



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 06:21 AM UTC

PDB ID : 6G4G / pdb_00006g4g
Title : Full length ectodomain of ectonucleotide phosphodiesterase/pyrophosphatase
-3 (NPP3) including the SMB domains but with a partially disordered active
site structure
Authors : Dohler, C.; Zebisch, M.; Strater, N.
Deposited on : 2018-03-27
Resolution : 2.80 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
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

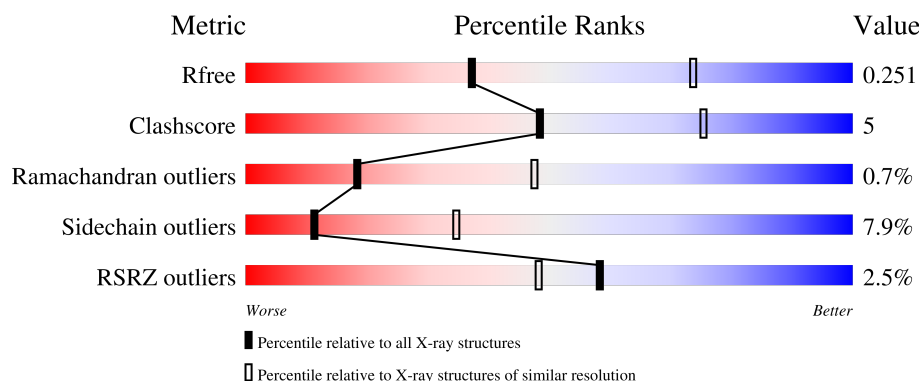
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

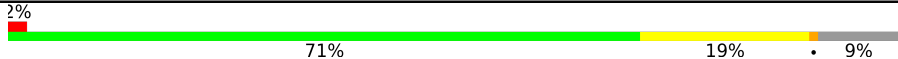
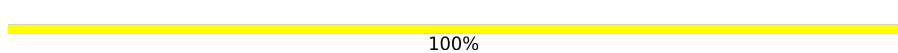
The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



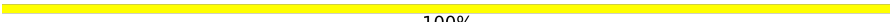
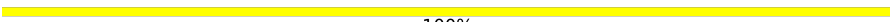
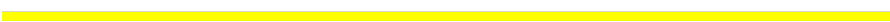
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	840	
1	B	840	
1	C	840	
1	D	840	
2	E	2	

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Mol	Chain	Length	Quality of chain
2	F	2	 100%
2	G	2	 100%
2	H	2	 100%
2	I	2	 100%
2	J	2	 100%
2	K	2	 100%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 24786 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 Ectonucleotide pyrophosphatase/phosphodiesterase family member 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	765	Total	C	N	O	S	0	0	0
			6131	3903	1040	1140	48			
1	B	759	Total	C	N	O	S	0	0	0
			6087	3871	1035	1134	47			
1	C	742	Total	C	N	O	S	0	0	0
			5982	3818	1016	1102	46			
1	D	781	Total	C	N	O	S	0	0	0
			6274	3991	1064	1171	48			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	45	ALA	-	expression tag	UNP P97675
A	46	GLU	-	expression tag	UNP P97675
A	47	THR	-	expression tag	UNP P97675
A	48	GLY	-	expression tag	UNP P97675
A	201	VAL	MET	variant	UNP P97675
A	596	ASN	SER	variant	UNP P97675
A	597	ARG	GLY	variant	UNP P97675
A	876	GLY	-	expression tag	UNP P97675
A	877	THR	-	expression tag	UNP P97675
A	878	LYS	-	expression tag	UNP P97675
A	879	HIS	-	expression tag	UNP P97675
A	880	HIS	-	expression tag	UNP P97675
A	881	HIS	-	expression tag	UNP P97675
A	882	HIS	-	expression tag	UNP P97675
A	883	HIS	-	expression tag	UNP P97675
A	884	HIS	-	expression tag	UNP P97675
B	45	ALA	-	expression tag	UNP P97675
B	46	GLU	-	expression tag	UNP P97675
B	47	THR	-	expression tag	UNP P97675
B	48	GLY	-	expression tag	UNP P97675

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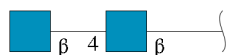
Chain	Residue	Modelled	Actual	Comment	Reference
B	201	VAL	MET	variant	UNP P97675
B	596	ASN	SER	variant	UNP P97675
B	597	ARG	GLY	variant	UNP P97675
B	876	GLY	-	expression tag	UNP P97675
B	877	THR	-	expression tag	UNP P97675
B	878	LYS	-	expression tag	UNP P97675
B	879	HIS	-	expression tag	UNP P97675
B	880	HIS	-	expression tag	UNP P97675
B	881	HIS	-	expression tag	UNP P97675
B	882	HIS	-	expression tag	UNP P97675
B	883	HIS	-	expression tag	UNP P97675
B	884	HIS	-	expression tag	UNP P97675
C	45	ALA	-	expression tag	UNP P97675
C	46	GLU	-	expression tag	UNP P97675
C	47	THR	-	expression tag	UNP P97675
C	48	GLY	-	expression tag	UNP P97675
C	201	VAL	MET	variant	UNP P97675
C	596	ASN	SER	variant	UNP P97675
C	597	ARG	GLY	variant	UNP P97675
C	876	GLY	-	expression tag	UNP P97675
C	877	THR	-	expression tag	UNP P97675
C	878	LYS	-	expression tag	UNP P97675
C	879	HIS	-	expression tag	UNP P97675
C	880	HIS	-	expression tag	UNP P97675
C	881	HIS	-	expression tag	UNP P97675
C	882	HIS	-	expression tag	UNP P97675
C	883	HIS	-	expression tag	UNP P97675
C	884	HIS	-	expression tag	UNP P97675
D	45	ALA	-	expression tag	UNP P97675
D	46	GLU	-	expression tag	UNP P97675
D	47	THR	-	expression tag	UNP P97675
D	48	GLY	-	expression tag	UNP P97675
D	201	VAL	MET	variant	UNP P97675
D	596	ASN	SER	variant	UNP P97675
D	597	ARG	GLY	variant	UNP P97675
D	876	GLY	-	expression tag	UNP P97675
D	877	THR	-	expression tag	UNP P97675
D	878	LYS	-	expression tag	UNP P97675
D	879	HIS	-	expression tag	UNP P97675
D	880	HIS	-	expression tag	UNP P97675
D	881	HIS	-	expression tag	UNP P97675
D	882	HIS	-	expression tag	UNP P97675

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Chain	Residue	Modelled	Actual	Comment	Reference
D	883	HIS	-	expression tag	UNP P97675
D	884	HIS	-	expression tag	UNP P97675

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

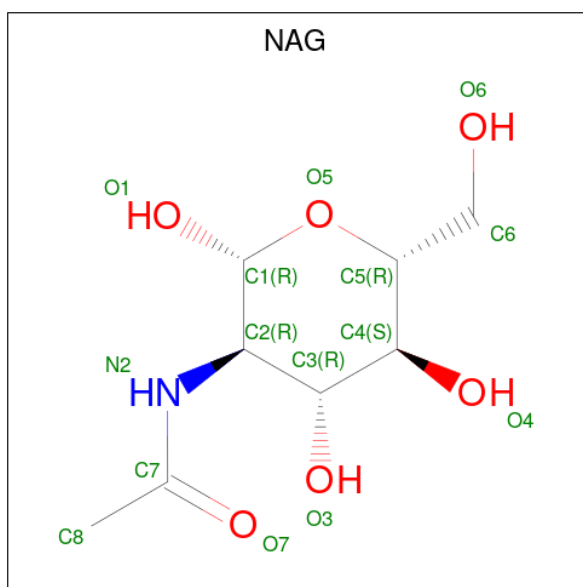


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	J	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	K	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		
3	B	1	Total	Ca	0	0
			1	1		
3	C	1	Total	Ca	0	0
			1	1		
3	D	1	Total	Ca	0	0
			1	1		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

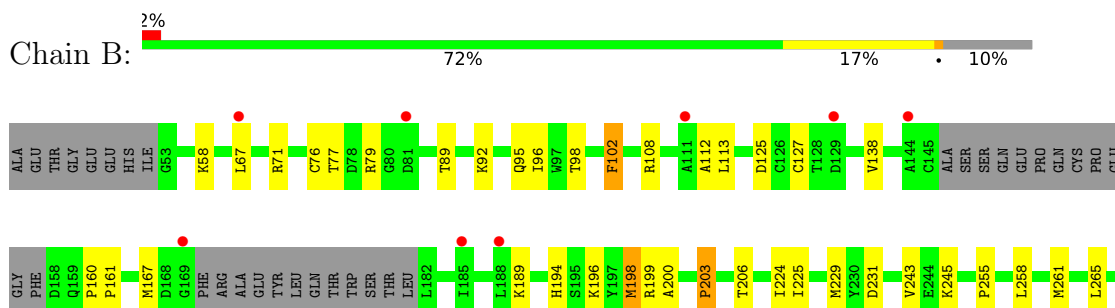
3 Residue-property plots

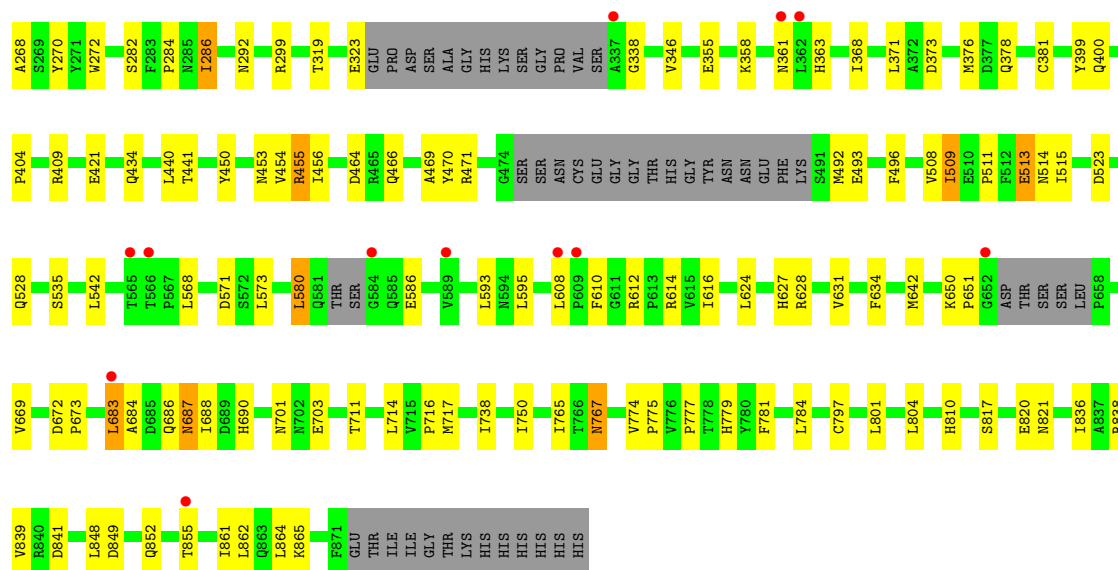
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Ectonucleotide pyrophosphatase/phosphodiesterase family member 3

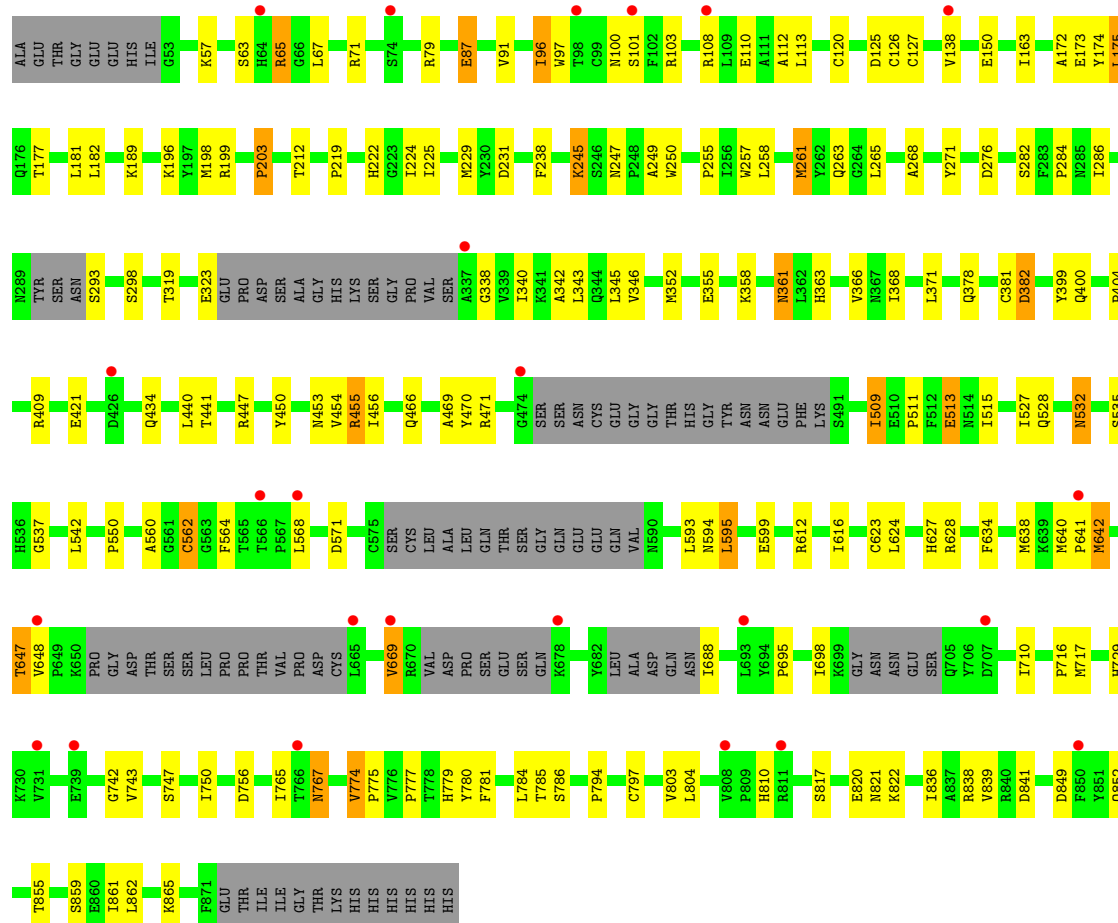


- Molecule 1: Ectonucleotide pyrophosphatase/phosphodiesterase family member 3





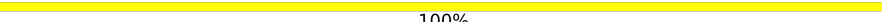
- Molecule 1: Ectonucleotide pyrophosphatase/phosphodiesterase family member 3



