



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 7, 2020 – 12:17 PM EDT

PDB ID : 6WXZ
Title : CRYSTAL STRUCTURE OF MYELOPEROXIDASE SUBFORM C (MPO)
COMPLEX WITH Compound-29 A.K.A 7-(1,2-DIPHENYLETHYL)-1H-[1,2
,3]TRIAZOLO[4,5-B]PYRIDIN-5-AMINE
Authors : Khan, J.A.
Deposited on : 2020-05-12
Resolution : 2.23 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 : 2.14.6
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) : 2.14.6

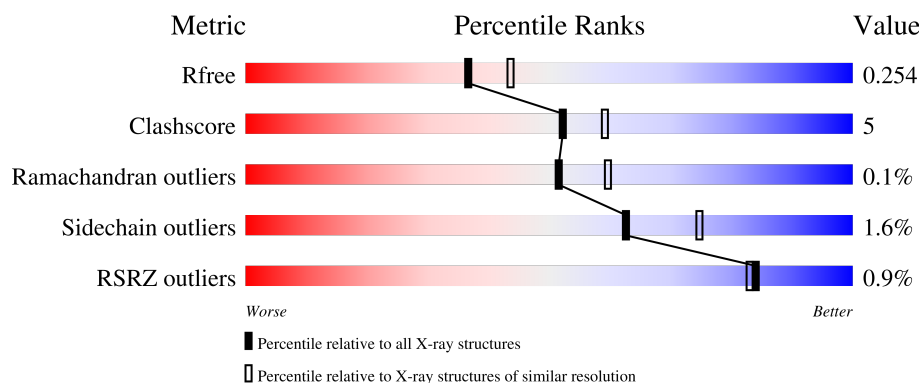
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

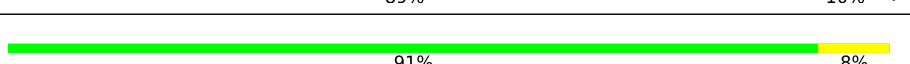
The reported resolution of this entry is 2.23 Å.

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.




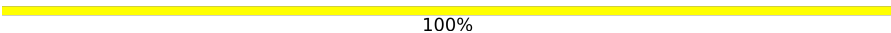
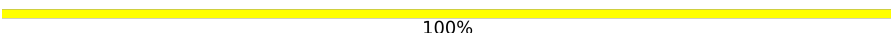
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5912 (2.24-2.20)
Clashscore	141614	6646 (2.24-2.20)
Ramachandran outliers	138981	6543 (2.24-2.20)
Sidechain outliers	138945	6544 (2.24-2.20)
RSRZ outliers	127900	5797 (2.24-2.20)

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	105	
1	D	105	
2	B	467	
2	E	467	
3	C	2	

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Mol	Chain	Length	Quality of chain
3	H	2	 <div>50%50%</div>
4	F	2	 <div>100%</div>
4	G	2	 <div>100%</div>

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
10	MAN	B	611	-	-	X	-
4	BMA	F	1	-	-	X	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 9836 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 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	103	Total	C	N	O	S	0	0	0
			818	519	145	149	5			
1	D	103	Total	C	N	O	S	0	0	0
			820	520	145	150	5			

- Molecule 2 is a protein called Myeloperoxidase heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	464	Total	C	N	O	S	18	0	0
			3689	2328	670	664	27			
2	E	465	Total	C	N	O	S	27	0	0
			3711	2341	679	664	27			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	2	Total	C	N	O	0	0	0
			24	14	1	9			
3	H	2	Total	C	N	O	0	0	0
			24	14	1	9			

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
4	F	2	Total	C	O	0	0	0
			22	12	10			
4	G	2	Total	C	O	0	0	0
			22	12	10			

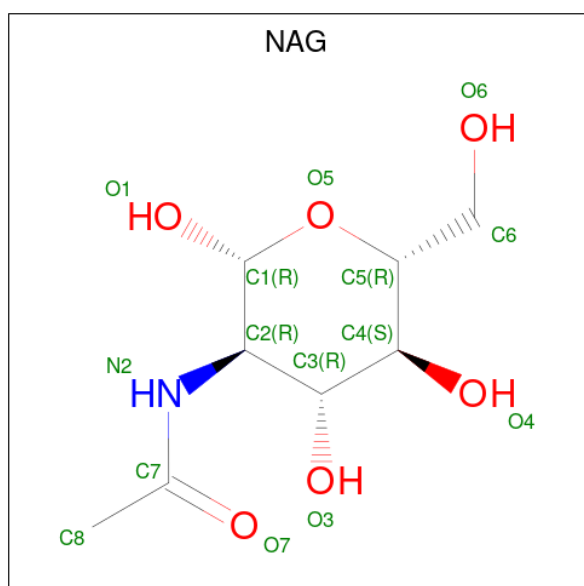
- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Cl	0	0
			1	1		
5	A	1	Total	Cl	0	0
			1	1		
5	D	1	Total	Cl	0	0
			1	1		
5	E	1	Total	Cl	0	0
			1	1		

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

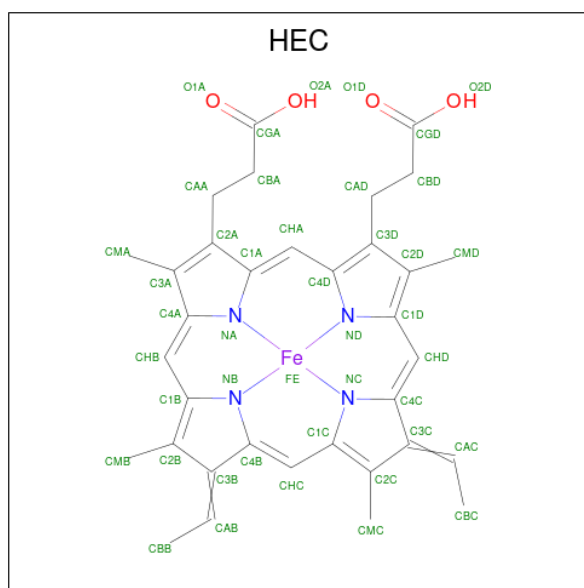
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Ca	0	0
			1	1		
6	D	1	Total	Ca	0	0
			1	1		

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



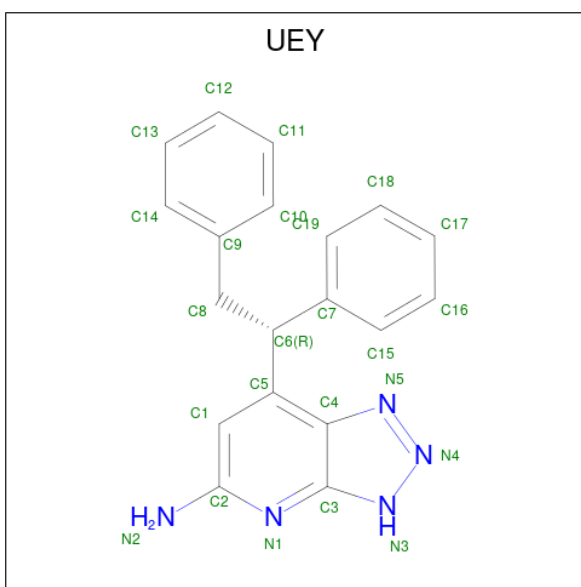
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total 14	C 8	N 1	O 5	0	0
7	B	1	Total 14	C 8	N 1	O 5	0	0
7	B	1	Total 14	C 8	N 1	O 5	0	0
7	B	1	Total 14	C 8	N 1	O 5	0	0
7	E	1	Total 14	C 8	N 1	O 5	0	0
7	E	1	Total 14	C 8	N 1	O 5	0	0
7	E	1	Total 14	C 8	N 1	O 5	0	0
7	E	1	Total 14	C 8	N 1	O 5	0	0

- Molecule 8 is HEME C (three-letter code: HEC) (formula: $\text{C}_{34}\text{H}_{34}\text{FeN}_4\text{O}_4$).



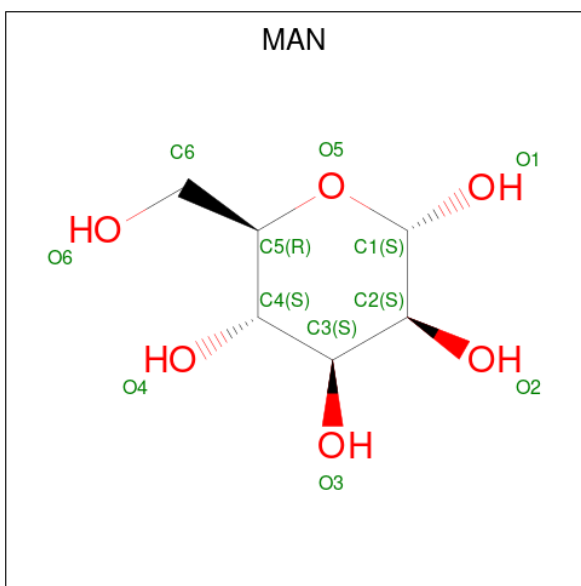
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
8	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 9 is 7-[(1R)-1,2-diphenylethyl]-3H-[1,2,3]triazolo[4,5-b]pyridin-5-amine (three-letter code: UEY) (formula: C₁₉H₁₇N₅) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	N	0	0
			24	19	5		
9	E	1	Total	C	N	0	0
			24	19	5		

- Molecule 10 is alpha-D-mannopyranose (three-letter code: MAN) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	B	1	Total	C	O	0	0
			11	6	5		
10	E	1	Total	C	O	0	0
			11	6	5		

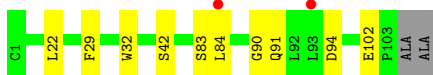
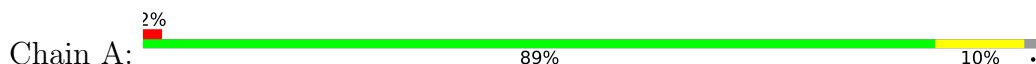
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	55	Total 55	O 55	0	0
11	B	155	Total 155	O 155	0	0
11	D	51	Total 51	O 51	0	0
11	E	171	Total 171	O 171	0	0

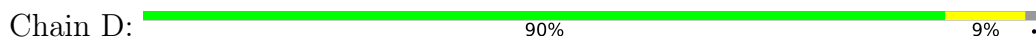
3 Residue-property plots [i](#)

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.

