Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 07:16 PM EDT

PDB ID	:	1F8R
Title	:	CRYSTAL STRUCTURE OF L-AMINO ACID OXIDASE FROM CALLOSELASMA RHODOSTOMA COMPLEXED WITH CITRATE
Authors	:	Pawelek, P.D.; Cheah, J.; Coulombe, R.; Macheroux, P.; Ghisla, S.; Vrielink, A.
Deposited on	:	2000-07-04
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 (i)) were used in the production of this report:

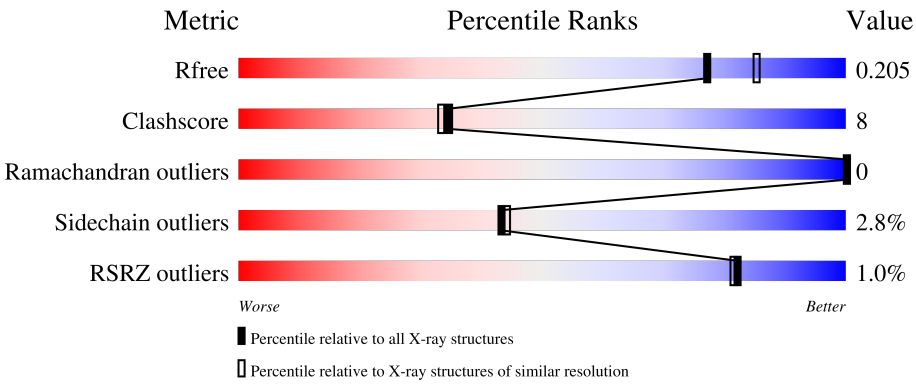
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (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% 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	498	82% 14% • •
1	B	498	% 77% 19% • •
1	C	498	% 82% 14% • •
1	D	498	2% 80% 17% • •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	E	3	33% 33% 33%
2	F	3	67% 33%
2	G	3	67% 33%
2	H	3	33% 33% 33%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	E	1	X	-	-	-
2	FUC	E	3	X	-	-	-
2	NAG	F	2	-	-	-	X
2	FUC	F	3	X	-	-	-
2	NAG	G	2	X	-	-	-
2	FUC	G	3	X	-	-	-
2	FUC	H	3	X	-	-	-
3	NAG	A	522	X	-	-	-
3	NAG	B	522	X	-	-	-
3	NAG	C	522	X	-	-	X
3	NAG	D	522	X	-	-	X
4	CIT	A	526	-	X	-	-
4	CIT	B	526	-	X	-	-
4	CIT	C	526	-	X	-	-
4	CIT	D	526	-	X	-	X

2 Entry composition (i)

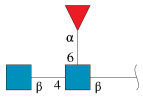
There are 6 unique types of molecules in this entry. The entry contains 17632 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 L-AMINO ACID OXIDASE.

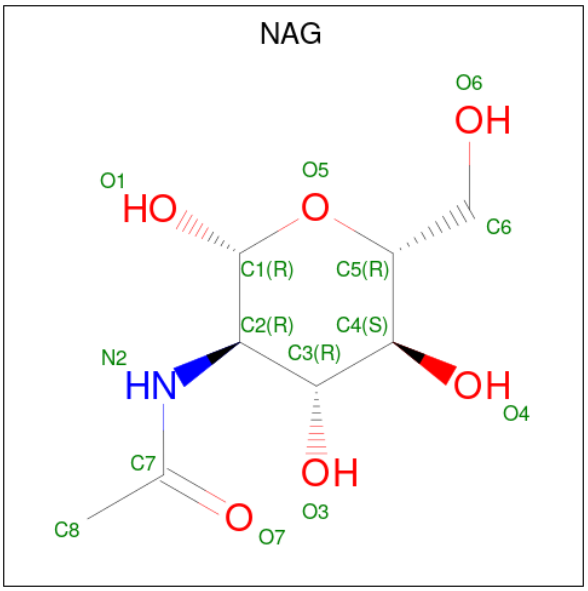
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	483	3804	2434	640	718	12	0	0	0
1	B	483	3847	2456	652	727	12	0	0	0
1	C	483	3813	2437	644	720	12	0	0	0
1	D	483	3827	2445	646	724	12	0	0	0

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



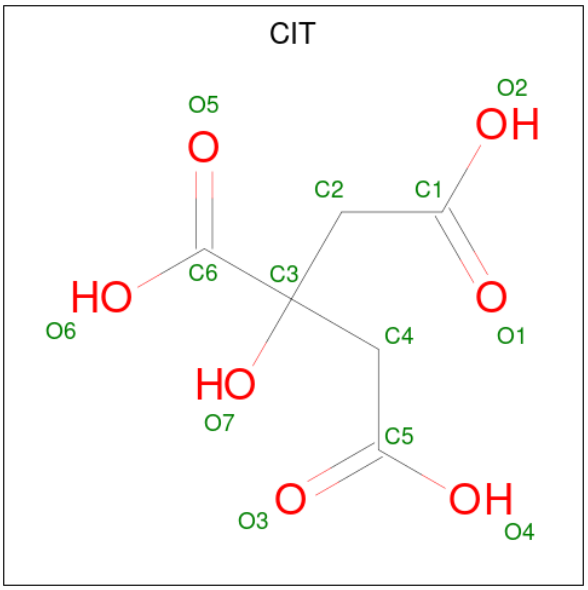
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	E	3	38	22	2	14	0	0	0
2	F	3	38	22	2	14	0	0	0
2	G	3	38	22	2	14	0	0	0
2	H	3	38	22	2	14	0	0	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



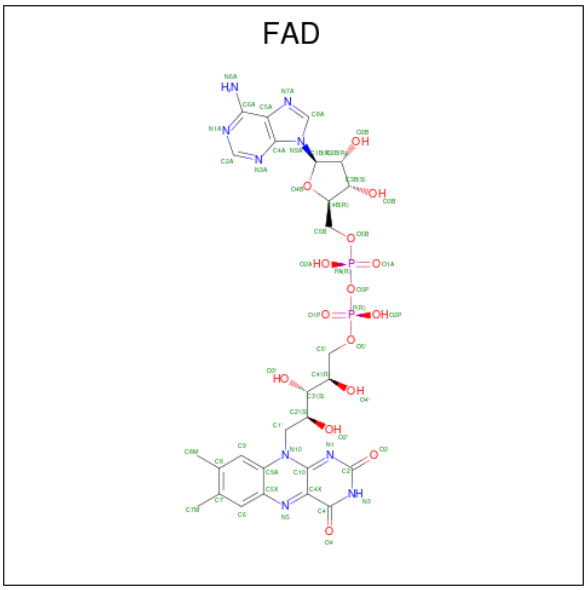
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	14	8	1	5	0	0
3	B	1	14	8	1	5	0	0
3	C	1	14	8	1	5	0	0
3	D	1	14	8	1	5	0	0

- Molecule 4 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
4	A	1	13	6	7		0	0
			Total	C	O			
4	B	1	13	6	7		0	0
			Total	C	O			
4	C	1	13	6	7		0	0
			Total	C	O			
4	D	1	13	6	7		0	0

- Molecule 5 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	466	466	466	0	0

Continued on next page...

Continued from previous page...

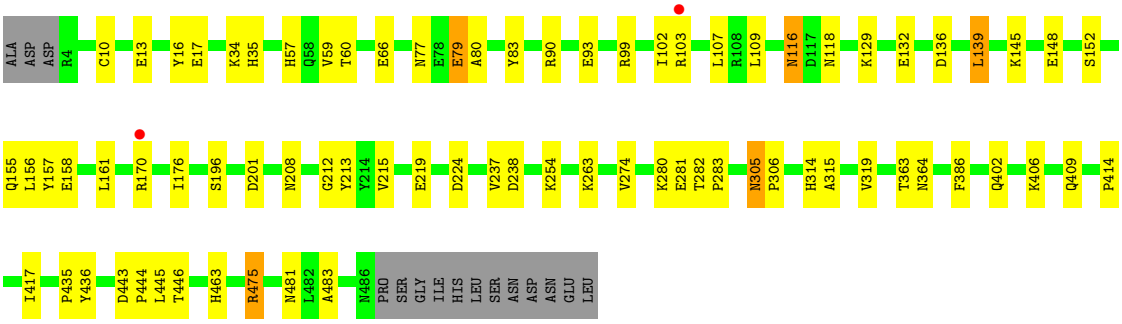
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	B	497	497	497	0	0
			Total	O		
6	C	461	461	461	0	0
			Total	O		
6	D	445	445	445	0	0

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 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.

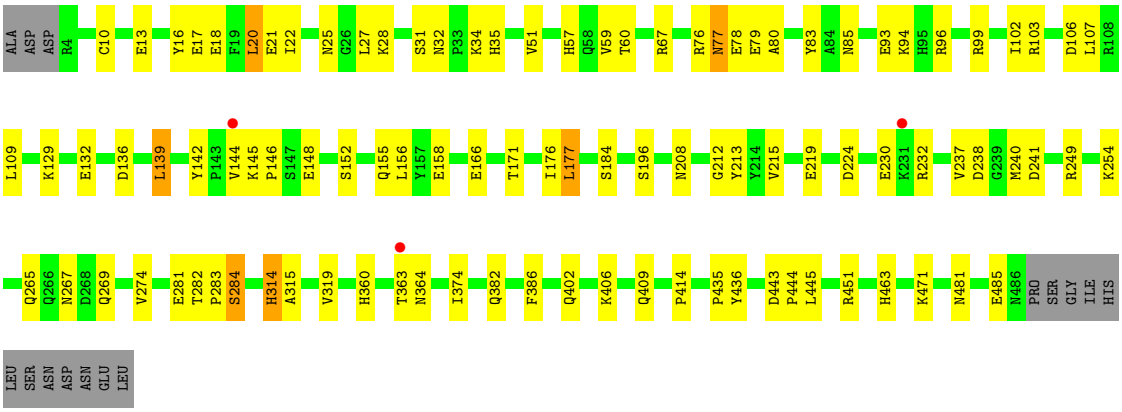
• Molecule 1: L-AMINO ACID OXIDASE

Chain A: 82% 14% • •



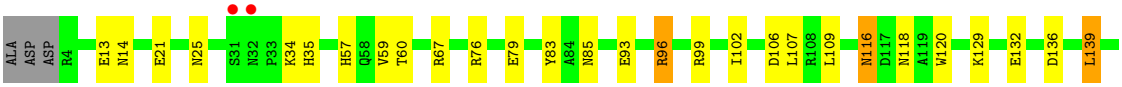
• Molecule 1: L-AMINO ACID OXIDASE

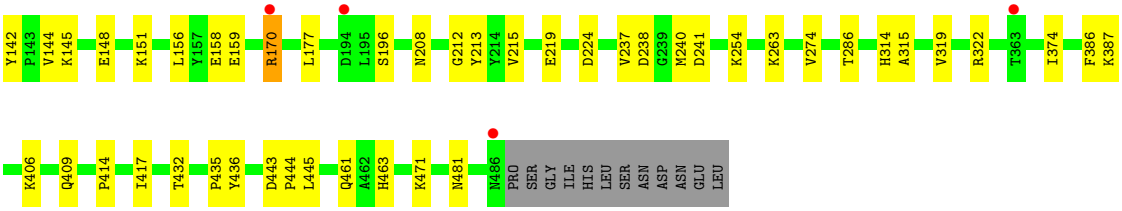
Chain B: % 77% 19% • •



• Molecule 1: L-AMINO ACID OXIDASE

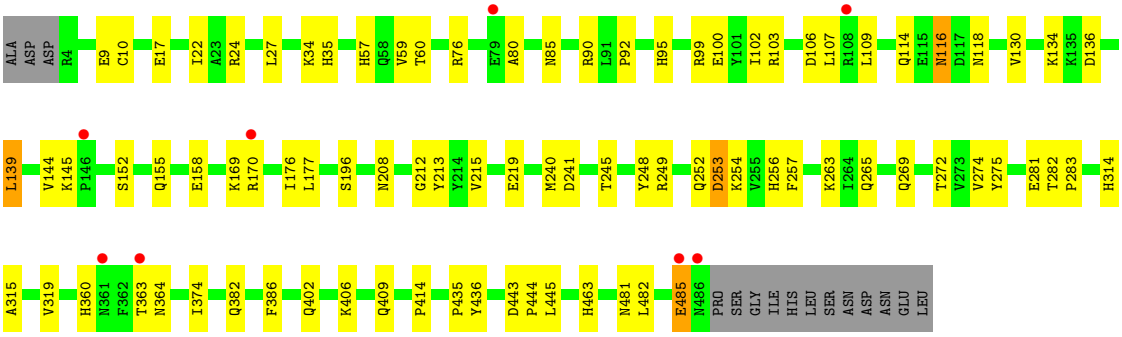
Chain C: % 82% 14% • •





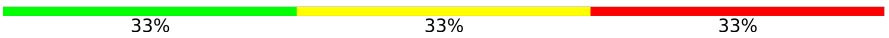
• Molecule 1: L-AMINO ACID OXIDASE

Chain D:



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

Chain E:

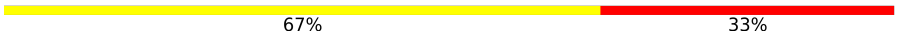


• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:

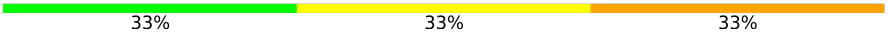
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:



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

Chain H:



NAG1
NAG2
FUC3

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	79.50Å 154.96Å 102.95Å 90.00° 109.49° 90.00°	Depositor
Resolution (Å)	500.00 – 2.00 48.52 – 2.00	Depositor EDS
% Data completeness (in resolution range)	88.1 (500.00-2.00) 88.1 (48.52-2.00)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.58 (at 2.00Å)	Xtriage
Refinement program	CNS 0.5	Depositor
R, R_{free}	0.185 , 0.210 0.180 , 0.205	Depositor DCC
R_{free} test set	13919 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å^2)	19.6	Xtriage
Anisotropy	0.517	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 57.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	17632	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 3.41% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, CIT, 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	0.33	0/3895	0.59	0/5282
1	B	0.35	0/3938	0.60	0/5332
1	C	0.33	0/3903	0.59	0/5291
1	D	0.34	0/3918	0.59	0/5309
All	All	0.34	0/15654	0.59	0/21214

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3804	0	3673	53	0
1	B	3847	0	3756	83	0
1	C	3813	0	3697	59	0
1	D	3827	0	3717	58	0
2	E	38	0	34	1	0
2	F	38	0	34	5	0
2	G	38	0	34	1	0
2	H	38	0	34	0	0
3	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
3	B	14	0	13	1	0
3	C	14	0	13	2	0
3	D	14	0	13	1	0
4	A	13	0	5	1	0
4	B	13	0	5	0	0
4	C	13	0	5	0	0
4	D	13	0	5	1	0
5	A	53	0	31	0	0
5	B	53	0	31	0	0
5	C	53	0	31	0	0
5	D	53	0	31	0	0
6	A	466	0	0	7	0
6	B	497	0	0	16	0
6	C	461	0	0	12	0
6	D	445	0	0	8	0
All	All	17632	0	15175	257	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 (257) 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:144:VAL:CG1	1:C:148:GLU:HB2	1.87	1.05
1:B:265:GLN:HE21	1:B:267:ASN:HD21	1.01	0.98
1:A:446:THR:HB	1:A:475:ARG:HH22	1.32	0.93
1:B:144:VAL:HG12	1:B:148:GLU:HB2	1.51	0.91
1:B:13:GLU:OE1	1:B:471:LYS:HE2	1.74	0.87
1:A:446:THR:HB	1:A:475:ARG:NH2	1.94	0.83
1:B:34:LYS:H	1:B:57:HIS:HD2	1.26	0.83
1:B:144:VAL:CG1	1:B:148:GLU:HB2	2.08	0.83
1:C:116:ASN:HD22	1:C:118:ASN:H	1.27	0.81
2:F:1:NAG:O3	2:F:2:NAG:H4	1.82	0.79
1:D:116:ASN:HD22	1:D:118:ASN:H	1.25	0.79
1:A:116:ASN:HD22	1:A:118:ASN:H	1.28	0.78
1:B:94:LYS:HG2	1:B:230:GLU:OE1	1.85	0.77
1:C:144:VAL:HG12	1:C:148:GLU:HB2	1.65	0.76
1:C:13:GLU:OE1	1:C:471:LYS:HE2	1.85	0.76
1:A:34:LYS:H	1:A:57:HIS:HD2	1.34	0.76
1:B:145:LYS:HG3	1:B:196:SER:HB3	1.69	0.74
1:A:475:ARG:NH2	6:A:1795:HOH:O	2.22	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:319:VAL:HG21	1:B:445:LEU:HD11	1.72	0.72
1:D:34:LYS:H	1:D:57:HIS:HD2	1.37	0.71
1:D:116:ASN:ND2	1:D:118:ASN:H	1.87	0.71
1:C:144:VAL:HG11	1:C:148:GLU:HB2	1.69	0.71
1:C:471:LYS:HE2	6:C:2083:HOH:O	1.90	0.70
1:B:219:GLU:OE2	1:B:463:HIS:HD2	1.74	0.70
1:A:116:ASN:ND2	1:A:118:ASN:H	1.90	0.70
1:C:34:LYS:H	1:C:57:HIS:HD2	1.40	0.69
1:B:28:LYS:HE3	6:B:2404:HOH:O	1.91	0.69
2:F:2:NAG:H61	2:F:3:FUC:O2	1.92	0.69
1:C:96:ARG:NH1	6:C:1060:HOH:O	2.26	0.68
1:C:116:ASN:ND2	1:C:118:ASN:H	1.90	0.68
1:C:219:GLU:OE2	1:C:463:HIS:HD2	1.76	0.68
1:D:145:LYS:HG3	1:D:196:SER:HB3	1.76	0.68
1:D:152:SER:OG	1:D:155:GLN:HG3	1.95	0.67
1:A:463:HIS:HE1	6:A:575:HOH:O	1.77	0.66
1:A:201:ASP:HA	6:A:1429:HOH:O	1.94	0.66
1:B:34:LYS:H	1:B:57:HIS:CD2	2.13	0.66
1:A:219:GLU:OE2	1:A:463:HIS:HD2	1.79	0.66
1:B:17:GLU:HB2	6:B:1104:HOH:O	1.96	0.65
1:B:265:GLN:HE21	1:B:267:ASN:ND2	1.85	0.65
1:A:34:LYS:H	1:A:57:HIS:CD2	2.14	0.65
1:D:219:GLU:OE2	1:D:463:HIS:HD2	1.80	0.65
1:C:461:GLN:OE1	6:C:2083:HOH:O	2.15	0.64
1:A:152:SER:OG	1:A:155:GLN:HG3	1.98	0.64
1:B:142:TYR:O	1:B:144:VAL:HG23	1.98	0.63
1:A:145:LYS:HG3	1:A:196:SER:HB3	1.80	0.63
1:D:90:ARG:HH11	1:D:114:GLN:HE22	1.47	0.63
1:B:463:HIS:HE1	6:B:692:HOH:O	1.82	0.62
1:B:269:GLN:HA	1:B:451:ARG:HE	1.63	0.62
3:C:522:NAG:O7	3:C:522:NAG:H3	2.00	0.62
1:A:315:ALA:O	1:A:319:VAL:HG23	2.00	0.61
1:C:129:LYS:HB2	1:C:132:GLU:HG3	1.82	0.60
1:B:27:LEU:HD13	1:B:51:VAL:HB	1.83	0.60
1:B:77:ASN:ND2	1:B:80:ALA:H	1.99	0.60
2:F:2:NAG:C1	2:F:2:NAG:O7	2.48	0.60
1:C:96:ARG:HD3	6:C:2078:HOH:O	2.01	0.60
1:D:34:LYS:H	1:D:57:HIS:CD2	2.18	0.60
1:A:129:LYS:HB2	1:A:132:GLU:HG3	1.84	0.60
1:C:322:ARG:NH1	1:C:374:ILE:HD13	2.17	0.60
1:B:166:GLU:HG2	6:B:2305:HOH:O	2.01	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:152:SER:OG	1:B:155:GLN:HG3	2.02	0.59
1:D:57:HIS:HE1	1:D:481:ASN:OD1	1.84	0.59
1:C:319:VAL:HG21	1:C:445:LEU:HD11	1.83	0.59
1:D:170:ARG:NH1	6:D:1880:HOH:O	2.34	0.59
1:B:77:ASN:C	1:B:77:ASN:HD22	2.06	0.58
1:D:17:GLU:OE2	6:D:2082:HOH:O	2.17	0.58
1:A:319:VAL:HG21	1:A:445:LEU:HD11	1.85	0.58
1:B:22:ILE:HG23	1:B:27:LEU:HD12	1.85	0.58
1:C:57:HIS:HE1	1:C:481:ASN:OD1	1.86	0.58
1:D:360:HIS:HA	3:D:522:NAG:H82	1.85	0.58
1:A:57:HIS:HE1	1:A:481:ASN:OD1	1.87	0.58
1:C:85:ASN:HD21	1:C:240:MET:H	1.51	0.58
1:D:319:VAL:HG21	1:D:445:LEU:HD11	1.85	0.58
1:A:17:GLU:HB2	6:A:1494:HOH:O	2.02	0.58
1:A:402:GLN:HG3	6:A:622:HOH:O	2.04	0.57
1:B:78:GLU:OE1	1:B:78:GLU:HA	2.04	0.57
1:C:34:LYS:H	1:C:57:HIS:CD2	2.21	0.57
1:A:90:ARG:NH2	4:A:526:CIT:O6	2.38	0.57
1:C:142:TYR:O	1:C:144:VAL:HG23	2.06	0.56
1:C:136:ASP:OD2	1:C:139:LEU:HD13	2.06	0.56
1:A:446:THR:CB	1:A:475:ARG:HH22	2.13	0.56
1:C:386:PHE:CD1	1:C:417:ILE:HD12	2.39	0.56
1:C:463:HIS:HE1	6:C:806:HOH:O	1.87	0.56
1:B:59:VAL:CG2	1:B:254:LYS:HD2	2.36	0.55
1:D:402:GLN:HG2	6:D:955:HOH:O	2.06	0.55
1:C:144:VAL:HG12	1:C:145:LYS:N	2.20	0.55
2:F:2:NAG:H61	2:F:3:FUC:HO2	1.70	0.55
1:B:103:ARG:NH2	6:B:1263:HOH:O	2.37	0.55
1:B:96:ARG:NH1	6:B:2330:HOH:O	2.39	0.55
1:B:274:VAL:HG22	1:B:284:SER:OG	2.07	0.55
1:B:146:PRO:HD2	6:B:1960:HOH:O	2.07	0.54
1:B:85:ASN:HD21	1:B:240:MET:H	1.55	0.54
1:C:471:LYS:CE	6:C:2083:HOH:O	2.51	0.54
1:C:14:ASN:N	6:C:2083:HOH:O	2.40	0.54
1:C:406:LYS:HA	1:C:409:GLN:HE21	1.73	0.54
1:C:471:LYS:NZ	6:C:2083:HOH:O	2.40	0.54
1:A:116:ASN:HD22	1:A:116:ASN:C	2.11	0.54
1:B:57:HIS:HE1	1:B:481:ASN:OD1	1.91	0.53
1:B:102:ILE:HG23	1:B:107:LEU:HB2	1.90	0.53
1:D:85:ASN:HD21	1:D:240:MET:H	1.55	0.53
1:D:315:ALA:O	1:D:319:VAL:HG23	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:ARG:O	1:A:103:ARG:HG3	2.08	0.53
1:B:144:VAL:HG12	1:B:148:GLU:OE1	2.09	0.53
1:B:269:GLN:HA	1:B:451:ARG:NE	2.23	0.53
1:C:79:GLU:HB2	6:C:2168:HOH:O	2.09	0.52
1:C:144:VAL:HG13	1:C:148:GLU:OE1	2.09	0.52
1:B:129:LYS:HB2	1:B:132:GLU:HG3	1.90	0.52
1:D:116:ASN:HD22	1:D:116:ASN:C	2.13	0.52
1:D:463:HIS:HE1	6:D:913:HOH:O	1.92	0.52
1:C:59:VAL:HG22	1:C:254:LYS:HD3	1.92	0.52
1:D:443:ASP:HB2	1:D:444:PRO:HD3	1.92	0.51
1:D:90:ARG:NH2	4:D:526:CIT:O6	2.43	0.51
1:A:102:ILE:HD13	1:A:109:LEU:HD21	1.92	0.51
1:B:212:GLY:O	1:B:215:VAL:HG22	2.11	0.51
1:B:59:VAL:HG22	1:B:254:LYS:HD2	1.92	0.51
1:D:9:GLU:HB2	6:D:2209:HOH:O	2.10	0.51
1:D:263:LYS:HB2	1:D:274:VAL:HB	1.92	0.51
1:B:99:ARG:O	1:B:103:ARG:HG3	2.10	0.51
1:D:212:GLY:O	1:D:215:VAL:HG22	2.10	0.50
1:A:212:GLY:O	1:A:215:VAL:HG22	2.11	0.50
1:D:406:LYS:HA	1:D:409:GLN:HE21	1.76	0.50
1:B:171:THR:HG22	2:F:3:FUC:H5	1.93	0.50
1:C:102:ILE:HD13	1:C:109:LEU:HD21	1.93	0.50
1:A:305:ASN:HD22	1:A:306:PRO:HA	1.77	0.50
1:A:406:LYS:HA	1:A:409:GLN:HE21	1.76	0.50
1:C:116:ASN:HD22	1:C:116:ASN:C	2.15	0.49
1:B:76:ARG:NH2	1:B:241:ASP:OD1	2.44	0.49
1:B:79:GLU:HB3	6:C:2337:HOH:O	2.12	0.49
1:B:34:LYS:N	1:B:57:HIS:HD2	2.02	0.49
1:D:76:ARG:NH2	1:D:241:ASP:OD1	2.42	0.49
1:D:102:ILE:HG23	1:D:107:LEU:HB2	1.95	0.48
1:D:256:HIS:HB3	6:D:2308:HOH:O	2.12	0.48
1:D:245:THR:O	1:D:249:ARG:HG3	2.13	0.48
1:B:136:ASP:OD2	1:B:139:LEU:HD13	2.13	0.48
1:C:212:GLY:O	1:C:215:VAL:HG22	2.14	0.48
1:C:148:GLU:HB3	1:C:156:LEU:HD21	1.95	0.48
1:C:315:ALA:O	1:C:319:VAL:HG23	2.13	0.48
1:A:386:PHE:CD1	1:A:417:ILE:HD12	2.49	0.48
1:B:148:GLU:HB3	1:B:156:LEU:HD21	1.96	0.48
1:B:144:VAL:HG11	1:B:148:GLU:HB2	1.92	0.47
1:A:79:GLU:CD	1:D:257:PHE:CD2	2.87	0.47
1:C:170:ARG:HG2	1:C:170:ARG:HH11	1.80	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:281:GLU:HG2	1:D:283:PRO:HD3	1.97	0.47
1:C:35:HIS:HE1	1:C:60:THR:OG1	1.97	0.47
1:C:145:LYS:HD3	1:C:196:SER:HB3	1.97	0.47
1:D:374:ILE:HD12	1:D:374:ILE:O	2.14	0.47
1:A:10:CYS:SG	1:A:176:ILE:HD11	2.55	0.47
1:A:34:LYS:N	1:A:57:HIS:HD2	2.07	0.47
1:A:93:GLU:HA	1:A:99:ARG:CZ	2.45	0.47
1:C:374:ILE:HD12	1:C:374:ILE:O	2.15	0.47
1:B:93:GLU:HA	1:B:99:ARG:CZ	2.44	0.47
1:B:319:VAL:CG2	1:B:445:LEU:HD11	2.44	0.47
1:C:76:ARG:NH2	1:C:241:ASP:OD1	2.45	0.47
1:B:265:GLN:NE2	1:B:267:ASN:HD21	1.86	0.46
1:B:374:ILE:HD12	1:B:374:ILE:O	2.15	0.46
1:C:102:ILE:HG23	1:C:107:LEU:HB2	1.98	0.46
1:D:92:PRO:HD2	1:D:95:HIS:ND1	2.29	0.46
1:D:34:LYS:N	1:D:57:HIS:HD2	2.10	0.46
1:A:280:LYS:HG3	1:D:409:GLN:HB3	1.97	0.46
1:B:102:ILE:HD13	1:B:109:LEU:HD21	1.97	0.46
1:D:265:GLN:HG3	1:D:272:THR:HB	1.97	0.46
1:D:35:HIS:HE1	1:D:60:THR:OG1	1.99	0.46
1:C:151:LYS:HE2	1:C:159:GLU:OE2	2.16	0.46
1:B:79:GLU:HB2	6:B:1822:HOH:O	2.16	0.45
1:D:275:TYR:CZ	1:D:283:PRO:HB2	2.51	0.45
1:B:32:ASN:HB2	6:B:1970:HOH:O	2.17	0.45
1:B:360:HIS:HA	3:B:522:NAG:H82	1.98	0.45
1:D:386:PHE:CE2	1:D:414:PRO:HB2	2.52	0.45
1:D:482:LEU:O	1:D:485:GLU:HG3	2.16	0.45
1:B:22:ILE:CG2	1:B:27:LEU:HD12	2.46	0.45
1:B:443:ASP:HB2	1:B:444:PRO:HD3	1.98	0.45
1:C:435:PRO:O	1:C:436:TYR:HB2	2.17	0.45
2:G:1:NAG:H4	2:G:3:FUC:O2	2.17	0.45
1:A:386:PHE:CE2	1:A:414:PRO:HB2	2.52	0.45
1:A:281:GLU:HG2	1:A:283:PRO:HD3	1.98	0.45
1:A:483:ALA:HA	6:A:1598:HOH:O	2.16	0.45
1:B:158:GLU:OE2	1:B:224:ASP:OD1	2.35	0.45
1:C:443:ASP:HB2	1:C:444:PRO:HD3	1.99	0.45
1:C:85:ASN:ND2	1:C:240:MET:H	2.15	0.45
1:D:435:PRO:O	1:D:436:TYR:HB2	2.17	0.45
1:C:21:GLU:OE2	1:C:25:ASN:ND2	2.41	0.45
1:A:435:PRO:O	1:A:436:TYR:HB2	2.16	0.44
1:B:21:GLU:OE2	1:B:25:ASN:ND2	2.40	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:34:LYS:N	1:C:57:HIS:HD2	2.13	0.44
1:C:136:ASP:O	1:C:139:LEU:HB2	2.17	0.44
1:B:20:LEU:HD12	1:B:20:LEU:O	2.17	0.44
1:B:282:THR:HG23	1:B:282:THR:O	2.17	0.44
1:D:253:ASP:OD1	1:D:253:ASP:N	2.51	0.44
1:A:443:ASP:HB2	1:A:444:PRO:HD3	1.99	0.44
1:B:35:HIS:HE1	1:B:60:THR:OG1	2.00	0.44
1:D:319:VAL:CG2	1:D:445:LEU:HD11	2.48	0.44
1:C:83:TYR:CD1	1:C:83:TYR:C	2.92	0.44
1:A:306:PRO:HG2	6:A:1280:HOH:O	2.17	0.44
1:C:158:GLU:OE2	1:C:224:ASP:OD1	2.36	0.44
1:B:83:TYR:CD1	1:B:83:TYR:C	2.92	0.44
1:B:184:SER:HB3	6:B:1235:HOH:O	2.17	0.43
1:D:282:THR:O	1:D:282:THR:OG1	2.33	0.43
1:A:59:VAL:HG22	1:A:254:LYS:HD3	1.99	0.43
1:B:249:ARG:HD2	6:B:1754:HOH:O	2.19	0.43
1:B:485:GLU:HG2	6:B:1551:HOH:O	2.17	0.43
1:D:136:ASP:O	1:D:139:LEU:HB2	2.18	0.43
1:A:237:VAL:O	1:A:238:ASP:HB2	2.19	0.43
1:B:67:ARG:NH2	6:B:1238:HOH:O	2.48	0.43
1:C:120:TRP:CH2	1:C:129:LYS:HE2	2.53	0.43
1:D:130:VAL:O	1:D:134:LYS:HG3	2.18	0.43
1:A:263:LYS:HB2	1:A:274:VAL:HB	2.00	0.43
1:B:93:GLU:HA	1:B:99:ARG:NE	2.33	0.43
1:B:232:ARG:HD2	6:B:2264:HOH:O	2.18	0.43
1:B:315:ALA:O	1:B:319:VAL:HG23	2.19	0.43
1:D:59:VAL:HG22	1:D:254:LYS:HD3	1.99	0.43
1:D:136:ASP:OD2	1:D:139:LEU:HD13	2.19	0.43
1:C:93:GLU:HA	1:C:99:ARG:CZ	2.49	0.43
1:B:13:GLU:HB2	1:B:16:TYR:CD1	2.53	0.42
1:B:402:GLN:HG2	6:B:740:HOH:O	2.17	0.42
1:A:319:VAL:CG2	1:A:445:LEU:HD11	2.48	0.42
1:D:85:ASN:ND2	1:D:240:MET:H	2.15	0.42
1:D:248:TYR:CZ	1:D:252:GLN:HG3	2.55	0.42
1:C:67:ARG:NH2	6:C:1430:HOH:O	2.45	0.42
1:B:374:ILE:HD12	1:B:374:ILE:C	2.39	0.42
1:C:386:PHE:CE2	1:C:414:PRO:HB2	2.54	0.42
1:A:148:GLU:HB3	1:A:156:LEU:HD21	2.01	0.42
1:A:157:TYR:O	1:A:161:LEU:HD13	2.20	0.42
1:B:10:CYS:SG	1:B:176:ILE:HD11	2.60	0.42
1:B:386:PHE:CE2	1:B:414:PRO:HB2	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:HIS:HE1	1:A:60:THR:OG1	2.03	0.41
1:D:22:ILE:HG23	1:D:27:LEU:HD12	2.02	0.41
1:D:374:ILE:HD12	1:D:374:ILE:C	2.40	0.41
1:B:281:GLU:HG2	1:B:283:PRO:HD3	2.02	0.41
1:C:263:LYS:HB2	1:C:274:VAL:HB	2.01	0.41
1:B:176:ILE:HG13	1:B:177:LEU:N	2.35	0.41
1:B:406:LYS:HA	1:B:409:GLN:HE21	1.85	0.41
1:A:136:ASP:O	1:A:139:LEU:HB2	2.21	0.41
1:C:237:VAL:O	1:C:238:ASP:HB2	2.21	0.41
1:D:102:ILE:HD13	1:D:109:LEU:HD21	2.02	0.41
1:C:148:GLU:HB3	1:C:156:LEU:CD2	2.50	0.41
1:B:136:ASP:O	1:B:139:LEU:HB2	2.19	0.41
1:B:435:PRO:O	1:B:436:TYR:HB2	2.20	0.41
1:D:24:ARG:HG2	1:D:100:GLU:OE1	2.21	0.41
1:D:99:ARG:O	1:D:103:ARG:HG3	2.21	0.41
1:A:139:LEU:HD12	1:A:139:LEU:HA	1.92	0.41
1:A:158:GLU:OE2	1:A:224:ASP:OD1	2.38	0.41
1:B:144:VAL:CG1	1:B:148:GLU:OE1	2.68	0.41
1:C:322:ARG:HG2	1:C:432:THR:OG1	2.21	0.41
1:A:13:GLU:HB2	1:A:16:TYR:CD1	2.55	0.41
1:D:10:CYS:SG	1:D:176:ILE:HD11	2.61	0.41
1:A:170:ARG:HD3	2:E:3:FUC:H62	2.02	0.41
3:C:522:NAG:O7	3:C:522:NAG:C3	2.63	0.41
1:D:80:ALA:O	1:D:364:ASN:ND2	2.54	0.40
1:A:102:ILE:HG23	1:A:107:LEU:HB2	2.03	0.40
1:A:83:TYR:CD1	1:A:83:TYR:C	2.95	0.40
1:B:80:ALA:O	1:B:364:ASN:ND2	2.54	0.40
1:C:387:LYS:HD2	6:C:2179:HOH:O	2.20	0.40
1:B:382:GLN:NE2	1:D:382:GLN:HE22	2.20	0.40
1:D:169:LYS:HG3	6:D:2218:HOH:O	2.20	0.40
1:A:80:ALA:O	1:A:364:ASN:ND2	2.55	0.40
1:B:18:GLU:HG3	6:B:1104:HOH:O	2.21	0.40
1:B:237:VAL:O	1:B:238:ASP:HB2	2.21	0.40
1:B:314:HIS:HD2	6:D:914:HOH:O	2.03	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	481/498 (97%)	468 (97%)	13 (3%)	0	100	100
1	B	481/498 (97%)	467 (97%)	14 (3%)	0	100	100
1	C	481/498 (97%)	470 (98%)	11 (2%)	0	100	100
1	D	481/498 (97%)	467 (97%)	14 (3%)	0	100	100
All	All	1924/1992 (97%)	1872 (97%)	52 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	398/427 (93%)	386 (97%)	12 (3%)	41	41
1	B	410/427 (96%)	399 (97%)	11 (3%)	44	46
1	C	402/427 (94%)	392 (98%)	10 (2%)	47	49
1	D	405/427 (95%)	392 (97%)	13 (3%)	39	38
All	All	1615/1708 (95%)	1569 (97%)	46 (3%)	43	44

