



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:27 AM UTC

PDB ID : 3L1R / pdb_00003l1r
Title : X-ray structure of the mutant lys300met of polyamine oxidase from zea mays
in complex with spermidine
Authors : Fiorillo, A.; Ilari, A.; Tavladoraki, P.
Deposited on : 2009-12-14
Resolution : 3.20 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

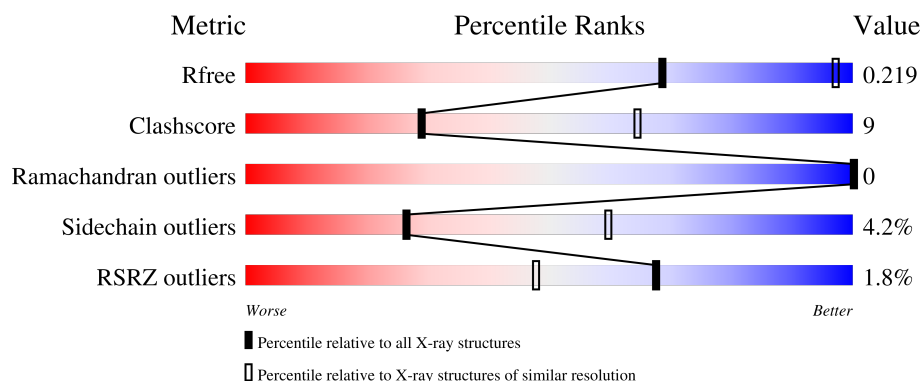
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	478	2% 78% 18% ..
1	B	478	% 76% 21% ..
2	C	2	100%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 7687 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 Polyamine oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	467	Total	C	N	O	S	20	0	0
			3748	2394	632	707	15			
1	B	466	Total	C	N	O	S	20	1	0
			3747	2394	633	705	15			

There are 14 discrepancies between the modelled and reference sequences:

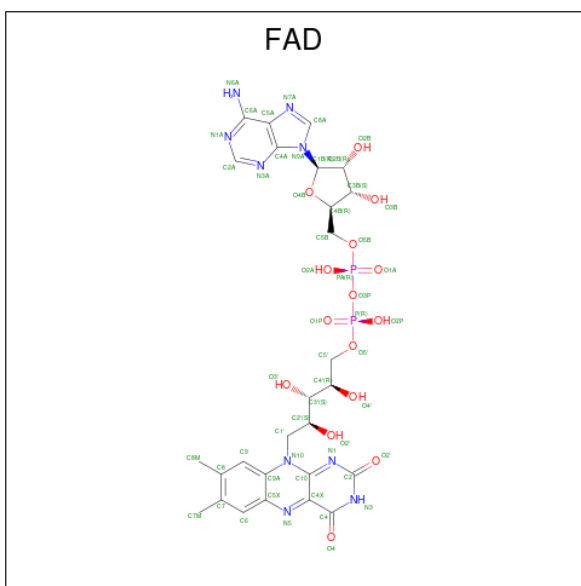
Chain	Residue	Modelled	Actual	Comment	Reference
A	300	MET	LYS	engineered mutation	UNP O64411
A	473	HIS	-	expression tag	UNP O64411
A	474	HIS	-	expression tag	UNP O64411
A	475	HIS	-	expression tag	UNP O64411
A	476	HIS	-	expression tag	UNP O64411
A	477	HIS	-	expression tag	UNP O64411
A	478	HIS	-	expression tag	UNP O64411
B	300	MET	LYS	engineered mutation	UNP O64411
B	473	HIS	-	expression tag	UNP O64411
B	474	HIS	-	expression tag	UNP O64411
B	475	HIS	-	expression tag	UNP O64411
B	476	HIS	-	expression tag	UNP O64411
B	477	HIS	-	expression tag	UNP O64411
B	478	HIS	-	expression tag	UNP O64411

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



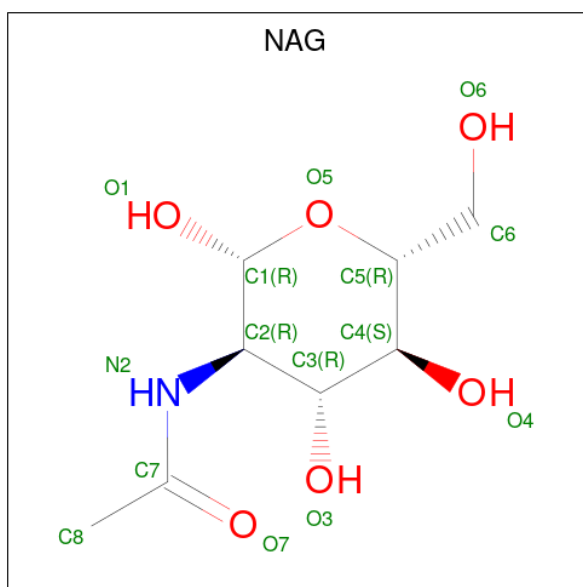
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $\text{C}_{27}\text{H}_{33}\text{N}_9\text{O}_{15}\text{P}_2$).



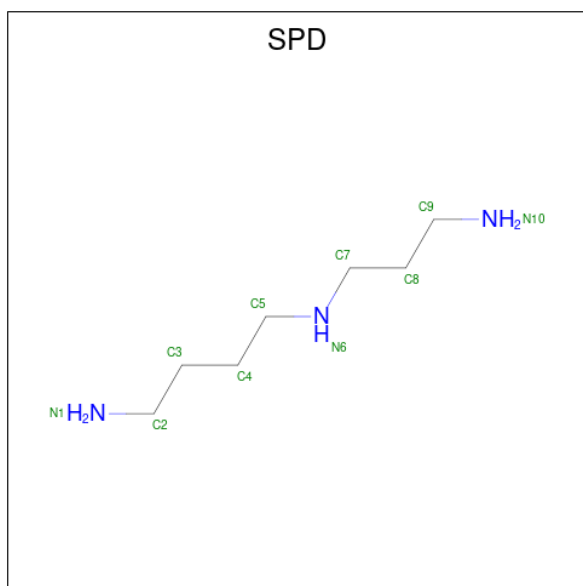
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 53	C 27	N 9	O 15	P 2	0	0
3	B	1	Total 53	C 27	N 9	O 15	P 2	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $\text{C}_8\text{H}_{15}\text{NO}_6$).



