



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 6, 2025 – 01:31 pm BST

PDB ID : 9SDS / pdb_00009sds
Title : Structure of native leukocyte myeloperoxidase in complex with a truncated version of the Staphylococcal Peroxidase Inhibitor SPIN and chloride at pH 5.5
Authors : Leitgeb, U.; Pfanzagl, V.
Deposited on : 2025-08-14
Resolution : 2.49 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	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
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)	:	2.46

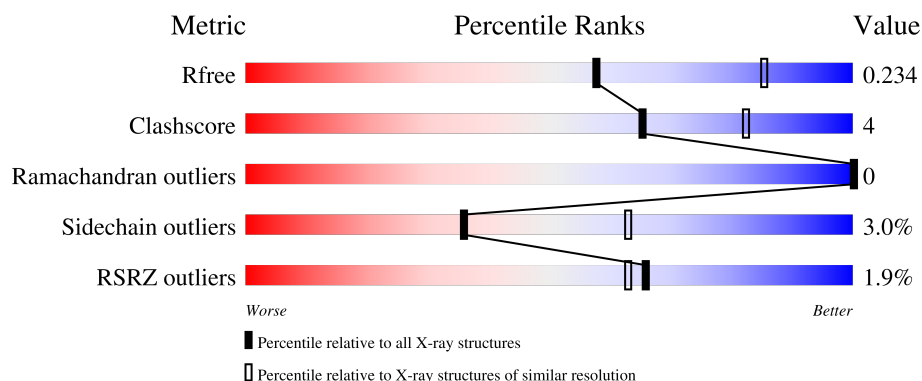
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.49 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}	164625	5504 (2.50-2.50)
Clashscore	180529	6282 (2.50-2.50)
Ramachandran outliers	177936	6191 (2.50-2.50)
Sidechain outliers	177891	6193 (2.50-2.50)
RSRZ outliers	164620	5504 (2.50-2.50)

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	114	<div> <div>18%</div> <div>74% 18% 8%</div> </div>
1	B	114	<div> <div>3%</div> <div>72% 19% 8%</div> </div>
2	E	60	<div> <div>73% 13% 5% 8%</div> </div>
2	F	60	<div> <div>18%</div> <div>62% 23% 10%</div> </div>

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Mol	Chain	Length	Quality of chain
3	C	467	<div><div>%</div><div><div></div><div>81%</div><div>16%</div><div>.</div></div></div>
3	D	467	<div><div>%</div><div><div></div><div>81%</div><div>16%</div><div>..</div></div></div>
4	G	6	<div><div><div></div><div>33%</div><div>67%</div></div></div>
4	J	6	<div><div><div></div><div>17%</div><div>67%</div><div>17%</div></div></div>
5	H	2	<div><div><div></div><div>100%</div></div></div>
5	I	2	<div><div><div></div><div>100%</div></div></div>
5	K	2	<div><div><div></div><div>100%</div></div></div>

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 10651 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 Myeloperoxidase light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	105	Total	C	N	O	S	0	0	0
			842	532	149	156	5			
1	B	105	Total	C	N	O	S	0	0	0
			842	532	149	156	5			

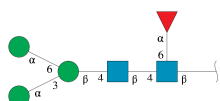
- Molecule 2 is a protein called Myeloperoxidase inhibitor SPIN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	55	Total	C	N	O	0	0	0
			448	284	75	89			
2	F	54	Total	C	N	O	0	0	0
			436	275	74	87			

- Molecule 3 is a protein called Myeloperoxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	465	Total	C	N	O	S	0	0	0
			3726	2348	686	665	27			
3	D	465	Total	C	N	O	S	0	0	0
			3726	2348	686	665	27			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	6	Total	C	N	O	0	0	0
			71	40	2	29			

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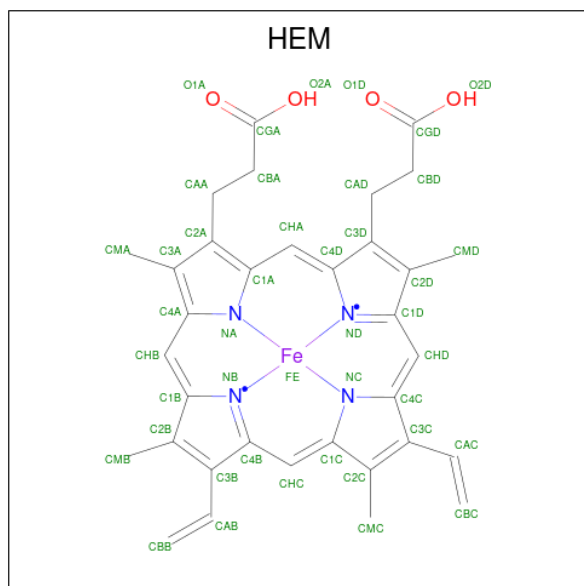
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	J	6	Total	C	N	O	0	0	0
			71	40	2	29			

- Molecule 5 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
5	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	K	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 6 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
6	B	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 7 is IODIDE ION (CCD ID: IOD) (formula: I).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total I 1 1	0	0
7	B	1	Total I 1 1	0	0

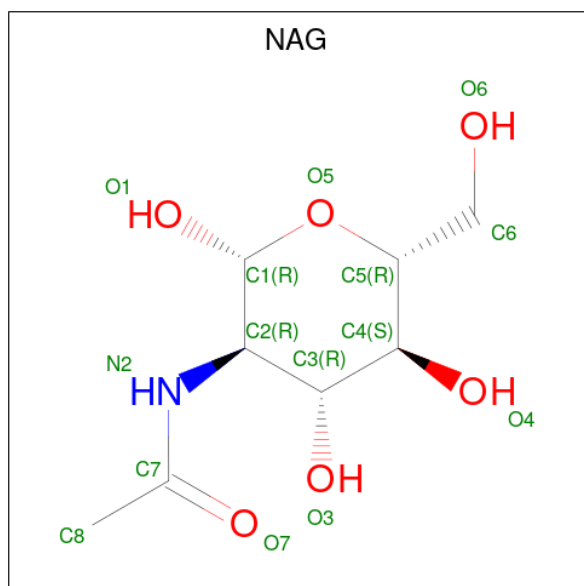
- Molecule 8 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	C	1	Total Ca 1 1	0	0
8	D	1	Total Ca 1 1	0	0

- Molecule 9 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	C	2	Total Cl 2 2	0	0
9	D	1	Total Cl 1 1	0	0

- Molecule 10 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	42	Total	O	0	0
			42	42		
11	E	3	Total	O	0	0
			3	3		
11	C	137	Total	O	0	0
			137	137		
11	B	28	Total	O	0	0
			28	28		
11	D	87	Total	O	0	0
			87	87		
11	F	1	Total	O	0	0
			1	1		

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.

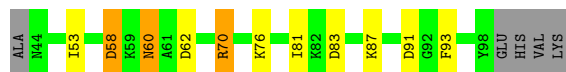
- Molecule 1: Myeloperoxidase light chain



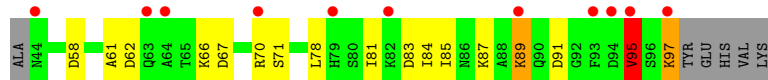
- Molecule 1: Myeloperoxidase light chain



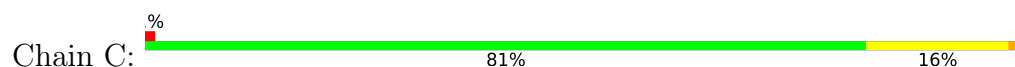
- Molecule 2: Myeloperoxidase inhibitor SPIN

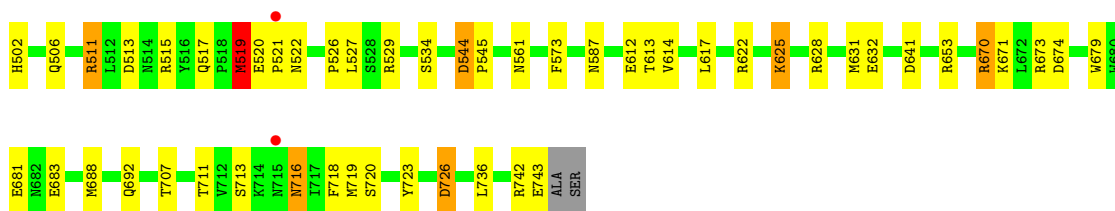


- Molecule 2: Myeloperoxidase inhibitor SPIN

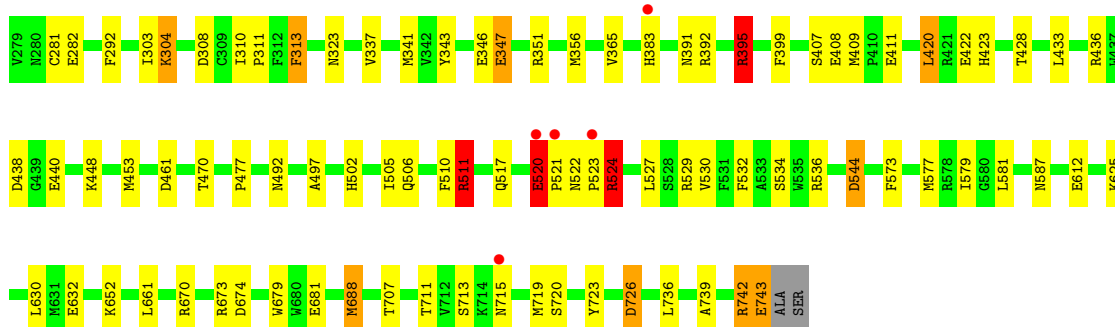
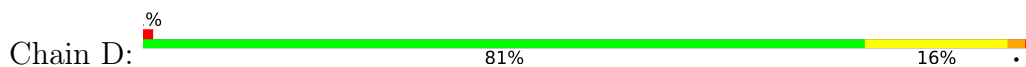


- Molecule 3: Myeloperoxidase

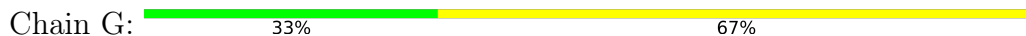




• Molecule 3: Myeloperoxidase



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




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



• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose




• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  100%

MAG1
MAG2

- Molecule 5: 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 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	111.16Å 111.16Å 241.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.74 – 2.49 48.74 – 2.49	Depositor EDS
% Data completeness (in resolution range)	98.0 (48.74-2.49) 98.0 (48.74-2.49)	Depositor EDS
R_{merge}	0.70	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.13 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, R_{free}	0.188 , 0.234 0.188 , 0.234	Depositor DCC
R_{free} test set	2639 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	19.3	Xtriage
Anisotropy	0.077	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 25.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10651	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.36% 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: FUC, BMA, CA, CL, MAN, HEM, IOD, NAG

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	0.77	0/867	1.56	14/1181 (1.2%)
1	B	0.74	0/867	1.55	15/1181 (1.3%)
2	E	0.70	0/455	1.85	11/610 (1.8%)
2	F	0.66	0/442	1.87	9/592 (1.5%)
3	C	0.77	0/3812	1.55	56/5173 (1.1%)
3	D	0.72	0/3812	1.55	50/5173 (1.0%)
All	All	0.74	0/10255	1.58	155/13910 (1.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
2	E	0	1
3	C	0	6
3	D	0	5
All	All	0	13

There are no bond length outliers.

