



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 7, 2024 – 03:45 PM EDT

PDB ID : 4PZF  
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](mailto: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>.

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

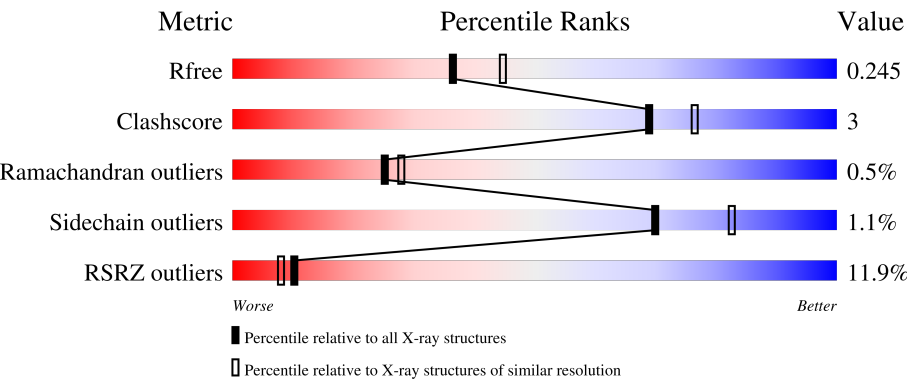
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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.



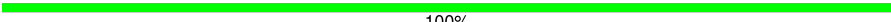
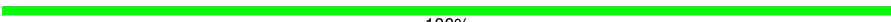

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	5791 (2.20-2.20)
Clashscore	180529	6634 (2.20-2.20)
Ramachandran outliers	177936	6560 (2.20-2.20)
Sidechain outliers	177891	6561 (2.20-2.20)
RSRZ outliers	164620	5791 (2.20-2.20)

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  $\geq 3$ , 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	<div><div>5%</div><div>86%6%7%</div></div>
1	B	538	<div><div>11%</div><div>85%7%7%</div></div>
1	C	538	<div><div>12%</div><div>80%12%8%</div></div>
1	D	538	<div><div>16%</div><div>84%8%8%</div></div>
2	E	2	<div><div></div><div>100%</div></div>

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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:

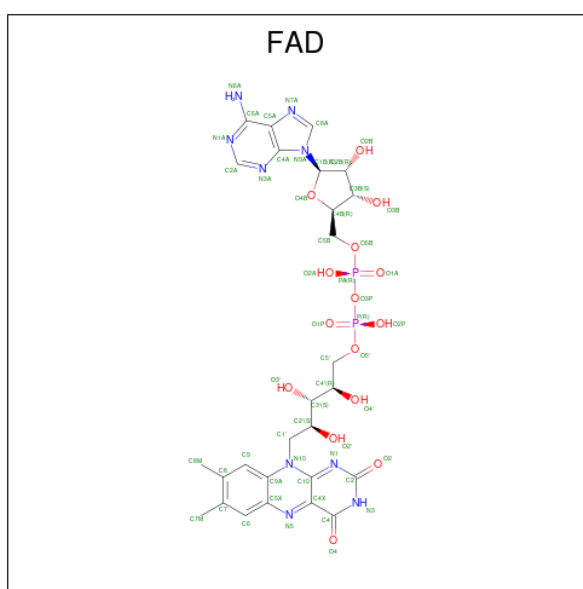
Chain	Residue	Modelled	Actual	Comment	Reference
A	22	GLU	LEU	SEE REMARK 999	UNP P30986
A	23	ALA	GLY	SEE REMARK 999	UNP P30986
A	164	ALA	GLY	engineered mutation	UNP P30986
B	22	GLU	LEU	SEE REMARK 999	UNP P30986
B	23	ALA	GLY	SEE REMARK 999	UNP P30986
B	164	ALA	GLY	engineered mutation	UNP P30986
C	22	GLU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

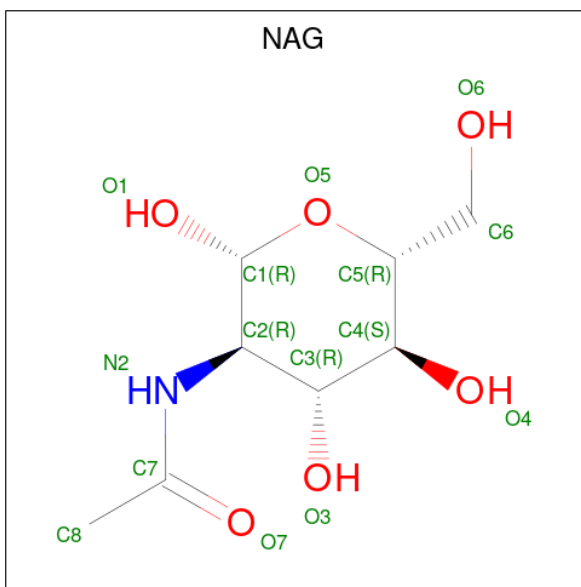
- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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			

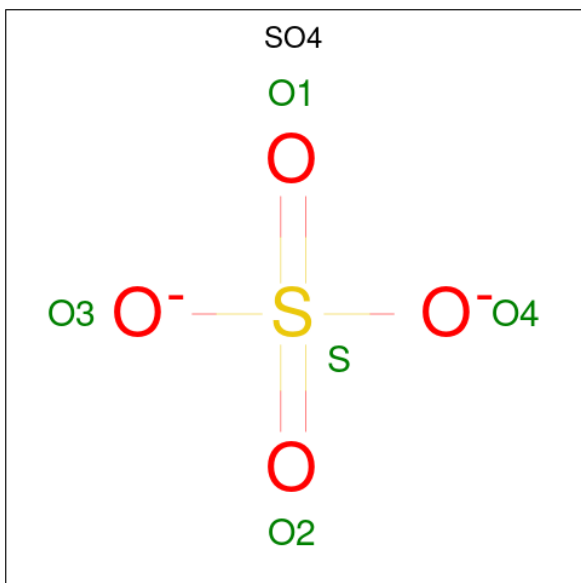
- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ).





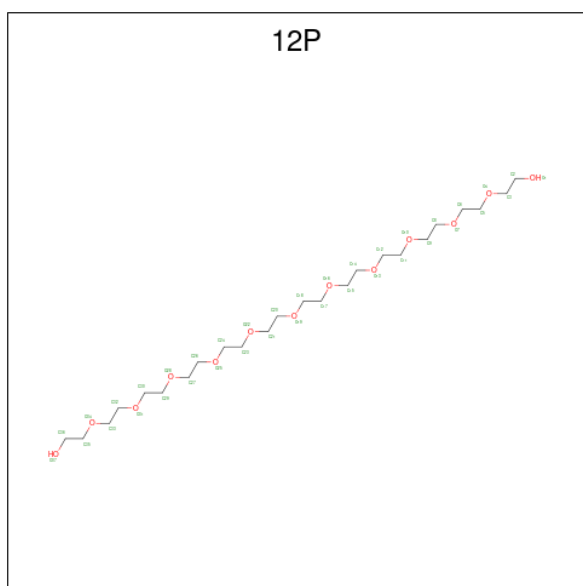
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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 (three-letter code: 12P) (formula: C<sub>24</sub>H<sub>50</sub>O<sub>13</sub>).



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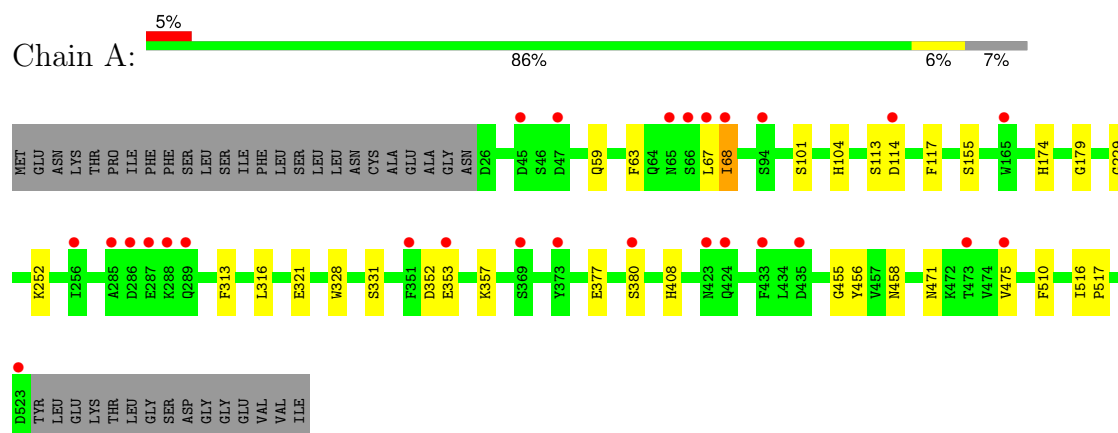
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	60	Total	O	0	0
			60	60		

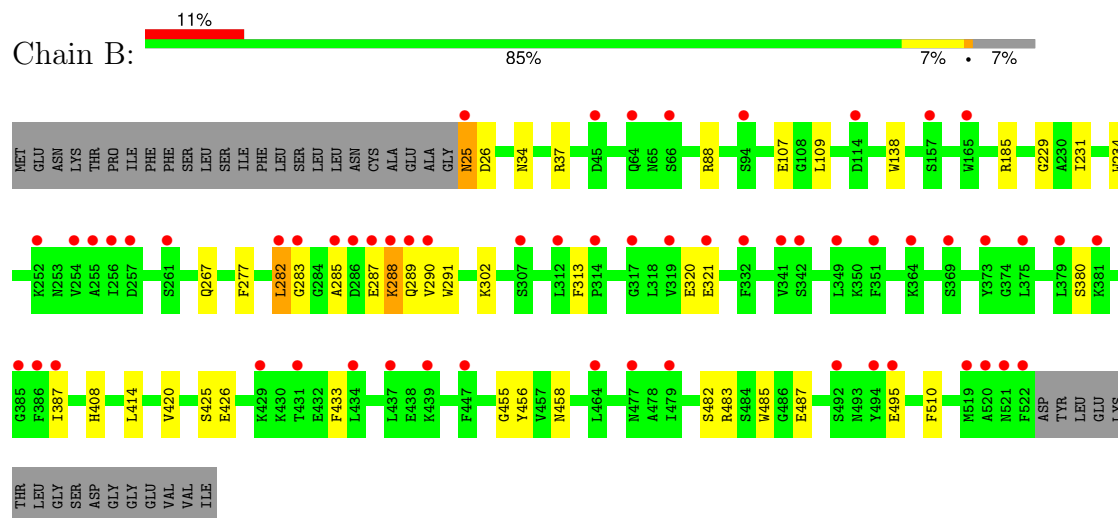
### 3 Residue-property plots [i](#)

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.

