



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 15, 2024 – 08:43 PM EST

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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

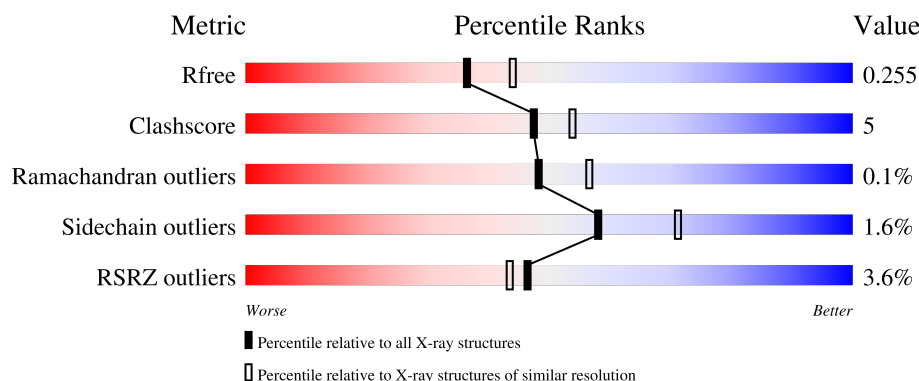
1 Overall quality at a glance

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.





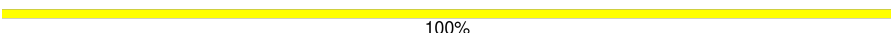
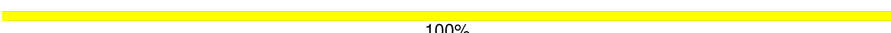
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	7167 (2.24-2.20)
Clashscore	180529	8096 (2.24-2.20)
Ramachandran outliers	177936	8010 (2.24-2.20)
Sidechain outliers	177891	8011 (2.24-2.20)
RSRZ outliers	164620	7166 (2.24-2.20)

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 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 $\leq 5\%$. 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	<div> <div>5%</div> <div> <div></div> <div>89%</div> <div>10%</div> <div></div> </div> </div>
1	D	105	<div> <div></div> <div>90%</div> <div>9%</div> <div></div> </div>
2	B	467	<div> <div>6%</div> <div> <div></div> <div>89%</div> <div>10%</div> <div></div> </div> </div>
2	E	467	<div> <div>2%</div> <div> <div></div> <div>91%</div> <div>8%</div> <div></div> </div> </div>

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Mol	Chain	Length	Quality of chain
3	C	2	 50% 50%
3	H	2	 50% 50%
4	F	2	 100%
4	G	2	 100%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	MAN	B	608	-	-	X	-
4	BMA	F	1	-	-	X	-

2 Entry composition [i](#)

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			

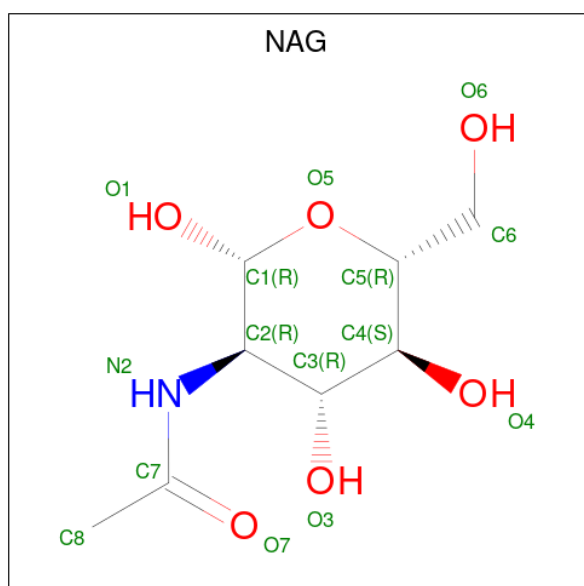
- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Cl	0	0
			1	1		
5	B	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).

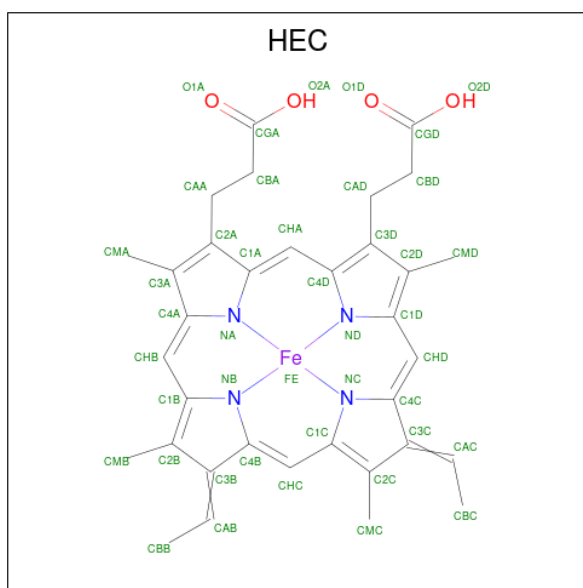
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Ca	0	0
			1	1		
6	E	1	Total	Ca	0	0
			1	1		

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



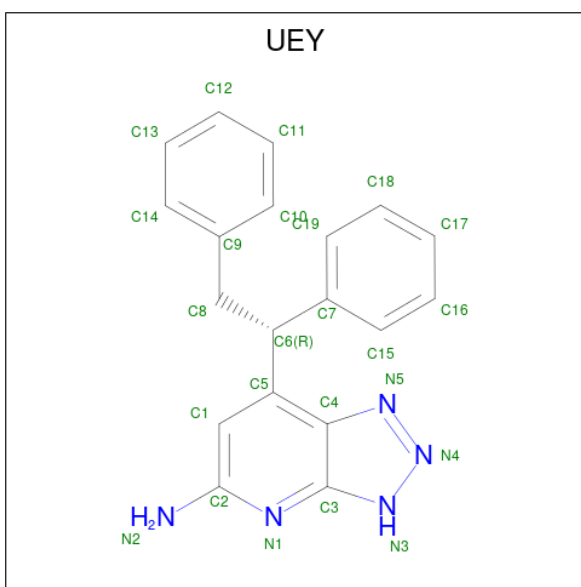
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	N	O	0	0
			14	8	1	5		
7	B	1	Total	C	N	O	0	0
			14	8	1	5		
7	B	1	Total	C	N	O	0	0
			14	8	1	5		
7	B	1	Total	C	N	O	0	0
			14	8	1	5		
7	E	1	Total	C	N	O	0	0
			14	8	1	5		
7	E	1	Total	C	N	O	0	0
			14	8	1	5		
7	E	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 8 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



