WORLDWIDE PDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Oct 19, 2023 – 12:30 AM EDT

PDB ID	:	2R5L
Title	:	Crystal structure of lactoperoxidase at 2.4A resolution
Authors	:	Singh, A.K.; Singh, N.; Sharma, S.; Kaur, P.; Srinivasan, A.; Singh, T.P.
Deposited on	:	2007-09-04
Resolution	:	2.40 Å(reported)

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	:	2.36
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 2.40 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.
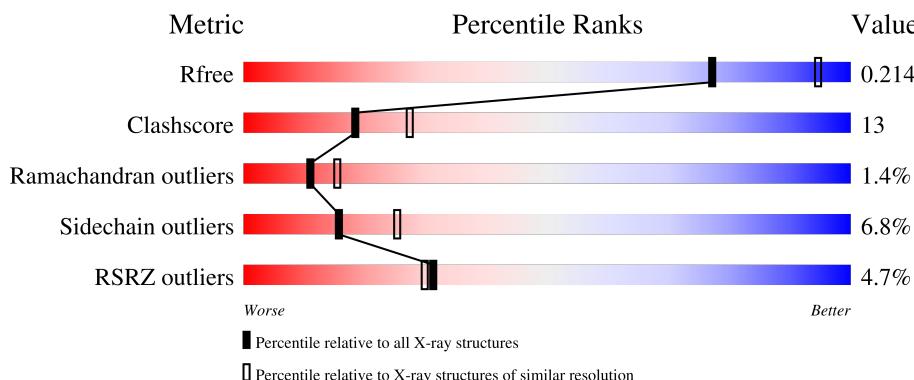
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	A	595	5% / 75% / 20% / 5%
2	B	3	33% / 67%
2	C	3	100%
2	D	3	67% / 33%
3	E	2	50% / 50%
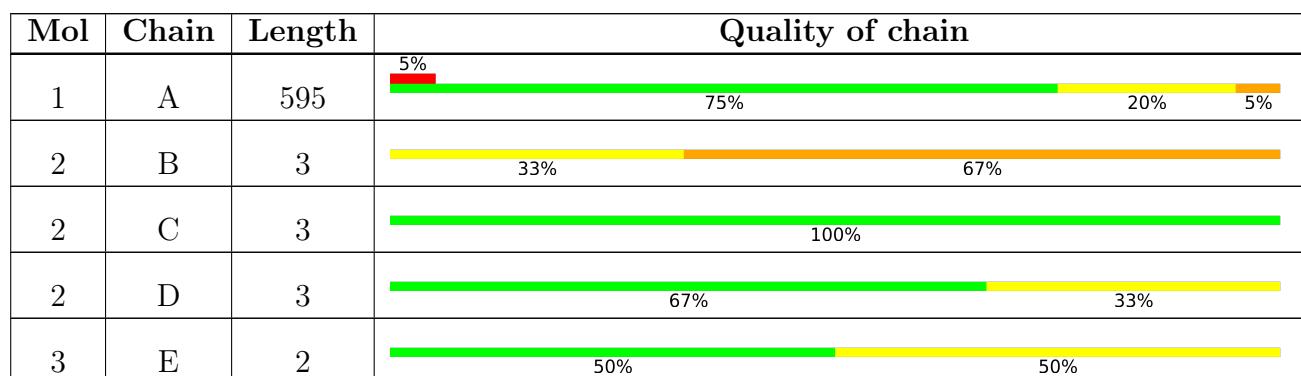
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MAN	B	3	-	-	-	X
2	MAN	C	3	-	-	-	X
2	MAN	D	3	-	-	-	X
3	NAG	E	2	-	-	-	X
5	IOD	A	617	-	-	X	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 5377 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Lactoperoxidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	595	Total 4757	C 3021	N 844	O 865	P 1	S 26	0	0	0

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.
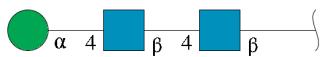
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	3	Total 39	C 22	N 2	O 15	0	0	0
2	C	3	Total 39	C 22	N 2	O 15	0	0	0
2	D	3	Total 39	C 22	N 2	O 15	0	0	0

- Molecule 3 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
3	E	2	Total 28	C 16	N 2	O 10	0	0	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 5 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	10	Total I 10 10		0	0

- Molecule 6 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).
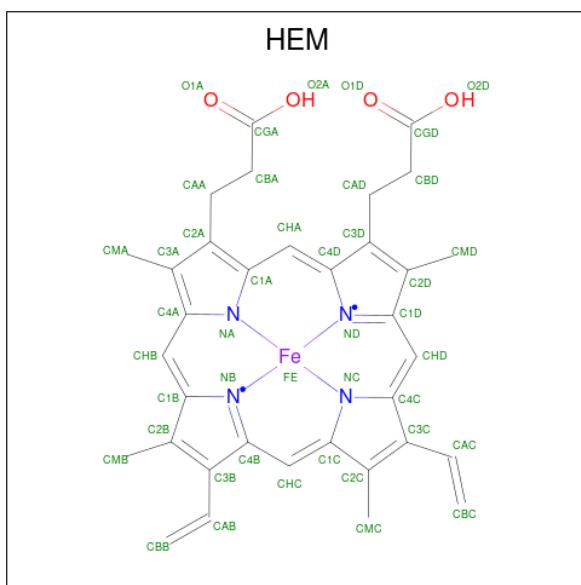
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	421	Total O 421 421		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 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
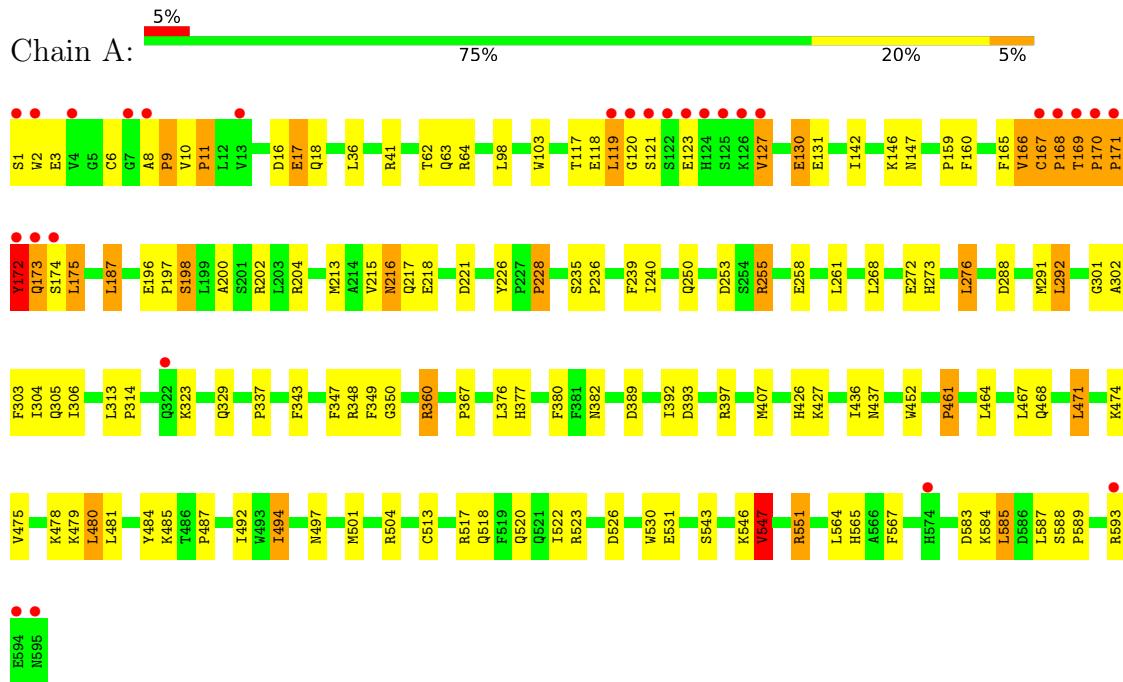
• Molecule 2: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

