Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 04:50 PM UTC

PDB ID	:	9QJO / pdb_00009qjo
Title	:	Structure of native leukocyte myeloperoxidase in complex with the Staphylococcal Peroxidase Inhibitor SPIN and bromide at pH 5.5
Authors	:	Leitgeb, U.; Pfanzagl, V.
Deposited on	:	2025-03-19
Resolution	:	2.18 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

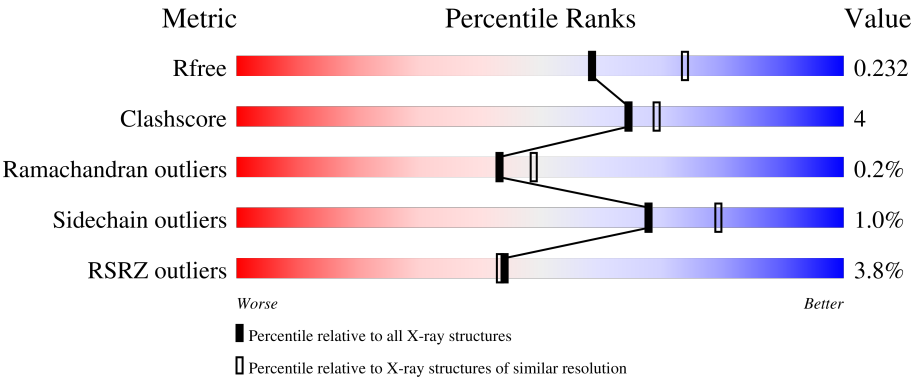
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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 2.18 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}	180053	8975 (2.20-2.16)
Clashscore	190562	9786 (2.20-2.16)
Ramachandran outliers	187476	9664 (2.20-2.16)
Sidechain outliers	187428	9664 (2.20-2.16)
RSRZ outliers	180081	8979 (2.20-2.16)

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% 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	B	467	91% 7% •
1	D	467	89% 10%
2	A	114	81% 11% • 8%
2	C	114	3% 82% 10% 8%
3	E	73	14% 89% • • 5%

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Mol	Chain	Length	Quality of chain
3	F	73	37% 84% 12%
4	G	2	50% 50%
5	H	6	67% 33%
5	I	6	100%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	BR	A	306	-	-	X	-
7	BR	B	810	-	-	X	-
7	BR	B	823	-	-	X	-
7	BR	B	826	-	-	X	-
7	BR	B	827	-	-	X	-
7	BR	D	809	-	-	X	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 11121 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Myeloperoxidase heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	465	Total	C	N	O	S	0	0	0
			3727	2348	686	666	27			
1	D	465	Total	C	N	O	S	0	0	0
			3727	2348	686	666	27			

- Molecule 2 is a protein called Myeloperoxidase light chain.

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

- Molecule 3 is a protein called Myeloperoxidase inhibitor SPIN.

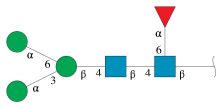
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	69	Total	C	N	O	0	0	0
			557	352	94	111			
3	F	70	Total	C	N	O	0	0	0
			566	357	95	114			

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



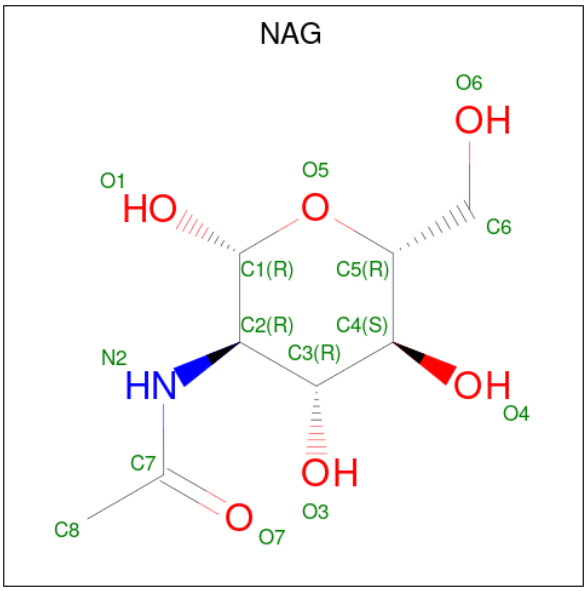
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
5	H	6	Total C N O 71 40 2 29	0	0	0
5	I	6	Total C N O 71 40 2 29	0	0	0

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



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

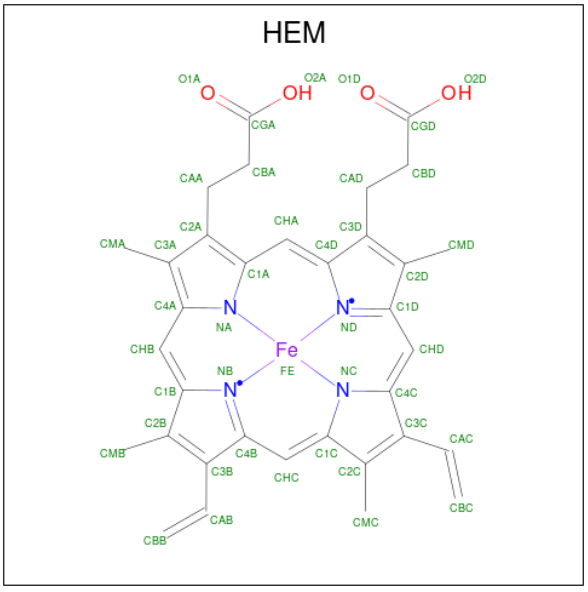
- Molecule 7 is BROMIDE ION (CCD ID: BR) (formula: Br).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	27	Total Br 27 27	0	0
7	D	15	Total Br 15 15	0	0
7	A	7	Total Br 7 7	0	0
7	C	6	Total Br 6 6	0	0
7	F	1	Total Br 1 1	0	0

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

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

- Molecule 9 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 10 is water.

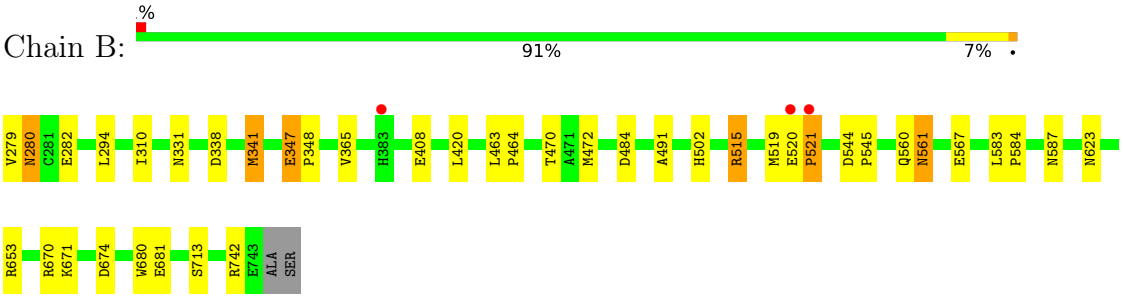
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	195	Total O 197 197	0	2
10	D	184	Total O 184 184	0	0
10	A	56	Total O 56 56	0	0
10	C	51	Total O 51 51	0	0
10	E	10	Total O 10 10	0	0
10	F	6	Total O 6 6	0	0

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 and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

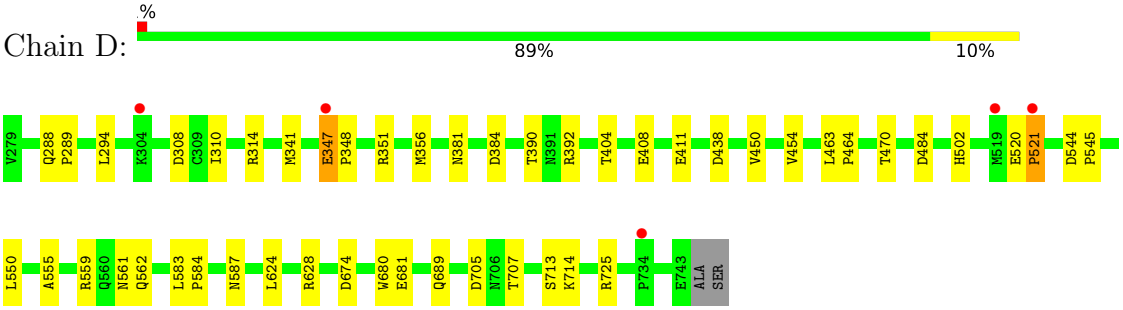
• Molecule 1: Myeloperoxidase heavy chain

Chain B:



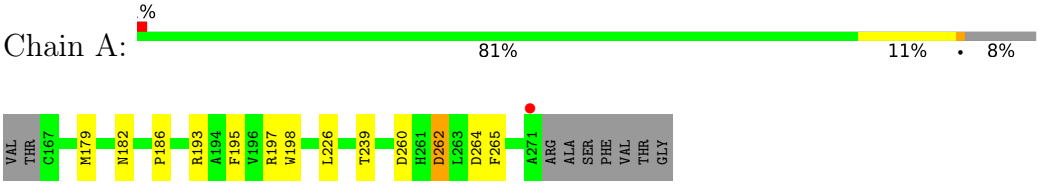
• Molecule 1: Myeloperoxidase heavy chain

Chain D:



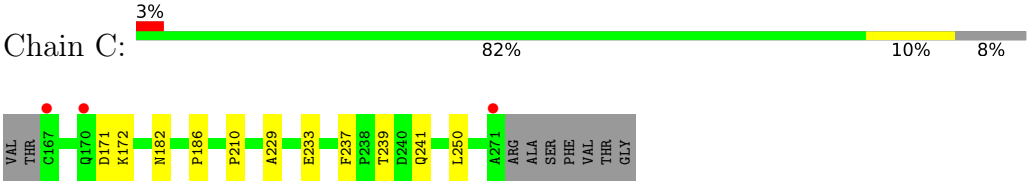
• Molecule 2: Myeloperoxidase light chain

Chain A:



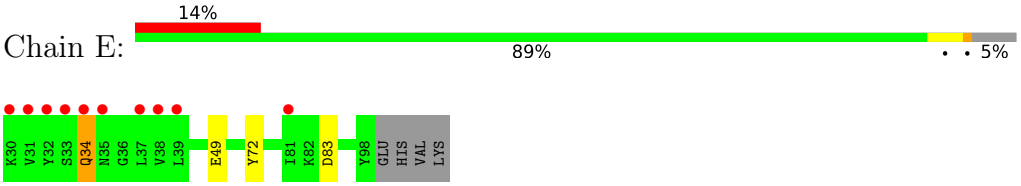
• Molecule 2: Myeloperoxidase light chain

Chain C:



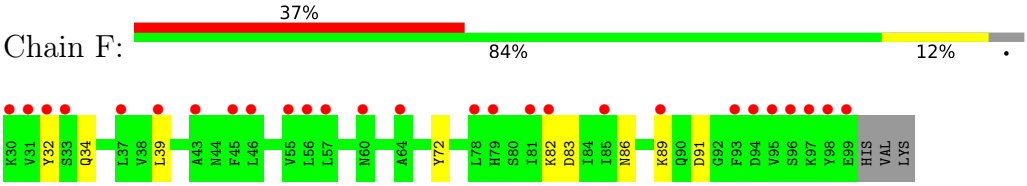
• Molecule 3: Myeloperoxidase inhibitor SPIN

Chain E:



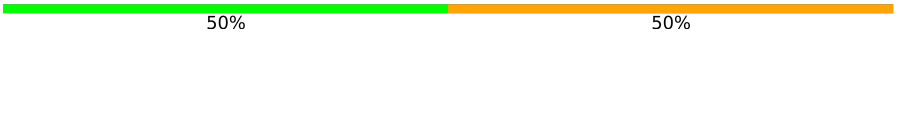
• Molecule 3: Myeloperoxidase inhibitor SPIN

Chain F:



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

Chain G:



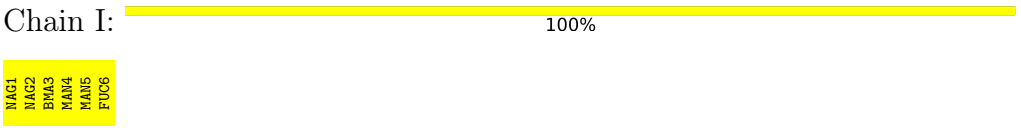
• Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:



• Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	110.88Å 110.88Å 240.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.61 – 2.18 48.61 – 2.18	Depositor EDS
% Data completeness (in resolution range)	66.5 (48.61-2.18) 66.7 (48.61-2.18)	Depositor EDS
R_{merge}	0.28	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.65 (at 2.18Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, R_{free}	0.178 , 0.232 0.182 , 0.232	Depositor DCC
R_{free} test set	2623 reflections (3.31%)	wwPDB-VP
Wilson B-factor (Å^2)	36.7	Xtriage
Anisotropy	0.088	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 34.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	11121	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.84% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CSO, BMA, CA, FUC, BR, HEM, MAN, NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	B	0.63	0/3805	1.07	7/5161 (0.1%)
1	D	0.59	0/3805	1.05	7/5161 (0.1%)
2	A	0.70	0/867	1.18	4/1181 (0.3%)
2	C	0.62	0/867	1.15	1/1181 (0.1%)
3	E	0.57	0/566	1.15	2/761 (0.3%)
3	F	0.54	0/575	1.13	1/773 (0.1%)
All	All	0.62	0/10485	1.09	22/14218 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2
1	D	0	2
All	All	0	4

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	674	ASP	CA-CB-CG	6.22	118.82	112.60
1	B	347	GLU	N-CA-CB	6.10	121.23	110.37
1	D	308	ASP	CA-CB-CG	6.01	118.61	112.60
3	E	83	ASP	CA-CB-CG	5.98	118.58	112.60
1	B	484	ASP	CA-CB-CG	5.93	118.53	112.60
3	E	34	GLN	CB-CA-C	-5.71	101.90	110.24
2	A	262	ASP	CA-CB-CG	5.62	118.22	112.60
3	F	83	ASP	CA-CB-CG	5.57	118.17	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	670	ARG	CA-CB-CG	-5.57	102.96	114.10
1	D	714	LYS	CB-CA-C	-5.35	99.70	109.54
1	B	338	ASP	CA-CB-CG	5.31	117.91	112.60
2	A	197	ARG	CB-CA-C	-5.30	101.50	110.19
1	D	470	THR	CA-CB-OG1	-5.24	101.75	109.60
2	A	260	ASP	CA-CB-CG	5.19	117.79	112.60
1	D	705	ASP	CA-CB-CG	5.14	117.74	112.60
1	D	674	ASP	CA-CB-CG	5.11	117.71	112.60
1	D	484	ASP	CA-CB-CG	5.10	117.70	112.60
1	B	472	MET	CG-SD-CE	-5.08	89.73	100.90
2	A	264	ASP	CA-CB-CG	5.07	117.67	112.60
1	B	561	ASN	CB-CA-C	-5.06	100.84	109.65
2	C	171	ASP	CA-CB-CG	5.06	117.66	112.60
1	D	438	ASP	CA-CB-CG	5.00	117.60	112.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	653	ARG	Sidechain
1	B	742	ARG	Sidechain
1	D	392	ARG	Sidechain
1	D	559	ARG	Sidechain