All (155) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	520	GLU	N-CA-CB	12.11	124.68	110.03
3	D	506	GLN	CB-CA-C	11.57	125.53	108.86
3	C	506	GLN	CB-CA-C	11.03	125.49	108.61
3	C	625	LYS	N-CA-CB	10.16	125.07	109.94
3	D	625	LYS	CB-CA-C	10.12	127.59	110.79
3	C	519	MET	CG-SD-CE	9.98	122.85	100.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	391	ASN	CA-CB-CG	9.36	121.95	112.60
3	D	506	GLN	N-CA-CB	-9.25	98.84	110.03
2	E	83	ASP	CA-CB-CG	8.83	121.43	112.60
1	A	220	ASN	CB-CA-C	8.82	124.25	111.73
3	D	524	ARG	CA-CB-CG	8.80	131.70	114.10
1	A	169	GLU	CB-CG-CD	8.45	126.96	112.60
1	A	233	GLU	CB-CG-CD	8.30	126.72	112.60
1	B	220	ASN	CB-CA-C	8.22	123.40	111.73
3	C	719	MET	CG-SD-CE	8.18	118.90	100.90
3	D	743	GLU	CB-CG-CD	8.07	126.31	112.60
3	D	470	THR	CA-CB-OG1	-8.04	97.54	109.60
3	D	356	MET	CG-SD-CE	7.88	118.23	100.90
3	C	292	PHE	CB-CA-C	7.86	121.51	111.21
3	D	742	ARG	CA-CB-CG	7.71	129.52	114.10
3	C	625	LYS	CB-CA-C	-7.68	98.51	110.81
3	C	282	GLU	CB-CG-CD	7.68	125.65	112.60
3	D	308	ASP	CA-CB-CG	7.66	120.26	112.60
3	C	632	GLU	N-CA-CB	-7.62	98.92	110.12
3	C	742	ARG	CA-CB-CG	7.36	128.82	114.10
3	C	428	THR	CA-CB-OG1	-7.20	98.80	109.60
3	D	670	ARG	CA-CB-CG	-7.14	99.83	114.10
3	C	612	GLU	N-CA-CB	7.13	120.88	110.26
3	D	625	LYS	N-CA-CB	-7.08	99.71	110.12
3	C	313	PHE	CA-CB-CG	7.07	120.87	113.80
3	C	506	GLN	N-CA-CB	-7.07	98.36	110.10
1	B	167	CYS	CB-CA-C	-7.00	96.81	110.10
3	D	612	GLU	N-CA-CB	6.95	121.05	110.42
1	B	241	GLN	CB-CA-C	-6.94	97.52	110.01
3	C	323	ASN	CB-CA-C	6.91	121.67	109.65
3	C	692	GLN	N-CA-CB	6.91	120.02	110.01
3	D	351	ARG	CD-NE-CZ	6.86	134.00	124.40
3	D	323	ASN	CB-CA-C	6.85	121.57	109.65
3	D	304	LYS	CB-CG-CD	6.83	127.01	111.30
3	C	351	ARG	CD-NE-CZ	6.82	133.95	124.40
3	C	391	ASN	CA-CB-CG	6.80	119.40	112.60
1	A	215	PRO	CB-CA-C	6.72	120.14	111.46
2	E	87	LYS	CG-CD-CE	-6.63	96.06	111.30
3	C	625	LYS	CA-CB-CG	6.62	127.34	114.10
3	D	674	ASP	CA-CB-CG	6.61	119.21	112.60
3	D	652	LYS	CB-CG-CD	6.60	126.47	111.30
3	D	292	PHE	CB-CA-C	6.59	121.42	111.14
3	D	346	GLU	CB-CG-CD	6.53	123.70	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	67	ASP	CA-CB-CG	6.50	119.10	112.60
2	E	60	ASN	CB-CA-C	-6.49	99.88	110.79
2	F	95	VAL	N-CA-CB	6.49	120.91	112.28
3	D	544	ASP	CA-CB-CG	6.43	119.03	112.60
2	F	83	ASP	CA-CB-CG	6.42	119.02	112.60
1	A	167	CYS	CB-CA-C	-6.32	98.10	110.10
3	C	674	ASP	CA-CB-CG	6.31	118.91	112.60
3	C	683	GLU	CB-CG-CD	6.28	123.28	112.60
3	D	383	HIS	CB-CA-C	6.28	119.93	109.89
3	D	470	THR	OG1-CB-CG2	-6.24	96.82	109.30
3	C	438	ASP	CA-CB-CG	6.24	118.84	112.60
3	D	719	MET	CG-SD-CE	6.21	114.55	100.90
3	C	573	PHE	CA-CB-CG	6.20	120.00	113.80
3	C	632	GLU	CB-CA-C	6.19	121.07	110.79
3	C	351	ARG	CB-CG-CD	6.14	125.43	111.30
3	D	313	PHE	CA-CB-CG	6.13	119.93	113.80
3	D	395	ARG	CD-NE-CZ	6.11	132.95	124.40
3	D	477	PRO	CB-CA-C	-6.10	103.25	111.12
3	C	711	THR	CA-CB-OG1	-6.09	100.47	109.60
1	A	267	PRO	CB-CA-C	6.08	119.01	111.23
3	C	544	ASP	CA-CB-CG	6.07	118.67	112.60
1	A	174	ARG	CB-CG-CD	-6.07	97.35	111.30
2	E	93	PHE	N-CA-CB	5.99	119.39	110.29
3	C	283	THR	CA-CB-OG1	-5.96	100.66	109.60
3	C	641	ASP	CA-CB-CG	5.91	118.51	112.60
3	D	440	GLU	CB-CG-CD	5.91	122.64	112.60
1	A	184	ARG	CD-NE-CZ	5.89	132.65	124.40
3	D	438	ASP	CA-CB-CG	5.89	118.50	112.60
1	A	266	THR	CA-CB-OG1	-5.87	100.80	109.60
1	B	234	ILE	CB-CA-C	5.86	116.65	110.91
2	E	58	ASP	CA-CB-CG	5.86	118.46	112.60
3	D	492	ASN	CB-CA-C	5.84	120.15	110.81
1	B	247	GLU	CB-CA-C	5.83	120.66	110.64
3	D	573	PHE	CA-CB-CG	5.78	119.58	113.80
3	C	346	GLU	CB-CG-CD	5.76	122.39	112.60
2	E	62	ASP	CA-CB-CG	5.75	118.36	112.60
1	A	211	TYR	N-CA-CB	5.71	118.34	109.48
3	C	383	HIS	CB-CA-C	5.71	119.15	109.84
3	D	422	GLU	CB-CG-CD	5.71	122.31	112.60
3	C	511	ARG	CB-CG-CD	-5.63	98.34	111.30
3	C	308	ASP	CA-CB-CG	5.63	118.23	112.60
3	C	613	THR	CA-CB-OG1	-5.61	101.18	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	473	ARG	CD-NE-CZ	5.59	132.23	124.40
1	B	208	SER	CA-CB-OG	-5.59	99.92	111.10
3	D	438	ASP	CA-C-N	5.59	126.18	119.98
3	D	438	ASP	C-N-CA	5.59	126.18	119.98
2	F	91	ASP	CB-CA-C	5.57	120.28	110.37
3	C	631	MET	CA-C-N	5.55	127.71	120.28
3	C	631	MET	C-N-CA	5.55	127.71	120.28
3	D	536	ARG	CD-NE-CZ	5.47	132.07	124.40
1	B	268	GLU	CB-CA-C	-5.46	100.92	109.22
3	D	726	ASP	CA-CB-CG	5.46	118.06	112.60
3	C	742	ARG	N-CA-CB	-5.45	102.64	110.44
3	C	480	ARG	CD-NE-CZ	5.45	132.03	124.40
1	B	246	GLN	CB-CA-C	-5.40	100.64	110.63
3	C	561	ASN	CB-CA-C	5.39	119.80	111.28
3	D	428	THR	CA-CB-OG1	-5.38	101.53	109.60
3	C	688	MET	CG-SD-CE	5.36	112.69	100.90
3	D	715	ASN	CA-CB-CG	5.36	117.96	112.60
3	C	395	ARG	CD-NE-CZ	5.34	131.88	124.40
1	A	208	SER	CA-CB-OG	-5.34	100.42	111.10
1	B	230	VAL	N-CA-CB	5.34	116.79	110.55
3	C	723	TYR	CB-CA-C	5.32	116.38	108.87
3	D	461	ASP	CA-CB-CG	5.32	117.92	112.60
1	B	238	PRO	CA-C-N	5.32	127.94	120.28
1	B	238	PRO	C-N-CA	5.32	127.94	120.28
1	A	220	ASN	CA-CB-CG	5.32	117.92	112.60
3	D	530	VAL	N-CA-CB	5.30	119.73	111.57
3	D	511	ARG	CB-CG-CD	-5.29	99.13	111.30
3	C	529	ARG	CD-NE-CZ	5.29	131.80	124.40
3	D	408	GLU	CB-CA-C	5.27	120.39	110.63
2	E	62	ASP	CA-C-N	5.26	127.32	120.28
2	E	62	ASP	C-N-CA	5.26	127.32	120.28
3	C	526	PRO	CB-CA-C	5.23	118.21	111.46
1	A	179	MET	CG-SD-CE	5.23	112.40	100.90
2	F	62	ASP	CB-CA-C	5.20	119.03	109.46
3	D	347	GLU	N-CA-CB	5.20	118.04	110.30
3	C	517	GLN	CB-CA-C	5.19	116.56	108.61
1	B	169	GLU	CB-CA-C	5.19	118.74	109.29
1	B	211	TYR	N-CA-CB	5.18	117.51	109.48
3	C	492	ASN	CB-CA-C	5.17	119.32	110.74
3	C	622	ARG	CB-CA-C	5.16	119.66	111.51
2	F	87	LYS	CB-CG-CD	5.15	123.14	111.30
3	D	681	GLU	CB-CA-C	-5.15	101.50	110.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	171	ASP	CA-CB-CG	5.14	117.74	112.60
1	A	230	VAL	N-CA-CB	5.13	116.55	110.55
3	C	422	GLU	CB-CG-CD	5.11	121.29	112.60
3	C	726	ASP	CA-CB-CG	5.10	117.70	112.60
3	D	529	ARG	CD-NE-CZ	5.08	131.51	124.40
2	F	97	LYS	CA-CB-CG	5.07	124.24	114.10
3	C	408	GLU	CB-CA-C	5.06	120.00	110.63
1	B	192	ASN	CB-CA-C	5.06	118.30	111.82
3	C	614	VAL	CA-C-N	5.06	125.71	119.99
3	C	614	VAL	C-N-CA	5.06	125.71	119.99
3	D	517	GLN	CB-CA-C	5.06	116.35	108.61
2	E	91	ASP	CB-CA-C	5.06	119.11	110.56
3	C	282	GLU	CB-CA-C	5.04	119.96	110.63
3	D	448	LYS	CB-CA-C	5.04	119.16	110.79
3	C	681	GLU	CB-CA-C	-5.03	101.70	110.09
2	E	53	ILE	CA-C-N	5.02	127.01	120.28
2	E	53	ILE	C-N-CA	5.02	127.01	120.28
3	D	711	THR	CA-CB-OG1	-5.02	102.07	109.60
2	F	71	SER	CA-C-N	5.02	127.00	120.28
2	F	71	SER	C-N-CA	5.02	127.00	120.28
3	C	617	LEU	CA-C-N	5.00	125.65	119.99
3	C	617	LEU	C-N-CA	5.00	125.65	119.99
3	D	723	TYR	CB-CA-C	5.00	115.93	108.87

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	183	ARG	Sidechain
3	C	314	ARG	Sidechain
3	C	351	ARG	Sidechain
3	C	436	ARG	Sidechain
3	C	515	ARG	Sidechain
3	C	653	ARG	Sidechain
3	C	670	ARG	Sidechain
3	D	392	ARG	Sidechain
3	D	395	ARG	Sidechain
3	D	436	ARG	Sidechain
3	D	511	ARG	Sidechain
3	D	524	ARG	Sidechain
2	E	70	ARG	Sidechain

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	842	0	800	6	0
1	B	842	0	800	7	0
2	E	448	0	436	7	0
2	F	436	0	427	7	0
3	C	3726	0	3720	25	0
3	D	3726	0	3721	28	0
4	G	71	0	61	0	0
4	J	71	0	61	1	0
5	H	28	0	25	0	0
5	I	28	0	25	0	0
5	K	28	0	25	0	0
6	A	43	0	30	2	0
6	B	43	0	30	1	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
8	C	1	0	0	0	0
8	D	1	0	0	0	0
9	C	2	0	0	0	0
9	D	1	0	0	0	0
10	D	14	0	13	0	0
11	A	42	0	0	0	0
11	B	28	0	0	0	0
11	C	137	0	0	0	0
11	D	87	0	0	0	0
11	E	3	0	0	2	0
11	F	1	0	0	0	0
All	All	10651	0	10174	76	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 4.

