



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:02 AM UTC

PDB ID : 4PZF / pdb_00004pzf
Title : Berberine bridge enzyme G164A variant, a reticuline dehydrogenase
Authors : Zafred, D.; Wallner, S.; Steiner, B.; Macheroux, P.
Deposited on : 2014-03-30
Resolution : 2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

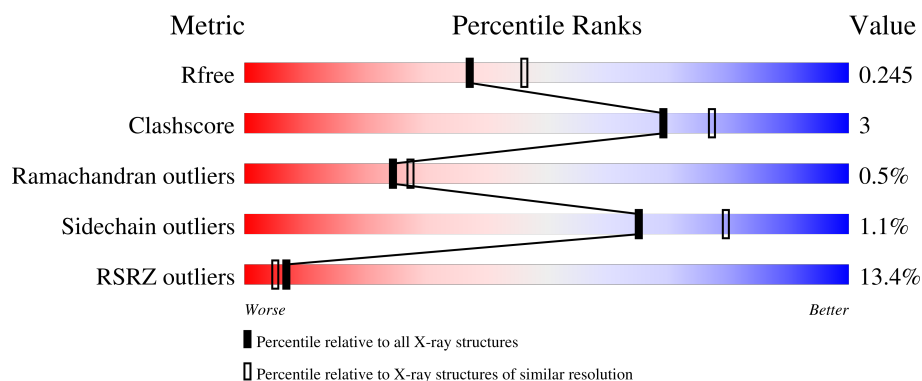
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	538	 6% 86% 6% 7%
1	B	538	 13% 84% 8% 7%
1	C	538	 14% 80% 11% 8%
1	D	538	 17% 84% 8% 8%
2	E	2	 100%

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Mol	Chain	Length	Quality of chain
2	F	2	 100%
2	G	2	 100%
2	H	2	 50% 50%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	SO4	B	605	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 16476 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 Reticuline oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	498	Total	C	N	O	S	0	0	0
			3935	2531	653	738	13			
1	B	498	Total	C	N	O	S	0	0	0
			3935	2531	654	737	13			
1	C	496	Total	C	N	O	S	0	0	0
			3916	2518	651	734	13			
1	D	497	Total	C	N	O	S	0	0	0
			3927	2527	652	735	13			

There are 12 discrepancies between the modelled and reference sequences:

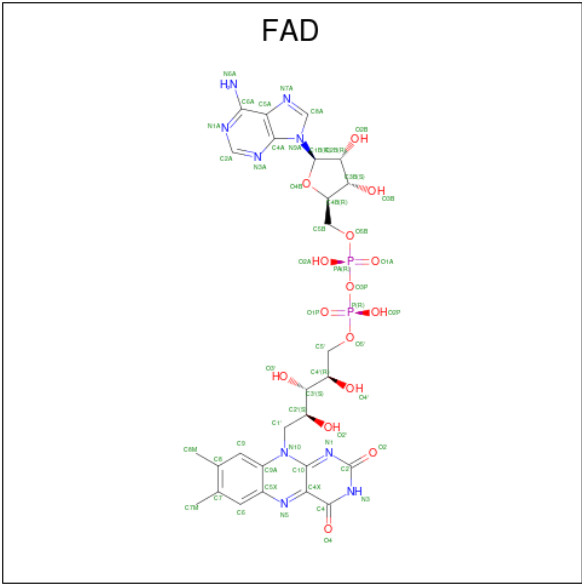
Chain	Residue	Modelled	Actual	Comment	Reference
A	22	GLU	LEU	SEE REMARK 999	UNP P30986
A	23	ALA	GLY	SEE REMARK 999	UNP P30986
A	164	ALA	GLY	engineered mutation	UNP P30986
B	22	GLU	LEU	SEE REMARK 999	UNP P30986
B	23	ALA	GLY	SEE REMARK 999	UNP P30986
B	164	ALA	GLY	engineered mutation	UNP P30986
C	22	GLU	LEU	SEE REMARK 999	UNP P30986
C	23	ALA	GLY	SEE REMARK 999	UNP P30986
C	164	ALA	GLY	engineered mutation	UNP P30986
D	22	GLU	LEU	SEE REMARK 999	UNP P30986
D	23	ALA	GLY	SEE REMARK 999	UNP P30986
D	164	ALA	GLY	engineered mutation	UNP P30986

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	H	2	Total	C	N	O	0	0	0
			28	16	2	10			

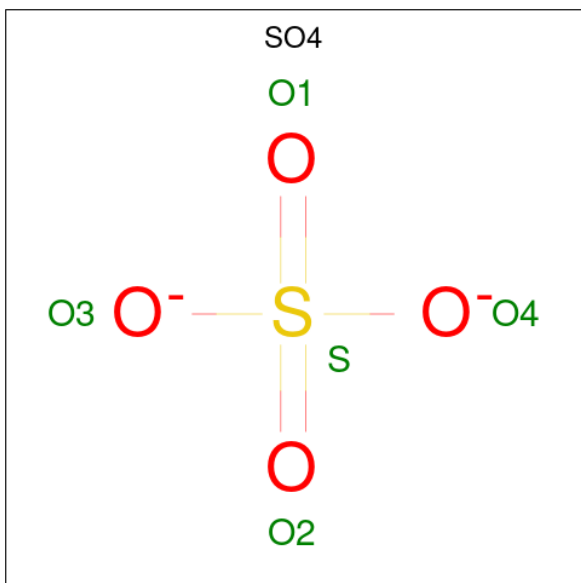
- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).





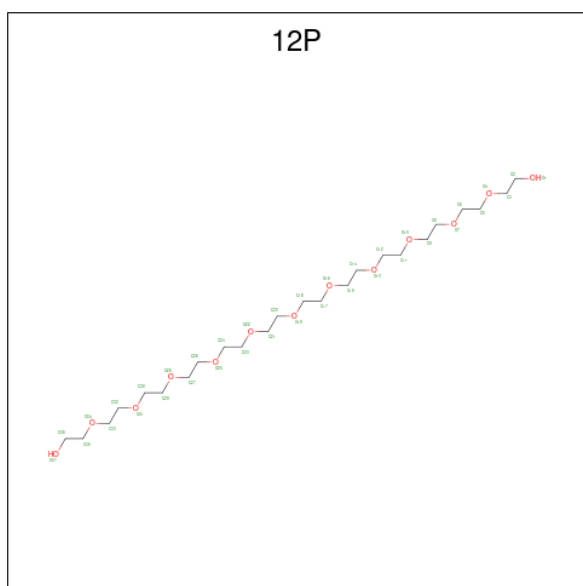
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total O S 5 4 1	0	0
5	C	1	Total O S 5 4 1	0	0
5	C	1	Total O S 5 4 1	0	0
5	D	1	Total O S 5 4 1	0	0
5	D	1	Total O S 5 4 1	0	0

- Molecule 6 is DODECAETHYLENE GLYCOL (CCD ID: 12P) (formula: $C_{24}H_{50}O_{13}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total C O 28 18 10	0	0
6	D	1	Total C O 22 14 8	0	0

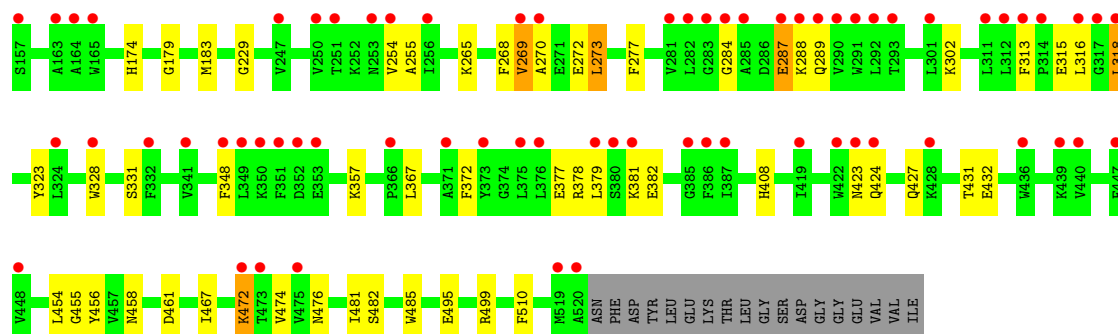
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	105	Total O 105 105	0	0
7	B	71	Total O 71 71	0	0
7	C	72	Total O 72 72	0	0

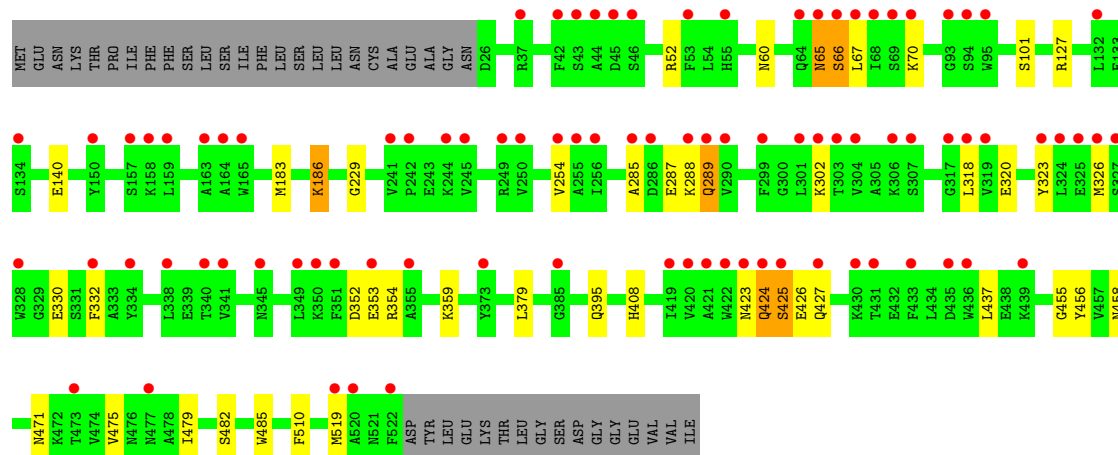
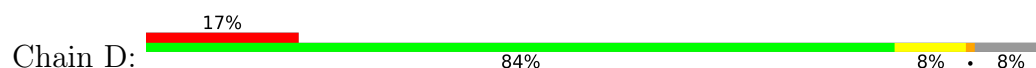
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	60	Total	O	0	0
			60	60		



• Molecule 1: Reticuline oxidase



• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



MAG2

- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:  50% 50%

MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	80.82Å 175.44Å 195.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.38 – 2.20 47.38 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.9 (47.38-2.20) 99.0 (47.38-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.96 (at 1.50Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.220 , 0.242 0.224 , 0.245	Depositor DCC
R_{free} test set	13609 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	33.7	Xtriage
Anisotropy	0.406	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 35.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16476	wwPDB-VP
Average B, all atoms (Å ²)	53.0	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 32.00 % 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 1.0087e-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: NAG, SO4, 12P, FAD

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	0.31	0/4033	0.72	1/5465 (0.0%)
1	B	0.31	0/4033	0.70	0/5465
1	C	0.32	0/4013	0.72	2/5438 (0.0%)
1	D	0.31	0/4025	0.73	3/5454 (0.1%)
All	All	0.31	0/16104	0.72	6/21822 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	65	ASN	N-CA-C	5.39	117.25	108.63
1	D	60	ASN	CA-C-N	5.19	126.33	119.84
1	D	60	ASN	C-N-CA	5.19	126.33	119.84
1	C	382	GLU	CA-C-N	5.01	124.67	119.56
1	C	382	GLU	C-N-CA	5.01	124.67	119.56
1	A	491	LEU	CB-CA-C	-5.00	110.79	116.54

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	3935	0	3861	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3935	0	3863	30	0
1	C	3916	0	3848	39	1
1	D	3927	0	3857	24	0
2	E	28	0	25	0	0
2	F	28	0	25	0	0
2	G	28	0	25	0	0
2	H	28	0	25	1	0
3	A	53	0	29	1	0
3	B	53	0	29	0	0
3	C	53	0	29	1	0
3	D	53	0	28	2	0
4	A	14	0	13	0	0
4	B	14	0	13	0	0
4	C	14	0	13	0	0
4	D	14	0	13	0	0
5	B	5	0	0	3	0
5	C	10	0	0	0	0
5	D	10	0	0	0	0
6	C	28	0	37	1	0
6	D	22	0	29	1	0
7	A	105	0	0	1	0
7	B	71	0	0	0	0
7	C	72	0	0	0	0
7	D	60	0	0	0	0
All	All	16476	0	15762	111	1

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 3.

