



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 2, 2023 – 01:27 AM EDT

PDB ID : 3TGY  
Title : Crystal structure of the complex of Bovine Lactoperoxidase with Ascorbic acid at 2.35 Å resolution  
Authors : Yamini, S.; Singh, R.P.; Singh, A.K.; Pandey, N.; Sinha, M.; Kaur, P.; Sharma, S.; Singh, T.P.  
Deposited on : 2011-08-18  
Resolution : 2.35 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

---

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) : 1.13  
EDS : 2.36  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

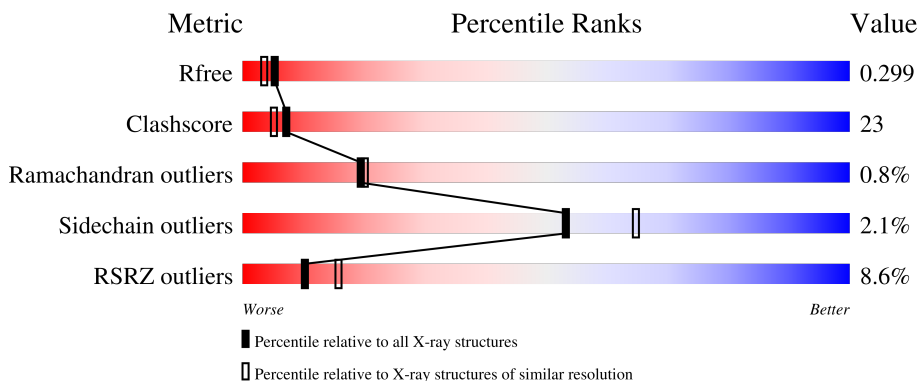
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.35 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	595	
2	B	2	
2	C	2	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	ASC	A	800	-	-	X	-
6	IOD	A	707	-	-	X	-

## 2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 5328 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Lactoperoxidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	595	4774	3037	847	863	1	26	0	0	0

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	2	28	16	2	10	0	0	0
2	C	2	28	16	2	10	0	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

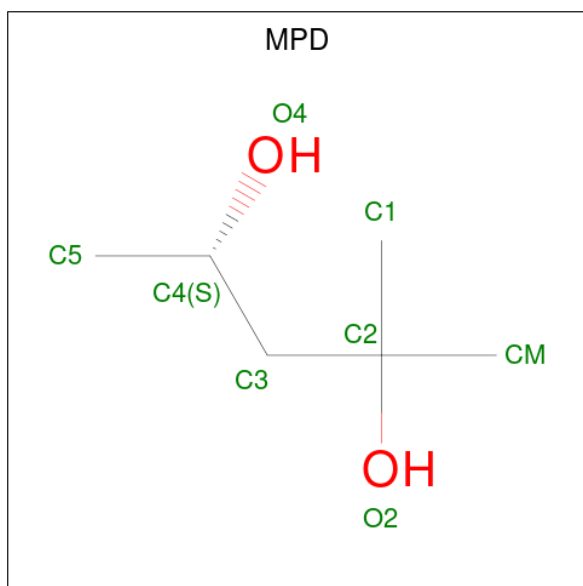
- Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C<sub>34</sub>H<sub>32</sub>FeN<sub>4</sub>O<sub>4</sub>).



- Molecule 6 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	9	Total I 9 9	0	0

- Molecule 7 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>2</sub>).



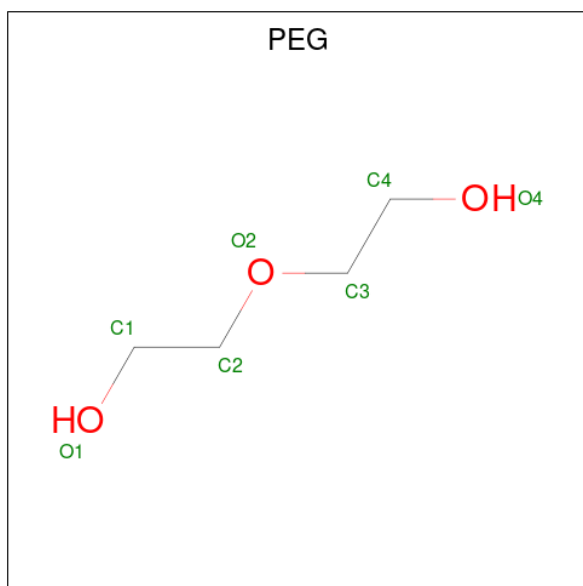
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 8 6 2	0	0

- Molecule 8 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 9 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $C_4H_{10}O_3$ ).



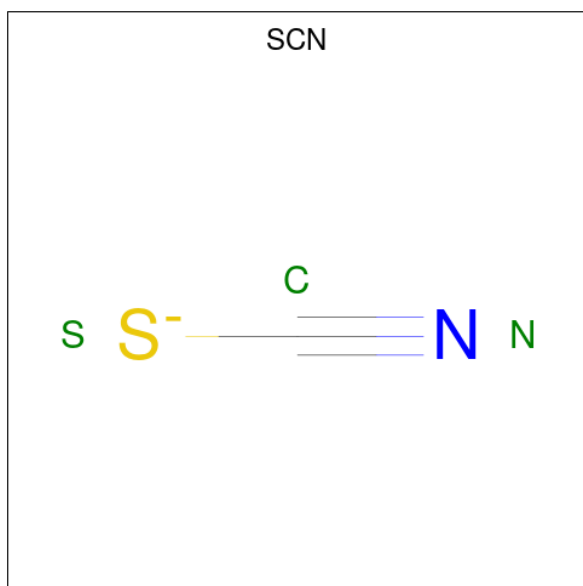
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 10 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

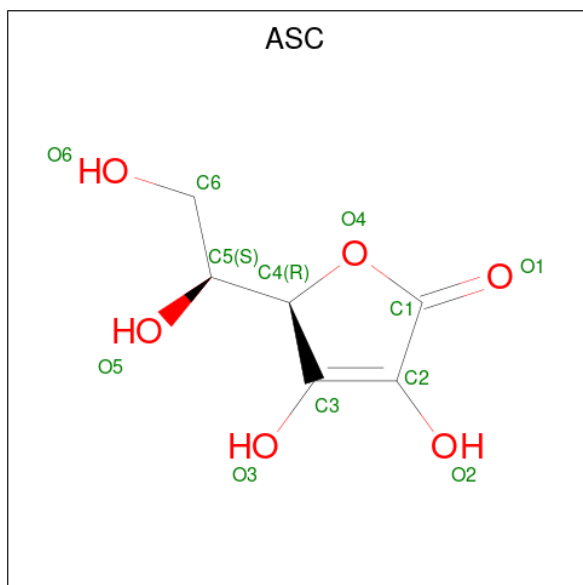
- Molecule 11 is THIOCYANATE ION (three-letter code: SCN) (formula: CNS).



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

- Molecule 12 is ASCORBIC ACID (three-letter code: ASC) (formula: C<sub>6</sub>H<sub>8</sub>O<sub>6</sub>).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	A	1	Total	C	O	0	0
			12	6	6		