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	GLU
1	A	77	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	79	GLU
1	A	116	ASN
1	A	139	LEU
1	A	208	ASN
1	A	213	TYR
1	A	282	THR
1	A	305	ASN
1	A	314	HIS
1	A	363	THR
1	A	475	ARG
1	B	20	LEU
1	B	31	SER
1	B	77	ASN
1	B	106	ASP
1	B	139	LEU
1	B	177	LEU
1	B	208	ASN
1	B	213	TYR
1	B	284	SER
1	B	314	HIS
1	B	363	THR
1	C	96	ARG
1	C	106	ASP
1	C	116	ASN
1	C	139	LEU
1	C	170	ARG
1	C	177	LEU
1	C	208	ASN
1	C	213	TYR
1	C	286	THR
1	C	314	HIS
1	D	106	ASP
1	D	116	ASN
1	D	139	LEU
1	D	144	VAL
1	D	158	GLU
1	D	177	LEU
1	D	208	ASN
1	D	213	TYR
1	D	253	ASP
1	D	269	GLN
1	D	314	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	363	THR
1	D	485	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	HIS
1	A	57	HIS
1	A	58	GLN
1	A	77	ASN
1	A	116	ASN
1	A	118	ASN
1	A	208	ASN
1	A	252	GLN
1	A	305	ASN
1	A	409	GLN
1	A	463	HIS
1	B	35	HIS
1	B	57	HIS
1	B	77	ASN
1	B	85	ASN
1	B	178	ASN
1	B	208	ASN
1	B	265	GLN
1	B	305	ASN
1	B	314	HIS
1	B	342	HIS
1	B	409	GLN
1	B	463	HIS
1	C	35	HIS
1	C	57	HIS
1	C	85	ASN
1	C	116	ASN
1	C	208	ASN
1	C	314	HIS
1	C	382	GLN
1	C	409	GLN
1	C	463	HIS
1	D	35	HIS
1	D	57	HIS
1	D	85	ASN
1	D	114	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	116	ASN
1	D	208	ASN
1	D	252	GLN
1	D	269	GLN
1	D	382	GLN
1	D	409	GLN
1	D	463	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)

12 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	E	1	2,1	14,14,15	0.91	0	17,19,21	0.96	1 (5%)
2	NAG	E	2	2	14,14,15	0.59	0	17,19,21	0.78	0
2	FUC	E	3	2	10,10,11	0.73	0	14,14,16	2.21	3 (21%)
2	NAG	F	1	2,1	14,14,15	0.53	0	17,19,21	1.02	1 (5%)
2	NAG	F	2	2	14,14,15	0.69	0	17,19,21	2.06	3 (17%)
2	FUC	F	3	2	10,10,11	0.67	0	14,14,16	1.75	3 (21%)
2	NAG	G	1	2,1	14,14,15	0.77	0	17,19,21	0.97	0
2	NAG	G	2	2	14,14,15	0.68	1 (7%)	17,19,21	0.86	1 (5%)
2	FUC	G	3	2	10,10,11	0.64	0	14,14,16	2.01	3 (21%)
2	NAG	H	1	2,1	14,14,15	0.67	0	17,19,21	0.66	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	H	2	2	14,14,15	0.56	0	17,19,21	0.92	1 (5%)
2	FUC	H	3	2	10,10,11	0.71	0	14,14,16	2.11	3 (21%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	E	1	2,1	1/1/5/7	1/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	FUC	E	3	2	2/2/4/5	-	0/1/1/1
2	NAG	F	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	3/6/23/26	0/1/1/1
2	FUC	F	3	2	2/2/4/5	-	0/1/1/1
2	NAG	G	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	G	2	2	1/1/5/7	2/6/23/26	0/1/1/1
2	FUC	G	3	2	3/3/4/5	-	0/1/1/1
2	NAG	H	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	H	2	2	-	2/6/23/26	0/1/1/1
2	FUC	H	3	2	2/2/4/5	-	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	2	NAG	C1-C2	2.03	1.55	1.52