- Molecule 1: Ectonucleotide pyrophosphatase/phosphodiesterase family member 3

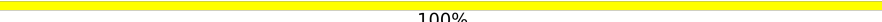


- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E: 

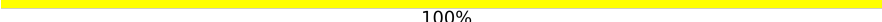
MAG1
MAG2

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

Chain F: 

MAG1
MAG2

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

Chain G: 

MAG1
MAG2

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

Chain H:  100%

MAG1
MAG2

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

Chain I:  100%

MAG1
MAG2

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

Chain J:  100%

MAG1
MAG2

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

Chain K:  100%

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	76.36Å 116.30Å 124.16Å 86.77° 87.76° 88.20°	Depositor
Resolution (Å)	47.22 – 2.80 47.22 – 2.80	Depositor EDS
% Data completeness (in resolution range)	65.3 (47.22-2.80) 65.3 (47.22-2.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.35 (at 2.81Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.196 , 0.237 0.209 , 0.251	Depositor DCC
R_{free} test set	3360 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	59.9	Xtriage
Anisotropy	0.168	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 75.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.044 for h,-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	24786	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% 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, CA

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	2/6303 (0.0%)	1.34	37/8565 (0.4%)
1	B	0.81	0/6254	1.32	27/8495 (0.3%)
1	C	0.85	1/6148 (0.0%)	1.33	23/8345 (0.3%)
1	D	0.88	1/6449 (0.0%)	1.37	49/8763 (0.6%)
All	All	0.86	4/25154 (0.0%)	1.34	136/34168 (0.4%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	198	MET	SD-CE	-8.95	1.57	1.79
1	A	114	CYS	CA-C	6.57	1.61	1.53
1	D	758	HIS	CA-C	-5.72	1.45	1.52
1	C	261	MET	SD-CE	-5.08	1.66	1.79

All (136) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	101	SER	CA-C-N	8.41	132.38	120.28
1	D	101	SER	C-N-CA	8.41	132.38	120.28
1	A	516	GLU	CA-C-N	8.14	131.10	120.60
1	A	516	GLU	C-N-CA	8.14	131.10	120.60
1	C	767	ASN	CA-CB-CG	7.62	120.22	112.60
1	D	767	ASN	CA-CB-CG	7.42	120.02	112.60
1	B	767	ASN	CA-CB-CG	7.29	119.89	112.60
1	D	99	CYS	CA-C-N	-7.25	107.69	121.54
1	D	99	CYS	C-N-CA	-7.25	107.69	121.54
1	B	687	ASN	CA-CB-CG	7.20	119.80	112.60
1	A	492	MET	CA-C-N	7.18	131.96	121.26
1	A	492	MET	C-N-CA	7.18	131.96	121.26
1	C	440	LEU	N-CA-C	-6.98	98.23	109.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	338	GLY	CA-C-N	6.91	129.40	120.56
1	A	338	GLY	C-N-CA	6.91	129.40	120.56
1	D	198	MET	CA-C-N	6.86	131.18	121.02
1	D	198	MET	C-N-CA	6.86	131.18	121.02
1	D	440	LEU	N-CA-C	-6.81	98.52	109.96
1	A	440	LEU	N-CA-C	-6.72	98.66	109.96
1	D	516	GLU	CA-C-N	6.71	129.25	120.60
1	D	516	GLU	C-N-CA	6.71	129.25	120.60
1	D	101	SER	N-CA-C	-6.67	103.93	111.07
1	B	440	LEU	N-CA-C	-6.60	98.87	109.96
1	A	203	PRO	CA-C-N	-6.52	112.03	122.66
1	A	203	PRO	C-N-CA	-6.52	112.03	122.66
1	D	338	GLY	CA-C-N	6.38	129.86	120.74
1	D	338	GLY	C-N-CA	6.38	129.86	120.74
1	D	189	LYS	CA-C-N	6.37	129.06	120.65
1	D	189	LYS	C-N-CA	6.37	129.06	120.65
1	C	532	ASN	CA-CB-CG	6.36	118.95	112.60
1	A	841	ASP	CA-C-N	6.25	128.51	120.70
1	A	841	ASP	C-N-CA	6.25	128.51	120.70
1	D	323	GLU	CB-CG-CD	6.18	123.11	112.60
1	D	756	ASP	CA-CB-CG	6.11	118.71	112.60
1	B	203	PRO	CA-C-N	-6.11	112.71	122.66
1	B	203	PRO	C-N-CA	-6.11	112.71	122.66
1	D	203	PRO	CA-C-N	-6.10	112.71	122.66
1	D	203	PRO	C-N-CA	-6.10	112.71	122.66
1	C	203	PRO	CA-C-N	-6.06	112.78	122.66
1	C	203	PRO	C-N-CA	-6.06	112.78	122.66
1	C	642	MET	N-CA-C	-6.05	106.03	113.41
1	D	94	THR	N-CA-C	-6.05	106.54	114.04
1	C	189	LYS	CA-C-N	6.01	128.58	120.65
1	C	189	LYS	C-N-CA	6.01	128.58	120.65
1	C	112	ALA	CA-C-N	6.00	128.61	120.44
1	C	112	ALA	C-N-CA	6.00	128.61	120.44
1	B	189	LYS	CA-C-N	5.99	128.55	120.65
1	B	189	LYS	C-N-CA	5.99	128.55	120.65
1	B	686	GLN	N-CA-C	-5.97	101.37	110.14
1	B	492	MET	CA-C-N	5.92	130.07	121.26
1	B	492	MET	C-N-CA	5.92	130.07	121.26
1	D	537	GLY	CA-C-N	5.87	128.40	120.65
1	D	537	GLY	C-N-CA	5.87	128.40	120.65
1	B	642	MET	N-CA-C	-5.85	106.05	113.43
1	C	125	ASP	CA-CB-CG	5.78	118.38	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	338	GLY	CA-C-N	5.78	129.00	120.74
1	C	338	GLY	C-N-CA	5.78	129.00	120.74
1	D	102	PHE	N-CA-C	5.78	118.35	111.71
1	C	454	VAL	CA-C-N	5.65	128.42	120.28
1	C	454	VAL	C-N-CA	5.65	128.42	120.28
1	D	109	LEU	N-CA-C	5.62	120.42	113.50
1	C	756	ASP	CA-CB-CG	5.62	118.22	112.60
1	B	454	VAL	CA-C-N	5.57	128.31	120.28
1	B	454	VAL	C-N-CA	5.57	128.31	120.28
1	D	112	ALA	CA-C-N	5.56	128.00	120.44
1	D	112	ALA	C-N-CA	5.56	128.00	120.44
1	C	562	CYS	CA-C-N	5.55	125.38	120.10
1	C	562	CYS	C-N-CA	5.55	125.38	120.10
1	A	125	ASP	CA-CB-CG	5.53	118.13	112.60
1	D	851	TYR	CA-C-N	5.52	128.44	120.38
1	D	851	TYR	C-N-CA	5.52	128.44	120.38
1	B	338	GLY	CA-C-N	5.52	128.63	120.74
1	B	338	GLY	C-N-CA	5.52	128.63	120.74
1	D	346	VAL	N-CA-CB	5.50	118.84	110.58
1	C	399	TYR	N-CA-C	-5.47	100.19	108.67
1	A	635	GLY	CA-C-N	5.46	127.92	120.54
1	A	635	GLY	C-N-CA	5.46	127.92	120.54
1	C	382	ASP	CA-CB-CG	5.45	118.05	112.60
1	C	571	ASP	CA-CB-CG	5.44	118.04	112.60
1	D	782	VAL	N-CA-CB	5.43	120.03	111.99
1	B	112	ALA	CA-C-N	5.43	127.82	120.44
1	B	112	ALA	C-N-CA	5.43	127.82	120.44
1	A	517	VAL	N-CA-C	5.41	116.04	110.36
1	B	634	PHE	N-CA-C	5.38	117.28	108.52
1	D	454	VAL	CA-C-N	5.37	128.01	120.28
1	D	454	VAL	C-N-CA	5.37	128.01	120.28
1	A	454	VAL	CA-C-N	5.37	128.01	120.28
1	A	454	VAL	C-N-CA	5.37	128.01	120.28
1	D	339	VAL	N-CA-C	-5.36	105.62	110.82
1	B	571	ASP	CA-CB-CG	5.34	117.94	112.60
1	A	681	PHE	CA-CB-CG	5.34	119.14	113.80
1	B	821	ASN	CA-C-N	5.33	129.25	121.31
1	B	821	ASN	C-N-CA	5.33	129.25	121.31
1	B	125	ASP	CA-CB-CG	5.32	117.92	112.60
1	D	803	VAL	N-CA-CB	-5.30	102.69	112.43
1	A	178	TRP	CA-C-N	5.29	128.15	120.79
1	A	178	TRP	C-N-CA	5.29	128.15	120.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	399	TYR	N-CA-C	-5.27	99.92	108.41
1	D	760	ASP	CA-CB-CG	5.26	117.86	112.60
1	A	189	LYS	CA-C-N	5.25	127.58	120.65
1	A	189	LYS	C-N-CA	5.25	127.58	120.65
1	D	856	GLN	N-CA-C	-5.21	103.53	108.22
1	B	102	PHE	CA-CB-CG	5.20	119.00	113.80
1	D	687	ASN	N-CA-C	-5.20	106.62	113.17
1	A	276	ASP	CA-CB-CG	5.18	117.78	112.60
1	B	464	ASP	CA-CB-CG	5.16	117.76	112.60
1	D	492	MET	CA-C-N	5.15	131.37	121.54
1	D	492	MET	C-N-CA	5.15	131.37	121.54
1	A	339	VAL	N-CA-C	-5.14	105.70	110.53
1	D	125	ASP	CA-CB-CG	5.14	117.74	112.60
1	A	844	LEU	CA-C-N	5.13	129.28	120.72
1	A	844	LEU	C-N-CA	5.13	129.28	120.72
1	D	399	TYR	N-CA-C	-5.13	100.72	108.67
1	D	571	ASP	CA-CB-CG	5.12	117.72	112.60
1	A	113	LEU	CA-C-N	5.12	130.79	122.39
1	A	113	LEU	C-N-CA	5.12	130.79	122.39
1	C	276	ASP	CA-CB-CG	5.11	117.71	112.60
1	A	399	TYR	N-CA-C	-5.08	100.23	108.41
1	A	64	HIS	N-CA-C	-5.08	107.12	113.72
1	A	374	HIS	CA-C-N	5.07	124.79	119.92
1	A	374	HIS	C-N-CA	5.07	124.79	119.92
1	D	642	MET	CA-C-N	5.07	131.35	121.63
1	D	642	MET	C-N-CA	5.07	131.35	121.63
1	A	142	THR	CA-C-N	5.04	128.22	120.82
1	A	142	THR	C-N-CA	5.04	128.22	120.82
1	A	464	ASP	CA-CB-CG	5.03	117.63	112.60
1	A	634	PHE	N-CA-C	5.03	116.47	108.67
1	C	647	THR	CB-CA-C	5.03	118.51	110.16
1	D	91	VAL	CA-C-N	5.03	127.33	120.54
1	D	91	VAL	C-N-CA	5.03	127.33	120.54
1	D	710	ILE	CA-C-N	5.03	127.72	120.38
1	D	710	ILE	C-N-CA	5.03	127.72	120.38
1	D	464	ASP	CA-CB-CG	5.01	117.61	112.60
1	A	746	VAL	N-CA-CB	5.01	118.21	111.90
1	B	292	ASN	CA-C-N	5.00	126.94	120.44
1	B	292	ASN	C-N-CA	5.00	126.94	120.44

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	6131	0	5886	65	0
1	B	6087	0	5850	55	0
1	C	5982	0	5757	77	0
1	D	6274	0	6017	69	0
2	E	28	0	25	0	0
2	F	28	0	25	0	0
2	G	28	0	25	0	0
2	H	28	0	25	0	0
2	I	28	0	25	0	0
2	J	28	0	25	0	0
2	K	28	0	25	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	42	0	39	0	0
4	B	28	0	26	0	0
4	C	14	0	13	0	0
4	D	28	0	26	1	0
All	All	24786	0	23789	266	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 5.

