Full wwPDB X-ray Structure Validation Report (i)

Aug 9, 2020 – 03:13 PM BST

PDB ID	:	1QPA
Title	:	LIGNIN PEROXIDASE ISOZYME LIP4.65 (PI 4.65)
Authors	:	Choinowski, T.H.; Piontek, K.
Deposited on	:	1996-10-08
Resolution	:	1.80 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 (i) symbol.

The following versions of software and data (see references (i)) 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	:	2.13.1
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)	:	2.13.1

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 1.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.
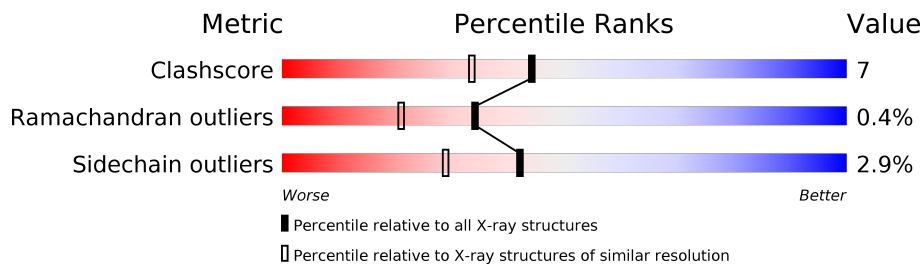
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)

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 on 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%

Mol	Chain	Length	Quality of chain
1	A	345	77% 19% · ·
1	B	345	80% 17% ·
2	C	3	67% 33%
3	D	2	50% 50%

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
2	FUC	C	3	X	-	X	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 5821 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 LIGNIN PEROXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	344	Total 2569	C 1630	N 432	O 492	S 15	0	0	0
1	B	344	Total 2569	C 1630	N 432	O 492	S 15	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	105	PRO	ARG	conflict	UNP P11542
A	171	HTR	TRP	modified residue	UNP P11542
A	283	ILE	THR	conflict	UNP P11542
B	105	PRO	ARG	conflict	UNP P11542
B	171	HTR	TRP	modified residue	UNP P11542
B	283	ILE	THR	conflict	UNP P11542

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.
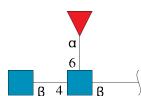
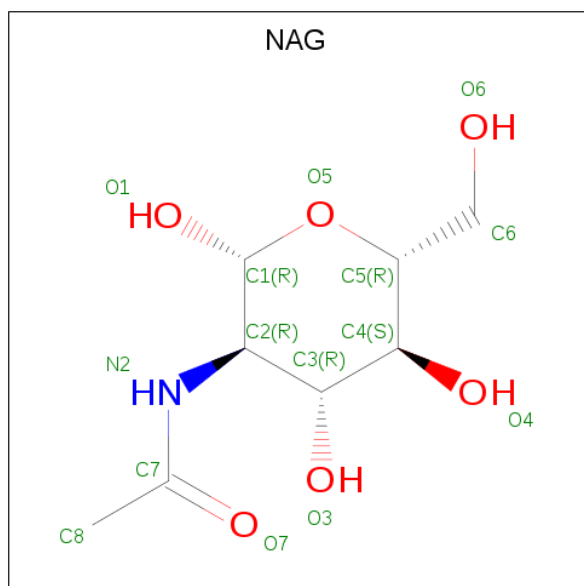| Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	3	Total 38	C 22	N 2	O 14	0	0	0

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-4)-alpha-D-mannopyranose.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	D	2	Total C O			0	0	0
			22 12	10				

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total C N O				0	0
			14 8 1	5				

- Molecule 5 is alpha-D-mannopyranose (three-letter code: MAN) (formula: $C_6H_{12}O_6$).
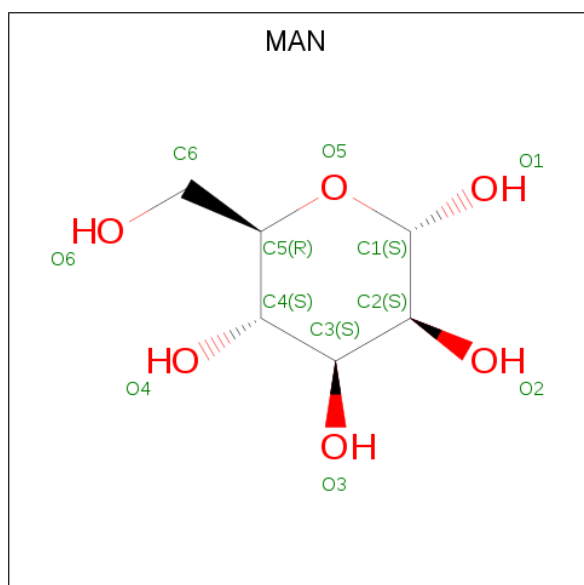
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total 11	C 6	O 5	0	0
5	A	1	Total 11	C 6	O 5	0	0
5	B	1	Total 11	C 6	O 5	0	0
5	B	1	Total 11	C 6	O 5	0	0
5	B	1	Total 11	C 6	O 5	0	0

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	2	Total 2	Ca 2	0	0
6	A	2	Total 2	Ca 2	0	0

- Molecule 7 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).
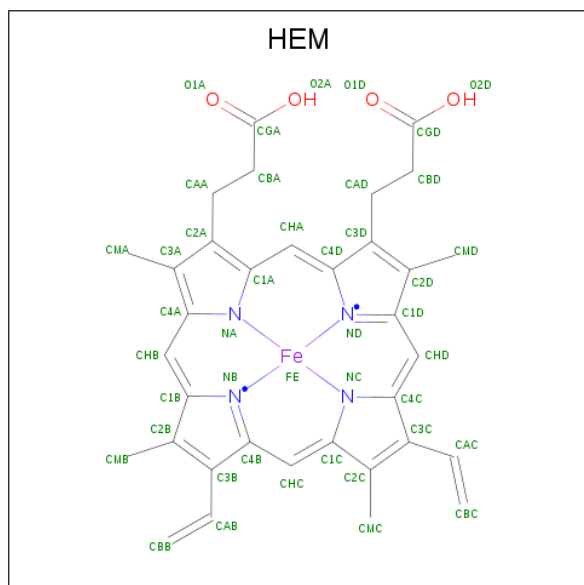
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
7	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	267	Total 267	O 267	0	0
8	B	197	Total 197	O 197	0	0

3 Residue-property plots ⓘ

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

• Molecule 1: LIGNIN PEROXIDASE

Chain A:

• Molecule 1: LIGNIN PEROXIDASE

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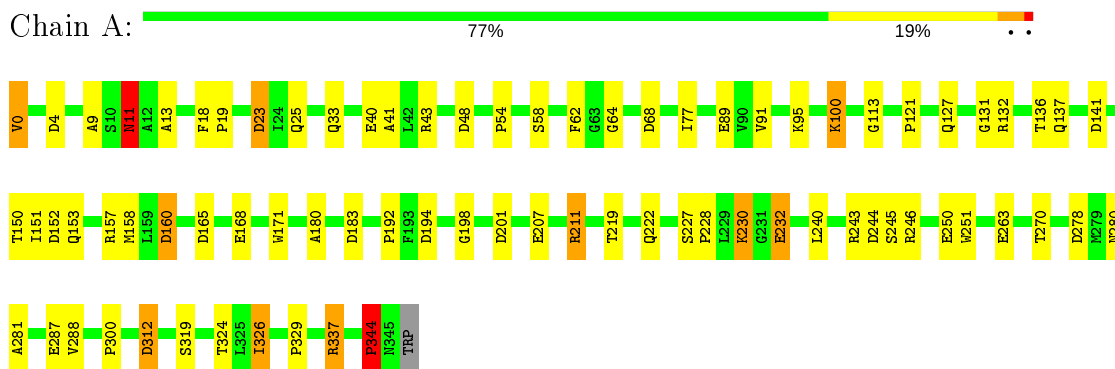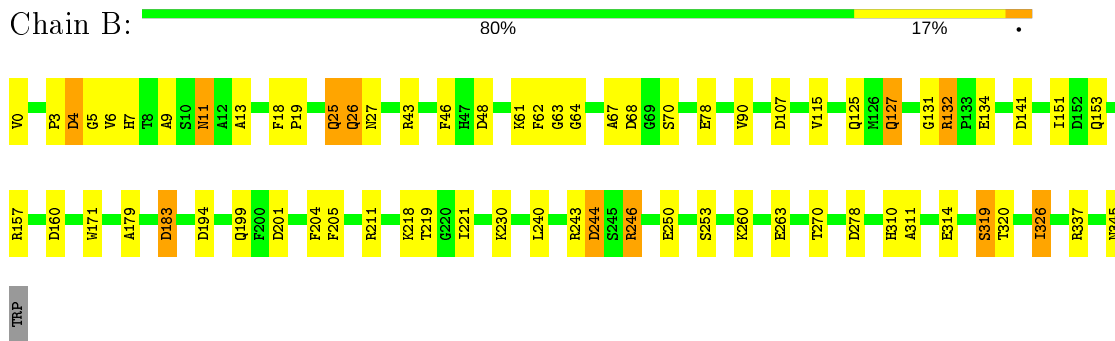
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:

• Molecule 3: alpha-D-mannopyranose-(1-4)-alpha-D-mannopyranose

Chain D:

4   Data and refinement statistics (i)

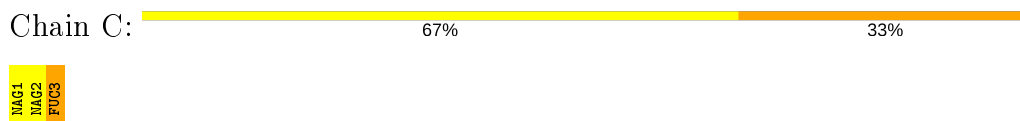| Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	57.79Å 94.02Å 81.26Å 90.00° 106.47° 90.00°	Depositor
Resolution (Å)	10.00 – 1.80 24.70 – 1.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-1.80) 96.1 (24.70-1.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.55 (at 1.80Å)	Xtriage
Refinement program	PROLSQ, X-PLOR	Depositor
R, R_{free}	(Not available) , (Not available) 0.163 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	20.8	Xtriage
Anisotropy	0.330	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 82.2	EDS
L-test for twinning[2]	$<\|L\|> = 0.50, <L^2> = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	5821	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.25% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (i)

5.1 Standard geometry (i)

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

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	0.98	1/2625 (0.0%)	1.93	64/3581 (1.8%)
1	B	0.87	2/2625 (0.1%)	1.99	53/3581 (1.5%)
All	All	0.92	3/5250 (0.1%)	1.96	117/7162 (1.6%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	11	ASN	CG-OD1	5.69	1.36	1.24
1	B	153	GLN	CD-OE1	5.51	1.36	1.24
1	B	26	GLN	CD-OE1	5.25	1.35	1.24

All (117) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	246	ARG	NE-CZ-NH1	41.65	141.12	120.30
1	B	337	ARG	CD-NE-CZ	23.20	156.09	123.60
1	A	160	ASP	CB-CG-OD2	19.84	136.16	118.30
1	B	246	ARG	NE-CZ-NH2	-18.94	110.83	120.30
1	A	246	ARG	NE-CZ-NH2	18.63	129.62	120.30
1	B	337	ARG	NE-CZ-NH1	17.08	128.84	120.30
1	B	48	ASP	CB-CG-OD2	15.69	132.42	118.30
1	A	68	ASP	CB-CG-OD2	11.69	128.82	118.30
1	A	152	ASP	CB-CG-OD2	-11.29	108.14	118.30
1	B	132	ARG	NE-CZ-NH1	11.09	125.85	120.30
1	A	152	ASP	CB-CG-OD1	10.70	127.93	118.30
1	B	246	ARG	NH1-CZ-NH2	-10.32	108.05	119.40
1	A	23	ASP	CB-CG-OD2	10.07	127.36	118.30
1	A	43	ARG	NE-CZ-NH2	9.89	125.25	120.30
1	B	160	ASP	CB-CG-OD2	9.83	127.14	118.30
1	A	337	ARG	NE-CZ-NH2	9.75	125.18	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	134	GLU	OE1-CD-OE2	9.64	134.87	123.30
1	A	337	ARG	CD-NE-CZ	9.55	136.97	123.60
1	A	165	ASP	CB-CG-OD2	9.30	126.67	118.30
1	A	250	GLU	OE1-CD-OE2	-9.25	112.20	123.30
1	A	168	GLU	OE1-CD-OE2	-9.14	112.33	123.30
1	A	141	ASP	CB-CG-OD2	-9.10	110.11	118.30
1	B	68	ASP	CB-CG-OD1	8.98	126.38	118.30
1	A	278	ASP	CB-CG-OD1	8.37	125.83	118.30
1	A	194	ASP	N-CA-CB	8.35	125.63	110.60
1	B	141	ASP	CB-CG-OD1	8.34	125.81	118.30
1	B	3	PRO	C-N-CA	8.29	142.43	121.70
1	B	157	ARG	NE-CZ-NH1	8.23	124.41	120.30
1	B	201	ASP	CB-CG-OD2	8.16	125.65	118.30
1	A	244	ASP	CB-CG-OD2	-8.09	111.02	118.30
1	A	278	ASP	CB-CG-OD2	-7.92	111.17	118.30
1	B	183	ASP	CB-CG-OD2	7.91	125.42	118.30
1	A	160	ASP	CB-CG-OD1	-7.77	111.31	118.30
1	A	201	ASP	CB-CG-OD1	7.56	125.10	118.30
1	A	211	ARG	CD-NE-CZ	-7.51	113.09	123.60
1	B	337	ARG	CB-CA-C	-7.47	95.47	110.40
1	A	201	ASP	CB-CG-OD2	7.32	124.88	118.30
1	A	157	ARG	NE-CZ-NH2	7.31	123.96	120.30
1	A	0	VAL	CG1-CB-CG2	-7.24	99.31	110.90
1	A	201	ASP	OD1-CG-OD2	-6.99	110.01	123.30
1	B	337	ARG	NH1-CZ-NH2	-6.98	111.72	119.40
1	B	157	ARG	CD-NE-CZ	6.97	133.35	123.60
1	A	100	LYS	CA-CB-CG	6.92	128.62	113.40
1	A	243	ARG	NE-CZ-NH1	6.89	123.74	120.30
1	A	43	ARG	NE-CZ-NH1	-6.84	116.88	120.30
1	B	179	ALA	N-CA-CB	-6.60	100.86	110.10
1	A	11	ASN	CB-CG-ND2	6.55	132.43	116.70
1	B	141	ASP	CB-CG-OD2	-6.50	112.45	118.30
1	A	141	ASP	CB-CG-OD1	6.31	123.97	118.30
1	A	11	ASN	CB-CG-OD1	-6.25	109.10	121.60
1	A	40	GLU	OE1-CD-OE2	-6.16	115.91	123.30
1	A	43	ARG	CD-NE-CZ	6.15	132.21	123.60
1	A	41	ALA	N-CA-CB	6.13	118.68	110.10
1	A	344	PRO	CA-N-CD	-6.11	102.95	111.50
1	B	199	GLN	OE1-CD-NE2	6.10	135.93	121.90
1	B	107	ASP	CB-CG-OD1	6.10	123.79	118.30
1	A	329	PRO	CA-C-O	6.09	134.82	120.20
1	B	278	ASP	CB-CG-OD1	6.09	123.78	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	132	ARG	NE-CZ-NH2	6.07	123.33	120.30
1	B	263	GLU	CG-CD-OE2	-6.07	106.17	118.30
1	B	199	GLN	O-C-N	6.05	132.38	122.70
1	A	246	ARG	NH1-CZ-NH2	-6.04	112.75	119.40
1	B	115	VAL	C-N-CA	6.03	134.95	122.30
1	B	205	PHE	CB-CG-CD1	-6.01	116.59	120.80
1	B	63	GLY	C-N-CA	5.96	134.82	122.30
1	B	314	GLU	CG-CD-OE1	5.94	130.18	118.30
1	B	48	ASP	OD1-CG-OD2	-5.93	112.04	123.30
1	B	68	ASP	OD1-CG-OD2	-5.92	112.06	123.30
1	B	43	ARG	NE-CZ-NH1	5.91	123.26	120.30
1	B	204	PHE	CB-CG-CD2	-5.91	116.66	120.80
1	B	153	GLN	N-CA-CB	-5.86	100.06	110.60
1	B	132	ARG	NE-CZ-NH2	-5.79	117.40	120.30
1	A	232	GLU	CG-CD-OE1	5.78	129.86	118.30
1	B	244	ASP	CB-CG-OD1	-5.77	113.11	118.30
1	A	89	GLU	CA-CB-CG	-5.74	100.77	113.40
1	B	134	GLU	N-CA-CB	-5.73	100.29	110.60
1	A	160	ASP	OD1-CG-OD2	-5.71	112.44	123.30
1	A	158	MET	CG-SD-CE	-5.68	91.11	100.20
1	A	278	ASP	O-C-N	5.67	131.77	122.70
1	A	113	GLY	O-C-N	-5.66	113.65	122.70
1	A	222	GLN	CG-CD-OE1	-5.61	110.37	121.60
1	B	205	PHE	CB-CG-CD2	5.60	124.72	120.80
1	A	280	ASN	CB-CA-C	5.57	121.54	110.40
1	A	77	ILE	CA-CB-CG1	-5.57	100.43	111.00
1	A	344	PRO	CB-CA-C	5.56	125.89	112.00
1	B	46	PHE	CB-CG-CD1	-5.53	116.93	120.80
1	B	125	GLN	CB-CG-CD	5.53	125.97	111.60
1	A	324	THR	CA-CB-CG2	-5.51	104.68	112.40
1	A	319	SER	CA-CB-OG	5.49	126.03	111.20
1	B	141	ASP	CA-C-N	5.48	127.16	116.20
1	A	243	ARG	N-CA-CB	-5.46	100.78	110.60
1	B	90	VAL	O-C-N	-5.42	114.03	122.70
1	A	246	ARG	NE-CZ-NH1	-5.39	117.61	120.30
1	B	127	GLN	CG-CD-OE1	-5.35	110.91	121.60
1	B	243	ARG	NE-CZ-NH2	5.33	122.96	120.30
1	A	137	GLN	N-CA-CB	-5.33	101.01	110.60
1	B	314	GLU	OE1-CD-OE2	-5.31	116.93	123.30
1	A	344	PRO	N-CA-C	5.27	125.80	112.10
1	A	263	GLU	OE1-CD-OE2	5.25	129.60	123.30
1	A	33	GLN	CA-CB-CG	5.23	124.91	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	48	ASP	C-N-CA	5.20	134.71	121.70
1	B	250	GLU	OE1-CD-OE2	-5.18	117.08	123.30
1	A	281	ALA	CB-CA-C	-5.17	102.34	110.10
1	B	46	PHE	CB-CG-CD2	5.17	124.42	120.80
1	A	4	ASP	CA-C-N	5.16	126.51	116.20
1	B	194	ASP	N-CA-CB	5.13	119.84	110.60
1	A	244	ASP	OD1-CG-OD2	5.13	133.04	123.30
1	A	251	TRP	CE3-CZ3-CH2	5.11	126.83	121.20
1	B	27	ASN	CB-CG-OD1	-5.10	111.40	121.60
1	B	278	ASP	CB-CG-OD2	-5.09	113.72	118.30
1	B	4	ASP	CA-C-N	-5.09	106.02	116.20
1	A	132	ARG	CD-NE-CZ	5.06	130.69	123.60
1	A	312	ASP	O-C-N	5.06	130.80	122.70
1	A	287	GLU	CA-C-N	5.05	128.32	117.20
1	B	5	GLY	N-CA-C	-5.05	100.47	113.10
1	B	4	ASP	CA-C-O	5.04	130.67	120.10
1	A	337	ARG	CB-CA-C	5.01	120.43	110.40

