



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:46 AM UTC

PDB ID : 2EFB / pdb\_00002efb  
Title : Crystal structure of the complex of goat lactoperoxidase with phosphate at 2.94 Å resolution  
Authors : Singh, A.K.; Hariprasad, G.; Prem Kumar, R.; Singh, N.; Bhushan, A.; Sharma, S.; Kaur, P.; Singh, T.P.  
Deposited on : 2007-02-22  
Resolution : 2.94 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](mailto: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>.

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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)  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

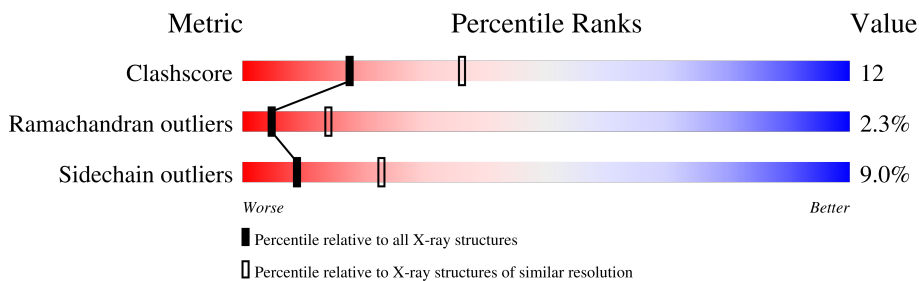
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.94 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1184 (2.96-2.92)
Ramachandran outliers	187476	1131 (2.96-2.92)
Sidechain outliers	187428	1131 (2.96-2.92)

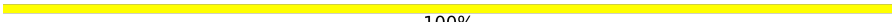
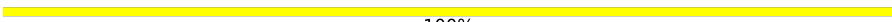
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria 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  $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	595	74% 21% . .
1	B	595	76% 18% 5% .
2	C	3	33% 33% 33%
2	D	3	100%
2	G	3	100%
3	E	3	100%
3	H	3	100%
3	I	3	100%

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Mol	Chain	Length	Quality of chain
4	F	2	 100%
4	J	2	 100%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	PO4	A	2001	-	-	X	-
5	PO4	B	2003	-	-	X	-
5	PO4	B	2004	-	-	X	-
9	CYN	A	2011	-	-	X	-

## 2 Entry composition [i](#)

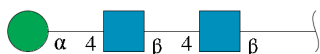
There are 12 unique types of molecules in this entry. The entry contains 10287 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Lactoperoxidase.

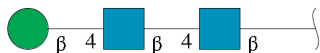
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	595	4754	3021	844	863	26	0	0	0
1	B	595	4754	3021	844	863	26	0	0	0

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	C	3	39	22	2	15	0	0	0
2	D	3	39	22	2	15	0	0	0
2	G	3	39	22	2	15	0	0	0

- Molecule 3 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	E	3	39	22	2	15	0	0	0
3	H	3	39	22	2	15	0	0	0

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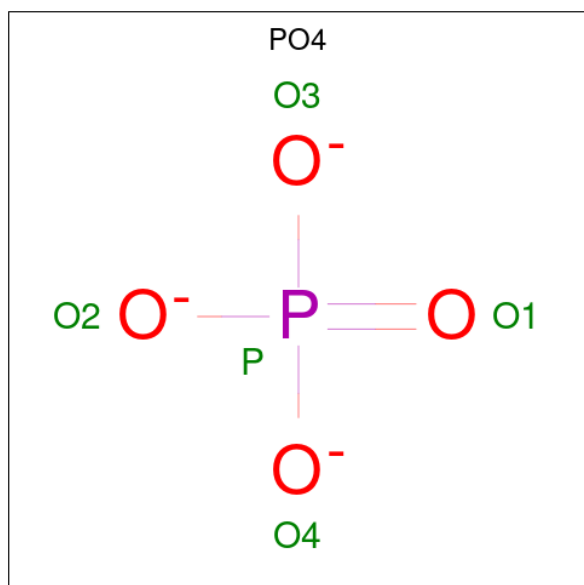
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	I	3	39	22	2	15	0	0	0

- Molecule 4 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
			Total	C	N	O			
4	F	2	28	16	2	10	0	0	0
4	J	2	28	16	2	10	0	0	0

- Molecule 5 is PHOSPHATE ION (CCD ID: PO4) (formula: O<sub>4</sub>P).



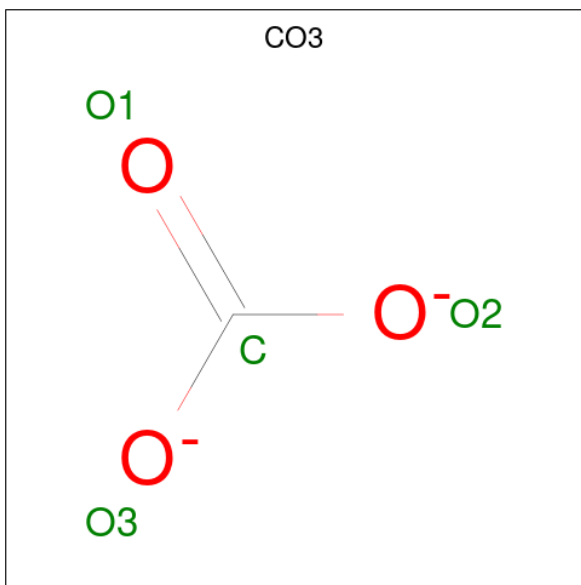
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	P		
5	A	1	5	4	1	0	0
5	A	1	5	4	1	0	0
5	A	1	5	4	1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total O P 5 4 1	0	0
5	B	1	Total O P 5 4 1	0	0

- Molecule 6 is CARBONATE ION (CCD ID: CO3) (formula: CO<sub>3</sub>).



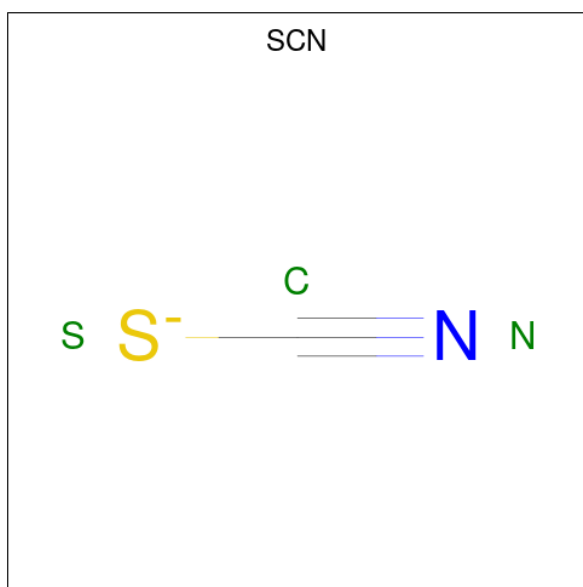
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 4 1 3	0	0
6	B	1	Total C O 4 1 3	0	0

- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

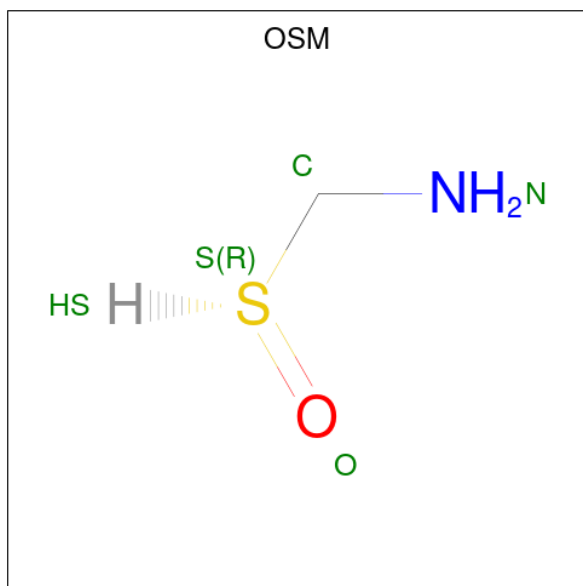
- Molecule 8 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C<sub>34</sub>H<sub>32</sub>FeN<sub>4</sub>O<sub>4</sub>).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
			Total	C	N			S
10	A	1	3	1	1	1	0	0

- Molecule 11 is 1-(OXIDOSULFANYL)METHANAMINE (CCD ID: OSM) (formula: CH<sub>5</sub>NOS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	N	O			S
11	B	1	4	1	1	1	1	0	0

- Molecule 12 is water.

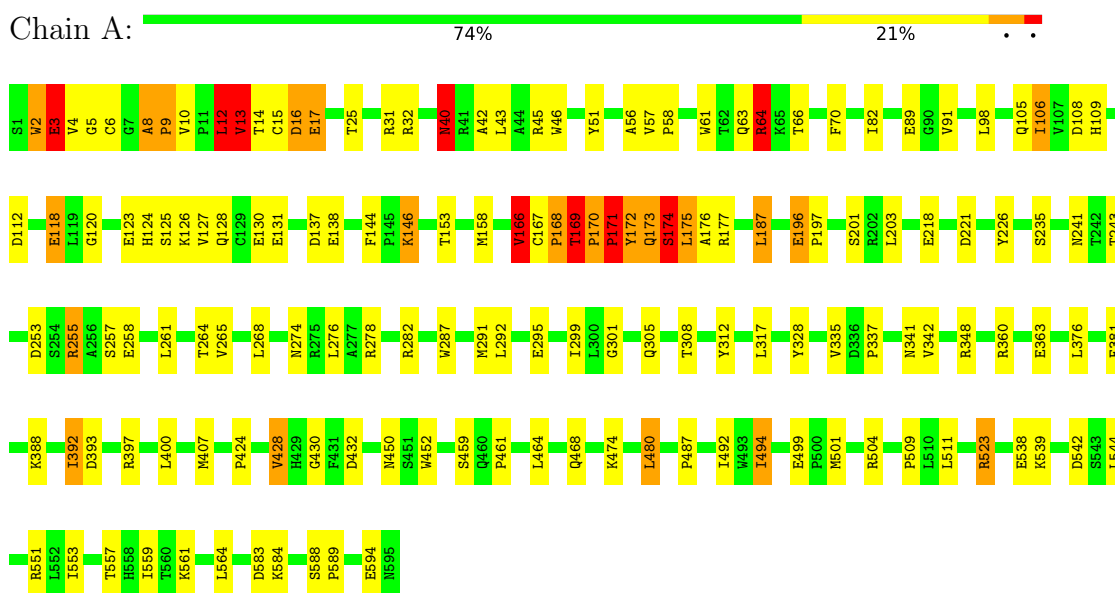
<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
12	A	188	Total 188	O 188	0	0
12	B	171	Total 171	O 171	0	0