All (266) 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:247:ASN:HD21	1:C:249:ALA:HB3	1.48	0.78
1:B:750:ILE:HD11	1:B:781:PHE:HB3	1.69	0.72
1:A:198:MET:HE1	1:A:517:VAL:HG21	1.73	0.70
1:A:509:ILE:HD13	1:A:542:LEU:HD11	1.77	0.66
1:A:409:ARG:HH22	1:A:471:ARG:NE	1.94	0.66
1:A:550:PRO:HB2	1:A:858:VAL:HG12	1.78	0.65
1:D:840:ARG:O	1:D:844:LEU:HD12	1.97	0.65
1:B:688:ILE:HD11	1:B:716:PRO:HB2	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:231:ASP:HB2	1:C:455:ARG:HD2	1.79	0.64
1:B:231:ASP:HB2	1:B:455:ARG:HD2	1.79	0.64
1:D:224:ILE:HA	1:D:229:MET:HE1	1.78	0.64
1:A:409:ARG:HH22	1:A:471:ARG:HE	1.44	0.64
1:C:409:ARG:HH22	1:C:471:ARG:HE	1.45	0.64
1:B:509:ILE:HD13	1:B:542:LEU:HD11	1.78	0.64
1:A:231:ASP:HB2	1:A:455:ARG:HD2	1.79	0.64
1:C:409:ARG:HH22	1:C:471:ARG:NE	1.95	0.63
1:B:224:ILE:HA	1:B:229:MET:HE1	1.79	0.63
1:B:849:ASP:HB3	1:B:852:GLN:HE21	1.63	0.63
1:B:409:ARG:HH22	1:B:471:ARG:NE	1.96	0.63
1:B:409:ARG:HH22	1:B:471:ARG:HE	1.47	0.62
1:A:198:MET:CE	1:A:517:VAL:HG21	2.29	0.62
1:A:224:ILE:HA	1:A:229:MET:HE1	1.80	0.62
1:C:224:ILE:HA	1:C:229:MET:HE1	1.81	0.62
1:C:638:MET:HE2	1:C:642:MET:HG2	1.81	0.62
1:D:231:ASP:HB2	1:D:455:ARG:HD2	1.82	0.61
1:C:378:GLN:HB3	1:C:466:GLN:HG2	1.82	0.61
1:C:509:ILE:HD13	1:C:542:LEU:HD11	1.82	0.61
1:B:690:HIS:HB2	1:B:714:LEU:HD22	1.82	0.61
1:B:711:THR:HA	1:B:714:LEU:HD12	1.82	0.61
1:A:638:MET:HE2	1:A:642:MET:HG2	1.84	0.60
1:A:258:LEU:HD23	1:A:261:MET:HE3	1.84	0.60
1:D:509:ILE:HD13	1:D:542:LEU:HD11	1.83	0.60
1:A:783:VAL:HG22	1:A:805:PRO:HB3	1.84	0.59
1:C:172:ALA:HA	1:C:175:LEU:HD12	1.84	0.59
1:B:270:TYR:CE1	1:B:299:ARG:HG2	2.37	0.59
1:C:258:LEU:HD23	1:C:261:MET:HE3	1.85	0.59
1:B:608:LEU:HD11	1:B:631:VAL:HG11	1.84	0.58
1:D:666:ARG:HG3	1:D:710:ILE:HG22	1.86	0.58
1:D:172:ALA:HA	1:D:175:LEU:HD12	1.85	0.58
1:D:701:ASN:HD21	1:D:703:GLU:HG2	1.67	0.58
1:A:210:HIS:HB2	1:A:273:PRO:HG2	1.84	0.58
1:A:378:GLN:HB3	1:A:466:GLN:HG2	1.85	0.58
1:B:378:GLN:HB3	1:B:466:GLN:HG2	1.85	0.58
1:D:258:LEU:HD23	1:D:261:MET:HE3	1.85	0.57
1:A:203:PRO:HD3	1:A:450:TYR:CE1	2.40	0.57
1:B:701:ASN:HD21	1:B:703:GLU:HG2	1.69	0.57
1:B:203:PRO:HD3	1:B:450:TYR:CE1	2.40	0.57
1:C:163:ILE:HD12	1:C:366:VAL:HG11	1.85	0.57
1:B:258:LEU:HD23	1:B:261:MET:HE3	1.85	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:784:LEU:HB2	1:B:804:LEU:HB3	1.86	0.56
1:C:196:LYS:HB2	1:C:511:PRO:HG3	1.86	0.56
1:A:78:ASP:O	4:D:907:NAG:H4	2.05	0.56
1:A:860:GLU:O	1:A:863:GLN:HB2	2.05	0.56
1:A:849:ASP:HB3	1:A:852:GLN:HE21	1.70	0.56
1:C:400:GLN:HG2	1:C:470:TYR:HA	1.88	0.56
1:B:400:GLN:HG2	1:B:470:TYR:HA	1.88	0.56
1:C:638:MET:CE	1:C:642:MET:HG2	2.36	0.56
1:A:701:ASN:HD21	1:A:703:GLU:HG2	1.70	0.55
1:B:89:THR:HG22	1:B:102:PHE:HB3	1.89	0.55
1:D:759:PHE:HB3	1:D:845:LEU:O	2.06	0.55
1:D:400:GLN:HG2	1:D:470:TYR:HA	1.89	0.55
1:D:203:PRO:HD3	1:D:450:TYR:CE1	2.42	0.55
1:D:378:GLN:HB3	1:D:466:GLN:HG2	1.88	0.55
1:A:400:GLN:HG2	1:A:470:TYR:HA	1.89	0.55
1:D:608:LEU:HD22	1:D:612:ARG:HA	1.89	0.55
1:C:225:ILE:HG12	1:C:455:ARG:HB3	1.89	0.54
1:D:163:ILE:HD12	1:D:366:VAL:HG11	1.90	0.54
1:A:642:MET:O	1:A:749:PRO:HD2	2.08	0.54
1:B:861:ILE:HG22	1:B:865:LYS:HE3	1.89	0.54
1:C:203:PRO:HD3	1:C:450:TYR:CE1	2.43	0.54
1:C:849:ASP:HB3	1:C:852:GLN:HE21	1.73	0.53
1:C:97:TRP:HB3	1:C:352:MET:HE1	1.90	0.53
1:A:225:ILE:HG12	1:A:455:ARG:HB3	1.90	0.53
1:C:803:VAL:HG21	1:C:839:VAL:HG21	1.90	0.53
1:D:225:ILE:HG12	1:D:455:ARG:HB3	1.91	0.53
1:A:255:PRO:HD2	1:A:258:LEU:HD12	1.91	0.53
1:B:92:LYS:O	1:B:96:ILE:HG12	2.09	0.53
1:C:786:SER:HA	1:C:794:PRO:HG3	1.90	0.53
1:C:247:ASN:ND2	1:C:249:ALA:HB3	2.21	0.53
1:C:263:GLN:NE2	1:C:527:ILE:HB	2.24	0.53
1:C:96:ILE:HD11	1:C:103:ARG:HD2	1.91	0.53
1:B:750:ILE:HB	1:B:779:HIS:HB2	1.91	0.52
1:D:716:PRO:HG2	1:D:777:PRO:HD3	1.92	0.52
1:B:225:ILE:HG12	1:B:455:ARG:HB3	1.90	0.52
1:A:210:HIS:CB	1:A:273:PRO:HG2	2.40	0.52
1:D:698:ILE:HG23	1:D:699:LYS:HG3	1.91	0.51
1:D:839:VAL:O	1:D:842:VAL:HB	2.10	0.51
1:B:261:MET:HA	1:B:265:LEU:O	2.10	0.51
1:D:728:PHE:HZ	1:D:784:LEU:HD11	1.75	0.51
1:C:100:ASN:O	1:C:101:SER:C	2.54	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:716:PRO:HG2	1:A:777:PRO:HD3	1.93	0.51
1:D:783:VAL:HG22	1:D:805:PRO:HB3	1.93	0.51
1:D:861:ILE:HG22	1:D:865:LYS:HE2	1.92	0.50
1:C:648:VAL:O	1:C:742:GLY:HA2	2.11	0.50
1:D:198:MET:HE1	1:D:514:ASN:HA	1.94	0.50
1:A:784:LEU:HD12	1:A:804:LEU:HD23	1.94	0.49
1:B:716:PRO:HG2	1:B:777:PRO:HD3	1.94	0.49
1:C:784:LEU:HB2	1:C:804:LEU:HB3	1.95	0.49
1:D:537:GLY:HA3	1:D:550:PRO:HG3	1.95	0.49
1:D:651:PRO:HD2	1:D:738:ILE:HG13	1.94	0.49
1:A:453:ASN:OD1	1:A:455:ARG:HB2	2.13	0.49
1:C:747:SER:HA	1:C:781:PHE:O	2.13	0.49
1:C:784:LEU:HD12	1:C:804:LEU:HD23	1.94	0.49
1:B:580:LEU:HD23	1:B:586:GLU:HG3	1.95	0.48
1:A:71:ARG:CZ	1:A:79:ARG:HE	2.27	0.48
1:A:784:LEU:HB2	1:A:804:LEU:HB3	1.94	0.48
1:B:651:PRO:HD2	1:B:738:ILE:HG13	1.93	0.48
1:B:453:ASN:OD1	1:B:455:ARG:HB2	2.13	0.48
1:B:255:PRO:HD2	1:B:258:LEU:HD12	1.94	0.48
1:C:513:GLU:HG2	1:C:515:ILE:HG12	1.96	0.48
1:C:255:PRO:HD2	1:C:258:LEU:HD12	1.95	0.48
1:B:801:LEU:HB2	1:B:864:LEU:HD21	1.96	0.48
1:A:163:ILE:HD12	1:A:366:VAL:HG11	1.96	0.48
1:C:258:LEU:HA	1:C:261:MET:HE3	1.96	0.48
1:C:247:ASN:HD22	1:C:250:TRP:CD1	2.32	0.48
1:C:743:VAL:HG23	1:C:786:SER:HB3	1.96	0.48
1:A:651:PRO:HD2	1:A:738:ILE:HG13	1.96	0.47
1:C:765:ILE:HG21	1:C:775:PRO:HB3	1.96	0.47
1:D:765:ILE:HG21	1:D:775:PRO:HB3	1.96	0.47
1:A:261:MET:HE1	1:A:284:PRO:HA	1.96	0.47
1:A:550:PRO:HB2	1:A:858:VAL:CG1	2.45	0.47
1:D:255:PRO:HD2	1:D:258:LEU:HD12	1.97	0.47
1:A:270:TYR:CE1	1:A:299:ARG:HG2	2.49	0.47
1:C:404:PRO:HG2	1:C:469:ALA:HB3	1.97	0.47
1:C:174:TYR:HB3	1:C:181:LEU:HD12	1.95	0.47
1:A:441:THR:HG21	1:A:456:ILE:HG22	1.96	0.46
1:C:560:ALA:O	1:C:623:CYS:HB3	2.16	0.46
1:C:100:ASN:H	1:C:103:ARG:HB2	1.79	0.46
1:A:743:VAL:HA	1:A:794:PRO:HG2	1.98	0.46
1:A:747:SER:HA	1:A:781:PHE:O	2.15	0.46
1:B:535:SER:HB3	1:B:862:LEU:HD22	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:290:TYR:OH	1:D:323:GLU:HG3	2.16	0.46
1:B:258:LEU:HA	1:B:261:MET:HE3	1.97	0.46
1:D:258:LEU:HA	1:D:261:MET:HE3	1.98	0.46
1:A:634:PHE:HA	1:A:641:PRO:HA	1.98	0.46
1:B:198:MET:HE2	1:B:371:LEU:HD22	1.97	0.46
1:D:261:MET:HE1	1:D:284:PRO:HA	1.98	0.45
1:A:641:PRO:HG2	1:A:693:LEU:HD23	1.97	0.45
1:A:89:THR:HG22	1:A:102:PHE:HB3	1.98	0.45
1:C:750:ILE:HD11	1:C:781:PHE:HB3	1.99	0.45
1:A:198:MET:HE2	1:A:514:ASN:HA	1.98	0.45
1:C:695:PRO:HG3	1:C:729:HIS:HD2	1.82	0.45
1:C:838:ARG:O	1:C:841:ASP:HB2	2.17	0.45
1:C:839:VAL:HB	1:C:865:LYS:HA	1.99	0.45
1:D:361:ASN:HD22	1:D:361:ASN:HA	1.64	0.45
1:D:643:TRP:HA	1:D:747:SER:O	2.16	0.45
1:A:765:ILE:HG21	1:A:775:PRO:HB3	1.97	0.45
1:A:225:ILE:HG13	1:A:229:MET:SD	2.57	0.45
1:C:71:ARG:CZ	1:C:79:ARG:HE	2.30	0.45
1:C:634:PHE:HA	1:C:641:PRO:HA	1.98	0.45
1:D:779:HIS:CD2	1:D:809:PRO:HA	2.52	0.45
1:A:198:MET:CE	1:A:517:VAL:CG2	2.94	0.45
1:C:453:ASN:OD1	1:C:455:ARG:HB2	2.16	0.45
1:D:573:LEU:HD21	1:D:673:PRO:HB3	1.99	0.45
1:D:843:GLU:HG2	1:D:850:PHE:CD2	2.52	0.45
1:B:71:ARG:CZ	1:B:79:ARG:HE	2.30	0.44
1:B:441:THR:HG21	1:B:456:ILE:HG22	1.99	0.44
1:C:198:MET:HE1	1:C:371:LEU:HD22	1.99	0.44
1:C:716:PRO:HG2	1:C:777:PRO:HD3	1.98	0.44
1:D:404:PRO:HG2	1:D:469:ALA:HB3	1.99	0.44
1:A:779:HIS:CD2	1:A:809:PRO:HA	2.52	0.44
1:A:785:THR:HG21	1:A:851:TYR:CE1	2.51	0.44
1:C:441:THR:HG21	1:C:456:ILE:HG22	2.00	0.44
1:D:441:THR:HG21	1:D:456:ILE:HG22	1.99	0.44
1:A:717:MET:HA	1:A:810:HIS:NE2	2.33	0.44
1:B:573:LEU:HD21	1:B:673:PRO:HB3	2.00	0.44
1:B:765:ILE:HG21	1:B:775:PRO:HB3	2.00	0.44
1:D:225:ILE:HG13	1:D:229:MET:SD	2.57	0.44
1:A:95:GLN:HE21	1:A:95:GLN:HB3	1.40	0.44
1:B:614:ARG:O	1:B:848:LEU:HA	2.17	0.44
1:D:380:SER:HB2	1:D:383:ARG:NH2	2.33	0.44
1:D:87:GLU:O	1:D:91:VAL:HG12	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:174:TYR:HB3	1:D:181:LEU:HD12	2.00	0.43
1:B:160:PRO:HA	1:B:161:PRO:HD3	1.95	0.43
1:C:717:MET:HA	1:C:810:HIS:NE2	2.33	0.43
1:A:861:ILE:HG22	1:A:865:LYS:HE3	1.99	0.43
1:C:225:ILE:HG13	1:C:229:MET:SD	2.58	0.43
1:C:695:PRO:HG3	1:C:729:HIS:CD2	2.53	0.43
1:D:73:ASP:CG	1:D:79:ARG:HH22	2.27	0.43
1:D:595:LEU:HD13	1:D:599:GLU:HB3	2.00	0.43
1:D:555:GLU:HG3	1:D:615:VAL:N	2.34	0.43
1:D:717:MET:HA	1:D:810:HIS:NE2	2.33	0.43
1:D:160:PRO:HA	1:D:161:PRO:HD3	1.90	0.43
1:A:682:TYR:C	1:A:683:LEU:HG	2.44	0.43
1:B:404:PRO:HG2	1:B:469:ALA:HB3	2.00	0.43
1:C:261:MET:HE1	1:C:284:PRO:HA	2.01	0.43
1:C:535:SER:HB3	1:C:862:LEU:HD22	2.00	0.43
1:C:777:PRO:HG2	1:C:780:TYR:CZ	2.53	0.43
1:A:258:LEU:HA	1:A:261:MET:HE3	2.00	0.43
1:B:198:MET:HG3	1:B:496:PHE:HB2	2.00	0.43
1:D:91:VAL:CG1	1:D:92:LYS:N	2.81	0.43
1:B:225:ILE:HG13	1:B:229:MET:SD	2.59	0.43
1:D:87:GLU:OE1	1:D:91:VAL:HG11	2.18	0.43
1:A:743:VAL:HG23	1:A:786:SER:HB3	2.01	0.43
1:B:199:ARG:HB3	1:B:513:GLU:HG3	2.00	0.43
1:D:196:LYS:HB2	1:D:511:PRO:HG3	1.99	0.43
1:A:268:ALA:HA	1:A:286:ILE:O	2.18	0.42
1:B:96:ILE:HG22	1:B:98:THR:H	1.83	0.42
1:B:268:ALA:HA	1:B:286:ILE:O	2.19	0.42
1:C:562:CYS:HB2	1:C:623:CYS:HB2	1.87	0.42
1:D:838:ARG:HG3	1:D:841:ASP:OD2	2.19	0.42
1:A:358:LYS:HA	1:A:363:HIS:ND1	2.35	0.42
1:D:261:MET:CE	1:D:284:PRO:HA	2.49	0.42
1:A:261:MET:CE	1:A:284:PRO:HA	2.49	0.42
1:C:750:ILE:HB	1:C:779:HIS:HB2	2.00	0.42
1:D:861:ILE:O	1:D:865:LYS:HG3	2.20	0.42
1:C:199:ARG:HB3	1:C:513:GLU:HA	2.01	0.42
1:C:261:MET:HA	1:C:265:LEU:O	2.19	0.42
1:B:261:MET:CE	1:B:284:PRO:HA	2.50	0.42
1:C:688:ILE:HD11	1:C:716:PRO:HB2	2.01	0.42
1:D:120:CYS:C	1:D:126:CYS:SG	3.02	0.42
1:D:627:HIS:CD2	1:D:670:ARG:HH12	2.37	0.42
1:C:63:SER:C	1:C:65:ARG:H	2.26	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:87:GLU:O	1:C:91:VAL:HB	2.19	0.42
1:C:182:LEU:HD21	1:C:343:LEU:HB3	2.01	0.42
1:B:200:ALA:HA	1:B:514:ASN:ND2	2.34	0.42
1:B:261:MET:HE1	1:B:284:PRO:HA	2.01	0.42
1:D:650:LYS:HA	1:D:651:PRO:HD3	1.86	0.42
1:C:861:ILE:HG22	1:C:865:LYS:HE3	2.02	0.42
1:C:238:PHE:CE2	1:C:245:LYS:HA	2.55	0.42
1:C:695:PRO:O	1:C:698:ILE:HG22	2.20	0.42
1:D:539:LEU:HB3	1:D:542:LEU:HD13	2.02	0.42
1:B:717:MET:HA	1:B:810:HIS:NE2	2.34	0.41
1:C:358:LYS:HA	1:C:363:HIS:ND1	2.35	0.41
1:D:747:SER:HA	1:D:781:PHE:O	2.19	0.41
1:A:261:MET:HA	1:A:265:LEU:O	2.21	0.41
1:D:210:HIS:HB2	1:D:273:PRO:HG2	2.02	0.41
1:D:695:PRO:O	1:D:698:ILE:HG22	2.20	0.41
1:A:688:ILE:HD11	1:A:716:PRO:HB2	2.02	0.41
1:B:358:LYS:HA	1:B:363:HIS:ND1	2.35	0.41
1:A:271:TYR:CD1	1:A:290:TYR:HA	2.56	0.41
1:B:838:ARG:O	1:B:841:ASP:HB2	2.20	0.41
1:C:564:PHE:CE1	1:C:594:ASN:HB2	2.55	0.41
1:C:219:PRO:HA	1:C:222:HIS:CE1	2.56	0.41
1:B:196:LYS:HB2	1:B:511:PRO:HG3	2.03	0.41
1:C:257:TRP:O	1:C:261:MET:HG3	2.20	0.41
1:D:358:LYS:HA	1:D:363:HIS:ND1	2.35	0.41
1:A:247:ASN:HB3	1:A:250:TRP:HD1	1.86	0.41
1:C:361:ASN:HD22	1:C:361:ASN:HA	1.72	0.41
1:C:640:MET:HE2	1:C:774:VAL:HG23	2.03	0.41
1:D:784:LEU:HD12	1:D:804:LEU:HD23	2.02	0.41
1:A:97:TRP:HB3	1:A:352:MET:HE1	2.03	0.41
1:A:194:HIS:CE1	1:A:508:VAL:HG22	2.56	0.41
1:B:650:LYS:HA	1:B:651:PRO:HD3	1.86	0.41
1:D:535:SER:O	1:D:538:SER:HB3	2.20	0.41
1:A:573:LEU:HD21	1:A:673:PRO:HB3	2.03	0.41
1:D:194:HIS:CE1	1:D:508:VAL:HG22	2.56	0.41
1:D:197:TYR:HE1	1:D:374:HIS:HB2	1.86	0.41
1:C:342:ALA:HA	1:C:345:LEU:HD12	2.03	0.41
1:A:217:LEU:HB2	1:A:222:HIS:HB3	2.03	0.40
1:A:219:PRO:HA	1:A:222:HIS:CE1	2.56	0.40
1:C:261:MET:CE	1:C:284:PRO:HA	2.51	0.40
1:D:198:MET:HE3	1:D:198:MET:HB2	1.88	0.40
1:C:120:CYS:C	1:C:126:CYS:SG	3.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:614:ARG:HD3	1:D:852:GLN:HG3	2.03	0.40
1:A:695:PRO:O	1:A:698:ILE:HG22	2.21	0.40
1:B:71:ARG:HH12	1:B:76:CYS:HA	1.87	0.40
1:B:194:HIS:CE1	1:B:508:VAL:HG22	2.56	0.40
1:D:219:PRO:HA	1:D:222:HIS:CE1	2.57	0.40
1:D:257:TRP:O	1:D:261:MET:HG3	2.22	0.40
1:A:257:TRP:O	1:A:261:MET:HG3	2.21	0.40
1:C:537:GLY:HA3	1:C:550:PRO:HG3	2.03	0.40
1:C:268:ALA:HA	1:C:286:ILE:O	2.21	0.40
1:C:595:LEU:HD13	1:C:599:GLU:HB3	2.04	0.40
1:D:199:ARG:HB3	1:D:513:GLU:HG3	2.03	0.40
1:D:453:ASN:OD1	1:D:455:ARG:HB2	2.22	0.40

