Full wwPDB X-ray Structure Validation Report ⓘ

Oct 16, 2023 – 12:51 AM EDT

PDB ID	:	2E9E
Title	:	Crystal structure of the complex of goat lactoperoxidase with Nitrate at 3.25 A resolution
Authors	:	Singh, A.K.; Prem kumar, R.; Singh, N.; Sharma, S.; Singh, S.B.; Bhushan, A.; Kaur, P.; Singh, T.P.
Deposited on	:	2007-01-25
Resolution	:	3.25 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:

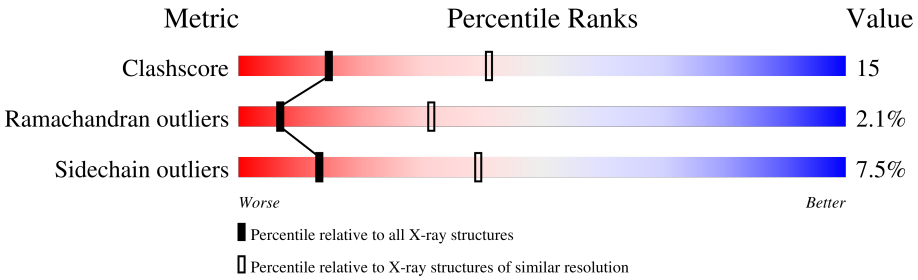
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 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	141614	1251 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	595	73% 23%
1	B	595	72% 24%
2	C	3	100%
2	D	3	67% 33%
2	G	3	67% 33%
3	E	3	100%
3	H	3	33% 67%
3	I	3	33% 67%

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

2 Entry composition

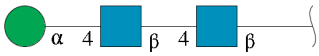
There are 12 unique types of molecules in this entry. The entry contains 10299 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

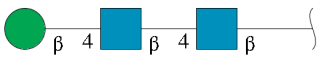
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	595	Total	C	N	O	S	0	0	0
			4754	3021	844	863	26			
1	B	595	Total	C	N	O	S	0	0	0
			4754	3021	844	863	26			

- 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
2	C	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	D	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	G	3	Total	C	N	O	0	0	0
			39	22	2	15			

- 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
3	E	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	H	3	Total	C	N	O	0	0	0
			39	22	2	15			

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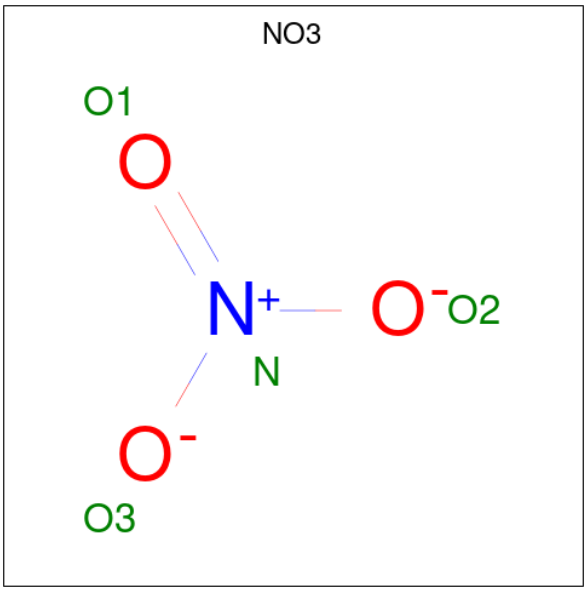
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	I	3	Total C N O 39 22 2 15	0	0	0

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

- Molecule 5 is NITRATE ION (three-letter code: NO3) (formula: NO_3).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total N O 4 1 3	0	0
5	A	1	Total N O 4 1 3	0	0
5	B	1	Total N O 4 1 3	0	0

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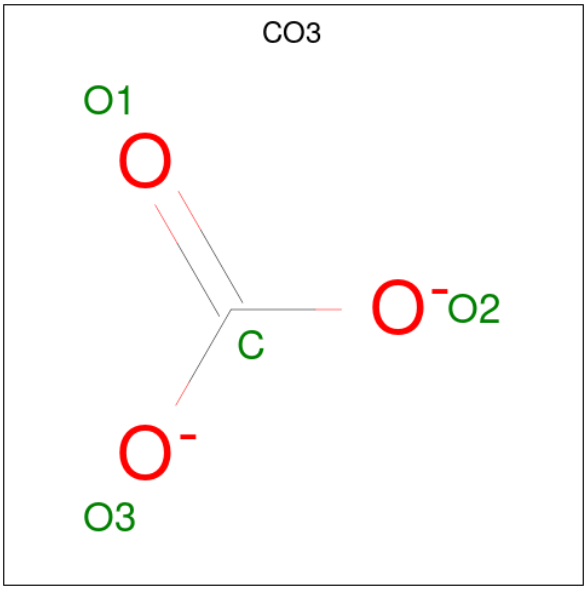
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total N O 4 1 3	0	0

- Molecule 6 is CARBONATE ION (three-letter code: CO3) (formula: CO_3).

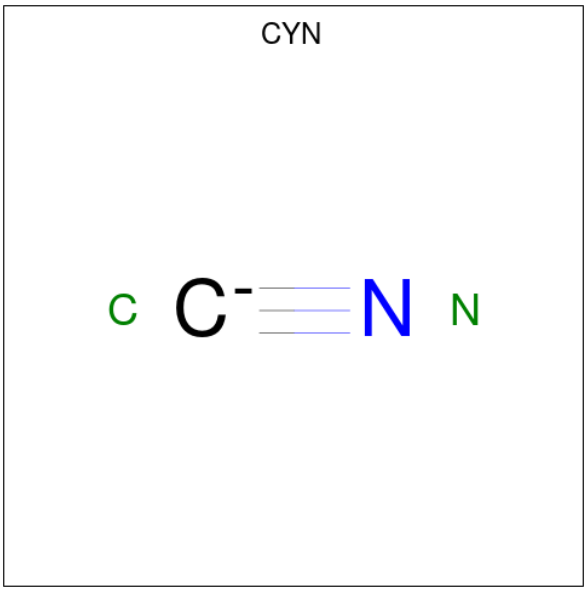


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 4 1 3	0	0
6	B	1	Total C O 4 1 3	0	0

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

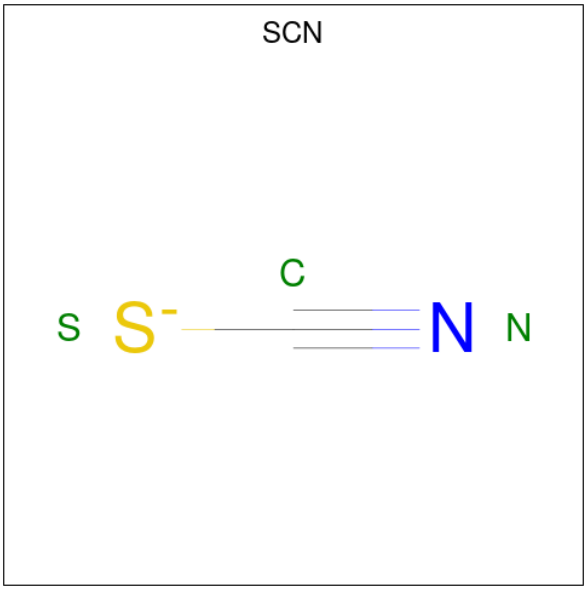
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Ca 1 1	0	0
7	B	1	Total Ca 1 1	0	0

- Molecule 8 is CYANIDE ION (three-letter code: CYN) (formula: CN).



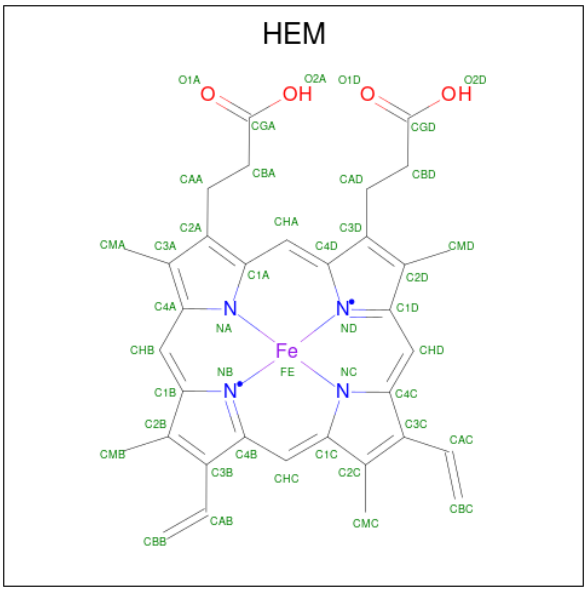
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C N 2 1 1	0	0

- Molecule 9 is THIOCYANATE ION (three-letter code: SCN) (formula: CNS).



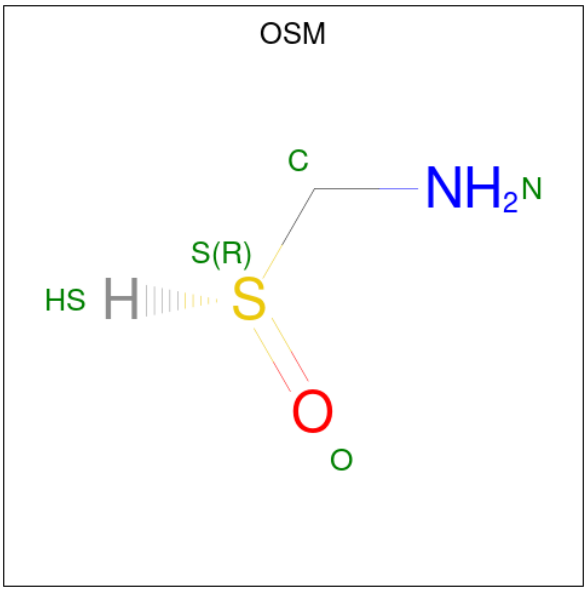
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C N S 3 1 1 1	0	0

- Molecule 10 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 11 is 1-(OXIDOSULFANYL)METHANAMINE (three-letter code: OSM) (formula: CH_5NOS).



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

- Molecule 12 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	180	Total O 180 180	0	0
12	B	200	Total O 200 200	0	0

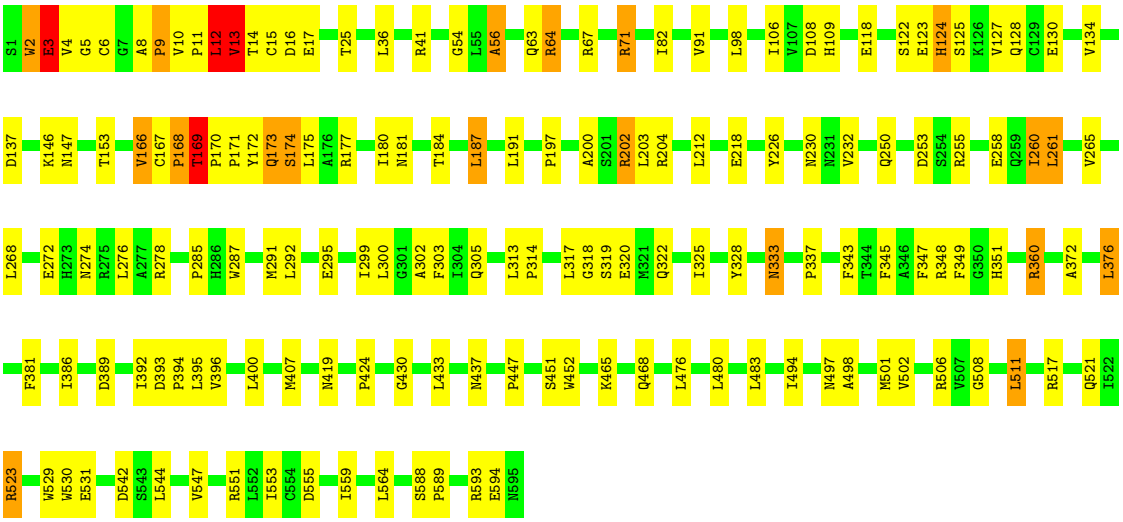
3 Residue-property plots (i)

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. 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.

