



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:11 PM UTC

PDB ID : 1B5Q / pdb_00001b5q
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 : 1999-01-07
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

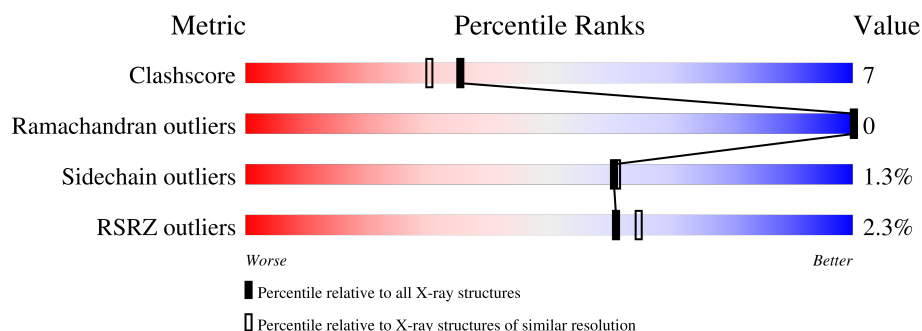
1 Overall quality at a glance

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	3% 76% 19% • •
1	B	472	2% 82% 14% • •
1	C	472	2% 83% 14% • •
2	D	2	100%
2	E	2	100%
3	F	5	100%

2 Entry composition [i](#)

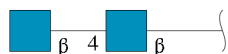
There are 6 unique types of molecules in this entry. The entry contains 12059 atoms, of which 0 are hydrogens and 0 are deuteriums.

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).

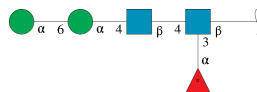
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	459	Total	C	N	O	S	60	0	0
			3684	2353	621	696	14			
1	B	462	Total	C	N	O	S	53	0	0
			3715	2374	627	700	14			
1	C	462	Total	C	N	O	S	44	0	0
			3715	2374	627	700	14			

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



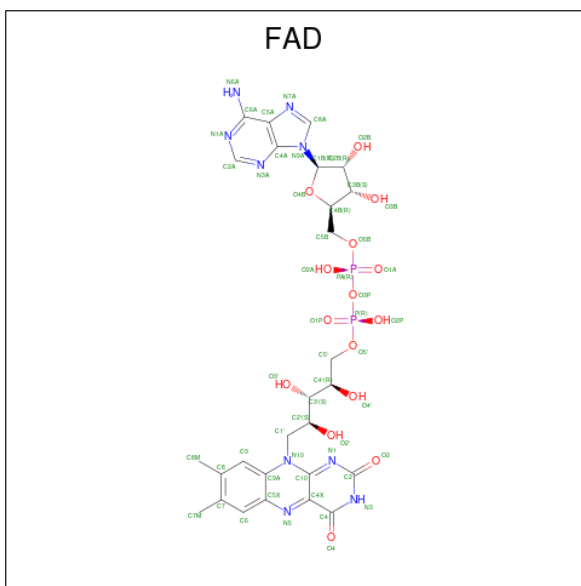
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			

- 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.



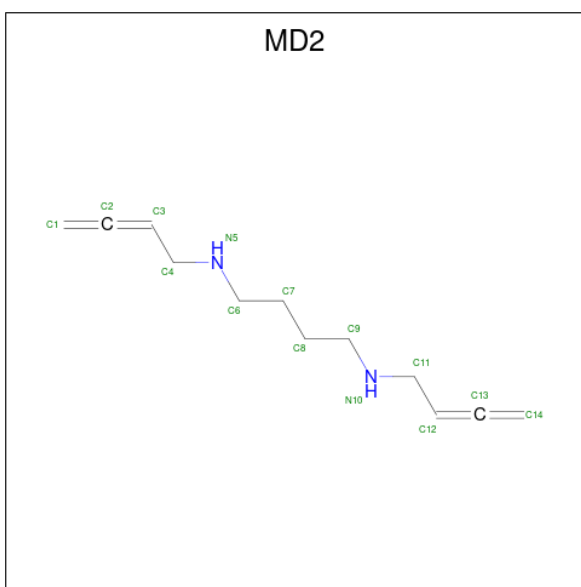
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	F	5	Total	C	N	O	0	0	0
			60	34	2	24			

- 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 53	C 27	N 9	O 15	P 2	0	0
4	B	1	Total 53	C 27	N 9	O 15	P 2	0	0
4	C	1	Total 53	C 27	N 9	O 15	P 2	0	0

- Molecule 5 is N,N'-BIS(2,3-BUTADIENYL)-1,4-BUTANE-DIAMINE (CCD ID: MD2) (formula: $C_{12}H_{20}N_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	N	0	0
			14	12	2		
5	B	1	Total	C	N	0	0
			14	12	2		
5	C	1	Total	C	N	0	0
			14	12	2		

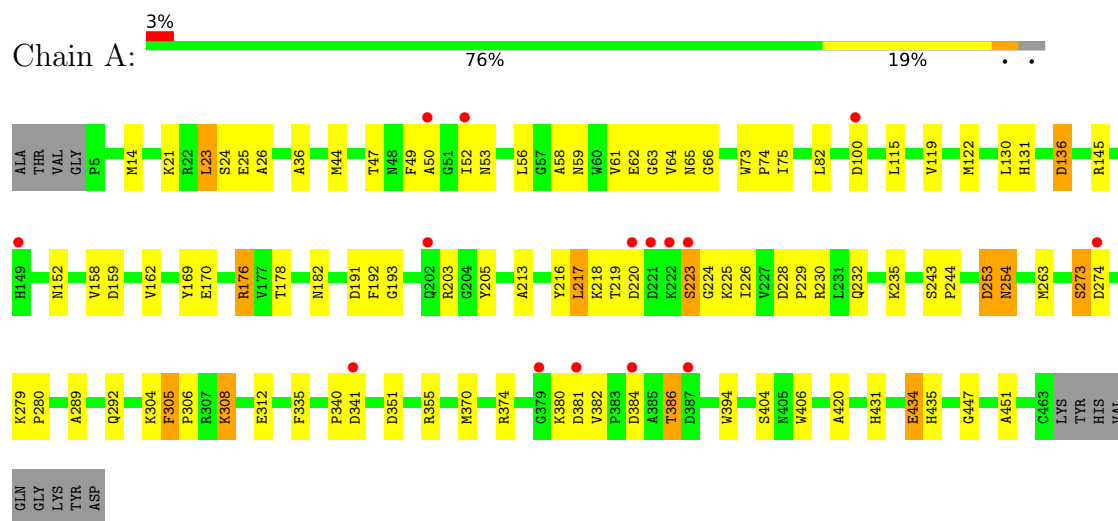
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	197	Total	O	0	0
			197	197		
6	B	207	Total	O	0	0
			207	207		
6	C	224	Total	O	0	0
			224	224		

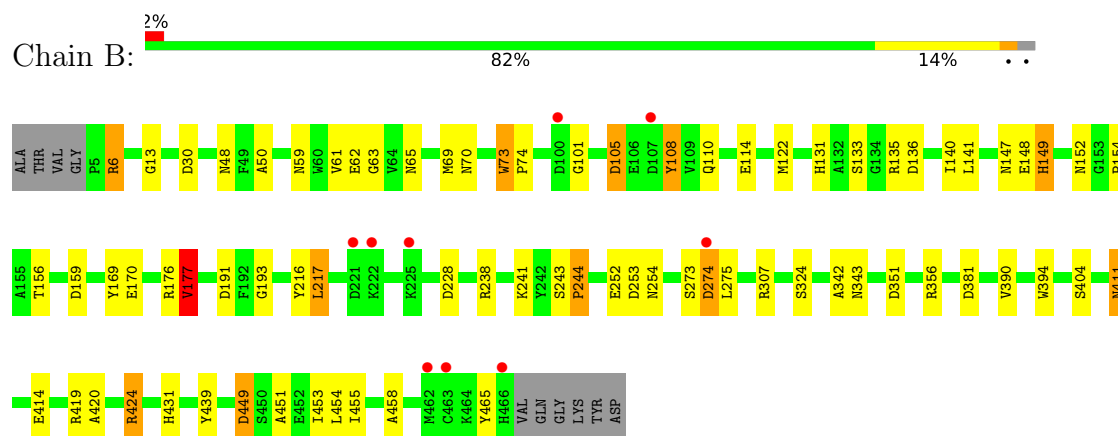
3 Residue-property plots [i](#)

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.

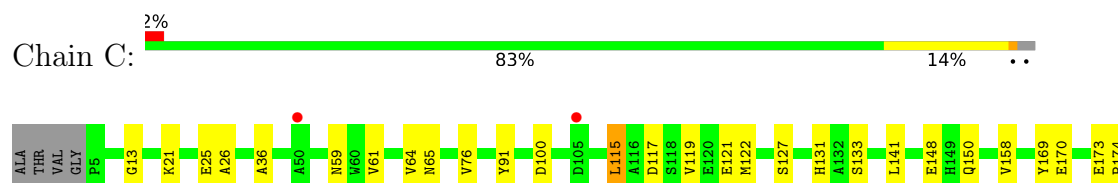
• Molecule 1: PROTEIN (POLYAMINE OXIDASE)

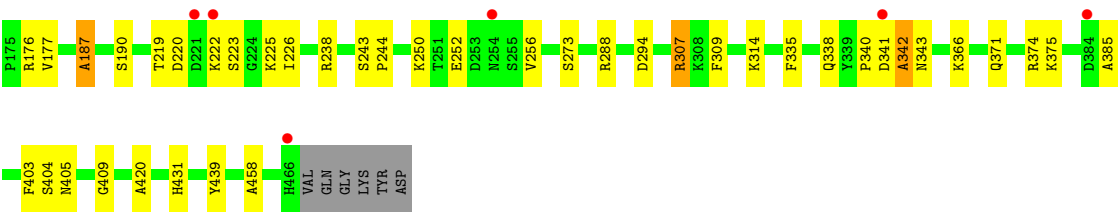


• Molecule 1: PROTEIN (POLYAMINE OXIDASE)



• Molecule 1: PROTEIN (POLYAMINE OXIDASE)





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



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



● 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



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	184.60Å 184.60Å 281.50Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 1.90 50.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	96.0 (50.00-1.90) 95.9 (50.00-1.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.95 (at 1.90Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.193 , (Not available) 0.182 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	19.3	Xtriage
Anisotropy	0.117	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 65.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12059	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.60% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MD2, NAG, FCA, FAD, MAN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.76	3/3775 (0.1%)	1.62	47/5116 (0.9%)
1	B	0.76	0/3808	1.59	41/5160 (0.8%)
1	C	0.77	0/3808	1.57	30/5160 (0.6%)
All	All	0.76	3/11391 (0.0%)	1.59	118/15436 (0.8%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	263	MET	SD-CE	7.25	1.97	1.79
1	A	14	MET	SD-CE	5.21	1.92	1.79
1	A	382	VAL	CA-C	-5.13	1.49	1.53