There are no symmetry-related clashes.

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	751/840 (89%)	700 (93%)	47 (6%)	4 (0%)	24	55
1	B	745/840 (89%)	694 (93%)	44 (6%)	7 (1%)	14	41
1	C	724/840 (86%)	674 (93%)	44 (6%)	6 (1%)	16	44
1	D	769/840 (92%)	710 (92%)	54 (7%)	5 (1%)	18	47
All	All	2989/3360 (89%)	2778 (93%)	189 (6%)	22 (1%)	18	47

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	683	LEU
1	B	820	GLU
1	D	148	SER

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Mol	Chain	Res	Type
1	A	820	GLU
1	C	820	GLU
1	D	290	TYR
1	A	148	SER
1	A	434	GLN
1	B	434	GLN
1	C	271	TYR
1	C	434	GLN
1	C	855	THR
1	D	434	GLN
1	B	373	ASP
1	B	684	ALA
1	C	821	ASN
1	D	93	SER
1	B	855	THR
1	D	272	TRP
1	C	669	VAL
1	A	616	ILE
1	B	272	TRP

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	686/749 (92%)	634 (92%)	52 (8%)	12	36
1	B	680/749 (91%)	629 (92%)	51 (8%)	12	37
1	C	665/749 (89%)	611 (92%)	54 (8%)	11	33
1	D	701/749 (94%)	642 (92%)	59 (8%)	10	32
All	All	2732/2996 (91%)	2516 (92%)	216 (8%)	11	35

All (216) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	LEU
1	A	77	THR

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Mol	Chain	Res	Type
1	A	87	GLU
1	A	92	LYS
1	A	95	GLN
1	A	96	ILE
1	A	113	LEU
1	A	127	CYS
1	A	138	VAL
1	A	155	GLU
1	A	243	VAL
1	A	245	LYS
1	A	282	SER
1	A	286	ILE
1	A	298	SER
1	A	319	THR
1	A	323	GLU
1	A	346	VAL
1	A	355	GLU
1	A	361	ASN
1	A	368	ILE
1	A	376	MET
1	A	381	CYS
1	A	413	GLN
1	A	421	GLU
1	A	447	ARG
1	A	455	ARG
1	A	493	GLU
1	A	509	ILE
1	A	513	GLU
1	A	515	ILE
1	A	528	GLN
1	A	538	SER
1	A	568	LEU
1	A	593	LEU
1	A	595	LEU
1	A	610	PHE
1	A	612	ARG
1	A	624	LEU
1	A	627	HIS
1	A	628	ARG
1	A	644	SER
1	A	669	VAL
1	A	672	ASP

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Mol	Chain	Res	Type
1	A	683	LEU
1	A	774	VAL
1	A	797	CYS
1	A	817	SER
1	A	820	GLU
1	A	836	ILE
1	A	854	LYS
1	A	859	SER
1	B	58	LYS
1	B	67	LEU
1	B	77	THR
1	B	95	GLN
1	B	108	ARG
1	B	113	LEU
1	B	127	CYS
1	B	138	VAL
1	B	167	MET
1	B	198	MET
1	B	206	THR
1	B	243	VAL
1	B	245	LYS
1	B	282	SER
1	B	286	ILE
1	B	319	THR
1	B	323	GLU
1	B	346	VAL
1	B	355	GLU
1	B	361	ASN
1	B	368	ILE
1	B	376	MET
1	B	381	CYS
1	B	421	GLU
1	B	455	ARG
1	B	493	GLU
1	B	509	ILE
1	B	513	GLU
1	B	515	ILE
1	B	523	ASP
1	B	528	GLN
1	B	568	LEU
1	B	580	LEU
1	B	593	LEU

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Mol	Chain	Res	Type
1	B	595	LEU
1	B	610	PHE
1	B	612	ARG
1	B	616	ILE
1	B	624	LEU
1	B	627	HIS
1	B	628	ARG
1	B	669	VAL
1	B	672	ASP
1	B	683	LEU
1	B	687	ASN
1	B	767	ASN
1	B	774	VAL
1	B	797	CYS
1	B	817	SER
1	B	836	ILE
1	B	839	VAL
1	C	57	LYS
1	C	65	ARG
1	C	67	LEU
1	C	87	GLU
1	C	96	ILE
1	C	108	ARG
1	C	110	GLU
1	C	113	LEU
1	C	127	CYS
1	C	138	VAL
1	C	150	GLU
1	C	173	GLU
1	C	175	LEU
1	C	177	THR
1	C	212	THR
1	C	245	LYS
1	C	282	SER
1	C	293	SER
1	C	298	SER
1	C	319	THR
1	C	323	GLU
1	C	340	ILE
1	C	346	VAL
1	C	355	GLU
1	C	361	ASN

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Mol	Chain	Res	Type
1	C	368	ILE
1	C	381	CYS
1	C	382	ASP
1	C	421	GLU
1	C	447	ARG
1	C	455	ARG
1	C	509	ILE
1	C	513	GLU
1	C	528	GLN
1	C	532	ASN
1	C	568	LEU
1	C	593	LEU
1	C	595	LEU
1	C	612	ARG
1	C	616	ILE
1	C	624	LEU
1	C	627	HIS
1	C	628	ARG
1	C	647	THR
1	C	669	VAL
1	C	710	ILE
1	C	767	ASN
1	C	774	VAL
1	C	785	THR
1	C	797	CYS
1	C	817	SER
1	C	822	LYS
1	C	836	ILE
1	C	859	SER
1	D	67	LEU
1	D	71	ARG
1	D	77	THR
1	D	91	VAL
1	D	92	LYS
1	D	96	ILE
1	D	113	LEU
1	D	127	CYS
1	D	138	VAL
1	D	155	GLU
1	D	168	ASP
1	D	173	GLU
1	D	175	LEU

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Mol	Chain	Res	Type
1	D	198	MET
1	D	243	VAL
1	D	245	LYS
1	D	266	LYS
1	D	282	SER
1	D	298	SER
1	D	319	THR
1	D	340	ILE
1	D	346	VAL
1	D	355	GLU
1	D	361	ASN
1	D	368	ILE
1	D	381	CYS
1	D	409	ARG
1	D	421	GLU
1	D	447	ARG
1	D	455	ARG
1	D	465	ARG
1	D	493	GLU
1	D	509	ILE
1	D	515	ILE
1	D	528	GLN
1	D	568	LEU
1	D	580	LEU
1	D	593	LEU
1	D	595	LEU
1	D	606	THR
1	D	612	ARG
1	D	616	ILE
1	D	624	LEU
1	D	627	HIS
1	D	628	ARG
1	D	644	SER
1	D	669	VAL
1	D	672	ASP
1	D	688	ILE
1	D	758	HIS
1	D	767	ASN
1	D	774	VAL
1	D	782	VAL
1	D	785	THR
1	D	797	CYS

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Mol	Chain	Res	Type
1	D	803	VAL
1	D	817	SER
1	D	820	GLU
1	D	854	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	95	GLN
1	A	135	GLN
1	A	152	GLN
1	A	194	HIS
1	A	227	ASN
1	A	292	ASN
1	A	361	ASN
1	A	419	ASN
1	A	526	HIS
1	A	528	GLN
1	A	594	ASN
1	A	622	HIS
1	A	687	ASN
1	A	701	ASN
1	A	852	GLN
1	A	856	GLN
1	B	95	GLN
1	B	135	GLN
1	B	194	HIS
1	B	227	ASN
1	B	359	GLN
1	B	361	ASN
1	B	419	ASN
1	B	514	ASN
1	B	528	GLN
1	B	541	HIS
1	B	552	HIS
1	B	591	GLN
1	B	594	ASN
1	B	622	HIS
1	B	701	ASN
1	B	702	ASN
1	B	741	ASN
1	B	792	HIS