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	2	NAG	C1-O5-C5	6.34	120.78	112.19
2	E	3	FUC	C1-C2-C3	5.63	116.58	109.67
2	H	3	FUC	C1-C2-C3	5.07	115.90	109.67
2	G	3	FUC	C1-C2-C3	4.30	114.95	109.67
2	G	3	FUC	C3-C4-C5	4.27	116.42	109.77
2	E	3	FUC	C2-C3-C4	4.20	118.17	110.89
2	F	2	NAG	O5-C1-C2	4.19	117.90	111.29
2	G	3	FUC	C2-C3-C4	4.09	117.97	110.89
2	H	3	FUC	C3-C4-C5	4.08	116.14	109.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	3	FUC	C2-C3-C4	4.06	117.91	110.89
2	E	3	FUC	C3-C4-C5	3.93	115.89	109.77
2	F	3	FUC	C1-C2-C3	3.92	114.48	109.67
2	F	3	FUC	C3-C4-C5	3.72	115.56	109.77
2	F	3	FUC	C2-C3-C4	3.23	116.49	110.89
2	E	1	NAG	C1-O5-C5	2.91	116.13	112.19
2	F	2	NAG	C4-C3-C2	-2.84	106.86	111.02
2	G	2	NAG	C1-O5-C5	2.24	115.23	112.19
2	H	2	NAG	C1-O5-C5	2.16	115.12	112.19
2	F	1	NAG	C6-C5-C4	2.15	118.04	113.00

All (11) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	E	1	NAG	C1
2	E	3	FUC	C3
2	E	3	FUC	C4
2	F	3	FUC	C3
2	F	3	FUC	C4
2	G	2	NAG	C1
2	G	3	FUC	C4
2	G	3	FUC	C3
2	G	3	FUC	C1
2	H	3	FUC	C3
2	H	3	FUC	C4

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	2	NAG	C1-C2-N2-C7
2	G	1	NAG	C4-C5-C6-O6
2	G	1	NAG	O5-C5-C6-O6
2	G	2	NAG	C4-C5-C6-O6
2	F	2	NAG	O5-C5-C6-O6
2	H	2	NAG	O5-C5-C6-O6
2	F	2	NAG	C4-C5-C6-O6
2	H	2	NAG	C4-C5-C6-O6
2	G	2	NAG	O5-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
2	E	1	NAG	C4-C5-C6-O6

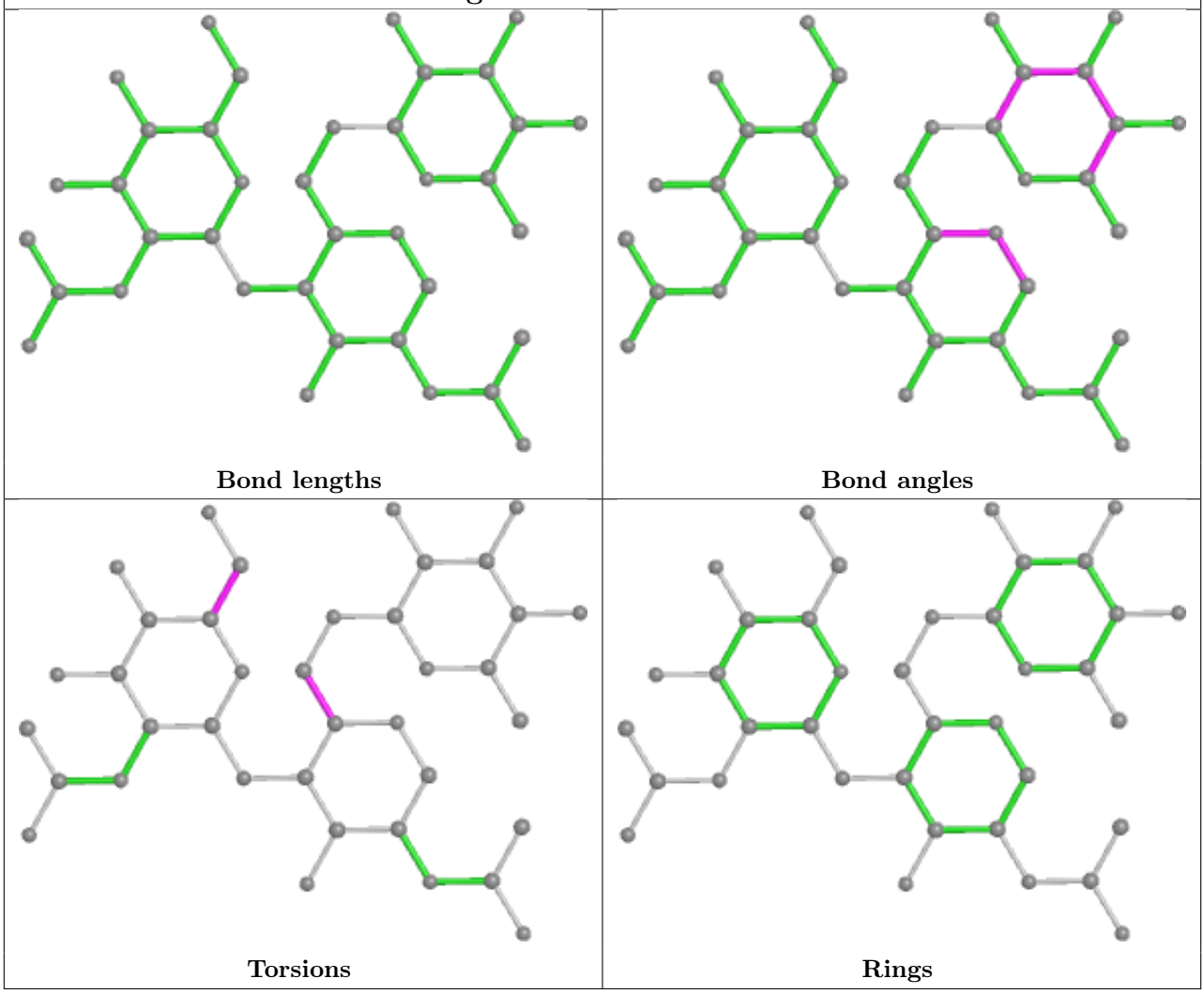
There are no ring outliers.

6 monomers are involved in 7 short contacts:

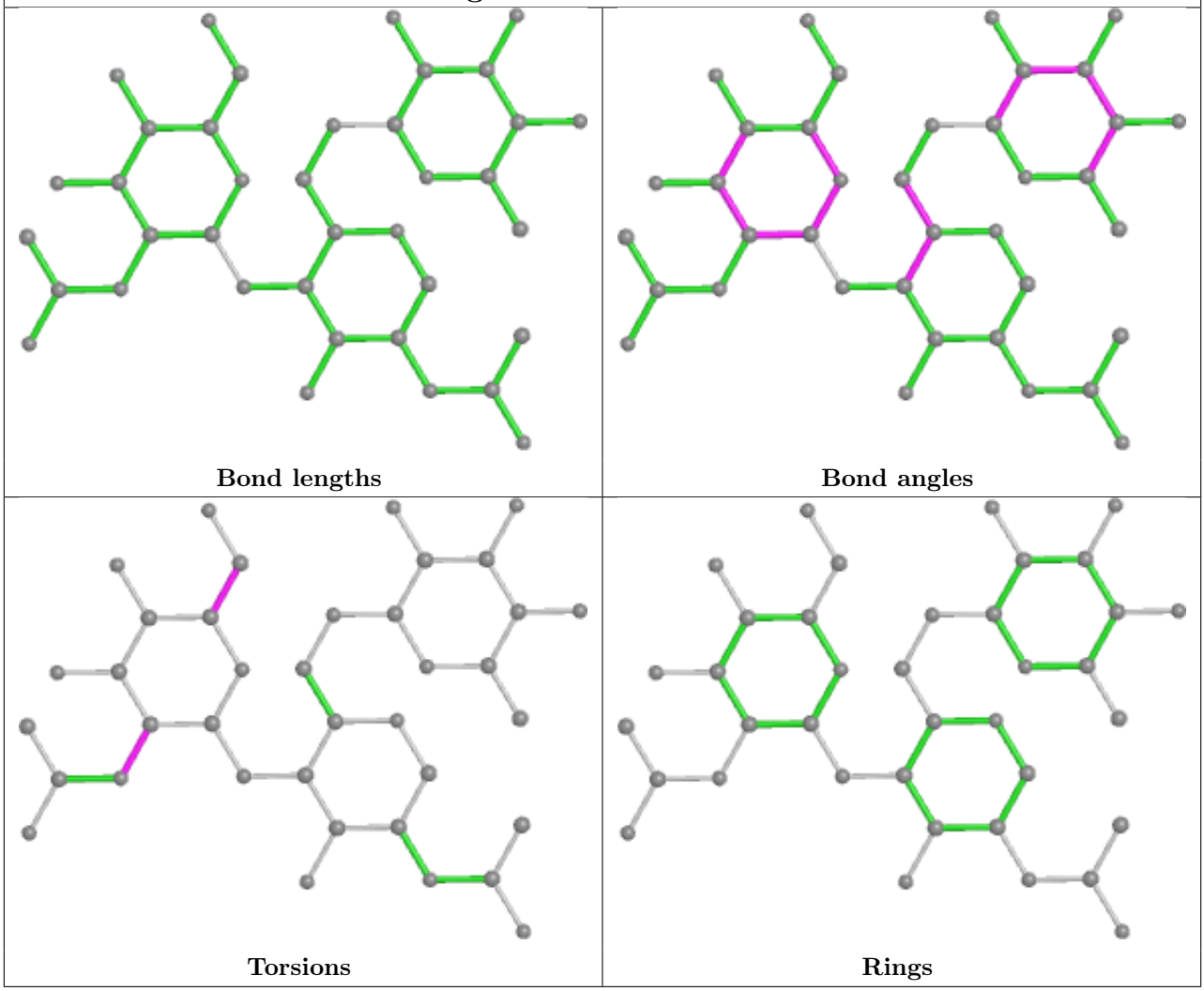
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	3	FUC	3	0
2	G	1	NAG	1	0
2	F	2	NAG	4	0
2	F	1	NAG	1	0
2	E	3	FUC	1	0
2	G	3	FUC	1	0