All (111) 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:483:ARG:NH2	1:B:495:GLU:OE2	2.11	0.83
1:D:52:ARG:NH2	2:H:2:NAG:O7	2.19	0.76
1:D:65:ASN:O	1:D:67:LEU:N	2.25	0.69
1:D:424:GLN:O	1:D:426:GLU:N	2.24	0.68
1:C:287:GLU:O	1:C:289:GLN:N	2.25	0.68
1:C:316:LEU:HB3	1:C:318:LEU:HD12	1.77	0.66
1:B:302:LYS:HE2	1:B:320:GLU:HG3	1.81	0.62
1:C:472:LYS:HE2	1:C:476:ASN:HD21	1.65	0.62
1:B:37:ARG:NH1	5:B:605:SO4:O4	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:472:LYS:O	1:C:476:ASN:ND2	2.32	0.62
1:D:66:SER:HA	1:D:70:LYS:HE2	1.83	0.61
1:C:269:VAL:HG12	1:C:273:LEU:HD11	1.84	0.59
1:C:357:LYS:NZ	1:C:461:ASP:OD1	2.36	0.59
1:C:287:GLU:C	1:C:289:GLN:H	2.10	0.59
1:D:352:ASP:OD1	1:D:353:GLU:N	2.36	0.58
1:B:288:LYS:H	1:B:380:SER:HB3	1.70	0.57
1:B:25:ASN:N	1:B:25:ASN:OD1	2.36	0.57
1:C:378:ARG:HA	1:C:381:LYS:HE2	1.86	0.56
1:D:359:LYS:HG3	1:D:437:LEU:HD21	1.87	0.55
1:B:483:ARG:HG3	1:B:487:GLU:HG3	1.88	0.55
1:D:302:LYS:HD3	1:D:323:TYR:HB2	1.89	0.55
1:C:265:LYS:NZ	1:C:315:GLU:OE1	2.38	0.55
1:A:321:GLU:OE1	1:A:321:GLU:N	2.41	0.54
1:C:273:LEU:HD22	1:C:277:PHE:HB3	1.89	0.53
1:D:254:VAL:O	1:D:289:GLN:HG3	2.07	0.53
1:B:34:ASN:OD1	1:B:88:ARG:NH2	2.42	0.53
1:D:186:LYS:O	1:D:395:GLN:HG3	2.10	0.51
1:C:367:LEU:HB2	1:C:372:PHE:CE2	2.46	0.51
1:D:482:SER:HA	1:D:485:TRP:CZ2	2.45	0.51
1:A:377:GLU:O	1:A:380:SER:OG	2.27	0.51
1:B:285:ALA:HB2	1:B:290:VAL:HG13	1.93	0.51
1:C:456:TYR:CZ	1:C:458:ASN:HB2	2.46	0.50
1:D:479:ILE:HD11	1:D:519:MET:HA	1.92	0.50
1:D:456:TYR:CZ	1:D:458:ASN:HB2	2.46	0.50
1:B:456:TYR:CZ	1:B:458:ASN:HB2	2.46	0.49
1:B:375:LEU:HB2	1:B:444:MET:HE2	1.94	0.49
1:A:229:GLY:HA2	1:A:510:PHE:CE2	2.47	0.49
1:C:423:ASN:OD1	1:C:424:GLN:N	2.39	0.49
1:D:302:LYS:HD2	1:D:320:GLU:HG3	1.95	0.49
1:C:472:LYS:HG2	1:C:476:ASN:HD21	1.78	0.49
1:D:127:ARG:NH1	1:D:140:GLU:OE1	2.46	0.49
1:D:229:GLY:HA2	1:D:510:PHE:CE2	2.48	0.49
1:B:229:GLY:HA2	1:B:510:PHE:CE2	2.48	0.48
1:B:287:GLU:C	1:B:289:GLN:H	2.21	0.48
1:C:183:MET:HE1	1:C:328:TRP:CD1	2.48	0.48
1:D:352:ASP:OD2	1:D:354:ARG:NH2	2.43	0.48
1:B:408:HIS:HE1	1:B:455:GLY:O	1.97	0.48
1:B:138:TRP:HB3	6:D:605:12P:H172	1.96	0.48
1:B:267:GLN:HB2	1:B:414:LEU:HD11	1.96	0.47
1:A:63:PHE:HA	1:A:68:ILE:HD13	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:282:LEU:HB3	1:B:283:GLY:H	1.60	0.47
1:C:127:ARG:NH1	1:C:140:GLU:OE1	2.46	0.47
1:C:268:PHE:O	1:C:270:ALA:N	2.48	0.47
1:C:467:ILE:HG12	1:C:485:TRP:HZ2	1.79	0.47
1:A:328:TRP:O	1:A:331:SER:OG	2.28	0.47
1:B:282:LEU:O	1:B:387:ILE:HG13	2.14	0.47
1:C:90:ILE:HG23	1:C:95:TRP:HB2	1.96	0.46
1:C:302:LYS:HD2	1:C:323:TYR:O	2.15	0.46
1:C:254:VAL:HG12	1:C:255:ALA:O	2.14	0.46
1:D:354:ARG:HG2	1:D:423:ASN:N	2.30	0.46
1:D:408:HIS:HE1	1:D:455:GLY:O	1.99	0.46
1:B:283:GLY:HA2	1:B:291:TRP:O	2.16	0.45
1:C:65:ASN:OD1	1:C:67:LEU:HB2	2.16	0.45
1:C:269:VAL:O	1:C:272:GLU:N	2.45	0.45
1:B:321:GLU:OE1	1:B:321:GLU:N	2.38	0.45
1:C:284:GLY:HA2	1:C:379:LEU:HD22	1.98	0.45
1:C:482:SER:HA	1:C:485:TRP:CZ2	2.52	0.45
1:D:318:LEU:HB3	1:D:323:TYR:HE2	1.82	0.45
1:A:357:LYS:HD2	7:A:766:HOH:O	2.17	0.45
1:A:456:TYR:CZ	1:A:458:ASN:HB2	2.52	0.45
1:C:408:HIS:HE1	1:C:455:GLY:O	2.00	0.45
1:A:352:ASP:OD1	1:A:353:GLU:N	2.50	0.45
1:C:138:TRP:CG	6:C:605:12P:H171	2.52	0.45
1:C:229:GLY:HA2	1:C:510:PHE:CE2	2.51	0.45
1:A:252:LYS:NZ	1:A:316:LEU:O	2.50	0.45
1:D:183:MET:HG3	1:D:332:PHE:HZ	1.81	0.44
1:C:424:GLN:O	1:C:427:GLN:HB2	2.18	0.44
1:B:420:VAL:HG21	1:B:433:PHE:HB3	2.00	0.44
1:B:288:LYS:H	1:B:380:SER:CB	2.30	0.44
1:B:482:SER:HA	1:B:485:TRP:CZ2	2.53	0.44
1:C:270:ALA:HA	1:C:273:LEU:HD12	2.00	0.44
1:A:101:SER:HB3	3:A:601:FAD:O1P	2.18	0.43
1:C:269:VAL:C	1:C:273:LEU:HD12	2.43	0.43
1:C:474:VAL:HG13	1:C:481:ILE:HD12	1.99	0.43
1:D:471:ASN:O	1:D:475:VAL:HG23	2.18	0.43
1:B:185:ARG:NH1	1:B:277:PHE:O	2.51	0.43
1:D:101:SER:HB3	3:D:601:FAD:O1P	2.18	0.43
1:A:408:HIS:HE1	1:A:455:GLY:O	2.02	0.43
1:B:37:ARG:NH1	5:B:605:SO4:S	2.72	0.42
1:A:174:HIS:CE1	1:A:179:GLY:HA2	2.54	0.42
1:A:471:ASN:O	1:A:475:VAL:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:113:SER:HB3	1:C:117:PHE:CD2	2.55	0.42
1:C:174:HIS:CE1	1:C:179:GLY:HA2	2.54	0.42
1:D:285:ALA:HB2	1:D:379:LEU:O	2.19	0.42
1:B:37:ARG:NH2	5:B:605:SO4:O1	2.47	0.42
1:C:50:PHE:CE1	1:C:74:ILE:HG13	2.54	0.42
1:B:25:ASN:HB2	1:B:26:ASP:H	1.57	0.42
1:C:313:PHE:CD1	1:C:316:LEU:HG	2.54	0.42
1:A:113:SER:HB3	1:A:117:PHE:CD2	2.55	0.41
1:B:352:ASP:CG	1:B:354:ARG:HH21	2.28	0.41
1:C:408:HIS:CD2	1:C:454:LEU:HD13	2.56	0.41
1:A:59:GLN:HG3	1:A:104:HIS:CD2	2.56	0.41
1:B:231:ILE:HG21	1:B:234:TRP:CE2	2.56	0.41
1:C:56:LEU:HG	1:C:348:PHE:CE1	2.56	0.41
1:A:516:ILE:HA	1:A:517:PRO:HD3	1.87	0.41
1:B:107:GLU:HB2	1:B:109:LEU:HG	2.03	0.41
1:B:287:GLU:O	1:B:289:GLN:N	2.53	0.40
3:C:601:FAD:H9	3:C:601:FAD:H1'2	1.86	0.40
1:D:326:MET:HB2	1:D:330:GLU:HB2	2.02	0.40
3:D:601:FAD:H9	3:D:601:FAD:H1'2	1.86	0.40
1:C:328:TRP:O	1:C:331:SER:OG	2.31	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:495:GLU:OE1	1:C:499:ARG:NH1[3_556]	2.18	0.02

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	496/538 (92%)	475 (96%)	19 (4%)	2 (0%)	30 34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	496/538 (92%)	468 (94%)	27 (5%)	1 (0%)	43	51
1	C	494/538 (92%)	469 (95%)	22 (4%)	3 (1%)	21	23
1	D	495/538 (92%)	467 (94%)	24 (5%)	4 (1%)	16	16
All	All	1981/2152 (92%)	1879 (95%)	92 (5%)	10 (0%)	24	27

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	68	ILE
1	B	288	LYS
1	C	288	LYS
1	D	66	SER
1	D	424	GLN
1	A	67	LEU
1	C	269	VAL
1	C	287	GLU
1	D	425	SER
1	D	287	GLU

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	426/460 (93%)	424 (100%)	2 (0%)	81	90
1	B	426/460 (93%)	421 (99%)	5 (1%)	63	78
1	C	424/460 (92%)	417 (98%)	7 (2%)	53	69
1	D	425/460 (92%)	420 (99%)	5 (1%)	63	78
All	All	1701/1840 (92%)	1682 (99%)	19 (1%)	65	79

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	155	SER

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Mol	Chain	Res	Type
1	A	311	LEU
1	B	25	ASN
1	B	282	LEU
1	B	313	PHE
1	B	425	SER
1	B	426	GLU
1	C	67	LEU
1	C	273	LEU
1	C	318	LEU
1	C	377	GLU
1	C	431	THR
1	C	432	GLU
1	C	472	LYS
1	D	186	LYS
1	D	288	LYS
1	D	289	GLN
1	D	425	SER
1	D	427	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	HIS
1	A	346	ASN
1	A	408	HIS
1	A	476	ASN
1	B	25	ASN
1	B	253	ASN
1	B	408	HIS
1	C	55	HIS
1	C	203	ASN
1	C	408	HIS
1	C	476	ASN
1	D	210	GLN
1	D	408	HIS
1	D	476	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 ⓘ

8 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	NAG	E	1	2,1	14,14,15	0.29	0	17,19,21	0.43	0
2	NAG	E	2	2	14,14,15	0.41	0	17,19,21	0.38	0
2	NAG	F	1	2,1	14,14,15	0.35	0	17,19,21	0.40	0
2	NAG	F	2	2	14,14,15	0.22	0	17,19,21	0.43	0
2	NAG	G	1	2,1	14,14,15	0.38	0	17,19,21	0.46	0
2	NAG	G	2	2	14,14,15	0.29	0	17,19,21	0.35	0
2	NAG	H	1	2,1	14,14,15	0.43	0	17,19,21	0.39	0
2	NAG	H	2	2	14,14,15	0.22	0	17,19,21	0.42	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	NAG	E	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	NAG	F	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	2/6/23/26	0/1/1/1
2	NAG	G	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	G	2	2	-	1/6/23/26	0/1/1/1
2	NAG	H	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	H	2	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