All (76) 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)
3:C:502:HIS:HD1	3:C:587:ASN:HD21	1.33	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:502:HIS:HD1	3:D:587:ASN:HD21	1.33	0.76
2:E:70:ARG:HH12	2:E:81:ILE:HD11	1.50	0.76
3:C:716:ASN:HD22	3:C:718:PHE:H	1.38	0.70
2:E:58:ASP:OD1	2:E:60:ASN:HB2	1.95	0.66
2:F:58:ASP:HB3	2:F:61:ALA:HB2	1.78	0.65
3:D:343:TYR:OH	3:D:423:HIS:HD2	1.81	0.62
3:C:343:TYR:OH	3:C:423:HIS:HD2	1.83	0.61
2:E:76:LYS:HE2	11:E:201:HOH:O	1.99	0.61
6:B:301:HEM:HBC2	6:B:301:HEM:HMC2	1.83	0.60
6:A:301:HEM:HMC2	6:A:301:HEM:HBC2	1.84	0.59
2:F:61:ALA:HB3	2:F:66:LYS:HE3	1.84	0.58
1:A:179:MET:HE1	1:A:193:ARG:HH21	1.68	0.58
3:C:716:ASN:ND2	3:C:718:PHE:H	2.01	0.58
3:D:453:MET:HE3	3:D:736:LEU:HD22	1.87	0.57
3:C:519:MET:HE3	3:C:545:PRO:HG3	1.88	0.55
2:E:76:LYS:CE	11:E:201:HOH:O	2.54	0.54
3:D:523:PRO:O	3:D:524:ARG:HB2	2.07	0.54
3:D:544:ASP:OD1	3:D:707:THR:HB	2.07	0.54
3:C:720:SER:HB3	3:C:726:ASP:HB3	1.91	0.53
3:D:520:GLU:HB3	3:D:521:PRO:HA	1.92	0.52
3:C:513:ASP:HA	3:C:519:MET:HE2	1.92	0.52
3:C:628:ARG:HH11	3:C:628:ARG:HG3	1.74	0.52
3:C:453:MET:HE3	3:C:736:LEU:HD22	1.91	0.51
3:D:343:TYR:OH	3:D:423:HIS:CD2	2.63	0.51
1:B:254:GLN:OE1	3:D:411:GLU:HB2	2.10	0.51
2:F:89:LYS:HG2	2:F:95:VAL:HG23	1.93	0.51
3:C:544:ASP:OD1	3:C:707:THR:HB	2.10	0.50
3:C:671:LYS:HE3	4:J:5:MAN:H61	1.94	0.50
3:C:475:TYR:O	3:C:670:ARG:HD2	2.10	0.50
1:B:179:MET:O	1:B:180:CYS:HB2	2.13	0.48
3:D:502:HIS:HA	3:D:505:ILE:HD12	1.95	0.48
3:D:720:SER:HB3	3:D:726:ASP:HB3	1.95	0.48
3:D:520:GLU:HG3	3:D:523:PRO:HG3	1.95	0.47
2:F:78:LEU:HD23	2:F:84:ILE:HA	1.95	0.47
3:C:673:ARG:HG3	3:C:679:TRP:CE2	2.49	0.47
3:C:520:GLU:OE1	3:C:521:PRO:HA	2.15	0.47
2:E:70:ARG:HH12	2:E:81:ILE:CD1	2.24	0.47
3:C:628:ARG:HG3	3:C:628:ARG:NH1	2.30	0.47
3:D:520:GLU:CB	3:D:521:PRO:HA	2.46	0.46
3:D:673:ARG:HG3	3:D:679:TRP:CE2	2.50	0.46
2:F:81:ILE:HG22	2:F:85:ILE:HD12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:ILE:HD13	3:D:630:LEU:HD23	1.98	0.46
3:C:343:TYR:OH	3:C:423:HIS:CD2	2.67	0.45
1:B:263:LEU:HD21	3:D:337:VAL:HG22	1.98	0.45
3:D:311:PRO:HG2	3:D:581:LEU:HD21	1.99	0.45
3:C:716:ASN:HD22	3:C:716:ASN:C	2.24	0.45
2:E:76:LYS:NZ	3:C:352:ASN:OD1	2.50	0.44
3:C:436:ARG:CZ	3:C:436:ARG:HB2	2.48	0.44
2:E:70:ARG:NH1	2:E:81:ILE:HD11	2.24	0.44
1:B:177:THR:O	1:B:190:ALA:HA	2.18	0.44
3:D:510:PHE:CE2	3:D:524:ARG:HG2	2.53	0.43
3:C:399:PHE:CE2	3:C:534:SER:HB2	2.53	0.43
1:A:177:THR:O	1:A:190:ALA:HA	2.18	0.43
3:D:282:GLU:OE2	3:D:577:MET:HE3	2.19	0.43
1:A:254:GLN:OE1	3:C:411:GLU:HB2	2.18	0.43
1:A:271:ALA:HB1	3:C:280:ASN:OD1	2.18	0.43
3:D:281:CYS:HB2	3:D:313:PHE:CZ	2.54	0.42
3:C:281:CYS:HB2	3:C:313:PHE:CZ	2.55	0.42
3:D:303:ILE:HG12	3:D:579:ILE:HD11	2.01	0.42
3:D:395:ARG:HH11	3:D:395:ARG:HG3	1.85	0.42
2:F:58:ASP:HB3	2:F:61:ALA:CB	2.47	0.42
6:A:301:HEM:HBC2	6:A:301:HEM:CMC	2.50	0.42
3:D:365:VAL:HG12	3:D:420:LEU:HD21	2.02	0.42
3:D:688:MET:HB3	3:D:688:MET:HE3	1.70	0.42
3:D:310:ILE:HA	3:D:311:PRO:HD2	1.97	0.42
3:D:739:ALA:O	3:D:742:ARG:HB3	2.20	0.41
3:D:399:PHE:CE2	3:D:534:SER:HB2	2.55	0.41
1:A:206:GLY:HA2	1:B:186:PRO:HD2	2.03	0.41
1:A:179:MET:O	1:A:180:CYS:HB2	2.21	0.40
1:B:250:LEU:HD23	1:B:250:LEU:HA	1.94	0.40
3:D:497:ALA:HB1	3:D:661:LEU:HD22	2.02	0.40
2:F:70:ARG:HH22	2:F:81:ILE:HD11	1.86	0.40
3:C:544:ASP:HB2	3:C:545:PRO:HD3	2.03	0.40
3:C:361:GLY:O	3:C:423:HIS:HE1	2.05	0.40
3:D:407:SER:O	3:D:532:PHE:HA	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	103/114 (90%)	99 (96%)	4 (4%)	0	100	100
1	B	103/114 (90%)	97 (94%)	6 (6%)	0	100	100
2	E	53/60 (88%)	53 (100%)	0	0	100	100
2	F	52/60 (87%)	51 (98%)	1 (2%)	0	100	100
3	C	463/467 (99%)	448 (97%)	15 (3%)	0	100	100
3	D	463/467 (99%)	445 (96%)	18 (4%)	0	100	100
All	All	1237/1282 (96%)	1193 (96%)	44 (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	90/97 (93%)	89 (99%)	1 (1%)	70	87
1	B	90/97 (93%)	90 (100%)	0	100	100
2	E	49/53 (92%)	49 (100%)	0	100	100
2	F	48/53 (91%)	45 (94%)	3 (6%)	15	30
3	C	411/412 (100%)	397 (97%)	14 (3%)	32	58
3	D	411/412 (100%)	396 (96%)	15 (4%)	30	56
All	All	1099/1124 (98%)	1066 (97%)	33 (3%)	36	63

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	170	GLN
3	C	347	GLU
3	C	383	HIS
3	C	409	MET
3	C	420	LEU
3	C	429	GLU
3	C	480	ARG
3	C	511	ARG
3	C	519	MET
3	C	522	ASN
3	C	527	LEU
3	C	625	LYS
3	C	713	SER
3	C	716	ASN
3	C	743	GLU
3	D	304	LYS
3	D	341	MET
3	D	347	GLU
3	D	395	ARG
3	D	409	MET
3	D	420	LEU
3	D	433	LEU
3	D	511	ARG
3	D	520	GLU
3	D	522	ASN
3	D	527	LEU
3	D	632	GLU
3	D	688	MET
3	D	713	SER
3	D	743	GLU
2	F	89	LYS
2	F	95	VAL
2	F	97	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	192	ASN
3	C	288	GLN
3	C	423	HIS
3	C	562	GLN

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Mol	Chain	Res	Type
3	C	716	ASN
1	B	192	ASN
3	D	287	GLN
3	D	305	ASN
3	D	423	HIS
3	D	562	GLN
3	D	575	GLN

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 ⓘ

18 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	$\# Z > 2$
4	NAG	G	1	4,3	14,14,15	0.48	0	17,19,21	1.30	2 (11%)
4	NAG	G	2	4	14,14,15	0.40	0	17,19,21	1.01	0
4	BMA	G	3	4	11,11,12	0.64	0	15,15,17	1.06	1 (6%)
4	MAN	G	4	4	11,11,12	1.40	2 (18%)	15,15,17	1.17	1 (6%)
4	MAN	G	5	4	11,11,12	0.77	0	15,15,17	1.66	1 (6%)
4	FUC	G	6	4	10,10,11	0.65	0	14,14,16	0.87	0
5	NAG	H	1	5,3	14,14,15	0.52	0	17,19,21	1.84	3 (17%)
5	NAG	H	2	5	14,14,15	0.75	0	17,19,21	1.75	4 (23%)
5	NAG	I	1	5,3	14,14,15	0.41	0	17,19,21	1.15	1 (5%)
5	NAG	I	2	5	14,14,15	0.56	0	17,19,21	1.11	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	J	1	4,3	14,14,15	0.42	0	17,19,21	1.05	0
4	NAG	J	2	4	14,14,15	0.39	0	17,19,21	1.25	2 (11%)
4	BMA	J	3	4	11,11,12	0.66	0	15,15,17	1.57	3 (20%)
4	MAN	J	4	4	11,11,12	1.40	1 (9%)	15,15,17	2.40	4 (26%)
4	MAN	J	5	4	11,11,12	0.95	1 (9%)	15,15,17	1.90	2 (13%)
4	FUC	J	6	4	10,10,11	1.01	0	14,14,16	1.05	1 (7%)
5	NAG	K	1	5,3	14,14,15	0.50	0	17,19,21	1.31	1 (5%)
5	NAG	K	2	5	14,14,15	0.65	0	17,19,21	2.32	4 (23%)