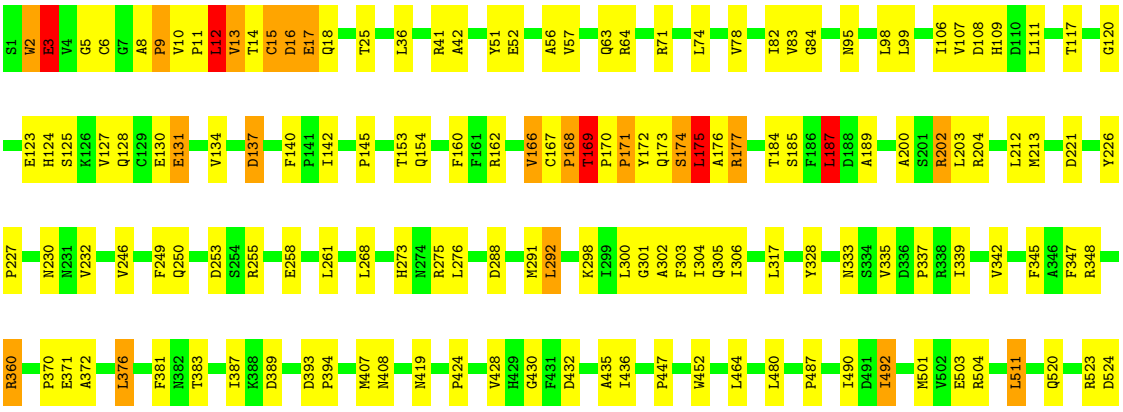
• Molecule 1: Lactoperoxidase

Chain A:



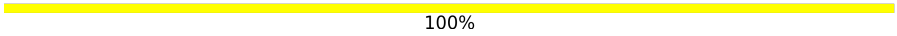
• Molecule 1: Lactoperoxidase

Chain B:



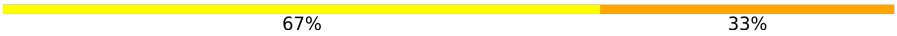
• Molecule 2: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:



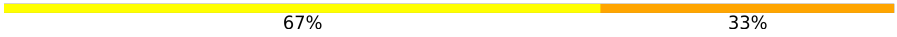
• Molecule 2: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:



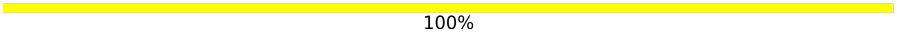
• Molecule 2: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:



• 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:



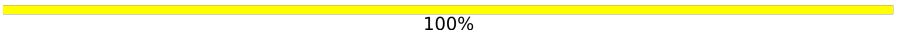
• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:

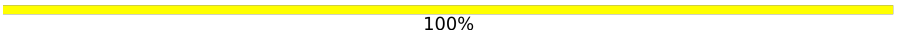
• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:

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

Chain F: 

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

Chain J: 

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	58.52Å 72.54Å 83.98Å 85.30° 84.06° 75.68°	Depositor
Resolution (Å)	20.00 – 3.25	Depositor
% Data completeness (in resolution range)	94.8 (20.00-3.25)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.15	Depositor
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.169 , 0.203	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10299	wwPDB-VP
Average B, all atoms (Å^2)	18.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CYN, BMA, OSM, MAN, NO3, CO3, CA, NAG, HEM, SCN

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	0.55	0/4883	0.73	5/6632 (0.1%)
1	B	0.54	0/4883	0.74	7/6632 (0.1%)
All	All	0.54	0/9766	0.73	12/13264 (0.1%)

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	A	0	1

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	175	LEU	CA-CB-CG	7.01	131.42	115.30
1	A	13	VAL	CA-CB-CG2	-6.31	101.43	110.90
1	A	15	CYS	CA-CB-SG	-6.10	103.03	114.00
1	B	13	VAL	CA-CB-CG1	6.03	119.94	110.90
1	B	13	VAL	CB-CA-C	-6.00	100.01	111.40
1	B	12	LEU	CA-CB-CG	5.84	128.73	115.30
1	B	13	VAL	N-CA-C	5.78	126.59	111.00
1	B	13	VAL	CA-CB-CG2	-5.44	102.75	110.90
1	B	15	CYS	CA-CB-SG	-5.43	104.23	114.00
1	A	13	VAL	N-CA-C	5.42	125.63	111.00
1	A	12	LEU	CA-CB-CG	5.21	127.28	115.30
1	A	13	VAL	CA-CB-CG1	5.01	118.42	110.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	12	LEU	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	4647	127	0
1	B	4754	0	4645	152	0
2	C	39	0	34	1	0
2	D	39	0	34	2	0
2	G	39	0	34	4	0
3	E	39	0	34	0	0
3	H	39	0	34	4	0
3	I	39	0	34	2	0
4	F	28	0	25	0	0
4	J	28	0	25	0	0
5	A	8	0	0	0	0
5	B	8	0	0	1	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	2	0	0	1	0
9	A	3	0	0	0	0
10	A	43	0	30	7	0
10	B	43	0	30	8	0
11	B	4	0	5	1	0
12	A	180	0	0	14	0
12	B	200	0	0	15	0
All	All	10299	0	9611	292	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 15.

