



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 6, 2026 – 04:03 pm BST

PDB ID : 9HVZ / pdb_00009hvz
Title : Bacterial protein - 4_5
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Deposited on : 2025-01-02
Resolution : 2.15 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:

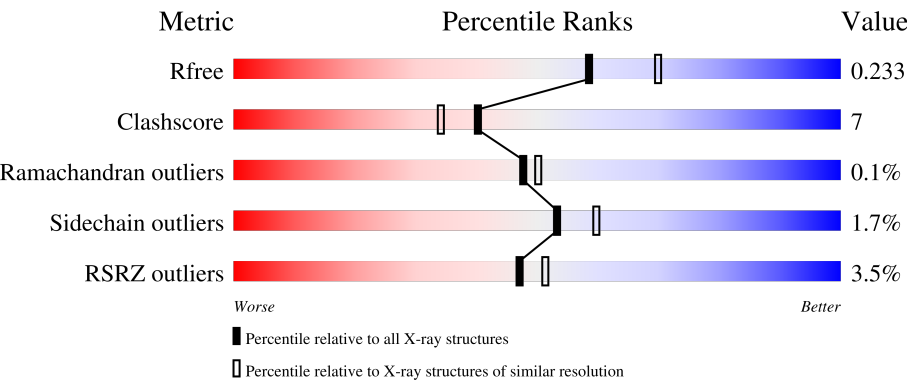
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	354	5% 83% 14% ..
1	B	354	2% 84% 13% .
1	C	354	4% 80% 17% ..
1	D	354	2% 85% 11% ..

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Mol	Chain	Length	Quality of chain
2	E	3	 100%
3	F	3	 33%67%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11692 atoms, of which 214 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 XcbB/CpsF family capsular polysaccharide biosynthesis protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	346	Total	C	N	O	S	0	0	0
			2741	1755	452	525	9			
1	B	344	Total	C	N	O	S	0	0	0
			2754	1767	455	523	9			
1	C	344	Total	C	N	O	S	0	0	0
			2734	1754	448	523	9			
1	D	344	Total	C	N	O	S	0	0	0
			2747	1763	453	522	9			

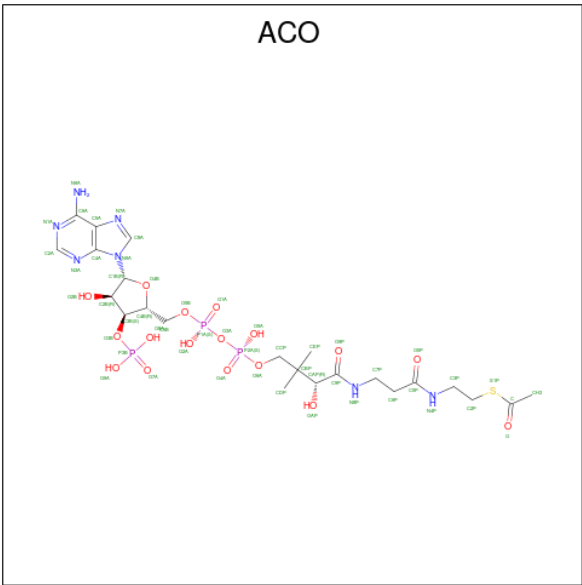
- Molecule 2 is an oligosaccharide called (2R)-2-(alpha-D-galactopyranosyloxy)-3-dihydroxypropyl phosphate-(7-4)-(2R)-2-(alpha-D-galactopyranosyloxy)-3-dihydroxypropyl phosphate-(7-4)-(2R)-2-(alpha-D-galactopyranosyloxy)-3-dihydroxypropyl phosphate.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	3	Total	C	H	O	P	0	0	0
			112	27	51	31	3			

- Molecule 3 is an oligosaccharide called (2R)-2-(alpha-D-galactopyranosyloxy)-3-dihydroxypropyl phosphate-(4-7)-(2R)-2-(alpha-D-galactopyranosyloxy)-3-dihydroxypropyl phosphate-(4-7)-(2R)-2-(alpha-D-galactopyranosyloxy)-3-dihydroxypropyl phosphate.

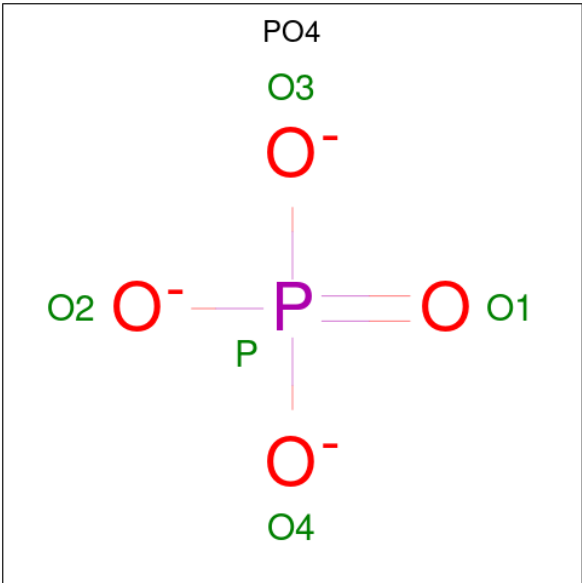
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	3	Total	C	H	O	P	0	0	0
			75	18	34	21	2			

- Molecule 4 is ACETYL COENZYME *A (CCD ID: ACO) (formula: C₂₃H₃₈N₇O₁₇P₃S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
4	A	1	Total	C	H	N	O	P	S	0	0
			85	23	34	7	17	3	1		
4	B	1	Total	C	H	N	O	P	S	0	0
			85	23	34	7	17	3	1		
4	C	1	Total	C	H	N	O	P	S	0	0
			85	23	34	7	17	3	1		
4	D	1	Total	C	H	N	O	P		0	0
			72	19	27	7	16	3			

- Molecule 5 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	P	0	0
			5	4	1		

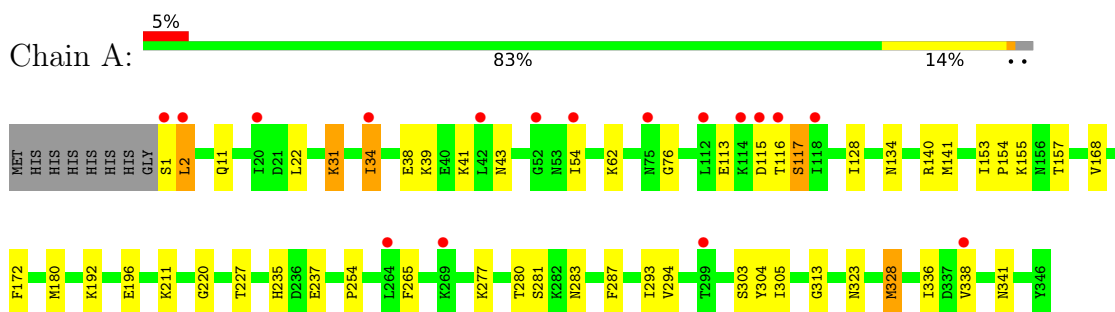
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	37	Total	O	0	0
			37	37		
6	B	57	Total	O	0	0
			57	57		
6	C	56	Total	O	0	0
			56	56		
6	D	47	Total	O	0	0
			47	47		

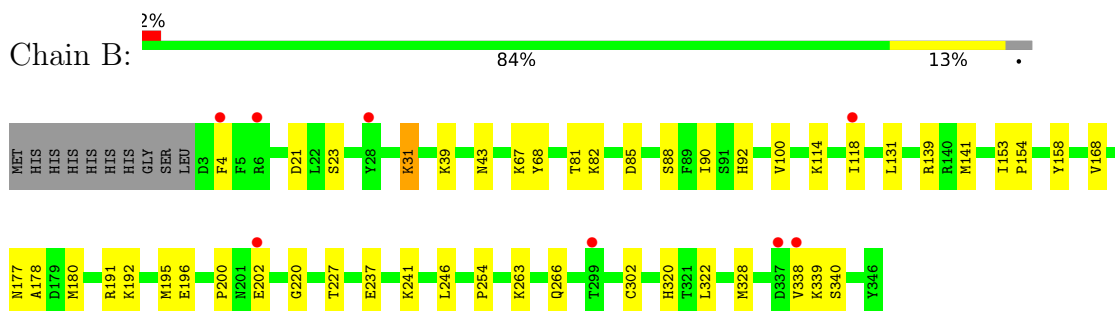
3 Residue-property plots [i](#)

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.