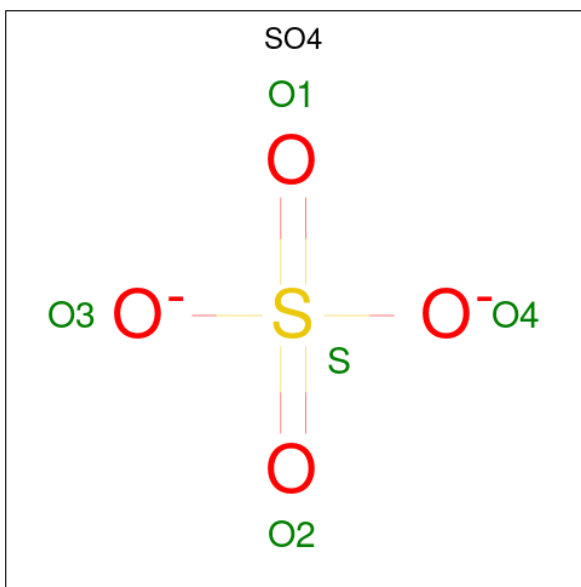
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	N	O	
			14	8	1	5	
							0
							0

- Molecule 5 is SPERMIDINE (CCD ID: SPD) (formula: $C_7H_{19}N_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	N		
			10	7	3	0	0
5	B	1	Total	C	N		
			10	7	3	0	0

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



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

- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Cl	0	0
			1	1		

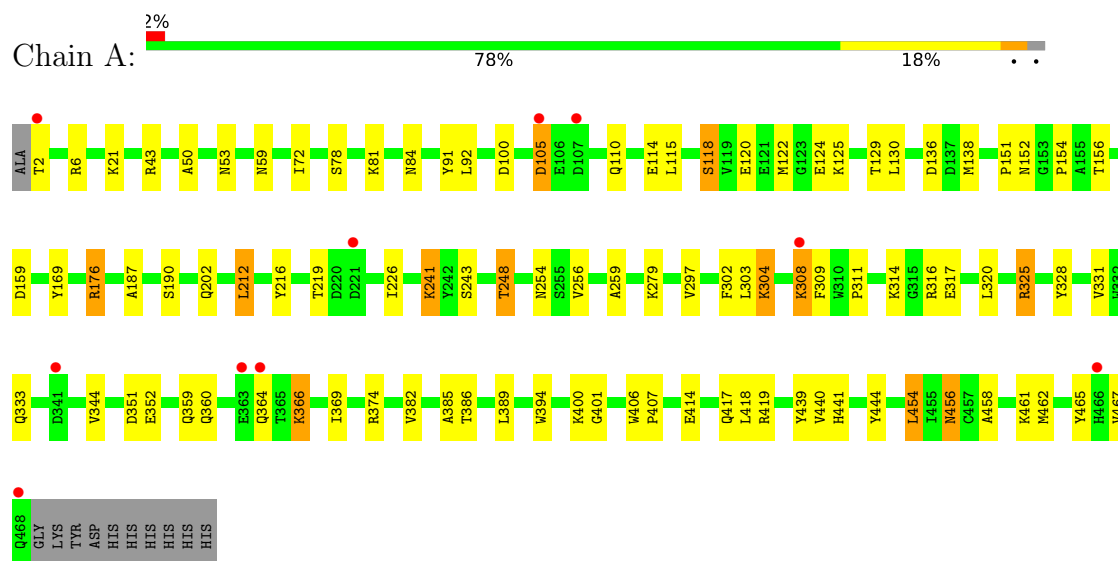
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	11	Total	O	0	0
			11	11		
8	B	7	Total	O	0	0
			7	7		

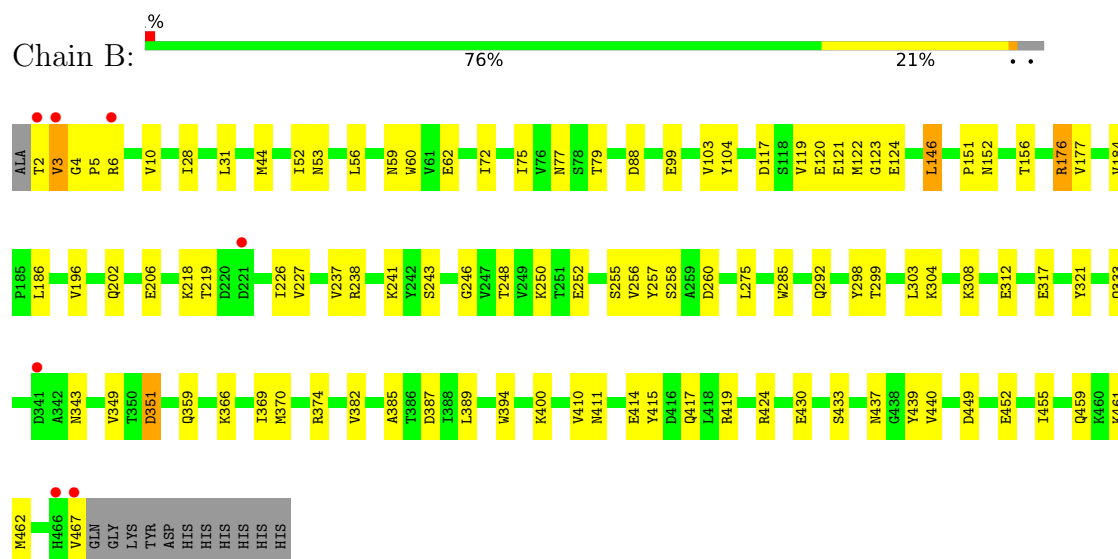
3 Residue-property plots

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: Polyamine oxidase



• Molecule 1: Polyamine oxidase



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

Chain C:

100%

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	137.68Å 137.68Å 189.15Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.50 – 3.20 46.50 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (46.50-3.20) 99.9 (46.50-3.20)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.46 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.5.0043	Depositor
R, R_{free}	0.192 , 0.216 0.197 , 0.219	Depositor DCC
R_{free} test set	1749 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	36.5	Xtriage
Anisotropy	0.539	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 43.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.029 for -h,-k,l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	7687	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.69% 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: CL, FAD, SPD, 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	0.54	0/3841	0.85	0/5207
1	B	0.56	0/3843	0.83	3/5209 (0.1%)
All	All	0.55	0/7684	0.84	3/10416 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	3	VAL	N-CA-C	5.78	116.78	111.81
1	B	351	ASP	CB-CA-C	-5.58	110.13	116.54
1	B	77	ASN	N-CA-C	5.13	117.66	111.40

