



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:19 AM UTC

PDB ID : 1B37 / pdb_00001b37
Title : A 30 ANGSTROM U-SHAPED CATALYTIC TUNNEL IN THE CRYSTAL
STRUCTURE OF POLYAMINE OXIDASE
Authors : Binda, C.; Coda, A.; Angelini, R.; Federico, R.; Ascenzi, P.; Mattevi, A.
Deposited on : 1998-12-17
Resolution : 1.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

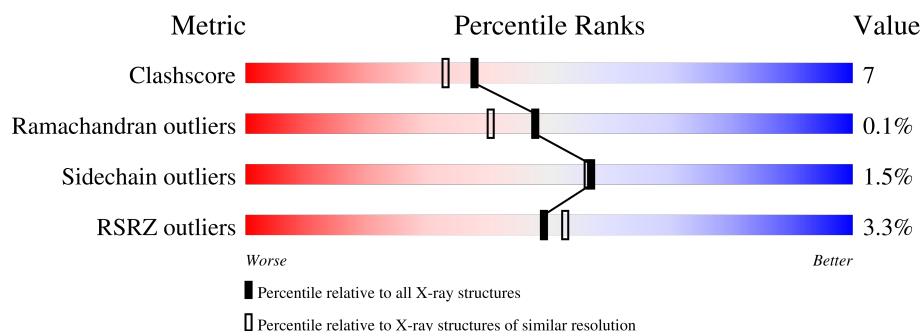
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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

Mol	Chain	Length	Quality of chain
1	A	472	4% 74% 20% • •
1	B	472	4% 78% 18% • •
1	C	472	2% 82% 15% • •
2	D	2	100%
2	E	2	50% 50%
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 criteria:

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

2 Entry composition [i](#)

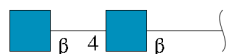
There are 5 unique types of molecules in this entry. The entry contains 12067 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PROTEIN (POLYAMINE OXIDASE).

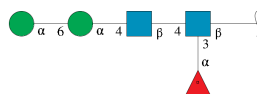
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	459	Total	C	N	O	S	57	0	0
			3684	2353	621	696	14			
1	B	462	Total	C	N	O	S	59	0	0
			3715	2374	627	700	14			
1	C	462	Total	C	N	O	S	55	0	0
			3715	2374	627	700	14			

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



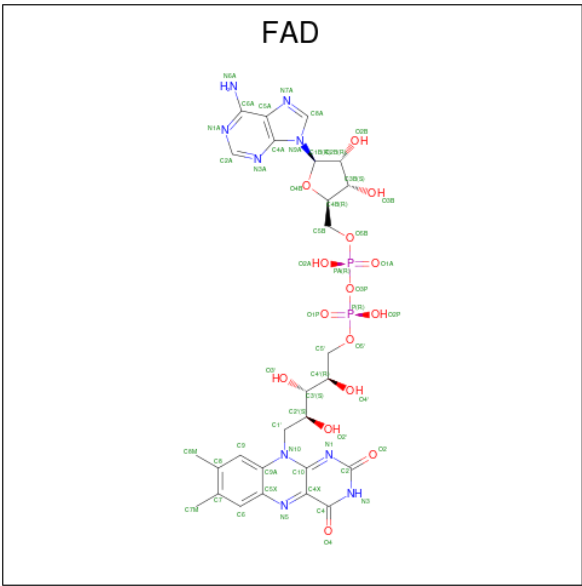
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			

- 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
3	F	5	Total	C	N	O	0	0	0
			60	34	2	24			

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



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

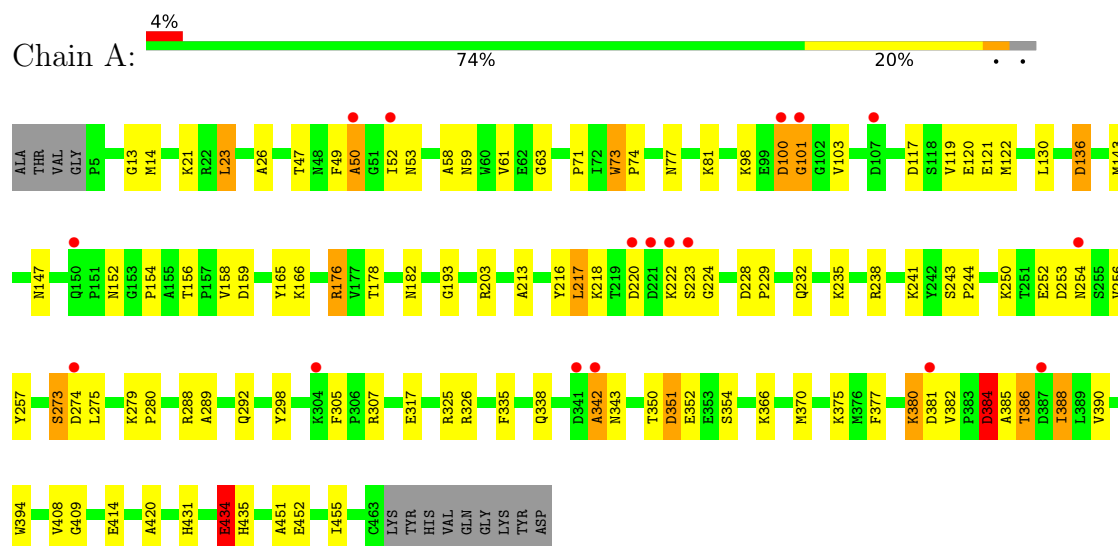
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	209	Total	O	0	0
			209	209		
5	B	220	Total	O	0	0
			220	220		
5	C	249	Total	O	0	0
			249	249		

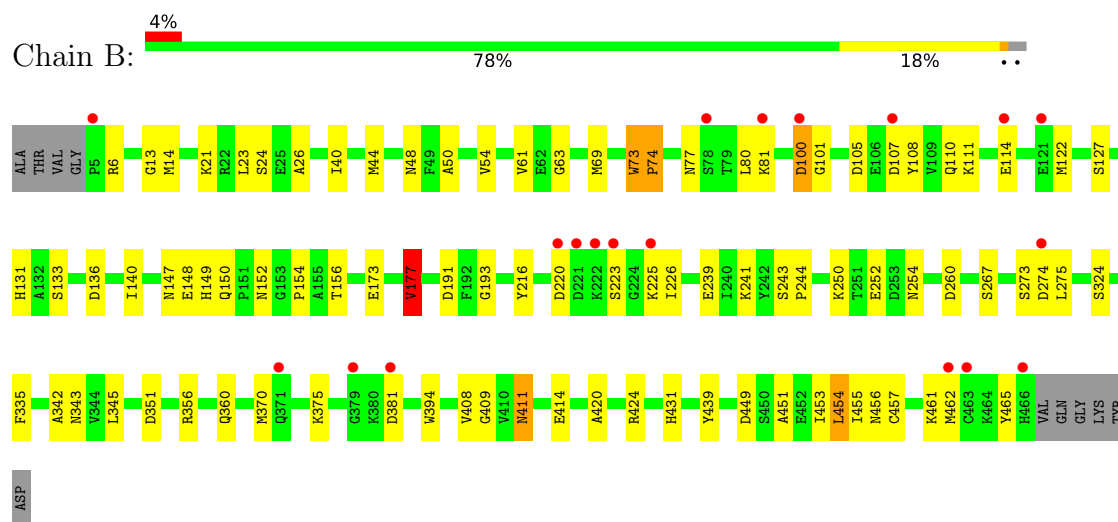
3 Residue-property plots

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

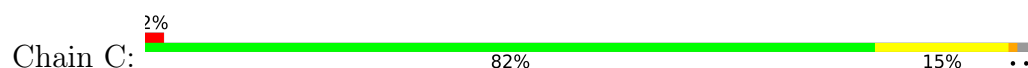
• Molecule 1: PROTEIN (POLYAMINE OXIDASE)

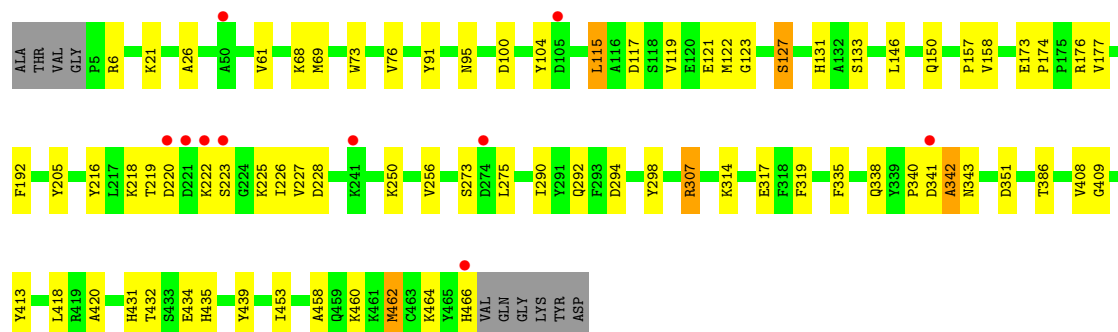


• Molecule 1: PROTEIN (POLYAMINE OXIDASE)

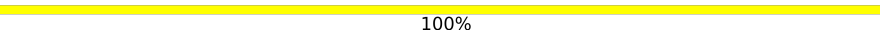


• Molecule 1: PROTEIN (POLYAMINE OXIDASE)





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

Chain D:  100%



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

Chain E:  50%



- 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:  40%



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	184.80Å 184.80Å 282.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 1.90 50.00 – 1.91	Depositor EDS
% Data completeness (in resolution range)	98.0 (50.00-1.90) 98.5 (50.00-1.91)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.43 (at 1.91Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.199 , (Not available) 0.188 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	19.8	Xtriage
Anisotropy	0.023	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 56.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12067	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.12% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, FCA, MAN, 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	0.89	2/3775 (0.1%)	1.62	46/5116 (0.9%)
1	B	0.88	3/3808 (0.1%)	1.62	45/5160 (0.9%)
1	C	0.90	1/3808 (0.0%)	1.62	42/5160 (0.8%)
All	All	0.89	6/11391 (0.1%)	1.62	133/15436 (0.9%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	1	0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	370	MET	SD-CE	6.20	1.95	1.79
1	B	149	HIS	CA-C	-6.04	1.46	1.53
1	C	462	MET	SD-CE	-5.70	1.65	1.79
1	A	14	MET	SD-CE	5.58	1.93	1.79
1	A	382	VAL	CA-C	-5.41	1.48	1.53
1	B	149	HIS	CA-CB	-5.33	1.45	1.53