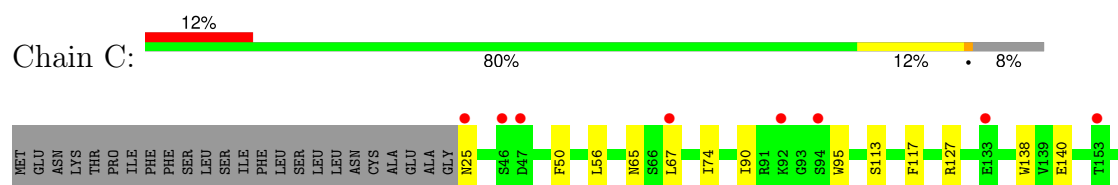
#### • Molecule 1: Reticuline oxidase

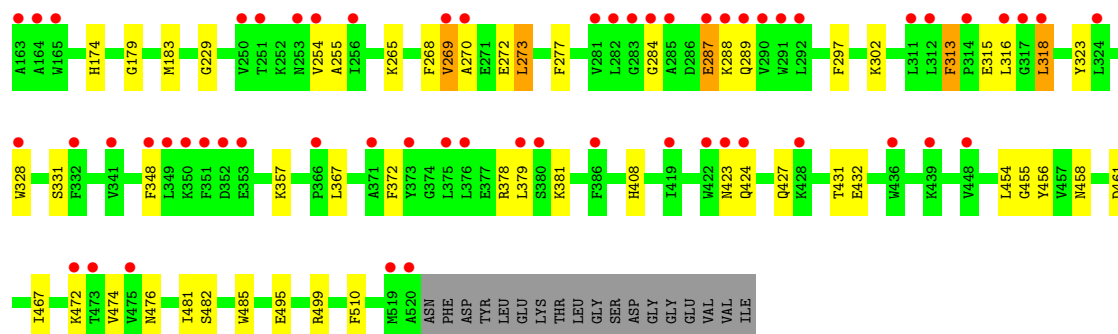


#### • Molecule 1: Reticuline oxidase

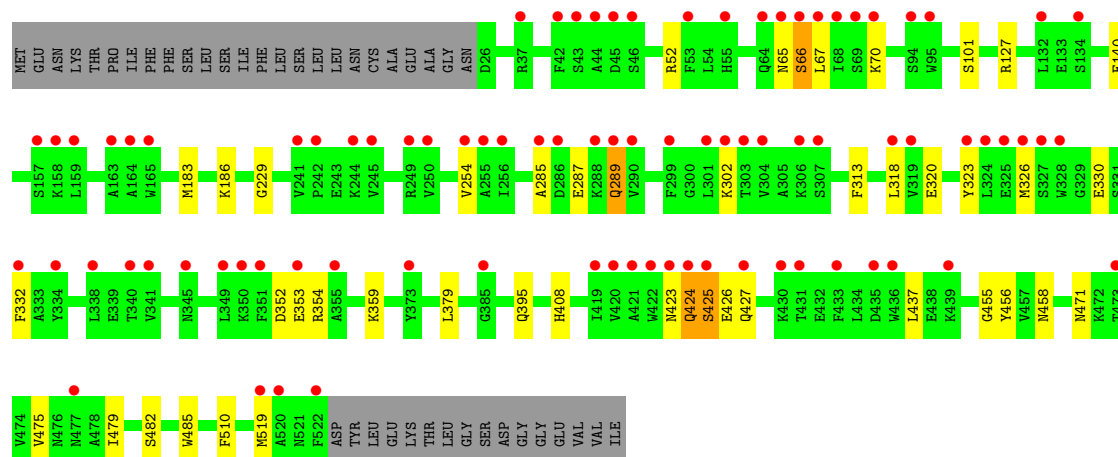
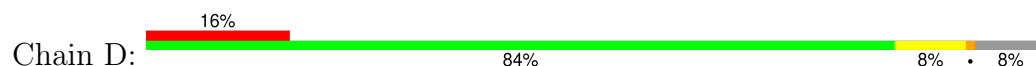


#### • Molecule 1: Reticuline oxidase





• 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



MAG1  
MAG2

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

Chain H:



MAG1  
MAG2

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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	7017 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.7	Xtriage
Anisotropy	0.406	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 35.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: 12P, FAD, NAG, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.25	0/4033	0.43	0/5465
1	B	0.25	0/4033	0.43	0/5465
1	C	0.25	0/4013	0.44	0/5438
1	D	0.25	0/4025	0.43	0/5454
All	All	0.25	0/16104	0.43	0/21822

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	3935	0	3861	16	0
1	B	3935	0	3863	28	0
1	C	3916	0	3848	38	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	108	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 (108) 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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:357:LYS:NZ	1:C:461:ASP:OD1	2.36	0.54
1:C:287:GLU:C	1:C:289:GLN:H	2.10	0.54
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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:328:TRP:O	1:C:331:SER:OG	2.31	0.44
1:B:288:LYS:H	1:B:380:SER:CB	2.30	0.44
1:B:287:GLU:C	1:B:289:GLN:H	2.21	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: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:C:183:MET:HE2	1:C:297:PHE:CZ	2.54	0.42
1:A:471:ASN:O	1:A:475:VAL:HG23	2.19	0.42
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:C:408:HIS:CD2	1:C:454:LEU:HD13	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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

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 [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	496/538 (92%)	475 (96%)	19 (4%)	2 (0%)	30	34
1	B	496/538 (92%)	468 (94%)	27 (5%)	1 (0%)	44	52
1	C	494/538 (92%)	469 (95%)	22 (4%)	3 (1%)	22	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%)	25	28

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	68	ILE

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Mol	Chain	Res	Type
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%)	423 (99%)	3 (1%)	81	90
1	B	426/460 (93%)	421 (99%)	5 (1%)	67	80
1	C	424/460 (92%)	418 (99%)	6 (1%)	62	77
1	D	425/460 (92%)	421 (99%)	4 (1%)	75	86
All	All	1701/1840 (92%)	1683 (99%)	18 (1%)	70	82

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	114	ASP
1	A	155	SER
1	A	313	PHE
1	B	25	ASN
1	B	282	LEU
1	B	313	PHE
1	B	425	SER
1	B	426	GLU
1	C	25	ASN
1	C	273	LEU
1	C	313	PHE
1	C	318	LEU

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Mol	Chain	Res	Type
1	C	431	THR
1	C	432	GLU
1	D	289	GLN
1	D	313	PHE
1	D	425	SER
1	D	427	GLN

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

Mol	Chain	Res	Type
1	A	39	HIS
1	A	408	HIS
1	B	25	ASN
1	B	55	HIS
1	B	408	HIS
1	B	459	HIS
1	C	55	HIS
1	C	408	HIS
1	C	459	HIS
1	C	476	ASN
1	D	408	HIS
1	D	459	HIS

### 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](#)

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:

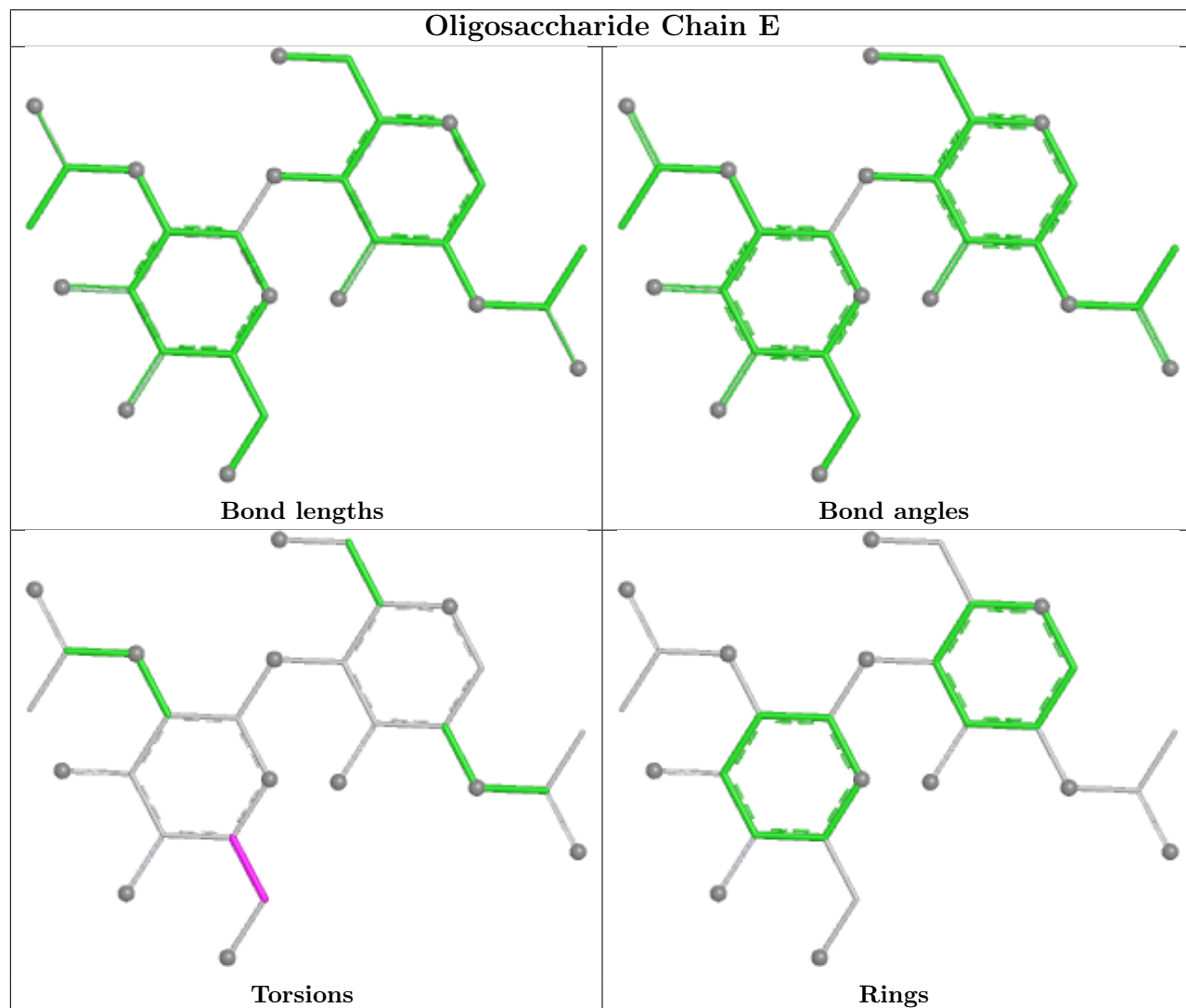
Mol	Chain	Res	Type	Atoms
2	E	2	NAG	O5-C5-C6-O6
2	F	2	NAG	O5-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
2	F	2	NAG	C4-C5-C6-O6
2	G	2	NAG	O5-C5-C6-O6
2	H	1	NAG	C4-C5-C6-O6