### 3 Residue-property plots

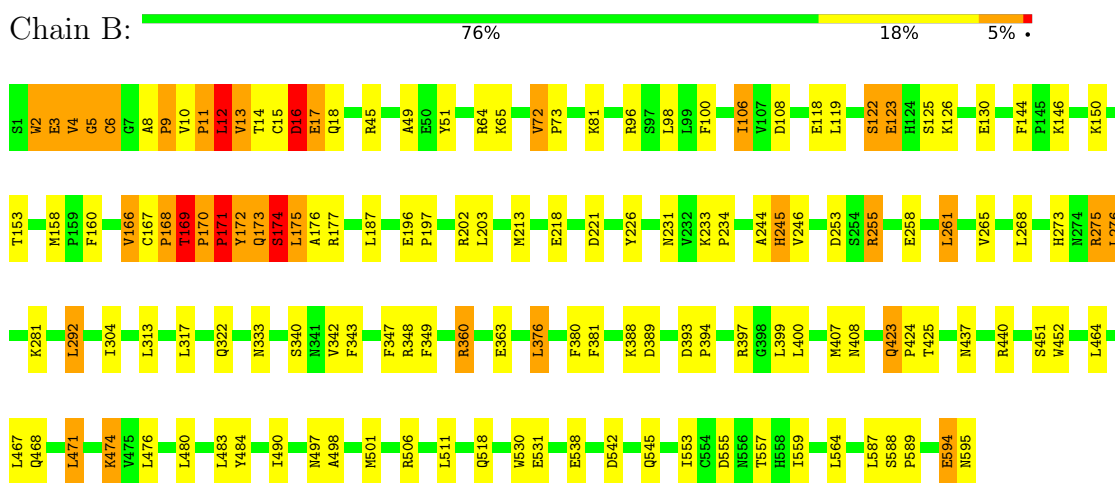
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

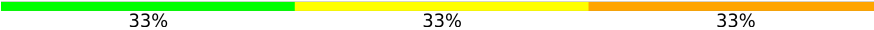
- Molecule 1: Lactoperoxidase



- Molecule 1: Lactoperoxidase

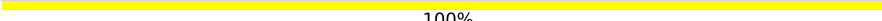


- Molecule 2: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:  33% 33% 33%

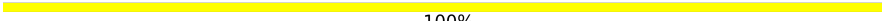
MAG1  
MAG2  
MAN3

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

Chain D:  100%

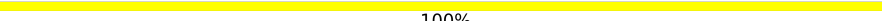
MAG1  
MAG2  
MAN3

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

Chain G:  100%

MAG1  
MAG2  
MAN3

- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  100%

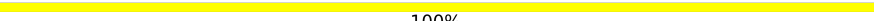
MAG1  
MAG2  
BMA3

- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:  100%

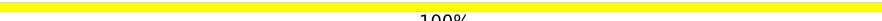
MAG1  
MAG2  
BMA3

- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  100%

MAG1  
MAG2  
BMA3

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

Chain F:  100%

MAG1  
MAG2

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

Chain J:

100%

MAG1  
MAG2

## 4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	59.20Å 75.59Å 83.81Å 79.93° 77.86° 72.50°	Depositor
Resolution (Å)	20.00 – 2.94	Depositor
% Data completeness (in resolution range)	95.3 (20.00-2.94)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.12	Depositor
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.180 , 0.219	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	10287	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	15.0	wwPDB-VP

## 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: SCN, NAG, CYN, HEM, CA, CO3, MAN, OSM, PO4, BMA

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	0.72	4/4883 (0.1%)	1.03	23/6632 (0.3%)
1	B	0.67	0/4883	1.00	16/6632 (0.2%)
All	All	0.69	4/9766 (0.0%)	1.01	39/13264 (0.3%)

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	A	0	3
1	B	0	3
All	All	0	6

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	63	GLN	C-N	10.33	1.48	1.33
1	A	120	GLY	N-CA	7.80	1.56	1.45
1	A	64	ARG	N-CA	6.19	1.54	1.46
1	A	63	GLN	CA-C	5.66	1.60	1.52

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	174	SER	N-CA-C	15.08	127.72	111.28
1	A	174	SER	O-C-N	-10.66	108.41	122.59
1	B	123	GLU	N-CA-C	9.98	125.63	108.76
1	B	170	PRO	CA-C-N	9.93	132.25	119.84
1	B	170	PRO	C-N-CA	9.93	132.25	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	170	PRO	CA-C-N	9.81	132.10	119.84
1	A	170	PRO	C-N-CA	9.81	132.10	119.84
1	A	173	GLN	OE1-CD-NE2	-9.74	112.86	122.60
1	A	172	TYR	N-CA-C	9.19	125.17	108.17
1	B	172	TYR	N-CA-C	9.12	123.21	108.63
1	A	63	GLN	OE1-CD-NE2	-8.70	113.91	122.60
1	B	13	VAL	N-CA-C	7.71	119.91	108.96
1	A	63	GLN	CA-C-N	7.33	135.54	121.54
1	A	63	GLN	C-N-CA	7.33	135.54	121.54
1	A	63	GLN	CG-CD-NE2	7.03	126.94	116.40
1	A	173	GLN	CG-CD-NE2	6.94	126.80	116.40
1	A	16	ASP	N-CA-C	-6.89	104.86	113.20
1	A	171	PRO	N-CA-C	6.80	126.48	112.47
1	B	246	VAL	N-CA-C	6.72	115.30	107.77
1	B	423	GLN	CA-C-N	6.70	126.20	119.24
1	B	423	GLN	C-N-CA	6.70	126.20	119.24
1	B	171	PRO	N-CA-C	6.61	126.08	112.47
1	B	169	THR	CA-C-N	6.28	126.85	120.38
1	B	169	THR	C-N-CA	6.28	126.85	120.38
1	B	16	ASP	N-CA-C	-6.02	105.06	113.37
1	A	492	ILE	N-CA-C	5.67	115.86	110.42
1	A	196	GLU	CA-C-N	5.53	125.62	119.32
1	A	196	GLU	C-N-CA	5.53	125.62	119.32
1	A	174	SER	N-CA-C	5.50	122.52	110.80
1	A	40	ASN	N-CA-C	5.48	122.48	110.80
1	B	12	LEU	N-CA-C	5.38	122.27	110.80
1	A	13	VAL	N-CA-C	5.28	120.32	109.34
1	B	173	GLN	CA-C-N	5.18	127.23	120.28
1	B	173	GLN	C-N-CA	5.18	127.23	120.28
1	A	112	ASP	N-CA-C	5.18	117.80	108.48
1	A	137	ASP	N-CA-C	-5.15	105.08	112.13
1	A	173	GLN	CA-C-N	5.15	131.38	121.54
1	A	173	GLN	C-N-CA	5.15	131.38	121.54
1	A	166	VAL	N-CA-C	5.14	120.02	109.34

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	12	LEU	Peptide
1	A	169	THR	Peptide
1	A	171	PRO	Peptide

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Mol	Chain	Res	Type	Group
1	B	12	LEU	Peptide
1	B	169	THR	Peptide
1	B	171	PRO	Peptide

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4754	0	4645	106	0
1	B	4754	0	4645	126	0
2	C	39	0	34	2	0
2	D	39	0	34	0	0
2	G	39	0	34	0	0
3	E	39	0	34	0	0
3	H	39	0	34	0	0
3	I	39	0	34	0	0
4	F	28	0	25	0	0
4	J	28	0	25	0	0
5	A	15	0	0	5	0
5	B	10	0	0	6	0
6	A	4	0	0	0	0
6	B	4	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
8	A	43	0	30	14	0
8	B	43	0	30	15	0
9	A	2	0	0	3	0
10	A	3	0	0	1	0
11	B	4	0	5	1	0
12	A	188	0	0	12	0
12	B	171	0	0	16	0
All	All	10287	0	9609	242	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 12.