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	G	1	4,3	-	0/6/23/26	0/1/1/1
4	NAG	G	2	4	-	0/6/23/26	0/1/1/1
4	BMA	G	3	4	-	0/2/19/22	0/1/1/1
4	MAN	G	4	4	-	1/2/19/22	0/1/1/1
4	MAN	G	5	4	-	1/2/19/22	0/1/1/1
4	FUC	G	6	4	-	-	0/1/1/1
5	NAG	H	1	5,3	-	0/6/23/26	0/1/1/1
5	NAG	H	2	5	-	2/6/23/26	0/1/1/1
5	NAG	I	1	5,3	-	2/6/23/26	0/1/1/1
5	NAG	I	2	5	-	2/6/23/26	0/1/1/1
4	NAG	J	1	4,3	-	0/6/23/26	0/1/1/1
4	NAG	J	2	4	-	0/6/23/26	0/1/1/1
4	BMA	J	3	4	-	0/2/19/22	0/1/1/1
4	MAN	J	4	4	-	2/2/19/22	0/1/1/1
4	MAN	J	5	4	-	0/2/19/22	0/1/1/1
4	FUC	J	6	4	-	-	0/1/1/1
5	NAG	K	1	5,3	-	2/6/23/26	0/1/1/1
5	NAG	K	2	5	-	1/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	4	MAN	O5-C5	3.00	1.49	1.43
4	G	4	MAN	C4-C5	2.81	1.58	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	5	MAN	C2-C3	2.32	1.55	1.52
4	G	4	MAN	O5-C5	2.19	1.47	1.43

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	K	2	NAG	C2-N2-C7	6.05	131.52	122.90
4	J	4	MAN	C1-O5-C5	5.59	119.77	112.19
4	G	5	MAN	C1-O5-C5	5.47	119.60	112.19
4	J	5	MAN	O2-C2-C3	5.26	120.67	110.14
5	K	2	NAG	C1-C2-N2	-4.84	102.22	110.49
5	H	1	NAG	C2-N2-C7	4.76	129.69	122.90
4	J	4	MAN	O2-C2-C3	4.74	119.63	110.14
5	H	1	NAG	C1-O5-C5	4.18	117.85	112.19
4	J	5	MAN	C1-O5-C5	4.13	117.79	112.19
5	H	2	NAG	C1-O5-C5	3.93	117.51	112.19
5	K	2	NAG	C4-C3-C2	3.69	116.42	111.02
5	H	2	NAG	C2-N2-C7	3.57	127.99	122.90
4	J	4	MAN	O3-C3-C4	3.50	118.44	110.35
4	J	3	BMA	C1-O5-C5	3.27	116.62	112.19
4	G	1	NAG	C2-N2-C7	3.14	127.38	122.90
5	I	2	NAG	C1-O5-C5	3.07	116.35	112.19
5	K	1	NAG	C2-N2-C7	-3.06	118.54	122.90
4	G	4	MAN	O3-C3-C4	2.99	117.27	110.35
5	H	2	NAG	C1-C2-N2	2.95	115.53	110.49
4	J	3	BMA	O3-C3-C2	-2.72	104.79	109.99
4	J	2	NAG	C2-N2-C7	2.70	126.75	122.90
4	G	3	BMA	C1-O5-C5	2.69	115.83	112.19
5	I	1	NAG	C6-C5-C4	2.67	119.25	113.00
4	G	1	NAG	C1-O5-C5	2.52	115.61	112.19
5	I	2	NAG	C1-C2-N2	2.32	114.46	110.49
5	H	2	NAG	C4-C3-C2	2.30	114.39	111.02
4	J	3	BMA	O5-C5-C6	-2.26	103.66	107.20
4	J	6	FUC	C3-C4-C5	-2.20	106.34	109.77
5	H	1	NAG	C1-C2-N2	2.19	114.23	110.49
4	J	4	MAN	C1-C2-C3	-2.14	107.04	109.67
5	K	2	NAG	O4-C4-C5	2.13	114.60	109.30
4	J	2	NAG	C8-C7-N2	-2.04	112.65	116.10

There are no chirality outliers.

All (13) torsion outliers are listed below:

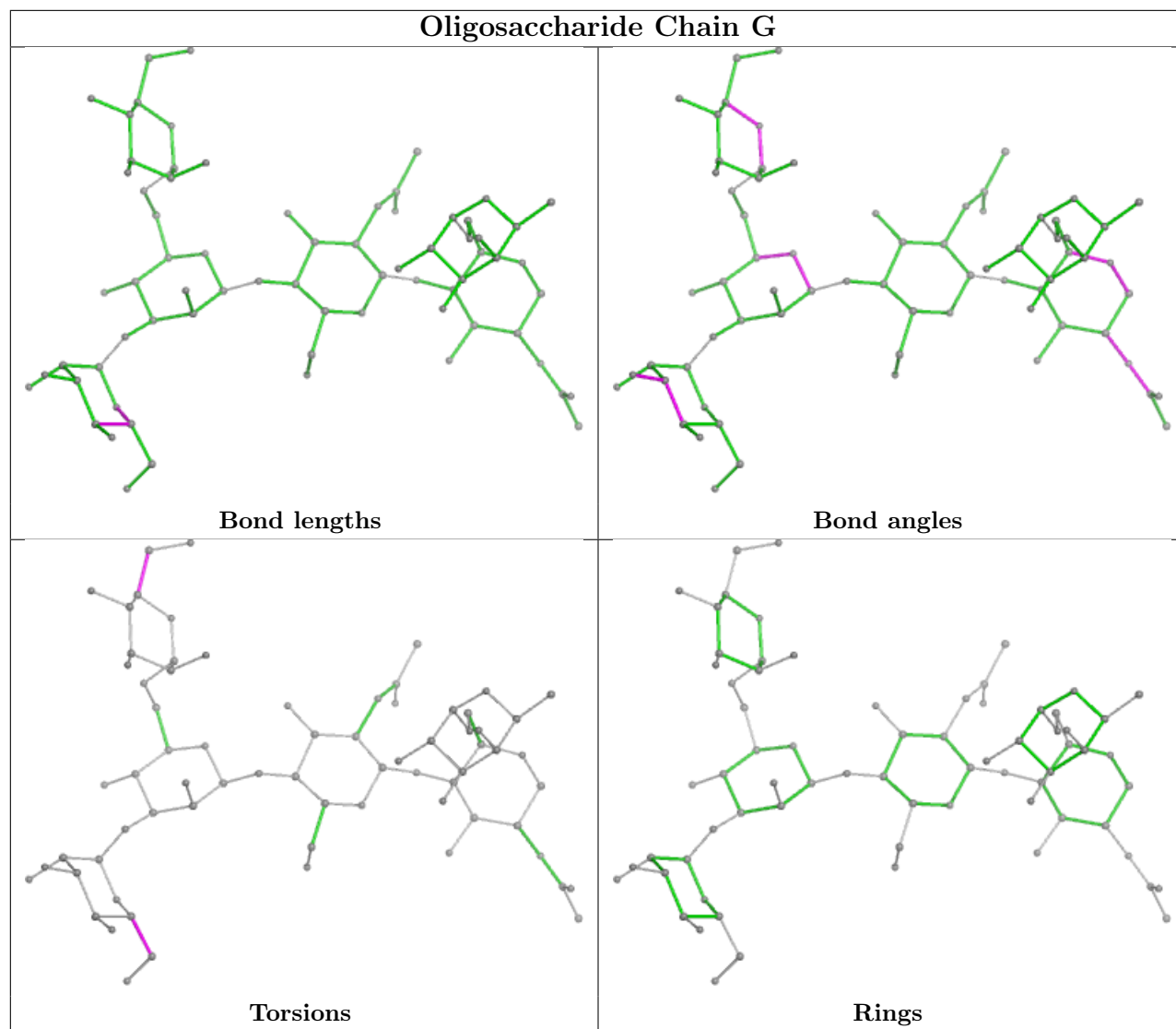
Mol	Chain	Res	Type	Atoms
4	J	4	MAN	O5-C5-C6-O6
5	K	1	NAG	O5-C5-C6-O6
5	I	1	NAG	C8-C7-N2-C2
4	J	4	MAN	C4-C5-C6-O6
5	K	1	NAG	C4-C5-C6-O6
5	H	2	NAG	C8-C7-N2-C2
5	I	1	NAG	O7-C7-N2-C2
5	H	2	NAG	O7-C7-N2-C2
5	I	2	NAG	C4-C5-C6-O6
5	I	2	NAG	O5-C5-C6-O6
4	G	5	MAN	C4-C5-C6-O6
5	K	2	NAG	O5-C5-C6-O6
4	G	4	MAN	C4-C5-C6-O6

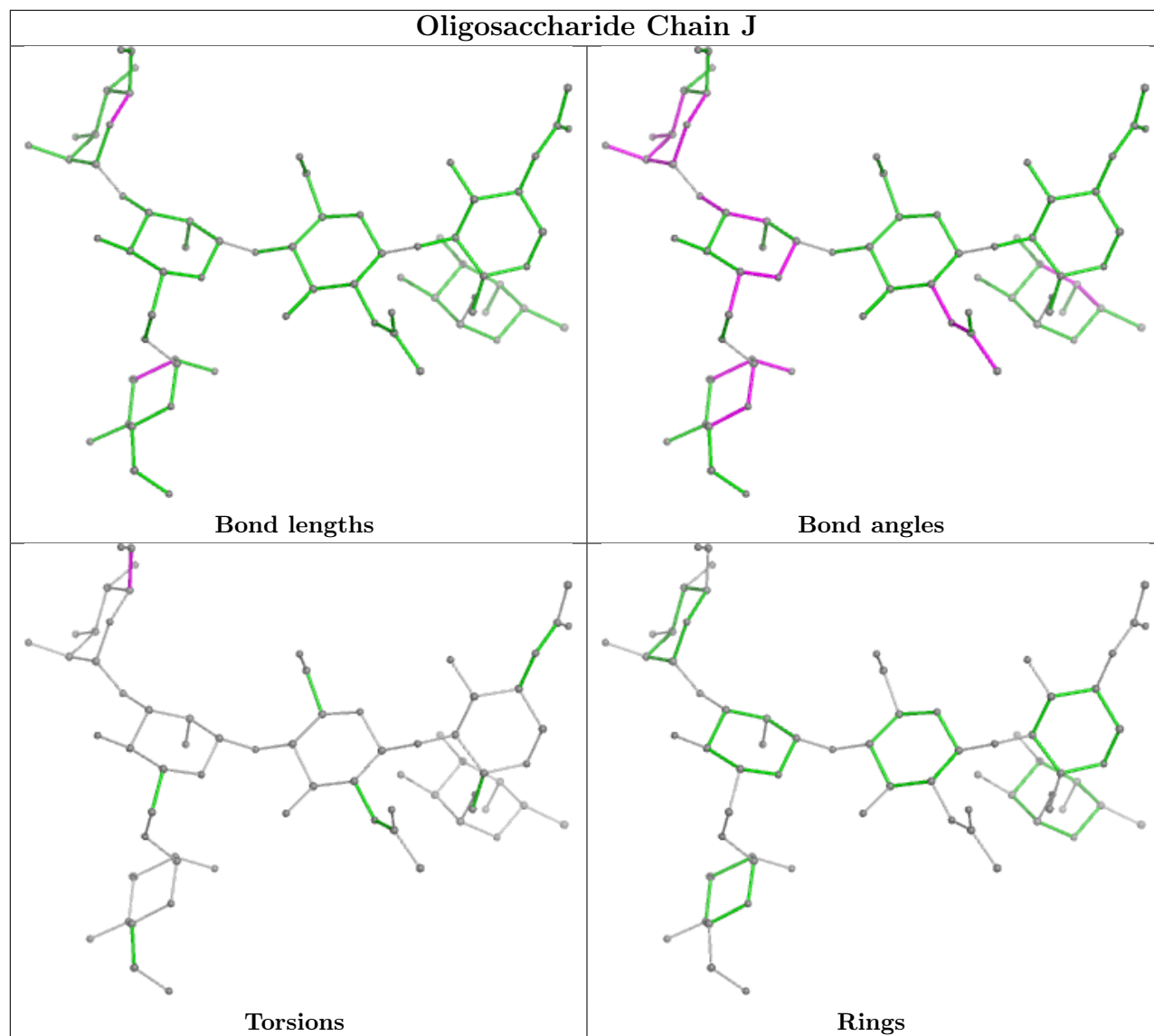
There are no ring outliers.