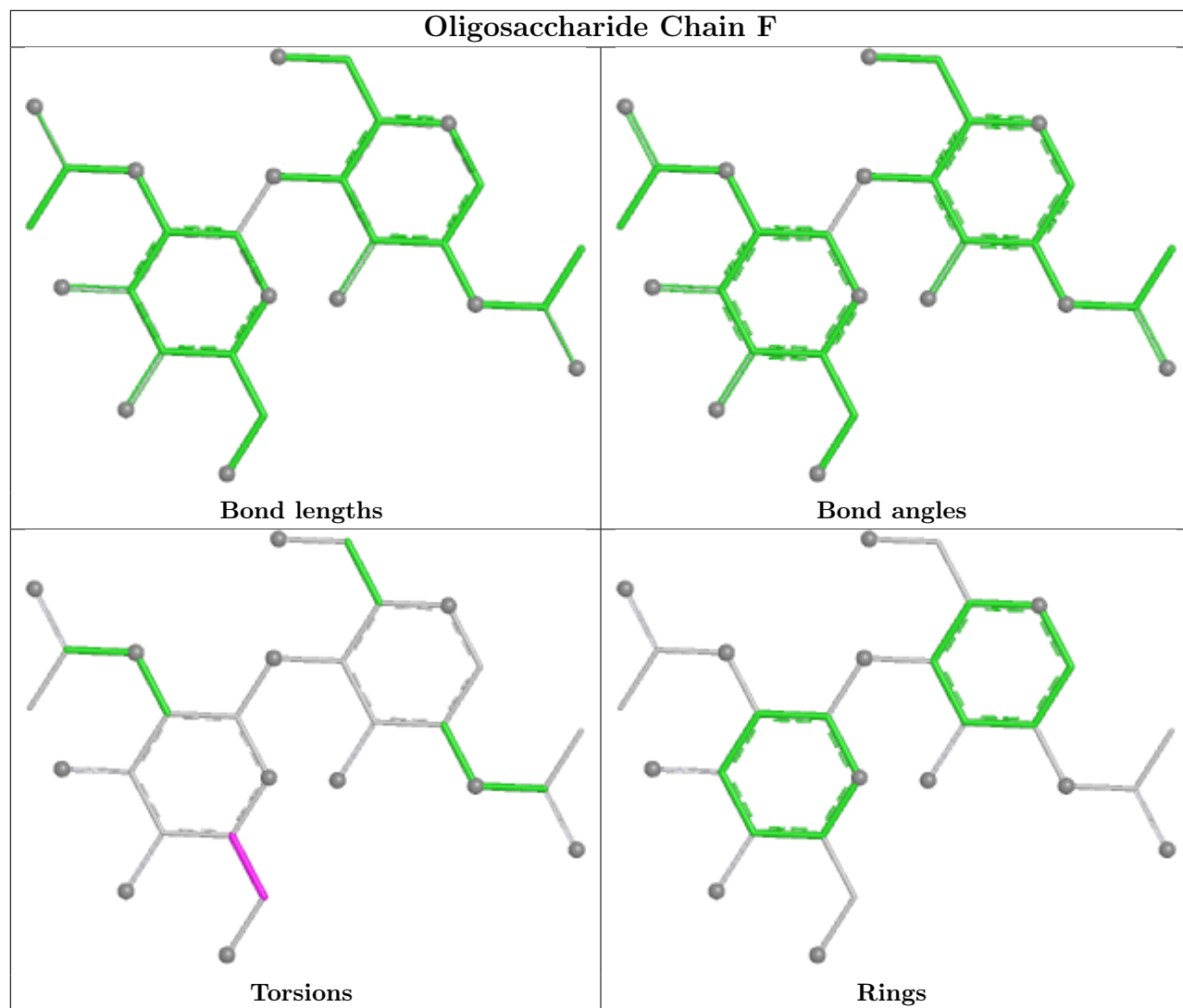
There are no ring outliers.

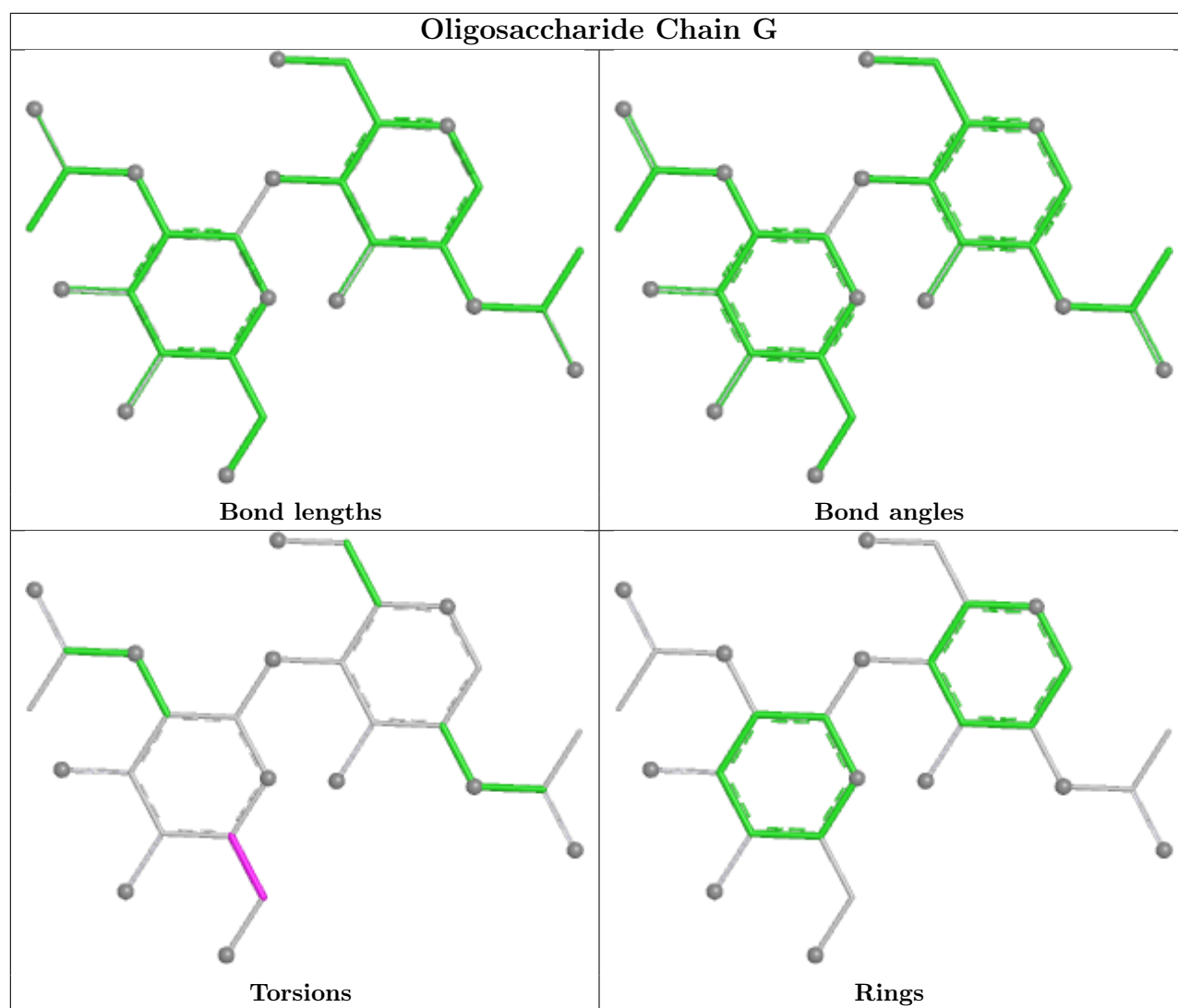
1 monomer is involved in 1 short contact:

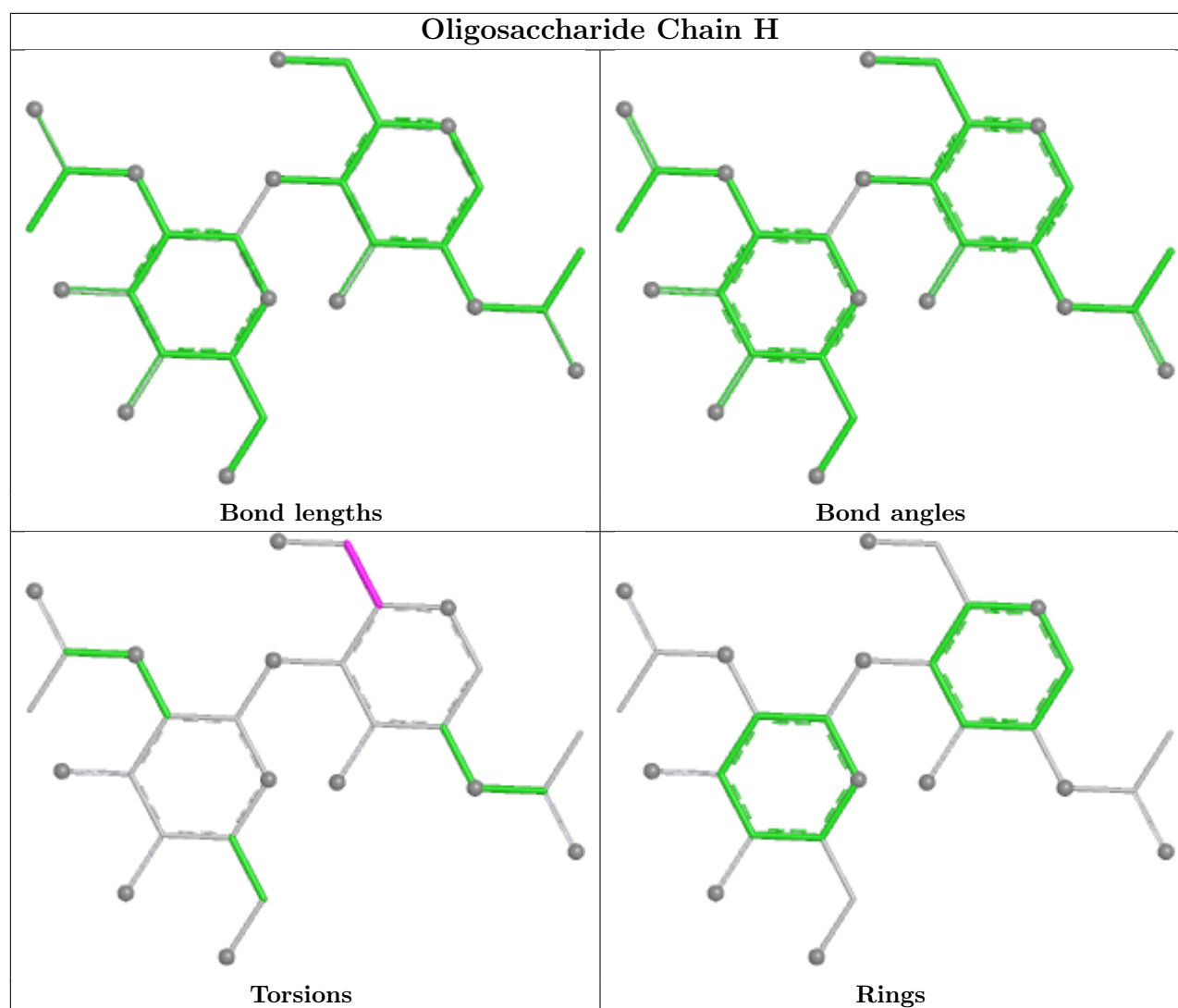
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	2	NAG	1	0

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	$\# Z  > 2$
3	FAD	A	601	1	54,58,58	1.30	5 (9%)	71,89,89	1.24	7 (9%)
3	FAD	B	601	1	54,58,58	1.27	4 (7%)	71,89,89	1.27	6 (8%)
5	SO4	C	606	-	4,4,4	0.25	0	6,6,6	0.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	D	604	1	14,14,15	0.22	0	17,19,21	0.42	0
5	SO4	C	607	-	4,4,4	0.25	0	6,6,6	0.09	0
4	NAG	C	604	1	14,14,15	0.42	0	17,19,21	0.42	0
4	NAG	A	604	1	14,14,15	0.20	0	17,19,21	0.47	0
5	SO4	D	607	-	4,4,4	0.23	0	6,6,6	0.08	0
3	FAD	D	601	1	54,58,58	1.29	5 (9%)	71,89,89	1.28	7 (9%)
6	12P	C	605	-	27,27,36	0.40	0	26,26,35	0.62	0
3	FAD	C	601	1	54,58,58	1.28	5 (9%)	71,89,89	1.26	6 (8%)
5	SO4	B	605	-	4,4,4	0.23	0	6,6,6	0.08	0
4	NAG	B	604	1	14,14,15	0.31	0	17,19,21	0.37	0
6	12P	D	605	-	21,21,36	0.42	0	20,20,35	0.47	0
5	SO4	D	606	-	4,4,4	0.24	0	6,6,6	0.10	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	A	601	1	-	5/30/50/50	0/6/6/6
3	FAD	B	601	1	-	3/30/50/50	0/6/6/6
4	NAG	D	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	A	604	1	-	2/6/23/26	0/1/1/1
3	FAD	D	601	1	-	5/30/50/50	0/6/6/6
6	12P	C	605	-	-	15/25/25/34	-
3	FAD	C	601	1	-	0/30/50/50	0/6/6/6
4	NAG	B	604	1	-	0/6/23/26	0/1/1/1
6	12P	D	605	-	-	8/19/19/34	-

All (19) 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	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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	C5X-N5	-2.79	1.34	1.39
3	C	601	FAD	C5X-N5	-2.75	1.34	1.39
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	B	601	FAD	C4-N3	-2.48	1.34	1.38
3	D	601	FAD	C4-N3	-2.44	1.34	1.38
3	A	601	FAD	O4B-C1B	2.36	1.44	1.40
3	A	601	FAD	C4-N3	-2.33	1.34	1.38
3	D	601	FAD	O4B-C1B	2.19	1.43	1.40
3	C	601	FAD	O4B-C1B	2.11	1.43	1.40

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	601	FAD	N3A-C2A-N1A	-3.92	123.36	128.67
3	C	601	FAD	N3A-C2A-N1A	-3.74	123.60	128.67
3	D	601	FAD	N3A-C2A-N1A	-3.72	123.62	128.67
3	A	601	FAD	N3A-C2A-N1A	-3.59	123.80	128.67
3	C	601	FAD	C4A-C5A-N7A	-3.05	106.12	109.34
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	D	601	FAD	C4A-C5A-N7A	-2.92	106.25	109.34
3	B	601	FAD	C4-C4X-N5	2.80	122.08	118.21
3	A	601	FAD	C4A-C5A-N7A	-2.79	106.39	109.34
3	C	601	FAD	C4-C4X-N5	2.71	121.95	118.21
3	B	601	FAD	C4A-C5A-N7A	-2.65	106.54	109.34
3	A	601	FAD	C4'-C3'-C2'	-2.62	109.21	113.57
3	B	601	FAD	C4X-C10-N1	-2.50	118.46	124.59
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	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	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	B	601	FAD	O4-C4-C4X	-2.15	120.87	126.53

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
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

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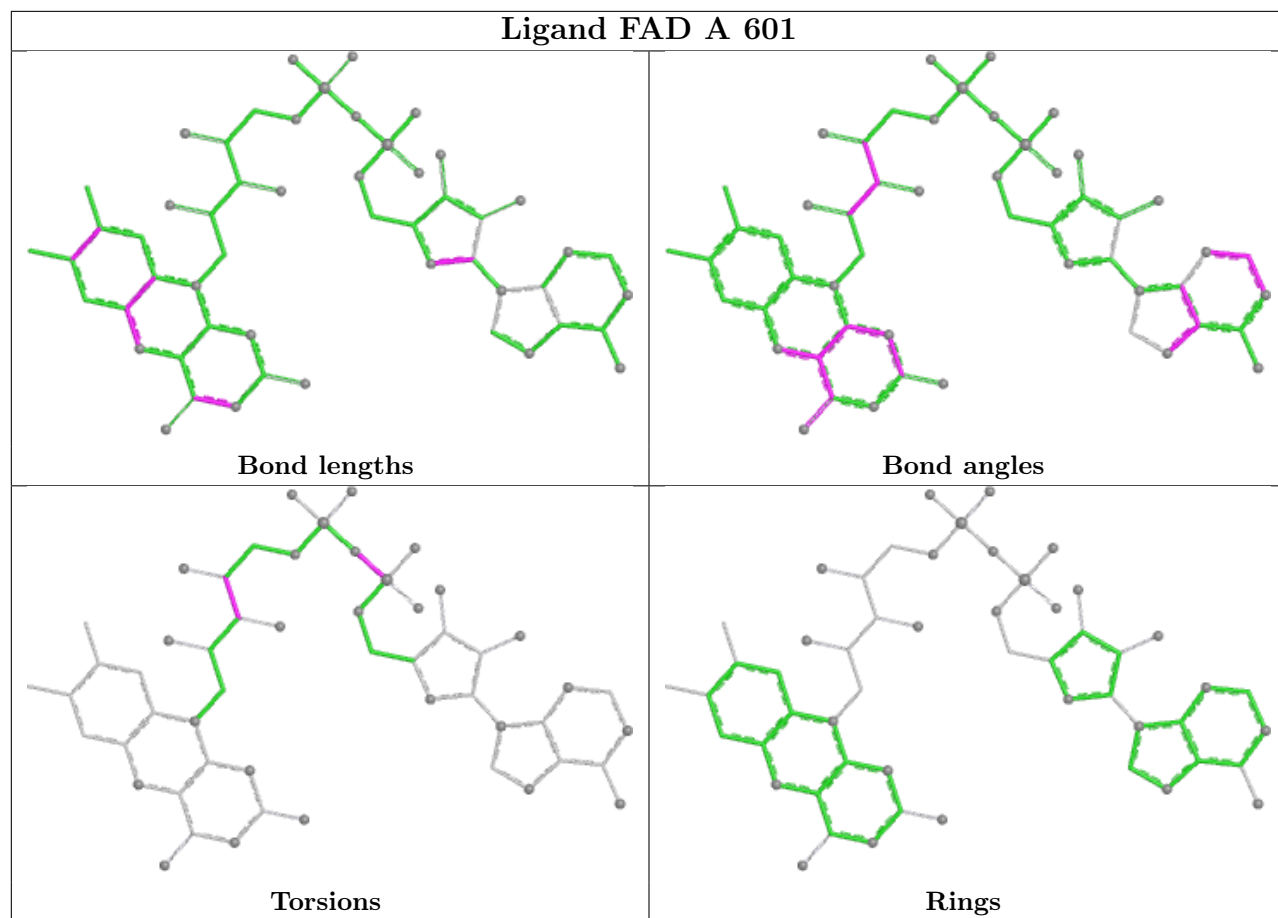
Mol	Chain	Res	Type	Atoms
3	B	601	FAD	PA-O3P-P-O2P
3	D	601	FAD	PA-O3P-P-O2P

There are no ring outliers.

