



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:59 AM UTC

PDB ID : 5TS5 / pdb_00005ts5
Title : Crystal structure of L-amino acid oxidase from Bothrops atrox
Authors : Feliciano, P.R.; Nonato, M.C.
Deposited on : 2016-10-27
Resolution : 2.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

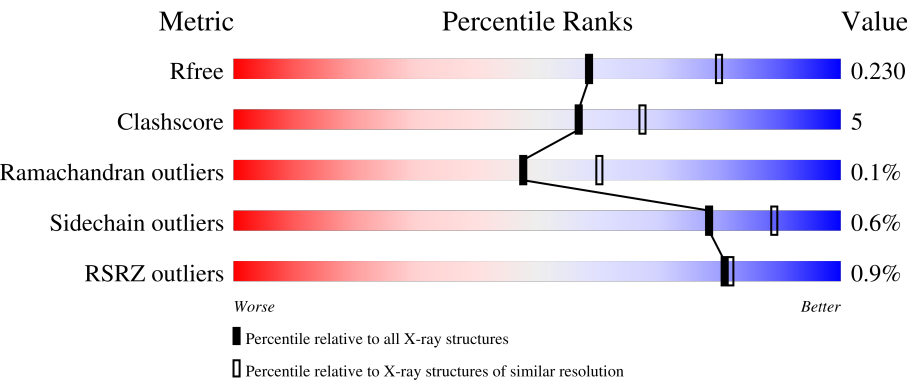
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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

Mol	Chain	Length	Quality of chain
1	A	484	% 89%11%
1	B	484	% 89%10%
1	C	484	87%12%
1	D	484	% 88%11%
2	E	2	100%

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Mol	Chain	Length	Quality of chain
2	F	2	 100%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 16605 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 Amine oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	483	Total	C	N	O	S	0	3	0
			3786	2408	643	721	14			
1	B	481	Total	C	N	O	S	0	8	0
			3814	2424	651	724	15			
1	C	480	Total	C	N	O	S	0	3	0
			3764	2400	635	715	14			
1	D	479	Total	C	N	O	S	0	3	0
			3755	2390	638	713	14			

There are 4 discrepancies between the modelled and reference sequences:

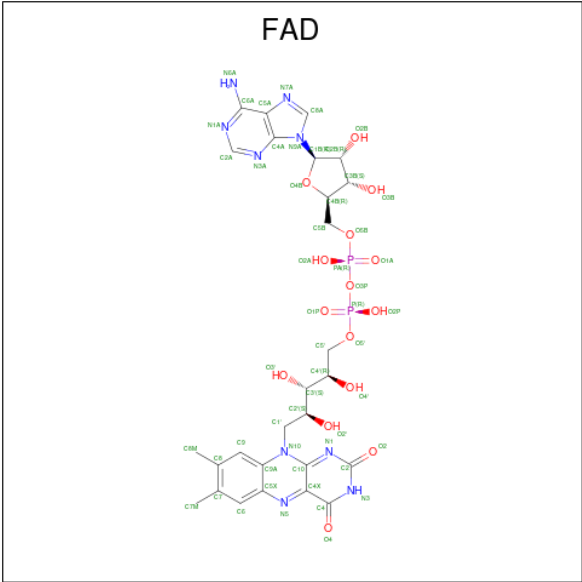
Chain	Residue	Modelled	Actual	Comment	Reference
A	409	GLN	HIS	conflict	UNP A0A0S1LJ33
B	409	GLN	HIS	conflict	UNP A0A0S1LJ33
C	409	GLN	HIS	conflict	UNP A0A0S1LJ33
D	409	GLN	HIS	conflict	UNP A0A0S1LJ33

- Molecule 2 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	2	Total	C	N	O	0	0	0
			24	14	1	9			
2	F	2	Total	C	N	O	0	0	0
			24	14	1	9			

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

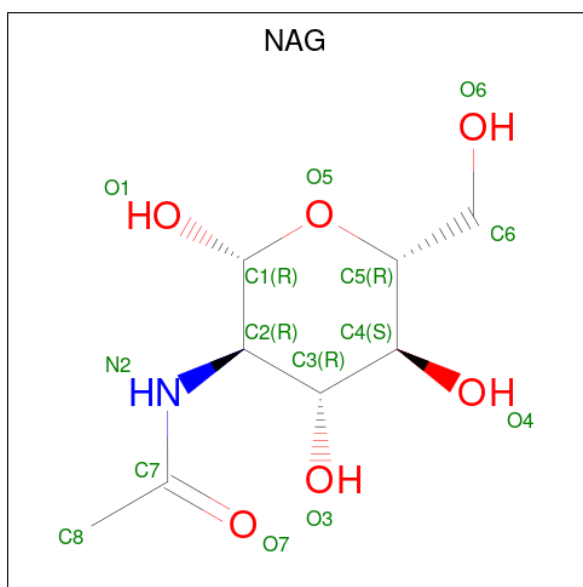


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

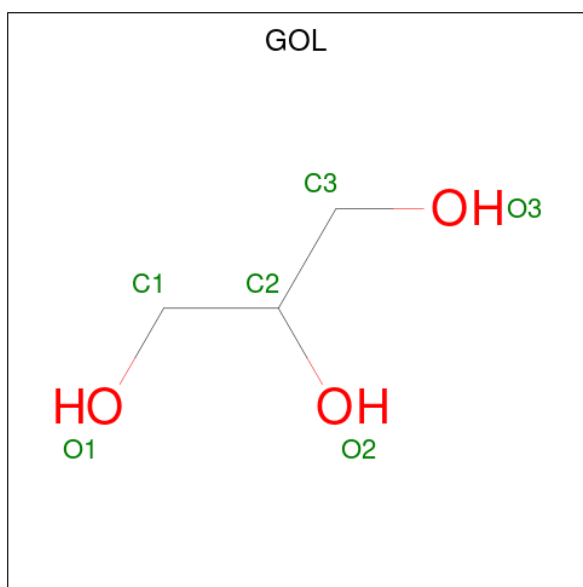
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	Zn	0	0
			3	3		
4	B	3	Total	Zn	0	1
			4	4		
4	C	3	Total	Zn	0	0
			3	3		
4	D	2	Total	Zn	0	0
			2	2		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		

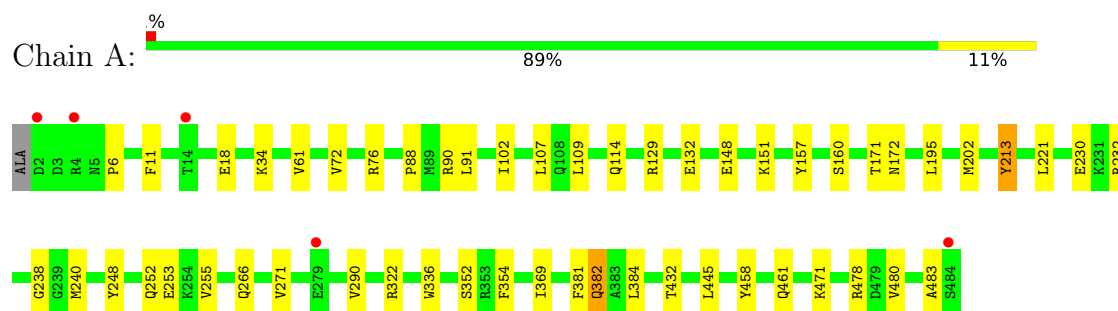
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	296	Total 297	O 297	0	1
7	B	279	Total 279	O 279	0	0
7	C	290	Total 290	O 290	0	0
7	D	299	Total 300	O 300	0	1

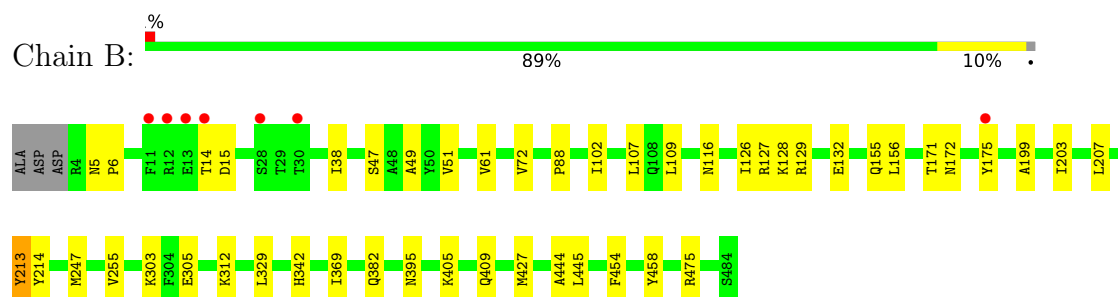
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

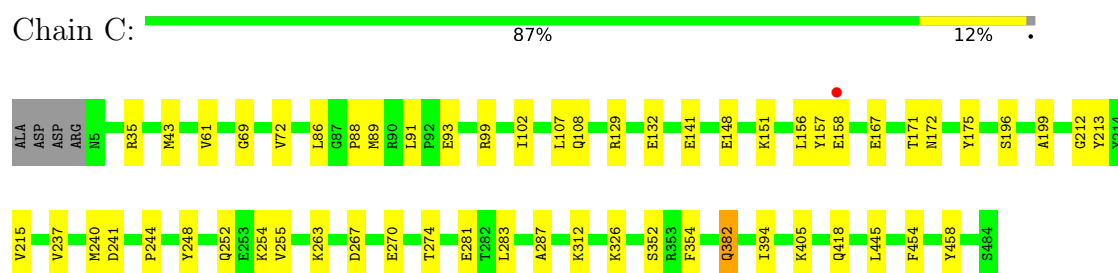
• Molecule 1: Amine oxidase



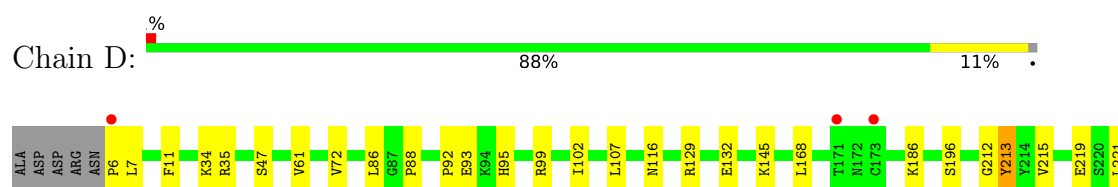
• Molecule 1: Amine oxidase



• Molecule 1: Amine oxidase



• Molecule 1: Amine oxidase





- Molecule 2: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  100%



- Molecule 2: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  100%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	73.64Å 123.92Å 105.08Å 90.00° 96.03° 90.00°	Depositor
Resolution (Å)	34.57 – 2.30 34.57 – 2.30	Depositor EDS
% Data completeness (in resolution range)	96.1 (34.57-2.30) 87.8 (34.57-2.30)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 2.29Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.180 , 0.230 0.181 , 0.230	Depositor DCC
R_{free} test set	3989 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å ²)	16.1	Xtriage
Anisotropy	0.150	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 46.8	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	0.93	EDS
Total number of atoms	16605	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.69% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, ZN, GOL, FUC, 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	0.17	1/3872 (0.0%)	0.32	0/5255
1	B	0.20	2/3899 (0.1%)	0.34	0/5287
1	C	0.17	0/3850	0.44	7/5227 (0.1%)
1	D	0.17	0/3840	0.33	0/5208
All	All	0.18	3/15461 (0.0%)	0.36	7/20977 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	214	TYR	C-O	-6.33	1.15	1.24
1	A	213	TYR	C-O	-5.14	1.17	1.24
1	B	213	TYR	C-O	-5.03	1.17	1.24