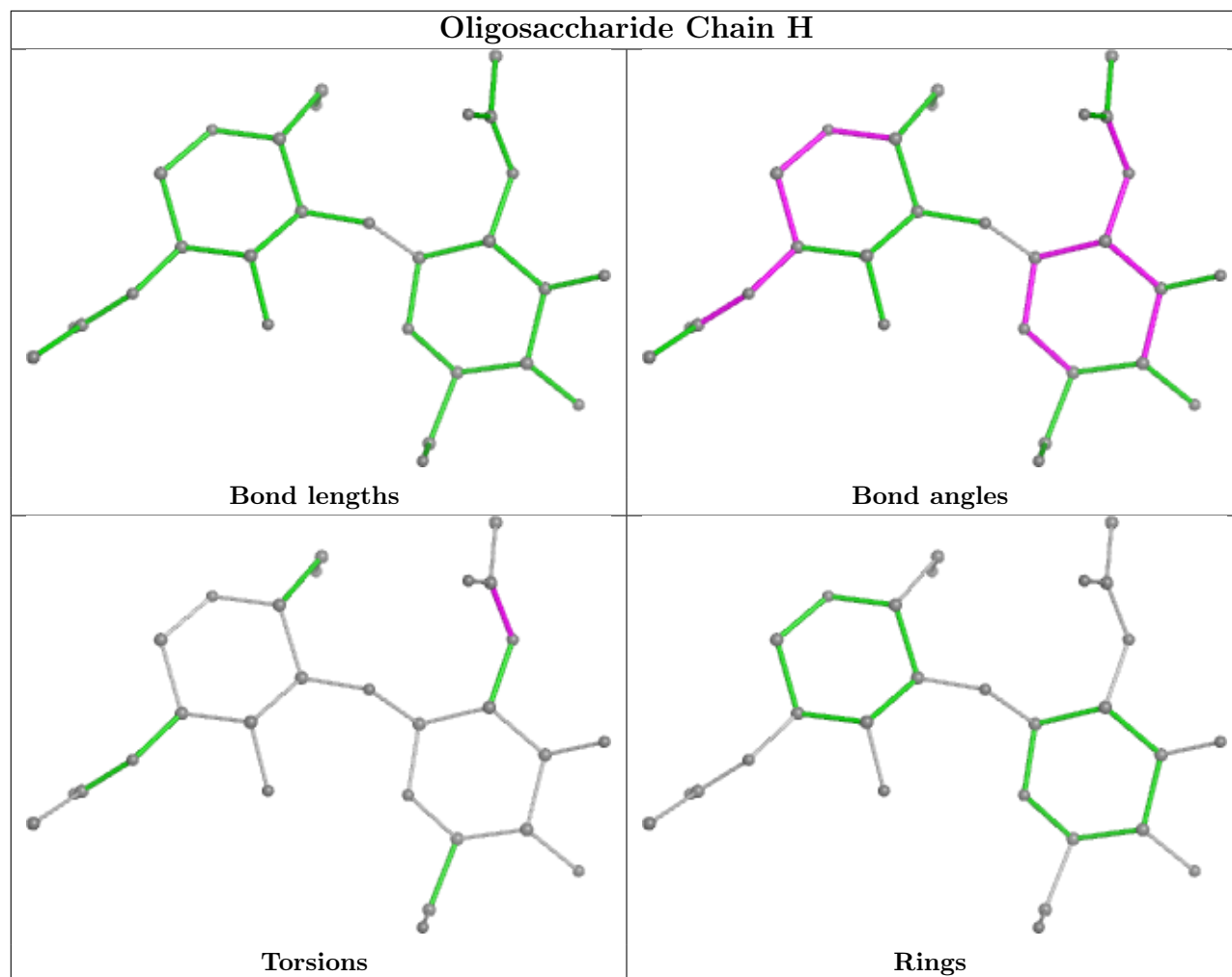
1 monomer is involved in 1 short contact:

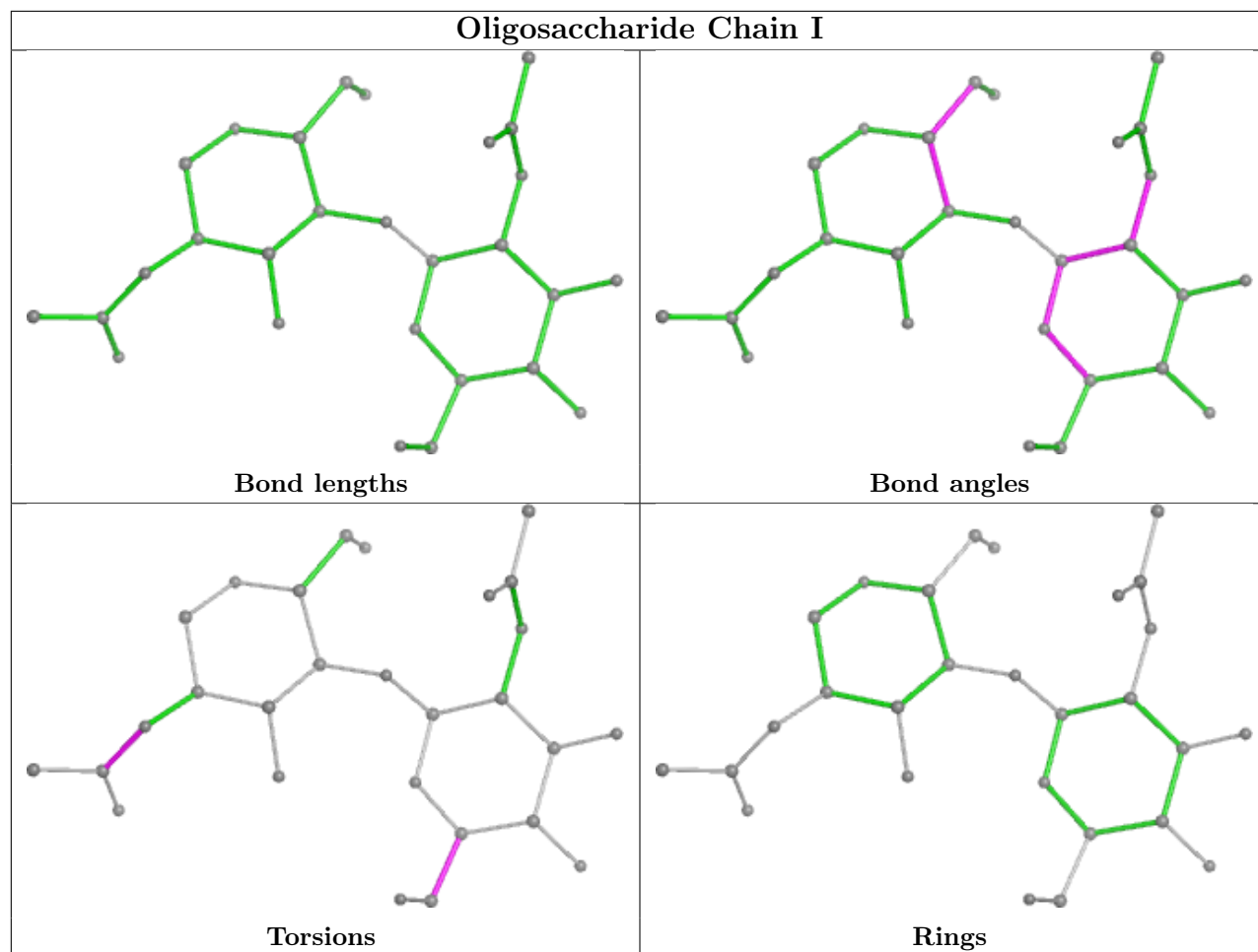
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	J	5	MAN	1	0

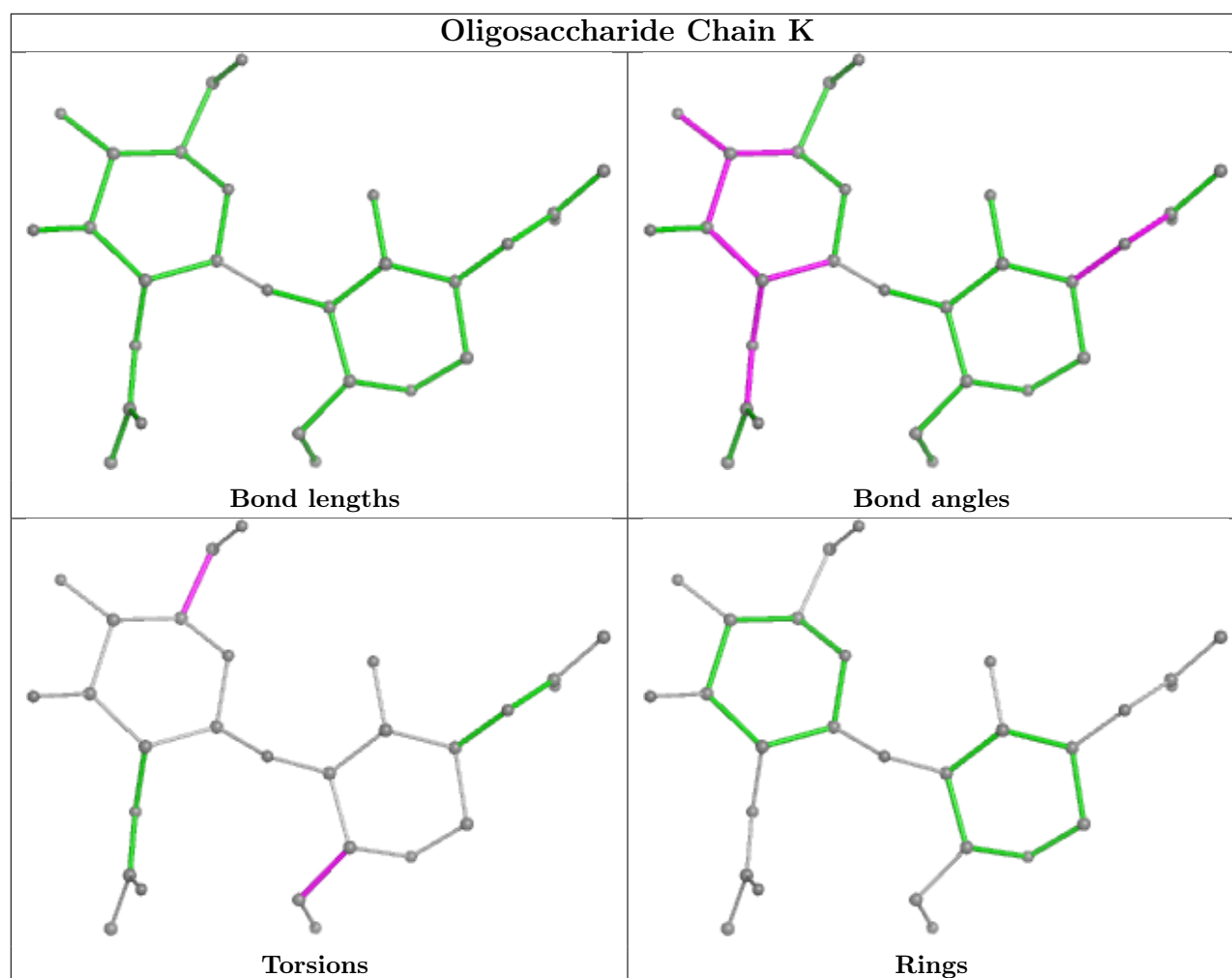
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 7 are monoatomic - leaving 3 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
10	NAG	D	801	3	14,14,15	0.83	0	17,19,21	2.38	6 (35%)
6	HEM	A	301	3,1	41,50,50	1.57	8 (19%)	45,82,82	1.90	11 (24%)
6	HEM	B	301	3,1	41,50,50	1.74	8 (19%)	45,82,82	1.44	4 (8%)

