



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 03:12 PM BST

PDB ID : 1D2V
Title : CRYSTAL STRUCTURE OF BROMIDE-BOUND HUMAN MYELOPER-
OXIDASE ISOFORM C AT PH 5.5
Authors : Fiedler, T.J.; Davey, C.A.; Fenna, R.E.
Deposited on : 1999-09-28
Resolution : 1.75 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
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

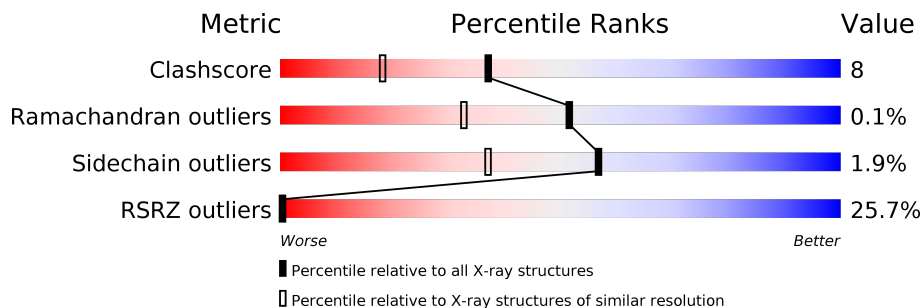
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	104	
1	B	104	
2	C	466	
2	D	466	
3	E	6	
3	F	6	

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
5	BR	A	843	-	-	X	-
9	ACT	C	1606	-	-	X	-
9	ACT	D	2604	-	-	X	X

2 Entry composition i

There are 10 unique types of molecules in this entry. The entry contains 10306 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	104	Total 838	C 529	N 148	O 156	S 5	0	0	0
1	B	104	Total 838	C 529	N 148	O 156	S 5	0	0	0

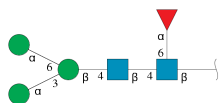
- Molecule 2 is a protein called MYELOPEROXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	466	Total 3733	C 2351	N 687	O 668	S 27	0	0	0
2	D	466	Total 3733	C 2351	N 687	O 668	S 27	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	150	CSO	CYS	modified residue	UNP P05164
D	150	CSO	CYS	modified residue	UNP P05164

- Molecule 3 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
			Total	C	N	O			
3	E	6	Total 71	C 40	N 2	O 29	0	0	0
3	F	6	Total 71	C 40	N 2	O 29	0	0	0

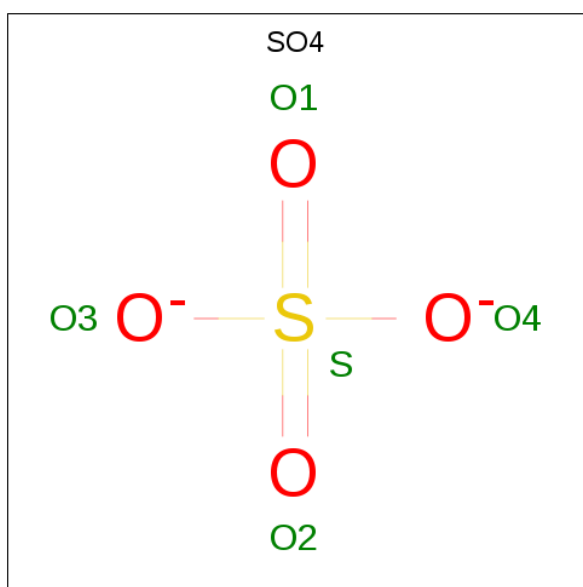
- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 5 is BROMIDE ION (three-letter code: BR) (formula: Br).

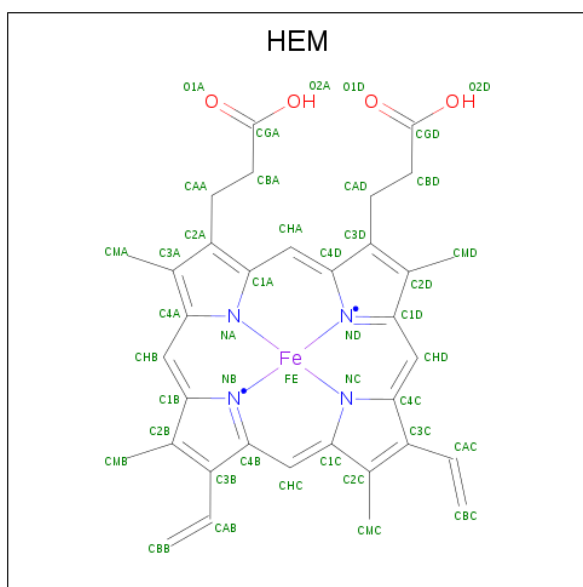
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	4	Total Br 4 4	0	0
5	A	4	Total Br 4 4	0	0

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



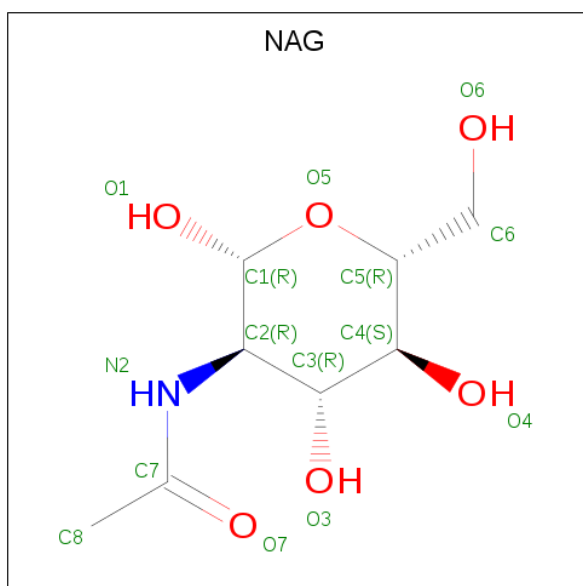
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O S 5 4 1	0	0
6	C	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0

- Molecule 7 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C₃₄H₃₂FeN₄O₄).



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

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



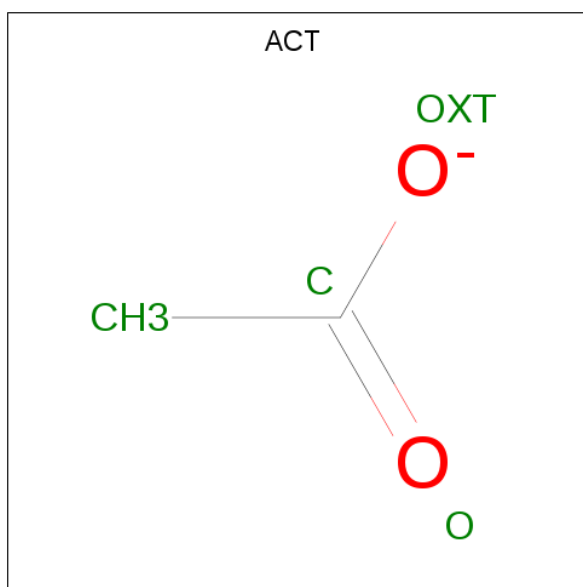
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
8	C	1	Total	C	N	O	0	0
			14	8	1	5		

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

- Molecule 9 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	C	1	Total	C O	0	0
			4	2 2		
9	C	1	Total	C O	0	0
			4	2 2		
9	C	1	Total	C O	0	0
			4	2 2		
9	D	1	Total	C O	0	0
			4	2 2		
9	D	1	Total	C O	0	0
			4	2 2		
9	D	1	Total	C O	0	0
			4	2 2		

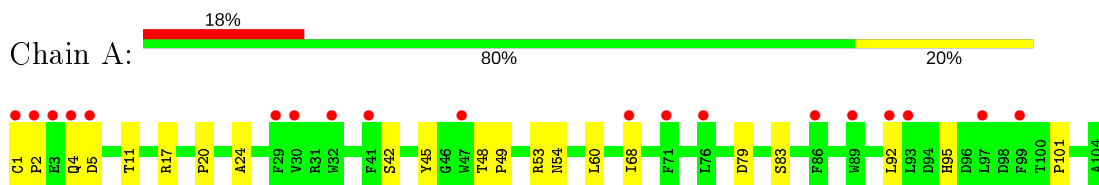
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	98	Total 98	O 98	0	0
10	C	319	Total 319	O 319	0	0
10	B	100	Total 100	O 100	0	0
10	D	314	Total 314	O 314	0	0

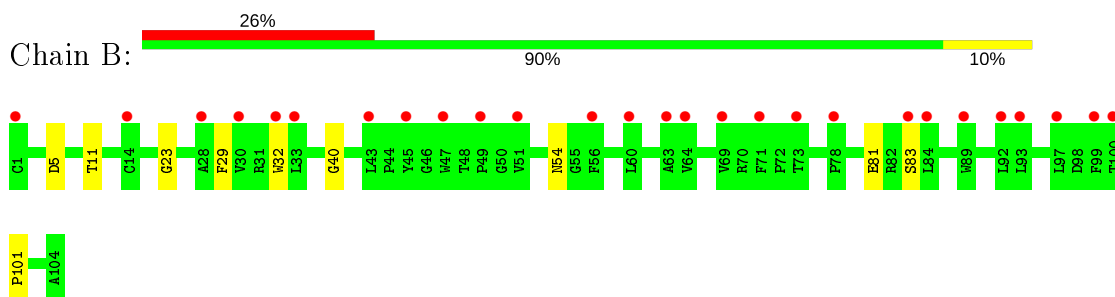
3 Residue-property plots [i](#)