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	3748	0	3645	70	0
1	B	3747	0	3650	73	0
2	C	28	0	25	0	0
3	A	53	0	31	2	0
3	B	53	0	31	1	0
4	A	14	0	13	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	10	0	19	0	0
5	B	10	0	19	3	0
6	B	5	0	0	0	0
7	B	1	0	0	0	0
8	A	11	0	0	1	0
8	B	7	0	0	0	0
All	All	7687	0	7433	131	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (131) 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:146:LEU:HD12	1:B:146:LEU:O	1.38	1.22
1:A:138:MET:HB3	1:B:292:GLN:HE21	1.13	1.09
1:B:146:LEU:HD12	1:B:146:LEU:C	1.80	1.04
1:A:138:MET:HB3	1:B:292:GLN:NE2	1.84	0.92
1:A:454:LEU:HD23	1:A:454:LEU:C	2.01	0.85
1:B:62:GLU:OE1	1:B:439:TYR:CE2	2.32	0.81
1:A:176:ARG:HD2	1:B:177:VAL:HG11	1.62	0.81
1:B:62:GLU:OE1	1:B:439:TYR:HE2	1.63	0.81
1:A:454:LEU:HD23	1:A:454:LEU:O	1.81	0.78
1:A:366:LYS:HE3	1:A:385:ALA:O	1.87	0.74
1:B:117:ASP:O	1:B:121:GLU:HG3	1.89	0.72
1:A:311:PRO:HB2	1:A:316:ARG:HD2	1.71	0.71
1:B:146:LEU:O	1:B:146:LEU:CD1	2.30	0.71
1:A:454:LEU:C	1:A:454:LEU:CD2	2.67	0.68
1:B:146:LEU:C	1:B:146:LEU:CD1	2.58	0.67
1:A:417:GLN:HG2	1:A:467:VAL:HG11	1.77	0.67
1:B:3:VAL:N	1:B:4:GLY:HA3	2.10	0.66
1:B:5:PRO:HD2	1:B:258:SER:O	1.94	0.65
1:A:308:LYS:HG2	1:A:308:LYS:O	1.98	0.64
1:B:2:THR:HG22	1:B:260:ASP:OD1	1.98	0.64
1:A:458:ALA:O	1:A:461:LYS:HE3	1.98	0.63
1:A:212:LEU:HD21	1:A:444:TYR:HE1	1.65	0.61
1:B:370:MET:HA	1:B:370:MET:HE2	1.81	0.61
1:B:6[A]:ARG:NH1	1:B:260:ASP:CG	2.57	0.61
1:A:53:ASN:H	1:A:202:GLN:NE2	1.98	0.61
1:A:400:LYS:HB3	1:B:151:PRO:HG3	1.82	0.60
1:A:414:GLU:HA	1:A:417:GLN:HG3	1.82	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3:VAL:H	1:B:4:GLY:HA3	1.67	0.59
1:B:119:VAL:HA	1:B:122:MET:HE3	1.84	0.58
1:A:138:MET:CB	1:B:292:GLN:HE21	2.02	0.58
1:B:410:VAL:HG13	1:B:414:GLU:HG3	1.85	0.58
1:B:219:THR:HG22	1:B:226:ILE:HA	1.85	0.57
1:B:299:THR:HB	1:B:349:VAL:HG23	1.87	0.57
1:B:124:GLU:HG3	1:B:184:VAL:HG12	1.86	0.56
1:A:394:TRP:HE1	1:B:152:ASN:ND2	2.03	0.56
1:B:60:TRP:CZ3	5:B:700:SPD:H41	2.40	0.56
1:A:53:ASN:H	1:A:202:GLN:HE22	1.52	0.56
1:A:302:PHE:HB2	1:A:389:LEU:HB3	1.88	0.55
1:A:130:LEU:HD22	1:A:136:ASP:O	2.06	0.55
1:A:78:SER:O	1:A:81:LYS:HE2	2.07	0.55
1:B:6[A]:ARG:HH12	1:B:260:ASP:CG	2.15	0.55
1:A:212:LEU:HD21	1:A:444:TYR:CE1	2.42	0.54
1:A:359:GLN:HE22	1:B:156:THR:HG22	1.72	0.54
1:B:6[B]:ARG:HG2	1:B:28:ILE:HG23	1.89	0.54
1:B:241:LYS:HB2	1:B:248:THR:HB	1.89	0.54
1:A:456:ASN:ND2	1:A:462:MET:HE3	2.23	0.54
1:B:62:GLU:HG2	1:B:196:VAL:CG1	2.38	0.54
1:A:303:LEU:HD11	1:A:369:ILE:HG21	1.90	0.53
1:B:99:GLU:HA	1:B:321:TYR:CE1	2.44	0.53
1:A:325:ARG:HD2	1:A:328:TYR:HB2	1.91	0.53
1:B:298:TYR:OH	5:B:700:SPD:H51	2.09	0.53
1:A:351:ASP:CG	1:A:352:GLU:H	2.15	0.52
1:B:255:SER:HB3	1:B:257:TYR:CE1	2.45	0.52
1:A:50:ALA:CB	1:A:304:LYS:HD2	2.40	0.51
1:A:394:TRP:HE1	1:B:152:ASN:HD22	1.58	0.51
1:A:351:ASP:CG	1:B:176:ARG:HH22	2.19	0.51
1:B:218:LYS:HG3	1:B:227:VAL:HG23	1.93	0.51
1:B:250:LYS:HG2	1:B:256:VAL:HG22	1.92	0.51
1:A:176:ARG:NH2	1:B:351:ASP:OD1	2.40	0.50
3:A:500:FAD:O2A	8:A:487:HOH:O	2.19	0.50
1:A:110:GLN:HE21	1:A:114:GLU:HG3	1.75	0.49
1:A:151:PRO:HG3	1:B:400:LYS:HB3	1.95	0.49
1:A:118:SER:O	1:A:122:MET:HG3	2.13	0.49
1:A:419:ARG:NH2	1:A:465:TYR:OH	2.45	0.49
1:A:187:ALA:HA	1:A:190:SER:HB2	1.95	0.48
1:B:75:ILE:HA	1:B:79:THR:HB	1.96	0.48
1:A:72:ILE:HD13	1:A:441:HIS:HA	1.95	0.48
1:A:50:ALA:HB1	1:A:304:LYS:HD2	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:GLU:HG2	1:B:196:VAL:HG11	1.96	0.47
1:B:246:GLY:HA2	1:B:424:ARG:CD	2.44	0.47
1:A:72:ILE:HG12	1:A:440:VAL:HG12	1.96	0.47
1:B:308:LYS:HE2	1:B:343:ASN:OD1	2.14	0.47
1:A:351:ASP:CG	1:A:352:GLU:N	2.72	0.47
1:B:2:THR:HA	1:B:260:ASP:OD1	2.13	0.47
1:A:359:GLN:NE2	1:B:156:THR:HG22	2.29	0.47
1:A:92:LEU:HD22	1:A:320:LEU:HG	1.97	0.47
1:B:6[B]:ARG:HG2	1:B:28:ILE:CG2	2.45	0.46
1:B:303:LEU:HD11	1:B:369:ILE:HG21	1.98	0.46
1:B:455:ILE:O	1:B:459:GLN:HB3	2.16	0.46
1:A:91:TYR:OH	1:A:314:LYS:HE2	2.16	0.46
1:A:309:PHE:CG	1:A:382:VAL:HG12	2.50	0.46
1:B:62:GLU:OE1	1:B:439:TYR:CD2	2.70	0.45
1:B:10:VAL:HG22	1:B:237:VAL:HG21	1.97	0.45
1:A:125:LYS:O	1:A:129:THR:HG23	2.17	0.45
1:B:56:LEU:HD21	1:B:389:LEU:HD21	1.98	0.45
1:B:366:LYS:HD2	1:B:385:ALA:HB3	1.98	0.45
1:A:120:GLU:O	1:A:124:GLU:HG3	2.16	0.45
1:A:241:LYS:HA	1:A:279:LYS:O	2.17	0.45
1:A:456:ASN:HD21	1:A:462:MET:HE3	1.81	0.45
1:A:136:ASP:OD1	1:A:136:ASP:N	2.50	0.45
1:A:374:ARG:HE	1:A:382:VAL:HG23	1.81	0.44
1:A:151:PRO:HG2	1:A:152:ASN:HD22	1.83	0.44
1:A:241:LYS:HG3	1:A:279:LYS:HB3	1.98	0.44
1:B:186:LEU:HD21	1:B:439:TYR:OH	2.18	0.44
1:B:238:ARG:HG3	1:B:252:GLU:HG3	1.98	0.44
1:B:103:VAL:HG12	1:B:104:TYR:O	2.18	0.44
1:A:169:TYR:CE1	1:A:331:VAL:HG11	2.52	0.44
1:A:303:LEU:O	1:A:344:VAL:HA	2.18	0.43
1:B:298:TYR:CZ	5:B:700:SPD:H51	2.52	0.43
1:B:452:GLU:HA	1:B:455:ILE:HD12	1.99	0.43
1:B:88:ASP:OD1	1:B:88:ASP:C	2.60	0.43
1:B:285:TRP:HE3	1:B:417:GLN:HE21	1.66	0.43
1:A:439:TYR:HB3	1:A:441:HIS:CE1	2.52	0.43
1:A:297:VAL:HG22	1:A:401:GLY:HA2	1.99	0.43
1:A:219:THR:HG22	1:A:226:ILE:HA	2.00	0.43
1:B:238:ARG:CG	1:B:252:GLU:HG3	2.49	0.42
1:A:72:ILE:CD1	1:A:441:HIS:HA	2.49	0.42
1:A:21:LYS:HB2	1:A:216:TYR:CE2	2.55	0.42
1:A:105:ASP:N	1:A:105:ASP:OD1	2.52	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:72:ILE:HG13	1:B:440:VAL:HG12	2.01	0.42
1:A:43:ARG:HB3	3:A:500:FAD:HM81	2.02	0.42
1:B:308:LYS:HD2	1:B:312:GLU:OE1	2.20	0.41
1:A:317:GLU:O	1:A:333:GLN:HA	2.20	0.41
1:B:317:GLU:O	1:B:333:GLN:HA	2.20	0.41
1:A:84:ASN:OD1	1:A:84:ASN:C	2.63	0.41
1:A:406:TRP:HA	1:A:407:PRO:HD3	1.89	0.41
1:A:154:PRO:HB3	1:A:159:ASP:HB3	2.01	0.41
1:B:415:TYR:OH	1:B:433:SER:O	2.37	0.41
1:A:6:ARG:O	1:A:259:ALA:HB1	2.20	0.41
1:B:394:TRP:O	1:B:400:LYS:HA	2.21	0.41
1:B:430:GLU:O	1:B:437:ASN:HA	2.21	0.41
1:A:241:LYS:HB3	1:A:248:THR:HB	2.02	0.41
1:A:297:VAL:HG21	1:A:394:TRP:HB2	2.03	0.41
1:B:304:LYS:HB3	1:B:387:ASP:HB2	2.03	0.41
1:A:304:LYS:HG3	1:A:386:THR:OG1	2.21	0.40
1:B:275:LEU:CD2	3:B:500:FAD:H61A	2.34	0.40
1:B:44:MET:O	1:B:206:GLU:HB3	2.21	0.40
1:B:374:ARG:HG2	1:B:382:VAL:HB	2.03	0.40
1:B:53:ASN:H	1:B:202:GLN:HE22	1.68	0.40
1:A:156:THR:HG22	1:B:359:GLN:HE22	1.85	0.40
1:B:120:GLU:O	1:B:123:GLY:N	2.55	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	465/478 (97%)	441 (95%)	24 (5%)	0	100	100
1	B	465/478 (97%)	441 (95%)	24 (5%)	0	100	100
All	All	930/956 (97%)	882 (95%)	48 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	401/410 (98%)	379 (94%)	22 (6%)	19	52
1	B	401/410 (98%)	389 (97%)	12 (3%)	36	66
All	All	802/820 (98%)	768 (96%)	34 (4%)	26	60