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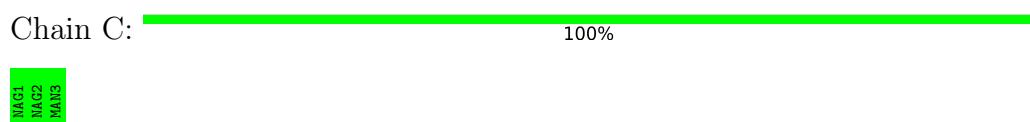
• Molecule 2: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:

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

Chain E:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	54.19Å 80.81Å 77.04Å 90.00° 102.95° 90.00°	Depositor
Resolution (Å)	19.98 – 2.40 24.88 – 2.40	Depositor EDS
% Data completeness (in resolution range)	97.8 (19.98-2.40) 97.8 (24.88-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.60 (at 2.39Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.196 , 0.203 0.178 , 0.214	Depositor DCC
R_{free} test set	1274 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å^2)	22.3	Xtriage
Anisotropy	0.279	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 53.4	EDS
L-test for twinning[2]	$< \lvert L \rvert > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5377	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.44% 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 $< \lvert L \rvert >$, $< L^2 >$ 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: NAG, IOD, SEP, CA, MAN, HEM

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	0.49	1/4875 (0.0%)	0.82	10/6621 (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	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	170	PRO	N-CA	6.27	1.57	1.47

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	172	TYR	CA-CB-CG	-9.13	96.05	113.40
1	A	585	LEU	CA-CB-CG	6.88	131.13	115.30
1	A	461	PRO	CA-N-CD	-6.60	102.26	111.50
1	A	6	CYS	CA-CB-SG	5.94	124.69	114.00
1	A	228	PRO	CA-N-CD	-5.88	103.28	111.50
1	A	171	PRO	CA-N-CD	-5.80	103.38	111.50
1	A	547	VAL	CB-CA-C	-5.57	100.82	111.40
1	A	11	PRO	N-CA-C	5.48	126.35	112.10
1	A	172	TYR	CB-CG-CD2	-5.14	117.91	121.00
1	A	587	LEU	CB-CG-CD1	-5.13	102.28	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	172	TYR	Sidechain

5.2 Too-close contacts ⓘ

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	4757	0	4645	126	0
2	B	39	0	34	2	0
2	C	39	0	34	0	0
2	D	39	0	34	0	0
3	E	28	0	25	0	0
4	A	1	0	0	0	0
5	A	10	0	0	4	0
6	A	43	0	30	3	0
7	A	421	0	0	18	0
All	All	5377	0	4802	130	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 13.