All (118) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	273	SER	CA-C-N	-11.71	104.80	122.83
1	C	273	SER	C-N-CA	-11.71	104.80	122.83
1	C	342	ALA	N-CA-C	10.69	124.22	111.82
1	C	307	ARG	NE-CZ-NH1	-10.33	111.17	121.50
1	C	340	PRO	CA-C-N	-10.29	106.19	122.65
1	C	340	PRO	C-N-CA	-10.29	106.19	122.65
1	A	223	SER	CB-CA-C	-9.61	95.64	110.92
1	A	381	ASP	CA-C-N	-9.47	115.77	122.59
1	A	381	ASP	C-N-CA	-9.47	115.77	122.59
1	C	307	ARG	NE-CZ-NH2	9.23	127.51	119.20
1	A	273	SER	CA-C-N	-8.98	108.83	124.82
1	A	273	SER	C-N-CA	-8.98	108.83	124.82
1	B	177	VAL	N-CA-CB	-8.67	102.67	112.21
1	A	224	GLY	N-CA-C	-8.24	103.94	115.32
1	C	61	VAL	N-CA-C	-7.82	95.86	107.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	149	HIS	CB-CA-C	-7.54	101.10	112.11
1	B	13	GLY	N-CA-C	-7.50	101.17	112.41
1	B	241	LYS	CD-CE-NZ	7.40	135.57	111.90
1	A	355	ARG	NE-CZ-NH2	-7.33	112.61	119.20
1	A	341	ASP	N-CA-C	7.26	123.66	113.56
1	A	205	TYR	N-CA-C	-7.26	103.36	111.71
1	A	100	ASP	N-CA-C	7.25	122.24	112.88
1	A	136	ASP	CB-CA-C	-7.22	98.52	110.72
1	C	420	ALA	N-CA-C	7.20	118.78	109.64
1	C	307	ARG	CD-NE-CZ	-7.02	114.58	124.40
1	A	386	THR	N-CA-CB	-6.96	99.59	110.30
1	C	338	GLN	N-CA-C	6.94	118.63	111.14
1	B	135	ARG	NE-CZ-NH1	-6.93	114.57	121.50
1	A	61	VAL	N-CA-C	-6.90	97.91	107.99
1	C	115	LEU	CB-CG-CD1	-6.84	90.18	110.70
1	B	73	TRP	N-CA-C	6.79	121.98	112.75
1	C	150	GLN	CB-CA-C	-6.76	99.49	109.97
1	B	351	ASP	N-CA-CB	-6.75	99.09	110.49
1	A	380	LYS	CA-C-N	-6.71	114.12	122.84
1	A	380	LYS	C-N-CA	-6.71	114.12	122.84
1	B	61	VAL	N-CA-C	-6.62	97.64	107.51
1	B	420	ALA	N-CA-C	6.53	117.11	109.60
1	B	140	ILE	N-CA-C	-6.53	104.13	110.72
1	A	406	TRP	CA-C-O	6.47	124.11	119.32
1	B	136	ASP	CB-CA-C	-6.45	100.63	111.02
1	B	65	ASN	CA-C-N	-6.44	115.04	122.83
1	B	65	ASN	C-N-CA	-6.44	115.04	122.83
1	C	177	VAL	N-CA-CB	-6.38	103.55	112.35
1	A	44	MET	N-CA-C	-6.35	97.34	108.20
1	C	458	ALA	N-CA-C	6.34	118.27	111.36
1	B	465	TYR	N-CA-C	6.34	124.30	110.80
1	B	149	HIS	CA-CB-CG	-6.33	107.47	113.80
1	A	420	ALA	N-CA-C	6.33	118.59	109.48
1	A	253	ASP	CA-C-N	-6.22	117.10	126.86
1	A	253	ASP	C-N-CA	-6.22	117.10	126.86
1	A	381	ASP	N-CA-C	-6.13	97.72	108.20
1	A	305	PHE	CA-C-N	5.99	125.54	119.19
1	A	305	PHE	C-N-CA	5.99	125.54	119.19
1	A	36	ALA	N-CA-C	5.98	117.80	111.28
1	B	424	ARG	CG-CD-NE	-5.92	98.97	112.00
1	C	26	ALA	N-CA-C	-5.86	105.90	113.16
1	A	178	THR	N-CA-C	5.85	119.44	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	289	ALA	N-CA-C	-5.81	105.03	111.36
1	A	115	LEU	N-CA-C	-5.76	104.90	111.07
1	B	191	ASP	N-CA-C	5.74	118.40	111.40
1	B	274	ASP	N-CA-C	5.72	119.83	112.86
1	A	203	ARG	N-CA-C	-5.67	105.86	112.89
1	C	13	GLY	N-CA-C	-5.66	103.92	112.41
1	B	6	ARG	N-CA-C	-5.59	100.60	109.76
1	A	176	ARG	CB-CG-CD	-5.54	98.56	111.30
1	A	374	ARG	NE-CZ-NH2	5.54	124.18	119.20
1	A	75	ILE	CB-CA-C	-5.53	104.59	112.22
1	B	122	MET	N-CA-C	-5.52	105.36	111.71
1	A	230	ARG	N-CA-C	-5.51	106.51	113.18
1	B	275	LEU	N-CA-C	-5.50	105.36	111.36
1	C	187	ALA	N-CA-C	5.50	117.27	111.28
1	C	36	ALA	N-CA-C	5.49	117.27	111.28
1	A	351	ASP	N-CA-CB	-5.45	101.28	110.49
1	C	409	GLY	N-CA-C	-5.45	107.75	113.58
1	B	238	ARG	N-CA-C	-5.44	107.01	113.97
1	C	174	PRO	CB-CA-C	-5.43	104.30	110.92
1	C	273	SER	O-C-N	-5.43	115.47	122.20
1	C	76	VAL	N-CA-C	5.40	115.61	110.53
1	A	191	ASP	N-CA-C	5.38	117.96	111.40
1	B	50	ALA	CA-C-N	-5.37	112.33	122.05
1	B	50	ALA	C-N-CA	-5.37	112.33	122.05
1	A	254	ASN	N-CA-C	5.37	121.67	113.51
1	B	244	PRO	CB-CA-C	-5.36	103.84	112.21
1	B	6	ARG	NE-CZ-NH2	5.36	124.02	119.20
1	A	145	ARG	NE-CZ-NH2	5.35	124.02	119.20
1	B	356	ARG	CA-C-O	5.33	126.18	120.70
1	A	335	PHE	N-CA-C	5.32	120.00	111.81
1	A	182	ASN	N-CA-C	5.31	119.45	112.92
1	A	162	VAL	N-CA-C	-5.30	105.36	110.72
1	C	309	PHE	N-CA-C	-5.27	105.92	114.09
1	C	288	ARG	CG-CD-NE	-5.24	100.48	112.00
1	A	447	GLY	N-CA-C	-5.23	106.46	112.73
1	C	374	ARG	CG-CD-NE	-5.21	100.54	112.00
1	B	135	ARG	CA-CB-CG	-5.18	103.75	114.10
1	B	147	ASN	CA-C-N	-5.17	113.31	122.26
1	B	147	ASN	C-N-CA	-5.17	113.31	122.26
1	B	228	ASP	CA-C-O	5.17	124.61	119.75
1	B	390	VAL	CB-CA-C	-5.15	106.19	111.08
1	B	449	ASP	N-CA-C	5.14	116.88	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	335	PHE	N-CA-C	5.14	121.74	110.80
1	C	341	ASP	CB-CA-C	5.13	119.23	110.56
1	B	253	ASP	N-CA-C	-5.12	107.19	112.93
1	B	156	THR	CA-C-N	5.12	124.56	119.24
1	B	156	THR	C-N-CA	5.12	124.56	119.24
1	A	24	SER	N-CA-C	-5.10	105.72	111.28
1	A	26	ALA	N-CA-C	-5.10	106.84	113.16
1	A	203	ARG	NE-CZ-NH1	-5.10	116.40	121.50
1	A	340	PRO	CA-C-N	-5.09	115.81	124.31
1	A	340	PRO	C-N-CA	-5.09	115.81	124.31
1	B	108	TYR	N-CA-C	-5.08	105.64	111.07
1	A	82	LEU	N-CA-C	-5.05	103.00	110.48
1	B	324	SER	N-CA-C	-5.03	107.09	113.18
1	B	458	ALA	CA-C-N	-5.02	113.10	122.09
1	B	458	ALA	C-N-CA	-5.02	113.10	122.09
1	C	341	ASP	N-CA-CB	5.02	117.89	110.56
1	A	273	SER	N-CA-C	5.02	119.26	113.18
1	B	101	GLY	N-CA-C	5.02	125.08	113.18
1	C	371	GLN	CA-CB-CG	5.01	124.11	114.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3684	0	3585	57	0
1	B	3715	0	3614	60	1
1	C	3715	0	3614	36	0
2	D	28	0	26	3	0
2	E	28	0	26	4	1
3	F	60	0	52	5	0
4	A	53	0	31	1	0
4	B	53	0	31	0	0
4	C	53	0	31	0	0
5	A	14	0	20	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	14	0	20	5	0
5	C	14	0	20	6	0
6	A	197	0	0	7	0
6	B	207	0	0	2	0
6	C	224	0	0	3	0
All	All	12059	0	11070	160	1