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



- Molecule 1: MYELOPEROXIDASE



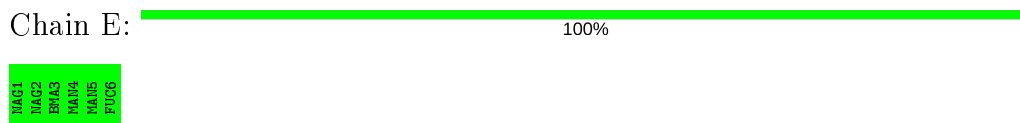
- Molecule 2: MYELOPEROXIDASE



- Molecule 2: MYELOPEROXIDASE



- Molecule 3: 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-acetamid o-2-deoxy-beta-D-glucopyranose



- Molecule 3: 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-acetamid o-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	111.16Å 63.49Å 92.48Å 90.00° 97.36° 90.00°	Depositor
Resolution (Å)	30.00 – 1.75 44.41 – 1.76	Depositor EDS
% Data completeness (in resolution range)	87.3 (30.00-1.75) 90.4 (44.41-1.76)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.37 (at 1.76Å)	Xtrriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.243 , 0.296 0.237 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	12.2	Xtrriage
Anisotropy	0.122	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 56.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	10306	wwPDB-VP
Average B, all atoms (Å ²)	10.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.13% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CSO, BMA, NAG, CA, FUC, BR, ACT, HEM, MAN, SO4

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	0.75	0/863	0.73	0/1174
1	B	0.76	0/863	0.72	0/1174
2	C	0.73	1/3811 (0.0%)	0.65	0/5168
2	D	0.70	0/3811	0.63	0/5168
All	All	0.72	1/9348 (0.0%)	0.66	0/12684

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	114	ASN	C-N	-6.21	1.19	1.34

There are no bond angle outliers.

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	838	0	798	17	0
1	B	838	0	798	8	0
2	C	3733	0	3723	65	0
2	D	3733	0	3725	65	0
3	E	71	0	61	0	0
3	F	71	0	61	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	4	0	0	3	0
5	B	4	0	0	1	0
6	A	5	0	0	0	0
6	B	5	0	0	0	0
6	C	5	0	0	0	0
7	A	43	0	30	3	0
7	B	43	0	30	2	0
8	C	28	0	26	1	0
8	D	28	0	26	0	0
9	C	12	0	9	4	0
9	D	12	0	9	3	0
10	A	98	0	0	4	0
10	B	100	0	0	1	0
10	C	319	0	0	10	0
10	D	314	0	0	4	0
All	All	10306	0	9296	147	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 8.

All (147) 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)
2:C:355:PRO:HG2	2:C:356:ASN:HD22	1.44	0.82
2:D:333:ARG:HH11	2:D:421:ASN:HD22	1.31	0.78
2:C:132:PRO:HG3	2:C:140:GLN:NE2	2.04	0.72
2:C:355:PRO:HG2	2:C:356:ASN:ND2	2.05	0.71
2:C:200:ASN:HD22	2:C:203:PHE:H	1.36	0.70
2:C:123:PRO:HB3	9:C:1606:ACT:H3	1.74	0.69
2:D:122:GLN:HA	2:D:122:GLN:HE21	1.55	0.69
2:D:349:ARG:HG3	2:D:351:GLN:HG2	1.73	0.69
2:C:349:ARG:HG3	2:C:351:GLN:HG2	1.76	0.69
8:C:1620:NAG:H5	10:C:1250(A):HOH:O	1.92	0.68
2:D:211:LEU:HD23	2:D:254:LEU:HD22	1.76	0.66
2:D:333:ARG:HH11	2:D:421:ASN:ND2	1.94	0.65
10:A:1243(A):HOH:O	2:C:129:LYS:HD3	1.98	0.64
2:D:128:LEU:HB2	2:D:144:ILE:HB	1.80	0.64
2:D:411:MET:HE2	2:D:415:LEU:HD21	1.80	0.63
2:C:514:TRP:CE2	2:C:515:GLU:HG3	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:5:ASP:HB3	10:B:1272(B):HOH:O	1.99	0.62
2:D:548:LYS:HE2	2:D:562:VAL:HG13	1.83	0.61
7:A:605:HEM:HBB2	2:C:242:GLU:OE1	2.00	0.61
2:C:200:ASN:ND2	2:C:203:PHE:H	1.98	0.60
2:D:122:GLN:HA	2:D:122:GLN:NE2	2.17	0.59
5:A:843:BR:BR	2:C:242:GLU:HG3	2.57	0.59
2:D:263:GLU:HG3	10:D:921(B):HOH:O	2.02	0.58
1:A:2:PRO:HD2	10:A:791(A):HOH:O	2.04	0.58
2:D:522:MET:HG3	9:D:2604:ACT:H1	1.84	0.58
2:D:122:GLN:HE21	2:D:123:PRO:CD	2.15	0.58
2:C:333:ARG:HH11	2:C:421:ASN:HD22	1.52	0.57
2:C:135:PRO:HG2	10:C:1204(A):HOH:O	2.05	0.56
2:D:122:GLN:HE21	2:D:123:PRO:HD3	1.71	0.56
5:A:843:BR:BR	10:C:957(A):HOH:O	2.73	0.56
2:C:354:GLU:HB3	2:C:355:PRO:HA	1.88	0.56
1:A:101:PRO:HB2	10:A:1247(A):HOH:O	2.05	0.55
2:C:382:ARG:NH1	10:C:777(A):HOH:O	2.37	0.54
1:A:83:SER:HB3	2:C:554:SER:O	2.08	0.54
2:C:485:LEU:HD13	2:C:490:ARG:HA	1.88	0.53
2:C:128:LEU:HB2	2:C:144:ILE:HB	1.91	0.53
2:D:378:ASP:HB2	2:D:379:PRO:HD3	1.91	0.53
2:D:548:LYS:HE2	2:D:562:VAL:CG1	2.38	0.53
2:D:271:TRP:HE1	2:D:577:GLU:CD	2.12	0.52
2:D:382:ARG:HG3	2:D:543:ILE:CD1	2.39	0.52
2:D:411:MET:CE	2:D:415:LEU:HD21	2.40	0.51
2:D:138:LYS:HZ3	2:D:138:LYS:HA	1.76	0.51
2:D:417:LEU:HB3	2:D:418:PRO:HD3	1.92	0.51
1:B:83:SER:HB3	2:D:554:SER:O	2.10	0.51
2:C:113:VAL:HG12	2:C:114:ASN:N	2.26	0.51
2:C:521:SER:OG	2:C:523:GLN:HG2	2.10	0.51
2:C:114:ASN:HA	10:C:973(A):HOH:O	2.11	0.51
2:C:507:ARG:HG3	2:C:513:TRP:CE2	2.46	0.51
2:D:255:ARG:NH1	2:D:377:ILE:HD11	2.26	0.51
2:C:139:ASN:HB2	2:C:142:ASP:OD1	2.11	0.50
2:D:138:LYS:NZ	2:D:138:LYS:HA	2.25	0.50
2:D:328:PHE:CD1	2:D:502:GLN:HG2	2.46	0.50
2:D:244:PRO:HB2	2:D:343:MET:SD	2.51	0.50
7:A:605:HEM:HBC2	7:A:605:HEM:HMC2	1.94	0.49
2:C:465:MET:CE	2:C:471:PRO:HD3	2.42	0.49
2:D:116:GLU:OE1	2:D:411:MET:HE3	2.11	0.49
2:C:394:GLN:HB3	2:C:460:LEU:HD22	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:416:ASP:O	2:D:420:LEU:HG	2.11	0.49
2:C:548:LYS:HD2	2:C:560:ASP:HA	1.94	0.49
1:A:20:PRO:HG2	1:B:40:GLY:HA3	1.95	0.48
1:A:92:LEU:HD22	2:C:249:MET:HB3	1.96	0.48
1:A:17:ARG:HB3	10:A:915(B):HOH:O	2.13	0.48
2:D:416:ASP:OD2	2:D:418:PRO:HD2	2.13	0.48
2:C:549:ASN:HB3	10:C:1232(A):HOH:O	2.13	0.48
2:C:116:GLU:HG3	2:C:147:PHE:CZ	2.48	0.47
2:C:549:ASN:ND2	10:C:829(A):HOH:O	2.46	0.47
2:D:514:TRP:CE2	2:D:515:GLU:HG3	2.49	0.47
2:D:213:PHE:CD2	2:D:231:PRO:HG2	2.50	0.47
2:D:554:SER:HB3	2:D:560:ASP:HB3	1.95	0.47
2:C:173:ALA:HA	2:C:175:MET:SD	2.55	0.47
2:D:548:LYS:HG2	2:D:562:VAL:HG13	1.96	0.47
2:D:354:GLU:HB3	2:D:355:PRO:HA	1.97	0.47
2:C:123:PRO:CB	9:C:1606:ACT:H3	2.42	0.46
2:D:394:GLN:HG3	10:D:850(B):HOH:O	2.15	0.46
2:C:462:ARG:O	2:C:466:GLU:HG2	2.15	0.46
2:D:345:ARG:NH1	10:D:762(B):HOH:O	2.48	0.46
2:D:378:ASP:O	2:D:543:ILE:HD11	2.15	0.46
2:C:333:ARG:HD3	2:C:421:ASN:ND2	2.30	0.46
2:C:361:LEU:O	2:C:364:VAL:HG22	2.16	0.46
5:A:758:BR:BR	2:C:543:ILE:HG23	2.70	0.46
2:D:533:LEU:HB3	2:D:534:PRO:HD3	1.98	0.46
2:C:297:LEU:HD11	2:C:503:PHE:CD1	2.51	0.46
1:B:32:TRP:CE2	2:D:325:ALA:HB2	2.51	0.46
1:A:1:CYS:SG	1:A:20:PRO:HB3	2.56	0.45
2:C:181:GLU:HB2	2:C:182:PRO:HD3	1.98	0.45
2:C:200:ASN:ND2	2:C:202:ARG:H	2.14	0.45
2:D:260:LEU:O	2:D:264:LEU:HG	2.17	0.45
2:C:416:ASP:OD2	2:C:418:PRO:HD2	2.15	0.45
2:D:115:CYS:HB2	2:D:147:PHE:CZ	2.51	0.45
2:C:255:ARG:NH1	2:C:377:ILE:HD11	2.32	0.45
2:D:122:GLN:HE21	2:D:122:GLN:CA	2.25	0.45
2:D:123:PRO:HA	2:D:124:PRO:HA	1.83	0.45
2:C:199:VAL:HG12	2:C:254:LEU:HD21	1.99	0.45
2:D:223:LEU:HD22	2:D:226:ARG:NH1	2.31	0.45
2:C:491:VAL:HB	2:C:495:LEU:HB2	1.99	0.45
2:C:265:LYS:HD3	2:C:276:LEU:HD11	1.98	0.44
7:A:605:HEM:HBC2	7:A:605:HEM:CMC	2.46	0.44
2:C:135:PRO:CG	10:C:1204(A):HOH:O	2.63	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:TYR:CE1	1:A:53:ARG:HG3	2.53	0.44
2:D:241:SER:O	2:D:366:PHE:HA	2.18	0.44
2:C:259:ARG:O	2:C:263:GLU:HG3	2.17	0.44
2:C:378:ASP:HB2	2:C:379:PRO:HD3	2.00	0.44
2:C:513:TRP:CD1	2:C:515:GLU:HB2	2.53	0.43
2:D:533:LEU:N	2:D:534:PRO:CD	2.81	0.43
5:B:843:BR:BR	2:D:242:GLU:HG3	2.74	0.43
1:B:101:PRO:HD2	2:D:164:ILE:O	2.19	0.43
2:C:229:ARG:HG2	2:C:229:ARG:HH11	1.84	0.43
1:A:68:ILE:HD13	2:C:464:LEU:HD23	2.00	0.43
1:A:101:PRO:HD2	2:C:164:ILE:O	2.18	0.43
2:D:194:LEU:HD13	10:D:948(B):HOH:O	2.18	0.43
1:A:79:ASP:O	2:C:388:PRO:HB3	2.19	0.43
2:D:526:GLN:NE2	2:D:530:GLN:HE21	2.17	0.43
7:B:605:HEM:CBC	2:D:335:GLY:HA3	2.48	0.43
2:C:124:PRO:HA	9:C:1606:ACT:H1	2.00	0.43
2:C:244:PRO:HD3	2:C:364:VAL:O	2.18	0.43
1:B:23:GLY:HA2	2:D:169:SER:OG	2.19	0.42
2:C:533:LEU:HB3	2:C:534:PRO:HD3	2.01	0.42
2:C:501:THR:HA	10:C:814(A):HOH:O	2.19	0.42
1:A:45:TYR:CZ	1:A:53:ARG:HG3	2.55	0.42
2:C:282:LYS:HG2	2:C:520:PHE:CZ	2.54	0.42
2:D:344:PHE:CD1	2:D:387:THR:HG21	2.55	0.42
2:C:242:GLU:O	2:C:365:PHE:HA	2.20	0.42
2:C:526:GLN:NE2	2:C:530:GLN:NE2	2.68	0.42
2:D:313:TYR:CZ	2:D:315:SER:HA	2.54	0.42
2:D:116:GLU:OE2	2:D:411:MET:HB2	2.20	0.42
7:B:605:HEM:HBB2	2:D:242:GLU:OE1	2.20	0.42
9:C:1606:ACT:H2	10:C:1213(A):HOH:O	2.19	0.41
1:B:11:THR:O	2:D:168:THR:HG22	2.20	0.41
2:D:332:PHE:C	2:D:334:TYR:H	2.24	0.41
1:A:4:GLN:HG2	1:A:5:ASP:N	2.35	0.41
2:D:430:LEU:HA	2:D:431:PRO:HD3	1.97	0.41
2:C:547:SER:HB2	2:C:551:ILE:HG13	2.03	0.41
1:A:48:THR:HA	1:A:49:PRO:HD3	1.92	0.41
1:A:11:THR:O	1:A:24:ALA:HA	2.20	0.41
1:B:29:PHE:CZ	2:D:329:THR:HG21	2.56	0.41
2:D:309:TYR:CZ	2:D:497:CYS:HA	2.55	0.41
1:A:60:LEU:HD12	1:A:60:LEU:N	2.36	0.41
1:A:95:HIS:CD2	2:C:239:ARG:CZ	3.04	0.41
2:D:525:ARG:HH21	9:D:2604:ACT:CH3	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:267:LEU:HD12	2:C:576:ARG:HB2	2.03	0.40
2:C:309:TYR:CZ	2:C:497:CYS:HA	2.56	0.40
2:C:328:PHE:CD1	2:C:502:GLN:HG2	2.56	0.40
2:C:489:GLY:O	2:C:490:ARG:HD3	2.21	0.40
2:D:363:ARG:HG2	2:D:409:GLN:NE2	2.36	0.40
2:D:370:ARG:O	2:D:374:GLU:HB2	2.21	0.40
2:D:525:ARG:HH21	9:D:2604:ACT:C	2.34	0.40
2:D:466:GLU:HG2	2:D:466:GLU:O	2.22	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	102/104 (98%)	100 (98%)	1 (1%)	1 (1%)	15	4
1	B	102/104 (98%)	100 (98%)	2 (2%)	0	100	100
2	C	463/466 (99%)	445 (96%)	18 (4%)	0	100	100
2	D	463/466 (99%)	449 (97%)	14 (3%)	0	100	100
All	All	1130/1140 (99%)	1094 (97%)	35 (3%)	1 (0%)	51	33