All (130) 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:2:TRP:HB2	1:A:175:LEU:HD12	1.23	1.20
1:A:168:PRO:HG2	1:A:172:TYR:CE1	1.85	1.11
1:A:167:CYS:HB3	1:A:168:PRO:HD2	1.34	1.09
1:A:169:THR:CG2	1:A:170:PRO:HD3	1.89	1.02
1:A:2:TRP:HA	7:A:998:HOH:O	1.65	0.95
1:A:167:CYS:HB3	1:A:168:PRO:CD	1.97	0.95
1:A:169:THR:HG22	1:A:170:PRO:HD3	1.49	0.93
1:A:481:LEU:HD21	1:A:487:PRO:HD3	1.50	0.93
1:A:169:THR:HG22	1:A:170:PRO:CD	2.00	0.91
1:A:481:LEU:CD2	1:A:487:PRO:HD3	2.03	0.89
1:A:119:LEU:H	1:A:119:LEU:HD12	1.39	0.88
1:A:303:PHE:HD1	1:A:547:VAL:HG11	1.39	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:CYS:CB	1:A:168:PRO:HD2	2.07	0.84
1:A:169:THR:HG23	1:A:170:PRO:HD3	1.61	0.81
1:A:119:LEU:H	1:A:119:LEU:CD1	1.93	0.81
1:A:196:GLU:HB3	1:A:198:SEP:O3P	1.84	0.77
1:A:169:THR:CG2	1:A:170:PRO:CD	2.59	0.76
1:A:118:GLU:HG3	7:A:1000:HOH:O	1.86	0.76
1:A:119:LEU:HD13	7:A:997:HOH:O	1.86	0.76
1:A:119:LEU:HD21	1:A:169:THR:HG23	1.71	0.73
1:A:119:LEU:CD1	1:A:119:LEU:N	2.51	0.72
1:A:167:CYS:CB	1:A:168:PRO:CD	2.63	0.72
1:A:216:ASN:HD22	1:A:218:GLU:H	1.39	0.71
1:A:547:VAL:HG12	7:A:696:HOH:O	1.90	0.70
1:A:567:PHE:HB2	5:A:617:IOD:I	2.61	0.69
1:A:1:SER:HB2	7:A:995:HOH:O	1.93	0.68
1:A:253:ASP:OD2	1:A:255:ARG:HD3	1.95	0.67
1:A:169:THR:HG22	1:A:170:PRO:HD2	1.77	0.66
1:A:130:GLU:HG3	7:A:935:HOH:O	1.96	0.66
2:B:1:NAG:H61	2:B:2:NAG:C1	2.26	0.66
1:A:130:GLU:HG2	1:A:159:PRO:HG3	1.78	0.65
1:A:169:THR:H	1:A:170:PRO:HD2	1.61	0.64
1:A:118:GLU:O	1:A:120:GLY:N	2.30	0.64
1:A:240:ILE:HD11	1:A:382:ASN:HA	1.79	0.64
1:A:127:VAL:HG13	1:A:131:GLU:HG3	1.80	0.63
1:A:172:TYR:HD2	1:A:173:GLN:H	1.45	0.63
1:A:168:PRO:CG	1:A:172:TYR:CE1	2.75	0.63
1:A:9:PRO:HG3	1:A:41:ARG:CZ	2.29	0.62
1:A:494:ILE:HD13	1:A:494:ILE:O	1.99	0.62
1:A:480:LEU:HD11	1:A:494:ILE:HD12	1.81	0.62
1:A:168:PRO:HG2	1:A:172:TYR:HE1	1.58	0.61
1:A:565:HIS:HB3	5:A:617:IOD:I	2.71	0.60
1:A:2:TRP:HB2	1:A:175:LEU:CD1	2.15	0.60
1:A:16:ASP:HB3	7:A:923:HOH:O	2.02	0.60
1:A:216:ASN:ND2	1:A:218:GLU:H	2.00	0.60
1:A:8:ALA:HB3	7:A:972:HOH:O	2.02	0.59
1:A:142:ILE:HD12	1:A:160:PHE:HB2	1.85	0.59
1:A:303:PHE:HD1	1:A:547:VAL:CG1	2.15	0.59
1:A:103:TRP:HH2	1:A:304:ILE:HD13	1.67	0.59
1:A:323:LYS:HE2	7:A:1012:HOH:O	2.02	0.59
2:B:2:NAG:H3	2:B:3:MAN:O5	2.01	0.59
1:A:481:LEU:HD21	1:A:487:PRO:CD	2.29	0.58
1:A:215:VAL:HA	1:A:228:PRO:HD3	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:GLN:HG2	7:A:913:HOH:O	2.02	0.58
1:A:467:LEU:HG	1:A:471:LEU:HD22	1.86	0.58
1:A:120:GLY:HA3	1:A:123:GLU:HB2	1.86	0.57
1:A:169:THR:H	1:A:170:PRO:CD	2.18	0.57
1:A:468:GLN:HG2	1:A:474:LYS:HA	1.86	0.57
1:A:146:LYS:O	1:A:147:ASN:HB2	2.05	0.56
1:A:215:VAL:CA	1:A:228:PRO:HD3	2.36	0.56
1:A:348:ARG:HH11	1:A:437:ASN:ND2	2.04	0.56
1:A:103:TRP:CH2	1:A:304:ILE:HD13	2.41	0.56
1:A:551:ARG:HD3	1:A:583:ASP:O	2.06	0.56
1:A:530:TRP:CE2	1:A:531:GLU:HG3	2.40	0.55
1:A:543:SER:HB3	1:A:585:LEU:HD12	1.88	0.55
1:A:303:PHE:CD1	1:A:547:VAL:HG11	2.31	0.55
1:A:17:GLU:N	7:A:923:HOH:O	2.40	0.55
1:A:239:PHE:CZ	1:A:427:LYS:HB3	2.42	0.54
1:A:588:SER:N	1:A:589:PRO:CD	2.70	0.54
1:A:215:VAL:C	1:A:228:PRO:HD3	2.28	0.54
1:A:288:ASP:O	1:A:292:LEU:HD22	2.08	0.53
1:A:551:ARG:HD3	1:A:584:LYS:HA	1.89	0.53
1:A:62:THR:HG22	1:A:64:ARG:HG2	1.89	0.53
1:A:360:ARG:NH2	1:A:389:ASP:OD2	2.42	0.52
1:A:146:LYS:HE2	7:A:980:HOH:O	2.09	0.52
1:A:452:TRP:CD1	1:A:492:ILE:HD13	2.45	0.52
1:A:301:GLY:O	1:A:305:GLN:HG3	2.10	0.52
1:A:272:GLU:O	1:A:276:LEU:HD22	2.10	0.51
1:A:349:PHE:CB	1:A:497:ASN:HD21	2.24	0.51
1:A:426:HIS:HB3	7:A:936:HOH:O	2.10	0.50
1:A:273:HIS:O	1:A:276:LEU:HB2	2.11	0.50
1:A:343:PHE:CD1	1:A:518:GLN:HG2	2.46	0.50
6:A:618:HEM:HBC2	6:A:618:HEM:HMC2	1.93	0.50
1:A:216:ASN:HD22	1:A:217:GLN:N	2.10	0.49
1:A:165:PHE:HZ	1:A:170:PRO:O	1.94	0.49
1:A:481:LEU:HD22	1:A:487:PRO:HD3	1.89	0.49
1:A:349:PHE:HA	1:A:497:ASN:HD21	1.77	0.49
1:A:197:PRO:O	1:A:198:SEP:C	2.59	0.49
1:A:187:LEU:HD13	1:A:305:GLN:HA	1.94	0.49
1:A:393:ASP:O	1:A:397:ARG:HG3	2.13	0.48
1:A:593:ARG:HD3	1:A:593:ARG:HA	1.71	0.48
1:A:302:ALA:O	1:A:306:ILE:HG13	2.14	0.48
1:A:494:ILE:HD13	1:A:494:ILE:C	2.34	0.48
1:A:475:VAL:HG12	1:A:479:LYS:HE3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:585:LEU:HA	7:A:669:HOH:O	2.14	0.47
1:A:175:LEU:HD11	7:A:995:HOH:O	2.15	0.47
1:A:407:MET:HB3	1:A:501:MET:CE	2.45	0.47
1:A:160:PHE:HD2	1:A:436:ILE:CD1	2.28	0.47
1:A:171:PRO:O	1:A:172:TYR:HB2	2.14	0.47
1:A:513:CYS:O	1:A:517:ARG:HG2	2.15	0.47
1:A:119:LEU:HD12	1:A:119:LEU:N	2.09	0.46
1:A:392:ILE:C	1:A:392:ILE:HD12	2.37	0.45
1:A:169:THR:N	1:A:170:PRO:HD2	2.31	0.45
1:A:213:MET:HG2	1:A:273:HIS:CD2	2.52	0.45
1:A:258:GLU:HG3	5:A:608:IOD:I	2.87	0.44
1:A:584:LYS:HB3	7:A:761:HOH:O	2.16	0.44
1:A:202:ARG:HD2	1:A:250:GLN:HE22	1.82	0.44
1:A:377:HIS:HA	1:A:380:PHE:CE2	2.53	0.44
1:A:119:LEU:HD13	1:A:119:LEU:N	2.33	0.43
1:A:216:ASN:ND2	5:A:610:IOD:I	3.22	0.43
1:A:221:ASP:HB2	1:A:226:TYR:CZ	2.53	0.43
1:A:174:SER:OG	1:A:175:LEU:N	2.52	0.42
1:A:478:LYS:HE3	1:A:478:LYS:HB2	1.69	0.42
1:A:522:ILE:HD12	1:A:522:ILE:C	2.39	0.42
1:A:142:ILE:HD11	1:A:160:PHE:CD2	2.55	0.42
1:A:522:ILE:O	1:A:526:ASP:HB2	2.19	0.42
1:A:350:GLY:HA3	6:A:618:HEM:CBC	2.50	0.42
1:A:484:TYR:O	1:A:485:LYS:HB2	2.19	0.42
1:A:10:VAL:HA	1:A:11:PRO:HD3	1.67	0.41
1:A:118:GLU:C	1:A:120:GLY:H	2.24	0.41
1:A:8:ALA:N	1:A:9:PRO:HD3	2.35	0.41
1:A:36:LEU:HG	1:A:337:PRO:HD2	2.03	0.41
1:A:63:GLN:HB2	7:A:987:HOH:O	2.20	0.41
1:A:313:LEU:N	1:A:314:PRO:CD	2.83	0.41
1:A:142:ILE:CD1	1:A:160:PHE:HB2	2.49	0.41
1:A:166:VAL:H	1:A:166:VAL:HG22	1.68	0.40
1:A:142:ILE:HD11	1:A:436:ILE:HD13	2.03	0.40
1:A:200:ALA:O	1:A:204:ARG:HG3	2.21	0.40
1:A:235:SER:HA	1:A:236:PRO:HD3	1.93	0.40
6:A:618:HEM:HAA1	7:A:685:HOH:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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%)	553 (93%)	31 (5%)	8 (1%)	11	15

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	119	LEU
1	A	167	CYS
1	A	168	PRO
1	A	169	THR
1	A	172	TYR
1	A	166	VAL
1	A	17	GLU
1	A	9	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	516/516 (100%)	481 (93%)	35 (7%)	16	25

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLU
1	A	18	GLN
1	A	98	LEU

Continued on next page...

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Mol	Chain	Res	Type
1	A	117	THR
1	A	121	SER
1	A	127	VAL
1	A	130	GLU
1	A	172	TYR
1	A	173	GLN
1	A	175	LEU
1	A	187	LEU
1	A	216	ASN
1	A	255	ARG
1	A	261	LEU
1	A	268	LEU
1	A	276	LEU
1	A	291	MET
1	A	292	LEU
1	A	329	GLN
1	A	347	PHE
1	A	360	ARG
1	A	367	PRO
1	A	376	LEU
1	A	461	PRO
1	A	464	LEU
1	A	471	LEU
1	A	480	LEU
1	A	494	ILE
1	A	504	ARG
1	A	520	GLN
1	A	523	ARG
1	A	546	LYS
1	A	547	VAL
1	A	551	ARG
1	A	564	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	216	ASN
1	A	217	GLN
1	A	222	HIS
1	A	329	GLN
1	A	423	GLN
1	A	437	ASN

Continued from previous page...