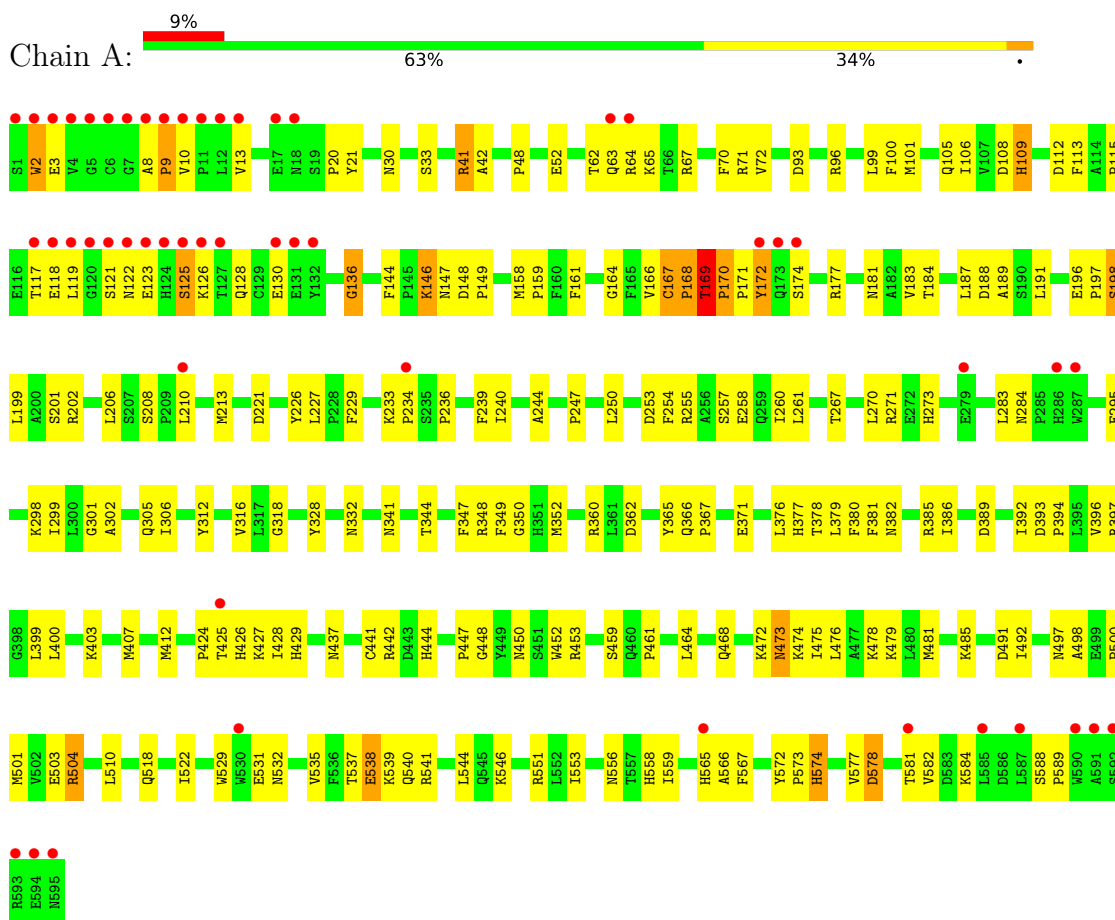
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	377	Total	O	0	0
			377	377		

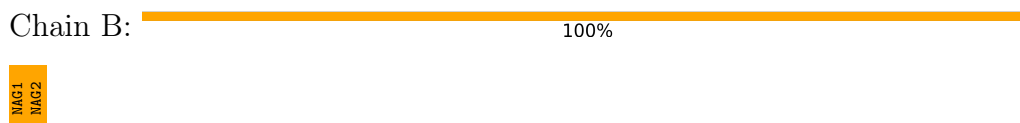
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

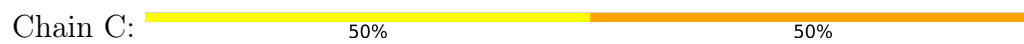
- Molecule 1: Lactoperoxidase



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



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



MAG1  
MAG2

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	53.71Å 79.61Å 65.78Å 90.00° 93.23° 90.00°	Depositor
Resolution (Å)	50.00 – 2.35 44.47 – 2.36	Depositor EDS
% Data completeness (in resolution range)	90.7 (50.00-2.35) 90.8 (44.47-2.36)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.92 (at 2.37Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.226 , 0.250 0.226 , 0.299	Depositor DCC
$R_{free}$ test set	1076 reflections (5.18%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	36.8	Xtrriage
Anisotropy	0.664	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 62.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5328	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.25% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, EDO, HEM, SEP, ASC, PEG, MPD, NAG, GOL, SCN, IOD

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	0.66	2/4891 (0.0%)	0.88	18/6634 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	48	PRO	N-CD	-13.07	1.29	1.47
1	A	9	PRO	N-CD	-11.58	1.31	1.47

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	109	HIS	N-CA-CB	-14.00	85.40	110.60
1	A	169	THR	C-N-CD	-9.56	99.58	120.60
1	A	2	TRP	CB-CA-C	-9.09	92.21	110.40
1	A	371	GLU	N-CA-C	-7.72	90.14	111.00
1	A	136	GLY	N-CA-C	7.29	131.32	113.10
1	A	187	LEU	N-CA-C	-7.06	91.95	111.00
1	A	109	HIS	CB-CA-C	6.70	123.81	110.40
1	A	574	HIS	N-CA-C	6.19	127.71	111.00
1	A	112	ASP	CB-CA-C	-6.17	98.07	110.40
1	A	412	MET	N-CA-C	6.03	127.28	111.00
1	A	13	VAL	N-CA-C	-5.93	94.98	111.00
1	A	125	SER	N-CA-C	-5.47	96.23	111.00
1	A	574	HIS	CB-CA-C	-5.41	99.58	110.40
1	A	473	ASN	CB-CA-C	5.25	120.91	110.40
1	A	532	ASN	N-CA-C	-5.07	97.30	111.00
1	A	504	ARG	CB-CA-C	-5.06	100.28	110.40
1	A	174	SER	CB-CA-C	-5.05	100.50	110.10
1	A	577	VAL	CB-CA-C	-5.01	101.89	111.40

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	A	4774	0	4686	216	0
2	B	28	0	25	3	0
2	C	28	0	25	1	0
3	A	1	0	0	0	0
4	A	43	0	30	11	0
5	A	28	0	26	0	0
6	A	9	0	0	4	0
7	A	8	0	13	4	0
8	A	4	0	6	1	0
9	A	7	0	9	0	0
10	A	6	0	8	0	0
11	A	3	0	0	0	0
12	A	12	0	6	6	0
13	A	377	0	0	3	0
All	All	5328	0	4834	221	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 23.

All (221) 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:119:LEU:O	1:A:119:LEU:HD23	1.42	1.14
1:A:170:PRO:HB2	1:A:171:PRO:CD	1.77	1.13
1:A:172:TYR:HE2	1:A:177:ARG:HA	1.09	1.10
1:A:166:VAL:O	1:A:168:PRO:HD3	1.54	1.06
1:A:170:PRO:CB	1:A:171:PRO:HD3	1.84	1.05
1:A:541:ARG:HA	1:A:544:LEU:HD12	1.41	1.02
1:A:118:GLU:HB2	1:A:121:SER:HB3	1.38	1.02
1:A:172:TYR:CE2	1:A:177:ARG:HA	1.98	0.99
1:A:425:THR:HG23	1:A:426:HIS:CE1	1.98	0.99

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:ALA:HB3	1:A:9:PRO:HD3	1.44	0.96
1:A:213:MET:HG2	1:A:273:HIS:CD2	2.03	0.94
1:A:424:PRO:O	1:A:425:THR:HG22	1.69	0.90
1:A:119:LEU:HD12	1:A:170:PRO:HG3	1.55	0.88
1:A:170:PRO:HB2	1:A:171:PRO:HD3	0.90	0.88
1:A:559:ILE:HG23	6:A:711:IOD:I	2.44	0.87
1:A:425:THR:CG2	1:A:426:HIS:CE1	2.58	0.86
1:A:172:TYR:HE2	1:A:177:ARG:CA	1.90	0.85
1:A:537:THR:H	1:A:540:GLN:HE21	1.24	0.83
1:A:117:THR:CG2	1:A:164:GLY:HA2	2.09	0.82
1:A:295:GLU:O	1:A:299:ILE:HG13	1.81	0.81
1:A:121:SER:HA	1:A:126:LYS:HD3	1.63	0.80
1:A:122:ASN:H	1:A:126:LYS:HE2	1.45	0.79
1:A:258:GLU:OE2	4:A:605:HEM:HMB3	1.82	0.79
1:A:166:VAL:O	1:A:168:PRO:CD	2.30	0.79
1:A:117:THR:HG23	1:A:164:GLY:HA2	1.65	0.78
1:A:146:LYS:HD3	1:A:147:ASN:ND2	1.98	0.77
1:A:348:ARG:HH11	1:A:437:ASN:ND2	1.82	0.77
1:A:108:ASP:OD2	4:A:605:HEM:CMD	2.33	0.77
1:A:117:THR:HG23	1:A:164:GLY:CA	2.16	0.76
1:A:197:PRO:HD2	1:A:198:SEP:O2P	1.85	0.75
1:A:257:SER:O	1:A:381:PHE:HA	1.86	0.75
1:A:255:ARG:HG2	12:A:800:ASC:H4	1.69	0.75
1:A:551:ARG:HD3	1:A:584:LYS:HA	1.67	0.75
1:A:130:GLU:OE1	1:A:426:HIS:HD2	1.69	0.74
1:A:407:MET:HB3	1:A:501:MET:HE3	1.71	0.73
1:A:166:VAL:C	1:A:168:PRO:HD3	2.09	0.73
1:A:199:LEU:HD22	1:A:254:PHE:CZ	2.24	0.73
2:B:1:NAG:H62	2:B:2:NAG:C7	2.19	0.72
1:A:108:ASP:OD2	4:A:605:HEM:HMD3	1.91	0.70
1:A:529:TRP:NE1	1:A:531:GLU:HG2	2.07	0.69
1:A:167:CYS:HB2	1:A:168:PRO:HD3	1.74	0.69
1:A:119:LEU:CD1	1:A:170:PRO:HG3	2.23	0.69
1:A:537:THR:HG23	1:A:540:GLN:NE2	2.08	0.69
1:A:475:ILE:O	1:A:479:LYS:HG3	1.92	0.68
1:A:328:TYR:CD2	1:A:531:GLU:HG3	2.28	0.68
1:A:258:GLU:OE2	4:A:605:HEM:CMB	2.41	0.68
4:A:605:HEM:HMB1	4:A:605:HEM:HBB2	1.74	0.68
1:A:122:ASN:H	1:A:126:LYS:CE	2.05	0.68
1:A:349:PHE:HA	1:A:497:ASN:HD21	1.59	0.68
1:A:425:THR:HG23	1:A:426:HIS:ND1	2.08	0.68