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	B	3727	0	3720	26	0
1	D	3727	0	3720	29	0
2	A	842	0	800	8	0
2	C	842	0	800	7	0
3	E	557	0	540	2	0
3	F	566	0	546	6	0
4	G	28	0	25	3	0
5	H	71	0	61	0	0
5	I	71	0	61	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	14	0	13	0	0
6	D	28	0	26	0	0
7	A	7	0	0	4	0
7	B	27	0	0	15	0
7	C	6	0	0	3	0
7	D	15	0	0	4	0
7	F	1	0	0	0	0
8	B	1	0	0	0	0
8	D	1	0	0	0	0
9	B	43	0	30	1	0
9	D	43	0	30	2	0
10	A	56	0	0	0	0
10	B	197	0	0	3	0
10	C	51	0	0	0	0
10	D	184	0	0	4	0
10	E	10	0	0	1	0
10	F	6	0	0	1	0
All	All	11121	0	10372	81	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (81) 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)
7:B:806:BR:BR	7:B:826:BR:BR	2.51	1.39
7:D:810:BR:BR	7:A:307:BR:BR	2.80	1.08
7:B:813:BR:BR	7:C:305:BR:BR	2.82	1.08
7:B:828:BR:BR	7:A:305:BR:BR	2.96	0.94
1:B:502:HIS:HD1	1:B:587:ASN:HD21	1.16	0.92
1:D:502:HIS:HD1	1:D:587:ASN:HD21	1.14	0.91
1:B:470:THR:HG22	7:B:826:BR:BR	2.26	0.91
7:B:827:BR:BR	4:G:1:NAG:H82	2.27	0.88
7:B:810:BR:BR	10:E:210:HOH:O	2.47	0.87
9:D:803:HEM:HMC2	9:D:803:HEM:HBC2	1.63	0.81
7:D:816:BR:BR	7:C:306:BR:BR	3.13	0.76
1:B:561:ASN:OD1	7:B:805:BR:BR	2.62	0.73
7:D:809:BR:BR	10:F:306:HOH:O	2.66	0.68
2:A:179:MET:HE1	2:A:193:ARG:HH21	1.58	0.68
7:B:827:BR:BR	4:G:1:NAG:C8	2.97	0.68
1:D:356:MET:HE2	1:D:356:MET:HA	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:B:830:HEM:HMC2	9:B:830:HEM:HBC2	1.78	0.64
1:B:341:MET:HE3	2:A:262:ASP:HB2	1.80	0.64
1:B:560:GLN:NE2	1:B:623:ASN:HD22	1.96	0.63
1:B:515:ARG:HH21	1:B:515:ARG:HG2	1.61	0.63
1:B:347:GLU:N	1:B:348:PRO:HD2	2.20	0.56
1:B:331:ASN:HB2	2:A:195:PHE:CE1	2.40	0.56
1:B:583:LEU:HB3	1:B:584:PRO:HD3	1.90	0.54
1:D:689:GLN:HG2	10:D:1049:HOH:O	2.07	0.54
1:B:519:MET:HE1	7:B:823:BR:BR	2.63	0.54
1:D:347:GLU:N	1:D:348:PRO:HD2	2.22	0.53
1:B:515:ARG:HH21	1:B:515:ARG:CG	2.21	0.53
1:D:356:MET:HG3	3:F:72:TYR:CD2	2.43	0.53
1:D:725:ARG:HD3	10:D:905:HOH:O	2.08	0.52
7:B:825:BR:BR	2:A:226:LEU:HD22	2.64	0.52
9:D:803:HEM:HBC2	9:D:803:HEM:CMC	2.37	0.52
1:B:347:GLU:HG2	10:B:1074:HOH:O	2.09	0.51
1:B:544:ASP:HB2	1:B:545:PRO:HD3	1.92	0.51
1:B:280:ASN:HA	10:B:996:HOH:O	2.10	0.51
1:D:408:GLU:HG3	7:D:809:BR:BR	2.66	0.50
7:B:823:BR:BR	10:B:1071:HOH:O	2.74	0.50
1:B:567:GLU:HG2	7:A:306:BR:BR	2.66	0.50
7:B:814:BR:BR	4:G:1:NAG:H81	2.67	0.49
1:D:463:LEU:N	1:D:464:PRO:CD	2.76	0.49
1:D:583:LEU:HB3	1:D:584:PRO:HD3	1.95	0.49
1:B:347:GLU:N	1:B:348:PRO:CD	2.76	0.48
2:C:182:ASN:O	2:C:186:PRO:HA	2.13	0.48
2:C:239:THR:HG21	7:C:302:BR:BR	2.69	0.48
1:B:463:LEU:N	1:B:464:PRO:CD	2.76	0.48
1:D:411:GLU:HB3	1:D:550:LEU:HD11	1.94	0.48
2:C:229:ALA:O	2:C:233:GLU:HG2	2.13	0.48
2:A:265:PHE:CE2	3:E:34:GLN:HG2	2.50	0.47
1:D:404:THR:HG21	3:F:32:TYR:CG	2.51	0.47
1:D:544:ASP:HB2	1:D:545:PRO:HD3	1.97	0.47
1:D:450:VAL:O	1:D:454:VAL:HG23	2.15	0.46
1:D:347:GLU:N	1:D:348:PRO:CD	2.79	0.46
1:D:561:ASN:OD1	1:D:562:GLN:HG3	2.15	0.46
1:B:294:LEU:HB2	1:B:310:ILE:HB	1.97	0.45
1:B:491:ALA:HB2	2:A:198:TRP:CE2	2.50	0.45
1:D:294:LEU:HB2	1:D:310:ILE:HB	1.98	0.45
1:D:384:ASP:HB2	10:D:1045:HOH:O	2.17	0.45
1:B:408:GLU:HG3	7:B:810:BR:BR	2.71	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:239:THR:HG21	7:A:306:BR:BR	2.72	0.44
1:D:314:ARG:CZ	2:C:210:PRO:HD3	2.48	0.44
1:D:680:TRP:CE2	1:D:681:GLU:HG3	2.52	0.44
1:B:470:THR:CG2	7:B:826:BR:BR	3.11	0.44
3:E:49:GLU:OE1	3:E:72:TYR:OH	2.33	0.44
3:F:82:LYS:O	3:F:86:ASN:HB2	2.17	0.44
1:D:544:ASP:OD1	1:D:707:THR:HB	2.18	0.43
1:B:365:VAL:HG12	1:B:420:LEU:HD21	2.00	0.43
1:D:381:ASN:HD21	3:F:91:ASP:HB3	1.83	0.43
1:D:562:GLN:HA	2:C:237:PHE:CG	2.53	0.43
2:C:172:LYS:HG2	2:C:172:LYS:O	2.19	0.43
1:B:680:TRP:CE2	1:B:681:GLU:HG3	2.54	0.43
1:D:725:ARG:NH1	10:D:905:HOH:O	2.46	0.42
2:A:182:ASN:O	2:A:186:PRO:HA	2.19	0.42
1:B:671:LYS:HE3	7:B:804:BR:BR	2.75	0.42
1:B:280:ASN:OD1	1:B:282:GLU:OE2	2.38	0.42
3:F:34:GLN:HB2	3:F:39:LEU:HD11	2.02	0.42
1:D:555:ALA:HA	2:C:250:LEU:HD13	2.01	0.41
1:B:520:GLU:N	1:B:521:PRO:HD2	2.36	0.41
1:D:584:PRO:O	1:D:587:ASN:HB2	2.20	0.41
1:D:624:LEU:HD21	1:D:628:ARG:NH2	2.36	0.41
1:D:288:GLN:O	1:D:289:PRO:C	2.64	0.40
1:D:520:GLU:N	1:D:521:PRO:HD2	2.36	0.40
1:D:356:MET:HG3	3:F:72:TYR:CE2	2.56	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	B	462/467 (99%)	446 (96%)	15 (3%)	1 (0%)	43 49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	D	462/467 (99%)	449 (97%)	11 (2%)	2 (0%)	30 31
2	A	103/114 (90%)	100 (97%)	3 (3%)	0	100 100
2	C	103/114 (90%)	100 (97%)	3 (3%)	0	100 100
3	E	67/73 (92%)	65 (97%)	2 (3%)	0	100 100
3	F	68/73 (93%)	66 (97%)	2 (3%)	0	100 100
All	All	1265/1308 (97%)	1226 (97%)	36 (3%)	3 (0%)	43 49

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	390	THR
1	B	521	PRO
1	D	521	PRO

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	B	410/411 (100%)	405 (99%)	5 (1%)	63 75
1	D	410/411 (100%)	406 (99%)	4 (1%)	68 79
2	A	90/97 (93%)	90 (100%)	0	100 100
2	C	90/97 (93%)	89 (99%)	1 (1%)	65 77
3	E	61/65 (94%)	61 (100%)	0	100 100
3	F	62/65 (95%)	61 (98%)	1 (2%)	55 68
All	All	1123/1146 (98%)	1112 (99%)	11 (1%)	68 79

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

Mol	Chain	Res	Type
1	B	279	VAL
1	B	280	ASN
1	B	341	MET

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Mol	Chain	Res	Type
1	B	515	ARG
1	B	713	SER
1	D	341	MET
1	D	347	GLU
1	D	351	ARG
1	D	713	SER
2	C	241	GLN
3	F	89	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	280	ASN
1	B	492	ASN
1	B	517	GLN
1	B	522	ASN
1	B	560	GLN
1	B	639	ASN
1	B	692	GLN
1	B	696	GLN
1	B	715	ASN
1	D	492	ASN
1	D	517	GLN
1	D	633	GLN
2	A	241	GLN
2	A	246	GLN
2	C	241	GLN
3	E	60	ASN
3	E	63	GLN
3	F	35	ASN
3	F	63	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	CSO	D	316	1	3,6,7	0.56	0	1,6,8	0.49	0
1	CSO	B	316	1	3,6,7	0.67	0	1,6,8	0.83	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
1	CSO	D	316	1	-	0/1/5/7	-
1	CSO	B	316	1	-	0/1/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

14 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	G	1	1,4	14,14,15	0.48	0	17,19,21	1.01	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	G	2	4	14,14,15	0.38	0	17,19,21	0.90	0
5	NAG	H	1	5,1	14,14,15	0.35	0	17,19,21	0.76	0
5	NAG	H	2	5	14,14,15	0.38	0	17,19,21	0.94	1 (5%)
5	BMA	H	3	5	11,11,12	0.43	0	15,15,17	0.64	0
5	MAN	H	4	5	11,11,12	0.55	0	15,15,17	0.69	0
5	MAN	H	5	5	11,11,12	0.62	0	15,15,17	1.27	1 (6%)
5	FUC	H	6	5	10,10,11	0.48	0	14,14,16	0.72	0
5	NAG	I	1	5,1	14,14,15	0.35	0	17,19,21	1.17	1 (5%)
5	NAG	I	2	5	14,14,15	0.58	0	17,19,21	1.26	1 (5%)
5	BMA	I	3	5	11,11,12	0.43	0	15,15,17	1.10	1 (6%)
5	MAN	I	4	5	11,11,12	0.37	0	15,15,17	0.95	1 (6%)
5	MAN	I	5	5	11,11,12	0.48	0	15,15,17	1.74	3 (20%)
5	FUC	I	6	5	10,10,11	0.46	0	14,14,16	1.03	1 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	G	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	G	2	4	-	2/6/23/26	0/1/1/1
5	NAG	H	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	H	2	5	-	0/6/23/26	0/1/1/1
5	BMA	H	3	5	-	0/2/19/22	0/1/1/1
5	MAN	H	4	5	-	1/2/19/22	0/1/1/1
5	MAN	H	5	5	-	1/2/19/22	0/1/1/1
5	FUC	H	6	5	-	-	0/1/1/1
5	NAG	I	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	I	2	5	-	0/6/23/26	0/1/1/1
5	BMA	I	3	5	-	0/2/19/22	0/1/1/1
5	MAN	I	4	5	-	0/2/19/22	0/1/1/1
5	MAN	I	5	5	-	2/2/19/22	0/1/1/1
5	FUC	I	6	5	-	-	0/1/1/1

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	I	2	NAG	O5-C1-C2	-4.37	104.53	111.29
5	I	5	MAN	C1-O5-C5	4.32	117.97	112.19
5	H	5	MAN	O2-C2-C3	3.96	118.35	110.15
5	I	5	MAN	O2-C2-C3	3.87	118.16	110.15
5	I	1	NAG	C1-C2-N2	3.13	115.37	110.43
5	I	6	FUC	C2-C3-C4	-2.40	106.64	110.86
5	I	5	MAN	C3-C4-C5	2.34	114.47	110.23
5	I	4	MAN	C1-O5-C5	2.19	115.13	112.19
4	G	1	NAG	C1-C2-N2	-2.10	107.12	110.43
5	H	2	NAG	C2-N2-C7	2.07	125.67	122.90
5	I	3	BMA	C1-O5-C5	2.07	114.95	112.19

There are no chirality outliers.