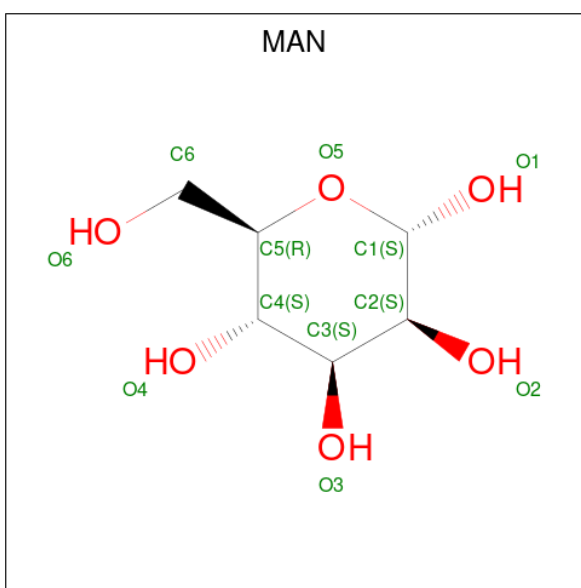
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	B	1	Total	C	Fe	N	O	0
			43	34	1	4	4	0
8	E	1	Total	C	Fe	N	O	0
			43	34	1	4	4	0

- Molecule 9 is 7-[(1R)-1,2-diphenylethyl]-3H-[1,2,3]triazolo[4,5-b]pyridin-5-amine (three-letter code: UEY) (formula: $C_{19}H_{17}N_5$) (labeled as "Ligand of Interest" by depositor).



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		

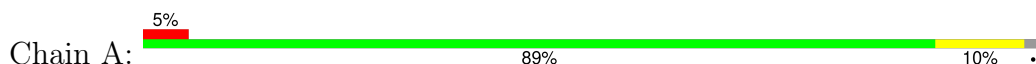
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	55	Total 55	O 55	0	0
11	B	156	Total 156	O 156	0	0
11	D	51	Total 51	O 51	0	0
11	E	170	Total 170	O 170	0	0

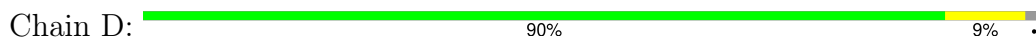
3 Residue-property plots [i](#)

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.

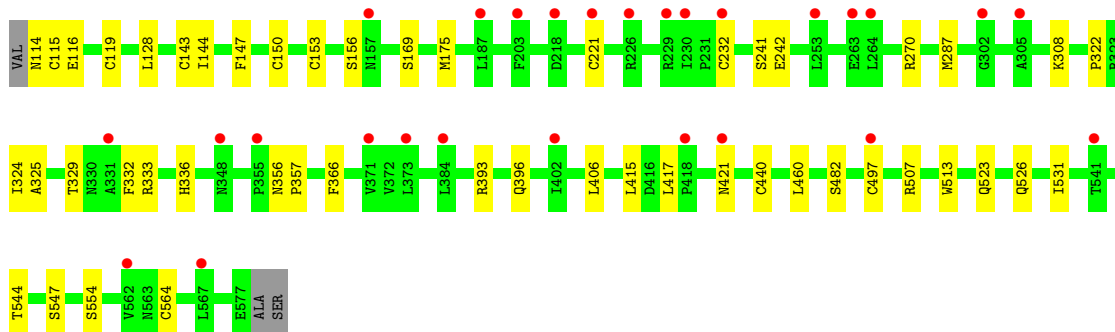
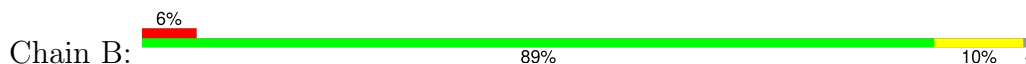
- Molecule 1: Myeloperoxidase light chain



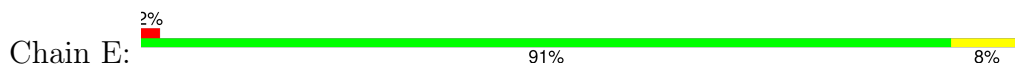
- Molecule 1: Myeloperoxidase light chain

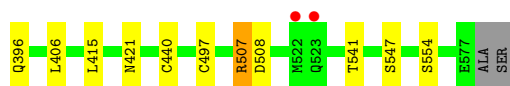


- Molecule 2: Myeloperoxidase heavy chain



- Molecule 2: Myeloperoxidase heavy chain





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

Chain C: 50% 50%



- 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)	Xtrriage
Refinement program	BUSTER 2.11.7 (17-DEC-2019)	Depositor
R, R_{free}	0.211 , 0.242 0.221 , 0.255	Depositor DCC
R_{free} test set	3514 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	42.6	Xtrriage
Anisotropy	0.548	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 61.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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: CL, UEY, MAN, BMA, CA, CSO, HEC, NAG, FUC

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	B	1	0	0	0	0
6	E	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	156	0	0	1	0
11	D	51	0	0	0	0
11	E	170	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:607:HEC:CMD	1.76	1.31
2:E:242:GLU:OE2	8:E:607:HEC:HMB3	1.31	1.28
1:A:94:ASP:OD2	8:B:604:HEC:HMD3	1.04	1.20
7:B:607:NAG:O4	4:F:1:BMA:C1	1.90	1.19
1:A:94:ASP:OD2	8:B:604:HEC:CMD	1.99	1.09
2:B:242:GLU:OE2	8:B:604:HEC:HMB3	1.57	1.04
7:E:602:NAG:O4	4:G:1:BMA:C1	2.06	1.03
1:D:94:ASP:CG	8:E:607:HEC:HMD3	1.81	1.01
1:D:94:ASP:OD2	8:E:607:HEC:HMD3	0.81	0.98
7:E:602: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:607:NAG:C1	3:H:1:NAG:O4	2.15	0.94
10:B:608:MAN:H2	4:F:1:BMA:O3	1.69	0.92
2:E:242:GLU:OE2	8:E:607: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:607: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:604:HEC:HMD3	2.06	0.70
2:B:119:CYS:HG	2:B:143:CYS:HG	1.33	0.69
7:E:602: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:SG	2:E:150:CSO:OD	2.55	0.64
1:D:90:GLY:C	8:E:607:HEC:HBC3	2.19	0.63
1:A:90:GLY:C	8:B:604:HEC:HBC3	2.21	0.61
2:B:308:LYS:HZ1	10:B:608:MAN:H62	1.65	0.60
2:E:308:LYS:HZ1	10:E:603:MAN:C1	2.16	0.59
10:E:603:MAN:H5	4:G:1:BMA:H2	1.85	0.58
5:B:609:CL:CL	11:B:764:HOH:O	2.54	0.57
10:E:603:MAN:H3	4:G:1:BMA:O3	2.04	0.57
10:B:608:MAN:C1	4:F:1:BMA:H3	2.36	0.55
7:B:607:NAG:C1	3:H:1:NAG:C4	2.84	0.55
7:E:602: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:603:MAN:C1	2.71	0.54
2:B:544:THR:HA	2:B:564:CYS:SG	2.48	0.53
7:E:602: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:607: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:604:HEC:HMC3	1.95	0.48
2:B:308:LYS:HZ1	10:B:608: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
1:A:32:TRP:CE2	2:B:325:ALA:HB2	2.51	0.46
2:B:308:LYS:NZ	10:B:608:MAN:C1	2.79	0.46
1:D:91:GLN:HB2	8:E:607: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:604: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:605:UEY:N5	2.33	0.43
8:E:607:HEC:HBC2	8:E:607:HEC:HMC1	1.99	0.43
2:B:150:CSO:OD	2:B:150:CSO:SG	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
10:B:608:MAN:C2	4:F:1:BMA:O3	2.53	0.42
1:D:83:SER:HB3	2:E:554:SER:O	2.19	0.42
7:E:605:NAG:O4	7:E:606:NAG:H2	2.19	0.41
7:B:602:NAG:O4	7:B:603:NAG:H2	2.20	0.41
1:A:29:PHE:CZ	2:B:329:THR:HG21	2.56	0.41
8:B:604:HEC:HMC1	8:B:604: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:608: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%)	44	51
All	All	1125/1144 (98%)	1091 (97%)	33 (3%)	1 (0%)	48	56