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Mol	Chain	Res	Type
1	C	64	HIS
1	C	186	ASN
1	C	194	HIS
1	C	227	ASN
1	C	247	ASN
1	C	359	GLN
1	C	361	ASN
1	C	419	ASN
1	C	434	GLN
1	C	435	HIS
1	C	594	ASN
1	C	622	HIS
1	C	741	ASN
1	C	852	GLN
1	D	149	GLN
1	D	194	HIS
1	D	227	ASN
1	D	361	ASN
1	D	419	ASN
1	D	514	ASN
1	D	528	GLN
1	D	541	HIS
1	D	594	ASN
1	D	622	HIS
1	D	686	GLN
1	D	687	ASN
1	D	701	ASN
1	D	702	ASN
1	D	741	ASN
1	D	758	HIS
1	D	792	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 ⓘ

14 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	1,2	14,14,15	0.37	0	17,19,21	1.49	2 (11%)
2	NAG	E	2	2	14,14,15	0.35	0	17,19,21	1.09	1 (5%)
2	NAG	F	1	1,2	14,14,15	0.34	0	17,19,21	1.76	3 (17%)
2	NAG	F	2	2	14,14,15	0.39	0	17,19,21	1.15	1 (5%)
2	NAG	G	1	1,2	14,14,15	0.35	0	17,19,21	1.49	2 (11%)
2	NAG	G	2	2	14,14,15	0.33	0	17,19,21	1.05	1 (5%)
2	NAG	H	1	1,2	14,14,15	0.36	0	17,19,21	1.45	2 (11%)
2	NAG	H	2	2	14,14,15	0.33	0	17,19,21	1.01	1 (5%)
2	NAG	I	1	1,2	14,14,15	0.29	0	17,19,21	1.38	3 (17%)
2	NAG	I	2	2	14,14,15	0.34	0	17,19,21	0.83	1 (5%)
2	NAG	J	1	1,2	14,14,15	0.38	0	17,19,21	1.51	2 (11%)
2	NAG	J	2	2	14,14,15	0.34	0	17,19,21	1.05	1 (5%)
2	NAG	K	1	1,2	14,14,15	0.26	0	17,19,21	1.26	2 (11%)
2	NAG	K	2	2	14,14,15	0.35	0	17,19,21	1.20	1 (5%)

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	H	2	2	-	0/6/23/26	0/1/1/1
2	NAG	I	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	I	2	2	-	0/6/23/26	0/1/1/1
2	NAG	J	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	J	2	2	-	0/6/23/26	0/1/1/1
2	NAG	K	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	K	2	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1	NAG	C1-O5-C5	5.85	120.02	112.19
2	G	1	NAG	O5-C1-C2	-5.33	103.05	111.29
2	J	1	NAG	O5-C1-C2	-5.29	103.11	111.29
2	E	1	NAG	O5-C1-C2	-4.99	103.57	111.29
2	H	1	NAG	O5-C1-C2	-4.83	103.81	111.29
2	E	2	NAG	C1-O5-C5	4.04	117.59	112.19
2	K	2	NAG	C1-O5-C5	3.97	117.51	112.19
2	G	2	NAG	C1-O5-C5	3.89	117.41	112.19
2	I	1	NAG	C1-O5-C5	3.68	117.12	112.19
2	J	2	NAG	C1-O5-C5	3.66	117.09	112.19
2	K	1	NAG	C1-O5-C5	3.60	117.01	112.19
2	H	2	NAG	C1-O5-C5	3.59	116.99	112.19
2	F	2	NAG	C1-O5-C5	3.51	116.89	112.19
2	E	1	NAG	C1-O5-C5	2.55	115.60	112.19
2	I	2	NAG	C1-O5-C5	2.54	115.59	112.19
2	F	1	NAG	C1-C2-N2	-2.49	106.51	110.43
2	I	1	NAG	O5-C1-C2	-2.46	107.48	111.29
2	K	1	NAG	O5-C1-C2	-2.34	107.66	111.29
2	H	1	NAG	C1-O5-C5	2.33	115.31	112.19
2	F	1	NAG	C3-C4-C5	2.25	114.31	110.23
2	I	1	NAG	C1-C2-N2	-2.17	107.01	110.43
2	G	1	NAG	C1-O5-C5	2.13	115.03	112.19
2	J	1	NAG	C1-C2-N2	2.11	113.75	110.43

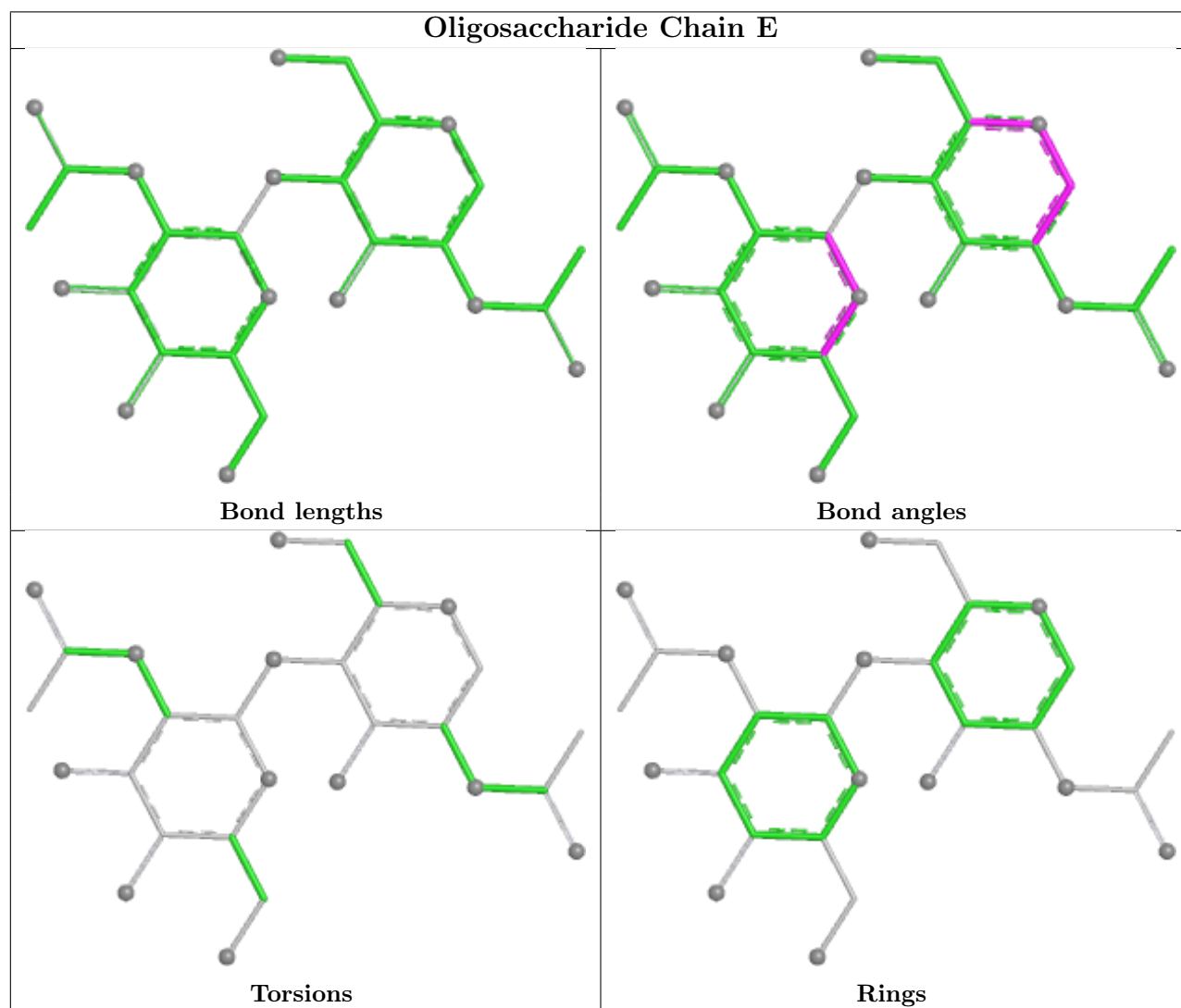
There are no chirality outliers.

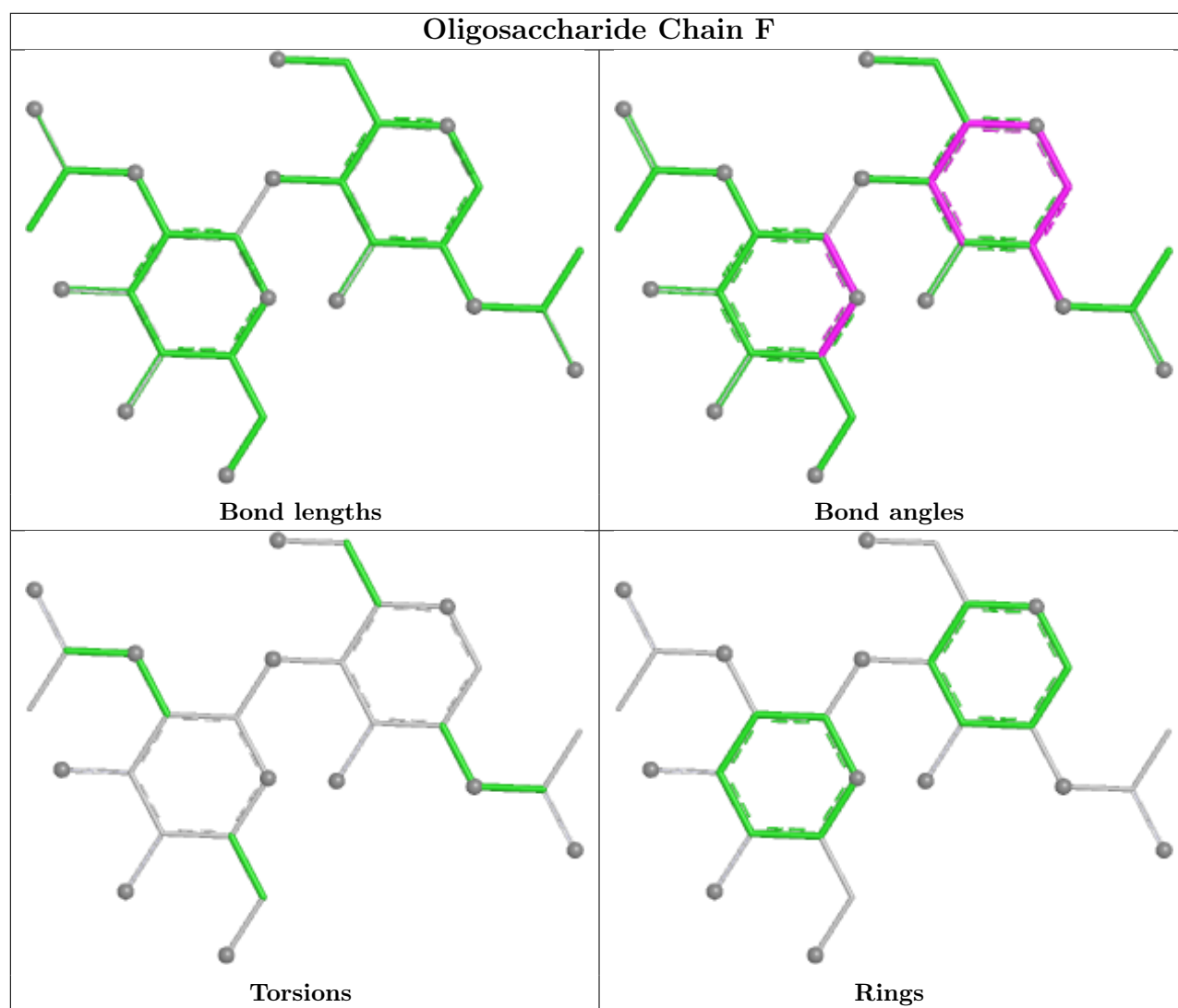
There are no torsion outliers.