All (292) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:LEU:HB2	1:A:13:VAL:HG23	1.21	1.19
1:A:8:ALA:HB1	1:A:9:PRO:HD2	1.36	1.08
1:B:12:LEU:HB2	1:B:13:VAL:HG23	1.13	1.08
1:B:258:GLU:OE2	10:B:821:HEM:HMB3	1.54	1.06
1:A:13:VAL:HG12	1:A:14:THR:H	1.16	1.05
1:B:13:VAL:HG12	1:B:14:THR:H	1.16	1.05
1:B:175:LEU:HD12	1:B:176:ALA:H	1.17	1.05
1:A:258:GLU:OE2	10:A:801:HEM:HMB3	1.54	1.04
1:B:487:PRO:HA	1:B:490:ILE:HD13	1.37	1.02
1:B:8:ALA:HB1	1:B:9:PRO:HD2	1.41	0.99
1:A:167:CYS:HB2	1:A:168:PRO:HD3	1.43	0.97
1:B:12:LEU:HB2	1:B:13:VAL:CG2	1.97	0.95
1:A:108:ASP:OD2	10:A:801:HEM:HMD3	1.66	0.94
1:B:175:LEU:CD1	1:B:176:ALA:H	1.82	0.93
1:A:12:LEU:HB2	1:A:13:VAL:CG2	1.99	0.92
1:B:167:CYS:HB2	1:B:168:PRO:HD3	1.51	0.92
1:B:13:VAL:CG1	1:B:14:THR:H	1.79	0.91
1:A:8:ALA:CB	1:A:9:PRO:HD2	2.01	0.90
1:B:108:ASP:OD2	10:B:821:HEM:HMD3	1.71	0.89
1:A:109:HIS:NE2	8:A:901:CYN:C	2.37	0.87
1:A:13:VAL:CG1	1:A:14:THR:H	1.81	0.87
1:A:230:ASN:HD21	1:A:232:VAL:HG12	1.42	0.84
1:A:134:VAL:HG12	12:A:951:HOH:O	1.78	0.83
1:A:230:ASN:ND2	1:A:232:VAL:HG12	1.93	0.83
1:B:8:ALA:CB	1:B:9:PRO:HD2	2.08	0.82
1:B:487:PRO:HA	1:B:490:ILE:CD1	2.11	0.81
1:B:52:GLU:HB3	1:B:57:VAL:HG12	1.61	0.80
1:A:13:VAL:HG12	1:A:14:THR:N	1.97	0.80
1:B:381:PHE:CZ	1:B:424:PRO:HG3	2.16	0.80
1:B:13:VAL:HG12	1:B:14:THR:N	1.95	0.80
1:A:169:THR:H	1:A:170:PRO:CD	1.96	0.77
1:A:123:GLU:HG3	1:A:125:SER:H	1.50	0.77
1:B:2:TRP:HB3	1:B:175:LEU:HD23	1.66	0.77
1:A:8:ALA:HB1	1:A:9:PRO:CD	2.15	0.75
1:B:2:TRP:HZ3	1:B:174:SER:HB3	1.53	0.74
12:A:945:HOH:O	2:D:3:MAN:H4	1.88	0.74
1:B:12:LEU:CB	1:B:13:VAL:HG23	2.06	0.74
1:A:253:ASP:OD2	1:A:255:ARG:HD3	1.87	0.73
1:B:169:THR:H	1:B:170:PRO:CD	2.01	0.73
1:A:2:TRP:HZ3	1:A:174:SER:HB3	1.53	0.73
1:A:260:ILE:HD12	1:A:395:LEU:HD13	1.70	0.73
1:B:2:TRP:CB	1:B:175:LEU:HD23	2.19	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:ARG:CZ	1:B:250:GLN:HE22	2.01	0.73
1:B:109:HIS:NE2	11:B:921:OSM:S	2.62	0.72
1:A:260:ILE:HD11	1:A:386:ILE:HG12	1.69	0.72
1:A:2:TRP:CB	1:A:175:LEU:HD12	2.19	0.72
1:A:230:ASN:HD21	1:A:232:VAL:CG1	2.02	0.71
1:A:63:GLN:O	1:A:71:ARG:NH2	2.23	0.71
1:A:124:HIS:HB2	1:B:137:ASP:CG	2.12	0.70
12:B:999:HOH:O	3:H:3:BMA:H4	1.91	0.70
1:A:2:TRP:HB2	1:A:175:LEU:CD1	2.22	0.69
1:B:432:ASP:O	1:B:436:ILE:HG12	1.91	0.69
1:B:56:ALA:HB1	1:B:177:ARG:HD3	1.75	0.69
1:B:8:ALA:HB1	1:B:9:PRO:CD	2.20	0.68
1:B:169:THR:H	1:B:170:PRO:HD2	1.57	0.68
1:B:173:GLN:HG2	12:B:986:HOH:O	1.92	0.68
3:I:2:NAG:H62	3:I:3:BMA:O2	1.94	0.67
1:A:124:HIS:HD2	1:A:127:VAL:HG21	1.59	0.67
1:A:260:ILE:CD1	1:A:395:LEU:HD13	2.25	0.66
1:A:169:THR:H	1:A:170:PRO:HD2	1.60	0.66
1:B:95:ASN:ND2	1:B:95:ASN:O	2.28	0.66
1:B:487:PRO:CA	1:B:490:ILE:HD13	2.22	0.66
1:B:10:VAL:HG11	1:B:41:ARG:CZ	2.26	0.65
10:A:801:HEM:HMB1	10:A:801:HEM:HBB2	1.76	0.65
1:B:407:MET:HB3	1:B:501:MET:CE	2.26	0.65
1:B:123:GLU:HG3	1:B:125:SER:H	1.59	0.65
3:H:2:NAG:H61	3:H:3:BMA:O2	1.97	0.65
1:A:2:TRP:HB3	1:A:175:LEU:HD12	1.77	0.65
1:A:106:ILE:HD11	1:A:265:VAL:HG11	1.79	0.64
1:A:300:LEU:O	1:A:303:PHE:HB3	1.97	0.64
1:A:260:ILE:HD13	1:A:260:ILE:O	1.98	0.64
1:A:465:LYS:HD2	1:A:468:GLN:NE2	2.13	0.64
1:B:8:ALA:C	1:B:10:VAL:H	2.01	0.64
1:B:246:VAL:HG11	1:B:387:ILE:HD13	1.80	0.64
1:B:108:ASP:CG	10:B:821:HEM:HMD3	2.18	0.63
1:B:407:MET:HB3	1:B:501:MET:HE3	1.80	0.63
1:A:82:ILE:HD11	1:A:483:LEU:HD12	1.79	0.62
1:A:260:ILE:HG23	1:A:261:LEU:HD13	1.80	0.62
10:A:801:HEM:HBC2	10:A:801:HEM:HMC2	1.82	0.61
1:A:360:ARG:NH2	1:A:389:ASP:OD2	2.33	0.61
1:A:407:MET:HB3	1:A:501:MET:CE	2.30	0.61
1:A:447:PRO:HD2	1:A:452:TRP:HE1	1.64	0.61
1:A:530:TRP:CE2	1:A:531:GLU:HG3	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:253:ASP:OD2	1:B:255:ARG:HD3	2.01	0.61
1:A:376:LEU:HD22	1:A:376:LEU:O	2.00	0.61
1:B:108:ASP:OD2	10:B:821:HEM:HMD2	2.00	0.61
12:A:1082:HOH:O	2:C:1:NAG:H3	2.00	0.61
1:B:134:VAL:HA	12:B:995:HOH:O	2.01	0.60
10:B:821:HEM:HMC1	10:B:821:HEM:HBC2	1.83	0.60
10:B:821:HEM:HMB1	10:B:821:HEM:HBB2	1.83	0.60
1:B:12:LEU:C	1:B:13:VAL:CG2	2.69	0.60
1:B:13:VAL:CG1	1:B:14:THR:N	2.56	0.60
1:B:175:LEU:HD12	1:B:176:ALA:N	2.02	0.60
1:A:106:ILE:HD11	1:A:265:VAL:CG1	2.32	0.59
1:A:260:ILE:CD1	1:A:395:LEU:CD1	2.81	0.59
1:B:230:ASN:CG	1:B:232:VAL:HG12	2.23	0.59
1:A:202:ARG:NH1	1:A:250:GLN:HE22	2.01	0.59
1:B:51:TYR:OH	1:B:177:ARG:HB3	2.03	0.59
1:B:227:PRO:HD2	12:B:949:HOH:O	2.02	0.59
1:A:2:TRP:HB2	1:A:175:LEU:HD12	1.85	0.58
1:B:568:GLN:HB3	2:G:1:NAG:C5	2.33	0.58
1:B:503:GLU:HG2	1:B:504:ARG:HG3	1.85	0.58
1:B:212:LEU:HB2	12:B:958:HOH:O	2.03	0.57
1:A:108:ASP:CG	10:A:801:HEM:HMD3	2.24	0.57
1:A:106:ILE:CD1	1:A:265:VAL:HG11	2.35	0.56
1:A:128:GLN:NE2	1:B:170:PRO:HB3	2.20	0.56
1:A:274:ASN:O	1:A:278:ARG:HG2	2.06	0.56
1:B:551:ARG:HD3	1:B:583:ASP:O	2.04	0.56
1:A:8:ALA:C	1:A:10:VAL:H	2.08	0.56
1:A:167:CYS:HB2	1:A:168:PRO:CD	2.28	0.56
1:B:168:PRO:HB2	1:B:170:PRO:HD2	1.87	0.56
1:B:202:ARG:CZ	1:B:250:GLN:NE2	2.68	0.56
1:A:8:ALA:CB	1:A:9:PRO:CD	2.80	0.56
1:A:106:ILE:HG23	1:A:191:LEU:HD11	1.86	0.56
1:A:169:THR:N	1:A:170:PRO:CD	2.66	0.56
1:A:2:TRP:HZ3	1:A:174:SER:CB	2.19	0.56
1:B:8:ALA:O	1:B:10:VAL:N	2.39	0.55
1:B:249:PHE:CE2	12:B:949:HOH:O	2.60	0.55
1:B:11:PRO:HB2	1:B:12:LEU:HD12	1.88	0.55
1:A:13:VAL:CG1	1:A:14:THR:N	2.59	0.55
1:B:2:TRP:CZ3	1:B:174:SER:HB3	2.38	0.55
1:B:2:TRP:HZ3	1:B:174:SER:CB	2.19	0.55
1:A:476:LEU:HD21	1:A:498:ALA:HB1	1.89	0.54
1:B:169:THR:N	1:B:170:PRO:CD	2.69	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:568:GLN:OE1	2:G:1:NAG:H5	2.08	0.54
1:A:285:PRO:HB3	12:A:1025:HOH:O	2.07	0.54
1:B:10:VAL:HG11	1:B:41:ARG:NH2	2.23	0.54
1:A:544:LEU:O	1:A:547:VAL:HG22	2.08	0.53
1:A:260:ILE:HD12	1:A:395:LEU:CD1	2.35	0.53
1:A:381:PHE:CZ	1:A:424:PRO:HG3	2.42	0.53
1:A:12:LEU:HD11	1:A:197:PRO:HG2	1.91	0.53
1:B:383:THR:O	1:B:387:ILE:HD12	2.09	0.53
2:D:2:NAG:H61	2:D:3:MAN:H2	1.91	0.53
1:A:529:TRP:CD1	1:A:531:GLU:HB2	2.44	0.53
1:B:302:ALA:O	1:B:306:ILE:HG13	2.08	0.53
1:B:15:CYS:C	1:B:17:GLU:H	2.13	0.52
1:B:13:VAL:HB	12:B:1084:HOH:O	2.10	0.52
1:B:16:ASP:O	1:B:18:GLN:N	2.40	0.52
1:B:230:ASN:ND2	1:B:232:VAL:HG12	2.25	0.52
1:B:213:MET:HG2	1:B:273:HIS:CD2	2.45	0.52
1:B:300:LEU:O	1:B:303:PHE:HB3	2.10	0.52
1:A:10:VAL:HG11	1:A:41:ARG:CZ	2.40	0.51
1:B:78:VAL:HG13	1:B:82:ILE:HD12	1.92	0.51
1:B:301:GLY:O	1:B:305:GLN:HG3	2.10	0.51
1:A:118:GLU:HA	12:A:932:HOH:O	2.10	0.51
1:A:12:LEU:C	1:A:13:VAL:CG2	2.79	0.51
1:A:348:ARG:HH11	1:A:437:ASN:ND2	2.09	0.51
1:B:166:VAL:O	1:B:167:CYS:C	2.48	0.51