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	59	ASN
1	A	100	ASP
1	A	105	ASP
1	A	115	LEU
1	A	118	SER
1	A	176	ARG
1	A	212	LEU
1	A	241	LYS
1	A	243	SER
1	A	248	THR
1	A	254	ASN
1	A	256	VAL
1	A	304	LYS
1	A	308	LYS
1	A	325	ARG
1	A	360	GLN
1	A	364	GLN
1	A	366	LYS
1	A	418	LEU
1	A	454	LEU
1	A	456	ASN
1	B	31	LEU
1	B	52	ILE
1	B	59	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	146	LEU
1	B	176	ARG
1	B	243	SER
1	B	411	ASN
1	B	419	ARG
1	B	449	ASP
1	B	461	LYS
1	B	462	MET
1	B	467	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	HIS
1	A	110	GLN
1	A	144	GLN
1	A	152	ASN
1	A	202	GLN
1	A	232	GLN
1	A	359	GLN
1	A	360	GLN
1	A	456	ASN
1	A	466	HIS
1	B	39	HIS
1	B	59	ASN
1	B	152	ASN
1	B	215	GLN
1	B	234	ASN
1	B	292	GLN
1	B	359	GLN
1	B	360	GLN
1	B	417	GLN
1	B	437	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 ⓘ

2 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	C	1	1,2	14,14,15	1.51	1 (7%)	17,19,21	1.67	4 (23%)
2	NAG	C	2	2	14,14,15	0.70	0	17,19,21	1.39	1 (5%)

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	C	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	NAG	O5-C1	-5.29	1.34	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	NAG	C1-O5-C5	-4.98	105.51	112.19
2	C	2	NAG	C4-C3-C2	4.72	117.93	111.02
2	C	1	NAG	O5-C1-C2	-2.33	107.68	111.29
2	C	1	NAG	O5-C5-C6	2.13	111.80	107.66
2	C	1	NAG	C2-N2-C7	-2.04	120.17	122.90

There are no chirality outliers.