All (242) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:8:ALA:HB1	1:B:9:PRO:HD2	1.32	1.11
1:A:8:ALA:HB1	1:A:9:PRO:HD2	1.28	1.09
1:A:175:LEU:HD22	1:A:176:ALA:H	1.15	1.09
1:A:2:TRP:HZ3	1:A:174:SER:HB3	1.25	1.00
1:B:168:PRO:HB2	1:B:170:PRO:HD2	1.44	0.98
1:A:13:VAL:HG12	1:A:14:THR:H	1.28	0.97
1:B:12:LEU:HB2	1:B:13:VAL:HG23	1.46	0.96
1:A:2:TRP:CZ3	1:A:174:SER:HB3	2.02	0.95
1:A:258:GLU:OE2	8:A:1001:HEM:HMB3	1.67	0.94
1:B:169:THR:H	1:B:170:PRO:CD	1.81	0.93
1:B:167:CYS:HB2	1:B:168:PRO:HD3	1.54	0.90
1:A:8:ALA:HB1	1:A:9:PRO:CD	2.02	0.89
1:A:108:ASP:OD2	8:A:1001:HEM:HMD3	1.73	0.89
1:A:108:ASP:CG	8:A:1001:HEM:HMD3	1.98	0.87
1:B:2:TRP:CZ3	1:B:174:SER:HB2	2.11	0.86
1:B:108:ASP:OD2	8:B:1021:HEM:HMD3	1.77	0.85
1:B:594:GLU:HG2	1:B:595:ASN:N	1.90	0.84
1:A:8:ALA:CB	1:A:9:PRO:HD2	2.09	0.83
1:B:381:PHE:CZ	1:B:424:PRO:HG3	2.14	0.83
1:B:258:GLU:OE2	8:B:1021:HEM:HMB3	1.79	0.82
8:B:1021:HEM:HMB1	8:B:1021:HEM:HBB2	1.62	0.82
1:B:14:THR:HG22	1:B:15:CYS:H	1.44	0.81
1:B:244:ALA:O	1:B:245:HIS:HB2	1.80	0.81
1:B:13:VAL:HG12	1:B:14:THR:N	1.96	0.81
1:B:13:VAL:CG1	1:B:14:THR:H	1.95	0.80
1:B:169:THR:H	1:B:170:PRO:HD2	1.44	0.80
1:A:2:TRP:HZ3	1:A:174:SER:CB	1.94	0.80
1:A:108:ASP:OD1	8:A:1001:HEM:HMD3	1.80	0.80
1:A:253:ASP:OD2	1:A:255:ARG:HD3	1.81	0.79
1:B:108:ASP:CG	8:B:1021:HEM:HMD3	2.07	0.79
1:A:108:ASP:OD2	8:A:1001:HEM:CMD	2.32	0.78
8:A:1001:HEM:HMB1	8:A:1001:HEM:HBB2	1.67	0.77
1:A:13:VAL:HG12	1:A:14:THR:N	1.99	0.76
1:A:13:VAL:CG1	1:A:14:THR:H	2.00	0.75
1:A:82:ILE:HG21	1:A:494:ILE:HD11	1.66	0.75
1:A:551:ARG:HD3	1:A:584:LYS:HA	1.67	0.75
1:B:258:GLU:OE2	8:B:1021:HEM:CMB	2.35	0.74
1:A:175:LEU:CD2	1:A:176:ALA:H	1.99	0.74
1:B:8:ALA:HB1	1:B:9:PRO:CD	2.16	0.74
1:A:258:GLU:OE2	8:A:1001:HEM:CMB	2.36	0.73
1:B:108:ASP:OD1	8:B:1021:HEM:HMD3	1.88	0.73
1:B:468:GLN:OE1	1:B:474:LYS:HG3	1.87	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:LEU:HD22	1:A:176:ALA:N	1.99	0.73
1:B:342:VAL:HB	5:B:2004:PO4:O2	1.88	0.72
1:A:14:THR:HG22	1:A:15:CYS:H	1.56	0.71
1:A:169:THR:H	1:A:170:PRO:CD	2.02	0.71
1:B:108:ASP:OD2	8:B:1021:HEM:CMD	2.37	0.71
1:B:171:PRO:HB2	1:B:172:TYR:HD2	1.56	0.71
1:B:2:TRP:CZ3	1:B:174:SER:CB	2.74	0.71
1:A:124:HIS:HD2	1:A:127:VAL:HG21	1.55	0.71
1:A:167:CYS:HB2	1:A:168:PRO:HD3	1.72	0.70
1:A:169:THR:H	1:A:170:PRO:HD2	1.55	0.70
1:B:13:VAL:CG1	1:B:14:THR:N	2.53	0.70
1:B:13:VAL:HG12	1:B:14:THR:H	1.56	0.69
1:A:397:ARG:HG3	1:A:559:ILE:HD12	1.75	0.69
12:A:2148:HOH:O	2:C:2:NAG:H5	1.93	0.69
1:A:196:GLU:HB3	12:A:2044:HOH:O	1.94	0.68
1:A:388:LYS:HD3	12:A:2037:HOH:O	1.93	0.68
1:A:45:ARG:HA	5:A:2001:PO4:O4	1.94	0.67
1:A:124:HIS:CD2	1:A:127:VAL:HG21	2.28	0.67
1:A:171:PRO:HB2	1:A:172:TYR:HD2	1.59	0.67
1:B:126:LYS:HD2	12:B:2039:HOH:O	1.95	0.67
1:A:381:PHE:CZ	1:A:424:PRO:HG3	2.29	0.66
1:A:168:PRO:HB2	1:A:170:PRO:HD2	1.78	0.66
1:A:407:MET:HB3	1:A:501:MET:HE3	1.75	0.66
1:B:253:ASP:OD2	1:B:255:ARG:HD3	1.97	0.65
1:B:538:GLU:HG3	12:B:2059:HOH:O	1.96	0.65
1:B:8:ALA:C	1:B:10:VAL:H	2.05	0.65
1:B:2:TRP:HZ3	1:B:174:SER:CB	2.10	0.64
1:B:119:LEU:HD11	1:B:169:THR:HG23	1.80	0.64
1:A:138:GLU:HA	1:A:138:GLU:OE2	1.98	0.64
1:B:14:THR:CG2	1:B:15:CYS:H	2.11	0.64
1:A:282:ARG:HD3	12:A:2073:HOH:O	1.98	0.63
1:B:11:PRO:HB2	1:B:12:LEU:HD12	1.81	0.63
1:A:12:LEU:HB2	1:A:13:VAL:HG23	1.78	0.63
1:B:15:CYS:C	1:B:17:GLU:H	2.02	0.63
1:B:169:THR:N	1:B:170:PRO:CD	2.58	0.62
1:B:14:THR:HG22	1:B:15:CYS:N	2.15	0.61
1:A:257:SER:O	1:A:381:PHE:HA	2.00	0.61
1:B:213:MET:HG2	1:B:273:HIS:CD2	2.37	0.60
1:B:322:GLN:HG3	12:B:2105:HOH:O	2.01	0.60
1:A:450:ASN:HD21	1:A:487:PRO:HB2	1.67	0.60
1:B:594:GLU:HG2	1:B:595:ASN:H	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:8:ALA:O	1:B:10:VAL:N	2.34	0.60
1:B:45:ARG:HD3	5:B:2004:PO4:O1	2.02	0.60
1:B:400:LEU:HD11	1:B:553:ILE:HD13	1.84	0.59
1:A:539:LYS:HB3	1:A:589:PRO:HB3	1.85	0.59
1:B:388:LYS:HD3	12:B:2062:HOH:O	2.03	0.59
1:B:407:MET:HB3	1:B:501:MET:HE3	1.85	0.58
1:A:499:GLU:OE1	1:A:509:PRO:HD2	2.03	0.58
1:B:348:ARG:HH11	1:B:437:ASN:ND2	2.02	0.58
12:A:2135:HOH:O	2:C:2:NAG:H62	2.03	0.57
1:A:106:ILE:HD11	1:A:265:VAL:HB	1.86	0.57
1:B:2:TRP:HZ3	1:B:174:SER:HB2	1.61	0.57
1:B:258:GLU:CD	8:B:1021:HEM:HMB3	2.28	0.57
1:B:275:ARG:NH2	12:B:2135:HOH:O	2.36	0.57
1:A:42:ALA:HB2	1:A:166:VAL:HG11	1.85	0.57
1:A:123:GLU:HG3	1:A:125:SER:H	1.68	0.57
1:B:276:LEU:HD12	1:B:587:LEU:HD11	1.87	0.56
1:B:594:GLU:CG	1:B:595:ASN:N	2.68	0.56
1:A:14:THR:HG22	1:A:15:CYS:N	2.21	0.56
1:A:171:PRO:CB	1:A:172:TYR:HD2	2.17	0.56
9:A:2011:CYN:N	10:A:2012:SCN:N	2.54	0.56
1:A:468:GLN:HG2	1:A:474:LYS:HA	1.88	0.56
1:A:56:ALA:HB1	1:A:177:ARG:HD3	1.89	0.55
1:A:12:LEU:HB2	1:A:13:VAL:CG2	2.35	0.55
1:A:118:GLU:HA	12:A:2018:HOH:O	2.06	0.55
1:A:264:THR:HG23	1:A:392:ILE:HB	1.89	0.55
1:B:376:LEU:HD13	1:B:380:PHE:CZ	2.42	0.55
1:B:11:PRO:HD2	12:B:2139:HOH:O	2.07	0.54
8:B:1021:HEM:HMC2	8:B:1021:HEM:HBC2	1.88	0.54
1:A:393:ASP:OD1	1:A:557:THR:HB	2.07	0.54
1:B:452:TRP:HH2	5:B:2004:PO4:O3	1.89	0.54
1:B:168:PRO:HG2	1:B:170:PRO:O	2.07	0.54
1:B:108:ASP:OD1	8:B:1021:HEM:CMD	2.54	0.54
1:B:15:CYS:C	1:B:17:GLU:N	2.67	0.53
1:A:258:GLU:CD	8:A:1001:HEM:HMB3	2.31	0.53
1:A:14:THR:CG2	1:A:15:CYS:H	2.20	0.53
1:A:108:ASP:CG	8:A:1001:HEM:CMD	2.76	0.53
1:B:108:ASP:OD1	8:B:1021:HEM:C2D	2.61	0.53
1:B:244:ALA:O	1:B:245:HIS:CB	2.54	0.53
1:A:168:PRO:HG2	1:A:170:PRO:O	2.08	0.53
1:B:108:ASP:CG	8:B:1021:HEM:CMD	2.78	0.53
1:B:106:ILE:HD11	1:B:265:VAL:HB	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:322:GLN:HG2	12:B:2119:HOH:O	2.09	0.53
1:A:10:VAL:HB	12:A:2119:HOH:O	2.09	0.52
1:B:81:LYS:HD2	1:B:483:LEU:HD21	1.91	0.52
1:B:8:ALA:CB	1:B:9:PRO:HD2	2.20	0.52
1:B:123:GLU:HG3	1:B:125:SER:H	1.74	0.52
1:A:342:VAL:HB	5:A:2001:PO4:O1	2.10	0.51
1:A:328:TYR:CD1	1:A:523:ARG:HD3	2.45	0.51
1:A:588:SER:OG	1:A:589:PRO:HD3	2.09	0.51
1:A:8:ALA:O	1:A:10:VAL:N	2.43	0.51
8:A:1001:HEM:HMC2	8:A:1001:HEM:HBC2	1.93	0.51
1:B:144:PHE:HE2	1:B:158:MET:HE3	1.74	0.51
1:B:118:GLU:HA	12:B:2061:HOH:O	2.10	0.51
1:A:221:ASP:HB2	1:A:226:TYR:CZ	2.45	0.51
1:A:109:HIS:CE1	1:A:255:ARG:HB2	2.46	0.50
1:B:196:GLU:HB3	12:B:2050:HOH:O	2.11	0.50
1:B:16:ASP:O	1:B:18:GLN:N	2.37	0.50
1:A:299:ILE:HG23	1:A:544:LEU:HD21	1.94	0.50
1:A:146:LYS:HB2	12:A:2046:HOH:O	2.12	0.50
1:B:12:LEU:HD12	1:B:12:LEU:N	2.27	0.50
1:B:467:LEU:HG	1:B:471:LEU:HD22	1.94	0.50
1:A:58:PRO:HG2	1:A:61:TRP:HB2	1.92	0.50
1:B:167:CYS:CB	1:B:168:PRO:HD3	2.36	0.49
1:B:440:ARG:HD2	12:B:2026:HOH:O	2.11	0.49
1:B:340:SER:HB2	5:B:2004:PO4:O4	2.12	0.49
1:A:450:ASN:ND2	1:A:487:PRO:HB2	2.26	0.49
1:B:530:TRP:CE2	1:B:531:GLU:HG3	2.48	0.49
1:A:31:ARG:HD3	12:A:2038:HOH:O	2.12	0.49
1:B:106:ILE:CD1	1:B:265:VAL:HG11	2.43	0.49
1:B:476:LEU:HD21	1:B:498:ALA:HB1	1.95	0.49
1:B:12:LEU:HD11	1:B:197:PRO:HG2	1.94	0.48
1:B:349:PHE:HB2	1:B:497:ASN:HD21	1.77	0.48
1:B:468:GLN:HG2	1:B:474:LYS:HA	1.95	0.48
1:B:45:ARG:CZ	1:B:49:ALA:HB2	2.43	0.48
1:A:274:ASN:O	1:A:278:ARG:HG2	2.14	0.48
1:A:561:LYS:HE3	12:A:2052:HOH:O	2.12	0.48
1:A:66:THR:HB	1:A:70:PHE:N	2.29	0.48
1:A:123:GLU:HB3	1:A:126:LYS:HE2	1.94	0.48
1:B:8:ALA:HB3	12:B:2133:HOH:O	2.14	0.48
1:A:8:ALA:C	1:A:10:VAL:H	2.23	0.47
1:A:158:MET:HE1	1:A:432:ASP:HB2	1.97	0.47
1:B:8:ALA:C	1:B:10:VAL:N	2.72	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4:VAL:HG23	12:B:2130:HOH:O	2.15	0.47
1:A:407:MET:HB3	1:A:501:MET:CE	2.44	0.47
8:A:1001:HEM:HMB1	8:A:1001:HEM:CBB	2.43	0.47
1:B:407:MET:SD	1:B:408:ASN:N	2.88	0.47
1:B:221:ASP:HB2	1:B:226:TYR:CZ	2.51	0.46
1:A:146:LYS:NZ	12:A:2197:HOH:O	2.49	0.46
1:B:501:MET:HE2	1:B:506:ARG:O	2.15	0.46
1:A:452:TRP:HH2	5:A:2001:PO4:O2	1.98	0.46
1:B:349:PHE:CB	1:B:497:ASN:HD21	2.29	0.46
1:A:400:LEU:HD11	1:A:553:ILE:HD13	1.97	0.46
8:B:1021:HEM:HBC2	8:B:1021:HEM:CMC	2.45	0.46
1:B:3:GLU:C	1:B:5:GLY:H	2.24	0.45
1:B:170:PRO:HA	1:B:171:PRO:HD3	1.51	0.45
1:B:393:ASP:HB2	1:B:394:PRO:HD3	1.99	0.45
1:A:43:LEU:HD13	1:A:341:ASN:HA	1.99	0.45
1:B:6:CYS:HA	12:B:2120:HOH:O	2.17	0.45
1:B:233:LYS:HA	1:B:234:PRO:C	2.41	0.45
1:B:150:LYS:HA	1:B:153:THR:HG22	1.98	0.44
1:B:360:ARG:NH2	1:B:389:ASP:OD2	2.51	0.44
1:A:25:THR:HG22	1:A:197:PRO:HD3	1.98	0.44
1:A:167:CYS:CB	1:A:168:PRO:HD3	2.44	0.44
1:B:171:PRO:HB2	1:B:172:TYR:CD2	2.44	0.44
1:B:349:PHE:HA	1:B:497:ASN:HD21	1.82	0.44
1:A:301:GLY:O	1:A:305:GLN:HG3	2.18	0.44
1:A:428:VAL:HG23	1:A:430:GLY:N	2.32	0.44
1:B:557:THR:OG1	1:B:559:ILE:HG12	2.17	0.44
1:B:381:PHE:HZ	1:B:424:PRO:HG3	1.75	0.44
1:B:363:GLU:HA	5:B:2003:PO4:O4	2.18	0.44
1:B:397:ARG:HG3	1:B:559:ILE:HD12	1.99	0.44
1:A:108:ASP:OD1	8:A:1001:HEM:CMD	2.58	0.44
1:B:51:TYR:OH	1:B:177:ARG:HB3	2.16	0.44
1:B:175:LEU:HD23	1:B:176:ALA:H	1.82	0.44
8:B:1021:HEM:HBA2	8:B:1021:HEM:HHA	1.99	0.44
1:A:8:ALA:CB	1:A:9:PRO:CD	2.74	0.44
1:A:168:PRO:HB2	1:A:169:THR:H	1.67	0.44
1:A:82:ILE:CG2	1:A:494:ILE:HD11	2.41	0.43
1:A:108:ASP:OD2	8:A:1001:HEM:HMD2	2.14	0.43
1:A:308:THR:O	1:A:312:TYR:HB3	2.19	0.43
1:A:348:ARG:HG2	8:A:1001:HEM:C2D	2.54	0.43
1:B:588:SER:N	1:B:589:PRO:CD	2.81	0.43
1:B:51:TYR:CZ	1:B:177:ARG:HB3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:GLU:C	1:A:5:GLY:H	2.25	0.43
1:A:105:GLN:HE21	9:A:2011:CYN:C	2.32	0.42
1:A:89:GLU:HB3	12:A:2174:HOH:O	2.20	0.42
1:B:173:GLN:HB3	1:B:174:SER:H	1.53	0.42
1:B:231:ASN:HA	12:B:2090:HOH:O	2.19	0.42
1:B:343:PHE:CG	1:B:518:GLN:HG2	2.54	0.42
1:A:15:CYS:C	1:A:17:GLU:H	2.28	0.42
1:A:46:TRP:N	5:A:2001:PO4:O2	2.53	0.42
1:B:72:VAL:HA	1:B:73:PRO:HD2	1.84	0.42
1:B:106:ILE:HD13	1:B:265:VAL:HG11	2.01	0.42
1:B:258:GLU:HG3	11:B:2021:OSM:C	2.49	0.42
1:A:109:HIS:NE2	9:A:2011:CYN:C	2.83	0.41
1:A:287:TRP:CZ3	1:A:295:GLU:HG3	2.55	0.41
1:B:275:ARG:HD2	1:B:555:ASP:HB3	2.02	0.41
1:B:168:PRO:HB2	1:B:169:THR:H	1.58	0.41
1:B:261:LEU:HD12	1:B:261:LEU:HA	1.85	0.41
1:A:291:MET:HE3	1:A:291:MET:HB3	1.97	0.41
1:B:397:ARG:NE	5:B:2003:PO4:O4	2.52	0.41
1:B:484:TYR:CD1	1:B:490:ILE:HA	2.56	0.41
1:A:144:PHE:HE2	1:A:158:MET:HE3	1.86	0.41
1:A:450:ASN:OD1	1:A:461:PRO:HD2	2.21	0.41
1:A:45:ARG:HD3	5:A:2001:PO4:O4	2.21	0.41
1:B:172:TYR:HE2	12:B:2093:HOH:O	2.03	0.41
1:A:335:VAL:O	1:A:337:PRO:HD3	2.21	0.41
1:B:108:ASP:OD2	8:B:1021:HEM:HMD2	2.20	0.41
1:B:160:PHE:HA	12:B:2151:HOH:O	2.19	0.41
1:A:51:TYR:HB3	1:A:57:VAL:O	2.21	0.41
1:B:281:LYS:HD3	1:B:292:LEU:HD21	2.03	0.41
1:A:187:LEU:HD23	1:A:187:LEU:HA	1.91	0.40
1:B:407:MET:CB	1:B:501:MET:HE3	2.51	0.40
1:A:480:LEU:HD12	1:A:480:LEU:HA	1.91	0.40
1:B:12:LEU:HD12	1:B:12:LEU:H	1.87	0.40
1:B:96:ARG:HD2	1:B:100:PHE:CG	2.56	0.40
1:B:261:LEU:HG	1:B:399:LEU:HD21	2.03	0.40
1:B:313:LEU:HA	1:B:313:LEU:HD23	1.84	0.40
1:B:343:PHE:CD1	1:B:518:GLN:HG2	2.56	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	593/595 (100%)	539 (91%)	38 (6%)	16 (3%)	4	11
1	B	593/595 (100%)	541 (91%)	41 (7%)	11 (2%)	6	17
All	All	1186/1190 (100%)	1080 (91%)	79 (7%)	27 (2%)	5	14