1:A:260:ILE:HD11	1:A:386:ILE:CG1	2.39	0.51
1:B:84:GLY:HA2	12:B:963:HOH:O	2.11	0.50
1:A:187:LEU:HD13	1:A:305:GLN:HA	1.93	0.50
1:A:272:GLU:HA	1:A:272:GLU:OE1	2.11	0.50
1:B:568:GLN:HB3	2:G:1:NAG:C6	2.42	0.50
12:B:971:HOH:O	3:H:3:BMA:H62	2.11	0.50
1:A:396:VAL:HB	1:A:559:ILE:HD11	1.92	0.50
1:B:169:THR:HB	12:B:926:HOH:O	2.10	0.49
1:B:249:PHE:CZ	12:B:949:HOH:O	2.54	0.49
1:B:588:SER:OG	1:B:589:PRO:HD3	2.13	0.49
1:A:333:ASN:C	1:A:333:ASN:HD22	2.15	0.49
1:B:436:ILE:HD13	1:B:436:ILE:N	2.27	0.49
12:B:1101:HOH:O	3:I:3:BMA:H4	2.12	0.49
1:A:56:ALA:HB1	1:A:177:ARG:HD3	1.94	0.49
1:B:2:TRP:HB2	1:B:175:LEU:HD23	1.92	0.49
1:B:56:ALA:CB	1:B:177:ARG:HD3	2.42	0.49
1:A:124:HIS:HD2	1:A:127:VAL:CG2	2.25	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:490:ILE:HD12	1:B:490:ILE:H	1.77	0.49
1:B:246:VAL:CG1	1:B:387:ILE:HD13	2.43	0.49
1:B:393:ASP:HB2	1:B:394:PRO:HD3	1.95	0.49
1:B:588:SER:N	1:B:589:PRO:CD	2.76	0.48
1:A:260:ILE:HD11	1:A:395:LEU:CD1	2.43	0.48
1:A:168:PRO:HB2	1:A:170:PRO:HD2	1.96	0.48
1:B:52:GLU:OE1	1:B:57:VAL:HG11	2.14	0.48
1:B:360:ARG:NH1	1:B:372:ALA:HA	2.28	0.48
1:B:594:GLU:H	1:B:594:GLU:CD	2.15	0.48
1:A:8:ALA:O	1:A:10:VAL:N	2.46	0.48
1:A:328:TYR:CD1	1:A:523:ARG:HD3	2.48	0.48
1:B:370:PRO:HG2	1:B:371:GLU:HG3	1.95	0.48
1:B:108:ASP:OD1	10:B:821:HEM:HMD3	2.13	0.48
1:A:8:ALA:O	1:A:10:VAL:HG23	2.13	0.48
1:B:360:ARG:NH2	1:B:389:ASP:OD2	2.47	0.48
1:A:2:TRP:HB2	1:A:175:LEU:HD11	1.96	0.47
1:B:298:LYS:HG2	1:B:536:PHE:CZ	2.50	0.47
1:B:328:TYR:CD1	1:B:523:ARG:HD3	2.49	0.47
1:A:258:GLU:CD	10:A:801:HEM:HMB3	2.29	0.47
1:A:392:ILE:O	1:A:396:VAL:HG23	2.14	0.47
1:A:25:THR:O	1:A:184:THR:HG22	2.13	0.47
1:B:12:LEU:C	1:B:13:VAL:HG22	2.35	0.47
1:B:335:VAL:O	1:B:337:PRO:HD3	2.15	0.47
1:B:523:ARG:HD2	1:B:524:ASP:OD1	2.15	0.47
1:A:588:SER:OG	1:A:589:PRO:HD3	2.15	0.47
1:B:8:ALA:O	1:B:10:VAL:HG23	2.15	0.47
1:A:180:ILE:HG22	1:A:181:ASN:N	2.30	0.47
1:A:349:PHE:HA	1:A:497:ASN:HD21	1.79	0.47
1:B:142:ILE:HD12	1:B:160:PHE:HB2	1.97	0.47
1:B:328:TYR:HD1	1:B:523:ARG:HD3	1.80	0.47
1:A:212:LEU:HB2	12:A:937:HOH:O	2.15	0.47
1:B:2:TRP:HB2	1:B:175:LEU:CD2	2.45	0.47
1:B:120:GLY:HA2	1:B:123:GLU:HB2	1.96	0.47
1:A:299:ILE:O	1:A:302:ALA:HB3	2.15	0.46
1:B:3:GLU:C	1:B:5:GLY:H	2.18	0.46
1:B:8:ALA:CB	1:B:9:PRO:CD	2.86	0.46
10:A:801:HEM:HBC2	10:A:801:HEM:CMC	2.45	0.46
1:B:432:ASP:HB3	1:B:435:ALA:HB3	1.98	0.46
1:A:360:ARG:NH1	1:A:372:ALA:HA	2.31	0.46
1:A:400:LEU:HD11	1:A:553:ILE:HD13	1.97	0.46
1:A:517:ARG:O	1:A:521:GLN:HG3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:GLU:C	1:A:5:GLY:H	2.20	0.46
1:B:42:ALA:HB2	1:B:166:VAL:HG11	1.98	0.46
1:A:2:TRP:CZ3	1:A:174:SER:HB3	2.40	0.46
1:B:511:LEU:HD12	1:B:511:LEU:HA	1.77	0.46
1:B:568:GLN:HB3	2:G:1:NAG:H5	1.98	0.45
1:A:407:MET:HB3	1:A:501:MET:HE3	1.97	0.45
1:A:551:ARG:NH2	1:A:555:ASP:OD1	2.45	0.45
1:A:594:GLU:HG2	12:A:931:HOH:O	2.15	0.45
1:A:10:VAL:CG1	1:A:41:ARG:CZ	2.94	0.45
1:B:529:TRP:CD1	1:B:531:GLU:HB2	2.52	0.45
1:B:111:LEU:O	1:B:339:ILE:HD13	2.16	0.45
1:A:167:CYS:N	12:A:1000:HOH:O	2.50	0.45
1:B:106:ILE:HG22	1:B:107:VAL:N	2.31	0.45
1:A:325:ILE:HG22	1:A:325:ILE:O	2.17	0.45
1:A:502:VAL:HG13	1:A:508:GLY:HA2	1.99	0.45
1:B:360:ARG:NH1	1:B:371:GLU:O	2.48	0.45
1:A:200:ALA:O	1:A:204:ARG:HG3	2.16	0.44
1:A:593:ARG:NH2	12:A:1011:HOH:O	2.50	0.44
10:B:821:HEM:HBB2	10:B:821:HEM:CMB	2.47	0.44
1:A:67:ARG:NH1	12:A:966:HOH:O	2.43	0.44
1:A:393:ASP:HB2	1:A:394:PRO:HD3	1.99	0.44
1:A:447:PRO:HD2	1:A:452:TRP:NE1	2.30	0.44
1:B:127:VAL:CG1	1:B:131:GLU:HG3	2.48	0.44
1:B:490:ILE:HD12	1:B:490:ILE:N	2.32	0.44
1:A:123:GLU:HG2	1:A:125:SER:HB3	2.00	0.44
1:A:511:LEU:HA	1:A:511:LEU:HD12	1.66	0.44
1:B:8:ALA:C	1:B:10:VAL:N	2.70	0.44
1:B:117:THR:HG23	1:B:162:ARG:O	2.18	0.44
1:A:64:ARG:H	1:A:64:ARG:HG3	1.68	0.43
1:B:288:ASP:O	1:B:292:LEU:HD22	2.18	0.43
1:B:221:ASP:HB2	1:B:226:TYR:CZ	2.54	0.43
1:B:530:TRP:CE2	1:B:531:GLU:HG3	2.53	0.43
1:B:538:GLU:HG2	1:B:541:ARG:NH2	2.33	0.43
1:B:99:LEU:HD23	1:B:566:ALA:O	2.18	0.43
1:B:170:PRO:HB3	1:B:171:PRO:HD2	2.00	0.43
3:H:2:NAG:H61	3:H:3:BMA:C2	2.49	0.43
1:A:12:LEU:CB	1:A:13:VAL:HG23	2.16	0.43
1:A:260:ILE:HD11	1:A:395:LEU:HD11	2.01	0.43
1:B:168:PRO:HB2	1:B:169:THR:H	1.53	0.43
1:B:551:ARG:O	1:B:552:LEU:C	2.56	0.43
1:B:230:ASN:ND2	1:B:232:VAL:CG1	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:ARG:HG3	12:A:1013:HOH:O	2.19	0.42
1:B:172:TYR:O	1:B:173:GLN:HG3	2.19	0.42
1:B:189:ALA:HB2	1:B:304:ILE:HD12	2.01	0.42
1:B:345:PHE:HA	1:B:348:ARG:HG3	2.01	0.42
1:B:83:VAL:O	1:B:83:VAL:HG12	2.20	0.42
1:A:146:LYS:O	1:A:147:ASN:HB2	2.20	0.42
1:B:175:LEU:CD1	1:B:176:ALA:N	2.66	0.42
1:B:185:SER:HA	1:B:339:ILE:CD1	2.50	0.42
1:B:452:TRP:CD1	1:B:492:ILE:HG13	2.55	0.42
1:B:63:GLN:O	1:B:71:ARG:NH2	2.52	0.42
1:B:74:LEU:HD12	1:B:145:PRO:HB3	2.01	0.42
1:B:95:ASN:HB3	12:B:996:HOH:O	2.20	0.42
1:B:140:PHE:O	1:B:160:PHE:HB3	2.20	0.42
1:B:127:VAL:HG13	1:B:131:GLU:HG3	2.00	0.42
1:B:154:GLN:HE21	1:B:154:GLN:HB3	1.56	0.42
1:B:298:LYS:NZ	1:B:535:VAL:O	2.34	0.42
1:A:506:ARG:HD2	12:A:1020:HOH:O	2.20	0.41
1:B:187:LEU:HD13	1:B:305:GLN:HA	2.02	0.41
1:A:291:MET:HE1	12:A:984:HOH:O	2.21	0.41
1:B:342:VAL:HG12	5:B:608:NO3:O1	2.20	0.41
1:B:490:ILE:CD1	1:B:490:ILE:H	2.33	0.41
1:A:419:ASN:O	1:A:430:GLY:HA2	2.21	0.41
1:A:588:SER:N	1:A:589:PRO:CD	2.84	0.41
1:A:36:LEU:HG	1:A:337:PRO:HD2	2.02	0.41
1:A:287:TRP:CZ3	1:A:295:GLU:HG3	2.56	0.41
1:A:343:PHE:O	1:A:345:PHE:N	2.53	0.41
1:B:447:PRO:HD2	1:B:452:TRP:HE1	1.85	0.41
1:A:41:ARG:NH1	12:A:1005:HOH:O	2.49	0.41
1:A:318:GLY:C	1:A:320:GLU:H	2.23	0.41
1:B:2:TRP:HZ3	1:B:174:SER:HG	1.68	0.41
1:B:95:ASN:OD1	12:B:977:HOH:O	2.22	0.41
1:A:172:TYR:O	1:A:173:GLN:HG3	2.21	0.40
1:A:318:GLY:C	1:A:320:GLU:N	2.74	0.40
1:B:407:MET:SD	1:B:408:ASN:N	2.94	0.40
1:B:36:LEU:HD12	1:B:36:LEU:HA	1.87	0.40
1:B:419:ASN:O	1:B:430:GLY:HA2	2.22	0.40
1:B:523:ARG:CD	1:B:524:ASP:OD1	2.69	0.40
1:A:261:LEU:HD12	1:A:261:LEU:HA	1.90	0.40
1:B:25:THR:O	1:B:184:THR:HG22	2.21	0.40
1:B:376:LEU:O	1:B:376:LEU:HD22	2.20	0.40
1:A:351:HIS:CE1	1:A:433:LEU:HD21	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:PRO:HB2	1:A:169:THR:H	1.61	0.40
1:A:313:LEU:N	1:A:314:PRO:CD	2.84	0.40
1:B:200:ALA:O	1:B:204:ARG:HG3	2.21	0.40
1:B:275:ARG:NH1	12:B:1045:HOH:O	2.53	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	593/595 (100%)	538 (91%)	40 (7%)	15 (2%)	5	28
1	B	593/595 (100%)	541 (91%)	42 (7%)	10 (2%)	9	36
All	All	1186/1190 (100%)	1079 (91%)	82 (7%)	25 (2%)	7	32

