



## Full wwPDB EM Validation Report ⓘ

Jul 27, 2025 – 12:32 AM JST

PDB ID : 8XMP / pdb\_00008xmp  
EMDB ID : EMD-38485  
Title : Structure of CD163 in complex with Hb-Hp  
Authors : Xu, H.; Su, X.D.  
Deposited on : 2023-12-27  
Resolution : 3.11 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>

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:

EMDB validation analysis : **FAILED**  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0rc1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : **FAILED**  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.45.1

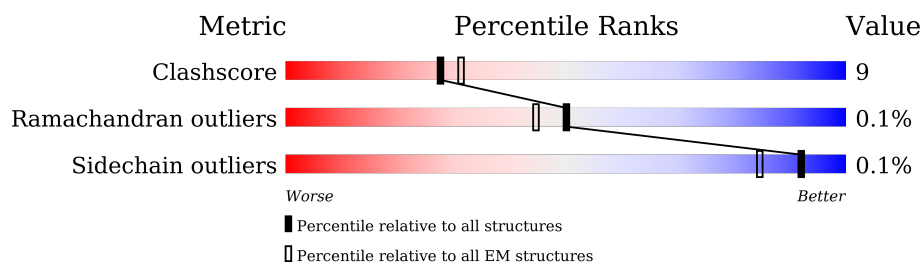
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.11 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)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	2	347	
2	D	1009	
2	E	1009	
2	F	1009	
3	C	142	
4	G	147	
5	A	2	
5	X	2	
5	Y	2	

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 22949 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Isoform 2 of Haptoglobin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	288	Total	C	N	O	S	0	0
			2263	1444	382	425	12		

- Molecule 2 is a protein called Scavenger receptor cysteine-rich type 1 protein M130.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	718	Total	C	N	O	S	0	0
			5455	3354	987	1054	60		
2	F	841	Total	C	N	O	S	0	0
			6370	3908	1158	1234	70		
2	D	841	Total	C	N	O	S	0	0
			6369	3908	1158	1233	70		

- Molecule 3 is a protein called Hemoglobin subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	141	Total	C	N	O	S	0	0
			1068	685	187	193	3		

- Molecule 4 is a protein called Hemoglobin subunit beta.

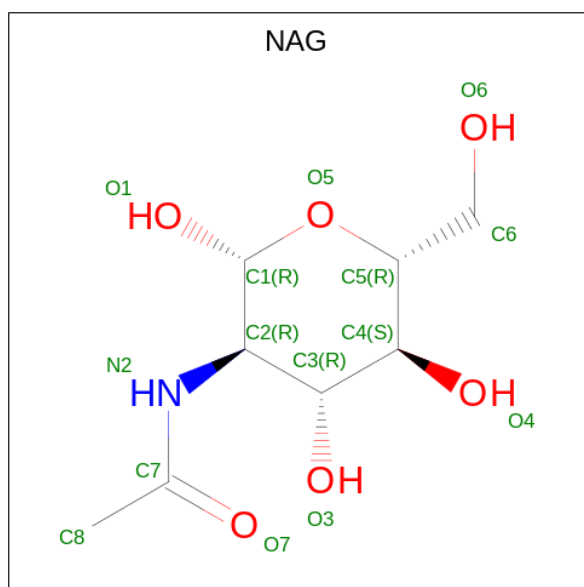
Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	143	Total	C	N	O	S	0	0
			1091	703	189	196	3		

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
5	Y	2	Total	C	N	O	0	0
			28	16	2	10		
5	A	2	Total	C	N	O	0	0
			28	16	2	10		
5	X	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				AltConf
6	2	1	Total	C	N	O	0
			14	8	1	5	
6	2	1	Total	C	N	O	0
			14	8	1	5	
6	E	1	Total	C	N	O	0
			14	8	1	5	
6	E	1	Total	C	N	O	0
			14	8	1	5	
6	F	1	Total	C	N	O	0
			14	8	1	5	
6	F	1	Total	C	N	O	0
			14	8	1	5	
6	F	1	Total	C	N	O	0
			14	8	1	5	
6	D	1	Total	C	N	O	0
			14	8	1	5	

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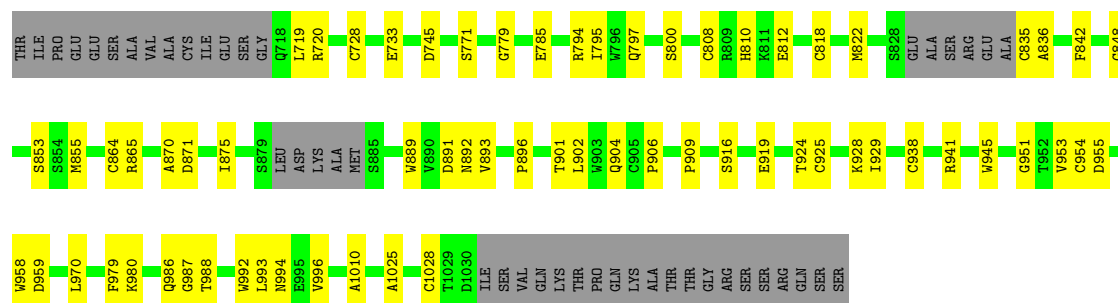
Mol	Chain	Residues	Atoms				AltConf
6	D	1	Total 14	C 8	N 1	O 5	0
6	D	1	Total 14	C 8	N 1	O 5	0

- | Mol | Chain | Residues | Atoms      |         | AltConf |
|-----|-------|----------|------------|---------|---------|
| 7   | E     | 5        | Total<br>5 | Ca<br>5 | 0       |
| 7   | F     | 9        | Total<br>9 | Ca<br>9 | 0       |
| 7   | D     | 9        | Total<br>9 | Ca<br>9 | 0       |

- # HEM

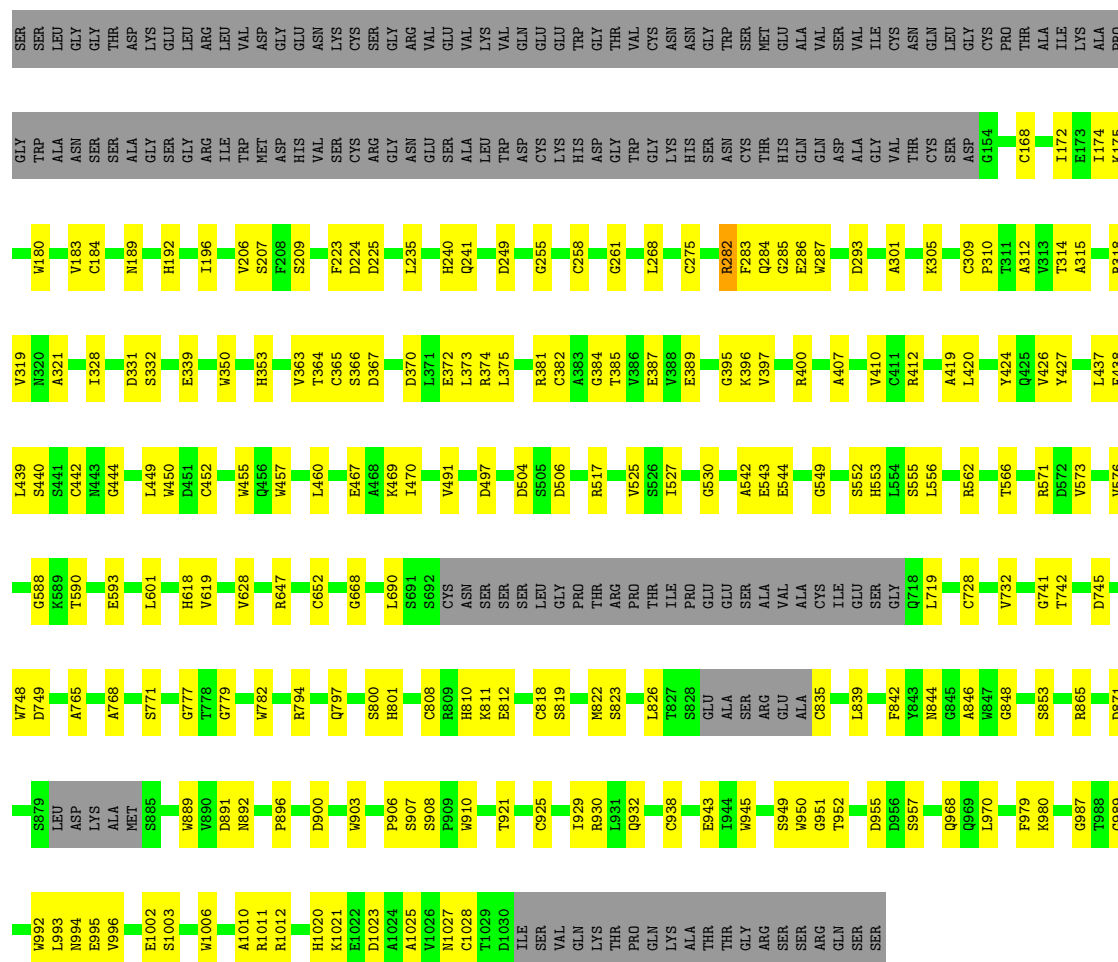
Mol	Chain	Residues	Atoms					AltConf
8	C	1	Total 43	C 34	Fe 1	N 4	O 4	0
8	G	1	Total 43	C 34	Fe 1	N 4	O 4	0





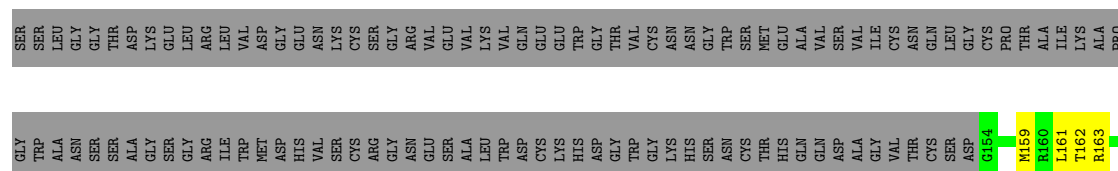
• Molecule 2: Scavenger receptor cysteine-rich type 1 protein M130

