Full wwPDB X-ray Structure Validation Report (i)

Dec 2, 2023 – 02:12 pm GMT

PDB ID	:	1H84
Title	:	COVALENT ADDUCT BETWEEN POLYAMINE OXIDASE AND N1ethyl N11((cycloheptyl)methyl)4,8diazaundecane at pH 4.6
Authors	:	Binda, C.; Coda, A.; Angelini, R.; Federico, R.; Ascenzi, P.; Mattevi, A.
Deposited on	:	2001-01-24
Resolution	:	2.00 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 (i) 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 (1)) were used in the production of this report:

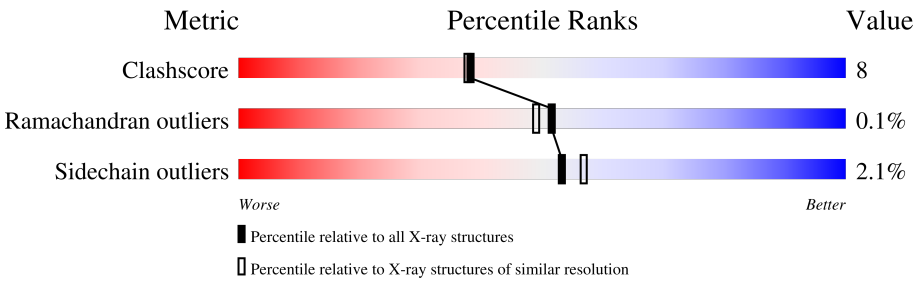
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.00 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))
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	472	78% 18% • •
1	B	472	81% 16% • •
1	C	472	82% 15% • •
2	D	2	100%
2	E	2	100%
3	F	5	40% 60%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	F	1	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 12174 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.

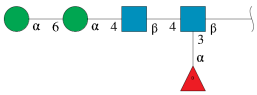
- Molecule 1 is a protein called POLYAMINE OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	459	3684	2353	621	696	14	56	0	0
1	B	462	3715	2374	627	700	14	54	0	0
1	C	462	3715	2374	627	700	14	56	0	0

- 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
			Total	C	N	O			
2	D	2	28	16	2	10	0	0	0
2	E	2	28	16	2	10	0	0	0

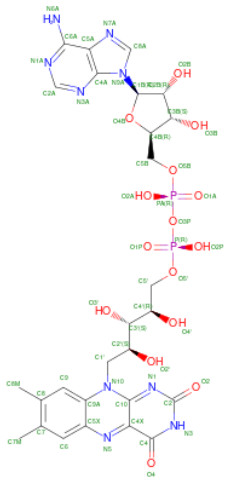
- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-D-fucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	F	5	60	34	2	24	0	0	0

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).

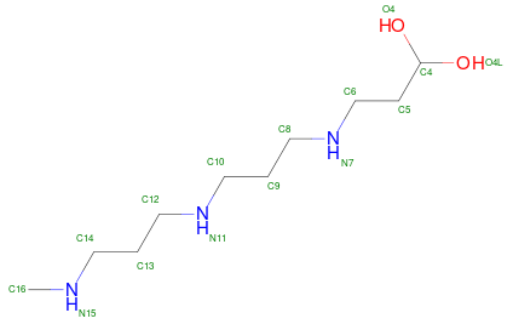
FAD



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

- Molecule 5 is 3-[(3-{[3-(METHYLAMINO)PROPYL]AMINO}PROPYL)AMINO]PROPANE-1,1-DIOL (three-letter code: NBA) (formula: $C_{10}H_{25}N_3O_2$).

NBA



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	A	1	14	10	3	1	0	0
5	B	1	14	10	3	1	0	0
5	C	1	14	10	3	1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	235	235	235	0	0
6	B	245	245	245	0	0
6	C	263	263	263	0	0

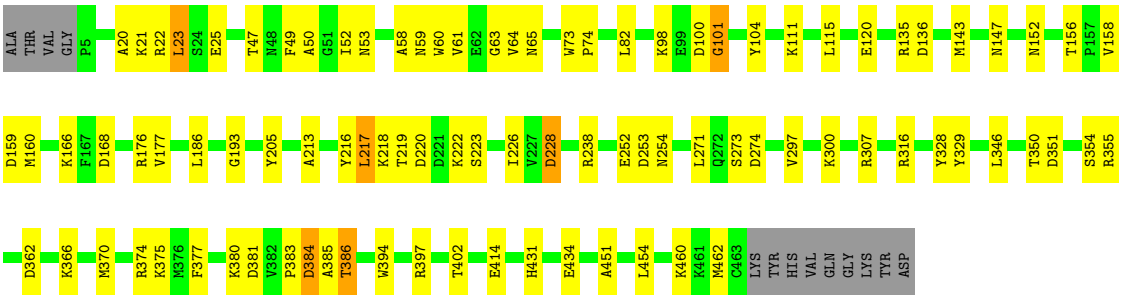
3 Residue-property plots (i)

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. 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. 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.

Note EDS was not executed.

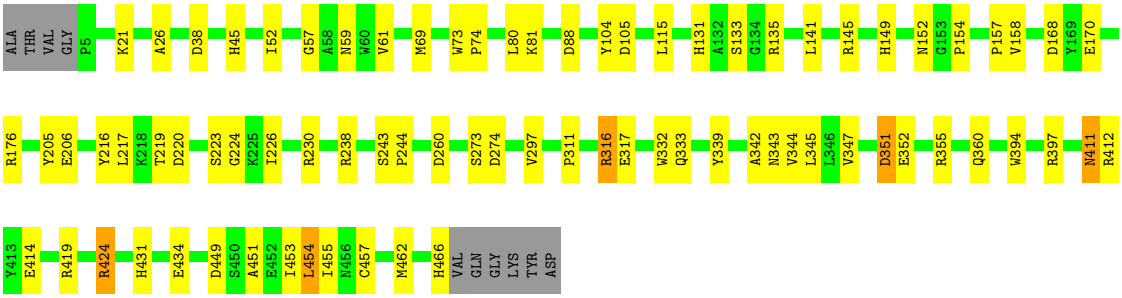
• Molecule 1: POLYAMINE OXIDASE

Chain A:



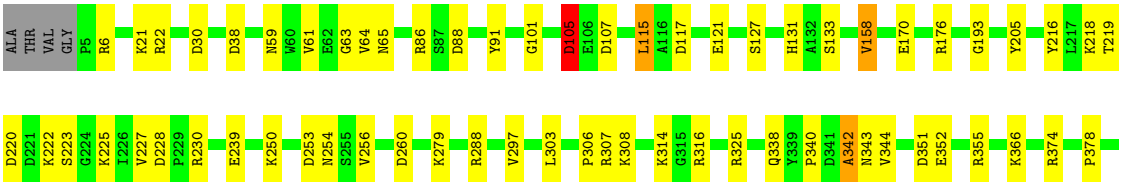
• Molecule 1: POLYAMINE OXIDASE

Chain B:



• Molecule 1: POLYAMINE OXIDASE

Chain C:



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

Chain D:

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

Chain E:

• Molecule 3: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-D-fucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α, β, γ	184.04Å 184.04Å 280.80Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.00	Depositor
% Data completeness (in resolution range)	93.5 (20.00-2.00)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT 5D	Depositor
R, R_{free}	0.189 , 0.227	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12174	wwPDB-VP
Average B, all atoms (Å^2)	15.0	wwPDB-VP

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: NBA, FCA, NAG, FAD, MAN

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	0.57	0/3775	1.27	21/5116 (0.4%)
1	B	0.55	0/3808	1.23	18/5160 (0.3%)
1	C	0.57	0/3808	1.25	25/5160 (0.5%)
All	All	0.57	0/11391	1.25	64/15436 (0.4%)

There are no bond length outliers.