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%)	31	39
1	D	86/90 (96%)	84 (98%)	2 (2%)	45	57
2	B	401/411 (98%)	396 (99%)	5 (1%)	67	79
2	E	405/411 (98%)	399 (98%)	6 (2%)	60	73
All	All	978/1002 (98%)	962 (98%)	16 (2%)	58	71

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

Sometimes 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	0.49	0	1,6,8	0.32	0
2	CSO	B	150	2	3,6,7	0.94	0	1,6,8	0.40	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	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	0.34	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	0.37	0	14,14,16	0.61	0
4	BMA	F	1	4	11,11,12	0.27	0	15,15,17	0.70	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	0.73	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	0.37	0	14,14,16	0.58	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	3.34	116.66	112.19
4	F	2	MAN	C1-O5-C5	3.10	116.34	112.19
3	H	1	NAG	O4-C4-C3	-2.64	104.16	110.38
3	C	1	NAG	O5-C1-C2	-2.38	107.61	111.29
3	C	1	NAG	O4-C4-C3	-2.33	104.88	110.38
3	H	1	NAG	O5-C1-C2	-2.28	107.77	111.29

There are no chirality outliers.

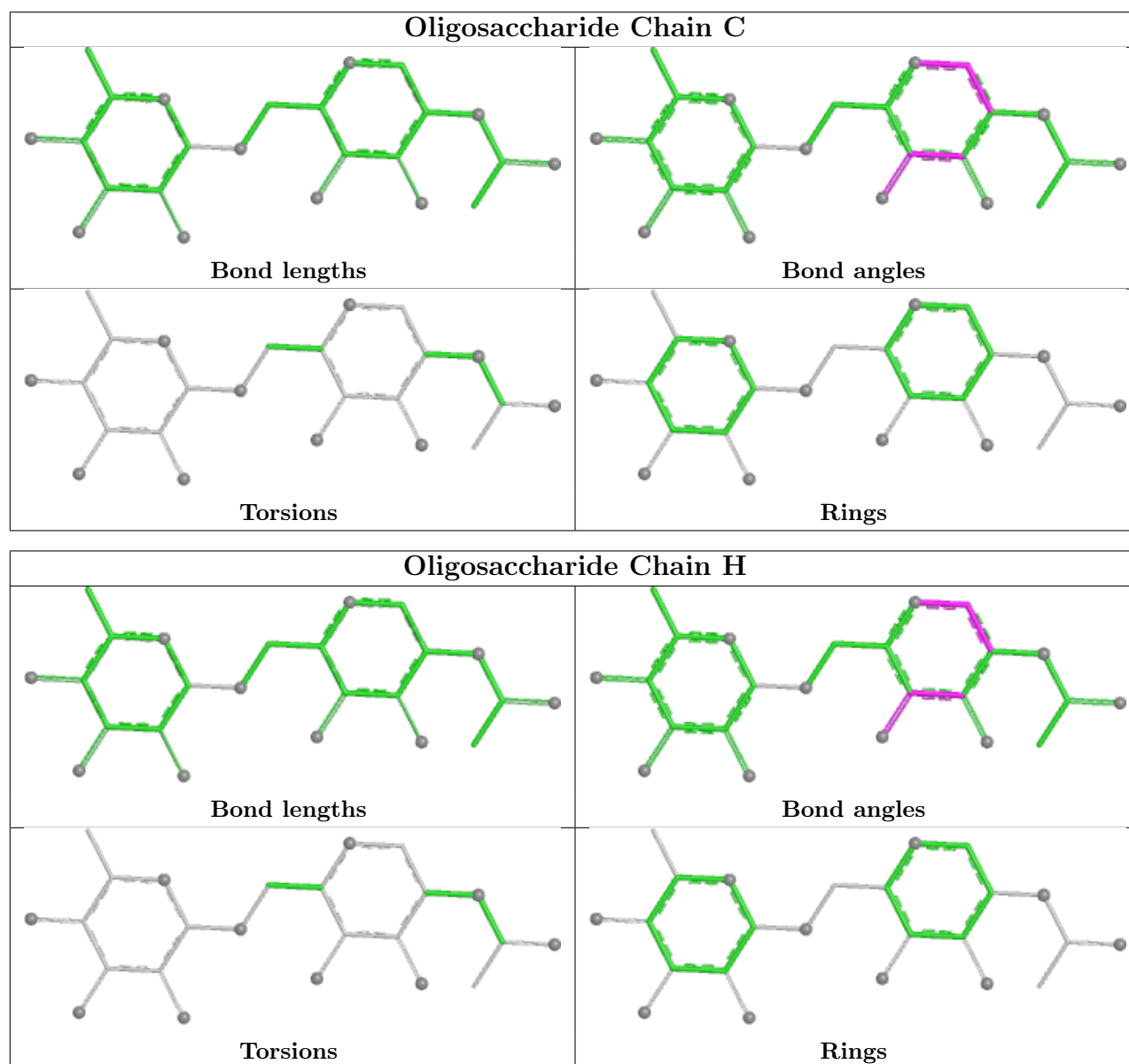
There are no torsion outliers.