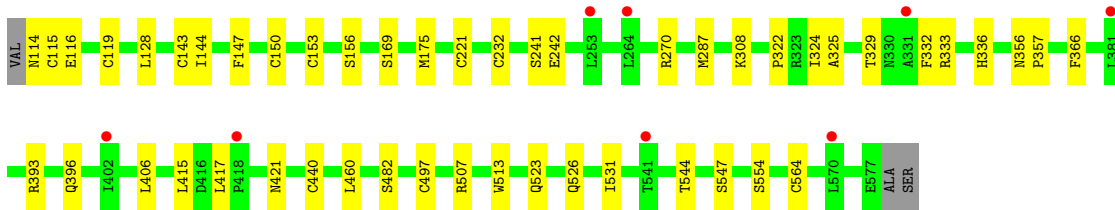
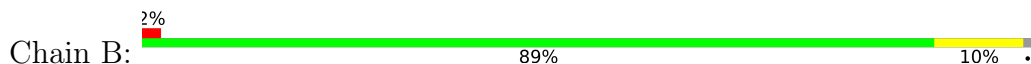
- Molecule 1: Myeloperoxidase light chain



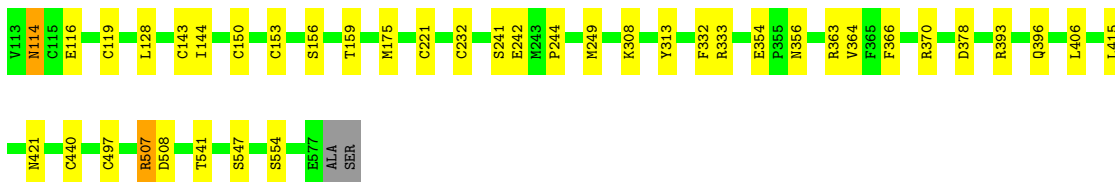
- Molecule 1: Myeloperoxidase light chain



- Molecule 2: Myeloperoxidase heavy chain



- Molecule 2: Myeloperoxidase heavy chain



- Molecule 3: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose





- Molecule 3: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H: 50% 50%



- Molecule 4: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose

Chain F: 100%



- Molecule 4: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose

Chain G: 100%



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	107.42Å 107.42Å 239.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	98.02 – 2.23 98.02 – 2.23	Depositor EDS
% Data completeness (in resolution range)	100.0 (98.02-2.23) 100.0 (98.02-2.23)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.16 (at 2.22Å)	Xtriage
Refinement program	BUSTER 2.11.7 (17-DEC-2019)	Depositor
R, R_{free}	0.211 , 0.242 0.221 , 0.254	Depositor DCC
R_{free} test set	3514 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	42.6	Xtriage
Anisotropy	0.548	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 50.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9836	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.38% 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, CL, CA, UEY, FUC, HEC, 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	0.43	0/843	0.63	0/1150
1	D	0.42	0/845	0.63	0/1153
2	B	0.42	0/3767	0.55	0/5113
2	E	0.41	0/3789	0.57	0/5141
All	All	0.42	0/9244	0.58	0/12557

There are no bond length outliers.

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	818	0	774	9	0
1	D	820	0	773	8	0
2	B	3689	0	3660	34	0
2	E	3711	0	3700	28	0
3	C	24	0	22	2	0
3	H	24	0	22	2	0
4	F	22	0	19	6	0
4	G	22	0	19	5	0
5	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	1	0	0	1	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
6	A	1	0	0	0	0
6	D	1	0	0	0	0
7	B	56	0	52	5	0
7	E	56	0	52	6	0
8	B	43	0	30	8	0
8	E	43	0	30	9	0
9	B	24	0	0	1	0
9	E	24	0	0	0	0
10	B	11	0	10	7	0
10	E	11	0	10	4	0
11	A	55	0	0	0	0
11	B	155	0	0	1	0
11	D	51	0	0	0	0
11	E	171	0	0	0	0
All	All	9836	0	9173	92	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 5.

All (92) 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:D:94:ASP:OD2	8:E:610:HEC:CMD	1.76	1.31
2:E:242:GLU:OE2	8:E:610:HEC:HMB3	1.31	1.28
1:A:94:ASP:OD2	8:B:605:HEC:HMD3	1.04	1.20
7:B:608:NAG:O4	4:F:1:BMA:C1	1.90	1.19
1:A:94:ASP:OD2	8:B:605:HEC:CMD	1.99	1.09
2:B:242:GLU:OE2	8:B:605:HEC:HMB3	1.57	1.04
7:E:601:NAG:O4	4:G:1:BMA:C1	2.06	1.03
1:D:94:ASP:CG	8:E:610:HEC:HMD3	1.81	1.01
1:D:94:ASP:OD2	8:E:610:HEC:HMD3	0.81	0.98
7:E:601:NAG:C1	3:C:1:NAG:O4	2.14	0.95
2:B:221:CYS:HG	2:B:232:CYS:HG	1.03	0.94
7:B:608:NAG:C1	3:H:1:NAG:O4	2.15	0.94
10:B:611:MAN:H2	4:F:1:BMA:O3	1.69	0.92
2:E:242:GLU:OE2	8:E:610:HEC:CMB	2.20	0.89
2:E:221:CYS:HG	2:E:232:CYS:HG	0.86	0.85
2:E:440:CYS:HG	2:E:497:CYS:HG	1.12	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:608:NAG:HO4	4:F:1:BMA:C1	1.95	0.78
2:B:440:CYS:HG	2:B:497:CYS:HG	1.26	0.77
1:A:94:ASP:CG	8:B:605:HEC:HMD3	2.06	0.70
2:B:119:CYS:HG	2:B:143:CYS:HG	1.33	0.69
7:E:601:NAG:HO4	4:G:1:BMA:C1	2.06	0.69
2:E:119:CYS:HG	2:E:143:CYS:HG	1.40	0.69
2:E:333:ARG:HH11	2:E:421:ASN:HD22	1.41	0.67
2:E:333:ARG:HH11	2:E:421:ASN:ND2	1.94	0.66
2:B:333:ARG:HH11	2:B:421:ASN:HD22	1.41	0.66
2:B:333:ARG:HH11	2:B:421:ASN:ND2	1.95	0.64
2:E:150:CSO:OD	2:E:150:CSO:SG	2.55	0.64
1:D:90:GLY:C	8:E:610:HEC:HBC3	2.19	0.63
1:A:90:GLY:C	8:B:605:HEC:HBC3	2.21	0.61
2:B:308:LYS:HZ1	10:B:611:MAN:H62	1.65	0.60
2:E:308:LYS:HZ1	10:E:604:MAN:C1	2.16	0.59
10:E:604:MAN:H5	4:G:1:BMA:H2	1.85	0.58
5:B:612:CL:CL	11:B:765:HOH:O	2.54	0.57
10:E:604:MAN:H3	4:G:1:BMA:O3	2.04	0.57
10:B:611:MAN:C1	4:F:1:BMA:H3	2.36	0.55
7:B:608:NAG:C1	3:H:1:NAG:C4	2.84	0.55
7:E:601:NAG:C1	3:C:1:NAG:C4	2.84	0.55
2:E:363:ARG:O	2:E:370:ARG:NH1	2.40	0.55
2:E:308:LYS:NZ	10:E:604:MAN:C1	2.71	0.54
2:B:544:THR:HA	2:B:564:CYS:SG	2.48	0.53
7:E:601:NAG:C4	4:G:1:BMA:C1	2.87	0.52
2:B:128:LEU:HB2	2:B:144:ILE:HB	1.93	0.51
2:E:128:LEU:HB2	2:E:144:ILE:HB	1.92	0.51
2:B:153:CYS:CB	2:E:153:CYS:HG	2.24	0.49
2:E:153:CYS:SG	2:E:156:SER:HB2	2.53	0.49
2:E:241:SER:O	2:E:366:PHE:HA	2.12	0.49
2:E:332:PHE:O	8:E:610:HEC:HAC	2.13	0.48
2:B:523:GLN:O	2:B:526:GLN:HG2	2.13	0.48
2:B:460:LEU:HD21	2:B:482:SER:HB3	1.95	0.48
1:A:91:GLN:HB2	8:B:605:HEC:HMC3	1.95	0.48
2:B:308:LYS:HZ1	10:B:611:MAN:C1	2.26	0.48
2:B:393:ARG:HB2	2:B:396:GLN:HB2	1.96	0.48
2:E:313:TYR:HD1	2:E:507:ARG:HD3	1.79	0.48
1:D:1:CYS:HG	1:D:14:CYS:HG	1.58	0.47
2:B:115:CYS:SG	2:B:147:PHE:CD2	3.04	0.47
2:E:244:PRO:HD3	2:E:364:VAL:O	2.15	0.47
2:E:393:ARG:HB2	2:E:396:GLN:HB2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:287:MET:HG2	2:B:531:ILE:HD13	1.95	0.47
2:E:378:ASP:OD1	2:E:541:THR:HB	2.15	0.47
2:E:406:LEU:HB3	2:E:415:LEU:HB2	1.97	0.46
2:E:114:ASN:ND2	2:E:116:GLU:H	2.12	0.46
2:B:308:LYS:NZ	10:B:611:MAN:C1	2.79	0.46
1:A:32:TRP:CE2	2:B:325:ALA:HB2	2.51	0.46
1:D:91:GLN:HB2	8:E:610:HEC:HMC3	1.97	0.46
2:E:221:CYS:CB	2:E:232:CYS:HG	2.29	0.45
2:E:221:CYS:SG	2:E:366:PHE:O	2.74	0.45
2:B:406:LEU:HB3	2:B:415:LEU:HB2	1.98	0.45
2:B:153:CYS:SG	2:B:156:SER:HB2	2.57	0.45
2:B:332:PHE:O	8:B:605:HEC:HAC	2.17	0.44
2:E:507:ARG:HD3	2:E:508:ASP:OD1	2.17	0.44
2:B:356:ASN:N	2:B:357:PRO:HD3	2.32	0.44
2:B:221:CYS:CB	2:B:232:CYS:HG	2.27	0.43
2:B:242:GLU:HG3	9:B:606:UEY:N5	2.33	0.43
8:E:610:HEC:HMC1	8:E:610:HEC:HBC2	1.99	0.43
2:B:150:CSO:SG	2:B:150:CSO:OD	2.77	0.43
2:B:333:ARG:HD3	2:B:421:ASN:ND2	2.34	0.42
1:A:83:SER:HB3	2:B:554:SER:O	2.18	0.42
2:B:241:SER:O	2:B:366:PHE:HA	2.19	0.42
2:B:507:ARG:HG3	2:B:513:TRP:CE2	2.54	0.42
1:D:92:LEU:HD22	2:E:249:MET:HB3	2.02	0.42
2:E:333:ARG:HD3	2:E:421:ASN:ND2	2.34	0.42
1:D:83:SER:HB3	2:E:554:SER:O	2.19	0.42
10:B:611:MAN:C2	4:F:1:BMA:O3	2.53	0.42
7:E:606:NAG:O4	7:E:607:NAG:H2	2.19	0.41
7:B:601:NAG:O4	7:B:602:NAG:H2	2.20	0.41
1:A:29:PHE:CZ	2:B:329:THR:HG21	2.56	0.41
8:B:605:HEC:HMC1	8:B:605:HEC:HBC2	2.01	0.41
2:B:336:HIS:CE1	2:B:417:LEU:HD21	2.56	0.41
1:A:22:LEU:HB3	2:B:322:PRO:HD2	2.03	0.41
2:B:169:SER:HB2	2:B:324:ILE:HG12	2.03	0.41
10:B:611:MAN:C1	4:F:1:BMA:C3	2.99	0.40
2:B:333:ARG:NH1	2:B:421:ASN:HD22	2.14	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	101/105 (96%)	99 (98%)	2 (2%)	0	100	100
1	D	101/105 (96%)	99 (98%)	2 (2%)	0	100	100
2	B	461/467 (99%)	449 (97%)	12 (3%)	0	100	100
2	E	462/467 (99%)	444 (96%)	17 (4%)	1 (0%)	47	54
All	All	1125/1144 (98%)	1091 (97%)	33 (3%)	1 (0%)	51	60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	354	GLU

