-C8
4	B	8	C8E	C13-C14-O15-C16
4	C	494	C8E	C11-C10-O9-C8
4	C	498	C8E	C13-C14-O15-C16
4	C	495	C8E	C7-C8-O9-C10
4	D	9	C8E	C7-C8-O9-C10
4	C	498	C8E	C10-C11-O12-C13
4	D	499	C8E	C10-C11-O12-C13
4	D	5	C8E	C20-C19-O18-C17
4	C	497	C8E	C2-C3-C4-C5
4	B	497	C8E	C6-C7-C8-O9
4	B	500	C8E	C5-C6-C7-C8
4	D	498	C8E	C2-C3-C4-C5
4	C	497	C8E	C4-C5-C6-C7
4	D	9	C8E	C17-C16-O15-C14
4	C	494	C8E	C4-C5-C6-C7
4	D	494	C8E	C13-C14-O15-C16
4	B	499	C8E	C3-C4-C5-C6
4	D	495	C8E	C1-C2-C3-C4
4	B	8	C8E	C1-C2-C3-C4
4	D	494	C8E	C7-C8-O9-C10
4	C	498	C8E	C11-C10-O9-C8
4	D	498	C8E	C1-C2-C3-C4
4	D	9	C8E	C16-C17-O18-C19
4	B	497	C8E	C7-C8-O9-C10
4	B	500	C8E	C7-C8-O9-C10
4	C	496	C8E	C7-C8-O9-C10
4	D	500	C8E	C7-C8-O9-C10
4	D	494	C8E	C14-C13-O12-C11
3	C	493	EDO	O1-C1-C2-O2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	C	498	C8E	C7-C8-O9-C10
4	D	499	C8E	C4-C5-C6-C7
4	D	9	C8E	C13-C14-O15-C16
4	B	8	C8E	O9-C10-C11-O12
4	C	7	C8E	C11-C10-O9-C8
4	A	11	C8E	C3-C4-C5-C6
4	B	497	C8E	C11-C10-O9-C8
4	D	498	C8E	C4-C5-C6-C7
4	B	8	C8E	C20-C19-O18-C17
4	C	494	C8E	C1-C2-C3-C4
4	C	494	C8E	O15-C16-C17-O18
4	B	8	C8E	O15-C16-C17-O18
4	D	5	C8E	O15-C16-C17-O18
4	B	502	C8E	C10-C11-O12-C13
4	D	501	C8E	C4-C5-C6-C7
3	B	4	EDO	O1-C1-C2-O2
4	A	10	C8E	C11-C10-O9-C8
4	B	497	C8E	C1-C2-C3-C4
4	C	494	C8E	C7-C8-O9-C10
4	B	8	C8E	C16-C17-O18-C19
4	D	500	C8E	C3-C4-C5-C6
4	D	497	C8E	C7-C8-O9-C10
4	D	494	C8E	C10-C11-O12-C13
4	B	502	C8E	O9-C10-C11-O12
3	A	8	EDO	O1-C1-C2-O2
3	B	495	EDO	O1-C1-C2-O2
3	D	491	EDO	O1-C1-C2-O2
4	D	498	C8E	O9-C10-C11-O12
4	C	495	C8E	O9-C10-C11-O12
4	C	494	C8E	C16-C17-O18-C19
4	D	493	C8E	C1-C2-C3-C4
4	D	5	C8E	O9-C10-C11-O12
4	D	9	C8E	O12-C13-C14-O15
4	A	494	C8E	C4-C5-C6-C7
4	D	495	C8E	C5-C6-C7-C8
4	D	493	C8E	C11-C10-O9-C8
4	A	10	C8E	C3-C4-C5-C6
4	C	498	C8E	O12-C13-C14-O15
4	D	501	C8E	C6-C7-C8-O9
4	D	494	C8E	C1-C2-C3-C4
4	D	496	C8E	C3-C4-C5-C6
4	C	494	C8E	C17-C16-O15-C14

Continued on next page...

Continued from previous page...

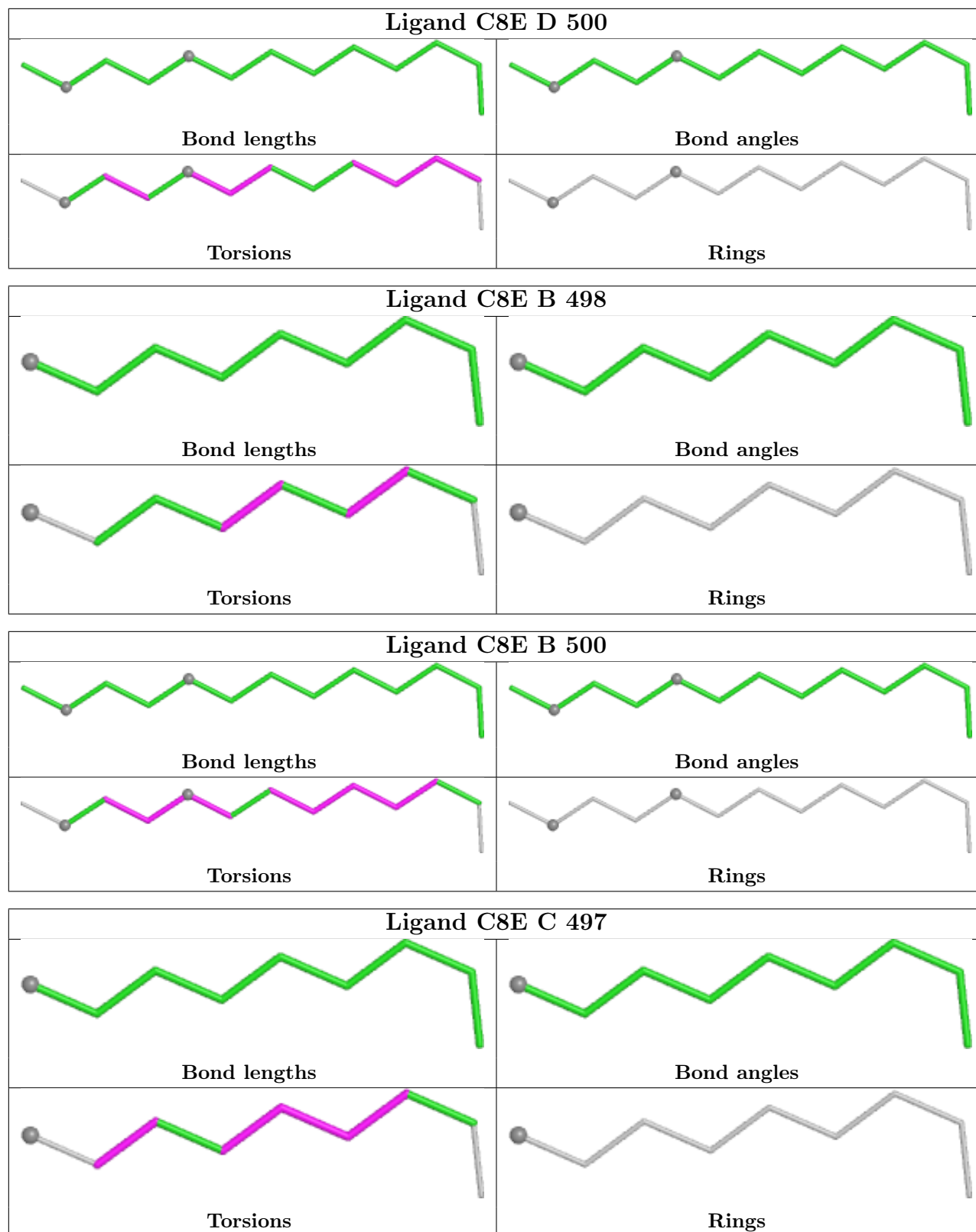
Mol	Chain	Res	Type	Atoms
4	B	500	C8E	O9-C10-C11-O12