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	42	SER

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	90/90 (100%)	89 (99%)	1 (1%)	73	60
1	B	90/90 (100%)	88 (98%)	2 (2%)	52	29
2	C	410/410 (100%)	401 (98%)	9 (2%)	52	29
2	D	410/410 (100%)	403 (98%)	7 (2%)	60	42
All	All	1000/1000 (100%)	981 (98%)	19 (2%)	57	37

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
2	C	122	GLN
2	C	175	MET
2	C	217	HIS
2	C	218	ASP
2	C	254	LEU
2	C	318	ASP
2	C	470	THR
2	C	497	CYS
2	C	523	GLN
1	B	54	ASN
1	B	81	GLU
2	D	124	PRO
2	D	138	LYS
2	D	175	MET
2	D	267	LEU
2	D	318	ASP
2	D	497	CYS
2	D	523	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
2	C	140	GLN
2	C	200	ASN
2	C	201	GLN
2	C	356	ASN
2	C	526	GLN

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Mol	Chain	Res	Type
2	C	530	GLN
2	C	549	ASN
1	B	54	ASN
2	D	122	GLN
2	D	421	ASN
2	D	526	GLN
2	D	549	ASN

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
2	CSO	D	150	2	3,6,7	0.93	0	0,6,8	0.00	-
2	CSO	C	150	2	3,6,7	0.75	0	0,6,8	0.00	-

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	CSO	D	150	2	-	0/1/5/7	-
2	CSO	C	150	2	-	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

12 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
3	NAG	E	1	3,2	14,14,15	0.85	0	17,19,21	0.93	0
3	NAG	E	2	3	14,14,15	0.75	0	17,19,21	0.79	0
3	BMA	E	3	3	11,11,12	0.70	0	15,15,17	0.62	0
3	MAN	E	4	3	11,11,12	0.67	0	15,15,17	0.85	0
3	MAN	E	5	3	11,11,12	0.57	0	15,15,17	0.72	0
3	FUC	E	6	3	10,10,11	0.69	0	14,14,16	0.61	0
3	NAG	F	1	3,2	14,14,15	0.71	0	17,19,21	1.15	1 (5%)
3	NAG	F	2	3	14,14,15	0.87	0	17,19,21	0.92	1 (5%)
3	BMA	F	3	3	11,11,12	0.85	0	15,15,17	0.62	0
3	MAN	F	4	3	11,11,12	0.80	0	15,15,17	0.98	1 (6%)
3	MAN	F	5	3	11,11,12	0.77	0	15,15,17	0.76	0
3	FUC	F	6	3	10,10,11	0.94	0	14,14,16	0.68	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
3	NAG	E	1	3,2	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	0/6/23/26	0/1/1/1
3	BMA	E	3	3	-	0/2/19/22	0/1/1/1
3	MAN	E	4	3	-	0/2/19/22	0/1/1/1
3	MAN	E	5	3	-	0/2/19/22	0/1/1/1
3	FUC	E	6	3	-	-	0/1/1/1

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

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	1	NAG	C2-N2-C7	-3.11	118.48	122.90
3	F	4	MAN	C1-O5-C5	3.02	116.28	112.19
3	F	2	NAG	C2-N2-C7	-2.68	119.09	122.90

There are no chirality outliers.