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	9	PRO
1	A	12	LEU
1	A	168	PRO
1	A	169	THR
1	A	171	PRO
1	A	174	SER
1	B	9	PRO
1	B	12	LEU
1	B	17	GLU
1	B	168	PRO
1	B	169	THR
1	B	171	PRO
1	A	594	GLU
1	B	4	VAL
1	A	8	ALA
1	A	17	GLU
1	A	40	ASN
1	A	64	ARG
1	A	118	GLU
1	A	241	ASN
1	B	122	SER
1	B	166	VAL
1	A	3	GLU
1	B	11	PRO
1	A	4	VAL

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Mol	Chain	Res	Type
1	A	166	VAL
1	B	5	GLY

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	517/517 (100%)	470 (91%)	47 (9%)	9 22
1	B	517/517 (100%)	471 (91%)	46 (9%)	9 23
All	All	1034/1034 (100%)	941 (91%)	93 (9%)	9 23

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	TRP
1	A	3	GLU
1	A	6	CYS
1	A	12	LEU
1	A	13	VAL
1	A	16	ASP
1	A	32	ARG
1	A	40	ASN
1	A	64	ARG
1	A	91	VAL
1	A	98	LEU
1	A	106	ILE
1	A	128	GLN
1	A	130	GLU
1	A	131	GLU
1	A	146	LYS
1	A	153	THR
1	A	173	GLN
1	A	175	LEU
1	A	187	LEU
1	A	201	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	203	LEU
1	A	218	GLU
1	A	235	SER
1	A	243	THR
1	A	255	ARG
1	A	261	LEU
1	A	268	LEU
1	A	276	LEU
1	A	292	LEU
1	A	317	LEU
1	A	360	ARG
1	A	363	GLU
1	A	376	LEU
1	A	392	ILE
1	A	428	VAL
1	A	459	SER
1	A	464	LEU
1	A	480	LEU
1	A	494	ILE
1	A	504	ARG
1	A	511	LEU
1	A	523	ARG
1	A	538	GLU
1	A	542	ASP
1	A	564	LEU
1	A	583	ASP
1	B	2	TRP
1	B	3	GLU
1	B	6	CYS
1	B	12	LEU
1	B	16	ASP
1	B	64	ARG
1	B	65	LYS
1	B	72	VAL
1	B	98	LEU
1	B	106	ILE
1	B	122	SER
1	B	130	GLU
1	B	146	LYS
1	B	166	VAL
1	B	169	THR
1	B	174	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	175	LEU
1	B	187	LEU
1	B	202	ARG
1	B	203	LEU
1	B	218	GLU
1	B	245	HIS
1	B	255	ARG
1	B	261	LEU
1	B	268	LEU
1	B	275	ARG
1	B	276	LEU
1	B	292	LEU
1	B	304	ILE
1	B	317	LEU
1	B	333	ASN
1	B	347	PHE
1	B	360	ARG
1	B	376	LEU
1	B	423	GLN
1	B	425	THR
1	B	451	SER
1	B	464	LEU
1	B	471	LEU
1	B	474	LYS
1	B	480	LEU
1	B	511	LEU
1	B	542	ASP
1	B	545	GLN
1	B	564	LEU
1	B	594	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	124	HIS
1	A	128	GLN
1	A	147	ASN
1	A	305	GLN
1	A	322	GLN
1	A	341	ASN
1	A	410	ASN
1	A	426	HIS

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Mol	Chain	Res	Type
1	A	429	HIS
1	A	460	GLN
1	A	468	GLN
1	A	497	ASN
1	A	545	GLN
1	B	128	GLN
1	B	173	GLN
1	B	179	GLN
1	B	230	ASN
1	B	333	ASN
1	B	341	ASN
1	B	437	ASN
1	B	460	GLN
1	B	497	ASN
1	B	520	GLN
1	B	570	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