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	9	PRO
1	A	12	LEU
1	A	169	THR
1	A	171	PRO
1	B	9	PRO
1	B	12	LEU
1	B	17	GLU
1	B	168	PRO
1	B	169	THR
1	B	174	SER
1	A	168	PRO
1	B	171	PRO
1	A	3	GLU
1	A	174	SER

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Mol	Chain	Res	Type
1	B	3	GLU
1	A	17	GLU
1	A	54	GLY
1	A	56	ALA
1	B	187	LEU
1	A	166	VAL
1	A	173	GLN
1	A	319	SER
1	B	166	VAL
1	A	11	PRO
1	A	4	VAL

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%)	477 (92%)	40 (8%)	13	38
1	B	517/517 (100%)	479 (93%)	38 (7%)	13	40
All	All	1034/1034 (100%)	956 (92%)	78 (8%)	13	39

All (78) 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	64	ARG
1	A	71	ARG
1	A	91	VAL
1	A	98	LEU
1	A	122	SER
1	A	124	HIS

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Mol	Chain	Res	Type
1	A	130	GLU
1	A	137	ASP
1	A	153	THR
1	A	166	VAL
1	A	169	THR
1	A	187	LEU
1	A	202	ARG
1	A	203	LEU
1	A	218	GLU
1	A	226	TYR
1	A	260	ILE
1	A	261	LEU
1	A	268	LEU
1	A	276	LEU
1	A	292	LEU
1	A	317	LEU
1	A	322	GLN
1	A	333	ASN
1	A	347	PHE
1	A	360	ARG
1	A	376	LEU
1	A	451	SER
1	A	480	LEU
1	A	494	ILE
1	A	511	LEU
1	A	523	ARG
1	A	542	ASP
1	A	564	LEU
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	98	LEU
1	B	124	HIS
1	B	128	GLN
1	B	130	GLU
1	B	131	GLU
1	B	137	ASP
1	B	153	THR
1	B	169	THR

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Mol	Chain	Res	Type
1	B	175	LEU
1	B	177	ARG
1	B	187	LEU
1	B	202	ARG
1	B	203	LEU
1	B	261	LEU
1	B	268	LEU
1	B	276	LEU
1	B	291	MET
1	B	292	LEU
1	B	317	LEU
1	B	333	ASN
1	B	347	PHE
1	B	360	ARG
1	B	376	LEU
1	B	428	VAL
1	B	464	LEU
1	B	480	LEU
1	B	492	ILE
1	B	511	LEU
1	B	520	GLN
1	B	538	GLU
1	B	542	ASP
1	B	564	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	124	HIS
1	A	128	GLN
1	A	147	ASN
1	A	217	GLN
1	A	222	HIS
1	A	230	ASN
1	A	250	GLN
1	A	333	ASN
1	A	341	ASN
1	A	364	ASN
1	A	408	ASN
1	A	437	ASN
1	A	468	GLN
1	A	497	ASN

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Mol	Chain	Res	Type
1	A	520	GLN
1	A	545	GLN
1	A	558	HIS
1	A	571	ASN
1	B	250	GLN
1	B	333	ASN
1	B	341	ASN
1	B	366	GLN
1	B	408	ASN
1	B	437	ASN
1	B	468	GLN
1	B	497	ASN
1	B	521	GLN
1	B	571	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