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	86/90 (96%)	83 (96%)	3 (4%)	36	44
1	D	86/90 (96%)	84 (98%)	2 (2%)	50	62
2	B	401/411 (98%)	396 (99%)	5 (1%)	71	82
2	E	405/411 (98%)	399 (98%)	6 (2%)	65	76
All	All	978/1002 (98%)	962 (98%)	16 (2%)	62	75

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

Mol	Chain	Res	Type
1	A	42	SER
1	A	84	LEU
1	A	102	GLU
2	B	114	ASN
2	B	116	GLU
2	B	175	MET
2	B	270	ARG
2	B	547	SER
1	D	4	GLN
1	D	42	SER
2	E	114	ASN
2	E	159	THR
2	E	175	MET
2	E	356	ASN
2	E	507	ARG
2	E	547	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	121	GLN
2	B	421	ASN
2	B	563	ASN
2	E	114	ASN
2	E	121	GLN
2	E	421	ASN
2	E	563	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	E	150	2	3,6,7	0.48	0	0,6,8	0.00	-
2	CSO	B	150	2	3,6,7	0.90	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	E	150	2	-	0/1/5/7	-
2	CSO	B	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.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	150	CSO	1	0
2	B	150	CSO	1	0

5.5 Carbohydrates [i](#)

8 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	C	1	3,2	14,14,15	0.33	0	17,19,21	0.89	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	FUC	C	2	3	10,10,11	0.36	0	14,14,16	0.66	0
4	BMA	F	1	4	11,11,12	0.27	0	15,15,17	0.75	0
4	MAN	F	2	4	11,11,12	0.32	0	15,15,17	0.89	1 (6%)
4	BMA	G	1	4	11,11,12	0.25	0	15,15,17	0.81	0
4	MAN	G	2	4	11,11,12	0.30	0	15,15,17	0.93	1 (6%)
3	NAG	H	1	3,2	14,14,15	0.30	0	17,19,21	1.01	2 (11%)
3	FUC	H	2	3	10,10,11	0.36	0	14,14,16	0.62	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	C	1	3,2	-	0/6/23/26	0/1/1/1
3	FUC	C	2	3	-	-	0/1/1/1
4	BMA	F	1	4	-	0/2/19/22	0/1/1/1
4	MAN	F	2	4	-	0/2/19/22	0/1/1/1
4	BMA	G	1	4	-	0/2/19/22	0/1/1/1
4	MAN	G	2	4	-	0/2/19/22	0/1/1/1
3	NAG	H	1	3,2	-	0/6/23/26	0/1/1/1
3	FUC	H	2	3	-	-	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	2	MAN	C1-O5-C5	3.30	116.66	112.19
4	F	2	MAN	C1-O5-C5	3.06	116.34	112.19
3	H	1	NAG	O4-C4-C3	-2.68	104.16	110.35
3	C	1	NAG	O4-C4-C3	-2.37	104.88	110.35
3	C	1	NAG	O5-C1-C2	-2.33	107.61	111.29
3	H	1	NAG	O5-C1-C2	-2.23	107.77	111.29

There are no chirality outliers.

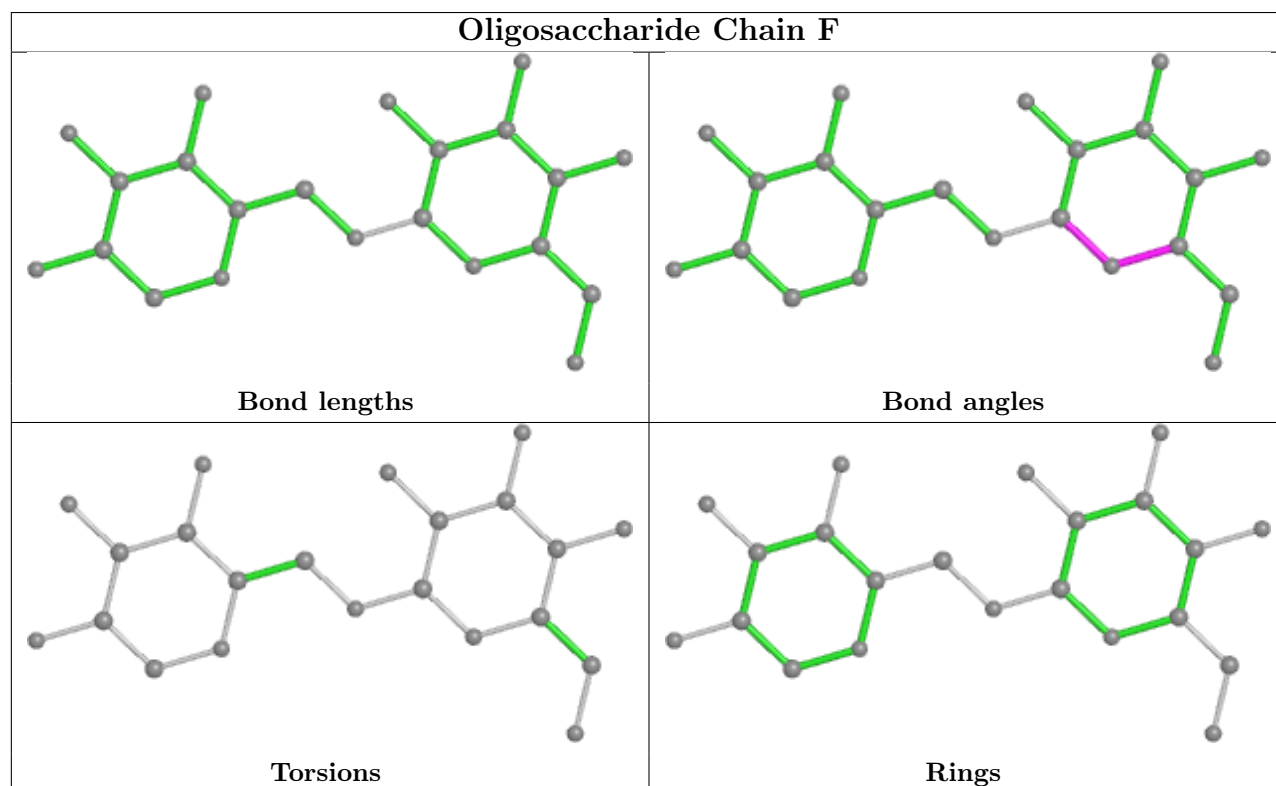
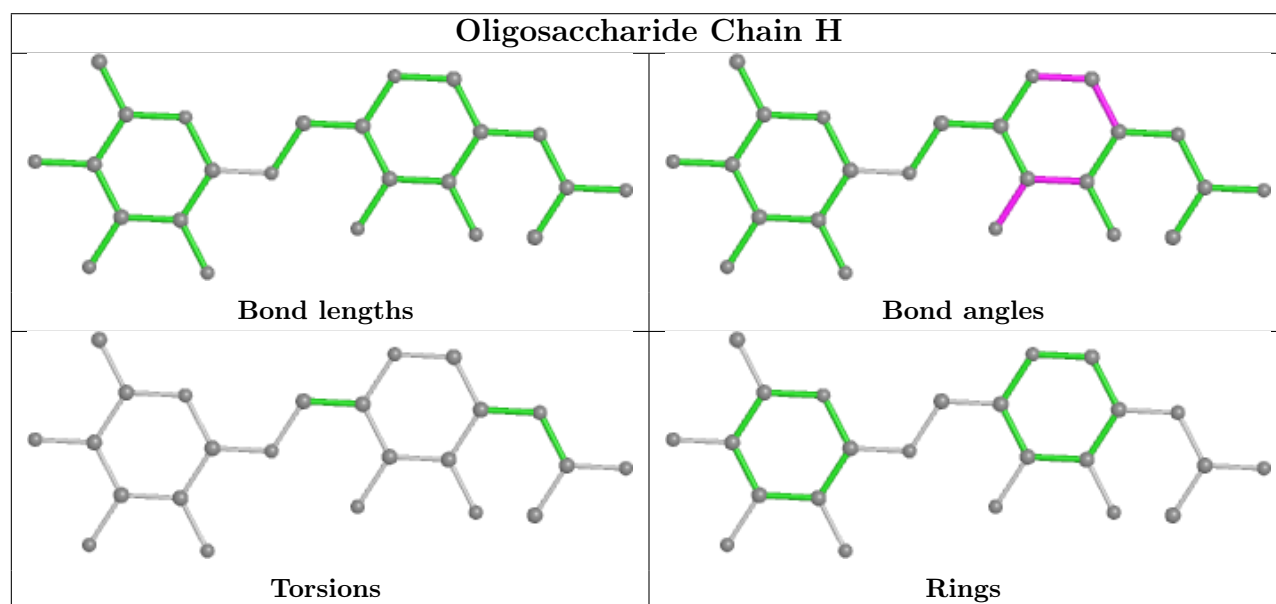
There are no torsion outliers.