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

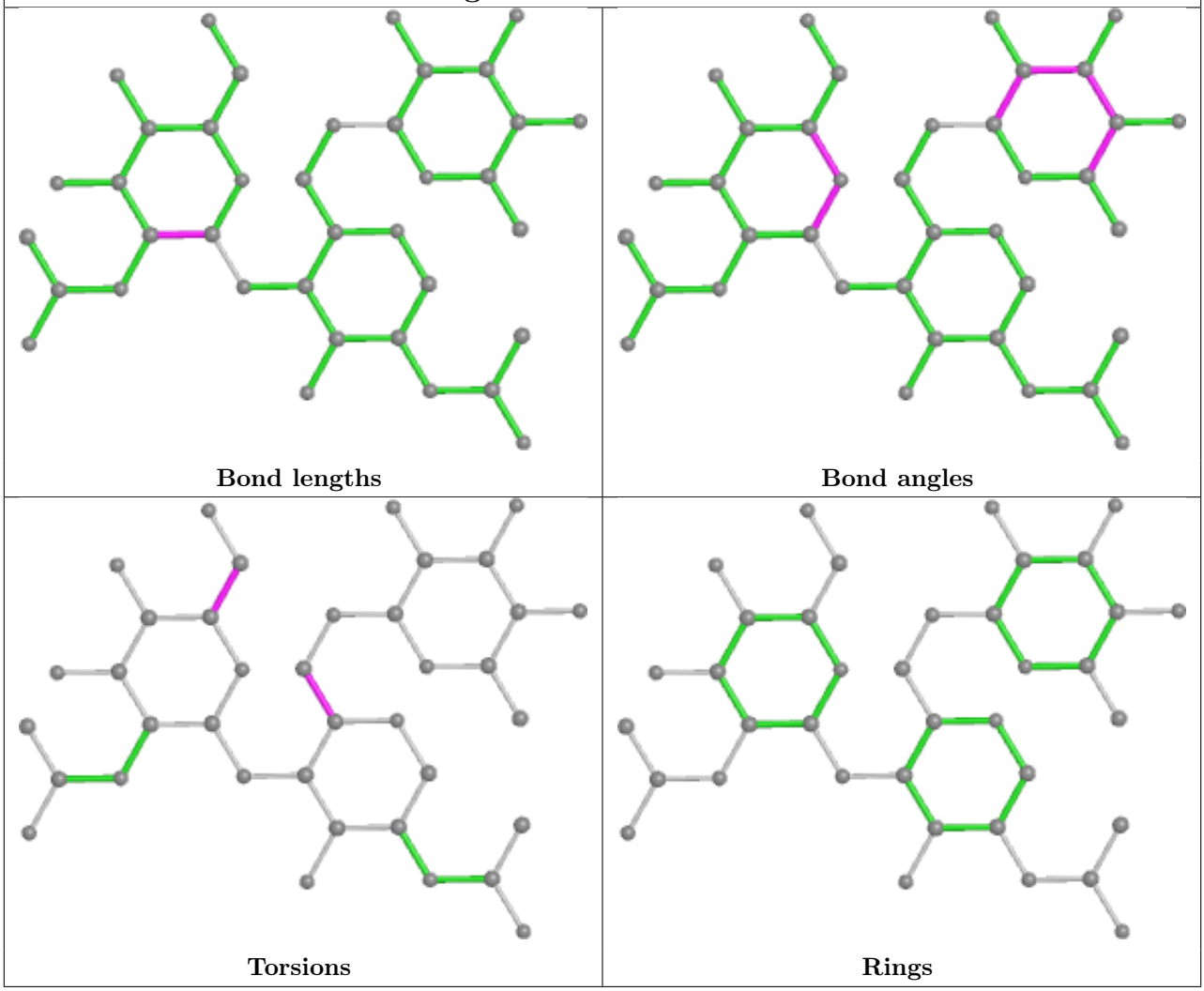
Oligosaccharide Chain E



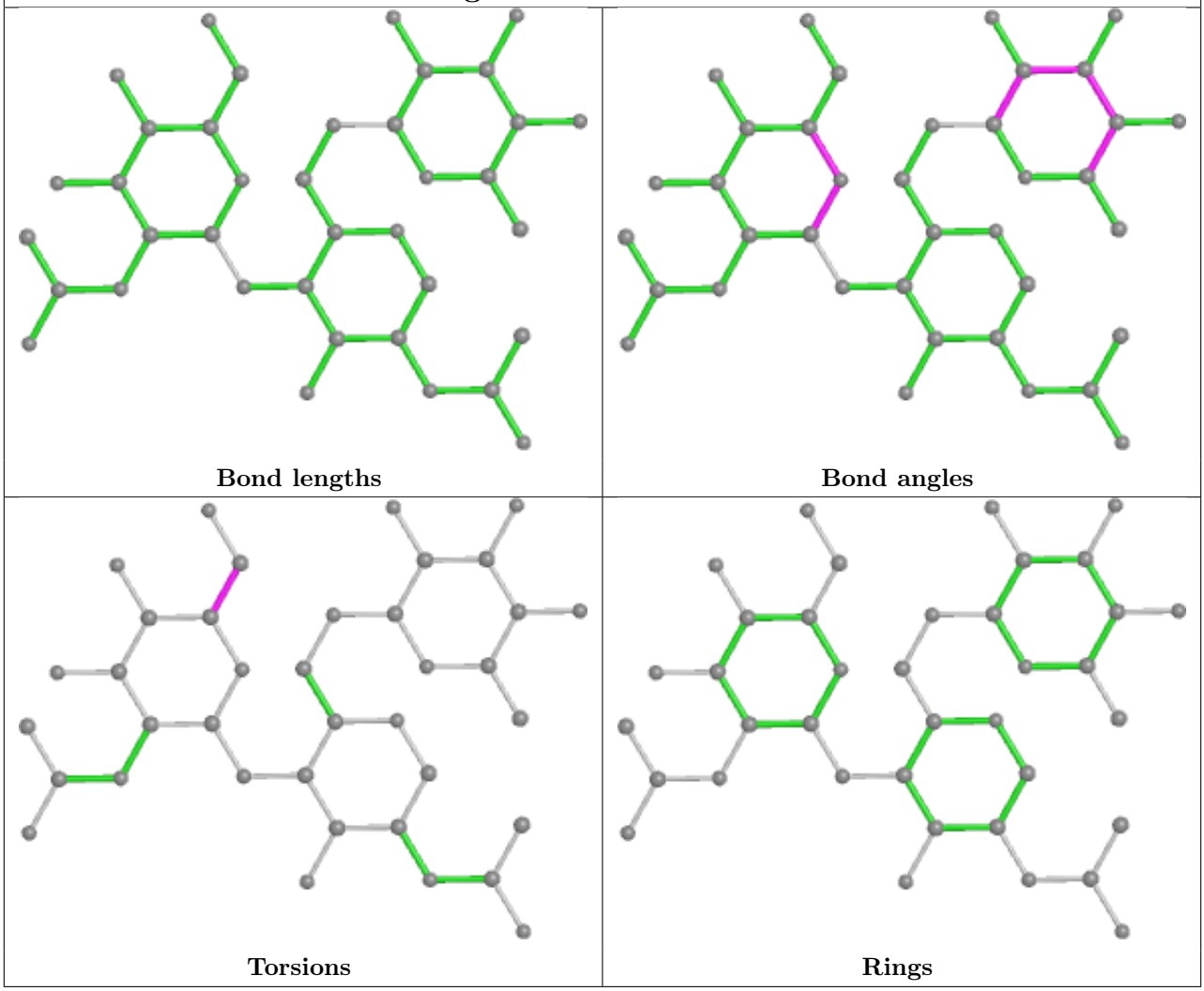
Oligosaccharide Chain F



Oligosaccharide Chain G



Oligosaccharide Chain H



5.6 Ligand geometry (i)

12 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	$\#\|Z\| > 2$
4	CIT	D	526	-	12,12,12	5.05	10 (83%)	17,17,17	2.24	6 (35%)
5	FAD	A	527	-	53,58,58	1.77	14 (26%)	68,89,89	1.28	6 (8%)
3	NAG	B	522	1	14,14,15	0.61	0	17,19,21	0.65	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	FAD	C	527	-	53,58,58	1.76	15 (28%)	68,89,89	1.25	7 (10%)
5	FAD	D	527	-	53,58,58	1.76	13 (24%)	68,89,89	1.29	7 (10%)
4	CIT	C	526	-	12,12,12	5.31	11 (91%)	17,17,17	2.30	7 (41%)
5	FAD	B	527	-	53,58,58	1.81	14 (26%)	68,89,89	1.26	7 (10%)
4	CIT	A	526	-	12,12,12	5.25	9 (75%)	17,17,17	2.14	6 (35%)
4	CIT	B	526	-	12,12,12	3.20	7 (58%)	17,17,17	2.30	7 (41%)
3	NAG	D	522	1	14,14,15	0.65	0	17,19,21	0.69	0
3	NAG	C	522	1	14,14,15	0.57	0	17,19,21	0.55	0
3	NAG	A	522	1	14,14,15	0.74	0	17,19,21	1.03	2 (11%)

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
4	CIT	D	526	-	-	9/16/16/16	-
5	FAD	A	527	-	-	3/30/50/50	0/6/6/6
3	NAG	B	522	1	1/1/5/7	2/6/23/26	0/1/1/1
5	FAD	C	527	-	-	6/30/50/50	0/6/6/6
5	FAD	D	527	-	-	3/30/50/50	0/6/6/6
4	CIT	C	526	-	-	6/16/16/16	-
5	FAD	B	527	-	-	6/30/50/50	0/6/6/6
4	CIT	A	526	-	-	10/16/16/16	-
4	CIT	B	526	-	-	8/16/16/16	-
3	NAG	D	522	1	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	C	522	1	1/1/5/7	3/6/23/26	0/1/1/1
3	NAG	A	522	1	1/1/5/7	0/6/23/26	0/1/1/1

All (93) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	526	CIT	C2-C3	13.47	1.70	1.53
4	D	526	CIT	C2-C3	9.27	1.65	1.53
4	A	526	CIT	C4-C3	8.67	1.64	1.53
4	A	526	CIT	C2-C3	8.60	1.64	1.53
4	A	526	CIT	C3-C6	8.03	1.61	1.53
4	D	526	CIT	C4-C3	7.53	1.63	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	526	CIT	C2-C1	7.35	1.73	1.50
4	D	526	CIT	C3-C6	7.17	1.60	1.53
4	D	526	CIT	C2-C1	7.01	1.72	1.50
4	B	526	CIT	C2-C3	6.28	1.61	1.53
4	C	526	CIT	C2-C1	5.50	1.67	1.50
4	C	526	CIT	O3-C5	5.21	1.39	1.22
4	B	526	CIT	C2-C1	5.18	1.66	1.50
4	C	526	CIT	C3-C6	5.11	1.58	1.53
5	B	527	FAD	O4B-C1B	4.78	1.47	1.41
5	D	527	FAD	O4B-C1B	4.75	1.47	1.41
5	A	527	FAD	O4B-C1B	4.61	1.47	1.41
4	D	526	CIT	O3-C5	4.49	1.37	1.22
5	C	527	FAD	O4B-C1B	4.48	1.47	1.41
4	A	526	CIT	O3-C5	4.41	1.36	1.22
5	A	527	FAD	PA-O2A	-3.95	1.36	1.55
5	C	527	FAD	PA-O2A	-3.94	1.36	1.55
5	B	527	FAD	PA-O2A	-3.86	1.37	1.55
5	D	527	FAD	PA-O2A	-3.84	1.37	1.55
5	C	527	FAD	O5'-C5'	3.82	1.59	1.44
5	A	527	FAD	O5'-C5'	3.79	1.59	1.44
4	C	526	CIT	O7-C3	3.72	1.50	1.43
5	B	527	FAD	O5'-C5'	3.72	1.59	1.44
4	A	526	CIT	O5-C6	3.69	1.34	1.22
5	D	527	FAD	O5'-C5'	3.69	1.59	1.44
4	B	526	CIT	O3-C5	3.65	1.34	1.22
5	A	527	FAD	C1'-C2'	3.65	1.57	1.52
4	C	526	CIT	O1-C1	-3.55	1.10	1.22
5	B	527	FAD	P-O2P	-3.46	1.39	1.55
4	C	526	CIT	O5-C6	3.44	1.33	1.22
4	D	526	CIT	O5-C6	3.42	1.33	1.22
5	D	527	FAD	P-O2P	-3.36	1.39	1.55
5	B	527	FAD	C4X-N5	3.34	1.37	1.30
4	B	526	CIT	O1-C1	-3.34	1.11	1.22
4	A	526	CIT	O2-C1	-3.33	1.19	1.30
4	C	526	CIT	O4-C5	-3.32	1.19	1.30
5	B	527	FAD	C1'-C2'	3.32	1.57	1.52
5	C	527	FAD	P-O2P	-3.28	1.39	1.55
5	D	527	FAD	C1'-C2'	3.25	1.57	1.52
5	A	527	FAD	P-O2P	-3.24	1.40	1.55
5	C	527	FAD	C4X-N5	3.22	1.37	1.30
4	C	526	CIT	O2-C1	-3.12	1.20	1.30
5	A	527	FAD	C4X-N5	2.96	1.36	1.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	526	CIT	O2-C1	-2.92	1.20	1.30
4	D	526	CIT	O2-C1	-2.92	1.20	1.30
5	D	527	FAD	C4X-N5	2.90	1.36	1.30
5	C	527	FAD	C1'-C2'	2.87	1.56	1.52
5	D	527	FAD	C8-C7	2.81	1.47	1.40
4	C	526	CIT	C4-C3	2.77	1.57	1.53
5	C	527	FAD	C9A-N10	2.76	1.46	1.41
4	D	526	CIT	O4-C5	-2.71	1.21	1.30
5	B	527	FAD	C8-C7	2.67	1.47	1.40
4	B	526	CIT	O4-C5	-2.67	1.21	1.30
4	A	526	CIT	O1-C1	-2.67	1.13	1.22
4	D	526	CIT	O1-C1	-2.65	1.13	1.22
4	A	526	CIT	O4-C5	-2.60	1.22	1.30
5	D	527	FAD	O2-C2	-2.58	1.19	1.24
5	A	527	FAD	O2-C2	-2.55	1.19	1.24
5	A	527	FAD	C8-C7	2.54	1.47	1.40
5	B	527	FAD	C9A-N10	2.53	1.45	1.41
5	D	527	FAD	C2B-C1B	-2.50	1.50	1.53
5	A	527	FAD	C9A-N10	2.49	1.45	1.41
5	C	527	FAD	C4A-N3A	2.47	1.39	1.35
5	C	527	FAD	C8-C7	2.46	1.47	1.40
5	D	527	FAD	C9A-N10	2.45	1.45	1.41
5	B	527	FAD	C2B-C1B	-2.44	1.50	1.53
5	B	527	FAD	C9A-C5X	2.43	1.45	1.41
5	A	527	FAD	C10-N1	2.41	1.38	1.33
5	C	527	FAD	O2-C2	-2.38	1.19	1.24
4	B	526	CIT	O5-C6	2.31	1.29	1.22
4	D	526	CIT	C4-C5	2.29	1.57	1.50
5	C	527	FAD	C6-C5X	2.28	1.43	1.40
5	D	527	FAD	C4A-N3A	2.26	1.38	1.35
5	A	527	FAD	C9A-C5X	2.24	1.44	1.41
5	B	527	FAD	O2-C2	-2.21	1.20	1.24
5	B	527	FAD	C6-C5X	2.20	1.43	1.40
4	C	526	CIT	C4-C5	2.19	1.57	1.50
5	C	527	FAD	C2A-N3A	2.17	1.35	1.32
5	B	527	FAD	C10-N1	2.17	1.37	1.33
5	A	527	FAD	C4A-N3A	2.15	1.38	1.35
5	B	527	FAD	C4A-N3A	2.12	1.38	1.35
5	D	527	FAD	C9A-C5X	2.07	1.44	1.41
5	C	527	FAD	C2B-C1B	-2.06	1.50	1.53
5	D	527	FAD	C10-N1	2.04	1.37	1.33
5	A	527	FAD	C2A-N3A	2.03	1.35	1.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	527	FAD	C10-N1	2.02	1.37	1.33
5	C	527	FAD	C2A-N1A	2.01	1.37	1.33
5	A	527	FAD	C6-C5X	2.01	1.43	1.40