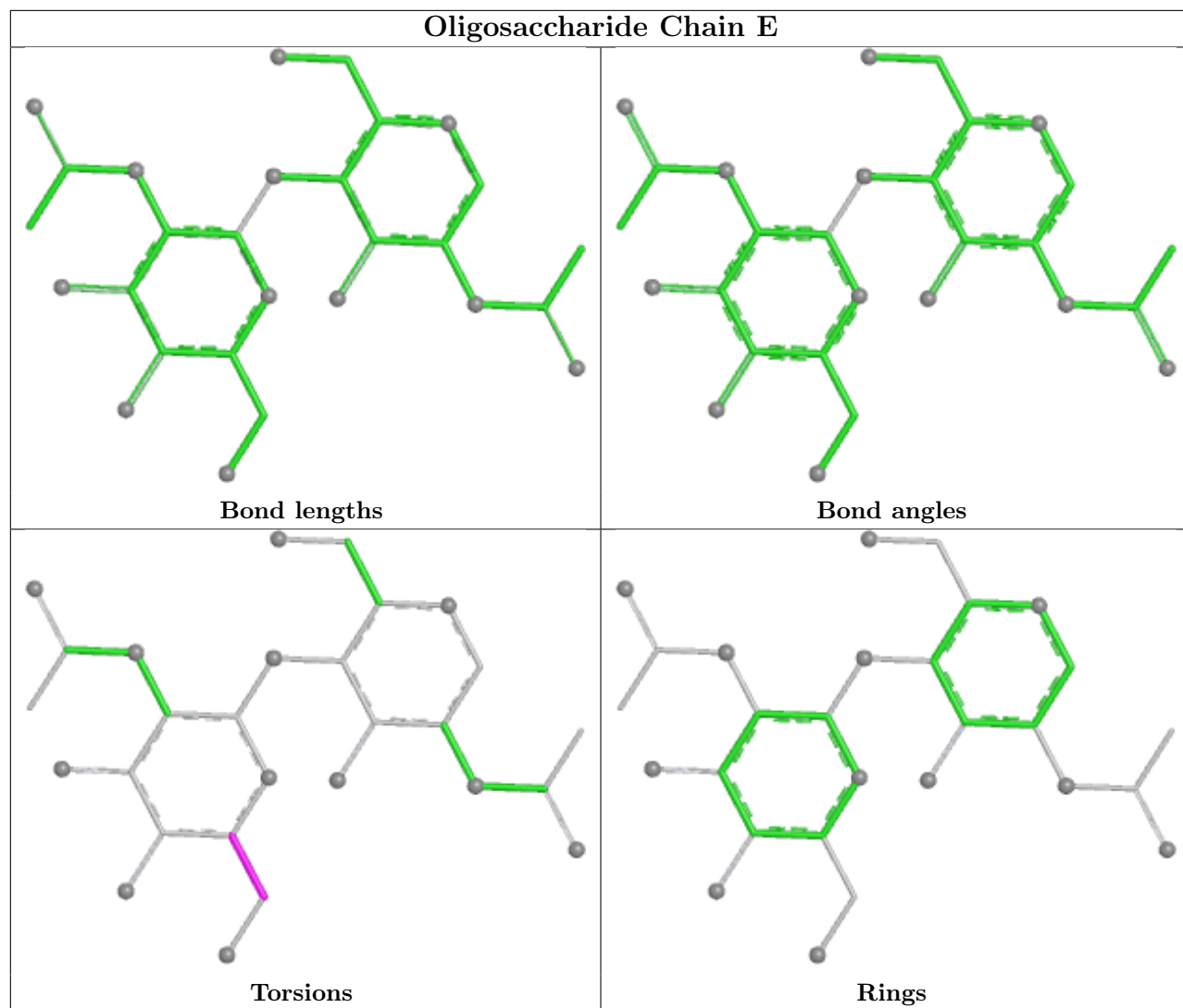
Mol	Chain	Res	Type	Atoms
2	E	2	NAG	O5-C5-C6-O6
2	F	2	NAG	O5-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
2	F	2	NAG	C4-C5-C6-O6
2	G	2	NAG	O5-C5-C6-O6
2	H	1	NAG	C4-C5-C6-O6

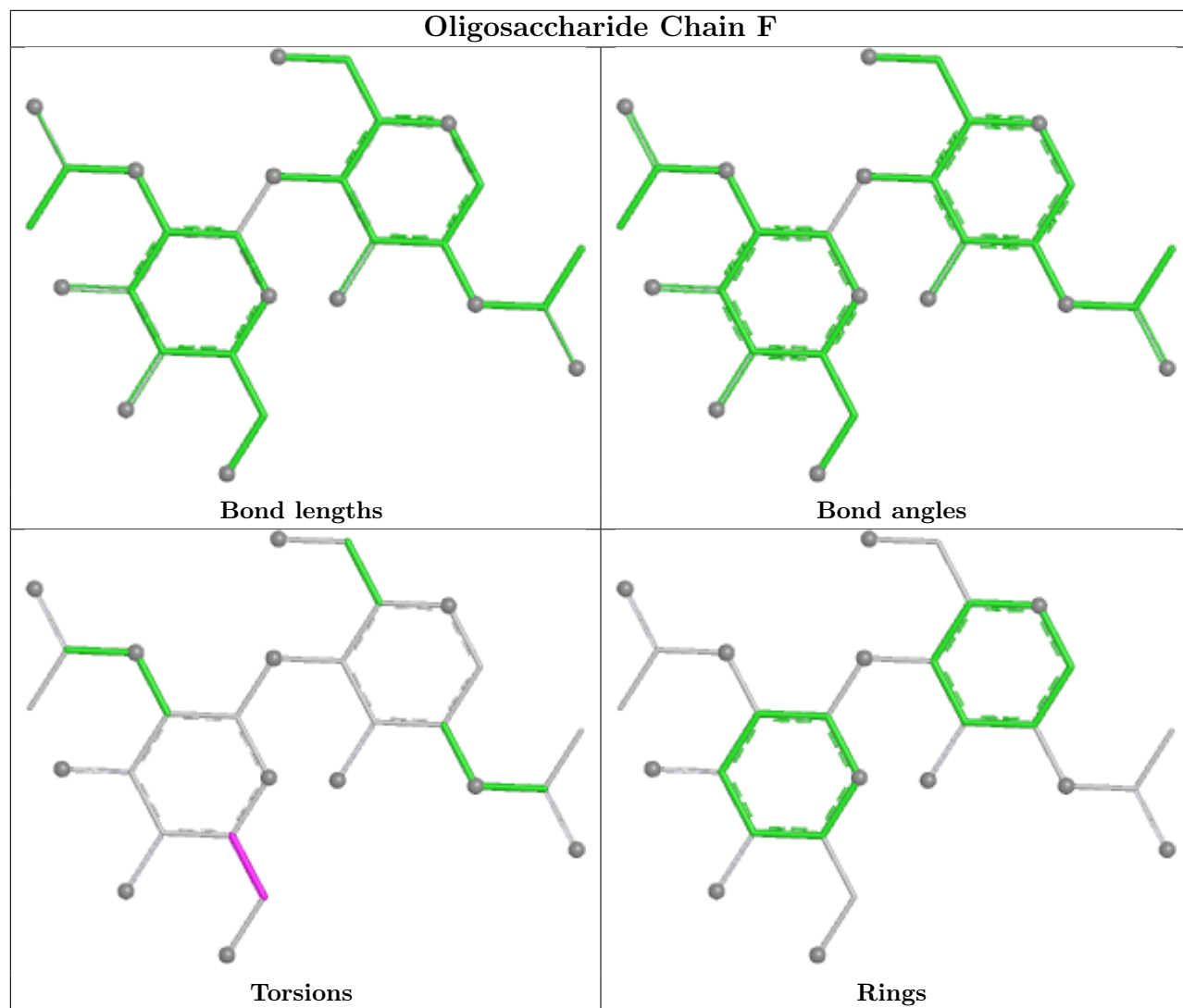
There are no ring outliers.

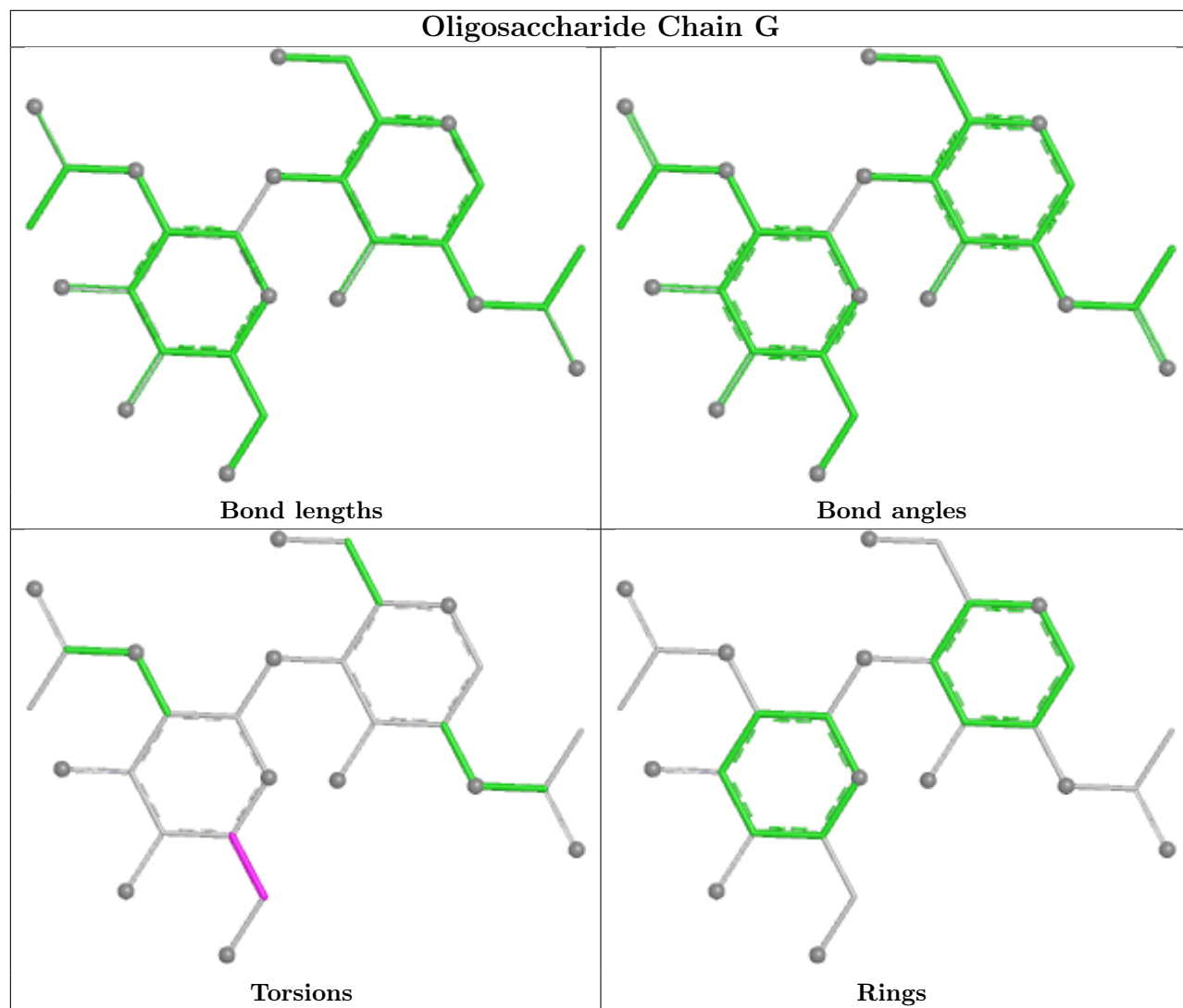
1 monomer is involved in 1 short contact:

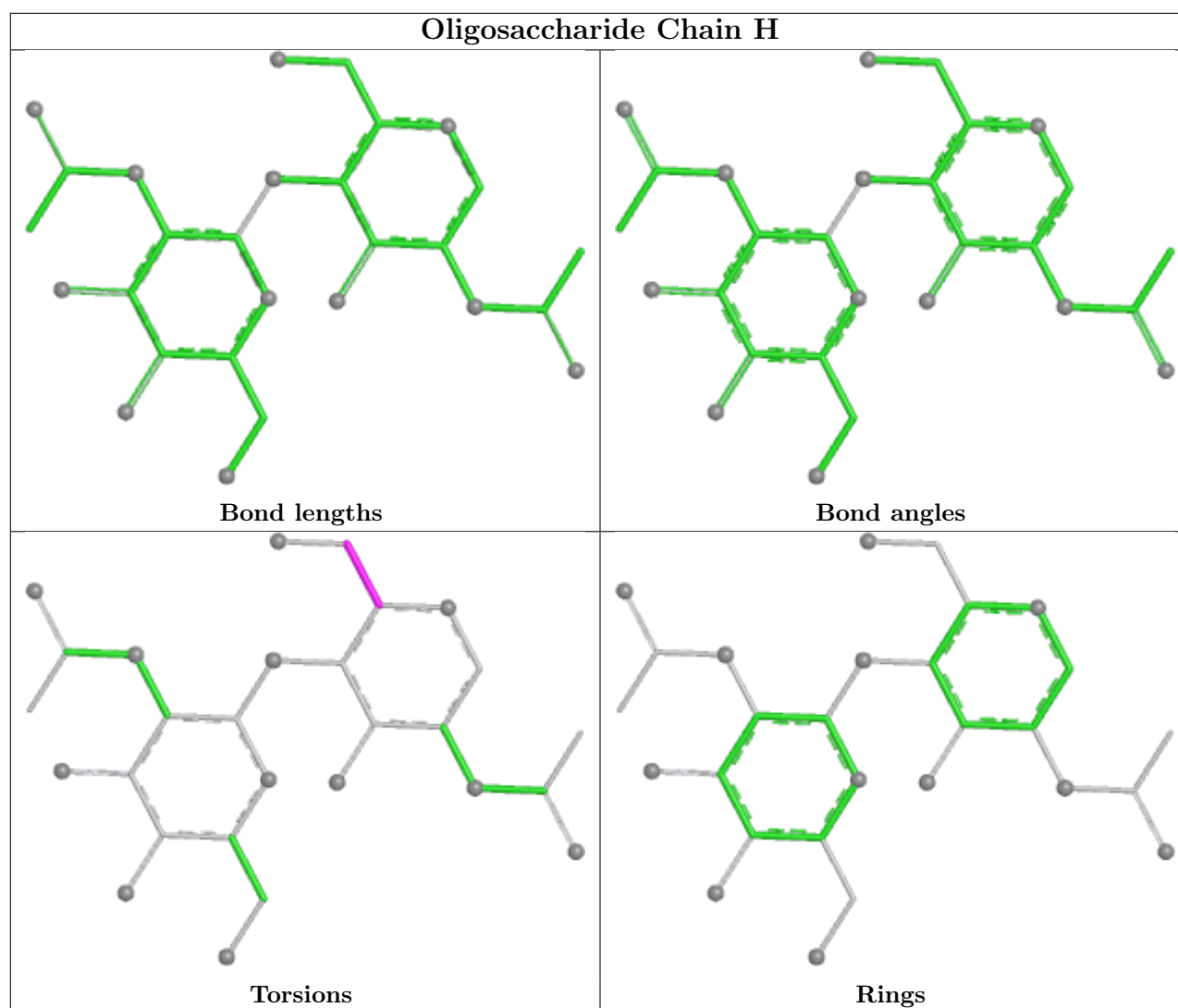
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	2	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.









5.6 Ligand geometry [i](#)

15 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	$\# Z > 2$
6	12P	C	605	-	27,27,36	0.40	0	26,26,35	0.62	0
5	SO4	C	607	-	4,4,4	0.25	0	6,6,6	0.09	0
5	SO4	D	606	-	4,4,4	0.24	0	6,6,6	0.10	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	FAD	D	601	1	58,58,58	1.47	8 (13%)	85,89,89	1.58	14 (16%)
5	SO4	C	606	-	4,4,4	0.25	0	6,6,6	0.08	0
4	NAG	A	604	1	14,14,15	0.20	0	17,19,21	0.47	0
4	NAG	C	604	1	14,14,15	0.42	0	17,19,21	0.42	0
4	NAG	D	604	1	14,14,15	0.22	0	17,19,21	0.42	0
4	NAG	B	604	1	14,14,15	0.31	0	17,19,21	0.37	0
3	FAD	B	601	1	58,58,58	1.46	8 (13%)	85,89,89	1.55	14 (16%)
3	FAD	C	601	1	58,58,58	1.47	9 (15%)	85,89,89	1.55	13 (15%)
3	FAD	A	601	1	58,58,58	1.47	8 (13%)	85,89,89	1.56	14 (16%)
6	12P	D	605	-	21,21,36	0.42	0	20,20,35	0.47	0
5	SO4	B	605	-	4,4,4	0.23	0	6,6,6	0.08	0
5	SO4	D	607	-	4,4,4	0.23	0	6,6,6	0.08	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FAD	D	601	1	-	5/34/50/50	0/6/6/6
4	NAG	A	604	1	-	2/6/23/26	0/1/1/1
4	NAG	C	604	1	-	2/6/23/26	0/1/1/1
4	NAG	D	604	1	-	2/6/23/26	0/1/1/1
4	NAG	B	604	1	-	0/6/23/26	0/1/1/1
3	FAD	B	601	1	-	3/34/50/50	0/6/6/6
3	FAD	C	601	1	-	0/34/50/50	0/6/6/6
3	FAD	A	601	1	-	5/34/50/50	0/6/6/6
6	12P	D	605	-	-	8/19/19/34	-
6	12P	C	605	-	-	15/25/25/34	-

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	601	FAD	C9A-C5X	5.29	1.49	1.41
3	A	601	FAD	C9A-C5X	5.28	1.49	1.41
3	B	601	FAD	C9A-C5X	5.25	1.49	1.41
3	C	601	FAD	C9A-C5X	5.21	1.49	1.41
3	C	601	FAD	C5A-C4A	4.76	1.47	1.39
3	A	601	FAD	C5A-C4A	4.70	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	601	FAD	C5A-C4A	4.68	1.47	1.39
3	B	601	FAD	C5A-C4A	4.57	1.47	1.39
3	A	601	FAD	C8-C7	3.49	1.49	1.40
3	B	601	FAD	C8-C7	3.42	1.49	1.40
3	C	601	FAD	C8-C7	3.40	1.49	1.40
3	D	601	FAD	C8-C7	3.38	1.49	1.40
3	A	601	FAD	C5X-N5	-2.84	1.34	1.39
3	B	601	FAD	C5A-C6A	2.81	1.48	1.41
3	D	601	FAD	C5A-C6A	2.80	1.48	1.41
3	B	601	FAD	C5X-N5	-2.79	1.34	1.39
3	C	601	FAD	C5A-C6A	2.77	1.48	1.41
3	C	601	FAD	C5X-N5	-2.75	1.34	1.39
3	A	601	FAD	C5A-C6A	2.72	1.48	1.41
3	D	601	FAD	C5X-N5	-2.61	1.34	1.39
3	C	601	FAD	C4-N3	-2.52	1.34	1.38
3	C	601	FAD	C8A-N7A	2.50	1.36	1.31
3	B	601	FAD	C4-N3	-2.48	1.34	1.38
3	D	601	FAD	C4-N3	-2.44	1.34	1.38
3	D	601	FAD	C8A-N7A	2.41	1.36	1.31
3	A	601	FAD	C8A-N7A	2.37	1.36	1.31
3	B	601	FAD	C8A-N7A	2.35	1.36	1.31
3	A	601	FAD	C4-N3	-2.33	1.34	1.38
3	B	601	FAD	C4A-N9A	-2.21	1.33	1.37
3	A	601	FAD	C5A-N7A	-2.09	1.35	1.39
3	D	601	FAD	C4A-N9A	-2.06	1.33	1.37
3	C	601	FAD	C5A-N7A	-2.06	1.35	1.39
3	C	601	FAD	C4A-N9A	-2.05	1.33	1.37

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	FAD	C5A-C4A-N3A	-5.86	118.64	126.72
3	D	601	FAD	C5A-C4A-N3A	-5.81	118.72	126.72
3	C	601	FAD	C5A-C4A-N3A	-5.50	119.14	126.72
3	B	601	FAD	C5A-C4A-N3A	-5.23	119.51	126.72
3	A	601	FAD	N3A-C4A-N9A	4.54	134.89	127.17
3	D	601	FAD	N3A-C4A-N9A	4.39	134.64	127.17
3	B	601	FAD	N3A-C4A-N9A	4.09	134.12	127.17
3	C	601	FAD	N3A-C4A-N9A	4.05	134.06	127.17
3	C	601	FAD	C4A-C5A-N7A	-3.90	106.12	110.58
3	D	601	FAD	C4A-C5A-N7A	-3.79	106.25	110.58
3	D	601	FAD	C2A-N3A-C4A	3.70	120.86	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	FAD	C2A-N3A-C4A	3.68	120.81	111.83
3	A	601	FAD	C4A-C5A-N7A	-3.67	106.39	110.58
3	C	601	FAD	C2A-N3A-C4A	3.62	120.68	111.83
3	B	601	FAD	C2A-N3A-C4A	3.57	120.55	111.83
3	B	601	FAD	C4A-C5A-N7A	-3.54	106.54	110.58
3	B	601	FAD	N3A-C2A-N1A	-3.45	123.36	128.58
3	C	601	FAD	N3A-C2A-N1A	-3.29	123.60	128.58
3	D	601	FAD	N3A-C2A-N1A	-3.28	123.62	128.58
3	A	601	FAD	N3A-C2A-N1A	-3.16	123.80	128.58
3	B	601	FAD	C4A-N9A-C8A	3.05	108.94	105.74
3	D	601	FAD	C4-C4X-N5	3.00	122.35	118.21
3	A	601	FAD	C4-C4X-N5	2.92	122.24	118.21
3	B	601	FAD	C4-C4X-N5	2.80	122.08	118.21
3	A	601	FAD	C4A-N9A-C8A	2.80	108.68	105.74
3	D	601	FAD	C4A-N9A-C8A	2.78	108.66	105.74
3	C	601	FAD	C4-C4X-N5	2.71	121.95	118.21
3	C	601	FAD	C5A-N7A-C8A	2.66	107.63	103.45
3	C	601	FAD	C4A-N9A-C8A	2.64	108.51	105.74
3	A	601	FAD	C4'-C3'-C2'	-2.62	109.21	113.57
3	D	601	FAD	C5A-N7A-C8A	2.61	107.56	103.45
3	A	601	FAD	C5A-N7A-C8A	2.60	107.54	103.45
3	C	601	FAD	C6A-C5A-N7A	2.57	137.04	132.09
3	B	601	FAD	C4X-C10-N1	-2.50	118.46	124.59
3	B	601	FAD	C5A-N7A-C8A	2.49	107.37	103.45
3	B	601	FAD	C6A-C5A-N7A	2.48	136.87	132.09
3	C	601	FAD	C4X-C10-N1	-2.40	118.70	124.59
3	A	601	FAD	C4X-C10-N1	-2.34	118.85	124.59
3	D	601	FAD	C6A-C5A-N7A	2.31	136.54	132.09
3	D	601	FAD	C4X-C10-N1	-2.31	118.94	124.59
3	D	601	FAD	C4'-C3'-C2'	-2.30	109.74	113.57
3	B	601	FAD	C10-N1-C2	2.23	121.68	116.85
3	B	601	FAD	N9A-C8A-N7A	-2.22	110.78	113.94
3	A	601	FAD	C6A-C5A-N7A	2.22	136.37	132.09
3	D	601	FAD	O4-C4-C4X	-2.20	120.72	126.53
3	C	601	FAD	C10-N1-C2	2.19	121.60	116.85
3	A	601	FAD	O4-C4-C4X	-2.18	120.78	126.53
3	D	601	FAD	C10-N1-C2	2.17	121.54	116.85
3	C	601	FAD	O4-C4-C4X	-2.16	120.83	126.53
3	A	601	FAD	C10-N1-C2	2.15	121.51	116.85
3	D	601	FAD	N9A-C8A-N7A	-2.15	110.89	113.94
3	B	601	FAD	O4-C4-C4X	-2.15	120.87	126.53
3	B	601	FAD	C2A-N1A-C6A	2.12	122.21	118.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	FAD	N9A-C8A-N7A	-2.12	110.93	113.94
3	C	601	FAD	N9A-C8A-N7A	-2.11	110.94	113.94

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	605	12P	O25-C26-C27-O28
6	D	605	12P	O31-C32-C33-O34
6	C	605	12P	O22-C23-C24-O25
4	C	604	NAG	O5-C5-C6-O6
6	C	605	12P	O19-C20-C21-O22
4	C	604	NAG	C4-C5-C6-O6
3	A	601	FAD	O3'-C3'-C4'-O4'
3	A	601	FAD	O3'-C3'-C4'-C5'
3	D	601	FAD	O3'-C3'-C4'-O4'
4	A	604	NAG	C4-C5-C6-O6
6	D	605	12P	O25-C26-C27-O28
4	A	604	NAG	O5-C5-C6-O6
3	A	601	FAD	C2'-C3'-C4'-O4'
6	D	605	12P	O22-C23-C24-O25
3	D	601	FAD	C2'-C3'-C4'-O4'
6	C	605	12P	O16-C17-C18-O19
6	C	605	12P	O13-C14-C15-O16
3	A	601	FAD	C2'-C3'-C4'-C5'
3	D	601	FAD	C2'-C3'-C4'-C5'
6	C	605	12P	O31-C32-C33-O34
3	D	601	FAD	O3'-C3'-C4'-C5'
6	C	605	12P	O28-C29-C30-O31
4	D	604	NAG	C4-C5-C6-O6
6	C	605	12P	C24-C23-O22-C21
4	D	604	NAG	O5-C5-C6-O6
6	C	605	12P	C20-C21-O22-C23
6	D	605	12P	C29-C30-O31-C32
6	C	605	12P	C21-C20-O19-C18
6	D	605	12P	C36-C35-O34-C33
6	D	605	12P	C20-C21-O22-C23
6	C	605	12P	C11-C12-O13-C14
6	C	605	12P	C29-C30-O31-C32
3	B	601	FAD	O3'-C3'-C4'-O4'
6	C	605	12P	C15-C14-O13-C12
6	C	605	12P	C30-C29-O28-C27