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	158	GLU	CA-CB-CG	10.72	135.53	114.10
1	C	158	GLU	N-CA-CB	-9.73	95.90	110.01
1	C	158	GLU	CB-CA-C	7.47	122.60	110.88
1	C	158	GLU	CG-CD-OE1	-7.41	101.37	118.40
1	C	158	GLU	CG-CD-OE2	7.36	135.34	118.40
1	C	157	TYR	CA-C-N	5.34	127.38	120.44
1	C	157	TYR	C-N-CA	5.34	127.38	120.44

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3786	0	3613	34	0
1	B	3814	0	3654	34	0
1	C	3764	0	3587	40	0
1	D	3755	0	3604	33	0
2	E	24	0	21	0	0
2	F	24	0	22	0	0
3	A	53	0	30	2	0
3	B	53	0	30	2	0
3	C	53	0	30	2	0
3	D	53	0	30	2	0
4	A	3	0	0	0	0
4	B	4	0	0	0	0
4	C	3	0	0	0	0
4	D	2	0	0	0	0
5	A	14	0	13	0	0
5	B	14	0	13	0	0
5	D	14	0	13	0	0
6	A	6	0	8	0	0
7	A	297	0	0	2	0
7	B	279	0	0	2	0
7	C	290	0	0	1	0
7	D	300	0	0	1	0
All	All	16605	0	14668	137	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (137) 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:C:167:GLU:O	1:C:171:THR:HG22	1.87	0.75
1:C:129:ARG:HB2	1:C:132:GLU:HG3	1.71	0.72
1:A:72:VAL:HG22	1:A:88:PRO:HG2	1.72	0.71
1:D:129:ARG:HB2	1:D:132:GLU:HG3	1.73	0.71
1:B:303:LYS:NZ	1:B:305:GLU:OE2	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:ILE:HG23	1:A:107:LEU:HB2	1.74	0.70
1:C:102:ILE:HG23	1:C:107:LEU:HB2	1.74	0.69
1:C:382:GLN:OE1	1:D:382:GLN:NE2	2.27	0.67
1:B:312:LYS:NZ	1:B:444:ALA:O	2.28	0.66
1:A:129:ARG:HB2	1:A:132:GLU:HG3	1.77	0.66
1:C:72:VAL:HG22	1:C:88:PRO:HG2	1.76	0.66
1:D:7:LEU:HD23	1:D:168:LEU:HD22	1.78	0.65
1:C:43:MET:HE2	1:C:43:MET:HA	1.78	0.64
1:A:18:GLU:OE1	1:A:478:ARG:NH2	2.30	0.64
1:B:102:ILE:HG23	1:B:107:LEU:HB2	1.79	0.63
1:C:254:LYS:NZ	7:C:602:HOH:O	2.29	0.62
1:D:72:VAL:HG22	1:D:88:PRO:HG2	1.80	0.62
1:A:271:VAL:HG21	1:A:290:VAL:HG23	1.80	0.62
1:D:312:LYS:NZ	1:D:444:ALA:O	2.31	0.62
1:B:72:VAL:HG22	1:B:88:PRO:HG2	1.79	0.62
1:B:129:ARG:HB2	1:B:132:GLU:HG3	1.81	0.62
1:A:381:PHE:HA	1:A:384:LEU:HD23	1.82	0.61
1:B:171:THR:HG21	1:B:175:TYR:CD1	2.36	0.61
1:B:156:LEU:HD13	1:B:199:ALA:HB1	1.81	0.61
1:D:265:GLN:NE2	7:D:602:HOH:O	2.29	0.60
1:D:102:ILE:HG23	1:D:107:LEU:HB2	1.86	0.58
1:B:171:THR:HG21	1:B:175:TYR:CG	2.40	0.57
1:C:171:THR:HG23	1:C:172:ASN:H	1.71	0.56
1:D:145:LYS:HG3	1:D:196:SER:HB3	1.87	0.56
1:D:47:SER:HA	1:D:247:MET:HE1	1.88	0.56
1:A:266:GLN:HG3	1:A:271:VAL:HG12	1.89	0.55
1:A:322:ARG:HD2	1:A:432:THR:OG1	2.06	0.54
1:A:102:ILE:HD13	1:A:109:LEU:HD21	1.90	0.54
1:D:312:LYS:HE2	1:D:454:PHE:CE2	2.43	0.53
1:A:61:VAL:HB	1:A:255:VAL:HA	1.90	0.53
1:C:312:LYS:HE2	1:C:454:PHE:CE2	2.44	0.52
1:B:329:LEU:HB2	1:B:369:ILE:HG13	1.91	0.52
1:A:148:GLU:HA	1:A:151:LYS:HD2	1.93	0.51
1:B:445:LEU:HD22	1:B:458:TYR:CD2	2.46	0.51
1:C:89:MET:HE3	1:C:326:LYS:NZ	2.26	0.51
1:C:61:VAL:HB	1:C:255:VAL:HA	1.92	0.50
1:A:11:PHE:HZ	1:A:221:LEU:HB3	1.75	0.50
1:B:128:LYS:NZ	1:C:141:GLU:OE1	2.44	0.50
1:C:91:LEU:HD11	1:C:240:MET:HE1	1.94	0.49
1:B:312:LYS:HE2	1:B:454:PHE:CD2	2.47	0.49
1:C:171:THR:OG1	1:C:172:ASN:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:88:PRO:HA	3:C:501:FAD:C4X	2.43	0.49
1:C:171:THR:HG23	1:C:172:ASN:N	2.28	0.49
1:A:88:PRO:HA	3:A:501:FAD:N5	2.27	0.49
1:D:445:LEU:HD22	1:D:458:TYR:CD2	2.48	0.49
1:D:61:VAL:HB	1:D:255:VAL:HA	1.96	0.48
1:B:445:LEU:HD22	1:B:458:TYR:HD2	1.78	0.48
1:A:253:GLU:H	1:A:253:GLU:CD	2.21	0.48
1:A:461:GLN:OE1	1:A:471:LYS:NZ	2.46	0.48
1:B:127:ARG:O	1:B:128:LYS:HD2	2.14	0.48
1:A:34:LYS:NZ	1:A:480:VAL:O	2.46	0.47
1:C:263:LYS:HB3	1:C:274:THR:HB	1.95	0.47
1:C:171:THR:CG2	1:C:172:ASN:H	2.27	0.47
1:C:394:ILE:HG22	1:C:405:LYS:HG3	1.97	0.47
1:B:312:LYS:HE2	1:B:454:PHE:CE2	2.49	0.47
1:B:475:ARG:NH1	7:B:620:HOH:O	2.47	0.47
1:D:445:LEU:HD22	1:D:458:TYR:HD2	1.80	0.47
1:C:43:MET:HE3	1:C:244:PRO:HG3	1.96	0.46
1:B:61:VAL:HB	1:B:255:VAL:HA	1.98	0.46
1:C:93:GLU:HA	1:C:99:ARG:CZ	2.45	0.46
1:D:382:GLN:OE1	1:D:421[B]:SER:OG	2.28	0.46
1:A:382:GLN:OE1	1:B:382:GLN:NE2	2.47	0.46
1:C:88:PRO:HA	3:C:501:FAD:N5	2.30	0.46
1:C:445:LEU:HD22	1:C:458:TYR:CD2	2.50	0.46
1:A:445:LEU:HD22	1:A:458:TYR:HD2	1.81	0.45
1:C:171:THR:OG1	1:C:175:TYR:HB3	2.16	0.45
1:B:38:ILE:HD12	1:B:49:ALA:HB2	1.98	0.45
1:B:88:PRO:HA	3:B:501:FAD:N5	2.30	0.45
1:C:241:ASP:C	1:C:244:PRO:HD2	2.41	0.45
1:D:11:PHE:CZ	1:D:221:LEU:HB3	2.51	0.45
1:B:88:PRO:HA	3:B:501:FAD:C4X	2.46	0.45
1:D:116:ASN:ND2	1:D:342:HIS:H	2.15	0.45
1:A:11:PHE:CZ	1:A:221:LEU:HB3	2.51	0.45
1:C:445:LEU:HD22	1:C:458:TYR:HD2	1.81	0.45
1:D:88:PRO:HA	3:D:501:FAD:N5	2.32	0.45
1:B:47:SER:O	1:B:51:VAL:HG22	2.17	0.44
1:C:86:LEU:HB3	1:C:418:GLN:HG2	1.99	0.44
1:B:203:ILE:HG23	1:B:207:LEU:HD12	1.99	0.44
1:C:281:GLU:OE2	1:C:283:LEU:HD21	2.17	0.44
1:D:266:GLN:HA	1:D:271:VAL:HA	2.00	0.44
1:C:212:GLY:O	1:C:215:VAL:HG22	2.18	0.44
1:C:248:TYR:CZ	1:C:252:GLN:HG3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:ARG:NH2	1:A:238:GLY:O	2.49	0.43
1:A:160:SER:HB3	1:A:195:LEU:HD11	2.01	0.43
1:A:157:TYR:O	1:A:160:SER:OG	2.34	0.43
1:B:116:ASN:ND2	1:B:342:HIS:H	2.16	0.43
1:C:89:MET:HE3	1:C:326:LYS:HZ2	1.83	0.43
1:A:90:ARG:NH1	1:A:114:GLN:OE1	2.50	0.43
1:D:99:ARG:NH2	1:D:234:ASP:OD1	2.42	0.43
1:D:186:LYS:HB2	1:D:213:TYR:CG	2.53	0.43
1:D:219:GLU:OE2	1:D:432:THR:HA	2.18	0.43
1:A:6:PRO:O	7:A:601:HOH:O	2.21	0.43
1:A:91:LEU:HD11	1:A:240:MET:HE1	2.00	0.43
1:B:405:LYS:HE3	1:B:409:GLN:NE2	2.33	0.43
1:D:34:LYS:HD3	1:D:289:TYR:CE2	2.54	0.43
1:A:336:TRP:CE3	1:A:369:ILE:HD11	2.54	0.42
1:D:88:PRO:HA	3:D:501:FAD:C4X	2.48	0.42
1:B:171:THR:HB	1:B:172:ASN:H	1.59	0.42
1:C:108:GLN:HG2	1:C:237:VAL:HG21	2.02	0.42
1:C:148:GLU:HA	1:C:151:LYS:HD2	2.02	0.42
1:A:266:GLN:NE2	7:A:629:HOH:O	2.52	0.42
1:A:72:VAL:HA	1:A:88:PRO:HD2	2.02	0.42
1:B:126:ILE:HG22	1:B:128:LYS:HD3	2.01	0.42
1:B:395[B]:ASN:OD1	1:B:405:LYS:NZ	2.42	0.42
1:A:248:TYR:CZ	1:A:252:GLN:HG3	2.55	0.42
1:D:247:MET:HE2	1:D:247:MET:HB3	1.94	0.42
1:B:247:MET:HE3	1:B:247:MET:HB2	1.92	0.41
1:D:35:ARG:O	1:D:287:ALA:HB1	2.20	0.41
1:B:14:THR:HA	1:B:15:ASP:HA	1.77	0.41
1:D:6:PRO:HB2	1:D:7:LEU:H	1.58	0.41
1:B:155:GLN:OE1	7:B:601:HOH:O	2.22	0.41
1:C:156:LEU:HD13	1:C:199:ALA:HB1	2.02	0.41
1:D:86:LEU:HB3	1:D:418:GLN:HG2	2.03	0.41
1:A:88:PRO:HA	3:A:501:FAD:C4X	2.50	0.41
1:C:352:SER:O	1:C:354:PHE:N	2.49	0.41
1:A:384:LEU:HD21	1:B:427:MET:HE3	2.03	0.41
1:B:5:ASN:HA	1:B:6:PRO:HD2	1.95	0.41
1:C:171:THR:HG21	1:C:175:TYR:HD2	1.86	0.41
1:D:352:SER:O	1:D:354:PHE:N	2.51	0.41
1:A:171:THR:OG1	1:A:172:ASN:N	2.53	0.41
1:A:230:GLU:HG3	1:A:232:ARG:H	1.86	0.41
1:D:92:PRO:HG2	1:D:95:HIS:CE1	2.56	0.41
1:D:416:MET:HE3	1:D:416:MET:HB2	1.88	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:ILE:HD13	1:B:109:LEU:HD21	2.03	0.40
1:C:35:ARG:O	1:C:287:ALA:HB1	2.22	0.40
1:D:212:GLY:O	1:D:215:VAL:HG22	2.22	0.40
1:C:148:GLU:OE1	1:C:196:SER:OG	2.36	0.40
1:C:267:ASP:OD1	1:C:270:GLU:N	2.45	0.40
1:D:95:HIS:O	1:D:99:ARG:HD2	2.21	0.40
1:A:352:SER:O	1:A:354:PHE:N	2.50	0.40
1:C:69:GLY:HA2	1:C:244:PRO:HB3	2.03	0.40
1:D:348:THR:O	1:D:353:ARG:HA	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	484/484 (100%)	469 (97%)	14 (3%)	1 (0%)	43	55
1	B	487/484 (101%)	471 (97%)	16 (3%)	0	100	100
1	C	481/484 (99%)	465 (97%)	16 (3%)	0	100	100
1	D	480/484 (99%)	465 (97%)	15 (3%)	0	100	100
All	All	1932/1936 (100%)	1870 (97%)	61 (3%)	1 (0%)	48	60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	483	ALA