22 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	C	1	1,2	14,14,15	0.62	0	17,19,21	0.82	0
2	NAG	C	2	2	14,14,15	0.68	0	17,19,21	1.36	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	MAN	C	3	2	11,11,12	0.64	0	15,15,17	1.35	1 (6%)
2	NAG	D	1	1,2	14,14,15	0.62	0	17,19,21	0.97	1 (5%)
2	NAG	D	2	2	14,14,15	0.55	0	17,19,21	1.66	3 (17%)
2	MAN	D	3	2	11,11,12	0.64	0	15,15,17	1.39	2 (13%)
3	NAG	E	1	1,3	14,14,15	0.65	0	17,19,21	1.48	3 (17%)
3	NAG	E	2	3	14,14,15	0.57	0	17,19,21	1.31	2 (11%)
3	BMA	E	3	3	11,11,12	0.58	0	15,15,17	1.68	1 (6%)
4	NAG	F	1	4,1	14,14,15	0.66	0	17,19,21	1.39	2 (11%)
4	NAG	F	2	4	14,14,15	0.65	0	17,19,21	1.59	3 (17%)
2	NAG	G	1	1,2	14,14,15	0.80	0	17,19,21	1.37	1 (5%)
2	NAG	G	2	2	14,14,15	0.78	1 (7%)	17,19,21	2.58	3 (17%)
2	MAN	G	3	2	11,11,12	0.64	0	15,15,17	1.29	3 (20%)
3	NAG	H	1	1,3	14,14,15	0.57	0	17,19,21	1.29	3 (17%)
3	NAG	H	2	3	14,14,15	0.67	0	17,19,21	1.23	2 (11%)
3	BMA	H	3	3	11,11,12	0.62	0	15,15,17	2.04	1 (6%)
3	NAG	I	1	1,3	14,14,15	0.48	0	17,19,21	1.64	3 (17%)
3	NAG	I	2	3	14,14,15	0.54	0	17,19,21	1.97	3 (17%)
3	BMA	I	3	3	11,11,12	0.60	0	15,15,17	1.42	3 (20%)
4	NAG	J	1	4,1	14,14,15	0.64	0	17,19,21	1.37	2 (11%)
4	NAG	J	2	4	14,14,15	0.49	0	17,19,21	0.79	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	C	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	4/6/23/26	0/1/1/1
2	MAN	C	3	2	-	2/2/19/22	1/1/1/1
2	NAG	D	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	MAN	D	3	2	-	0/2/19/22	0/1/1/1
3	NAG	E	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	E	2	3	-	4/6/23/26	0/1/1/1
3	BMA	E	3	3	-	2/2/19/22	1/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	F	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	F	2	4	-	2/6/23/26	0/1/1/1
2	NAG	G	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	G	2	2	-	1/6/23/26	0/1/1/1
2	MAN	G	3	2	-	0/2/19/22	0/1/1/1
3	NAG	H	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	H	2	3	-	2/6/23/26	0/1/1/1
3	BMA	H	3	3	-	2/2/19/22	0/1/1/1
3	NAG	I	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	I	2	3	-	2/6/23/26	0/1/1/1
3	BMA	I	3	3	-	2/2/19/22	1/1/1/1
4	NAG	J	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	J	2	4	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	2	NAG	C1-C2	2.22	1.55	1.52

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	2	NAG	C1-O5-C5	8.94	124.17	112.19
3	H	3	BMA	C1-O5-C5	7.00	121.56	112.19
3	I	2	NAG	C1-O5-C5	6.30	120.62	112.19
3	E	3	BMA	C1-O5-C5	5.57	119.65	112.19
2	D	2	NAG	C4-C3-C2	4.70	117.90	111.02
2	G	1	NAG	C4-C3-C2	4.66	117.85	111.02
3	I	1	NAG	C1-O5-C5	4.40	118.08	112.19
4	F	1	NAG	C4-C3-C2	4.32	117.34	111.02
2	C	3	MAN	C1-O5-C5	4.28	117.92	112.19
3	I	3	BMA	C1-O5-C5	4.25	117.88	112.19
4	J	1	NAG	C4-C3-C2	4.16	117.12	111.02
2	G	3	MAN	C1-O5-C5	3.82	117.30	112.19
4	F	2	NAG	C1-O5-C5	3.80	117.28	112.19
4	F	2	NAG	C4-C3-C2	3.79	116.57	111.02
3	E	1	NAG	C1-O5-C5	3.68	117.12	112.19
2	G	2	NAG	O4-C4-C3	3.53	118.69	110.38
2	D	3	MAN	C1-O5-C5	3.49	116.86	112.19
3	E	2	NAG	C1-O5-C5	3.43	116.78	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	2	NAG	O5-C1-C2	3.17	116.20	111.29
3	H	2	NAG	C4-C3-C2	3.08	115.54	111.02
3	I	1	NAG	C4-C3-C2	3.04	115.48	111.02
3	I	2	NAG	O5-C1-C2	-2.97	106.70	111.29
3	E	1	NAG	C4-C3-C2	2.83	115.17	111.02
2	C	2	NAG	C4-C3-C2	2.82	115.15	111.02
2	D	3	MAN	C1-C2-C3	2.79	113.71	109.64
2	D	2	NAG	O4-C4-C3	-2.71	103.98	110.38
3	E	2	NAG	O5-C1-C2	-2.69	107.12	111.29
2	D	2	NAG	C1-O5-C5	2.57	115.63	112.19
3	H	1	NAG	C1-O5-C5	2.53	115.57	112.19
2	C	2	NAG	C1-O5-C5	2.52	115.57	112.19
3	H	1	NAG	O7-C7-C8	-2.47	117.65	122.05
2	D	1	NAG	C4-C3-C2	2.41	114.55	111.02
4	J	1	NAG	C3-C4-C5	2.35	114.49	110.23
4	F	2	NAG	O5-C1-C2	2.29	114.83	111.29
4	F	1	NAG	C3-C4-C5	2.27	114.35	110.23
3	I	1	NAG	O5-C1-C2	-2.19	107.89	111.29
3	I	2	NAG	O5-C5-C4	2.17	116.11	110.83
3	H	2	NAG	O5-C1-C2	-2.14	107.98	111.29
2	G	3	MAN	C1-C2-C3	2.14	112.76	109.64
3	H	1	NAG	C4-C3-C2	2.08	114.06	111.02
3	I	3	BMA	O5-C5-C6	2.06	111.67	107.66
4	J	2	NAG	C1-O5-C5	2.06	114.94	112.19
3	I	3	BMA	C1-C2-C3	2.02	112.59	109.64
2	C	2	NAG	C3-C4-C5	2.01	113.88	110.23
3	E	1	NAG	O5-C1-C2	-2.01	108.18	111.29
2	G	3	MAN	O5-C5-C6	2.01	111.57	107.66

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	F	2	NAG	C8-C7-N2-C2
4	F	2	NAG	O7-C7-N2-C2
4	J	2	NAG	C8-C7-N2-C2
4	J	2	NAG	O7-C7-N2-C2
3	I	3	BMA	O5-C5-C6-O6
3	E	2	NAG	C8-C7-N2-C2
3	E	2	NAG	O7-C7-N2-C2
3	I	2	NAG	C8-C7-N2-C2
3	I	2	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
2	C	2	NAG	O5-C5-C6-O6
3	H	3	BMA	O5-C5-C6-O6
3	E	3	BMA	O5-C5-C6-O6
3	E	3	BMA	C4-C5-C6-O6
3	I	3	BMA	C4-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6
3	E	1	NAG	C8-C7-N2-C2
3	H	3	BMA	C4-C5-C6-O6
3	I	1	NAG	C4-C5-C6-O6
2	G	1	NAG	C8-C7-N2-C2
3	E	1	NAG	O7-C7-N2-C2
2	C	3	MAN	C4-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
3	I	1	NAG	O5-C5-C6-O6
2	C	2	NAG	C8-C7-N2-C2
2	G	1	NAG	O7-C7-N2-C2
3	E	2	NAG	C4-C5-C6-O6
2	C	2	NAG	O7-C7-N2-C2
2	G	2	NAG	C4-C5-C6-O6
3	H	2	NAG	C4-C5-C6-O6
2	G	1	NAG	O5-C5-C6-O6
2	C	3	MAN	O5-C5-C6-O6
2	G	1	NAG	C4-C5-C6-O6
3	H	2	NAG	O5-C5-C6-O6
2	C	1	NAG	C4-C5-C6-O6
2	C	1	NAG	O5-C5-C6-O6

All (3) ring outliers are listed below:

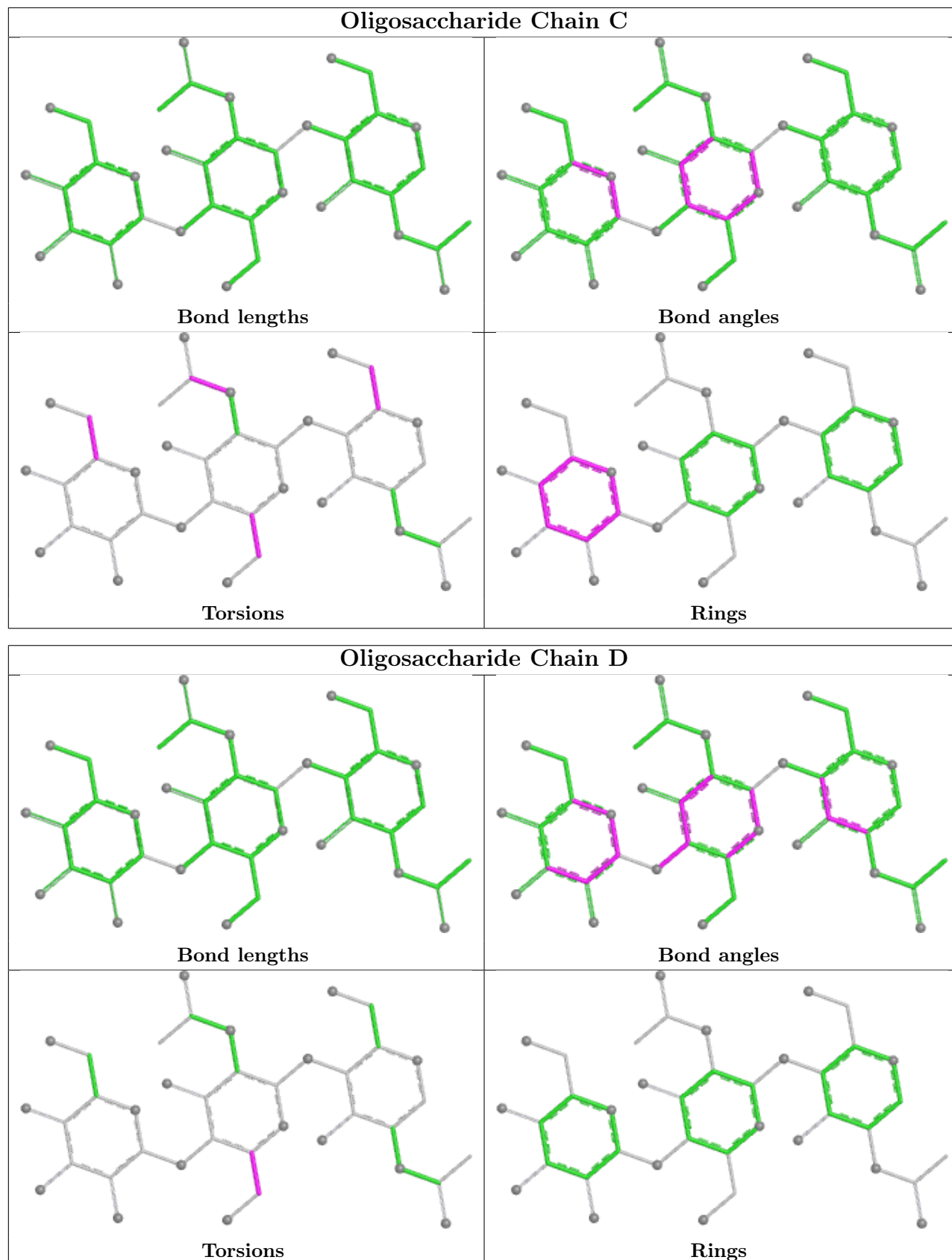
Mol	Chain	Res	Type	Atoms
2	C	3	MAN	C1-C2-C3-C4-C5-O5
3	I	3	BMA	C1-C2-C3-C4-C5-O5
3	E	3	BMA	C1-C2-C3-C4-C5-O5