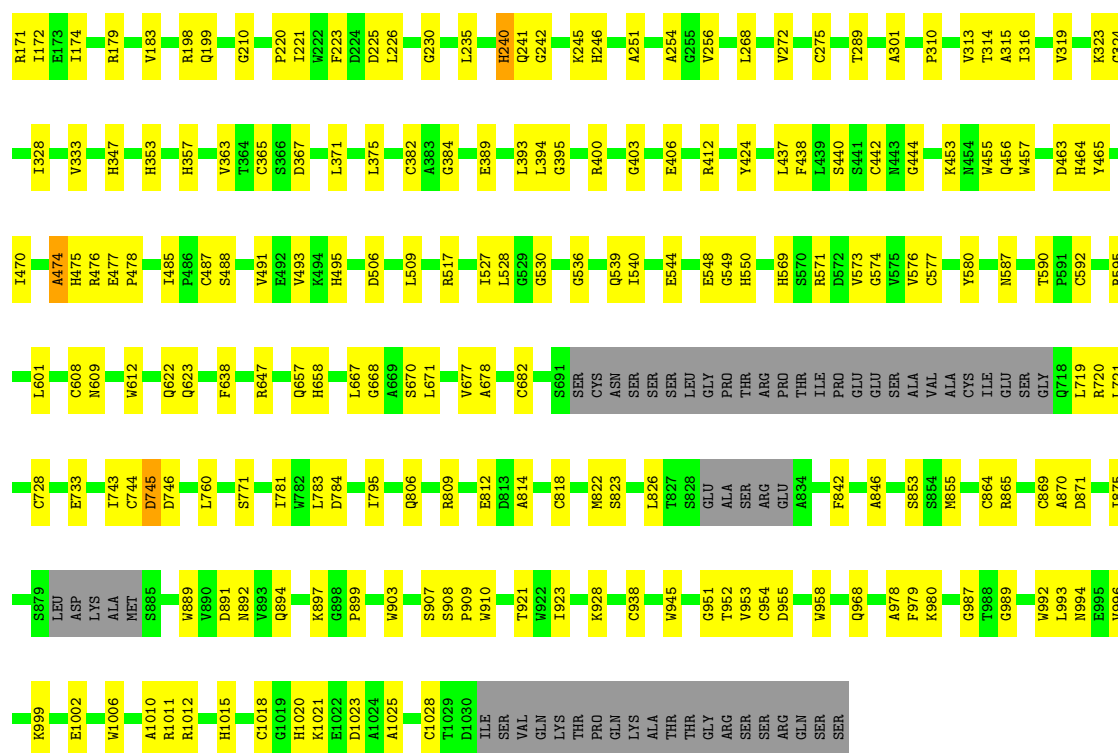
Chain F: 63% 20% 17%



• Molecule 2: Scavenger receptor cysteine-rich type 1 protein M130

Chain D: 63% 20% 17%





• Molecule 3: Hemoglobin subunit alpha

Chain C: 87% 12%



• Molecule 4: Hemoglobin subunit beta

Chain G: 78% 20%



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

Chain Y: 100%



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

Chain A: 100%



MAG  
120  
MAG 120

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

Chain X:

100%MAG  
120  
MAG 120

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	432933	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

## 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: HEM, NAG, CA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	2	0.15	0/2316	0.30	0/3142
2	D	0.15	0/6516	0.33	2/8822 (0.0%)
2	E	0.12	0/5580	0.27	0/7560
2	F	0.13	0/6517	0.31	0/8823
3	C	0.13	0/1096	0.26	0/1491
4	G	0.13	0/1119	0.25	0/1522
All	All	0.14	0/23144	0.30	2/31360 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	475	HIS	N-CA-C	-8.57	101.63	110.97
2	D	474	ALA	N-CA-C	-5.99	103.62	113.50

There are no chirality outliers.

There are no planarity outliers.

### 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	2	2263	0	2224	46	0
2	D	6369	0	5910	122	0
2	E	5455	0	5081	99	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	6370	0	5910	132	0
3	C	1068	0	1073	13	0
4	G	1091	0	1089	22	0
5	A	28	0	25	0	0
5	X	28	0	25	0	0
5	Y	28	0	25	0	0
6	2	28	0	26	1	0
6	D	42	0	39	0	0
6	E	28	0	26	0	0
6	F	42	0	39	0	0
7	D	9	0	0	0	0
7	E	5	0	0	0	0
7	F	9	0	0	0	0
8	C	43	0	30	2	0
8	G	43	0	30	2	0
All	All	22949	0	21552	422	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 9.