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:GLY:CA	1:A:504:ARG:O	2.44	0.66
1:A:130:GLU:CD	1:A:426:HIS:HD2	1.98	0.66
1:A:529:TRP:HE1	1:A:531:GLU:HG2	1.60	0.64
1:A:8:ALA:CB	1:A:9:PRO:HD3	2.17	0.63
1:A:472:LYS:HD2	1:A:500:PRO:HG2	1.81	0.63
1:A:122:ASN:N	1:A:126:LYS:CE	2.61	0.63
1:A:118:GLU:CB	1:A:121:SER:HB3	2.22	0.63
1:A:229:PHE:CD1	1:A:247:PRO:HG2	2.34	0.63
1:A:425:THR:CG2	1:A:426:HIS:ND1	2.61	0.62
1:A:332:ASN:OD1	1:A:332:ASN:C	2.34	0.62
1:A:117:THR:HG21	1:A:164:GLY:HA2	1.80	0.62
2:B:1:NAG:H62	2:B:2:NAG:C8	2.30	0.62
1:A:407:MET:HB3	1:A:501:MET:CE	2.29	0.62
1:A:221:ASP:HB2	1:A:226:TYR:CZ	2.35	0.61
1:A:122:ASN:N	1:A:126:LYS:HE3	2.15	0.61
1:A:208:SER:O	1:A:210:LEU:N	2.28	0.61
1:A:267:THR:O	1:A:271:ARG:HB2	2.00	0.61
1:A:464:LEU:HD12	1:A:481:MET:HG3	1.82	0.61
1:A:123:GLU:O	1:A:126:LYS:HG2	2.01	0.61
1:A:529:TRP:CD1	1:A:531:GLU:HG2	2.35	0.61
1:A:2:TRP:HE3	1:A:3:GLU:H	1.46	0.60
2:B:1:NAG:H62	2:B:2:NAG:H82	1.83	0.60
1:A:169:THR:H	1:A:170:PRO:HD3	1.66	0.60
1:A:52:GLU:OE1	1:A:65:LYS:HB2	2.01	0.60
1:A:52:GLU:OE1	1:A:62:THR:HB	2.02	0.60
1:A:318:GLY:HA3	1:A:504:ARG:O	2.02	0.60
1:A:113:PHE:CZ	1:A:115:PRO:HB3	2.37	0.59
1:A:227:LEU:HD22	1:A:250:LEU:O	2.02	0.59
1:A:227:LEU:HD21	1:A:270:LEU:HD13	1.84	0.59
1:A:301:GLY:O	1:A:305:GLN:HG3	2.02	0.59
1:A:118:GLU:O	1:A:118:GLU:HG2	2.03	0.58
1:A:397:ARG:CG	1:A:559:ILE:HD13	2.33	0.58
1:A:169:THR:N	1:A:170:PRO:HD3	2.18	0.58
1:A:202:ARG:HD3	7:A:598:MPD:H11	1.86	0.58
1:A:119:LEU:O	1:A:119:LEU:CD2	2.35	0.58
1:A:424:PRO:O	1:A:425:THR:CG2	2.47	0.58
1:A:119:LEU:HD23	1:A:119:LEU:C	2.20	0.58
1:A:10:VAL:HG13	1:A:10:VAL:O	2.03	0.58
1:A:169:THR:N	1:A:170:PRO:CD	2.66	0.58
1:A:362:ASP:O	1:A:365:TYR:N	2.36	0.58
1:A:99:LEU:HG	1:A:567:PHE:CE1	2.40	0.57