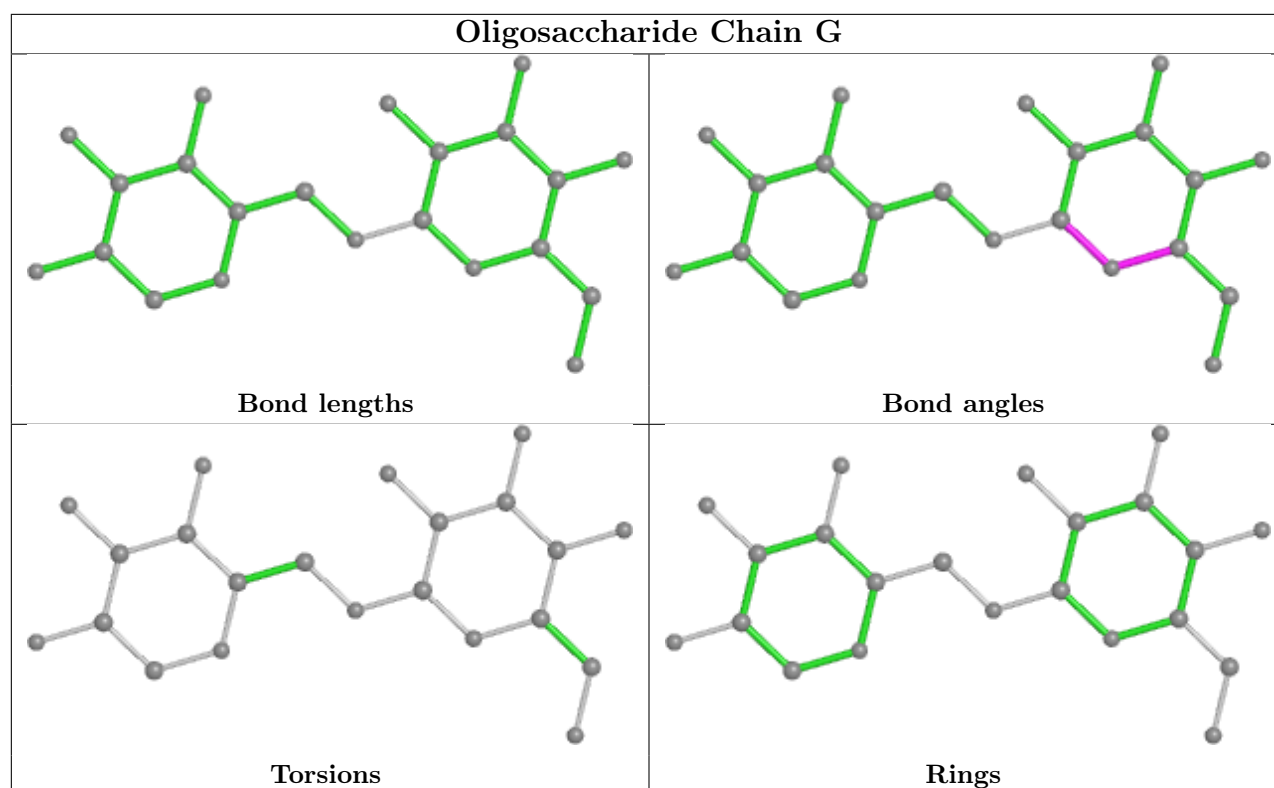
There are no ring outliers.

4 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	1	NAG	2	0
4	F	1	BMA	6	0
4	G	1	BMA	5	0
3	C	1	NAG	2	0

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





5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 6 are monoatomic - leaving 14 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	$\# Z > 2$
10	MAN	E	604	-	11,11,12	0.26	0	15,15,17	0.48	0
7	NAG	B	608	-	14,14,15	0.34	0	17,19,21	0.59	0
9	UEY	E	611	-	25,27,27	0.70	0	26,37,37	0.92	3 (11%)
7	NAG	B	607	2	14,14,15	0.34	0	17,19,21	0.58	0
8	HEC	E	610	2	26,50,50	2.18	5 (19%)	18,82,82	2.31	7 (38%)
7	NAG	E	606	2	14,14,15	0.31	0	17,19,21	0.56	0
8	HEC	B	605	2	26,50,50	2.19	6 (23%)	18,82,82	1.93	6 (33%)
7	NAG	E	601	-	14,14,15	0.33	0	17,19,21	0.68	0
9	UEY	B	606	-	25,27,27	0.71	1 (4%)	26,37,37	0.77	2 (7%)
7	NAG	E	605	2	14,14,15	0.32	0	17,19,21	0.69	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	B	601	2	14,14,15	0.28	0	17,19,21	0.59	0
10	MAN	B	611	-	11,11,12	0.54	0	15,15,17	1.14	2 (13%)
7	NAG	B	602	-	14,14,15	0.30	0	17,19,21	1.21	3 (17%)
7	NAG	E	607	-	14,14,15	0.29	0	17,19,21	1.18	3 (17%)

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
10	MAN	E	604	-	-	1/2/19/22	0/1/1/1
7	NAG	B	608	-	-	0/6/23/26	0/1/1/1
9	UEY	E	611	-	-	2/12/12/12	0/4/4/4
7	NAG	B	607	2	-	0/6/23/26	0/1/1/1
8	HEC	E	610	2	-	0/6/54/54	-
7	NAG	E	606	2	-	2/6/23/26	0/1/1/1
8	HEC	B	605	2	-	0/6/54/54	-
7	NAG	E	601	-	-	0/6/23/26	0/1/1/1
9	UEY	B	606	-	-	0/12/12/12	0/4/4/4
7	NAG	E	605	2	-	0/6/23/26	0/1/1/1
7	NAG	B	601	2	-	2/6/23/26	0/1/1/1
10	MAN	B	611	-	-	1/2/19/22	0/1/1/1
7	NAG	B	602	-	-	0/6/23/26	0/1/1/1
7	NAG	E	607	-	-	0/6/23/26	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	605	HEC	C3B-C2B	-8.18	1.32	1.40
8	E	610	HEC	C3B-C2B	-7.83	1.32	1.40
8	E	610	HEC	CBB-CAB	-3.94	1.34	1.49
8	E	610	HEC	CBC-CAC	-3.85	1.35	1.49
8	B	605	HEC	CBB-CAB	-3.63	1.35	1.49
8	B	605	HEC	CBC-CAC	-3.52	1.36	1.49
8	E	610	HEC	C3C-C2C	-3.21	1.37	1.40
8	B	605	HEC	C3D-C2D	-2.67	1.29	1.37
8	E	610	HEC	C3B-C4B	2.28	1.47	1.43
8	B	605	HEC	C1C-NC	2.17	1.40	1.36
8	B	605	HEC	C3B-C4B	2.08	1.46	1.43
9	B	606	UEY	C2-N1	2.03	1.36	1.33