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	355	ARG	NE-CZ-NH2	-12.83	113.89	120.30
1	B	355	ARG	NE-CZ-NH2	-11.10	114.75	120.30
1	C	355	ARG	NE-CZ-NH2	-10.31	115.14	120.30
1	C	307	ARG	NE-CZ-NH1	-8.95	115.82	120.30
1	A	355	ARG	NE-CZ-NH1	8.85	124.73	120.30
1	B	135	ARG	NE-CZ-NH1	-8.51	116.04	120.30
1	A	307	ARG	NE-CZ-NH2	-8.14	116.23	120.30
1	C	86	ARG	NE-CZ-NH1	8.08	124.34	120.30
1	C	176	ARG	NE-CZ-NH2	-7.83	116.39	120.30
1	A	228	ASP	CB-CG-OD2	-7.57	111.49	118.30
1	C	374	ARG	NE-CZ-NH2	-7.17	116.72	120.30
1	B	115	LEU	CB-CG-CD1	-7.15	98.84	111.00
1	B	170	GLU	OE1-CD-OE2	-6.98	114.93	123.30
1	C	397	ARG	NE-CZ-NH2	-6.89	116.86	120.30
1	A	101	GLY	N-CA-C	6.87	130.26	113.10
1	C	115	LEU	CB-CG-CD2	-6.76	99.50	111.00
1	C	316	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	C	340	PRO	C-N-CA	-6.36	105.81	121.70
1	C	230	ARG	NE-CZ-NH1	-6.22	117.19	120.30
1	A	297	VAL	CB-CA-C	-6.19	99.64	111.40
1	C	22	ARG	NE-CZ-NH2	-6.15	117.22	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	135	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	A	454	LEU	CB-CG-CD1	-5.98	100.84	111.00
1	C	325	ARG	NE-CZ-NH1	-5.94	117.33	120.30
1	A	316	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	C	308	LYS	CD-CE-NZ	5.92	125.32	111.70
1	B	115	LEU	CB-CG-CD2	-5.91	100.95	111.00
1	B	355	ARG	NE-CZ-NH1	5.87	123.24	120.30
1	C	288	ARG	NE-CZ-NH1	-5.83	117.39	120.30
1	A	381	ASP	N-CA-C	-5.82	95.27	111.00
1	C	61	VAL	N-CA-C	-5.72	95.55	111.00
1	B	412	ARG	NE-CZ-NH1	-5.72	117.44	120.30
1	C	260	ASP	CB-CG-OD2	5.72	123.44	118.30
1	C	22	ARG	NE-CZ-NH1	5.69	123.15	120.30
1	B	351	ASP	N-CA-CB	-5.67	100.39	110.60
1	B	316	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	C	88	ASP	CB-CG-OD1	5.60	123.34	118.30
1	A	22	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	B	424	ARG	NE-CZ-NH1	5.59	123.10	120.30
1	A	61	VAL	N-CA-C	-5.56	95.99	111.00
1	C	38	ASP	CB-CG-OD1	5.56	123.30	118.30
1	A	374	ARG	NE-CZ-NH1	-5.54	117.53	120.30
1	B	454	LEU	CA-CB-CG	5.54	128.03	115.30
1	B	230	ARG	NE-CZ-NH1	-5.50	117.55	120.30
1	C	307	ARG	NE-CZ-NH2	5.49	123.04	120.30
1	A	397	ARG	NE-CZ-NH1	5.47	123.04	120.30
1	B	38	ASP	CB-CG-OD2	-5.46	113.38	118.30
1	B	88	ASP	CB-CG-OD1	5.45	123.20	118.30
1	B	454	LEU	CB-CG-CD1	5.35	120.10	111.00
1	A	351	ASP	CB-CG-OD1	5.34	123.11	118.30
1	C	342	ALA	N-CA-C	5.33	125.40	111.00
1	A	397	ARG	NE-CZ-NH2	-5.29	117.65	120.30
1	C	297	VAL	CB-CA-C	-5.28	101.36	111.40
1	C	158	VAL	CG1-CB-CG2	-5.28	102.45	110.90
1	A	176	ARG	CB-CG-CD	-5.27	97.90	111.60
1	B	297	VAL	CB-CA-C	-5.24	101.45	111.40
1	C	397	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	A	362	ASP	CB-CG-OD1	5.17	122.95	118.30
1	B	61	VAL	N-CA-C	-5.17	97.05	111.00
1	A	386	THR	N-CA-CB	-5.16	100.49	110.30
1	A	60	TRP	CB-CA-C	-5.15	100.10	110.40
1	C	105	ASP	CB-CG-OD2	5.11	122.90	118.30
1	B	397	ARG	NE-CZ-NH2	5.10	122.85	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	186	LEU	CB-CG-CD2	-5.03	102.44	111.00

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	3684	0	3585	51	0
1	B	3715	0	3614	60	0
1	C	3715	0	3614	42	0
2	D	28	0	26	4	0
2	E	28	0	26	3	0
3	F	60	0	53	8	0
4	A	53	0	31	2	0
4	B	53	0	31	2	0
4	C	53	0	31	3	0
5	A	14	0	23	1	0
5	B	14	0	23	0	0
5	C	14	0	23	1	0
6	A	235	0	0	1	0
6	B	245	0	0	2	0
6	C	263	0	0	2	0
All	All	12174	0	11080	165	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 8.