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:ASP:OD2	4:A:605:HEM:HMD2	2.05	0.57
1:A:318:GLY:HA2	1:A:504:ARG:O	2.05	0.57
1:A:166:VAL:C	1:A:168:PRO:CD	2.72	0.57
1:A:169:THR:O	1:A:169:THR:HG22	2.05	0.57
1:A:397:ARG:HG3	1:A:559:ILE:CD1	2.35	0.56
1:A:93:ASP:O	1:A:403:LYS:HD3	2.06	0.56
1:A:537:THR:H	1:A:540:GLN:NE2	2.00	0.56
1:A:400:LEU:HD11	1:A:553:ILE:HD13	1.88	0.55
1:A:42:ALA:HB2	1:A:166:VAL:HG11	1.88	0.55
1:A:118:GLU:HB2	1:A:121:SER:CB	2.25	0.55
1:A:130:GLU:OE1	1:A:426:HIS:CD2	2.56	0.55
1:A:551:ARG:NH1	1:A:582:VAL:O	2.38	0.54
1:A:393:ASP:OD2	1:A:558:HIS:HB2	2.06	0.54
1:A:366:GLN:O	1:A:367:PRO:C	2.43	0.54
1:A:233:LYS:HA	1:A:234:PRO:C	2.28	0.54
1:A:381:PHE:HZ	12:A:800:ASC:H62	1.71	0.54
1:A:172:TYR:CE2	1:A:177:ARG:CA	2.77	0.54
1:A:428:ILE:HG13	1:A:429:HIS:H	1.72	0.54
1:A:244:ALA:HB2	2:C:1:NAG:O5	2.08	0.53
1:A:407:MET:CB	1:A:501:MET:CE	2.86	0.53
1:A:464:LEU:HD11	1:A:478:LYS:HA	1.91	0.53
1:A:312:TYR:O	1:A:316:VAL:HG23	2.09	0.53
1:A:565:HIS:HB3	6:A:720:IOD:I	2.78	0.53
1:A:344:THR:O	4:A:605:HEM:HMD1	2.08	0.52
1:A:202:ARG:HH11	7:A:598:MPD:H11	1.74	0.52
1:A:397:ARG:HG2	1:A:559:ILE:HD13	1.91	0.52
1:A:227:LEU:CD2	1:A:270:LEU:HD13	2.39	0.52
1:A:376:LEU:HA	1:A:379:LEU:HD12	1.91	0.52
1:A:546:LYS:HG3	13:A:889:HOH:O	2.09	0.51
1:A:108:ASP:CG	4:A:605:HEM:HMD3	2.30	0.51
1:A:63:GLN:HG3	1:A:71:ARG:HH12	1.74	0.51
1:A:169:THR:H	1:A:170:PRO:CD	2.22	0.51
1:A:106:ILE:HG23	1:A:191:LEU:HD11	1.93	0.50
1:A:72:VAL:O	1:A:72:VAL:HG23	2.12	0.50
1:A:20:PRO:HG2	1:A:21:TYR:CE1	2.47	0.49
1:A:70:PHE:CD1	1:A:485:LYS:HB2	2.47	0.49
1:A:352:MET:HB2	13:A:625:HOH:O	2.12	0.49
1:A:539:LYS:HB3	1:A:589:PRO:HB3	1.95	0.49
1:A:428:ILE:HG13	1:A:429:HIS:N	2.27	0.49
1:A:8:ALA:N	1:A:9:PRO:CD	2.75	0.49
1:A:30:ASN:HB3	1:A:33:SER:O	2.13	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:LYS:CD	1:A:147:ASN:ND2	2.71	0.49
1:A:442:ARG:NH2	1:A:491:ASP:OD2	2.46	0.49
1:A:328:TYR:CE2	1:A:531:GLU:HG3	2.47	0.48
1:A:474:LYS:HB3	1:A:478:LYS:NZ	2.27	0.48
1:A:378:THR:HG22	8:A:609:EDO:H21	1.96	0.48
1:A:428:ILE:CG1	1:A:429:HIS:N	2.76	0.48
1:A:159:PRO:HG3	1:A:426:HIS:CD2	2.49	0.48
1:A:184:THR:OG1	1:A:188:ASP:OD2	2.31	0.48
1:A:392:ILE:O	1:A:396:VAL:HG23	2.14	0.47
1:A:253:ASP:OD2	1:A:255:ARG:HB2	2.15	0.47
1:A:574:HIS:C	1:A:574:HIS:HD1	2.19	0.46
1:A:255:ARG:HD2	12:A:800:ASC:C2	2.45	0.46
1:A:348:ARG:C	1:A:350:GLY:N	2.69	0.46
1:A:397:ARG:HG3	1:A:559:ILE:HD13	1.96	0.46
1:A:283:LEU:O	1:A:284:ASN:ND2	2.47	0.46
1:A:108:ASP:OD1	4:A:605:HEM:HMD3	2.16	0.46
1:A:9:PRO:O	1:A:41:ARG:NH1	2.49	0.46
1:A:261:LEU:HD22	1:A:399:LEU:HG	1.98	0.46
1:A:267:THR:HG21	1:A:392:ILE:HD13	1.97	0.46
1:A:67:ARG:NH2	1:A:448:GLY:N	2.64	0.46
1:A:105:GLN:O	1:A:109:HIS:HB2	2.16	0.46
1:A:144:PHE:CE2	1:A:158:MET:HG3	2.50	0.46
1:A:476:LEU:HD21	1:A:498:ALA:HB1	1.98	0.46
1:A:199:LEU:HD13	7:A:598:MPD:H12	1.98	0.46
1:A:377:HIS:HA	1:A:380:PHE:CE2	2.51	0.46
1:A:397:ARG:HG3	1:A:559:ILE:HD11	1.96	0.46
1:A:123:GLU:H	1:A:126:LYS:HE3	1.81	0.46
1:A:239:PHE:CZ	1:A:427:LYS:HD3	2.51	0.46
1:A:213:MET:CG	1:A:273:HIS:CD2	2.90	0.45
1:A:468:GLN:O	1:A:472:LYS:N	2.49	0.45
1:A:62:THR:HG22	1:A:64:ARG:HG2	1.98	0.45
1:A:113:PHE:HB3	1:A:183:VAL:HG13	1.98	0.45
1:A:119:LEU:HD12	1:A:170:PRO:CG	2.36	0.45
1:A:172:TYR:CD2	1:A:177:ARG:HB2	2.52	0.45
1:A:229:PHE:CG	1:A:247:PRO:HG2	2.52	0.45
1:A:258:GLU:CD	4:A:605:HEM:HMB3	2.36	0.45
1:A:169:THR:O	1:A:169:THR:CG2	2.65	0.45
1:A:119:LEU:CD1	1:A:170:PRO:CG	2.94	0.45
1:A:166:VAL:HG23	1:A:172:TYR:OH	2.16	0.45
1:A:447:PRO:HG2	1:A:452:TRP:CE2	2.52	0.45
1:A:588:SER:N	1:A:589:PRO:CD	2.80	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:LYS:HE3	1:A:535:VAL:HG12	1.99	0.44
1:A:348:ARG:NH1	1:A:437:ASN:ND2	2.60	0.44
1:A:188:ASP:O	1:A:189:ALA:HB3	2.18	0.44
1:A:578:ASP:O	1:A:581:THR:OG1	2.36	0.44
1:A:126:LYS:HA	1:A:161:PHE:CZ	2.52	0.44
1:A:126:LYS:NZ	13:A:964:HOH:O	2.50	0.44
1:A:125:SER:HA	1:A:128:GLN:CB	2.49	0.43
1:A:452:TRP:HH2	6:A:707:IOD:I	2.72	0.43
1:A:518:GLN:O	1:A:522:ILE:HG12	2.19	0.43
1:A:453:ARG:NH2	1:A:459:SER:OG	2.52	0.43
1:A:538:GLU:O	1:A:539:LYS:C	2.55	0.43
1:A:239:PHE:CE1	1:A:427:LYS:HD3	2.53	0.43
1:A:240:ILE:HD11	1:A:382:ASN:HA	2.00	0.43
1:A:341:ASN:OD1	1:A:444:HIS:ND1	2.43	0.43
1:A:349:PHE:HA	1:A:497:ASN:ND2	2.31	0.43
1:A:121:SER:HA	1:A:126:LYS:CD	2.43	0.43
1:A:551:ARG:CZ	1:A:584:LYS:HG2	2.49	0.43
1:A:393:ASP:N	1:A:394:PRO:CD	2.82	0.42
1:A:166:VAL:O	1:A:167:CYS:HB2	2.19	0.42
1:A:109:HIS:HA	1:A:255:ARG:NH2	2.34	0.42
1:A:101:MET:SD	1:A:101:MET:C	2.98	0.42
1:A:522:ILE:HD13	1:A:522:ILE:HA	1.79	0.42
1:A:99:LEU:HD23	1:A:566:ALA:HB1	2.02	0.42
1:A:202:ARG:HD2	7:A:598:MPD:H4	2.01	0.42
1:A:572:TYR:CD1	1:A:573:PRO:HA	2.55	0.42
1:A:258:GLU:HG3	12:A:800:ASC:O4	2.19	0.41
1:A:468:GLN:HA	1:A:473:ASN:O	2.20	0.41
1:A:492:ILE:HD11	1:A:510:LEU:HD21	2.01	0.41
1:A:113:PHE:O	1:A:181:ASN:HA	2.21	0.41
1:A:196:GLU:HA	1:A:197:PRO:HD3	1.81	0.41
1:A:574:HIS:C	1:A:574:HIS:ND1	2.72	0.41
1:A:109:HIS:NE2	12:A:800:ASC:O1	2.51	0.41
1:A:474:LYS:O	1:A:478:LYS:HG3	2.21	0.41
1:A:170:PRO:CB	1:A:171:PRO:CD	2.60	0.41
1:A:348:ARG:HH11	1:A:437:ASN:HD22	1.64	0.41
1:A:302:ALA:O	1:A:306:ILE:HG13	2.20	0.41
4:A:605:HEM:CMB	4:A:605:HEM:HBB2	2.47	0.41
1:A:236:PRO:O	1:A:239:PHE:HB3	2.21	0.41
1:A:260:ILE:HD11	1:A:386:ILE:HG13	2.02	0.41
1:A:255:ARG:CD	12:A:800:ASC:C2	2.98	0.41
1:A:385:ARG:O	1:A:389:ASP:HB3	2.21	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:ARG:HD2	1:A:100:PHE:CG	2.56	0.41
1:A:119:LEU:CD2	1:A:119:LEU:C	2.87	0.40
1:A:148:ASP:HA	1:A:149:PRO:HD3	1.93	0.40
1:A:450:ASN:OD1	1:A:461:PRO:HD2	2.21	0.40
1:A:537:THR:N	1:A:540:GLN:HE21	2.05	0.40
1:A:271:ARG:HD3	1:A:556:ASN:O	2.21	0.40
1:A:452:TRP:CH2	6:A:707:IOD:I	3.45	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	592/595 (100%)	558 (94%)	29 (5%)	5 (1%)	19 20

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	167	CYS
1	A	168	PRO
1	A	170	PRO
1	A	136	GLY
1	A	169	THR

### 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%)	506 (98%)	11 (2%)	53 65

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	ARG
1	A	146	LYS
1	A	172	TYR
1	A	201	SER
1	A	206	LEU
1	A	347	PHE
1	A	360	ARG
1	A	441	CYS
1	A	503	GLU
1	A	538	GLU
1	A	578	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	147	ASN
1	A	273	HIS
1	A	284	ASN
1	A	364	ASN
1	A	426	HIS
1	A	437	ASN
1	A	497	ASN
1	A	521	GLN
1	A	540	GLN
1	A	545	GLN
1	A	558	HIS
1	A	565	HIS
1	A	570	ASN
1	A	595	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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
1	SEP	A	198	1	8,9,10	0.94	0	8,12,14	2.44	2 (25%)

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
1	SEP	A	198	1	-	4/5/8/10	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	198	SEP	OG-CB-CA	6.11	114.09	108.14
1	A	198	SEP	OG-P-O1P	2.39	113.18	106.47

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	198	SEP	CB-OG-P-O2P
1	A	198	SEP	CB-OG-P-O3P
1	A	198	SEP	CA-CB-OG-P
1	A	198	SEP	CB-OG-P-O1P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	198	SEP	1	0

## 5.5 Carbohydrates [i](#)

4 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	B	1	2,1	14,14,15	0.63	0	17,19,21	1.64	3 (17%)
2	NAG	B	2	2	14,14,15	0.60	0	17,19,21	1.13	2 (11%)
2	NAG	C	1	2,1	14,14,15	0.73	0	17,19,21	1.25	1 (5%)
2	NAG	C	2	2	14,14,15	0.47	0	17,19,21	1.65	2 (11%)