5.3.2 Protein sidechains [i](#)

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	390/416 (94%)	387 (99%)	3 (1%)	73	86
1	B	393/416 (94%)	392 (100%)	1 (0%)	86	93
1	C	385/416 (92%)	383 (100%)	2 (0%)	81	90
1	D	388/416 (93%)	384 (99%)	4 (1%)	68	82
All	All	1556/1664 (94%)	1546 (99%)	10 (1%)	78	89

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	202	MET
1	A	213	TYR
1	A	382	GLN
1	B	213	TYR
1	C	213	TYR
1	C	382	GLN
1	D	93	GLU
1	D	213	TYR
1	D	267	ASP
1	D	369	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	GLN
1	A	110	ASN
1	A	125	ASN
1	A	258	ASN
1	B	249	GLN
1	B	252	GLN
1	B	402	GLN
1	C	25	ASN
1	C	249	GLN
1	C	258	ASN
1	C	439	GLN
1	D	125	ASN
1	D	178	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 ⓘ

4 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	1,2	14,14,15	0.20	0	17,19,21	0.87	1 (5%)
2	FUC	E	2	2	10,10,11	0.93	1 (10%)	14,14,16	1.33	2 (14%)
2	NAG	F	1	1,2	14,14,15	0.36	0	17,19,21	0.45	0
2	FUC	F	2	2	10,10,11	0.96	0	14,14,16	1.00	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	1,2	-	1/6/23/26	0/1/1/1
2	FUC	E	2	2	-	-	0/1/1/1
2	NAG	F	1	1,2	-	2/6/23/26	0/1/1/1
2	FUC	F	2	2	-	-	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	2	FUC	O5-C5	2.22	1.48	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	2	FUC	C1-O5-C5	3.16	120.42	112.97
2	E	2	FUC	O5-C5-C4	2.97	114.89	109.55
2	E	1	NAG	C1-O5-C5	2.87	116.03	112.19

There are no chirality outliers.

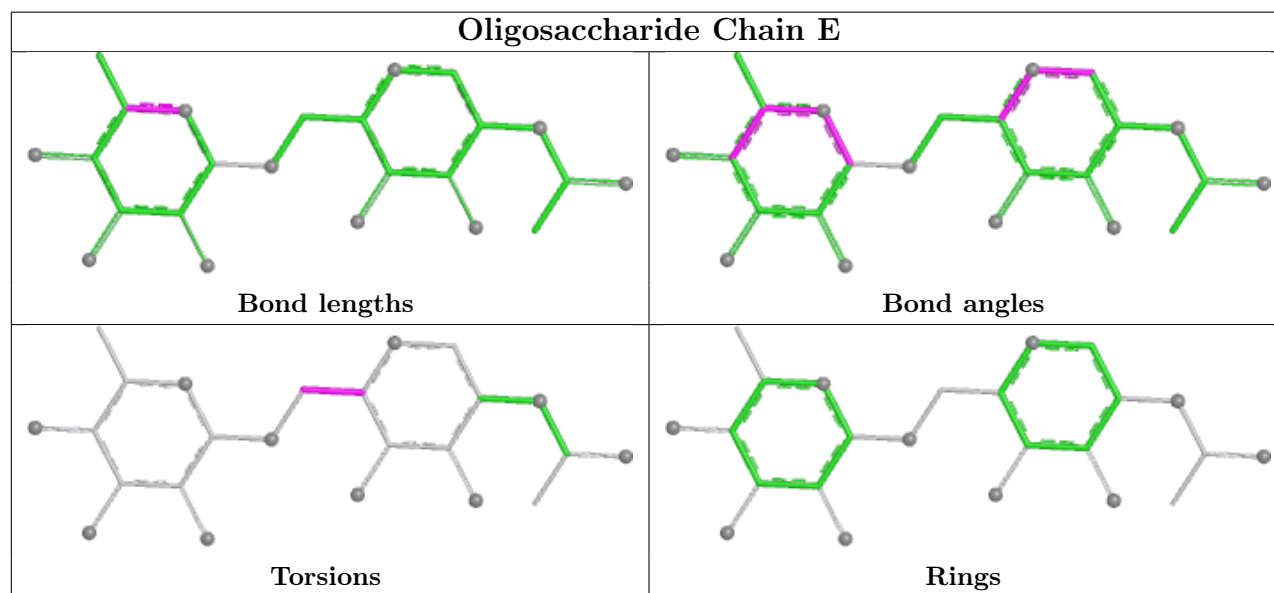
All (3) torsion outliers are listed below:

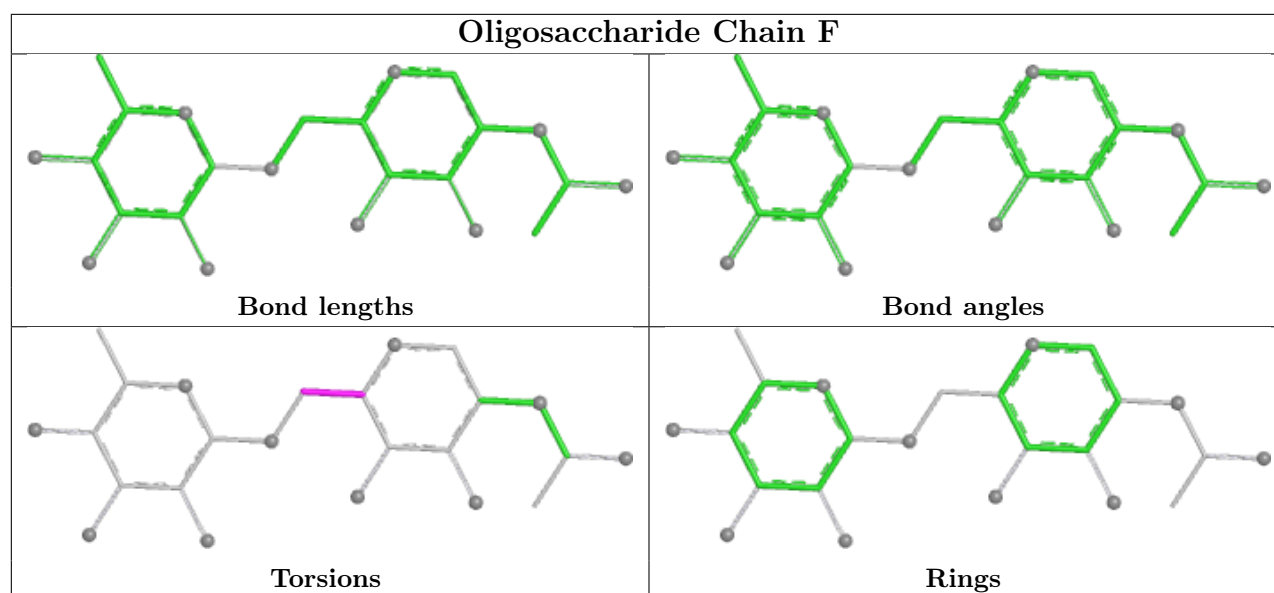
Mol	Chain	Res	Type	Atoms
2	F	1	NAG	O5-C5-C6-O6
2	F	1	NAG	C4-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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





5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 12 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	FAD	B	501	-	58,58,58	2.22	17 (29%)	85,89,89	1.90	24 (28%)
6	GOL	A	505	-	5,5,5	0.36	0	5,5,5	0.40	0
3	FAD	C	501	-	58,58,58	2.24	17 (29%)	85,89,89	1.91	24 (28%)
3	FAD	D	501	-	58,58,58	2.23	17 (29%)	85,89,89	1.87	23 (27%)
5	NAG	B	507	-	14,14,15	0.58	0	19,19,21	0.65	0
5	NAG	D	504	1	14,14,15	0.55	0	17,19,21	0.95	1 (5%)
3	FAD	A	501	-	58,58,58	2.23	17 (29%)	85,89,89	1.90	23 (27%)
5	NAG	A	504	1	14,14,15	0.36	0	17,19,21	0.51	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	B	501	-	-	11/34/50/50	0/6/6/6
6	GOL	A	505	-	-	2/4/4/4	-
3	FAD	C	501	-	-	7/34/50/50	0/6/6/6
3	FAD	D	501	-	-	7/34/50/50	0/6/6/6
5	NAG	B	507	-	-	4/6/22/26	1/1/1/1
5	NAG	D	504	1	-	1/6/23/26	0/1/1/1
3	FAD	A	501	-	-	8/34/50/50	0/6/6/6
5	NAG	A	504	1	-	2/6/23/26	0/1/1/1

All (68) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	501	FAD	O4-C4	7.93	1.38	1.23
3	B	501	FAD	O4-C4	7.88	1.38	1.23
3	A	501	FAD	O4-C4	7.87	1.38	1.23
3	C	501	FAD	O4-C4	7.85	1.38	1.23
3	C	501	FAD	C4X-N5	5.35	1.42	1.30
3	D	501	FAD	C4X-N5	5.34	1.42	1.30
3	B	501	FAD	C4X-N5	5.33	1.42	1.30
3	A	501	FAD	C4X-N5	5.30	1.42	1.30
3	C	501	FAD	O2B-C2B	-5.10	1.30	1.43
3	A	501	FAD	O2B-C2B	-5.09	1.30	1.43
3	D	501	FAD	O2B-C2B	-5.07	1.30	1.43
3	B	501	FAD	O2B-C2B	-4.97	1.30	1.43
3	B	501	FAD	C9-C9A	4.29	1.46	1.39
3	A	501	FAD	C9-C9A	4.26	1.46	1.39
3	D	501	FAD	C9-C9A	4.24	1.46	1.39
3	C	501	FAD	C9-C9A	4.23	1.46	1.39
3	C	501	FAD	C2B-C3B	-4.04	1.42	1.53
3	A	501	FAD	C2B-C3B	-3.99	1.42	1.53
3	B	501	FAD	C2B-C3B	-3.98	1.42	1.53
3	D	501	FAD	C2B-C3B	-3.97	1.42	1.53
3	D	501	FAD	C1B-N9A	3.97	1.57	1.46
3	C	501	FAD	C1B-N9A	3.93	1.57	1.46
3	A	501	FAD	C1B-N9A	3.91	1.57	1.46
3	B	501	FAD	C1B-N9A	3.89	1.57	1.46
3	B	501	FAD	C10-N1	3.73	1.40	1.33
3	A	501	FAD	C10-N1	3.71	1.40	1.33
3	C	501	FAD	C10-N1	3.70	1.40	1.33
3	D	501	FAD	C10-N1	3.68	1.40	1.33
3	D	501	FAD	C6-C5X	3.56	1.45	1.40
3	B	501	FAD	C6-C5X	3.51	1.45	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	501	FAD	C6-C5X	3.48	1.45	1.40
3	A	501	FAD	C6-C5X	3.48	1.45	1.40
3	B	501	FAD	C2B-C1B	3.38	1.64	1.53
3	C	501	FAD	C2B-C1B	3.37	1.64	1.53
3	A	501	FAD	C2B-C1B	3.35	1.64	1.53
3	D	501	FAD	C2B-C1B	3.33	1.63	1.53
3	A	501	FAD	C6A-N6A	2.69	1.41	1.34
3	C	501	FAD	C6A-N6A	2.64	1.40	1.34
3	D	501	FAD	C6A-N6A	2.63	1.40	1.34
3	B	501	FAD	C6A-N6A	2.61	1.40	1.34
3	A	501	FAD	O4'-C4'	-2.52	1.38	1.43
3	C	501	FAD	C9A-N10	2.49	1.45	1.41
3	C	501	FAD	C6-C7	2.46	1.43	1.39
3	A	501	FAD	C9A-N10	2.46	1.45	1.41
3	C	501	FAD	O4'-C4'	-2.44	1.38	1.43
3	B	501	FAD	O4'-C4'	-2.44	1.38	1.43
3	D	501	FAD	C6-C7	2.43	1.42	1.39
3	D	501	FAD	O4'-C4'	-2.39	1.38	1.43
3	B	501	FAD	C6-C7	2.36	1.42	1.39
3	B	501	FAD	C9A-N10	2.36	1.45	1.41
3	D	501	FAD	C9A-N10	2.28	1.45	1.41
3	A	501	FAD	C8A-N7A	2.27	1.36	1.31
3	A	501	FAD	C6-C7	2.24	1.42	1.39
3	B	501	FAD	C8A-N7A	2.23	1.36	1.31
3	C	501	FAD	C8A-N7A	2.19	1.35	1.31
3	D	501	FAD	C8A-N7A	2.18	1.35	1.31
3	A	501	FAD	C4A-N3A	2.16	1.38	1.34
3	C	501	FAD	C9-C8	2.16	1.42	1.39
3	D	501	FAD	C4A-N3A	2.14	1.38	1.34
3	C	501	FAD	C4A-N3A	2.13	1.38	1.34
3	B	501	FAD	O4B-C1B	2.12	1.46	1.42
3	B	501	FAD	C4A-N3A	2.09	1.38	1.34
3	C	501	FAD	O4B-C1B	2.07	1.46	1.42
3	A	501	FAD	C9-C8	2.07	1.42	1.39
3	A	501	FAD	O4B-C1B	2.06	1.46	1.42
3	B	501	FAD	C9-C8	2.04	1.42	1.39
3	D	501	FAD	O4B-C1B	2.03	1.46	1.42
3	D	501	FAD	C9-C8	2.01	1.42	1.39