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	E	610	HEC	CAA-CBA-CGA	4.80	120.72	112.67
8	E	610	HEC	CMC-C2C-C3C	4.05	130.58	125.82
8	E	610	HEC	CMC-C2C-C1C	-4.01	122.30	128.46
8	B	605	HEC	CMC-C2C-C1C	-3.71	122.77	128.46
8	B	605	HEC	CMC-C2C-C3C	3.69	130.16	125.82
8	E	610	HEC	CBA-CAA-C2A	-3.54	105.96	112.48
7	E	607	NAG	O5-C1-C2	-3.45	105.83	111.29
8	B	605	HEC	CBA-CAA-C2A	-3.35	106.30	112.48
7	B	602	NAG	O5-C1-C2	-3.35	106.00	111.29
8	B	605	HEC	CBD-CAD-C3D	-3.35	106.31	112.49
8	E	610	HEC	CMA-C3A-C2A	2.91	130.43	124.94
8	E	610	HEC	CBD-CAD-C3D	-2.85	107.22	112.49
10	B	611	MAN	C1-C2-C3	2.80	113.10	109.67
10	B	611	MAN	C1-O5-C5	2.66	115.80	112.19
8	B	605	HEC	CAA-CBA-CGA	2.63	117.09	112.67
7	E	605	NAG	C1-O5-C5	2.55	115.64	112.19
7	B	602	NAG	C1-C2-N2	2.54	114.82	110.49
7	E	607	NAG	C1-C2-N2	2.38	114.55	110.49
7	B	602	NAG	C1-O5-C5	2.32	115.33	112.19
8	E	610	HEC	CMD-C2D-C1D	-2.30	124.93	128.46
9	E	611	UEY	N2-C2-N1	-2.25	116.39	118.26
9	B	606	UEY	N2-C2-N1	-2.18	116.45	118.26
8	B	605	HEC	CMA-C3A-C2A	2.17	129.03	124.94
7	E	607	NAG	C1-O5-C5	2.14	115.09	112.19
9	E	611	UEY	C2-N1-C3	-2.09	116.02	119.22
9	B	606	UEY	N5-N4-N3	-2.07	108.56	111.25
9	E	611	UEY	N5-N4-N3	-2.03	108.61	111.25

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	601	NAG	C4-C5-C6-O6
7	E	606	NAG	C4-C5-C6-O6
7	B	601	NAG	O5-C5-C6-O6
9	E	611	UEY	C6-C8-C9-C10
10	E	604	MAN	O5-C5-C6-O6
7	E	606	NAG	O5-C5-C6-O6
10	B	611	MAN	O5-C5-C6-O6
9	E	611	UEY	C6-C8-C9-C14

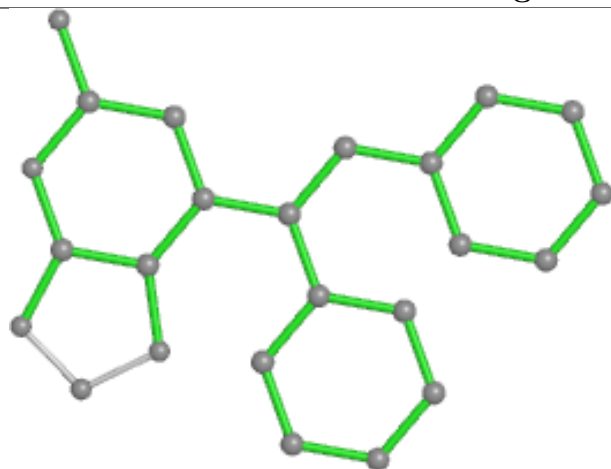
There are no ring outliers.

11 monomers are involved in 40 short contacts:

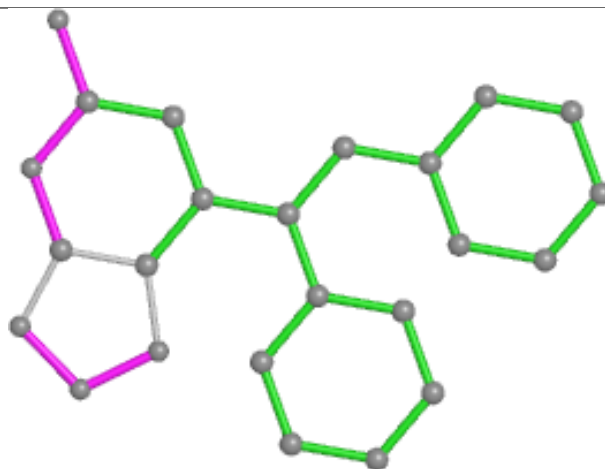
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	E	604	MAN	4	0
7	B	608	NAG	4	0
8	E	610	HEC	9	0
7	E	606	NAG	1	0
8	B	605	HEC	8	0
7	E	601	NAG	5	0
9	B	606	UEY	1	0
7	B	601	NAG	1	0
10	B	611	MAN	7	0
7	B	602	NAG	1	0
7	E	607	NAG	1	0