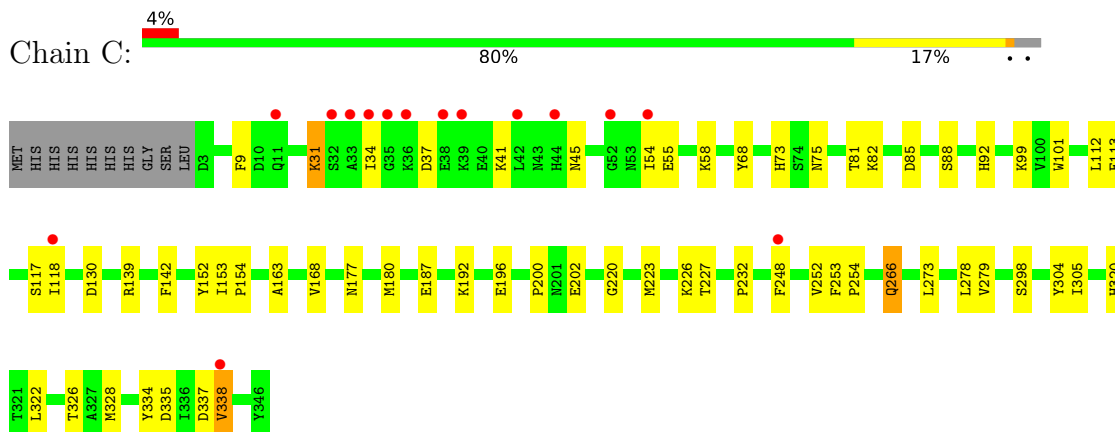
- Molecule 1: XcbB/CpsF family capsular polysaccharide biosynthesis protein



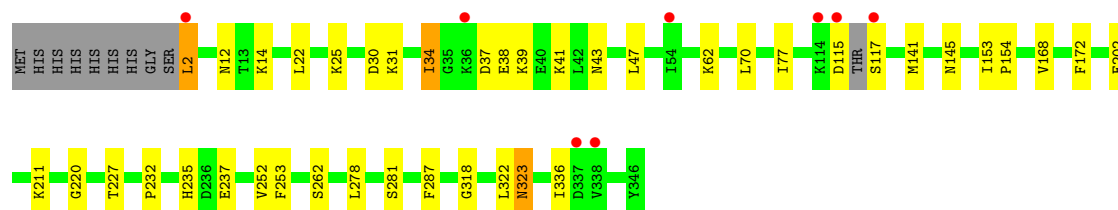
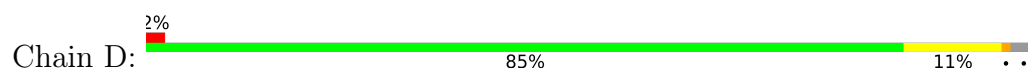
- Molecule 1: XcbB/CpsF family capsular polysaccharide biosynthesis protein



- Molecule 1: XcbB/CpsF family capsular polysaccharide biosynthesis protein



- Molecule 1: XcbB/CpsF family capsular polysaccharide biosynthesis protein



- Molecule 2: (2R)-2-(alpha-D-galactopyranosyloxy)-3-dihydroxypropyl phosphate-(7-4)-(2R)-2-(alpha-D-galactopyranosyloxy)-3-dihydroxypropyl phosphate-(7-4)-(2R)-2-(alpha-D-galactopyranosyloxy)-3-dihydroxypropyl phosphate



A110J1
A110J2
A110J3

- Molecule 3: (2R)-2-(alpha-D-galactopyranosyloxy)-3-dihydroxypropyl phosphate-(4-7)-(2R)-2-(alpha-D-galactopyranosyloxy)-3-dihydroxypropyl phosphate-(4-7)-(2R)-2-(alpha-D-galactopyranosyloxy)-3-dihydroxypropyl phosphate



A110J1
A110J2
A110J3

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	90.79Å 98.85Å 102.49Å 90.00° 106.31° 90.00°	Depositor
Resolution (Å)	42.99 – 2.15 42.99 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.6 (42.99-2.15) 99.9 (42.99-2.15)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.28 (at 2.16Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.198 , 0.233 0.198 , 0.233	Depositor DCC
R_{free} test set	2000 reflections (2.12%)	wwPDB-VP
Wilson B-factor (Å ²)	47.5	Xtriage
Anisotropy	0.796	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 40.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11692	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.91% 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: PO4, A1I0J, ACO

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	0.33	0/2799	0.49	0/3791
1	B	0.35	0/2812	0.51	0/3799
1	C	0.35	0/2792	0.48	0/3779
1	D	0.35	0/2804	0.51	0/3789
All	All	0.35	0/11207	0.50	0/15158

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2741	0	2632	35	0
1	B	2754	0	2698	37	0
1	C	2734	0	2641	46	0
1	D	2747	0	2670	31	0
2	E	61	51	0	0	0
3	F	41	34	0	0	0
4	A	51	34	34	2	0
4	B	51	34	34	2	0
4	C	51	34	34	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	45	27	26	6	0
5	A	5	0	0	0	0
6	A	37	0	0	1	0
6	B	57	0	0	3	0
6	C	56	0	0	2	0
6	D	47	0	0	0	0
All	All	11478	214	10769	146	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 7.