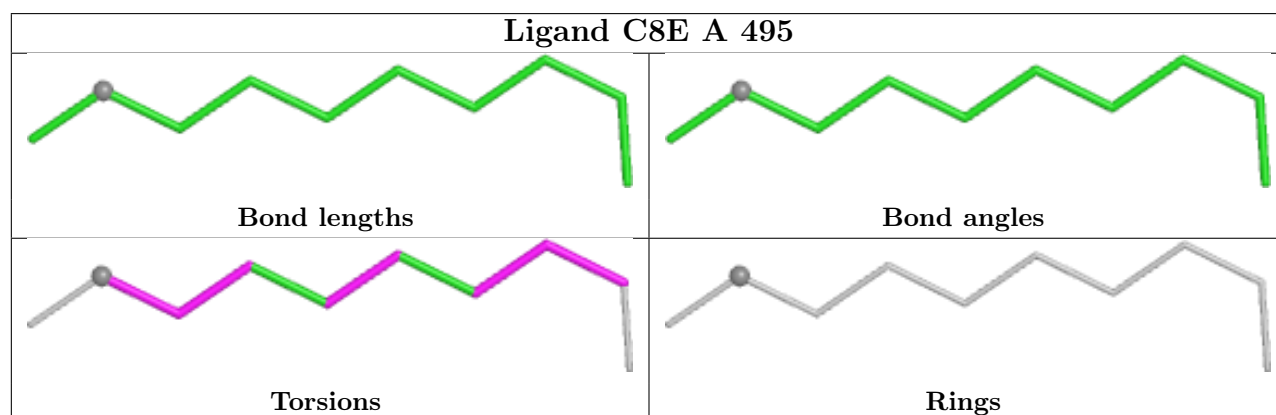
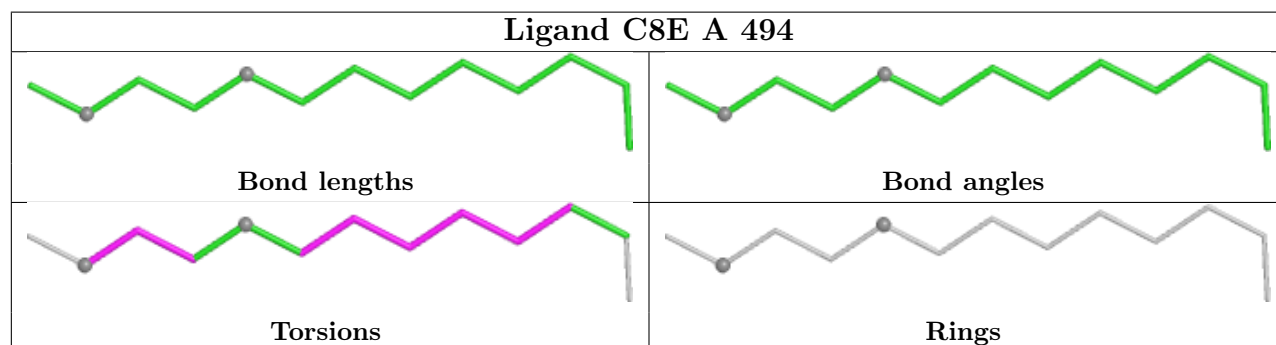
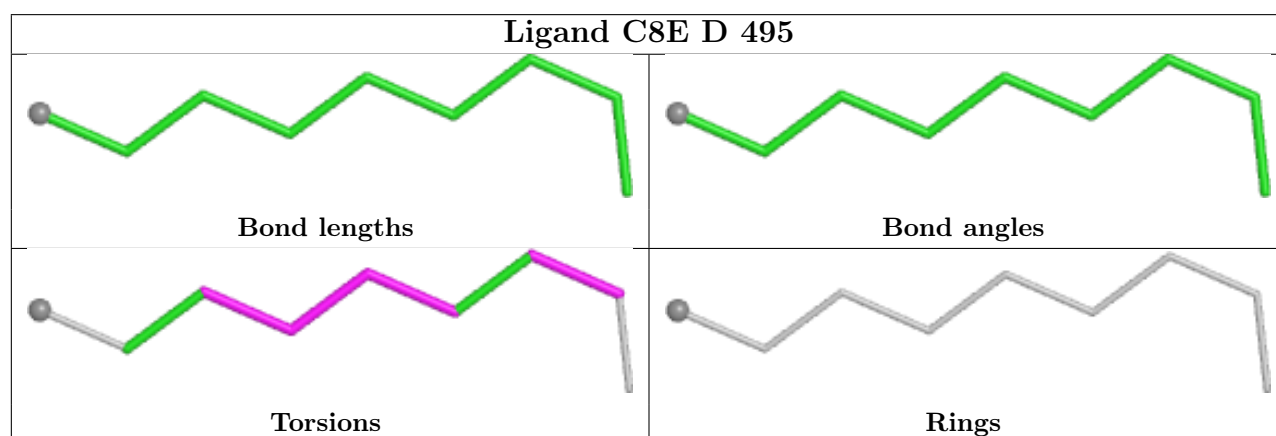
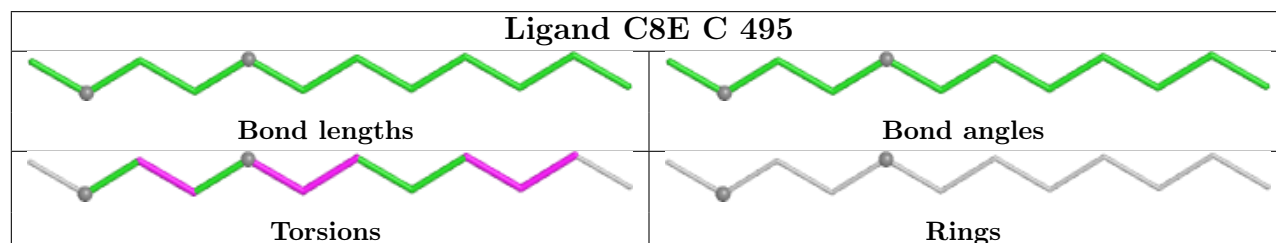
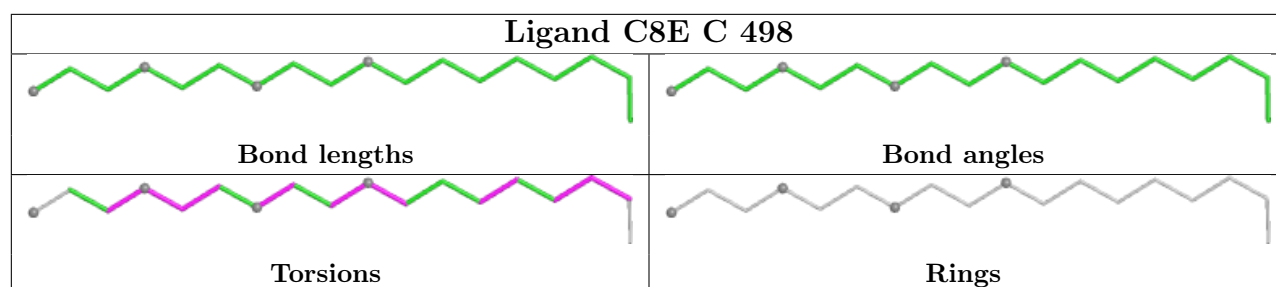
There are no ring outliers.

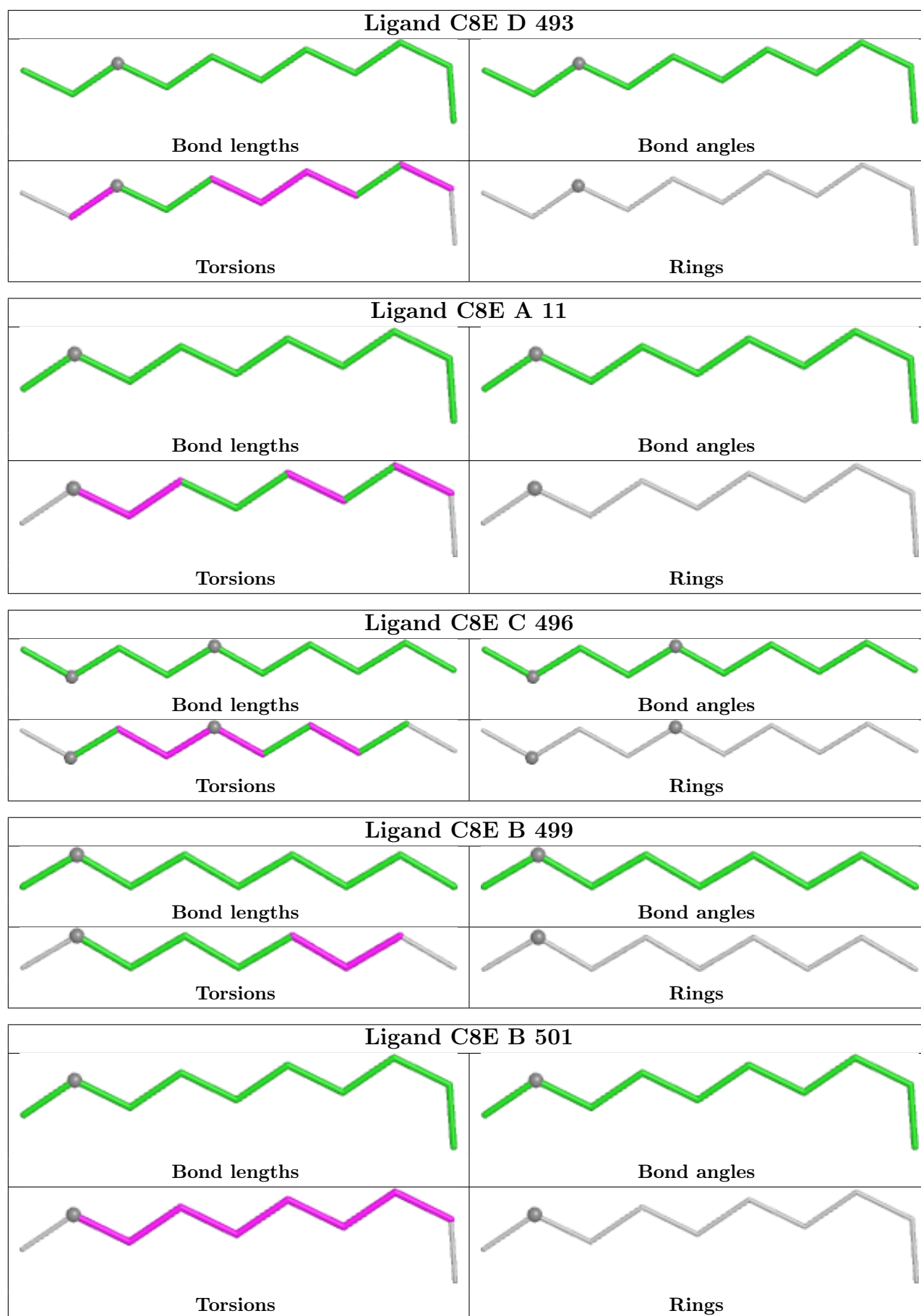
23 monomers are involved in 41 short contacts:

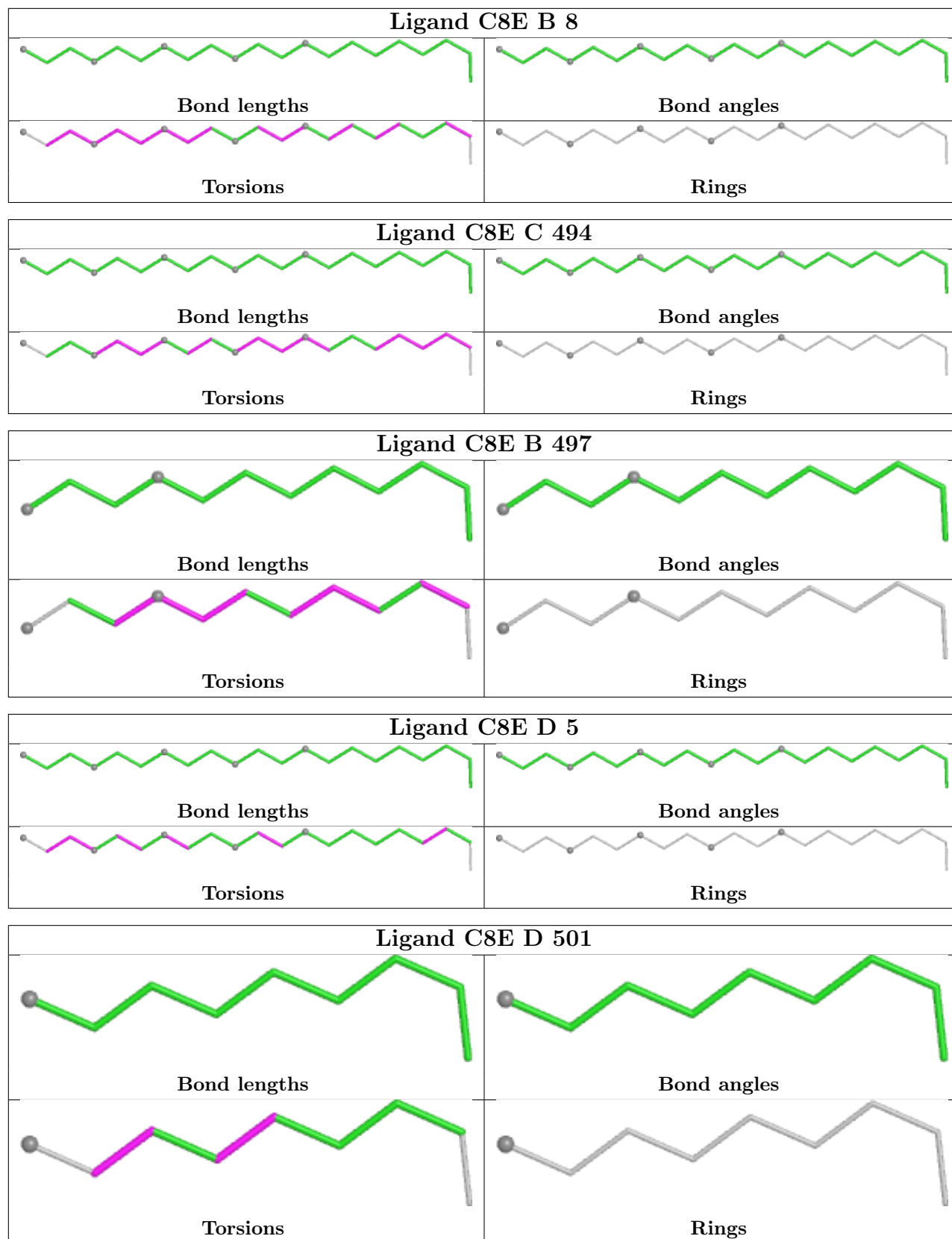
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	493	EDO	1	0
4	B	500	C8E	3	0
4	C	497	C8E	1	0
3	B	495	EDO	2	0
4	C	498	C8E	3	0
4	D	495	C8E	1	0
4	A	494	C8E	2	0
4	A	495	C8E	1	0
3	B	6	EDO	1	0
4	C	496	C8E	1	0
4	B	501	C8E	1	0
3	B	4	EDO	1	0
4	B	8	C8E	8	0
3	A	3	EDO	1	0
4	B	497	C8E	2	0
4	D	5	C8E	3	0
4	C	7	C8E	3	0
3	D	7	EDO	1	0
4	D	9	C8E	2	0
3	D	492	EDO	1	0
4	D	494	C8E	1	0
4	D	498	C8E	1	0
3	C	11	EDO	1	0

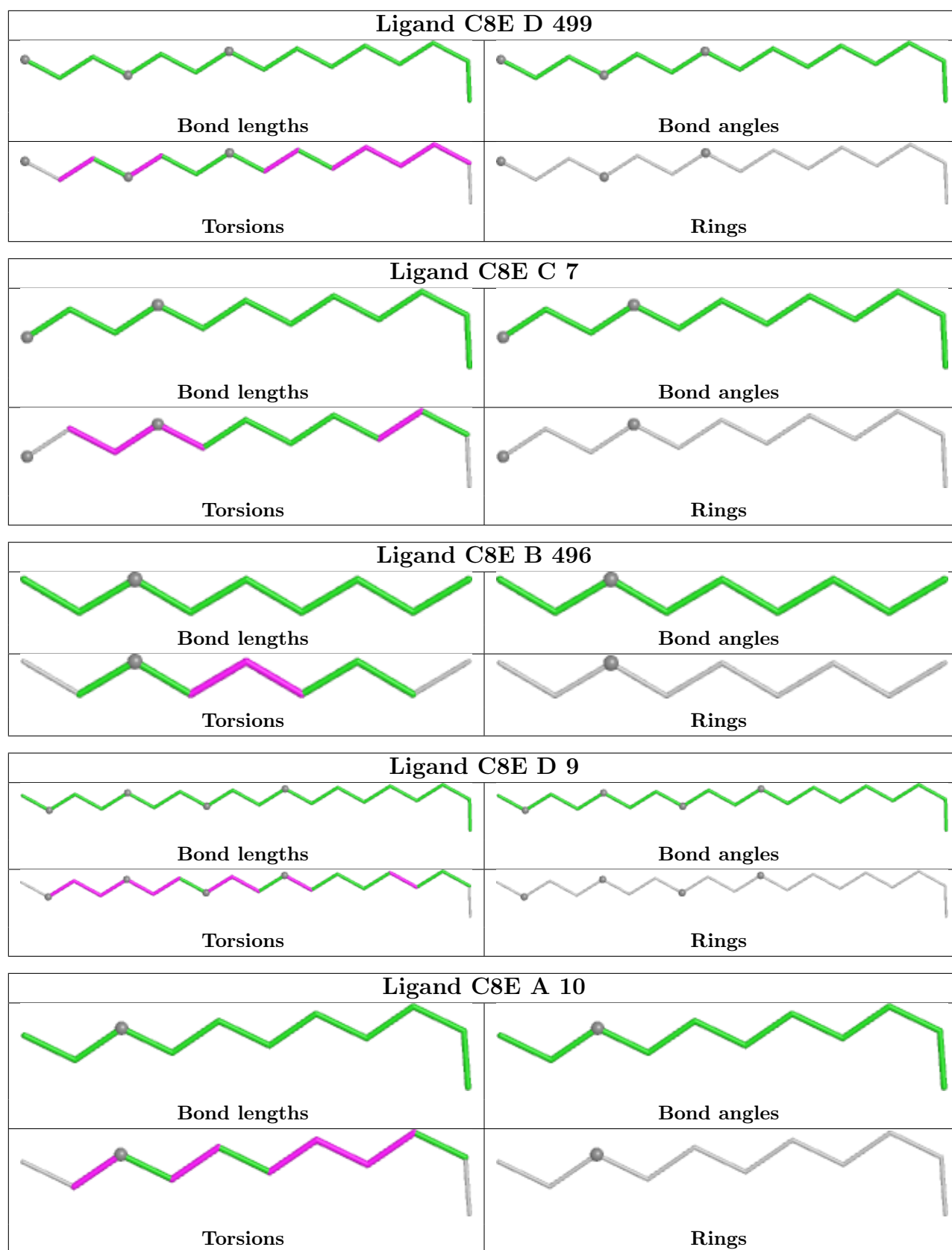
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