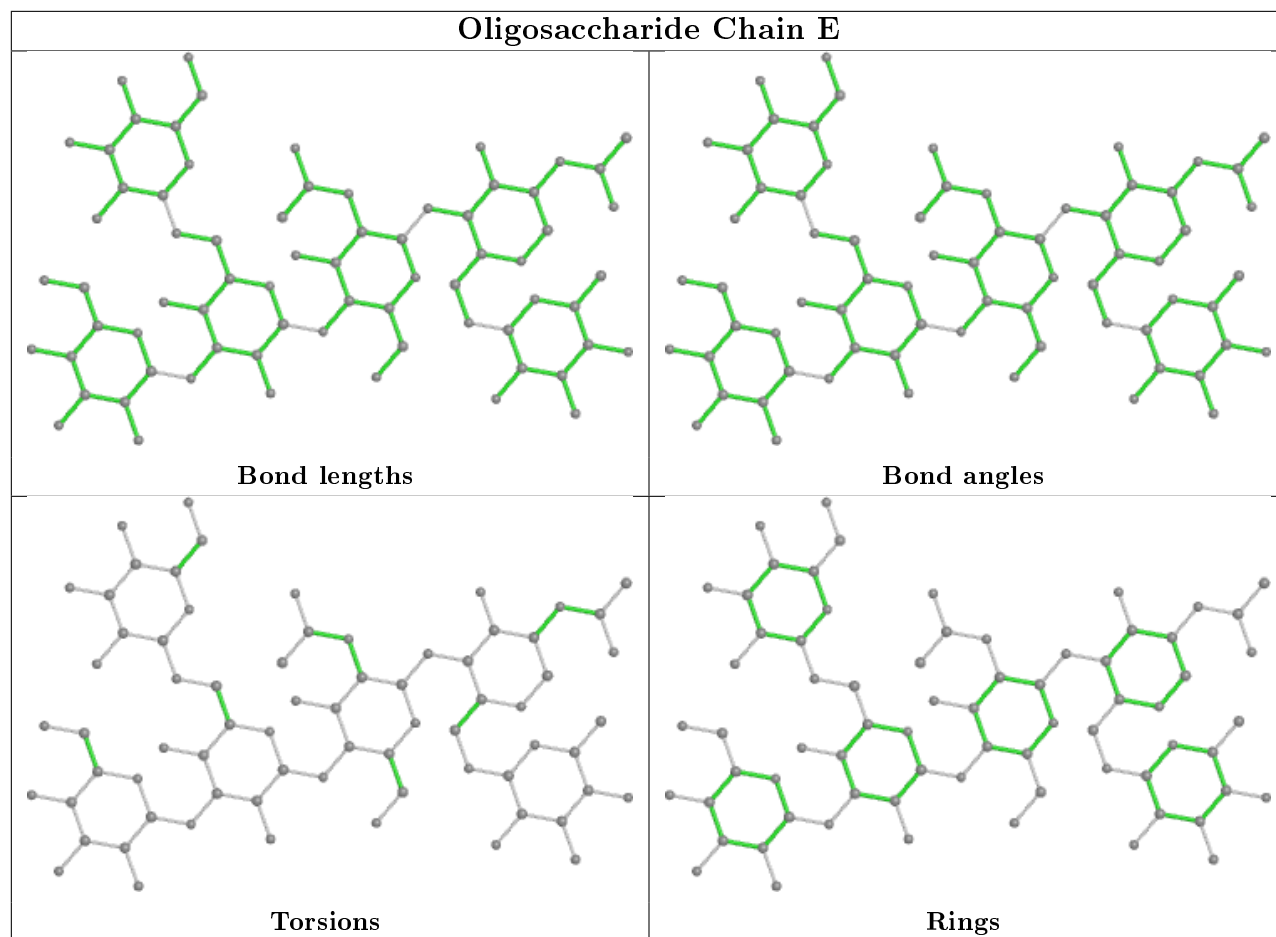
All (2) torsion outliers are listed below:

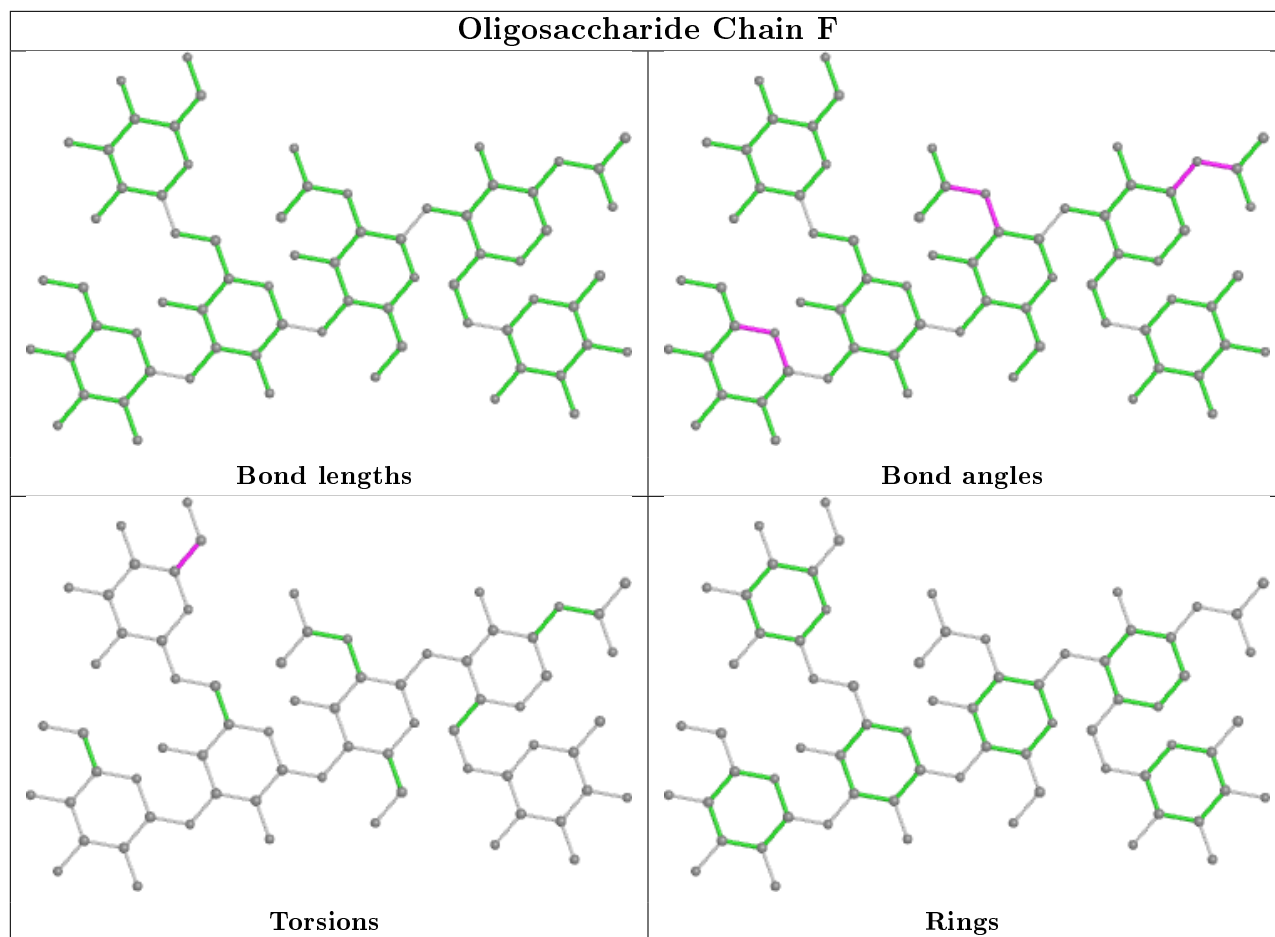
Mol	Chain	Res	Type	Atoms
3	F	5	MAN	O5-C5-C6-O6
3	F	5	MAN	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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





5.6 Ligand geometry [i](#)

Of 25 ligands modelled in this entry, 10 are monoatomic - leaving 15 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
8	NAG	C	1630	2	14,14,15	0.53	0	17,19,21	0.81	0
9	ACT	C	1604	-	1,3,3	3.48	1 (100%)	0,3,3	0.00	-
9	ACT	D	2607	-	1,3,3	3.46	1 (100%)	0,3,3	0.00	-
7	HEM	B	605	1,10,2	27,50,50	1.65	7 (25%)	17,82,82	1.17	1 (5%)
6	SO4	B	2602	-	4,4,4	0.29	0	6,6,6	0.06	0
6	SO4	C	1603	-	4,4,4	0.25	0	6,6,6	0.13	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	ACT	C	1606	-	1,3,3	2.72	1 (100%)	0,3,3	0.00	-
9	ACT	D	2604	-	1,3,3	3.42	1 (100%)	0,3,3	0.00	-
8	NAG	D	2620	2	14,14,15	0.53	0	17,19,21	0.74	0
8	NAG	D	2630	2	14,14,15	0.81	0	17,19,21	1.06	2 (11%)
6	SO4	A	1602	-	4,4,4	0.14	0	6,6,6	0.16	0
9	ACT	C	1607	-	1,3,3	3.91	1 (100%)	0,3,3	0.00	-
8	NAG	C	1620	2	14,14,15	0.67	0	17,19,21	1.12	2 (11%)
7	HEM	A	605	1,10,2	27,50,50	1.69	5 (18%)	17,82,82	1.20	1 (5%)
9	ACT	D	2606	-	1,3,3	2.30	1 (100%)	0,3,3	0.00	-