All (165) 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:69:MET:HE2	1:B:74:PRO:HD3	1.29	1.12
1:B:69:MET:CE	1:B:73:TRP:HB3	1.86	1.05
1:B:69:MET:HE3	1:B:73:TRP:HB3	1.42	1.00
1:B:69:MET:CE	1:B:74:PRO:HD3	1.92	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:131:HIS:CD2	1:C:133:SER:H	1.87	0.90
3:F:1:NAG:C4	3:F:2:NAG:C1	2.50	0.90
1:C:91:TYR:OH	1:C:314:LYS:HE2	1.74	0.85
1:A:273:SER:O	1:A:274:ASP:HB2	1.78	0.83
1:B:411:ASN:ND2	1:B:414:GLU:H	1.75	0.82
2:E:1:NAG:C4	2:E:2:NAG:C1	2.62	0.78
1:B:131:HIS:CD2	1:B:133:SER:H	2.02	0.77
1:A:394:TRP:HE1	1:B:152:ASN:ND2	1.82	0.76
1:C:131:HIS:HD2	1:C:133:SER:H	1.30	0.74
1:B:131:HIS:HD2	1:B:133:SER:H	1.35	0.73
2:D:1:NAG:C4	2:D:2:NAG:C1	2.66	0.73
1:A:431:HIS:CD2	1:A:431:HIS:H	2.09	0.67
1:C:117:ASP:O	1:C:121:GLU:HG3	1.94	0.67
3:F:1:NAG:O4	3:F:2:NAG:C2	2.43	0.66
1:A:394:TRP:HE1	1:B:152:ASN:HD22	1.43	0.66
3:F:1:NAG:H3	3:F:5:FCA:O2	1.97	0.65
1:A:216:TYR:CD1	1:A:217:LEU:HD13	2.32	0.64
1:A:238:ARG:NH1	1:A:252:GLU:OE2	2.29	0.64
2:D:1:NAG:HO4	2:D:2:NAG:C1	2.09	0.63
1:C:412:ARG:NH1	1:C:434:GLU:OE1	2.29	0.63
1:C:431:HIS:H	1:C:431:HIS:CD2	2.18	0.62
1:A:73:TRP:HB3	1:A:74:PRO:HD3	1.81	0.62
1:B:69:MET:HE3	1:B:73:TRP:CB	2.25	0.61
1:B:411:ASN:HD22	1:B:414:GLU:H	1.46	0.61
2:E:1:NAG:O4	2:E:2:NAG:C2	2.48	0.61
1:A:98:LYS:HG2	1:A:104:TYR:CE1	2.37	0.60
1:A:152:ASN:ND2	1:B:394:TRP:HE1	2.00	0.60
1:A:21:LYS:O	1:A:25:GLU:HG3	2.01	0.60
1:C:131:HIS:HD2	1:C:133:SER:OG	1.85	0.59
1:C:220:ASP:OD2	1:C:222:LYS:N	2.36	0.59
1:B:342:ALA:O	1:B:343:ASN:HB2	2.03	0.58
1:C:250:LYS:HG2	1:C:256:VAL:HG22	1.85	0.58
1:A:216:TYR:CE1	1:A:217:LEU:HD13	2.40	0.57
1:C:91:TYR:CZ	1:C:314:LYS:HE2	2.40	0.57
1:C:253:ASP:O	1:C:254:ASN:HB2	2.05	0.57
1:B:220:ASP:O	1:B:224:GLY:N	2.37	0.56
1:B:431:HIS:H	1:B:431:HIS:CD2	2.23	0.56
1:C:412:ARG:HD3	1:C:434:GLU:OE1	2.05	0.56
1:B:69:MET:HE2	1:B:73:TRP:HB3	1.86	0.55
1:C:158:VAL:HG12	6:C:2073:HOH:O	2.05	0.55
1:C:220:ASP:HB3	1:C:223:SER:OG	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:449:ASP:O	1:B:453:ILE:HG13	2.06	0.55
1:C:131:HIS:CD2	1:C:133:SER:OG	2.60	0.55
1:A:111:LYS:O	1:A:115:LEU:HG	2.07	0.54
1:C:131:HIS:HD2	1:C:133:SER:N	2.03	0.54
1:C:366:LYS:HD2	1:C:385:ALA:HB3	1.89	0.54
1:B:411:ASN:HD21	1:B:414:GLU:HG3	1.73	0.54
1:C:6:ARG:HH11	1:C:6:ARG:HG3	1.73	0.54
1:C:342:ALA:O	1:C:343:ASN:HB2	2.08	0.54
1:A:220:ASP:HB3	1:A:223:SER:OG	2.08	0.53
1:B:243:SER:HB2	1:B:244:PRO:HD2	1.90	0.53
1:B:26:ALA:HB2	1:B:455:ILE:HD13	1.91	0.53
1:A:152:ASN:HD22	1:B:394:TRP:HE1	1.56	0.52
1:A:366:LYS:HD2	1:A:385:ALA:HB3	1.91	0.52
1:A:253:ASP:O	1:A:254:ASN:HB2	2.08	0.52
1:C:219:THR:HA	1:C:225:LYS:O	2.09	0.52
1:B:451:ALA:O	1:B:455:ILE:HG13	2.10	0.51
1:B:243:SER:HB2	1:B:244:PRO:CD	2.40	0.51
1:C:131:HIS:HD2	1:C:133:SER:CB	2.24	0.51
3:F:1:NAG:HO4	3:F:2:NAG:C1	2.12	0.51
1:C:21:LYS:HB2	1:C:216:TYR:CE2	2.46	0.51
1:A:63:GLY:HA2	1:A:193:GLY:O	2.10	0.51
1:B:457:CYS:HA	1:B:462:MET:O	2.12	0.50
1:A:220:ASP:OD1	1:A:222:LYS:N	2.36	0.49
1:C:306:PRO:HD3	1:C:386:THR:HG23	1.94	0.49
1:B:411:ASN:HD22	1:B:411:ASN:C	2.16	0.49
1:C:170:GLU:OE2	5:C:591:NBA:H122	2.13	0.49
1:B:419:ARG:HD3	6:B:2219:HOH:O	2.13	0.49
1:A:218:LYS:H	1:A:228:ASP:HB2	1.78	0.48
1:B:45:HIS:HA	1:B:206:GLU:OE2	2.13	0.48
1:C:402:THR:CB	4:C:590:FAD:HM83	2.44	0.48
1:C:6:ARG:HA	1:C:30:ASP:O	2.13	0.48
1:A:47:THR:O	1:A:53:ASN:HA	2.13	0.48
1:C:218:LYS:H	1:C:228:ASP:HB2	1.78	0.48
1:A:219:THR:HG22	1:A:226:ILE:HA	1.96	0.48
1:A:49:PHE:O	1:A:50:ALA:HB3	2.13	0.47
1:B:219:THR:HG22	1:B:226:ILE:HA	1.95	0.47
1:B:220:ASP:HB3	1:B:223:SER:OG	2.14	0.47
1:A:414:GLU:O	1:A:414:GLU:HG3	2.13	0.47
1:B:131:HIS:HD2	1:B:133:SER:OG	1.98	0.47
1:C:402:THR:HB	4:C:590:FAD:HM83	1.96	0.47
2:E:1:NAG:O6	2:E:2:NAG:C1	2.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:GLU:OE1	1:A:166:LYS:NZ	2.46	0.47
1:A:217:LEU:HD12	1:A:217:LEU:HA	1.62	0.47
1:B:141:LEU:HD22	1:B:176:ARG:HB3	1.97	0.46
1:A:64:VAL:HG12	1:A:65:ASN:N	2.30	0.46
1:A:370:MET:HE2	1:A:384:ASP:HA	1.98	0.46
1:B:360:GLN:NE2	6:B:2188:HOH:O	2.49	0.46
3:F:1:NAG:C3	3:F:5:FCA:O2	2.63	0.46
1:A:143:MET:SD	1:A:147:ASN:ND2	2.89	0.46
1:B:411:ASN:ND2	1:B:414:GLU:HG3	2.31	0.45
1:A:156:THR:O	1:A:160:MET:HG3	2.16	0.45
3:F:1:NAG:O6	3:F:2:NAG:C1	2.64	0.45
3:F:2:NAG:H62	3:F:5:FCA:H5	1.98	0.45
1:B:69:MET:HE1	1:B:74:PRO:HD3	1.88	0.45
2:D:1:NAG:H4	2:D:2:NAG:C1	2.46	0.45
1:B:104:TYR:CZ	1:B:158:VAL:CG2	3.00	0.45
1:B:411:ASN:HD21	1:B:414:GLU:H	1.60	0.45
1:A:98:LYS:HG2	1:A:104:TYR:CD1	2.52	0.45
1:A:300:LYS:HB3	1:A:346:LEU:HD11	1.98	0.45
1:A:370:MET:HE1	1:A:383:PRO:O	2.18	0.44
1:B:131:HIS:CD2	1:B:133:SER:OG	2.71	0.44
3:F:1:NAG:H4	3:F:2:NAG:C1	2.42	0.44
1:B:220:ASP:CG	1:B:223:SER:HG	2.21	0.44
1:B:273:SER:O	1:B:274:ASP:HB2	2.18	0.44
1:C:131:HIS:CD2	1:C:133:SER:CB	3.00	0.44
1:B:344:VAL:HG12	1:B:345:LEU:N	2.32	0.44
1:A:82:LEU:HD23	1:A:82:LEU:HA	1.81	0.44
1:A:20:ALA:HB3	1:A:216:TYR:OH	2.19	0.43
1:B:260:ASP:O	1:B:424:ARG:HD3	2.18	0.43
1:C:63:GLY:HA2	1:C:193:GLY:O	2.17	0.43
1:C:438:GLY:O	4:C:590:FAD:H1'2	2.18	0.43
1:A:158:VAL:HG13	1:A:159:ASP:N	2.34	0.43
1:A:273:SER:O	1:A:274:ASP:CB	2.45	0.43
1:A:377:PHE:HB3	1:A:380:LYS:HG3	2.01	0.43
1:B:69:MET:CE	1:B:73:TRP:CB	2.77	0.43
1:A:100:ASP:OD1	1:A:375:LYS:HE2	2.19	0.43
1:A:460:LYS:HB3	1:A:462:MET:CE	2.49	0.43
1:C:338:GLN:OE1	1:C:338:GLN:N	2.51	0.43
1:C:101:GLY:HA3	1:C:378:PRO:HG3	2.00	0.43
1:A:58:ALA:HA	4:A:590:FAD:C4X	2.49	0.42
1:C:105:ASP:OD2	1:C:107:ASP:N	2.51	0.42
1:A:213:ALA:O	1:A:217:LEU:HB2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:LEU:O	1:B:81:LYS:HB2	2.19	0.42
1:B:351:ASP:CG	1:B:352:GLU:H	2.22	0.42
1:A:402:THR:HB	4:A:590:FAD:HM83	2.00	0.42
1:A:23:LEU:HD13	1:A:451:ALA:HB1	2.01	0.42
1:A:253:ASP:OD1	1:A:253:ASP:C	2.58	0.42
1:A:350:THR:HA	1:A:354:SER:OG	2.19	0.42
5:A:591:NBA:HC52	6:A:2228:HOH:O	2.19	0.42
1:B:26:ALA:CB	1:B:455:ILE:HD13	2.49	0.42
1:B:57:GLY:HA2	4:B:590:FAD:C7M	2.50	0.42
1:C:381:ASP:HB3	6:C:2206:HOH:O	2.20	0.42
1:B:311:PRO:HB2	1:B:316:ARG:HD2	2.01	0.42
1:C:91:TYR:CD1	1:C:91:TYR:N	2.87	0.42
1:B:69:MET:CE	1:B:73:TRP:CD1	3.03	0.42
1:B:145:ARG:O	1:B:149:HIS:N	2.51	0.42
1:B:104:TYR:CZ	1:B:158:VAL:HG23	2.55	0.41
1:B:69:MET:CE	1:B:74:PRO:CD	2.81	0.41
1:B:21:LYS:HB2	1:B:216:TYR:CE2	2.55	0.41
1:B:131:HIS:HD2	1:B:133:SER:N	2.12	0.41
1:A:218:LYS:N	1:A:228:ASP:HB2	2.36	0.41
1:B:220:ASP:O	1:B:224:GLY:HA2	2.21	0.41
1:C:351:ASP:CG	1:C:352:GLU:H	2.22	0.41
1:A:328:TYR:O	1:A:329:TYR:C	2.58	0.41
1:B:52:ILE:HD12	1:B:339:TYR:CD2	2.55	0.41
1:B:317:GLU:O	1:B:333:GLN:HA	2.21	0.41
1:B:332:TRP:CZ3	1:B:347:VAL:HB	2.56	0.41
1:C:454:LEU:HD12	1:C:454:LEU:O	2.21	0.41
2:D:1:NAG:O6	2:D:2:NAG:C1	2.69	0.41
1:A:177:VAL:HG12	1:A:177:VAL:O	2.21	0.41
1:A:220:ASP:OD1	1:A:220:ASP:C	2.59	0.41
1:C:218:LYS:O	1:C:227:VAL:N	2.47	0.41
1:C:303:LEU:O	1:C:344:VAL:HA	2.21	0.41
1:A:271:LEU:HD23	1:A:271:LEU:HA	1.85	0.41
1:B:57:GLY:HA2	4:B:590:FAD:HM72	2.03	0.41
1:C:239:GLU:OE2	1:C:279:LYS:HD2	2.21	0.40
1:A:136:ASP:OD1	1:A:136:ASP:N	2.48	0.40
1:B:217:LEU:HD23	1:B:217:LEU:HA	1.82	0.40
1:B:220:ASP:O	1:B:224:GLY:CA	2.70	0.40
1:C:64:VAL:O	1:C:65:ASN:HB2	2.20	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	457/472 (97%)	440 (96%)	16 (4%)	1 (0%)	47	44
1	B	460/472 (98%)	443 (96%)	17 (4%)	0	100	100
1	C	460/472 (98%)	443 (96%)	17 (4%)	0	100	100
All	All	1377/1416 (97%)	1326 (96%)	50 (4%)	1 (0%)	51	49