All (146) 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:177:ASN:HA	1:B:180:MET:HE2	1.23	1.13
1:C:177:ASN:HA	1:C:180:MET:HE2	1.43	0.97
1:C:130:ASP:CG	1:C:139:ARG:HH21	1.74	0.94
1:C:177:ASN:HA	1:C:180:MET:CE	2.08	0.84
1:B:177:ASN:HA	1:B:180:MET:CE	2.07	0.83
1:C:130:ASP:OD2	1:C:139:ARG:NH2	2.17	0.78
1:D:2:LEU:HD22	1:D:25:LYS:HD3	1.66	0.77
1:B:180:MET:HE1	1:B:254:PRO:HB3	1.70	0.73
1:D:22:LEU:HD11	1:D:62:LYS:HE2	1.72	0.72
1:C:55:GLU:OE2	1:C:58:LYS:NZ	2.14	0.71
1:A:1:SER:O	1:A:2:LEU:HD23	1.91	0.71
1:A:116:THR:HA	6:A:535:HOH:O	1.90	0.70
1:B:118:ILE:HD12	1:B:118:ILE:O	1.91	0.70
1:B:177:ASN:CA	1:B:180:MET:HE2	2.13	0.69
1:A:116:THR:O	1:A:117:SER:HB2	1.93	0.68
1:A:22:LEU:HD11	1:A:62:LYS:HE2	1.76	0.67
1:B:237:GLU:HG3	1:B:241:LYS:NZ	2.10	0.67
1:B:237:GLU:HG3	1:B:241:LYS:CE	2.24	0.67
1:D:2:LEU:O	1:D:2:LEU:HD13	1.95	0.67
1:C:31:LYS:O	1:C:31:LYS:HE3	1.95	0.65
1:B:302:CYS:SG	1:B:340:SER:HB3	2.38	0.64
1:D:318:GLY:HA3	4:D:401:ACO:O9P	1.98	0.64
1:C:200:PRO:HB2	1:C:202:GLU:OE1	1.99	0.63
1:A:1:SER:C	1:A:2:LEU:HD23	2.24	0.62
1:C:101:TRP:CE2	1:C:192:LYS:HD2	2.35	0.62
1:C:177:ASN:CA	1:C:180:MET:HE2	2.23	0.62
1:B:266:GLN:OE1	1:B:266:GLN:HA	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:GLN:NE2	1:A:34:ILE:HD13	2.15	0.61
1:C:180:MET:HE1	1:C:254:PRO:HB3	1.83	0.61
1:C:54:ILE:HG22	1:C:58:LYS:HE3	1.83	0.60
1:C:9:PHE:HD1	1:C:34:ILE:HD11	1.66	0.60
1:D:12:ASN:O	1:D:14:LYS:HE2	2.02	0.59
1:B:131:LEU:HD12	1:B:139:ARG:HH11	1.69	0.58
1:C:118:ILE:HD12	1:C:118:ILE:O	2.03	0.58
1:C:192:LYS:HE3	1:C:196:GLU:OE2	2.04	0.57
1:B:200:PRO:HB2	1:B:202:GLU:CD	2.30	0.56
1:C:54:ILE:O	1:C:58:LYS:HG3	2.05	0.56
1:C:37:ASP:O	1:C:41:LYS:HG3	2.05	0.56
1:B:39:LYS:O	1:B:43:ASN:HB2	2.06	0.56
1:B:328:MET:SD	1:B:338:VAL:HG21	2.45	0.56
1:B:263:LYS:NZ	6:B:501:HOH:O	2.35	0.55
1:B:85:ASP:OD1	1:B:88:SER:OG	2.23	0.55
1:A:180:MET:SD	1:A:254:PRO:HG3	2.47	0.55
1:A:117:SER:HB2	1:D:117:SER:N	2.23	0.54
1:D:153:ILE:HB	1:D:154:PRO:CD	2.37	0.54
1:B:31:LYS:HD3	1:B:31:LYS:C	2.33	0.54
1:B:141:MET:HE3	1:B:168:VAL:O	2.08	0.54
1:A:336:ILE:HA	1:B:339:LYS:HD2	1.90	0.54
1:A:31:LYS:O	1:A:31:LYS:HE3	2.08	0.54
4:D:401:ACO:O9P	4:D:401:ACO:H131	2.08	0.53
1:A:281:SER:O	1:A:287:PHE:HB2	2.08	0.53
1:C:9:PHE:CD1	1:C:34:ILE:HD11	2.44	0.53
1:D:37:ASP:O	1:D:41:LYS:HD2	2.09	0.53
1:D:2:LEU:CD2	1:D:25:LYS:HD3	2.36	0.52
1:A:34:ILE:O	1:A:41:LYS:HA	2.10	0.52
1:A:303:SER:H	1:A:341:ASN:ND2	2.08	0.52
1:B:191:ARG:O	1:B:195:MET:HE2	2.10	0.51
1:B:81:THR:HG21	1:B:92:HIS:CE1	2.45	0.51
1:A:304:TYR:C	1:A:305:ILE:HD13	2.36	0.51
1:B:4:PHE:C	1:B:4:PHE:CD1	2.87	0.51
1:A:153:ILE:HB	1:A:154:PRO:CD	2.41	0.51
1:D:30:ASP:HA	1:D:77:ILE:HD13	1.92	0.50
1:B:90:ILE:HD12	1:B:100:VAL:HB	1.94	0.50
1:A:172:PHE:CD2	1:A:211:LYS:HG3	2.47	0.50
1:A:220:GLY:HA3	1:A:227:THR:OG1	2.13	0.49
1:B:322:LEU:HD21	4:B:401:ACO:O4B	2.12	0.48
1:D:172:PHE:CD2	1:D:211:LYS:HG3	2.48	0.48
1:A:128:ILE:HB	4:A:401:ACO:H21	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:THR:O	1:D:115:ASP:OD1	2.32	0.48
1:C:99:LYS:NZ	6:C:505:HOH:O	2.45	0.48
1:A:192:LYS:O	1:A:196:GLU:HG3	2.14	0.48
1:A:280:THR:HG23	1:A:305:ILE:HD12	1.95	0.48
1:B:237:GLU:HG3	1:B:241:LYS:HE2	1.96	0.48
1:C:142:PHE:CD1	1:C:163:ALA:HA	2.49	0.48
1:C:273:LEU:HD12	1:C:298:SER:OG	2.13	0.48
1:A:305:ILE:HD13	1:A:305:ILE:N	2.28	0.47
1:D:30:ASP:HA	1:D:77:ILE:CD1	2.43	0.47
1:C:101:TRP:CD2	1:C:192:LYS:HD2	2.49	0.47
1:C:187:GLU:HG3	1:C:223:MET:HE3	1.96	0.47
1:C:322:LEU:O	1:C:326:THR:HG23	2.14	0.47
1:A:277:LYS:HG3	1:A:328:MET:HE3	1.97	0.47
1:B:114:LYS:HE2	1:B:158:TYR:OH	2.14	0.47
1:C:337:ASP:OD1	1:C:338:VAL:N	2.47	0.47
1:A:235:HIS:CE1	1:A:237:GLU:HB2	2.51	0.46
1:B:302:CYS:SG	1:B:340:SER:CB	3.03	0.46
1:C:68:TYR:CE1	1:C:82:LYS:HB2	2.50	0.46
1:C:130:ASP:OD1	1:C:139:ARG:NH2	2.43	0.46
1:B:263:LYS:NZ	6:B:502:HOH:O	2.49	0.46
1:D:235:HIS:CE1	1:D:237:GLU:HB2	2.51	0.46
1:C:232:PRO:HD2	1:C:278:LEU:HD21	1.98	0.46
1:B:21:ASP:OD1	1:B:23:SER:OG	2.33	0.46
1:C:154:PRO:HG3	1:C:334:TYR:CZ	2.51	0.45
1:B:153:ILE:HB	1:B:154:PRO:CD	2.45	0.45
1:D:220:GLY:HA3	1:D:227:THR:OG1	2.17	0.45
1:A:134:ASN:O	1:A:140:ARG:HD3	2.17	0.45
1:C:81:THR:HG21	1:C:92:HIS:CE1	2.52	0.45
1:A:31:LYS:HG3	1:A:76:GLY:O	2.18	0.44
1:C:85:ASP:OD1	1:C:88:SER:OG	2.18	0.44
1:D:202:GLU:H	1:D:202:GLU:CD	2.25	0.44
1:D:323:ASN:H	1:D:323:ASN:HD22	1.64	0.44
1:D:323:ASN:HA	4:D:401:ACO:N1A	2.32	0.44
1:C:45:ASN:HA	1:C:73:HIS:CE1	2.53	0.44
1:B:68:TYR:CE1	1:B:82:LYS:HB2	2.53	0.44
1:A:153:ILE:HD12	1:A:157:THR:HG21	2.00	0.44
1:D:47:LEU:HG	1:D:70:LEU:HD22	1.99	0.44
1:A:283:ASN:O	1:A:313:GLY:HA2	2.18	0.43
1:B:220:GLY:HA3	1:B:227:THR:OG1	2.17	0.43
1:D:153:ILE:HB	1:D:154:PRO:HD2	2.00	0.43
1:C:112:LEU:O	1:C:113:GLU:HG2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:220:GLY:HA3	1:C:227:THR:OG1	2.18	0.43
1:D:39:LYS:O	1:D:43:ASN:HB2	2.18	0.43
1:C:338:VAL:HG13	1:D:336:ILE:HB	2.00	0.43
1:D:2:LEU:HD22	1:D:2:LEU:HA	1.71	0.43
1:A:293:ILE:HD12	1:A:293:ILE:N	2.32	0.43
1:C:168:VAL:HB	1:C:248:PHE:HB2	2.00	0.43
1:D:145:ASN:HB3	4:D:401:ACO:OAP	2.18	0.43
1:B:4:PHE:C	1:B:4:PHE:HD1	2.26	0.43
1:A:323:ASN:HA	4:A:401:ACO:N1A	2.33	0.42
1:C:153:ILE:HB	1:C:154:PRO:CD	2.49	0.42
1:C:152:TYR:HA	4:D:401:ACO:N1A	2.35	0.42
1:B:180:MET:CE	1:B:254:PRO:HB3	2.46	0.42
1:B:320:HIS:HD2	6:B:525:HOH:O	2.01	0.42
1:C:118:ILE:H	1:C:118:ILE:HG13	1.71	0.42
1:D:281:SER:O	1:D:287:PHE:HB2	2.20	0.42
1:D:322:LEU:HD21	4:D:401:ACO:O4B	2.20	0.42
1:C:75:ASN:OD1	1:C:75:ASN:O	2.38	0.42
1:D:287:PHE:CD1	1:D:287:PHE:C	2.97	0.42
1:D:232:PRO:HD2	1:D:278:LEU:HD21	2.01	0.42
1:A:141:MET:HE3	1:A:168:VAL:O	2.19	0.42
1:D:34:ILE:O	1:D:41:LYS:HA	2.19	0.42
1:A:113:GLU:HG3	1:A:155:LYS:HB3	2.01	0.41
1:C:304:TYR:C	1:C:305:ILE:HD13	2.44	0.41
1:C:320:HIS:HD2	6:C:533:HOH:O	2.03	0.41
1:D:252:VAL:HG23	1:D:253:PHE:CD1	2.54	0.41
1:C:266:GLN:HA	1:C:266:GLN:OE1	2.19	0.41
1:A:265:PHE:CE2	1:A:294:VAL:HG22	2.55	0.41
1:B:67:LYS:HG2	1:B:178:ALA:HB1	2.03	0.41
1:C:278:LEU:HD23	1:C:279:VAL:N	2.35	0.41
1:C:278:LEU:HD23	1:C:278:LEU:C	2.45	0.41
1:A:39:LYS:O	1:A:43:ASN:HB2	2.21	0.41
1:A:280:THR:CG2	1:A:305:ILE:HD12	2.51	0.41
1:B:192:LYS:NZ	1:B:196:GLU:OE2	2.33	0.40
1:B:246:LEU:HD23	4:B:401:ACO:HH31	2.03	0.40
1:C:252:VAL:HG23	1:C:253:PHE:CD1	2.56	0.40
1:C:226:LYS:NZ	1:C:335:ASP:OD1	2.49	0.40
1:D:141:MET:HE3	1:D:168:VAL:O	2.21	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	344/354 (97%)	333 (97%)	10 (3%)	1 (0%)	36	34
1	B	342/354 (97%)	335 (98%)	7 (2%)	0	100	100
1	C	342/354 (97%)	335 (98%)	7 (2%)	0	100	100
1	D	340/354 (96%)	333 (98%)	7 (2%)	0	100	100
All	All	1368/1416 (97%)	1336 (98%)	31 (2%)	1 (0%)	48	50

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	117	SER

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	300/324 (93%)	292 (97%)	8 (3%)	39	41
1	B	307/324 (95%)	306 (100%)	1 (0%)	86	91
1	C	301/324 (93%)	296 (98%)	5 (2%)	53	60
1	D	303/324 (94%)	297 (98%)	6 (2%)	48	54
All	All	1211/1296 (93%)	1191 (98%)	20 (2%)	53	60

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LEU
1	A	31	LYS
1	A	34	ILE
1	A	38	GLU
1	A	54	ILE
1	A	115	ASP
1	A	328	MET
1	A	338	VAL
1	B	31	LYS
1	C	31	LYS
1	C	117	SER
1	C	266	GLN
1	C	328	MET
1	C	338	VAL
1	D	2	LEU
1	D	31	LYS
1	D	34	ILE
1	D	38	GLU
1	D	262	SER
1	D	323	ASN

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

Mol	Chain	Res	Type
1	A	66	ASN
1	A	267	ASN
1	A	310	ASN
1	A	341	ASN
1	B	73	HIS
1	B	92	HIS
1	C	66	ASN
1	C	92	HIS
1	C	310	ASN
1	D	19	ASN
1	D	119	ASN
1	D	323	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

6 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	A1I0J	E	1	2	20,20,21	0.63	1 (5%)	26,28,30	0.70	0
2	A1I0J	E	2	2	20,20,21	0.74	1 (5%)	26,28,30	1.27	4 (15%)
2	A1I0J	E	3	2	21,21,21	0.60	1 (4%)	29,30,30	1.25	3 (10%)
3	A1I0J	F	1	3	9,9,21	0.76	0	11,12,30	1.15	1 (9%)
3	A1I0J	F	2	3	20,20,21	1.17	2 (10%)	26,28,30	1.04	1 (3%)
3	A1I0J	F	3	3	11,11,21	0.28	0	15,15,30	0.58	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
2	A1I0J	E	1	2	-	1/14/30/34	0/1/1/1
2	A1I0J	E	2	2	-	2/14/30/34	0/1/1/1
2	A1I0J	E	3	2	-	7/14/34/34	0/1/1/1
3	A1I0J	F	1	3	-	3/8/8/34	-
3	A1I0J	F	2	3	-	2/14/30/34	0/1/1/1
3	A1I0J	F	3	3	-	0/2/18/34	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	2	A1I0J	P-O8	3.99	1.63	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	2	A1I0J	P-O9	2.65	1.65	1.54
2	E	2	A1I0J	P-O9	2.44	1.64	1.54
2	E	1	A1I0J	O10-CAQ	2.19	1.53	1.44
2	E	3	A1I0J	P-O9	2.13	1.63	1.54

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	3	A1I0J	O10-P-O8	4.56	119.26	106.47
3	F	2	A1I0J	O7-P-O10	3.28	115.47	106.73
2	E	2	A1I0J	O10-P-O8	3.21	115.48	106.47
3	F	1	A1I0J	O10-P-O8	3.07	115.09	106.47
2	E	3	A1I0J	P-O10-CAQ	3.06	126.71	118.30
2	E	2	A1I0J	O1-CAR-CAS	-2.88	99.87	108.47
2	E	2	A1I0J	O1-CAR-CAQ	2.82	117.94	109.03
2	E	2	A1I0J	O7-P-O10	-2.63	99.74	106.73
2	E	3	A1I0J	O1-CAR-CAQ	2.10	115.67	109.03

There are no chirality outliers.