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
10	NAG	D	801	3	-	2/6/23/26	0/1/1/1
6	HEM	A	301	3,1	-	4/12/54/54	-
6	HEM	B	301	3,1	-	4/12/54/54	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	301	HEM	C4D-ND	-5.36	1.31	1.40
6	B	301	HEM	C1D-C2D	-4.71	1.35	1.44
6	A	301	HEM	FE-ND	4.14	2.17	1.96
6	A	301	HEM	C4D-C3D	-4.07	1.38	1.45
6	B	301	HEM	C4D-C3D	-4.04	1.38	1.45
6	A	301	HEM	C1B-NB	-3.33	1.34	1.40
6	A	301	HEM	C1D-C2D	-3.25	1.38	1.44
6	A	301	HEM	CHA-C4D	3.02	1.42	1.35
6	A	301	HEM	C3B-C4B	-2.94	1.39	1.44
6	B	301	HEM	C3B-C4B	-2.91	1.39	1.44
6	B	301	HEM	C1B-NB	-2.76	1.35	1.40
6	A	301	HEM	C1B-C2B	-2.68	1.39	1.44
6	A	301	HEM	C4D-ND	-2.22	1.36	1.40
6	B	301	HEM	C3B-C2B	2.19	1.41	1.37
6	B	301	HEM	C1B-C2B	-2.19	1.40	1.44
6	B	301	HEM	FE-NB	2.13	2.07	1.96

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	301	HEM	C4B-CHC-C1C	6.32	130.90	122.56
10	D	801	NAG	C1-O5-C5	5.47	119.61	112.19
6	B	301	HEM	C4C-CHD-C1D	5.13	129.33	122.56
6	B	301	HEM	C4B-CHC-C1C	4.80	128.90	122.56
10	D	801	NAG	C1-C2-N2	4.51	118.19	110.49
6	A	301	HEM	C4C-CHD-C1D	4.37	128.33	122.56
10	D	801	NAG	O3-C3-C2	4.10	117.94	109.47
6	A	301	HEM	C4B-C3B-C2B	-3.74	104.14	107.11
6	A	301	HEM	C2C-C3C-C4C	-3.56	104.41	106.90
6	A	301	HEM	O1A-CGA-CBA	-3.52	111.78	123.08
10	D	801	NAG	C3-C4-C5	-3.09	104.73	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	301	HEM	CAD-CBD-CGD	-2.69	107.82	113.60
6	B	301	HEM	C4A-C3A-C2A	-2.69	105.13	107.00
6	A	301	HEM	O2A-CGA-CBA	2.63	122.49	114.03
6	B	301	HEM	C4D-ND-C1D	2.58	107.74	105.07
10	D	801	NAG	O4-C4-C5	2.32	115.05	109.30
6	A	301	HEM	CMA-C3A-C4A	-2.19	125.11	128.46
6	A	301	HEM	CBD-CAD-C3D	-2.11	106.76	112.63
6	A	301	HEM	O1D-CGD-CBD	-2.07	116.42	123.08
6	A	301	HEM	CHB-C1B-NB	-2.07	121.83	124.38
10	D	801	NAG	O5-C1-C2	-2.04	108.07	111.29

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	D	801	NAG	C8-C7-N2-C2
10	D	801	NAG	O7-C7-N2-C2
6	B	301	HEM	CAD-CBD-CGD-O2D
6	A	301	HEM	CAD-CBD-CGD-O1D
6	A	301	HEM	CAD-CBD-CGD-O2D
6	A	301	HEM	CAA-CBA-CGA-O1A
6	B	301	HEM	CAD-CBD-CGD-O1D
6	B	301	HEM	CAA-CBA-CGA-O2A
6	A	301	HEM	CAA-CBA-CGA-O2A
6	B	301	HEM	CAA-CBA-CGA-O1A

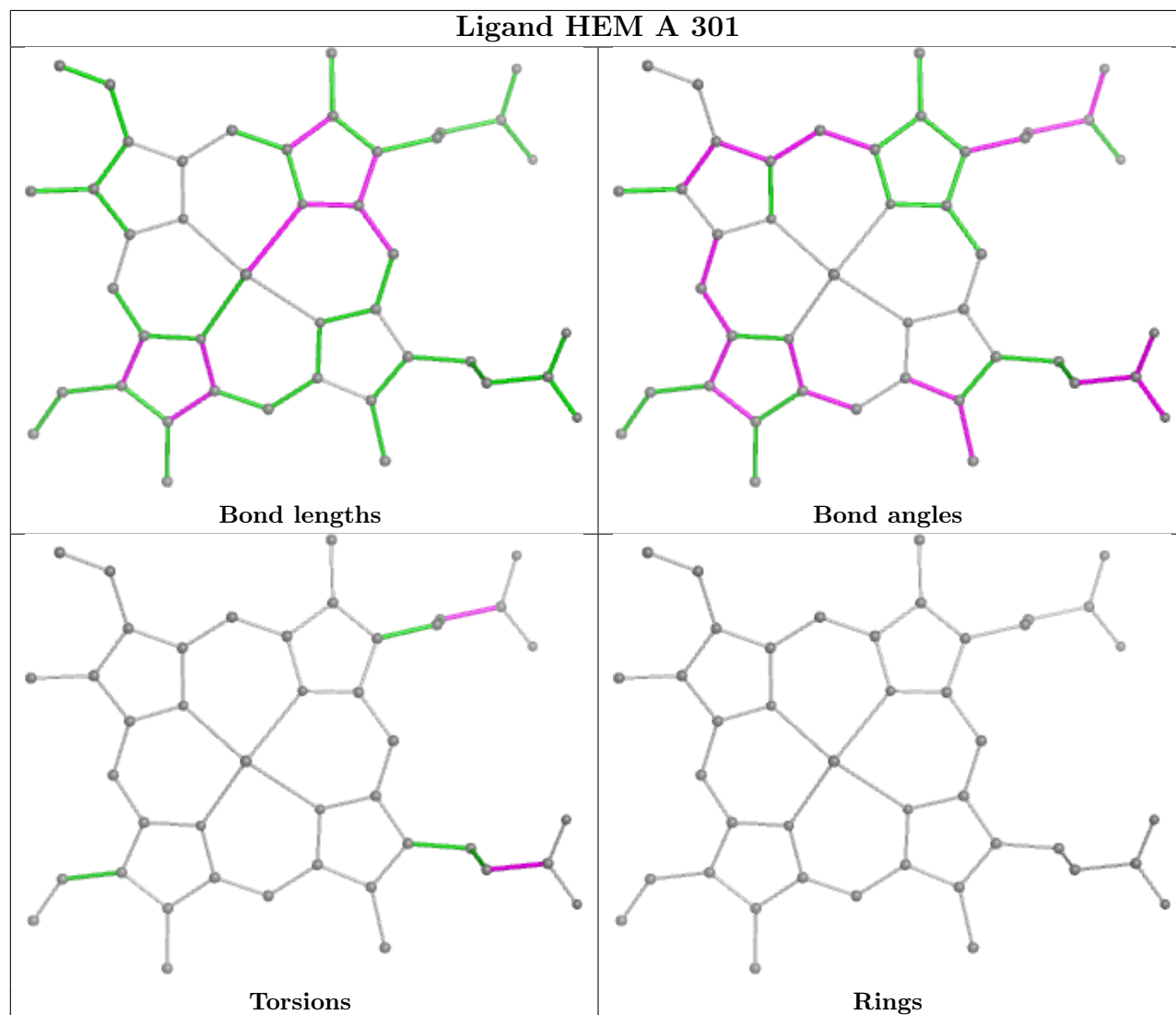
There are no ring outliers.

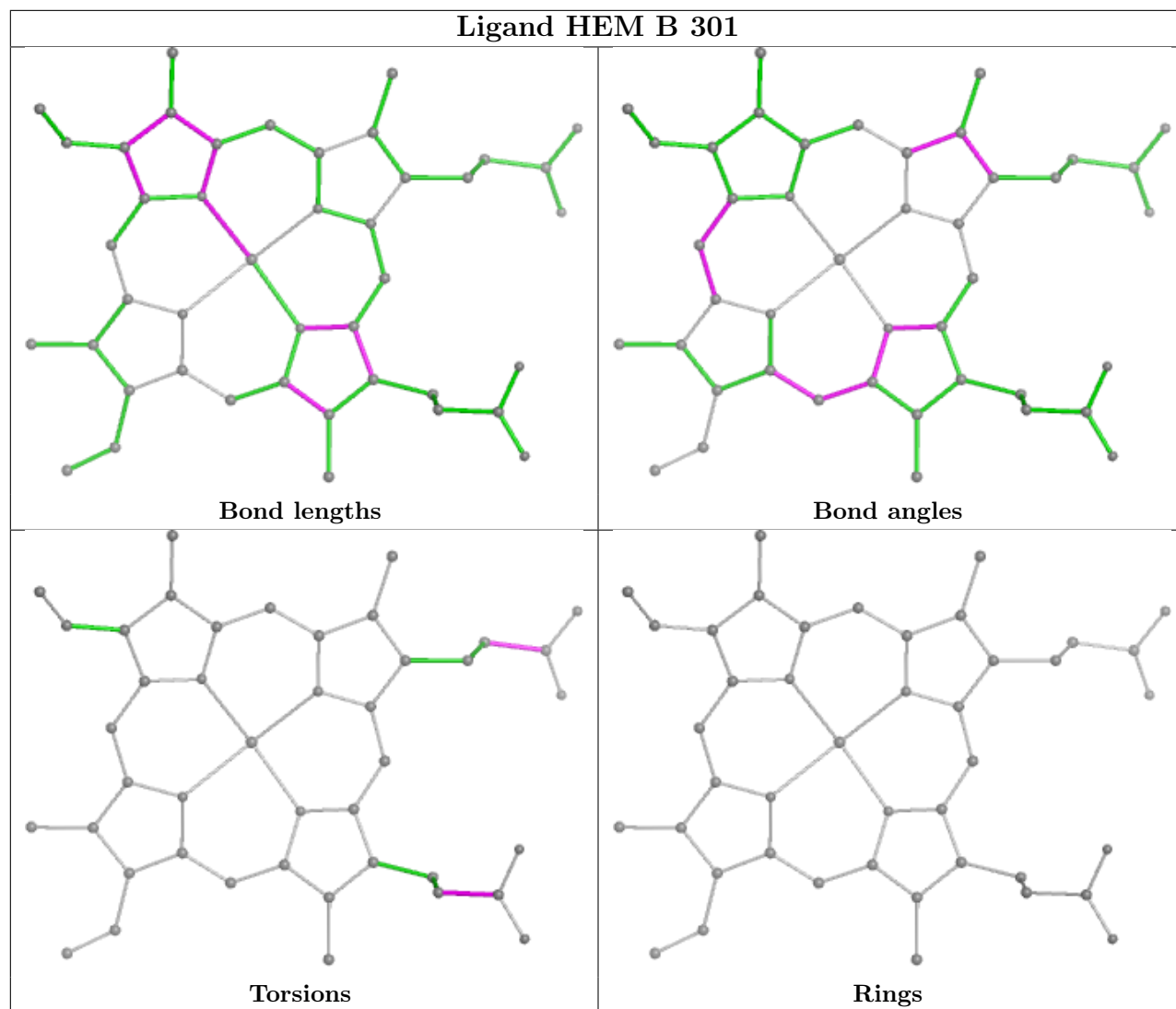
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	301	HEM	2	0
6	B	301	HEM	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	105/114 (92%)	-0.64	1 (0%) 79 76	8, 18, 42, 76	0
1	B	105/114 (92%)	-0.43	3 (2%) 54 50	13, 25, 52, 75	0
2	E	55/60 (91%)	-0.18	0 100 100	23, 40, 67, 74	0
2	F	54/60 (90%)	1.30	11 (20%) 3 3	54, 74, 98, 100	0
3	C	465/467 (99%)	-0.71	4 (0%) 81 78	7, 19, 39, 66	0
3	D	465/467 (99%)	-0.43	5 (1%) 77 74	11, 29, 53, 94	0
All	All	1249/1282 (97%)	-0.47	24 (1%) 66 63	7, 24, 61, 100	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	523	PRO	4.0
3	D	715	ASN	3.5
2	F	97	LYS	3.4
3	C	383	HIS	3.2
2	F	44	ASN	3.1
2	F	93	PHE	3.1
3	D	521	PRO	3.1
2	F	82	LYS	2.9
2	F	95	VAL	2.7
1	B	271	ALA	2.7
2	F	64	ALA	2.7
3	C	521	PRO	2.7
3	D	383	HIS	2.5
2	F	79	HIS	2.5
2	F	89	LYS	2.4
2	F	94	ASP	2.3
3	C	715	ASN	2.3
3	D	520	GLU	2.3
2	F	63	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	169	GLU	2.2
1	B	170	GLN	2.2
1	A	271	ALA	2.1
2	F	70	ARG	2.1
3	C	280	ASN	2.1