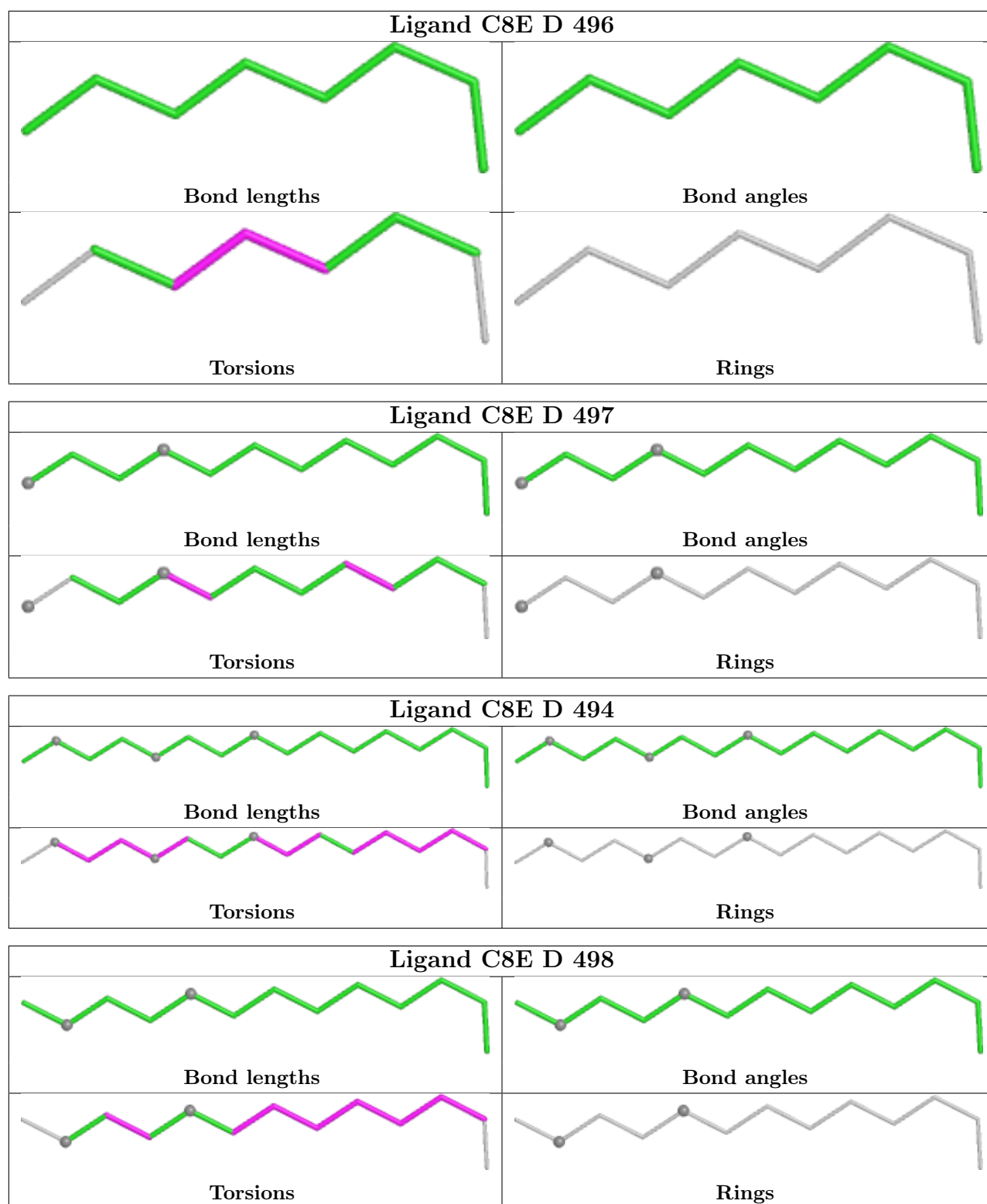


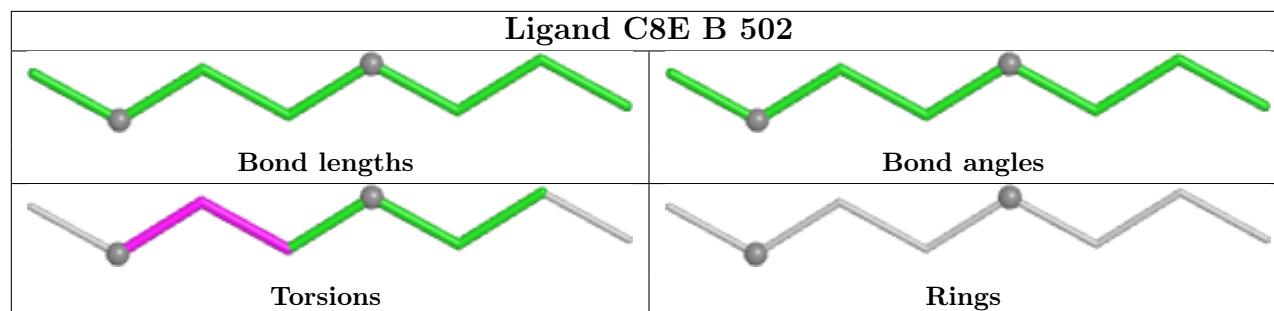












5.7 Other polymers [i](#)

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	424/479 (88%)	0.73	48 (11%) 10 11	10, 36, 78, 105	2 (0%)
1	B	425/479 (88%)	0.65	33 (7%) 19 21	9, 36, 72, 102	5 (1%)
1	C	405/479 (84%)	0.76	50 (12%) 8 9	18, 38, 73, 102	1 (0%)
1	D	406/479 (84%)	0.69	45 (11%) 10 11	16, 36, 68, 100	1 (0%)
All	All	1660/1916 (86%)	0.71	176 (10%) 11 12	9, 36, 74, 105	9 (0%)

All (176) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	238	GLY	5.5
1	C	79	GLY	5.2
1	C	231	SER	5.0
1	C	245	ASP	4.9
1	D	288	LEU	4.7
1	D	232	GLY	4.3
1	A	233	HIS	4.2
1	C	149	GLY	4.1
1	A	416	ASN	4.1
1	C	416	ASN	4.1
1	D	416	ASN	4.1
1	B	472	GLY	4.1
1	B	444	PRO	4.0
1	D	472	GLY	4.0
1	D	245	ASP	4.0
1	A	443	LEU	3.9
1	D	244	LEU	3.9
1	C	472	GLY	3.8
1	C	78	PHE	3.7
1	B	243	ASN	3.7
1	C	289	THR	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	237	PRO	3.7
1	C	121	PRO	3.7
1	B	448	SER	3.7
1	D	194	LEU	3.6
1	A	473	PRO	3.6
1	B	473	PRO	3.6
1	C	247	THR	3.5
1	A	411	GLY	3.5
1	A	234	LEU	3.5
1	A	448	SER	3.5
1	C	303	GLN	3.5
1	A	444	PRO	3.4
1	A	472	GLY	3.4
1	D	122	ASP	3.4
1	B	121	PRO	3.4
1	B	233	HIS	3.4
1	D	443	LEU	3.3
1	B	445	ALA	3.3
1	D	304	SER	3.3
1	A	232	GLY	3.3
1	C	230	ASP	3.3
1	A	175	THR	3.3
1	B	450	TYR	3.3
1	B	443	LEU	3.3
1	A	121	PRO	3.3
1	D	473	PRO	3.3
1	D	231	SER	3.3
1	C	339	ASP	3.2
1	D	243	ASN	3.2
1	C	103	THR	3.2
1	C	443	LEU	3.1
1	A	81	TRP	3.1
1	B	411	GLY	3.1
1	D	444	PRO	3.1
1	D	339	ASP	3.1
1	D	303	GLN	3.0
1	C	148	PHE	3.0
1	C	286	ASP	3.0
1	C	473	PRO	3.0
1	D	410	ILE	2.9
1	A	412	THR	2.9
1	D	452	ASP	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	444	PRO	2.8
1	C	104	LEU	2.8
1	B	242	ASP	2.8
1	A	446	SER	2.8
1	A	104	LEU	2.8
1	D	103	THR	2.8
1	A	63	GLY	2.8
1	D	248	TYR	2.8
1	A	98	THR	2.8
1	B	194	LEU	2.8
1	C	441	GLY	2.7
1	B	442	LEU	2.7
1	C	135	TYR	2.7
1	B	247	THR	2.7
1	B	449	GLN	2.7
1	D	175	THR	2.7
1	D	195	ASP	2.7
1	A	231	SER	2.7
1	A	243	ASN	2.7
1	B	300	THR	2.7
1	A	388	LEU	2.7
1	B	170	TRP	2.7
1	C	194	LEU	2.7
1	D	148	PHE	2.6
1	A	289	THR	2.6
1	D	337	GLY	2.6
1	D	104	LEU	2.6
1	C	170	TRP	2.6
1	A	299	ALA	2.6
1	B	248	TYR	2.6
1	C	134	ASP	2.6
1	D	133	VAL	2.6
1	C	41	ASN	2.6
1	A	64	GLY	2.6
1	B	446	SER	2.6
1	B	237	PRO	2.5
1	D	63	GLY	2.5
1	B	231	SER	2.5
1	B	413[A]	SER	2.5
1	C	133	VAL	2.5
1	D	200	GLU	2.5
1	D	60	THR	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	410	ILE	2.4
1	A	248	TYR	2.4
1	C	195	ASP	2.4
1	C	449	GLN	2.4
1	B	418	ALA	2.4
1	D	69	ILE	2.4
1	C	40	LYS	2.4
1	C	81	TRP	2.4
1	D	286	ASP	2.4
1	D	474	GLY	2.4
1	B	439	LYS	2.4
1	A	363	VAL	2.4
1	B	388	LEU	2.4
1	C	84	TRP	2.4
1	A	236	ARG	2.4
1	A	474	GLY	2.4
1	D	338	LYS	2.4
1	A	124	SER	2.4
1	A	170	TRP	2.4
1	B	81	TRP	2.4
1	B	103	THR	2.3
1	A	42	PHE	2.3
1	A	298	ILE	2.3
1	A	451	VAL	2.3
1	A	194	LEU	2.3
1	A	449	GLN	2.3
1	C	288	LEU	2.3
1	B	59	GLY	2.3
1	C	250	GLY	2.3
1	A	66	LEU	2.3
1	C	266	TYR	2.3
1	A	418	ALA	2.3
1	D	322	GLU	2.3
1	C	248	TYR	2.3
1	A	249	THR	2.3
1	C	304	SER	2.3
1	A	239	GLU	2.3
1	D	390	GLU	2.3
1	A	40	LYS	2.3
1	C	66	LEU	2.2
1	B	407	ASP	2.2
1	D	79	GLY	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	247	THR	2.2
1	D	66	LEU	2.2
1	A	339	ASP	2.2
1	C	474	GLY	2.2
1	C	445	ALA	2.2
1	D	445	ALA	2.2
1	A	439	LYS	2.2
1	C	60	THR	2.2
1	C	412	THR	2.2
1	C	452	ASP	2.2
1	D	451	VAL	2.2
1	D	453	GLU	2.2
1	D	336	GLY	2.2
1	A	230	ASP	2.1
1	B	122	ASP	2.1
1	D	64	GLY	2.1
1	A	445	ALA	2.1
1	C	85	SER	2.1
1	C	418	ALA	2.1
1	A	62	PRO	2.1
1	D	62	PRO	2.1
1	D	199	PRO	2.1
1	C	200	GLU	2.1
1	C	409	ASP	2.1
1	D	207	VAL	2.1
1	B	195	ASP	2.0
1	B	230	ASP	2.0
1	C	203	ASP	2.0
1	C	63	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	EDO	B	9	4/4	0.60	0.23	56,60,71,75	0
4	C8E	C	498	18/21	0.75	0.23	23,76,95,101	0
4	C8E	D	497	12/21	0.76	0.19	32,53,71,74	0
3	EDO	C	493	4/4	0.79	0.21	55,55,60,73	0
4	C8E	B	496	9/21	0.79	0.20	41,53,61,68	0
4	C8E	D	499	15/21	0.79	0.19	27,51,71,74	0
4	C8E	D	498	13/21	0.80	0.17	27,45,59,62	0
3	EDO	C	10	4/4	0.80	0.17	58,63,71,83	0
4	C8E	C	494	21/21	0.81	0.20	23,46,71,83	0
3	EDO	B	491	4/4	0.82	0.13	39,49,53,58	0
4	C8E	A	494	13/21	0.82	0.19	33,46,73,76	0
4	C8E	D	494	16/21	0.83	0.18	32,44,77,79	0
4	C8E	B	501	10/21	0.83	0.17	34,42,52,59	0
3	EDO	A	8	4/4	0.83	0.14	49,52,61,63	0
3	EDO	A	491	4/4	0.83	0.15	33,53,57,61	0
3	EDO	D	492	4/4	0.84	0.16	49,56,60,65	0
4	C8E	B	502	8/21	0.84	0.17	29,47,59,65	0
4	C8E	D	496	8/21	0.84	0.15	25,41,46,49	0
4	C8E	B	8	21/21	0.84	0.15	21,41,57,63	0
4	C8E	C	495	12/21	0.84	0.15	20,41,53,60	0
4	C8E	C	496	10/21	0.84	0.16	21,43,83,84	0
4	C8E	D	493	11/21	0.85	0.15	15,39,52,58	0
4	C8E	B	497	12/21	0.85	0.15	27,45,71,72	0
4	C8E	D	500	13/21	0.85	0.15	20,38,65,65	0
4	C8E	C	497	9/21	0.86	0.13	36,44,59,62	0
4	C8E	B	500	13/21	0.86	0.15	24,35,75,77	0
4	C8E	A	495	10/21	0.86	0.14	25,29,50,63	0
4	C8E	D	5	21/21	0.86	0.15	33,51,70,75	0
3	EDO	A	492	4/4	0.86	0.17	41,48,52,55	0
4	C8E	D	495	9/21	0.87	0.12	29,48,58,59	0
3	EDO	B	492	4/4	0.87	0.13	44,44,54,55	0
3	EDO	A	493	4/4	0.87	0.16	54,58,58,62	0
4	C8E	A	10	11/21	0.88	0.14	25,35,52,59	0
3	EDO	C	491	4/4	0.88	0.15	46,55,57,63	0
4	C8E	B	499	9/21	0.89	0.14	29,35,54,59	0
3	EDO	B	493	4/4	0.89	0.16	54,62,71,71	0
3	EDO	B	6	4/4	0.90	0.12	29,34,39,51	0