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
8	NAG	C	1630	2	-	0/6/23/26	0/1/1/1
7	HEM	B	605	1,10,2	-	0/6/54/54	-
8	NAG	D	2620	2	-	0/6/23/26	0/1/1/1
8	NAG	D	2630	2	-	1/6/23/26	0/1/1/1
8	NAG	C	1620	2	-	2/6/23/26	0/1/1/1
7	HEM	A	605	1,10,2	-	0/6/54/54	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	605	HEM	C3C-CAC	-4.13	1.39	1.47
7	B	605	HEM	C3B-C2B	-3.93	1.34	1.40
9	C	1607	ACT	CH3-C	3.91	1.53	1.48
7	A	605	HEM	C3B-CAB	-3.72	1.40	1.47
9	C	1604	ACT	CH3-C	3.48	1.53	1.48
9	D	2607	ACT	CH3-C	3.46	1.53	1.48
9	D	2604	ACT	CH3-C	3.42	1.53	1.48
7	A	605	HEM	C3B-C2B	-3.03	1.36	1.40
7	B	605	HEM	C3B-CAB	-3.02	1.41	1.47
9	C	1606	ACT	CH3-C	2.72	1.52	1.48
7	B	605	HEM	CBB-CAB	2.56	1.46	1.29
7	B	605	HEM	CBC-CAC	2.52	1.46	1.29
7	A	605	HEM	CBB-CAB	2.48	1.45	1.29
7	B	605	HEM	C3C-CAC	-2.48	1.42	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	D	2606	ACT	CH3-C	2.30	1.51	1.48
7	A	605	HEM	CBC-CAC	2.22	1.43	1.29
7	B	605	HEM	C1B-C2B	2.12	1.47	1.42
7	B	605	HEM	CAD-C3D	2.05	1.55	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	2630	NAG	C1-C2-N2	-2.56	106.12	110.49
8	C	1620	NAG	C2-N2-C7	-2.46	119.39	122.90
7	A	605	HEM	C3B-C4B-NB	2.46	112.38	109.21
8	D	2630	NAG	C1-O5-C5	-2.28	109.10	112.19
7	B	605	HEM	C3B-C4B-NB	2.19	112.03	109.21
8	C	1620	NAG	O5-C5-C6	-2.08	103.94	107.20

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	C	1620	NAG	O5-C5-C6-O6
8	C	1620	NAG	C4-C5-C6-O6
8	D	2630	NAG	C4-C5-C6-O6

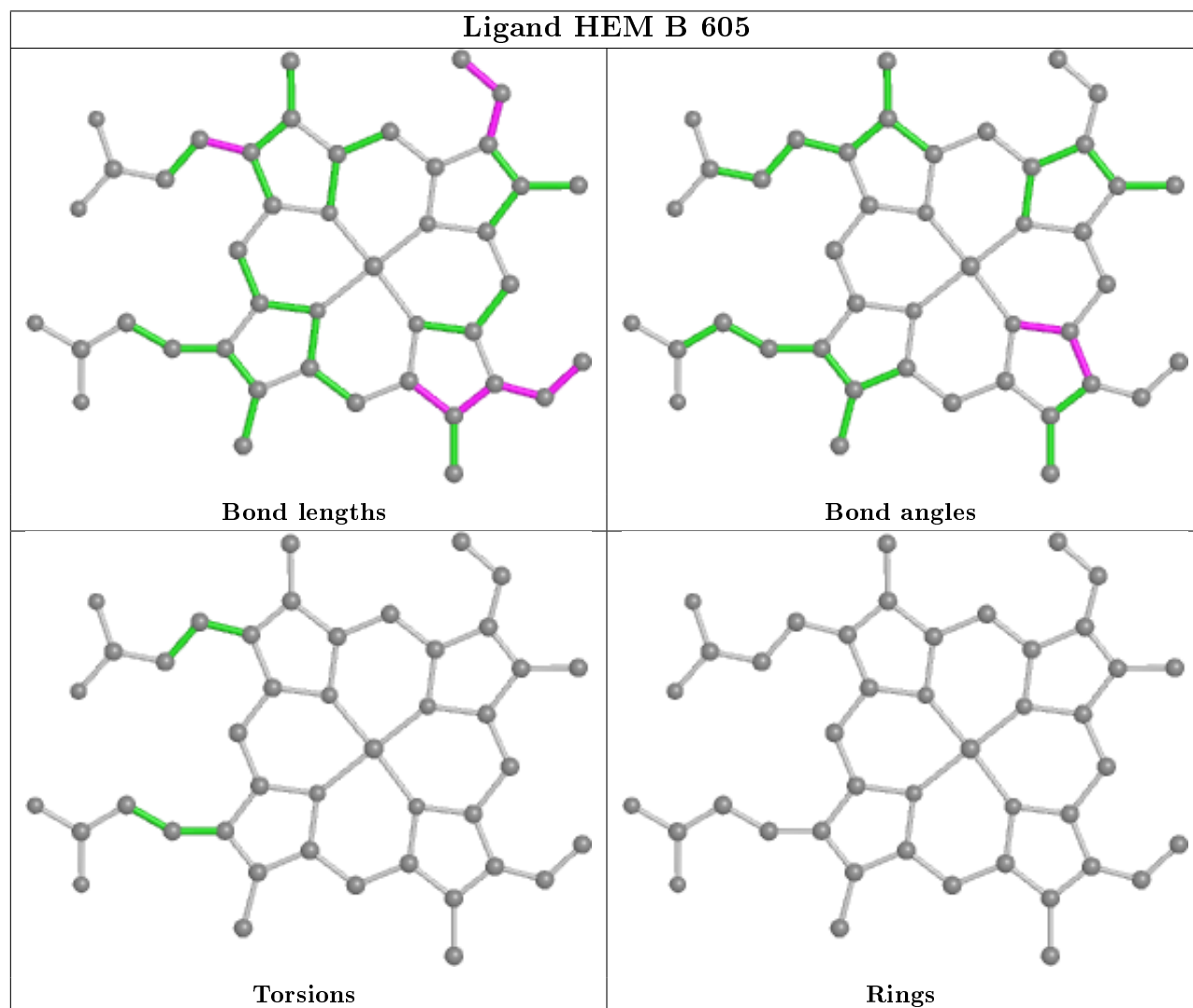
There are no ring outliers.

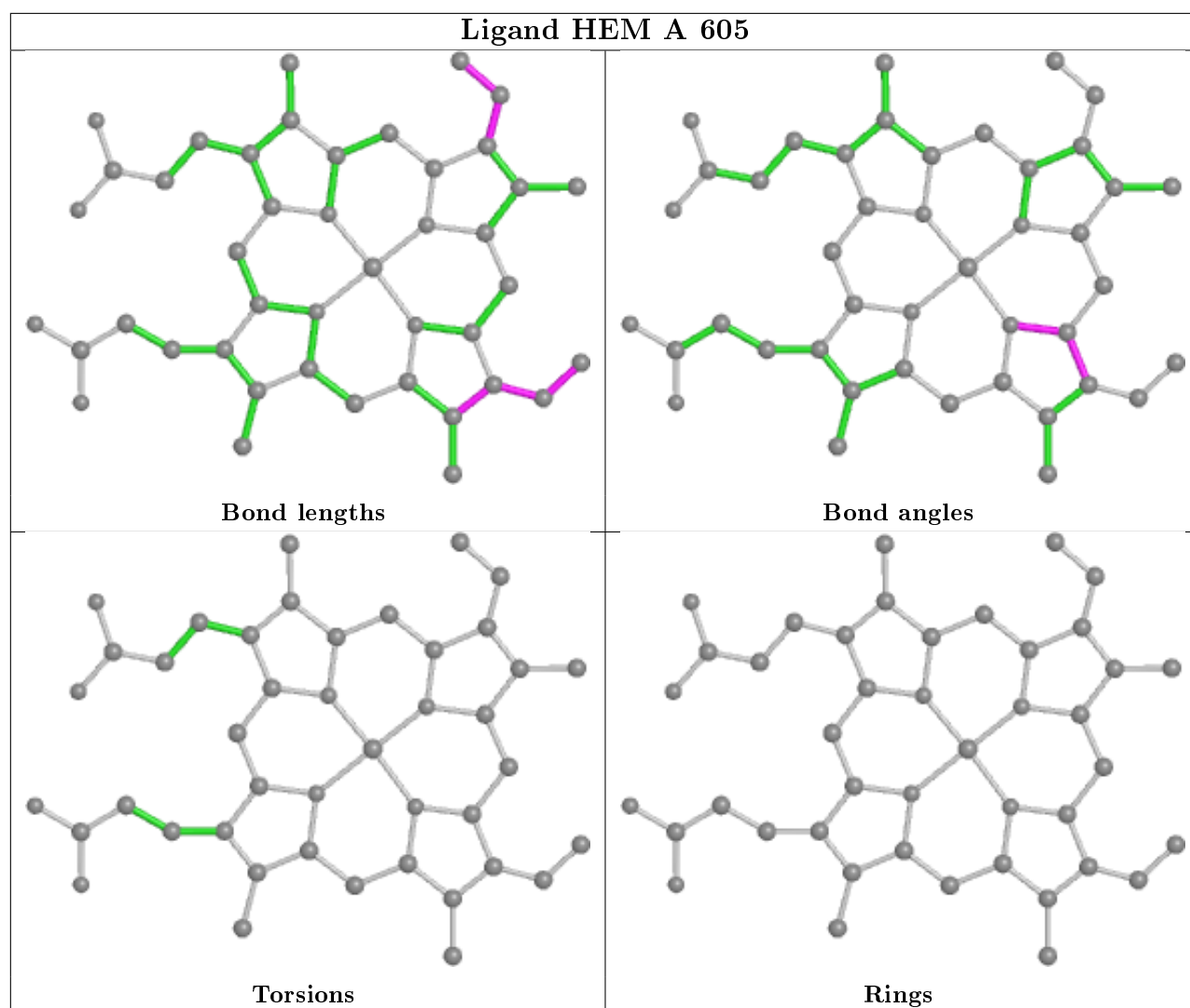
5 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	605	HEM	2	0
9	C	1606	ACT	4	0
9	D	2604	ACT	3	0
8	C	1620	NAG	1	0
7	A	605	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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	114:ASN	C	115:CYS	N	1.19