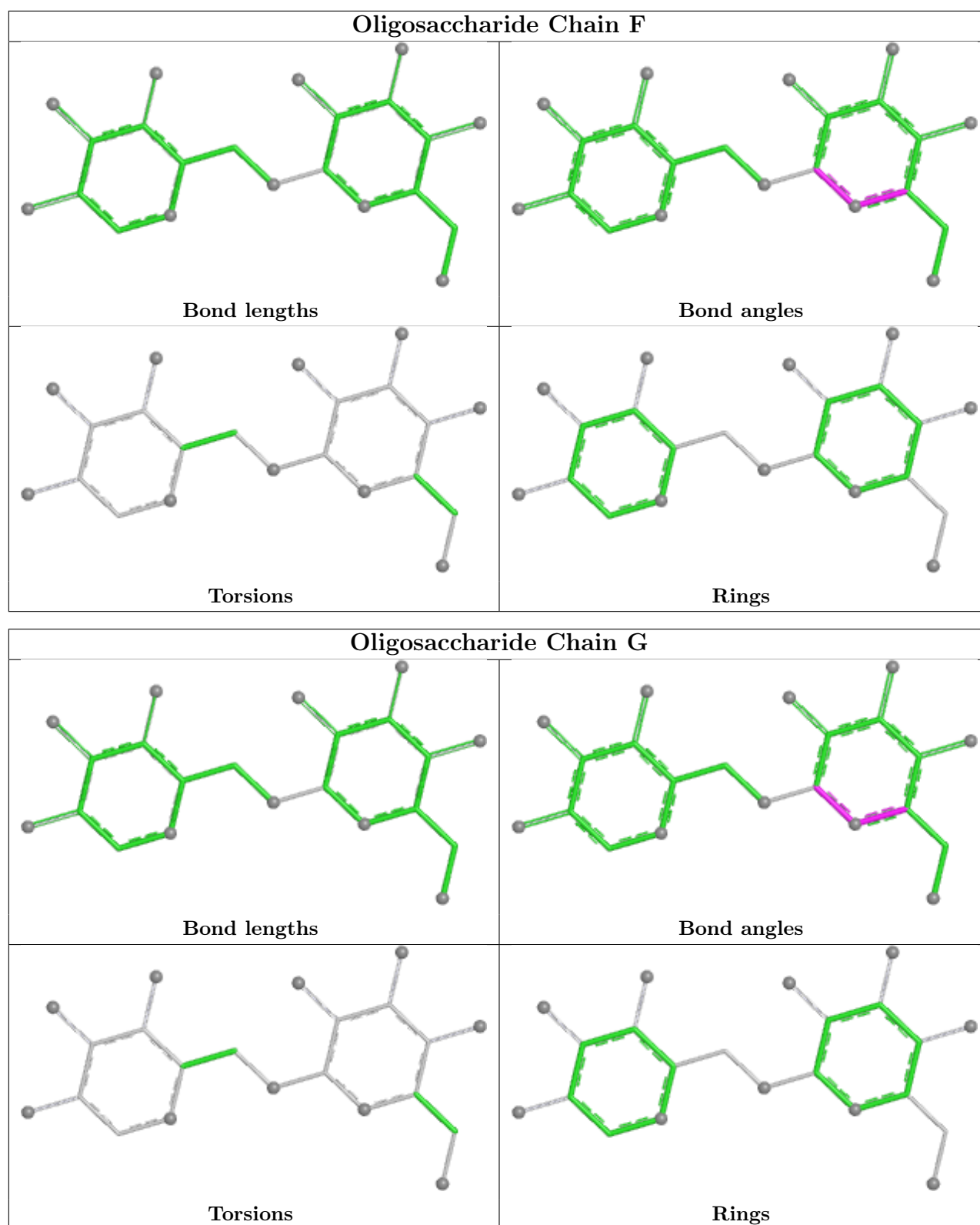
There are no ring outliers.

4 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	1	BMA	5	0
4	F	1	BMA	6	0
3	H	1	NAG	2	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	$\# Z > 2$
9	UEY	B	605	-	24,27,27	0.66	1 (4%)	27,37,37	0.81	2 (7%)
9	UEY	E	608	-	24,27,27	0.65	0	27,37,37	0.90	3 (11%)
7	NAG	E	604	2	14,14,15	0.33	0	17,19,21	0.70	1 (5%)
7	NAG	E	605	2	14,14,15	0.32	0	17,19,21	0.57	0
7	NAG	B	602	2	14,14,15	0.29	0	17,19,21	0.60	0
7	NAG	B	607	-	14,14,15	0.35	0	17,19,21	0.61	0
7	NAG	E	602	-	14,14,15	0.34	0	17,19,21	0.71	0
7	NAG	B	606	2	14,14,15	0.36	0	17,19,21	0.58	0
8	HEC	E	607	2	32,50,50	1.94	5 (15%)	30,82,82	1.95	9 (30%)
7	NAG	E	606	-	14,14,15	0.30	0	17,19,21	1.23	3 (17%)
10	MAN	E	603	-	11,11,12	0.26	0	15,15,17	0.48	0
8	HEC	B	604	2	32,50,50	1.96	6 (18%)	30,82,82	1.93	9 (30%)
7	NAG	B	603	-	14,14,15	0.31	0	17,19,21	1.26	3 (17%)
10	MAN	B	608	-	11,11,12	0.54	0	15,15,17	1.07	2 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	UEY	B	605	-	-	0/12/12/12	0/4/4/4
9	UEY	E	608	-	-	2/12/12/12	0/4/4/4
7	NAG	E	604	2	-	0/6/23/26	0/1/1/1
7	NAG	E	605	2	-	2/6/23/26	0/1/1/1
7	NAG	B	602	2	-	2/6/23/26	0/1/1/1
7	NAG	B	607	-	-	0/6/23/26	0/1/1/1
7	NAG	E	602	-	-	0/6/23/26	0/1/1/1
7	NAG	B	606	2	-	0/6/23/26	0/1/1/1
8	HEC	E	607	2	-	4/10/54/54	-
7	NAG	E	606	-	-	0/6/23/26	0/1/1/1
10	MAN	E	603	-	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	HEC	B	604	2	-	4/10/54/54	-
7	NAG	B	603	-	-	0/6/23/26	0/1/1/1
10	MAN	B	608	-	-	1/2/19/22	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	604	HEC	C2B-C3B	-7.61	1.32	1.40
8	E	607	HEC	C2B-C3B	-7.28	1.32	1.40
8	E	607	HEC	CBB-CAB	-3.99	1.34	1.49
8	E	607	HEC	CBC-CAC	-3.90	1.35	1.49
8	B	604	HEC	CBB-CAB	-3.68	1.35	1.49
8	B	604	HEC	CBC-CAC	-3.56	1.36	1.49
8	E	607	HEC	C3C-C2C	-2.98	1.37	1.40
8	B	604	HEC	C3D-C2D	-2.67	1.29	1.37
8	E	607	HEC	C4B-C3B	2.28	1.47	1.43
8	B	604	HEC	C1C-NC	2.10	1.40	1.36
8	B	604	HEC	C4B-C3B	2.08	1.46	1.43
9	B	605	UEY	C2-N1	2.03	1.36	1.33