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	2569	0	2448	27	0
1	B	2569	0	2447	33	0
2	C	38	0	34	7	0
3	D	22	0	19	4	0
4	A	14	0	13	0	0
5	A	22	0	20	0	0
5	B	33	0	30	5	0
6	A	2	0	0	0	0
6	B	2	0	0	0	0
7	A	43	0	30	4	0
7	B	43	0	30	4	0
8	A	267	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	B	197	0	0	1	0
All	All	5821	0	5071	69	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 7.

All (69) 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:11:ASN:HD22	1:A:13:ALA:H	0.99	0.93
1:B:260:LYS:HE3	2:C:3:FUC:H2	1.54	0.90
1:B:4:ASP:HB3	1:B:6:VAL:H	1.36	0.89
1:B:211:ARG:HB2	1:B:211:ARG:NH1	1.95	0.82
1:B:4:ASP:OD2	1:B:7:HIS:ND1	2.12	0.81
1:B:151:ILE:HD11	1:B:240:LEU:HB2	1.64	0.79
1:A:11:ASN:ND2	1:A:13:ALA:H	1.78	0.79
1:B:253:SER:HB2	2:C:3:FUC:H63	1.65	0.78
5:B:380:MAN:H62	2:C:3:FUC:H62	1.67	0.77
1:B:211:ARG:HH11	1:B:211:ARG:HB2	1.50	0.77
1:B:11:ASN:HD22	1:B:13:ALA:H	1.34	0.75
1:B:319:SER:HB2	5:B:380:MAN:H2	1.69	0.75
1:A:25:GLN:HE21	1:A:25:GLN:HA	1.51	0.74
5:B:380:MAN:C6	2:C:3:FUC:H62	2.20	0.72
1:A:11:ASN:HD22	1:A:13:ALA:N	1.83	0.71
1:B:25:GLN:HA	1:B:25:GLN:HE21	1.56	0.69
1:B:260:LYS:CE	2:C:3:FUC:H2	2.22	0.69
8:B:591:HOH:O	2:C:3:FUC:H61	1.92	0.68
1:A:150:THR:OG1	1:A:153:GLN:HG3	1.93	0.68
1:A:227:SER:HB2	1:A:228:PRO:HD2	1.79	0.65
1:B:311:ALA:HA	3:D:2:MAN:O4	1.98	0.64
1:A:127:GLN:NE2	1:A:270:THR:OG1	2.30	0.63
1:A:25:GLN:HA	1:A:25:GLN:NE2	2.15	0.62
1:A:23:ASP:OD2	1:A:100:LYS:HE3	2.01	0.60
1:A:300:PRO:HG3	1:B:326:ILE:HG13	1.85	0.59
7:A:350:HEM:HHC	7:A:350:HEM:HBB2	1.85	0.59
1:B:218:LYS:HB3	1:B:221:ILE:HD11	1.85	0.58
1:B:244:ASP:OD1	1:B:246:ARG:HD3	2.03	0.58
1:A:230:LYS:HD2	8:A:472:HOH:O	2.03	0.57
1:A:326:ILE:HD13	1:A:326:ILE:H	1.70	0.56
7:B:350:HEM:HHC	7:B:350:HEM:HBB2	1.88	0.56
1:B:151:ILE:HD11	1:B:240:LEU:CB	2.35	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:PHE:HB2	1:B:19:PRO:HD3	1.90	0.53
1:B:310:HIS:HB3	3:D:2:MAN:H5	1.91	0.53
1:B:11:ASN:ND2	1:B:13:ALA:H	2.03	0.52
1:B:25:GLN:NE2	1:B:25:GLN:HA	2.22	0.52
1:B:320:THR:HG21	5:B:380:MAN:O6	2.10	0.52
1:B:311:ALA:N	3:D:2:MAN:H62	2.26	0.50
7:A:350:HEM:HBB2	7:A:350:HEM:CHC	2.41	0.50
1:A:0:VAL:HG13	1:A:9:ALA:O	2.11	0.50
1:B:4:ASP:HB3	1:B:6:VAL:N	2.17	0.50
1:B:211:ARG:HH11	1:B:211:ARG:CB	2.23	0.47
1:A:151:ILE:HD11	1:A:240:LEU:HB2	1.96	0.46
1:B:62:PHE:CE2	1:B:64:GLY:HA2	2.51	0.45
1:B:0:VAL:HB	1:B:9:ALA:O	2.16	0.45
1:A:18:PHE:HB2	1:A:19:PRO:HD3	1.97	0.45
1:A:211:ARG:HG3	1:A:312:ASP:O	2.16	0.45
1:A:58:SER:HA	8:A:700:HOH:O	2.17	0.45
1:A:121:PRO:HD2	1:A:198:GLY:O	2.16	0.45
5:B:380:MAN:H61	2:C:3:FUC:H62	1.94	0.44
1:B:70:SER:OG	1:B:78:GLU:OE2	2.35	0.44
7:B:350:HEM:CHC	7:B:350:HEM:HBB2	2.48	0.44
1:A:207:GLU:OE1	1:A:232:GLU:OE1	2.35	0.44
1:A:230:LYS:HD3	1:A:230:LYS:HA	1.37	0.43
1:B:127:GLN:NE2	1:B:270:THR:OG1	2.48	0.43
1:A:62:PHE:CE2	1:A:64:GLY:HA2	2.54	0.42
1:A:91:VAL:HG12	1:A:95:LYS:HE3	2.01	0.42
1:B:311:ALA:H	3:D:2:MAN:H62	1.85	0.42
1:A:183:ASP:OD2	7:A:350:HEM:O2A	2.37	0.42
1:A:288:VAL:HG12	1:A:288:VAL:O	2.20	0.42
1:A:54:PRO:HD2	1:A:160:ASP:OD1	2.20	0.41
7:B:350:HEM:CBB	7:B:350:HEM:HHC	2.49	0.41
1:B:67:ALA:O	1:B:132:ARG:HD3	2.20	0.41
1:A:230:LYS:CD	8:A:472:HOH:O	2.67	0.41
1:B:183:ASP:OD2	7:B:350:HEM:O2A	2.39	0.41
1:B:26:GLN:O	1:B:26:GLN:HG2	2.19	0.41
1:B:62:PHE:CZ	1:B:64:GLY:HA2	2.56	0.41
7:A:350:HEM:HHC	7:A:350:HEM:CBB	2.49	0.41
1:A:180:ALA:HA	1:A:192:PRO:HA	2.02	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	341/345 (99%)	332 (97%)	7 (2%)	2 (1%)	25	12
1	B	341/345 (99%)	326 (96%)	14 (4%)	1 (0%)	41	27
All	All	682/690 (99%)	658 (96%)	21 (3%)	3 (0%)	34	21