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	101	GLY

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	394/404 (98%)	385 (98%)	9 (2%)	50	53
1	B	397/404 (98%)	386 (97%)	11 (3%)	43	44
1	C	397/404 (98%)	392 (99%)	5 (1%)	69	74
All	All	1188/1212 (98%)	1163 (98%)	25 (2%)	53	57

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LEU
1	A	52	ILE

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Mol	Chain	Res	Type
1	A	59	ASN
1	A	168	ASP
1	A	205	TYR
1	A	217	LEU
1	A	384	ASP
1	A	386	THR
1	A	434	GLU
1	B	59	ASN
1	B	105	ASP
1	B	154	PRO
1	B	157	PRO
1	B	168	ASP
1	B	205	TYR
1	B	238	ARG
1	B	411	ASN
1	B	434	GLU
1	B	454	LEU
1	B	466	HIS
1	C	59	ASN
1	C	105	ASP
1	C	115	LEU
1	C	127	SER
1	C	205	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	149	HIS
1	A	152	ASN
1	A	360	GLN
1	A	431	HIS
1	B	131	HIS
1	B	150	GLN
1	B	152	ASN
1	B	360	GLN
1	B	411	ASN
1	B	431	HIS
1	B	435	HIS
1	C	48	ASN
1	C	131	HIS
1	C	152	ASN
1	C	292	GLN

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Mol	Chain	Res	Type
1	C	360	GLN
1	C	431	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)

9 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	D	1	2,1	14,14,15	0.94	0	17,19,21	1.61	3 (17%)
2	NAG	D	2	2	14,14,15	0.90	1 (7%)	17,19,21	1.66	3 (17%)
2	NAG	E	1	2,1	14,14,15	1.20	2 (14%)	17,19,21	1.74	4 (23%)
2	NAG	E	2	2	14,14,15	0.91	1 (7%)	17,19,21	1.30	2 (11%)
3	NAG	F	1	1,3	14,14,15	1.02	0	17,19,21	1.93	6 (35%)
3	NAG	F	2	3	14,14,15	1.04	1 (7%)	17,19,21	1.57	4 (23%)
3	MAN	F	3	3	11,11,12	0.76	0	15,15,17	3.14	5 (33%)
3	MAN	F	4	3	11,11,12	0.54	0	15,15,17	1.62	3 (20%)
3	FCA	F	5	3	10,10,11	1.22	2 (20%)	14,14,16	2.02	6 (42%)

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	D	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	NAG	E	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
3	NAG	F	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1
3	MAN	F	3	3	-	0/2/19/22	0/1/1/1
3	MAN	F	4	3	-	2/2/19/22	0/1/1/1
3	FCA	F	5	3	-	-	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	2	NAG	O5-C1	-2.99	1.38	1.43
2	E	1	NAG	C1-C2	-2.75	1.48	1.52
3	F	5	FCA	C2-C3	-2.65	1.48	1.52
2	E	2	NAG	O5-C1	-2.62	1.39	1.43
2	E	1	NAG	O5-C1	-2.48	1.39	1.43
2	D	2	NAG	O5-C1	-2.23	1.40	1.43
3	F	5	FCA	O2-C2	2.09	1.47	1.43