All (133) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	420	ALA	N-CA-C	10.72	123.26	109.64
1	C	340	PRO	CA-C-N	-10.69	105.55	122.65
1	C	340	PRO	C-N-CA	-10.69	105.55	122.65
1	B	177	VAL	N-CA-CB	-9.73	101.50	112.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	342	ALA	N-CA-C	9.30	122.61	111.82
1	A	101	GLY	N-CA-C	9.20	134.97	113.18
1	C	273	SER	CA-C-N	-9.03	108.19	122.73
1	C	273	SER	C-N-CA	-9.03	108.19	122.73
1	A	61	VAL	N-CA-C	-8.87	95.05	107.99
1	A	273	SER	CA-C-N	-8.71	109.31	124.82
1	A	273	SER	C-N-CA	-8.71	109.31	124.82
1	B	149	HIS	CB-CA-C	-8.26	100.06	112.11
1	B	61	VAL	N-CA-C	-8.09	96.18	107.99
1	C	307	ARG	NE-CZ-NH1	-7.91	113.59	121.50
1	A	136	ASP	CB-CA-C	-7.72	97.67	110.72
1	C	61	VAL	N-CA-C	-7.71	96.03	107.51
1	B	465	TYR	N-CA-C	7.46	122.60	111.04
1	C	176	ARG	CA-C-N	-7.42	112.81	122.16
1	C	176	ARG	C-N-CA	-7.42	112.81	122.16
1	B	13	GLY	N-CA-C	-7.24	101.55	112.41
1	C	335	PHE	N-CA-C	7.04	121.83	112.25
1	B	409	GLY	CA-C-N	-6.91	114.23	122.93
1	B	409	GLY	C-N-CA	-6.91	114.23	122.93
1	C	307	ARG	CD-NE-CZ	-6.84	114.82	124.40
1	C	409	GLY	N-CA-C	-6.78	106.33	113.58
1	A	381	ASP	CA-C-N	-6.76	117.72	122.59
1	A	381	ASP	C-N-CA	-6.76	117.72	122.59
1	B	73	TRP	N-CA-C	6.71	121.97	113.25
1	A	77	ASN	N-CA-C	6.64	120.60	112.23
1	B	351	ASP	N-CA-CB	-6.62	99.29	110.49
1	A	224	GLY	N-CA-C	-6.60	106.22	115.32
1	C	26	ALA	N-CA-C	-6.49	105.11	113.16
1	B	356	ARG	CA-C-O	6.46	127.35	120.70
1	A	384	ASP	CB-CA-C	-6.37	98.23	109.62
1	A	390	VAL	CA-C-O	-6.34	116.57	120.88
1	C	317	GLU	N-CA-C	6.22	118.57	111.11
1	C	115	LEU	N-CA-CB	-6.19	101.00	110.16
1	A	351	ASP	N-CA-CB	-6.16	100.08	110.49
1	B	420	ALA	N-CA-C	6.14	117.44	109.64
1	A	335	PHE	N-CA-C	6.09	121.19	111.81
1	A	408	VAL	CA-C-N	-6.08	116.86	123.30
1	A	408	VAL	C-N-CA	-6.08	116.86	123.30
1	C	307	ARG	NE-CZ-NH2	6.07	124.67	119.20
1	C	76	VAL	N-CA-C	6.07	116.24	110.53
1	B	136	ASP	CB-CA-C	-6.06	101.27	111.02
1	C	338	GLN	N-CA-C	6.04	117.66	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	317	GLU	N-CA-C	6.02	117.85	111.28
1	A	73	TRP	CA-C-O	5.99	124.60	118.73
1	C	150	GLN	CB-CA-C	-5.98	100.70	109.97
1	C	408	VAL	CA-C-N	-5.98	116.96	123.30
1	C	408	VAL	C-N-CA	-5.98	116.96	123.30
1	A	380	LYS	CA-C-N	-5.97	114.55	122.85
1	A	380	LYS	C-N-CA	-5.97	114.55	122.85
1	A	434	GLU	N-CA-C	5.86	117.67	111.28
1	C	458	ALA	N-CA-C	5.86	117.74	111.36
1	C	177	VAL	N-CA-C	-5.85	107.06	113.43
1	C	205	TYR	N-CA-C	-5.81	105.03	111.71
1	C	351	ASP	N-CA-C	5.76	117.06	108.31
1	B	226	ILE	N-CA-C	-5.66	101.52	109.21
1	B	149	HIS	CA-CB-CG	-5.65	108.15	113.80
1	B	324	SER	N-CA-C	-5.63	106.36	113.18
1	C	409	GLY	CA-C-N	-5.62	115.85	122.93
1	C	409	GLY	C-N-CA	-5.62	115.85	122.93
1	B	6	ARG	N-CA-C	-5.62	100.54	109.59
1	C	104	TYR	N-CA-C	-5.62	103.29	110.53
1	C	275	LEU	N-CA-C	5.58	117.80	111.11
1	A	178	THR	N-CA-C	5.58	119.01	110.20
1	B	54	VAL	N-CA-C	-5.56	101.07	108.96
1	A	381	ASP	N-CA-C	-5.55	97.43	107.75
1	C	174	PRO	CB-CA-C	-5.54	104.16	110.92
1	A	298	TYR	N-CA-CB	-5.54	102.08	110.77
1	C	439	TYR	N-CA-C	5.53	118.27	110.14
1	B	44	MET	N-CA-C	-5.51	98.23	107.99
1	B	173	GLU	N-CA-C	-5.51	101.85	108.25
1	A	342	ALA	N-CA-C	5.51	119.26	112.54
1	B	267	SER	N-CA-C	5.50	117.42	110.33
1	A	26	ALA	N-CA-C	-5.48	106.44	113.02
1	A	338	GLN	N-CA-C	5.48	117.06	111.14
1	B	345	LEU	N-CA-C	-5.48	101.03	109.52
1	B	191	ASP	N-CA-C	5.46	118.41	111.69
1	A	156	THR	N-CA-C	-5.46	103.04	110.36
1	B	101	GLY	N-CA-C	5.45	126.09	113.18
1	A	386	THR	N-CA-CB	-5.45	101.92	110.30
1	A	100	ASP	CA-C-N	5.40	132.00	121.41
1	A	100	ASP	C-N-CA	5.40	132.00	121.41
1	A	414	GLU	CA-CB-CG	-5.39	103.33	114.10
1	C	432	THR	N-CA-C	-5.37	105.37	112.94
1	A	275	LEU	N-CA-C	-5.37	105.43	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	115	LEU	CB-CG-CD1	-5.34	94.67	110.70
1	B	335	PHE	N-CA-C	5.32	120.00	111.81
1	C	146	LEU	N-CA-C	-5.31	105.39	111.07
1	C	100	ASP	N-CA-C	5.31	118.77	112.72
1	A	305	PHE	CA-C-N	5.30	124.92	119.56
1	A	305	PHE	C-N-CA	5.30	124.92	119.56
1	A	289	ALA	N-CA-C	-5.30	105.58	111.36
1	B	147	ASN	CA-C-N	-5.30	113.09	122.26
1	B	147	ASN	C-N-CA	-5.30	113.09	122.26
1	B	177	VAL	N-CA-C	-5.30	107.65	113.43
1	A	288	ARG	CA-CB-CG	-5.27	103.56	114.10
1	C	192	PHE	N-CA-C	5.25	119.68	113.28
1	B	140	ILE	N-CA-C	-5.22	105.29	110.62
1	B	14	MET	N-CA-C	5.21	116.96	111.28
1	B	456	ASN	CB-CA-C	-5.18	102.18	110.79
1	B	50	ALA	CA-C-N	-5.18	112.67	122.05
1	B	50	ALA	C-N-CA	-5.18	112.67	122.05
1	C	413	TYR	N-CA-C	-5.18	105.52	111.07
1	B	156	THR	N-CA-C	-5.17	103.63	110.40
1	A	182	ASN	N-CA-C	5.16	119.26	112.92
1	B	461	LYS	CB-CA-C	5.15	119.64	111.51
1	A	388	ILE	CA-C-N	-5.13	115.53	122.77
1	A	388	ILE	C-N-CA	-5.13	115.53	122.77
1	B	408	VAL	N-CA-C	-5.12	102.97	109.58
1	A	71	PRO	CA-C-N	-5.12	112.24	120.64
1	A	71	PRO	C-N-CA	-5.12	112.24	120.64
1	B	439	TYR	N-CA-C	5.12	117.45	109.52
1	B	122	MET	N-CA-C	-5.11	105.84	111.71
1	A	13	GLY	N-CA-C	-5.11	104.75	112.41
1	C	95	ASN	N-CA-C	5.10	117.41	110.88
1	B	148	GLU	N-CA-C	-5.10	107.11	113.38
1	A	176	ARG	CB-CG-CD	-5.09	99.59	111.30
1	A	409	GLY	N-CA-C	-5.09	108.13	113.58
1	B	275	LEU	N-CA-C	-5.08	105.82	111.36
1	A	420	ALA	N-CA-C	5.07	116.96	109.50
1	C	68	LYS	N-CA-C	-5.07	101.67	109.52
1	B	100	ASP	CB-CA-C	5.06	120.49	110.42
1	C	341	ASP	N-CA-C	5.04	119.12	112.92
1	B	108	TYR	N-CA-C	-5.04	105.67	111.07
1	B	77	ASN	N-CA-C	5.03	119.41	113.28
1	B	122	MET	CA-C-N	-5.03	113.83	120.22
1	B	122	MET	C-N-CA	-5.03	113.83	120.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	298	TYR	N-CA-CB	-5.03	102.58	110.77
1	A	50	ALA	CB-CA-C	-5.01	104.62	111.73
1	B	381	ASP	N-CA-CB	5.01	118.92	110.46

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	C	386	THR	CB

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	3584	59	0
1	B	3715	0	3614	56	1
1	C	3715	0	3613	39	0
2	D	28	0	25	0	0
2	E	28	0	25	0	1
3	F	60	0	52	4	0
4	A	53	0	31	1	0
4	B	53	0	31	0	0
4	C	53	0	31	0	0
5	A	209	0	0	2	1
5	B	220	0	0	3	1
5	C	249	0	0	4	3
All	All	12067	0	11006	152	4

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 7.