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	104/104 (100%)	1.39	19 (18%) 1 1	2, 6, 17, 43	0
1	B	104/104 (100%)	1.44	27 (25%) 0 0	3, 7, 15, 23	0
2	C	465/466 (99%)	1.48	106 (22%) 0 0	2, 7, 19, 35	0
2	D	465/466 (99%)	1.64	141 (30%) 0 0	3, 9, 24, 41	0
All	All	1138/1140 (99%)	1.53	293 (25%) 0 0	2, 8, 22, 43	0

All (293) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	113	VAL	14.8
2	D	355	PRO	8.9
2	D	568	PRO	6.2
1	A	4	GLN	5.8
2	D	578	ALA	5.2
1	A	2	PRO	5.2
2	C	353	MET	5.1
2	D	218	ASP	5.0
2	D	543	ILE	4.9
2	C	223	LEU	4.9
2	C	355	PRO	4.8
2	D	562	VAL	4.6
2	D	217	HIS	4.6
2	C	190	MET	4.4
2	C	157	ASN	4.4
2	C	212	PRO	4.3
2	D	529	ALA	4.2
2	C	158	ILE	4.1
2	D	575	TRP	4.1
2	C	199	VAL	4.1
1	A	1	CYS	4.0

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Mol	Chain	Res	Type	RSRZ
2	D	113	VAL	4.0
1	B	1	CYS	4.0
2	D	261	ALA	4.0
2	D	315	SER	3.9
2	C	351	GLN	3.8
2	C	155	GLY	3.7
1	A	3	GLU	3.7
2	D	351	GLN	3.7
2	D	269	PRO	3.6
2	D	222	LEU	3.6
2	D	216	LEU	3.6
2	C	217	HIS	3.6
2	D	406	LEU	3.6
2	D	417	LEU	3.6
2	D	572	LEU	3.6
1	A	97	LEU	3.6
2	D	190	MET	3.5
2	D	227	SER	3.5
1	B	89	TRP	3.5
2	D	226	ARG	3.5
2	C	452	GLY	3.5
1	B	60	LEU	3.5
2	D	202	ARG	3.5
2	D	157	ASN	3.4
2	D	538	CYS	3.4
2	D	124	PRO	3.4
2	D	527	ALA	3.4
2	C	147	PHE	3.4
2	D	407	PHE	3.4
1	B	47	TRP	3.4
2	C	436	TRP	3.4
2	D	303	PRO	3.4
2	C	578	ALA	3.3
2	D	352	PRO	3.3
2	C	141	ALA	3.3
2	D	267	LEU	3.3
2	D	253	LEU	3.3
2	D	117	THR	3.2
2	D	328	PHE	3.2
2	C	379	PRO	3.2
2	C	357	PRO	3.2
1	B	51	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
2	C	128	LEU	3.2
2	D	185	ARG	3.1
2	D	567	LEU	3.1
2	C	561	PHE	3.0
2	C	324	ILE	3.0
2	D	173	ALA	3.0
2	C	369	TRP	3.0
2	D	471	PRO	3.0
2	D	557	TYR	3.0
2	D	302	GLY	3.0
2	D	360	PRO	3.0
2	C	557	TYR	2.9
2	D	271	TRP	2.9
1	B	33	LEU	2.9
2	C	359	VAL	2.9
2	D	264	LEU	2.9
2	D	410	VAL	2.9
2	D	357	PRO	2.9
2	C	133	ASN	2.9
2	C	327	VAL	2.9
1	B	63	ALA	2.9
2	D	272	ASP	2.9
2	D	499	ILE	2.9
2	D	576	ARG	2.9
2	D	309	TYR	2.9
2	D	348	ASN	2.9
1	B	92	LEU	2.9
2	C	216	LEU	2.9
2	C	543	ILE	2.9
2	D	542	GLY	2.8
2	D	212	PRO	2.8
2	C	462	ARG	2.8
2	D	296	TYR	2.8
1	A	30	VAL	2.8
2	D	546	VAL	2.8
2	C	140	GLN	2.8
2	D	561	PHE	2.8
2	C	114	ASN	2.8
2	D	356	ASN	2.8
2	D	566	THR	2.8
2	D	164	ILE	2.8
2	C	139	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
2	C	417	LEU	2.8
2	D	359	VAL	2.8
1	A	47	TRP	2.8
2	C	328	PHE	2.7
2	C	440	CYS	2.7
2	C	354	GLU	2.7
2	C	519	VAL	2.7
2	D	494	LEU	2.7
2	D	419	ALA	2.7
2	C	506	LEU	2.7
2	D	574	SER	2.7
1	A	76	LEU	2.7
2	C	320	VAL	2.7
1	A	89	TRP	2.7
2	C	211	LEU	2.7
2	D	120	VAL	2.7
2	C	352	PRO	2.7
2	C	283	ILE	2.6
2	D	397	ILE	2.6
2	C	171	VAL	2.6
2	C	313	TYR	2.6
2	D	350	TYR	2.6
2	D	485	LEU	2.6
2	D	544	THR	2.6
2	D	353	MET	2.6
2	D	220	PRO	2.6
2	C	461	ALA	2.6
2	D	147	PHE	2.6
1	A	93	LEU	2.6
2	C	386	ALA	2.6
2	D	221	CYS	2.6
1	B	100	THR	2.6
2	C	253	LEU	2.6
2	C	419	ALA	2.6
2	D	176	VAL	2.6
2	C	430	LEU	2.6
2	C	485	LEU	2.6
2	D	280	ALA	2.6
2	C	220	PRO	2.6
2	D	558	PRO	2.6
1	A	99	PHE	2.5
2	C	334	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
2	D	155	GLY	2.5
2	D	548	LYS	2.5
2	D	156	SER	2.5
2	D	565	SER	2.5
2	C	477	TRP	2.5
2	C	264	LEU	2.5
2	D	192	ASN	2.5
2	C	325	ALA	2.5
2	D	325	ALA	2.5
2	D	496	ALA	2.5
1	A	41	PHE	2.5
2	C	332	PHE	2.5
2	C	558	PRO	2.5
2	C	203	PHE	2.5
1	B	97	LEU	2.5
2	D	246	LEU	2.5
2	D	455	LEU	2.5
2	D	193	GLN	2.5
2	D	522	MET	2.4
2	D	545	THR	2.4
2	D	233	PHE	2.4
2	C	246	LEU	2.4
1	B	28	ALA	2.4
2	D	292	THR	2.4
1	A	29	PHE	2.4
1	A	71	PHE	2.4
1	A	92	LEU	2.4
2	D	169	SER	2.4
2	D	191	SER	2.4
2	D	254	LEU	2.4
2	C	329	THR	2.4
1	A	32	TRP	2.4
2	D	436	TRP	2.4
2	D	266	SER	2.4
2	D	125	CYS	2.4
2	C	458	LEU	2.4
2	D	211	LEU	2.4
2	D	337	THR	2.4
2	D	339	ILE	2.4
2	D	207	GLY	2.4
2	C	127	PRO	2.4
2	C	349	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
2	C	513	TRP	2.4
2	D	369	TRP	2.4
2	C	542	GLY	2.4
2	C	176	VAL	2.3
2	D	349	ARG	2.3
2	D	399	VAL	2.3
2	D	290	ILE	2.3
2	D	498	ILE	2.3
2	C	514	TRP	2.3
2	D	379	PRO	2.3
1	B	83	SER	2.3
2	D	354	GLU	2.3
1	B	32	TRP	2.3
2	C	576	ARG	2.3
2	D	300	VAL	2.3
1	B	84	LEU	2.3
2	C	130	ILE	2.3
2	C	125	CYS	2.3
2	C	170	PHE	2.3
2	C	304	THR	2.3
2	D	234	LEU	2.3
2	C	476	ILE	2.3
2	C	227	SER	2.3
2	C	552	PHE	2.3
2	D	520	PHE	2.3
2	D	310	LEU	2.2
2	D	476	ILE	2.2
1	B	99	PHE	2.2
2	C	213	PHE	2.2
2	D	314	ARG	2.2
1	B	30	VAL	2.2
2	C	448	VAL	2.2
2	C	276	LEU	2.2
2	C	409	GLN	2.2
2	D	492	GLY	2.2
2	C	537	ILE	2.2
2	C	538	CYS	2.2
2	C	173	ALA	2.2
2	D	225	ASN	2.2
1	B	64	VAL	2.2
2	D	223	LEU	2.2
1	B	49	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	78	PRO	2.2
1	A	86	PHE	2.2
2	C	365	PHE	2.2
1	B	14	CYS	2.2
2	C	221	CYS	2.2
2	C	568	PRO	2.2
2	D	373	LEU	2.2
2	D	381	LEU	2.2
1	B	45	TYR	2.1
2	C	285	GLY	2.1
2	C	391	LEU	2.1
2	D	201	GLN	2.1
2	C	228	ALA	2.1
2	C	398	ALA	2.1
2	D	563	ASN	2.1
2	D	154	PRO	2.1
2	D	182	PRO	2.1
2	C	284	VAL	2.1
1	B	43	LEU	2.1
2	D	262	THR	2.1
2	C	331	ALA	2.1
2	D	331	ALA	2.1
2	D	270	ARG	2.1
2	C	366	PHE	2.1
2	C	512	PHE	2.1
2	D	203	PHE	2.1
2	D	547	SER	2.1
2	C	545	THR	2.1
2	C	218	ASP	2.1
1	B	93	LEU	2.1
2	C	196	LEU	2.1
2	C	529	ALA	2.1
2	D	430	LEU	2.1
2	D	287	MET	2.1
2	D	402	ILE	2.1
2	C	350	TYR	2.1
2	D	559	ARG	2.1
2	C	198	ALA	2.1
2	C	194	LEU	2.1
2	D	252	LEU	2.1
2	D	338	LEU	2.1
2	D	174	SER	2.1