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	B	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	B	2	2	-	2/6/23/26	0/1/1/1
2	NAG	C	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2	NAG	C1-O5-C5	5.65	119.84	112.19
2	B	1	NAG	C3-C4-C5	4.15	117.64	110.24
2	B	1	NAG	C4-C3-C2	3.25	115.78	111.02
2	C	2	NAG	O5-C5-C6	2.94	111.81	107.20
2	C	1	NAG	C4-C3-C2	2.92	115.30	111.02

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	NAG	C4-C3-C2	2.64	114.88	111.02
2	B	1	NAG	C1-O5-C5	2.24	115.22	112.19
2	B	2	NAG	O5-C5-C6	2.17	110.61	107.20

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	2	NAG	O5-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
2	B	2	NAG	C4-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6
2	C	1	NAG	O5-C5-C6-O6
2	C	1	NAG	C4-C5-C6-O6

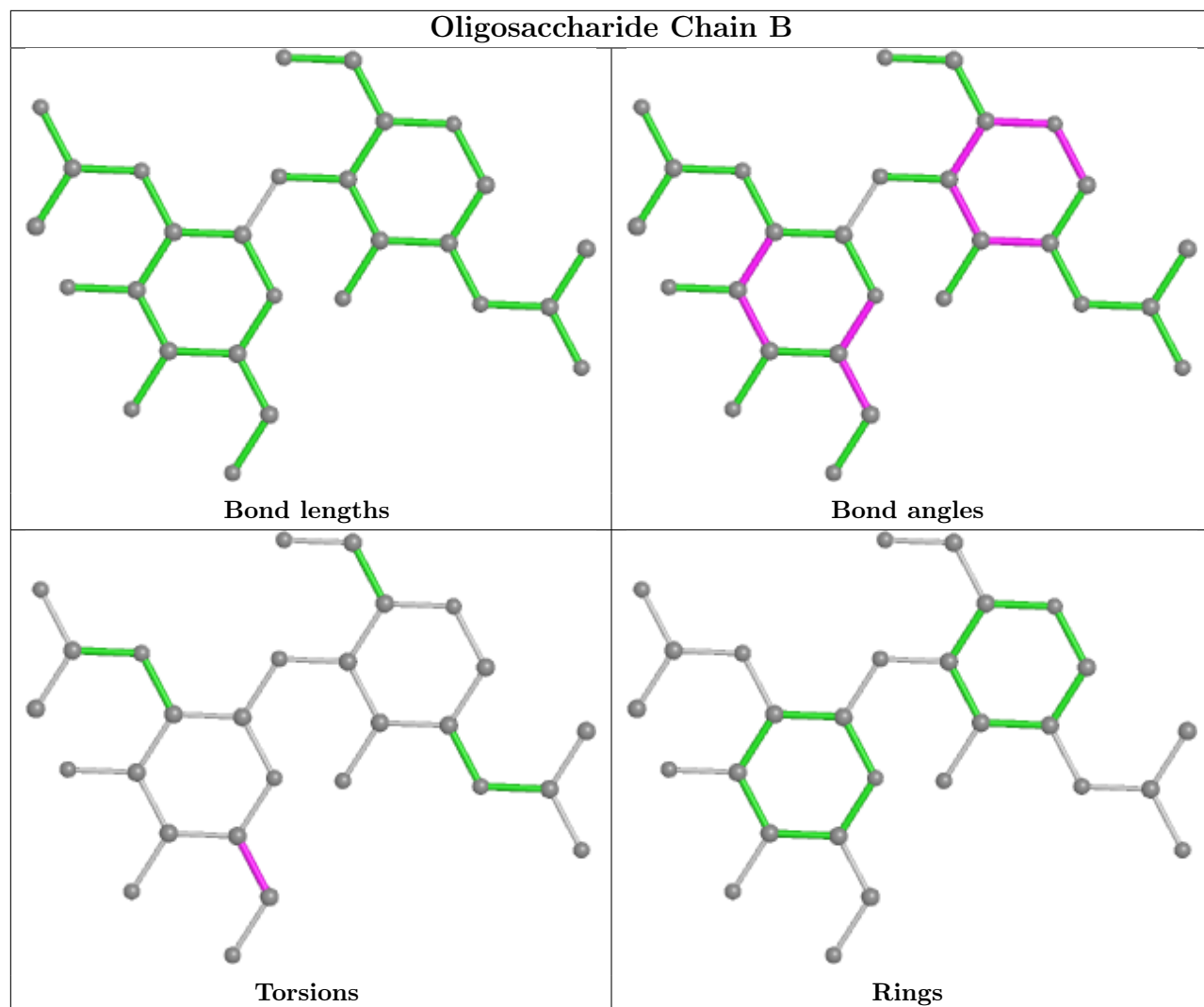
There are no ring outliers.

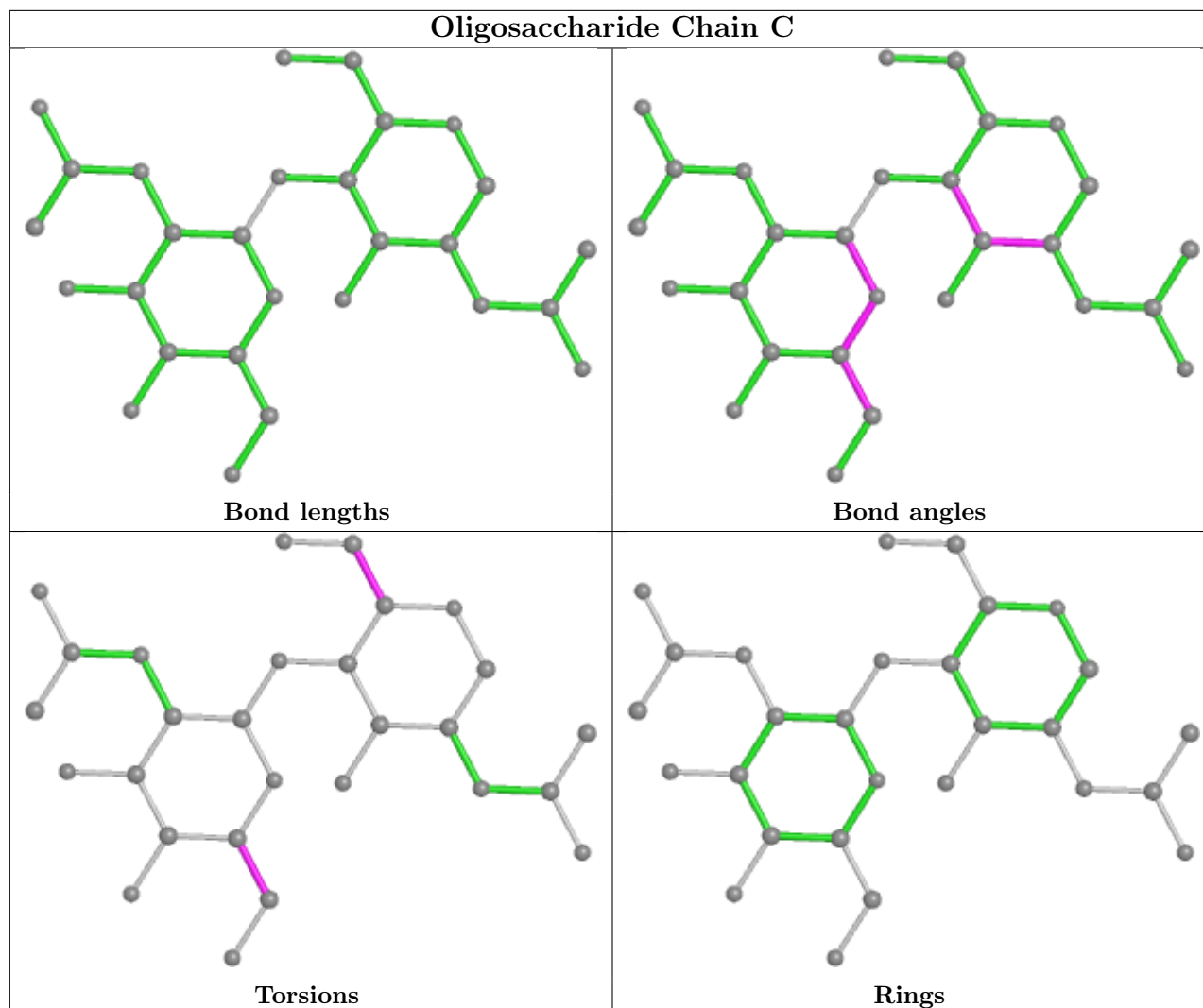
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	NAG	1	0
2	B	1	NAG	3	0
2	B	2	NAG	3	0