All (152) 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	1.35	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69:MET:CE	1:B:73:TRP:HB3	1.94	0.97
1:C:91:TYR:OH	1:C:314:LYS:HE2	1.70	0.92
1:B:69:MET:CE	1:B:74:PRO:HD3	2.01	0.90
1:C:131:HIS:CD2	1:C:133:SER:H	1.89	0.89
1:B:69:MET:HE1	1:B:73:TRP:CD1	2.07	0.89
3:F:1:NAG:C4	3:F:2:NAG:C1	2.51	0.89
1:B:69:MET:HE1	1:B:73:TRP:HD1	1.38	0.88
1:B:69:MET:HE3	1:B:73:TRP:HB3	1.58	0.85
1:A:273:SER:O	1:A:274:ASP:HB2	1.77	0.83
1:B:69:MET:HE2	1:B:74:PRO:CD	2.09	0.82
1:B:411:ASN:ND2	1:B:414:GLU:H	1.85	0.75
1:C:292:GLN:OE1	5:C:1019:HOH:O	2.02	0.75
1:A:431:HIS:CD2	1:A:431:HIS:H	2.03	0.75
1:B:131:HIS:CD2	1:B:133:SER:H	2.05	0.74
1:B:131:HIS:HD2	1:B:133:SER:H	1.37	0.72
1:C:131:HIS:HD2	1:C:133:SER:H	1.34	0.72
1:A:119:VAL:HA	1:A:122:MET:HE3	1.73	0.71
1:B:114:GLU:HA	1:B:114:GLU:OE1	1.91	0.70
1:C:117:ASP:O	1:C:121:GLU:HG3	1.91	0.70
1:B:220:ASP:HB3	1:B:223:SER:OG	1.92	0.70
1:A:130:LEU:HD22	1:A:136:ASP:HB2	1.76	0.68
1:A:394:TRP:HE1	1:B:152:ASN:ND2	1.93	0.65
1:A:434:GLU:HG2	1:A:435:HIS:CD2	2.31	0.65
1:B:411:ASN:HD22	1:B:414:GLU:H	1.45	0.65
1:C:119:VAL:HA	1:C:122:MET:HE3	1.78	0.64
1:A:370:MET:HE2	1:A:384:ASP:HA	1.79	0.63
1:A:73:TRP:HB3	1:A:74:PRO:HD3	1.81	0.63
1:A:216:TYR:CD1	1:A:217:LEU:HD13	2.33	0.63
1:A:229:PRO:O	1:A:232:GLN:NE2	2.32	0.62
1:C:220:ASP:HB3	1:C:223:SER:OG	2.00	0.62
1:B:431:HIS:H	1:B:431:HIS:CD2	2.18	0.61
1:C:220:ASP:OD2	1:C:222:LYS:N	2.35	0.60
3:F:1:NAG:H4	3:F:2:NAG:C1	2.33	0.58
1:B:69:MET:HE1	1:B:73:TRP:HB3	1.83	0.58
1:B:241:LYS:HE3	1:B:250:LYS:HE3	1.84	0.58
1:C:431:HIS:H	1:C:431:HIS:CD2	2.19	0.58
1:B:243:SER:HB2	1:B:244:PRO:CD	2.34	0.58
1:A:366:LYS:HD2	1:A:385:ALA:HB3	1.86	0.57
1:C:131:HIS:HD2	1:C:133:SER:OG	1.87	0.57
1:C:250:LYS:HG2	1:C:256:VAL:HG22	1.86	0.57
1:A:216:TYR:CE1	1:A:217:LEU:HD13	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:243:SER:HB2	1:B:244:PRO:HD2	1.88	0.56
1:B:81:LYS:NZ	1:B:81:LYS:HB3	2.21	0.55
1:C:460:LYS:HB3	1:C:462:MET:HE2	1.89	0.54
1:A:220:ASP:HB3	1:A:223:SER:OG	2.08	0.54
1:A:292:GLN:OE1	5:A:1029:HOH:O	2.19	0.53
1:B:457:CYS:HA	1:B:462:MET:O	2.09	0.53
1:C:342:ALA:O	1:C:343:ASN:HB2	2.09	0.53
1:B:449:ASP:O	1:B:453:ILE:HG13	2.08	0.52
1:C:131:HIS:CD2	1:C:133:SER:OG	2.62	0.52
1:C:91:TYR:HH	1:C:314:LYS:HE2	1.72	0.52
1:C:131:HIS:HD2	1:C:133:SER:CB	2.23	0.52
1:A:152:ASN:ND2	1:B:394:TRP:HE1	2.08	0.51
1:A:394:TRP:HE1	1:B:152:ASN:HD22	1.57	0.51
1:C:219:THR:HG22	1:C:226:ILE:HA	1.93	0.51
1:A:58:ALA:HA	4:A:800:FAD:C4X	2.41	0.51
1:B:451:ALA:O	1:B:455:ILE:HG13	2.11	0.51
1:C:464:LYS:HG2	1:C:466:HIS:O	2.10	0.51
1:B:100:ASP:OD2	1:B:375:LYS:NZ	2.43	0.51
1:C:131:HIS:HD2	1:C:133:SER:N	2.07	0.51
1:A:63:GLY:HA2	1:A:193:GLY:O	2.11	0.51
1:B:273:SER:O	1:B:274:ASP:HB2	2.11	0.50
1:A:218:LYS:H	1:A:228:ASP:HB2	1.77	0.50
1:A:220:ASP:OD1	1:A:222:LYS:N	2.44	0.50
1:A:243:SER:HB2	1:A:244:PRO:CD	2.40	0.50
1:B:131:HIS:HD2	1:B:133:SER:OG	1.95	0.50
1:B:360:GLN:NE2	5:B:934:HOH:O	2.44	0.50
1:A:23:LEU:HD13	1:A:451:ALA:HB1	1.93	0.49
1:B:114:GLU:OE1	5:B:1063:HOH:O	2.19	0.49
1:A:241:LYS:HE3	1:A:250:LYS:HE3	1.95	0.49
1:B:80:LEU:O	1:B:81:LYS:HB2	2.12	0.49
1:A:431:HIS:CD2	5:A:880:HOH:O	2.65	0.49
1:A:120:GLU:OE1	1:A:166:LYS:NZ	2.32	0.49
1:A:49:PHE:O	1:A:50:ALA:HB3	2.12	0.48
1:A:152:ASN:HD22	1:B:394:TRP:HE1	1.59	0.48
1:C:218:LYS:H	1:C:228:ASP:HB2	1.79	0.48
1:B:411:ASN:HD21	1:B:414:GLU:HG3	1.79	0.48
1:B:411:ASN:HD22	1:B:411:ASN:C	2.22	0.48
1:C:307:ARG:NH1	5:C:957:HOH:O	2.28	0.48
1:B:131:HIS:CD2	1:B:133:SER:OG	2.67	0.47
1:B:342:ALA:O	1:B:343:ASN:HB2	2.15	0.47
1:C:218:LYS:O	1:C:227:VAL:N	2.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:219:THR:HA	1:C:225:LYS:O	2.14	0.46
1:A:273:SER:O	1:A:274:ASP:CB	2.42	0.46
1:A:434:GLU:O	1:A:434:GLU:HG3	2.14	0.46
1:C:131:HIS:CD2	1:C:133:SER:CB	2.99	0.46
1:C:220:ASP:OD2	1:C:222:LYS:HB3	2.15	0.46
1:A:143:MET:SD	1:A:147:ASN:ND2	2.90	0.45
1:A:213:ALA:O	1:A:217:LEU:HB2	2.17	0.45
1:A:434:GLU:HG2	1:A:435:HIS:NE2	2.31	0.45
1:B:63:GLY:HA2	1:B:193:GLY:O	2.16	0.45
1:B:131:HIS:HD2	1:B:133:SER:CB	2.30	0.45
1:A:307:ARG:NH1	1:A:307:ARG:HG2	2.31	0.45
1:A:81:LYS:O	1:A:203:ARG:NH2	2.50	0.45
1:A:388:ILE:HD13	1:A:388:ILE:HG21	1.74	0.45
1:A:176:ARG:HD2	1:B:177:VAL:HG21	1.98	0.44
1:C:173:GLU:OE1	1:C:294:ASP:OD2	2.35	0.44
1:B:150:GLN:NE2	5:B:932:HOH:O	2.50	0.44
1:A:238:ARG:NH1	1:A:252:GLU:OE2	2.48	0.44
1:A:73:TRP:N	1:A:74:PRO:CD	2.81	0.44
1:B:252:GLU:C	1:B:254:ASN:H	2.26	0.44
1:B:114:GLU:OE1	1:B:114:GLU:CA	2.61	0.44
1:C:69:MET:HE2	1:C:69:MET:HB2	1.81	0.44
1:B:107:ASP:O	1:B:111:LYS:HG3	2.18	0.44
1:A:307:ARG:HG2	1:A:307:ARG:HH11	1.83	0.43
1:C:453:ILE:HA	1:C:453:ILE:HD13	1.62	0.43
1:B:69:MET:HE2	1:B:74:PRO:CG	2.48	0.43
1:C:158:VAL:HG12	5:C:995:HOH:O	2.17	0.43
1:B:110:GLN:O	1:B:114:GLU:HG2	2.17	0.43
1:A:243:SER:CB	1:A:244:PRO:CD	2.97	0.43
1:A:47:THR:O	1:A:53:ASN:HA	2.19	0.43
3:F:1:NAG:H3	3:F:5:FCA:O2	2.18	0.43
1:C:6:ARG:HH11	1:C:6:ARG:HG3	1.84	0.43
1:C:290:ILE:HA	1:C:418:LEU:HD21	2.01	0.42
1:C:431:HIS:CD2	5:C:810:HOH:O	2.72	0.42
1:B:23:LEU:O	1:B:24:SER:C	2.58	0.42
1:B:454:LEU:HD12	1:B:454:LEU:C	2.44	0.42
1:A:98:LYS:HE3	1:A:103:VAL:O	2.18	0.42
1:A:279:LYS:HA	1:A:280:PRO:C	2.43	0.42
1:B:81:LYS:NZ	1:B:81:LYS:CB	2.82	0.42
1:A:350:THR:HA	1:A:354:SER:OG	2.19	0.42
1:C:21:LYS:HB2	1:C:216:TYR:CE2	2.55	0.42
1:A:256:VAL:HG12	1:A:257:TYR:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:243:SER:CB	1:B:244:PRO:CD	2.95	0.42
1:B:223:SER:HB2	1:B:225:LYS:HG3	2.00	0.42
1:B:26:ALA:HB2	1:B:455:ILE:HD13	2.02	0.42
1:A:342:ALA:O	1:A:343:ASN:HB2	2.21	0.41
1:A:235:LYS:NZ	1:A:253:ASP:OD2	2.38	0.41
1:B:40:ILE:HD13	1:B:40:ILE:HG21	1.66	0.41
1:B:220:ASP:CB	1:B:223:SER:OG	2.64	0.41
1:B:239:GLU:OE2	1:B:241:LYS:HE2	2.20	0.41
1:A:351:ASP:CG	1:A:352:GLU:H	2.29	0.41
1:A:253:ASP:O	1:A:254:ASN:HB2	2.20	0.41
1:A:165:TYR:CD2	1:A:165:TYR:C	2.97	0.41
1:B:21:LYS:HB2	1:B:216:TYR:CE2	2.55	0.41
1:A:49:PHE:N	1:A:52:ILE:O	2.38	0.41
1:A:158:VAL:HG13	1:A:159:ASP:N	2.36	0.41
1:A:325:ARG:O	1:A:326:ARG:C	2.63	0.41
1:A:377:PHE:HB3	1:A:380:LYS:HG2	2.03	0.41
1:C:73:TRP:HE1	3:F:1:NAG:C7	2.34	0.41
1:C:218:LYS:N	1:C:228:ASP:HB2	2.36	0.41
1:A:117:ASP:O	1:A:121:GLU:HG3	2.21	0.40
1:A:452:GLU:HA	1:A:455:ILE:HD12	2.02	0.40
1:A:100:ASP:OD1	1:A:375:LYS:HE2	2.21	0.40
1:C:386:THR:H	1:C:386:THR:HG22	1.62	0.40
1:A:21:LYS:HB2	1:A:216:TYR:CE2	2.56	0.40
1:A:217:LEU:HD12	1:A:217:LEU:HA	1.77	0.40
1:C:418:LEU:HD23	1:C:418:LEU:HA	1.93	0.40
1:C:434:GLU:CG	1:C:435:HIS:CD2	3.04	0.40
1:B:260:ASP:O	1:B:424:ARG:HD3	2.21	0.40
1:C:123:GLY:O	1:C:127:SER:HB2	2.21	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:928:HOH:O	5:C:928:HOH:O[10_665]	0.94	1.26
5:B:943:HOH:O	5:C:1014:HOH:O[10_665]	1.82	0.38
5:A:1038:HOH:O	5:C:1017:HOH:O[8_665]	2.16	0.04
1:B:48:ASN:ND2	2:E:2:NAG:C8[9_765]	2.18	0.02