All (15) torsion outliers are listed below:

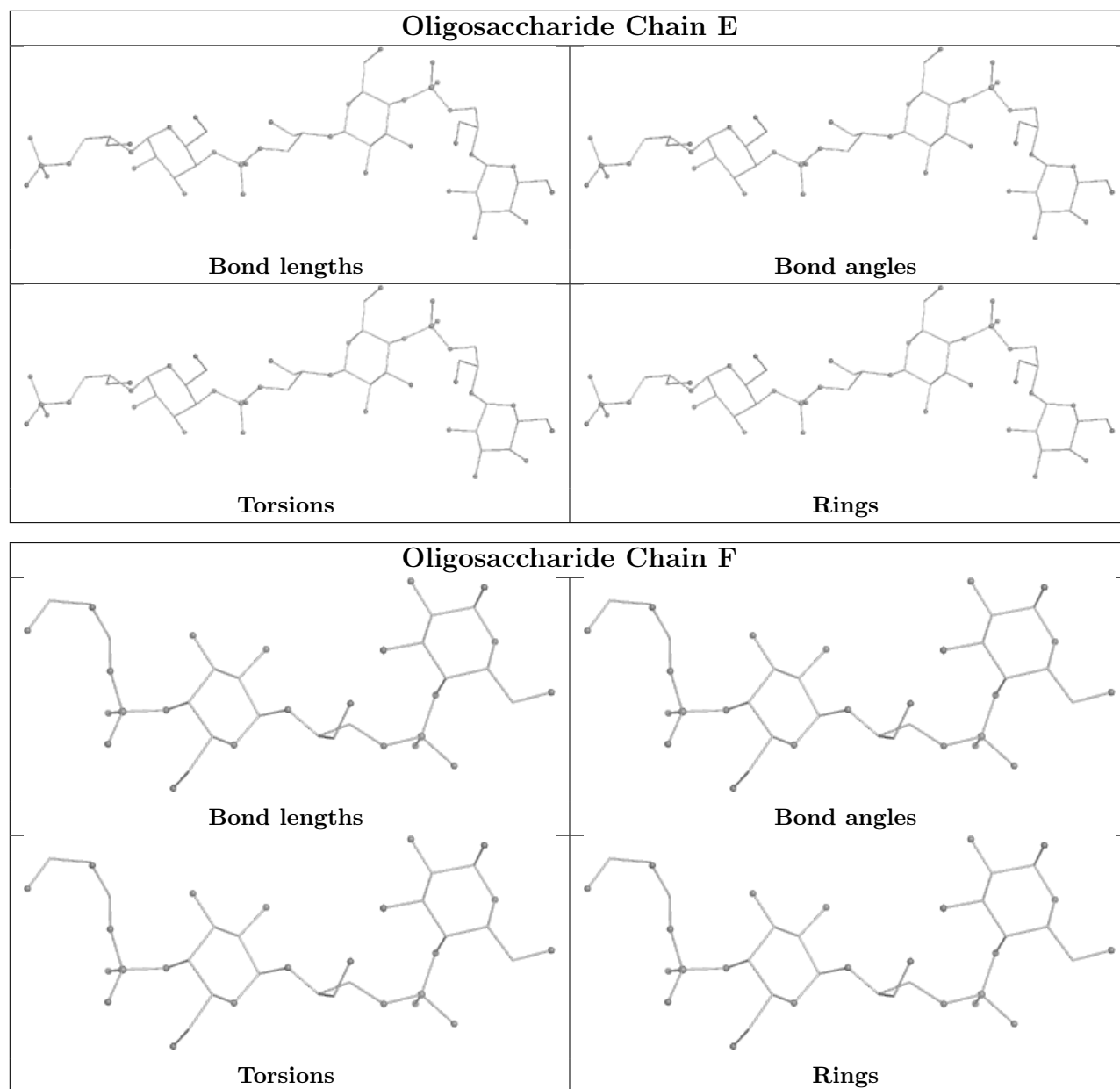
Mol	Chain	Res	Type	Atoms
2	E	2	A1I0J	O1-CAR-CAS-OAU
2	E	3	A1I0J	CAQ-O10-P-O9
3	F	1	A1I0J	O10-CAQ-CAR-O1
3	F	2	A1I0J	O5-C5-C6-O6
3	F	1	A1I0J	O10-CAQ-CAR-CAS
2	E	3	A1I0J	O5-C5-C6-O6
2	E	2	A1I0J	CAS-CAR-O1-C1
2	E	3	A1I0J	CAQ-CAR-O1-C1
2	E	3	A1I0J	CAS-CAR-O1-C1
2	E	3	A1I0J	O5-C1-O1-CAR
2	E	3	A1I0J	O1-CAR-CAS-OAU
2	E	1	A1I0J	CAQ-O10-P-O7
3	F	1	A1I0J	CAQ-O10-P-O9
2	E	3	A1I0J	C2-C1-O1-CAR
3	F	2	A1I0J	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for oligosaccharide.



5.6 Ligand geometry ⓘ

5 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	ACO	B	401	-	48,53,53	1.15	4 (8%)	69,79,79	1.86	16 (23%)
4	ACO	C	401	-	48,53,53	1.15	6 (12%)	69,79,79	1.80	15 (21%)
5	PO4	A	402	-	4,4,4	0.66	0	6,6,6	0.64	0
4	ACO	D	401	-	42,47,53	1.19	3 (7%)	62,72,79	2.03	14 (22%)
4	ACO	A	401	-	48,53,53	1.10	5 (10%)	69,79,79	1.84	15 (21%)

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	ACO	D	401	-	-	16/44/60/67	0/3/3/3
4	ACO	B	401	-	-	6/51/67/67	0/3/3/3
4	ACO	A	401	-	-	6/51/67/67	0/3/3/3
4	ACO	C	401	-	-	9/51/67/67	0/3/3/3

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	401	ACO	C5A-C4A	4.26	1.47	1.39
4	D	401	ACO	C5A-C4A	4.14	1.46	1.39
4	C	401	ACO	C5A-C4A	4.00	1.46	1.39
4	A	401	ACO	C5A-C4A	3.93	1.46	1.39
4	D	401	ACO	C5A-C6A	2.69	1.48	1.41
4	B	401	ACO	C5A-C6A	2.68	1.48	1.41
4	A	401	ACO	C5A-C6A	2.59	1.48	1.41
4	C	401	ACO	C5A-C6A	2.50	1.48	1.41
4	A	401	ACO	C8A-N9A	-2.46	1.33	1.37
4	D	401	ACO	C8A-N9A	-2.36	1.33	1.37
4	C	401	ACO	C8A-N7A	2.32	1.36	1.31
4	B	401	ACO	C8A-N9A	-2.20	1.33	1.37
4	C	401	ACO	C8A-N9A	-2.20	1.33	1.37
4	C	401	ACO	P3B-O3B	2.20	1.63	1.59
4	C	401	ACO	C5A-N7A	-2.18	1.34	1.39
4	B	401	ACO	C8A-N7A	2.16	1.35	1.31
4	A	401	ACO	C4A-N9A	-2.15	1.32	1.37
4	A	401	ACO	C5A-N7A	-2.12	1.35	1.39