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Mol	Chain	Res	Type	RSRZ
2	C	209	ALA	2.0
2	C	316	TYR	2.0
2	D	284	VAL	2.0
2	D	555	ASN	2.0
2	C	344	PHE	2.0
2	D	332	PHE	2.0
2	D	366	PHE	2.0
2	D	210	LEU	2.0
1	A	68	ILE	2.0
1	B	73	THR	2.0
2	D	564	CYS	2.0
2	C	309	TYR	2.0
1	B	69	VAL	2.0
1	B	56	PHE	2.0
1	B	71	PHE	2.0
2	C	260	LEU	2.0
2	D	276	LEU	2.0
2	D	342	PHE	2.0
1	A	5	ASP	2.0
2	D	268	ASN	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, 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	CSO	D	150	7/8	0.91	0.13	5,6,8,10	0
2	CSO	C	150	7/8	0.94	0.10	2,5,7,9	0

6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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.

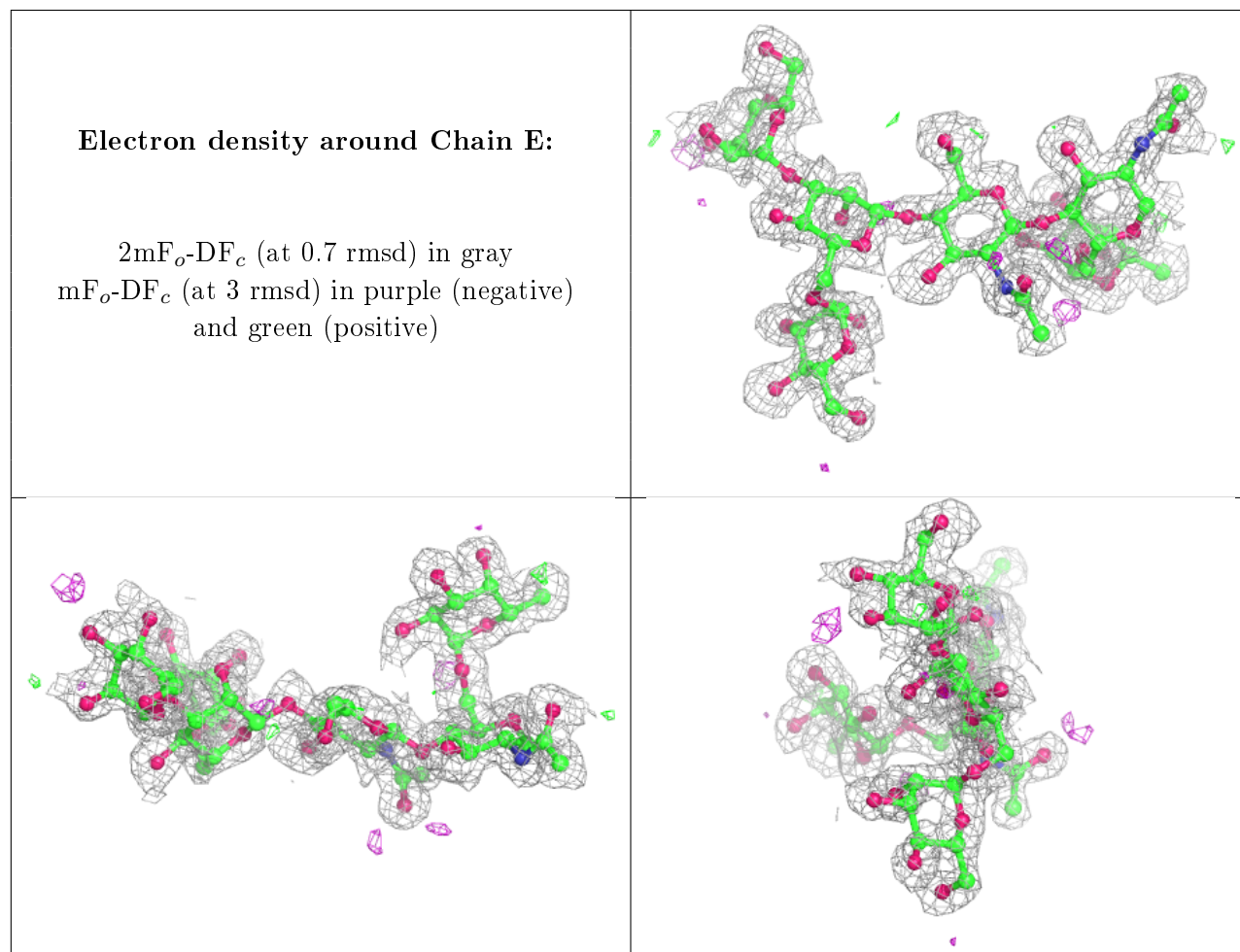
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MAN	F	4	11/12	0.68	0.26	17,20,22,23	0

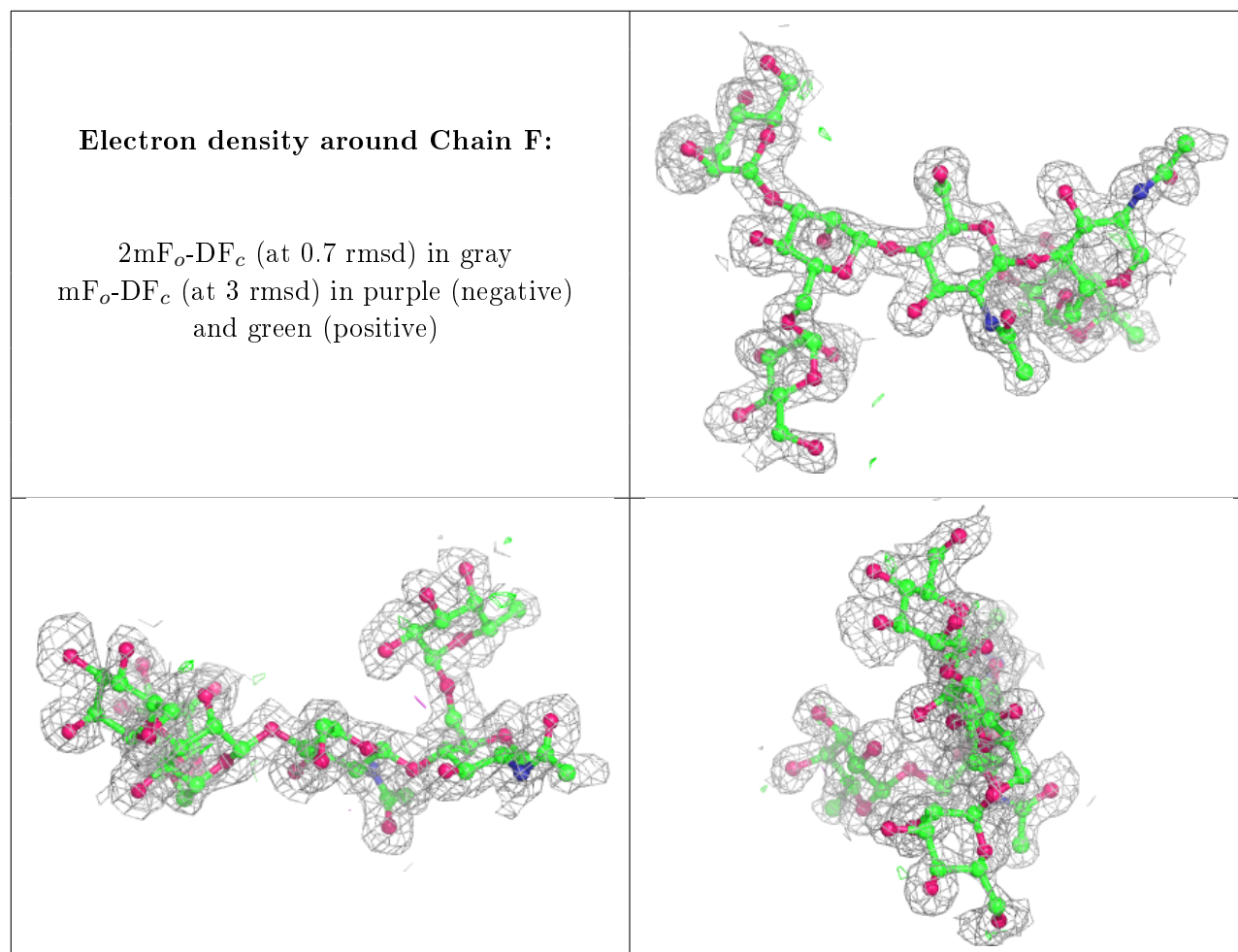
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	FUC	F	6	10/11	0.79	0.22	10,14,16,19	0
3	MAN	E	4	11/12	0.80	0.23	21,25,26,28	0
3	MAN	F	5	11/12	0.82	0.22	9,14,18,23	0
3	BMA	E	3	11/12	0.84	0.22	9,14,15,18	0
3	FUC	E	6	10/11	0.85	0.14	9,13,15,17	0
3	MAN	E	5	11/12	0.86	0.18	13,15,17,18	0
3	BMA	F	3	11/12	0.87	0.17	9,12,14,18	0
3	NAG	E	2	14/15	0.88	0.17	5,8,11,12	0
3	NAG	F	1	14/15	0.88	0.15	9,10,15,16	0
3	NAG	E	1	14/15	0.89	0.14	6,8,11,13	0
3	NAG	F	2	14/15	0.91	0.13	6,8,10,11	0