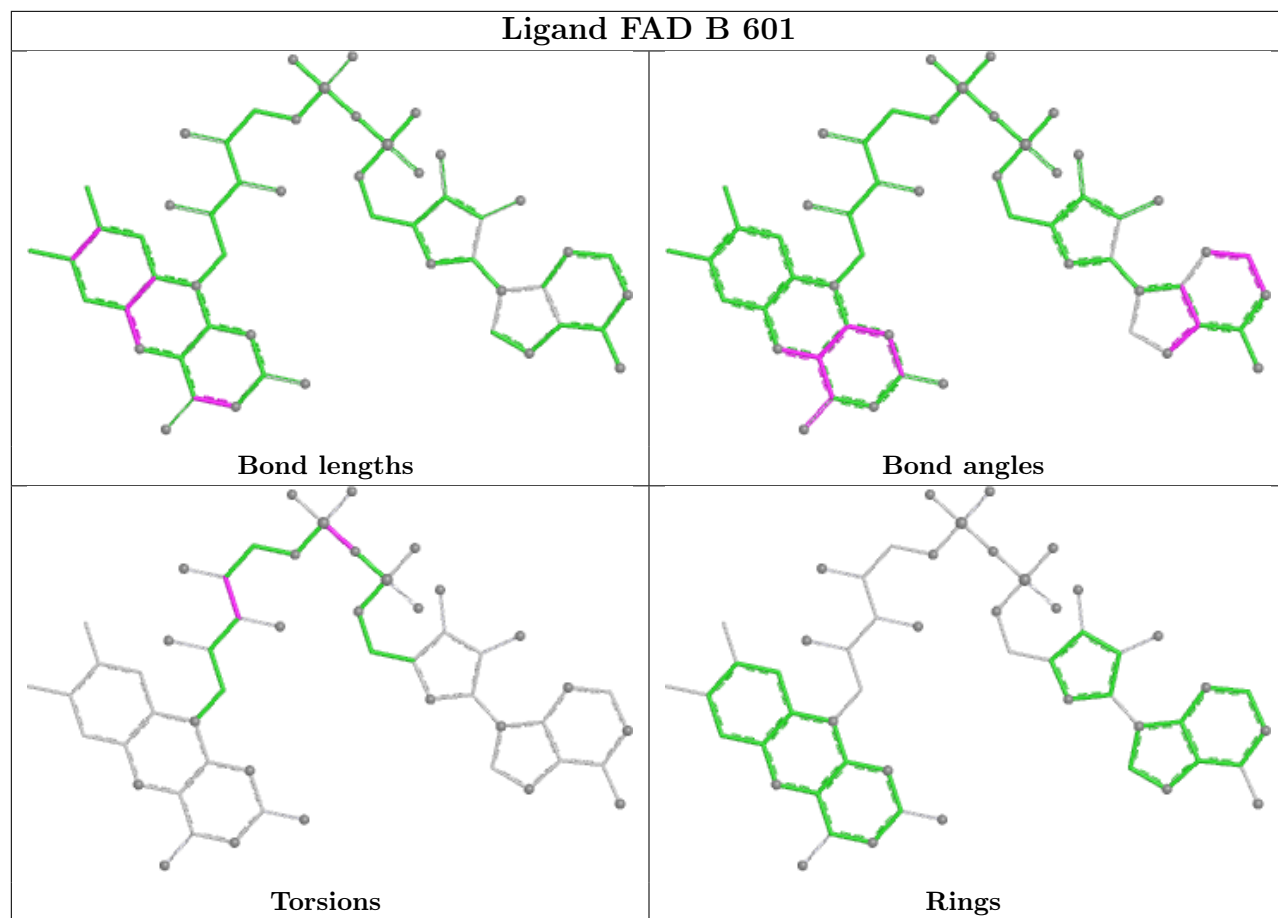
6 monomers are involved in 9 short contacts:

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

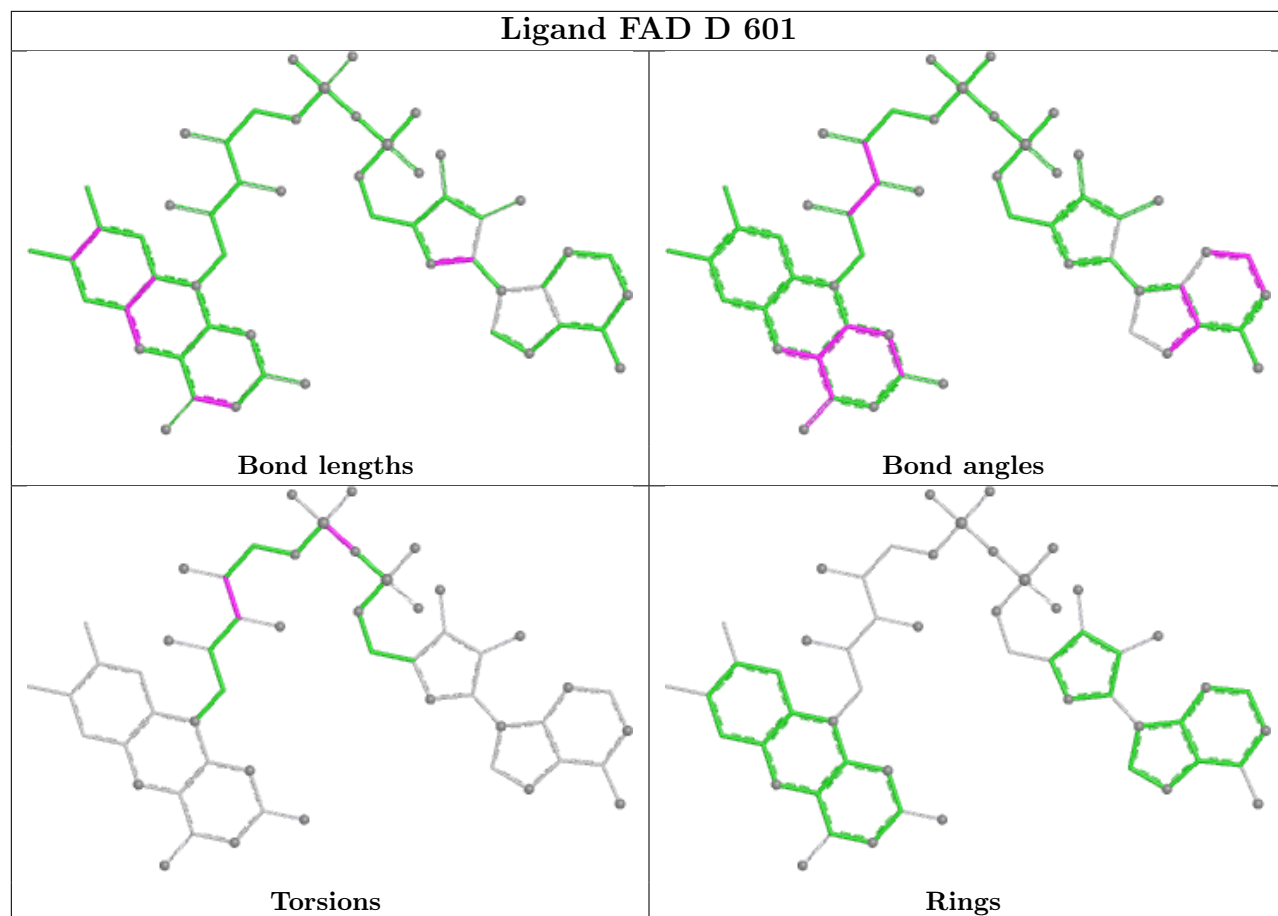
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