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	401	ACO	C5A-C4A-N3A	-6.07	118.83	126.75
4	B	401	ACO	C5A-C4A-N3A	-5.94	119.00	126.75
4	D	401	ACO	N3A-C4A-N9A	5.81	136.65	127.08
4	C	401	ACO	C5A-C4A-N3A	-5.69	119.33	126.75
4	A	401	ACO	C5A-C4A-N3A	-5.68	119.33	126.75
4	A	401	ACO	N3A-C4A-N9A	5.37	135.94	127.08
4	B	401	ACO	N3A-C4A-N9A	5.32	135.84	127.08
4	D	401	ACO	C4A-N9A-C8A	5.02	111.17	105.73
4	A	401	ACO	C4A-N9A-C8A	5.00	111.15	105.73
4	C	401	ACO	N3A-C4A-N9A	4.94	135.22	127.08
4	B	401	ACO	C4A-N9A-C8A	4.41	110.50	105.73
4	C	401	ACO	C4A-N9A-C8A	4.20	110.28	105.73
4	D	401	ACO	C2A-N3A-C4A	4.16	121.58	111.75
4	D	401	ACO	N3A-C2A-N1A	-4.05	122.27	128.60
4	C	401	ACO	N3A-C2A-N1A	-4.00	122.35	128.60
4	B	401	ACO	C2A-N3A-C4A	3.96	121.10	111.75
4	A	401	ACO	C2A-N3A-C4A	3.91	120.98	111.75
4	C	401	ACO	C2A-N3A-C4A	3.87	120.90	111.75
4	B	401	ACO	N3A-C2A-N1A	-3.86	122.57	128.60
4	A	401	ACO	N3A-C2A-N1A	-3.78	122.69	128.60
4	D	401	ACO	O4B-C1B-N9A	3.71	115.36	108.06
4	D	401	ACO	C5A-N7A-C8A	3.69	108.76	103.51
4	B	401	ACO	C4A-C5A-N7A	-3.58	106.25	110.62
4	B	401	ACO	C5A-N7A-C8A	3.54	108.53	103.51
4	D	401	ACO	C4A-C5A-N7A	-3.54	106.31	110.62
4	A	401	ACO	C5A-N7A-C8A	3.53	108.52	103.51
4	A	401	ACO	C4A-C5A-N7A	-3.49	106.37	110.62
4	C	401	ACO	C4A-C5A-N7A	-3.45	106.41	110.62
4	A	401	ACO	N9A-C8A-N7A	-3.42	109.23	113.91
4	D	401	ACO	N9A-C8A-N7A	-3.42	109.24	113.91
4	C	401	ACO	C5A-N7A-C8A	3.35	108.27	103.51
4	D	401	ACO	P2A-O3A-P1A	-3.21	121.83	132.83
4	B	401	ACO	N9A-C8A-N7A	-3.19	109.55	113.91
4	C	401	ACO	N9A-C8A-N7A	-3.17	109.58	113.91
4	B	401	ACO	O4B-C1B-N9A	3.07	114.12	108.06
4	C	401	ACO	O4B-C1B-N9A	3.05	114.07	108.06
4	D	401	ACO	CDP-CBP-CCP	2.92	112.99	108.23
4	D	401	ACO	C2B-C3B-C4B	2.82	108.23	103.22
4	B	401	ACO	P2A-O3A-P1A	-2.79	123.27	132.83
4	C	401	ACO	P2A-O3A-P1A	-2.77	123.30	132.83
4	C	401	ACO	C2A-N1A-C6A	2.61	123.24	118.77
4	C	401	ACO	C6P-C7P-N8P	2.58	117.10	111.90
4	A	401	ACO	C6A-C5A-N7A	2.55	136.77	132.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	401	ACO	C2B-C3B-C4B	2.52	107.68	103.22
4	B	401	ACO	C6A-C5A-N7A	2.47	136.61	132.02
4	B	401	ACO	C2A-N1A-C6A	2.43	122.94	118.77
4	D	401	ACO	C6A-C5A-N7A	2.42	136.53	132.02
4	A	401	ACO	CDP-CBP-CCP	2.41	112.17	108.23
4	A	401	ACO	O4B-C1B-N9A	2.35	112.70	108.06
4	C	401	ACO	C3P-N4P-C5P	-2.27	118.61	122.84
4	B	401	ACO	C6P-C7P-N8P	2.27	116.47	111.90
4	C	401	ACO	C6A-C5A-N7A	2.25	136.21	132.02
4	A	401	ACO	P2A-O3A-P1A	-2.23	125.19	132.83
4	C	401	ACO	CDP-CBP-CCP	2.21	111.84	108.23
4	B	401	ACO	O5P-C5P-C6P	-2.16	118.07	122.02
4	A	401	ACO	C2A-N1A-C6A	2.12	122.41	118.77
4	B	401	ACO	CDP-CBP-CCP	2.12	111.69	108.23
4	A	401	ACO	O5A-P2A-O4A	2.11	122.67	112.24
4	D	401	ACO	C2A-N1A-C6A	2.09	122.35	118.77
4	B	401	ACO	C7P-C6P-C5P	-2.02	109.00	112.36

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	401	ACO	C5B-O5B-P1A-O1A
4	D	401	ACO	C5B-O5B-P1A-O2A
4	D	401	ACO	P2A-O3A-P1A-O5B
4	D	401	ACO	CEP-CBP-CCP-O6A
4	D	401	ACO	CAP-CBP-CCP-O6A
4	D	401	ACO	O9P-C9P-CAP-CBP
4	D	401	ACO	N8P-C9P-CAP-CBP
4	D	401	ACO	O9P-C9P-CAP-OAP
4	D	401	ACO	N8P-C9P-CAP-OAP
4	B	401	ACO	O4B-C4B-C5B-O5B
4	C	401	ACO	O4B-C4B-C5B-O5B
4	D	401	ACO	C3B-C4B-C5B-O5B
4	D	401	ACO	O4B-C4B-C5B-O5B
4	D	401	ACO	CDP-CBP-CCP-O6A
4	A	401	ACO	S1P-C2P-C3P-N4P
4	B	401	ACO	C3B-C4B-C5B-O5B
4	C	401	ACO	C3B-C4B-C5B-O5B
4	B	401	ACO	S1P-C2P-C3P-N4P
4	A	401	ACO	P2A-O3A-P1A-O2A
4	C	401	ACO	P2A-O3A-P1A-O2A

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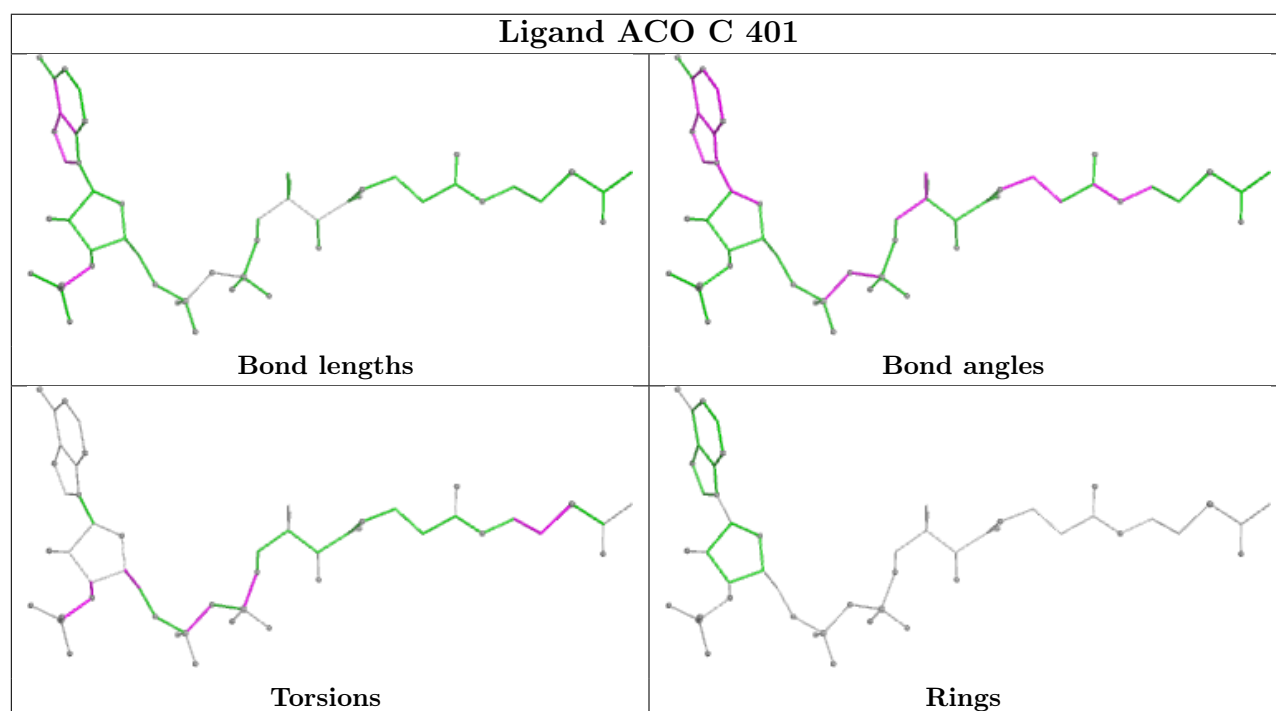
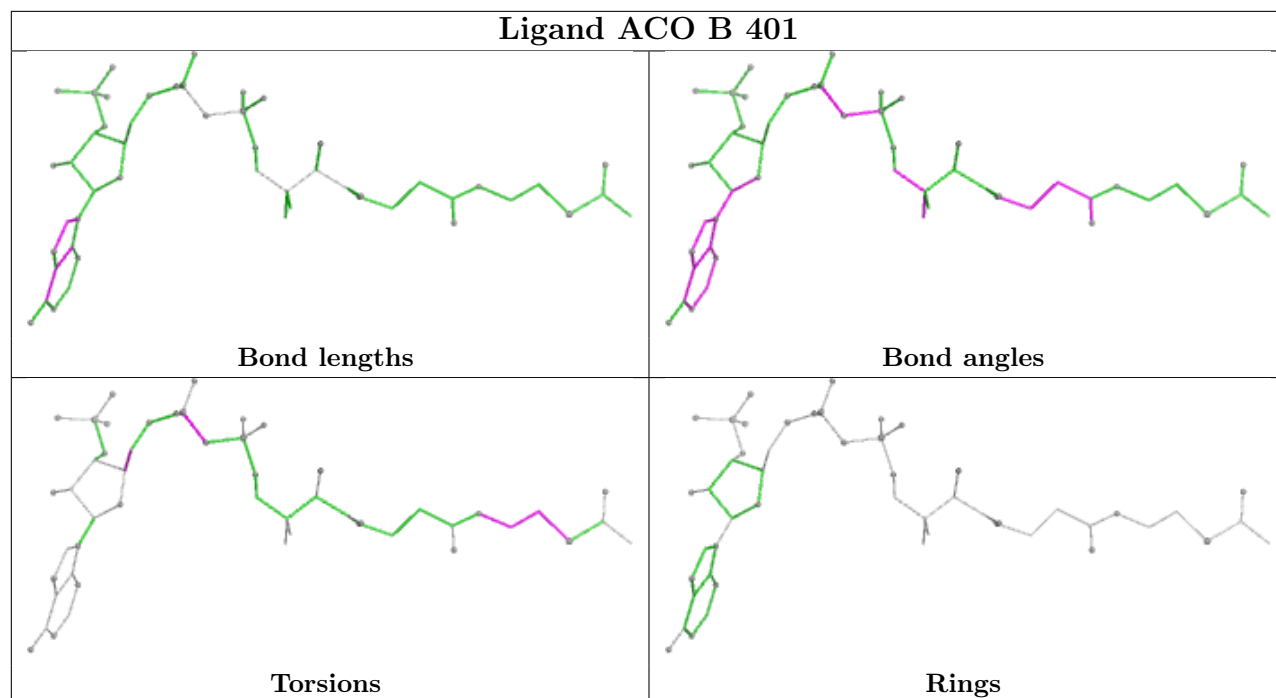
Mol	Chain	Res	Type	Atoms
4	C	401	ACO	C2B-C3B-O3B-P3B
4	B	401	ACO	C2P-C3P-N4P-C5P
4	A	401	ACO	C3P-C2P-S1P-C
4	B	401	ACO	C3P-C2P-S1P-C
4	C	401	ACO	C3P-C2P-S1P-C
4	A	401	ACO	P2A-O3A-P1A-O1A
4	C	401	ACO	P2A-O3A-P1A-O1A
4	C	401	ACO	S1P-C2P-C3P-N4P
4	A	401	ACO	C3B-O3B-P3B-O8A
4	C	401	ACO	C3B-O3B-P3B-O8A
4	C	401	ACO	CCP-O6A-P2A-O3A
4	D	401	ACO	C5B-O5B-P1A-O3A
4	B	401	ACO	P2A-O3A-P1A-O1A
4	D	401	ACO	P2A-O3A-P1A-O1A
4	D	401	ACO	CBP-CCP-O6A-P2A
4	D	401	ACO	C2B-C3B-O3B-P3B
4	A	401	ACO	O4B-C4B-C5B-O5B