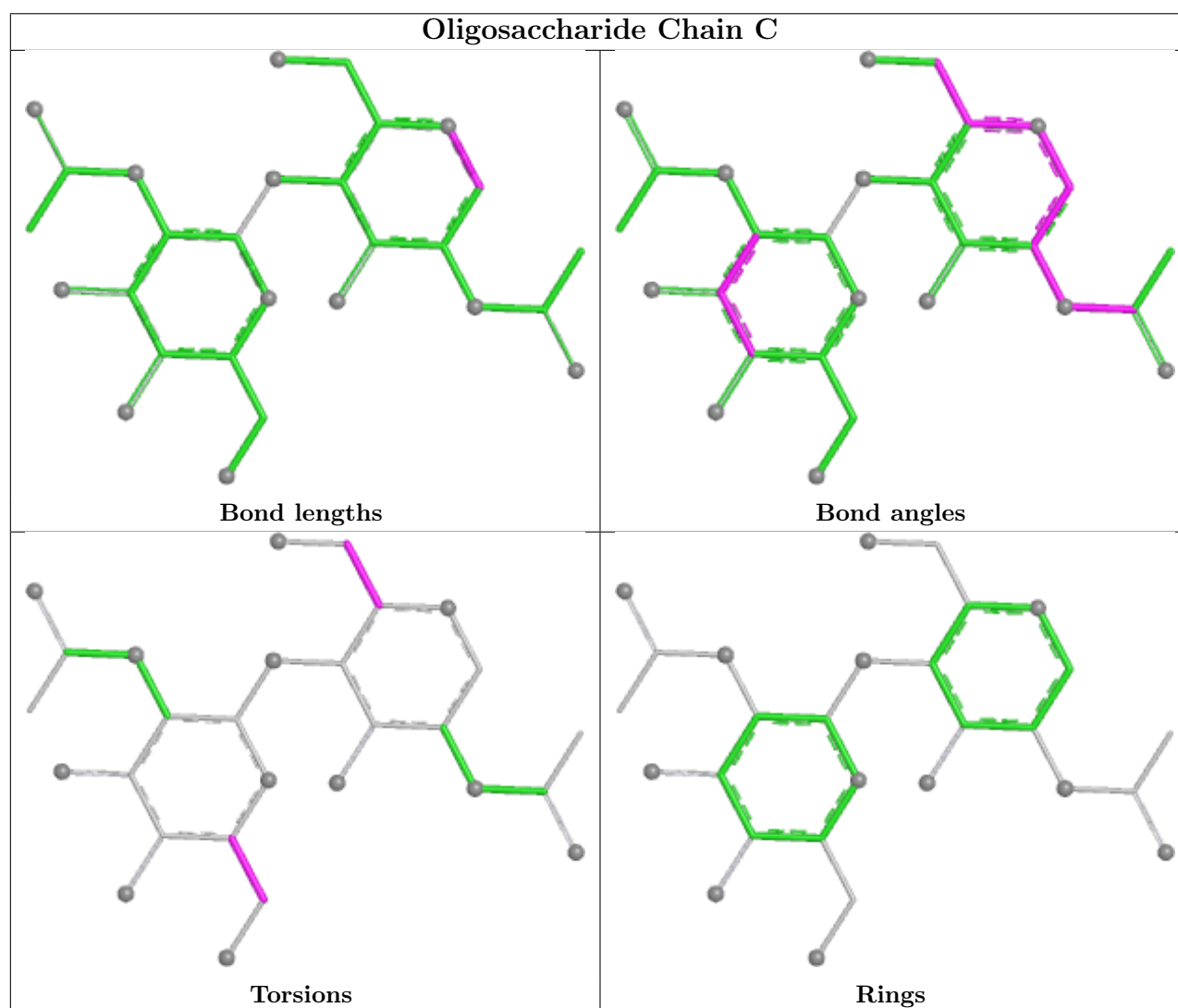
All (4) torsion outliers are listed below:

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

Of 7 ligands modelled in this entry, 1 is monoatomic - leaving 6 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
5	SPD	B	700	-	9,9,9	0.30	0	8,8,8	0.62	0
3	FAD	B	500	-	58,58,58	1.21	8 (13%)	85,89,89	1.60	16 (18%)
6	SO4	B	479	-	4,4,4	0.23	0	6,6,6	0.33	0
4	NAG	A	600	1	14,14,15	0.61	0	17,19,21	1.34	2 (11%)
3	FAD	A	500	-	58,58,58	1.10	5 (8%)	85,89,89	1.59	16 (18%)
5	SPD	A	700	-	9,9,9	0.28	0	8,8,8	0.71	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
5	SPD	B	700	-	-	4/7/7/7	-
3	FAD	B	500	-	-	8/34/50/50	0/6/6/6
4	NAG	A	600	1	-	1/6/23/26	0/1/1/1
3	FAD	A	500	-	-	8/34/50/50	0/6/6/6
5	SPD	A	700	-	-	5/7/7/7	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	500	FAD	C4X-N5	4.18	1.39	1.30
3	A	500	FAD	C4X-N5	3.78	1.38	1.30
3	B	500	FAD	C10-N1	3.14	1.39	1.33
3	B	500	FAD	C2A-N1A	2.89	1.39	1.33
3	A	500	FAD	C2A-N1A	2.72	1.38	1.33
3	B	500	FAD	C2A-N3A	2.72	1.38	1.33
3	A	500	FAD	C10-N1	2.60	1.38	1.33
3	A	500	FAD	C2A-N3A	2.48	1.38	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	500	FAD	P-O3P	2.48	1.62	1.59
3	B	500	FAD	C5A-N7A	-2.35	1.34	1.39
3	B	500	FAD	PA-O3P	2.16	1.61	1.59
3	B	500	FAD	C8A-N7A	2.03	1.35	1.31
3	A	500	FAD	C8A-N7A	2.01	1.35	1.31

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	500	FAD	N3A-C2A-N1A	-5.84	119.74	128.58
3	B	500	FAD	N3A-C2A-N1A	-5.83	119.76	128.58
3	B	500	FAD	C5A-C4A-N3A	-4.63	120.35	126.72
3	A	500	FAD	N9A-C8A-N7A	-4.37	107.73	113.94
3	A	500	FAD	C5A-C4A-N3A	-4.04	121.15	126.72
3	B	500	FAD	C9A-C5X-N5	-3.98	118.23	122.45
3	B	500	FAD	N9A-C8A-N7A	-3.59	108.84	113.94
4	A	600	NAG	C4-C3-C2	3.49	116.14	111.02
3	A	500	FAD	C4-N3-C2	-3.48	119.47	125.64
3	B	500	FAD	C4A-C5A-N7A	-3.44	106.65	110.58
3	B	500	FAD	C10-C4X-N5	-3.34	117.98	124.81
3	B	500	FAD	C2A-N3A-C4A	3.28	119.85	111.83
3	B	500	FAD	C5'-C4'-C3'	-3.24	106.11	112.22
3	A	500	FAD	C5'-C4'-C3'	-3.20	106.19	112.22
3	A	500	FAD	C5A-N7A-C8A	3.19	108.47	103.45
3	A	500	FAD	C2A-N3A-C4A	3.18	119.60	111.83
3	A	500	FAD	C9A-C5X-N5	-2.92	119.36	122.45
3	A	500	FAD	C4A-C5A-N7A	-2.91	107.25	110.58
3	B	500	FAD	N3A-C4A-N9A	2.85	132.01	127.17
3	B	500	FAD	C4-N3-C2	-2.84	120.61	125.64
3	A	500	FAD	C10-C4X-N5	-2.75	119.20	124.81
3	A	500	FAD	O4-C4-C4X	-2.58	119.71	126.53
4	A	600	NAG	O5-C5-C6	2.54	112.61	107.66
3	A	500	FAD	N3A-C4A-N9A	2.50	131.43	127.17
3	A	500	FAD	C4X-C4-N3	2.48	119.57	113.25
3	B	500	FAD	C4X-C4-N3	2.44	119.47	113.25
3	B	500	FAD	C5X-N5-C4X	2.37	121.92	118.09
3	B	500	FAD	C4-C4X-N5	2.36	121.47	118.21
3	A	500	FAD	C4X-C10-N1	-2.30	118.95	124.59
3	B	500	FAD	C5A-N7A-C8A	2.14	106.82	103.45
3	B	500	FAD	C4X-C10-N1	-2.09	119.46	124.59
3	A	500	FAD	C4X-C10-N10	2.09	119.48	116.48
3	B	500	FAD	O4-C4-C4X	-2.05	121.12	126.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	500	FAD	C4A-N9A-C1B	-2.02	121.92	126.63

There are no chirality outliers.