All (95) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	501	FAD	C5A-C4A-N3A	-4.65	120.31	126.72
3	D	501	FAD	C5A-C4A-N3A	-4.64	120.33	126.72
3	B	501	FAD	C5A-C4A-N3A	-4.60	120.38	126.72
3	A	501	FAD	O4B-C4B-C3B	4.49	114.07	105.15
3	B	501	FAD	C4A-N9A-C8A	4.49	110.45	105.74
3	A	501	FAD	C5A-C4A-N3A	-4.49	120.53	126.72
3	B	501	FAD	O4B-C4B-C3B	4.49	114.06	105.15
3	A	501	FAD	N3A-C2A-N1A	-4.48	121.80	128.58
3	C	501	FAD	O4B-C4B-C3B	4.44	113.97	105.15
3	C	501	FAD	C4A-N9A-C8A	4.43	110.39	105.74
3	C	501	FAD	N9A-C8A-N7A	-4.42	107.66	113.94
3	B	501	FAD	N9A-C8A-N7A	-4.41	107.68	113.94
3	D	501	FAD	O4B-C4B-C3B	4.40	113.89	105.15
3	A	501	FAD	C4A-N9A-C8A	4.40	110.36	105.74
3	D	501	FAD	N3A-C2A-N1A	-4.37	121.97	128.58
3	B	501	FAD	N3A-C2A-N1A	-4.36	121.98	128.58
3	D	501	FAD	C4A-N9A-C8A	4.36	110.31	105.74
3	A	501	FAD	N9A-C8A-N7A	-4.35	107.77	113.94
3	D	501	FAD	N9A-C8A-N7A	-4.29	107.85	113.94
3	C	501	FAD	N3A-C2A-N1A	-4.27	122.12	128.58
3	C	501	FAD	O4B-C1B-N9A	4.21	116.18	108.09
3	C	501	FAD	C2B-C1B-N9A	4.19	123.72	113.30
3	A	501	FAD	O4B-C1B-N9A	4.18	116.12	108.09
3	B	501	FAD	O4B-C1B-N9A	4.16	116.09	108.09
3	C	501	FAD	N3A-C4A-N9A	4.11	134.15	127.17
3	D	501	FAD	N3A-C4A-N9A	4.10	134.14	127.17
3	A	501	FAD	C2B-C1B-N9A	4.09	123.46	113.30
3	B	501	FAD	N3A-C4A-N9A	4.06	134.08	127.17
3	D	501	FAD	O4B-C1B-N9A	4.06	115.89	108.09
3	D	501	FAD	C2B-C1B-N9A	4.02	123.30	113.30
3	B	501	FAD	C2B-C1B-N9A	3.98	123.19	113.30
3	A	501	FAD	N3A-C4A-N9A	3.97	133.93	127.17
3	C	501	FAD	C5A-N7A-C8A	3.32	108.67	103.45
3	B	501	FAD	C5A-N7A-C8A	3.24	108.55	103.45
3	D	501	FAD	C5A-N7A-C8A	3.21	108.50	103.45
3	A	501	FAD	C5A-N7A-C8A	3.21	108.49	103.45
3	D	501	FAD	C2A-N3A-C4A	3.02	119.20	111.83
3	B	501	FAD	C2A-N3A-C4A	3.01	119.19	111.83
3	A	501	FAD	C2A-N3A-C4A	2.99	119.13	111.83
3	C	501	FAD	C2A-N3A-C4A	2.99	119.13	111.83
3	A	501	FAD	C4-N3-C2	-2.87	120.54	125.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	501	FAD	O2A-PA-O3P	2.86	115.01	107.27
3	B	501	FAD	O5'-C5'-C4'	2.85	116.96	109.36
3	B	501	FAD	O2A-PA-O3P	2.78	114.78	107.27
3	D	501	FAD	C4-N3-C2	-2.77	120.72	125.64
3	B	501	FAD	C4-N3-C2	-2.75	120.76	125.64
3	A	501	FAD	C4X-C10-N1	-2.74	117.87	124.59
3	C	501	FAD	C4-N3-C2	-2.73	120.79	125.64
3	A	501	FAD	C4X-C4-N3	2.70	120.12	113.25
3	B	501	FAD	C4X-C4-N3	2.70	120.12	113.25
3	C	501	FAD	C4X-C4-N3	2.70	120.11	113.25
3	C	501	FAD	O5'-C5'-C4'	2.69	116.55	109.36
3	A	501	FAD	C10-N1-C2	2.68	122.65	116.85
3	D	501	FAD	C4X-C4-N3	2.67	120.04	113.25
3	B	501	FAD	C10-N1-C2	2.66	122.61	116.85
3	D	501	FAD	C4X-C10-N1	-2.65	118.09	124.59
3	C	501	FAD	C4X-C10-N1	-2.65	118.09	124.59
3	C	501	FAD	C10-N1-C2	2.65	122.58	116.85
3	D	501	FAD	C10-N1-C2	2.64	122.56	116.85
3	D	501	FAD	O5'-C5'-C4'	2.63	116.38	109.36
3	B	501	FAD	C4X-C10-N1	-2.59	118.23	124.59
3	A	501	FAD	O2A-PA-O3P	2.54	114.14	107.27
3	A	501	FAD	O4-C4-C4X	-2.54	119.83	126.53
3	B	501	FAD	O4-C4-C4X	-2.52	119.88	126.53
3	A	501	FAD	O5'-C5'-C4'	2.51	116.06	109.36
3	A	501	FAD	C2'-C1'-N10	2.49	121.99	110.20
3	C	501	FAD	C4A-C5A-N7A	-2.49	107.73	110.58
3	C	501	FAD	O4-C4-C4X	-2.49	119.97	126.53
3	B	501	FAD	C2'-C1'-N10	2.46	121.84	110.20
3	C	501	FAD	C2'-C1'-N10	2.46	121.84	110.20
3	C	501	FAD	O2P-P-O1P	-2.46	101.01	112.44
3	D	501	FAD	O4-C4-C4X	-2.45	120.06	126.53
3	B	501	FAD	C4A-C5A-N7A	-2.45	107.78	110.58
3	D	501	FAD	C4A-C5A-N7A	-2.43	107.80	110.58
3	D	501	FAD	C2'-C1'-N10	2.40	121.53	110.20
3	A	501	FAD	C4A-C5A-N7A	-2.39	107.85	110.58
3	B	501	FAD	O2A-PA-O1A	-2.37	101.44	112.44
3	A	501	FAD	C4X-C10-N10	2.34	119.83	116.48
3	D	501	FAD	O2A-PA-O3P	2.32	113.54	107.27
3	A	501	FAD	O2P-P-O1P	-2.29	101.78	112.44
3	D	501	FAD	O2P-P-O1P	-2.29	101.79	112.44
3	B	501	FAD	O2P-P-O1P	-2.28	101.85	112.44
5	D	504	NAG	C2-N2-C7	2.27	125.94	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	501	FAD	C4X-C10-N10	2.27	119.72	116.48
3	D	501	FAD	C4X-C10-N10	2.25	119.71	116.48
3	A	501	FAD	O2A-PA-O1A	-2.24	102.00	112.44
3	D	501	FAD	O2A-PA-O1A	-2.24	102.05	112.44
3	C	501	FAD	O2A-PA-O1A	-2.23	102.06	112.44
3	C	501	FAD	C4X-C10-N10	2.21	119.64	116.48
3	A	501	FAD	C10-C4X-N5	-2.06	120.59	124.81
3	B	501	FAD	C10-C4X-N5	-2.06	120.60	124.81
3	C	501	FAD	C4B-O4B-C1B	-2.03	104.99	109.47
3	D	501	FAD	C10-C4X-N5	-2.02	120.67	124.81
3	C	501	FAD	C10-C4X-N5	-2.02	120.69	124.81
3	B	501	FAD	C4-C4X-N5	2.01	120.98	118.21

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	FAD	C5B-O5B-PA-O1A
3	C	501	FAD	C5B-O5B-PA-O1A
5	A	504	NAG	O5-C5-C6-O6
5	B	507	NAG	O5-C5-C6-O6
5	A	504	NAG	C4-C5-C6-O6
5	B	507	NAG	C8-C7-N2-C2
5	B	507	NAG	O7-C7-N2-C2
6	A	505	GOL	O1-C1-C2-O2
3	A	501	FAD	O3'-C3'-C4'-C5'
3	D	501	FAD	O3'-C3'-C4'-C5'
5	B	507	NAG	C4-C5-C6-O6
3	A	501	FAD	C2'-C3'-C4'-C5'
3	B	501	FAD	C2'-C3'-C4'-C5'
3	D	501	FAD	C2'-C3'-C4'-C5'
3	A	501	FAD	C2'-C3'-C4'-O4'
3	B	501	FAD	C2'-C3'-C4'-O4'
3	D	501	FAD	C2'-C3'-C4'-O4'
6	A	505	GOL	O1-C1-C2-C3
3	B	501	FAD	O3'-C3'-C4'-C5'
5	D	504	NAG	O5-C5-C6-O6
3	D	501	FAD	P-O3P-PA-O1A
3	A	501	FAD	O3'-C3'-C4'-O4'
3	B	501	FAD	PA-O3P-P-O5'
3	C	501	FAD	PA-O3P-P-O5'
3	D	501	FAD	PA-O3P-P-O5'

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Mol	Chain	Res	Type	Atoms
3	C	501	FAD	C2'-C3'-C4'-O4'
3	B	501	FAD	P-O3P-PA-O1A
3	D	501	FAD	O3'-C3'-C4'-O4'
3	B	501	FAD	O2'-C2'-C3'-O3'
3	B	501	FAD	O3'-C3'-C4'-O4'
3	C	501	FAD	C2'-C3'-C4'-C5'
3	B	501	FAD	C5B-O5B-PA-O1A
3	D	501	FAD	C5B-O5B-PA-O1A
3	C	501	FAD	P-O3P-PA-O2A
3	A	501	FAD	PA-O3P-P-O5'
3	B	501	FAD	C1'-C2'-C3'-O3'
3	B	501	FAD	O4B-C4B-C5B-O5B
3	C	501	FAD	O3'-C3'-C4'-C5'
3	A	501	FAD	P-O3P-PA-O1A
3	A	501	FAD	P-O3P-PA-O2A
3	C	501	FAD	P-O3P-PA-O1A
3	B	501	FAD	O2'-C2'-C3'-C4'

All (1) ring outliers are listed below:

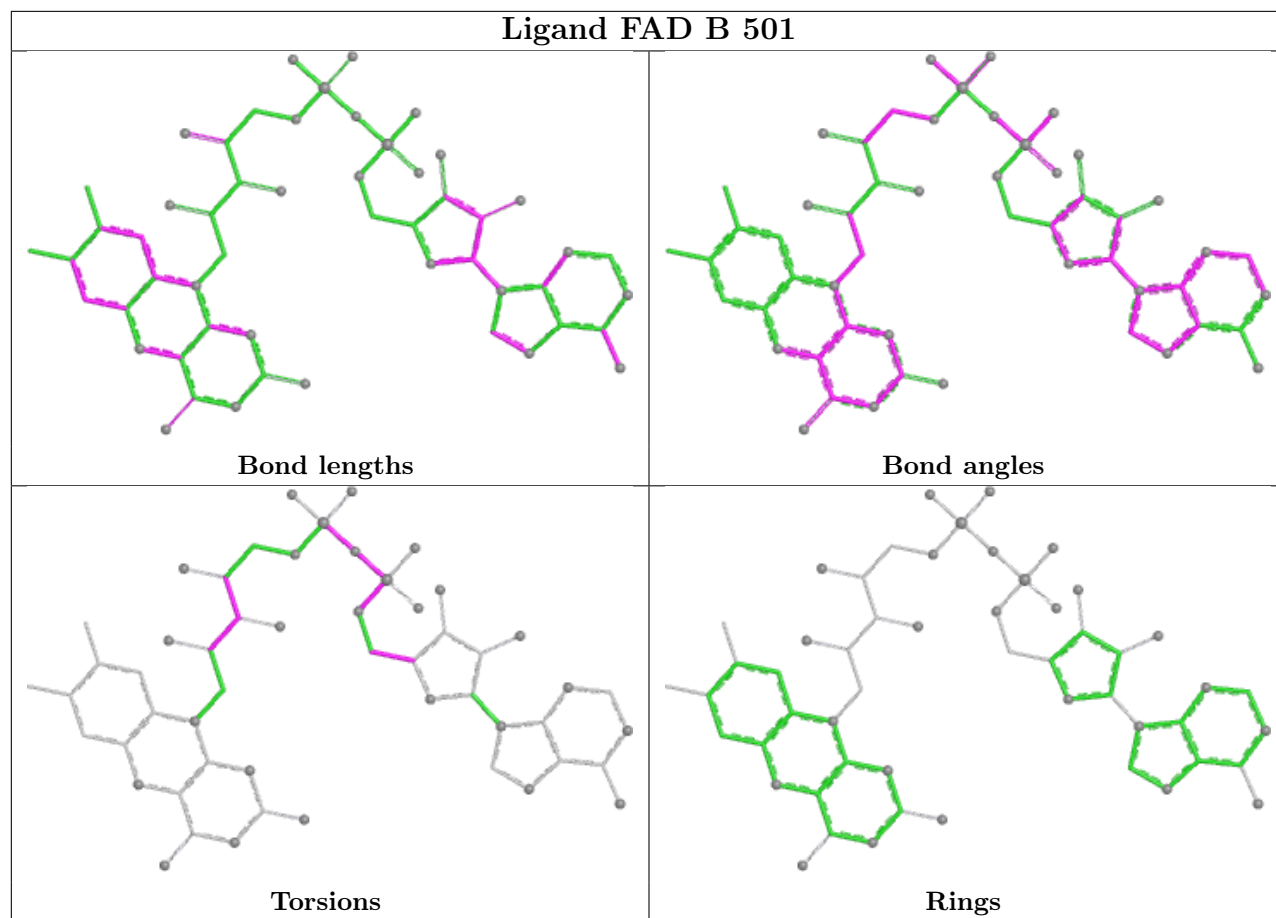
Mol	Chain	Res	Type	Atoms
5	B	507	NAG	C1-C2-C3-C4-C5-O5