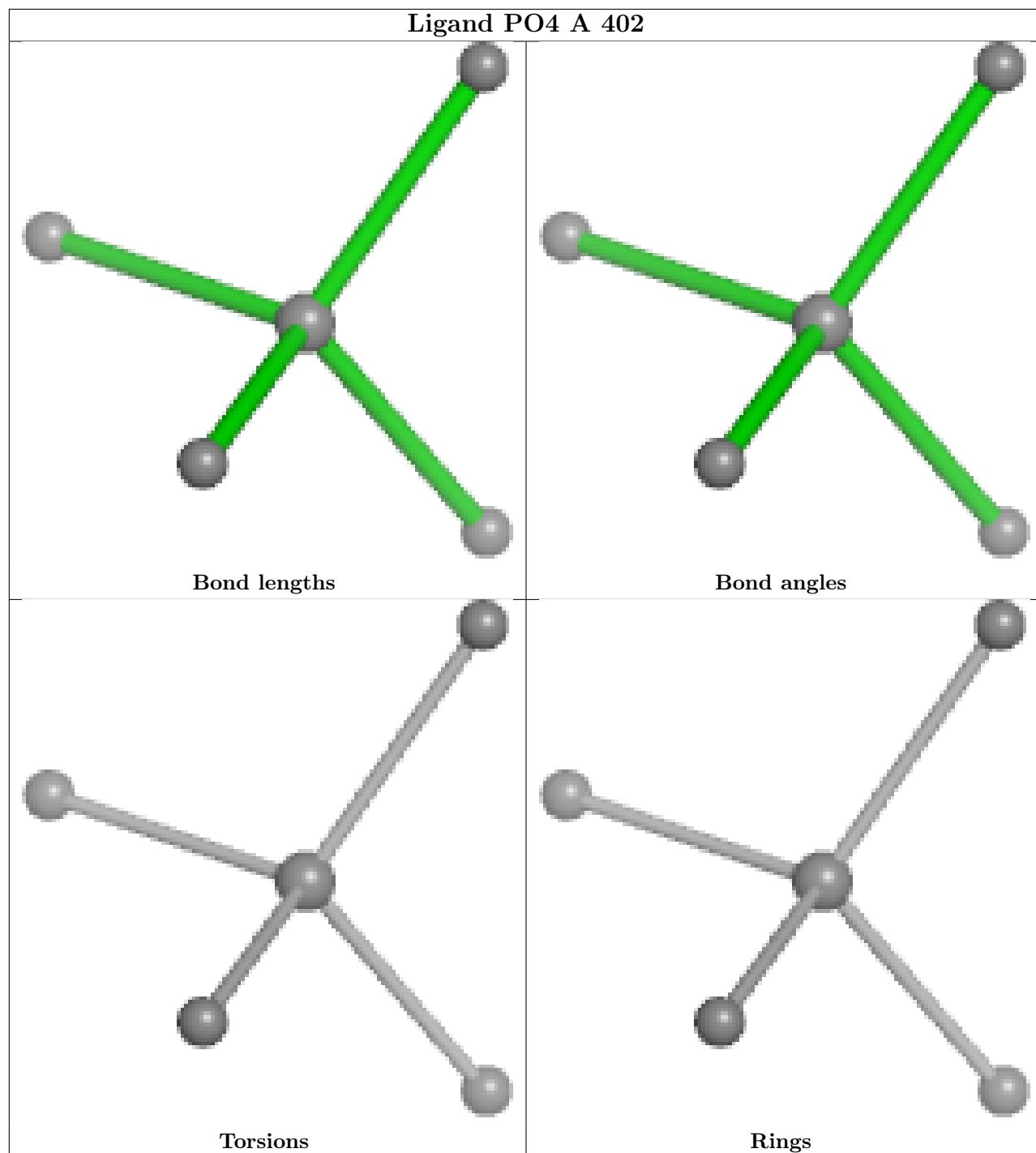
There are no ring outliers.

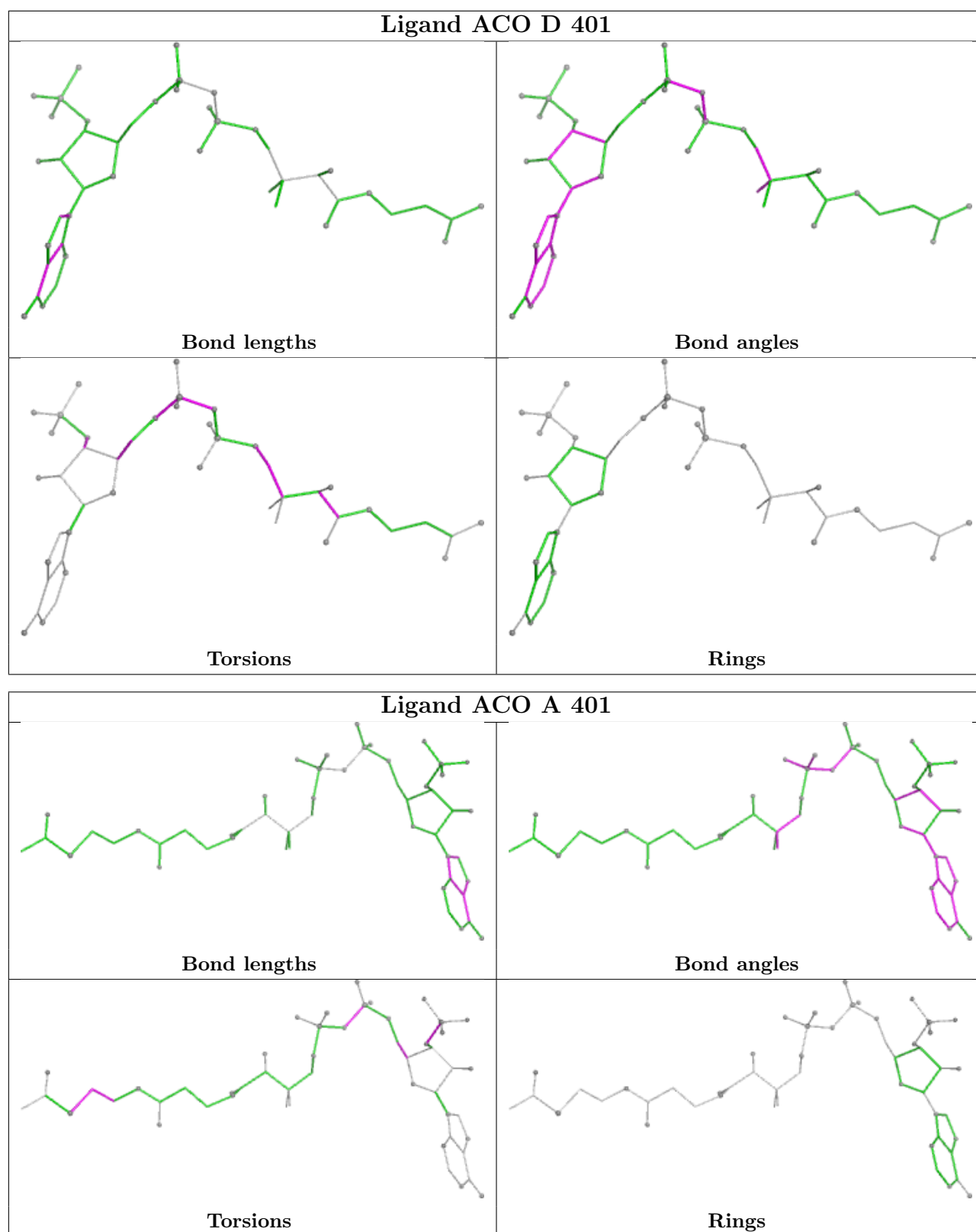
3 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	401	ACO	2	0
4	D	401	ACO	6	0
4	A	401	ACO	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	346/354 (97%)	0.63	17 (4%) 35 39	46, 60, 78, 93	0
1	B	344/354 (97%)	0.47	8 (2%) 61 64	45, 57, 75, 93	0
1	C	344/354 (97%)	0.52	15 (4%) 39 44	46, 57, 76, 92	0
1	D	344/354 (97%)	0.42	8 (2%) 61 64	46, 56, 71, 97	0
All	All	1378/1416 (97%)	0.51	48 (3%) 47 51	45, 57, 76, 97	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	2	LEU	4.5
1	A	116	THR	4.3
1	D	117	SER	4.0
1	B	118	ILE	3.8
1	C	118	ILE	3.4
1	D	338	VAL	3.4
1	D	54	ILE	3.3
1	B	4	PHE	3.0
1	A	118	ILE	3.0
1	C	35	GLY	3.0
1	C	54	ILE	2.9
1	B	338	VAL	2.8
1	A	1	SER	2.8
1	A	112	LEU	2.8
1	A	20	ILE	2.8
1	C	42	LEU	2.7
1	C	33	ALA	2.7
1	A	54	ILE	2.7
1	A	34	ILE	2.6
1	C	52	GLY	2.6
1	A	338	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	36	LYS	2.6
1	B	6	ARG	2.5
1	C	11	GLN	2.5
1	C	338	VAL	2.5
1	D	337	ASP	2.5
1	D	114	LYS	2.4
1	A	114	LYS	2.4
1	A	269	LYS	2.4
1	A	75	ASN	2.3
1	D	115	ASP	2.3
1	A	299	THR	2.3
1	A	2	LEU	2.3
1	A	42	LEU	2.3
1	C	32	SER	2.2
1	C	34	ILE	2.2
1	C	39	LYS	2.2
1	B	202	GLU	2.2
1	B	337	ASP	2.2
1	A	52	GLY	2.2
1	B	28	TYR	2.2
1	D	36	LYS	2.2
1	C	44	HIS	2.1
1	C	38	GLU	2.1
1	A	115	ASP	2.1
1	C	248	PHE	2.1
1	A	264	LEU	2.0
1	B	299	THR	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](#)