Continued on next page...

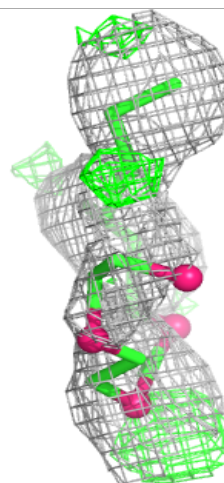
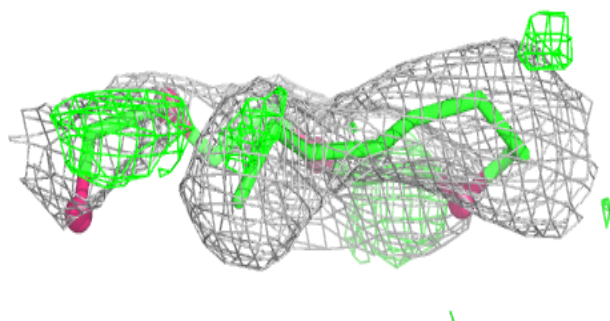
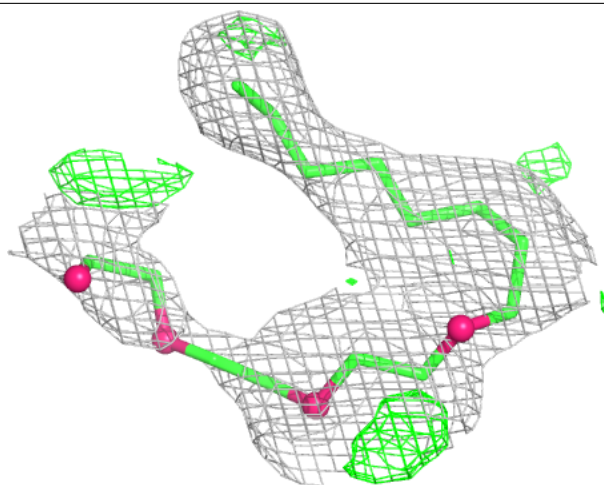
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	EDO	C	492	4/4	0.90	0.15	39,42,51,56	0
4	C8E	D	9	19/21	0.90	0.13	17,35,53,55	0
3	EDO	C	11	4/4	0.90	0.12	35,46,53,62	0
4	C8E	C	7	12/21	0.90	0.12	25,40,60,66	0
3	EDO	B	494	4/4	0.91	0.13	34,35,37,39	0
2	CA	C	3	1/1	0.92	0.12	71,71,71,71	0
4	C8E	A	11	10/21	0.92	0.10	28,36,46,61	0
4	C8E	D	501	9/21	0.92	0.13	26,34,46,47	0
4	C8E	B	498	9/21	0.93	0.11	27,33,42,45	0
3	EDO	C	5	4/4	0.94	0.09	24,25,27,37	0
3	EDO	A	3	4/4	0.94	0.11	20,28,33,41	0
3	EDO	D	491	4/4	0.94	0.11	39,53,53,62	0
3	EDO	D	7	4/4	0.95	0.07	16,19,21,26	0
2	CA	A	4	1/1	0.95	0.14	65,65,65,65	0
3	EDO	B	495	4/4	0.95	0.12	39,48,52,55	0
3	EDO	C	1	4/4	0.95	0.08	14,18,25,36	0
3	EDO	A	2	4/4	0.96	0.10	17,30,34,40	0
2	CA	D	1	1/1	0.97	0.10	58,58,58,58	0
3	EDO	B	4	4/4	0.97	0.06	18,23,28,40	0
2	CA	B	2	1/1	0.97	0.11	61,61,61,61	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.

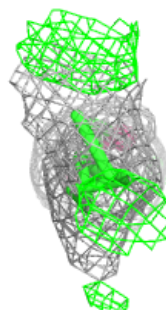
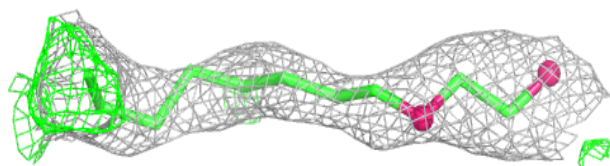
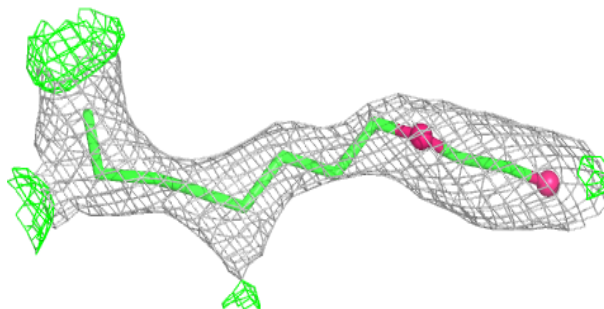
Electron density around C8E C 498:

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

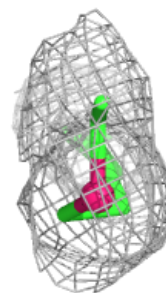
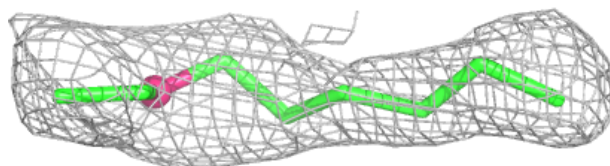
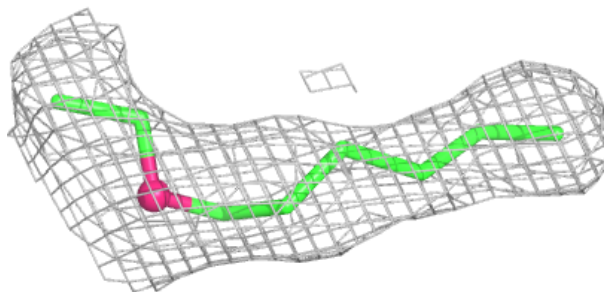


Electron density around C8E D 497:

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

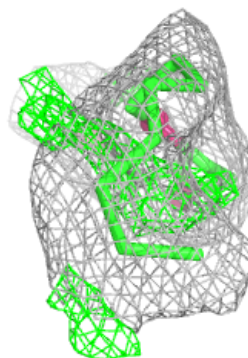
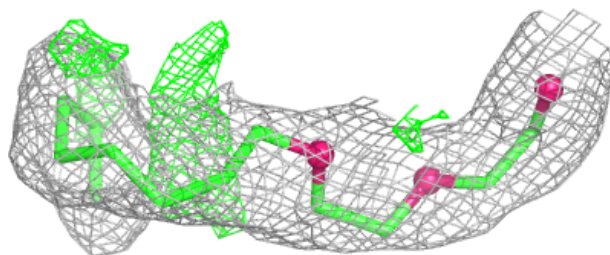
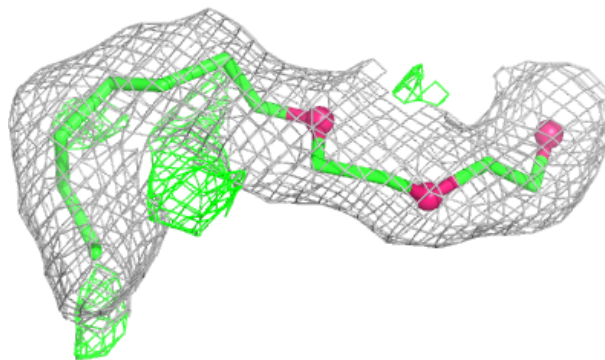
**Electron density around C8E B 496:**

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

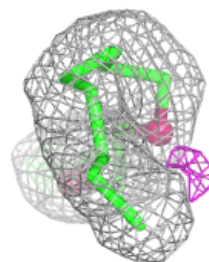
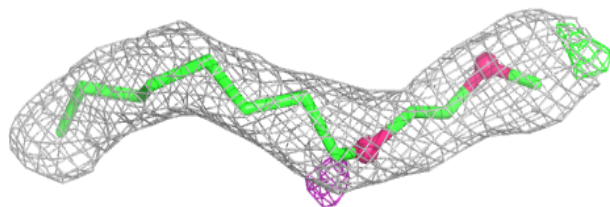
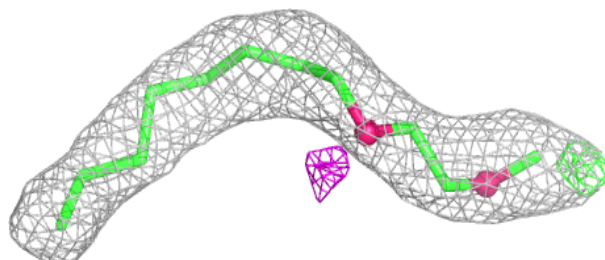


Electron density around C8E D 499:

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

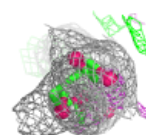
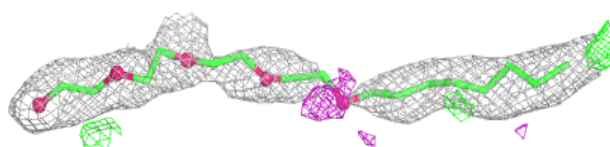
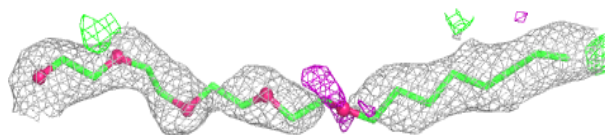
**Electron density around C8E D 498:**

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

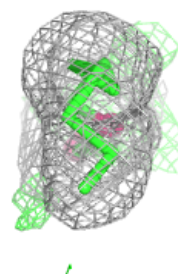
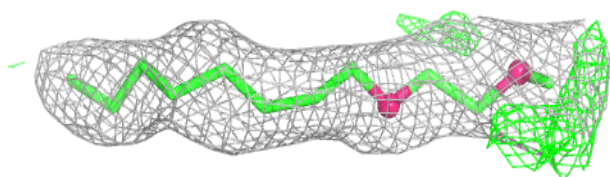
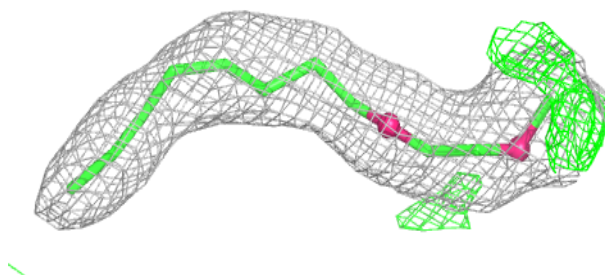


Electron density around C8E C 494:

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

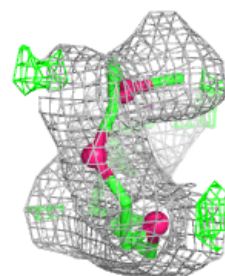
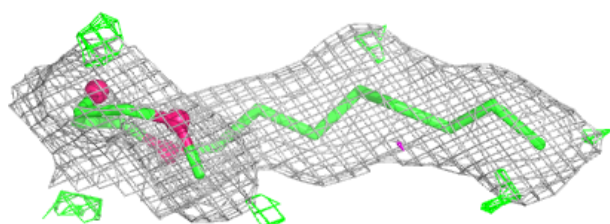
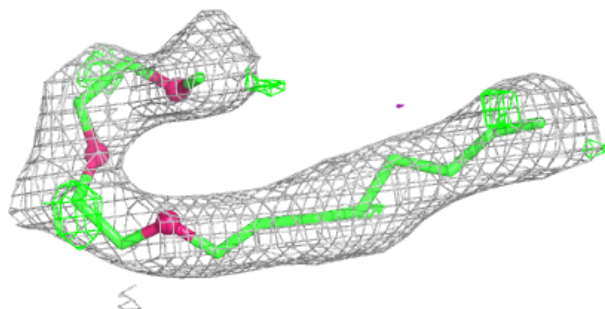
**Electron density around C8E A 494:**

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

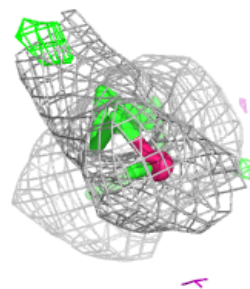
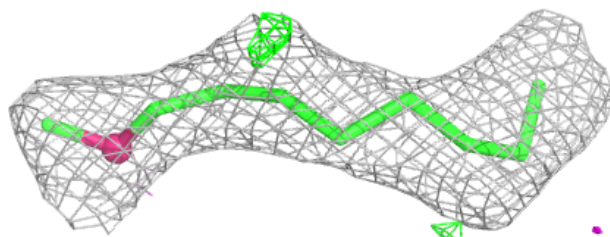
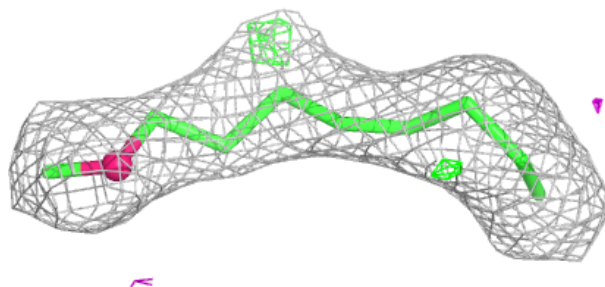


Electron density around C8E D 494:

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

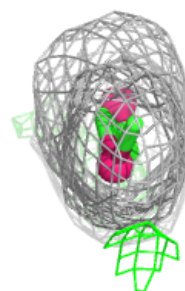
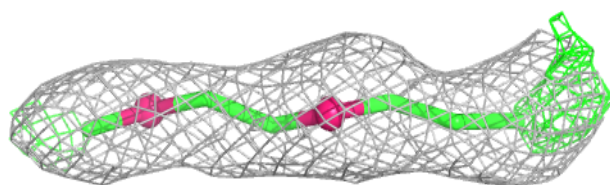
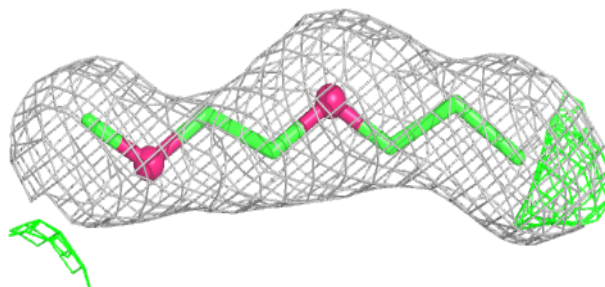
**Electron density around C8E B 501:**

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

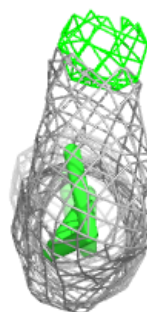
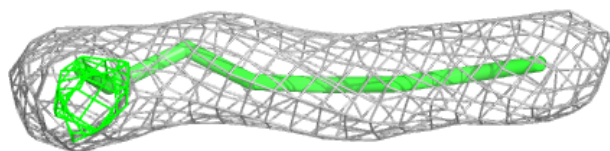
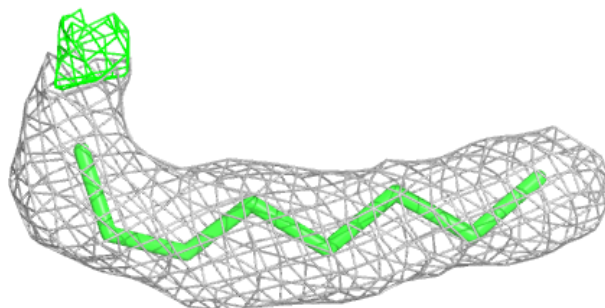


Electron density around C8E B 502:

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

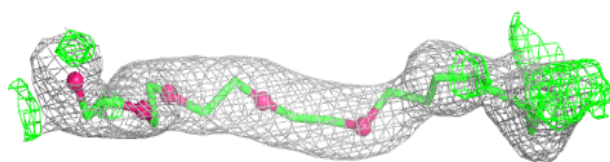
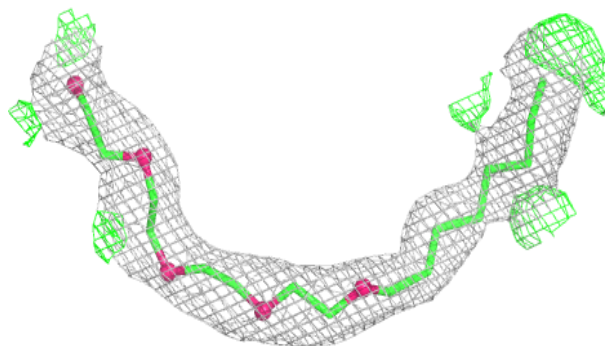
**Electron density around C8E D 496:**

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

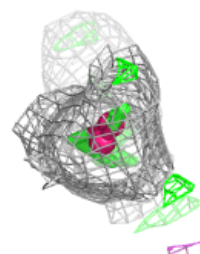
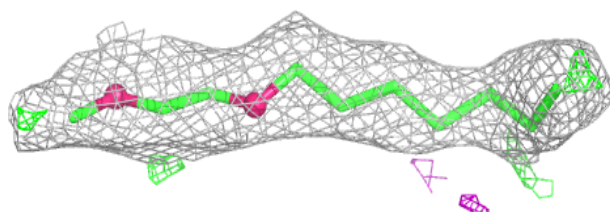
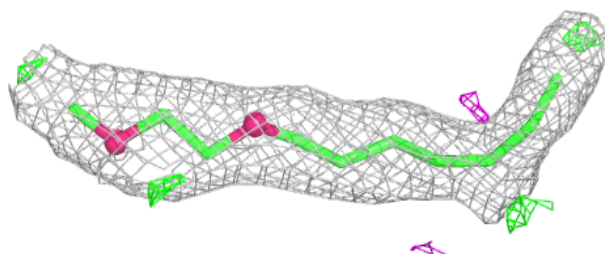


Electron density around C8E B 8:

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

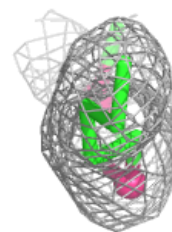
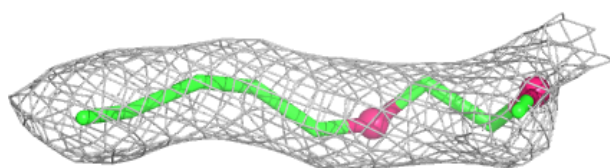
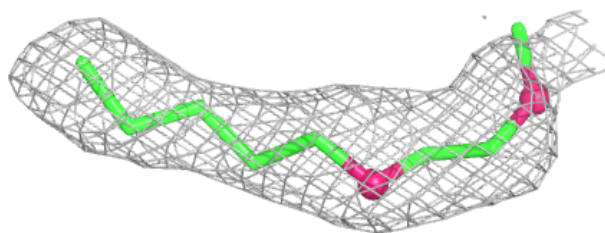
**Electron density around C8E C 495:**

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

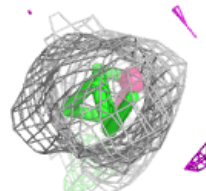
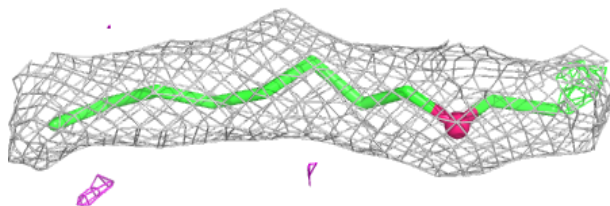
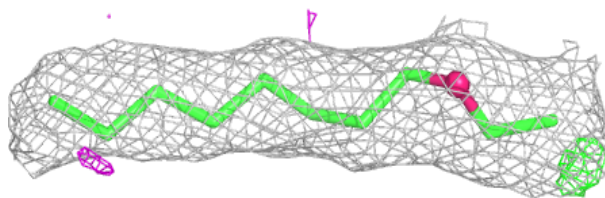


Electron density around C8E C 496:

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

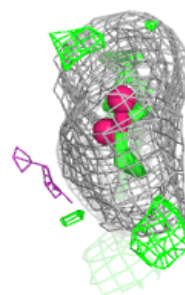
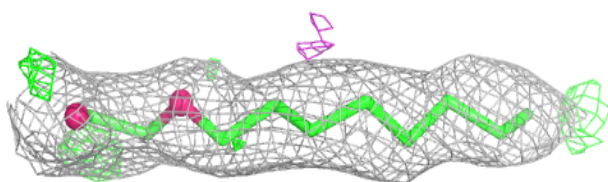
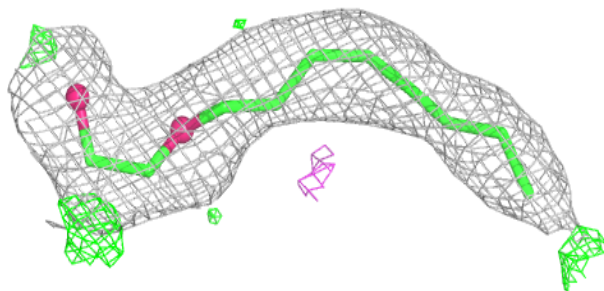
**Electron density around C8E D 493:**

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

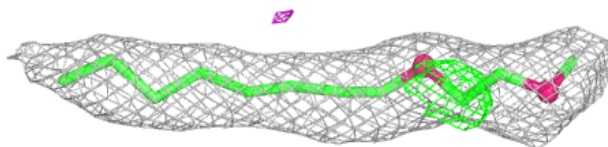
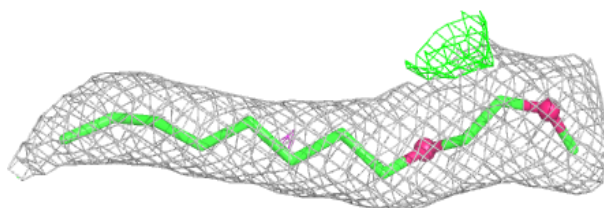


Electron density around C8E B 497:

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

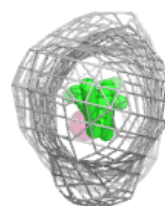
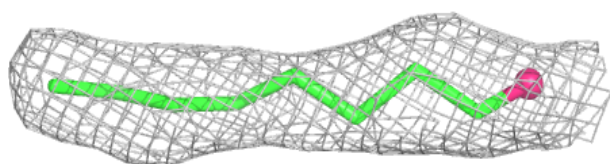
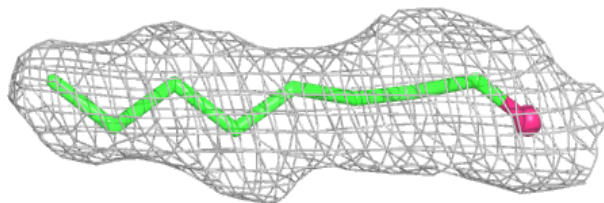
**Electron density around C8E D 500:**

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

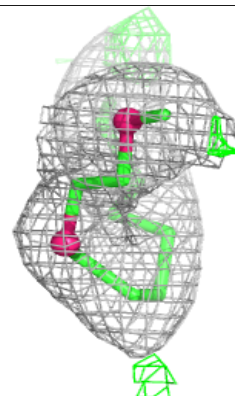
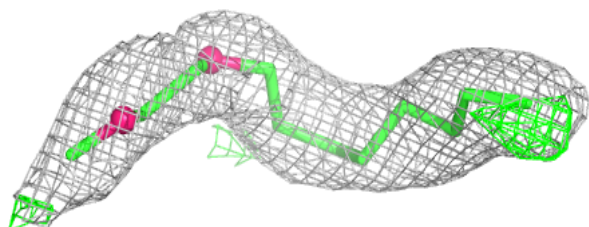
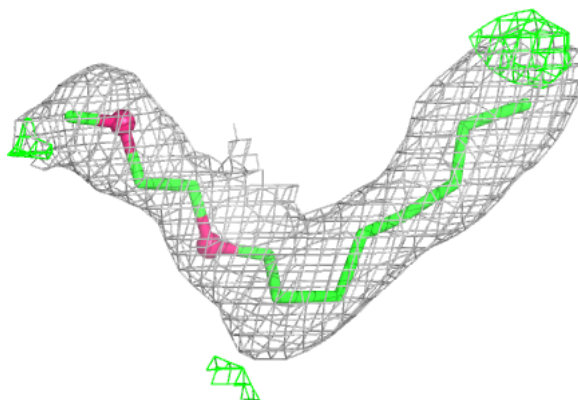


Electron density around C8E C 497:

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

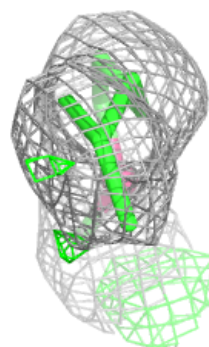
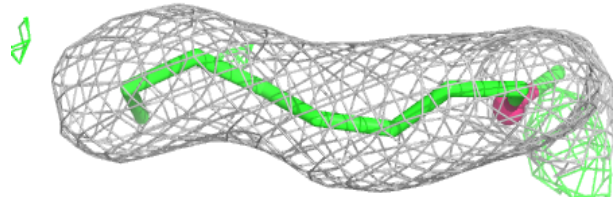
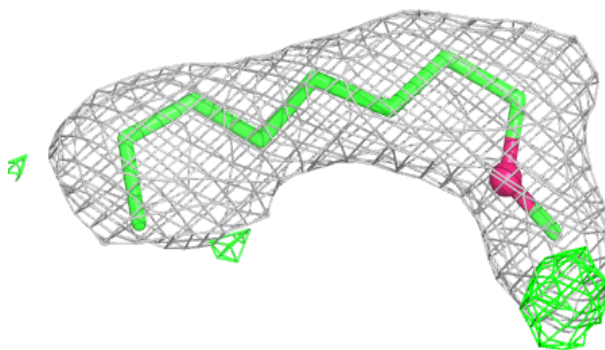
**Electron density around C8E B 500:**