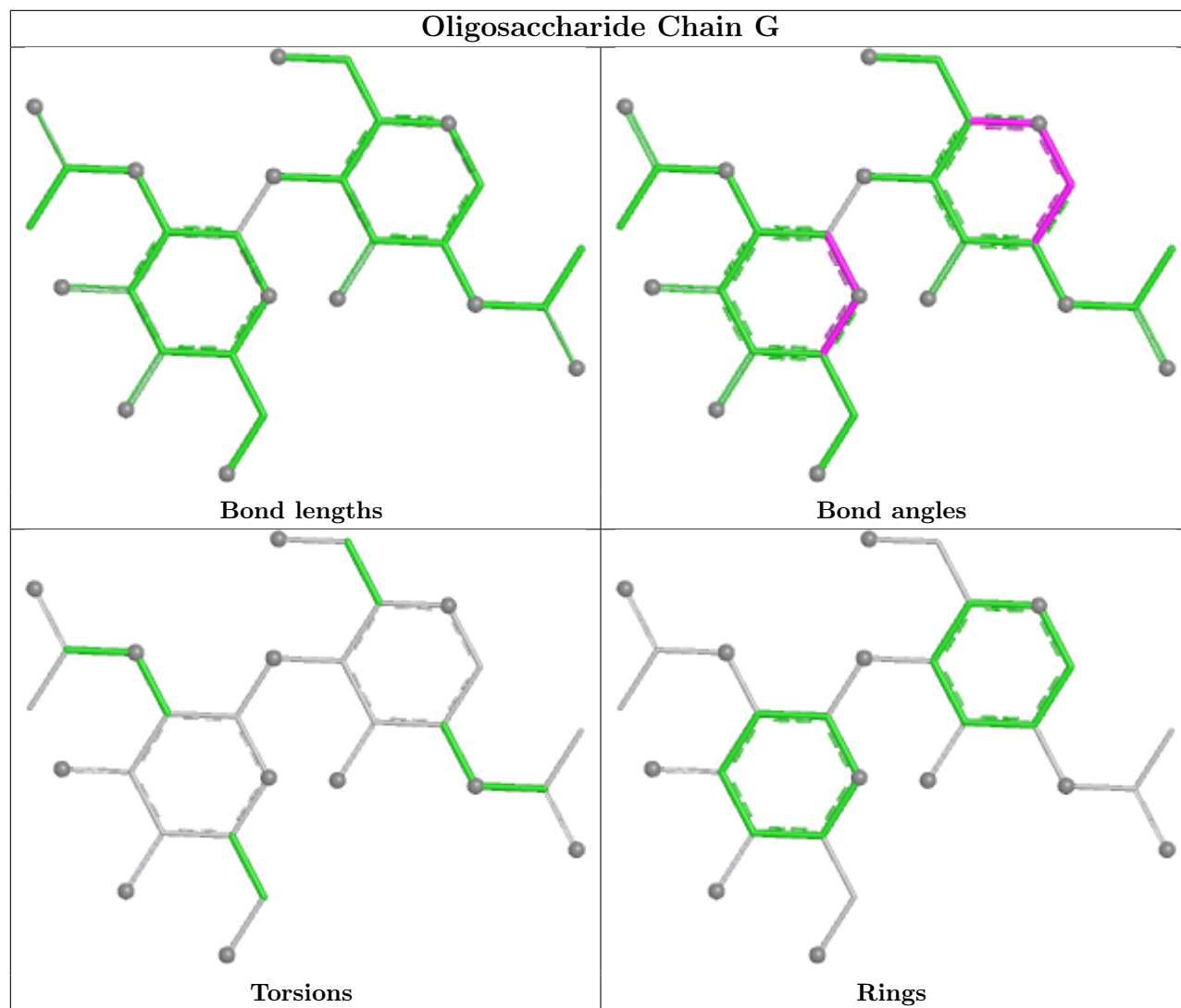
There are no ring outliers.

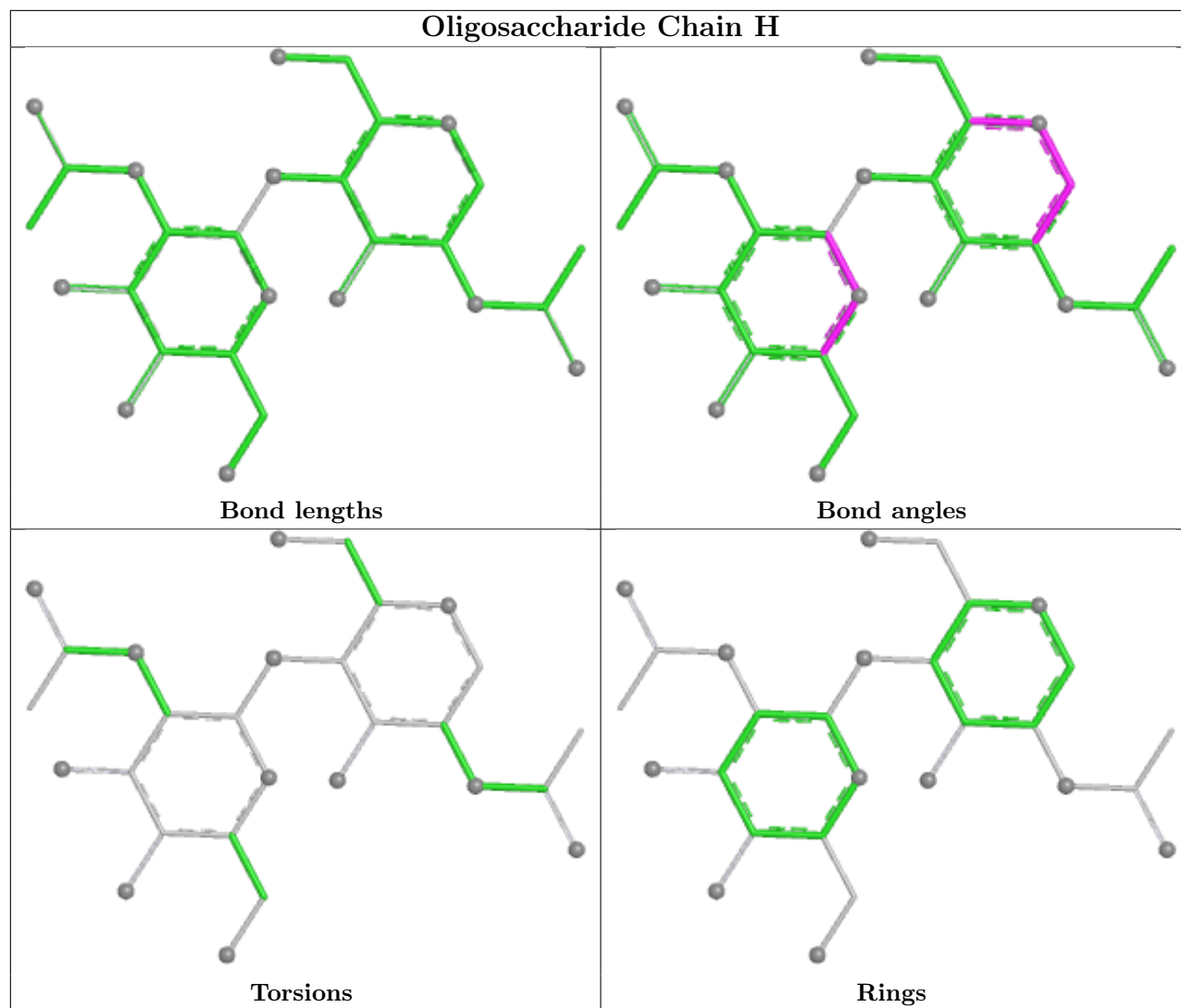
No monomer is involved in short contacts.

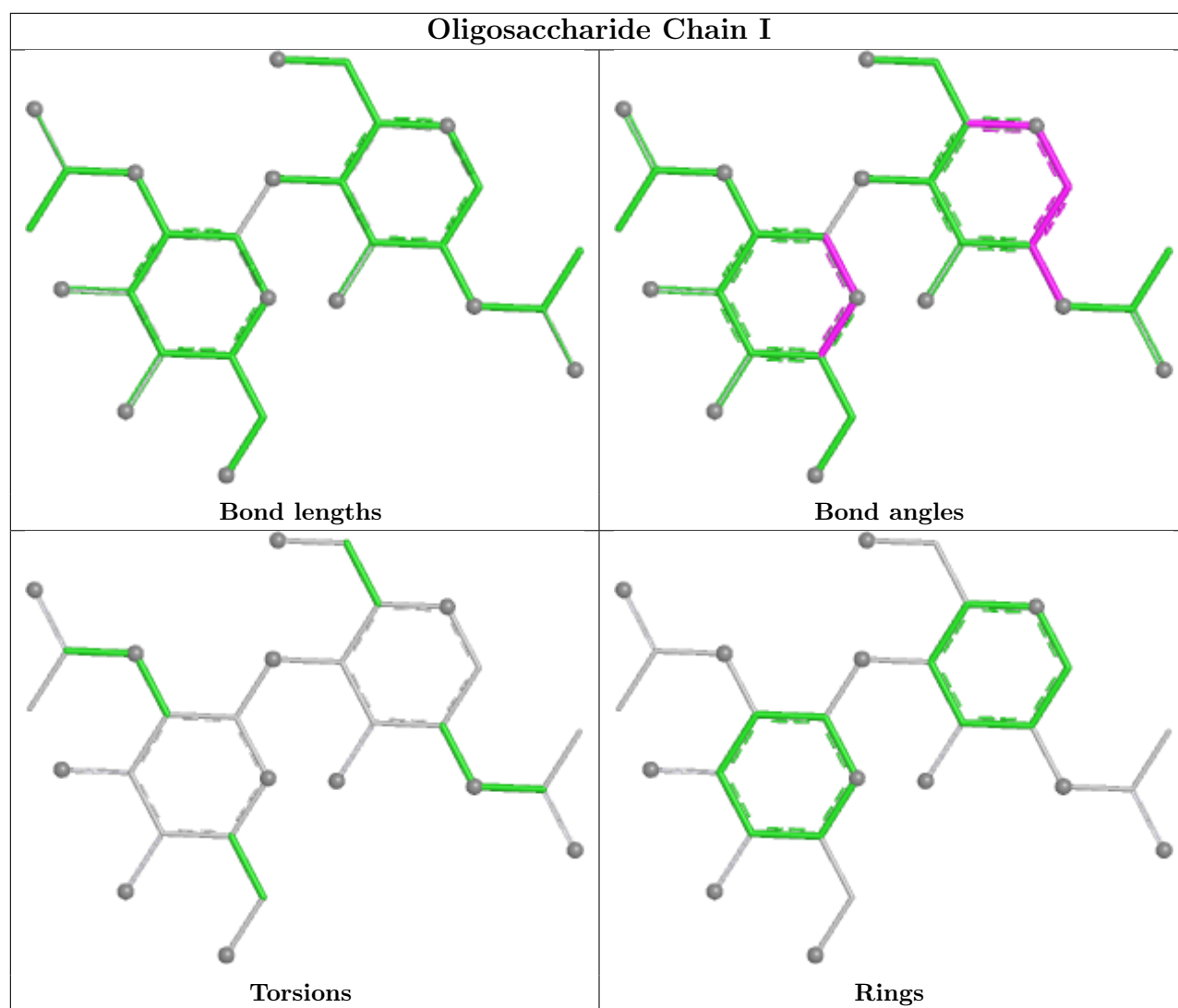
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