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 (160) 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:A:192:PHE:O	6:A:601:HOH:O	1.60	1.19
1:B:69:MET:CE	1:B:74:PRO:HD3	1.80	1.10
1:B:69:MET:HE2	1:B:74:PRO:HD3	1.35	1.06
1:B:69:MET:CE	1:B:73:TRP:HB3	1.88	1.02
1:B:69:MET:HE2	1:B:74:PRO:CD	1.94	0.97
1:A:220:ASP:HB3	1:A:223:SER:HB2	1.47	0.94
1:A:192:PHE:C	6:A:601:HOH:O	2.05	0.91
1:C:131:HIS:CD2	1:C:133:SER:H	1.90	0.88
1:C:91:TYR:OH	1:C:314:LYS:HE2	1.73	0.87
1:B:69:MET:HE3	1:B:73:TRP:HB3	1.56	0.87
2:E:1:NAG:C4	2:E:2:NAG:C1	2.54	0.85
1:B:69:MET:HE1	1:B:73:TRP:HB3	1.57	0.85
1:B:131:HIS:CD2	1:B:133:SER:H	1.98	0.81
2:D:1:NAG:C4	2:D:2:NAG:C1	2.59	0.80
1:B:69:MET:HE1	1:B:73:TRP:CD1	2.17	0.80
1:B:69:MET:HE3	1:B:74:PRO:HD3	1.64	0.79
1:B:69:MET:HE2	1:B:74:PRO:CG	2.14	0.77
1:B:131:HIS:HD2	1:B:133:SER:H	1.29	0.76
1:A:273:SER:O	1:A:274:ASP:HB2	1.84	0.76
3:F:1:NAG:C4	3:F:2:NAG:C1	2.64	0.76
1:C:117:ASP:O	1:C:121:GLU:HG3	1.85	0.76
1:A:431:HIS:CD2	1:A:431:HIS:H	2.04	0.75
1:C:404:SER:O	5:C:502:MD2:HC1A	1.86	0.74
1:B:114:GLU:HA	1:B:114:GLU:OE1	1.86	0.74
1:B:419:ARG:HG2	6:B:701:HOH:O	1.89	0.72
1:B:216:TYR:CD1	1:B:217:LEU:HD13	2.24	0.72
1:C:119:VAL:HA	1:C:122:MET:HE3	1.72	0.71
1:B:243:SER:HB2	1:B:244:PRO:HD2	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69:MET:HE1	1:B:73:TRP:HD1	1.57	0.69
1:B:411:ASN:ND2	1:B:414:GLU:H	1.90	0.68
1:A:292:GLN:OE1	6:A:602:HOH:O	2.12	0.68
2:D:1:NAG:HO4	2:D:2:NAG:C1	2.05	0.68
1:A:404:SER:O	5:A:502:MD2:HC1A	1.94	0.68
1:A:223:SER:HB3	1:A:225:LYS:H	1.59	0.67
1:C:148:GLU:OE2	6:C:601:HOH:O	2.13	0.67
1:C:131:HIS:HD2	1:C:133:SER:H	1.40	0.66
1:C:431:HIS:H	1:C:431:HIS:CD2	2.13	0.66
1:B:170:GLU:O	5:B:502:MD2:HC42	1.95	0.66
1:C:170:GLU:O	5:C:502:MD2:HC42	1.96	0.65
1:B:69:MET:HE2	1:B:74:PRO:HG3	1.78	0.64
1:A:131:HIS:ND1	1:A:136:ASP:OD2	2.30	0.64
1:A:170:GLU:O	5:A:502:MD2:HC42	1.99	0.62
1:A:130:LEU:HD22	1:A:136:ASP:HB2	1.82	0.62
1:B:431:HIS:H	1:B:431:HIS:CD2	2.17	0.62
1:C:131:HIS:HD2	1:C:133:SER:OG	1.82	0.61
3:F:1:NAG:H3	3:F:5:FCA:O2	2.00	0.60
1:A:394:TRP:HE1	1:B:152:ASN:ND2	1.99	0.60
1:A:119:VAL:HA	1:A:122:MET:HE3	1.84	0.59
1:B:69:MET:HE1	1:B:73:TRP:CB	2.31	0.58
1:A:64:VAL:O	1:A:65:ASN:HB2	2.02	0.58
1:B:243:SER:HB2	1:B:244:PRO:CD	2.34	0.58
1:A:62:GLU:OE2	5:A:502:MD2:HC91	2.02	0.57
1:C:131:HIS:CD2	1:C:133:SER:OG	2.58	0.56
1:A:216:TYR:CD1	1:A:217:LEU:HD13	2.40	0.56
1:B:404:SER:O	5:B:502:MD2:HC1A	2.06	0.56
1:A:169:TYR:CZ	5:A:502:MD2:HC12	2.42	0.55
1:C:405:ASN:OD1	5:C:502:MD2:HC11	2.06	0.55
1:A:273:SER:O	1:A:274:ASP:CB	2.45	0.54
1:A:50:ALA:HB1	1:A:304:LYS:HD2	1.90	0.54
1:C:366:LYS:HD2	1:C:385:ALA:HB3	1.90	0.54
1:A:50:ALA:CB	1:A:304:LYS:HD2	2.38	0.54
1:A:152:ASN:ND2	1:B:394:TRP:HE1	2.06	0.54
1:A:223:SER:CB	1:A:225:LYS:H	2.22	0.53
1:B:244:PRO:O	1:B:424:ARG:NH1	2.40	0.53
1:A:243:SER:HB2	1:A:244:PRO:CD	2.38	0.53
1:A:64:VAL:CA	6:A:601:HOH:O	2.57	0.53
1:A:73:TRP:HB3	1:A:74:PRO:HD3	1.91	0.53
1:A:370:MET:HE2	1:A:384:ASP:HA	1.90	0.52
1:A:21:LYS:O	1:A:25:GLU:HG3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:216:TYR:CE1	1:B:217:LEU:HD13	2.45	0.52
3:F:3:MAN:H61	3:F:4:MAN:C5	2.39	0.52
1:C:131:HIS:HD2	1:C:133:SER:CB	2.22	0.52
1:A:158:VAL:HG13	1:A:159:ASP:N	2.26	0.51
1:B:273:SER:O	1:B:274:ASP:HB2	2.10	0.51
1:B:342:ALA:O	1:B:343:ASN:HB2	2.10	0.51
1:B:411:ASN:HD22	1:B:414:GLU:H	1.55	0.51
1:C:220:ASP:OD2	1:C:222:LYS:N	2.39	0.51
1:A:23:LEU:HD13	1:A:451:ALA:HB1	1.91	0.51
1:A:63:GLY:C	6:A:601:HOH:O	2.53	0.51
1:A:394:TRP:HE1	1:B:152:ASN:HD22	1.57	0.51
1:A:431:HIS:CD2	6:A:637:HOH:O	2.63	0.51
1:C:342:ALA:O	1:C:343:ASN:HB2	2.12	0.50
3:F:3:MAN:H61	3:F:4:MAN:H5	1.93	0.50
1:C:307:ARG:NH1	6:C:602:HOH:O	2.31	0.50
2:E:1:NAG:H4	2:E:2:NAG:C1	2.39	0.50
1:C:21:LYS:O	1:C:25:GLU:HG3	2.11	0.50
1:B:148:GLU:O	1:B:149:HIS:HB2	2.11	0.50
1:A:308:LYS:HD2	1:A:312:GLU:CD	2.37	0.50
1:C:131:HIS:CD2	1:C:133:SER:CB	2.95	0.49
1:A:434:GLU:HG2	1:A:435:HIS:CD2	2.47	0.49
1:B:131:HIS:CD2	1:B:133:SER:OG	2.66	0.49
1:A:176:ARG:HD2	1:B:177:VAL:HG21	1.95	0.49
1:A:370:MET:HG3	1:A:384:ASP:OD2	2.13	0.49
1:A:216:TYR:CE1	1:A:217:LEU:HD13	2.48	0.48
1:B:216:TYR:CD1	1:B:217:LEU:CD1	2.96	0.48
1:C:64:VAL:O	1:C:65:ASN:HB2	2.12	0.48
1:A:66:GLY:N	1:A:192:PHE:O	2.43	0.48
1:B:307:ARG:NH2	1:B:381:ASP:OD2	2.45	0.48
1:A:235:LYS:NZ	1:A:253:ASP:OD2	2.32	0.48
1:C:220:ASP:HB3	1:C:223:SER:OG	2.13	0.48
2:E:1:NAG:HO4	2:E:2:NAG:C1	2.22	0.48
1:B:6:ARG:HA	1:B:30:ASP:O	2.14	0.48
1:A:64:VAL:N	6:A:601:HOH:O	2.46	0.48
1:B:63:GLY:HA2	1:B:193:GLY:O	2.14	0.47
1:C:169:TYR:O	5:C:502:MD2:H111	2.13	0.47
1:B:69:MET:HE1	1:B:73:TRP:CG	2.48	0.47
1:A:49:PHE:O	1:A:52:ILE:HG12	2.14	0.47
1:B:131:HIS:HD2	1:B:133:SER:N	2.05	0.47
1:B:131:HIS:HD2	1:B:133:SER:OG	1.97	0.47
1:A:229:PRO:O	1:A:232:GLN:NE2	2.41	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:243:SER:HB2	1:C:244:PRO:CD	2.44	0.47
3:F:1:NAG:C3	3:F:5:FCA:O2	2.63	0.47
1:A:63:GLY:HA2	1:A:193:GLY:O	2.14	0.47
1:A:131:HIS:HD1	1:A:136:ASP:CG	2.23	0.47
1:A:152:ASN:HD22	1:B:394:TRP:HE1	1.61	0.47
1:C:131:HIS:HD2	1:C:133:SER:N	2.11	0.47
1:B:114:GLU:OE1	1:B:114:GLU:CA	2.58	0.46
1:C:403:PHE:CZ	5:C:502:MD2:HC62	2.50	0.46
1:A:218:LYS:H	1:A:228:ASP:HB2	1.80	0.46
1:C:238:ARG:NH1	1:C:252:GLU:OE2	2.47	0.46
1:B:69:MET:HE3	1:B:70:ASN:O	2.15	0.46
1:B:169:TYR:CZ	5:B:502:MD2:HC12	2.51	0.46
1:A:243:SER:CB	1:A:244:PRO:CD	2.94	0.45
1:C:250:LYS:HG2	1:C:256:VAL:HG22	1.97	0.45
1:C:219:THR:HG22	1:C:226:ILE:HA	1.98	0.45
1:B:252:GLU:C	1:B:254:ASN:H	2.25	0.45
1:B:451:ALA:O	1:B:455:ILE:HG13	2.17	0.45
1:A:220:ASP:CB	1:A:223:SER:HB2	2.34	0.44
1:A:47:THR:O	1:A:53:ASN:HA	2.16	0.44
1:C:173:GLU:OE1	1:C:294:ASP:OD2	2.36	0.44
1:B:449:ASP:O	1:B:453:ILE:HG13	2.17	0.44
1:A:73:TRP:N	1:A:74:PRO:CD	2.81	0.44
1:C:439:TYR:CZ	5:C:502:MD2:HC41	2.53	0.43
1:B:419:ARG:HD3	6:B:615:HOH:O	2.18	0.43
1:C:158:VAL:HG12	6:C:800:HOH:O	2.19	0.43
1:B:110:GLN:O	1:B:114:GLU:HG2	2.17	0.43
1:B:133:SER:O	1:B:411:ASN:HB2	2.18	0.43
1:A:219:THR:HG22	1:A:226:ILE:HA	2.01	0.43
2:D:1:NAG:H4	2:D:2:NAG:C1	2.46	0.43
1:A:213:ALA:O	1:A:217:LEU:HB2	2.19	0.42
1:A:47:THR:HG21	1:A:56:LEU:HD21	2.00	0.42
1:C:431:HIS:CD2	1:C:431:HIS:N	2.85	0.42
1:B:243:SER:CB	1:B:244:PRO:CD	2.95	0.42
1:B:154:PRO:HB3	1:B:159:ASP:HB3	2.00	0.42
1:B:411:ASN:HD22	1:B:411:ASN:C	2.27	0.42
1:C:100:ASP:OD1	1:C:375:LYS:HE2	2.19	0.42
1:B:141:LEU:HD22	1:B:176:ARG:HB3	2.01	0.42
1:A:253:ASP:O	1:A:254:ASN:HB2	2.20	0.42
1:C:219:THR:HA	1:C:225:LYS:O	2.18	0.42
1:A:58:ALA:HA	4:A:501:FAD:C4X	2.50	0.41
1:B:131:HIS:HD2	1:B:133:SER:CB	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1:NAG:O4	2:E:2:NAG:C2	2.63	0.41
1:A:305:PHE:HB3	1:A:306:PRO:HD2	2.02	0.41
1:A:279:LYS:HA	1:A:280:PRO:HA	1.90	0.41
1:B:105:ASP:OD1	1:B:108:TYR:N	2.49	0.41
1:C:187:ALA:HA	1:C:190:SER:OG	2.20	0.41
1:B:62:GLU:OE2	5:B:502:MD2:HC91	2.21	0.41
1:B:439:TYR:CZ	5:B:502:MD2:HC41	2.56	0.40
1:C:141:LEU:HD22	1:C:176:ARG:HB3	2.03	0.40
1:B:216:TYR:CE1	1:B:217:LEU:CD1	3.04	0.40

All (1) 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)
1:B:48:ASN:ND2	2:E:2:NAG:C8[9_765]	2.02	0.18