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	E	607	HEC	CMC-C2C-C1C	-4.20	122.30	128.46
8	E	607	HEC	CMC-C2C-C3C	4.05	130.58	125.82
8	E	607	HEC	CBA-CAA-C2A	-4.00	105.96	112.55
8	B	604	HEC	O2A-CGA-O1A	-3.95	113.18	123.33
8	B	604	HEC	CMC-C2C-C1C	-3.88	122.77	128.46
8	B	604	HEC	CBA-CAA-C2A	-3.79	106.30	112.55
8	B	604	HEC	CBD-CAD-C3D	-3.70	106.31	112.54
8	B	604	HEC	CMC-C2C-C3C	3.69	130.16	125.82
7	E	606	NAG	O5-C1-C2	-3.53	105.83	111.29
7	B	603	NAG	O5-C1-C2	-3.42	106.00	111.29
8	E	607	HEC	CBD-CAD-C3D	-3.16	107.22	112.54
8	E	607	HEC	CMA-C3A-C2A	2.91	130.43	124.94
7	B	603	NAG	C1-C2-N2	2.79	114.82	110.43
8	E	607	HEC	O2A-CGA-O1A	-2.75	116.27	123.33
8	B	604	HEC	O2D-CGD-O1D	-2.72	116.33	123.33
10	B	608	MAN	C1-O5-C5	2.69	115.80	112.19
8	E	607	HEC	O2D-CGD-CBD	2.63	122.31	114.00
7	E	606	NAG	C1-C2-N2	2.62	114.55	110.43
7	E	604	NAG	C1-O5-C5	2.58	115.64	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	E	607	HEC	CAA-CBA-CGA	2.55	120.72	113.83
8	B	604	HEC	O2D-CGD-CBD	2.52	121.97	114.00
8	B	604	HEC	O2A-CGA-CBA	2.48	121.84	114.00
8	E	607	HEC	CMD-C2D-C1D	-2.40	124.93	128.46
10	B	608	MAN	C1-C2-C3	2.37	113.10	109.64
7	B	603	NAG	C1-O5-C5	2.35	115.33	112.19
9	E	608	UEY	N2-C2-N1	-2.23	116.39	118.24
7	E	606	NAG	C1-O5-C5	2.17	115.09	112.19
8	B	604	HEC	CMA-C3A-C2A	2.17	129.03	124.94
9	B	605	UEY	N2-C2-N1	-2.15	116.45	118.24
9	E	608	UEY	C2-N1-C3	-2.09	116.02	119.22
9	B	605	UEY	N5-N4-N3	-2.07	108.56	111.25
9	E	608	UEY	N5-N4-N3	-2.03	108.61	111.25

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	602	NAG	C4-C5-C6-O6
7	E	605	NAG	C4-C5-C6-O6
7	B	602	NAG	O5-C5-C6-O6
10	E	603	MAN	O5-C5-C6-O6
9	E	608	UEY	C6-C8-C9-C10
7	E	605	NAG	O5-C5-C6-O6
10	B	608	MAN	O5-C5-C6-O6
9	E	608	UEY	C6-C8-C9-C14
8	E	607	HEC	CAA-CBA-CGA-O2A
8	E	607	HEC	CAD-CBD-CGD-O1D
8	B	604	HEC	CAD-CBD-CGD-O1D
8	B	604	HEC	CAD-CBD-CGD-O2D
8	E	607	HEC	CAA-CBA-CGA-O1A
8	E	607	HEC	CAD-CBD-CGD-O2D
8	B	604	HEC	CAA-CBA-CGA-O2A
8	B	604	HEC	CAA-CBA-CGA-O1A

There are no ring outliers.

11 monomers are involved in 40 short contacts:

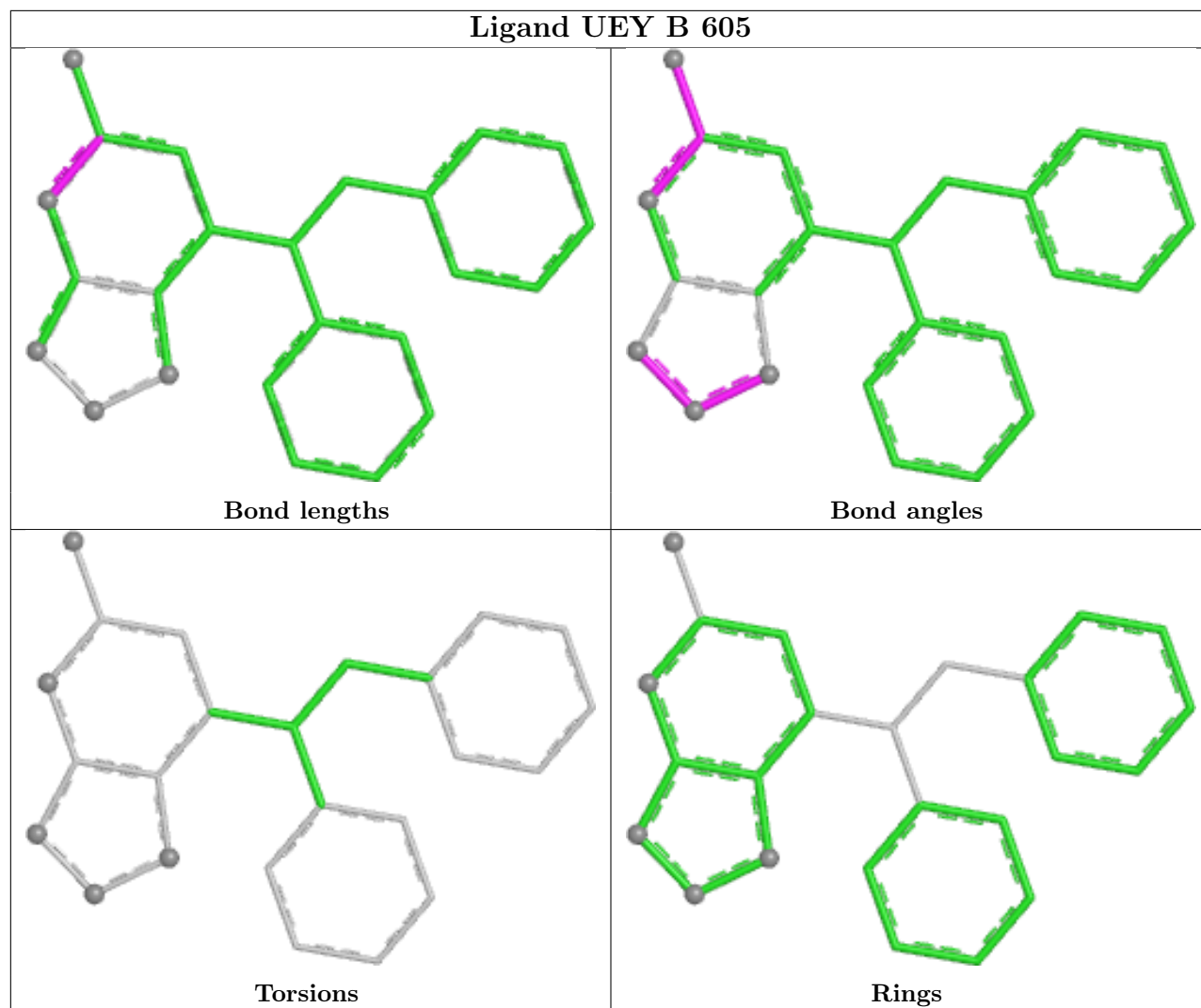
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	605	UEY	1	0
7	E	605	NAG	1	0