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	526	CIT	C3-C2-C1	5.91	128.13	113.81
4	B	526	CIT	C3-C2-C1	5.54	127.23	113.81
4	A	526	CIT	C3-C2-C1	5.43	126.95	113.81
4	C	526	CIT	C3-C2-C1	4.20	123.99	113.81
4	C	526	CIT	O6-C6-C3	3.92	119.86	113.05
4	B	526	CIT	O4-C5-C4	3.49	125.56	114.35
4	B	526	CIT	O5-C6-C3	-3.44	117.39	122.25
4	C	526	CIT	O5-C6-C3	-3.41	117.43	122.25
4	D	526	CIT	O4-C5-C4	3.29	124.93	114.35
5	D	527	FAD	C5'-C4'-C3'	-3.23	105.96	112.20
5	A	527	FAD	C5'-C4'-C3'	-3.22	105.98	112.20
4	C	526	CIT	O7-C3-C6	-3.17	104.42	108.86
4	A	526	CIT	O4-C5-C4	3.16	124.50	114.35
4	B	526	CIT	O6-C6-C3	3.14	118.50	113.05
4	C	526	CIT	O4-C5-C4	3.01	124.01	114.35
5	B	527	FAD	C5'-C4'-C3'	-2.96	106.50	112.20
4	A	526	CIT	C2-C3-C6	2.93	116.41	110.11
5	C	527	FAD	O5B-PA-O1A	-2.90	97.73	109.07
4	A	526	CIT	O4-C5-O3	-2.88	116.12	123.30
5	D	527	FAD	O4B-C1B-C2B	-2.85	102.76	106.93
5	A	527	FAD	O4B-C1B-C2B	-2.84	102.77	106.93
5	C	527	FAD	C5'-C4'-C3'	-2.81	106.78	112.20
4	D	526	CIT	O4-C5-O3	-2.72	116.51	123.30
5	B	527	FAD	O4B-C1B-C2B	-2.70	102.98	106.93
5	A	527	FAD	O5B-PA-O1A	-2.66	98.66	109.07
5	C	527	FAD	O4B-C1B-C2B	-2.66	103.04	106.93
5	B	527	FAD	O5B-PA-O1A	-2.64	98.77	109.07
5	C	527	FAD	C5A-C6A-N1A	-2.61	114.44	120.35
5	D	527	FAD	C5A-C6A-N1A	-2.59	114.49	120.35
5	B	527	FAD	C5A-C6A-N6A	2.58	124.28	120.35
5	D	527	FAD	C5A-C6A-N6A	2.57	124.25	120.35
4	D	526	CIT	C2-C3-C6	2.55	115.58	110.11
5	A	527	FAD	C5A-C6A-N6A	2.52	124.18	120.35
5	D	527	FAD	C2A-N1A-C6A	2.51	123.05	118.75
5	A	527	FAD	C5A-C6A-N1A	-2.51	114.67	120.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	527	FAD	O5B-PA-O1A	-2.50	99.29	109.07
5	B	527	FAD	C2A-N1A-C6A	2.47	122.98	118.75
5	A	527	FAD	C2A-N1A-C6A	2.46	122.96	118.75
5	C	527	FAD	C2A-N1A-C6A	2.45	122.95	118.75
5	B	527	FAD	C5A-C6A-N1A	-2.45	114.81	120.35
4	C	526	CIT	O7-C3-C4	-2.43	103.71	109.40
5	C	527	FAD	C5A-C6A-N6A	2.40	124.00	120.35
4	A	526	CIT	O7-C3-C4	-2.34	103.92	109.40
4	C	526	CIT	O4-C5-O3	-2.34	117.47	123.30
3	A	522	NAG	C1-O5-C5	2.31	115.32	112.19
4	B	526	CIT	O3-C5-C4	-2.30	116.22	122.94
5	D	527	FAD	C4-N3-C2	-2.29	121.42	125.64
4	D	526	CIT	O7-C3-C6	-2.17	105.81	108.86
5	C	527	FAD	C4-N3-C2	-2.15	121.67	125.64
5	B	527	FAD	C4-N3-C2	-2.09	121.79	125.64
4	D	526	CIT	O7-C3-C4	-2.08	104.54	109.40
4	B	526	CIT	O2-C1-O1	2.06	128.44	123.30
4	A	526	CIT	C4-C3-C6	-2.05	105.70	110.11
4	B	526	CIT	O4-C5-O3	-2.05	118.19	123.30
3	A	522	NAG	C2-N2-C7	-2.02	120.03	122.90

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	522	NAG	C1
3	B	522	NAG	C1
3	C	522	NAG	C1
3	D	522	NAG	C1

All (56) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	522	NAG	C3-C2-N2-C7
4	A	526	CIT	O7-C3-C6-O5
4	B	526	CIT	O7-C3-C6-O5
4	B	526	CIT	O7-C3-C6-O6
4	C	526	CIT	O7-C3-C6-O5
4	C	526	CIT	O7-C3-C6-O6
4	C	526	CIT	C4-C3-C6-O5
4	C	526	CIT	C4-C3-C6-O6
4	D	526	CIT	O7-C3-C6-O5
4	D	526	CIT	O7-C3-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	D	526	CIT	C4-C3-C6-O5
5	A	527	FAD	PA-O3P-P-O5'
5	B	527	FAD	PA-O3P-P-O5'
5	C	527	FAD	PA-O3P-P-O5'
3	B	522	NAG	O5-C5-C6-O6
3	C	522	NAG	O5-C5-C6-O6
3	B	522	NAG	C4-C5-C6-O6
3	C	522	NAG	C4-C5-C6-O6
5	C	527	FAD	O3'-C3'-C4'-O4'
5	C	527	FAD	O3'-C3'-C4'-C5'
5	C	527	FAD	C2'-C3'-C4'-C5'
5	C	527	FAD	C2'-C3'-C4'-O4'
4	B	526	CIT	C4-C3-C6-O5
4	D	526	CIT	C4-C3-C6-O6
4	B	526	CIT	C3-C4-C5-O3
5	B	527	FAD	O3'-C3'-C4'-C5'
5	B	527	FAD	C2'-C3'-C4'-O4'
4	A	526	CIT	C3-C4-C5-O4
4	B	526	CIT	C3-C4-C5-O4
4	C	526	CIT	C3-C4-C5-O3
4	C	526	CIT	C3-C4-C5-O4
4	D	526	CIT	C3-C4-C5-O4
4	A	526	CIT	O7-C3-C6-O6
4	A	526	CIT	C2-C3-C6-O6
4	A	526	CIT	C4-C3-C6-O5
4	A	526	CIT	C4-C3-C6-O6
4	B	526	CIT	C4-C3-C6-O6
4	A	526	CIT	C3-C4-C5-O3
4	D	526	CIT	C3-C4-C5-O3
5	D	527	FAD	PA-O3P-P-O5'
5	B	527	FAD	O3'-C3'-C4'-O4'
5	B	527	FAD	C2'-C3'-C4'-C5'
4	B	526	CIT	C2-C3-C6-O6
5	A	527	FAD	O4B-C4B-C5B-O5B
4	A	526	CIT	C2-C3-C6-O5
4	B	526	CIT	C2-C3-C6-O5
5	C	527	FAD	O4B-C4B-C5B-O5B
4	D	526	CIT	C2-C3-C6-O6
4	A	526	CIT	O1-C1-C2-C3
4	D	526	CIT	O1-C1-C2-C3
4	D	526	CIT	O2-C1-C2-C3
4	A	526	CIT	O2-C1-C2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	B	527	FAD	O4B-C4B-C5B-O5B
5	D	527	FAD	O4B-C4B-C5B-O5B
5	D	527	FAD	O3'-C3'-C4'-C5'
5	A	527	FAD	O3'-C3'-C4'-C5'

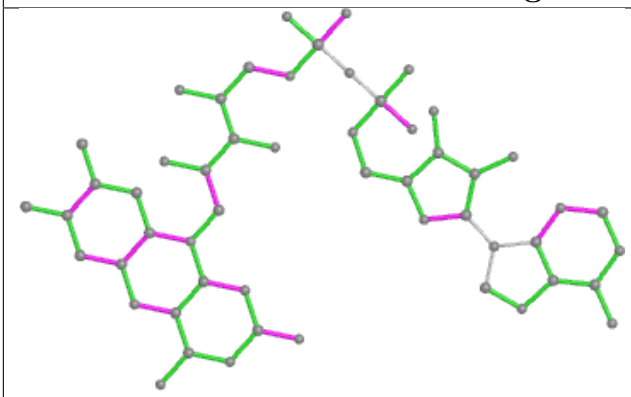
There are no ring outliers.

5 monomers are involved in 6 short contacts:

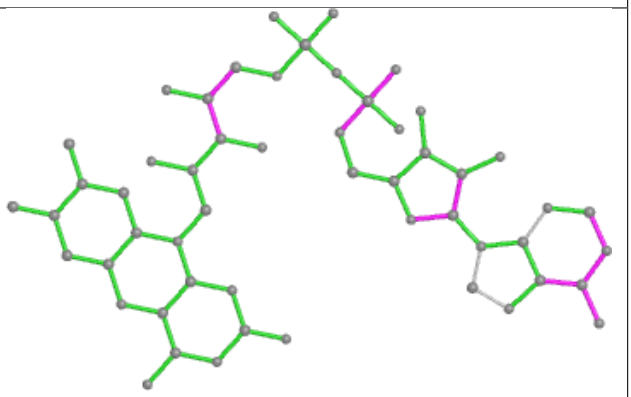
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	526	CIT	1	0
3	B	522	NAG	1	0
4	A	526	CIT	1	0
3	D	522	NAG	1	0
3	C	522	NAG	2	0

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.

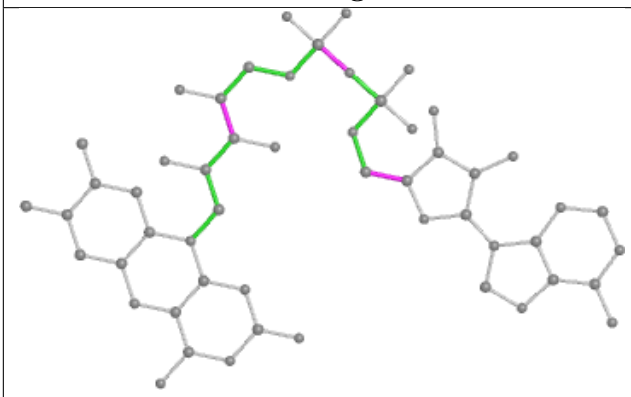
Ligand FAD A 527



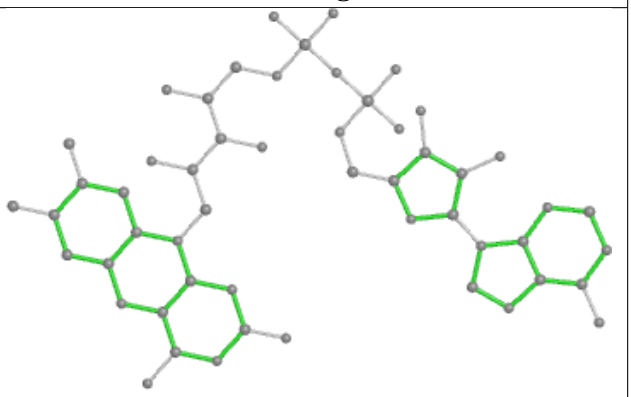
Bond lengths



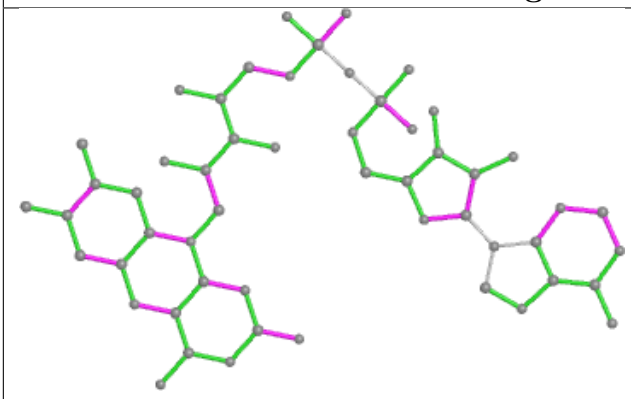
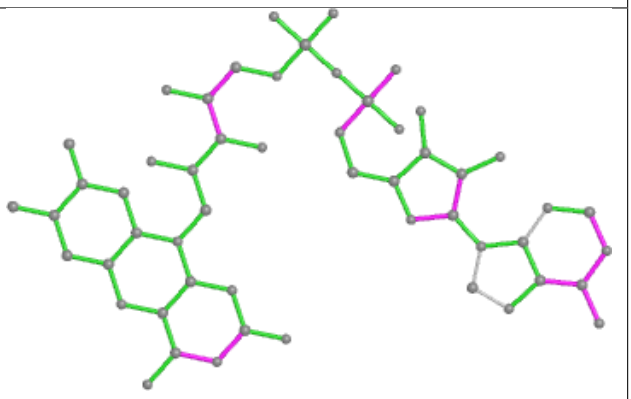
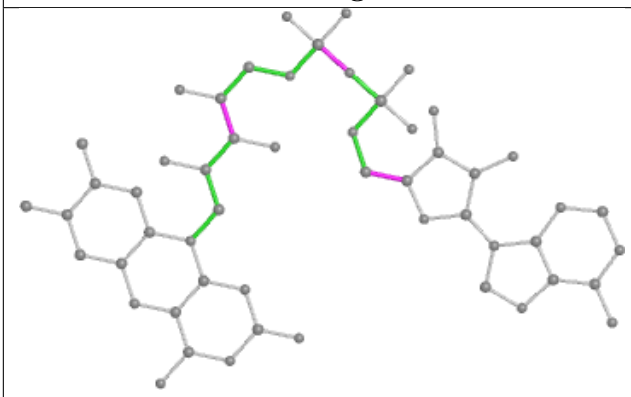
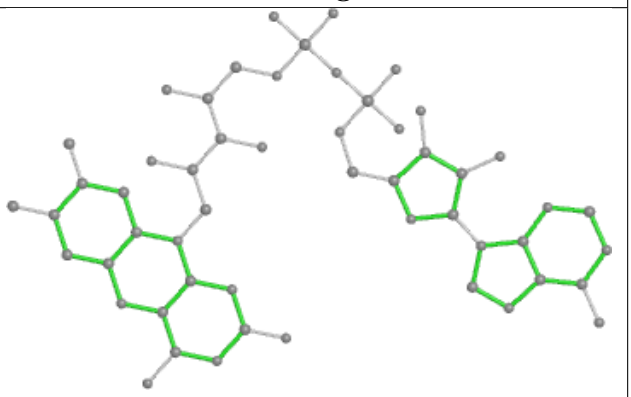
Bond angles