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	344	PRO
1	A	131	GLY
1	B	131	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	274/275 (100%)	266 (97%)	8 (3%)	42	29
1	B	274/275 (100%)	266 (97%)	8 (3%)	42	29
All	All	548/550 (100%)	532 (97%)	16 (3%)	42	29

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	136	THR
1	A	219	THR

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Mol	Chain	Res	Type
1	A	230	LYS
1	A	245	SER
1	A	326	ILE
1	A	337	ARG
1	A	344	PRO
1	B	11	ASN
1	B	25	GLN
1	B	61	LYS
1	B	219	THR
1	B	230	LYS
1	B	319	SER
1	B	326	ILE
1	B	345	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	25	GLN
1	A	59	GLN
1	A	94	GLN
1	A	119	ASN
1	A	127	GLN
1	B	11	ASN
1	B	25	GLN
1	B	33	GLN
1	B	59	GLN
1	B	94	GLN
1	B	119	ASN
1	B	127	GLN
1	B	199	GLN
1	B	222	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	HTR	B	171	1	14,16,17	1.20	1 (7%)	16,22,24	1.70	5 (31%)
1	HTR	A	171	1	14,16,17	1.49	1 (7%)	16,22,24	1.95	5 (31%)

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	HTR	B	171	1	-	2/5/10/12	0/2/2/2
1	HTR	A	171	1	-	3/5/10/12	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	171	HTR	CG-CD2	4.12	1.45	1.40
1	B	171	HTR	OH-CB	2.26	1.47	1.42

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	171	HTR	OH-CB-CA	4.16	116.07	107.28
1	A	171	HTR	CH2-CZ2-CE2	-3.45	115.11	120.08
1	A	171	HTR	OH-CB-CG	3.34	116.14	111.03
1	A	171	HTR	OH-CB-CA	3.28	114.20	107.28
1	A	171	HTR	O-C-CA	-2.99	116.93	124.78
1	A	171	HTR	CZ3-CH2-CZ2	2.73	124.26	120.44
1	B	171	HTR	CH2-CZ2-CE2	-2.45	116.56	120.08
1	B	171	HTR	O-C-CA	-2.44	118.39	124.78
1	B	171	HTR	OH-CB-CG	2.27	114.50	111.03
1	B	171	HTR	CG-CB-CA	2.24	114.49	111.49

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	171	HTR	O-C-CA-CB
1	A	171	HTR	O-C-CA-CB
1	B	171	HTR	N-CA-CB-OH
1	A	171	HTR	N-CA-CB-OH
1	A	171	HTR	N-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

5 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
2	NAG	C	1	1,2	14,14,15	1.39	2 (14%)	17,19,21	3.51	5 (29%)
2	NAG	C	2	2	14,14,15	1.21	1 (7%)	17,19,21	3.13	11 (64%)
2	FUC	C	3	2	10,10,11	1.52	2 (20%)	14,14,16	2.44	5 (35%)
3	MAN	D	1	1,3	11,11,12	0.71	0	15,15,17	2.36	6 (40%)
3	MAN	D	2	3	11,11,12	0.87	1 (9%)	15,15,17	1.98	4 (26%)

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MAN	D	2	3	-	0/2/19/22	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3	FUC	O5-C5	3.36	1.50	1.43
2	C	1	NAG	O7-C7	-3.12	1.16	1.23
2	C	2	NAG	O7-C7	-2.87	1.16	1.23
2	C	1	NAG	O6-C6	-2.45	1.32	1.42
3	D	2	MAN	C1-C2	2.26	1.57	1.52
2	C	3	FUC	O2-C2	2.09	1.47	1.43

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1	NAG	C1-O5-C5	8.95	124.31	112.19
2	C	1	NAG	C4-C3-C2	-6.81	101.04	111.02
2	C	1	NAG	O4-C4-C5	6.38	125.14	109.30
2	C	2	NAG	C1-O5-C5	-5.64	104.55	112.19
2	C	3	FUC	C3-C4-C5	5.22	117.91	109.77
2	C	2	NAG	C3-C4-C5	4.99	119.14	110.24
2	C	2	NAG	C1-C2-N2	4.99	119.01	110.49
2	C	1	NAG	O5-C5-C6	-4.67	99.88	107.20
2	C	2	NAG	O6-C6-C5	4.48	126.67	111.29
2	C	3	FUC	O5-C5-C4	4.28	117.20	109.52
3	D	2	MAN	O4-C4-C5	4.04	119.33	109.30
2	C	2	NAG	O5-C1-C2	-4.02	104.95	111.29
3	D	2	MAN	C6-C5-C4	3.99	122.34	113.00
2	C	2	NAG	C4-C3-C2	-3.86	105.37	111.02
3	D	1	MAN	O4-C4-C3	-3.78	101.61	110.35
3	D	1	MAN	O2-C2-C3	-3.73	102.66	110.14
3	D	1	MAN	C1-O5-C5	3.58	117.04	112.19
2	C	3	FUC	C1-O5-C5	-3.55	104.73	112.78
3	D	1	MAN	C2-C3-C4	3.48	116.92	110.89
2	C	3	FUC	C2-C3-C4	3.44	116.85	110.89
3	D	2	MAN	O5-C5-C6	-3.14	102.27	107.20
2	C	2	NAG	O3-C3-C2	3.10	115.88	109.47
3	D	1	MAN	C1-C2-C3	2.99	113.34	109.67
2	C	1	NAG	C3-C4-C5	-2.56	105.67	110.24
2	C	2	NAG	C8-C7-N2	-2.56	111.76	116.10
3	D	2	MAN	O4-C4-C3	-2.56	104.44	110.35
2	C	2	NAG	O7-C7-C8	2.30	126.33	122.06

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Full wwPDB X-ray Structure Validation Report

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	3	FUC	O4-C4-C5	2.17	114.48	109.67
2	C	2	NAG	O5-C5-C4	2.14	116.03	110.83
3	D	1	MAN	O3-C3-C2	-2.10	105.96	109.99
2	C	2	NAG	O4-C4-C3	-2.02	105.68	110.35

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	3	FUC	C1

All (8) torsion outliers are listed below:

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

There are no ring outliers.