All (26) torsion outliers are listed below:

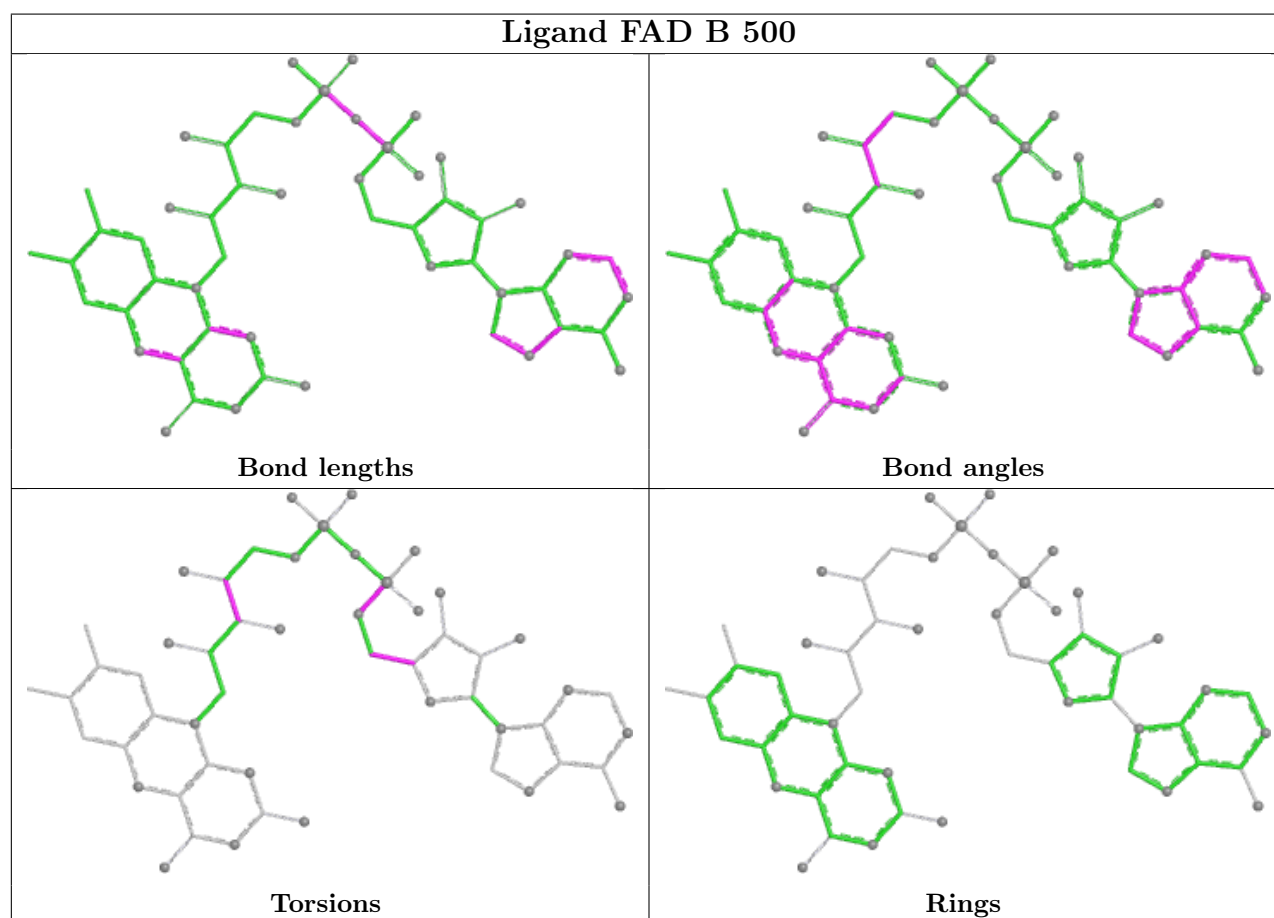
Mol	Chain	Res	Type	Atoms
3	A	500	FAD	C5B-O5B-PA-O1A
3	B	500	FAD	C5B-O5B-PA-O1A
3	B	500	FAD	C5B-O5B-PA-O3P
5	A	700	SPD	C3-C4-C5-N6
5	B	700	SPD	N6-C7-C8-C9
3	B	500	FAD	C2'-C3'-C4'-C5'
3	B	500	FAD	C2'-C3'-C4'-O4'
3	B	500	FAD	O3'-C3'-C4'-C5'
5	A	700	SPD	N6-C7-C8-C9
5	B	700	SPD	C2-C3-C4-C5
3	A	500	FAD	C2'-C3'-C4'-O4'
5	A	700	SPD	C2-C3-C4-C5
3	A	500	FAD	C2'-C3'-C4'-C5'
3	A	500	FAD	C5B-O5B-PA-O2A
3	A	500	FAD	C5B-O5B-PA-O3P
3	B	500	FAD	C5B-O5B-PA-O2A
3	B	500	FAD	O3'-C3'-C4'-O4'
3	A	500	FAD	O3'-C3'-C4'-C5'
5	B	700	SPD	C8-C7-N6-C5
3	B	500	FAD	O4B-C4B-C5B-O5B
5	A	700	SPD	C8-C7-N6-C5
3	A	500	FAD	O4B-C4B-C5B-O5B
5	A	700	SPD	C7-C8-C9-N10
5	B	700	SPD	C7-C8-C9-N10
3	A	500	FAD	O3'-C3'-C4'-O4'
4	A	600	NAG	C4-C5-C6-O6