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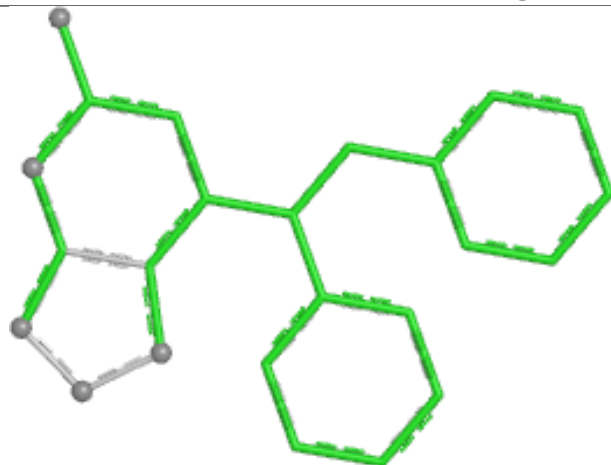
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	602	NAG	1	0
7	B	607	NAG	4	0
7	E	602	NAG	5	0
8	E	607	HEC	9	0
7	E	606	NAG	1	0
10	E	603	MAN	4	0
8	B	604	HEC	8	0
7	B	603	NAG	1	0
10	B	608	MAN	7	0

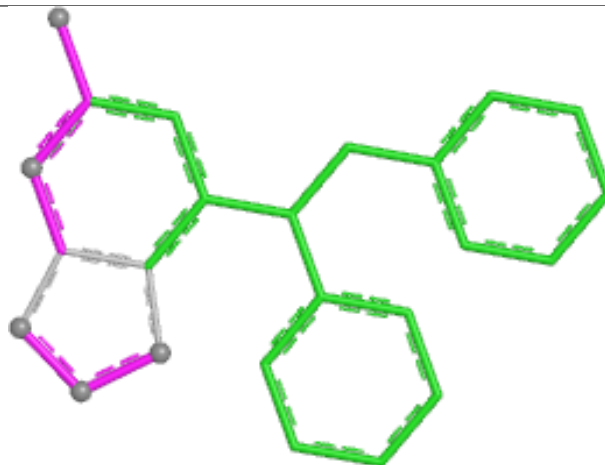
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