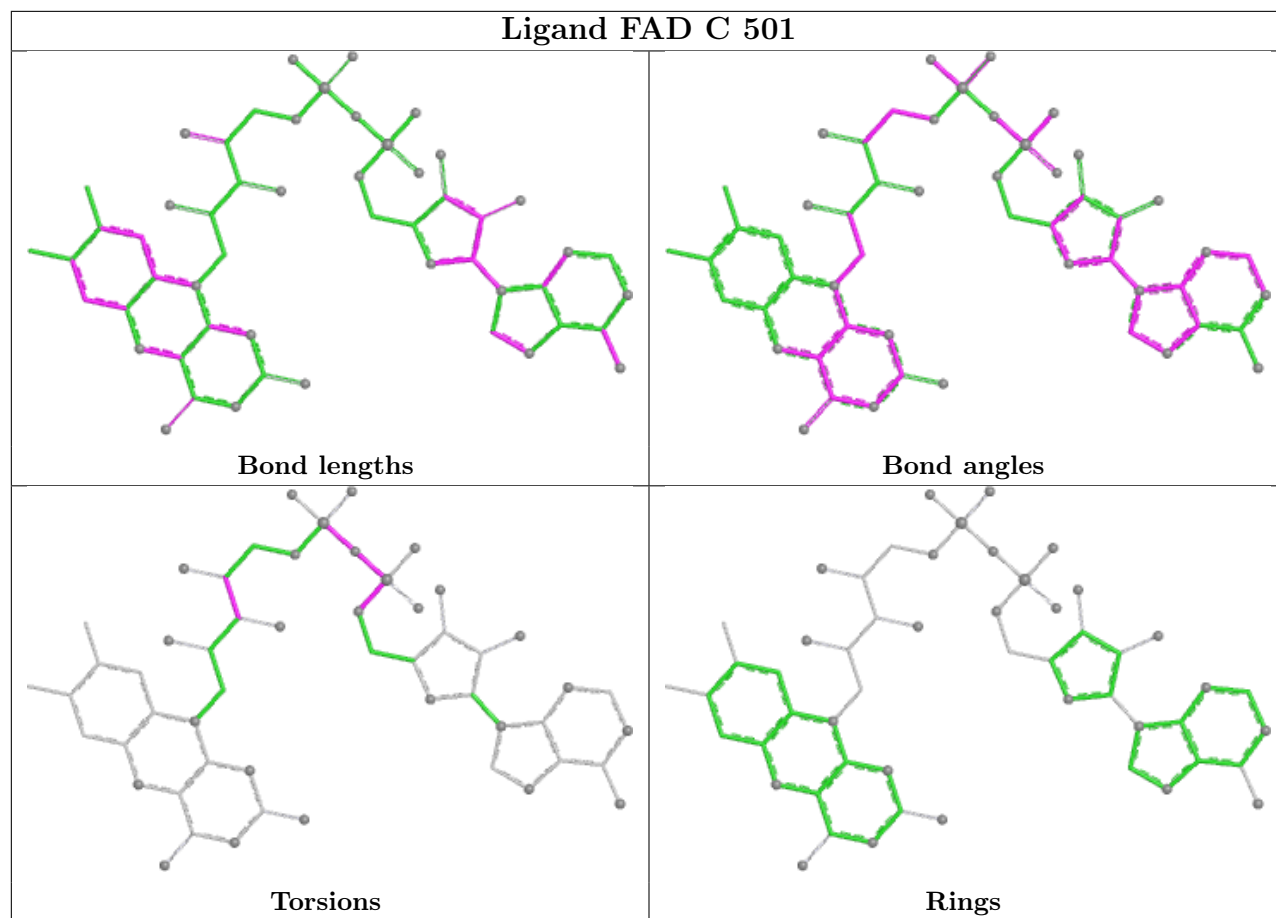
4 monomers are involved in 8 short contacts:

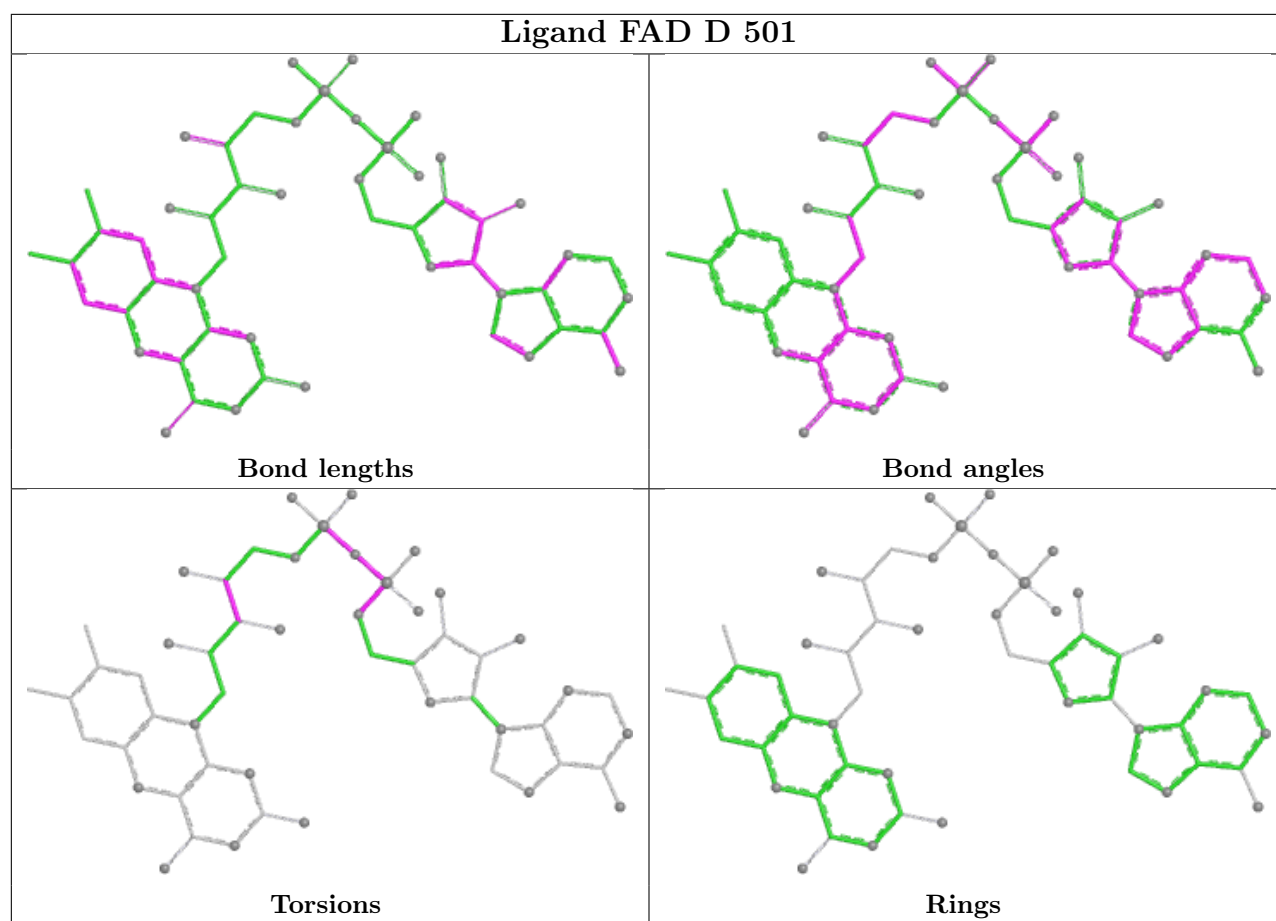
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	501	FAD	2	0
3	C	501	FAD	2	0
3	D	501	FAD	2	0
3	A	501	FAD	2	0