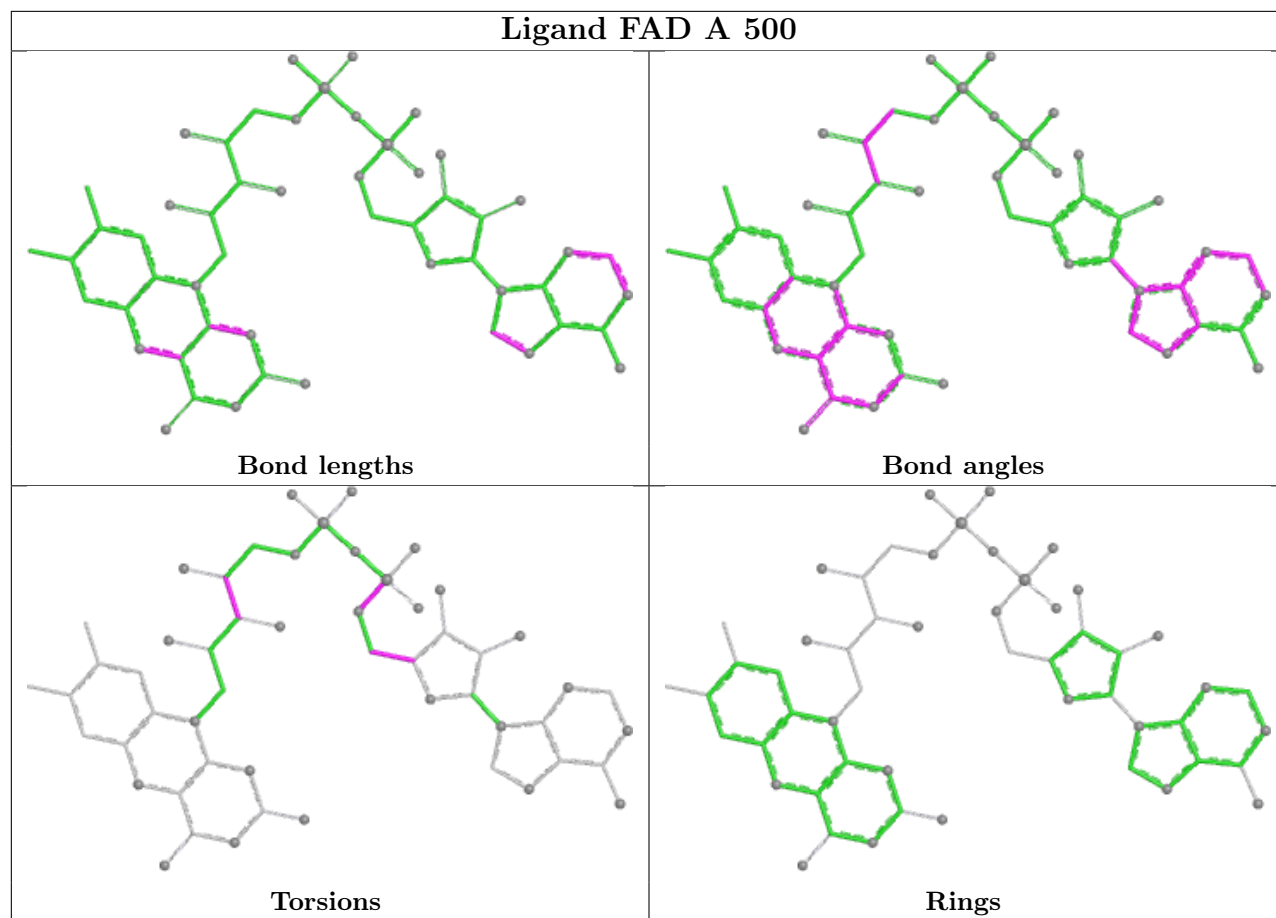
There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	700	SPD	3	0
3	B	500	FAD	1	0
3	A	500	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.





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, 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	467/478 (97%)	-0.20	10 (2%) 63 43	9, 29, 39, 52	21 (4%)
1	B	466/478 (97%)	-0.19	7 (1%) 72 52	9, 29, 39, 51	14 (3%)
All	All	933/956 (97%)	-0.19	17 (1%) 67 48	9, 29, 39, 52	35 (3%)

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2	THR	4.4
1	A	2	THR	4.2
1	A	466	HIS	4.1
1	B	3	VAL	4.0
1	A	105	ASP	3.9
1	A	221	ASP	3.8
1	A	107	ASP	3.7
1	A	364	GLN	3.0
1	A	341	ASP	2.9
1	B	466	HIS	2.8
1	B	6[A]	ARG	2.8
1	A	468	GLN	2.5
1	B	341	ASP	2.5
1	B	467	VAL	2.2
1	A	308	LYS	2.2
1	B	221	ASP	2.2
1	A	363	GLU	2.1

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

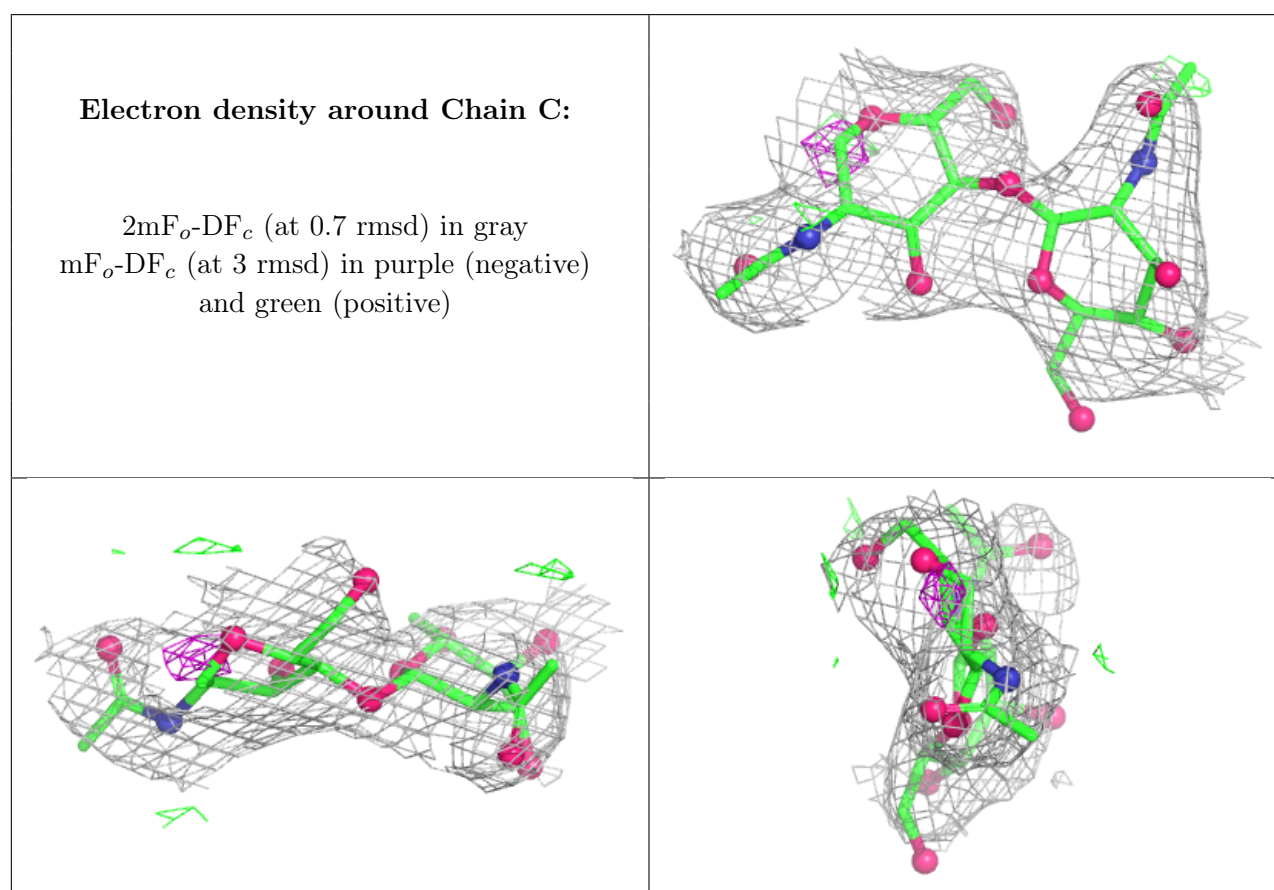
There are no non-standard protein/DNA/RNA residues in this entry.

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(Å ²)	Q<0.9
2	NAG	C	2	14/15	0.76	0.17	60,62,63,63	0
2	NAG	C	1	14/15	0.89	0.13	51,53,55,58	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.