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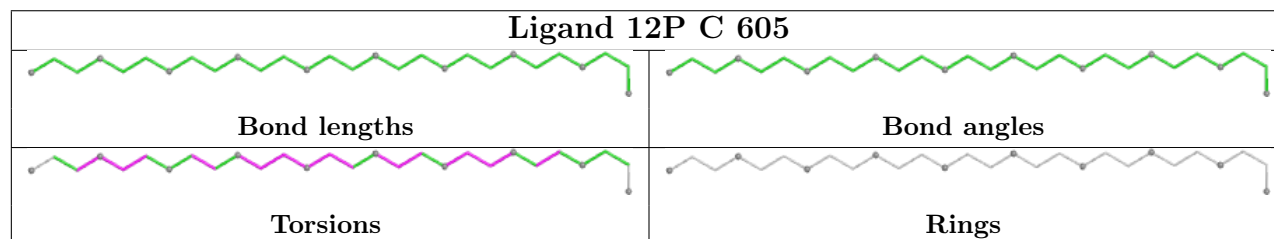
Mol	Chain	Res	Type	Atoms
6	C	605	12P	C27-C26-O25-C24
6	D	605	12P	C32-C33-O34-C35
3	B	601	FAD	C2'-C3'-C4'-O4'
6	D	605	12P	O19-C20-C21-O22
3	A	601	FAD	P-O3P-PA-O2A
3	B	601	FAD	PA-O3P-P-O2P
3	D	601	FAD	PA-O3P-P-O2P

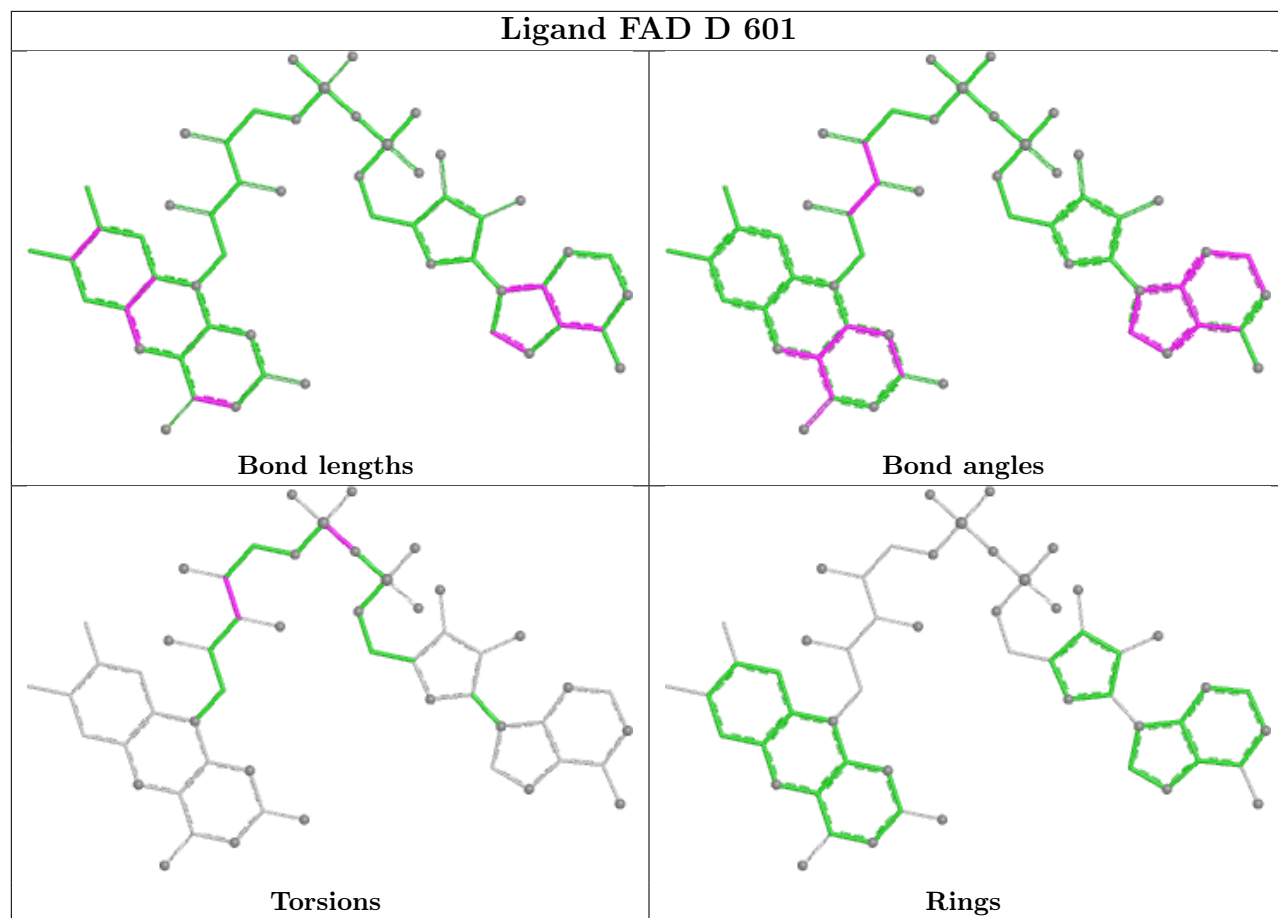
There are no ring outliers.

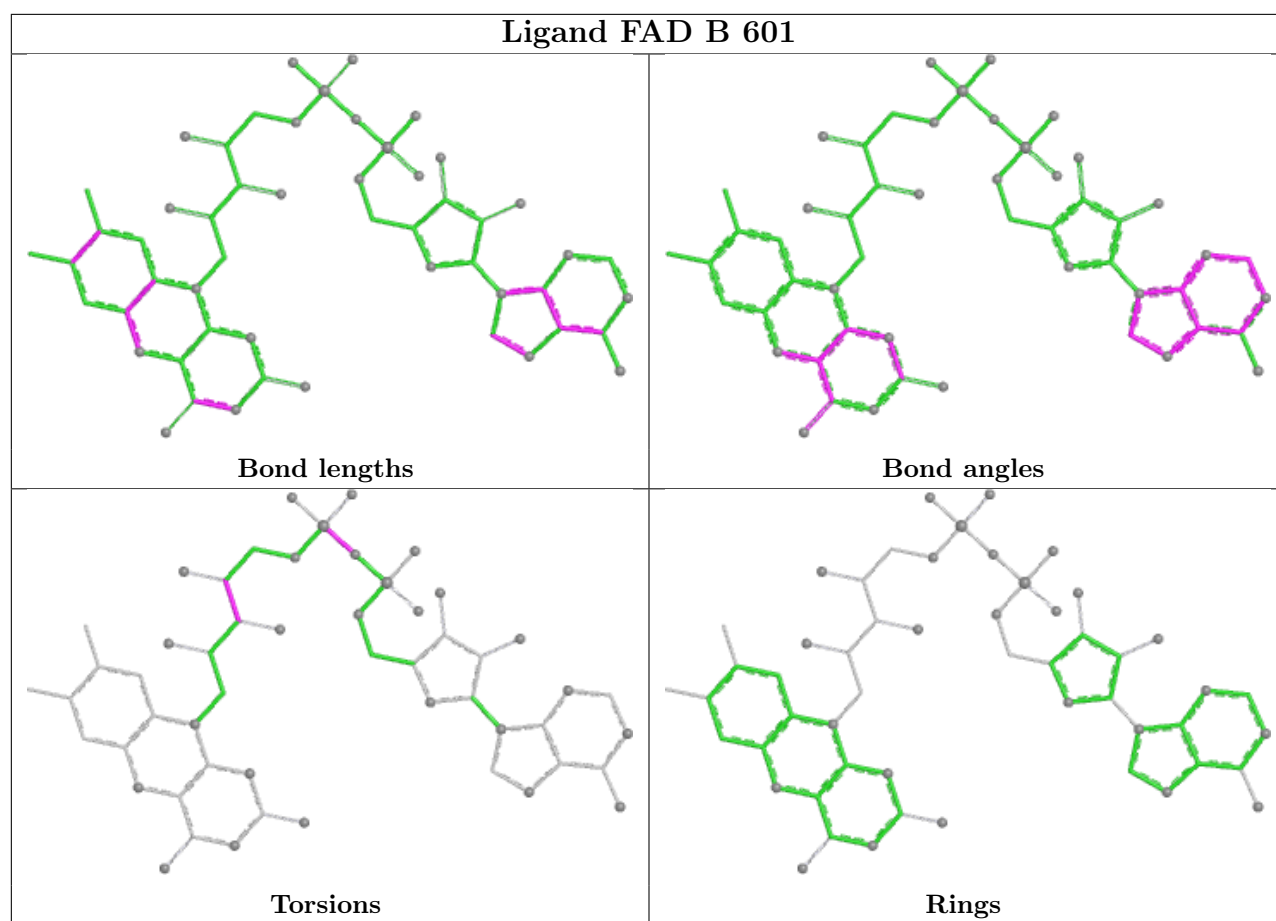
6 monomers are involved in 9 short contacts:

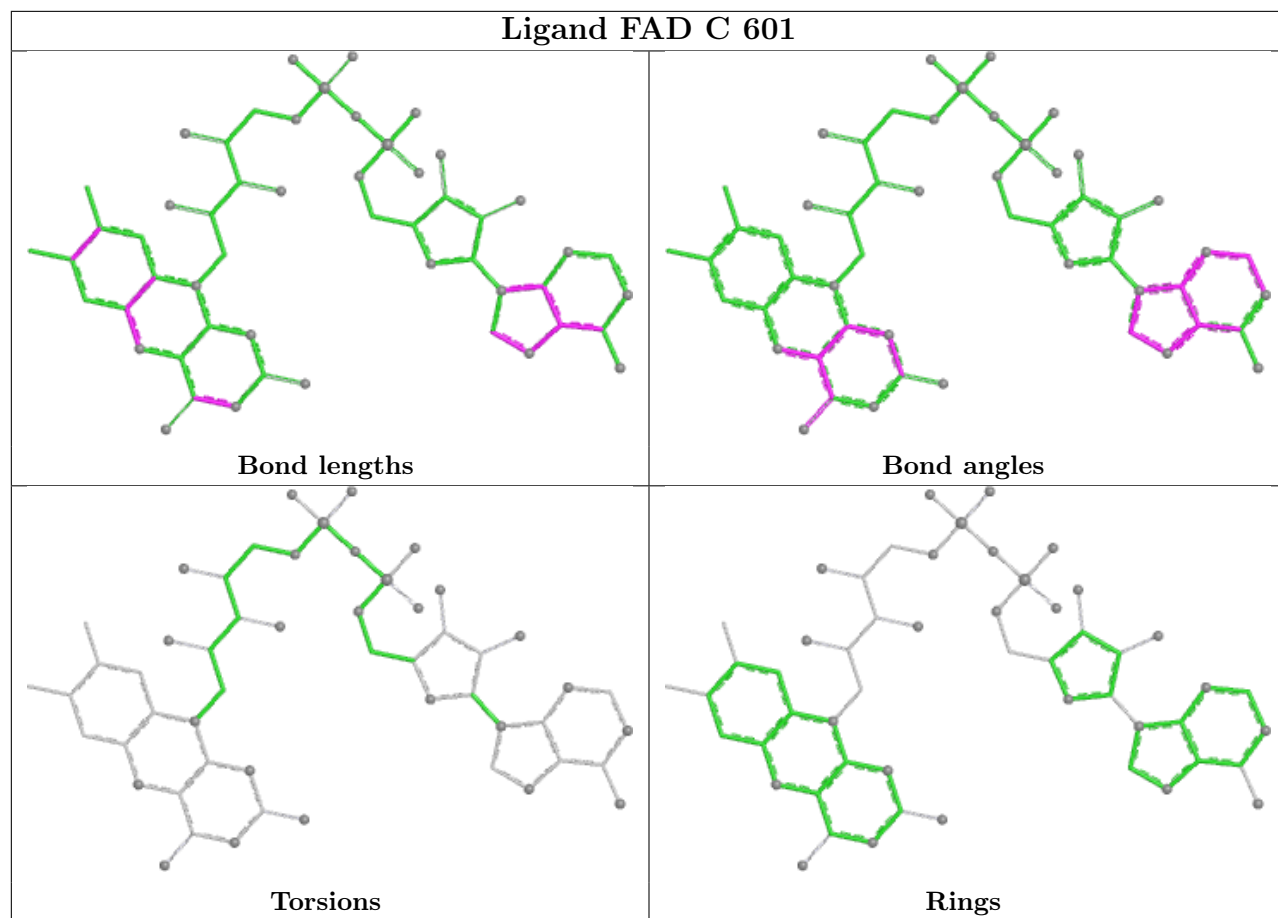
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	605	12P	1	0
3	D	601	FAD	2	0
3	C	601	FAD	1	0
3	A	601	FAD	1	0
6	D	605	12P	1	0
5	B	605	SO4	3	0