5.3 Torsion angles

5.3.1 Protein backbone

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%)	19 (4%)	0	100	100
1	B	460/472 (98%)	442 (96%)	18 (4%)	0	100	100
1	C	460/472 (98%)	442 (96%)	18 (4%)	0	100	100
All	All	1377/1416 (97%)	1322 (96%)	55 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	394/404 (98%)	388 (98%)	6 (2%)	57	56
1	B	397/404 (98%)	391 (98%)	6 (2%)	57	56
1	C	397/404 (98%)	394 (99%)	3 (1%)	73	75
All	All	1188/1212 (98%)	1173 (99%)	15 (1%)	61	61

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LEU
1	A	59	ASN
1	A	217	LEU
1	A	308	LYS
1	A	386	THR
1	A	434	GLU
1	B	59	ASN
1	B	105	ASP
1	B	177	VAL
1	B	217	LEU
1	B	411	ASN
1	B	454	LEU
1	C	59	ASN
1	C	115	LEU
1	C	127	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	152	ASN
1	A	234	ASN
1	A	359	GLN
1	A	360	GLN
1	A	431	HIS
1	A	456	ASN
1	B	131	HIS
1	B	149	HIS
1	B	152	ASN
1	B	360	GLN

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Mol	Chain	Res	Type
1	B	411	ASN
1	B	431	HIS
1	B	437	ASN
1	B	466	HIS
1	C	84	ASN
1	C	131	HIS
1	C	360	GLN
1	C	431	HIS
1	C	437	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

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	1.75	3 (21%)	17,19,21	3.27	10 (58%)
2	NAG	D	2	2	14,14,15	1.48	2 (14%)	17,19,21	2.19	5 (29%)
2	NAG	E	1	1,2	14,14,15	2.00	4 (28%)	17,19,21	3.11	11 (64%)
2	NAG	E	2	2	14,14,15	1.27	1 (7%)	17,19,21	3.18	6 (35%)
3	NAG	F	1	1,3	14,14,15	1.81	4 (28%)	17,19,21	4.29	12 (70%)
3	NAG	F	2	3	14,14,15	1.57	3 (21%)	17,19,21	2.82	5 (29%)
3	MAN	F	3	3	11,11,12	0.83	0	15,15,17	1.94	4 (26%)
3	MAN	F	4	3	11,11,12	0.77	0	15,15,17	1.51	4 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	FCA	F	5	3	10,10,11	1.55	1 (10%)	14,14,16	1.99	6 (42%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	D	1	1,2	-	0/6/23/26	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
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
3	NAG	F	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1
3	MAN	F	3	3	-	1/2/19/22	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 (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1	NAG	O5-C5	4.85	1.52	1.43
2	D	1	NAG	O5-C5	4.72	1.52	1.43
2	D	2	NAG	C1-C2	-3.72	1.47	1.52
3	F	2	NAG	O5-C5	3.59	1.50	1.43
2	E	1	NAG	C1-C2	-3.40	1.47	1.52
3	F	5	FCA	C2-C3	-3.35	1.47	1.52
3	F	1	NAG	C1-C2	-3.12	1.48	1.52
3	F	1	NAG	O5-C5	3.06	1.49	1.43
2	D	2	NAG	O5-C1	-2.97	1.38	1.43
2	D	1	NAG	O3-C3	2.88	1.50	1.43
3	F	2	NAG	O6-C6	2.76	1.54	1.42
3	F	1	NAG	C4-C3	-2.54	1.45	1.52
3	F	1	NAG	C6-C5	-2.53	1.43	1.51
2	E	2	NAG	C2-N2	2.51	1.50	1.46
2	E	1	NAG	O3-C3	2.45	1.49	1.43
2	E	1	NAG	C4-C3	-2.22	1.46	1.52
2	D	1	NAG	C1-C2	-2.08	1.49	1.52
3	F	2	NAG	O4-C4	-2.01	1.38	1.43

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	1	NAG	C8-C7-N2	-8.47	102.06	116.12
2	E	2	NAG	O6-C6-C5	8.14	139.05	111.33
3	F	2	NAG	O5-C5-C6	-7.85	92.39	107.66
3	F	1	NAG	C1-O5-C5	7.29	121.95	112.19
2	E	1	NAG	C2-N2-C7	-7.07	113.42	122.90
2	D	1	NAG	O6-C6-C5	6.85	134.65	111.33
3	F	1	NAG	O7-C7-C8	6.65	133.89	122.05
2	D	2	NAG	C2-N2-C7	-6.60	114.05	122.90
2	E	2	NAG	O5-C5-C6	-6.41	95.19	107.66
3	F	3	MAN	O2-C2-C3	5.81	122.19	110.15
3	F	1	NAG	O6-C6-C5	5.46	129.93	111.33
3	F	1	NAG	C6-C5-C4	5.03	125.36	113.02
2	D	1	NAG	C1-O5-C5	4.98	118.86	112.19
3	F	1	NAG	O5-C5-C6	-4.90	98.14	107.66
2	E	1	NAG	C1-O5-C5	4.77	118.58	112.19
3	F	2	NAG	O4-C4-C3	4.66	121.35	110.38
2	E	1	NAG	O6-C6-C5	4.60	126.98	111.33
2	D	1	NAG	C8-C7-N2	-4.43	108.78	116.12
3	F	2	NAG	C1-O5-C5	4.34	118.00	112.19
2	E	2	NAG	C2-N2-C7	-4.30	117.14	122.90
3	F	1	NAG	O4-C4-C3	4.22	120.31	110.38
2	D	1	NAG	O5-C5-C6	-4.17	99.54	107.66
2	D	1	NAG	C2-N2-C7	-3.84	117.75	122.90
2	D	1	NAG	O7-C7-C8	3.68	128.60	122.05
2	E	2	NAG	C6-C5-C4	3.60	121.87	113.02
2	D	1	NAG	C6-C5-C4	3.58	121.80	113.02
3	F	1	NAG	C4-C3-C2	3.42	116.04	111.02
3	F	2	NAG	O5-C5-C4	-3.42	102.50	110.83
2	E	1	NAG	O4-C4-C5	-3.41	100.92	109.32
2	E	1	NAG	O5-C5-C4	-3.32	102.75	110.83
2	E	2	NAG	C1-O5-C5	3.26	116.56	112.19
2	D	1	NAG	O4-C4-C5	-3.18	101.50	109.32
3	F	5	FCA	C1-C2-C3	3.17	114.26	109.64
3	F	1	NAG	O5-C1-C2	-3.13	106.44	111.29
3	F	4	MAN	O2-C2-C3	3.04	116.45	110.15
3	F	5	FCA	C1-O5-C5	3.02	120.09	112.97
3	F	1	NAG	C1-C2-N2	-3.02	105.68	110.43
3	F	5	FCA	C3-C4-C5	-2.99	105.27	109.81
3	F	5	FCA	O5-C5-C6	-2.97	100.95	107.40
2	E	1	NAG	O5-C5-C6	-2.97	101.88	107.66
3	F	4	MAN	C1-C2-C3	-2.79	105.58	109.64
3	F	1	NAG	C3-C4-C5	2.67	115.08	110.23
2	E	2	NAG	O4-C4-C3	2.67	116.66	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1	NAG	O3-C3-C4	2.56	116.40	110.38
2	E	1	NAG	O4-C4-C3	-2.49	104.51	110.38
3	F	5	FCA	O3-C3-C4	-2.47	104.55	110.38
2	E	1	NAG	O7-C7-C8	2.45	126.42	122.05
2	D	1	NAG	O3-C3-C4	2.45	116.15	110.38
3	F	3	MAN	C1-C2-C3	-2.44	106.10	109.64
2	E	1	NAG	O5-C1-C2	-2.37	107.62	111.29
2	D	1	NAG	C3-C4-C5	2.37	114.53	110.23
2	D	2	NAG	O4-C4-C5	2.36	115.13	109.32
2	D	2	NAG	O3-C3-C4	2.33	115.88	110.38
3	F	4	MAN	C3-C4-C5	-2.32	106.03	110.23
2	D	2	NAG	C8-C7-N2	-2.31	112.29	116.12
3	F	3	MAN	O5-C1-C2	2.28	116.23	110.79
3	F	1	NAG	O5-C5-C4	-2.28	105.28	110.83
3	F	2	NAG	O3-C3-C4	2.27	115.73	110.38
2	D	2	NAG	C6-C5-C4	2.25	118.55	113.02
3	F	4	MAN	O5-C1-C2	2.19	116.02	110.79
3	F	5	FCA	O3-C3-C2	2.11	114.36	110.05
3	F	3	MAN	C3-C4-C5	-2.07	106.48	110.23
2	E	1	NAG	C3-C4-C5	2.02	113.90	110.23

There are no chirality outliers.

All (11) torsion outliers are listed below:

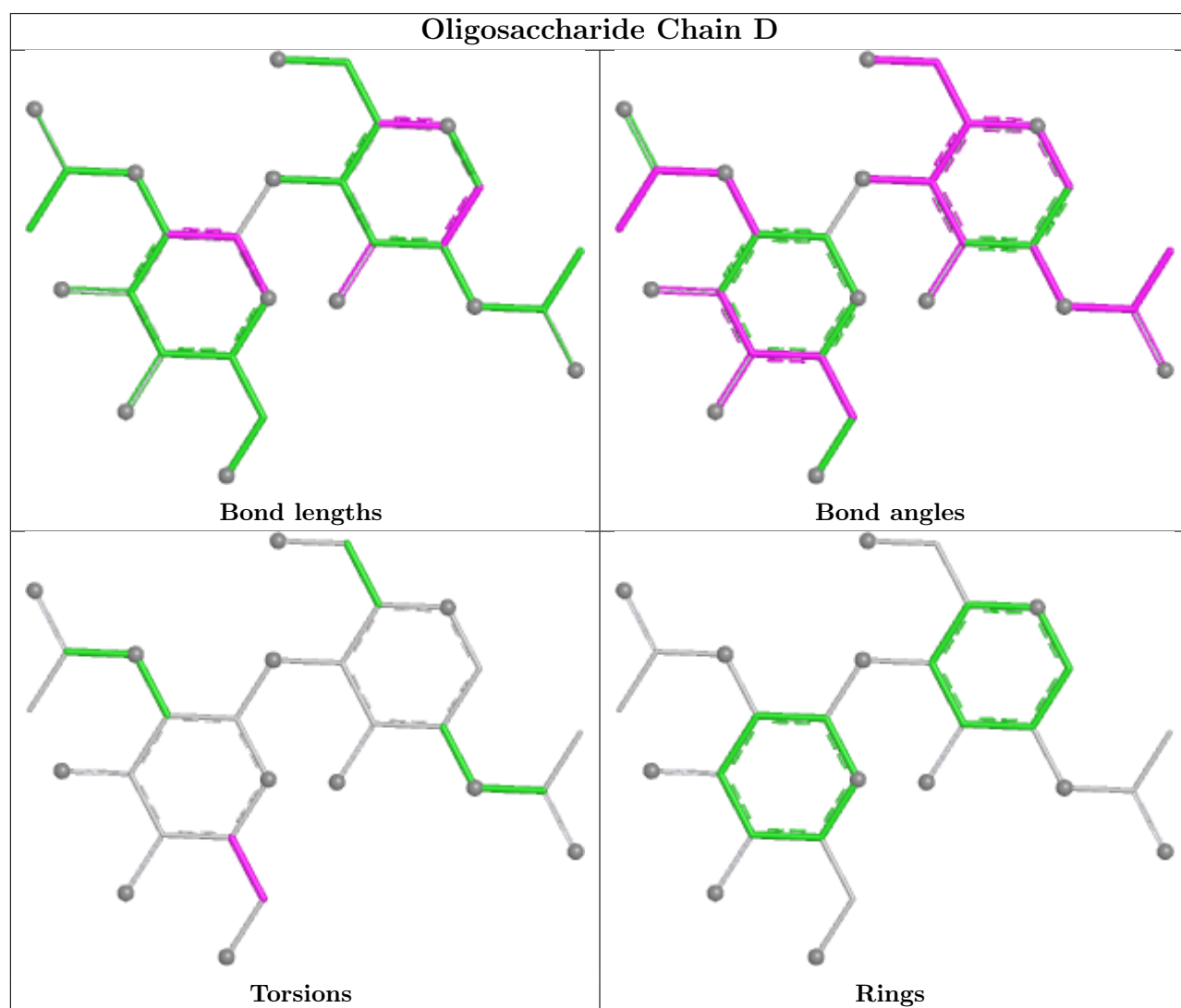
Mol	Chain	Res	Type	Atoms
2	D	2	NAG	C4-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
2	E	1	NAG	C4-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6
3	F	4	MAN	C4-C5-C6-O6
3	F	4	MAN	O5-C5-C6-O6
3	F	3	MAN	C4-C5-C6-O6