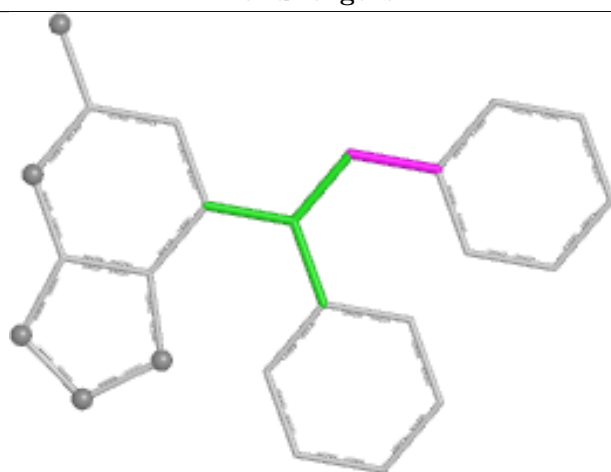
Ligand UEY E 608



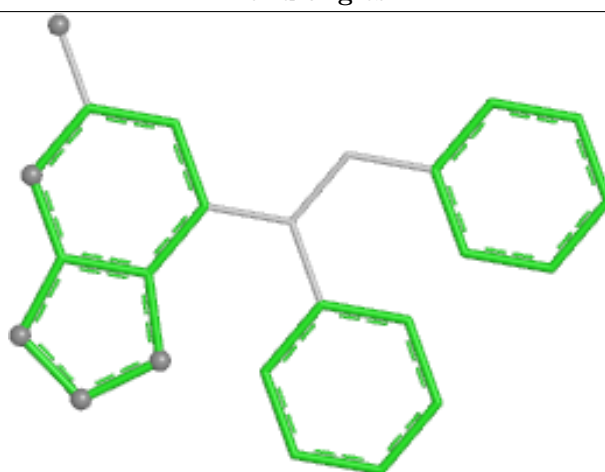
Bond lengths



Bond angles

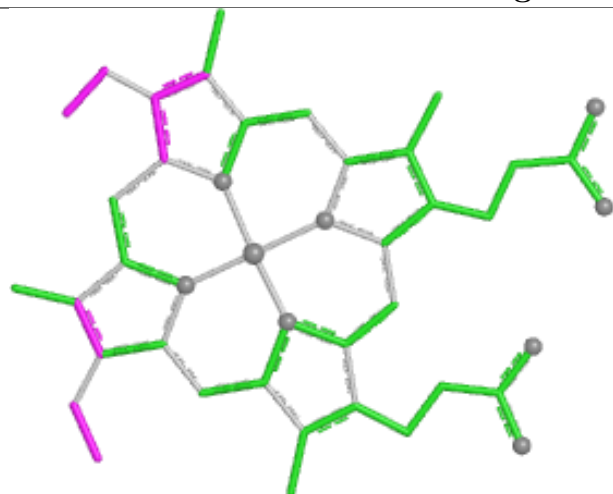


Torsions

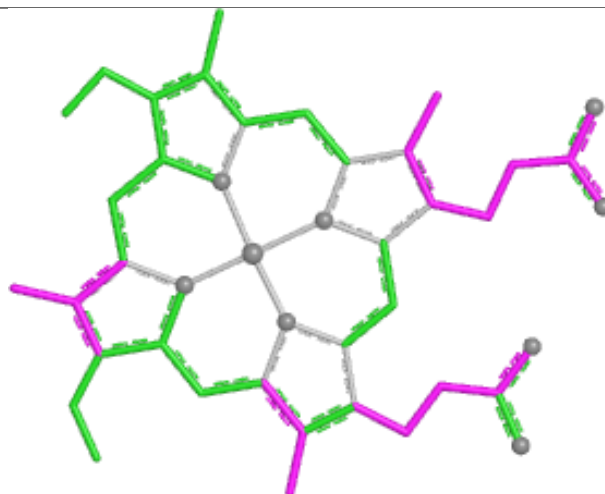


Rings

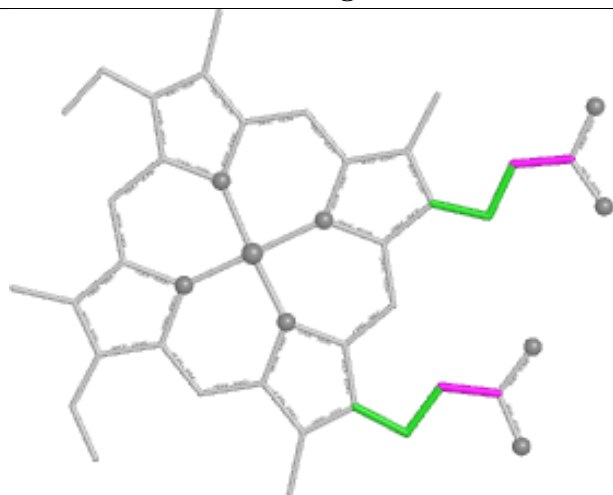
Ligand HEC E 607



Bond lengths



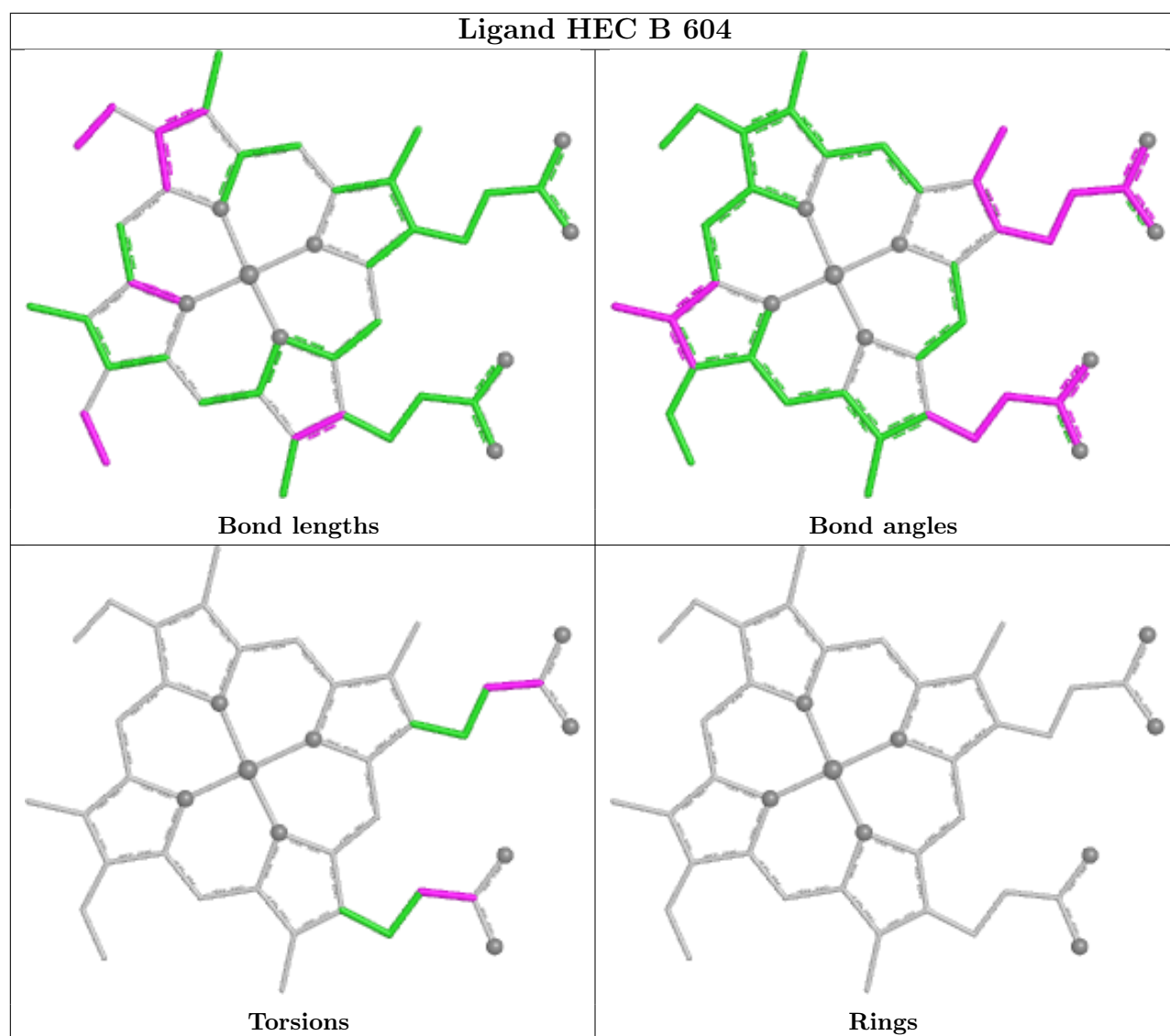
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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%)	0.41	5 (4%) 36 33	38, 50, 79, 82	0
1	D	103/105 (98%)	-0.01	0 100 100	35, 50, 71, 76	0
2	B	463/467 (99%)	0.71	27 (5%) 30 27	28, 62, 89, 102	5 (1%)
2	E	464/467 (99%)	0.23	9 (1%) 66 63	34, 55, 77, 100	10 (2%)
All	All	1133/1144 (99%)	0.42	41 (3%) 46 43	28, 57, 81, 102	15 (1%)

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	157	ASN	3.1
2	B	418	PRO	3.1
1	A	4	GLN	3.1
2	B	402	ILE	3.0
2	E	218	ASP	3.0
2	B	371	VAL	3.0
2	B	348	ASN	2.8
2	B	331	ALA	2.7
2	B	541	THR	2.7
2	B	226	ARG	2.7
1	A	1	CYS	2.6
1	A	72	PRO	2.6
2	B	230	ILE	2.6
2	B	373	LEU	2.4
2	B	253	LEU	2.4
2	B	305	ALA	2.4
2	B	263	GLU	2.4
2	E	156	SER	2.3
1	A	76	LEU	2.3
1	A	84	LEU	2.3
2	B	562	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
2	E	116	GLU	2.2
2	B	355	PRO	2.2
2	E	355	PRO	2.2
2	E	393	ARG	2.2
2	B	302	GLY	2.2
2	B	218	ASP	2.2
2	B	421	ASN	2.2
2	B	567	LEU	2.2
2	B	157	ASN	2.1
2	B	384	LEU	2.1
2	B	221	CYS	2.1
2	B	229	ARG	2.1
2	B	232	CYS	2.1
2	E	348	ASN	2.1
2	E	522	MET	2.1
2	B	497	CYS	2.1
2	E	523	GLN	2.1
2	B	203	PHE	2.0
2	B	187	LEU	2.0
2	B	264	LEU	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	B	150	7/8	0.90	0.11	41,41,49,90	0
2	CSO	E	150	7/8	0.96	0.07	39,39,40,46	0