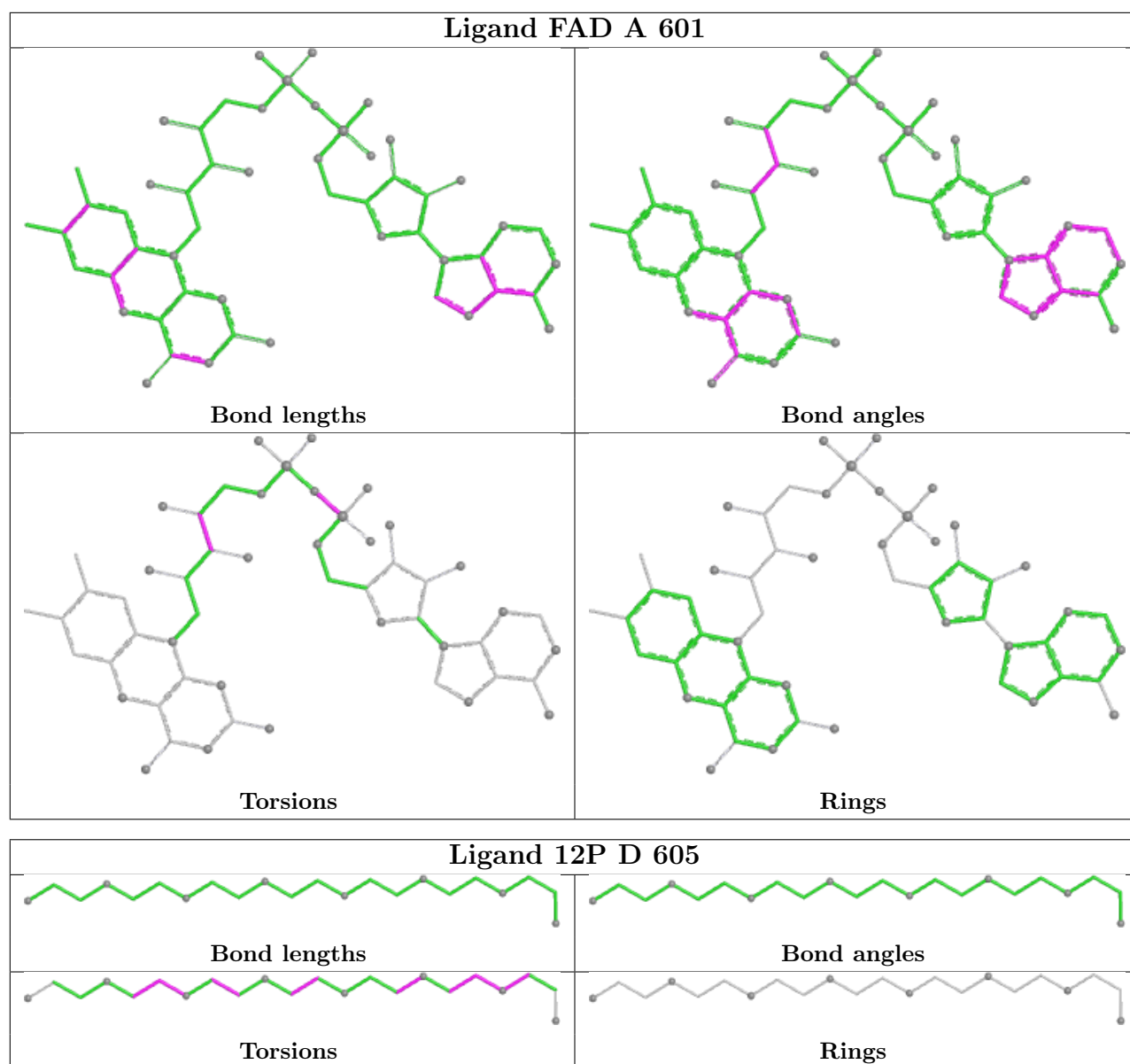
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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	498/538 (92%)	0.56	33 (6%) 24 21	28, 45, 76, 111	0
1	B	498/538 (92%)	0.94	68 (13%) 6 5	29, 56, 86, 114	0
1	C	496/538 (92%)	0.93	77 (15%) 5 4	30, 52, 80, 107	0
1	D	497/538 (92%)	0.94	89 (17%) 3 3	28, 50, 87, 114	0
All	All	1989/2152 (92%)	0.84	267 (13%) 7 5	28, 51, 84, 114	0

All (267) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	68	ILE	7.7
1	A	351	PHE	6.8
1	C	351	PHE	6.6
1	A	286	ASP	6.5
1	B	351	PHE	6.0
1	B	522	PHE	6.0
1	D	67	LEU	5.5
1	B	256	ILE	5.3
1	A	67	LEU	5.1
1	D	165	TRP	4.7
1	D	132	LEU	4.7
1	B	285	ALA	4.6
1	B	257	ASP	4.5
1	B	332	PHE	4.5
1	D	351	PHE	4.3
1	C	350	LYS	4.2
1	C	520	ALA	4.2
1	D	44	ALA	4.2
1	D	42	PHE	4.2
1	C	386	PHE	4.1
1	B	288	LYS	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	290	VAL	4.0
1	B	282	LEU	4.0
1	D	285	ALA	4.0
1	D	299	PHE	4.0
1	B	286	ASP	3.9
1	A	165	TRP	3.9
1	A	66	SER	3.9
1	D	66	SER	3.8
1	D	241	VAL	3.8
1	C	332	PHE	3.7
1	C	290	VAL	3.6
1	D	69	SER	3.6
1	C	282	LEU	3.6
1	C	165	TRP	3.6
1	C	291	TRP	3.6
1	D	289	GLN	3.6
1	C	288	LYS	3.5
1	A	424	GLN	3.5
1	C	473	THR	3.5
1	D	64	GLN	3.5
1	A	353	GLU	3.5
1	B	289	GLN	3.4
1	B	431	THR	3.4
1	B	492	SER	3.4
1	B	495	GLU	3.3
1	B	464	LEU	3.3
1	B	381	LYS	3.3
1	C	380	SER	3.3
1	D	286	ASP	3.3
1	D	159	LEU	3.3
1	D	473	THR	3.3
1	C	371	ALA	3.3
1	D	301	LEU	3.3
1	B	521	ASN	3.2
1	D	323	TYR	3.2
1	C	254	VAL	3.2
1	A	289	GLN	3.2
1	C	256	ILE	3.2
1	D	303	THR	3.2
1	C	439	LYS	3.2
1	D	65	ASN	3.2
1	A	65	ASN	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	288	LYS	3.1
1	A	287	GLU	3.1
1	C	284	GLY	3.1
1	C	316	LEU	3.1
1	D	328	TRP	3.0
1	D	327	SER	3.0
1	C	289	GLN	3.0
1	D	350	LYS	3.0
1	D	164	ALA	3.0
1	C	375	LEU	3.0
1	A	380	SER	3.0
1	B	283	GLY	3.0
1	C	353	GLU	3.0
1	B	165	TRP	3.0
1	C	270	ALA	3.0
1	D	318	LEU	3.0
1	D	427	GLN	3.0
1	D	302	LYS	2.9
1	C	251	THR	2.9
1	B	287	GLU	2.9
1	B	519	MET	2.9
1	B	25	ASN	2.9
1	C	25	ASN	2.9
1	C	423	ASN	2.9
1	D	522	PHE	2.9
1	D	304	VAL	2.9
1	A	68	ILE	2.9
1	C	163	ALA	2.9
1	D	254	VAL	2.8
1	D	422	TRP	2.8
1	D	435	ASP	2.8
1	C	283	GLY	2.8
1	B	312	LEU	2.8
1	D	288	LYS	2.8
1	D	421	ALA	2.8
1	B	387	ILE	2.7
1	C	311	LEU	2.7
1	A	114	ASP	2.7
1	D	423	ASN	2.7
1	C	472	LYS	2.7
1	D	307	SER	2.7
1	C	285	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	373	TYR	2.7
1	D	424	GLN	2.7
1	C	287	GLU	2.7
1	D	244	LYS	2.7
1	B	385	GLY	2.7
1	D	338	LEU	2.7
1	D	355	ALA	2.6
1	C	348	PHE	2.6
1	D	256	ILE	2.6
1	B	307	SER	2.6
1	C	318	LEU	2.6
1	C	324	LEU	2.6
1	B	157	SER	2.6
1	C	94	SER	2.6
1	D	349	LEU	2.6
1	D	255	ALA	2.6
1	B	261	SER	2.6
1	B	379	LEU	2.6
1	B	520	ALA	2.6
1	C	422	TRP	2.6
1	C	436	TRP	2.6
1	B	386	PHE	2.6
1	C	314	PRO	2.6
1	D	242	PRO	2.6
1	D	341	VAL	2.6
1	D	134	SER	2.6
1	D	163	ALA	2.5
1	B	477	ASN	2.5
1	C	47	ASP	2.5
1	D	326	MET	2.5
1	B	314	PRO	2.5
1	B	66	SER	2.5
1	B	429	LYS	2.5
1	C	269	VAL	2.5
1	D	46	SER	2.5
1	D	94	SER	2.5
1	D	70	LYS	2.5
1	B	64	GLN	2.5
1	C	424	GLN	2.5
1	B	254	VAL	2.5
1	B	479	ILE	2.5
1	C	328	TRP	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	319	VAL	2.5
1	B	252	LYS	2.5
1	C	92	LYS	2.5
1	A	285	ALA	2.5
1	B	321	GLU	2.4
1	D	43	SER	2.4
1	C	475	VAL	2.4
1	D	245	VAL	2.4
1	D	334	TYR	2.4
1	D	430	LYS	2.4
1	D	431	THR	2.4
1	B	94	SER	2.4
1	B	114	ASP	2.4
1	C	428	LYS	2.4
1	A	475	VAL	2.4
1	B	341	VAL	2.4
1	D	419	ILE	2.4
1	A	45	ASP	2.4
1	A	473	THR	2.4
1	B	342	SER	2.4
1	C	519	MET	2.4
1	C	133	GLU	2.4
1	A	523	ASP	2.3
1	C	253	ASN	2.3
1	D	373	TYR	2.3
1	C	366	PRO	2.3
1	B	364	LYS	2.3
1	C	317	GLY	2.3
1	B	447	PHE	2.3
1	C	250	VAL	2.3
1	C	448	VAL	2.3
1	D	420	VAL	2.3
1	D	37	ARG	2.3
1	D	324	LEU	2.3
1	A	47	ASP	2.3
1	A	373	TYR	2.3
1	B	369	SER	2.3
1	D	345	ASN	2.3
1	D	95	TRP	2.3
1	D	385	GLY	2.3
1	D	55	HIS	2.3
1	C	281	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	341	VAL	2.3
1	B	45	ASP	2.3
1	A	369	SER	2.3
1	D	158	LYS	2.3
1	C	67	LEU	2.2
1	D	433	PHE	2.2
1	D	325	GLU	2.2
1	A	256	ILE	2.2
1	C	292	LEU	2.2
1	C	312	LEU	2.2
1	D	250	VAL	2.2
1	D	290	VAL	2.2
1	B	317	GLY	2.2
1	B	255	ALA	2.2
1	B	439	LYS	2.2
1	C	164	ALA	2.2
1	A	94	SER	2.2
1	C	46	SER	2.2
1	D	436	TRP	2.2
1	B	349	LEU	2.2
1	B	375	LEU	2.2
1	C	349	LEU	2.2
1	B	319	VAL	2.2
1	A	433	PHE	2.2
1	C	352	ASP	2.2
1	D	520	ALA	2.2
1	B	373	TYR	2.2
1	B	494	TYR	2.2
1	C	379	LEU	2.2
1	D	45	ASP	2.2
1	D	477	ASN	2.2
1	D	519	MET	2.2
1	D	306	LYS	2.2
1	D	340	THR	2.2
1	C	376	LEU	2.1
1	A	435	ASP	2.1
1	D	53	PHE	2.1
1	D	332	PHE	2.1
1	D	353	GLU	2.1
1	A	163	ALA	2.1
1	C	153	THR	2.1
1	D	150	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	434	LEU	2.1
1	B	437	LEU	2.1
1	C	419	ILE	2.1
1	A	290	VAL	2.1
1	C	440	VAL	2.1
1	C	447	PHE	2.1
1	D	249	ARG	2.1
1	D	157	SER	2.1
1	A	423	ASN	2.1
1	A	42	PHE	2.1
1	C	313	PHE	2.1
1	C	385	GLY	2.1
1	D	425	SER	2.1
1	A	255	ALA	2.1
1	B	444	MET	2.1
1	B	292	LEU	2.1
1	B	376	LEU	2.1
1	C	387	ILE	2.1
1	B	323	TYR	2.1
1	C	247	VAL	2.1
1	D	93	GLY	2.1
1	D	439	LYS	2.0
1	C	293	THR	2.0
1	A	282	LEU	2.0
1	A	352	ASP	2.0
1	B	318	LEU	2.0
1	B	498	ILE	2.0
1	D	317	GLY	2.0
1	B	372	PHE	2.0
1	B	272	GLU	2.0
1	C	157	SER	2.0
1	B	427	GLN	2.0
1	B	476	ASN	2.0
1	C	65	ASN	2.0
1	C	301	LEU	2.0
1	C	381	LYS	2.0