All (8) torsion outliers are listed below:

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

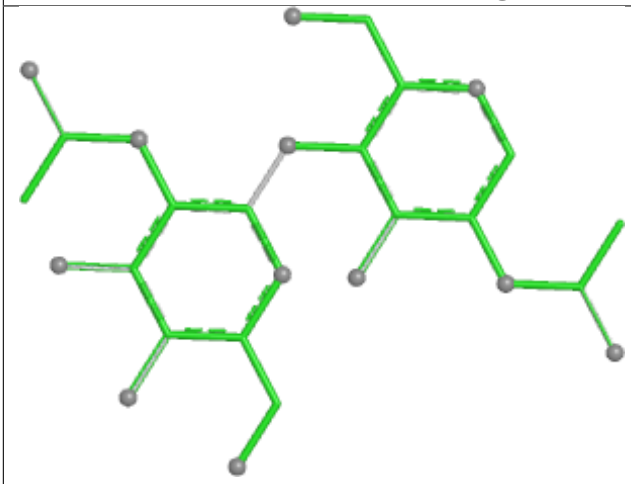
There are no ring outliers.

1 monomer is involved in 3 short contacts:

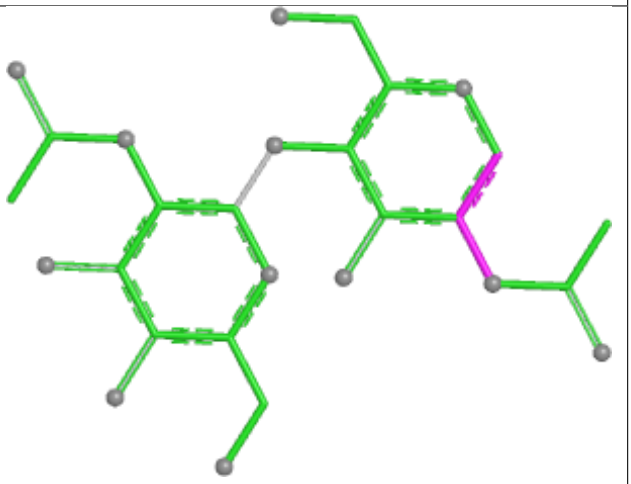
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	1	NAG	3	0