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





6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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(\AA^2)	Q<0.9
9	ACT	C	1606	4/4	0.46	0.28	22,23,24,25	0
6	SO4	B	2602	5/5	0.48	0.33	42,42,43,44	5
9	ACT	D	2607	4/4	0.49	0.29	29,30,30,31	0
9	ACT	D	2604	4/4	0.64	0.43	32,34,34,34	0
9	ACT	C	1604	4/4	0.73	0.23	17,17,20,22	0
8	NAG	C	1630	14/15	0.74	0.23	18,22,27,28	0
8	NAG	D	2630	14/15	0.75	0.26	26,30,34,35	0
9	ACT	C	1607	4/4	0.79	0.25	22,23,23,25	0
8	NAG	D	2620	14/15	0.79	0.24	16,21,26,28	0
8	NAG	C	1620	14/15	0.86	0.21	9,14,20,24	0
9	ACT	D	2606	4/4	0.91	0.13	13,14,14,18	0

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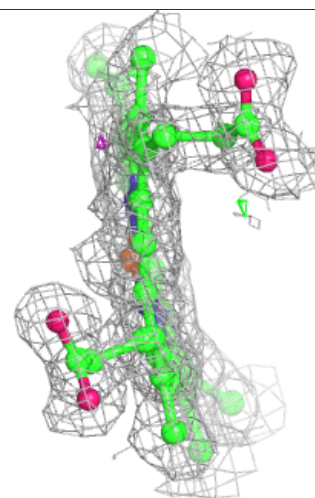
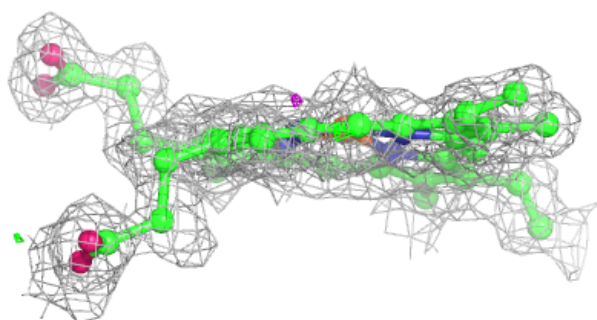
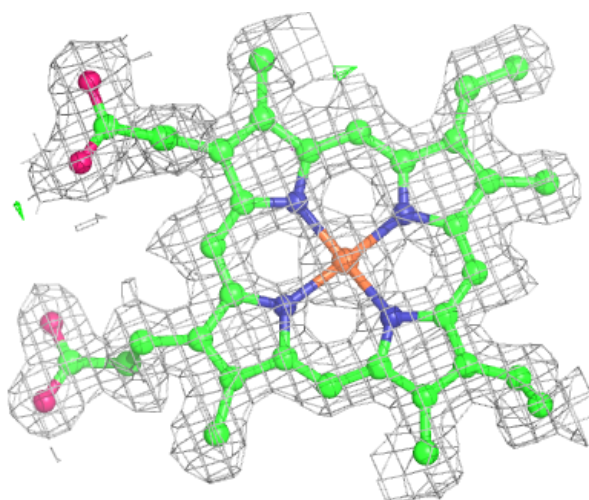
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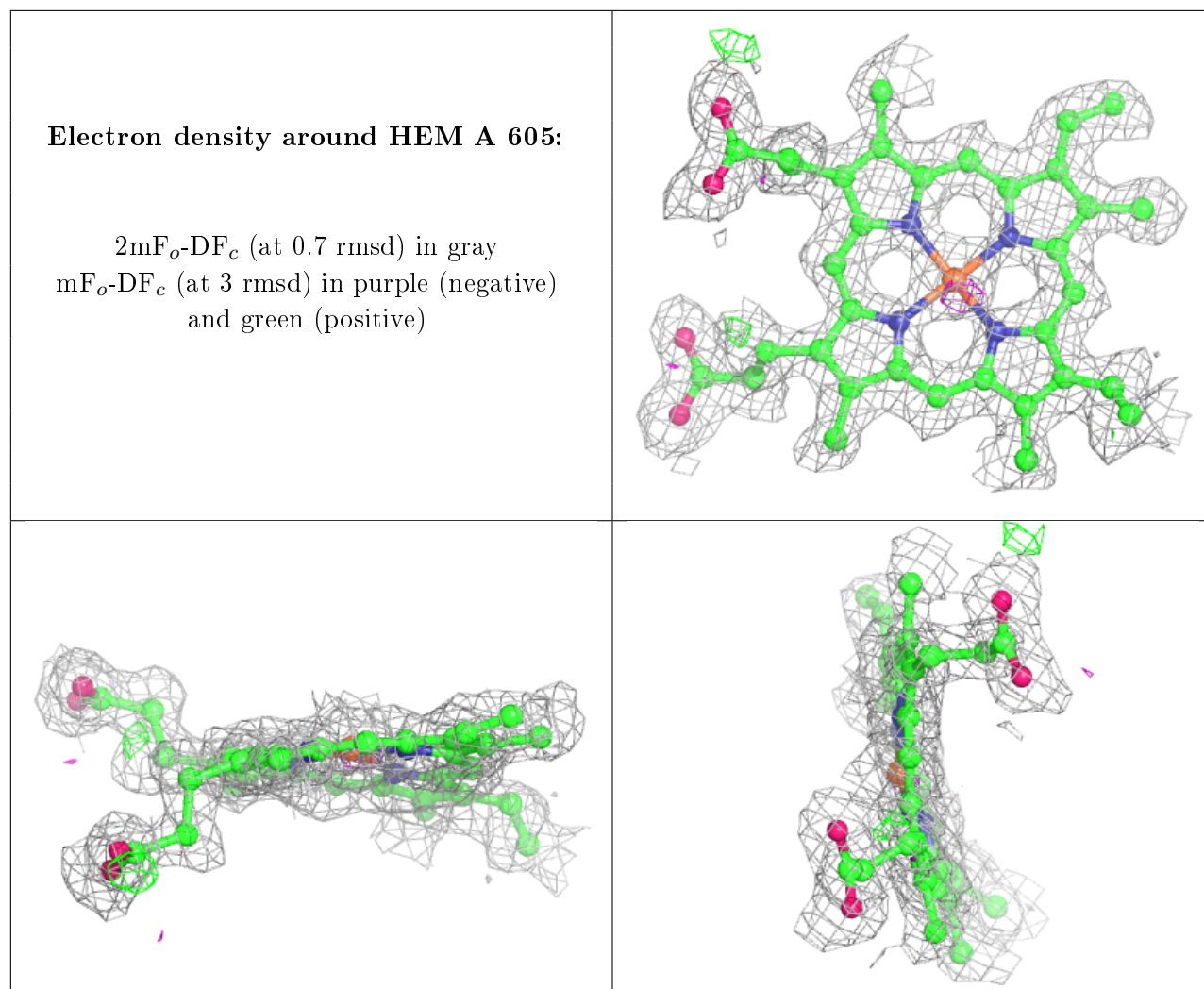
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	HEM	B	605	43/43	0.93	0.16	2,5,8,9	0
6	SO4	C	1603	5/5	0.93	0.12	20,21,23,25	0
7	HEM	A	605	43/43	0.94	0.17	2,5,8,8	0
5	BR	B	758	1/1	0.94	0.12	18,18,18,18	1
6	SO4	A	1602	5/5	0.96	0.10	19,19,21,22	0
5	BR	A	843	1/1	0.97	0.14	12,12,12,12	1
5	BR	A	758	1/1	0.98	0.07	16,16,16,16	1
5	BR	B	889	1/1	0.98	0.06	23,23,23,23	1
5	BR	A	889	1/1	0.99	0.06	24,24,24,24	1
5	BR	B	843	1/1	0.99	0.06	12,12,12,12	1
4	CA	A	600	1/1	1.00	0.10	5,5,5,5	0
4	CA	B	600	1/1	1.00	0.13	7,7,7,7	0
5	BR	A	601	1/1	1.00	0.09	6,6,6,6	0
5	BR	B	601	1/1	1.00	0.10	6,6,6,6	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 B 605:

$2mF_o-DF_c$ (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.