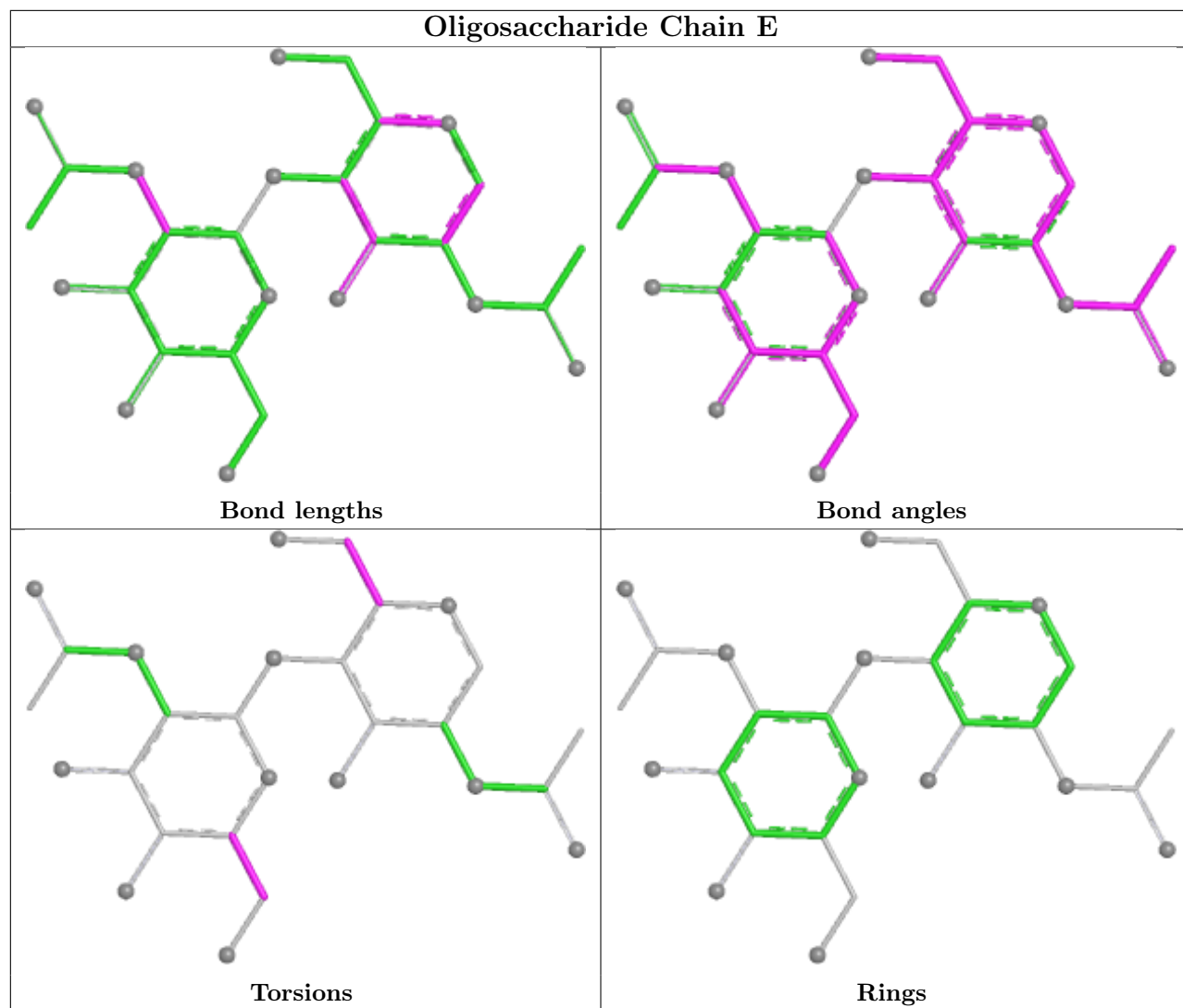
There are no ring outliers.

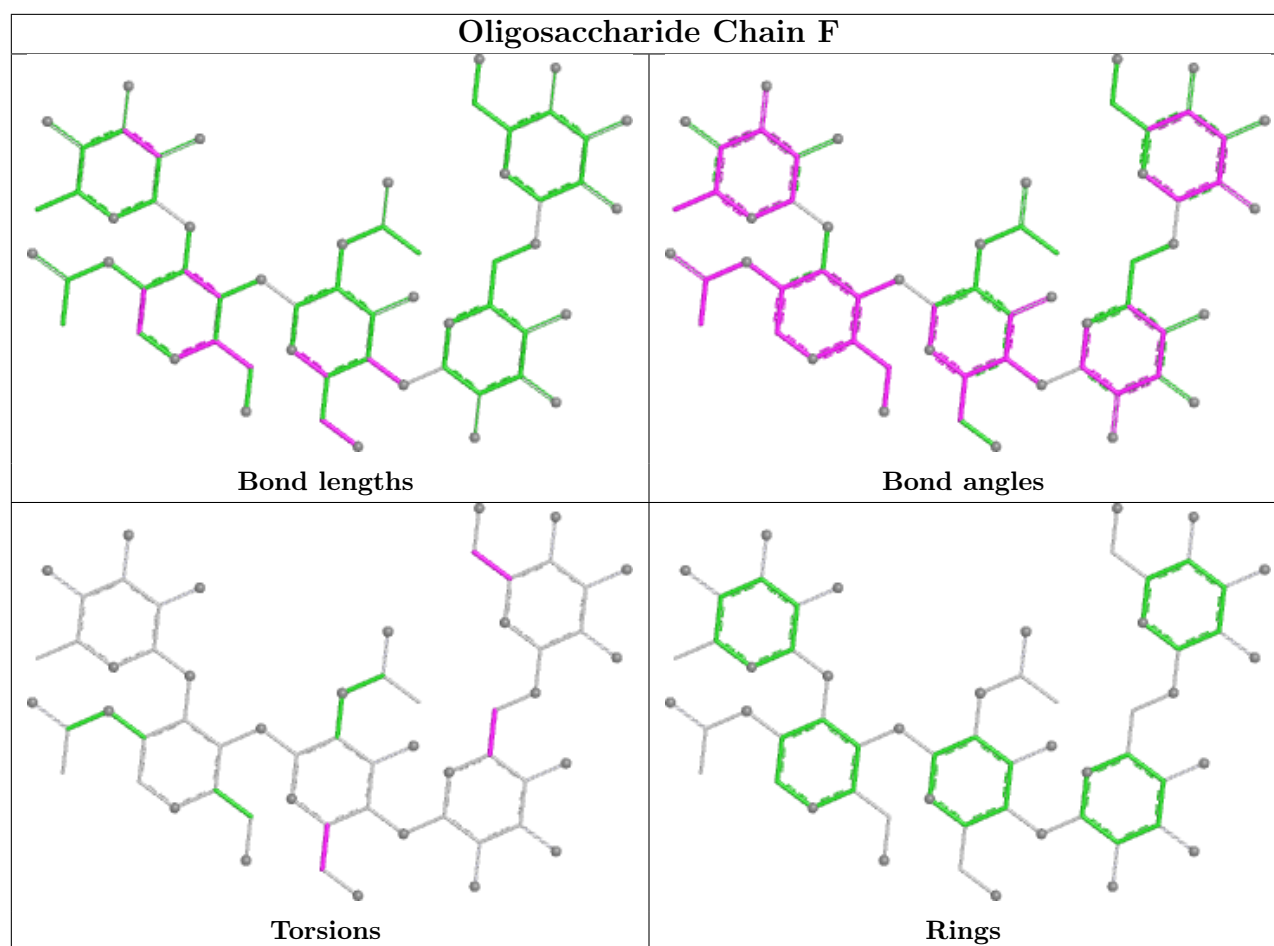
9 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	4	MAN	2	0
2	D	2	NAG	3	0
2	E	2	NAG	4	1
3	F	1	NAG	3	0
3	F	5	FCA	2	0
2	D	1	NAG	3	0
3	F	2	NAG	1	0
3	F	3	MAN	2	0
2	E	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](#)

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	MD2	C	502	-	11,13,13	1.00	1 (9%)	12,12,12	5.84	4 (33%)
5	MD2	A	502	-	11,13,13	0.88	0	12,12,12	3.86	4 (33%)
5	MD2	B	502	-	11,13,13	0.96	1 (9%)	12,12,12	3.07	4 (33%)
4	FAD	A	501	-	58,58,58	0.94	4 (6%)	85,89,89	1.28	12 (14%)
4	FAD	B	501	-	58,58,58	1.12	3 (5%)	85,89,89	1.25	11 (12%)
4	FAD	C	501	-	58,58,58	1.14	6 (10%)	85,89,89	1.20	9 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MD2	C	502	-	-	5/9/11/11	-
5	MD2	A	502	-	-	8/9/11/11	-
5	MD2	B	502	-	-	6/9/11/11	-
4	FAD	A	501	-	-	1/34/50/50	0/6/6/6
4	FAD	B	501	-	-	2/34/50/50	0/6/6/6
4	FAD	C	501	-	-	5/34/50/50	0/6/6/6

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	501	FAD	PA-O3P	5.01	1.64	1.59
4	C	501	FAD	PA-O3P	3.55	1.63	1.59
4	B	501	FAD	P-O3P	3.43	1.63	1.59
4	C	501	FAD	C4X-N5	3.15	1.37	1.30
4	A	501	FAD	C1'-C2'	2.54	1.56	1.52
4	A	501	FAD	C4X-N5	2.53	1.36	1.30
4	B	501	FAD	C4X-N5	2.49	1.36	1.30
4	C	501	FAD	C5'-C4'	2.36	1.55	1.51
5	C	502	MD2	C13-C12	2.35	1.34	1.29
4	C	501	FAD	C1'-C2'	2.29	1.55	1.52
4	C	501	FAD	C2-N1	-2.29	1.31	1.36
4	C	501	FAD	C9A-C5X	2.22	1.44	1.41
4	A	501	FAD	C5'-C4'	2.19	1.54	1.51
4	A	501	FAD	C5X-N5	-2.04	1.35	1.39
5	B	502	MD2	C13-C12	2.04	1.34	1.29