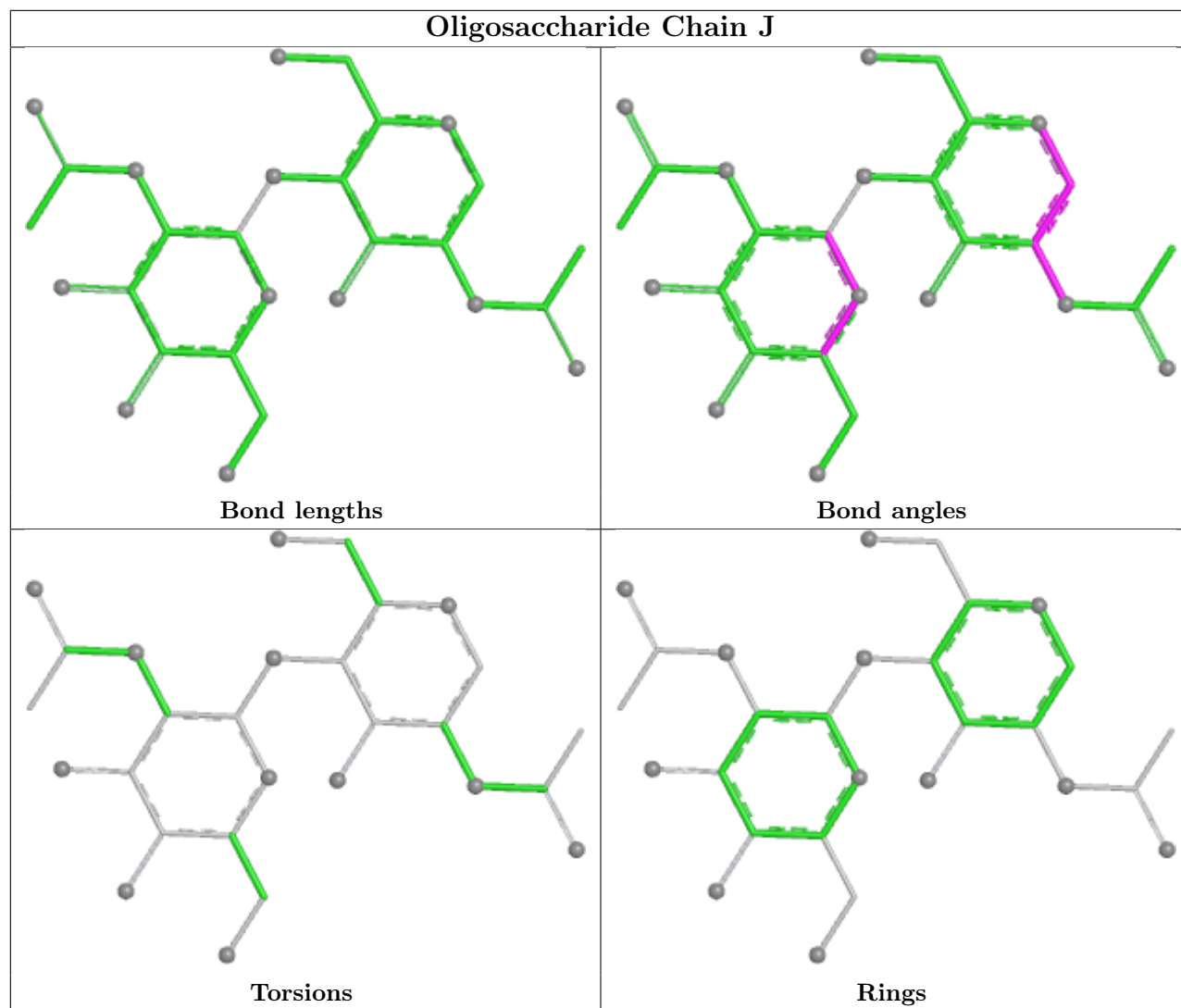


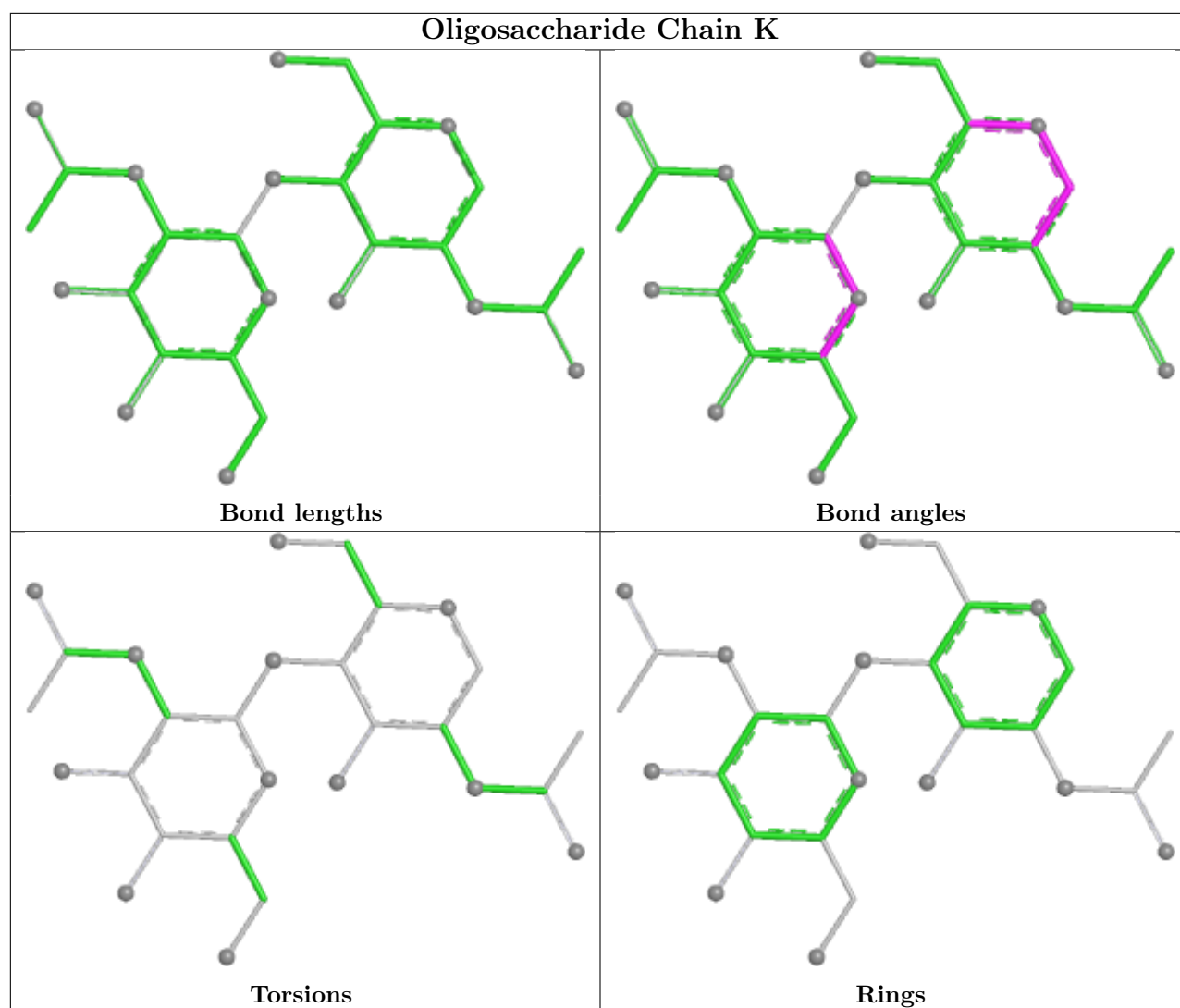












5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	A	908	1	14,14,15	0.41	0	17,19,21	1.29	3 (17%)
4	NAG	B	904	1	14,14,15	0.32	0	17,19,21	1.10	2 (11%)
4	NAG	D	907	1	14,14,15	0.41	0	17,19,21	1.38	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	B	905	1	14,14,15	0.33	0	17,19,21	1.09	2 (11%)
4	NAG	D	904	1	14,14,15	0.30	0	17,19,21	1.15	2 (11%)
4	NAG	C	904	1	14,14,15	0.33	0	17,19,21	1.12	2 (11%)
4	NAG	A	904	1	14,14,15	0.32	0	17,19,21	1.19	3 (17%)
4	NAG	A	905	1	14,14,15	0.39	0	17,19,21	1.21	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	908	1	-	1/6/23/26	0/1/1/1
4	NAG	B	904	1	-	1/6/23/26	0/1/1/1
4	NAG	D	907	1	-	3/6/23/26	0/1/1/1
4	NAG	B	905	1	-	0/6/23/26	0/1/1/1
4	NAG	D	904	1	-	1/6/23/26	0/1/1/1
4	NAG	C	904	1	-	1/6/23/26	0/1/1/1
4	NAG	A	904	1	-	1/6/23/26	0/1/1/1
4	NAG	A	905	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	907	NAG	C1-O5-C5	4.60	118.35	112.19
4	A	908	NAG	O5-C1-C2	-3.99	105.11	111.29
4	A	905	NAG	C1-O5-C5	3.64	117.07	112.19
4	D	904	NAG	O5-C1-C2	-3.25	106.26	111.29
4	A	904	NAG	O5-C1-C2	-3.16	106.40	111.29
4	C	904	NAG	O5-C1-C2	-3.03	106.60	111.29
4	B	905	NAG	C1-O5-C5	2.97	116.16	112.19
4	B	904	NAG	O5-C1-C2	-2.83	106.92	111.29
4	A	904	NAG	C1-O5-C5	2.66	115.75	112.19
4	B	904	NAG	C1-O5-C5	2.56	115.62	112.19
4	C	904	NAG	C1-O5-C5	2.51	115.55	112.19
4	D	904	NAG	C1-O5-C5	2.50	115.54	112.19
4	A	908	NAG	C1-C2-N2	2.20	113.91	110.43
4	A	908	NAG	C1-O5-C5	2.11	115.01	112.19
4	B	905	NAG	O5-C1-C2	-2.02	108.16	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	904	NAG	C1-C2-N2	2.00	113.59	110.43

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	907	NAG	O5-C5-C6-O6
4	D	907	NAG	C4-C5-C6-O6
4	A	905	NAG	O5-C5-C6-O6
4	A	905	NAG	C4-C5-C6-O6
4	A	908	NAG	O5-C5-C6-O6
4	B	904	NAG	O5-C5-C6-O6
4	C	904	NAG	O5-C5-C6-O6
4	D	904	NAG	O5-C5-C6-O6
4	A	904	NAG	O5-C5-C6-O6
4	D	907	NAG	O7-C7-N2-C2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	907	NAG	1	0

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	765/840 (91%)	-0.04	17 (2%)	62 52	28, 66, 114, 148	1 (0%)
1	B	759/840 (90%)	0.39	20 (2%)	57 47	56, 93, 127, 150	1 (0%)
1	C	742/840 (88%)	0.26	24 (3%)	50 40	43, 82, 126, 168	1 (0%)
1	D	781/840 (92%)	-0.07	16 (2%)	65 56	30, 61, 102, 130	1 (0%)
All	All	3047/3360 (90%)	0.13	77 (2%)	58 48	28, 76, 121, 168	4 (0%)

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	669	VAL	5.0
1	B	652	GLY	4.8
1	C	101	SER	4.5
1	D	474	GLY	4.3
1	D	110	GLU	4.0
1	B	185	ILE	3.9
1	D	584	GLY	3.7
1	A	579	ALA	3.6
1	C	648	VAL	3.5
1	C	766	THR	3.5
1	C	568	LEU	3.4
1	C	74	SER	3.4
1	D	98	THR	3.4
1	A	178	TRP	3.3
1	A	337	ALA	3.3
1	A	157	PHE	3.3
1	C	337	ALA	3.2
1	B	169	GLY	3.1
1	B	337	ALA	3.1
1	B	188	LEU	3.1
1	B	362	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	474	GLY	3.0
1	B	683	LEU	2.9
1	A	652	GLY	2.8
1	C	665	LEU	2.8
1	B	81	ASP	2.8
1	A	871	PHE	2.7
1	A	81	ASP	2.7
1	A	67	LEU	2.7
1	B	855	THR	2.7
1	C	731	VAL	2.7
1	B	111	ALA	2.6
1	A	658	PRO	2.6
1	D	148	SER	2.5
1	C	811	ARG	2.5
1	C	64	HIS	2.5
1	A	78	ASP	2.5
1	B	129	ASP	2.5
1	C	707	ASP	2.5
1	D	337	ALA	2.5
1	D	111	ALA	2.4
1	C	566	THR	2.4
1	B	608	LEU	2.4
1	B	589	VAL	2.4
1	D	697	ALA	2.4
1	B	584	GLY	2.4
1	B	144	ALA	2.3
1	C	739	GLU	2.3
1	A	589	VAL	2.3
1	C	474	GLY	2.3
1	D	281	GLY	2.3
1	A	855	THR	2.3
1	C	808	VAL	2.3
1	B	565	THR	2.2
1	D	151	PRO	2.2
1	D	64	HIS	2.2
1	B	67	LEU	2.2
1	A	98	THR	2.2
1	C	678	LYS	2.2
1	C	693	LEU	2.2
1	B	609	PRO	2.1
1	C	641	PRO	2.1
1	D	566	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	597	ARG	2.1
1	D	821	ASN	2.1
1	A	80	GLY	2.1
1	B	566	THR	2.1
1	D	170	PHE	2.1
1	C	108	ARG	2.1
1	A	568	LEU	2.1
1	A	169	GLY	2.1
1	C	850	PHE	2.1
1	C	426	ASP	2.1
1	D	63	SER	2.0
1	B	361	ASN	2.0
1	C	98	THR	2.0
1	C	138	VAL	2.0

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

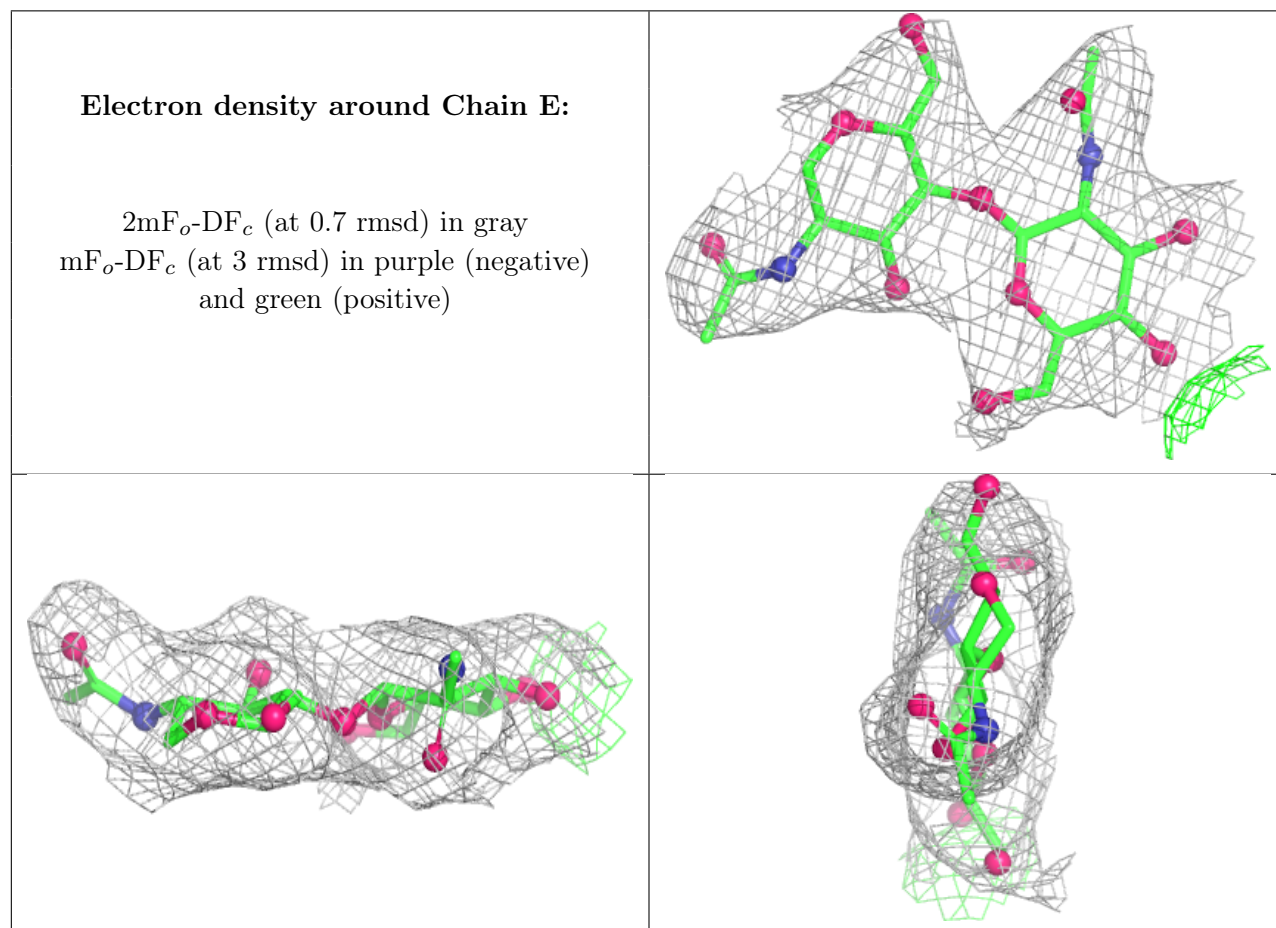
There are no non-standard protein/DNA/RNA residues in this entry.

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.