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	3	MAN	O2-C2-C3	10.60	131.38	110.14
2	E	1	NAG	C2-N2-C7	-4.36	116.70	122.90
2	D	2	NAG	C2-N2-C7	-3.93	117.31	122.90
3	F	1	NAG	C1-C2-N2	-3.92	103.79	110.49
2	D	1	NAG	O5-C5-C6	-3.90	101.09	107.20
3	F	4	MAN	C1-C2-C3	-3.87	104.91	109.67
3	F	2	NAG	O5-C5-C6	-3.87	101.14	107.20
3	F	5	FCA	O5-C1-C2	-3.79	104.92	110.77
3	F	1	NAG	C8-C7-N2	-3.47	110.23	116.10
3	F	5	FCA	C3-C4-C5	-3.25	104.72	109.77
3	F	4	MAN	C2-C3-C4	-3.13	105.48	110.89
3	F	3	MAN	O5-C5-C6	3.13	112.11	107.20
2	E	1	NAG	C1-C2-N2	-3.11	105.17	110.49
3	F	4	MAN	O2-C2-C3	3.09	116.32	110.14
2	D	2	NAG	C1-C2-N2	-3.01	105.34	110.49
2	D	1	NAG	C1-O5-C5	2.98	116.23	112.19
3	F	2	NAG	O5-C5-C4	-2.95	103.64	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	1	NAG	O4-C4-C3	-2.91	103.61	110.35
2	D	2	NAG	C8-C7-N2	-2.85	111.28	116.10
3	F	1	NAG	O5-C5-C6	-2.81	102.80	107.20
2	D	1	NAG	O3-C3-C4	2.68	116.55	110.35
3	F	5	FCA	O3-C3-C4	-2.60	104.33	110.35
3	F	2	NAG	C2-N2-C7	-2.57	119.24	122.90
3	F	3	MAN	O2-C2-C1	2.54	114.35	109.15
2	E	2	NAG	C1-O5-C5	2.51	115.60	112.19
3	F	3	MAN	C1-O5-C5	2.48	115.55	112.19
3	F	2	NAG	C3-C4-C5	2.47	114.64	110.24
2	E	1	NAG	C1-O5-C5	2.45	115.51	112.19
3	F	1	NAG	O7-C7-C8	2.33	126.39	122.06
3	F	3	MAN	O4-C4-C3	2.26	115.58	110.35
3	F	1	NAG	C1-O5-C5	2.17	115.13	112.19
2	E	1	NAG	O3-C3-C4	2.15	115.32	110.35
2	E	2	NAG	O5-C5-C6	-2.10	103.92	107.20
3	F	5	FCA	C2-C3-C4	-2.07	107.32	110.89
3	F	5	FCA	O2-C2-C1	-2.05	104.95	109.15
3	F	5	FCA	C1-O5-C5	2.04	117.40	112.78

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	2	NAG	C4-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
2	E	1	NAG	C4-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6
3	F	1	NAG	C4-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
3	F	4	MAN	O5-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
3	F	1	NAG	O5-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
3	F	4	MAN	C4-C5-C6-O6

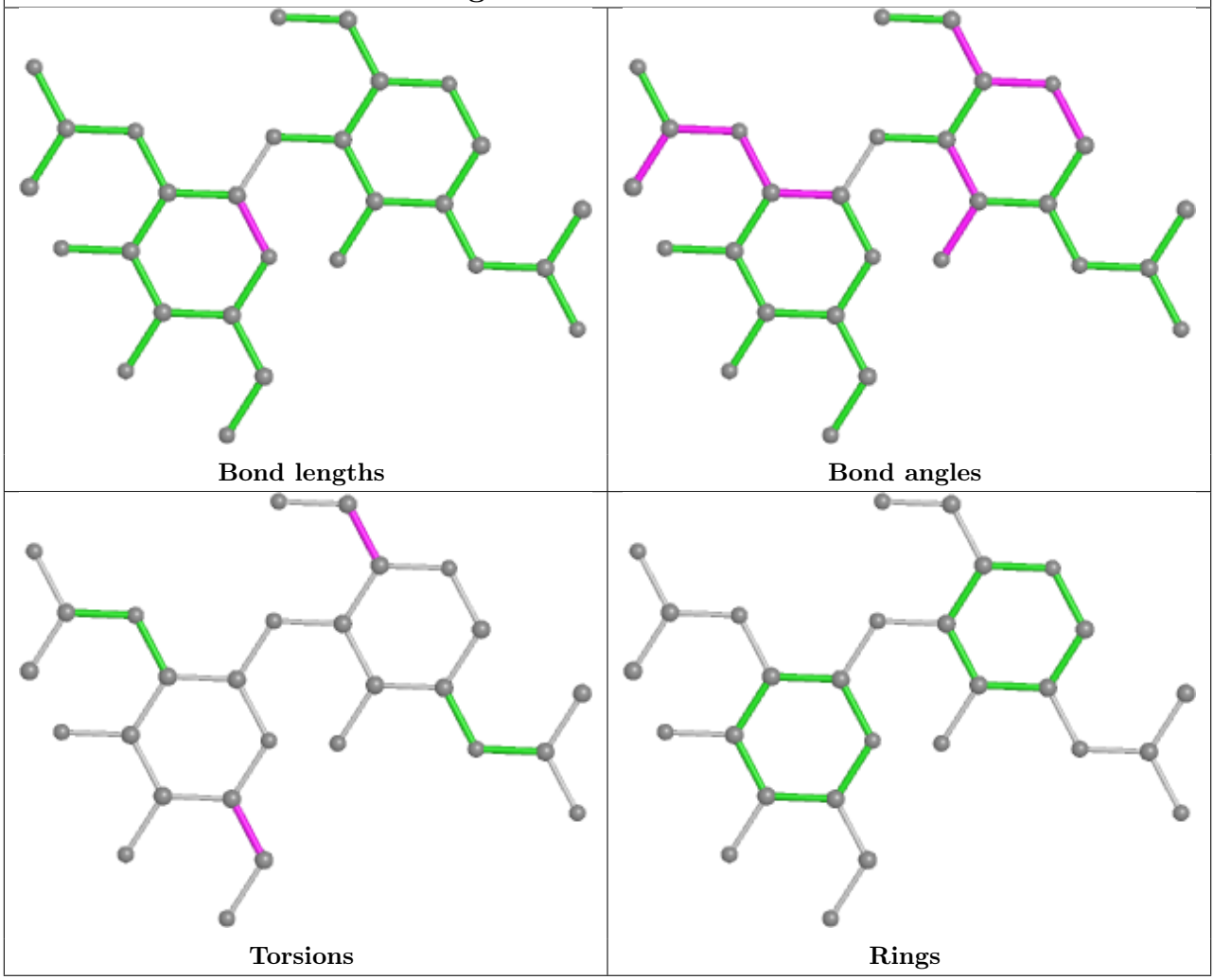
There are no ring outliers.

7 monomers are involved in 15 short contacts:

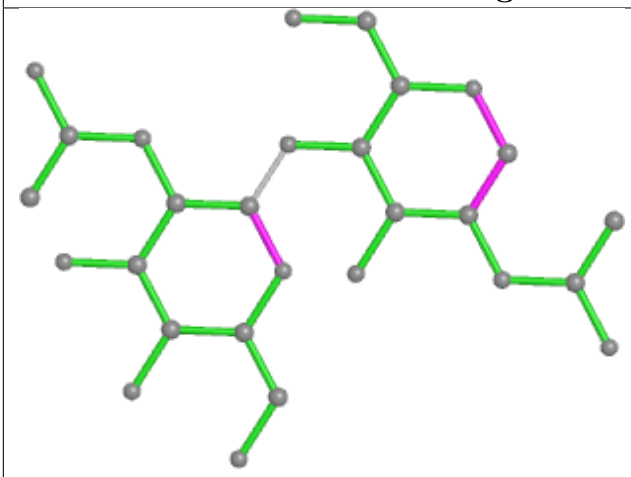
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1	NAG	4	0
2	E	2	NAG	3	0
2	D	2	NAG	4	0
3	F	5	FCA	3	0
3	F	2	NAG	6	0
2	E	1	NAG	3	0
3	F	1	NAG	7	0