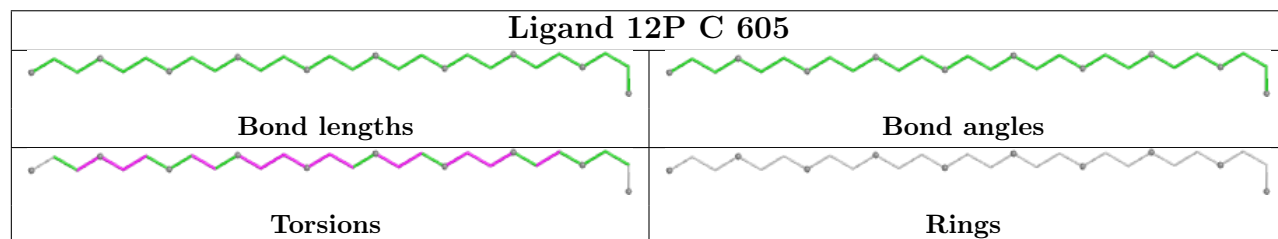
## Ligand FAD B 601

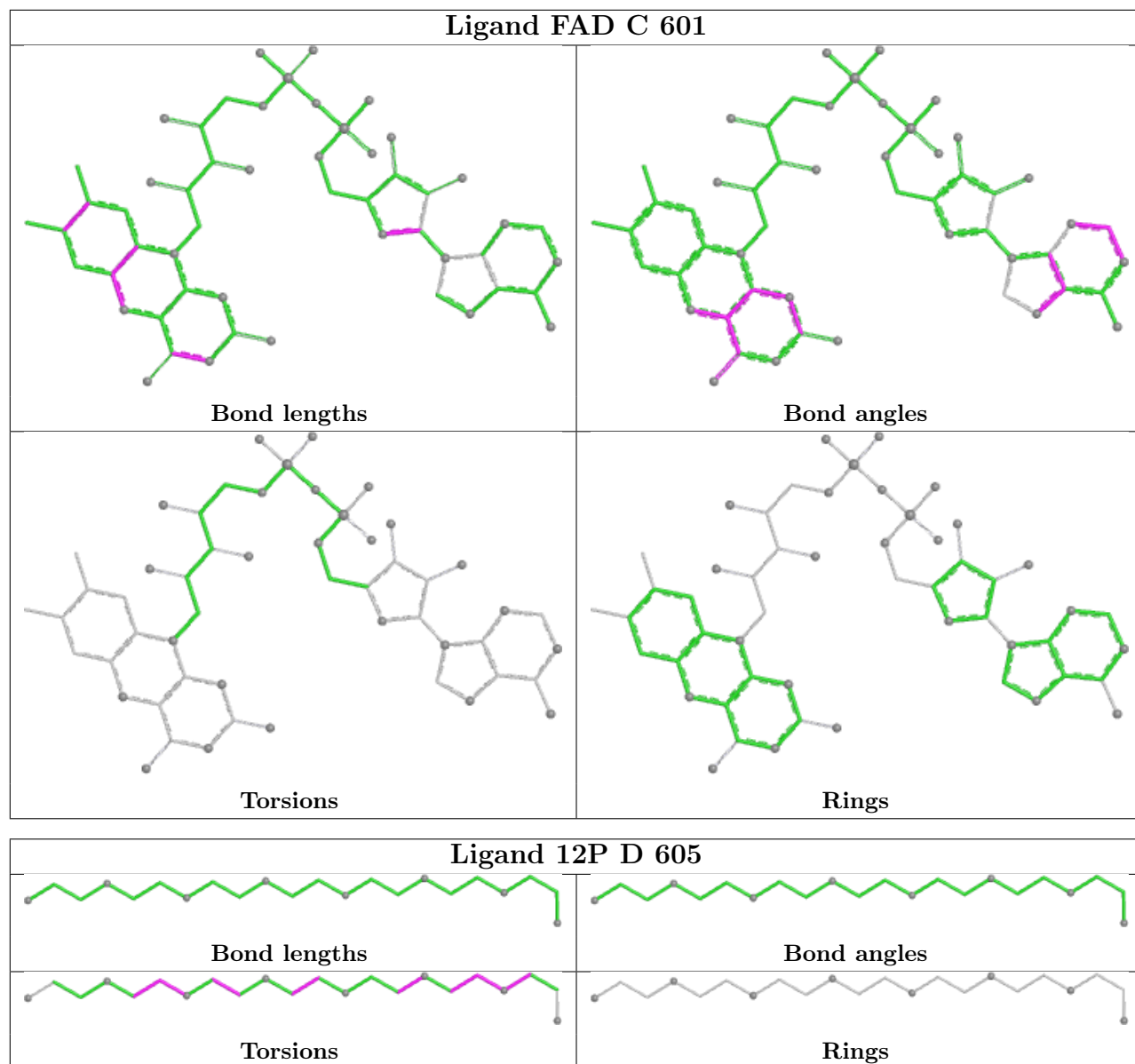


## Ligand FAD D 601



## Ligand 12P C 605





## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	498/538 (92%)	0.46	27 (5%) 32 29	28, 45, 76, 111	0
1	B	498/538 (92%)	0.84	58 (11%) 11 9	29, 56, 86, 114	0
1	C	496/538 (92%)	0.83	66 (13%) 8 7	30, 52, 80, 107	0
1	D	497/538 (92%)	0.84	86 (17%) 5 4	28, 50, 87, 114	0
All	All	1989/2152 (92%)	0.74	237 (11%) 10 8	28, 51, 84, 114	0

All (237) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	68	ILE	7.6
1	A	351	PHE	6.7
1	A	286	ASP	6.5
1	C	351	PHE	6.4
1	B	351	PHE	5.9
1	B	522	PHE	5.9
1	D	67	LEU	5.4
1	B	256	ILE	5.2
1	A	67	LEU	5.0
1	D	132	LEU	4.6
1	D	165	TRP	4.5
1	B	257	ASP	4.5
1	B	285	ALA	4.4
1	B	332	PHE	4.3
1	C	350	LYS	4.3
1	D	351	PHE	4.1
1	C	520	ALA	4.1
1	D	44	ALA	4.1
1	B	288	LYS	4.1
1	D	42	PHE	4.1
1	C	386	PHE	3.9

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

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Mol	Chain	Res	Type	RSRZ
1	A	287	GLU	3.1
1	D	350	LYS	3.0
1	A	65	ASN	3.0
1	C	353	GLU	3.0
1	C	289	GLN	3.0
1	D	327	SER	3.0
1	C	284	GLY	2.9
1	C	316	LEU	2.9
1	A	380	SER	2.9
1	D	302	LYS	2.9
1	C	375	LEU	2.9
1	D	427	GLN	2.9
1	D	164	ALA	2.9
1	B	287	GLU	2.9
1	B	283	GLY	2.9
1	D	328	TRP	2.9
1	D	318	LEU	2.9
1	C	270	ALA	2.8
1	C	251	THR	2.8
1	B	25	ASN	2.8
1	C	25	ASN	2.8
1	C	423	ASN	2.8
1	B	165	TRP	2.8
1	B	519	MET	2.8
1	A	68	ILE	2.8
1	D	288	LYS	2.8
1	D	435	ASP	2.8
1	D	522	PHE	2.8
1	D	304	VAL	2.8
1	C	163	ALA	2.7
1	D	254	VAL	2.7
1	C	283	GLY	2.7
1	C	472	LYS	2.7
1	B	312	LEU	2.7
1	D	422	TRP	2.7
1	D	244	LYS	2.7
1	C	287	GLU	2.6
1	B	387	ILE	2.6
1	A	114	ASP	2.6
1	D	421	ALA	2.6
1	D	423	ASN	2.6
1	D	307	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	424	GLN	2.6
1	C	311	LEU	2.6
1	B	307	SER	2.6
1	B	385	GLY	2.5
1	C	285	ALA	2.5
1	D	338	LEU	2.5
1	C	373	TYR	2.5
1	D	256	ILE	2.5
1	B	157	SER	2.5
1	C	94	SER	2.5
1	C	348	PHE	2.5
1	D	355	ALA	2.5
1	C	318	LEU	2.5
1	C	324	LEU	2.5
1	B	429	LYS	2.5
1	B	261	SER	2.5
1	D	349	LEU	2.5
1	D	134	SER	2.5
1	C	47	ASP	2.5
1	D	70	LYS	2.5
1	D	255	ALA	2.5
1	B	379	LEU	2.5
1	B	477	ASN	2.5
1	C	314	PRO	2.5
1	D	242	PRO	2.5
1	B	66	SER	2.4
1	D	326	MET	2.4
1	B	252	LYS	2.4
1	C	92	LYS	2.4
1	B	520	ALA	2.4
1	B	386	PHE	2.4
1	D	341	VAL	2.4
1	B	314	PRO	2.4
1	B	321	GLU	2.4
1	D	46	SER	2.4
1	D	94	SER	2.4
1	D	430	LYS	2.4
1	C	422	TRP	2.4
1	C	436	TRP	2.4
1	B	64	GLN	2.4
1	C	424	GLN	2.4
1	D	163	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	269	VAL	2.4
1	C	428	LYS	2.4
1	B	479	ILE	2.4
1	D	43	SER	2.4
1	B	254	VAL	2.3
1	D	319	VAL	2.3
1	B	94	SER	2.3
1	B	114	ASP	2.3
1	A	285	ALA	2.3
1	C	133	GLU	2.3
1	C	475	VAL	2.3
1	D	245	VAL	2.3
1	B	364	LYS	2.3
1	D	431	THR	2.3
1	C	328	TRP	2.3
1	A	45	ASP	2.3
1	D	334	TYR	2.3
1	D	37	ARG	2.3
1	A	523	ASP	2.3
1	B	342	SER	2.3
1	D	419	ILE	2.3
1	C	519	MET	2.3
1	C	253	ASN	2.3
1	A	473	THR	2.3
1	A	475	VAL	2.3
1	B	341	VAL	2.3
1	A	47	ASP	2.3
1	C	366	PRO	2.2
1	B	369	SER	2.2
1	C	317	GLY	2.2
1	D	158	LYS	2.2
1	D	324	LEU	2.2
1	D	345	ASN	2.2
1	D	373	TYR	2.2
1	C	250	VAL	2.2
1	C	448	VAL	2.2
1	D	420	VAL	2.2
1	B	447	PHE	2.2
1	B	45	ASP	2.2
1	D	325	GLU	2.2
1	A	373	TYR	2.2
1	D	55	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	281	VAL	2.2
1	B	439	LYS	2.2
1	A	369	SER	2.2
1	D	385	GLY	2.2
1	D	95	TRP	2.1
1	C	67	LEU	2.1
1	D	306	LYS	2.1
1	C	341	VAL	2.1
1	D	433	PHE	2.1
1	C	352	ASP	2.1
1	A	94	SER	2.1
1	C	46	SER	2.1
1	A	256	ILE	2.1
1	C	292	LEU	2.1
1	C	312	LEU	2.1
1	D	250	VAL	2.1
1	D	290	VAL	2.1
1	D	353	GLU	2.1
1	D	45	ASP	2.1
1	B	317	GLY	2.1
1	B	349	LEU	2.1
1	B	375	LEU	2.1
1	C	349	LEU	2.1
1	D	477	ASN	2.1
1	B	255	ALA	2.1
1	C	164	ALA	2.1
1	D	519	MET	2.1
1	B	319	VAL	2.1
1	A	433	PHE	2.1
1	A	435	ASP	2.1
1	C	379	LEU	2.1
1	D	436	TRP	2.1
1	D	340	THR	2.1
1	D	520	ALA	2.1
1	D	249	ARG	2.0
1	B	373	TYR	2.0
1	B	494	TYR	2.0
1	C	376	LEU	2.0
1	C	153	THR	2.0
1	D	53	PHE	2.0
1	D	332	PHE	2.0
1	D	157	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	425	SER	2.0
1	D	439	LYS	2.0
1	C	419	ILE	2.0
1	A	423	ASN	2.0
1	B	434	LEU	2.0
1	B	437	LEU	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](#)

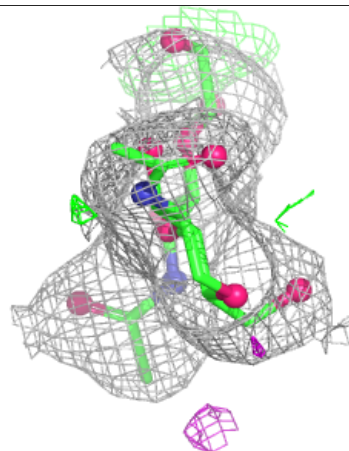
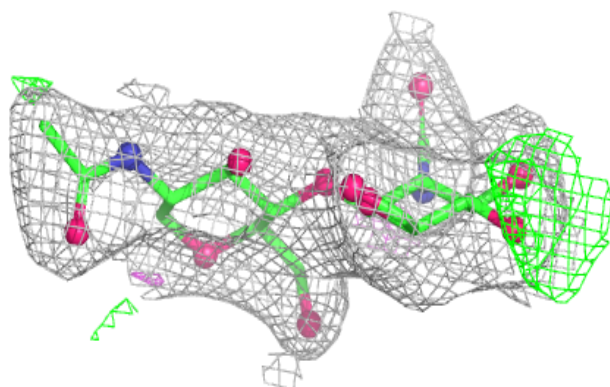
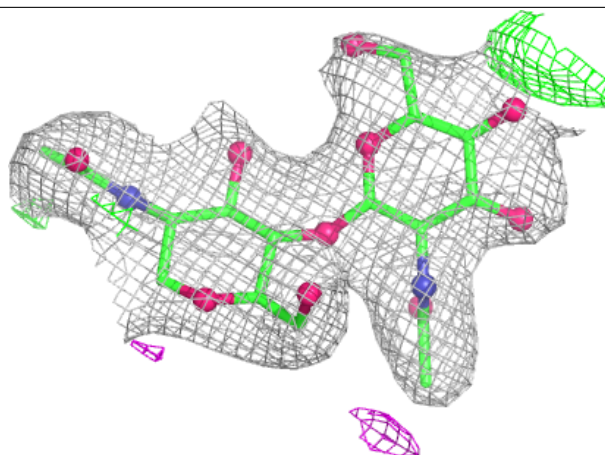
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	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.