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

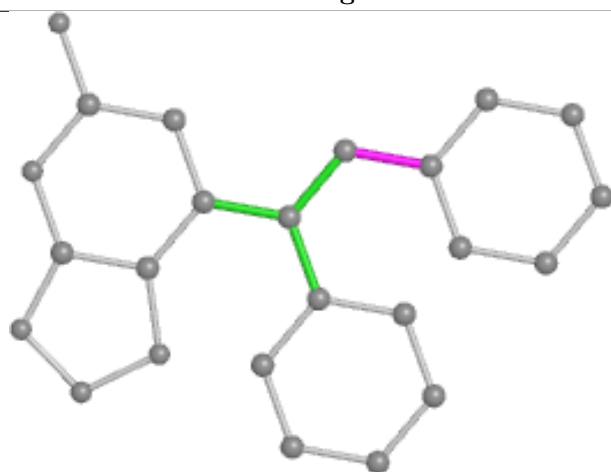
Ligand UEY E 611



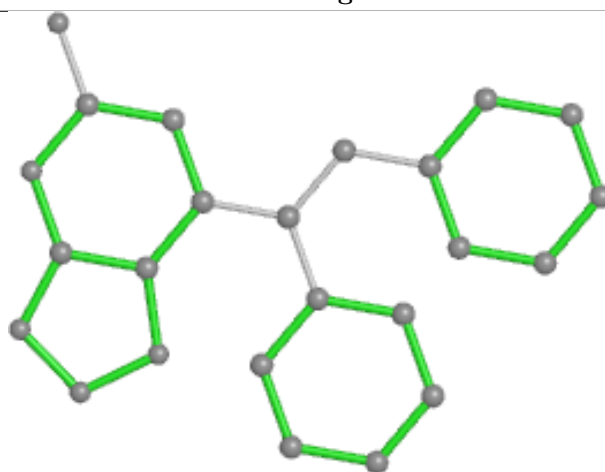
Bond lengths



Bond angles

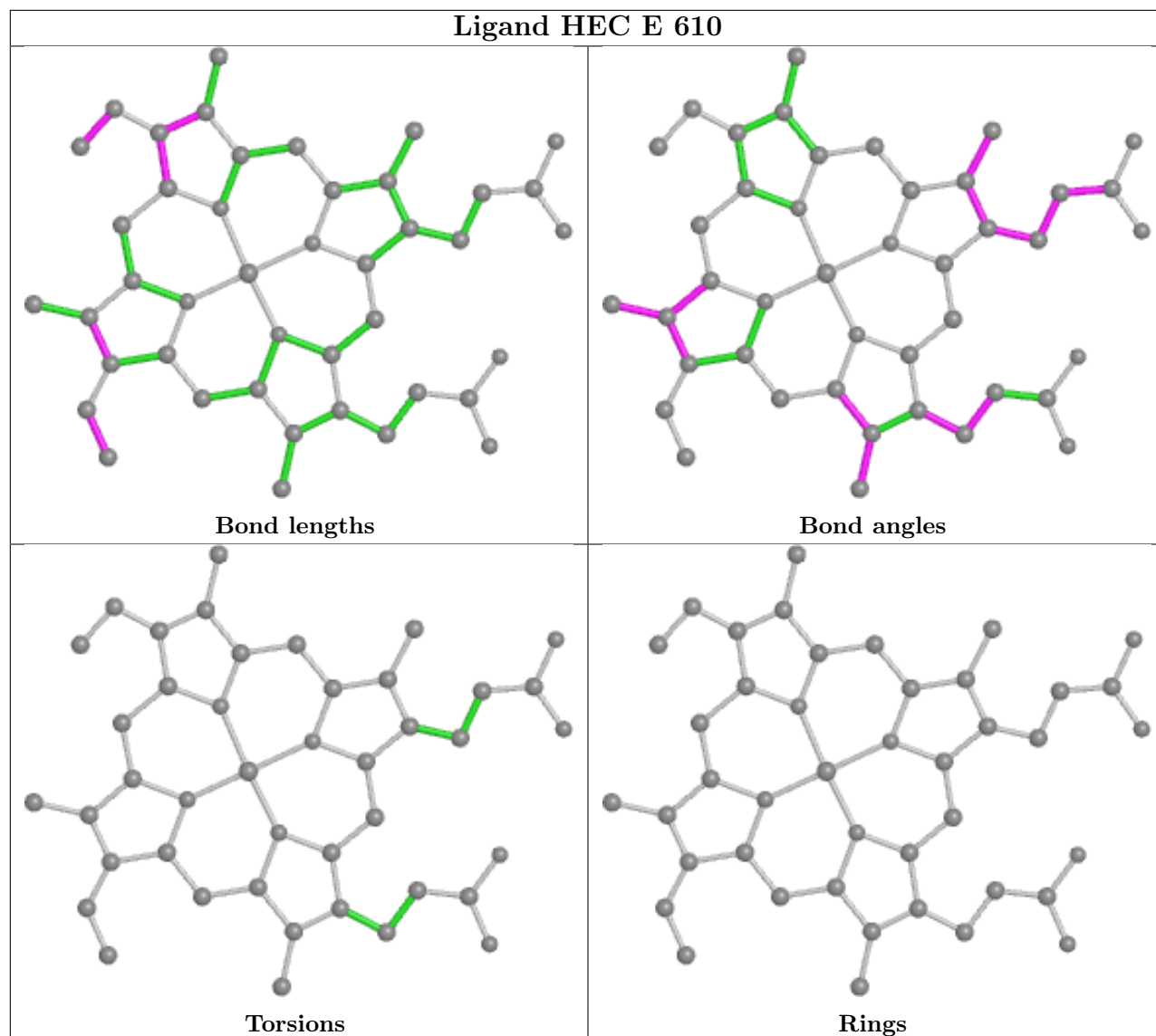


Torsions

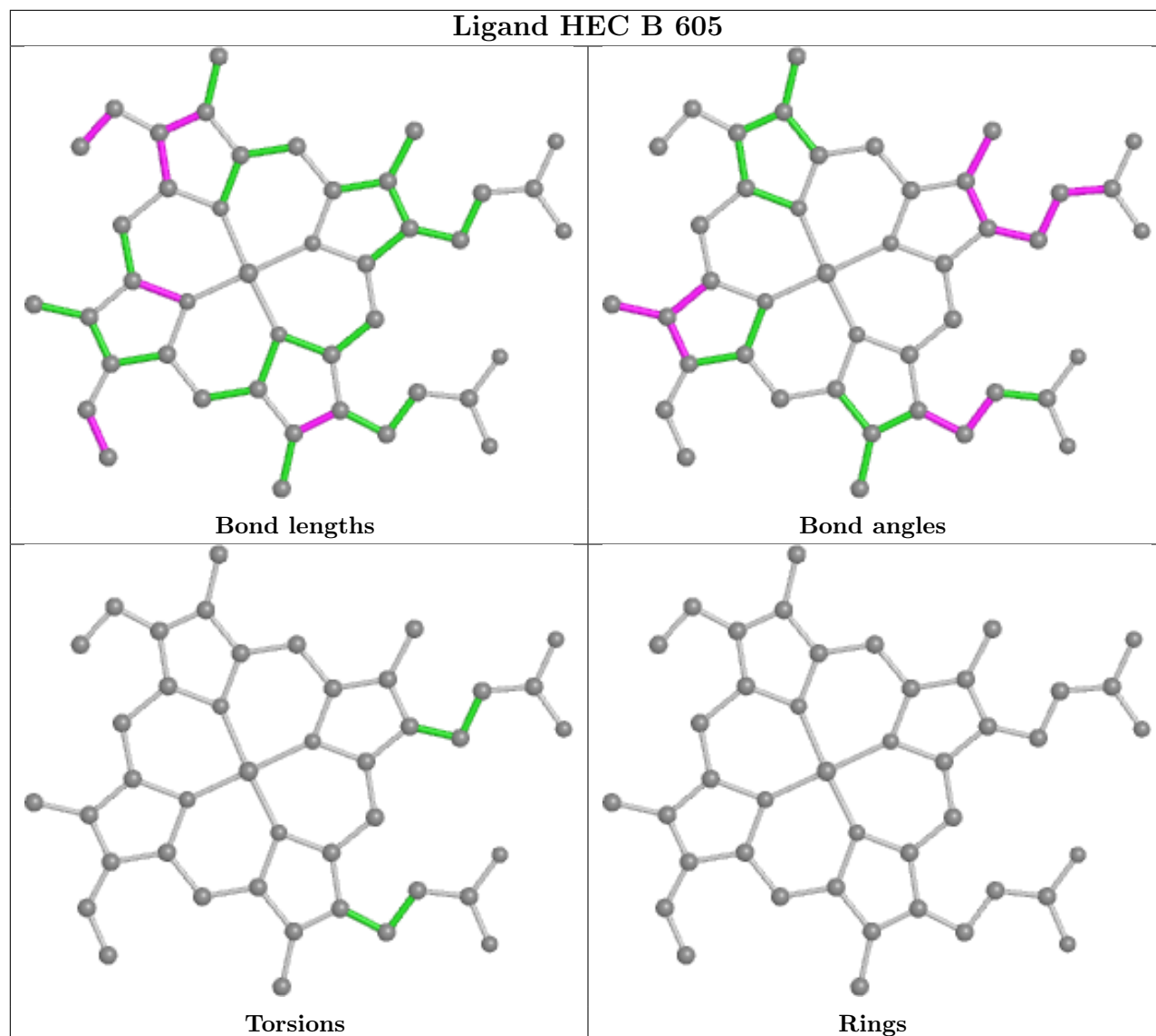


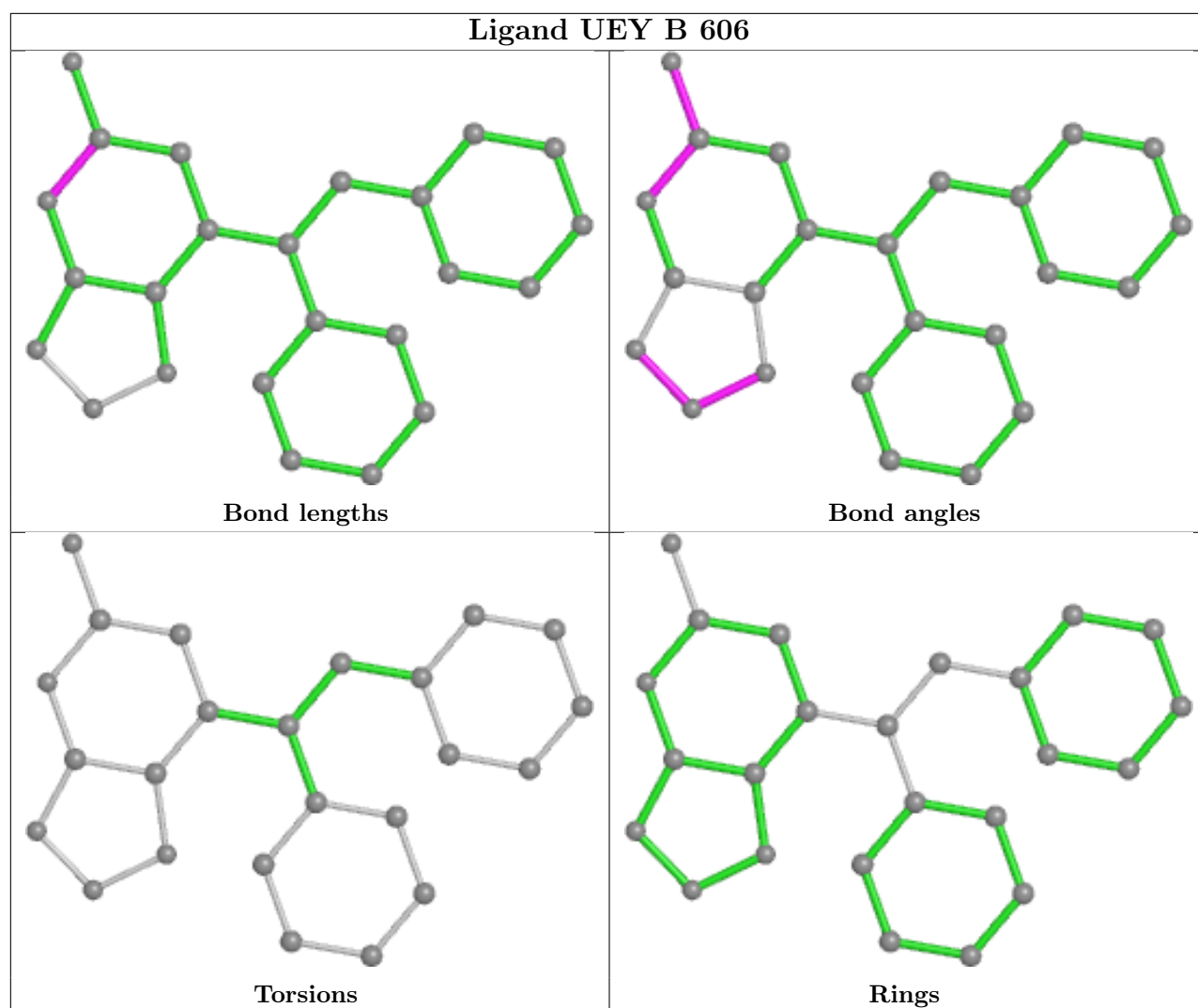
Rings

Ligand HEC E 610



Ligand HEC B 605





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	103/105 (98%)	0.17	2 (1%) 66 65	38, 50, 79, 82	0
1	D	103/105 (98%)	-0.06	0 100 100	35, 50, 71, 76	0
2	B	463/467 (99%)	0.24	8 (1%) 70 68	37, 62, 89, 102	5 (1%)
2	E	464/467 (99%)	-0.03	0 100 100	34, 56, 77, 100	10 (2%)
All	All	1133/1144 (99%)	0.10	10 (0%) 84 83	34, 57, 81, 102	15 (1%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	381	LEU	3.3
2	B	253	LEU	3.2
2	B	402	ILE	2.8
2	B	418	PRO	2.4
2	B	541	THR	2.4
1	A	84	LEU	2.3
2	B	331	ALA	2.3
2	B	264	LEU	2.2
1	A	93	LEU	2.2
2	B	570	LEU	2.0

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.