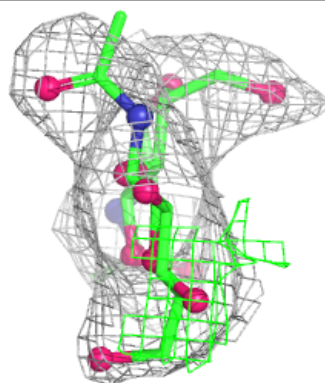
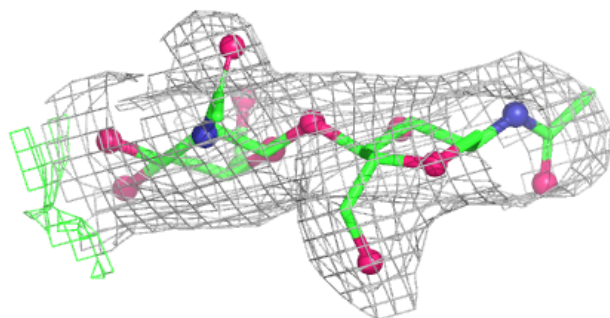
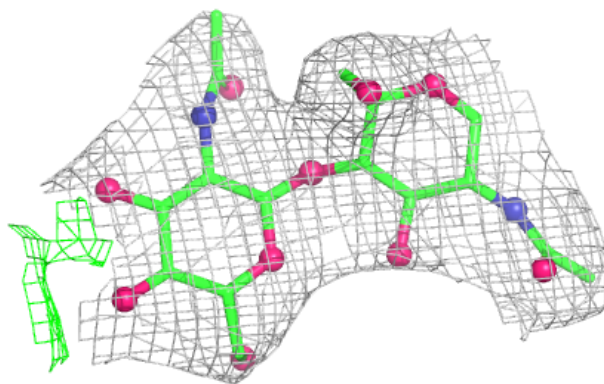
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	G	2	14/15	0.76	0.12	112,115,124,125	0
2	NAG	J	2	14/15	0.76	0.15	109,112,119,119	0
2	NAG	H	2	14/15	0.80	0.12	103,108,111,113	0
2	NAG	K	2	14/15	0.83	0.12	63,71,78,82	0
2	NAG	I	2	14/15	0.84	0.09	68,72,82,87	0
2	NAG	E	2	14/15	0.85	0.09	79,86,96,98	0
2	NAG	G	1	14/15	0.86	0.09	95,101,108,111	0
2	NAG	H	1	14/15	0.90	0.10	87,92,99,101	0
2	NAG	J	1	14/15	0.91	0.13	90,96,100,103	0
2	NAG	E	1	14/15	0.93	0.08	56,62,69,74	0
2	NAG	K	1	14/15	0.94	0.10	43,55,60,63	0
2	NAG	F	2	14/15	0.94	0.08	49,61,67,67	0
2	NAG	F	1	14/15	0.96	0.06	36,43,51,57	0
2	NAG	I	1	14/15	0.97	0.06	53,58,62,63	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.

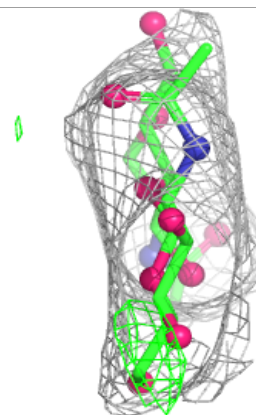
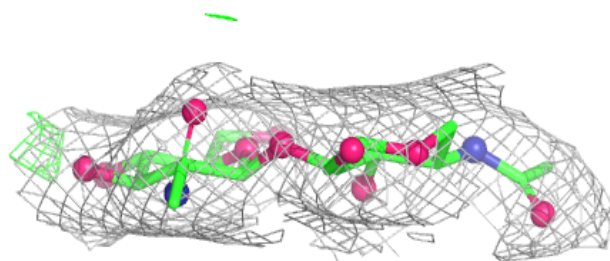
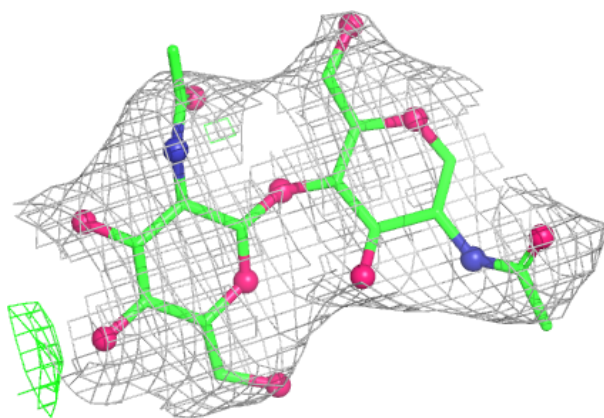


Electron density around Chain F:

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

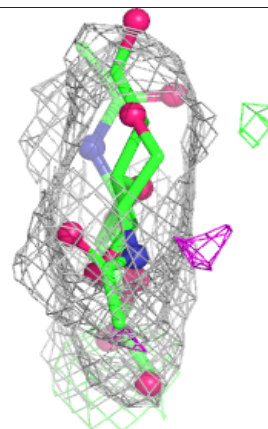
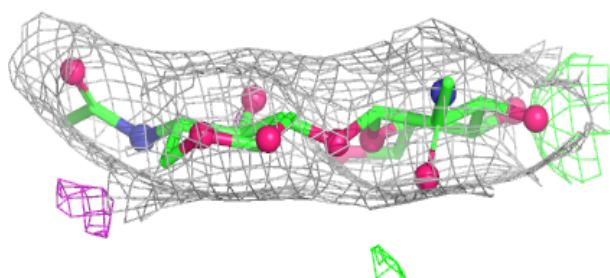
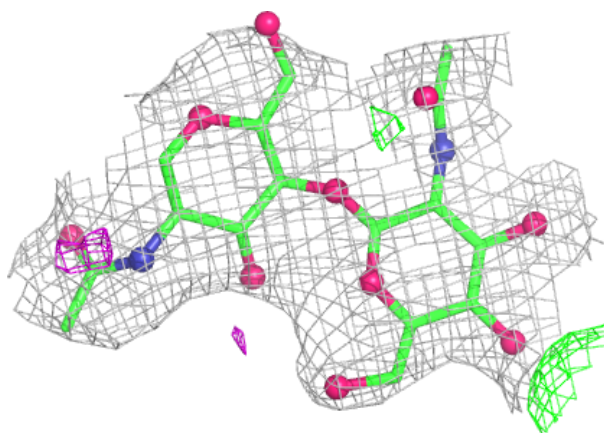
**Electron density around Chain G:**

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



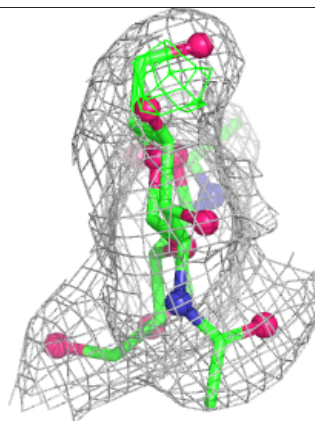
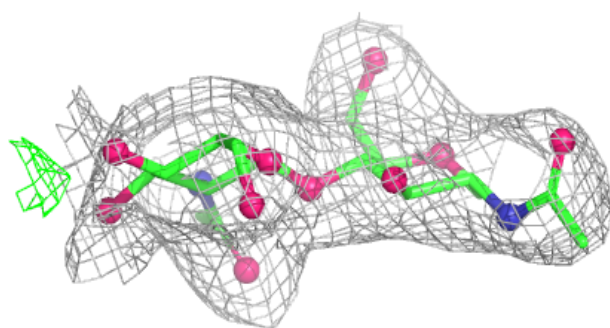
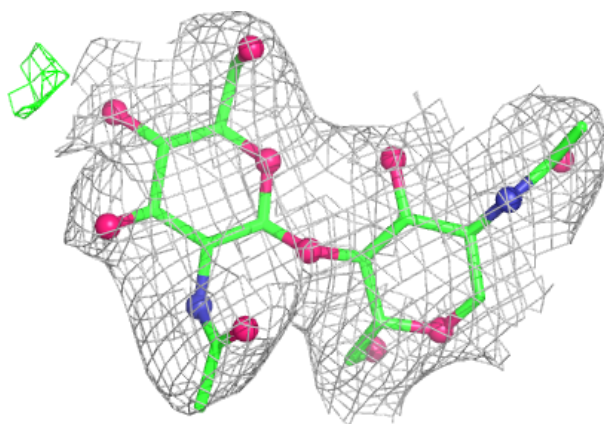
Electron density around Chain H:

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



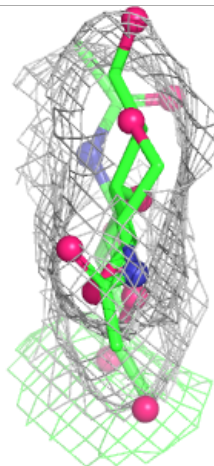
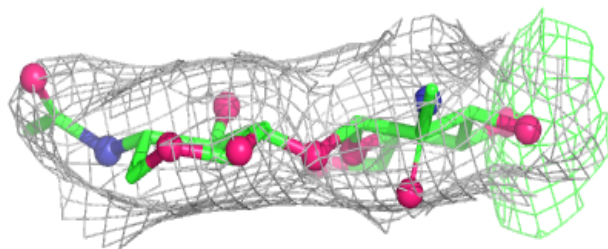
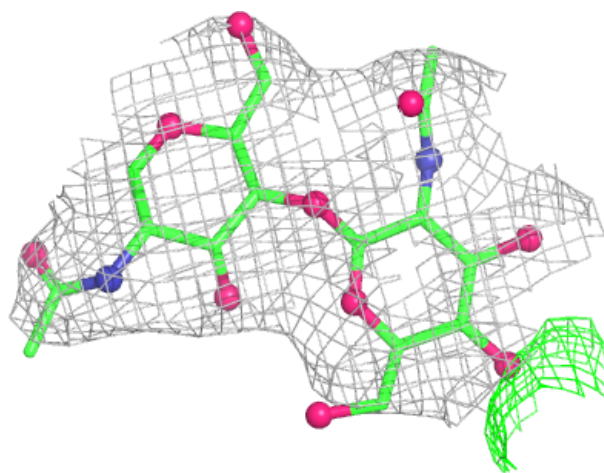
Electron density around Chain I:

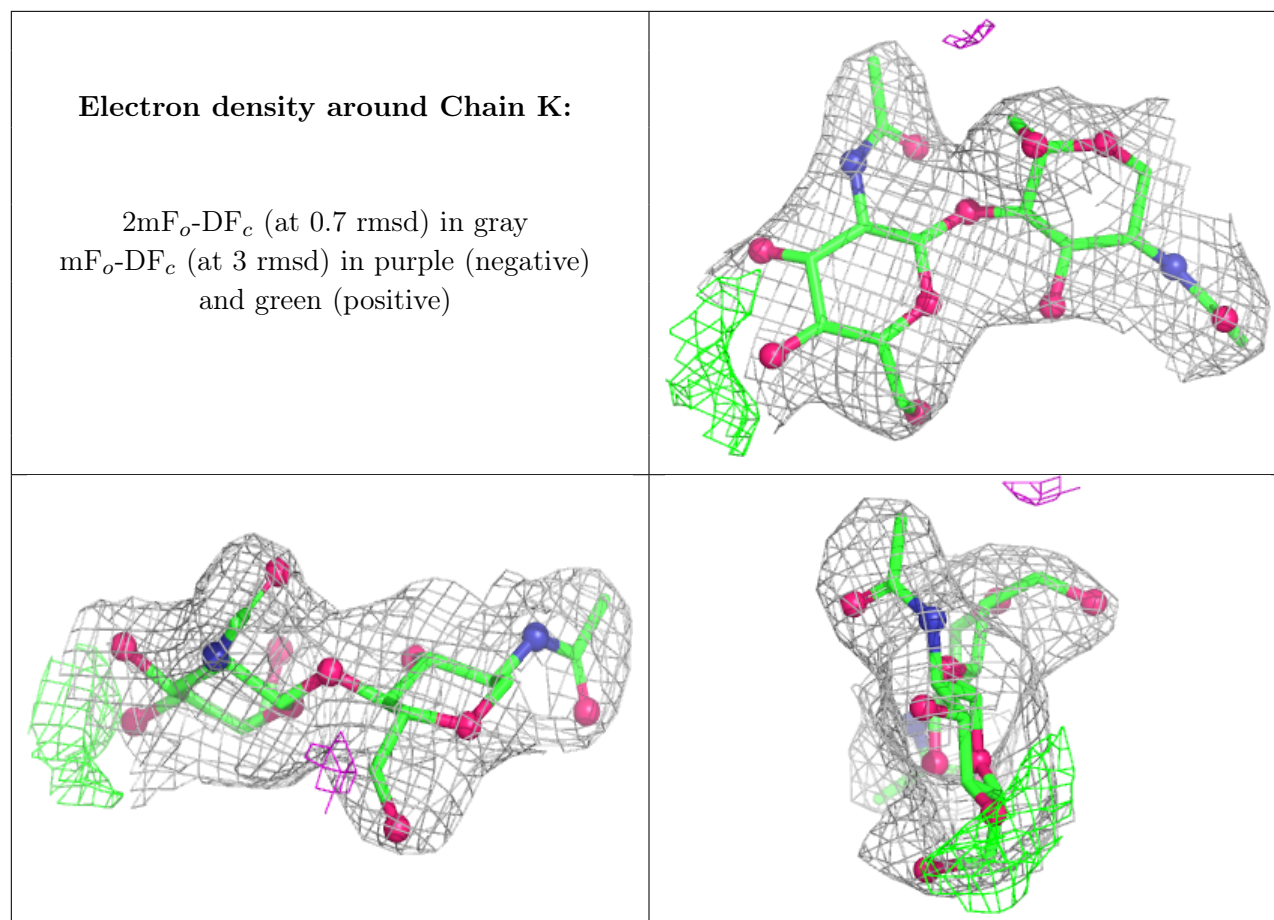
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain J:

$2mF_o-DF_c$ (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
4	NAG	A	908	14/15	0.67	0.11	96,103,112,113	0
4	NAG	D	907	14/15	0.76	0.11	77,84,89,91	0
4	NAG	A	905	14/15	0.81	0.10	45,62,74,75	0
4	NAG	B	904	14/15	0.82	0.13	117,120,124,124	0
4	NAG	C	904	14/15	0.84	0.11	74,86,94,97	0
4	NAG	B	905	14/15	0.84	0.13	79,85,91,92	0
4	NAG	D	904	14/15	0.87	0.12	58,65,73,76	0
4	NAG	A	904	14/15	0.90	0.10	63,70,73,75	0
3	CA	D	901	1/1	0.91	0.07	102,102,102,102	0
3	CA	B	901	1/1	0.97	0.03	95,95,95,95	0
3	CA	A	901	1/1	0.97	0.04	72,72,72,72	0
3	CA	C	901	1/1	0.98	0.07	87,87,87,87	0

6.5 Other polymers [i](#)

There are no such residues in this entry.