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	2,1	14,14,15	0.62	0	17,19,21	0.79	0
2	NAG	C	2	2	14,14,15	0.69	0	17,19,21	1.39	3 (17%)
2	MAN	C	3	2	11,11,12	0.50	0	15,15,17	1.43	1 (6%)
2	NAG	D	1	2,1	14,14,15	0.70	1 (7%)	17,19,21	1.04	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAG	D	2	2	14,14,15	0.81	0	17,19,21	1.29	2 (11%)
2	MAN	D	3	2	11,11,12	0.60	0	15,15,17	0.74	0
3	NAG	E	1	3,1	14,14,15	0.68	0	17,19,21	1.21	1 (5%)
3	NAG	E	2	3	14,14,15	0.56	0	17,19,21	1.56	2 (11%)
3	BMA	E	3	3	11,11,12	0.75	0	15,15,17	1.61	3 (20%)
4	NAG	F	1	4,1	14,14,15	0.62	0	17,19,21	1.61	3 (17%)
4	NAG	F	2	4	14,14,15	0.68	0	17,19,21	1.56	1 (5%)
2	NAG	G	1	2,1	14,14,15	0.76	0	17,19,21	1.74	6 (35%)
2	NAG	G	2	2	14,14,15	0.64	0	17,19,21	2.60	2 (11%)
2	MAN	G	3	2	11,11,12	0.90	0	15,15,17	1.95	3 (20%)
3	NAG	H	1	3,1	14,14,15	0.51	0	17,19,21	1.00	0
3	NAG	H	2	3	14,14,15	0.75	0	17,19,21	1.50	2 (11%)
3	BMA	H	3	3	11,11,12	0.74	0	15,15,17	2.32	4 (26%)
3	NAG	I	1	3,1	14,14,15	0.73	0	17,19,21	1.46	2 (11%)
3	NAG	I	2	3	14,14,15	0.73	0	17,19,21	1.38	2 (11%)
3	BMA	I	3	3	11,11,12	0.68	0	15,15,17	1.69	2 (13%)
4	NAG	J	1	4,1	14,14,15	0.64	0	17,19,21	1.65	4 (23%)
4	NAG	J	2	4	14,14,15	0.71	0	17,19,21	0.98	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	2,1	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
2	MAN	C	3	2	-	2/2/19/22	1/1/1/1
2	NAG	D	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	4/6/23/26	0/1/1/1
2	MAN	D	3	2	-	1/2/19/22	1/1/1/1
3	NAG	E	1	3,1	-	3/6/23/26	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
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	2,1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	G	2	2	-	2/6/23/26	0/1/1/1
2	MAN	G	3	2	-	1/2/19/22	1/1/1/1
3	NAG	H	1	3,1	-	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	3,1	-	2/6/23/26	0/1/1/1
3	NAG	I	2	3	-	3/6/23/26	0/1/1/1
3	BMA	I	3	3	-	1/2/19/22	1/1/1/1
4	NAG	J	1	4,1	-	2/6/23/26	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	D	1	NAG	C1-C2	2.16	1.55	1.52

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	2	NAG	C1-O5-C5	8.42	123.60	112.19
3	H	3	BMA	C1-O5-C5	7.03	121.72	112.19
2	G	3	MAN	C1-O5-C5	5.27	119.33	112.19
3	I	3	BMA	C1-O5-C5	5.12	119.13	112.19
4	F	1	NAG	C4-C3-C2	4.85	118.13	111.02
4	F	2	NAG	C4-C3-C2	4.72	117.93	111.02
2	C	3	MAN	C1-O5-C5	4.66	118.50	112.19
4	J	1	NAG	C4-C3-C2	4.64	117.81	111.02
3	H	2	NAG	C4-C3-C2	4.45	117.54	111.02
3	E	2	NAG	C1-O5-C5	4.43	118.19	112.19
3	E	3	BMA	C1-O5-C5	4.30	118.01	112.19
2	G	2	NAG	O5-C1-C2	4.08	117.74	111.29
3	I	2	NAG	C1-O5-C5	3.96	117.56	112.19
2	D	2	NAG	C4-C3-C2	3.74	116.50	111.02
2	G	1	NAG	C4-C3-C2	3.54	116.20	111.02
2	C	2	NAG	C4-C3-C2	3.35	115.92	111.02
3	I	1	NAG	C1-O5-C5	3.31	116.68	112.19
2	G	3	MAN	C1-C2-C3	3.26	113.67	109.67
3	H	3	BMA	O5-C1-C2	3.21	115.73	110.77
3	I	3	BMA	O5-C5-C6	3.12	112.10	107.20
3	E	2	NAG	O5-C1-C2	-3.10	106.39	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	1	NAG	C6-C5-C4	3.05	120.16	113.00
3	E	1	NAG	C1-O5-C5	2.96	116.20	112.19
2	G	3	MAN	O5-C5-C6	2.95	111.83	107.20
3	I	1	NAG	C4-C3-C2	2.77	115.08	111.02
3	H	3	BMA	C1-C2-C3	2.75	113.05	109.67
4	J	1	NAG	C3-C4-C5	2.75	115.15	110.24
3	E	3	BMA	O5-C5-C6	2.75	111.51	107.20
2	C	2	NAG	C3-C4-C5	2.73	115.11	110.24
4	F	1	NAG	O5-C5-C6	2.56	111.22	107.20
2	G	1	NAG	O5-C5-C6	2.56	111.21	107.20
2	D	1	NAG	C1-O5-C5	2.53	115.61	112.19
3	H	3	BMA	O2-C2-C1	2.47	114.20	109.15
3	I	2	NAG	O5-C1-C2	-2.31	107.65	111.29
4	J	2	NAG	C4-C3-C2	2.28	114.36	111.02
2	D	2	NAG	O5-C1-C2	-2.22	107.78	111.29
2	G	1	NAG	O4-C4-C5	-2.19	103.86	109.30
4	J	1	NAG	O5-C5-C6	2.17	110.60	107.20
4	F	1	NAG	C3-C4-C5	2.16	114.10	110.24
4	J	1	NAG	O3-C3-C4	-2.15	105.37	110.35
2	G	1	NAG	O7-C7-C8	-2.04	118.27	122.06
3	H	2	NAG	C1-O5-C5	2.02	114.93	112.19
2	G	1	NAG	O5-C1-C2	-2.00	108.12	111.29
3	E	3	BMA	O2-C2-C1	2.00	113.25	109.15
2	C	2	NAG	C1-O5-C5	2.00	114.90	112.19

There are no chirality outliers.

All (39) torsion outliers are listed below:

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

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

All (5) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	3	MAN	C1-C2-C3-C4-C5-O5
2	D	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
2	C	3	MAN	C1-C2-C3-C4-C5-O5

8 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	3	MAN	2	0
3	H	2	NAG	2	0
3	I	3	BMA	2	0

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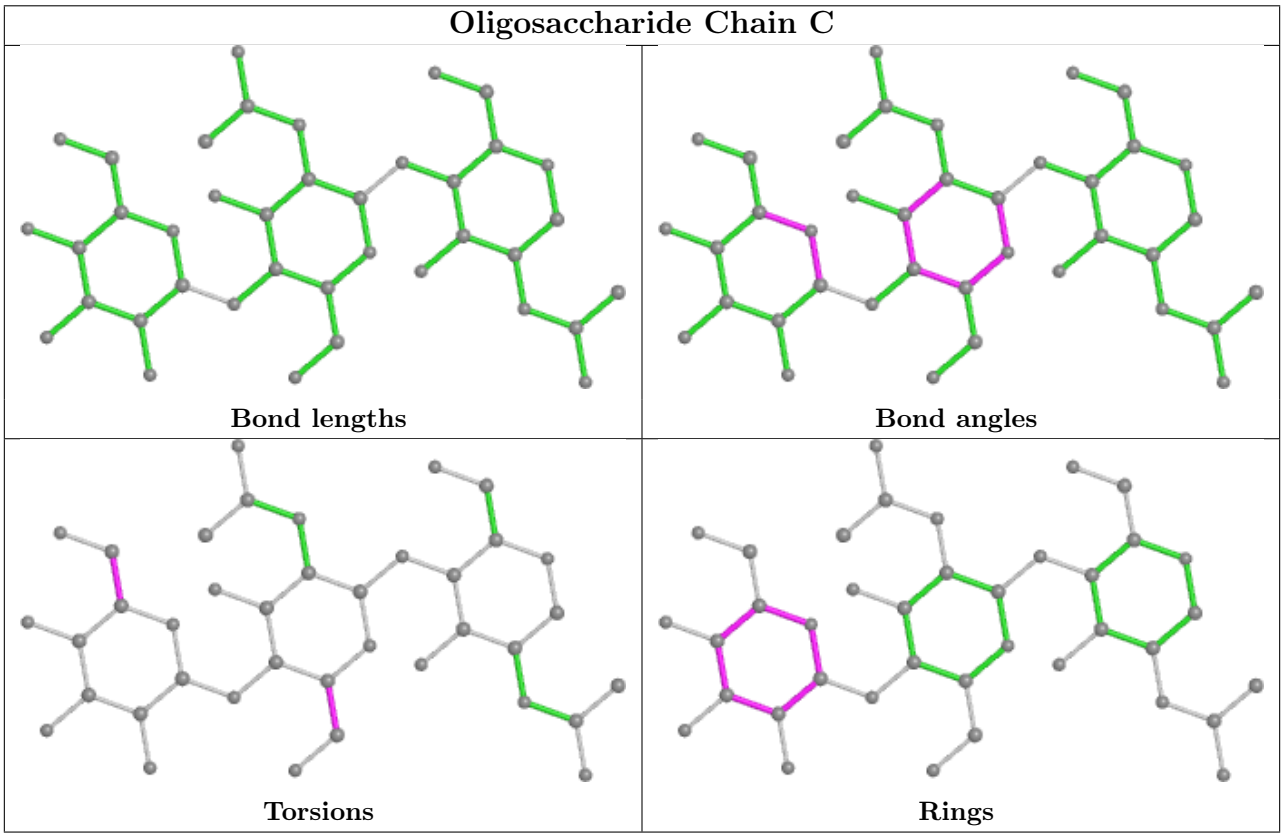
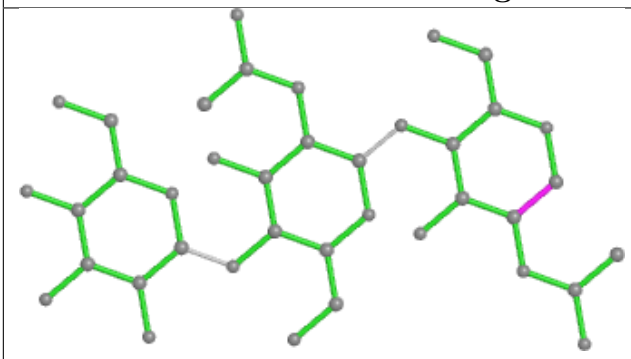
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	2	NAG	1	0
3	I	2	NAG	1	0
2	G	1	NAG	4	0
3	H	3	BMA	4	0
2	C	1	NAG	1	0

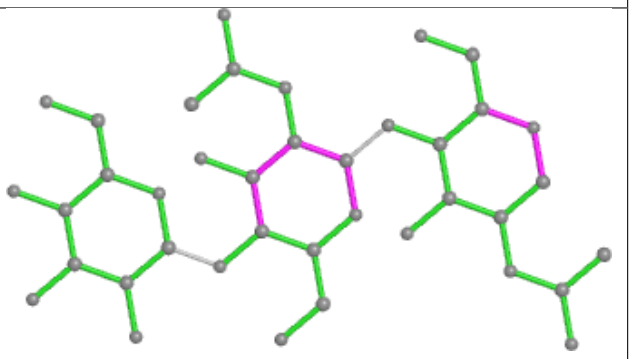
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