2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	2	MAN	4	0
2	C	3	FUC	7	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 C

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain D

Bond lengths

Bond angles

Torsions

Rings
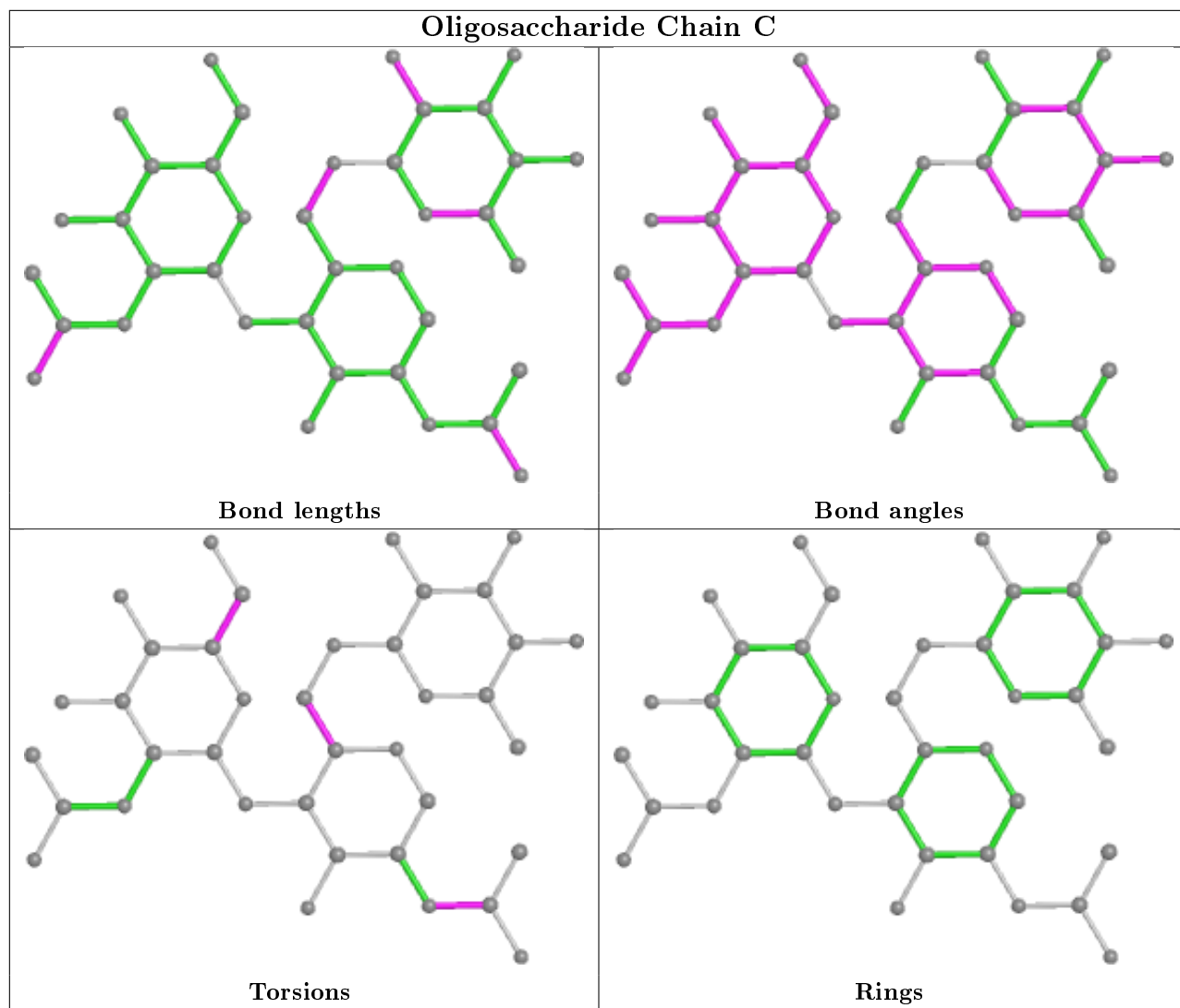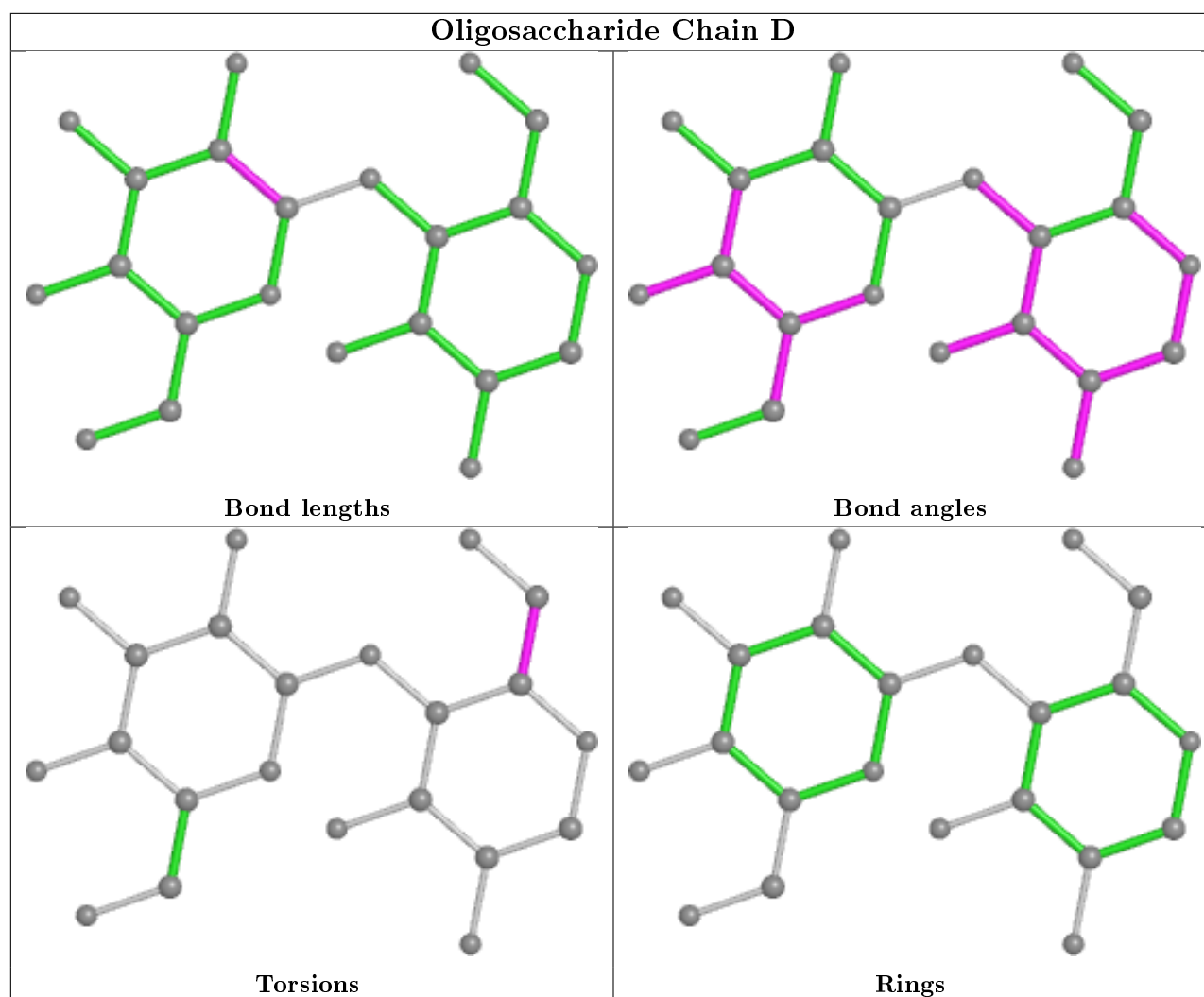
5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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	#$|Z| > 2$
5	MAN	A	370	1	11,11,12	1.22	1 (9%)	15,15,17	2.36	8 (53%)
7	HEM	B	350	1,8	27,50,50	1.97	8 (29%)	17,82,82	2.36	6 (35%)
7	HEM	A	350	1,8	27,50,50	2.13	8 (29%)	17,82,82	2.81	8 (47%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
4	NAG	A	360	1	14,14,15	1.01	1 (7%)	17,19,21	2.01	5 (29%)
5	MAN	B	380	1	11,11,12	0.92	1 (9%)	15,15,17	1.52	1 (6%)
5	MAN	B	370	1	11,11,12	1.21	1 (9%)	15,15,17	1.64	2 (13%)
5	MAN	A	375	1	11,11,12	1.12	2 (18%)	15,15,17	2.22	6 (40%)
5	MAN	B	375	1	11,11,12	1.12	1 (9%)	15,15,17	2.44	5 (33%)