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	502	MD2	C4-C3-C2	15.71	135.90	124.22
5	C	502	MD2	C11-C12-C13	-11.26	115.85	124.22
5	B	502	MD2	C11-C12-C13	-8.32	118.04	124.22
5	A	502	MD2	C11-C12-C13	-8.26	118.08	124.22
5	A	502	MD2	C4-C3-C2	-7.94	118.32	124.22
4	A	501	FAD	C9A-C5X-N5	-5.42	116.70	122.45
5	A	502	MD2	C11-N10-C9	-5.25	102.21	112.85
5	B	502	MD2	C4-C3-C2	-4.83	120.63	124.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	502	MD2	C4-N5-C6	4.60	122.18	112.85
5	A	502	MD2	C8-C9-N10	-3.36	103.06	112.07
4	B	501	FAD	C4-N3-C2	-3.15	120.05	125.64
4	C	501	FAD	O4B-C1B-C2B	-3.08	100.02	106.62
4	A	501	FAD	C5'-C4'-C3'	-3.04	106.48	112.22
4	C	501	FAD	O3'-C3'-C2'	-2.99	102.14	108.93
4	C	501	FAD	O3P-PA-O1A	-2.80	102.27	110.70
5	B	502	MD2	C12-C11-N10	2.68	117.13	110.70
4	C	501	FAD	C4'-C3'-C2'	2.64	117.97	113.57
4	C	501	FAD	C4-C4X-N5	2.63	121.85	118.21
4	B	501	FAD	O4B-C1B-C2B	-2.63	100.99	106.62
4	A	501	FAD	O2'-C2'-C3'	-2.61	103.14	109.25
5	C	502	MD2	C11-N10-C9	2.46	117.85	112.85
4	C	501	FAD	C9A-C5X-N5	-2.42	119.89	122.45
4	A	501	FAD	O4-C4-N3	2.36	124.56	120.11
4	B	501	FAD	O4B-C1B-N9A	-2.35	103.57	108.09
4	A	501	FAD	C2B-C3B-C4B	2.31	107.07	102.61
5	B	502	MD2	C7-C6-N5	2.29	118.21	112.07
4	C	501	FAD	C10-N1-C2	2.28	121.78	116.85
4	C	501	FAD	N3A-C2A-N1A	2.26	132.00	128.58
4	B	501	FAD	C4X-C10-N10	2.23	119.68	116.48
4	B	501	FAD	C6-C7-C8	-2.22	116.42	119.69
4	A	501	FAD	O2A-PA-O1A	2.22	122.77	112.44
4	B	501	FAD	O3P-PA-O1A	-2.21	104.05	110.70
4	A	501	FAD	C6-C5X-C9A	2.21	122.08	119.05
4	B	501	FAD	N6A-C6A-N1A	2.17	123.22	118.38
4	B	501	FAD	C4A-C5A-N7A	2.16	113.05	110.58
4	A	501	FAD	C8M-C8-C9	-2.14	115.79	119.57
4	A	501	FAD	O4-C4-C4X	-2.14	120.89	126.53
4	C	501	FAD	O2A-PA-O1A	2.11	122.28	112.44
4	B	501	FAD	C10-N1-C2	2.10	121.39	116.85
4	A	501	FAD	C4'-C3'-C2'	2.10	117.06	113.57
4	A	501	FAD	C9-C8-C7	2.08	122.74	119.69
4	B	501	FAD	C4X-C10-N1	-2.08	119.50	124.59
4	B	501	FAD	C10-C4X-N5	-2.02	120.69	124.81
4	A	501	FAD	C6-C7-C8	-2.00	116.75	119.69

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	501	FAD	C5B-O5B-PA-O1A

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Mol	Chain	Res	Type	Atoms
5	A	502	MD2	N10-C11-C12-C13
5	B	502	MD2	N10-C11-C12-C13
5	B	502	MD2	N5-C6-C7-C8
5	C	502	MD2	C3-C4-N5-C6
5	A	502	MD2	C8-C9-N10-C11
5	A	502	MD2	N5-C6-C7-C8
5	C	502	MD2	N5-C6-C7-C8
5	A	502	MD2	C3-C4-N5-C6
5	B	502	MD2	C3-C4-N5-C6
4	C	501	FAD	O3'-C3'-C4'-O4'
5	A	502	MD2	C6-C7-C8-C9
4	A	501	FAD	PA-O3P-P-O5'
5	A	502	MD2	C12-C11-N10-C9
5	C	502	MD2	N10-C11-C12-C13
5	A	502	MD2	C7-C8-C9-N10
5	C	502	MD2	C12-C11-N10-C9
5	C	502	MD2	C8-C9-N10-C11
5	A	502	MD2	C7-C6-N5-C4
5	B	502	MD2	C8-C9-N10-C11
5	B	502	MD2	C12-C11-N10-C9
5	B	502	MD2	C7-C6-N5-C4
4	C	501	FAD	C2B-C1B-N9A-C8A
4	C	501	FAD	O4B-C4B-C5B-O5B
4	C	501	FAD	O3'-C3'-C4'-C5'
4	B	501	FAD	C2'-C3'-C4'-O4'
4	B	501	FAD	O4B-C4B-C5B-O5B

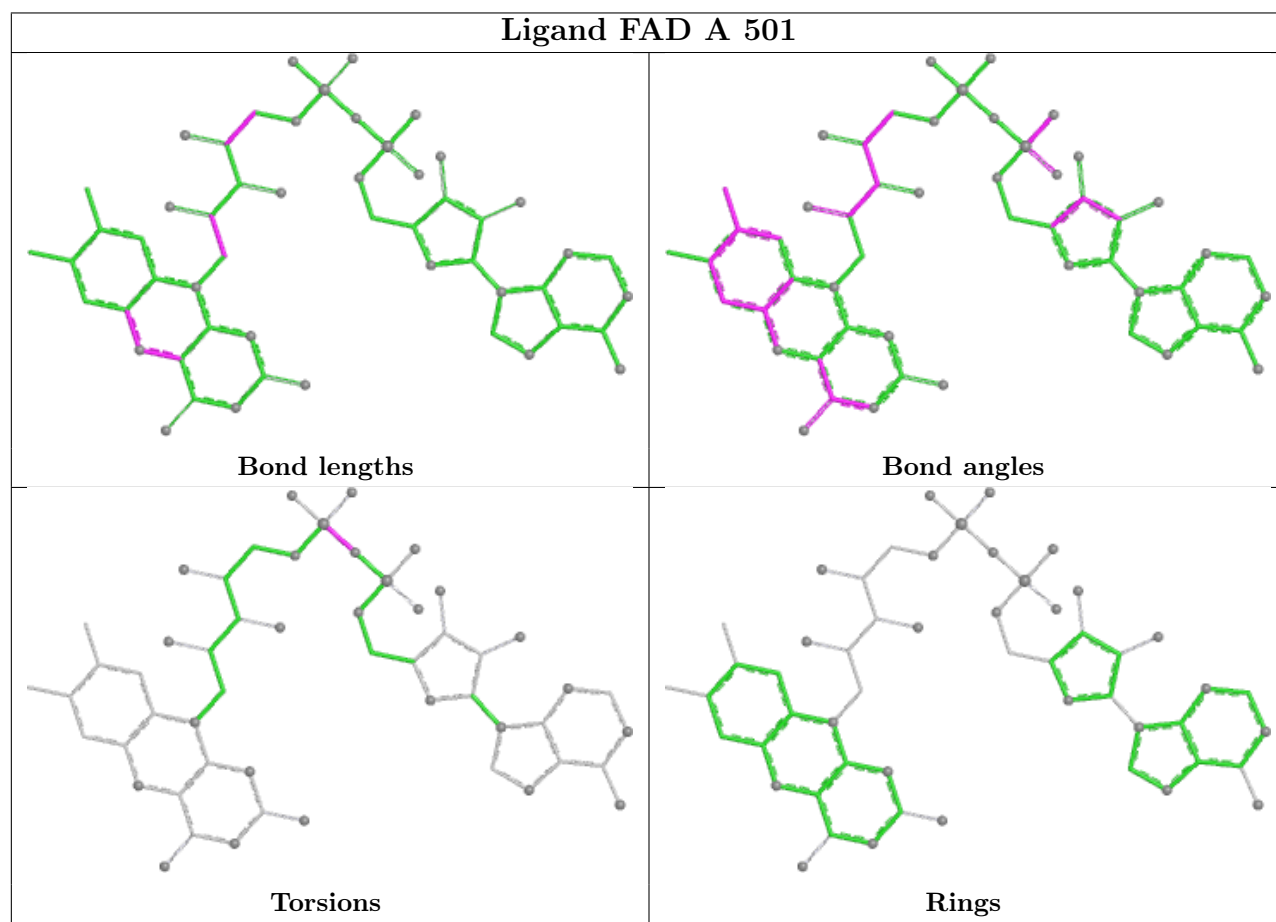
There are no ring outliers.

4 monomers are involved in 16 short contacts:

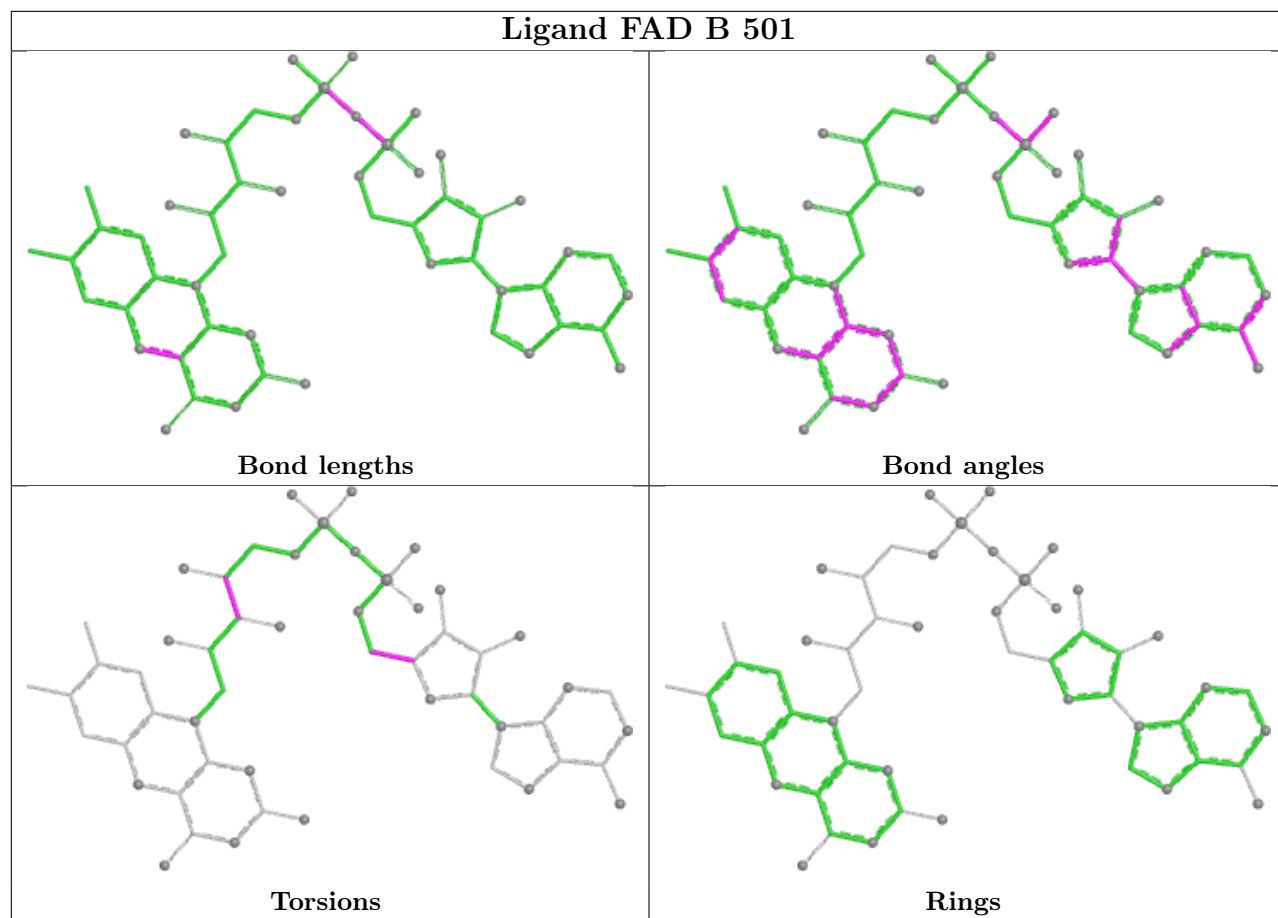
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	502	MD2	6	0
5	A	502	MD2	4	0
5	B	502	MD2	5	0
4	A	501	FAD	1	0