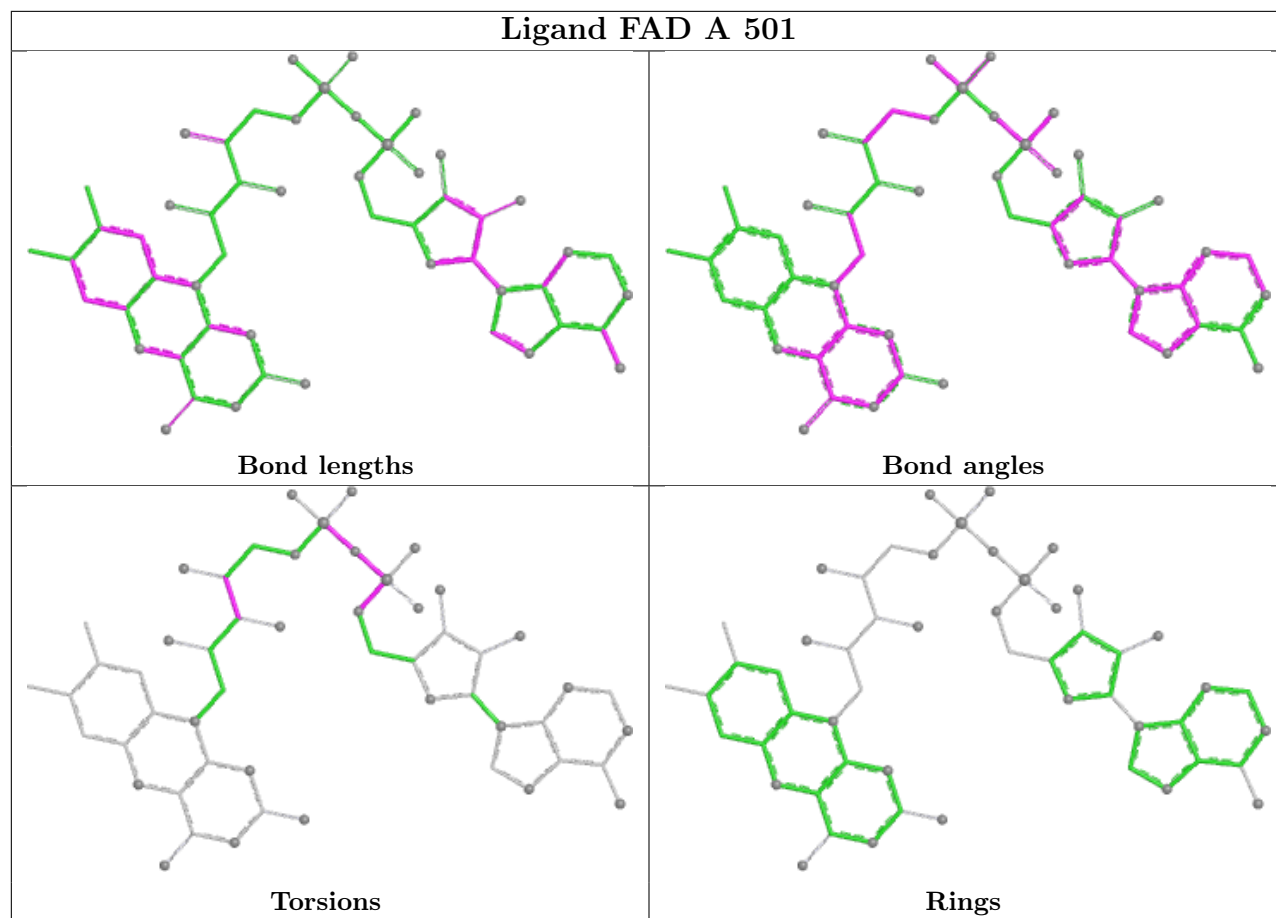
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand FAD B 501









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	483/484 (99%)	-0.08	5 (1%) 79 80	9, 21, 38, 56	3 (0%)
1	B	481/484 (99%)	-0.04	7 (1%) 72 73	7, 22, 39, 60	8 (1%)
1	C	480/484 (99%)	-0.08	1 (0%) 91 91	12, 23, 42, 63	3 (0%)
1	D	479/484 (98%)	-0.03	5 (1%) 79 80	8, 22, 42, 60	3 (0%)
All	All	1923/1936 (99%)	-0.06	18 (0%) 81 82	7, 22, 40, 63	17 (0%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	28	SER	3.6
1	B	14	THR	3.2
1	D	6	PRO	3.2
1	C	158	GLU	3.0
1	B	11	PHE	2.9
1	D	229	TYR	2.8
1	A	484	SER	2.6
1	D	173	CYS	2.5
1	D	228	ALA	2.5
1	A	2	ASP	2.4
1	A	4	ARG	2.4
1	D	171	THR	2.3
1	A	279	GLU	2.3
1	A	14	THR	2.3
1	B	13	GLU	2.3
1	B	175	TYR	2.2
1	B	12	ARG	2.2
1	B	30	THR	2.1

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

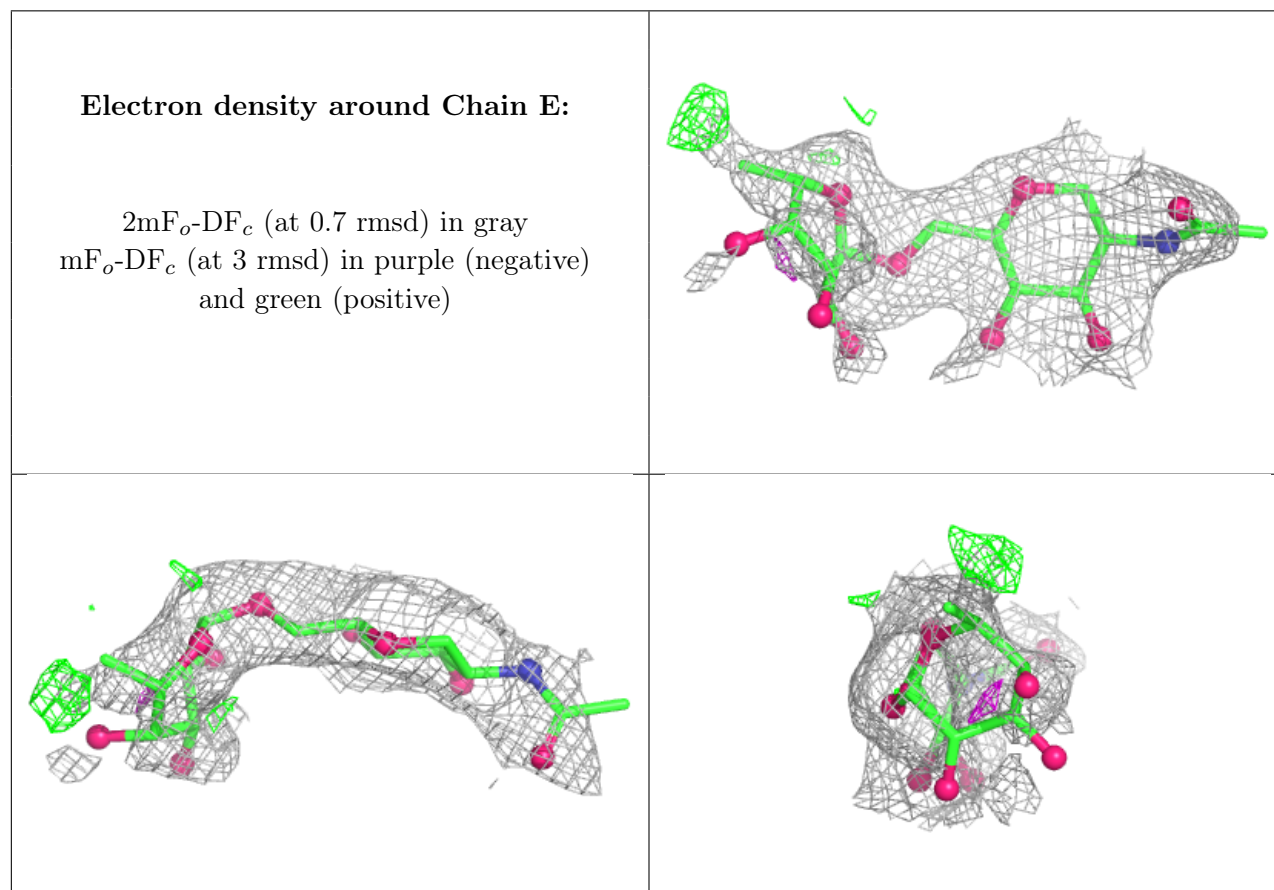
There are no non-standard protein/DNA/RNA residues in this entry.

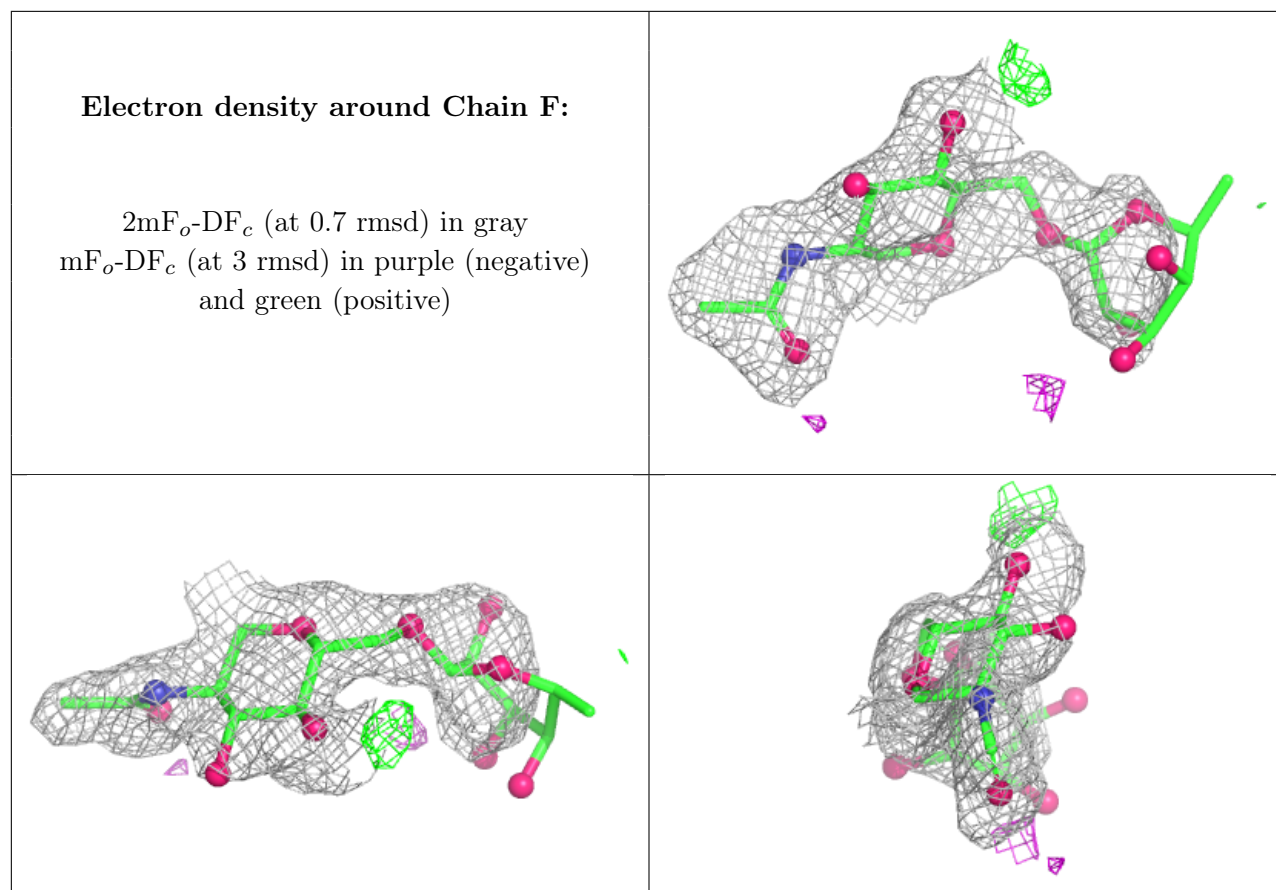
6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FUC	F	2	10/11	0.51	0.20	61,72,80,82	0
2	FUC	E	2	10/11	0.66	0.20	46,53,62,69	0
2	NAG	E	1	14/15	0.79	0.12	44,51,54,57	0
2	NAG	F	1	14/15	0.81	0.11	31,45,53,54	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.