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.

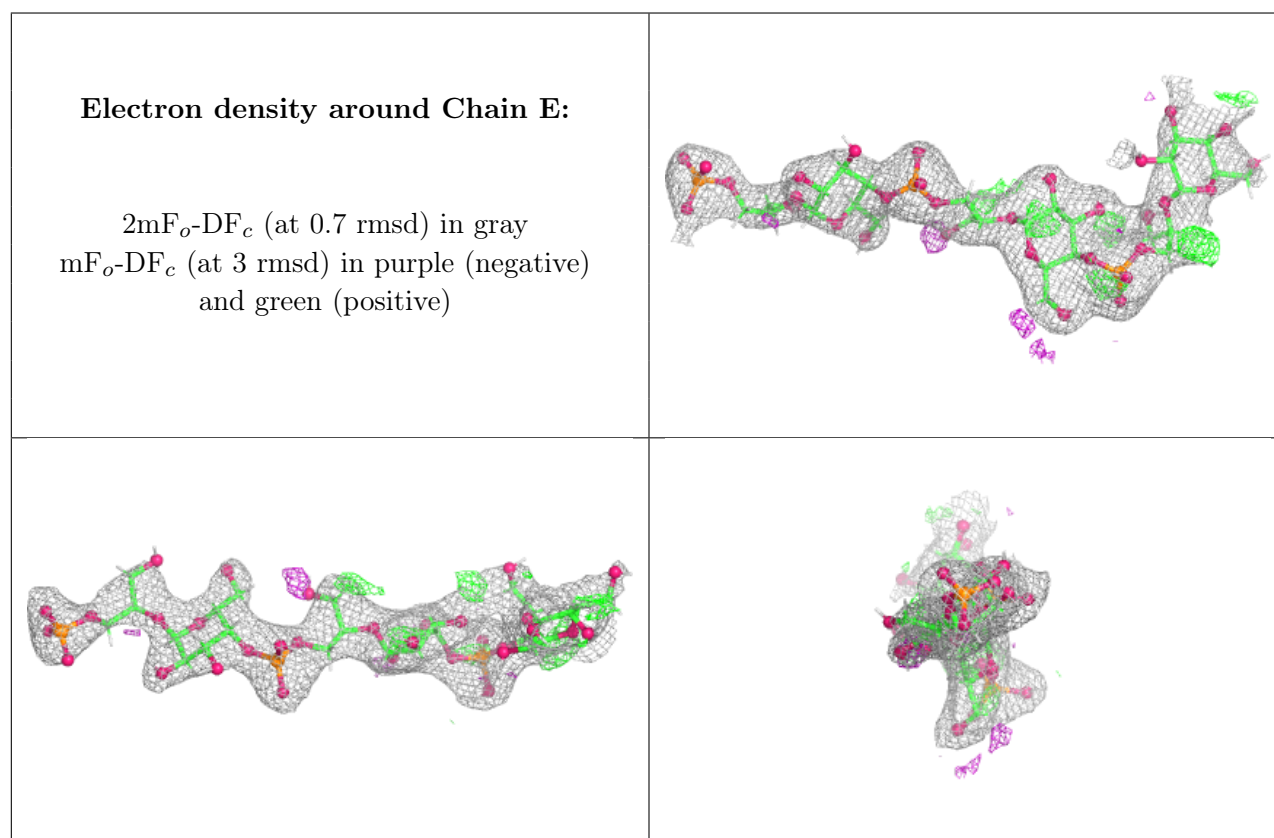
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	A1I0J	F	3	11/21	0.40	0.16	89,95,112,116	21

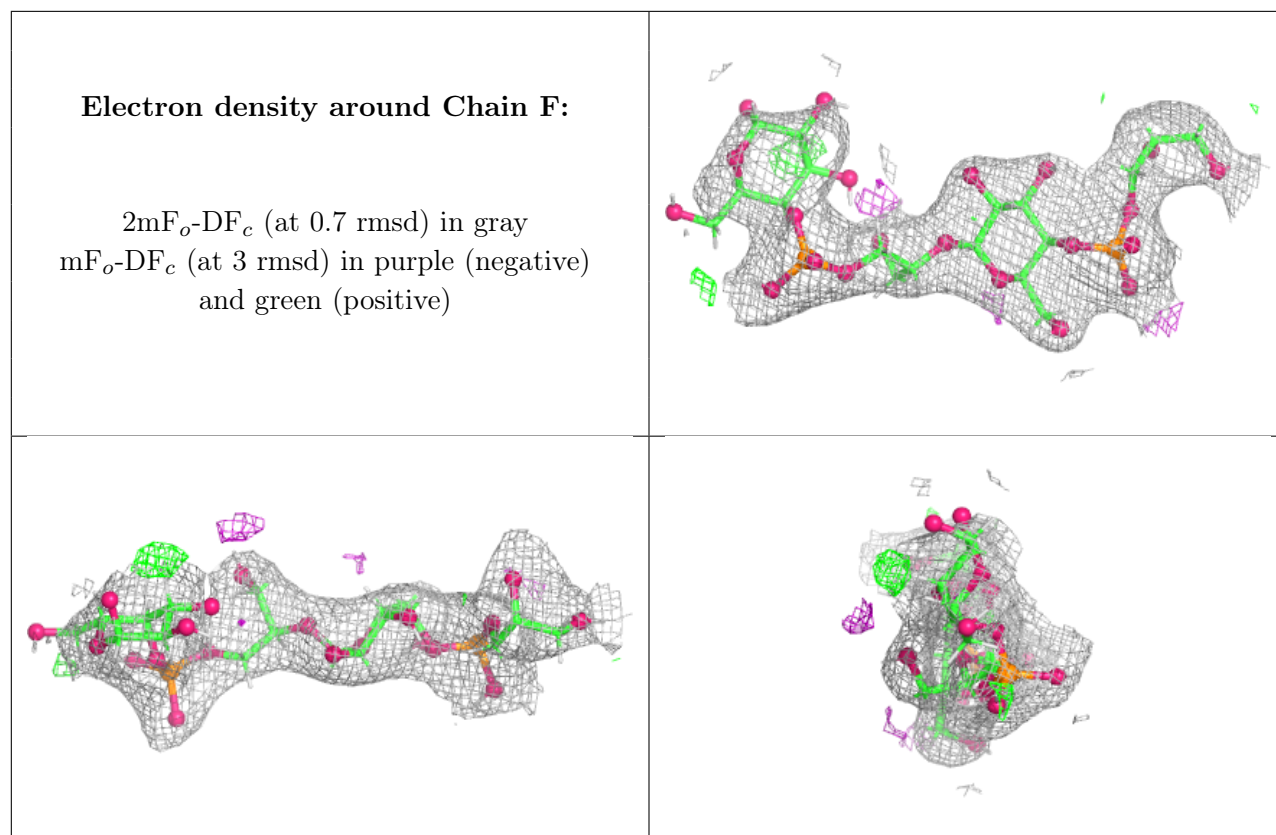
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	A1I0J	E	3	21/21	0.84	0.15	54,87,106,109	39
2	A1I0J	E	1	20/21	0.84	0.15	64,81,95,96	36
2	A1I0J	E	2	20/21	0.86	0.15	52,68,81,90	37
3	A1I0J	F	2	20/21	0.90	0.11	58,70,85,87	37
3	A1I0J	F	1	10/21	0.93	0.11	53,64,78,83	17

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.