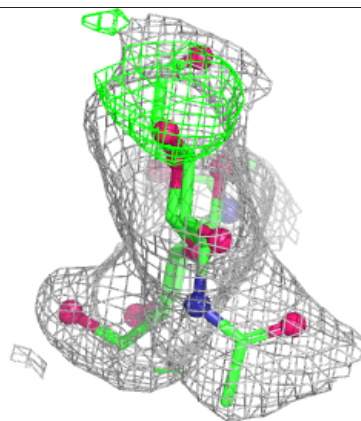
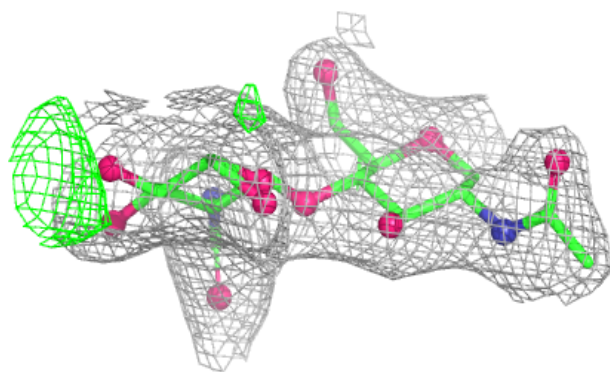
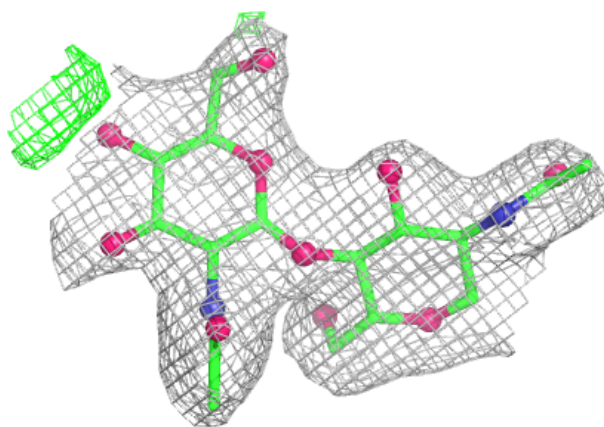
**Electron density around Chain E:**

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



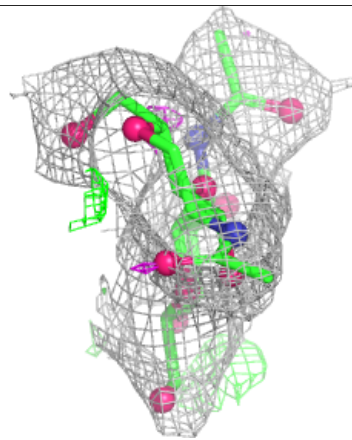
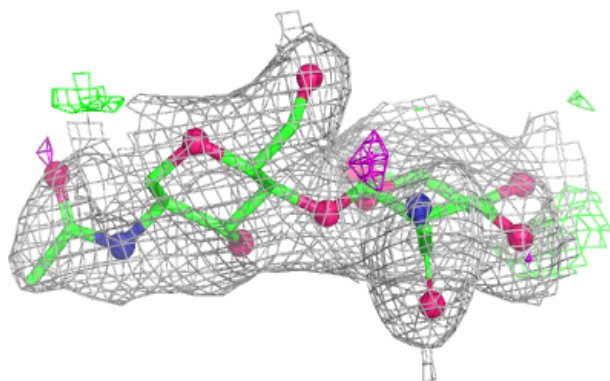
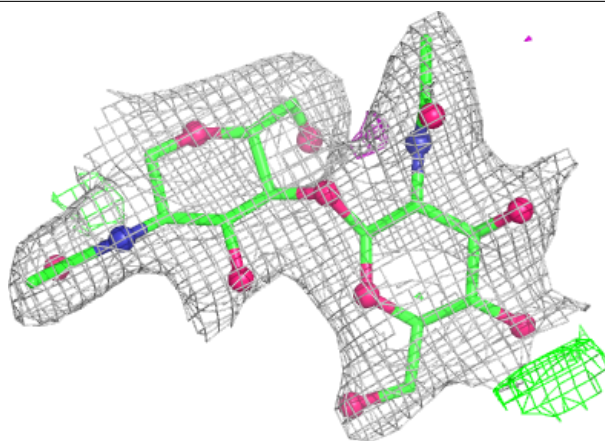
**Electron density around Chain F:**

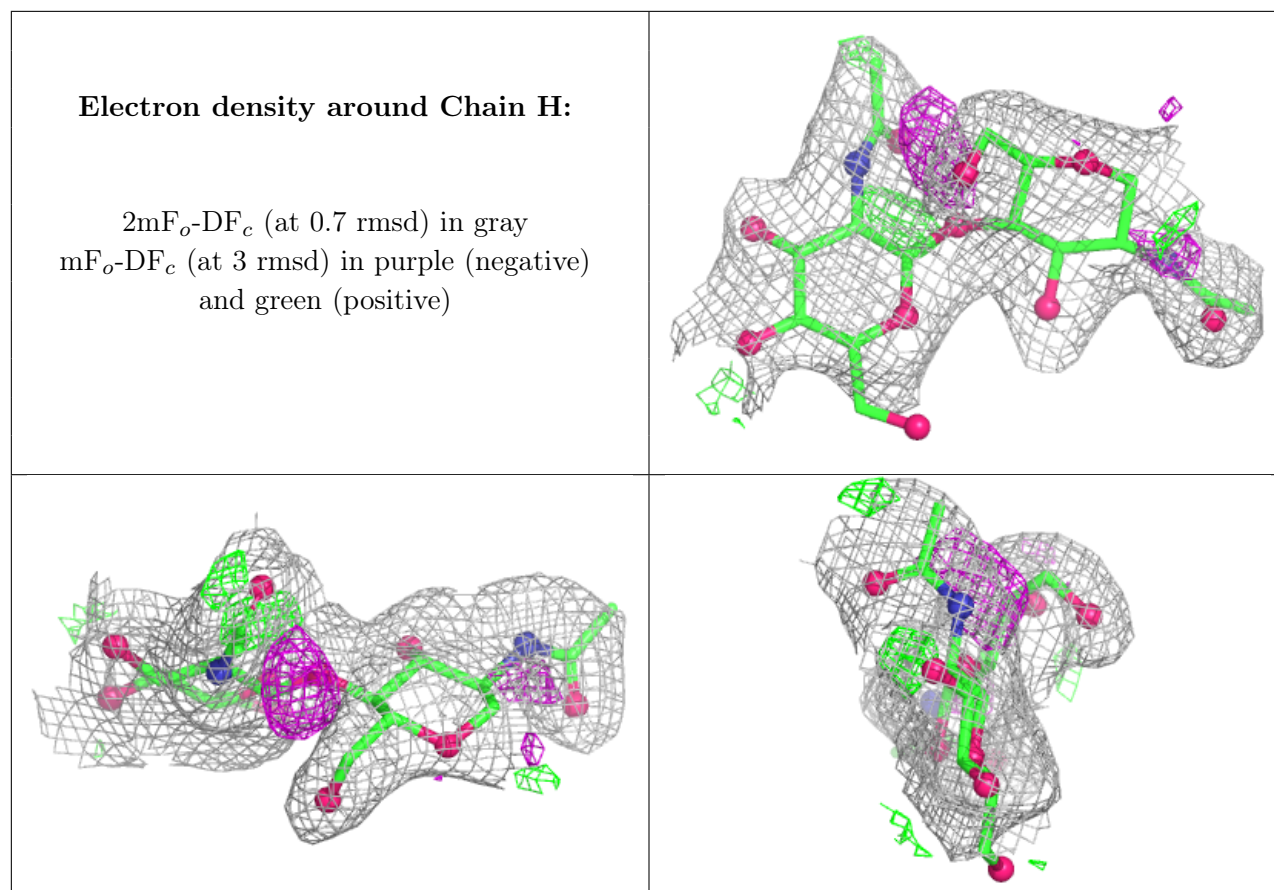
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



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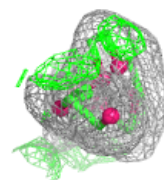
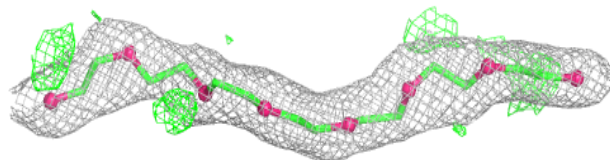
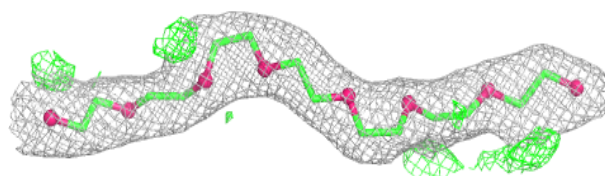
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	FAD	D	601	53/53	0.97	0.07	26,34,47,50	0
3	FAD	A	601	53/53	0.97	0.06	24,31,41,44	0

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.