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.

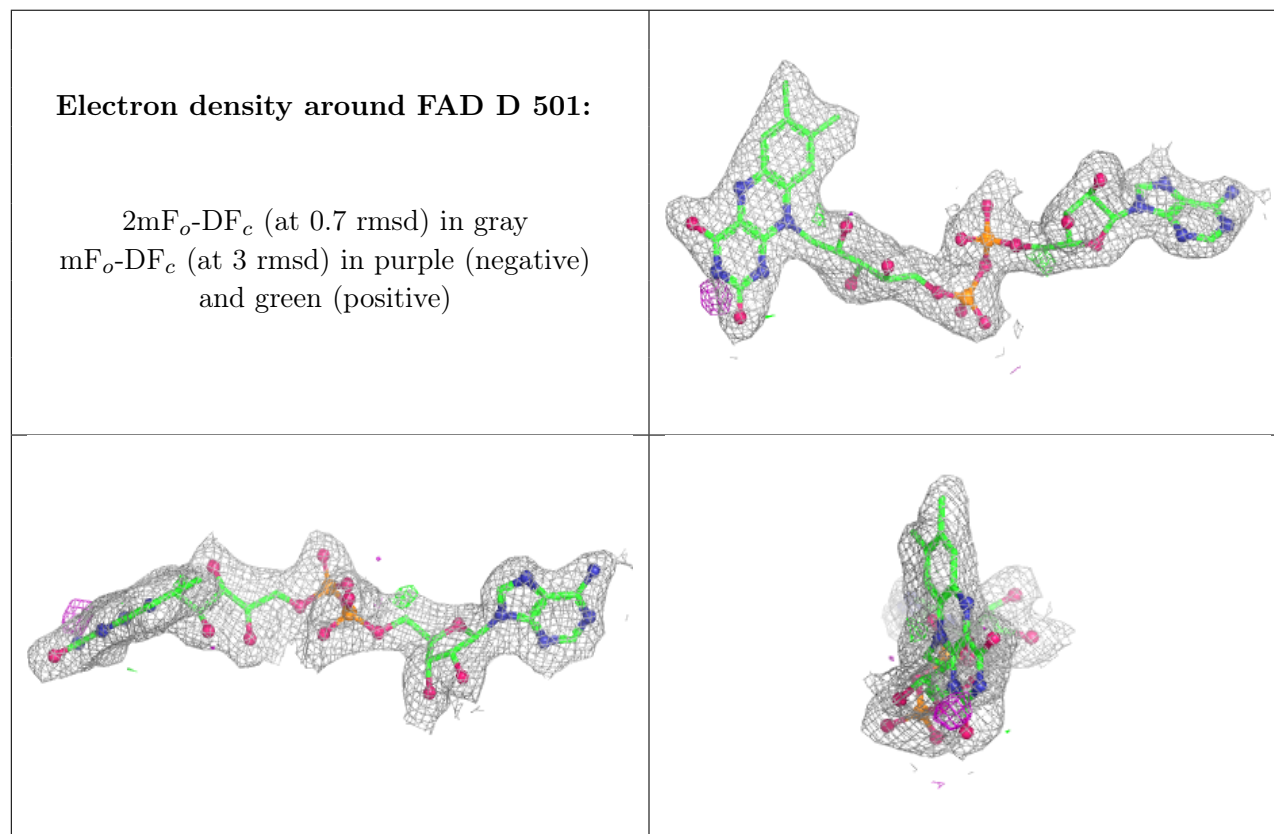
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	NAG	B	507	14/15	0.69	0.16	42,57,62,62	0
5	NAG	D	504	14/15	0.71	0.14	53,58,62,62	0
6	GOL	A	505	6/6	0.82	0.13	35,40,44,46	0
5	NAG	A	504	14/15	0.83	0.10	26,34,45,48	0
4	ZN	C	503	1/1	0.90	0.07	52,52,52,52	1
4	ZN	B	502[A]	1/1	0.93	0.08	41,41,41,41	1
4	ZN	C	506	1/1	0.93	0.07	65,65,65,65	0
4	ZN	B	502[B]	1/1	0.93	0.08	38,38,38,38	1
4	ZN	A	506	1/1	0.94	0.05	54,54,54,54	0
3	FAD	D	501	53/53	0.95	0.08	9,14,19,21	0
3	FAD	C	501	53/53	0.96	0.07	11,15,20,23	0
3	FAD	A	501	53/53	0.96	0.07	9,14,18,20	0
4	ZN	A	503	1/1	0.96	0.04	35,35,35,35	1

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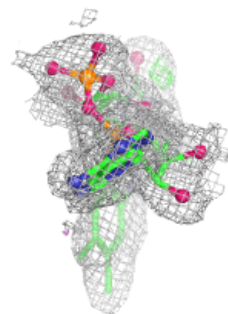
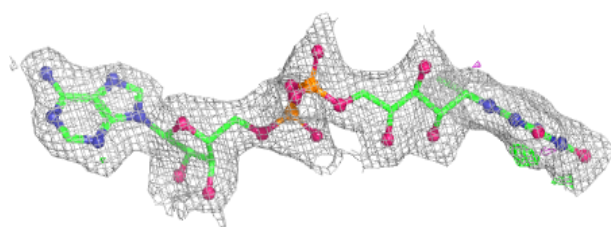
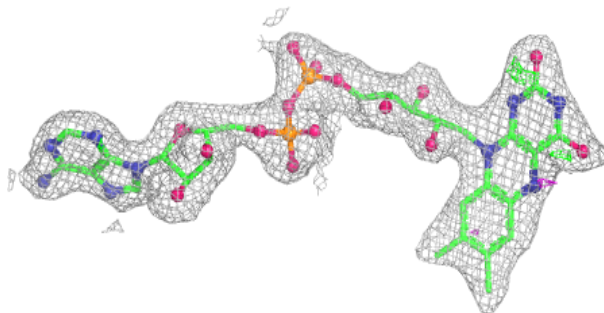
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	FAD	B	501	53/53	0.96	0.07	9,16,21,22	0
4	ZN	A	502	1/1	0.97	0.04	50,50,50,50	0
4	ZN	B	504	1/1	0.97	0.04	50,50,50,50	0
4	ZN	C	502	1/1	0.98	0.05	60,60,60,60	0
4	ZN	D	502	1/1	0.98	0.03	43,43,43,43	0
4	ZN	B	503	1/1	0.98	0.04	52,52,52,52	0
4	ZN	D	503	1/1	0.99	0.04	33,33,33,33	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.

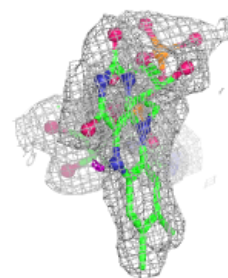
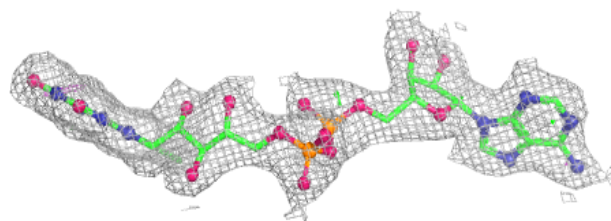
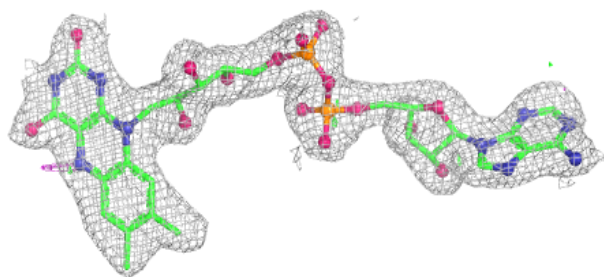


Electron density around FAD C 501:

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

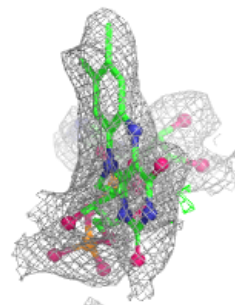
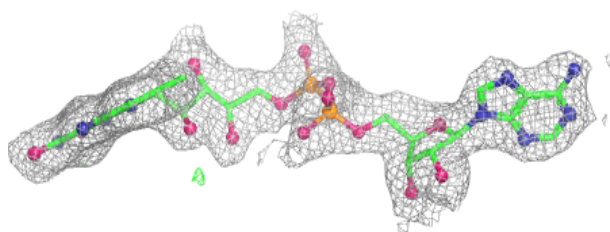
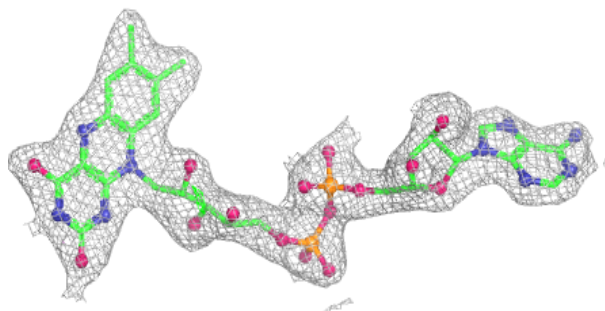
**Electron density around FAD A 501:**

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



Electron density around FAD B 501:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.