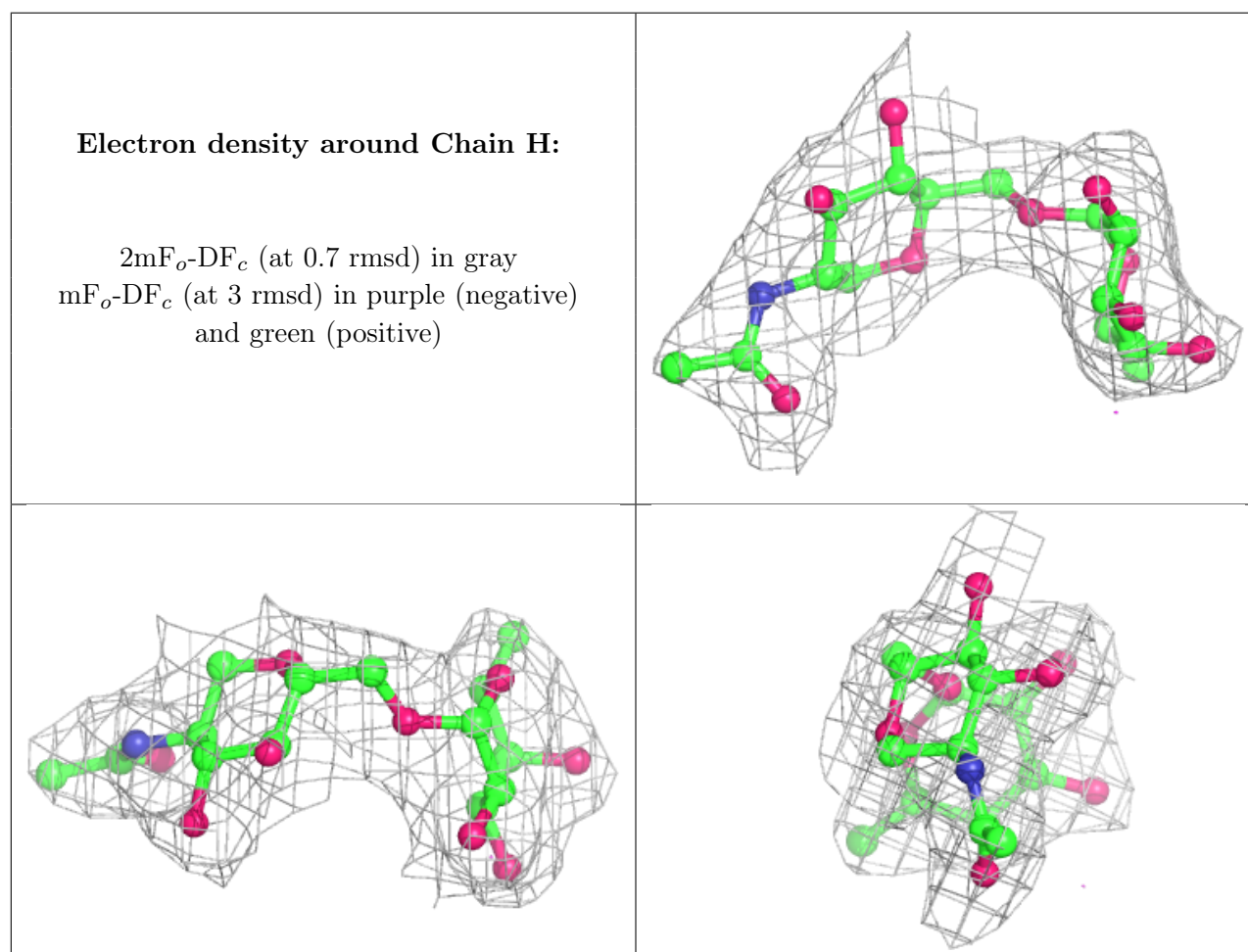
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	CSO	B	150	7/8	0.89	0.17	41,41,49,90	0
2	CSO	E	150	7/8	0.95	0.17	39,39,40,46	0

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.

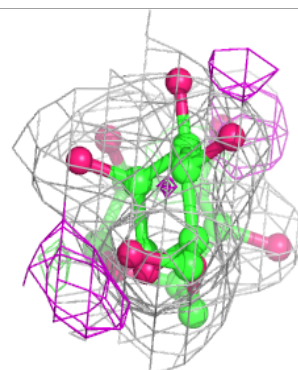
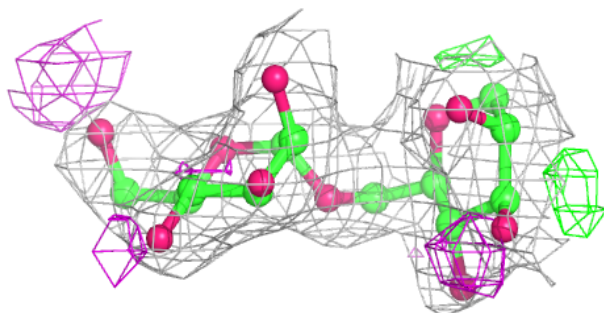
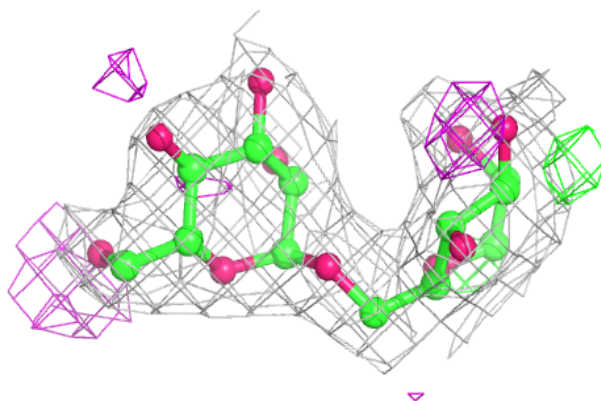
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	BMA	F	1	11/12	0.79	0.16	61,64,66,67	0
4	MAN	F	2	11/12	0.91	0.16	58,59,60,60	0
4	BMA	G	1	11/12	0.91	0.14	59,59,59,60	0
3	FUC	C	2	10/11	0.94	0.12	52,53,53,54	0
3	NAG	C	1	14/15	0.94	0.15	54,56,58,59	0
4	MAN	G	2	11/12	0.95	0.11	50,51,51,51	0
3	FUC	H	2	10/11	0.95	0.13	53,54,55,55	0
3	NAG	H	1	14/15	0.96	0.12	46,47,49,50	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.

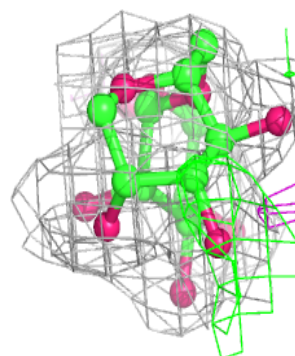
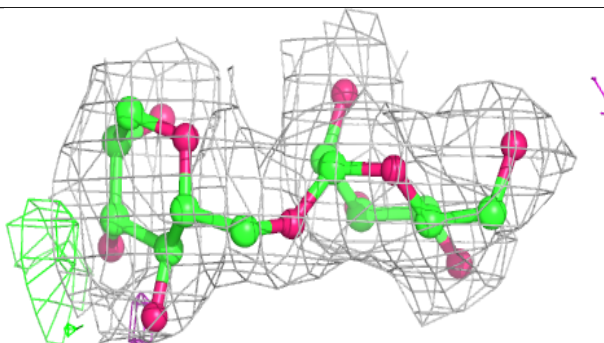
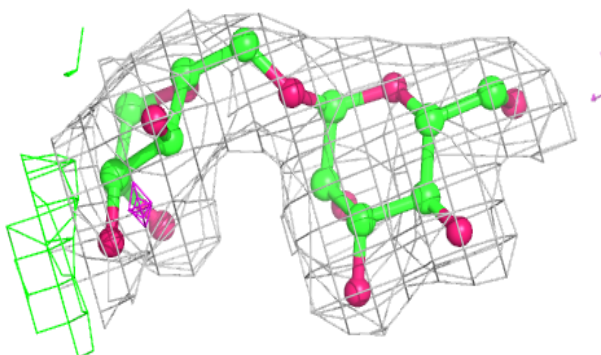


Electron density around Chain F:

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

**Electron density around Chain G:**

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



6.4 Ligands ⓘ

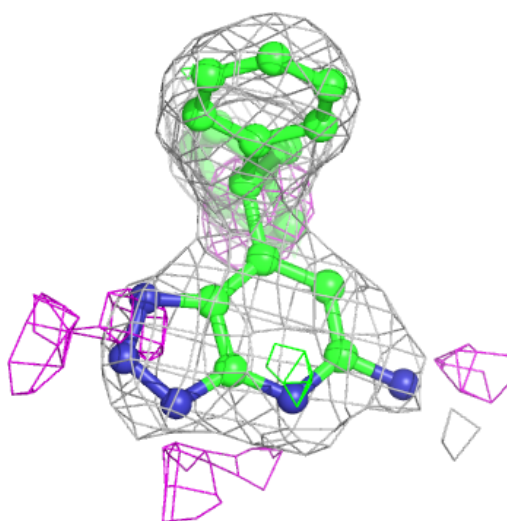
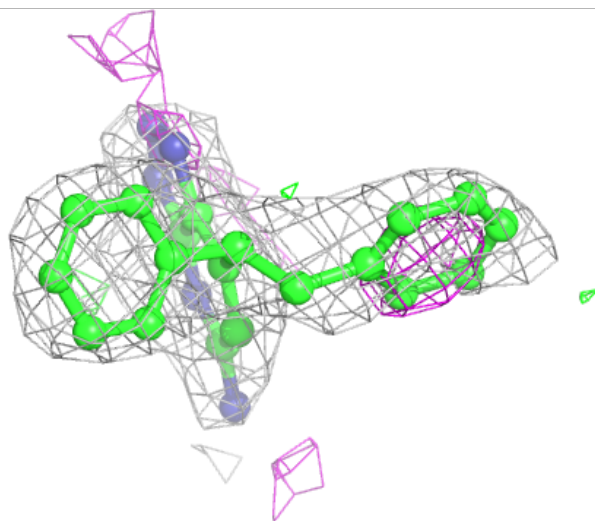
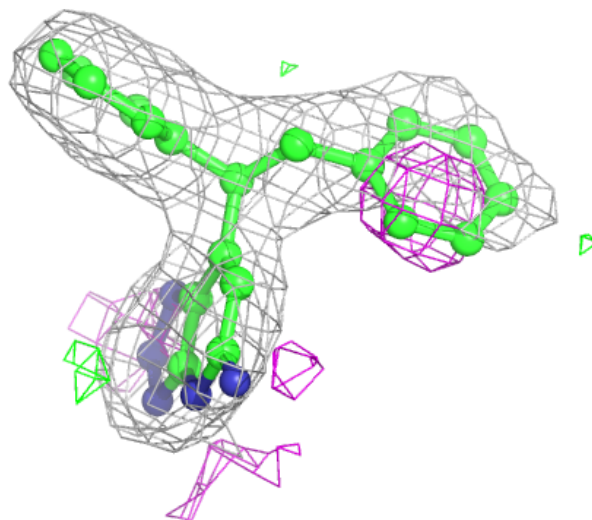
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
10	MAN	E	604	11/12	0.57	0.28	138,138,139,139	0
7	NAG	B	602	14/15	0.66	0.18	118,118,118,119	0
7	NAG	B	607	14/15	0.71	0.22	78,80,81,82	0
7	NAG	B	601	14/15	0.78	0.15	84,85,86,86	0
9	UEY	B	606	24/24	0.84	0.25	54,56,58,58	0
5	CL	B	612	1/1	0.86	0.27	76,76,76,76	0
7	NAG	E	605	14/15	0.86	0.13	67,72,73,74	0
10	MAN	B	611	11/12	0.87	0.16	97,98,98,99	0
7	NAG	E	607	14/15	0.87	0.18	110,112,113,113	0
7	NAG	E	606	14/15	0.88	0.17	81,83,84,85	0
9	UEY	E	611	24/24	0.94	0.22	44,47,57,57	0
8	HEC	B	605	43/43	0.94	0.20	45,49,50,52	0
7	NAG	E	601	14/15	0.95	0.14	45,49,51,52	0
5	CL	E	612	1/1	0.96	0.34	67,67,67,67	0
7	NAG	B	608	14/15	0.96	0.14	46,49,49,50	0
6	CA	D	202	1/1	0.96	0.11	38,38,38,38	0
8	HEC	E	610	43/43	0.97	0.15	40,45,47,49	0
5	CL	A	201	1/1	0.97	0.09	38,38,38,38	0
5	CL	D	201	1/1	0.98	0.10	36,36,36,36	0
6	CA	A	202	1/1	0.99	0.11	50,50,50,50	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.