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

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

6.3 Carbohydrates [i](#)

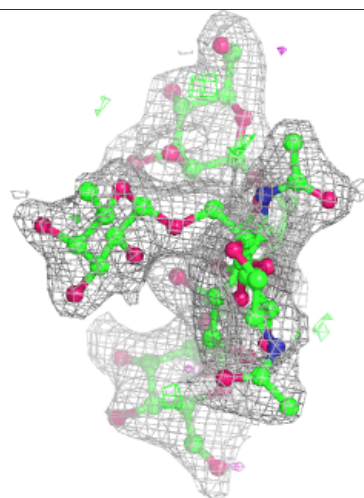
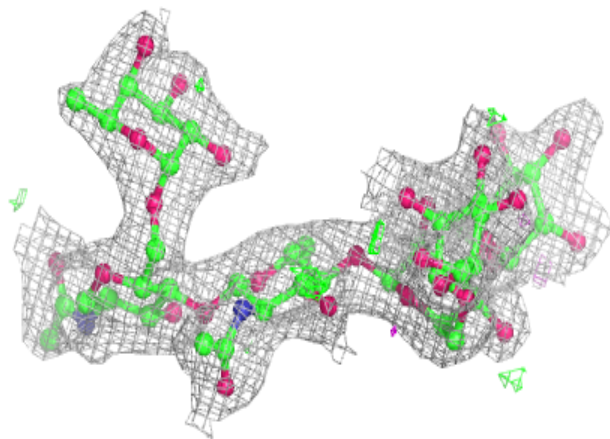
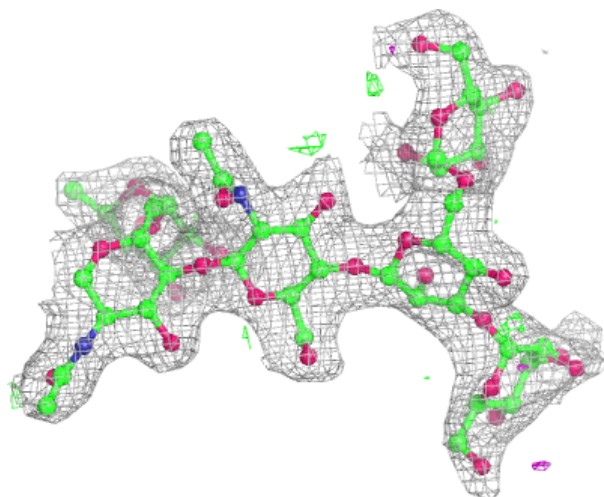
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MAN	J	4	11/12	0.77	0.14	51,57,61,61	0
5	NAG	I	2	14/15	0.77	0.16	49,65,76,77	0
5	NAG	K	2	14/15	0.79	0.13	62,65,68,72	0
4	MAN	G	4	11/12	0.82	0.13	49,51,54,58	0
5	NAG	H	2	14/15	0.83	0.13	45,50,54,55	0
5	NAG	K	1	14/15	0.91	0.10	42,49,53,58	0
4	MAN	J	5	11/12	0.91	0.07	26,28,29,30	0
4	FUC	J	6	10/11	0.92	0.10	34,39,43,43	0
5	NAG	I	1	14/15	0.93	0.08	32,37,43,51	0
4	MAN	G	5	11/12	0.94	0.08	30,33,35,39	0
4	FUC	G	6	10/11	0.94	0.07	26,29,31,33	0
4	BMA	G	3	11/12	0.95	0.07	32,33,38,42	0
4	NAG	G	1	14/15	0.95	0.06	22,25,26,27	0
4	NAG	J	2	14/15	0.95	0.07	21,22,26,26	0
4	BMA	J	3	11/12	0.95	0.06	29,29,34,40	0
5	NAG	H	1	14/15	0.96	0.07	26,31,34,40	0
4	NAG	J	1	14/15	0.96	0.06	22,23,25,28	0
4	NAG	G	2	14/15	0.96	0.07	22,26,29,29	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.

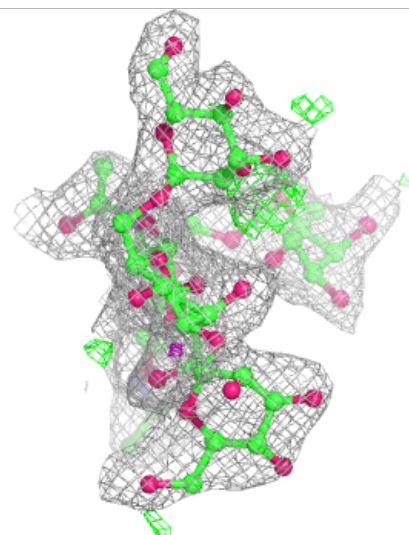
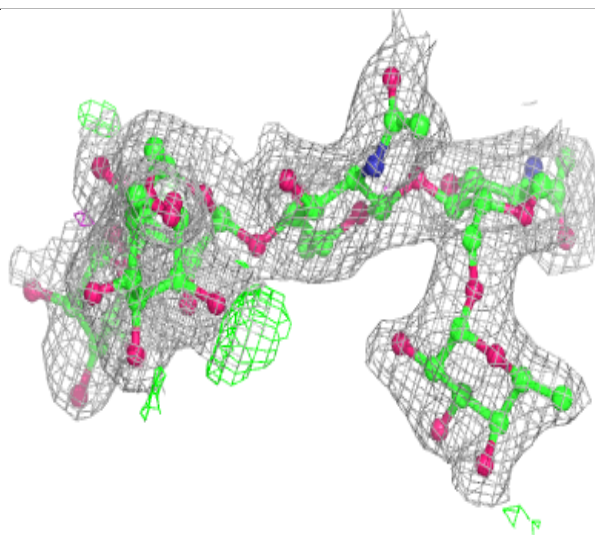
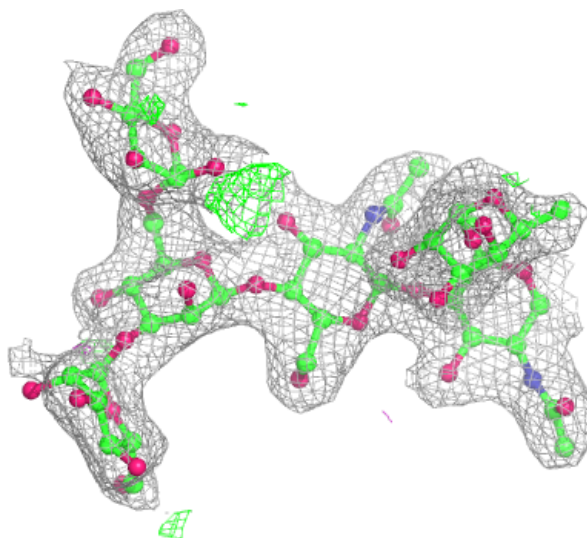
Electron density around Chain G:

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



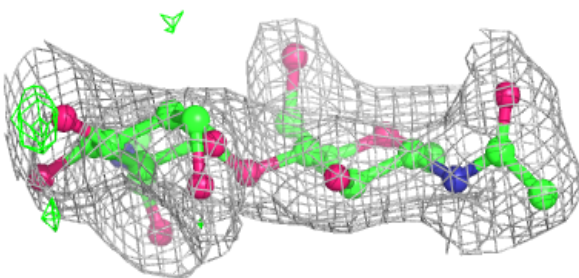
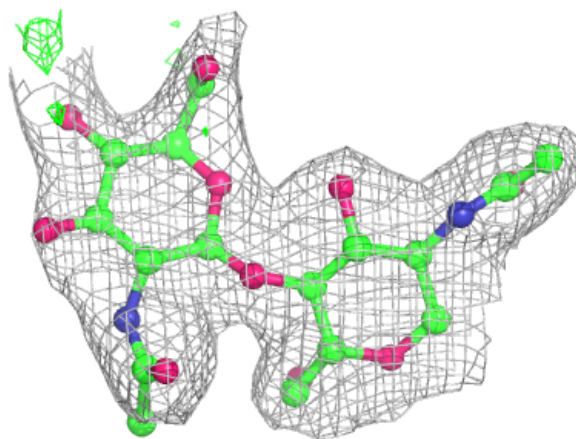
Electron density around Chain J:

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



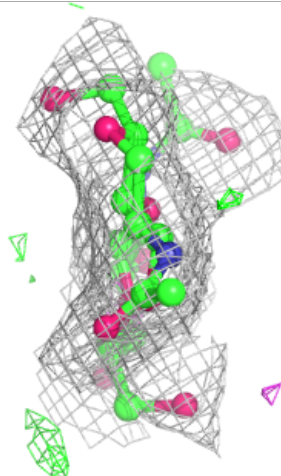
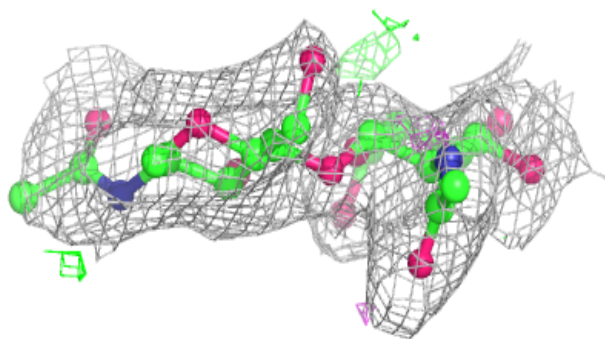
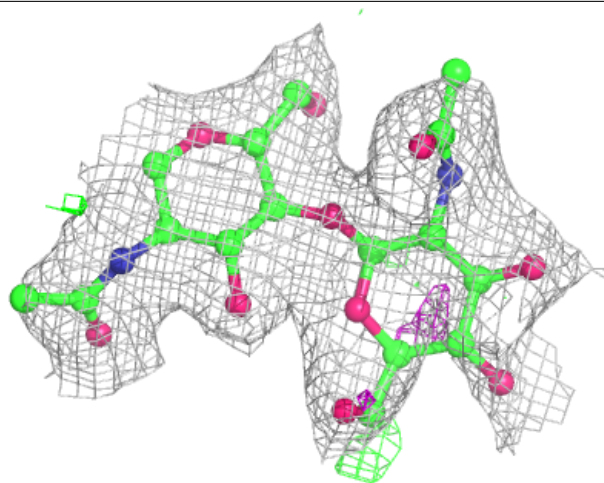
Electron density around Chain H:

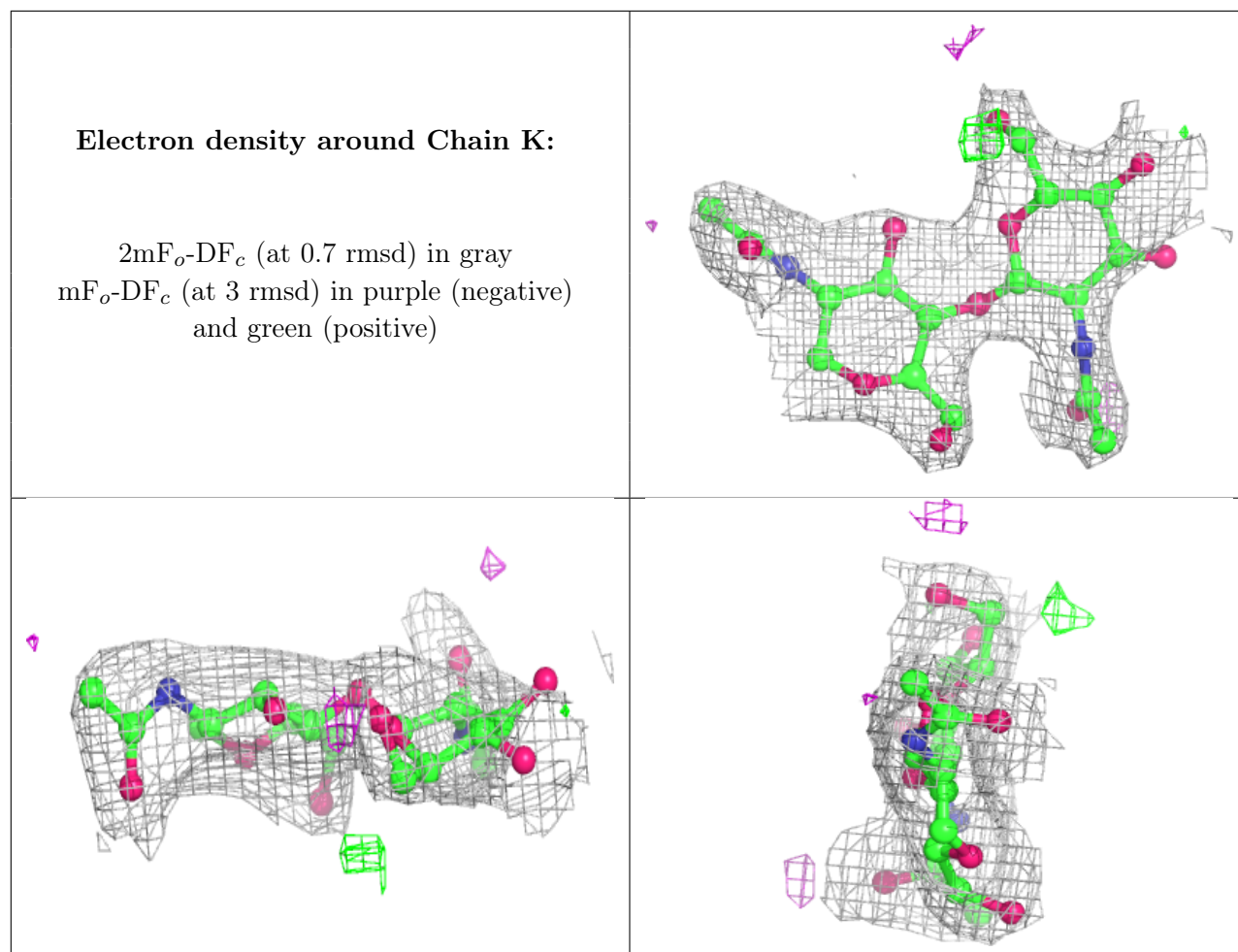
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





6.4 Ligands [i](#)

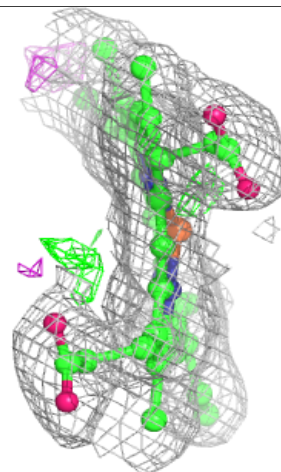
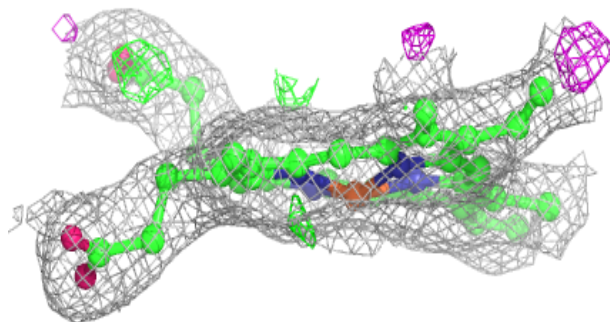
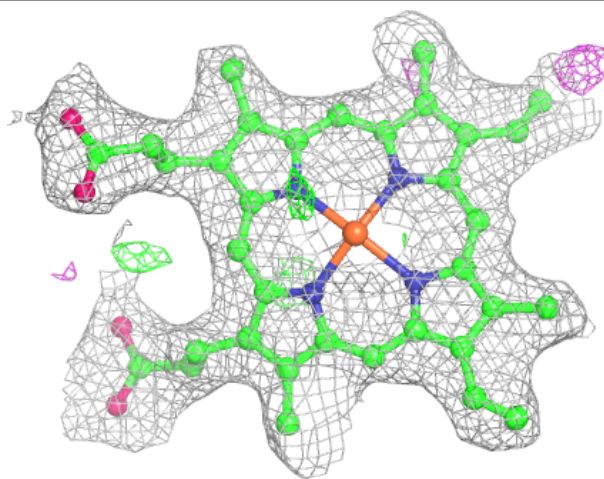
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

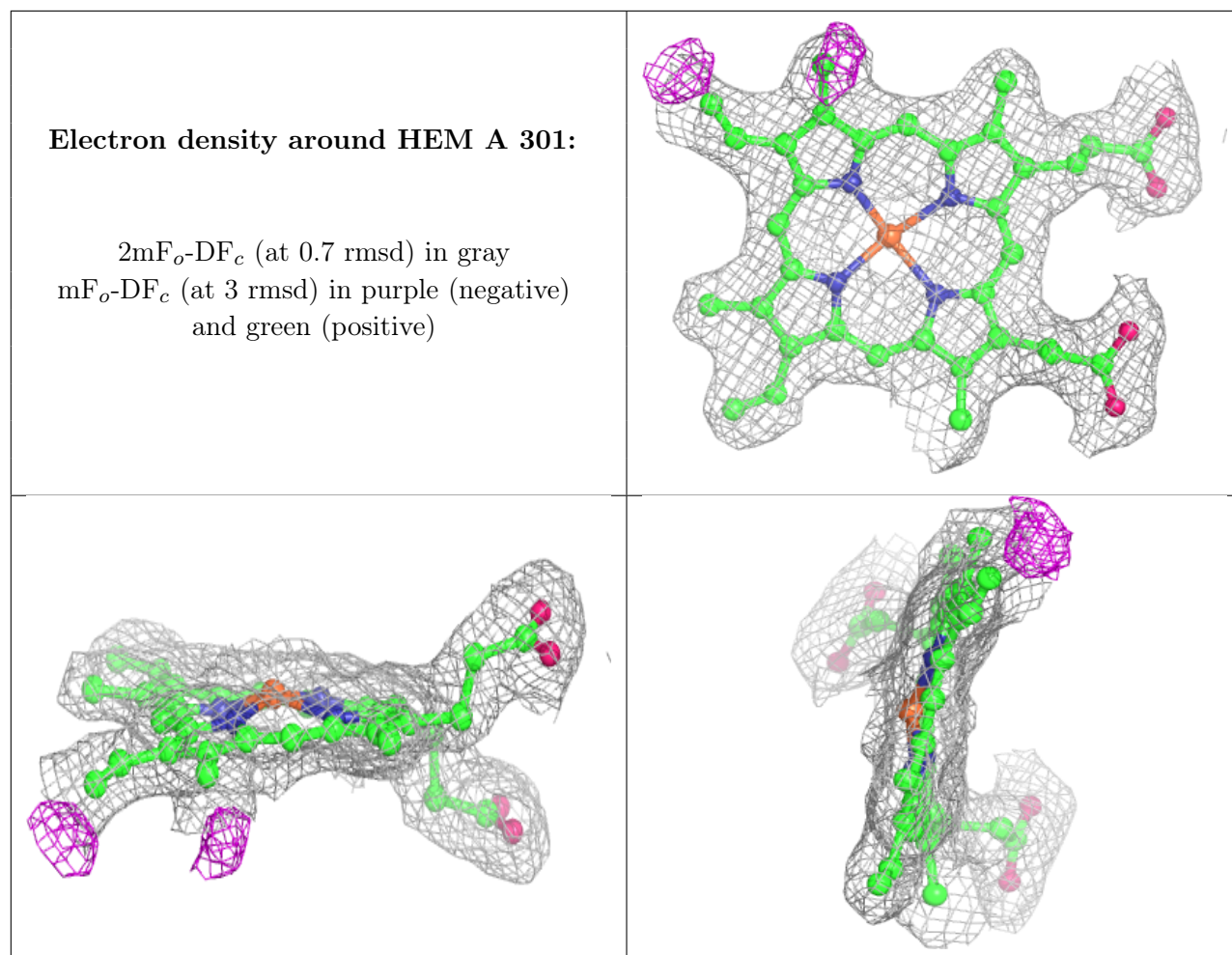
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
10	NAG	D	801	14/15	0.85	0.12	50,54,57,58	0
9	CL	D	803	1/1	0.93	0.08	46,46,46,46	0
9	CL	C	802	1/1	0.94	0.10	43,43,43,43	0
6	HEM	B	301	43/43	0.97	0.06	15,19,23,30	0
6	HEM	A	301	43/43	0.98	0.05	8,9,12,16	0
9	CL	C	803	1/1	0.98	0.04	24,24,24,24	0
8	CA	C	801	1/1	0.99	0.05	5,5,5,5	0
7	IOD	A	302	1/1	1.00	0.01	11,11,11,11	0
8	CA	D	802	1/1	1.00	0.07	10,10,10,10	0
7	IOD	B	302	1/1	1.00	0.01	15,15,15,15	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 HEM B 301:

$2mF_o-DF_c$ (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.