6.4 Ligands [i](#)

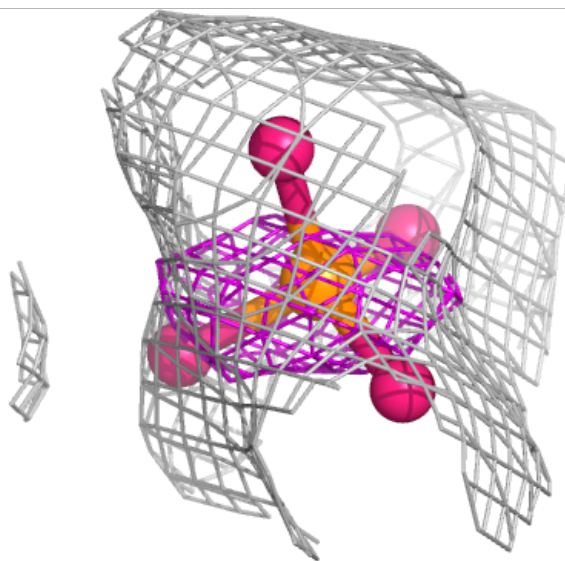
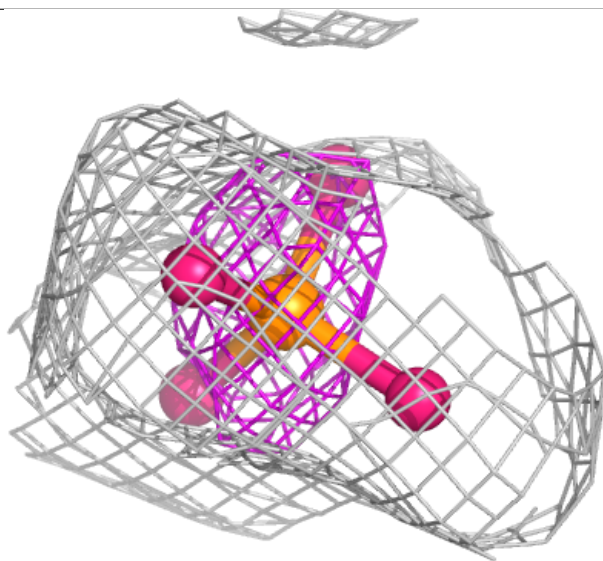
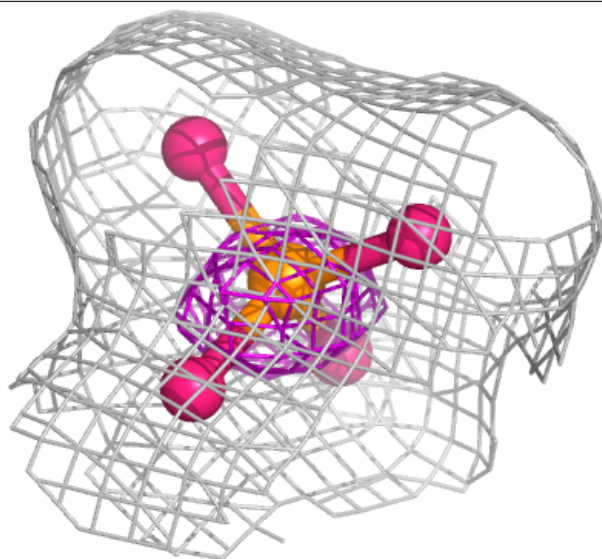
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	PO4	A	402	5/5	0.61	0.13	87,87,98,108	0
4	ACO	D	401	45/51	0.75	0.19	58,74,90,99	72
4	ACO	B	401	51/51	0.75	0.22	51,69,81,87	85
4	ACO	C	401	51/51	0.85	0.15	49,67,80,87	85
4	ACO	A	401	51/51	0.89	0.13	51,64,82,85	85

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.

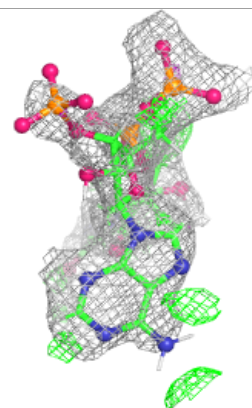
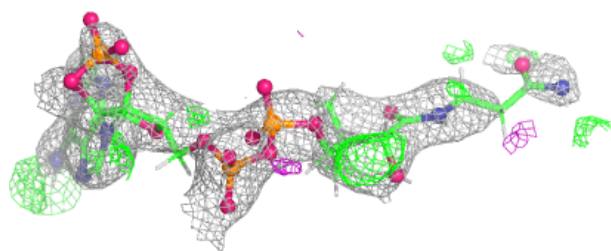
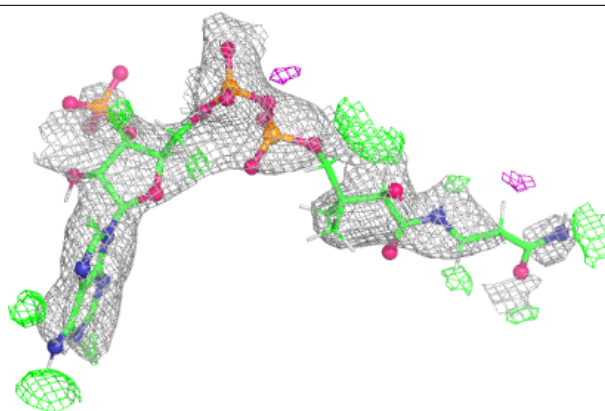
Electron density around PO4 A 402:

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

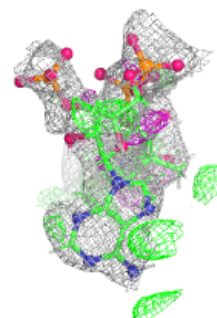
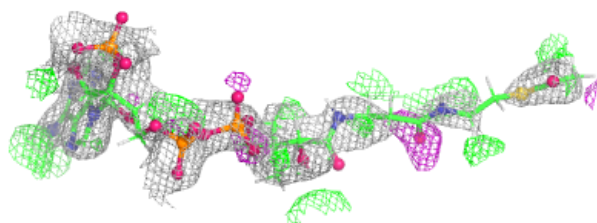
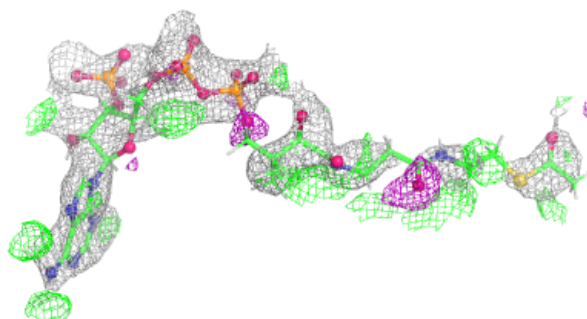


Electron density around ACO D 401:

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

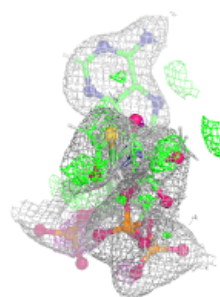
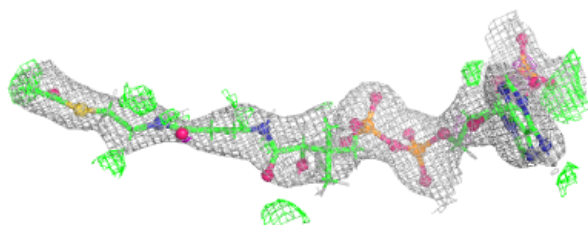
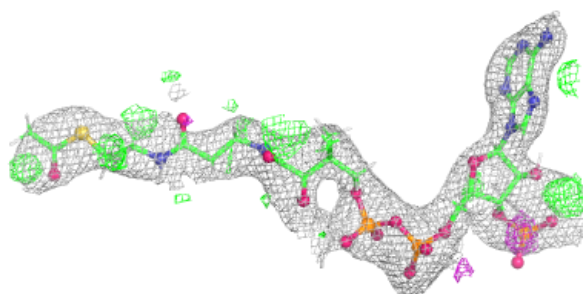
**Electron density around ACO B 401:**

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

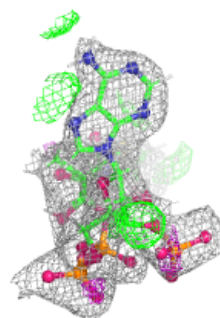
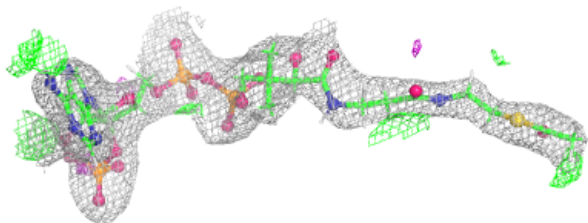
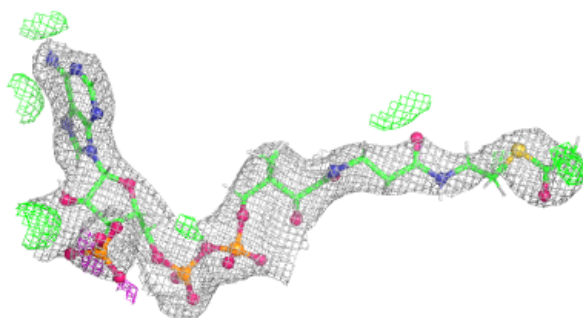


Electron density around ACO C 401:

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

**Electron density around ACO A 401:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.