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	457/472 (97%)	438 (96%)	18 (4%)	1 (0%)	43	36
1	B	460/472 (98%)	442 (96%)	18 (4%)	0	100	100
1	C	460/472 (98%)	443 (96%)	17 (4%)	0	100	100
All	All	1377/1416 (97%)	1323 (96%)	53 (4%)	1 (0%)	48	40

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%)	387 (98%)	7 (2%)	51	50
1	B	397/404 (98%)	390 (98%)	7 (2%)	51	50
1	C	397/404 (98%)	393 (99%)	4 (1%)	68	70
All	All	1188/1212 (98%)	1170 (98%)	18 (2%)	57	56

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

Mol	Chain	Res	Type
1	A	23	LEU
1	A	59	ASN

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Mol	Chain	Res	Type
1	A	154	PRO
1	A	217	LEU
1	A	384	ASP
1	A	386	THR
1	A	434	GLU
1	B	74	PRO
1	B	105	ASP
1	B	127	SER
1	B	154	PRO
1	B	177	VAL
1	B	411	ASN
1	B	454	LEU
1	C	115	LEU
1	C	127	SER
1	C	157	PRO
1	C	319	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	ASN
1	A	152	ASN
1	A	359	GLN
1	A	360	GLN
1	A	431	HIS
1	A	437	ASN
1	B	131	HIS
1	B	149	HIS
1	B	150	GLN
1	B	152	ASN
1	B	182	ASN
1	B	277	GLN
1	B	360	GLN
1	B	411	ASN
1	B	431	HIS
1	B	437	ASN
1	C	48	ASN
1	C	131	HIS
1	C	359	GLN
1	C	360	GLN
1	C	431	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

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	1,2	14,14,15	1.34	1 (7%)	17,19,21	3.07	5 (29%)
2	NAG	D	2	2	14,14,15	0.82	0	17,19,21	2.90	5 (29%)
2	NAG	E	1	1,2	14,14,15	1.44	2 (14%)	17,19,21	2.44	7 (41%)
2	NAG	E	2	2	14,14,15	1.47	3 (21%)	17,19,21	3.05	6 (35%)
3	NAG	F	1	1,3	14,14,15	1.55	2 (14%)	17,19,21	4.31	11 (64%)
3	NAG	F	2	3	14,14,15	1.02	1 (7%)	17,19,21	1.81	5 (29%)
3	MAN	F	3	3	11,11,12	0.89	0	15,15,17	3.16	2 (13%)
3	MAN	F	4	3	11,11,12	0.78	0	15,15,17	1.36	2 (13%)
3	FCA	F	5	3	10,10,11	1.25	1 (10%)	14,14,16	2.27	7 (50%)

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	1/1/4/5	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 (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1	NAG	C1-C2	-4.11	1.46	1.52
3	F	1	NAG	C1-C2	-3.97	1.46	1.52
3	F	1	NAG	O5-C1	-3.71	1.37	1.43
2	E	2	NAG	O5-C1	-3.53	1.37	1.43
2	D	1	NAG	O5-C1	-3.41	1.38	1.43
3	F	2	NAG	O5-C1	-2.92	1.38	1.43
3	F	5	FCA	C2-C3	-2.67	1.48	1.52
2	E	1	NAG	O5-C1	-2.23	1.39	1.43
2	E	2	NAG	C6-C5	-2.14	1.44	1.51
2	E	2	NAG	C4-C5	2.11	1.57	1.53

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	3	MAN	O2-C2-C3	10.86	132.64	110.15
2	E	2	NAG	C1-O5-C5	10.83	126.70	112.19
3	F	1	NAG	C8-C7-N2	-10.19	99.21	116.12
3	F	1	NAG	O5-C5-C6	-8.04	92.02	107.66
2	D	2	NAG	C2-N2-C7	-8.01	112.16	122.90
3	F	1	NAG	C1-O5-C5	7.46	122.18	112.19
2	D	1	NAG	O5-C5-C6	-7.35	93.36	107.66
2	E	1	NAG	C1-O5-C5	6.99	121.56	112.19
2	D	1	NAG	C1-O5-C5	6.95	121.51	112.19
2	D	2	NAG	C1-O5-C5	6.05	120.29	112.19
3	F	1	NAG	O7-C7-C8	5.78	132.34	122.05
2	D	1	NAG	C6-C5-C4	5.15	125.66	113.02
3	F	3	MAN	O2-C2-C1	-4.25	99.50	109.22
3	F	5	FCA	O5-C5-C6	-4.22	98.24	107.40
2	E	1	NAG	O5-C5-C6	-4.19	99.50	107.66
3	F	2	NAG	O5-C5-C6	-3.83	100.20	107.66
3	F	5	FCA	C3-C4-C5	-3.79	104.05	109.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	2	NAG	C2-N2-C7	-3.75	117.87	122.90
3	F	1	NAG	O7-C7-N2	3.63	128.40	121.98
3	F	2	NAG	C1-O5-C5	3.62	117.04	112.19
2	D	1	NAG	O4-C4-C5	-3.45	100.84	109.32
2	D	2	NAG	C6-C5-C4	3.25	120.99	113.02
3	F	1	NAG	O5-C5-C4	-3.02	103.49	110.83
3	F	5	FCA	C1-C2-C3	3.01	114.03	109.64
3	F	5	FCA	O5-C1-C2	-2.95	103.75	110.79
3	F	4	MAN	C3-C4-C5	-2.87	105.02	110.23
3	F	1	NAG	O6-C6-C5	2.78	120.78	111.33
3	F	1	NAG	C4-C3-C2	2.75	115.05	111.02
3	F	5	FCA	C1-O5-C5	2.60	119.11	112.97
3	F	2	NAG	O4-C4-C5	-2.58	102.96	109.32
2	D	2	NAG	O5-C5-C6	2.49	112.50	107.66
3	F	1	NAG	C3-C4-C5	-2.39	105.90	110.23
3	F	4	MAN	C1-C2-C3	-2.39	106.17	109.64
2	D	2	NAG	O5-C5-C4	2.38	116.61	110.83
2	E	2	NAG	C6-C5-C4	2.36	118.83	113.02
2	E	2	NAG	O5-C5-C4	-2.36	105.08	110.83
2	E	1	NAG	C8-C7-N2	-2.33	112.25	116.12
2	E	2	NAG	O6-C6-C5	2.25	119.00	111.33
2	E	2	NAG	O4-C4-C5	2.22	114.80	109.32
3	F	5	FCA	O3-C3-C4	-2.21	105.16	110.38
2	E	1	NAG	C2-N2-C7	-2.21	119.94	122.90
3	F	5	FCA	O2-C2-C3	-2.20	105.59	110.15
2	E	1	NAG	O6-C6-C5	2.20	118.82	111.33
2	D	1	NAG	C8-C7-N2	-2.18	112.50	116.12
2	E	1	NAG	C6-C5-C4	2.18	118.37	113.02
2	E	1	NAG	C1-C2-N2	-2.11	107.11	110.43
3	F	2	NAG	O3-C3-C4	2.06	115.23	110.38
3	F	1	NAG	O5-C1-C2	-2.06	108.11	111.29
3	F	2	NAG	C1-C2-N2	-2.05	107.20	110.43
3	F	1	NAG	C6-C5-C4	2.04	118.03	113.02

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	F	3	MAN	C1

All (14) torsion outliers are listed below:

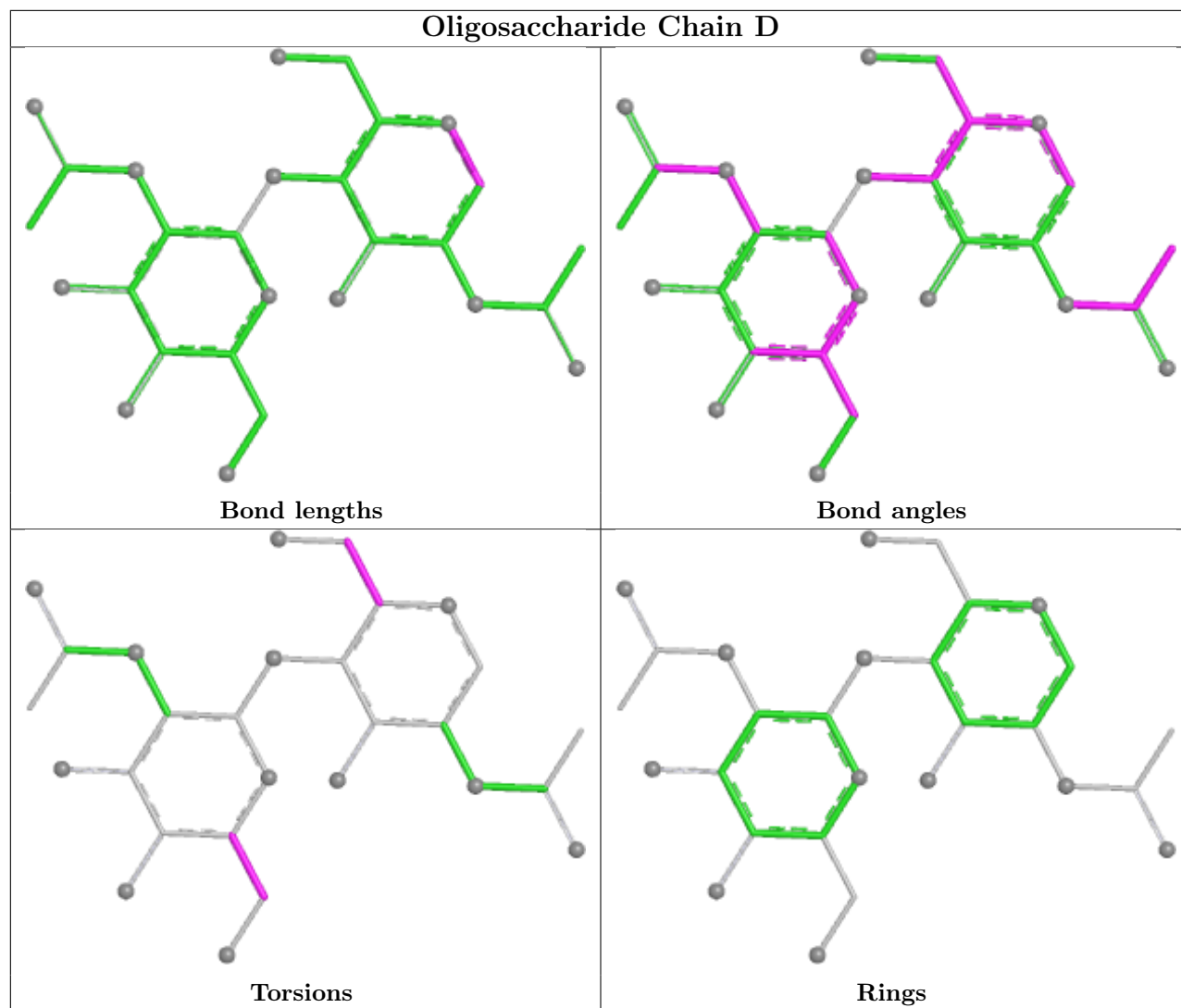
Mol	Chain	Res	Type	Atoms
3	F	1	NAG	C4-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6
2	E	1	NAG	C4-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
3	F	4	MAN	O5-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6
3	F	4	MAN	C4-C5-C6-O6
3	F	1	NAG	O5-C5-C6-O6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

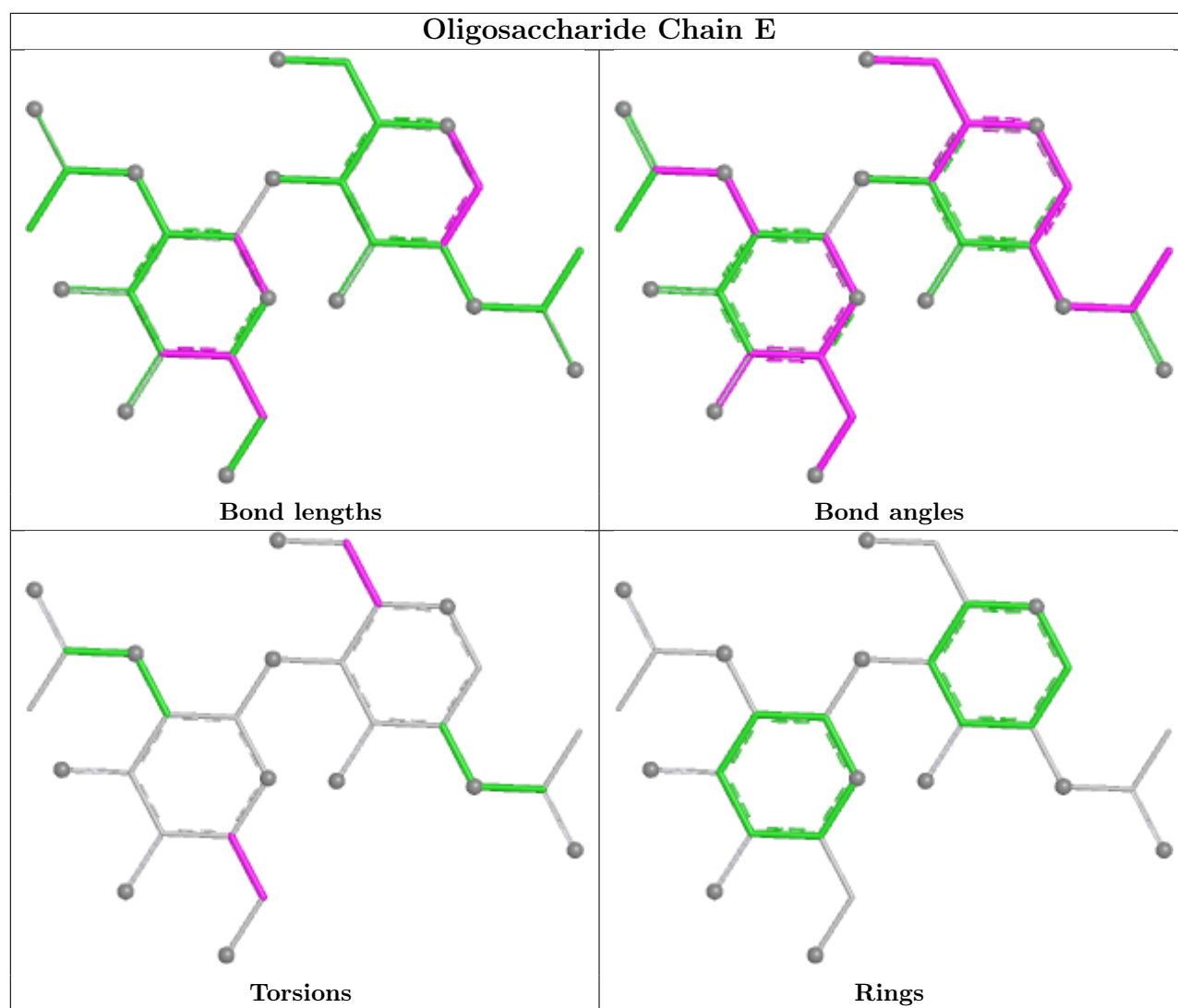
There are no ring outliers.

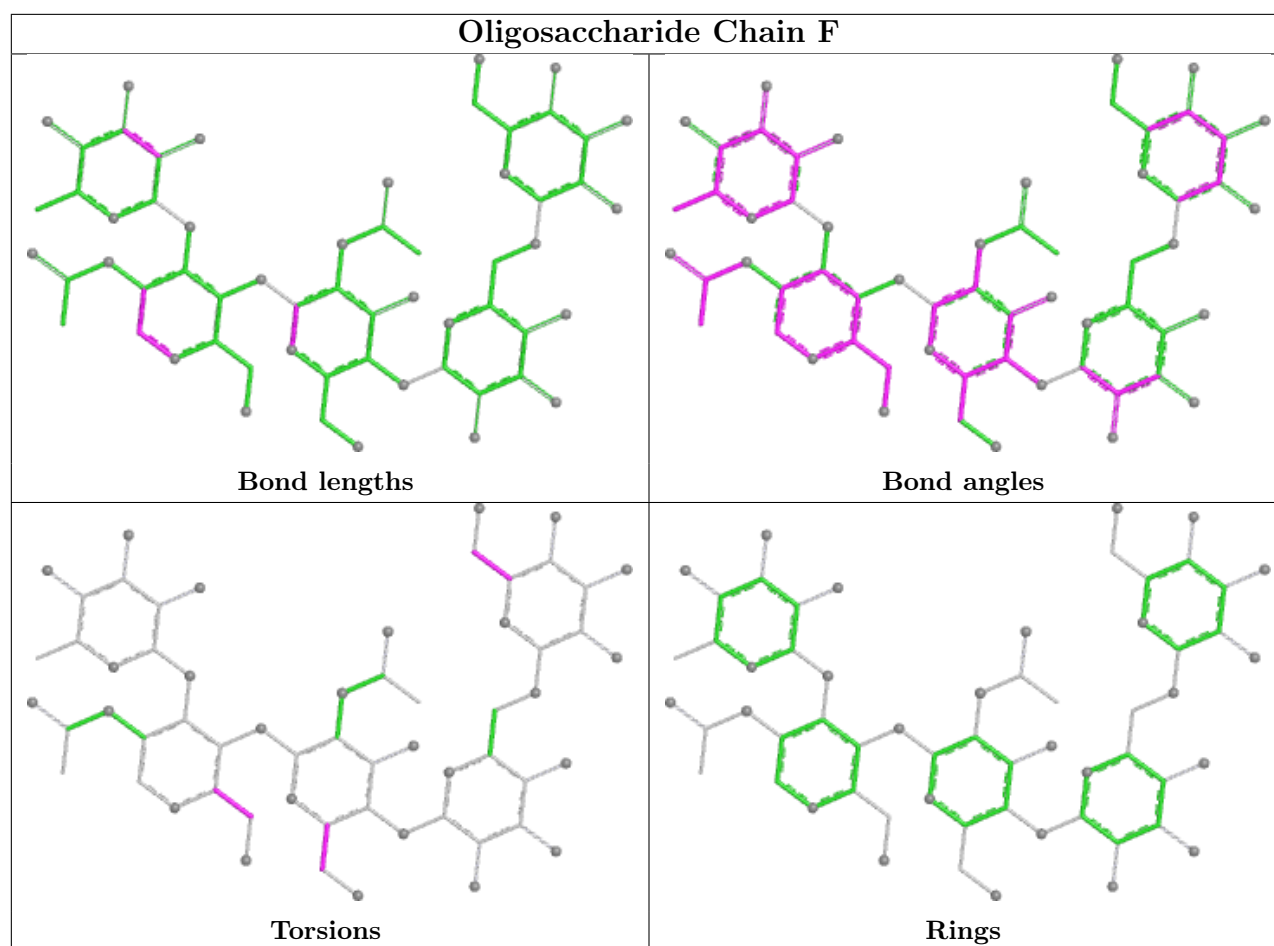
4 monomers are involved in 5 short contacts:

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

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







5.6 Ligand geometry [i](#)

3 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	FAD	B	801	-	58,58,58	1.01	3 (5%)	85,89,89	1.26	11 (12%)
4	FAD	A	800	-	58,58,58	1.04	7 (12%)	85,89,89	1.28	8 (9%)
4	FAD	C	802	-	58,58,58	1.27	8 (13%)	85,89,89	1.19	10 (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	FAD	B	801	-	-	5/34/50/50	0/6/6/6
4	FAD	A	800	-	-	1/34/50/50	0/6/6/6
4	FAD	C	802	-	-	1/34/50/50	0/6/6/6

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	802	FAD	PA-O3P	3.92	1.63	1.59
4	C	802	FAD	C4X-N5	3.74	1.38	1.30
4	B	801	FAD	PA-O3P	3.18	1.62	1.59
4	B	801	FAD	C4X-N5	2.99	1.37	1.30
4	B	801	FAD	P-O3P	2.76	1.62	1.59
4	C	802	FAD	C9A-C5X	2.62	1.45	1.41
4	A	800	FAD	P-O3P	2.61	1.62	1.59
4	C	802	FAD	C5'-C4'	2.41	1.55	1.51
4	C	802	FAD	P-O3P	2.37	1.62	1.59
4	A	800	FAD	C1'-C2'	2.35	1.55	1.52
4	C	802	FAD	C9-C8	2.32	1.42	1.39
4	A	800	FAD	C5'-C4'	2.25	1.54	1.51
4	A	800	FAD	C9A-N10	-2.16	1.37	1.41
4	A	800	FAD	PA-O3P	2.13	1.61	1.59
4	C	802	FAD	C7M-C7	2.08	1.54	1.51
4	C	802	FAD	C10-N1	2.07	1.37	1.33
4	A	800	FAD	C5X-N5	-2.04	1.35	1.39
4	A	800	FAD	C4X-N5	2.01	1.35	1.30

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	800	FAD	C9A-C5X-N5	-5.80	116.30	122.45
4	C	802	FAD	O4B-C1B-C2B	-3.21	99.75	106.62
4	B	801	FAD	C4-C4X-N5	3.20	122.63	118.21
4	A	800	FAD	C6-C5X-C9A	3.05	123.24	119.05
4	B	801	FAD	C10-C4X-N5	-2.96	118.76	124.81
4	B	801	FAD	C10-N1-C2	2.83	122.98	116.85
4	B	801	FAD	O3'-C3'-C4'	-2.80	102.56	108.93
4	A	800	FAD	C10-C4X-N5	-2.71	119.28	124.81
4	C	802	FAD	C5'-C4'-C3'	-2.63	107.25	112.22
4	A	800	FAD	C5'-C4'-C3'	-2.41	107.68	112.22
4	B	801	FAD	O2A-PA-O3P	2.38	113.71	107.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	801	FAD	C7M-C7-C8	2.36	125.57	120.76
4	A	800	FAD	O4'-C4'-C3'	2.34	114.72	109.25
4	C	802	FAD	C4-C4X-N5	2.28	121.36	118.21
4	C	802	FAD	C10-N1-C2	2.28	121.78	116.85
4	C	802	FAD	O3P-PA-O1A	-2.27	103.88	110.70
4	A	800	FAD	O4-C4-N3	2.22	124.30	120.11
4	C	802	FAD	O2A-PA-O1A	2.21	122.73	112.44
4	A	800	FAD	O2A-PA-O1A	2.18	122.60	112.44
4	B	801	FAD	O3P-PA-O1A	-2.16	104.22	110.70
4	B	801	FAD	O4B-C1B-C2B	-2.14	102.03	106.62
4	B	801	FAD	C6-C7-C8	-2.11	116.59	119.69
4	A	800	FAD	C8M-C8-C9	-2.09	115.89	119.57
4	C	802	FAD	N3A-C2A-N1A	2.08	131.74	128.58
4	C	802	FAD	C9-C8-C7	2.08	122.74	119.69
4	C	802	FAD	O2P-P-O3P	-2.06	101.70	107.27
4	B	801	FAD	C9-C8-C7	2.06	122.71	119.69
4	C	802	FAD	O2P-P-O1P	2.01	121.79	112.44
4	B	801	FAD	C4'-C3'-C2'	2.00	116.90	113.57

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	802	FAD	C2B-C1B-N9A-C8A
4	B	801	FAD	O3'-C3'-C4'-O4'
4	B	801	FAD	C2'-C3'-C4'-O4'
4	B	801	FAD	C2B-C1B-N9A-C8A
4	A	800	FAD	O4B-C4B-C5B-O5B
4	B	801	FAD	O3'-C3'-C4'-C5'
4	B	801	FAD	O4B-C4B-C5B-O5B

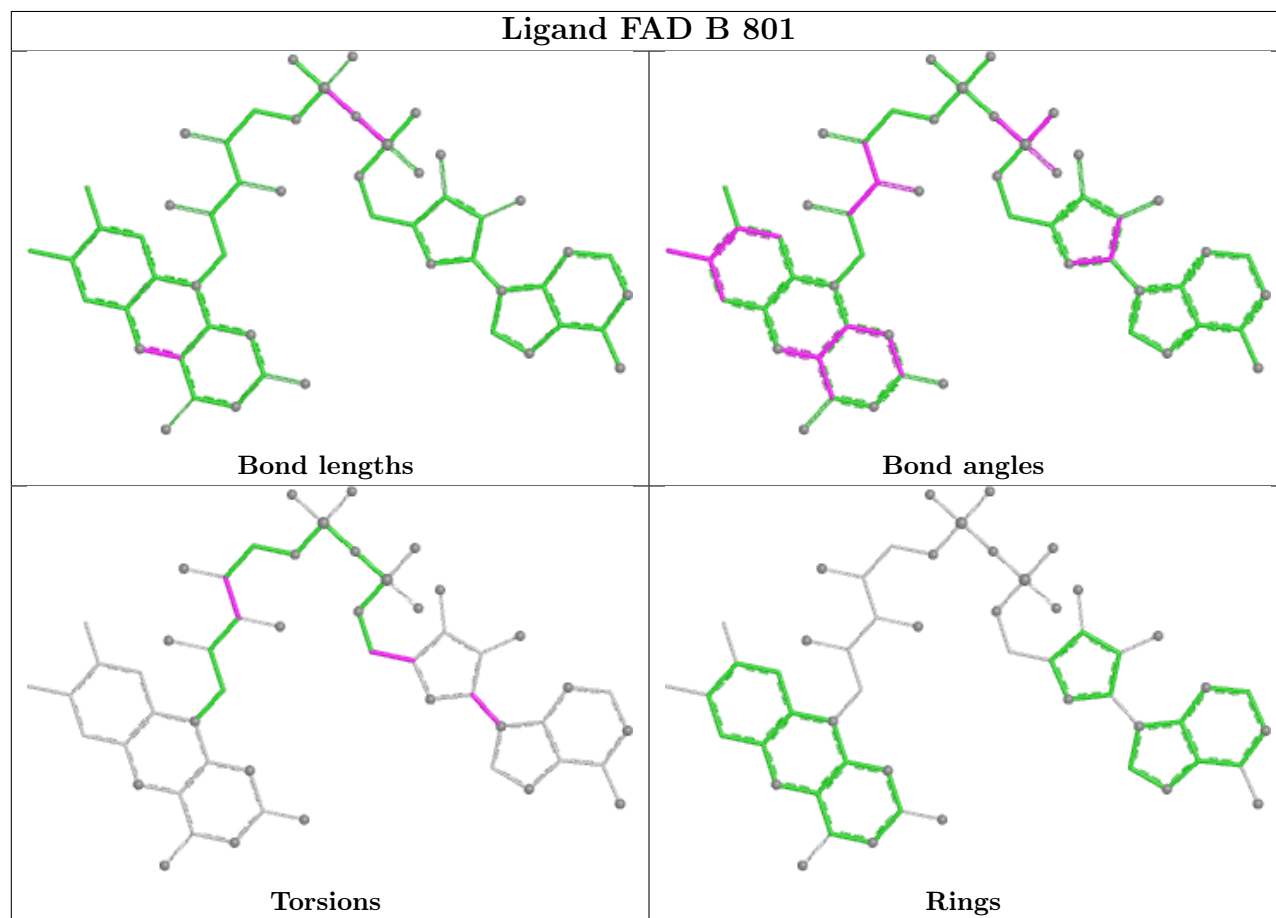
There are no ring outliers.

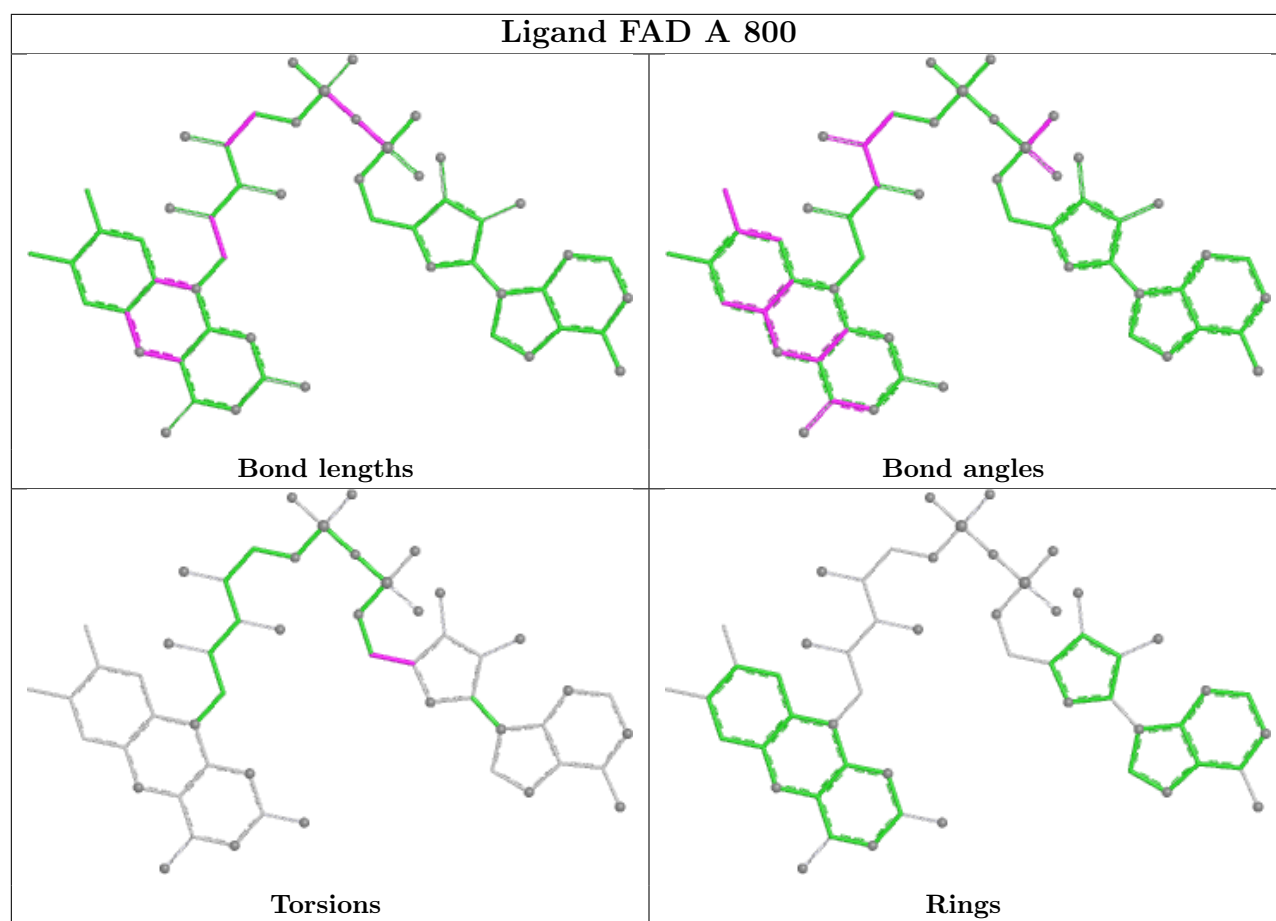
1 monomer is involved in 1 short contact:

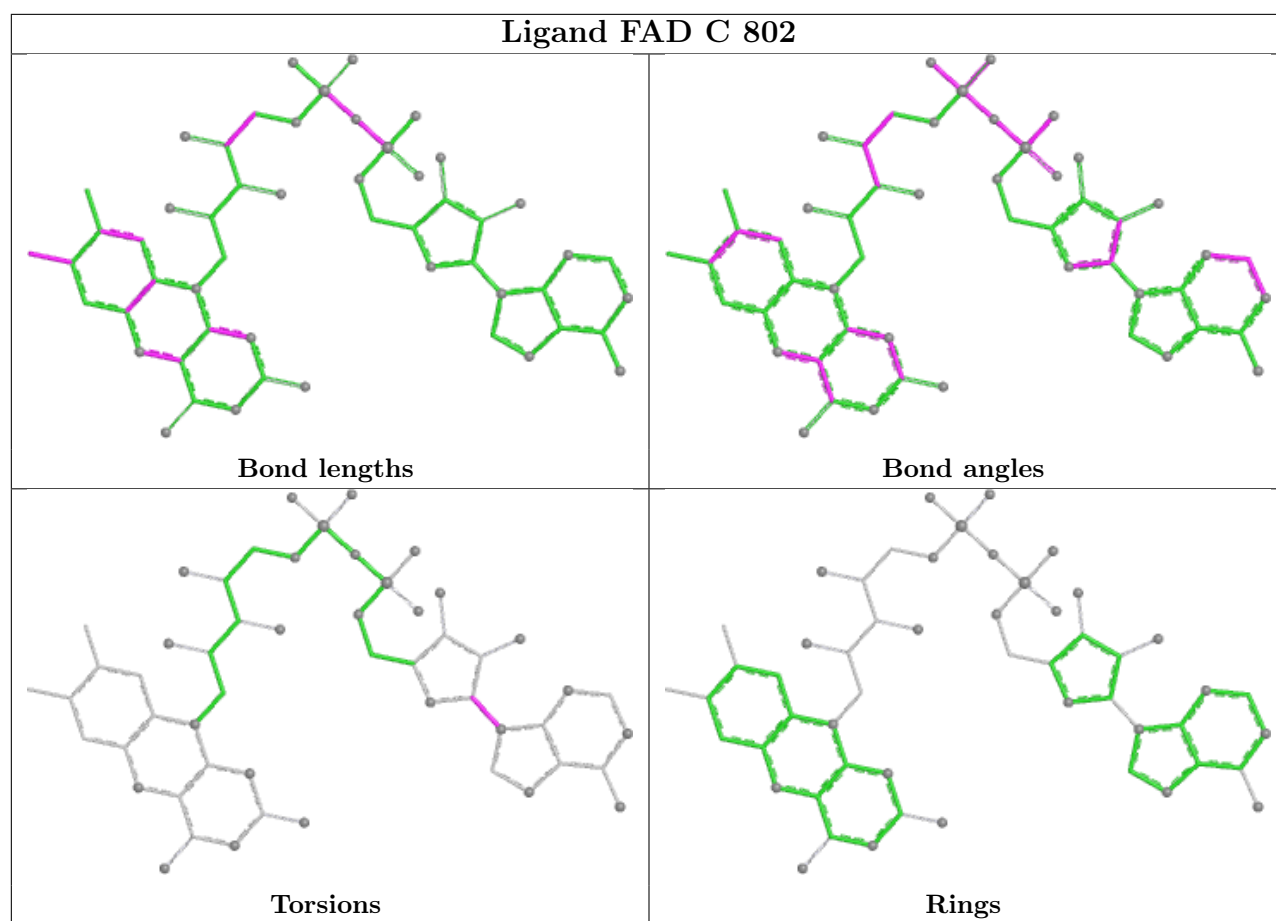
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	800	FAD	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	459/472 (97%)	-0.31	17 (3%) 45 48	4, 13, 34, 61	19 (4%)
1	B	462/472 (97%)	-0.41	19 (4%) 41 44	3, 12, 32, 67	20 (4%)
1	C	462/472 (97%)	-0.53	10 (2%) 62 66	3, 11, 29, 46	19 (4%)
All	All	1383/1416 (97%)	-0.42	46 (3%) 49 52	3, 12, 33, 67	58 (4%)

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	466	HIS	5.9
1	A	221	ASP	5.7
1	C	221	ASP	4.6
1	B	225	LYS	4.5
1	B	100	ASP	4.2
1	B	220	ASP	4.2
1	B	81	LYS	4.0
1	B	222	LYS	4.0
1	A	341	ASP	3.9
1	C	222	LYS	3.8
1	B	221	ASP	3.7
1	A	100	ASP	3.3
1	A	223	SER	3.3
1	A	220	ASP	3.3
1	A	50	ALA	3.2
1	C	50	ALA	3.2
1	B	78	SER	3.1
1	C	341	ASP	3.0
1	A	222	LYS	2.9
1	C	241	LYS	2.9
1	B	463	CYS	2.9
1	A	381	ASP	2.9
1	B	107	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	52	ILE	2.7
1	B	462	MET	2.7
1	B	274	ASP	2.6
1	A	274	ASP	2.6
1	B	371	GLN	2.6
1	B	381	ASP	2.5
1	A	342	ALA	2.5
1	B	223	SER	2.5
1	C	105	ASP	2.5
1	B	379	GLY	2.5
1	A	107	ASP	2.5
1	C	466	HIS	2.4
1	A	304	LYS	2.4
1	C	274	ASP	2.3
1	B	5	PRO	2.3
1	C	223	SER	2.2
1	B	114	GLU	2.2
1	A	387	ASP	2.2
1	B	121	GLU	2.2
1	A	254	ASN	2.1
1	C	220	ASP	2.1
1	A	150	GLN	2.0
1	A	101	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	D	2	14/15	0.74	0.23	22,45,94,100	0
3	MAN	F	3	11/12	0.81	0.22	25,43,66,74	0
3	MAN	F	4	11/12	0.82	0.22	31,44,73,100	0
2	NAG	E	2	14/15	0.84	0.21	18,52,100,100	0
2	NAG	D	1	14/15	0.85	0.16	23,35,59,59	0

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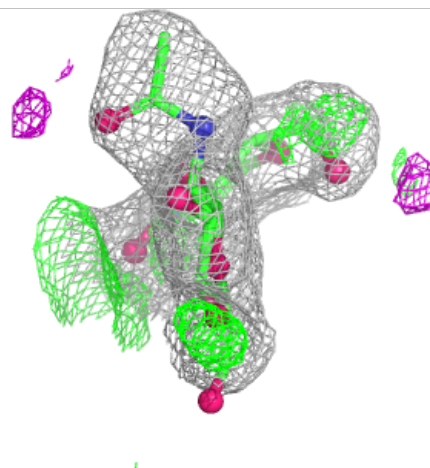
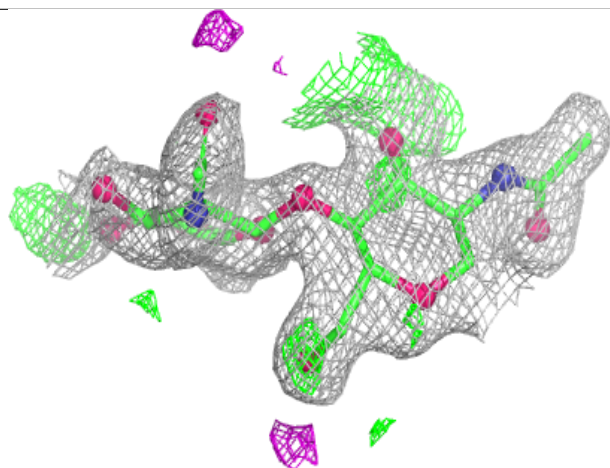
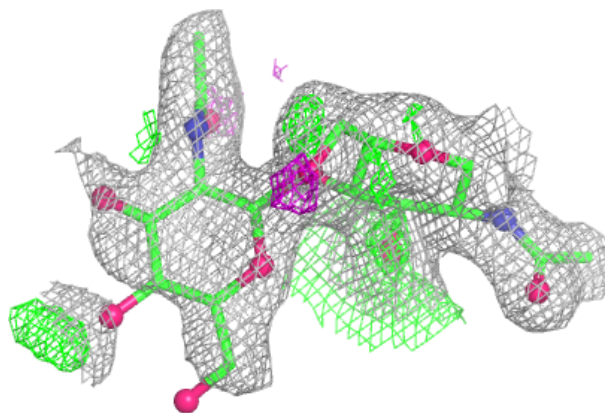
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	FCA	F	5	10/11	0.85	0.20	6,30,36,100	0
3	NAG	F	2	14/15	0.86	0.15	5,17,31,65	0
2	NAG	E	1	14/15	0.87	0.18	13,29,38,100	0
3	NAG	F	1	14/15	0.87	0.17	5,15,34,100	0

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.