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

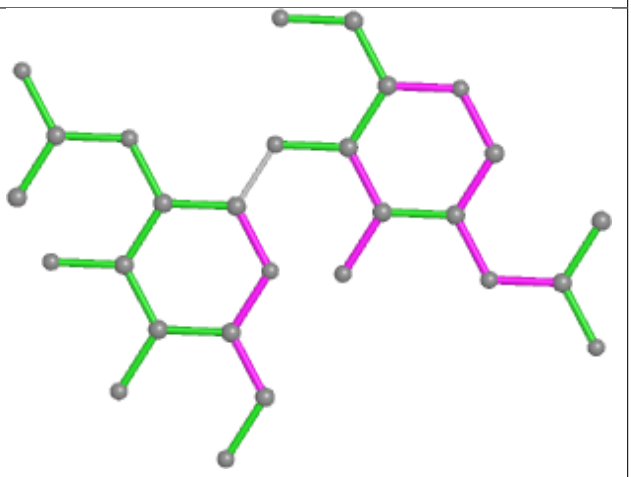
Oligosaccharide Chain D



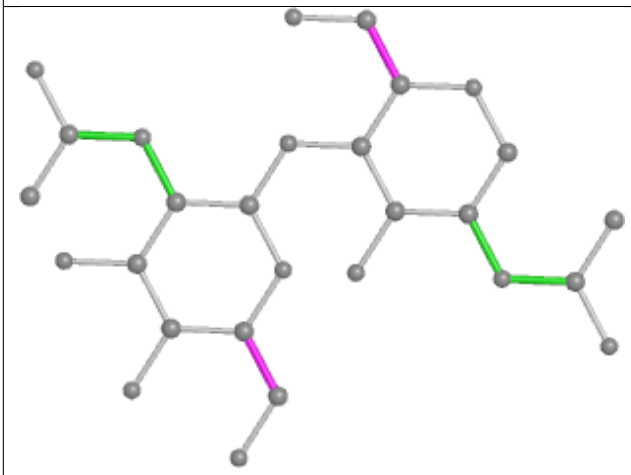
Oligosaccharide Chain E



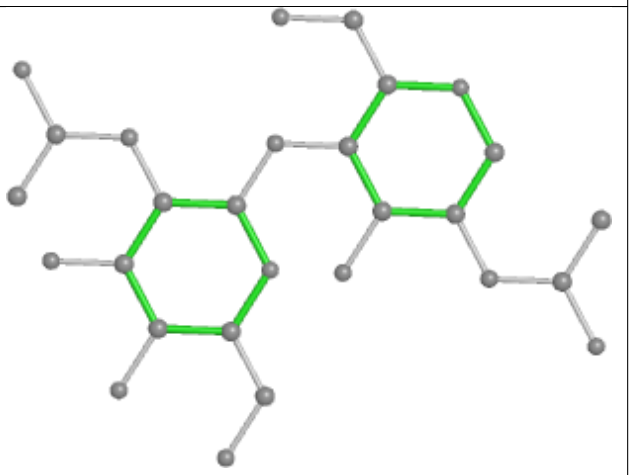
Bond lengths



Bond angles

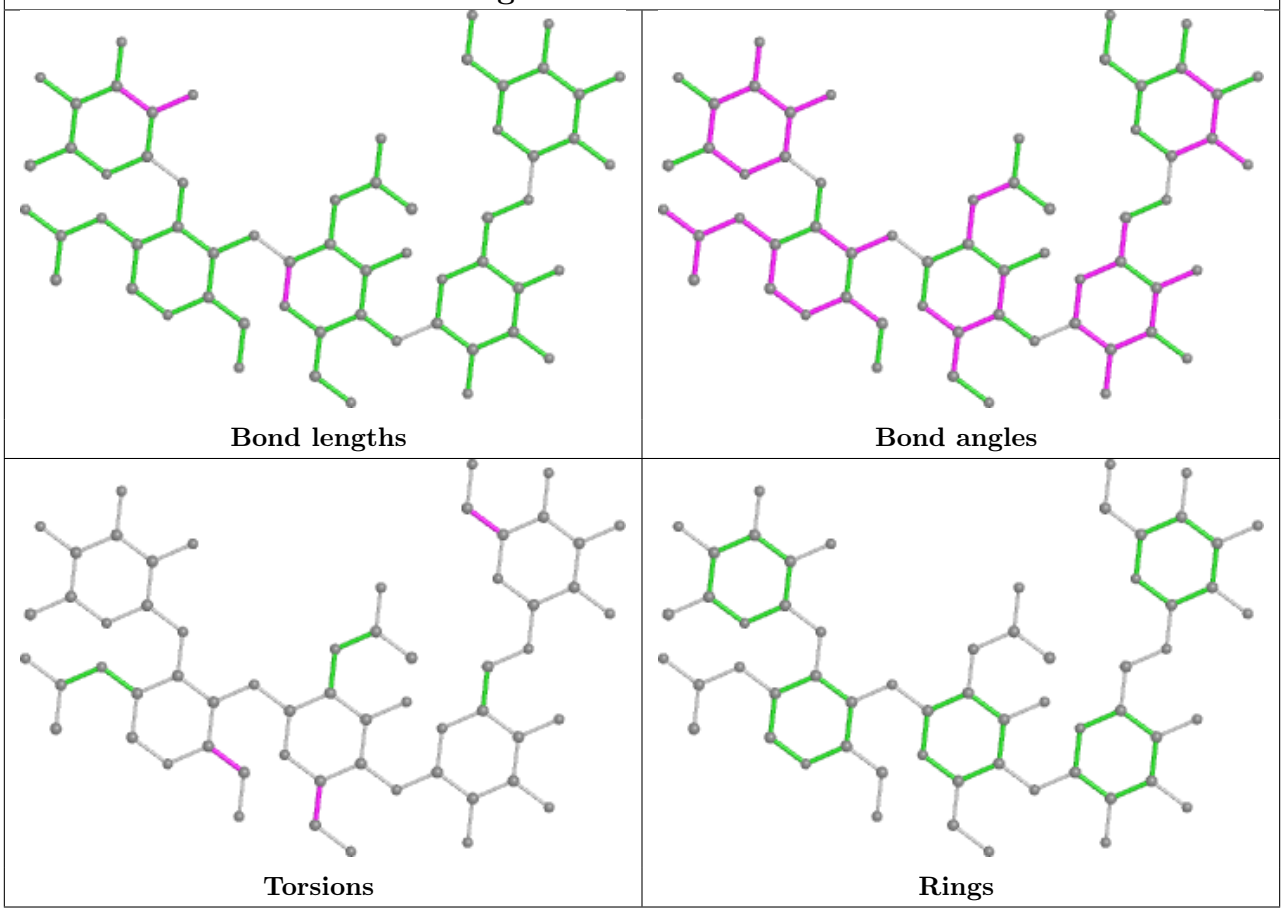


Torsions



Rings

Oligosaccharide Chain F



5.6 Ligand geometry (i)

6 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	$\#\|Z\| > 2$
5	NBA	A	591	4	13,13,14	0.69	0	12,12,14	1.54	1 (8%)
4	FAD	C	590	5	53,58,58	1.06	2 (3%)	68,89,89	1.40	11 (16%)
5	NBA	C	591	4	13,13,14	0.61	0	12,12,14	1.51	1 (8%)
5	NBA	B	591	4	13,13,14	0.56	0	12,12,14	1.99	5 (41%)
4	FAD	B	590	5	53,58,58	0.89	1 (1%)	68,89,89	1.28	11 (16%)
4	FAD	A	590	5	53,58,58	0.89	1 (1%)	68,89,89	1.41	13 (19%)

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	NBA	A	591	4	-	5/11/11/12	-
4	FAD	C	590	5	-	5/30/50/50	0/6/6/6
5	NBA	C	591	4	-	5/11/11/12	-
5	NBA	B	591	4	-	2/11/11/12	-
4	FAD	B	590	5	-	2/30/50/50	0/6/6/6
4	FAD	A	590	5	-	2/30/50/50	0/6/6/6

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	590	FAD	C4X-N5	3.85	1.38	1.30
4	A	590	FAD	C4X-N5	3.22	1.37	1.30
4	B	590	FAD	C4X-N5	3.11	1.36	1.30
4	C	590	FAD	C9A-C5X	2.64	1.45	1.41