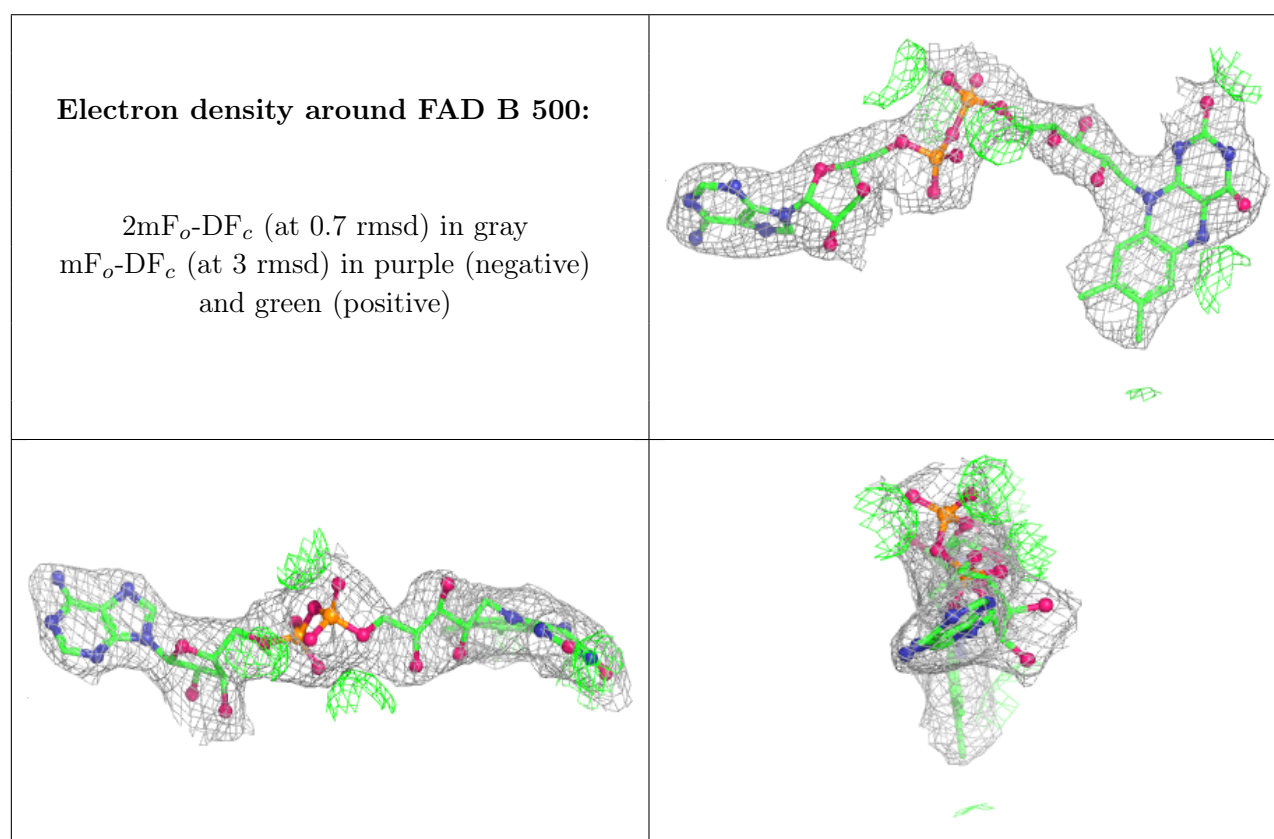


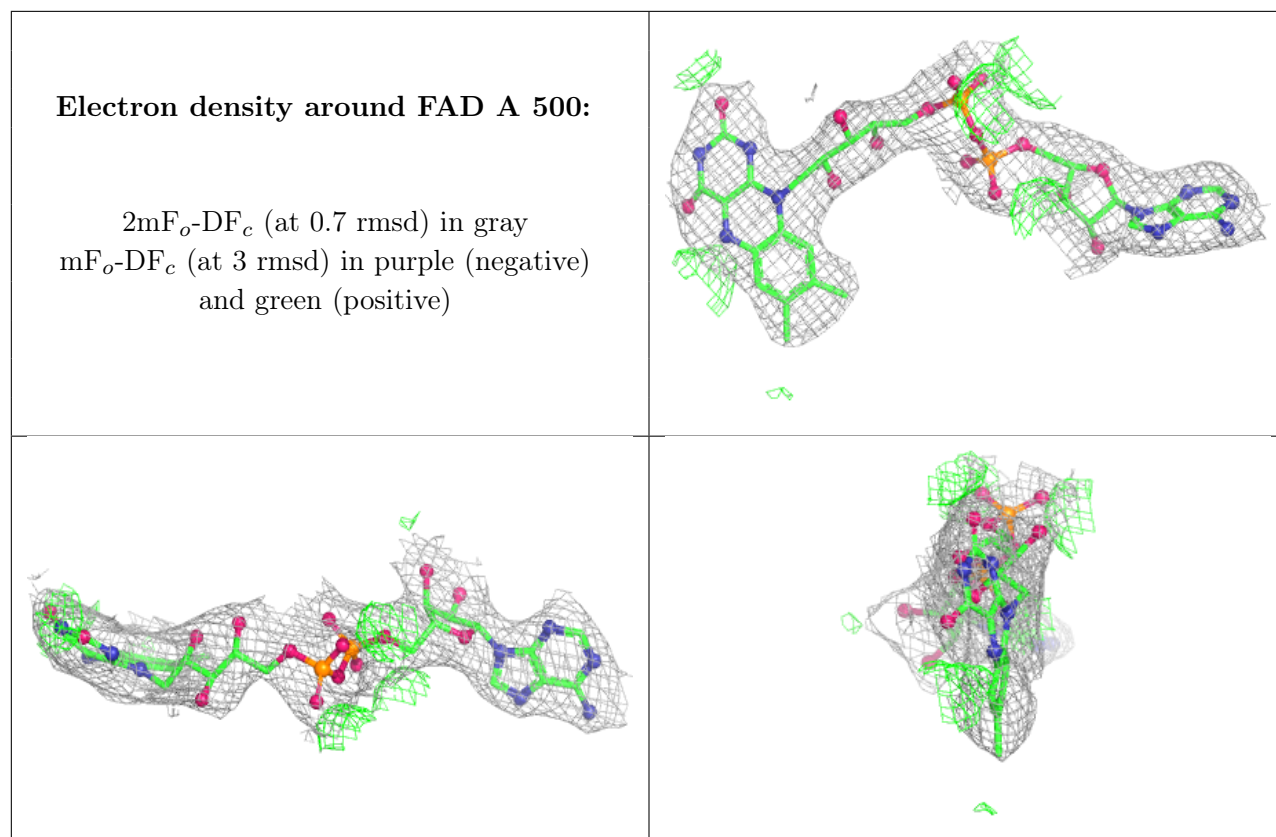
6.4 Ligands [i](#)

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
4	NAG	A	600	14/15	0.82	0.16	45,48,49,50	0
6	SO4	B	479	5/5	0.94	0.10	54,54,54,55	0
7	CL	B	480	1/1	0.94	0.12	31,31,31,31	0
5	SPD	B	700	10/10	0.95	0.14	34,36,40,40	0
5	SPD	A	700	10/10	0.96	0.12	33,39,42,43	0
3	FAD	B	500	53/53	0.98	0.07	22,25,27,27	0
3	FAD	A	500	53/53	0.98	0.06	18,22,25,27	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.