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







## 5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 10 are monoatomic - leaving 9 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	HEM	A	605	13,1	41,50,50	2.08	13 (31%)	45,82,82	2.20	20 (44%)
11	SCN	A	615	-	1,2,2	1.25	0	0,1,1	-	-
5	NAG	A	604	1	14,14,15	0.50	0	17,19,21	1.76	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	MPD	A	598	-	7,7,7	2.75	2 (28%)	9,10,10	1.56	3 (33%)
10	GOL	A	612	-	5,5,5	0.70	0	5,5,5	0.93	0
9	PEG	A	611	-	6,6,6	1.72	1 (16%)	5,5,5	0.97	0
8	EDO	A	609	-	3,3,3	0.29	0	2,2,2	0.11	0
5	NAG	A	596	1	14,14,15	0.63	0	17,19,21	1.33	4 (23%)
12	ASC	A	800	-	12,12,12	1.23	1 (8%)	17,17,17	2.90	9 (52%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	HEM	A	605	13,1	-	4/12/54/54	-
5	NAG	A	604	1	-	2/6/23/26	0/1/1/1
7	MPD	A	598	-	-	1/5/5/5	-
10	GOL	A	612	-	-	0/4/4/4	-
9	PEG	A	611	-	-	2/4/4/4	-
8	EDO	A	609	-	-	0/1/1/1	-
5	NAG	A	596	1	-	2/6/23/26	0/1/1/1
12	ASC	A	800	-	-	5/6/22/22	0/1/1/1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	598	MPD	C1-C2	-5.30	1.36	1.52
4	A	605	HEM	CMC-C2C	4.79	1.63	1.51
7	A	598	MPD	O2-C2	-4.78	1.32	1.44
4	A	605	HEM	C3C-C2C	-4.57	1.34	1.40
9	A	611	PEG	O1-C1	-4.04	1.21	1.42
4	A	605	HEM	C3D-C2D	4.01	1.45	1.36
4	A	605	HEM	CMB-C2B	3.76	1.58	1.50
12	A	800	ASC	O4-C4	-3.63	1.39	1.45
4	A	605	HEM	FE-NB	3.60	2.14	1.96
4	A	605	HEM	C3C-CAC	3.39	1.54	1.47
4	A	605	HEM	CBD-CGD	3.29	1.58	1.50
4	A	605	HEM	C1B-NB	-2.97	1.35	1.40
4	A	605	HEM	CHB-C1B	2.96	1.42	1.35
4	A	605	HEM	C2A-C3A	-2.91	1.29	1.37
4	A	605	HEM	CAD-C3D	2.42	1.57	1.51

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	605	HEM	O1D-CGD	2.10	1.29	1.22
4	A	605	HEM	C3B-C4B	-2.09	1.40	1.44

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	800	ASC	O1-C1-C2	-6.81	118.69	129.37
4	A	605	HEM	C4A-C3A-C2A	5.82	111.05	107.00
12	A	800	ASC	O4-C1-O1	5.80	128.10	121.25
5	A	604	NAG	C1-O5-C5	4.88	118.81	112.19
4	A	605	HEM	CMD-C2D-C1D	4.88	132.46	125.04
4	A	605	HEM	C1B-NB-C4B	4.25	109.46	105.07
12	A	800	ASC	O4-C4-C5	4.01	123.14	110.04
4	A	605	HEM	CHC-C4B-NB	3.87	128.64	124.43
4	A	605	HEM	CMC-C2C-C3C	3.47	131.16	124.68
4	A	605	HEM	CBD-CAD-C3D	-3.40	103.17	112.63
4	A	605	HEM	CAD-C3D-C4D	3.20	130.25	124.66
12	A	800	ASC	O5-C5-C6	3.12	116.45	109.14
4	A	605	HEM	CAA-C2A-C3A	3.01	135.88	127.25
4	A	605	HEM	CMA-C3A-C4A	-2.92	123.97	128.46
12	A	800	ASC	O6-C6-C5	2.83	117.24	111.07
5	A	596	NAG	C1-O5-C5	2.64	115.78	112.19
4	A	605	HEM	C3C-C4C-NC	-2.60	106.03	110.94
4	A	605	HEM	C3D-C4D-ND	2.59	113.05	110.17
5	A	596	NAG	O5-C5-C6	2.54	111.18	107.20
5	A	604	NAG	C3-C4-C5	2.50	114.69	110.24
12	A	800	ASC	C1-C2-C3	-2.50	104.63	107.80
4	A	605	HEM	O1D-CGD-CBD	-2.48	115.10	123.08
7	A	598	MPD	C5-C4-C3	2.48	123.38	111.69
12	A	800	ASC	O4-C4-C3	-2.38	101.26	103.71
5	A	604	NAG	C2-N2-C7	2.29	126.17	122.90
4	A	605	HEM	O2D-CGD-CBD	2.28	121.36	114.03
12	A	800	ASC	O3-C3-C4	2.27	124.00	118.08
4	A	605	HEM	C4D-C3D-C2D	-2.24	103.63	106.90
5	A	596	NAG	C4-C3-C2	2.20	114.25	111.02
4	A	605	HEM	CMD-C2D-C3D	-2.14	120.31	126.12
4	A	605	HEM	CHD-C1D-ND	2.13	126.74	124.43
7	A	598	MPD	CM-C2-C1	2.12	114.98	110.57
4	A	605	HEM	C4B-C3B-C2B	-2.08	105.46	107.11
7	A	598	MPD	C1-C2-C3	-2.06	100.37	109.96
4	A	605	HEM	C4C-CHD-C1D	-2.05	119.85	122.56
4	A	605	HEM	CHC-C4B-C3B	-2.02	121.47	124.57

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	596	NAG	O7-C7-C8	-2.02	118.31	122.06
4	A	605	HEM	C2C-C3C-C4C	2.02	108.31	106.90
12	A	800	ASC	O3-C3-C2	-2.00	127.03	132.29

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	598	MPD	C2-C3-C4-O4
12	A	800	ASC	C3-C4-C5-C6
12	A	800	ASC	C3-C4-C5-O5
12	A	800	ASC	O4-C4-C5-C6
12	A	800	ASC	O4-C4-C5-O5
5	A	596	NAG	O5-C5-C6-O6
5	A	596	NAG	C4-C5-C6-O6
12	A	800	ASC	O5-C5-C6-O6
5	A	604	NAG	C4-C5-C6-O6
5	A	604	NAG	O5-C5-C6-O6
9	A	611	PEG	O1-C1-C2-O2
9	A	611	PEG	O2-C3-C4-O4
4	A	605	HEM	CAA-CBA-CGA-O2A
4	A	605	HEM	CAA-CBA-CGA-O1A
4	A	605	HEM	CAD-CBD-CGD-O2D
4	A	605	HEM	CAD-CBD-CGD-O1D