Mol	Chain	Res	Type
1	A	468	GLN
1	A	497	ASN
1	A	520	GLN
1	A	521	GLN
1	A	545	GLN
1	A	570	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	1.29	1 (12%)	8,12,14	2.50	5 (62%)

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	-	1/5/8/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	198	SEP	OG-CB	2.10	1.52	1.44

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	198	SEP	O2P-P-O1P	-3.23	98.04	110.68
1	A	198	SEP	O3P-P-OG	3.20	115.26	106.73
1	A	198	SEP	P-OG-CB	3.15	126.97	118.30
1	A	198	SEP	O2P-P-OG	2.72	113.96	106.73
1	A	198	SEP	O3P-P-O1P	-2.31	101.65	110.68

There are no chirality outliers.

All (1) torsion outliers are listed below:

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

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	198	SEP	2	0

5.5 Carbohydrates ⓘ

11 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	1,2	14,14,15	0.67	0	17,19,21	0.82	0
2	NAG	B	2	2	14,14,15	0.79	0	17,19,21	0.89	1 (5%)
2	MAN	B	3	2	11,11,12	0.74	0	15,15,17	1.35	3 (20%)
2	NAG	C	1	1,2	14,14,15	0.52	0	17,19,21	0.74	0
2	NAG	C	2	2	14,14,15	0.46	0	17,19,21	0.80	0
2	MAN	C	3	2	11,11,12	0.59	0	15,15,17	0.59	0
2	NAG	D	1	1,2	14,14,15	0.53	0	17,19,21	0.84	0
2	NAG	D	2	2	14,14,15	0.71	0	17,19,21	1.39	3 (17%)
2	MAN	D	3	2	11,11,12	0.57	0	15,15,17	0.65	0
3	NAG	E	1	1,3	14,14,15	0.76	0	17,19,21	1.53	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
3	NAG	E	2	3	14,14,15	0.65	0	17,19,21	0.60	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
2	NAG	B	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	B	2	2	-	0/6/23/26	0/1/1/1
2	MAN	B	3	2	-	2/2/19/22	0/1/1/1
2	NAG	C	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
2	MAN	C	3	2	-	2/2/19/22	0/1/1/1
2	NAG	D	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1
2	MAN	D	3	2	-	1/2/19/22	0/1/1/1
3	NAG	E	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	0/6/23/26	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(^{o})	Ideal(^{o})
3	E	1	NAG	C4-C3-C2	5.19	118.62	111.02
2	D	2	NAG	C1-O5-C5	3.56	117.02	112.19
2	B	3	MAN	C1-C2-C3	3.43	113.88	109.67
2	B	3	MAN	C1-O5-C5	2.81	116.00	112.19
2	D	2	NAG	C4-C3-C2	-2.70	107.06	111.02
2	B	2	NAG	C4-C3-C2	2.56	114.77	111.02
2	D	2	NAG	C2-N2-C7	-2.39	119.50	122.90
2	B	3	MAN	O5-C1-C2	2.24	114.22	110.77

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	2	NAG	O5-C5-C6-O6
2	C	3	MAN	C4-C5-C6-O6
2	B	3	MAN	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	C	3	MAN	O5-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6
2	B	3	MAN	C4-C5-C6-O6
2	B	1	NAG	O5-C5-C6-O6
2	B	1	NAG	C4-C5-C6-O6
2	D	3	MAN	C4-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 2 short contacts:

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

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

Oligosaccharide Chain B

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain C

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain D

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain E

Bond lengths

Bond angles

Torsions

Rings
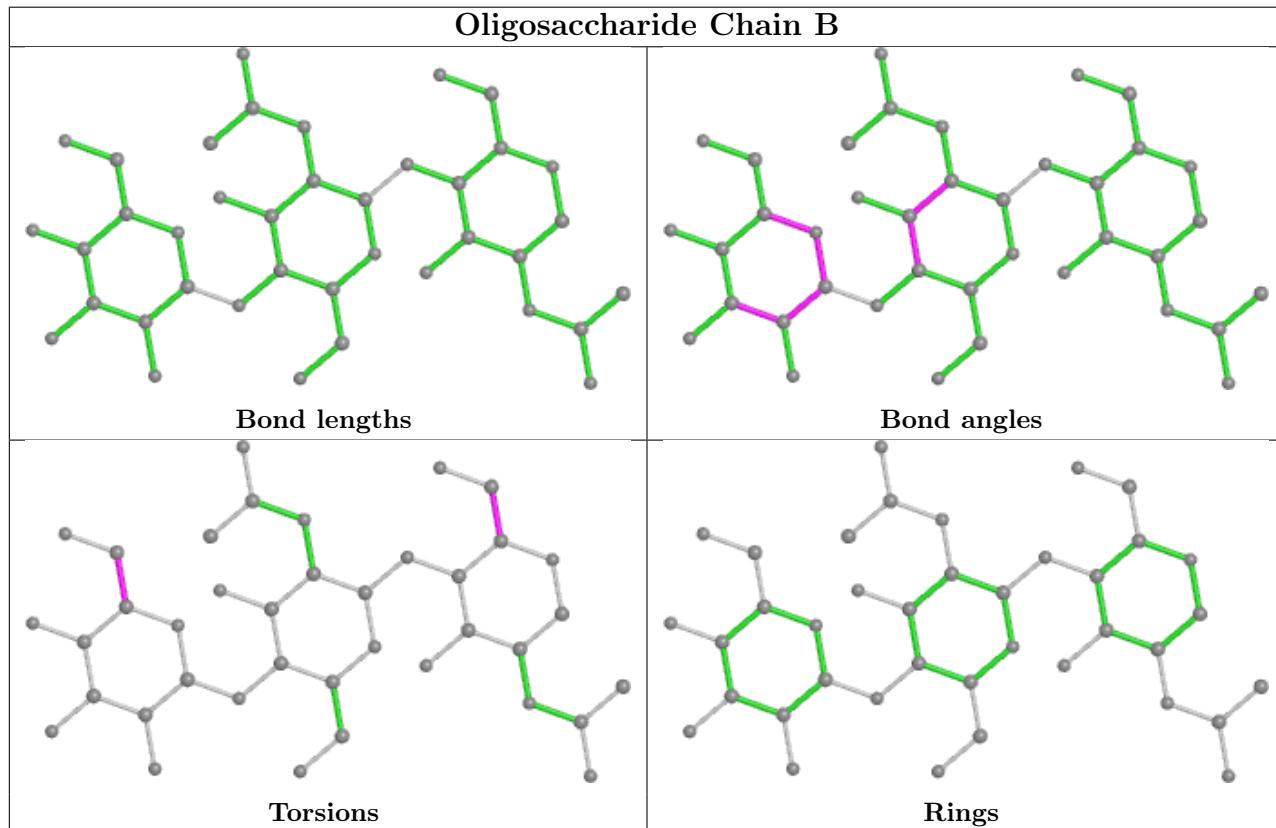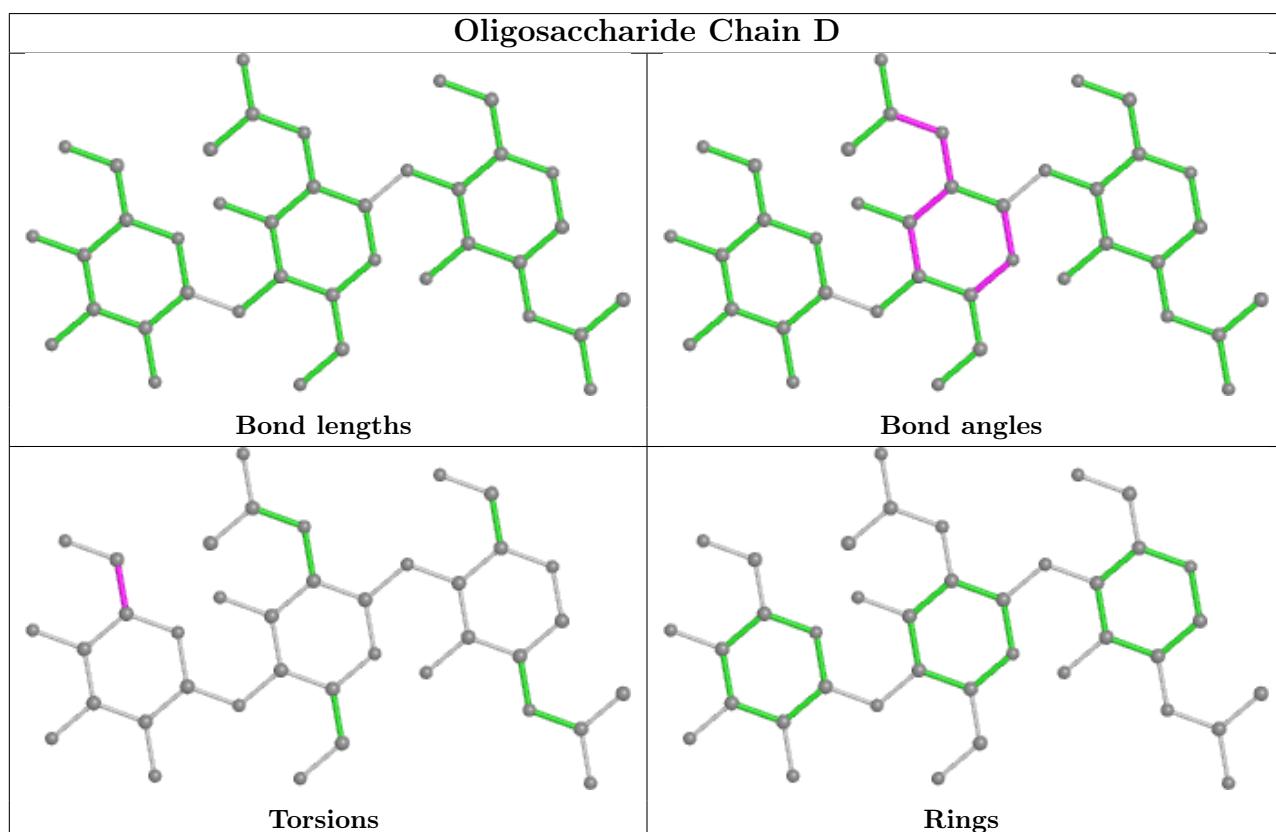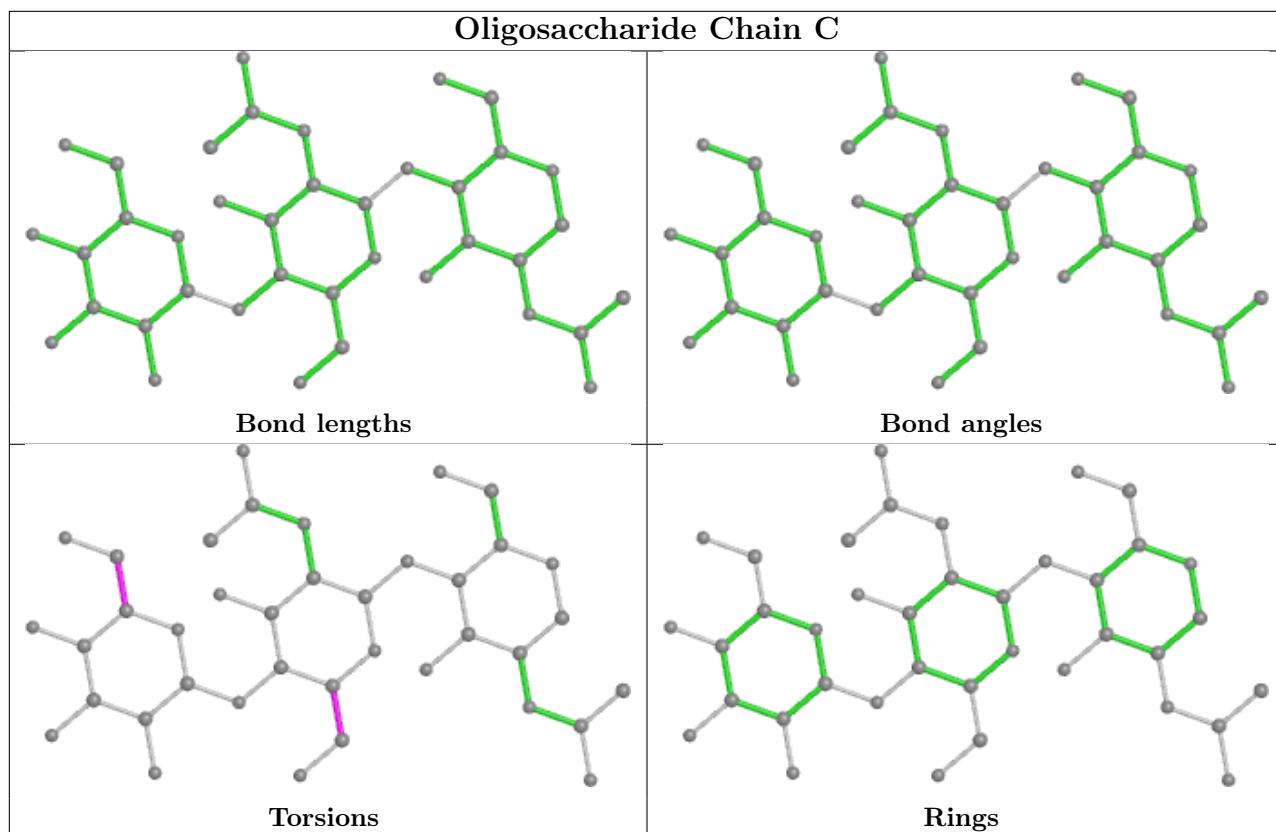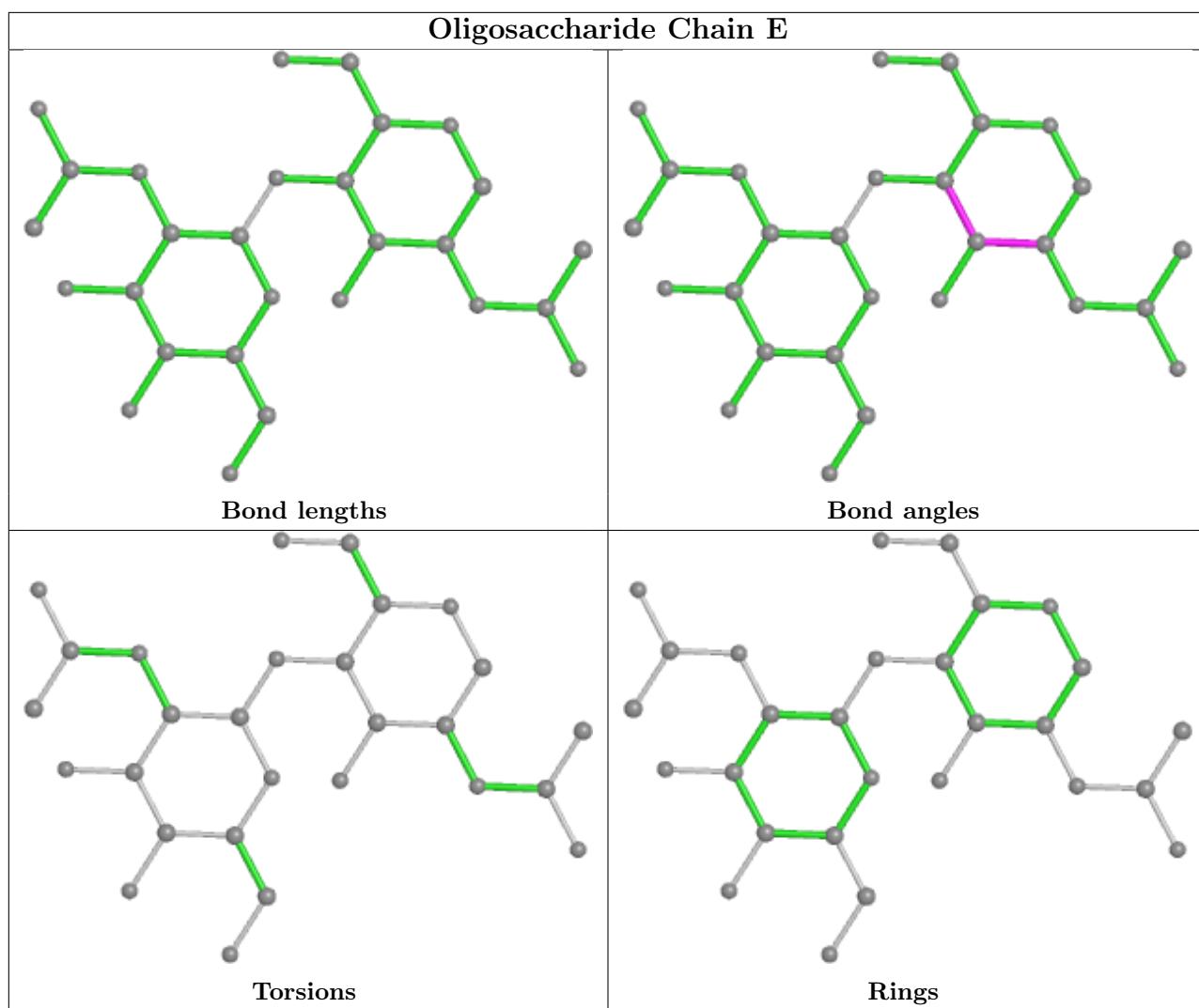
5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 11 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
6	HEM	A	618	1,7	41,50,50	1.90	6 (14%)	45,82,82	1.54	9 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	HEM	A	618	1,7	-	4/12/54/54	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	618	HEM	C3D-C2D	6.92	1.51	1.36
6	A	618	HEM	C3C-C2C	-4.52	1.34	1.40
6	A	618	HEM	C3C-CAC	3.92	1.55	1.47
6	A	618	HEM	CAA-C2A	2.85	1.56	1.52
6	A	618	HEM	CAB-C3B	2.83	1.55	1.47
6	A	618	HEM	CMB-C2B	2.06	1.55	1.50