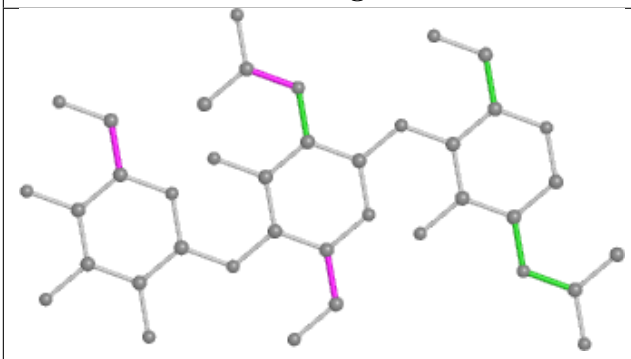
Oligosaccharide Chain D



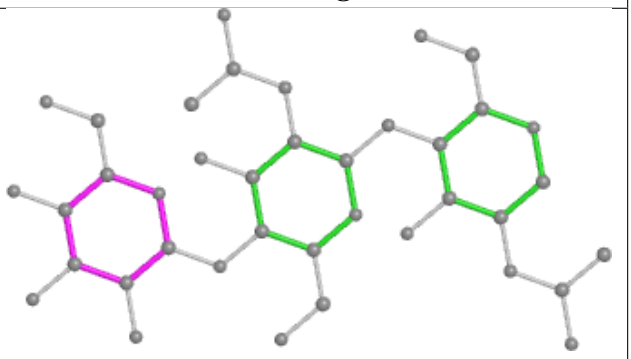
Bond lengths



Bond angles

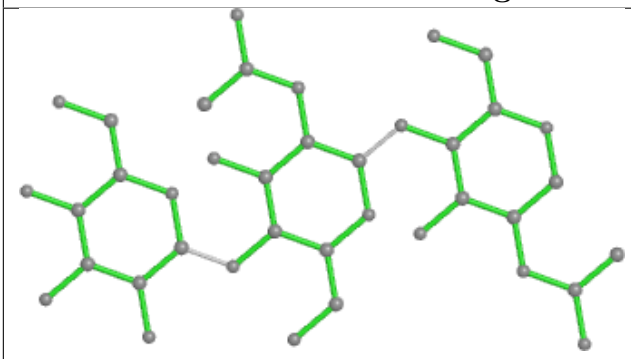


Torsions

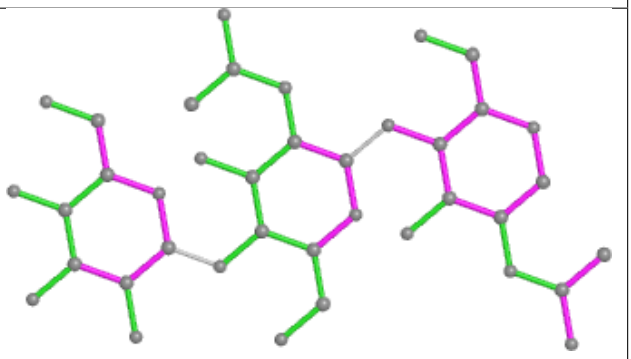


Rings

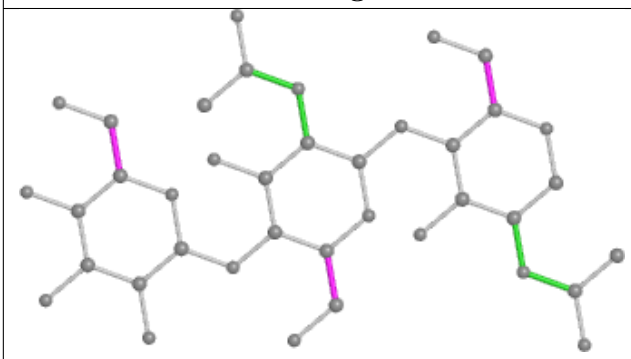
Oligosaccharide Chain G



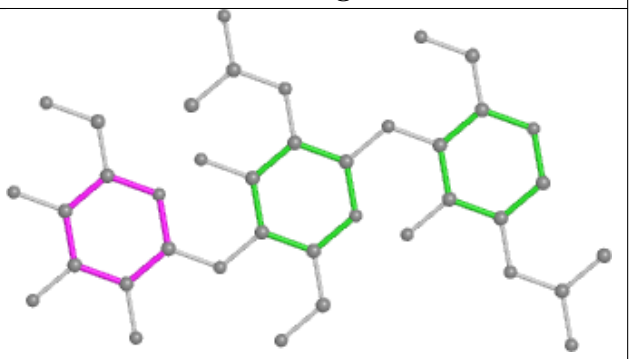
Bond lengths



Bond angles

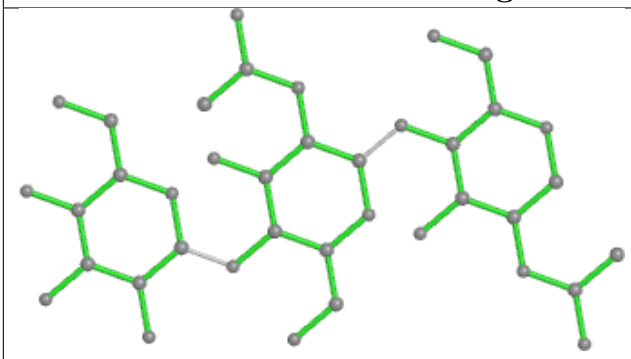


Torsions

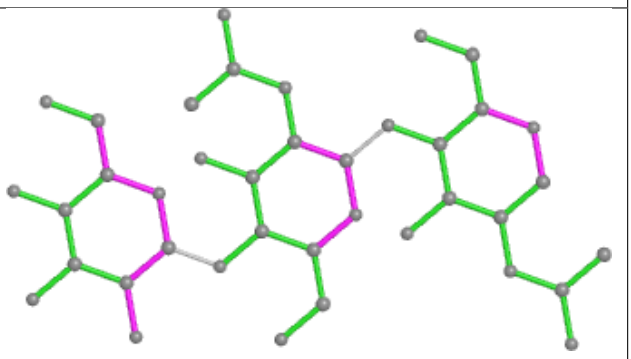


Rings

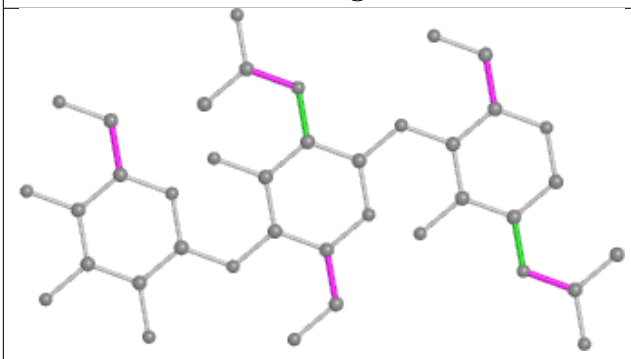
Oligosaccharide Chain E



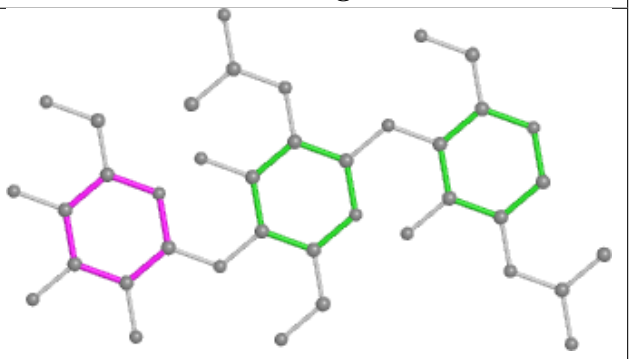
Bond lengths



Bond angles

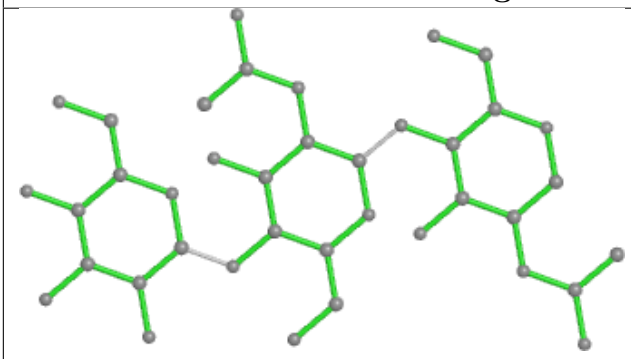


Torsions

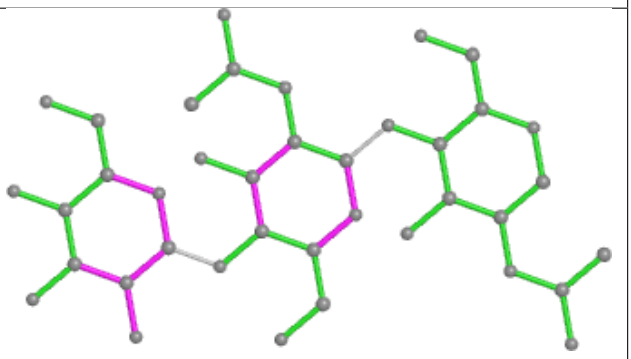


Rings

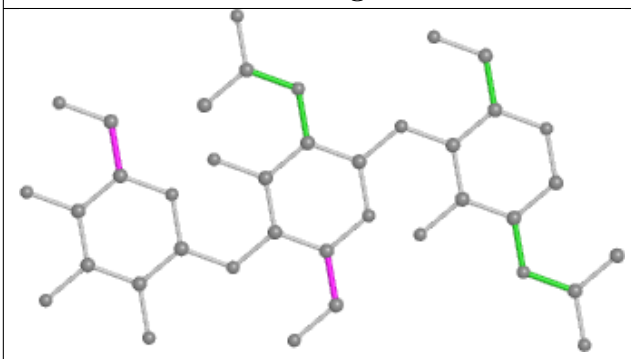
Oligosaccharide Chain H



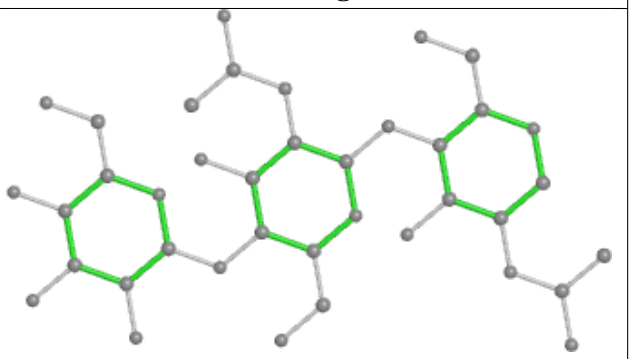
Bond lengths



Bond angles

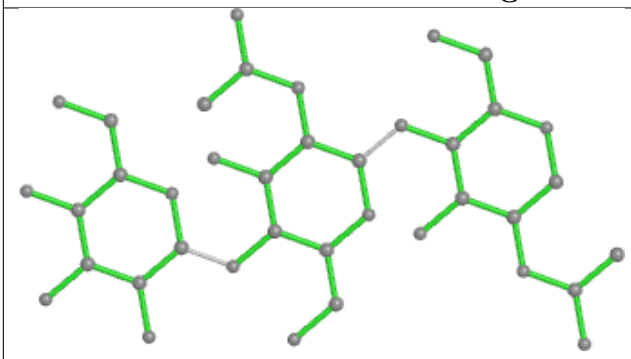


Torsions

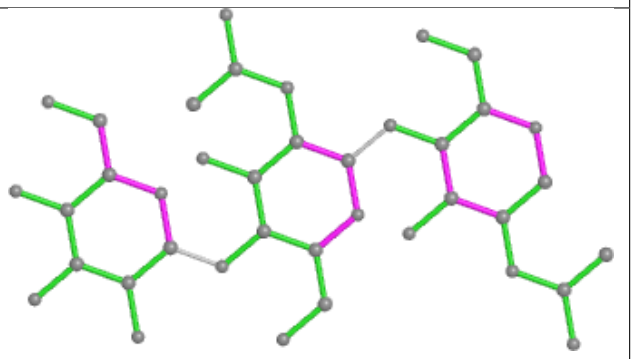


Rings

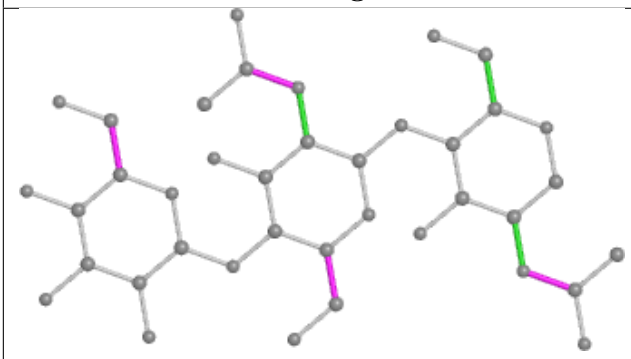
Oligosaccharide Chain I



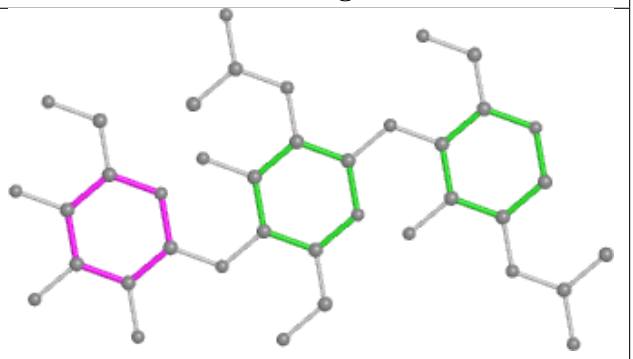
Bond lengths



Bond angles

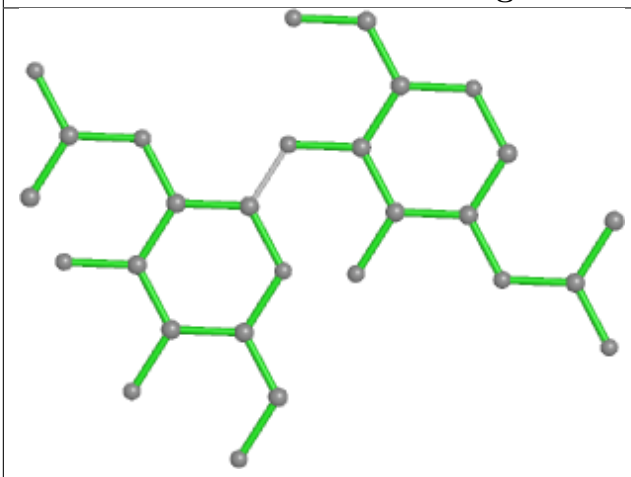


Torsions

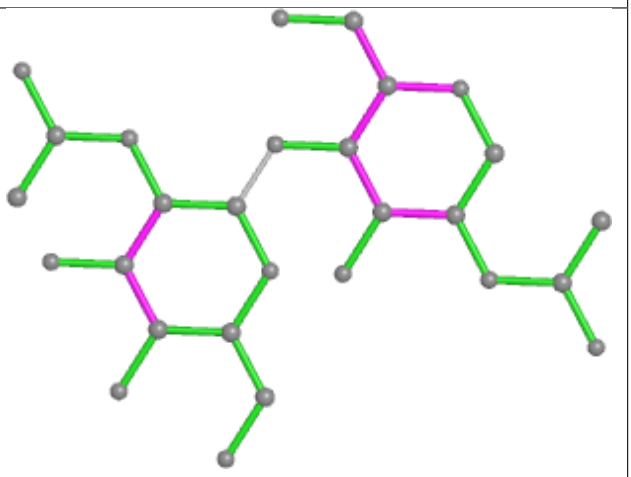


Rings

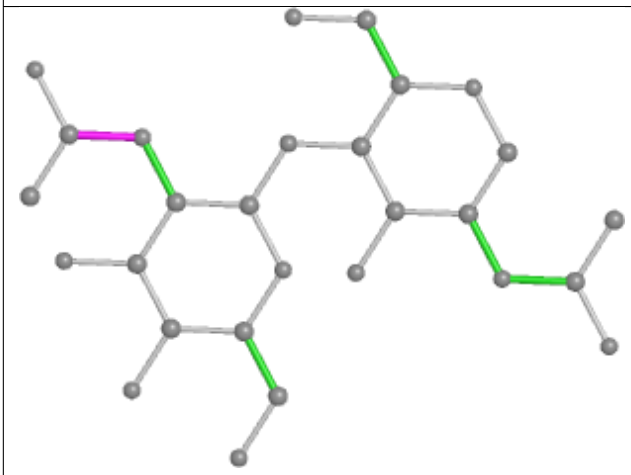
Oligosaccharide Chain F



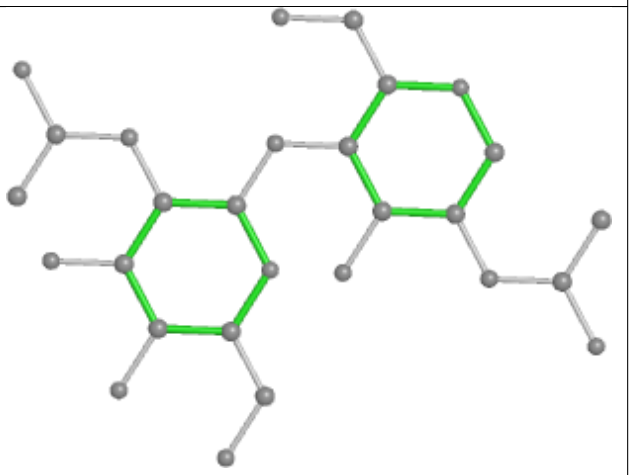
Bond lengths



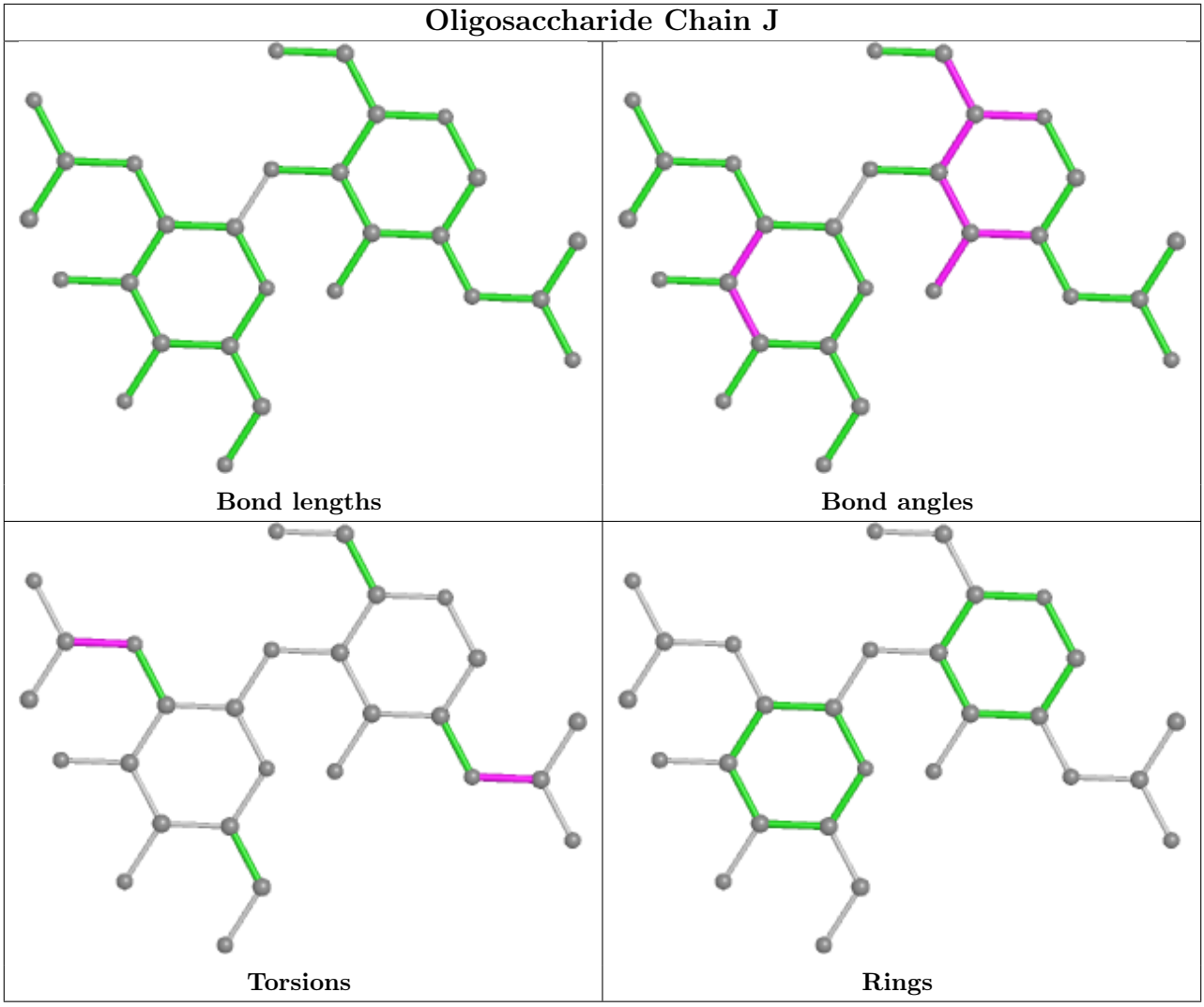
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

Of 13 ligands modelled in this entry, 2 are monoatomic - leaving 11 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	HEM	A	801	1,8	41,50,50	2.04	7 (17%)	45,82,82	2.05	13 (28%)
6	CO3	B	609	-	2,3,3	0.44	0	2,3,3	0.61	0
5	NO3	B	607	-	1,3,3	3.86	1 (100%)	0,3,3	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	CO3	A	609	-	2,3,3	0.42	0	2,3,3	0.44	0
5	NO3	A	607	-	1,3,3	3.86	1 (100%)	0,3,3	-	-
9	SCN	A	902	-	1,2,2	2.00	1 (100%)	0,1,1	-	-
8	CYN	A	901	10	0,1,1	-	-	-		
10	HEM	B	821	1,11	41,50,50	1.89	7 (17%)	45,82,82	2.08	15 (33%)
11	OSM	B	921	10	1,3,3	0.05	0	0,2,2	-	-
5	NO3	A	608	-	1,3,3	3.38	1 (100%)	0,3,3	-	-
5	NO3	B	608	-	1,3,3	3.21	1 (100%)	0,3,3	-	-

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	HEM	B	821	1,11	-	4/12/54/54	-
11	OSM	B	921	10	-	0/0/1/1	-
10	HEM	A	801	1,8	-	2/12/54/54	-