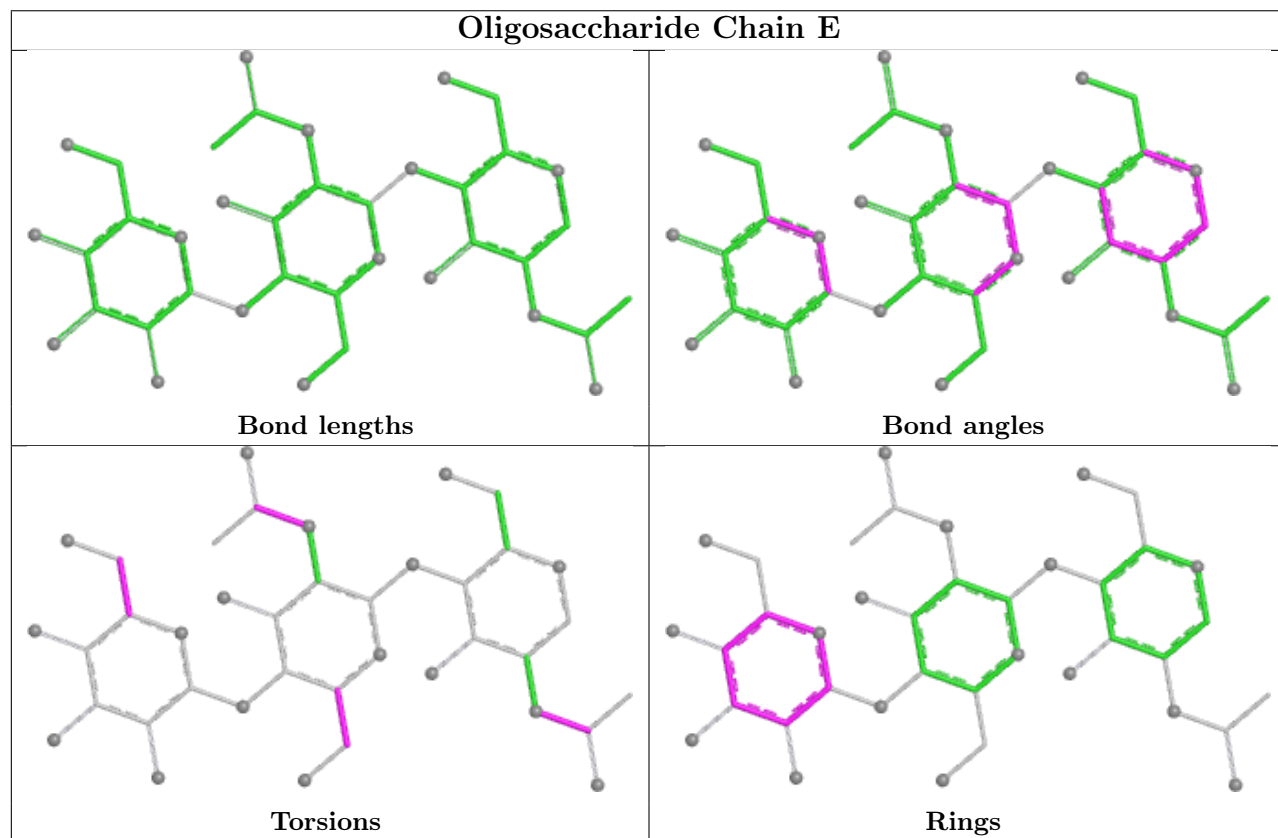
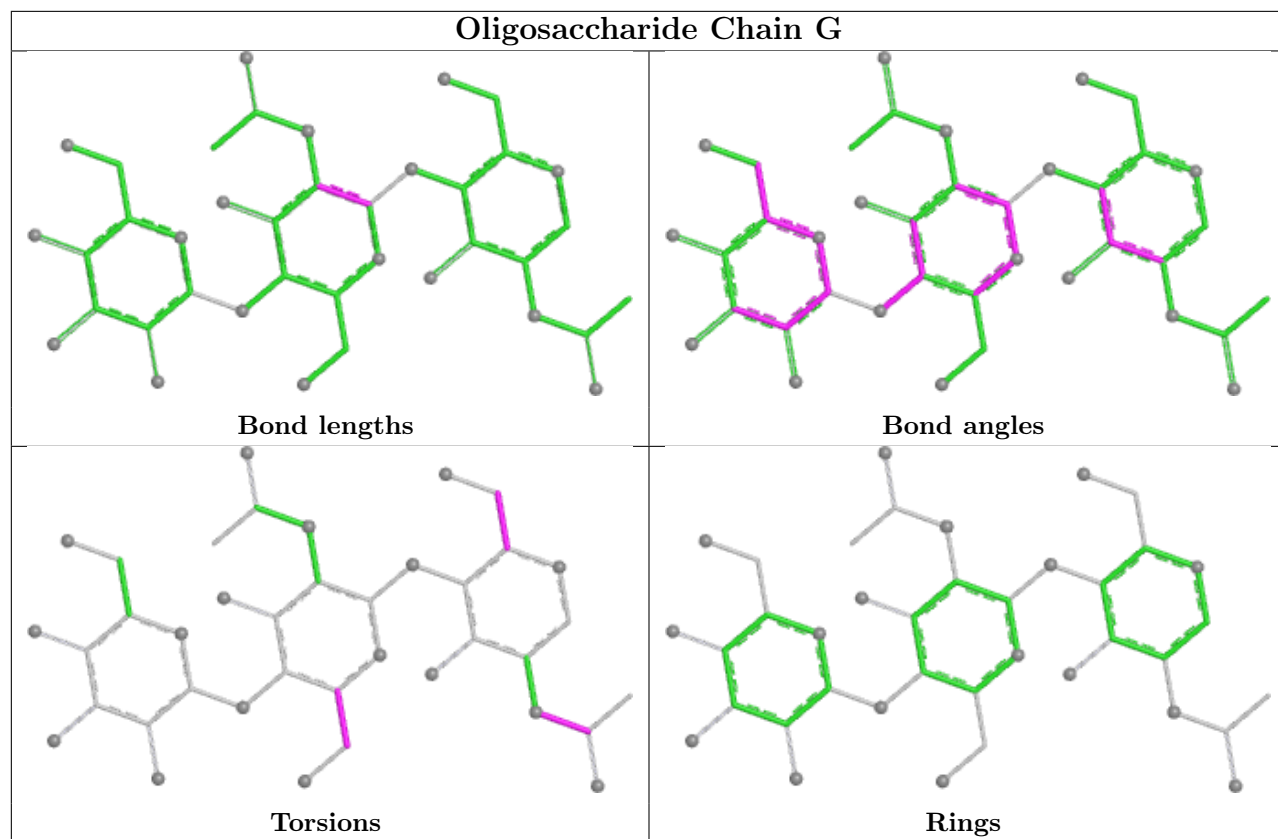
1 monomer is involved in 2 short contacts:

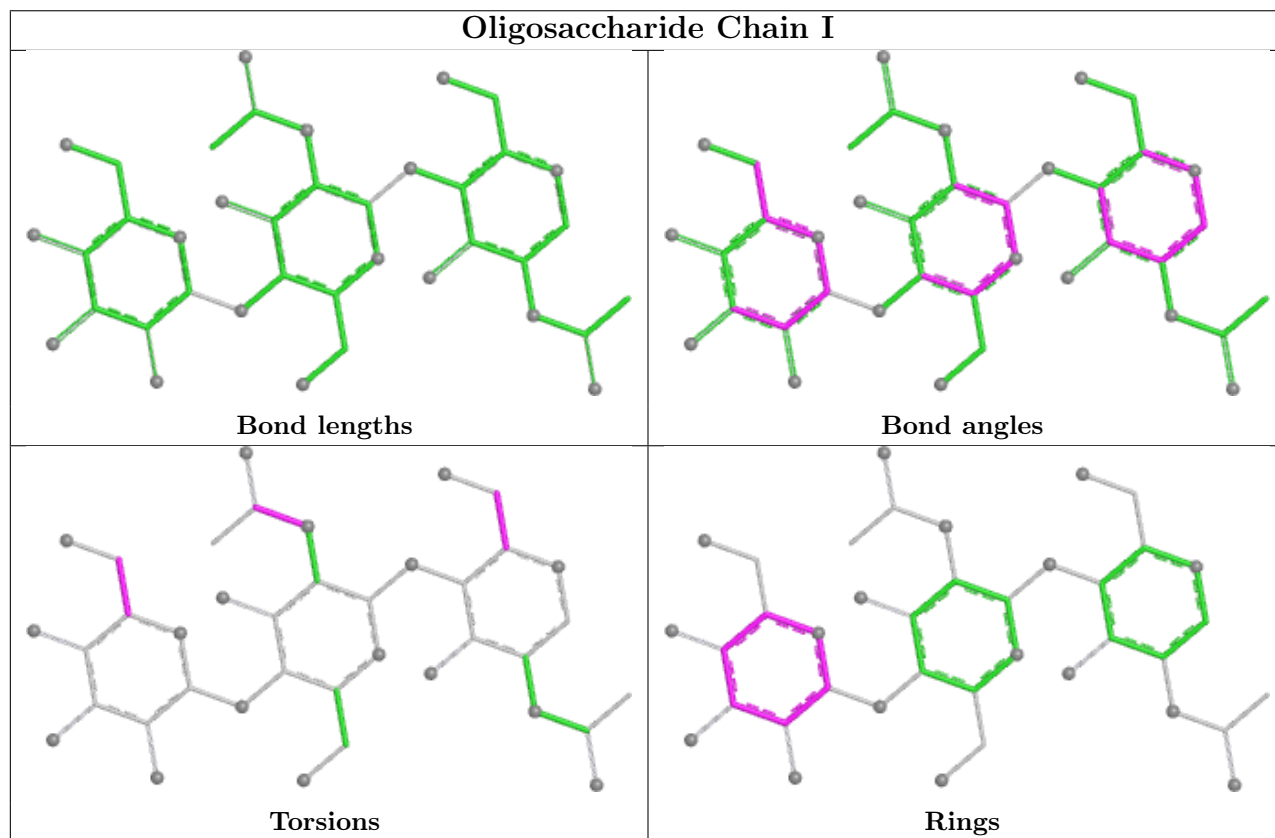
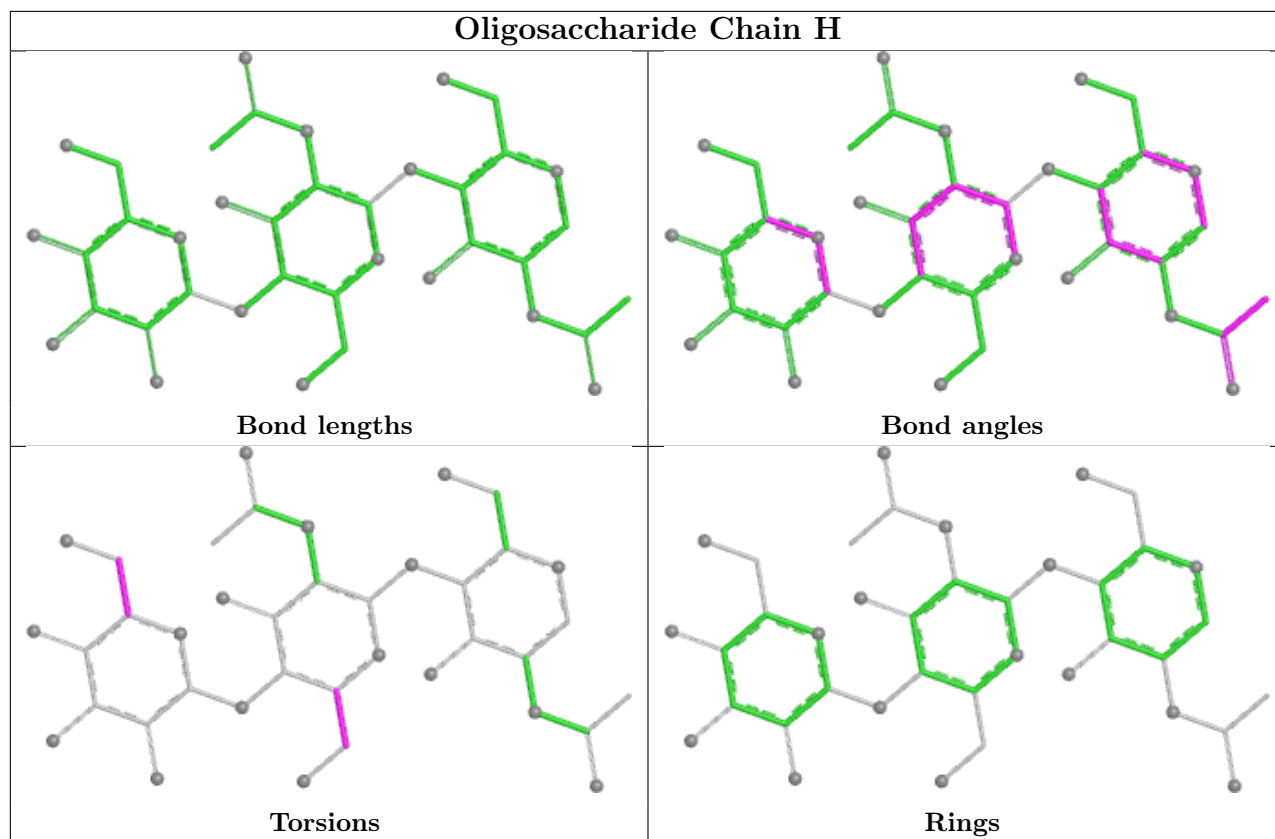
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2	NAG	2	0