All (422) 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)
1:2:252:ARG:HD3	2:D:251:ALA:HB2	1.62	0.81
3:C:117:PHE:O	4:G:30:ARG:NH2	2.19	0.75
8:G:201:HEM:HHC	8:G:201:HEM:HBB2	1.68	0.74
2:E:808:CYS:SG	2:F:1021:LYS:NZ	2.61	0.74
2:D:162:THR:HG22	2:D:163:ARG:HG3	1.71	0.71
2:F:282:ARG:HD2	2:F:285:GLY:HA2	1.73	0.71
2:F:527:ILE:H	2:F:949:SER:HB3	1.55	0.70
1:2:254:TYR:OH	1:2:327:TYR:O	2.09	0.70
2:D:313:VAL:HG21	2:D:371:LEU:HD11	1.73	0.70
2:F:381:ARG:NH1	2:F:497:ASP:OD2	2.24	0.69
2:D:822:MET:HB3	2:D:903:TRP:NE1	2.08	0.68
2:E:670:SER:HA	2:E:909:PRO:HB3	1.77	0.67
4:G:26:GLU:OE2	4:G:30:ARG:NH1	2.28	0.67
2:F:395:GLY:HA3	2:F:457:TRP:HH2	1.60	0.66
2:E:381:ARG:NH2	2:E:414:LEU:O	2.28	0.66
3:C:31:ARG:NH1	4:G:127:GLN:OE1	2.23	0.66
2:E:864:CYS:HB3	2:E:870:ALA:HB3	1.77	0.66
1:2:65:VAL:O	1:2:76:ASN:ND2	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:328:ILE:HD13	2:E:353:HIS:HD2	1.61	0.65
2:D:938:CYS:HB3	2:D:1028:CYS:HB2	1.77	0.65
2:D:517:ARG:NH2	2:D:549:GLY:O	2.29	0.65
2:D:781:ILE:HB	2:D:806:GLN:HG3	1.77	0.65
3:C:27:GLU:OE1	3:C:112:HIS:NE2	2.29	0.65
2:E:315:ALA:HB3	2:E:364:THR:HB	1.79	0.65
2:F:407:ALA:HB1	2:F:470:ILE:HD13	1.78	0.64
2:F:811:LYS:NZ	2:D:1018:CYS:SG	2.69	0.64
2:E:728:CYS:HB3	2:E:818:CYS:HB2	1.80	0.64
2:E:517:ARG:NH2	2:E:549:GLY:O	2.30	0.64
2:D:241:GLN:NE2	2:D:245:LYS:O	2.31	0.63
2:F:846:ALA:HB3	2:F:889:TRP:HZ2	1.63	0.63
2:D:968:GLN:NE2	2:D:1002:GLU:O	2.32	0.63
2:D:463:ASP:OD1	2:D:464:HIS:ND1	2.31	0.63
2:F:517:ARG:NH2	2:F:549:GLY:O	2.30	0.63
2:F:439:LEU:HD21	2:F:449:LEU:HD11	1.81	0.63
2:D:952:THR:HG21	2:D:987:GLY:HA3	1.81	0.62
2:E:413:GLN:HB3	2:E:448:SER:HA	1.79	0.62
2:D:720:ARG:HG2	2:D:733:GLU:HB2	1.82	0.62
2:E:779:GLY:O	2:E:810:HIS:NE2	2.22	0.62
2:F:420:LEU:HB3	2:F:556:LEU:HD21	1.80	0.62
2:F:374:ARG:HH22	2:F:389:GLU:HG3	1.64	0.62
1:2:123:HIS:HB2	1:2:161:THR:HG23	1.81	0.61
2:E:312:ALA:HB3	2:E:367:ASP:HA	1.83	0.61
2:F:779:GLY:O	2:F:810:HIS:NE2	2.25	0.61
2:F:275:CYS:HB3	2:F:365:CYS:HB2	1.83	0.61
2:D:601:LEU:HD21	2:D:894:GLN:HB3	1.83	0.61
2:D:744:CYS:O	2:D:745:ASP:HB3	2.00	0.60
2:D:979:PHE:HB2	2:D:1025:ALA:HB3	1.84	0.60
2:D:647:ARG:NH1	2:D:907:SER:O	2.34	0.60
2:F:618:HIS:HB3	2:F:690:LEU:HD11	1.82	0.60
2:F:184:CYS:HB2	2:F:224:ASP:HA	1.84	0.60
8:C:201:HEM:HMC2	8:C:201:HEM:HBC2	1.83	0.60
2:E:379:GLY:HA3	2:E:427:TYR:HD2	1.66	0.59
2:F:315:ALA:HB3	2:F:364:THR:HB	1.83	0.59
2:F:207:SER:HB3	2:F:283:PHE:HZ	1.67	0.59
2:D:323:LYS:HB3	2:D:357:HIS:HB3	1.83	0.59
2:E:301:ALA:HA	2:E:314:THR:HG21	1.83	0.59
2:D:587:ASN:ND2	2:D:638:PHE:O	2.36	0.59
2:D:721:LEU:HD13	2:D:760:LEU:HD11	1.84	0.59
2:E:996:VAL:HA	2:E:1010:ALA:HB2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:C:201:HEM:HMB2	8:C:201:HEM:HBB2	1.85	0.59
2:E:590:THR:HG22	2:E:592:CYS:H	1.67	0.59
2:F:366:SER:OG	2:F:370:ASP:OD1	2.21	0.58
2:D:159:MET:SD	2:D:199:GLN:NE2	2.76	0.58
2:F:318:ARG:HB2	2:F:321:ALA:HB3	1.86	0.58
2:D:437:LEU:HD11	2:D:455:TRP:HE3	1.69	0.58
2:F:952:THR:HG21	2:F:987:GLY:HA3	1.84	0.58
2:F:989:GLY:O	2:F:1020:HIS:NE2	2.27	0.57
2:F:590:THR:HB	2:F:593:GLU:OE2	2.04	0.57
2:D:548:GLU:OE1	2:D:550:HIS:ND1	2.33	0.57
4:G:20:VAL:HA	4:G:68:LEU:HD23	1.84	0.57
3:C:21:ALA:HB1	3:C:63:ALA:HB1	1.87	0.57
2:D:746:ASP:HB2	2:D:784:ASP:OD1	2.05	0.57
2:E:901:THR:OG1	2:E:904:GLN:NE2	2.34	0.57
2:E:958:TRP:O	2:E:980:LYS:NZ	2.32	0.57
2:F:955:ASP:HB2	2:F:980:LYS:HG2	1.87	0.56
2:E:333:VAL:HA	2:E:347:HIS:HB3	1.88	0.56
2:D:412:ARG:NH2	2:D:444:GLY:O	2.35	0.56
2:D:275:CYS:HB3	2:D:365:CYS:HB2	1.87	0.56
2:E:295:TRP:HD1	2:E:316:ILE:HG23	1.69	0.56
2:E:955:ASP:HB2	2:E:980:LYS:HG2	1.88	0.56
2:D:590:THR:HG22	2:D:592:CYS:H	1.70	0.56
2:F:312:ALA:HB3	2:F:367:ASP:HA	1.88	0.56
2:E:305:LYS:NZ	2:E:339:GLU:O	2.32	0.56
2:F:196:ILE:HD11	2:F:235:LEU:HD22	1.88	0.56
2:F:372:GLU:HB2	2:F:389:GLU:HB2	1.88	0.55
2:F:628:VAL:HG12	2:F:690:LEU:HG	1.88	0.55
2:D:198:ARG:NH2	2:D:230:GLY:O	2.33	0.55
2:D:316:ILE:HG13	2:D:456:GLN:HG2	1.88	0.55
2:E:567:CYS:SG	2:E:568:SER:N	2.79	0.55
2:E:938:CYS:HB3	2:E:1028:CYS:HB2	1.89	0.55
2:F:968:GLN:NE2	2:F:1002:GLU:O	2.40	0.55
2:D:406:GLU:HG3	2:D:442:CYS:HB2	1.88	0.55
2:F:282:ARG:HG3	2:F:287:TRP:CD2	2.42	0.55
2:F:183:VAL:HG13	2:F:223:PHE:HB2	1.89	0.55
2:F:823:SER:HB3	2:F:842:PHE:HB3	1.89	0.55
3:C:114:PRO:O	4:G:116:HIS:NE2	2.40	0.54
2:E:583:ILE:HG21	2:E:659:MET:HG3	1.88	0.54
2:F:552:SER:OG	2:F:553:HIS:ND1	2.37	0.54
2:F:979:PHE:HB2	2:F:1025:ALA:HB3	1.89	0.54
2:F:808:CYS:SG	2:D:1021:LYS:NZ	2.81	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:771:SER:HA	2:D:812:GLU:HA	1.89	0.54
2:F:268:LEU:HD21	2:F:363:VAL:HG12	1.89	0.54
1:2:340:VAL:O	1:2:344:ILE:HG12	2.07	0.54
2:D:953:VAL:HG13	2:D:993:LEU:HB2	1.89	0.54
2:D:463:ASP:OD1	2:D:464:HIS:N	2.35	0.54
2:D:864:CYS:HB3	2:D:870:ALA:HB3	1.90	0.53
2:F:172:ILE:HD13	2:F:196:ILE:HG13	1.91	0.53
1:2:284:MET:HE2	1:2:326:GLU:HA	1.89	0.53
2:F:293:ASP:OD2	4:G:82:LYS:NZ	2.35	0.53
2:E:477:GLU:HB3	2:E:494:LYS:HE2	1.91	0.53
2:D:671:LEU:HG	2:D:909:PRO:HG3	1.91	0.53
2:D:743:ILE:HG12	2:D:783:LEU:HD23	1.91	0.53
2:F:542:ALA:HB2	2:F:566:THR:HB	1.89	0.53
1:2:124:HIS:HA	6:2:401:NAG:H82	1.90	0.53
4:G:45:PHE:HA	4:G:59:LYS:HD2	1.90	0.52
1:2:103:ILE:N	1:2:295:ASP:OD2	2.42	0.52
2:E:509:LEU:HA	2:E:527:ILE:HD11	1.91	0.52
2:E:853:SER:OG	2:E:892:ASN:OD1	2.26	0.52
1:2:223:SER:HB2	1:2:237:LEU:HD21	1.92	0.52
2:E:474:ALA:HA	2:E:477:GLU:HB2	1.90	0.52
2:F:647:ARG:NH2	2:F:907:SER:O	2.43	0.52
2:D:608:CYS:HA	2:D:678:ALA:H	1.74	0.52
2:F:331:ASP:OD1	2:F:332:SER:N	2.43	0.52
2:F:822:MET:HB3	2:F:903:TRP:NE1	2.24	0.52
2:F:506:ASP:OD1	2:F:562:ARG:NH2	2.40	0.52
2:E:836:ALA:HB1	2:E:924:THR:HG22	1.92	0.52
2:E:954:CYS:HB3	2:E:994:ASN:HB3	1.90	0.52
2:D:174:ILE:HD11	2:D:235:LEU:HD23	1.92	0.52
2:E:278:ARG:NH1	2:E:322:SER:O	2.43	0.52
2:D:989:GLY:O	2:D:1020:HIS:NE2	2.34	0.52
1:2:178:VAL:HG11	1:2:343:THR:HG21	1.92	0.51
2:F:1006:TRP:O	2:F:1012:ARG:NH1	2.43	0.51
2:E:266:LEU:HD11	2:E:279:LEU:HD21	1.93	0.51
2:E:328:ILE:HD13	2:E:353:HIS:CD2	2.42	0.51
2:E:487:CYS:HB3	2:E:577:CYS:HB2	1.91	0.51
2:F:305:LYS:NZ	2:F:339:GLU:O	2.39	0.51
2:D:487:CYS:HB3	2:D:577:CYS:HB2	1.92	0.51
8:G:201:HEM:HBC2	8:G:201:HEM:HMC2	1.91	0.51
2:E:720:ARG:HG2	2:E:733:GLU:HB2	1.93	0.51
2:D:328:ILE:O	2:D:353:HIS:NE2	2.24	0.51