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	801	HEM	C3D-C2D	7.71	1.53	1.36
10	B	821	HEM	C3D-C2D	7.02	1.51	1.36
10	A	801	HEM	FE-NB	4.83	2.20	1.96
10	B	821	HEM	C3C-CAC	4.24	1.56	1.47
10	A	801	HEM	C3C-CAC	3.88	1.55	1.47
5	B	607	NO3	O1-N	3.86	1.41	1.24
5	A	607	NO3	O1-N	3.86	1.41	1.24
10	B	821	HEM	CAB-C3B	3.54	1.57	1.47
10	A	801	HEM	CAB-C3B	3.42	1.56	1.47
5	A	608	NO3	O1-N	3.38	1.39	1.24
5	B	608	NO3	O1-N	3.21	1.38	1.24
10	A	801	HEM	C3C-C2C	-3.18	1.36	1.40
10	A	801	HEM	CAA-C2A	3.11	1.56	1.52
10	B	821	HEM	FE-NB	2.77	2.10	1.96
10	B	821	HEM	CAA-C2A	2.68	1.56	1.52
10	B	821	HEM	C3C-C2C	-2.45	1.37	1.40
10	B	821	HEM	FE-ND	2.12	2.07	1.96
10	A	801	HEM	CMB-C2B	2.00	1.55	1.50
9	A	902	SCN	C-N	2.00	1.22	1.15

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	A	801	HEM	C4D-ND-C1D	7.09	112.40	105.07
10	B	821	HEM	C4D-ND-C1D	6.70	111.99	105.07
10	A	801	HEM	C4B-CHC-C1C	4.38	128.34	122.56
10	B	821	HEM	C4B-CHC-C1C	4.36	128.31	122.56
10	A	801	HEM	C4C-CHD-C1D	3.81	127.59	122.56
10	A	801	HEM	CMD-C2D-C1D	3.64	130.59	125.04
10	B	821	HEM	C3B-C2B-C1B	3.56	109.13	106.49
10	A	801	HEM	C1B-NB-C4B	3.54	108.73	105.07
10	B	821	HEM	C1B-NB-C4B	3.46	108.65	105.07
10	B	821	HEM	CMD-C2D-C1D	3.39	130.19	125.04
10	B	821	HEM	C4C-CHD-C1D	3.25	126.85	122.56
10	B	821	HEM	C4A-C3A-C2A	2.92	109.03	107.00
10	B	821	HEM	CAD-C3D-C4D	2.73	129.43	124.66
10	B	821	HEM	C2B-C1B-NB	-2.72	106.62	109.84
10	A	801	HEM	CHC-C4B-NB	2.68	127.35	124.43
10	B	821	HEM	CBA-CAA-C2A	-2.58	108.21	112.62
10	A	801	HEM	CHA-C4D-ND	2.54	127.51	124.38
10	A	801	HEM	CBD-CAD-C3D	-2.53	105.59	112.63
10	B	821	HEM	CHC-C4B-NB	2.49	127.14	124.43
10	B	821	HEM	CHA-C4D-ND	2.48	127.44	124.38
10	A	801	HEM	CAD-CBD-CGD	-2.43	108.38	113.60
10	A	801	HEM	C3B-C2B-C1B	2.40	108.26	106.49
10	B	821	HEM	CBD-CAD-C3D	-2.39	105.97	112.63
10	A	801	HEM	C2B-C1B-NB	-2.20	107.23	109.84
10	A	801	HEM	C4A-C3A-C2A	2.12	108.47	107.00
10	B	821	HEM	CAD-CBD-CGD	-2.12	109.04	113.60
10	B	821	HEM	CMC-C2C-C3C	2.09	128.59	124.68
10	A	801	HEM	C3D-C4D-ND	-2.02	107.92	110.17

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	B	821	HEM	CAD-CBD-CGD-O2D
10	B	821	HEM	CAD-CBD-CGD-O1D
10	B	821	HEM	CAA-CBA-CGA-O1A
10	B	821	HEM	CAA-CBA-CGA-O2A
10	A	801	HEM	CAD-CBD-CGD-O2D
10	A	801	HEM	CAD-CBD-CGD-O1D

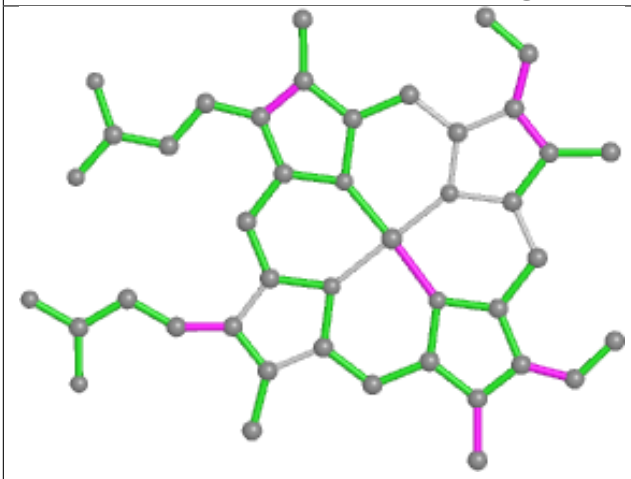
There are no ring outliers.

5 monomers are involved in 18 short contacts:

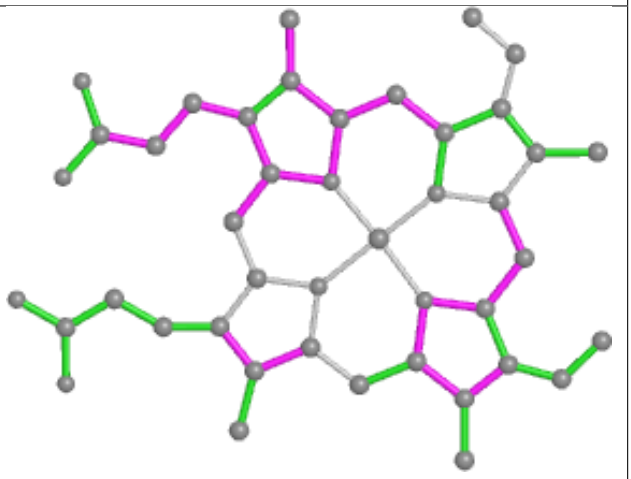
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	801	HEM	7	0
8	A	901	CYN	1	0
10	B	821	HEM	8	0
11	B	921	OSM	1	0
5	B	608	NO3	1	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

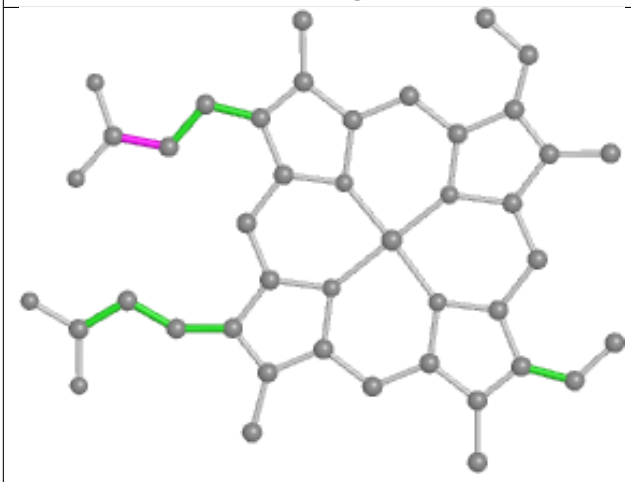
Ligand HEM A 801



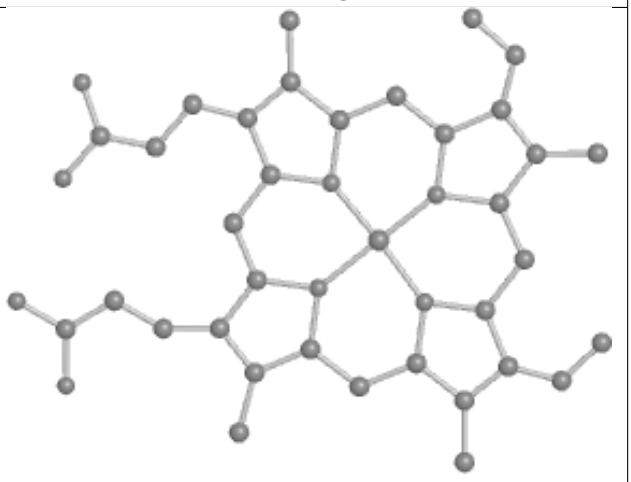
Bond lengths



Bond angles

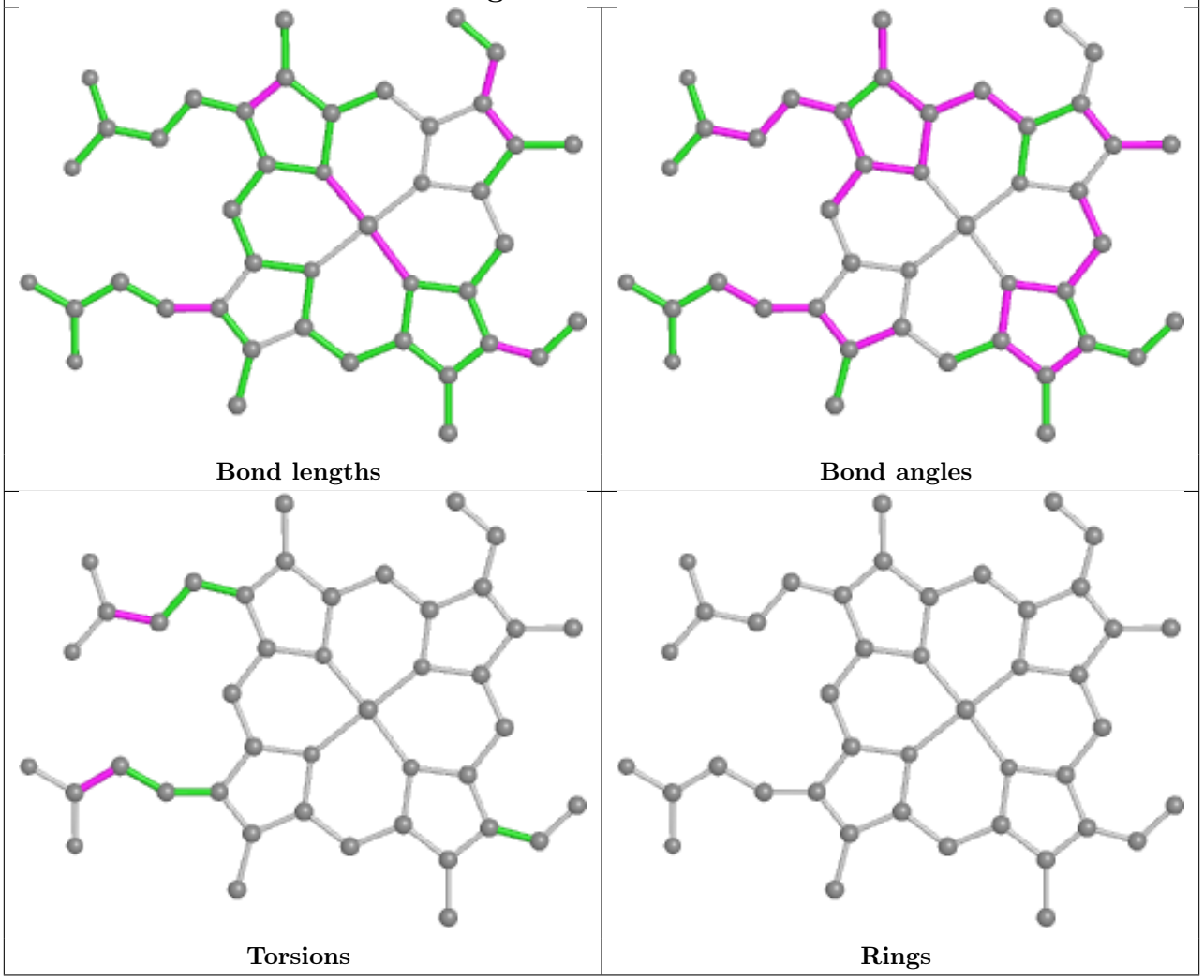


Torsions



Rings

Ligand HEM B 821



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.