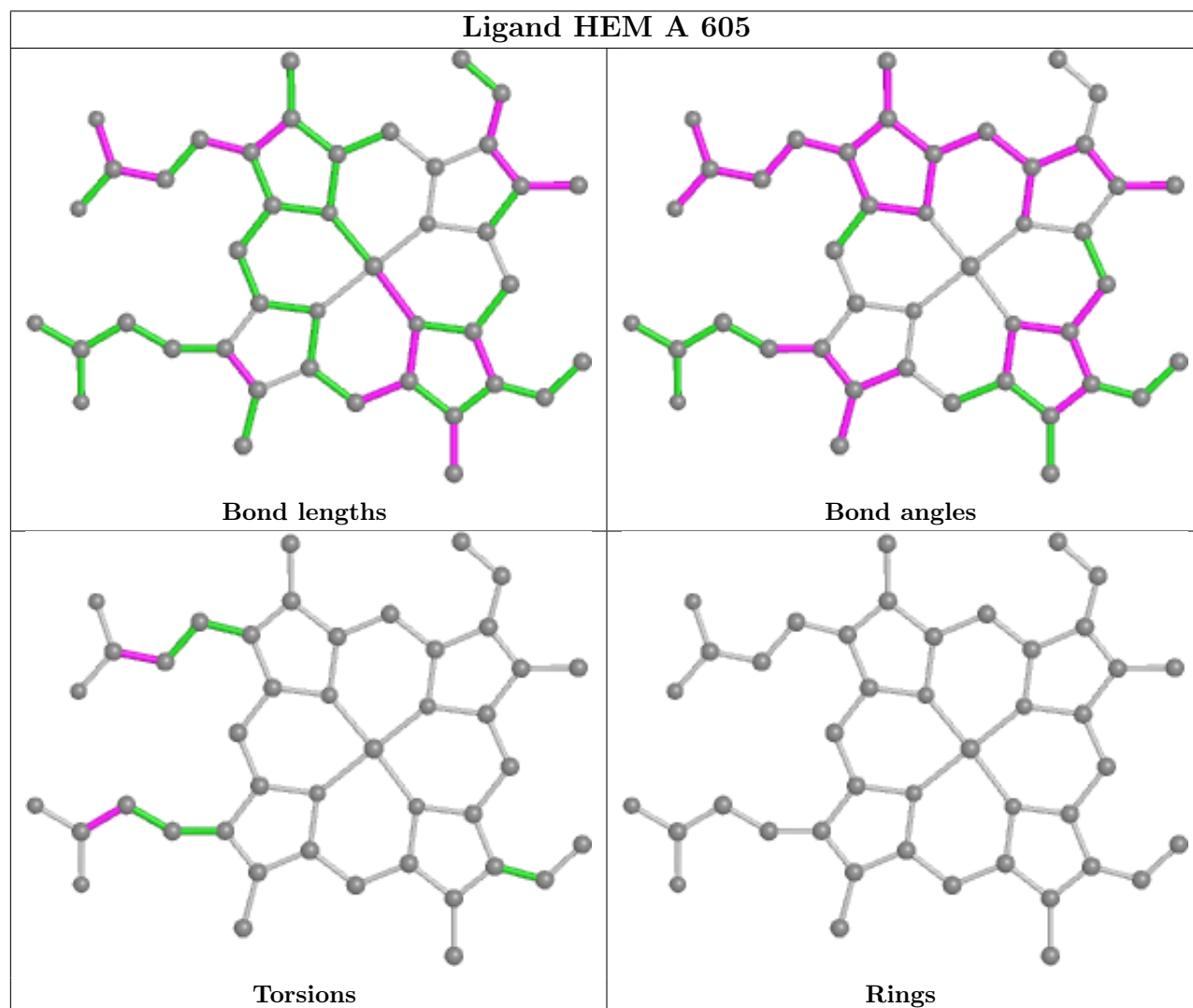
There are no ring outliers.

4 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	605	HEM	11	0
7	A	598	MPD	4	0
8	A	609	EDO	1	0
12	A	800	ASC	6	0

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

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



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	594/595 (99%)	0.53	51 (8%) <b>10</b> <b>16</b>	26, 47, 84, 100	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	TRP	12.4
1	A	122	ASN	11.3
1	A	172	TYR	9.7
1	A	119	LEU	8.1
1	A	120	GLY	7.1
1	A	173	GLN	6.9
1	A	121	SER	6.5
1	A	593	ARG	6.4
1	A	234	PRO	6.2
1	A	124	HIS	6.2
1	A	595	ASN	6.0
1	A	12	LEU	5.9
1	A	10	VAL	5.8
1	A	13	VAL	5.2
1	A	132	TYR	5.0
1	A	4	VAL	5.0
1	A	6	CYS	4.9
1	A	117	THR	4.7
1	A	587	LEU	4.4
1	A	123	GLU	4.1
1	A	1	SER	4.0
1	A	9	PRO	3.9
1	A	131	GLU	3.9
1	A	11	PRO	3.8
1	A	5	GLY	3.7
1	A	126	LYS	3.6
1	A	174	SER	3.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	530	TRP	3.5
1	A	591	ALA	3.4
1	A	594	GLU	3.3
1	A	8	ALA	3.2
1	A	125	SER	3.1
1	A	64	ARG	2.9
1	A	590	TRP	2.9
1	A	17	GLU	2.9
1	A	425	THR	2.8
1	A	581	THR	2.8
1	A	3	GLU	2.7
1	A	7	GLY	2.7
1	A	118	GLU	2.6
1	A	279	GLU	2.5
1	A	585	LEU	2.5
1	A	127	THR	2.5
1	A	210	LEU	2.5
1	A	287	TRP	2.5
1	A	130	GLU	2.3
1	A	565	HIS	2.3
1	A	63	GLN	2.3
1	A	286	HIS	2.2
1	A	592	SER	2.2
1	A	18	ASN	2.1

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
1	SEP	A	198	10/11	0.79	0.25	51,52,53,54	0

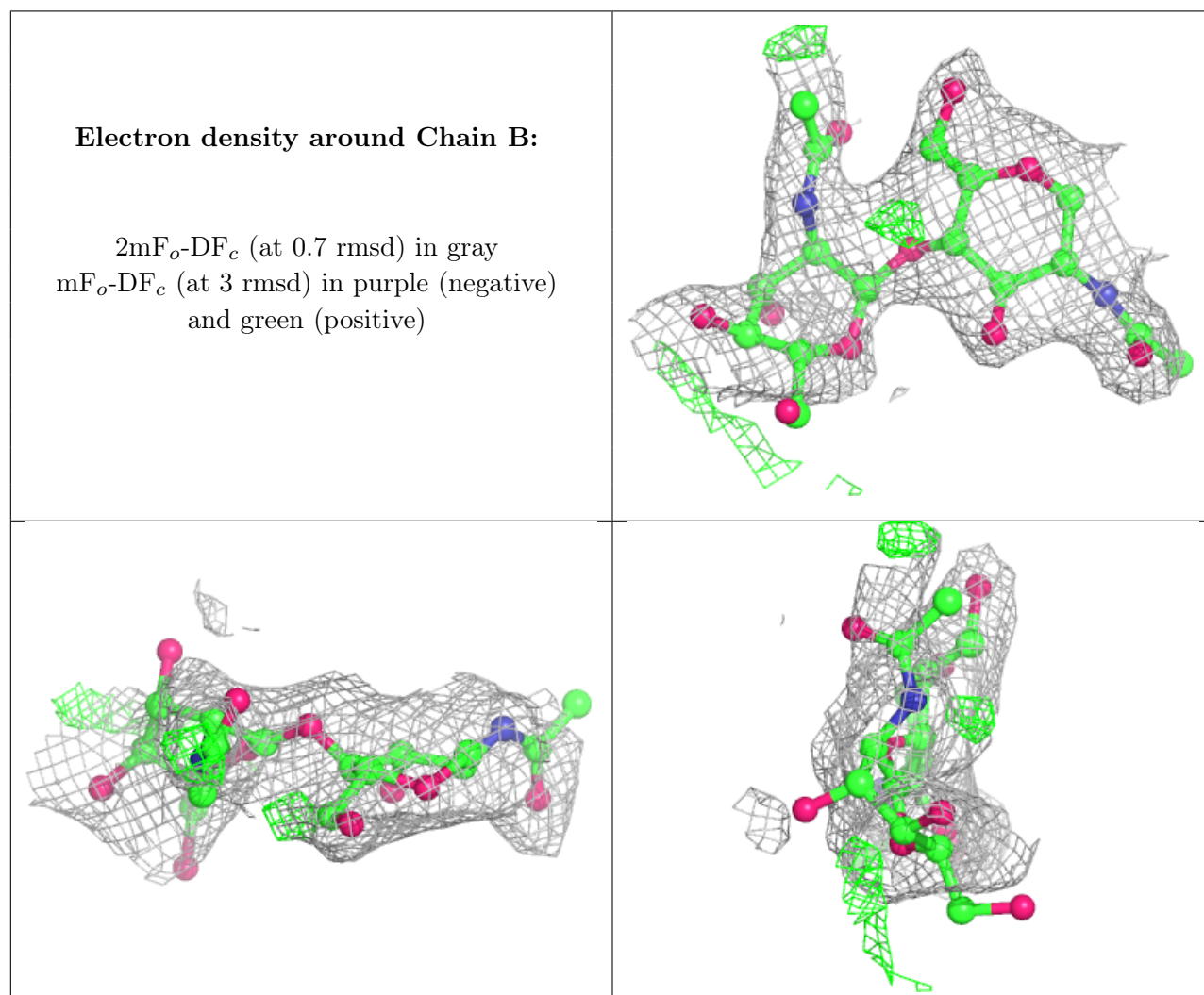
## 6.3 Carbohydrates [i](#)