2:D:875:ILE:HD13	2:D:923:ILE:HG22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:376:ARG:NH1	2:E:387:GLU:OE1	2.44	0.51
2:E:893:VAL:HG11	2:E:902:LEU:HD11	1.92	0.51
2:F:427:TYR:OH	2:F:543:GLU:OE2	2.28	0.51
4:G:55:MET:O	4:G:61:LYS:NZ	2.38	0.51
2:E:478:PRO:HB3	2:E:493:VAL:HG22	1.93	0.51
2:F:896:PRO:HD3	2:F:906:PRO:HD2	1.92	0.51
2:D:319:VAL:HG12	2:D:457:TRP:CD1	2.45	0.51
2:D:403:GLY:N	2:D:406:GLU:OE1	2.38	0.50
2:F:301:ALA:HA	2:F:314:THR:HG21	1.92	0.50
2:D:506:ASP:HB2	2:D:544:GLU:HA	1.92	0.50
2:F:412:ARG:NH2	2:F:444:GLY:O	2.32	0.50
2:E:979:PHE:HB2	2:E:1025:ALA:HB3	1.94	0.50
2:F:748:TRP:CD1	2:F:768:ALA:HB1	2.47	0.50
2:D:183:VAL:HG13	2:D:223:PHE:HB2	1.94	0.50
1:2:230:ASN:ND2	4:G:101:GLU:OE2	2.32	0.50
2:E:473:SER:C	2:E:475:HIS:H	2.19	0.50
2:D:301:ALA:HA	2:D:314:THR:HG21	1.92	0.50
2:E:473:SER:O	2:E:475:HIS:N	2.45	0.50
2:D:1011:ARG:NH2	2:D:1015:HIS:O	2.44	0.50
2:D:536:GLY:O	2:D:569:HIS:ND1	2.44	0.50
1:2:49:ARG:NH1	1:2:51:GLN:OE1	2.45	0.50
2:F:749:ASP:OD1	2:F:749:ASP:N	2.44	0.50
1:2:271:VAL:HG23	1:2:318:PHE:HE1	1.77	0.50
2:F:987:GLY:N	2:F:1023:ASP:OD2	2.41	0.50
2:E:848:GLY:HA3	2:E:889:TRP:HD1	1.76	0.49
2:E:526:SER:HB3	2:E:865:ARG:HH22	1.77	0.49
2:F:765:ALA:HA	2:F:818:CYS:HA	1.92	0.49
2:D:951:GLY:HA3	2:D:992:TRP:CD1	2.47	0.49
2:F:374:ARG:NH1	2:F:387:GLU:OE2	2.45	0.49
2:F:979:PHE:HE2	2:F:1027:ASN:HB2	1.76	0.49
1:2:93:PRO:HG2	1:2:96:PRO:HB3	1.94	0.49
2:F:826:LEU:HD12	2:F:835:CYS:HB3	1.93	0.49
2:D:226:LEU:HD23	2:D:240:HIS:HB3	1.93	0.49
2:D:743:ILE:HB	2:D:814:ALA:HB3	1.94	0.49
2:D:891:ASP:OD1	2:D:892:ASN:N	2.45	0.49
2:F:800:SER:OG	2:F:801:HIS:N	2.45	0.49
4:G:10:ALA:HB1	4:G:126:VAL:HG12	1.93	0.49
2:F:542:ALA:HB1	2:F:562:ARG:HG2	1.94	0.49
2:F:309:CYS:HB2	2:F:310:PRO:HD2	1.94	0.49
2:D:822:MET:HB3	2:D:903:TRP:CE2	2.47	0.49
2:E:794:ARG:HB2	2:E:797:GLN:HG3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:395:GLY:HA3	2:D:457:TRP:HH2	1.78	0.48
2:D:491:VAL:HB	2:D:573:VAL:HG13	1.94	0.48
2:E:434:ASN:OD1	2:E:435:THR:N	2.45	0.48
2:D:438:PHE:HB2	2:D:456:GLN:HB2	1.95	0.48
2:E:443:ASN:ND2	2:E:445:ASN:OD1	2.36	0.48
2:E:473:SER:C	2:E:475:HIS:N	2.71	0.48
2:E:951:GLY:HA3	2:E:992:TRP:CD1	2.49	0.48
2:F:206:VAL:CG1	2:F:283:PHE:HE1	2.26	0.48
2:D:328:ILE:HB	2:D:353:HIS:CE1	2.47	0.48
2:E:891:ASP:OD1	2:E:892:ASN:N	2.46	0.48
2:F:839:LEU:HB3	2:F:921:THR:HG23	1.96	0.48
2:F:929:ILE:HG12	2:F:970:LEU:HD11	1.96	0.48
2:D:994:ASN:HD21	2:D:1011:ARG:HH11	1.62	0.48
1:2:95:ASN:ND2	1:2:111:LYS:O	2.47	0.48
1:2:175:GLU:HB2	1:2:194:LYS:HA	1.94	0.48
2:F:437:LEU:HD11	2:F:455:TRP:HE3	1.79	0.48
2:F:957:SER:HB3	2:F:995:GLU:HA	1.96	0.48
3:C:96:VAL:O	3:C:100:LEU:HG	2.13	0.48
2:E:822:MET:HA	2:E:842:PHE:O	2.13	0.48
1:2:156:LYS:HZ3	2:E:355:CYS:HB3	1.79	0.47
2:D:172:ILE:HD11	2:D:256:VAL:HG13	1.96	0.47
2:D:400:ARG:HG3	2:D:465:TYR:CZ	2.49	0.47
2:E:618:HIS:HB3	2:E:690:LEU:HD11	1.95	0.47
2:F:491:VAL:HB	2:F:573:VAL:HG13	1.95	0.47
2:D:958:TRP:CD1	2:D:978:ALA:HB1	2.48	0.47
2:E:571:ARG:HH12	2:E:988:THR:HA	1.79	0.47
1:2:138:LEU:HD22	1:2:164:LEU:HD21	1.95	0.47
1:2:206:ILE:HG21	1:2:312:ALA:HB2	1.96	0.47
2:F:728:CYS:HB3	2:F:818:CYS:HB2	1.97	0.47
2:E:916:SER:HG	2:E:919:GLU:CD	2.23	0.47
1:2:221:TYR:CE1	1:2:241:MET:HG2	2.50	0.47
2:F:282:ARG:HA	2:F:286:GLU:O	2.14	0.47
2:D:375:LEU:HD12	2:D:382:CYS:C	2.40	0.47
2:F:930:ARG:HG3	2:F:943:GLU:HB2	1.96	0.47
2:D:1006:TRP:O	2:D:1012:ARG:NH2	2.48	0.47
2:F:240:HIS:O	2:F:241:GLN:HG3	2.14	0.47
2:F:601:LEU:HD22	2:F:896:PRO:HB3	1.97	0.47
2:D:994:ASN:HD21	2:D:1011:ARG:NH1	2.12	0.47
2:F:771:SER:HA	2:F:812:GLU:HA	1.96	0.47
1:2:273:PRO:HB3	1:2:318:PHE:CG	2.50	0.46
2:F:174:ILE:HD11	2:F:235:LEU:HD23	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:397:VAL:HG22	2:F:437:LEU:HB3	1.97	0.46
2:D:954:CYS:HB3	2:D:994:ASN:HB3	1.97	0.46
2:E:390:ILE:HG22	2:E:391:GLN:OE1	2.15	0.46
2:D:869:CYS:O	2:D:928:LYS:HG2	2.14	0.46
2:E:848:GLY:HA3	2:E:889:TRP:CD1	2.50	0.46
2:F:207:SER:HB2	2:F:350:TRP:CD1	2.50	0.46
2:F:384:GLY:HA2	2:F:424:TYR:CG	2.51	0.46
1:2:221:TYR:CD1	1:2:241:MET:HG2	2.51	0.46
2:F:619:VAL:HG21	2:F:652:CYS:HB3	1.96	0.46
2:F:741:GLY:HA3	2:F:782:TRP:CD1	2.51	0.46
2:D:272:VAL:HG11	2:D:393:LEU:HB2	1.96	0.46
1:2:269:VAL:HG13	3:C:134:THR:HG22	1.97	0.46
2:F:871:ASP:HB3	2:F:945:TRP:NE1	2.31	0.46
2:F:282:ARG:HD2	2:F:285:GLY:CA	2.42	0.46
1:2:321:SER:OG	1:2:325:ALA:O	2.34	0.46
2:E:397:VAL:HG22	2:E:437:LEU:HB3	1.97	0.46
2:F:175:LYS:HB2	2:F:180:TRP:CD2	2.51	0.46
2:F:375:LEU:HD12	2:F:382:CYS:HA	1.98	0.46
2:F:951:GLY:HA3	2:F:992:TRP:CD1	2.51	0.46
2:D:955:ASP:O	2:D:980:LYS:HE3	2.16	0.46
2:E:413:GLN:OE1	2:E:448:SER:OG	2.26	0.45
2:F:994:ASN:OD1	2:F:1011:ARG:HB3	2.16	0.45
2:D:530:GLY:HA2	2:D:571:ARG:HA	1.98	0.45
2:E:745:ASP:OD1	2:E:812:GLU:HB2	2.15	0.45
2:F:385:THR:HG22	2:F:469:LYS:HG3	1.97	0.45
2:F:442:CYS:HB2	2:F:452:CYS:HB2	1.53	0.45
2:D:268:LEU:HD21	2:D:363:VAL:HG22	1.98	0.45
2:E:310:PRO:HB3	2:E:367:ASP:HB3	1.98	0.45
2:E:397:VAL:HG22	2:E:437:LEU:HD23	1.98	0.45
2:E:439:LEU:HD11	2:E:449:LEU:HD11	1.97	0.45
2:F:209:SER:O	2:F:255:GLY:N	2.42	0.45
2:D:310:PRO:HB3	2:D:367:ASP:HB3	1.96	0.45
2:D:667:LEU:HB2	2:D:903:TRP:HA	1.97	0.45
2:D:744:CYS:O	2:D:744:CYS:SG	2.74	0.45
3:C:16:LYS:HD3	3:C:116:GLU:HG2	1.98	0.45
2:E:373:LEU:HD22	2:E:413:GLN:HE21	1.82	0.45
2:E:384:GLY:HA2	2:E:424:TYR:CG	2.51	0.45
2:E:608:CYS:HA	2:E:678:ALA:H	1.80	0.45
2:F:225:ASP:HB3	2:F:241:GLN:HG2	1.98	0.45
2:F:506:ASP:HB3	2:F:544:GLU:HA	1.99	0.45
2:D:225:ASP:O	2:D:240:HIS:HA	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:333:VAL:HA	1:2:336:ILE:HG12	1.98	0.45
2:E:353:HIS:NE2	2:E:355:CYS:O	2.50	0.45
2:F:932:GLN:HG3	2:F:943:GLU:HG3	1.99	0.45
2:E:290:ILE:O	2:E:361:ALA:N	2.37	0.45
2:F:419:ALA:HB1	2:F:470:ILE:HD11	1.99	0.45
2:F:440:SER:HB2	4:G:77:HIS:HD2	1.81	0.45
2:F:835:CYS:HB2	2:F:925:CYS:HB2	1.98	0.45
2:F:865:ARG:HH21	2:F:900:ASP:HA	1.82	0.45
2:D:389:GLU:HB2	2:D:394:LEU:HD13	1.99	0.45
2:E:601:LEU:HD22	2:E:896:PRO:HB3	1.99	0.45
2:F:283:PHE:O	2:F:284:GLN:C	2.60	0.45
2:F:319:VAL:HG12	2:F:457:TRP:CD1	2.52	0.45
2:F:822:MET:HA	2:F:842:PHE:O	2.17	0.45
2:D:509:LEU:HA	2:D:527:ILE:HD11	1.99	0.45
4:G:57:ASN:HB3	4:G:60:VAL:HB	1.98	0.45
1:2:134:ASN:HD21	1:2:137:TRP:HB2	1.82	0.44
2:E:318:ARG:HG2	2:E:459:GLY:HA2	1.98	0.44
2:E:953:VAL:HG22	2:E:993:LEU:HB2	1.99	0.44