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

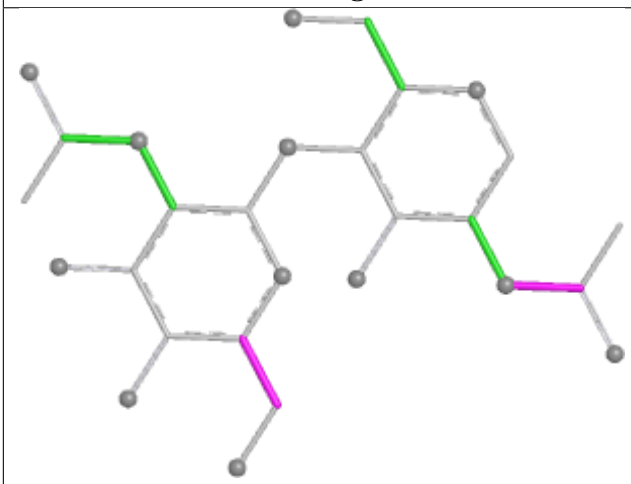
Oligosaccharide Chain G



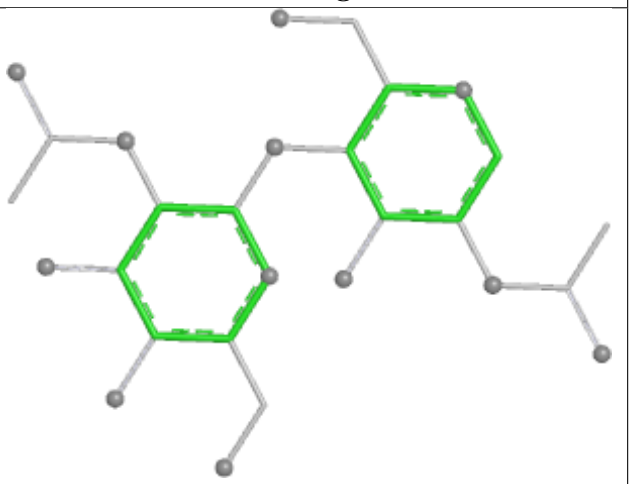
Bond lengths



Bond angles

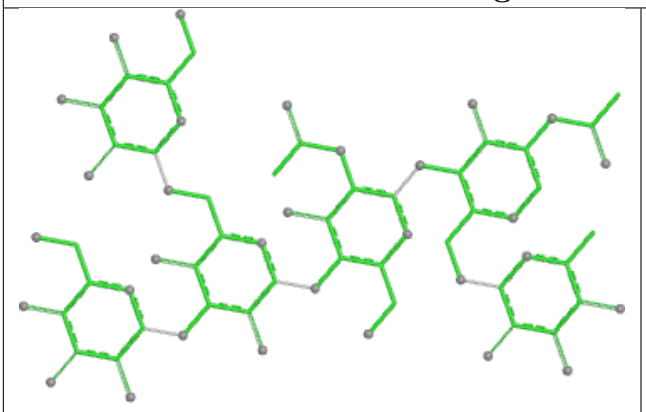


Torsions

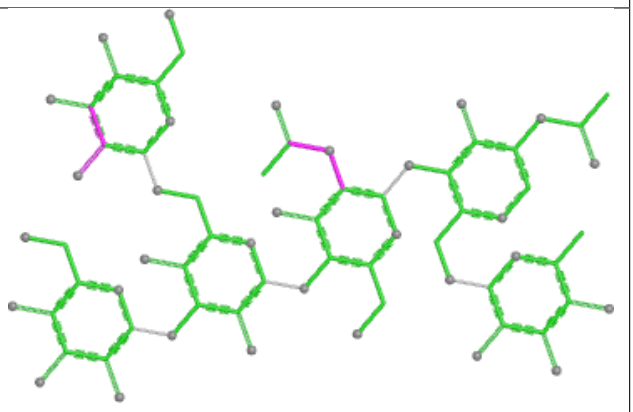


Rings

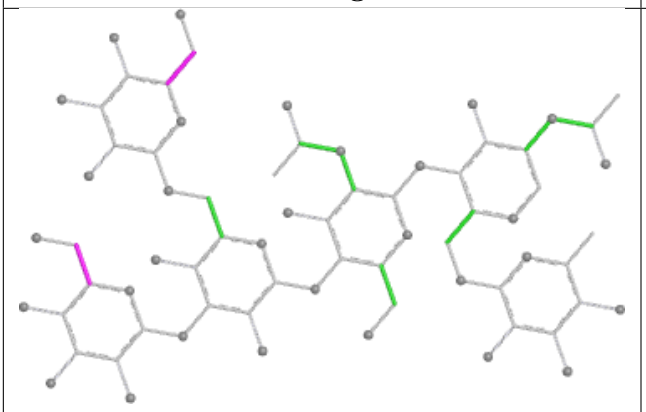
Oligosaccharide Chain H



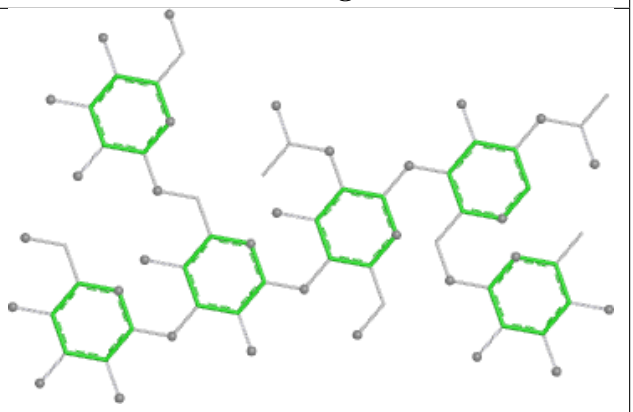
Bond lengths



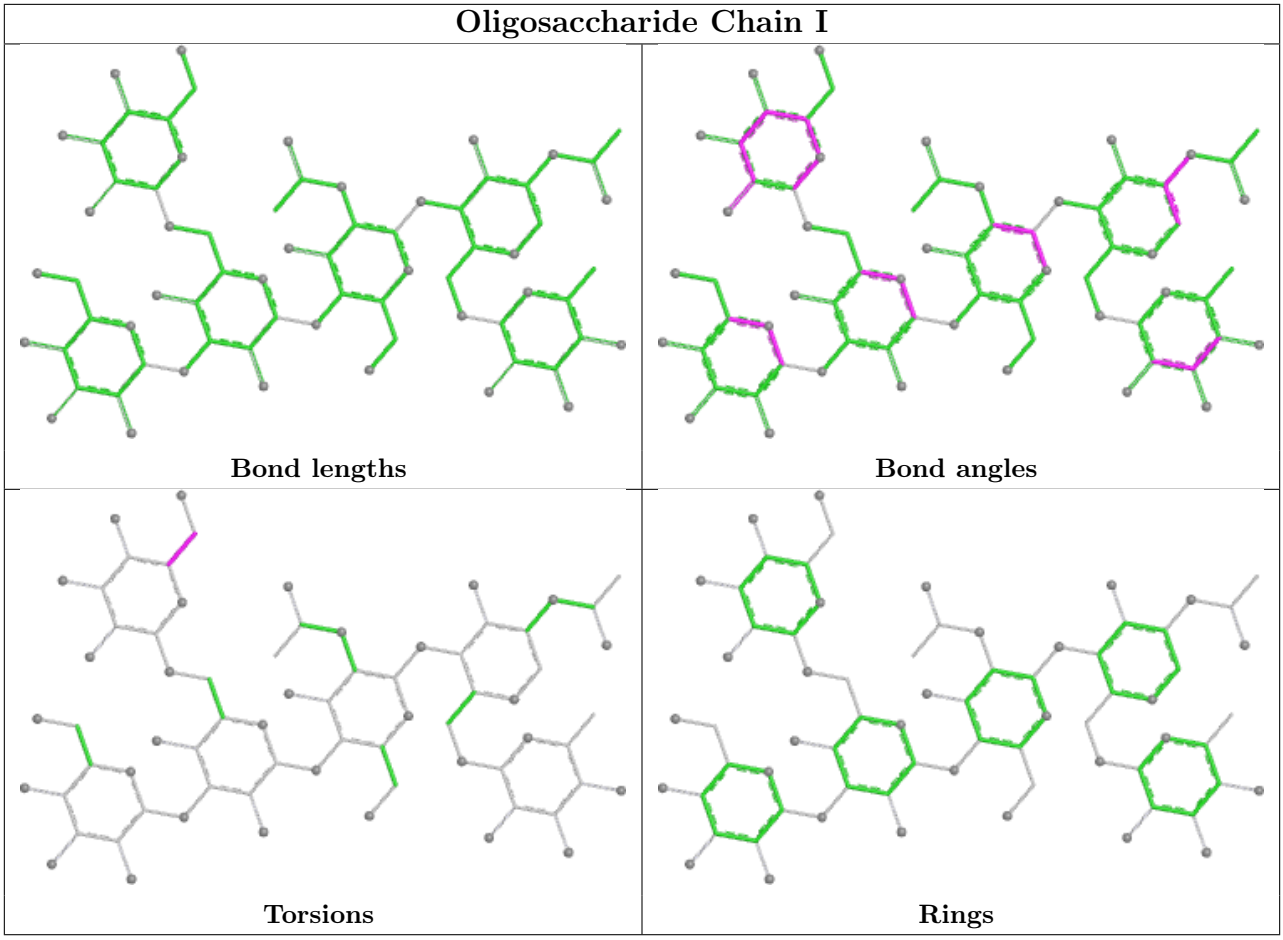
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

Of 63 ligands modelled in this entry, 58 are monoatomic - leaving 5 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	$\#\|Z\| > 2$
9	HEM	B	830	2,1	50,50,50	2.19	16 (32%)	67,82,82	1.27	5 (7%)
6	NAG	D	801	1	14,14,15	0.60	0	17,19,21	1.09	2 (11%)
9	HEM	D	803	2,1	50,50,50	2.24	16 (32%)	67,82,82	1.17	5 (7%)
6	NAG	D	802	1	14,14,15	0.47	0	17,19,21	1.17	1 (5%)
6	NAG	B	801	1	14,14,15	0.45	0	17,19,21	0.95	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
9	HEM	B	830	2,1	-	4/14/54/54	-
6	NAG	D	801	1	-	2/6/23/26	0/1/1/1
9	HEM	D	803	2,1	-	4/14/54/54	-
6	NAG	D	802	1	-	2/6/23/26	0/1/1/1
6	NAG	B	801	1	-	0/6/23/26	0/1/1/1

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	D	803	HEM	FE-ND	6.42	2.14	1.94
9	B	830	HEM	FE-ND	6.03	2.13	1.94
9	D	803	HEM	FE-NB	5.79	2.12	1.94
9	B	830	HEM	FE-NA	4.83	2.11	1.95
9	B	830	HEM	C1D-C2D	-4.83	1.34	1.44
9	B	830	HEM	C1B-NB	-4.77	1.32	1.40
9	B	830	HEM	C4D-C3D	-4.76	1.37	1.45
9	D	803	HEM	FE-NC	4.67	2.10	1.95
9	D	803	HEM	FE-NA	4.01	2.08	1.95
9	D	803	HEM	C1A-C2A	-3.89	1.36	1.44
9	B	830	HEM	C3C-C4C	-3.50	1.39	1.46
9	D	803	HEM	C3C-C4C	-3.50	1.39	1.46
9	D	803	HEM	C4A-C3A	-3.45	1.35	1.43
9	B	830	HEM	C4D-ND	-3.43	1.34	1.40
9	B	830	HEM	C1D-ND	-3.40	1.32	1.38
9	B	830	HEM	C3B-C4B	-3.23	1.38	1.44
9	D	803	HEM	C4D-ND	-3.08	1.34	1.40
9	D	803	HEM	C4D-C3D	-2.92	1.40	1.45
9	D	803	HEM	C1D-C2D	-2.86	1.38	1.44
9	D	803	HEM	C1B-C2B	-2.84	1.38	1.44
9	B	830	HEM	C1A-C2A	-2.73	1.39	1.44
9	D	803	HEM	C1B-NB	-2.65	1.35	1.40
9	D	803	HEM	C3B-C4B	-2.64	1.39	1.44
9	B	830	HEM	C4A-C3A	-2.60	1.37	1.43
9	B	830	HEM	C1C-C2C	-2.57	1.40	1.45
9	B	830	HEM	C1A-NA	-2.39	1.35	1.39
9	D	803	HEM	C1A-NA	-2.34	1.35	1.39
9	B	830	HEM	C1B-C2B	-2.30	1.39	1.44
9	B	830	HEM	O2A-CGA	-2.26	1.23	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	830	HEM	C1C-NC	-2.23	1.35	1.39
9	D	803	HEM	C1C-C2C	-2.17	1.41	1.45
9	D	803	HEM	O2D-CGD	-2.11	1.23	1.30

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	B	830	HEM	C3B-C4B-NB	4.34	112.58	109.47
9	B	830	HEM	C4B-C3B-C2B	-3.63	103.94	107.28
9	D	803	HEM	CAD-CBD-CGD	3.02	121.67	113.67
6	D	802	NAG	C1-C2-N2	-2.85	105.94	110.43
9	D	803	HEM	C4C-CHD-C1D	2.84	132.06	126.02
9	D	803	HEM	CHA-C4D-ND	-2.80	120.91	124.37
9	D	803	HEM	CHC-C1C-NC	-2.37	121.87	124.45
9	B	830	HEM	CHD-C4C-NC	-2.31	121.94	124.45
6	D	801	NAG	C1-C2-N2	2.28	114.02	110.43
9	D	803	HEM	CHD-C1D-C2D	2.21	128.52	125.03
6	D	801	NAG	C1-O5-C5	2.14	115.05	112.19
9	B	830	HEM	CHC-C1C-NC	-2.14	122.13	124.45
9	B	830	HEM	C4D-ND-C1D	2.06	107.65	105.21
6	B	801	NAG	C1-C2-N2	-2.02	107.25	110.43

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	D	802	NAG	C8-C7-N2-C2
6	D	801	NAG	C4-C5-C6-O6
6	D	802	NAG	O7-C7-N2-C2
6	D	801	NAG	O5-C5-C6-O6
9	B	830	HEM	CAA-CBA-CGA-O2A
9	B	830	HEM	CAA-CBA-CGA-O1A
9	B	830	HEM	CAD-CBD-CGD-O1D
9	B	830	HEM	CAD-CBD-CGD-O2D
9	D	803	HEM	CAD-CBD-CGD-O1D
9	D	803	HEM	CAA-CBA-CGA-O2A
9	D	803	HEM	CAA-CBA-CGA-O1A
9	D	803	HEM	CAD-CBD-CGD-O2D

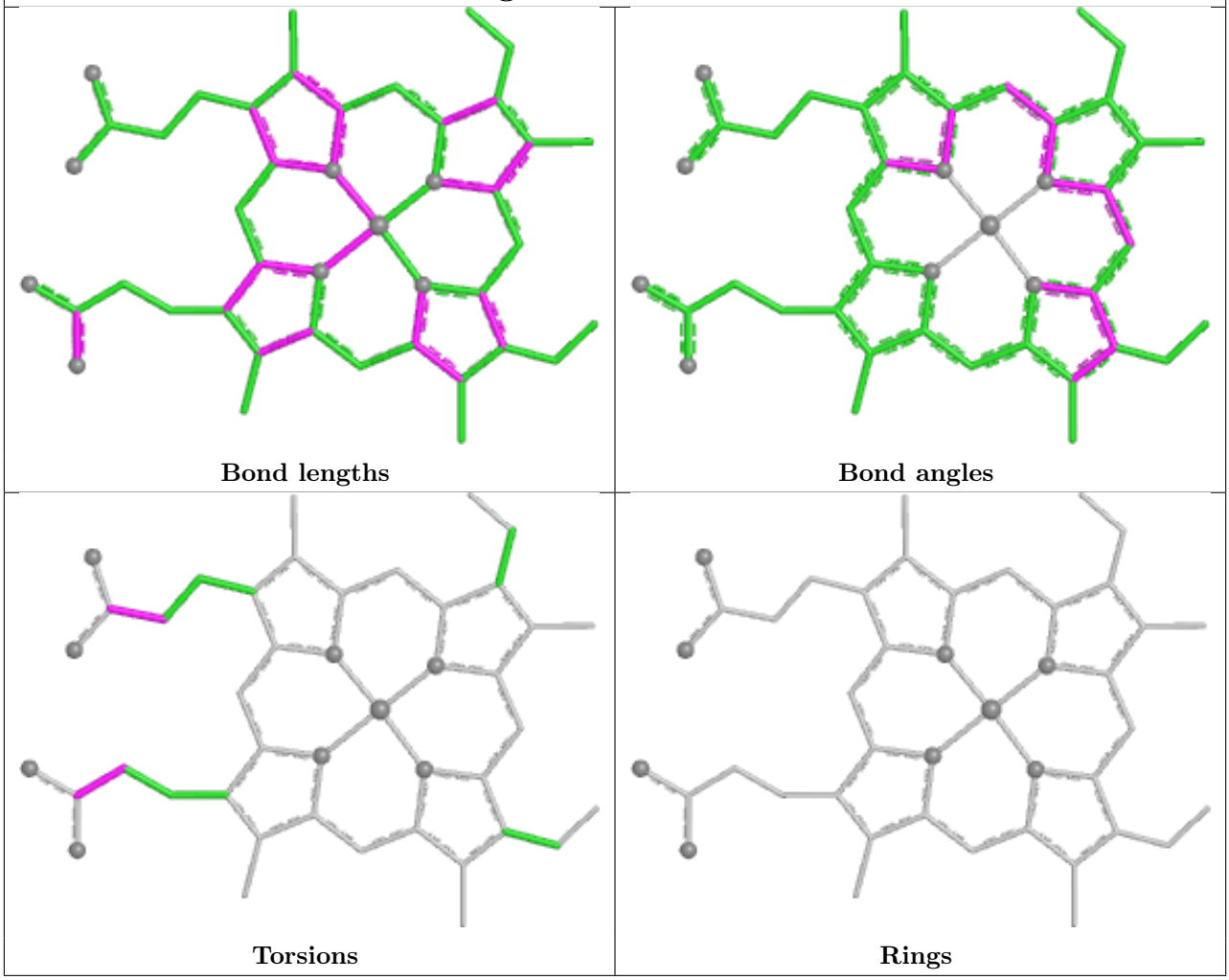
There are no ring outliers.