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	MAN	A	370	1	-	1/2/19/22	0/1/1/1
7	HEM	B	350	1,8	-	0/6/54/54	-
7	HEM	A	350	1,8	-	0/6/54/54	-
4	NAG	A	360	1	-	2/6/23/26	0/1/1/1
5	MAN	B	380	1	-	2/2/19/22	0/1/1/1
5	MAN	B	370	1	-	2/2/19/22	0/1/1/1
5	MAN	A	375	1	-	0/2/19/22	0/1/1/1
5	MAN	B	375	1	-	2/2/19/22	0/1/1/1

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	350	HEM	C1A-NA	6.39	1.49	1.36
7	B	350	HEM	C3C-C2C	-5.04	1.33	1.40
7	A	350	HEM	C3B-C2B	-3.76	1.35	1.40
7	A	350	HEM	C4A-NA	3.63	1.43	1.36
7	B	350	HEM	C3B-CAB	3.45	1.55	1.47
7	A	350	HEM	C3C-CAC	3.43	1.54	1.47
7	B	350	HEM	C3B-C2B	-3.40	1.35	1.40
4	A	360	NAG	O7-C7	-3.17	1.16	1.23
5	B	370	MAN	C1-C2	3.12	1.59	1.52
7	A	350	HEM	C3B-CAB	2.97	1.54	1.47
7	B	350	HEM	CMC-C2C	2.95	1.58	1.51
7	B	350	HEM	C4A-NA	2.87	1.42	1.36
5	A	370	MAN	C1-C2	2.76	1.58	1.52
7	A	350	HEM	C3C-C2C	-2.69	1.36	1.40
7	B	350	HEM	C3C-CAC	2.67	1.53	1.47
5	B	375	MAN	C1-C2	2.61	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	375	MAN	C4-C5	2.49	1.58	1.53
7	A	350	HEM	C1B-C2B	2.38	1.48	1.42
7	B	350	HEM	C1A-NA	2.22	1.40	1.36
5	A	375	MAN	C1-C2	2.16	1.57	1.52
7	B	350	HEM	C4B-NB	2.13	1.40	1.36
5	B	380	MAN	C1-C2	2.06	1.56	1.52
7	A	350	HEM	C4D-C3D	2.00	1.47	1.42

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	350	HEM	CAA-CBA-CGA	7.23	124.80	112.67
5	B	375	MAN	C1-O5-C5	6.27	120.69	112.19
7	A	350	HEM	CMD-C2D-C1D	-5.18	120.51	128.46
5	A	375	MAN	O3-C3-C2	-5.14	100.15	109.99
5	A	370	MAN	C6-C5-C4	4.89	124.47	113.00
7	B	350	HEM	CMD-C2D-C1D	-4.86	121.00	128.46
4	A	360	NAG	C2-N2-C7	4.70	129.60	122.90
5	B	370	MAN	C1-O5-C5	4.59	118.42	112.19
7	B	350	HEM	CMD-C2D-C3D	4.22	132.90	124.94
5	A	370	MAN	C2-C3-C4	4.15	118.08	110.89
5	B	380	MAN	C6-C5-C4	4.06	122.52	113.00
7	B	350	HEM	CMA-C3A-C4A	-3.83	122.57	128.46
5	B	375	MAN	C2-C3-C4	3.47	116.90	110.89
5	B	375	MAN	O5-C5-C6	-3.28	102.06	107.20
5	B	375	MAN	O2-C2-C1	-3.25	102.50	109.15
7	B	350	HEM	CMA-C3A-C2A	3.24	131.06	124.94
5	A	375	MAN	O6-C6-C5	-3.17	100.42	111.29
5	A	370	MAN	C1-C2-C3	3.05	113.41	109.67
7	B	350	HEM	CMB-C2B-C3B	3.00	130.29	124.68
7	A	350	HEM	CMD-C2D-C3D	2.95	130.50	124.94
7	A	350	HEM	CBA-CAA-C2A	2.93	117.89	112.49
4	A	360	NAG	O5-C5-C6	-2.87	102.70	107.20
5	A	375	MAN	C6-C5-C4	2.87	119.73	113.00
5	A	375	MAN	O2-C2-C1	-2.86	103.30	109.15
7	A	350	HEM	CMA-C3A-C4A	-2.84	124.10	128.46
4	A	360	NAG	O5-C5-C4	-2.81	104.00	110.83
4	A	360	NAG	O4-C4-C5	2.79	116.22	109.30
7	A	350	HEM	CMB-C2B-C3B	2.77	129.86	124.68
5	A	370	MAN	C1-O5-C5	2.68	115.83	112.19
5	A	370	MAN	O3-C3-C2	-2.63	104.95	109.99
4	A	360	NAG	O3-C3-C4	-2.56	104.42	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	350	HEM	C3B-C4B-NB	-2.55	105.92	109.21
5	A	375	MAN	O3-C3-C4	2.40	115.90	110.35
5	A	370	MAN	O2-C2-C3	2.30	114.74	110.14
5	A	375	MAN	C2-C3-C4	2.25	114.79	110.89
7	B	350	HEM	CAA-CBA-CGA	2.25	116.44	112.67
7	A	350	HEM	C4C-C3C-C2C	-2.21	105.36	106.90
5	A	370	MAN	O5-C5-C6	-2.18	103.78	107.20
5	B	375	MAN	C6-C5-C4	2.14	118.03	113.00
5	A	370	MAN	O3-C3-C4	2.11	115.23	110.35
5	B	370	MAN	O2-C2-C1	2.02	113.28	109.15

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	360	NAG	C8-C7-N2-C2
5	B	380	MAN	C4-C5-C6-O6
4	A	360	NAG	O7-C7-N2-C2
5	B	380	MAN	O5-C5-C6-O6
5	B	370	MAN	O5-C5-C6-O6
5	B	375	MAN	C4-C5-C6-O6
5	A	370	MAN	O5-C5-C6-O6
5	B	375	MAN	O5-C5-C6-O6
5	B	370	MAN	C4-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	350	HEM	4	0
7	A	350	HEM	4	0
5	B	380	MAN	5	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 350