2:F:891:ASP:OD1	2:F:892:ASN:N	2.48	0.44
2:D:474:ALA:HA	2:D:477:GLU:HB2	1.99	0.44
2:E:295:TRP:CD1	2:E:316:ILE:HG23	2.51	0.44
2:E:480:LEU:HD21	2:E:515:LEU:HD21	2.00	0.44
2:E:835:CYS:SG	2:E:925:CYS:HB2	2.58	0.44
2:D:384:GLY:HA2	2:D:424:TYR:CG	2.53	0.44
2:E:855:MET:HG2	2:E:875:ILE:HD11	1.99	0.44
2:F:889:TRP:HB3	2:F:910:TRP:CE3	2.52	0.44
2:D:622:GLN:NE2	2:D:657:GLN:OE1	2.50	0.44
2:F:437:LEU:HD11	2:F:455:TRP:CE3	2.53	0.44
2:F:668:GLY:HA2	2:F:908:SER:O	2.18	0.44
2:D:289:THR:HG21	2:D:324:GLY:HA3	1.99	0.44
4:G:24:GLY:HA3	4:G:68:LEU:HB2	2.00	0.44
2:D:315:ALA:HB2	2:D:455:TRP:CH2	2.53	0.44
1:2:119:LYS:HB3	1:2:165:TYR:HB2	1.99	0.44
1:2:132:LEU:HB3	1:2:205:PRO:HA	2.00	0.44
1:2:134:ASN:ND2	1:2:137:TRP:HB2	2.32	0.44
2:F:794:ARG:H	2:F:797:GLN:HE21	1.66	0.44
2:F:396:LYS:HD2	2:F:467:GLU:OE2	2.18	0.43
2:F:420:LEU:HD12	2:F:555:SER:HB2	1.99	0.43
2:F:530:GLY:HA2	2:F:571:ARG:HA	2.00	0.43
2:F:848:GLY:HA3	2:F:889:TRP:CD1	2.53	0.43
2:D:668:GLY:HA2	2:D:908:SER:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:846:ALA:HB3	2:D:889:TRP:HZ2	1.83	0.43
2:E:896:PRO:HD3	2:E:906:PRO:HD2	1.99	0.43
2:D:319:VAL:HG12	2:D:457:TRP:HD1	1.83	0.43
2:D:728:CYS:HB3	2:D:818:CYS:HB2	1.99	0.43
1:2:131:THR:HG21	1:2:299:ALA:HB2	1.99	0.43
2:D:595:ARG:HD2	2:D:677:VAL:HG21	2.00	0.43
2:D:670:SER:HA	2:D:909:PRO:HB3	2.00	0.43
2:E:871:ASP:HB2	2:E:945:TRP:CE2	2.53	0.43
2:F:996:VAL:HA	2:F:1010:ALA:HB2	1.99	0.43
2:D:823:SER:HB3	2:D:842:PHE:HB3	2.00	0.43
2:E:929:ILE:HG23	2:E:970:LEU:HD23	2.00	0.43
2:E:959:ASP:HB2	2:D:809:ARG:HE	1.83	0.43
2:D:161:LEU:HA	2:D:171:ARG:O	2.19	0.43
2:D:528:LEU:N	2:D:574:GLY:O	2.41	0.43
4:G:24:GLY:N	4:G:68:LEU:HD22	2.34	0.43
2:E:402:TRP:CE2	2:E:468:ALA:HB1	2.54	0.43
1:2:90:CYS:HB3	1:2:207:CYS:HB2	1.71	0.43
2:D:853:SER:OG	2:D:891:ASP:OD1	2.37	0.43
2:E:599:LYS:HB2	2:E:604:TRP:CD2	2.53	0.43
2:D:540:ILE:HD11	2:D:569:HIS:HA	2.01	0.43
1:2:154:THR:HG23	1:2:156:LYS:H	1.84	0.43
2:E:399:ASP:OD1	2:E:465:TYR:HB3	2.19	0.43
2:E:928:LYS:HE3	2:E:928:LYS:HB2	1.87	0.43
2:F:168:CYS:HB3	2:F:258:CYS:HB2	2.00	0.43
2:D:822:MET:HA	2:D:842:PHE:O	2.19	0.43
2:D:865:ARG:HG2	2:D:871:ASP:HA	2.01	0.43
2:D:476:ARG:HH11	2:D:495:HIS:HA	1.83	0.42
2:F:189:ASN:OD1	2:F:192:HIS:ND1	2.45	0.42
2:D:889:TRP:HB3	2:D:910:TRP:CE3	2.55	0.42
1:2:104:LEU:HD12	1:2:292:CYS:HB2	2.00	0.42
2:E:494:LYS:HB2	2:E:499:TRP:CD1	2.55	0.42
2:E:579:ARG:HD3	2:E:658:HIS:CG	2.54	0.42
1:2:247:GLN:HE21	1:2:251:ILE:HD11	1.84	0.42
2:F:249:ASP:OD1	2:F:249:ASP:N	2.52	0.42
2:F:993:LEU:HD23	2:F:1012:ARG:HA	2.01	0.42
2:D:333:VAL:HA	2:D:347:HIS:HB3	2.01	0.42
2:D:210:GLY:HA2	2:D:254:ALA:HA	2.01	0.42
4:G:51:PRO:O	4:G:55:MET:HG2	2.19	0.42
2:E:396:LYS:HD3	2:E:467:GLU:HB3	2.02	0.42
2:F:410:VAL:HG23	2:F:449:LEU:HD13	2.00	0.42
2:D:478:PRO:HB3	2:D:493:VAL:HG22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:592:CYS:HB3	2:D:682:CYS:HB2	2.02	0.42
1:2:141:THR:HG21	1:2:317:SER:HA	2.02	0.42
2:E:785:GLU:O	2:E:800:SER:HA	2.20	0.42
2:E:941:ARG:HH11	2:E:987:GLY:HA2	1.84	0.42
2:F:282:ARG:HG3	2:F:287:TRP:CE2	2.54	0.42
1:2:103:ILE:HD13	1:2:291:THR:HG22	2.02	0.42
1:2:107:HIS:HB2	1:2:239:TYR:O	2.19	0.42
1:2:132:LEU:HD23	1:2:138:LEU:HG	2.02	0.42
2:D:580:TYR:CE2	2:D:899:PRO:HD3	2.55	0.42
3:C:94:ASP:OD2	3:C:96:VAL:HG12	2.20	0.42
2:D:609:ASN:HA	2:D:612:TRP:HB3	2.02	0.42
2:E:916:SER:N	2:E:919:GLU:OE2	2.50	0.42
2:E:719:LEU:HD13	2:E:795:ILE:HG21	2.02	0.41
2:D:179:ARG:HE	2:D:220:PRO:HG3	1.84	0.41
2:D:996:VAL:HA	2:D:1010:ALA:HB2	2.02	0.41
1:2:168:LYS:HG2	1:2:202:ARG:HD2	2.02	0.41
1:2:236:HIS:NE2	4:G:100:PRO:HG2	2.35	0.41
2:E:424:TYR:HE1	2:E:469:LYS:HG2	1.84	0.41
2:F:745:ASP:OD1	2:F:812:GLU:HB2	2.19	0.41
2:D:999:LYS:HA	2:D:999:LYS:HD2	1.92	0.41
2:F:206:VAL:HG11	2:F:283:PHE:HE1	1.85	0.41
2:F:438:PHE:CE1	2:F:460:LEU:HB2	2.56	0.41
1:2:104:LEU:HD22	1:2:323:ALA:HB2	2.01	0.41
2:E:318:ARG:HH12	2:E:323:LYS:HA	1.86	0.41
2:F:938:CYS:HB3	2:F:1028:CYS:HB2	2.01	0.41
1:2:259:VAL:HG23	1:2:262:LYS:HB2	2.01	0.41
2:D:855:MET:HE3	2:D:921:THR:HG21	2.03	0.41
3:C:16:LYS:HE2	3:C:16:LYS:HB3	1.84	0.41
4:G:75:LEU:HD21	4:G:133:VAL:HG11	2.03	0.41
2:E:504:ASP:HA	2:E:573:VAL:HB	2.01	0.41
2:F:400:ARG:HD2	4:G:79:ASP:HB3	2.01	0.41
2:F:424:TYR:CE2	2:F:426:VAL:HA	2.56	0.41
2:F:504:ASP:HA	2:F:573:VAL:HB	2.02	0.41
2:F:968:GLN:HE22	2:F:1003:SER:C	2.28	0.41
2:D:437:LEU:HD11	2:D:455:TRP:CE3	2.53	0.41
3:C:84:SER:OG	3:C:135:VAL:O	2.34	0.41
2:E:425:GLN:OE1	2:E:427:TYR:OH	2.25	0.41
2:D:440:SER:OG	2:D:453:LYS:O	2.39	0.41
2:D:826:LEU:HD11	2:D:923:ILE:HD11	2.02	0.41
2:D:871:ASP:HB3	2:D:945:TRP:NE1	2.36	0.41
2:E:404:LEU:HD23	2:E:404:LEU:HA	1.95	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:608:CYS:HA	2:E:678:ALA:N	2.36	0.41
2:F:373:LEU:HB2	2:F:450:TRP:CZ2	2.56	0.41
2:F:384:GLY:HA2	2:F:424:TYR:CD2	2.56	0.41
2:D:242:GLY:HA3	2:D:245:LYS:HD3	2.03	0.41
2:D:375:LEU:HD13	2:D:470:ILE:HG23	2.02	0.41
2:E:623:GLN:HB2	2:E:658:HIS:HA	2.02	0.41
2:F:588:GLY:HA3	2:F:593:GLU:O	2.21	0.41
2:D:221:ILE:HB	2:D:246:HIS:CD2	2.55	0.41
2:D:488:SER:HB2	2:D:576:VAL:HG22	2.03	0.41
2:D:623:GLN:HG3	2:D:658:HIS:CD2	2.56	0.41
1:2:140:THR:HG21	1:2:145:LEU:HD21	2.03	0.40
2:E:771:SER:HA	2:E:812:GLU:HA	2.03	0.40
2:F:819:SER:OG	2:F:844:ASN:OD1	2.23	0.40
2:D:539:GLN:OE1	2:D:539:GLN:N	2.55	0.40
2:D:719:LEU:HD13	2:D:795:ILE:HG21	2.02	0.40
4:G:123:THR:HB	4:G:125:PRO:HD2	2.03	0.40
1:2:236:HIS:CD2	4:G:100:PRO:HG2	2.56	0.40
2:E:941:ARG:NH1	2:E:986:GLN:O	2.54	0.40
2:F:719:LEU:HD11	2:F:732:VAL:HG13	2.03	0.40
2:F:742:THR:HG21	2:F:777:GLY:HA3	2.03	0.40
2:F:889:TRP:HB3	2:F:910:TRP:HE3	1.85	0.40
2:F:930:ARG:HG2	2:F:950:TRP:CZ3	2.56	0.40
3:C:27:GLU:HG2	3:C:31:ARG:HE	1.85	0.40
1:2:218:ARG:O	1:2:244:VAL:HG22	2.21	0.40
2:F:328:ILE:HB	2:F:353:HIS:CD2	2.56	0.40
2:F:853:SER:OG	2:F:891:ASP:OD1	2.39	0.40
2:E:316:ILE:O	2:E:457:TRP:N	2.54	0.40
4:G:14:LEU:HD22	4:G:130:TYR:CE2	2.57	0.40
4:G:88:LEU:HB3	4:G:141:LEU:HD11	2.03	0.40
1:2:333:VAL:O	1:2:337:GLN:N	2.54	0.40
2:F:168:CYS:HB2	2:F:261:GLY:HA3	2.03	0.40
2:F:525:VAL:HB	2:F:576:VAL:HG12	2.03	0.40
2:D:485:ILE:HG21	2:D:897:LYS:O	2.22	0.40
2:D:987:GLY:N	2:D:1023:ASP:OD2	2.44	0.40
3:C:10:VAL:HG21	3:C:128:PHE:HB2	2.04	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 PDB entries followed by that with respect to all EM entries.