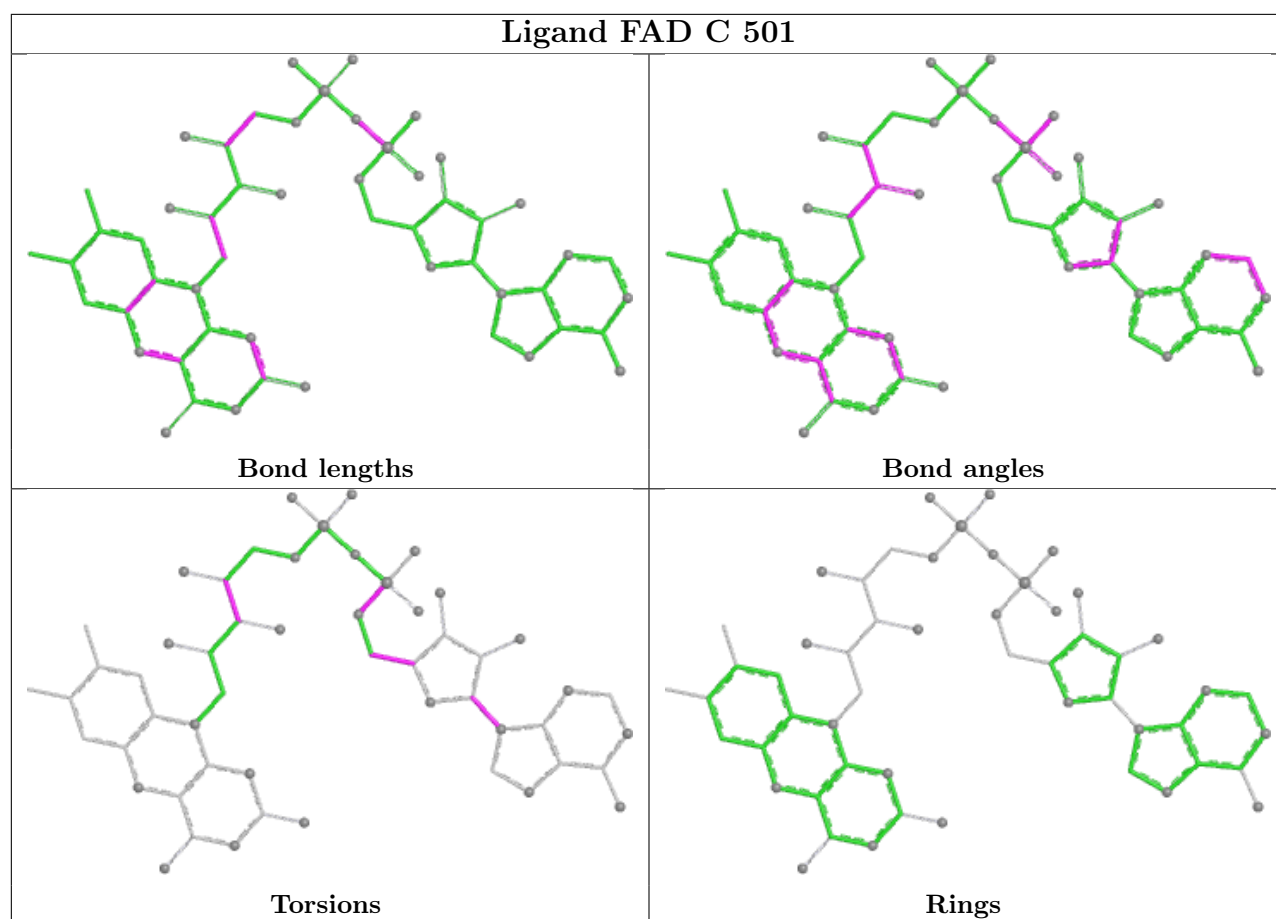
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



Ligand FAD B 501





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	459/472 (97%)	-0.38	15 (3%) 49 52	6, 14, 37, 69	20 (4%)
1	B	462/472 (97%)	-0.51	9 (1%) 66 70	4, 13, 35, 70	18 (3%)
1	C	462/472 (97%)	-0.56	8 (1%) 69 72	5, 12, 35, 57	15 (3%)
All	All	1383/1416 (97%)	-0.48	32 (2%) 61 65	4, 13, 36, 70	53 (3%)

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	466	HIS	5.3
1	A	221	ASP	5.1
1	C	221	ASP	4.7
1	A	100	ASP	4.0
1	A	341	ASP	3.9
1	B	463	CYS	3.8
1	A	222	LYS	3.7
1	C	50	ALA	3.6
1	C	341	ASP	3.6
1	A	381	ASP	3.1
1	C	466	HIS	3.1
1	B	462	MET	3.0
1	A	220	ASP	3.0
1	A	202	GLN	3.0
1	A	274	ASP	2.8
1	A	223	SER	2.7
1	C	222	LYS	2.7
1	B	221	ASP	2.6
1	A	52	ILE	2.5
1	B	100	ASP	2.5
1	C	254	ASN	2.5
1	C	105	ASP	2.5
1	A	50	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	222	LYS	2.4
1	A	384	ASP	2.3
1	B	274	ASP	2.3
1	B	225	LYS	2.3
1	C	384	ASP	2.2
1	B	107	ASP	2.1
1	A	149	HIS	2.1
1	A	379	GLY	2.0
1	A	387	ASP	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](#)

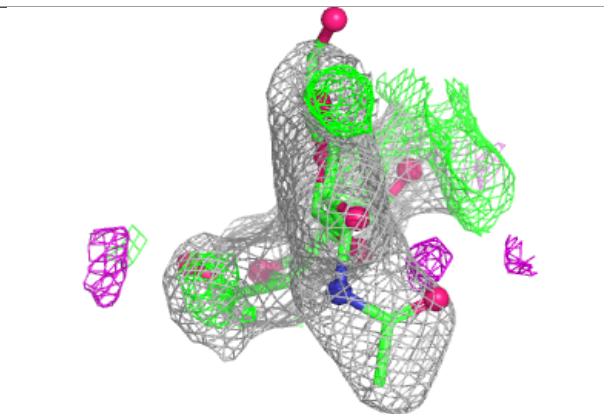
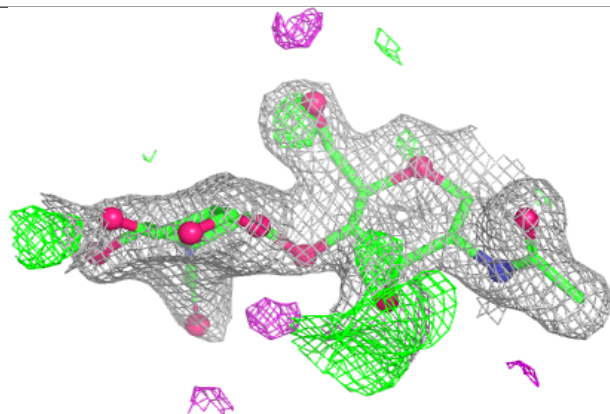
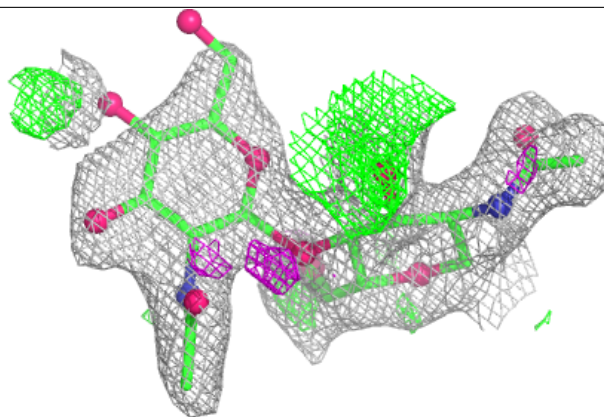
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MAN	F	3	11/12	0.76	0.18	24,36,53,55	0
3	FCA	F	5	10/11	0.77	0.20	9,34,42,75	0
3	MAN	F	4	11/12	0.79	0.18	30,40,63,96	0
3	NAG	F	2	14/15	0.79	0.17	3,12,39,74	0
2	NAG	D	2	14/15	0.81	0.18	26,53,100,100	0
2	NAG	D	1	14/15	0.84	0.17	17,35,71,100	0
2	NAG	E	2	14/15	0.84	0.20	14,46,98,100	0
2	NAG	E	1	14/15	0.89	0.15	9,24,38,100	0
3	NAG	F	1	14/15	0.89	0.13	1,12,24,57	0

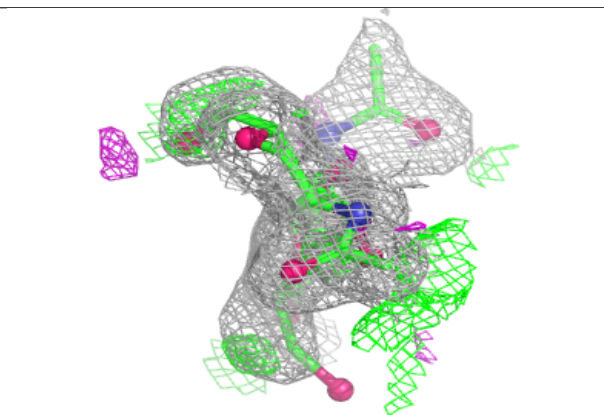
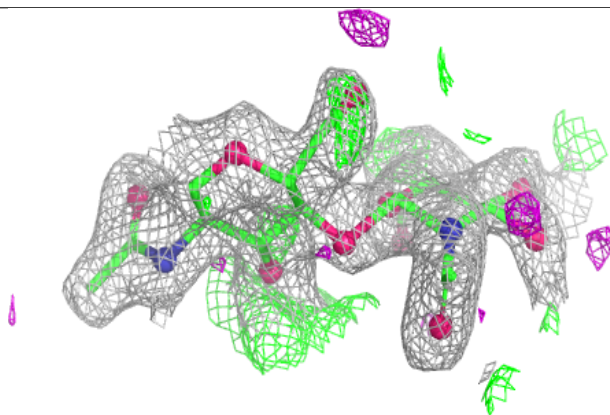
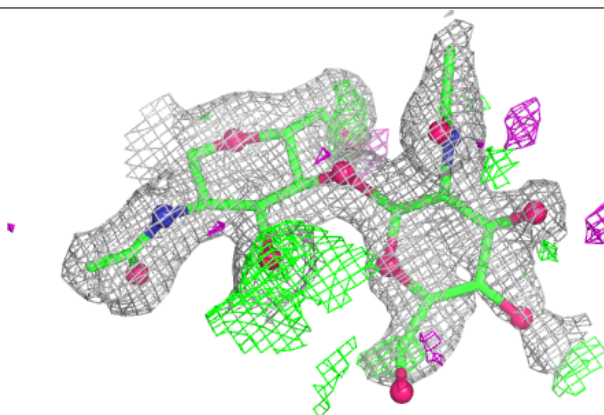
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