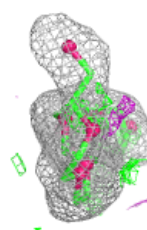
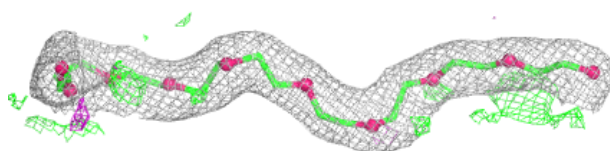
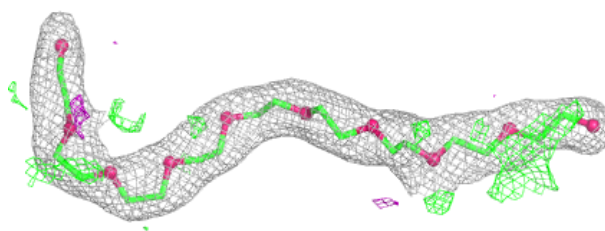
**Electron density around 12P D 605:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

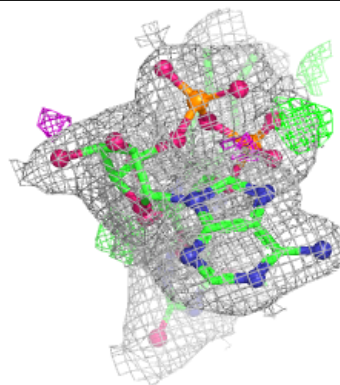
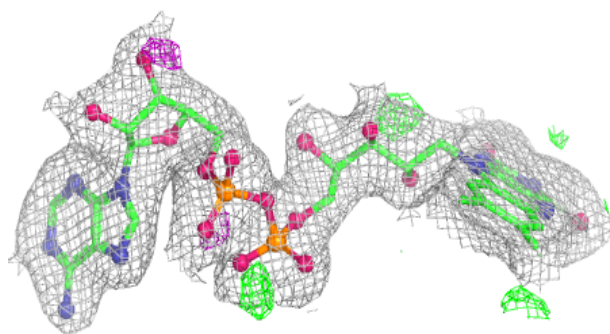
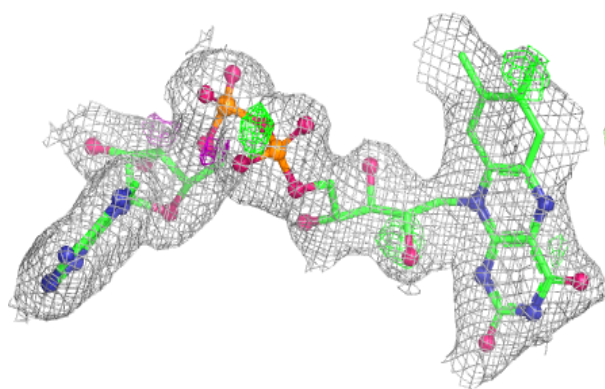


**Electron density around 12P C 605:**

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

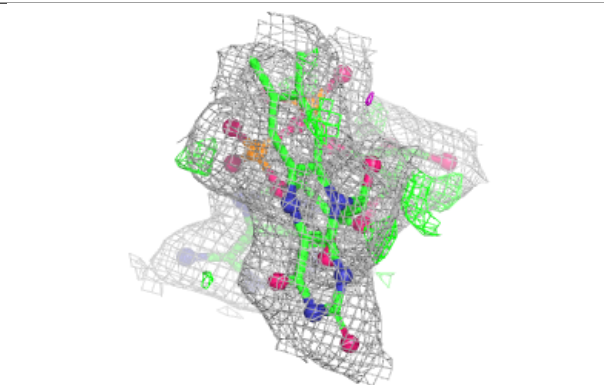
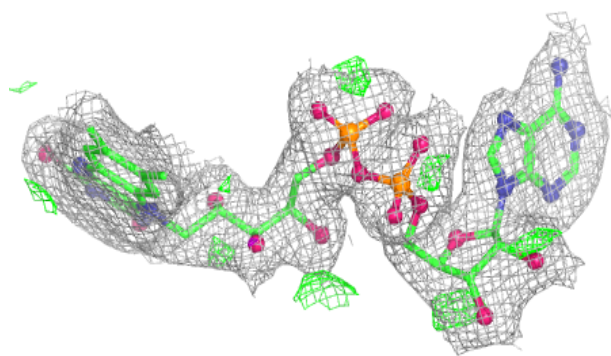
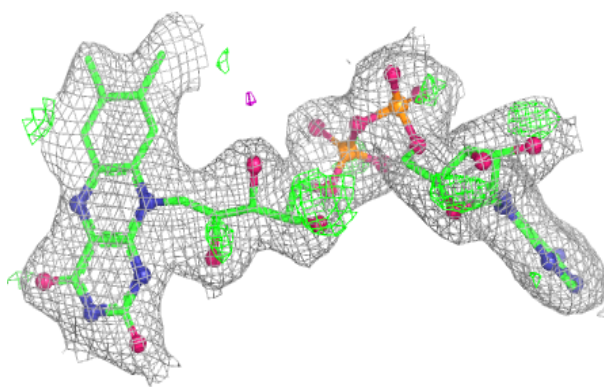
**Electron density around FAD C 601:**

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

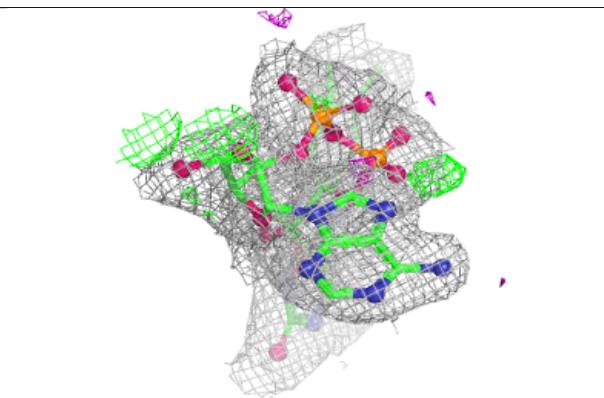
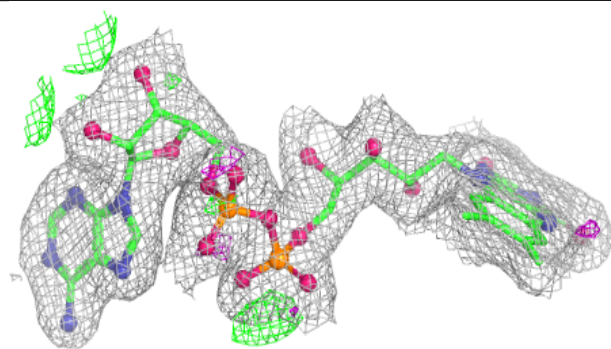
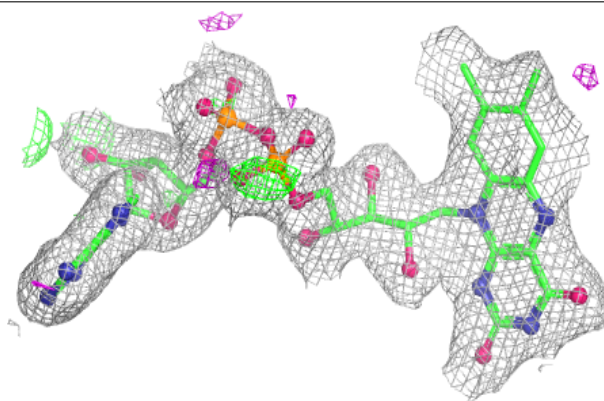


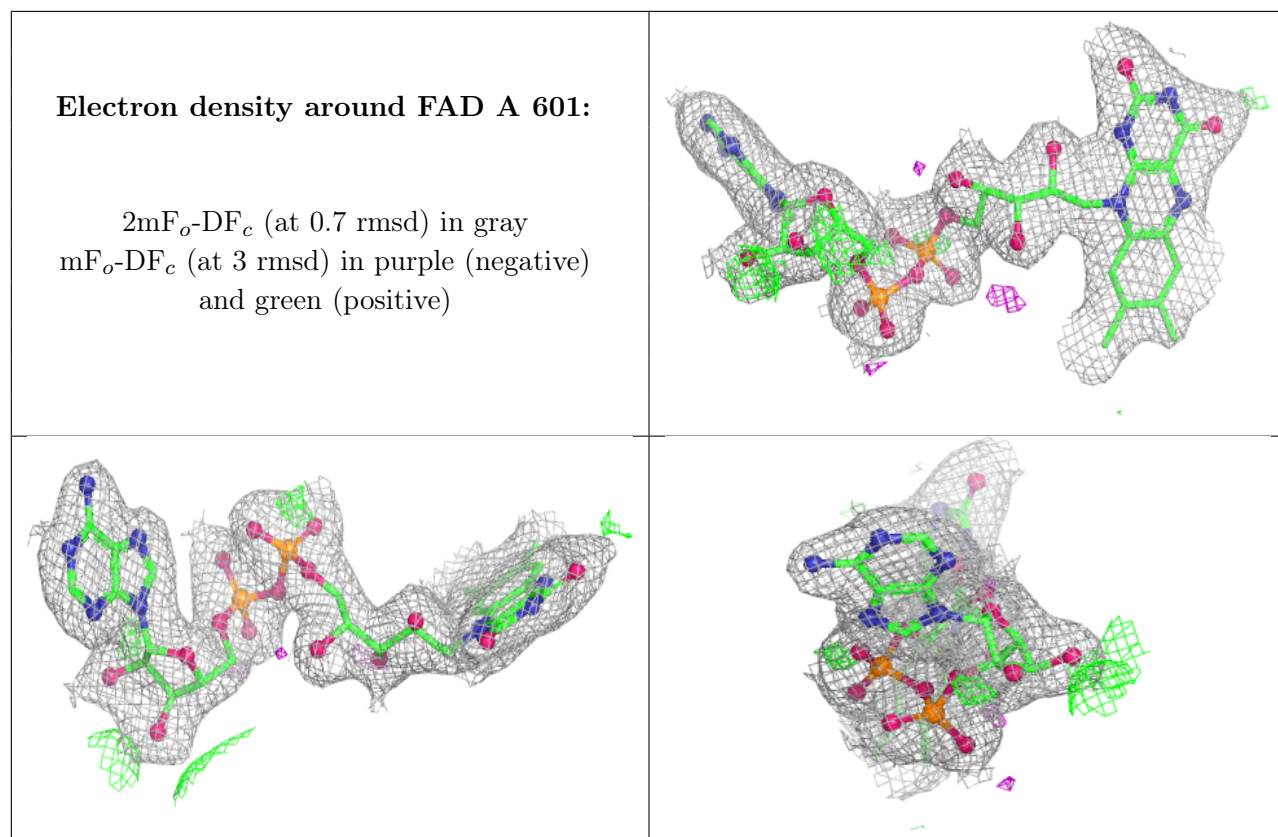
**Electron density around FAD B 601:**

$2mF_o-DF_c$  (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.