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	2	282/347 (81%)	257 (91%)	24 (8%)	1 (0%)	30	61
2	D	833/1009 (83%)	801 (96%)	31 (4%)	1 (0%)	48	78
2	E	706/1009 (70%)	686 (97%)	19 (3%)	1 (0%)	48	78
2	F	833/1009 (83%)	811 (97%)	22 (3%)	0	100	100
3	C	139/142 (98%)	137 (99%)	2 (1%)	0	100	100
4	G	141/147 (96%)	140 (99%)	1 (1%)	0	100	100
All	All	2934/3663 (80%)	2832 (96%)	99 (3%)	3 (0%)	50	78

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	240	HIS
2	E	474	ALA
1	2	63	ASP

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	2	246/294 (84%)	246 (100%)	0	100	100
2	D	684/823 (83%)	683 (100%)	1 (0%)	92	97
2	E	590/823 (72%)	589 (100%)	1 (0%)	92	96
2	F	685/823 (83%)	684 (100%)	1 (0%)	92	97

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	113/114 (99%)	113 (100%)	0	100	100
4	G	115/119 (97%)	115 (100%)	0	100	100
All	All	2433/2996 (81%)	2430 (100%)	3 (0%)	92	97

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	473	SER
2	F	282	ARG
2	D	745	ASP

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

Mol	Chain	Res	Type
1	2	107	HIS
1	2	117	GLN
1	2	185	GLN
1	2	236	HIS
2	E	475	HIS
2	E	539	GLN
2	E	622	GLN
2	E	773	HIS
2	E	805	GLN
2	F	284	GLN
2	F	306	GLN
2	F	327	HIS
2	F	338	HIS
2	F	495	HIS
2	F	611	HIS
2	F	648	HIS
2	F	773	HIS
2	F	797	GLN
2	F	932	GLN
2	D	327	HIS
2	D	475	HIS
2	D	688	GLN
2	D	773	HIS
2	D	892	ASN
2	D	946	HIS
3	C	68	ASN

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Mol	Chain	Res	Type
3	C	72	HIS
4	G	80	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 ⓘ

6 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	$\# Z  > 2$
5	NAG	A	1	5,1	14,14,15	0.23	0	17,19,21	0.41	0
5	NAG	A	2	5	14,14,15	0.19	0	17,19,21	0.39	0
5	NAG	X	1	5,2	14,14,15	0.28	0	17,19,21	0.43	0
5	NAG	X	2	5	14,14,15	0.17	0	17,19,21	0.41	0
5	NAG	Y	1	5,2	14,14,15	0.25	0	17,19,21	0.40	0
5	NAG	Y	2	5	14,14,15	0.24	0	17,19,21	0.39	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	1	5,1	-	4/6/23/26	0/1/1/1
5	NAG	A	2	5	-	2/6/23/26	0/1/1/1
5	NAG	X	1	5,2	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	X	2	5	-	0/6/23/26	0/1/1/1
5	NAG	Y	1	5,2	-	2/6/23/26	0/1/1/1
5	NAG	Y	2	5	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

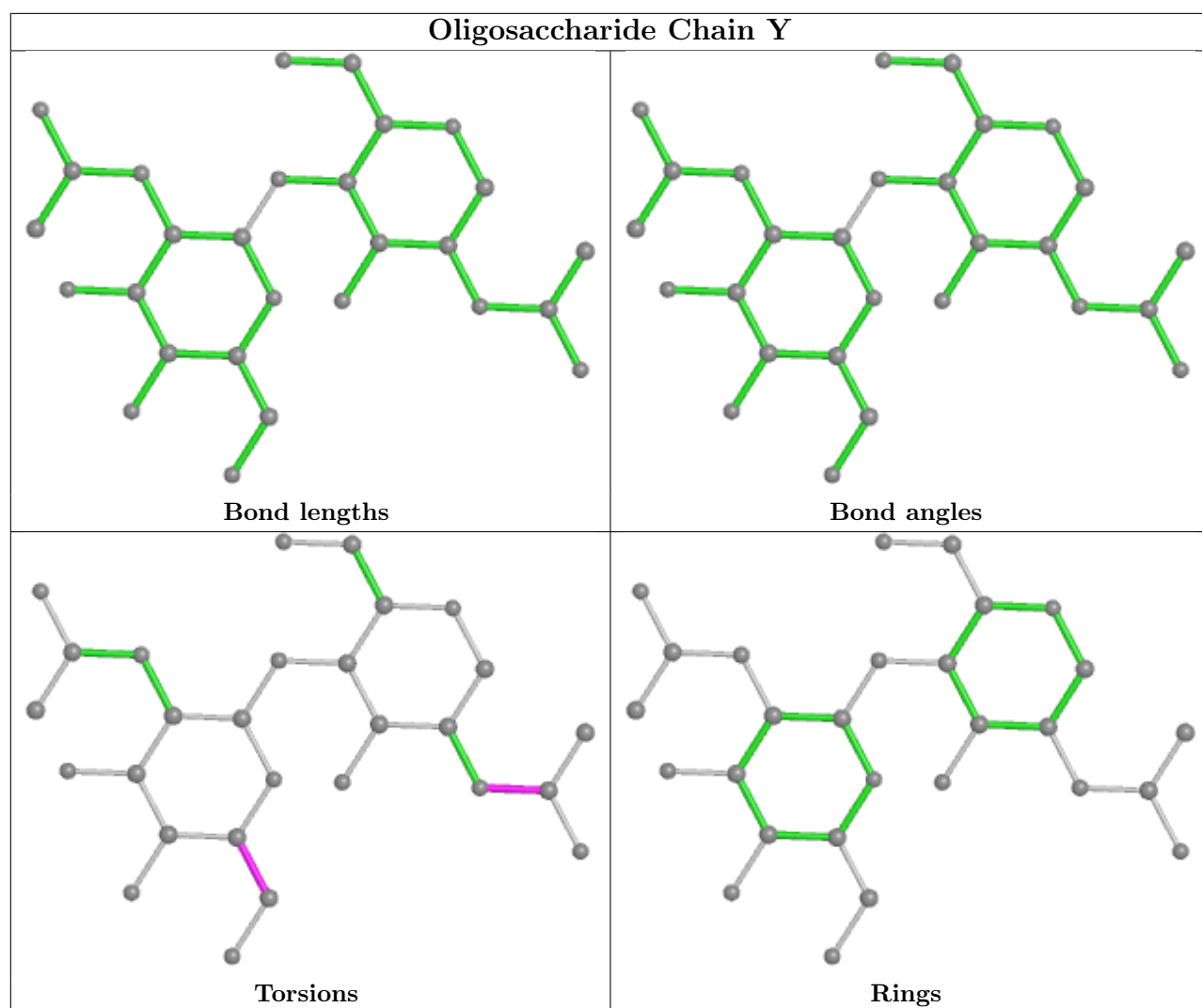
All (12) torsion outliers are listed below:

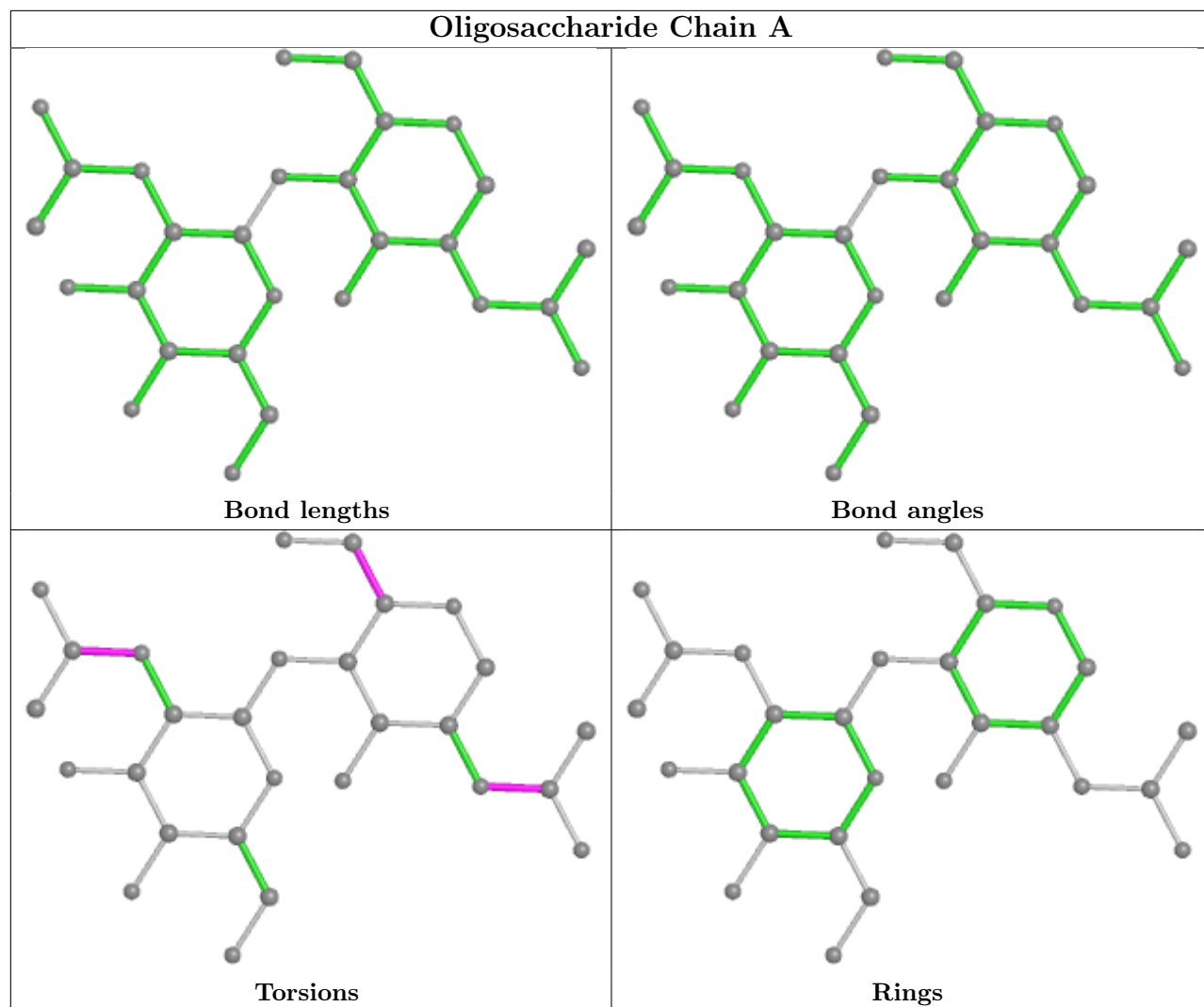
Mol	Chain	Res	Type	Atoms
5	Y	2	NAG	C4-C5-C6-O6
5	Y	1	NAG	C8-C7-N2-C2
5	Y	1	NAG	O7-C7-N2-C2
5	A	1	NAG	C8-C7-N2-C2
5	A	1	NAG	O7-C7-N2-C2
5	A	2	NAG	C8-C7-N2-C2
5	A	2	NAG	O7-C7-N2-C2
5	X	1	NAG	C8-C7-N2-C2
5	X	1	NAG	O7-C7-N2-C2
5	Y	2	NAG	O5-C5-C6-O6
5	A	1	NAG	C4-C5-C6-O6
5	A	1	NAG	O5-C5-C6-O6

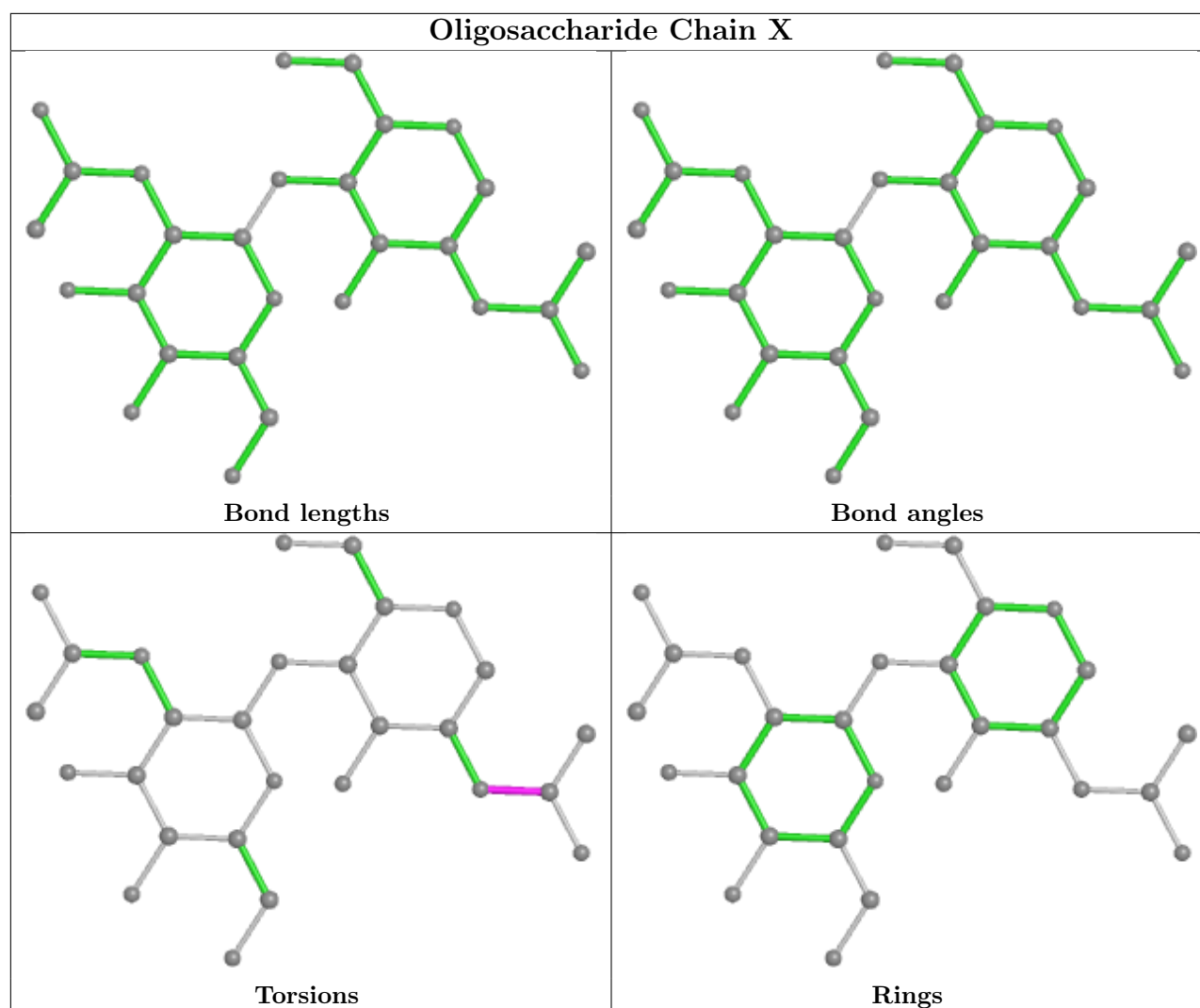
There are no ring outliers.

No monomer is involved in short contacts.

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







## 5.6 Ligand geometry [i](#)

Of 35 ligands modelled in this entry, 23 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	$\# Z  > 2$
6	NAG	D	1101	2	14,14,15	0.21	0	17,19,21	0.40	0
6	NAG	F	1101	2	14,14,15	0.24	0	17,19,21	0.39	0
6	NAG	E	1101	2	14,14,15	0.19	0	17,19,21	0.42	0
6	NAG	D	1103	2	14,14,15	0.23	0	17,19,21	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	NAG	E	1102	2	14,14,15	0.25	0	17,19,21	0.47	0
8	HEM	C	201	3	41,50,50	1.46	3 (7%)	45,82,82	1.36	9 (20%)
6	NAG	F	1103	2	14,14,15	0.22	0	17,19,21	0.43	0
6	NAG	2	402	1	14,14,15	0.26	0	17,19,21	0.51	0
6	NAG	D	1102	2	14,14,15	0.22	0	17,19,21	0.41	0
6	NAG	F	1102	2	14,14,15	0.19	0	17,19,21	0.41	0
8	HEM	G	201	4	41,50,50	1.46	3 (7%)	45,82,82	1.48	6 (13%)
6	NAG	2	401	1	14,14,15	0.24	0	17,19,21	0.41	0

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
6	NAG	D	1101	2	-	0/6/23/26	0/1/1/1
6	NAG	F	1101	2	-	2/6/23/26	0/1/1/1
6	NAG	E	1101	2	-	2/6/23/26	0/1/1/1
6	NAG	D	1103	2	-	2/6/23/26	0/1/1/1
6	NAG	E	1102	2	-	4/6/23/26	0/1/1/1
8	HEM	C	201	3	-	2/12/54/54	-
6	NAG	F	1103	2	-	1/6/23/26	0/1/1/1
6	NAG	2	402	1	-	2/6/23/26	0/1/1/1
6	NAG	D	1102	2	-	0/6/23/26	0/1/1/1
6	NAG	F	1102	2	-	2/6/23/26	0/1/1/1
8	HEM	G	201	4	-	1/12/54/54	-
6	NAG	2	401	1	-	0/6/23/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	201	HEM	C3C-C2C	-4.05	1.34	1.40
8	G	201	HEM	C3C-C2C	-3.95	1.34	1.40
8	C	201	HEM	C3C-CAC	3.76	1.55	1.47
8	G	201	HEM	C3C-CAC	3.67	1.55	1.47
8	C	201	HEM	CAB-C3B	3.03	1.55	1.47
8	G	201	HEM	CAB-C3B	2.89	1.55	1.47

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	G	201	HEM	C4B-CHC-C1C	3.14	126.70	122.56
8	G	201	HEM	C3B-C2B-C1B	3.00	108.71	106.49
8	G	201	HEM	C1B-NB-C4B	2.97	108.14	105.07
8	C	201	HEM	C4D-ND-C1D	2.73	107.89	105.07
8	G	201	HEM	C4D-ND-C1D	2.67	107.83	105.07
8	C	201	HEM	C1B-NB-C4B	2.55	107.71	105.07
8	G	201	HEM	CMC-C2C-C3C	2.40	129.16	124.68
8	G	201	HEM	C4C-CHD-C1D	2.31	125.61	122.56
8	C	201	HEM	C4C-CHD-C1D	2.21	125.48	122.56
8	C	201	HEM	CMC-C2C-C3C	2.18	128.76	124.68
8	C	201	HEM	CAD-CBD-CGD	-2.13	109.03	113.60
8	C	201	HEM	C4B-CHC-C1C	2.09	125.32	122.56
8	C	201	HEM	C3D-C4D-ND	-2.06	107.87	110.17
8	C	201	HEM	C4A-C3A-C2A	2.02	108.40	107.00
8	C	201	HEM	C3B-C2B-C1B	2.01	107.98	106.49

There are no chirality outliers.