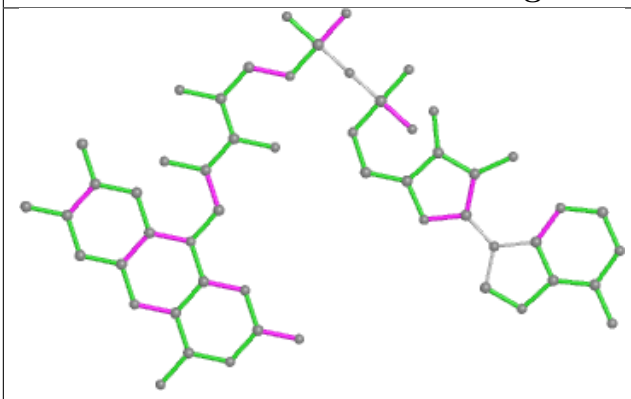
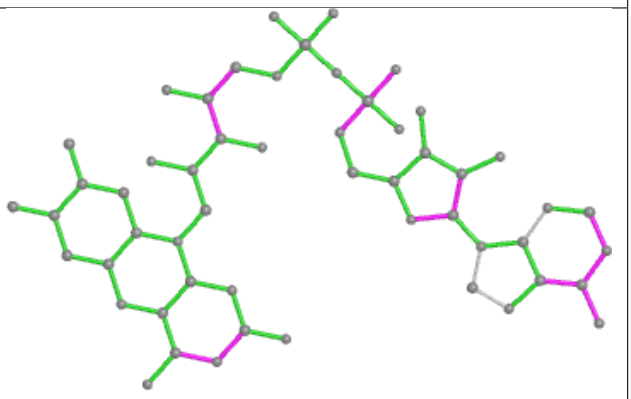
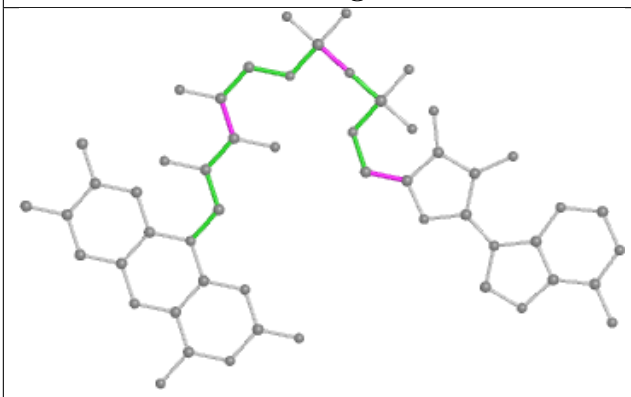
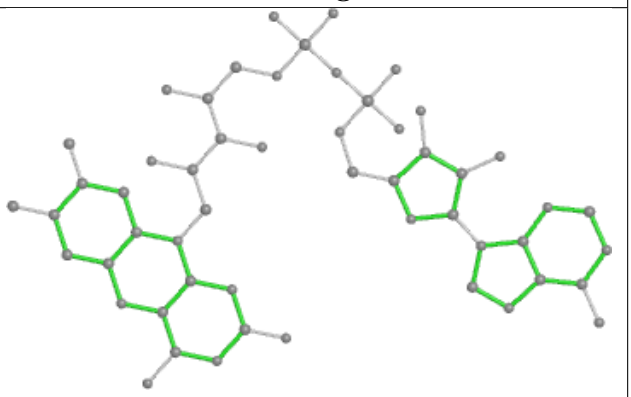


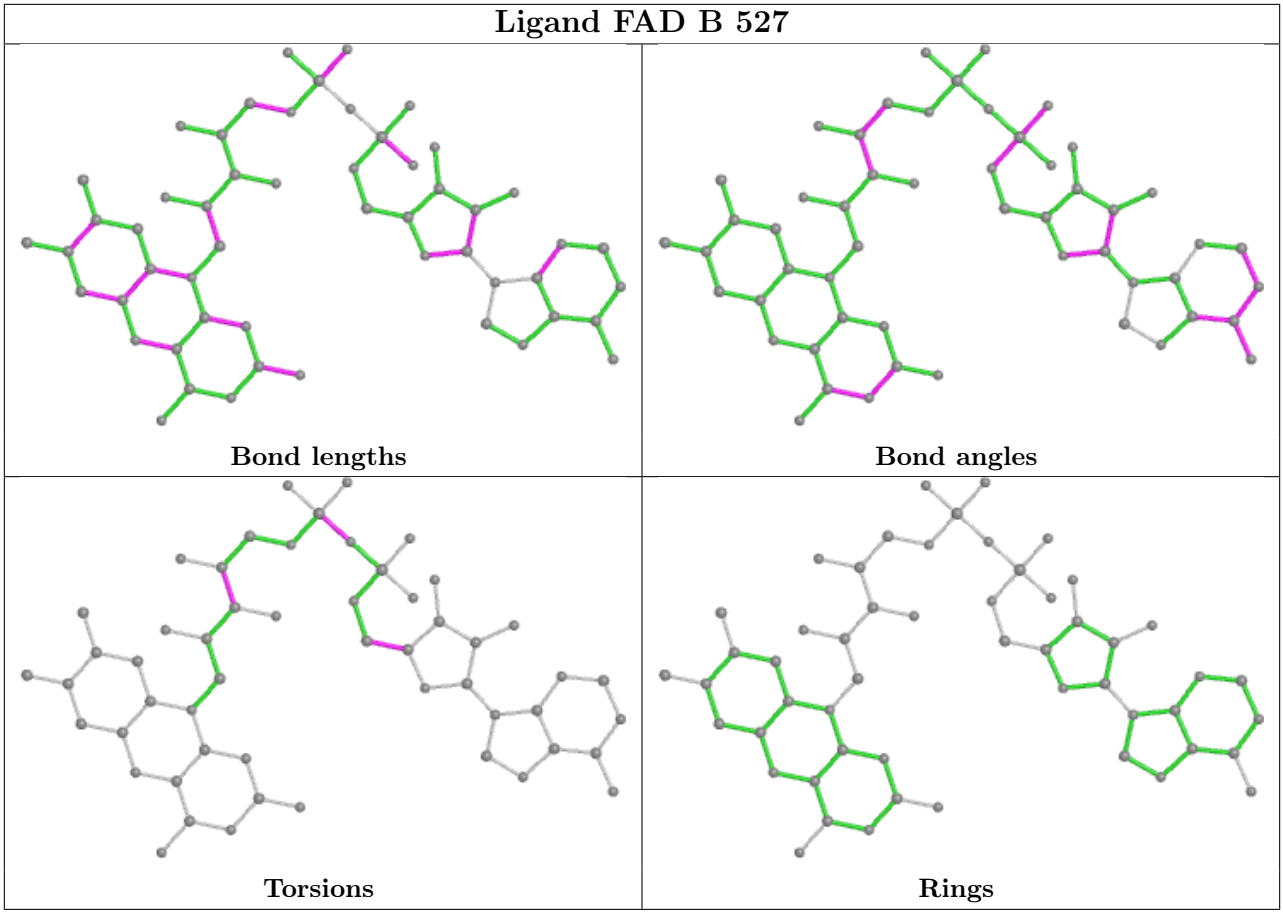
Torsions



Rings

Ligand FAD C 527	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand FAD D 527	
 Bond lengths	 Bond angles
 Torsions	 Rings



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	483/498 (96%)	-0.31	2 (0%)	92	92	13, 22, 35, 57	8 (1%)
1	B	483/498 (96%)	-0.31	3 (0%)	89	88	12, 21, 35, 58	7 (1%)
1	C	483/498 (96%)	-0.31	6 (1%)	79	78	12, 22, 35, 59	5 (1%)
1	D	483/498 (96%)	-0.30	8 (1%)	70	68	12, 22, 36, 59	4 (0%)
All	All	1932/1992 (96%)	-0.30	19 (0%)	82	81	12, 22, 35, 59	24 (1%)

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	363	THR	6.1
1	D	486	ASN	5.4
1	C	486	ASN	4.6
1	C	194	ASP	4.5
1	D	146	PRO	4.2
1	C	31	SER	3.9
1	C	363	THR	3.9
1	B	363	THR	3.0
1	D	108	ARG	2.9
1	D	361	ASN	2.6
1	D	170	ARG	2.5
1	C	32	ASN	2.4
1	B	231	LYS	2.4
1	A	170	ARG	2.3
1	D	79	GLU	2.3
1	A	103	ARG	2.2
1	C	170	ARG	2.1
1	D	485	GLU	2.1
1	B	144	VAL	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)

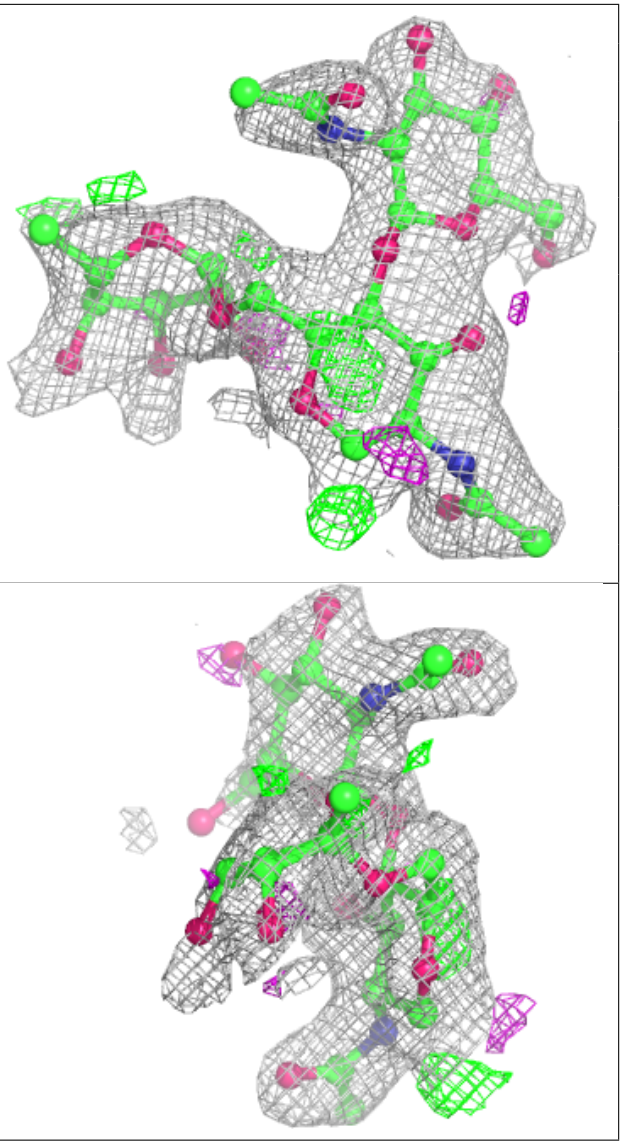
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	F	2	14/15	0.63	0.57	62,64,65,66	0
2	NAG	H	2	14/15	0.72	0.31	51,54,57,58	0
2	FUC	E	3	10/11	0.77	0.29	53,55,55,56	0
2	FUC	G	3	10/11	0.80	0.28	56,56,57,57	0
2	NAG	G	1	14/15	0.80	0.19	45,51,54,55	0
2	NAG	F	1	14/15	0.81	0.21	47,53,59,59	0
2	NAG	E	2	14/15	0.82	0.28	52,53,56,57	0
2	NAG	G	2	14/15	0.82	0.29	57,59,60,61	0
2	FUC	H	3	10/11	0.82	0.21	45,46,47,48	0
2	NAG	H	1	14/15	0.83	0.15	38,42,44,48	0
2	FUC	F	3	10/11	0.84	0.39	61,62,63,63	0
2	NAG	E	1	14/15	0.85	0.13	40,43,49,51	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

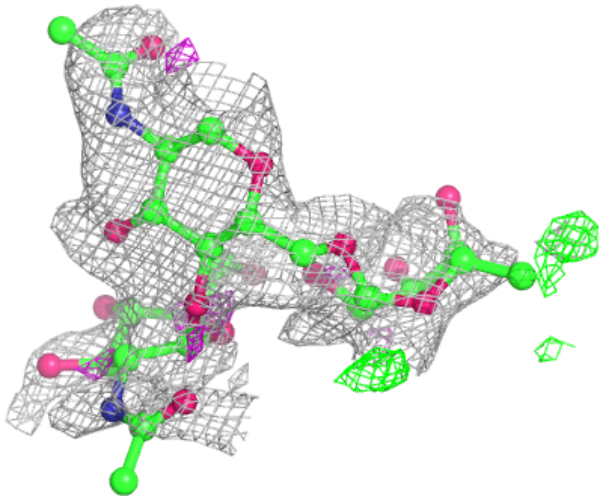
Electron density around Chain E:

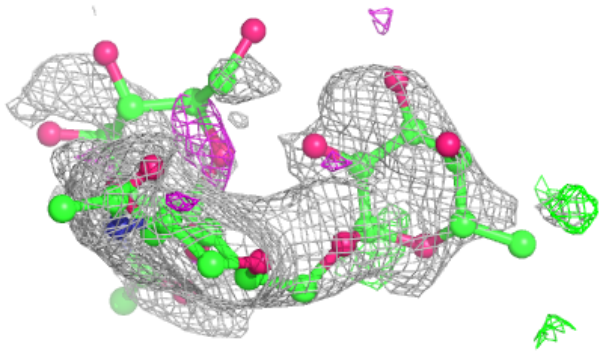
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

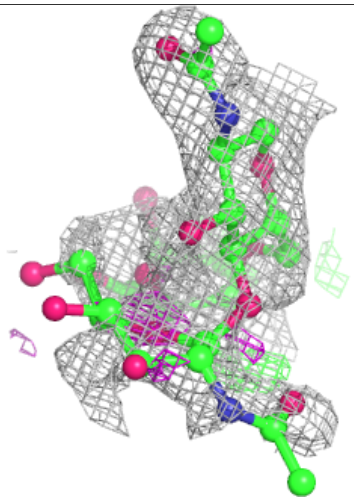


Electron density around Chain F:

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

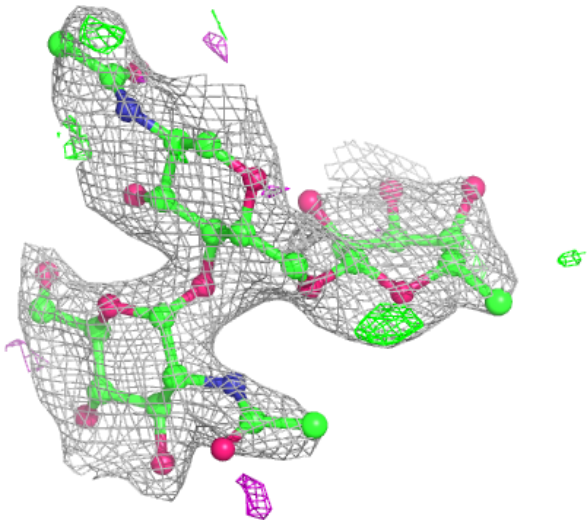


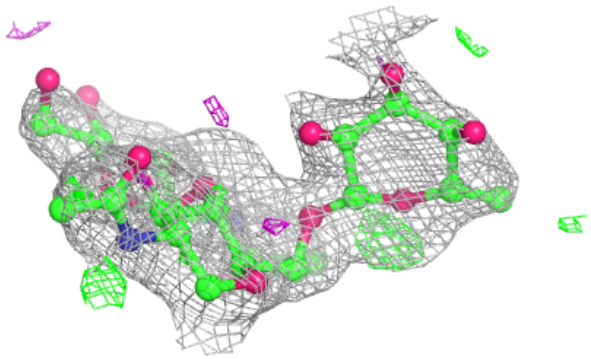


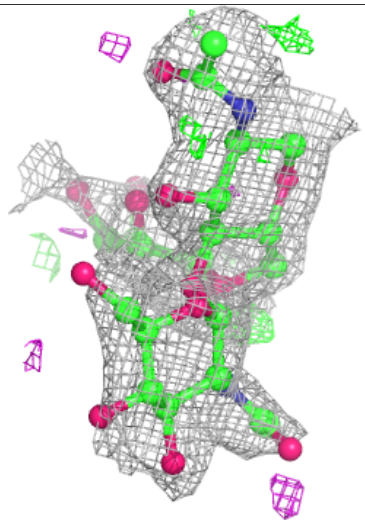


Electron density around Chain G:

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

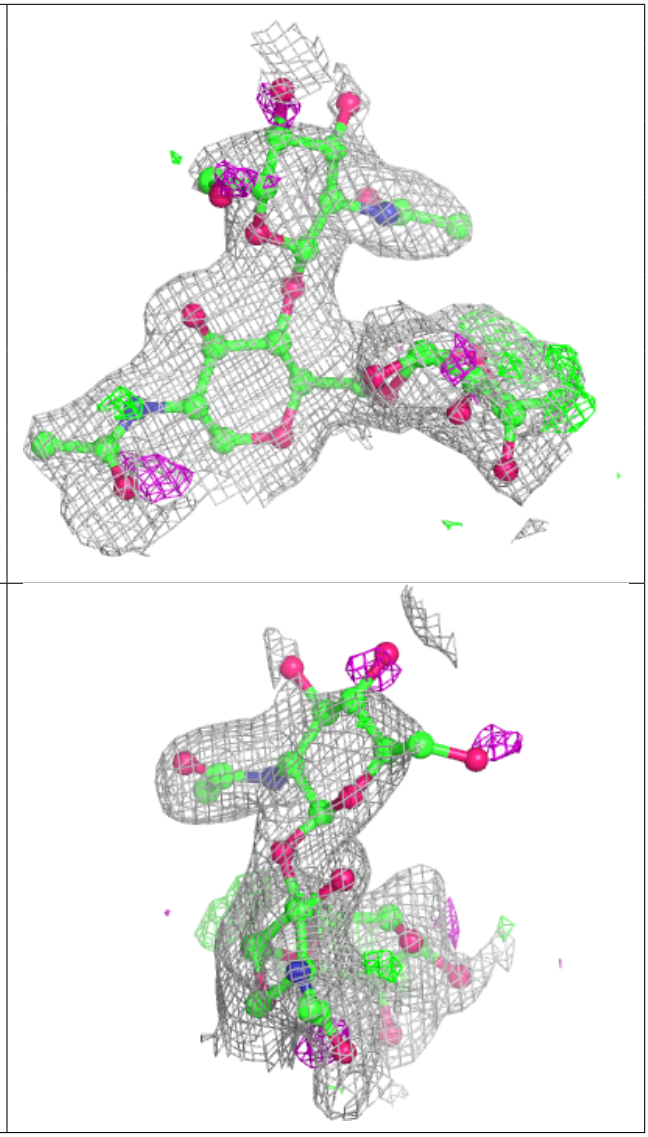






Electron density around Chain H:

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



6.4 Ligands (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
3	NAG	C	522	14/15	0.49	0.44	57,61,62,62	0
3	NAG	D	522	14/15	0.51	0.48	59,63,64,65	0
4	CIT	B	526	13/13	0.59	0.39	61,64,67,68	0
4	CIT	A	526	13/13	0.63	0.40	63,66,68,69	0
4	CIT	C	526	13/13	0.65	0.39	65,68,70,70	0
4	CIT	D	526	13/13	0.66	0.47	79,82,83,84	0
3	NAG	A	522	14/15	0.70	0.32	51,54,56,57	0

Continued on next page...

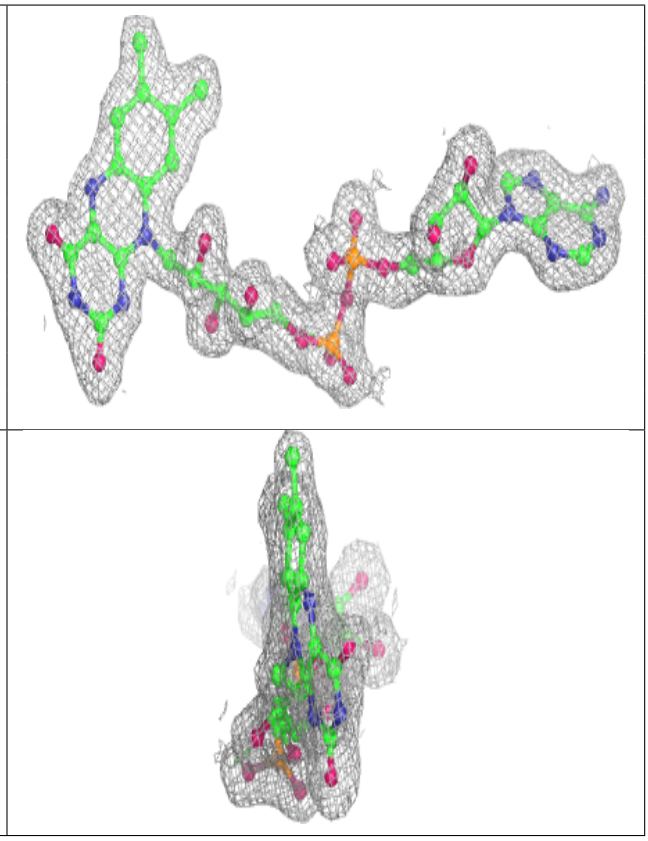
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	B	522	14/15	0.73	0.26	52,54,57,57	0
5	FAD	A	527	53/53	0.98	0.08	13,14,16,17	0
5	FAD	B	527	53/53	0.98	0.08	10,13,15,16	0
5	FAD	C	527	53/53	0.98	0.08	10,12,15,16	0
5	FAD	D	527	53/53	0.98	0.09	11,14,16,18	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.

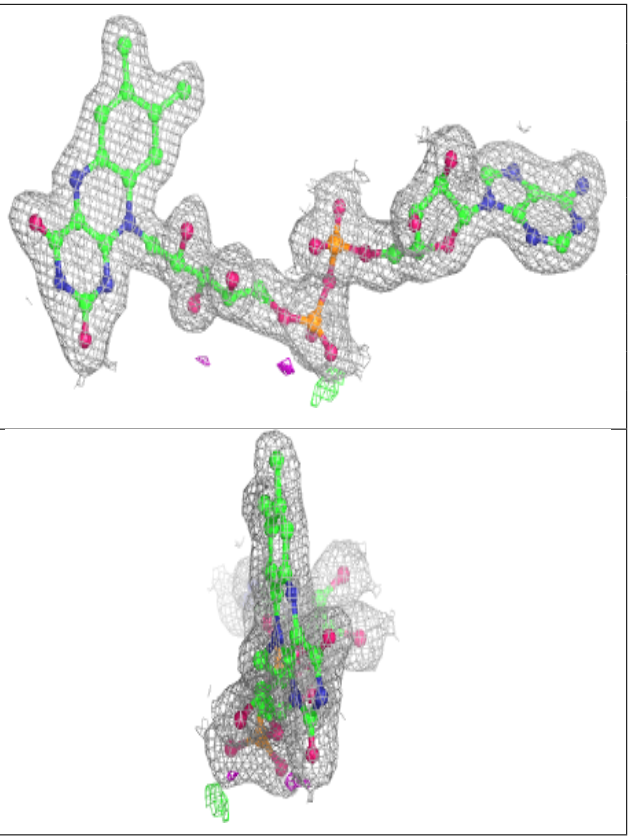
Electron density around FAD A 527:

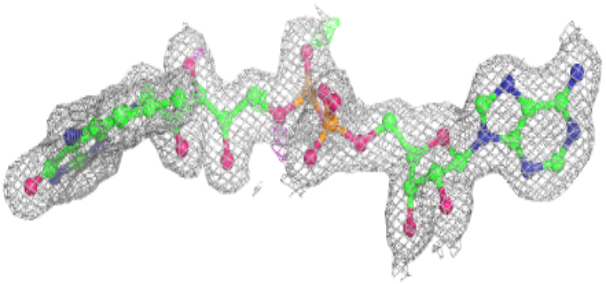
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)



Electron density around FAD B 527:

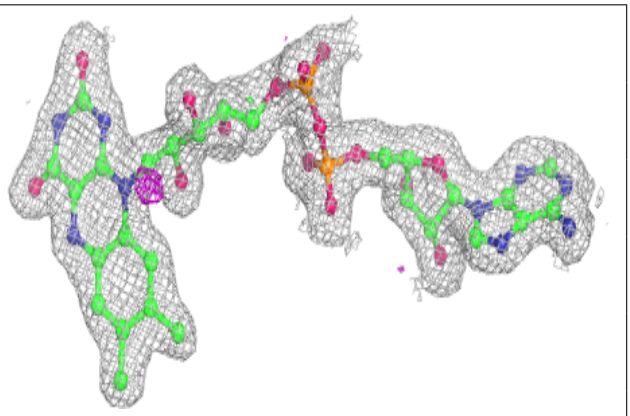
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

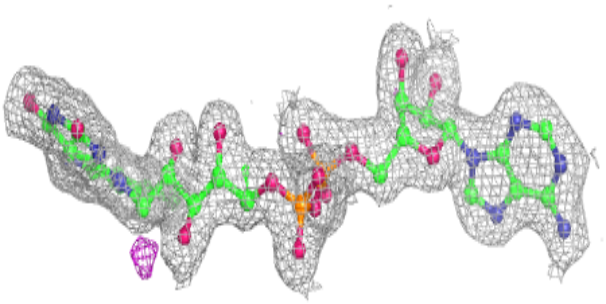


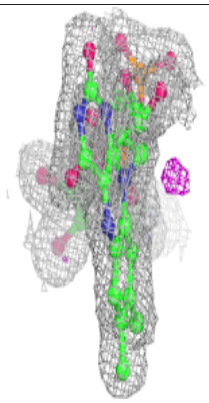


Electron density around FAD C 527:

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

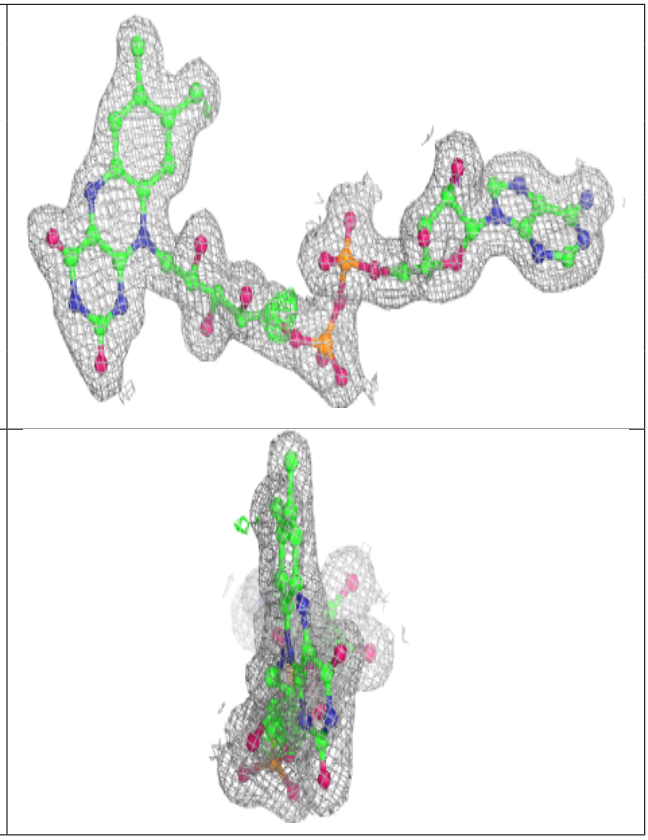






Electron density around FAD D 527:

$2mF_o$-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.