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

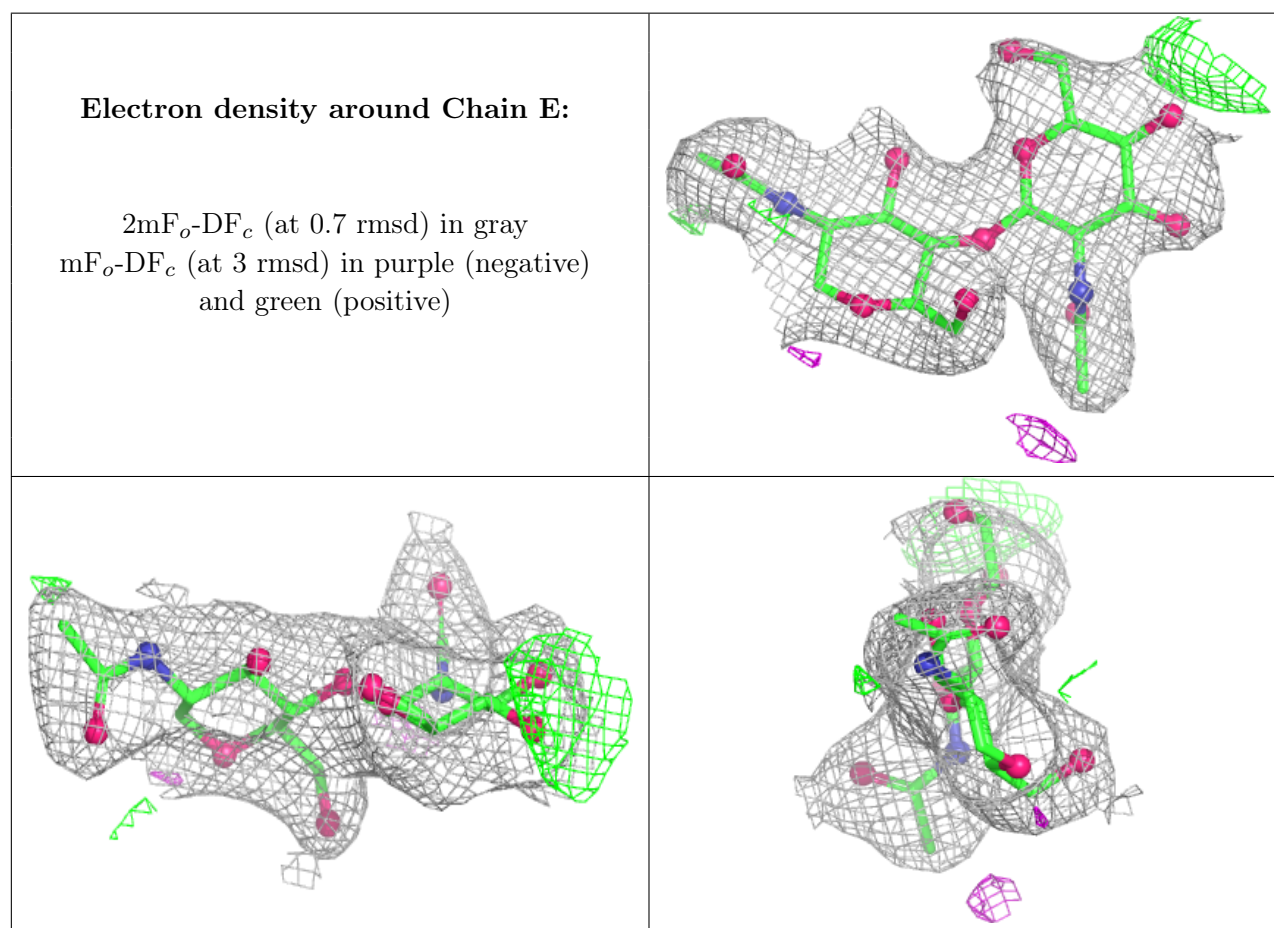
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

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.

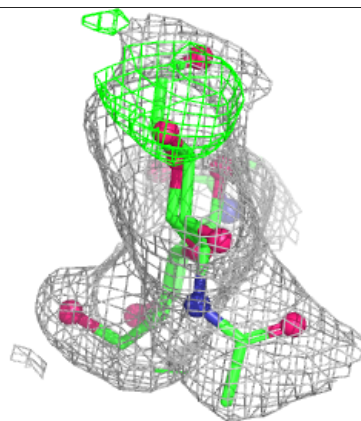
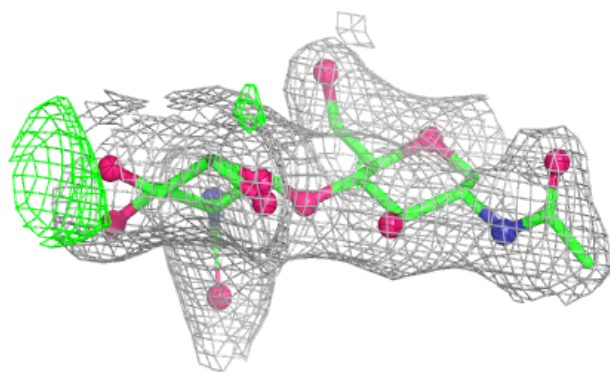
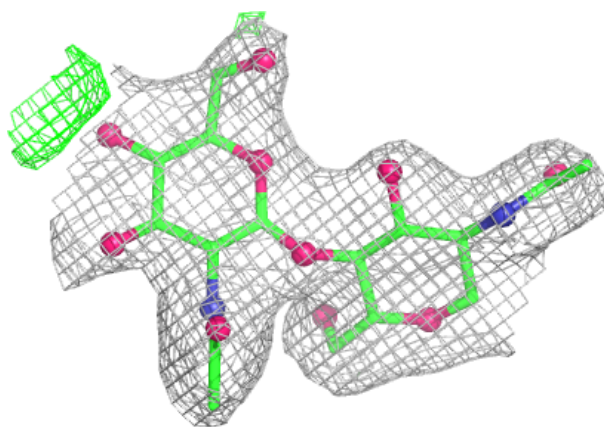
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	H	2	14/15	0.71	0.18	72,86,97,100	0
2	NAG	F	2	14/15	0.75	0.15	68,73,81,84	0
2	NAG	E	2	14/15	0.76	0.15	50,69,79,80	0
2	NAG	H	1	14/15	0.77	0.17	63,73,79,80	0
2	NAG	G	2	14/15	0.80	0.14	63,70,78,80	0
2	NAG	G	1	14/15	0.84	0.13	54,63,67,68	0
2	NAG	F	1	14/15	0.87	0.13	56,63,69,70	0
2	NAG	E	1	14/15	0.88	0.10	50,55,60,65	0

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.



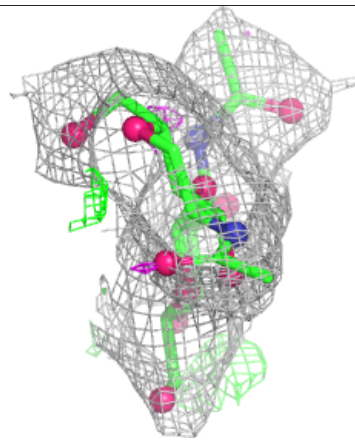
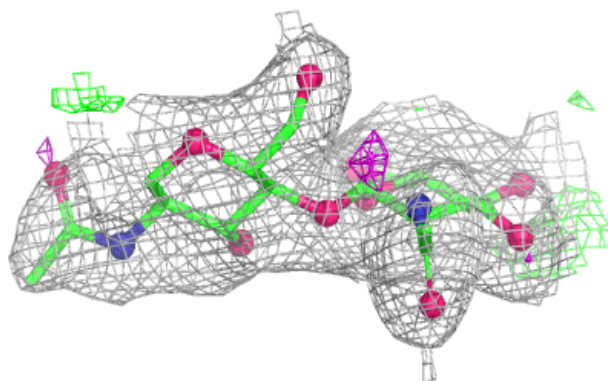
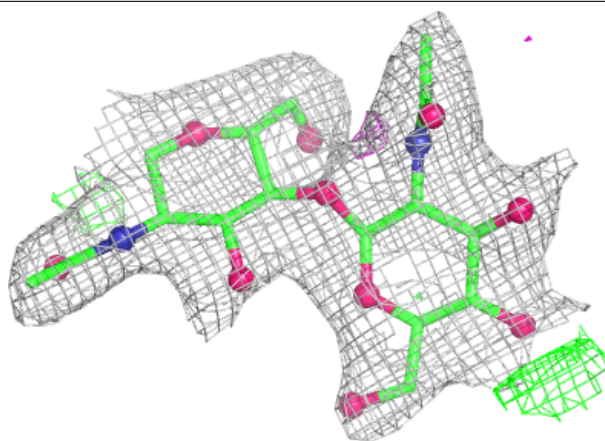
Electron density around Chain F:

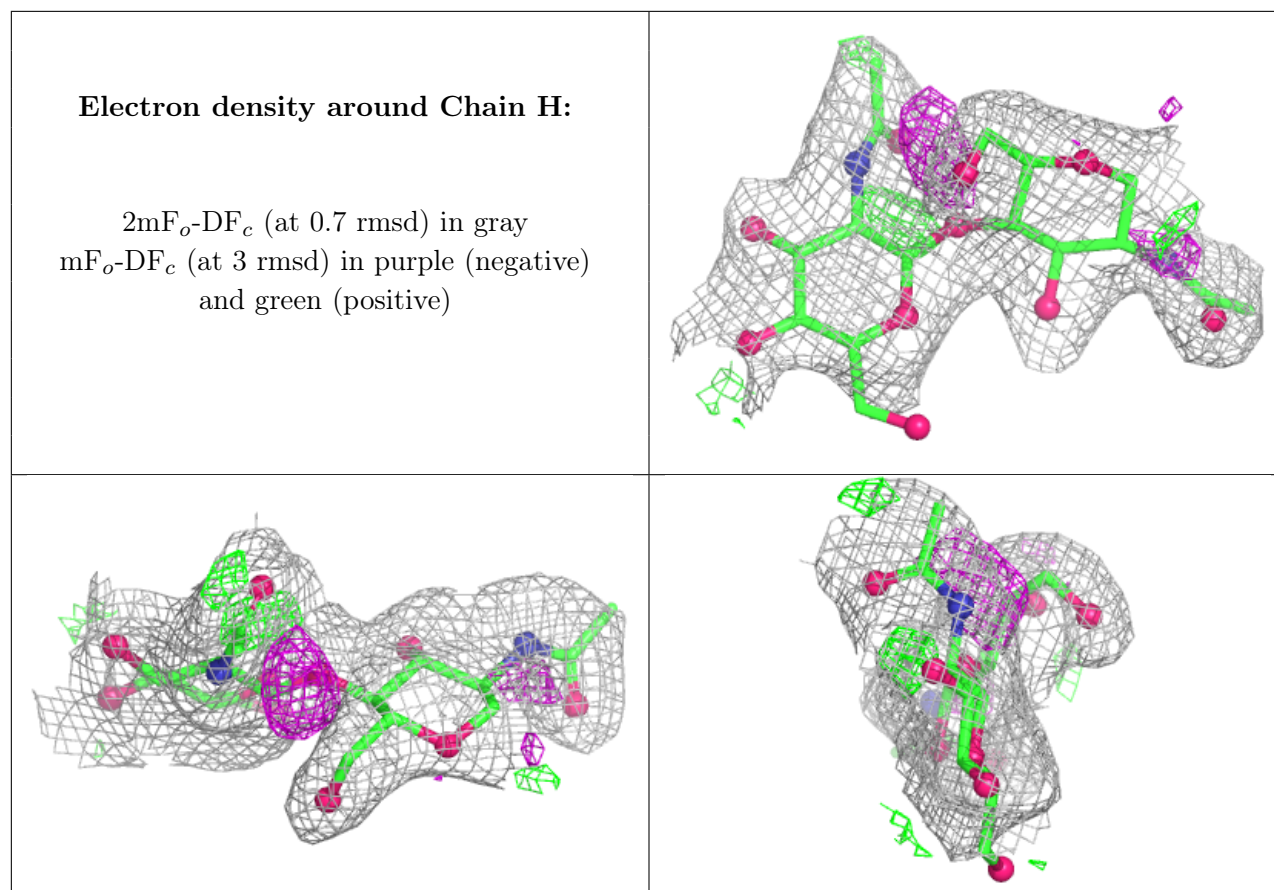
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain G:

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





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
4	NAG	C	604	14/15	0.47	0.19	83,93,99,103	0
4	NAG	B	604	14/15	0.55	0.17	93,97,102,106	0
4	NAG	D	604	14/15	0.64	0.16	90,95,96,98	0
4	NAG	A	604	14/15	0.67	0.17	78,82,87,87	0
5	SO4	C	607	5/5	0.77	0.13	56,57,63,69	5
5	SO4	D	606	5/5	0.80	0.18	48,52,57,59	5
5	SO4	D	607	5/5	0.83	0.14	46,50,55,64	5
5	SO4	B	605	5/5	0.87	0.09	60,66,72,73	0
6	12P	D	605	22/37	0.88	0.13	39,51,56,59	0
6	12P	C	605	28/37	0.89	0.13	36,50,60,68	0
5	SO4	C	606	5/5	0.89	0.09	60,62,73,73	0
3	FAD	C	601	53/53	0.95	0.08	28,38,50,53	0
3	FAD	B	601	53/53	0.96	0.07	28,36,45,49	0

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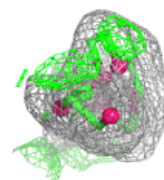
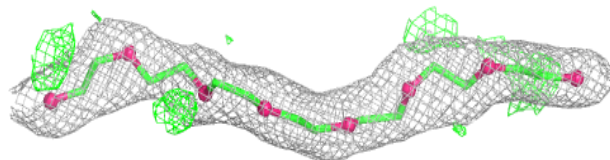
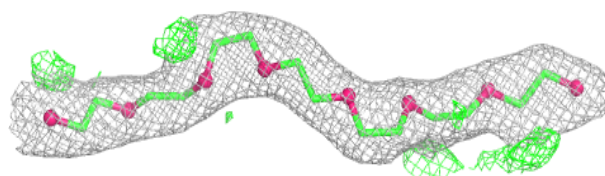
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	FAD	D	601	53/53	0.97	0.07	26,34,47,50	0
3	FAD	A	601	53/53	0.97	0.06	24,31,41,44	0

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.

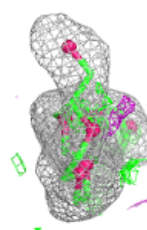
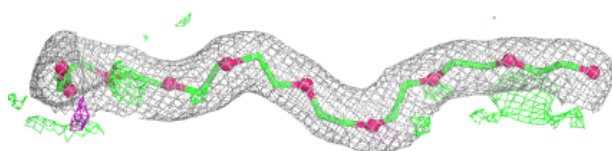
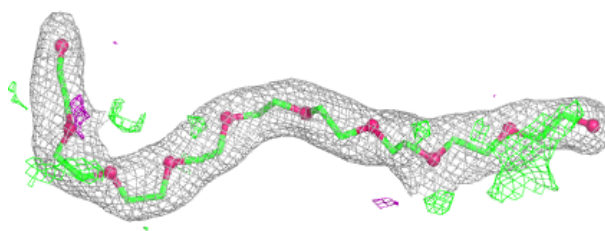
Electron density around 12P D 605:

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

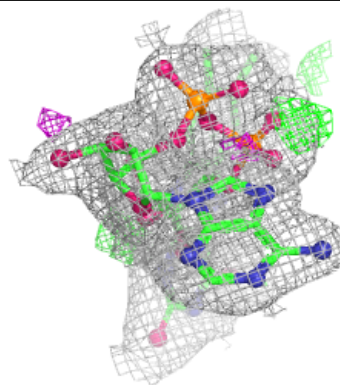
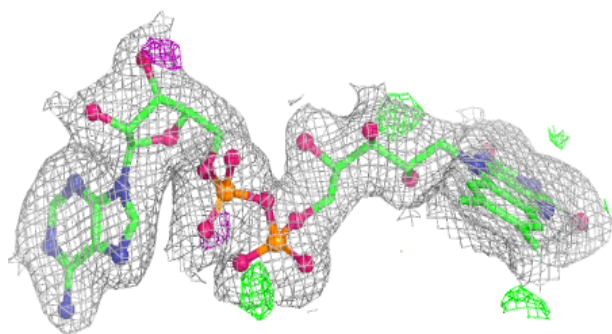
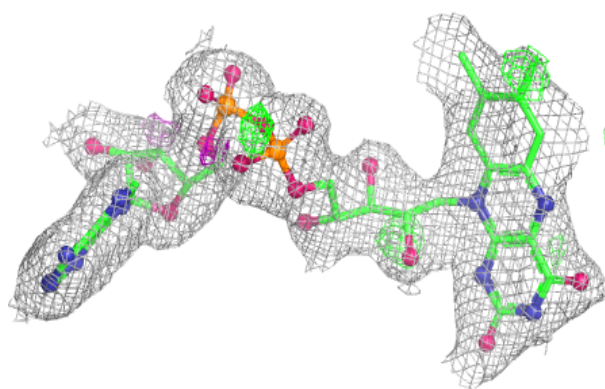


Electron density around 12P C 605:

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

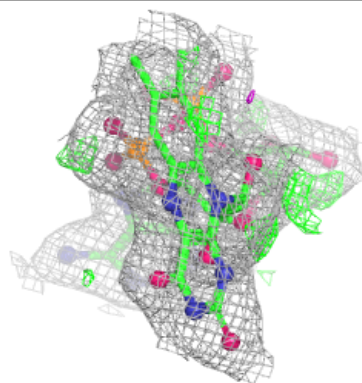
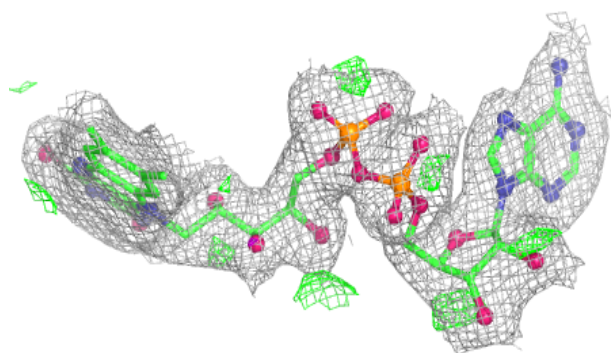
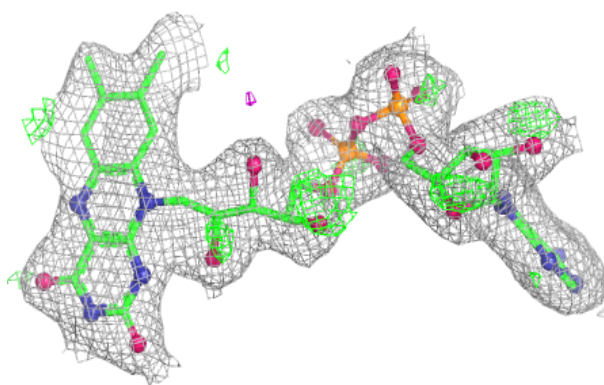
**Electron density around FAD C 601:**

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

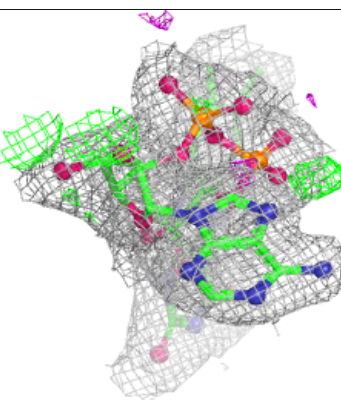
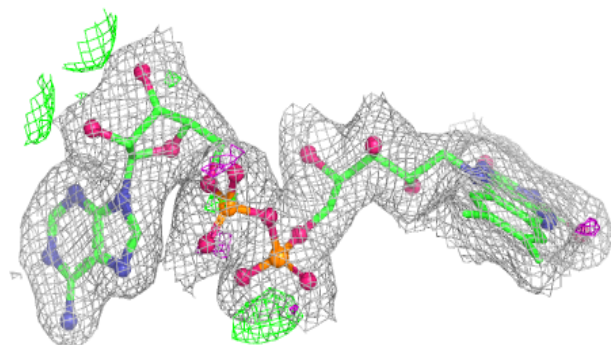
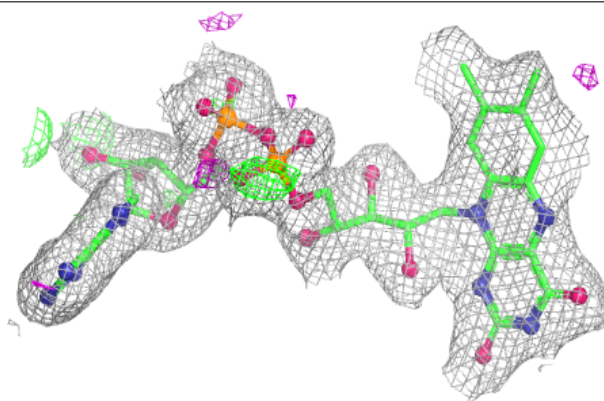


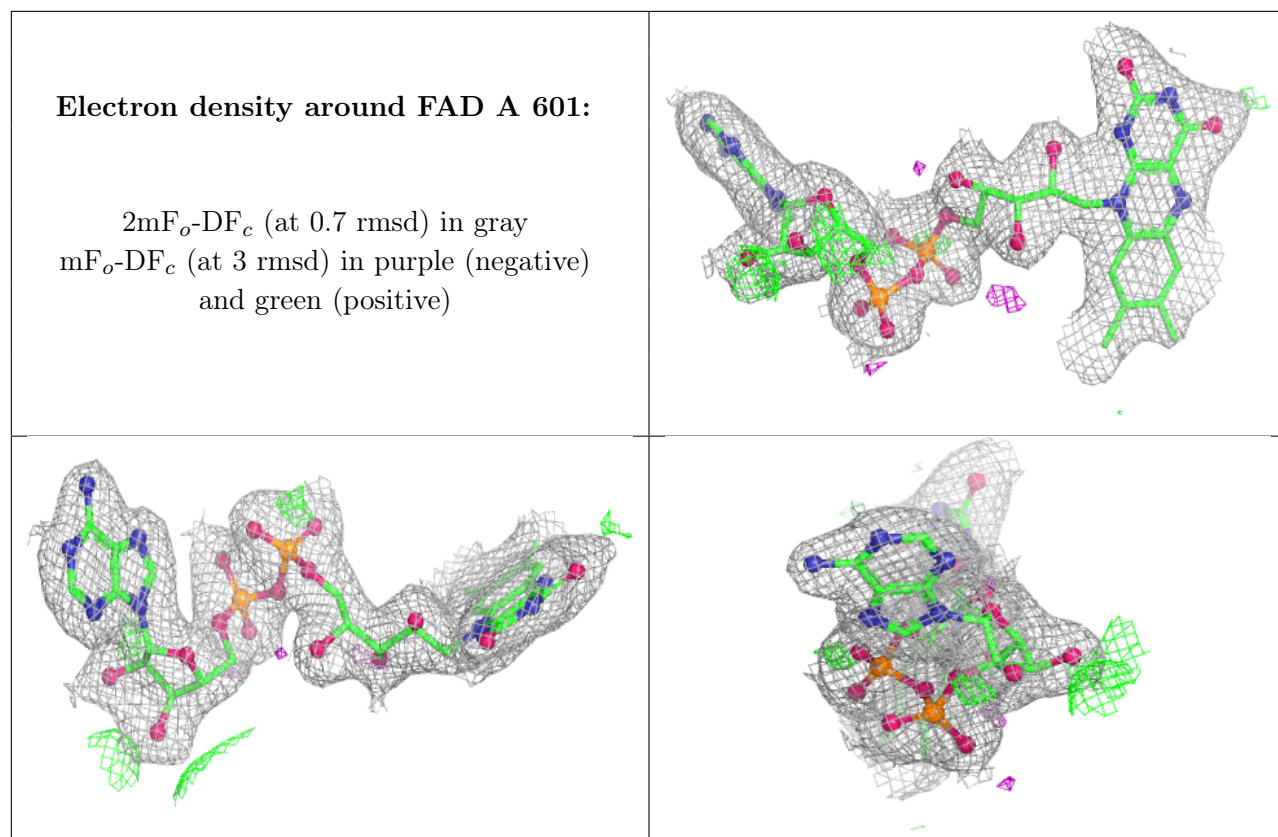
Electron density around FAD B 601:

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

**Electron density around FAD D 601:**

$2mF_o-DF_c$ (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.