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

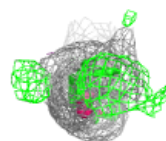
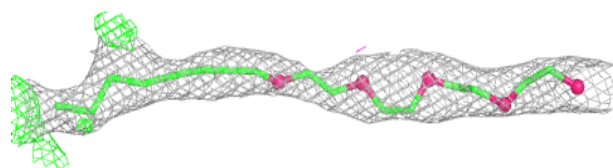
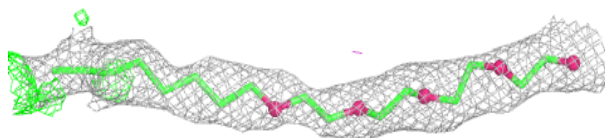


Electron density around C8E A 495:

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

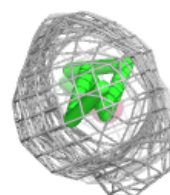
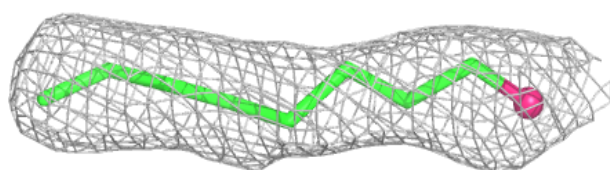
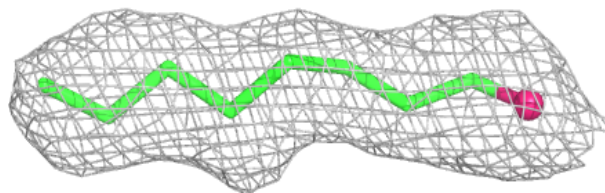
**Electron density around C8E D 5:**

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

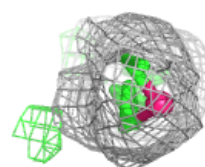
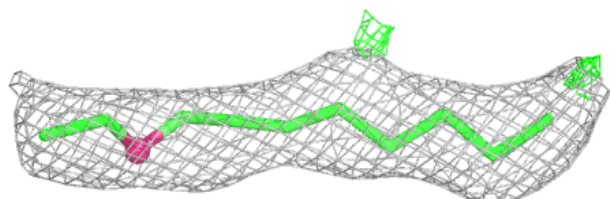
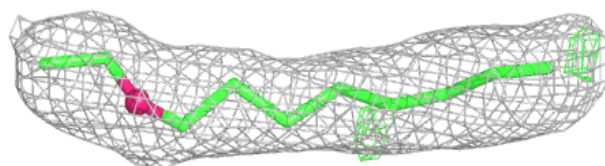


Electron density around C8E D 495:

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

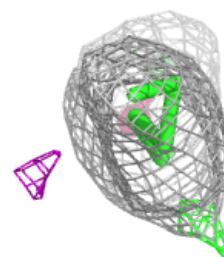
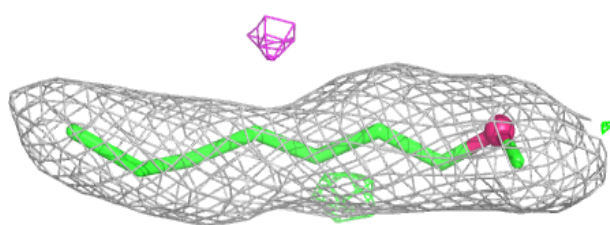
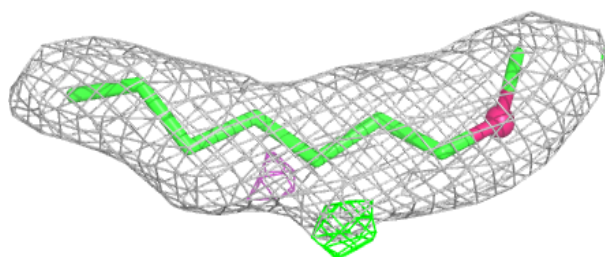
**Electron density around C8E A 10:**

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

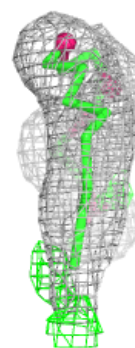
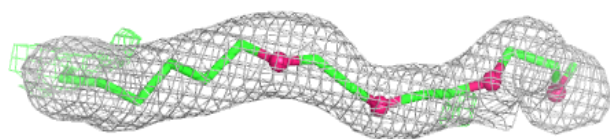
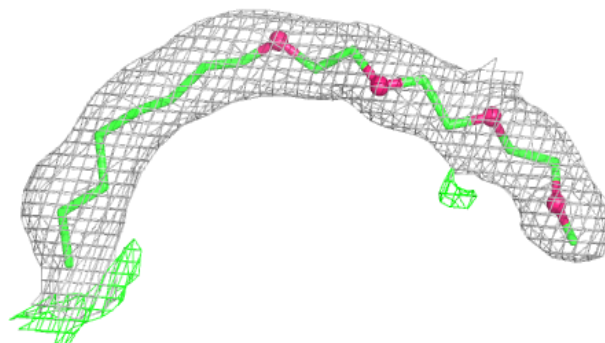


Electron density around C8E B 499:

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

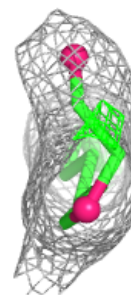
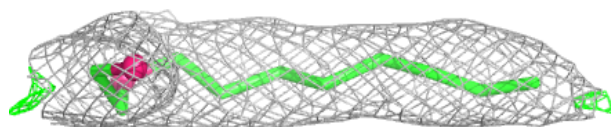
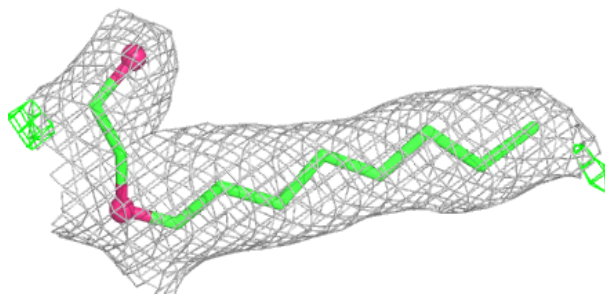
**Electron density around C8E D 9:**

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

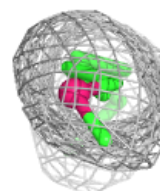
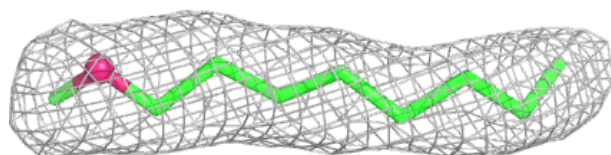
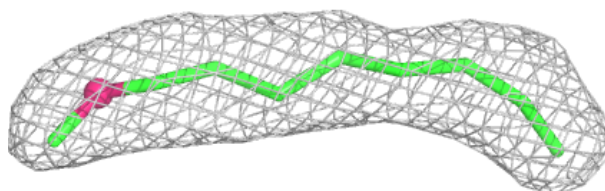


Electron density around C8E C 7:

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

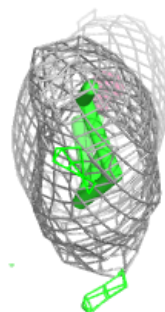
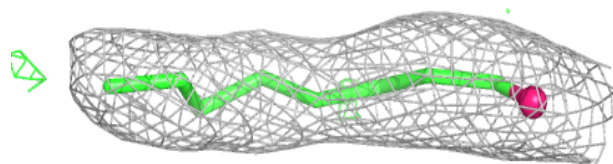
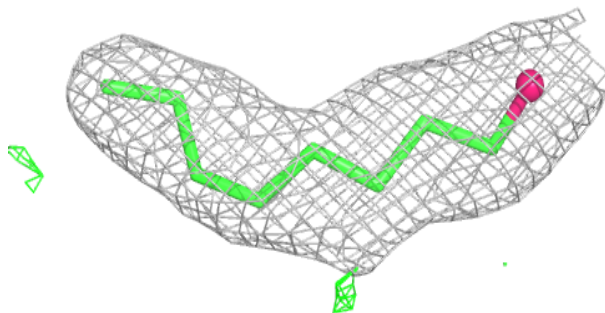
**Electron density around C8E A 11:**

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

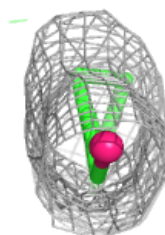
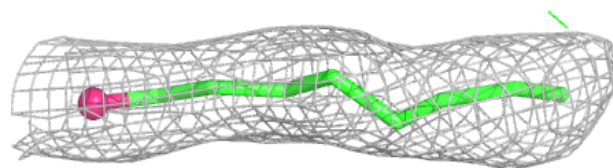
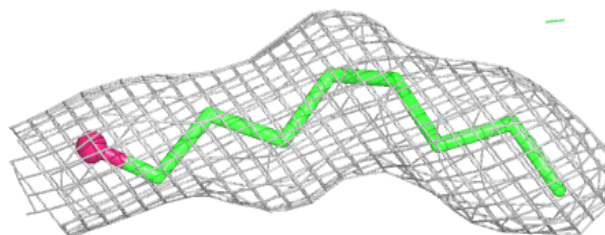


Electron density around C8E D 501:

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

**Electron density around C8E B 498:**

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



6.5 Other polymers ⓘ

There are no such residues in this entry.