2 monomers are involved in 3 short contacts:

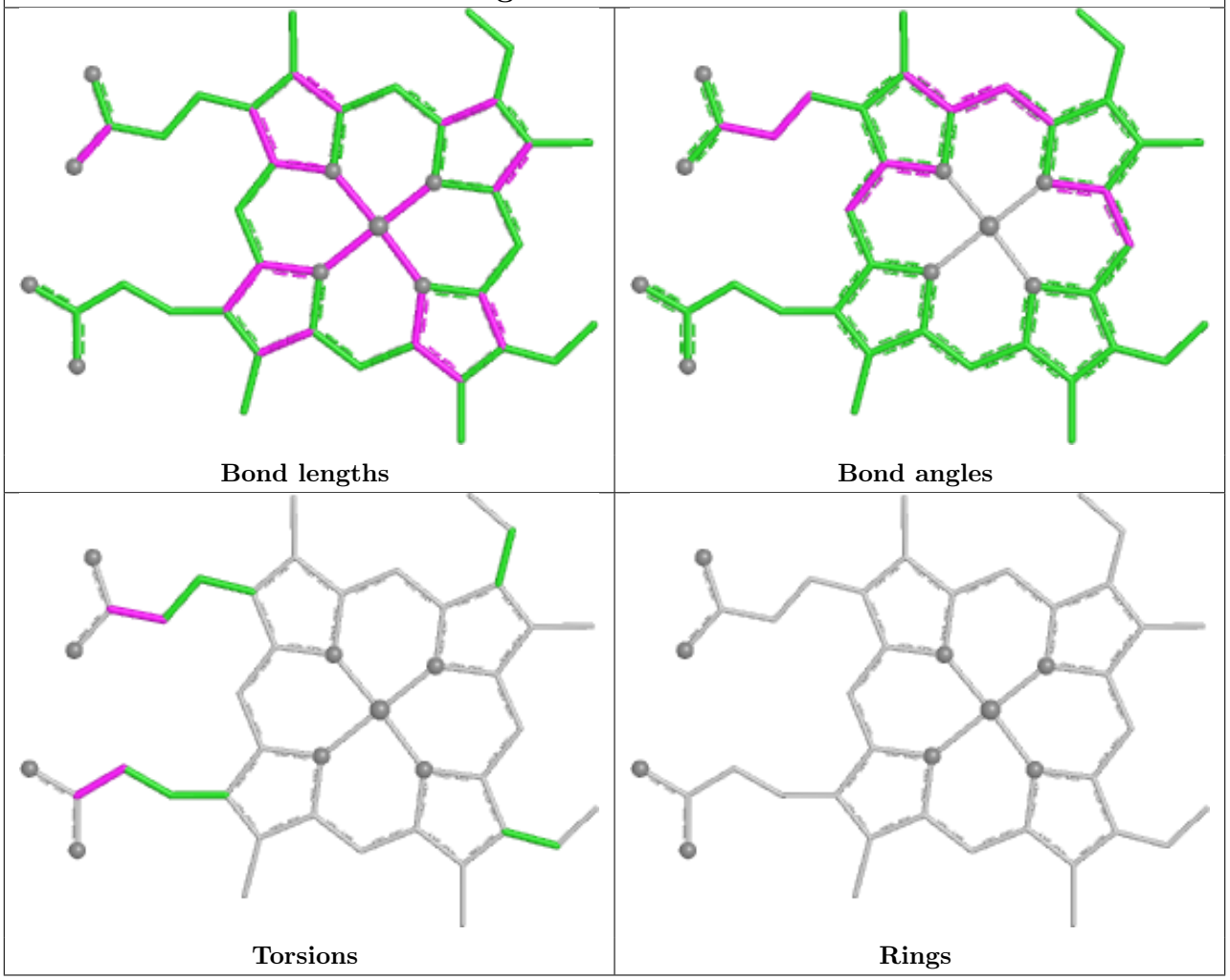
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	830	HEM	1	0
9	D	803	HEM	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for 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 B 830



Ligand HEM D 803



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	B	464/467 (99%)	-0.20	3 (0%) 85 84	22, 33, 58, 95	0
1	D	464/467 (99%)	0.02	5 (1%) 78 77	24, 40, 65, 103	0
2	A	105/114 (92%)	-0.23	1 (0%) 79 79	21, 31, 55, 94	0
2	C	105/114 (92%)	0.06	3 (2%) 53 53	23, 35, 67, 91	0
3	E	69/73 (94%)	0.71	10 (14%) 6 5	34, 56, 78, 87	0
3	F	70/73 (95%)	1.82	27 (38%) 1 1	61, 89, 118, 133	0
All	All	1277/1308 (97%)	0.06	49 (3%) 44 43	21, 37, 80, 133	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	521	PRO	5.1
1	B	521	PRO	4.5
3	F	95	VAL	4.1
1	D	734	PRO	3.9
3	F	39	LEU	3.8
3	F	99	GLU	3.8
3	F	30	LYS	3.5
1	B	383	HIS	3.5
3	E	38	VAL	3.5
3	F	82	LYS	3.4
3	F	31	VAL	3.3
3	E	39	LEU	3.3
3	E	31	VAL	3.3
3	F	96	SER	3.2
3	E	30	LYS	3.2
3	F	57	LEU	3.1
3	F	81	ILE	3.1
3	F	98	TYR	3.0
3	F	89	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
2	C	167	CYS	2.9
1	B	520	GLU	2.8
3	E	34	GLN	2.7
3	E	37	LEU	2.7
3	E	32	TYR	2.7
3	F	55	VAL	2.7
3	F	78	LEU	2.6
1	D	304	LYS	2.6
3	F	93	PHE	2.5
2	C	170	GLN	2.5
2	C	271	ALA	2.4
3	F	60	ASN	2.4
3	E	33	SER	2.4
3	F	97	LYS	2.3
3	F	32	TYR	2.3
1	D	347	GLU	2.3
3	F	64	ALA	2.3
3	F	46	LEU	2.3
3	F	37	LEU	2.2
3	F	56	LEU	2.2
3	F	79	HIS	2.2
2	A	271	ALA	2.2
3	E	35	ASN	2.2
3	E	81	ILE	2.2
3	F	45	PHE	2.2
3	F	85	ILE	2.2
3	F	94	ASP	2.1
3	F	43	ALA	2.1
3	F	33	SER	2.1
1	D	519	MET	2.0

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^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	CSO	D	316	7/8	0.96	0.06	26,27,28,32	0
1	CSO	B	316	7/8	0.98	0.05	22,23,25,26	1

6.3 Carbohydrates (i)

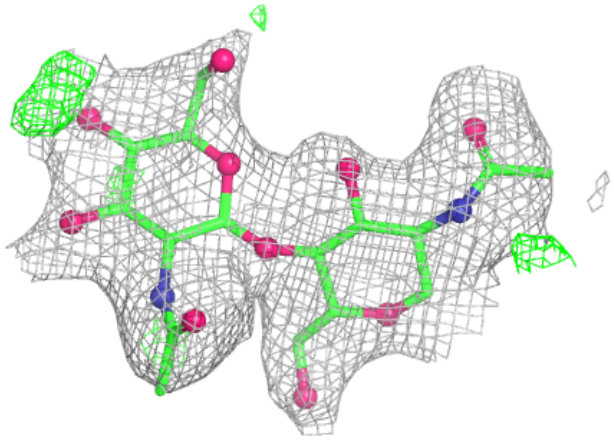
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