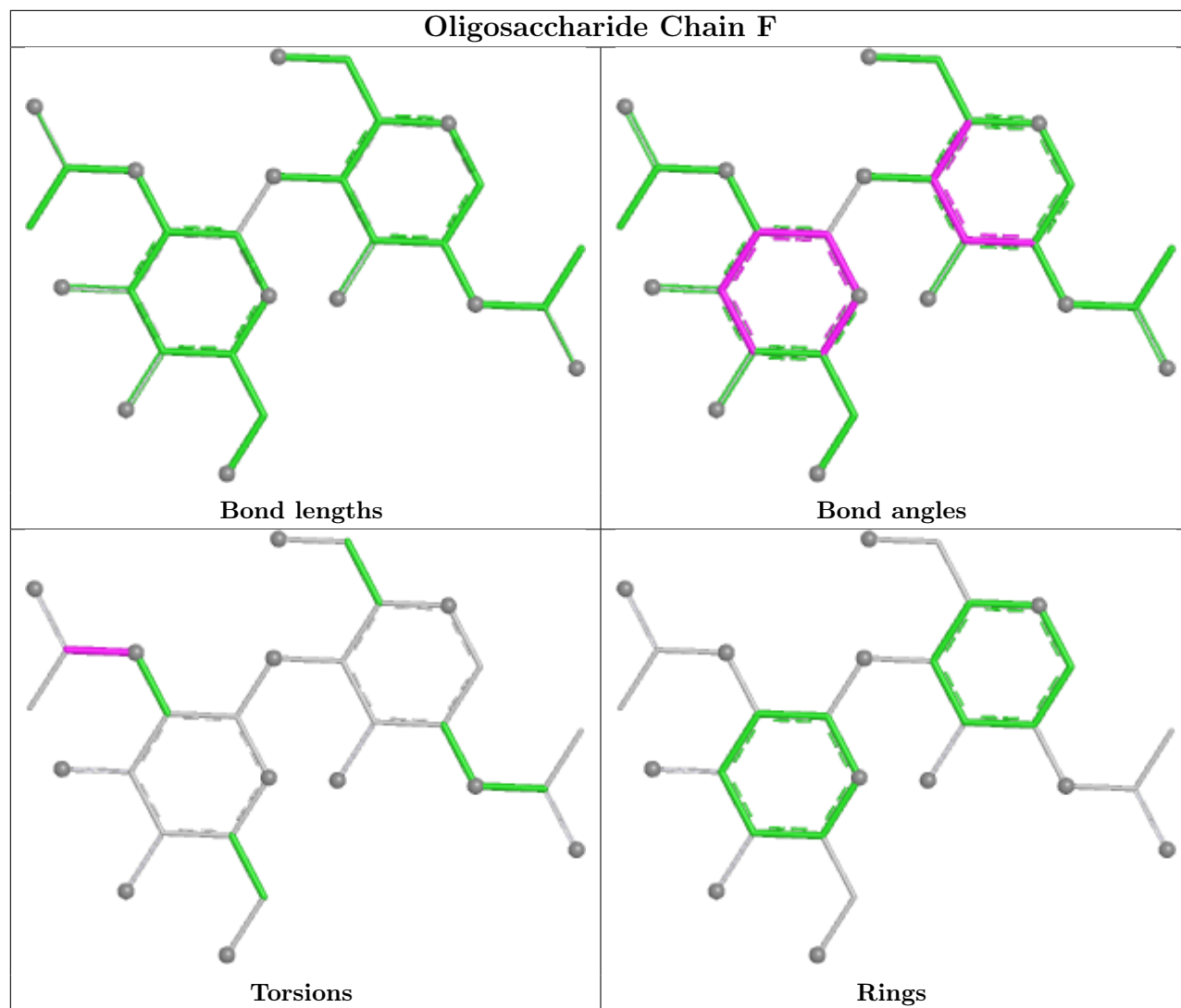
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

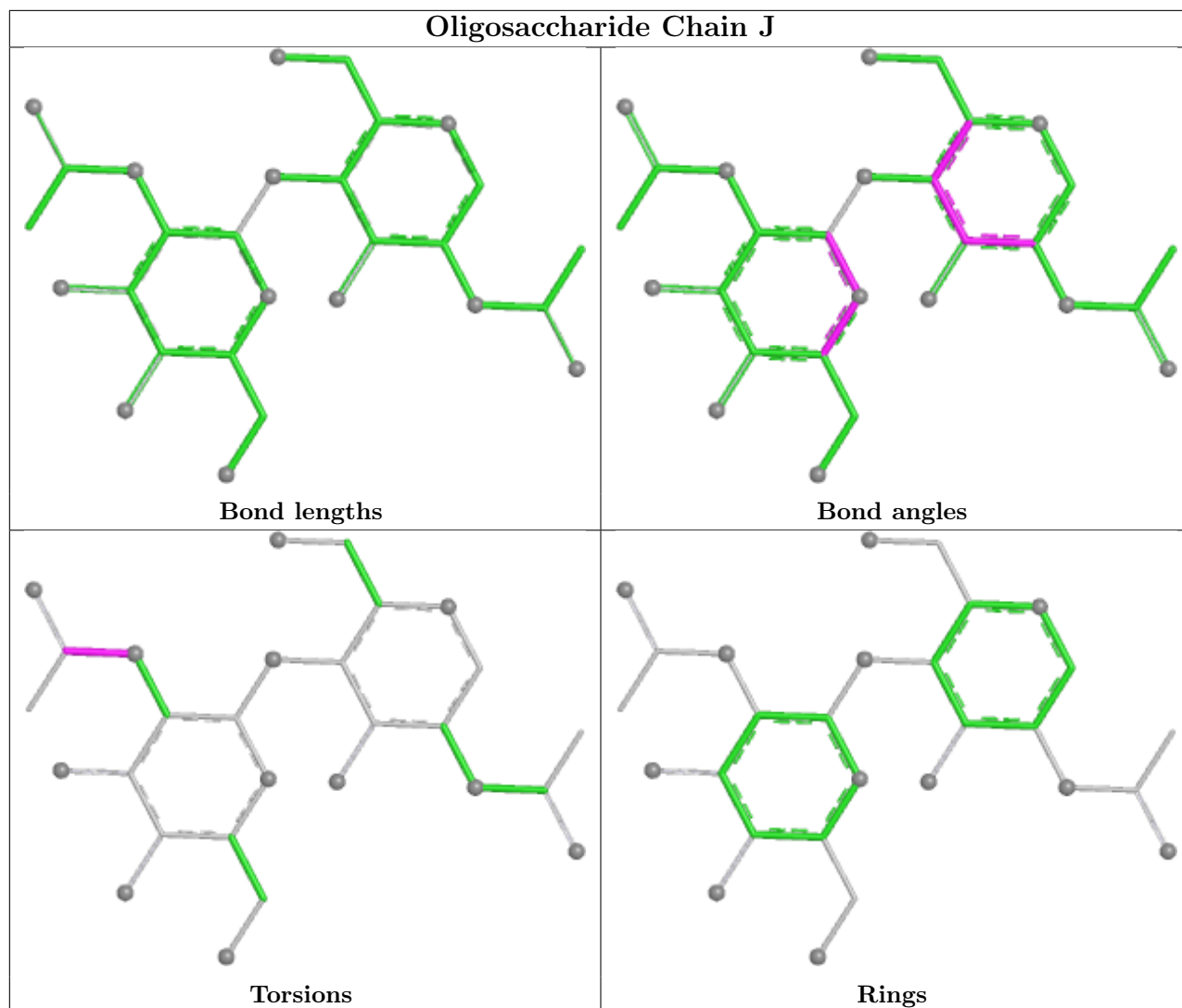
bond angles, torsion angles, and ring geometry for oligosaccharide.