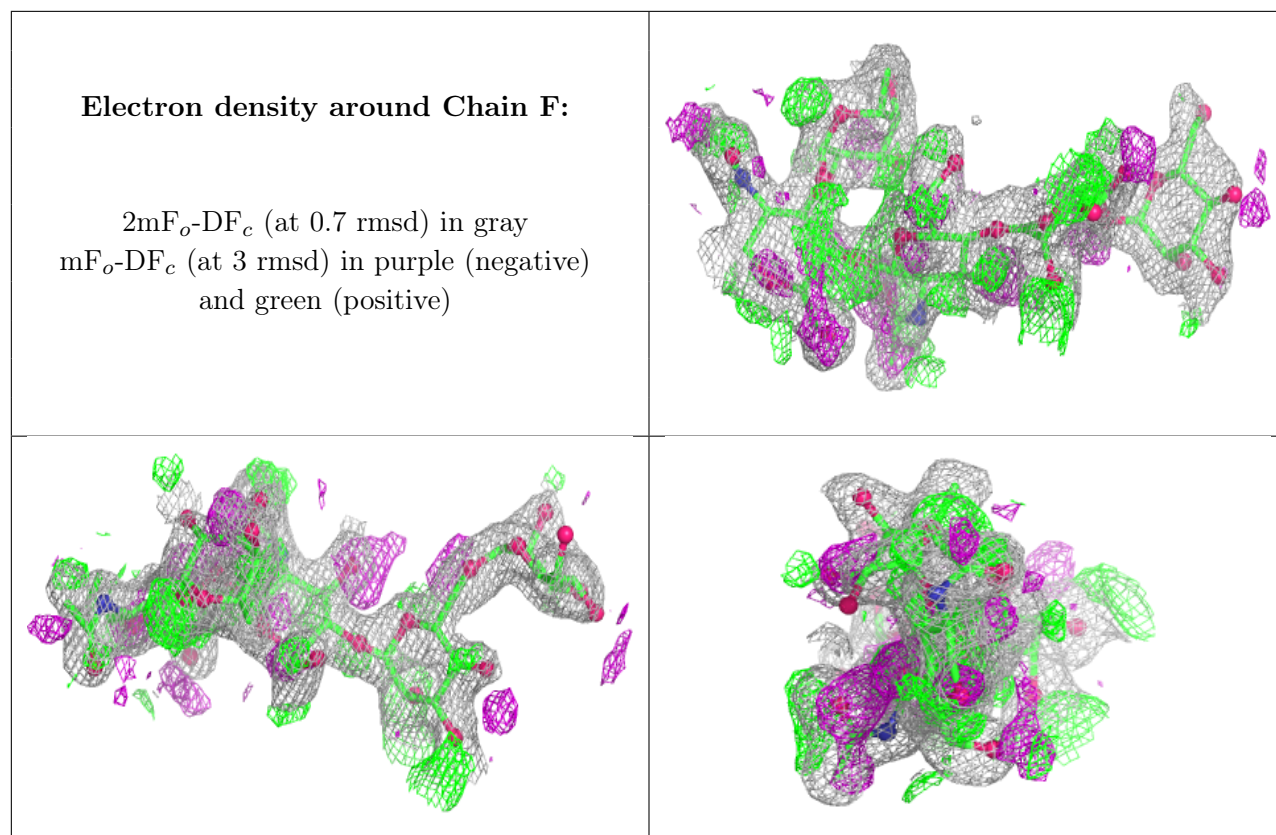
Electron density around Chain D:

$2mF_o-DF_c$ (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)





6.4 Ligands [i](#)

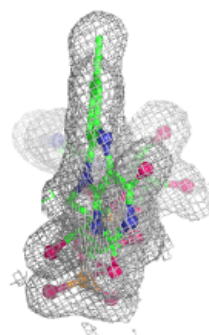
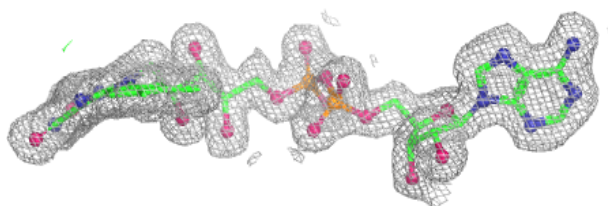
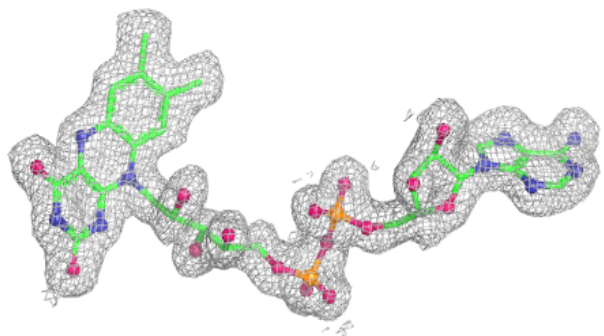
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	MD2	A	502	14/14	0.91	0.10	19,32,39,41	0
5	MD2	B	502	14/14	0.92	0.13	13,33,55,55	0
5	MD2	C	502	14/14	0.92	0.11	19,30,38,46	0
4	FAD	A	501	53/53	0.99	0.03	3,9,13,16	0
4	FAD	B	501	53/53	0.99	0.03	1,6,9,10	0
4	FAD	C	501	53/53	0.99	0.04	3,7,12,12	0

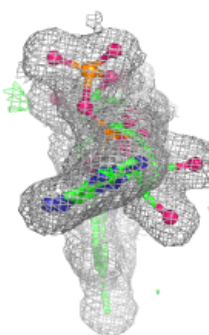
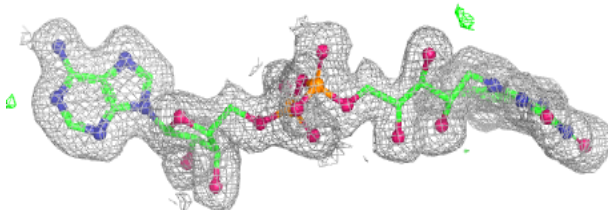
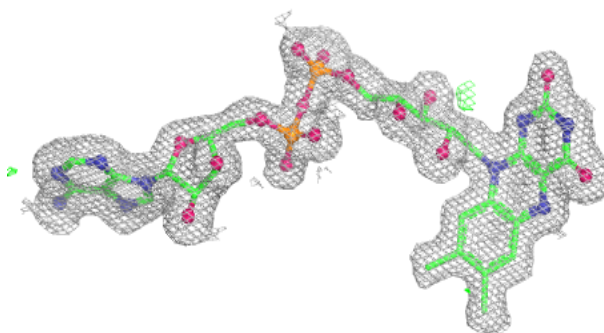
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

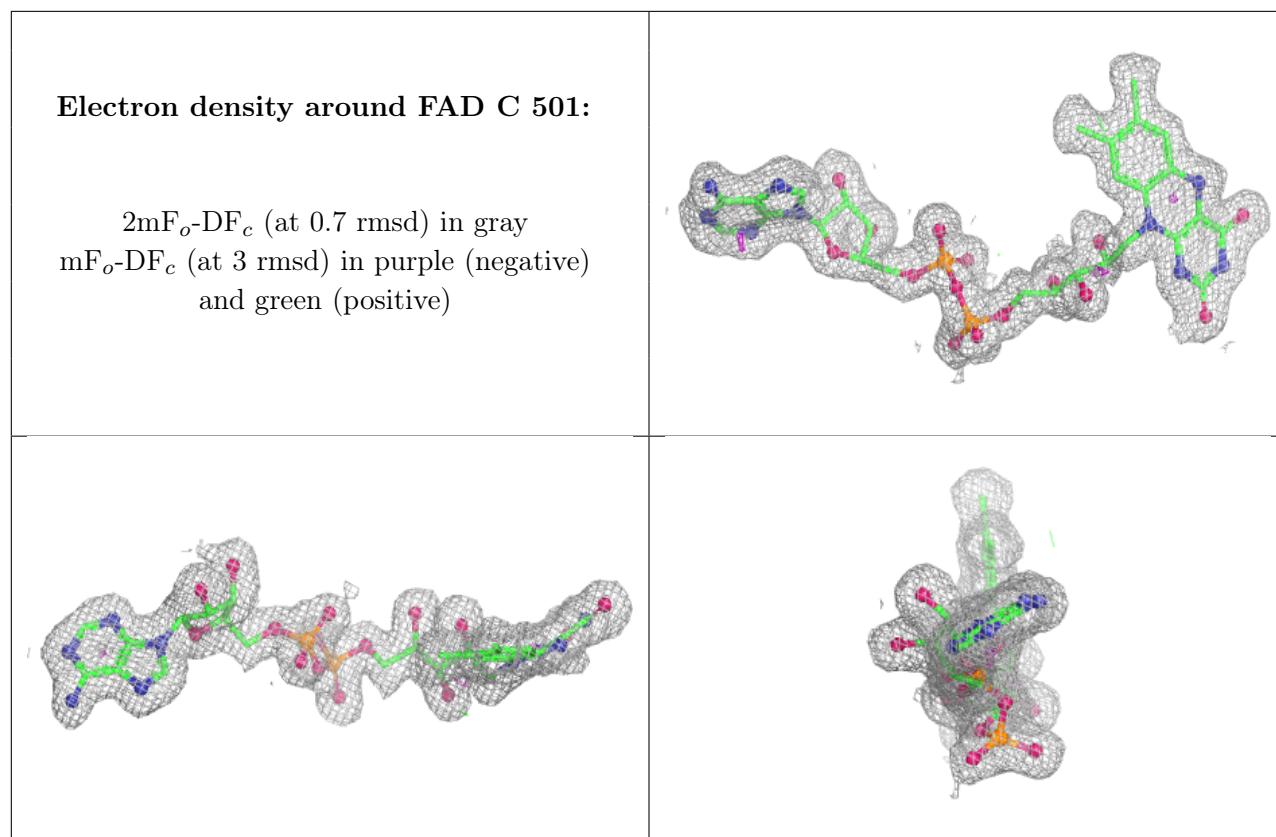
Electron density around FAD A 501:

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

**Electron density around FAD B 501:**

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





6.5 Other polymers [i](#)

There are no such residues in this entry.