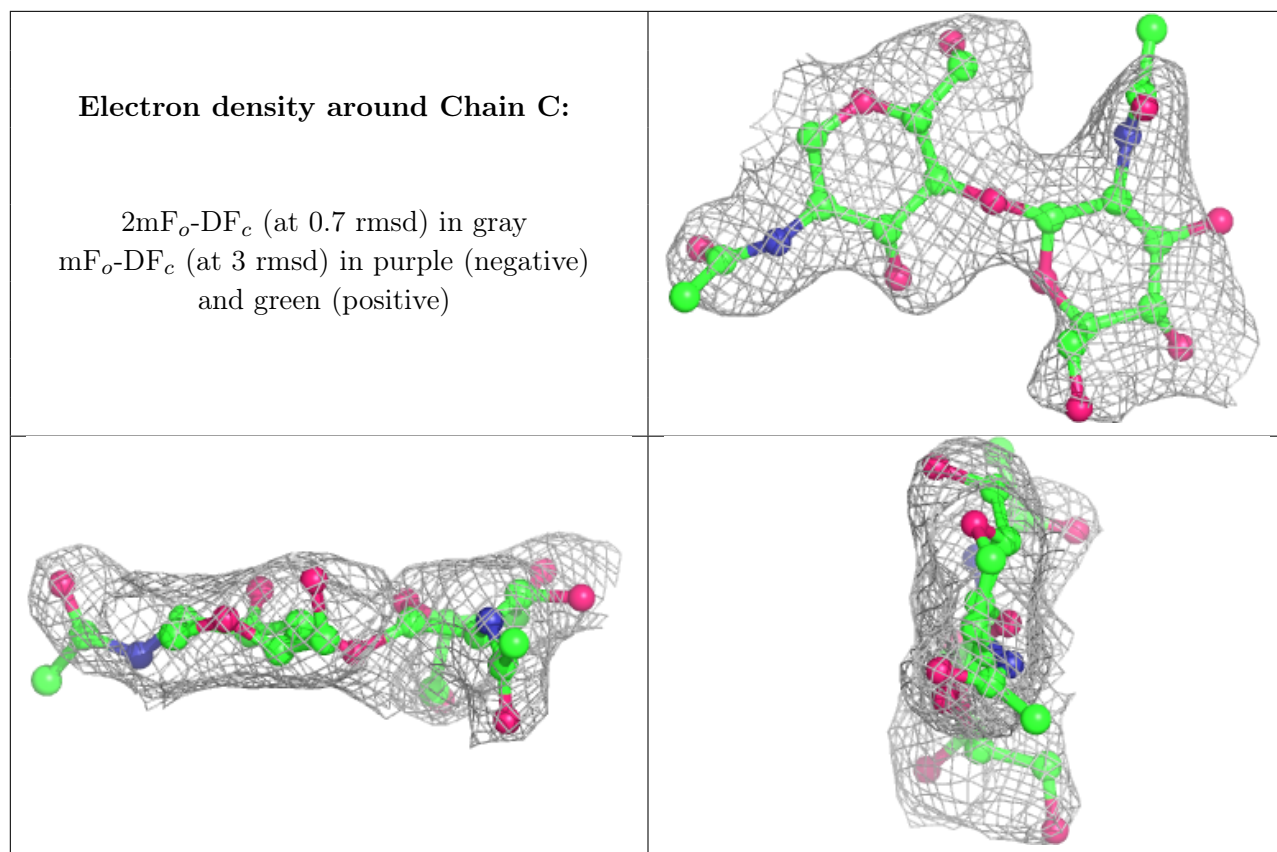
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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



Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAG	B	2	14/15	0.73	0.26	83,85,88,89	0
2	NAG	C	2	14/15	0.82	0.21	70,72,73,73	0
2	NAG	B	1	14/15	0.85	0.18	70,73,75,79	0
2	NAG	C	1	14/15	0.87	0.15	58,60,63,67	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.





## 6.4 Ligands [i](#)

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

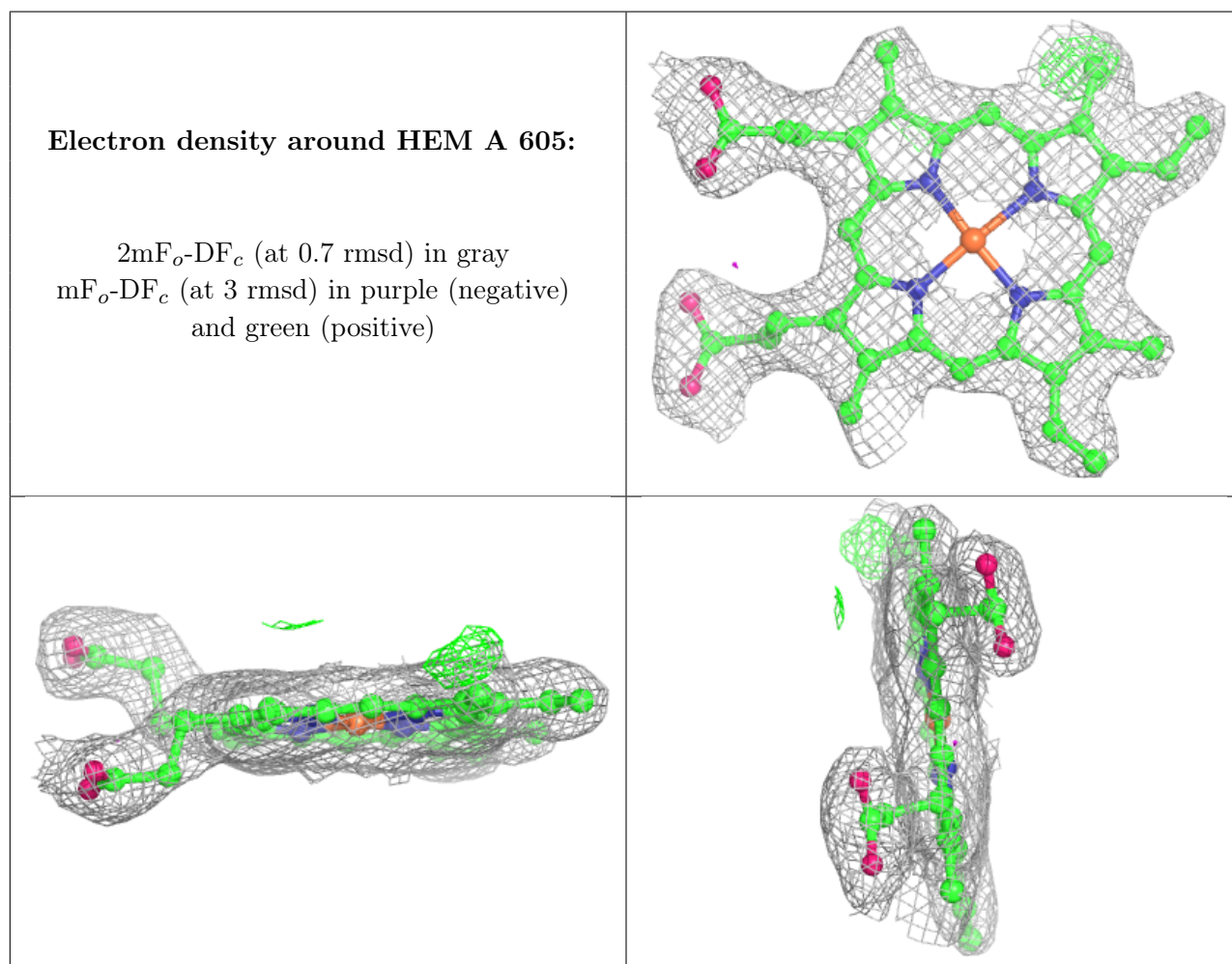
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
12	ASC	A	800	12/12	0.72	0.30	25,30,33,34	0
7	MPD	A	598	8/8	0.73	0.29	30,30,31,31	0
6	IOD	A	719	1/1	0.79	0.11	96,96,96,96	0
8	EDO	A	609	4/4	0.81	0.22	24,25,25,26	0
11	SCN	A	615	3/3	0.82	0.22	47,47,48,48	0
5	NAG	A	596	14/15	0.82	0.21	64,68,70,71	0
5	NAG	A	604	14/15	0.83	0.24	64,67,68,68	0
9	PEG	A	611	7/7	0.84	0.25	62,63,63,63	0
10	GOL	A	612	6/6	0.86	0.11	49,49,50,50	0
6	IOD	A	711	1/1	0.88	0.22	94,94,94,94	0
6	IOD	A	720	1/1	0.89	0.27	95,95,95,95	0
6	IOD	A	707	1/1	0.91	0.06	39,39,39,39	0
6	IOD	A	715	1/1	0.93	0.08	78,78,78,78	0
4	HEM	A	605	43/43	0.96	0.15	24,27,29,31	0

*Continued on next page...*

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	IOD	A	710	1/1	0.96	0.04	76,76,76,76	0
6	IOD	A	709	1/1	0.97	0.07	96,96,96,96	0
3	CA	A	606	1/1	0.97	0.15	33,33,33,33	0
6	IOD	A	708	1/1	0.98	0.05	68,68,68,68	0
6	IOD	A	718	1/1	0.98	0.03	66,66,66,66	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



## 6.5 Other polymers [i](#)

There are no such residues in this entry.