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM A 350

Bond lengths

Bond angles

Torsions

Rings
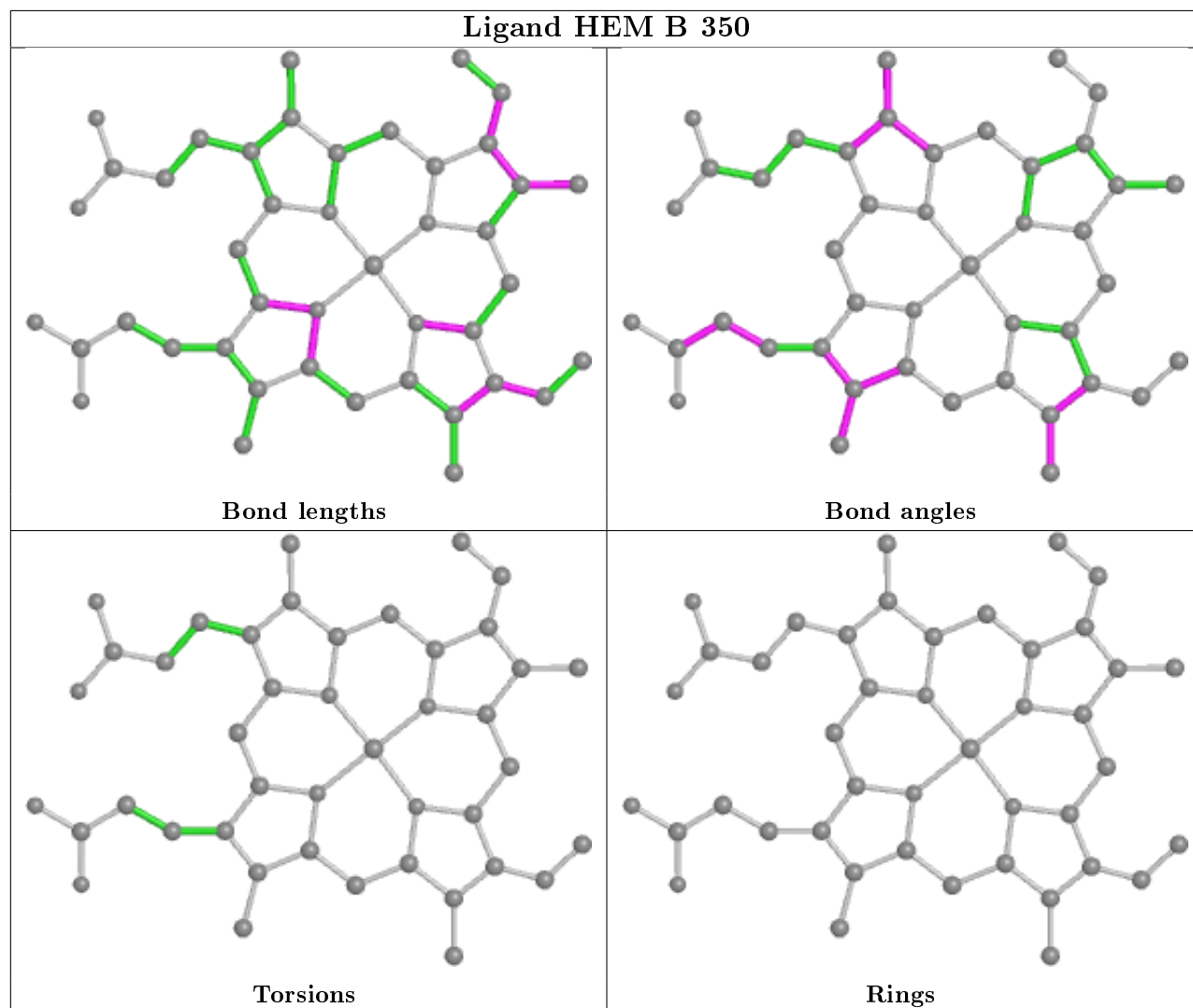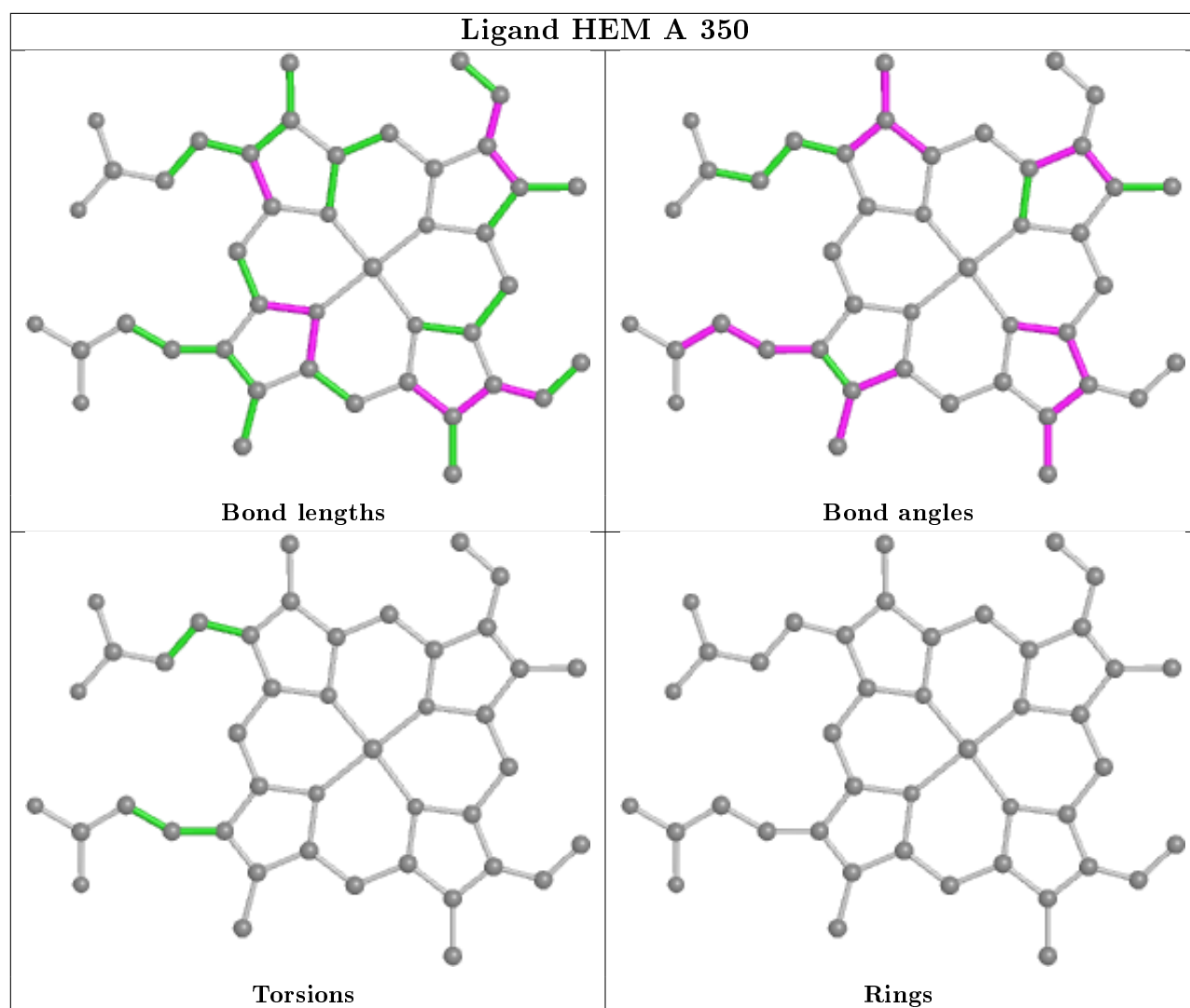
5.7　Other polymers (i)

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 (i)

6.1 Protein, DNA and RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

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 C:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
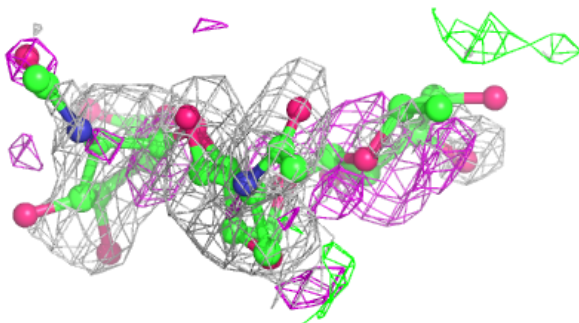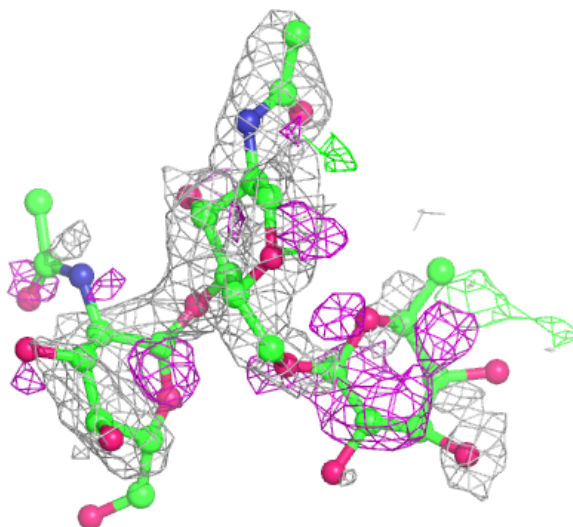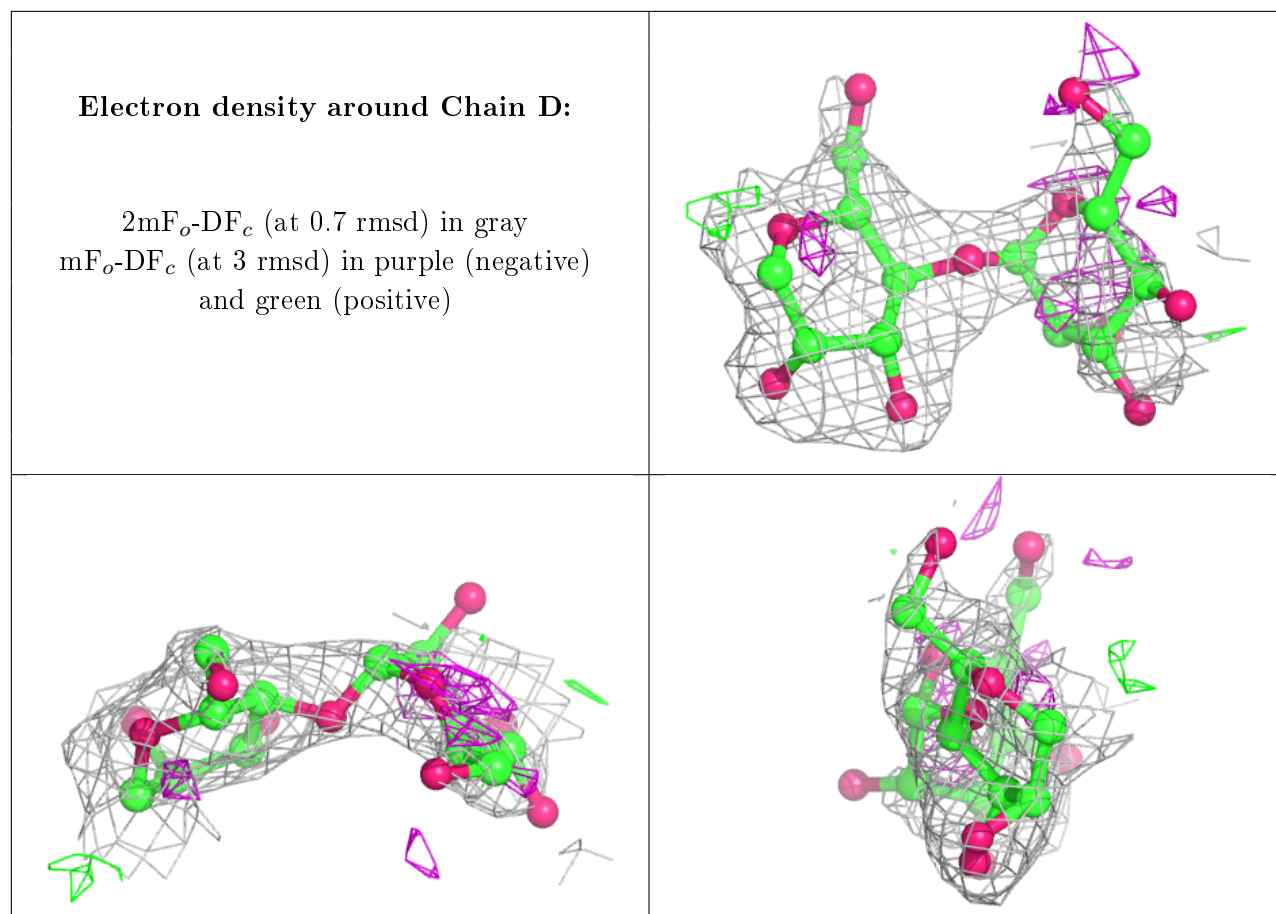
Electron density around Chain D:

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

6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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 A 350:

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

Electron density around HEM B 350:

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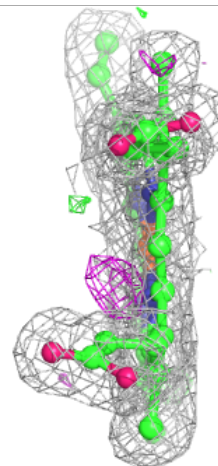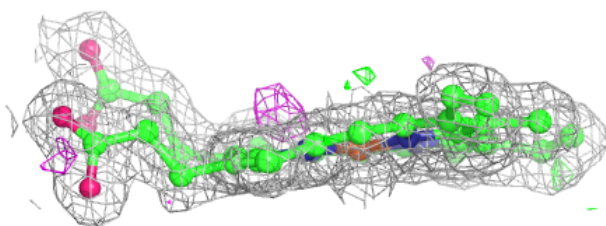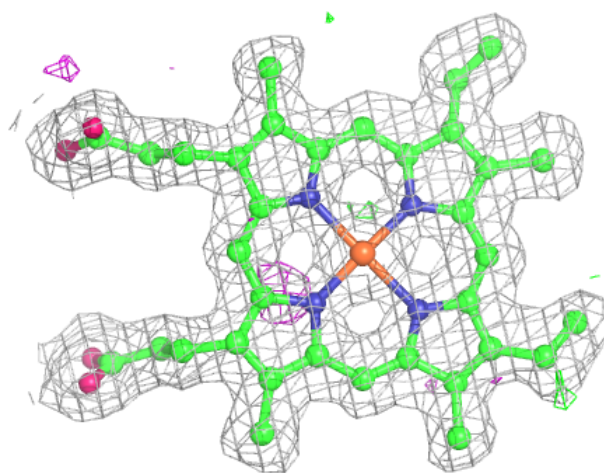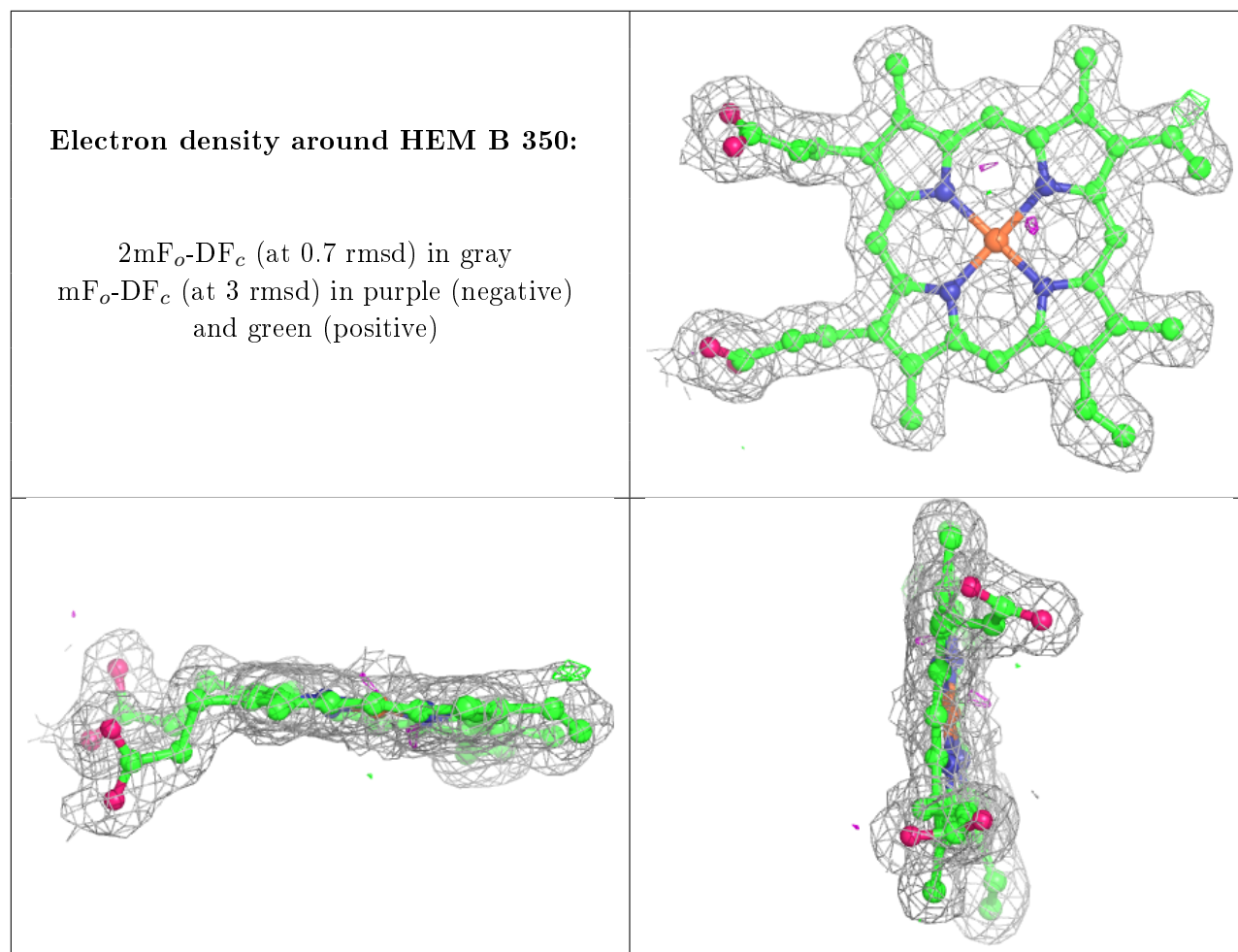
6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.