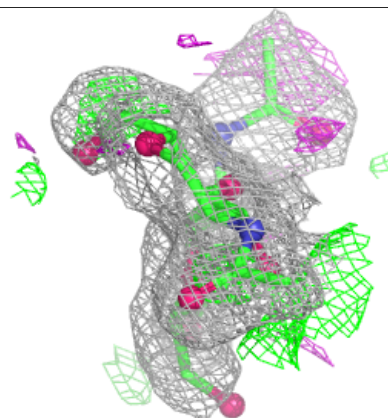
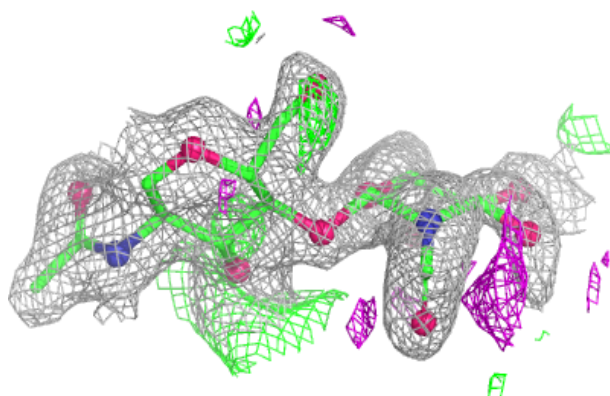
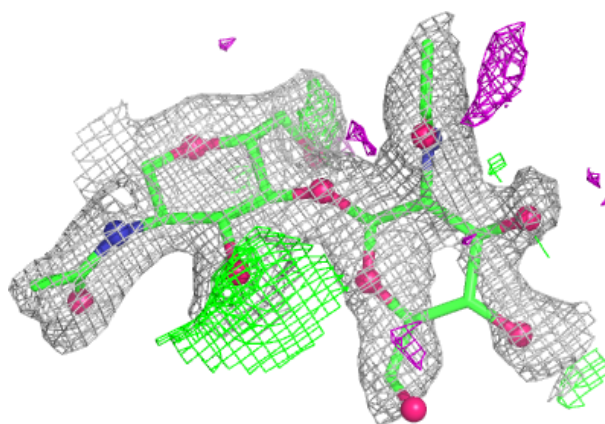
Electron density around Chain D:

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

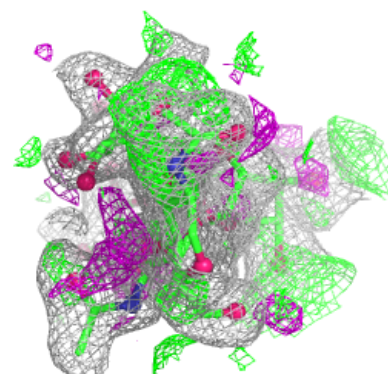
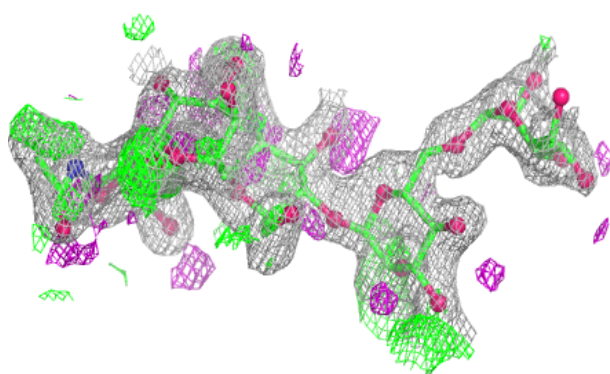
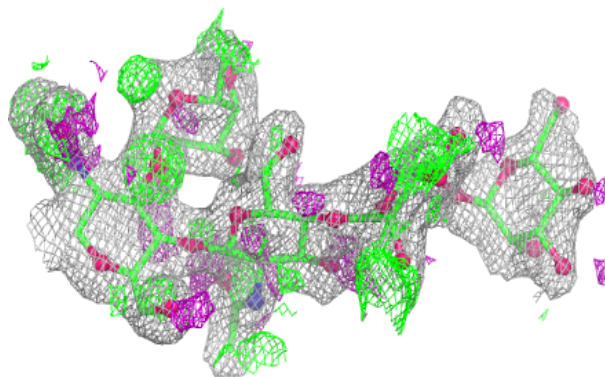


Electron density around Chain E:

$2mF_o-DF_c$ (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)

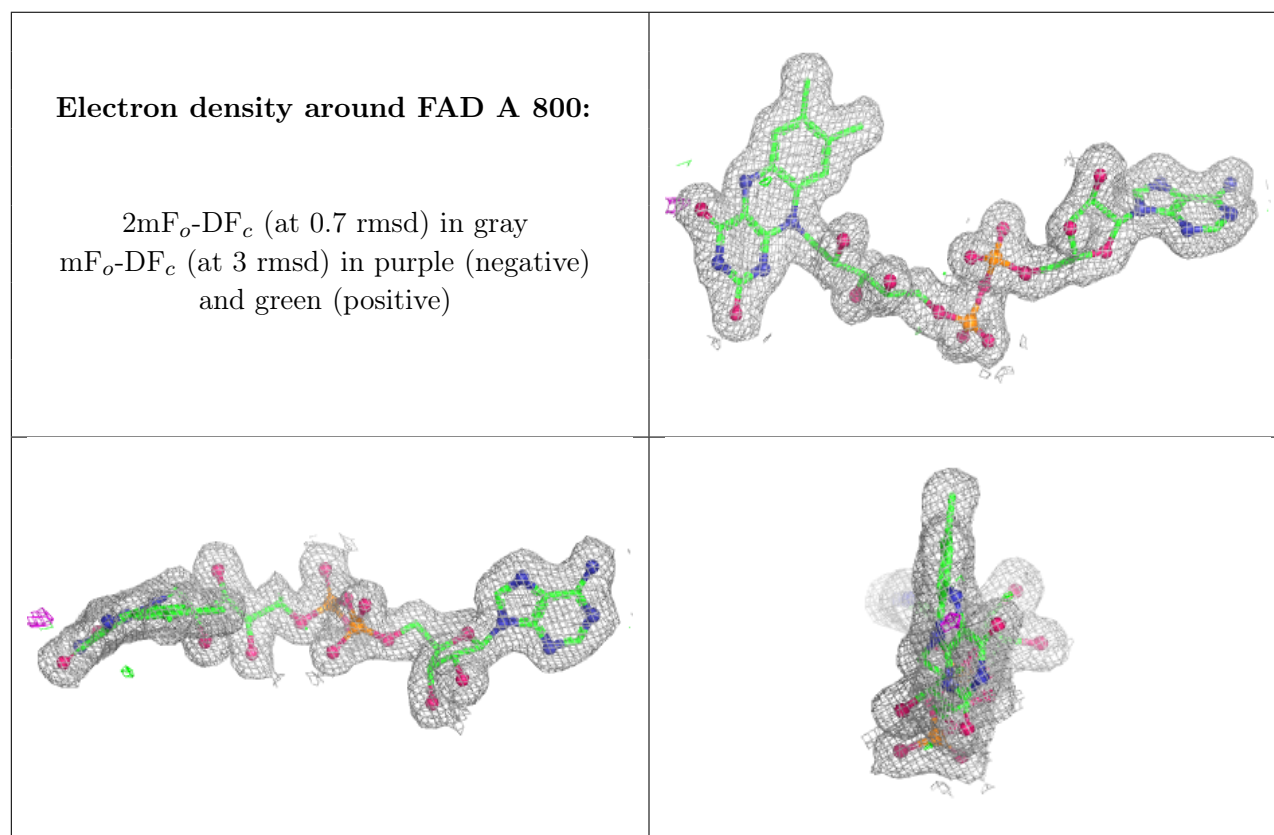


6.4 Ligands ⓘ

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

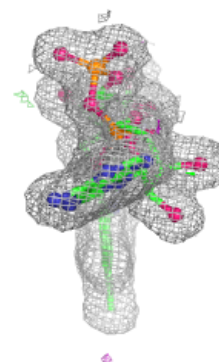
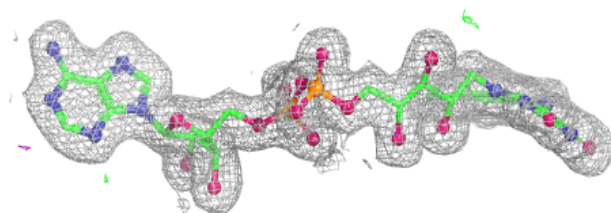
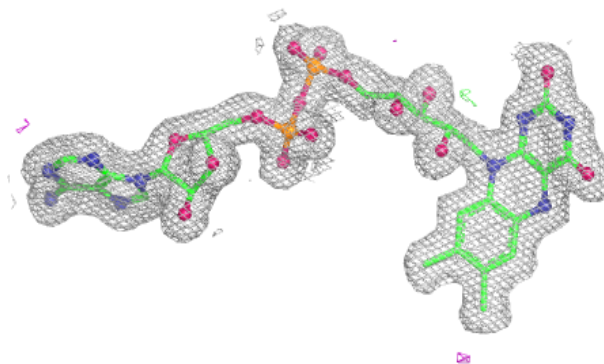
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	FAD	A	800	53/53	0.99	0.04	3,8,12,14	0
4	FAD	B	801	53/53	0.99	0.03	1,6,8,9	0
4	FAD	C	802	53/53	0.99	0.04	1,7,11,11	0

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.

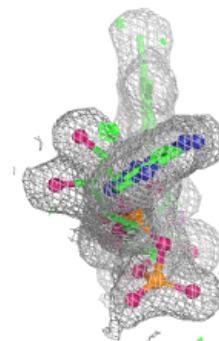
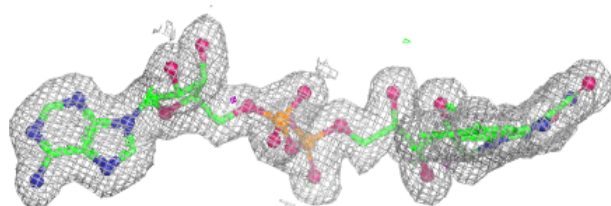
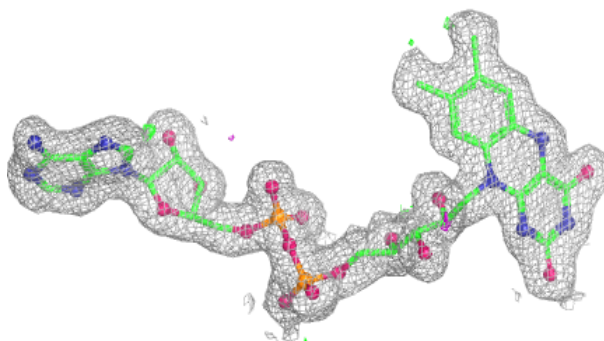


Electron density around FAD B 801:

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

**Electron density around FAD C 802:**

$2mF_o-DF_c$ (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.