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	591	NBA	C9-C8-N7	-4.13	101.00	112.14
4	A	590	FAD	C9A-C5X-N5	-4.10	117.97	122.43
5	C	591	NBA	C9-C8-N7	-3.72	102.10	112.14
4	C	590	FAD	C4-C4X-N5	3.59	123.35	118.23
4	C	590	FAD	C10-N1-C2	3.59	124.08	116.90
4	A	590	FAD	C4'-C3'-C2'	3.51	120.67	113.36
4	C	590	FAD	O4B-C1B-C2B	-3.13	102.35	106.93
4	C	590	FAD	O2A-PA-O1A	3.08	127.45	112.24
5	B	591	NBA	C16-N15-C14	-2.96	103.41	111.95
4	A	590	FAD	C1'-N10-C9A	2.93	125.39	120.51
5	B	591	NBA	C9-C8-N7	-2.90	104.32	112.14
5	B	591	NBA	C12-N11-C10	-2.86	99.96	113.45
5	B	591	NBA	C14-C13-C12	-2.86	103.83	114.26
4	B	590	FAD	O2-C2-N1	-2.79	117.21	121.83
4	A	590	FAD	C5X-N5-C4X	-2.78	113.46	118.07
4	A	590	FAD	C10-C4X-N5	-2.66	119.21	124.86
4	B	590	FAD	C5A-C6A-N6A	2.65	124.38	120.35
4	B	590	FAD	C1'-N10-C9A	-2.59	116.19	120.51
4	C	590	FAD	C5X-N5-C4X	-2.58	113.79	118.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	591	NBA	C10-C9-C8	-2.55	104.96	114.26
4	C	590	FAD	O2P-P-O1P	2.45	124.36	112.24
4	A	590	FAD	C8M-C8-C9	-2.45	114.96	119.49
4	C	590	FAD	C4X-C4-N3	2.41	119.32	113.19
4	B	590	FAD	O2B-C2B-C1B	-2.39	102.03	110.85
4	A	590	FAD	C4-C4X-N5	2.38	121.62	118.23
4	B	590	FAD	C5X-N5-C4X	-2.35	114.17	118.07
4	C	590	FAD	C5'-C4'-C3'	-2.34	107.67	112.20
4	B	590	FAD	O4B-C1B-C2B	-2.33	103.52	106.93
4	A	590	FAD	O4B-C1B-C2B	-2.25	103.64	106.93
4	A	590	FAD	C9A-N10-C10	-2.21	117.32	120.77
4	A	590	FAD	O2A-PA-O1A	2.17	122.98	112.24
4	B	590	FAD	C10-C4X-N5	-2.16	120.26	124.86
4	C	590	FAD	N3A-C2A-N1A	2.16	132.06	128.68
4	A	590	FAD	C6-C5X-C9A	2.15	121.97	118.94
4	C	590	FAD	C5A-C6A-N6A	2.14	123.60	120.35
4	B	590	FAD	O3'-C3'-C4'	-2.13	103.67	108.81
4	A	590	FAD	C9-C8-C7	2.12	122.71	119.67
4	B	590	FAD	O4-C4-C4X	-2.10	121.03	126.60
4	A	590	FAD	O4'-C4'-C3'	2.07	114.14	109.10
4	B	590	FAD	O2P-P-O1P	2.07	122.49	112.24
4	C	590	FAD	O4-C4-C4X	-2.06	121.13	126.60
4	B	590	FAD	O2-C2-N3	2.01	122.56	118.65

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	591	NBA	C12-C13-C14-N15
5	B	591	NBA	N11-C10-C9-C8
5	C	591	NBA	N11-C12-C13-C14
5	A	591	NBA	N11-C12-C13-C14
5	C	591	NBA	C12-C13-C14-N15
5	C	591	NBA	N11-C10-C9-C8
5	A	591	NBA	C9-C10-N11-C12
5	B	591	NBA	N11-C12-C13-C14
5	C	591	NBA	C9-C10-N11-C12
4	C	590	FAD	O3'-C3'-C4'-O4'
5	A	591	NBA	N11-C10-C9-C8
4	C	590	FAD	C5B-O5B-PA-O1A
4	C	590	FAD	C2'-C3'-C4'-O4'
5	C	591	NBA	C13-C12-N11-C10

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Mol	Chain	Res	Type	Atoms
4	A	590	FAD	C2'-C3'-C4'-O4'
5	A	591	NBA	C5-C6-N7-C8
4	B	590	FAD	O4B-C4B-C5B-O5B
4	C	590	FAD	O4B-C4B-C5B-O5B
4	A	590	FAD	O4B-C4B-C5B-O5B
4	B	590	FAD	O3'-C3'-C4'-O4'
4	C	590	FAD	O3'-C3'-C4'-C5'

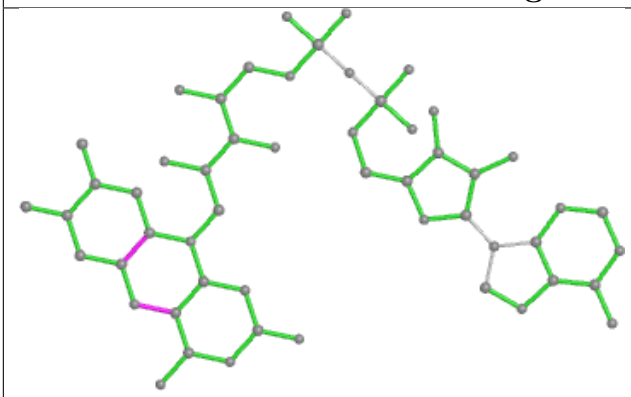
There are no ring outliers.

5 monomers are involved in 9 short contacts:

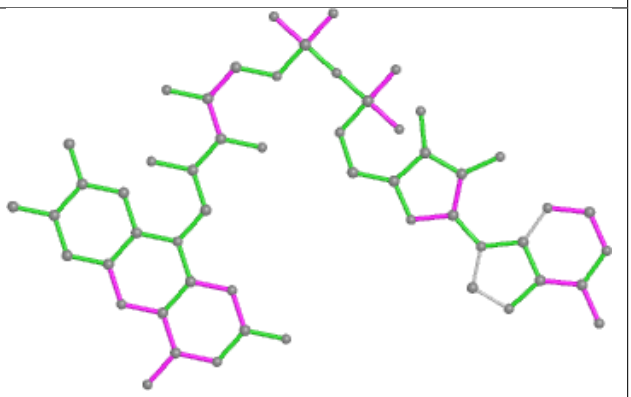
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	591	NBA	1	0
4	C	590	FAD	3	0
5	C	591	NBA	1	0
4	B	590	FAD	2	0
4	A	590	FAD	2	0

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 then 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.