All (18) torsion outliers are listed below:

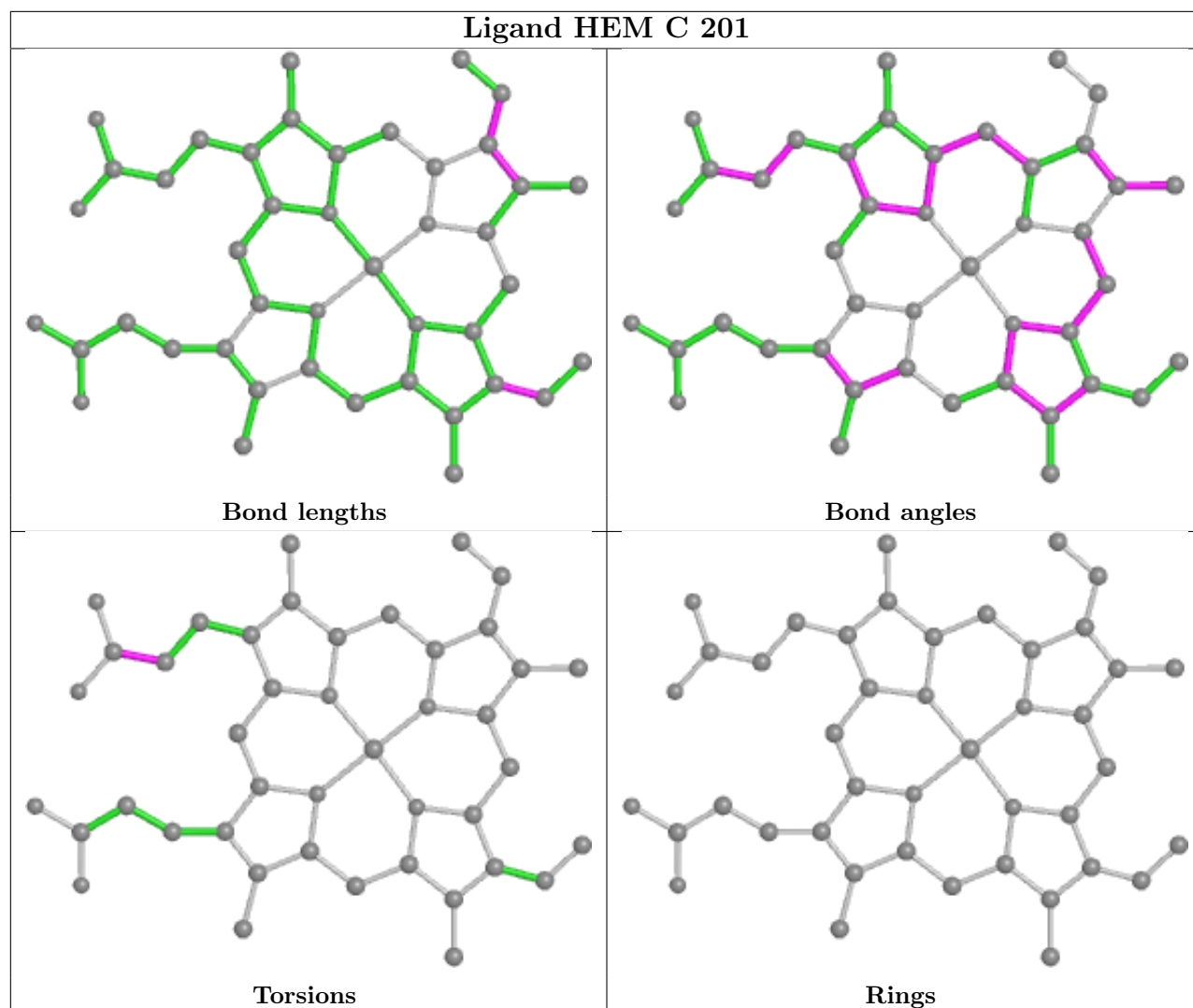
Mol	Chain	Res	Type	Atoms
6	E	1101	NAG	C4-C5-C6-O6
6	2	402	NAG	O5-C5-C6-O6
6	E	1101	NAG	O5-C5-C6-O6
6	E	1102	NAG	O5-C5-C6-O6
6	F	1101	NAG	C4-C5-C6-O6
6	F	1101	NAG	O5-C5-C6-O6
6	E	1102	NAG	C4-C5-C6-O6
6	2	402	NAG	C4-C5-C6-O6
6	E	1102	NAG	C8-C7-N2-C2
6	E	1102	NAG	O7-C7-N2-C2
8	G	201	HEM	C4B-C3B-CAB-CBB
6	D	1103	NAG	C4-C5-C6-O6
6	D	1103	NAG	O5-C5-C6-O6
6	F	1102	NAG	C4-C5-C6-O6
6	F	1102	NAG	O5-C5-C6-O6
6	F	1103	NAG	C4-C5-C6-O6
8	C	201	HEM	CAD-CBD-CGD-O2D
8	C	201	HEM	CAD-CBD-CGD-O1D

There are no ring outliers.

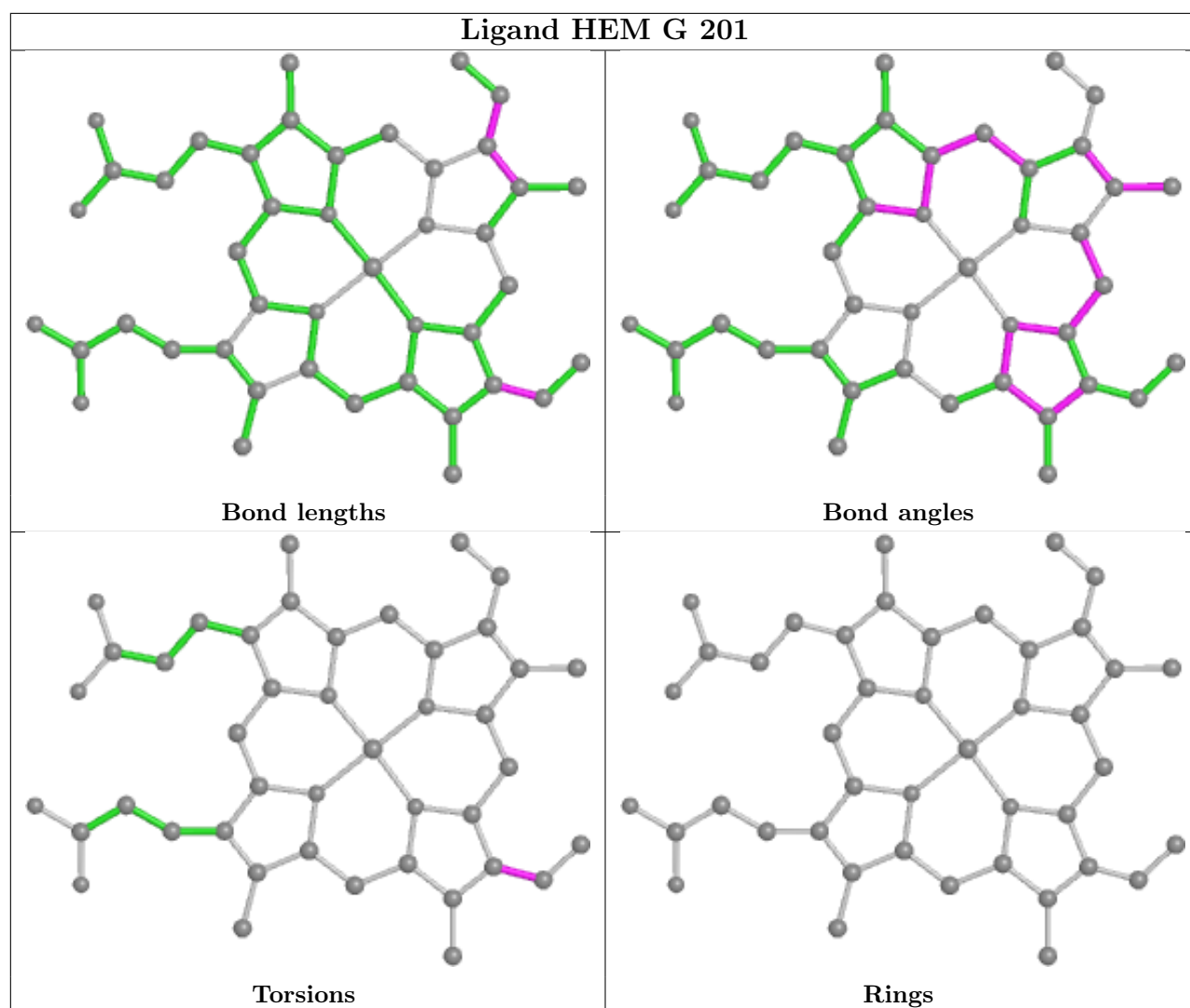
3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	201	HEM	2	0
8	G	201	HEM	2	0
6	2	401	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 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.