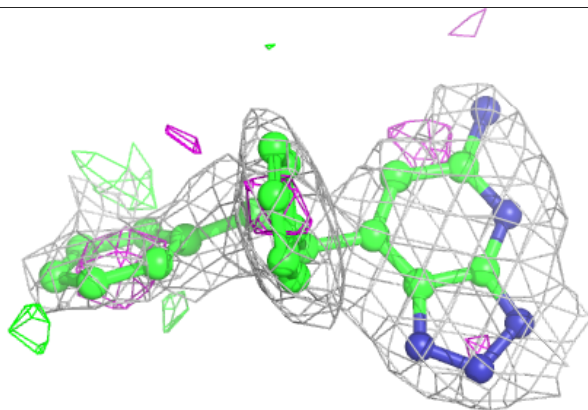
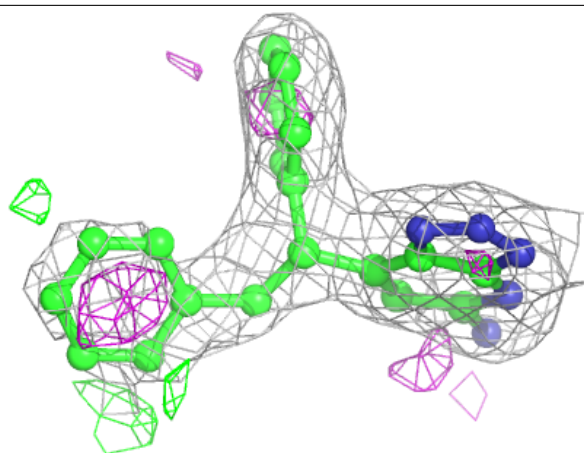
Electron density around UEY B 606:

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



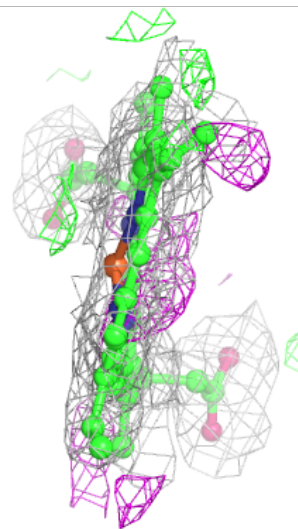
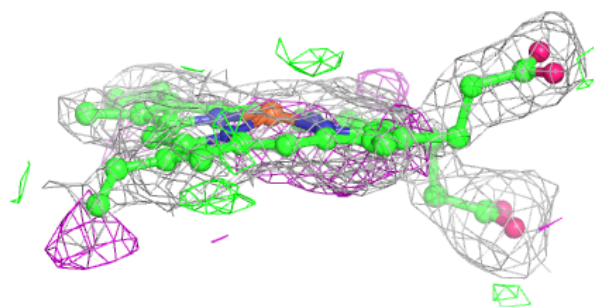
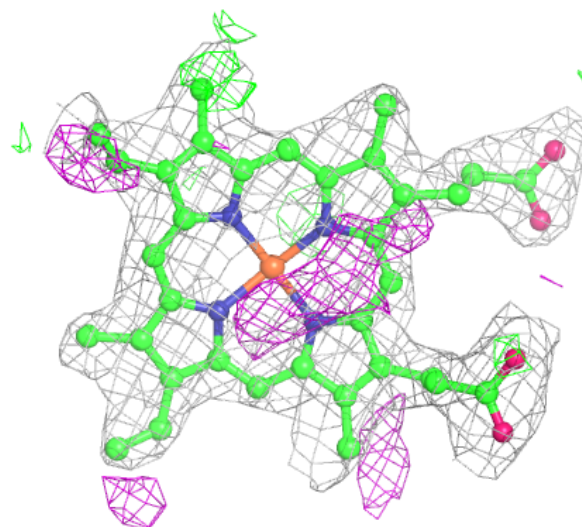
Electron density around UEY E 611:

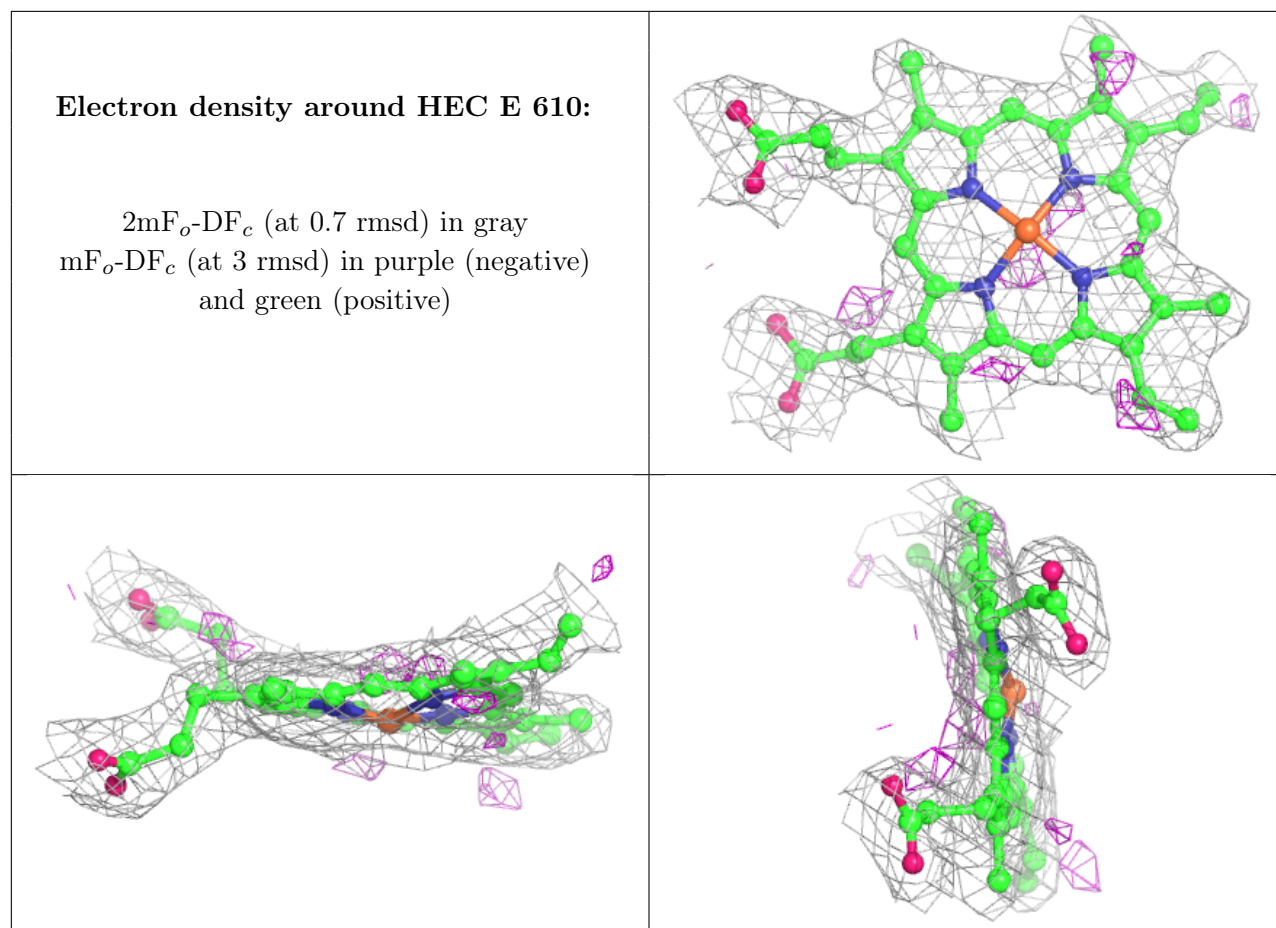
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEC 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 [i](#)

There are no such residues in this entry.