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	618	HEM	C4D-ND-C1D	4.63	109.85	105.07
6	A	618	HEM	C4B-CHC-C1C	3.70	127.45	122.56
6	A	618	HEM	CHC-C4B-NB	2.80	127.48	124.43
6	A	618	HEM	CHD-C1D-ND	2.73	127.40	124.43
6	A	618	HEM	C3B-C2B-C1B	2.66	108.46	106.49
6	A	618	HEM	CAD-C3D-C4D	2.59	129.18	124.66
6	A	618	HEM	C1B-NB-C4B	2.28	107.43	105.07
6	A	618	HEM	C4C-CHD-C1D	2.22	125.49	122.56
6	A	618	HEM	C4D-C3D-C2D	-2.07	103.88	106.90

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	618	HEM	CAD-CBD-CGD-O2D
6	A	618	HEM	CAD-CBD-CGD-O1D
6	A	618	HEM	CAA-CBA-CGA-O2A
6	A	618	HEM	CAA-CBA-CGA-O1A

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	618	HEM	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 all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand HEM A 618

Bond lengths   Bond angles

Torsions   Rings
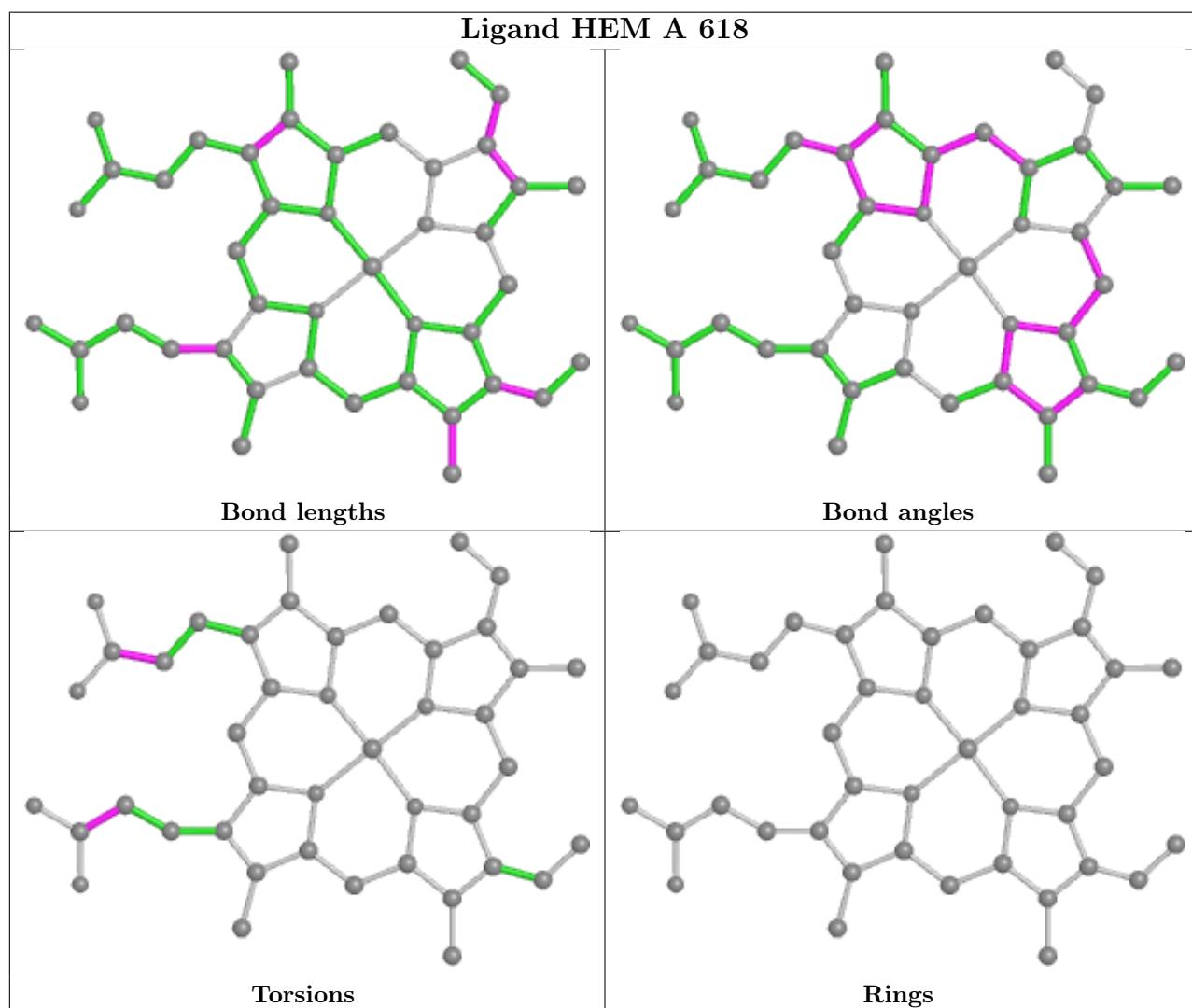
5.7 Other polymers ⓘ

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, 95th 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	A	594/595 (99%)	-0.13	28 (4%)	31	30	8, 22, 59, 85	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	7	GLY	10.7
1	A	174	SER	10.2
1	A	2	TRP	8.7
1	A	1	SER	8.6
1	A	173	GLN	8.0
1	A	121	SER	7.7
1	A	122	SER	7.4
1	A	595	ASN	6.6
1	A	119	LEU	6.5
1	A	120	GLY	6.0
1	A	593	ARG	5.6
1	A	594	GLU	4.9
1	A	171	PRO	4.5
1	A	172	TYR	4.3
1	A	124	HIS	4.2
1	A	170	PRO	3.9
1	A	169	THR	3.5
1	A	126	LYS	3.4
1	A	13	VAL	3.3
1	A	8	ALA	3.3
1	A	125	SER	3.1
1	A	123	GLU	2.5
1	A	322	GLN	2.4
1	A	127	VAL	2.4
1	A	168	PRO	2.3
1	A	4	VAL	2.3
1	A	167	CYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	574	HIS	2.1

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

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, 95th 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	SEP	A	198	10/11	0.92	0.21	2,22,24,28	0

6.3 Carbohydrates ⓘ

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, 95th 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
2	MAN	B	3	11/12	0.58	0.46	74,76,76,77	0
2	MAN	D	3	11/12	0.62	0.44	70,73,74,74	0
3	NAG	E	2	14/15	0.71	0.50	68,71,73,73	0
2	NAG	C	2	14/15	0.72	0.34	59,63,65,68	0
2	MAN	C	3	11/12	0.74	0.51	71,73,73,74	0
2	NAG	D	2	14/15	0.75	0.32	56,58,62,67	0
2	NAG	B	2	14/15	0.76	0.39	63,68,69,72	0
3	NAG	E	1	14/15	0.79	0.26	52,56,59,64	0
2	NAG	B	1	14/15	0.89	0.18	43,46,51,57	0
2	NAG	C	1	14/15	0.93	0.14	41,44,48,54	0
2	NAG	D	1	14/15	0.95	0.14	36,41,44,50	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 B:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
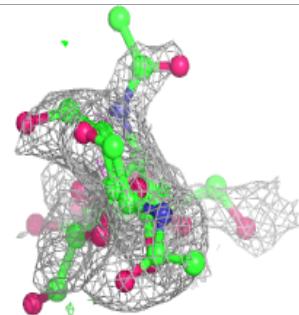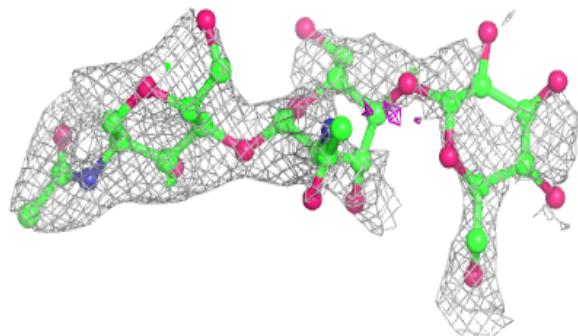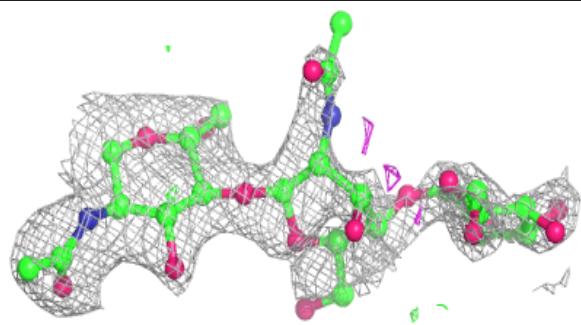
Electron density around Chain C:

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$_o$-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 E:

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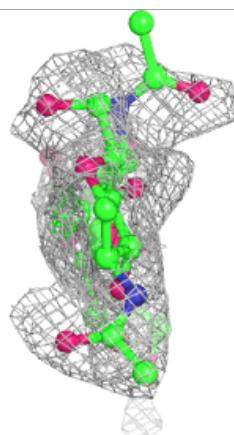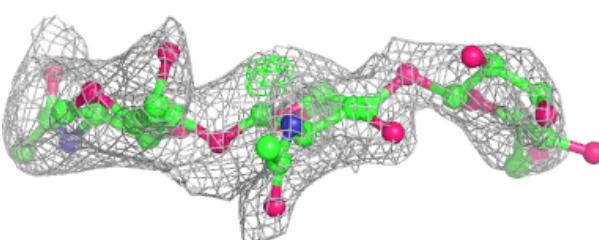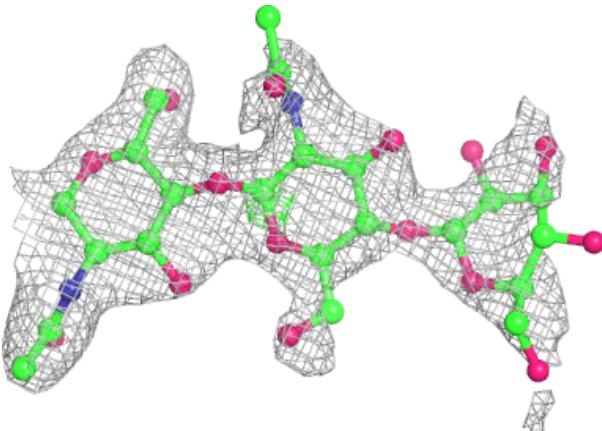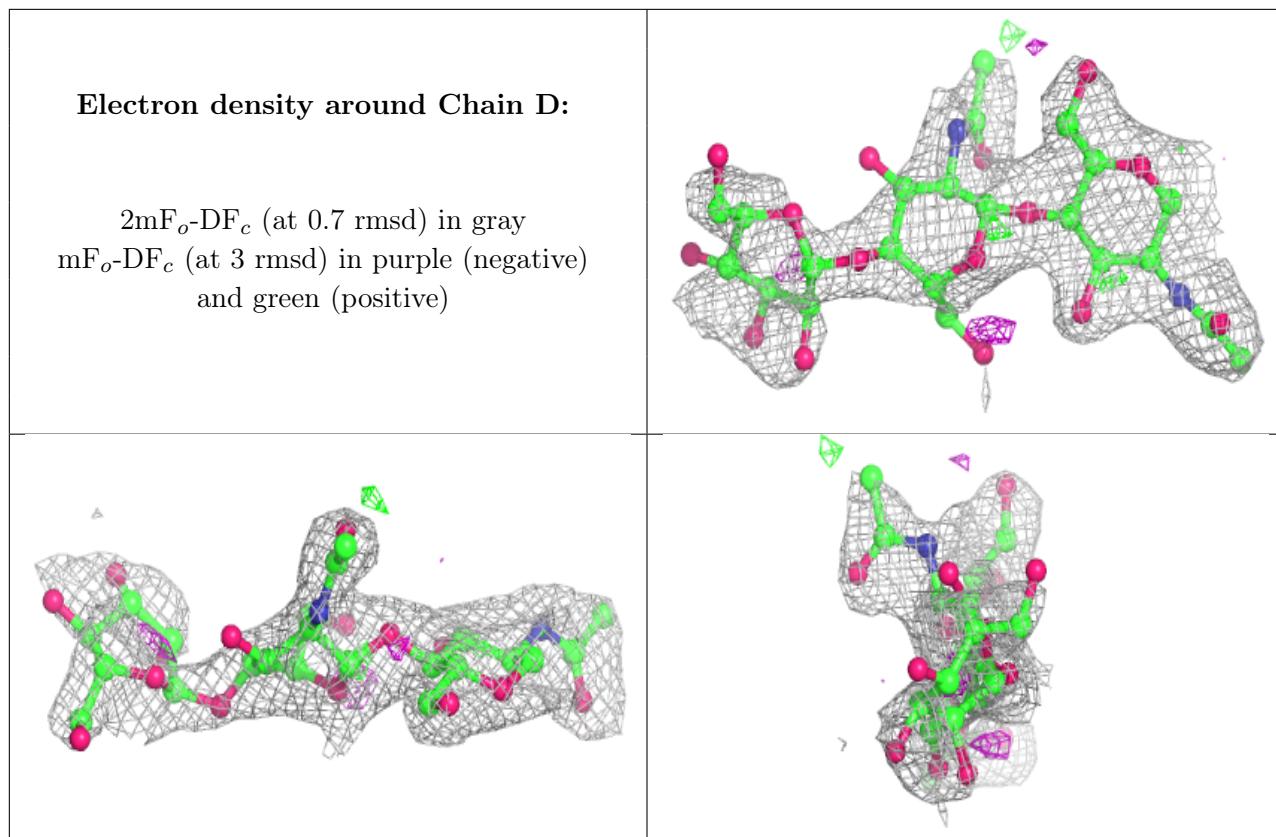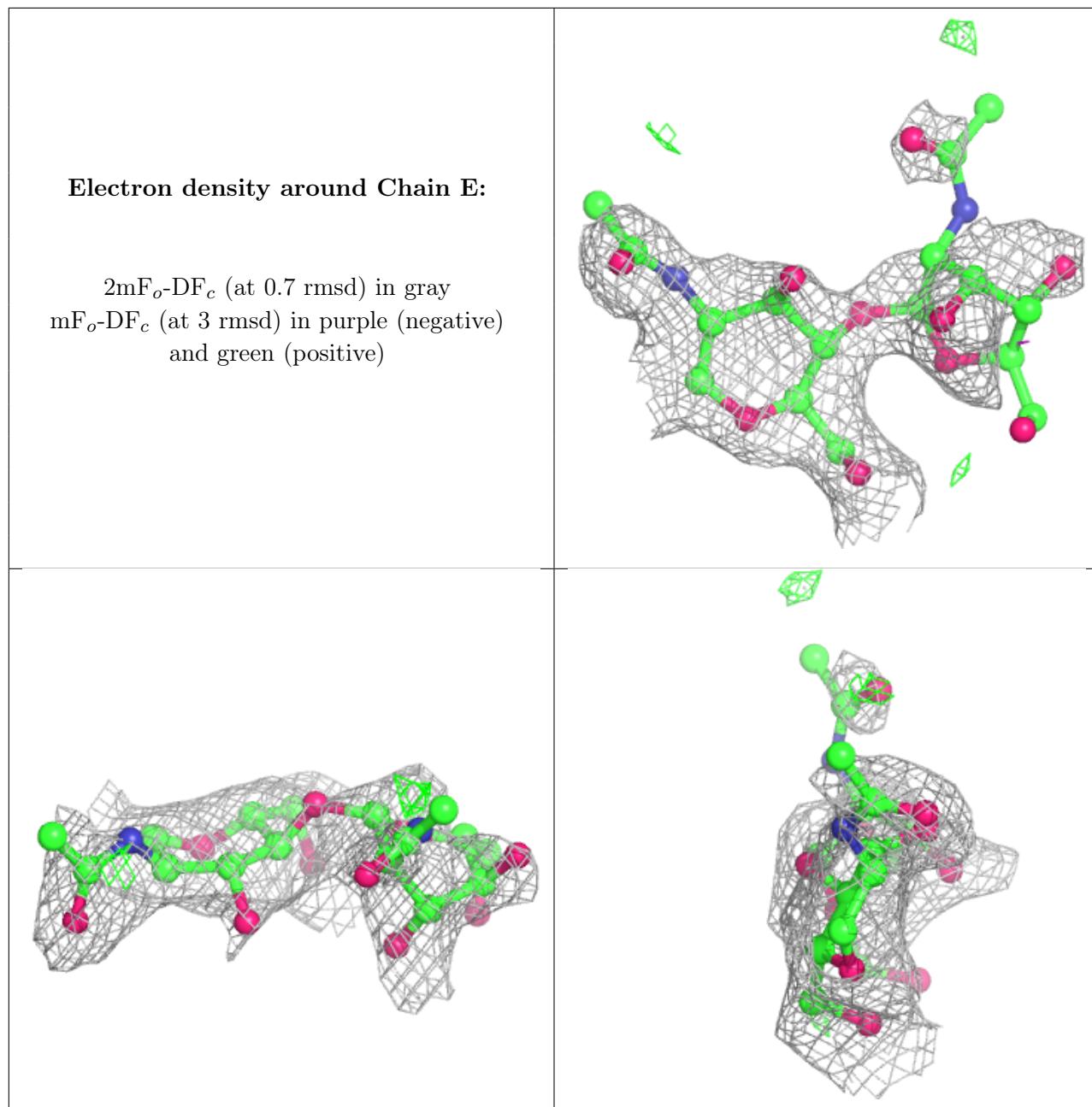
6.4 Ligands (i)

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, 95th 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	IOD	A	613	1/1	0.93	0.18	66,66,66,66	0
5	IOD	A	610	1/1	0.96	0.07	64,64,64,64	0
5	IOD	A	615	1/1	0.96	0.07	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å²)	Q<0.9
5	IOD	A	617	1/1	0.96	0.25	77,77,77,77	0
5	IOD	A	612	1/1	0.97	0.07	68,68,68,68	0
6	HEM	A	618	43/43	0.97	0.09	8,13,19,20	0
5	IOD	A	614	1/1	0.98	0.04	65,65,65,65	0
5	IOD	A	611	1/1	0.98	0.07	66,66,66,66	0
4	CA	A	607	1/1	0.99	0.08	16,16,16,16	0
5	IOD	A	616	1/1	1.00	0.04	52,52,52,52	0
5	IOD	A	608	1/1	1.00	0.07	51,51,51,51	0
5	IOD	A	609	1/1	1.00	0.09	21,21,21,21	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 A 618:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.