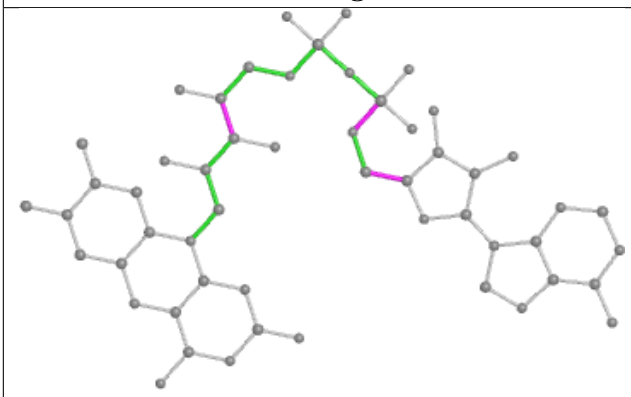
Ligand FAD C 590



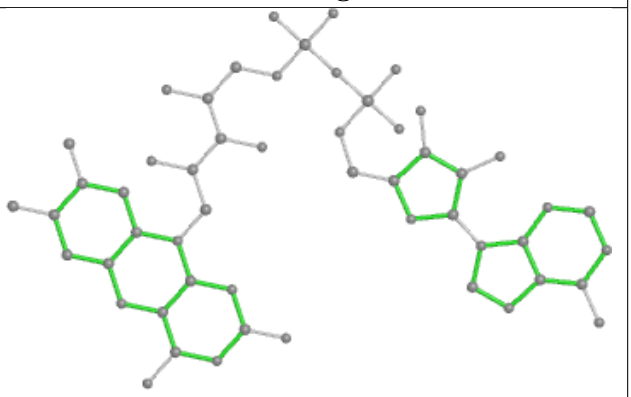
Bond lengths



Bond angles

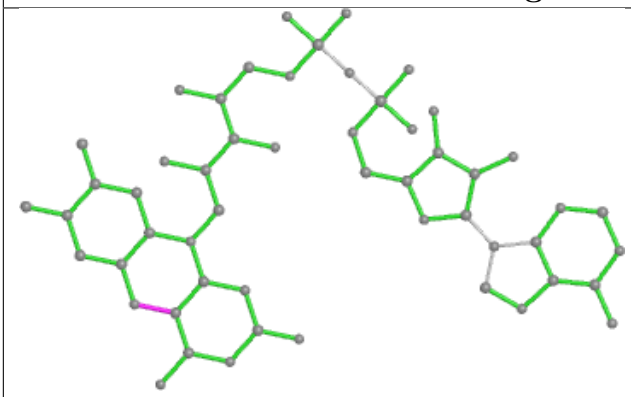


Torsions

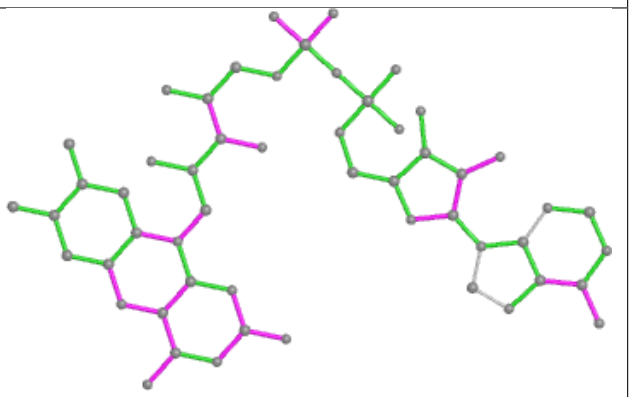


Rings

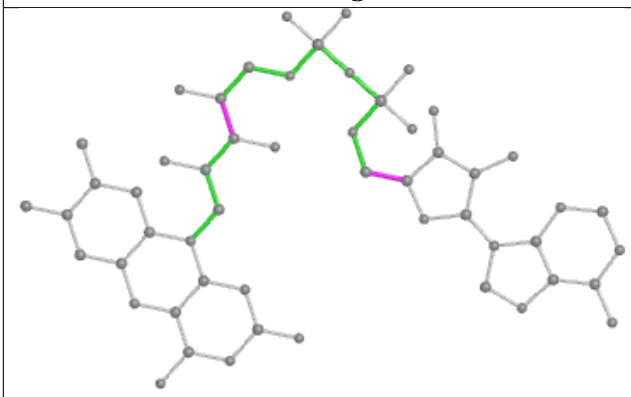
Ligand FAD B 590



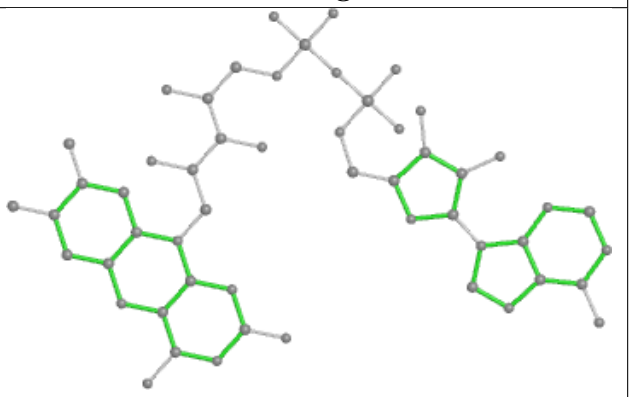
Bond lengths



Bond angles

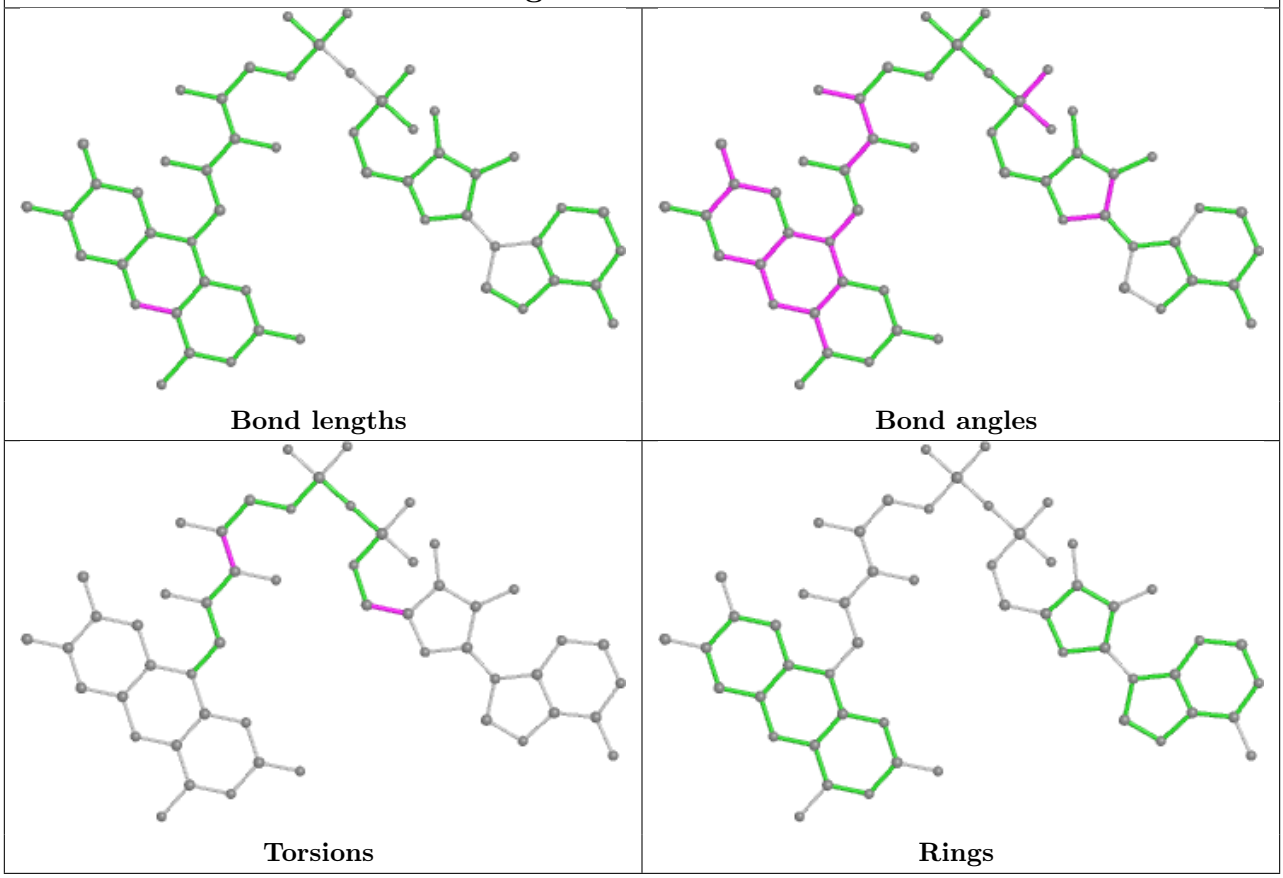


Torsions



Rings

Ligand FAD A 590



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)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.