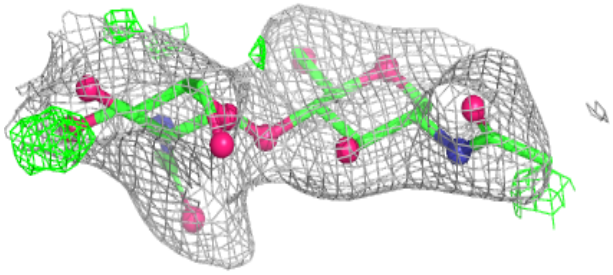
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	MAN	I	4	11/12	0.71	0.15	72,79,84,86	0
5	MAN	H	4	11/12	0.77	0.14	65,71,82,94	0
4	NAG	G	2	14/15	0.78	0.13	61,80,89,93	0
5	MAN	I	5	11/12	0.89	0.09	40,44,45,48	0
4	NAG	G	1	14/15	0.90	0.09	45,53,60,71	0
5	MAN	H	5	11/12	0.91	0.08	37,43,47,55	0
5	BMA	I	3	11/12	0.91	0.08	35,37,43,56	0
5	FUC	H	6	10/11	0.92	0.09	42,44,47,48	0
5	NAG	H	1	14/15	0.93	0.07	33,35,37,44	0
5	BMA	H	3	11/12	0.93	0.07	35,40,43,55	0
5	FUC	I	6	10/11	0.93	0.08	41,47,51,52	0
5	NAG	I	2	14/15	0.95	0.07	26,30,32,34	0
5	NAG	I	1	14/15	0.96	0.06	29,33,36,38	0
5	NAG	H	2	14/15	0.96	0.06	28,33,36,38	0

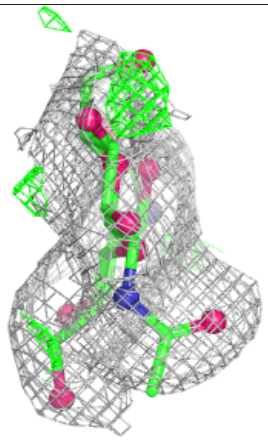
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain G:

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

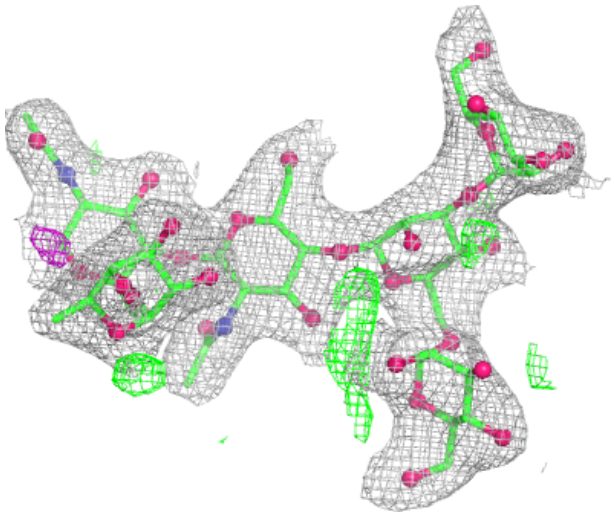


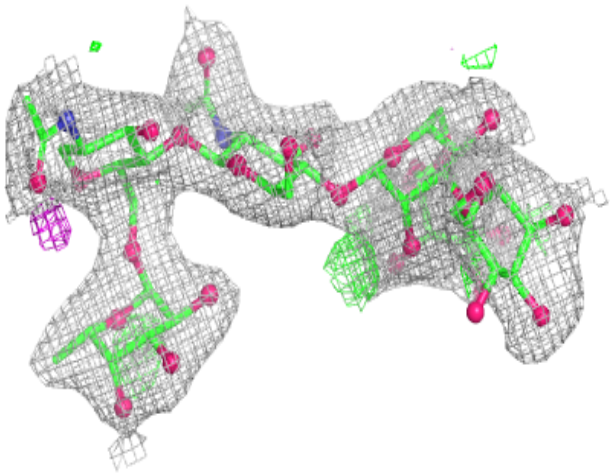


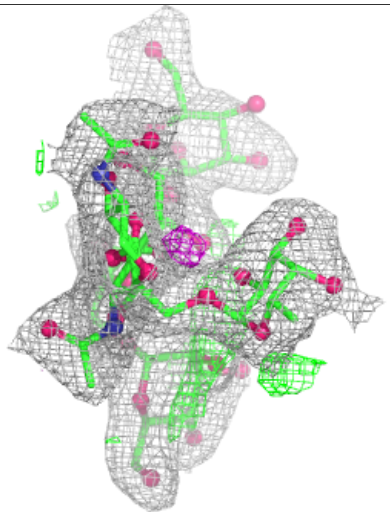


Electron density around Chain H:

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

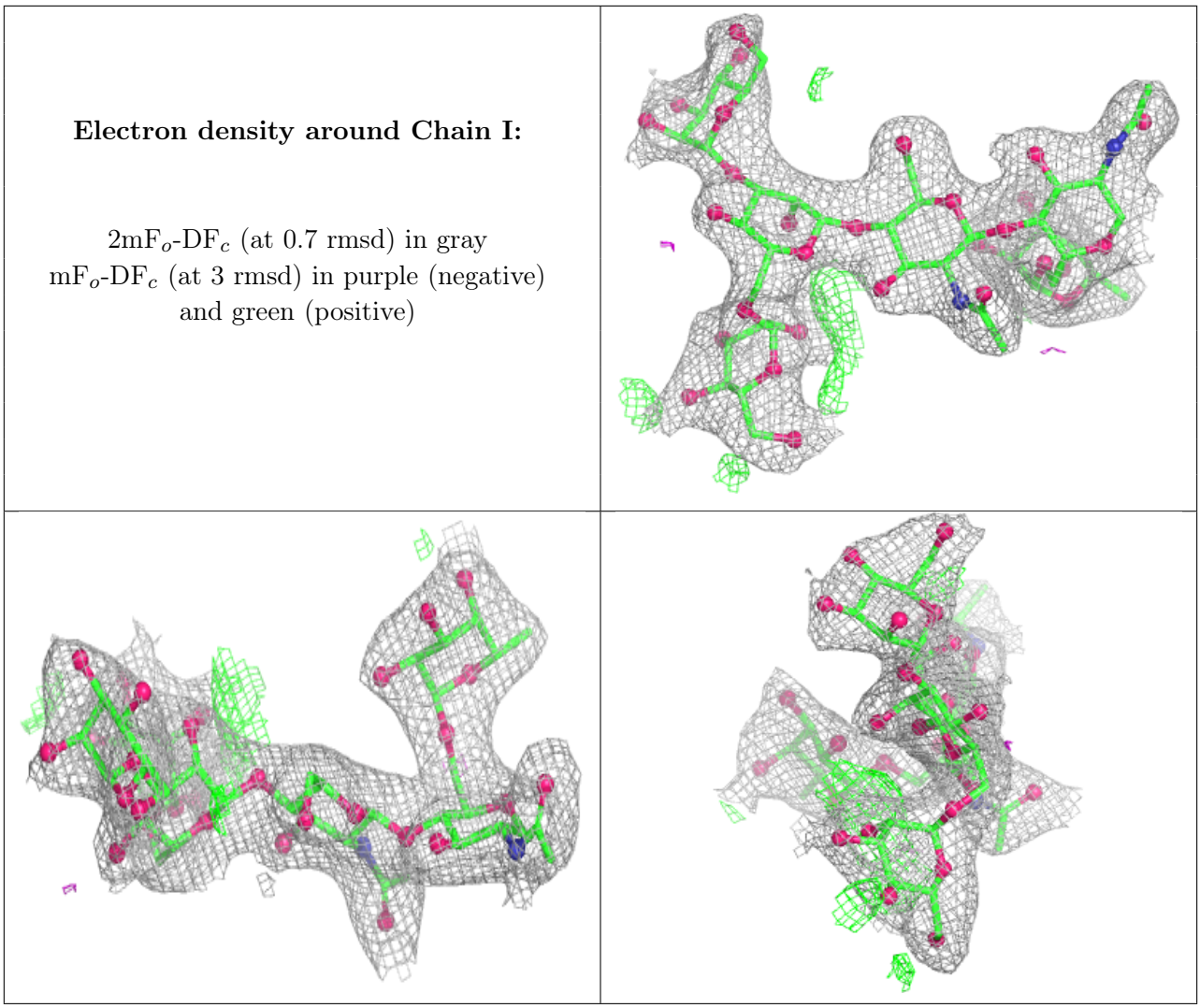






Electron density around Chain I:

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



6.4 Ligands

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^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	BR	A	305	1/1	0.81	0.15	51,51,51,51	1
7	BR	D	818	1/1	0.83	0.11	75,75,75,75	1
6	NAG	D	802	14/15	0.84	0.13	64,68,71,71	0
7	BR	B	823	1/1	0.84	0.12	61,61,61,61	1
6	NAG	D	801	14/15	0.85	0.10	44,52,56,56	0
7	BR	D	811	1/1	0.87	0.09	40,40,40,40	1
7	BR	B	810	1/1	0.88	0.14	65,65,65,65	1
6	NAG	B	801	14/15	0.88	0.09	34,41,47,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	BR	B	824	1/1	0.88	0.10	55,55,55,55	1
7	BR	B	819	1/1	0.89	0.08	47,47,47,47	1
7	BR	D	812	1/1	0.89	0.11	58,58,58,58	1
7	BR	B	809	1/1	0.89	0.10	51,51,51,51	1
7	BR	B	813	1/1	0.89	0.07	33,33,33,33	1
7	BR	B	806	1/1	0.91	0.09	54,54,54,54	1
7	BR	D	814	1/1	0.91	0.08	54,54,54,54	1
7	BR	D	810	1/1	0.92	0.09	48,48,48,48	1
7	BR	B	820	1/1	0.92	0.09	50,50,50,50	1
7	BR	D	806	1/1	0.92	0.11	50,50,50,50	1
7	BR	C	304	1/1	0.92	0.09	49,49,49,49	1
7	BR	C	306	1/1	0.92	0.10	64,64,64,64	1
7	BR	B	825	1/1	0.93	0.10	50,50,50,50	1
7	BR	D	817	1/1	0.93	0.09	52,52,52,52	1
7	BR	B	827	1/1	0.94	0.06	47,47,47,47	1
7	BR	D	815	1/1	0.94	0.11	55,55,55,55	1
7	BR	B	828	1/1	0.94	0.07	51,51,51,51	1
7	BR	B	815	1/1	0.94	0.06	47,47,47,47	1
7	BR	A	304	1/1	0.94	0.09	49,49,49,49	1
7	BR	B	816	1/1	0.94	0.07	49,49,49,49	1
7	BR	B	818	1/1	0.94	0.08	51,51,51,51	1
7	BR	B	814	1/1	0.94	0.07	46,46,46,46	1
7	BR	F	201	1/1	0.94	0.06	55,55,55,55	1
7	BR	B	822	1/1	0.95	0.07	53,53,53,53	1
7	BR	D	809	1/1	0.95	0.09	73,73,73,73	1
7	BR	C	303	1/1	0.95	0.08	53,53,53,53	1
7	BR	B	817	1/1	0.95	0.07	52,52,52,52	1
7	BR	A	302	1/1	0.95	0.10	46,46,46,46	1
7	BR	A	303	1/1	0.95	0.07	41,41,41,41	1
7	BR	D	804	1/1	0.96	0.06	47,47,47,47	0
7	BR	B	826	1/1	0.96	0.07	49,49,49,49	1
7	BR	B	811	1/1	0.96	0.07	35,35,35,35	1
7	BR	B	821	1/1	0.96	0.04	34,34,34,34	1
7	BR	D	816	1/1	0.96	0.05	48,48,48,48	1
7	BR	B	805	1/1	0.97	0.07	53,53,53,53	1
7	BR	C	305	1/1	0.97	0.07	41,41,41,41	1
9	HEM	D	803	43/43	0.97	0.07	25,33,39,43	0
7	BR	B	808	1/1	0.98	0.04	44,44,44,44	1
7	BR	B	804	1/1	0.98	0.08	41,41,41,41	1
7	BR	D	813	1/1	0.98	0.07	48,48,48,48	1
7	BR	A	306	1/1	0.98	0.03	44,44,44,44	1
7	BR	A	307	1/1	0.98	0.07	52,52,52,52	1

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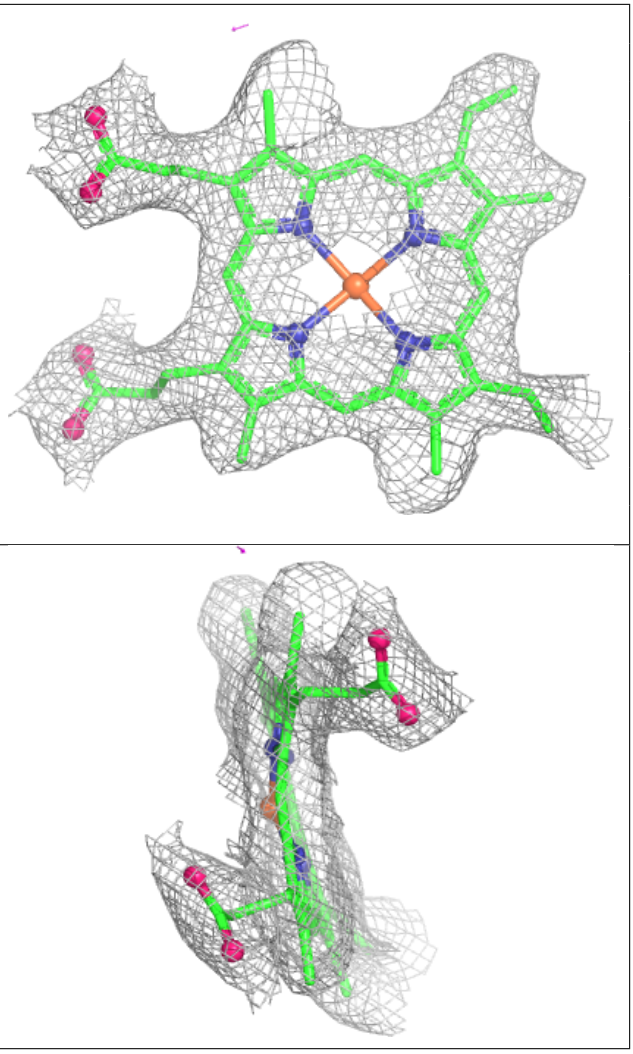
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	BR	C	302	1/1	0.98	0.06	45,45,45,45	1
7	BR	D	805	1/1	0.98	0.06	42,42,42,42	0
7	BR	B	802	1/1	0.98	0.04	37,37,37,37	0
7	BR	D	807	1/1	0.98	0.12	39,39,39,39	0
7	BR	D	808	1/1	0.98	0.06	45,45,45,45	1
7	BR	B	803	1/1	0.98	0.07	38,38,38,38	0
9	HEM	B	830	43/43	0.98	0.06	20,25,28,31	0
7	BR	B	812	1/1	0.98	0.05	42,42,42,42	1
8	CA	B	829	1/1	0.99	0.03	27,27,27,27	0
8	CA	D	819	1/1	0.99	0.01	32,32,32,32	0
7	BR	B	807	1/1	0.99	0.04	42,42,42,42	1
7	BR	A	301	1/1	0.99	0.03	23,23,23,23	0
7	BR	C	301	1/1	1.00	0.04	24,24,24,24	0

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

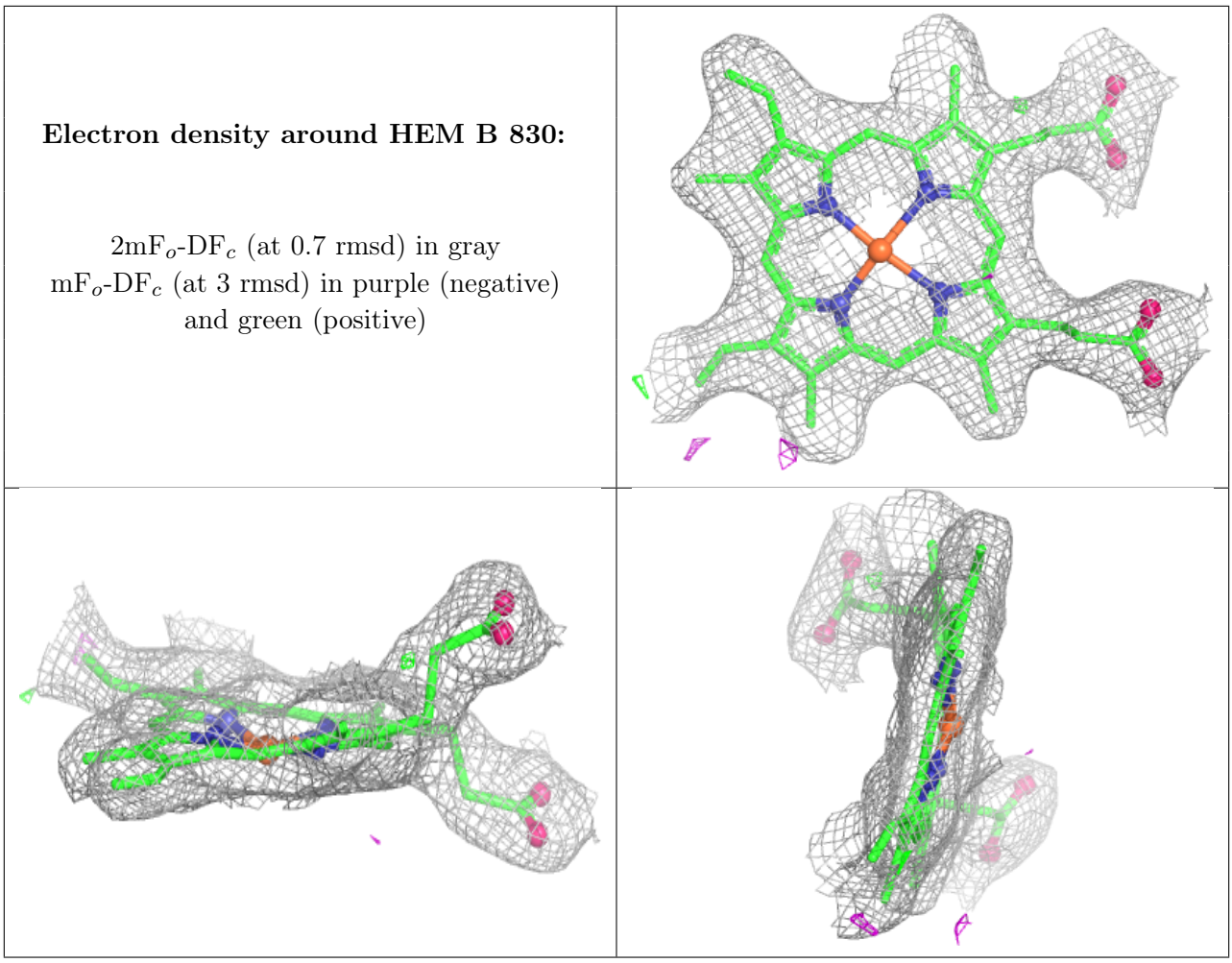
Electron density around HEM D 803:

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



Electron density around HEM B 830:

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



6.5 Other polymers

There are no such residues in this entry.