## 5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 2 are monoatomic - leaving 12 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	SCN	A	2012	-	1,2,2	1.92	0	0,1,1	-	-
6	CO3	B	2007	-	3,3,3	0.76	0	2,3,3	0.24	0
5	PO4	A	2005	-	4,4,4	0.89	0	6,6,6	0.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	CYN	A	2011	-	1,1,1	0.36	0	-		
5	PO4	B	2003	-	4,4,4	0.90	0	6,6,6	0.58	0
5	PO4	A	2001	-	4,4,4	0.80	0	6,6,6	0.81	0
6	CO3	A	2006	-	3,3,3	0.76	0	2,3,3	0.17	0
8	HEM	A	1001	1	50,50,50	2.12	7 (14%)	67,82,82	1.43	5 (7%)
8	HEM	B	1021	1	50,50,50	2.08	8 (16%)	67,82,82	1.44	7 (10%)
5	PO4	B	2004	-	4,4,4	1.10	0	6,6,6	0.56	0
5	PO4	A	2002	-	4,4,4	0.95	0	6,6,6	0.53	0
11	OSM	B	2021	-	1,3,3	0.09	0	0,2,2	-	-

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
11	OSM	B	2021	-	-	0/0/1/1	-
8	HEM	A	1001	1	-	2/14/54/54	-
8	HEM	B	1021	1	-	2/14/54/54	-

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	1021	HEM	FE-NB	8.62	2.21	1.94
8	A	1001	HEM	FE-NB	7.78	2.18	1.94
8	A	1001	HEM	C3D-C2D	7.35	1.52	1.36
8	B	1021	HEM	C3D-C2D	7.10	1.52	1.36
8	A	1001	HEM	FE-NA	7.02	2.18	1.95
8	B	1021	HEM	FE-NC	4.55	2.10	1.95
8	B	1021	HEM	CAB-C3B	3.28	1.56	1.47
8	A	1001	HEM	CAC-C3C	2.99	1.55	1.47
8	B	1021	HEM	CAC-C3C	2.96	1.55	1.47
8	A	1001	HEM	CAB-C3B	2.75	1.54	1.47
8	B	1021	HEM	CMB-C2B	2.33	1.55	1.50
8	B	1021	HEM	FE-NA	2.28	2.02	1.95
8	B	1021	HEM	FE-ND	2.20	2.01	1.94
8	A	1001	HEM	CMC-C2C	2.12	1.55	1.50
8	A	1001	HEM	FE-ND	2.09	2.01	1.94

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	1001	HEM	C4D-ND-C1D	6.31	112.67	105.21
8	B	1021	HEM	C4D-ND-C1D	5.66	111.91	105.21
8	B	1021	HEM	CMD-C2D-C1D	4.45	131.99	125.03
8	A	1001	HEM	CAD-C3D-C4D	3.32	130.48	124.70
8	B	1021	HEM	CAD-C3D-C4D	2.43	128.93	124.70
8	B	1021	HEM	C3A-C4A-NA	-2.36	106.36	110.14
8	B	1021	HEM	CHA-C4D-ND	2.30	127.21	124.37
8	A	1001	HEM	CMD-C2D-C1D	2.26	128.56	125.03
8	B	1021	HEM	C1B-NB-C4B	2.23	107.85	105.21
8	A	1001	HEM	CHC-C4B-NB	2.22	126.81	124.42
8	A	1001	HEM	C3D-C4D-ND	-2.21	107.75	110.17
8	B	1021	HEM	C3B-C2B-C1B	2.05	107.95	106.41

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	1001	HEM	CAD-CBD-CGD-O1D
8	A	1001	HEM	CAD-CBD-CGD-O2D
8	B	1021	HEM	CAD-CBD-CGD-O2D
8	B	1021	HEM	CAD-CBD-CGD-O1D

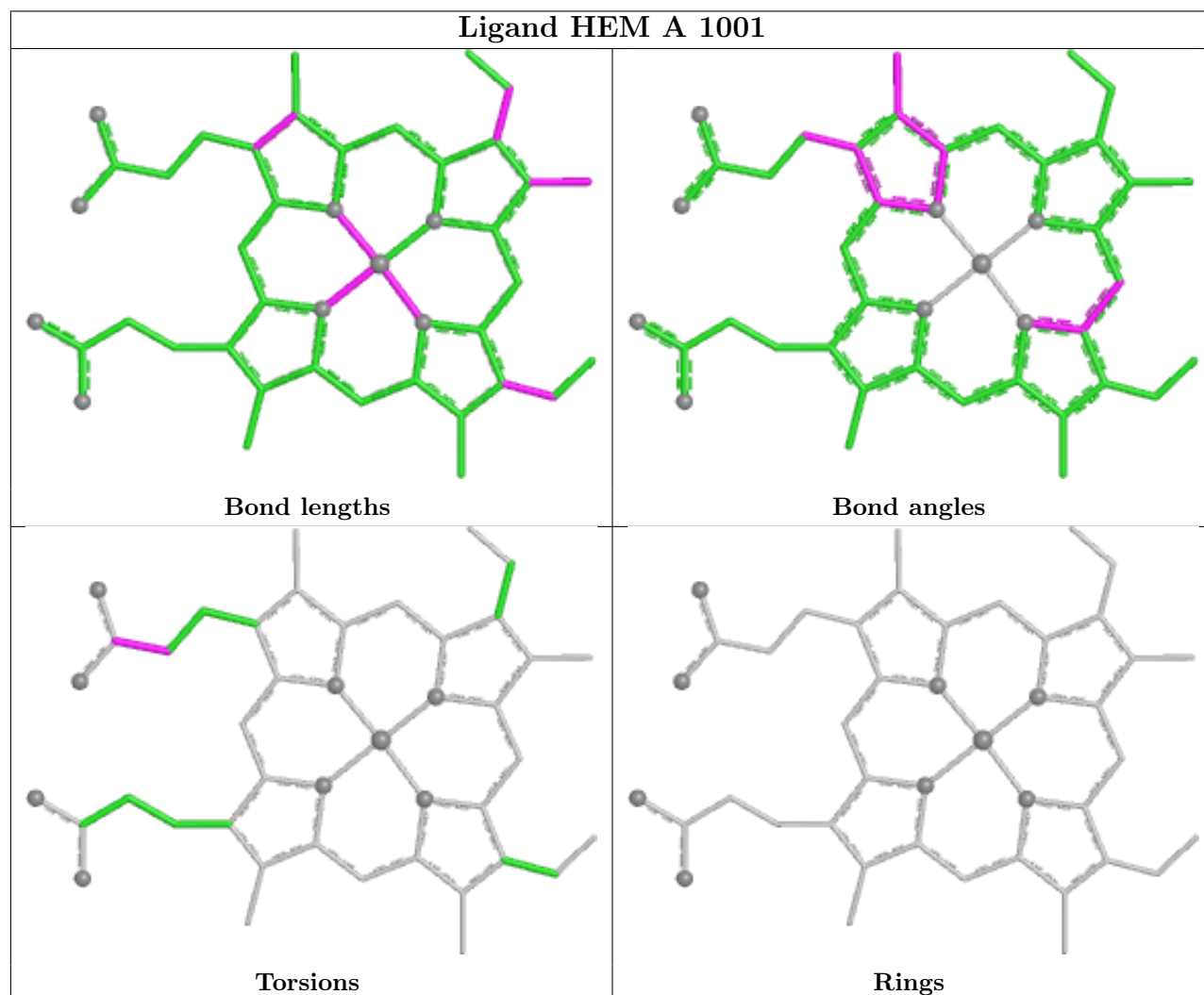
There are no ring outliers.

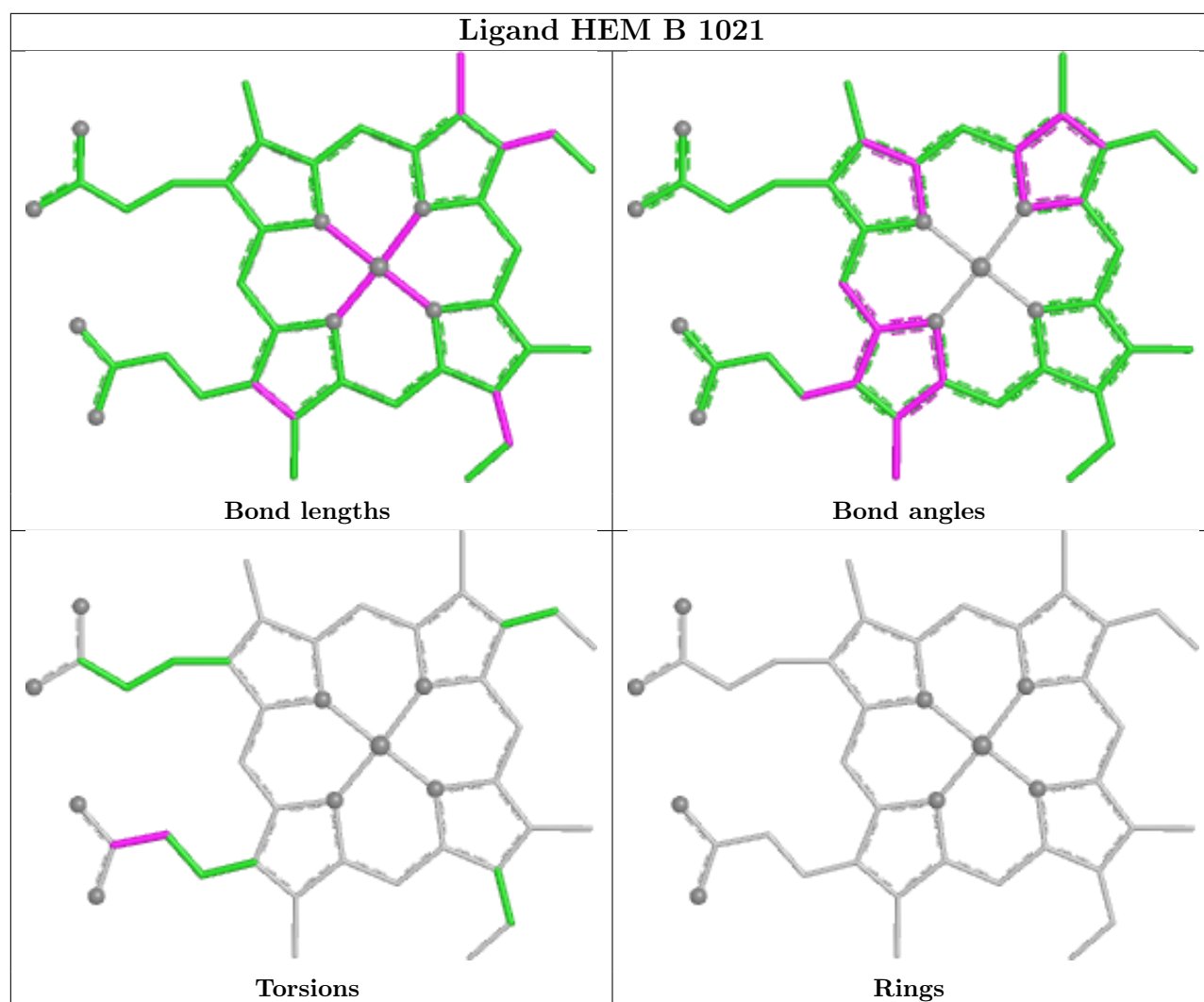
8 monomers are involved in 44 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	2012	SCN	1	0
9	A	2011	CYN	3	0
5	B	2003	PO4	2	0
5	A	2001	PO4	5	0
8	A	1001	HEM	14	0
8	B	1021	HEM	15	0
5	B	2004	PO4	4	0
11	B	2021	OSM	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

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.