6.3 Carbohydrates [i](#)

SUGAR-RSR INFOmissingINFO

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,

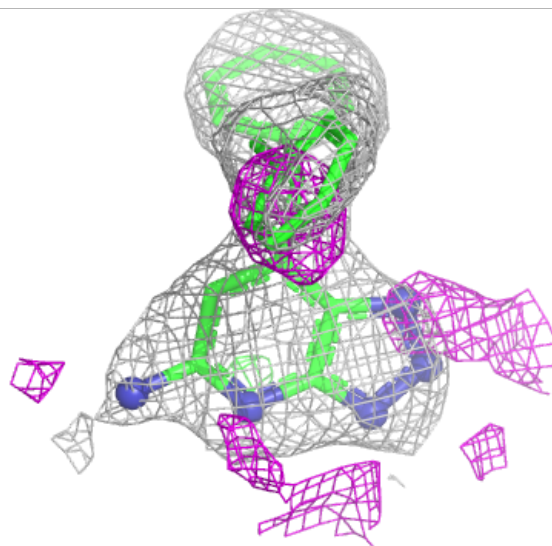
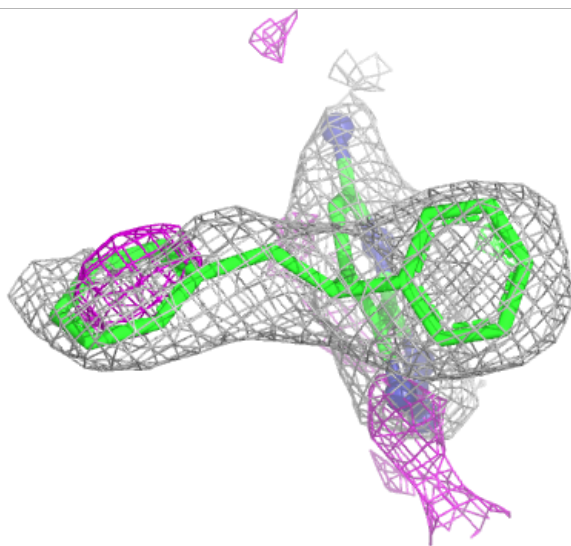
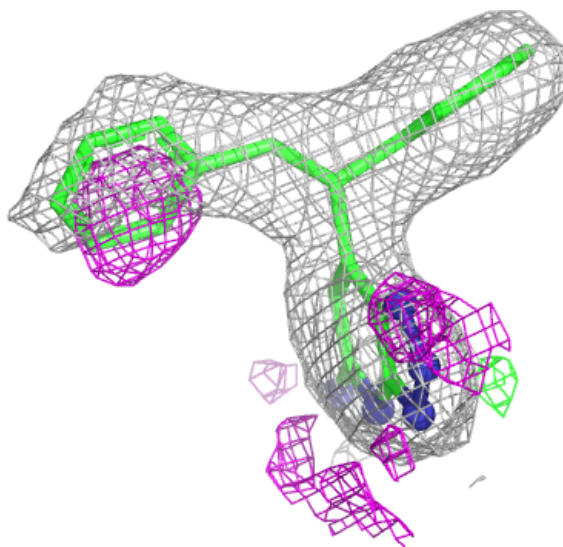
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
10	MAN	E	603	11/12	0.48	0.21	138,138,139,139	0
10	MAN	B	608	11/12	0.67	0.16	97,98,98,99	0
7	NAG	B	603	14/15	0.71	0.13	118,118,118,119	0
7	NAG	B	606	14/15	0.73	0.13	78,80,81,82	0
7	NAG	B	602	14/15	0.76	0.14	84,85,86,86	0
7	NAG	E	606	14/15	0.79	0.12	110,112,113,113	0
9	UEY	B	605	24/24	0.85	0.14	54,56,58,58	0
7	NAG	E	604	14/15	0.87	0.10	67,72,73,74	0
7	NAG	E	605	14/15	0.87	0.12	81,83,84,85	0
5	CL	B	609	1/1	0.89	0.22	76,76,76,76	0
9	UEY	E	608	24/24	0.90	0.10	44,47,57,57	0
8	HEC	B	604	43/43	0.94	0.10	45,49,50,52	0
7	NAG	E	602	14/15	0.95	0.08	45,49,51,52	0
5	CL	E	609	1/1	0.95	0.31	67,67,67,67	0
7	NAG	B	607	14/15	0.95	0.08	46,49,49,50	0
5	CL	D	201	1/1	0.97	0.08	36,36,36,36	0
8	HEC	E	607	43/43	0.97	0.08	40,45,47,49	0
5	CL	A	201	1/1	0.97	0.07	38,38,38,38	0
6	CA	E	601	1/1	0.98	0.03	38,38,38,38	0
6	CA	B	601	1/1	0.99	0.02	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.

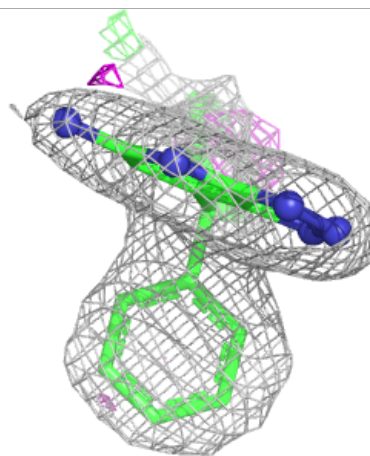
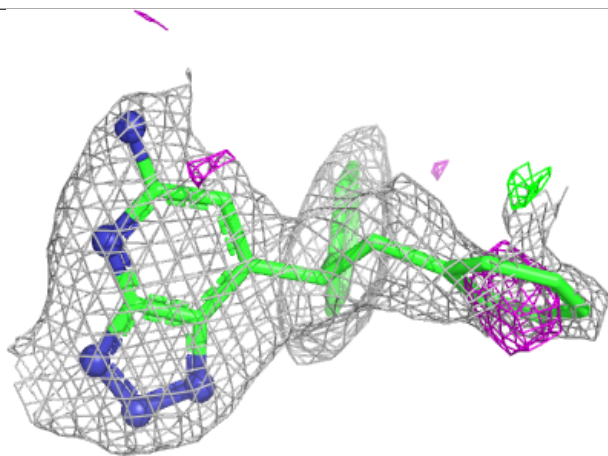
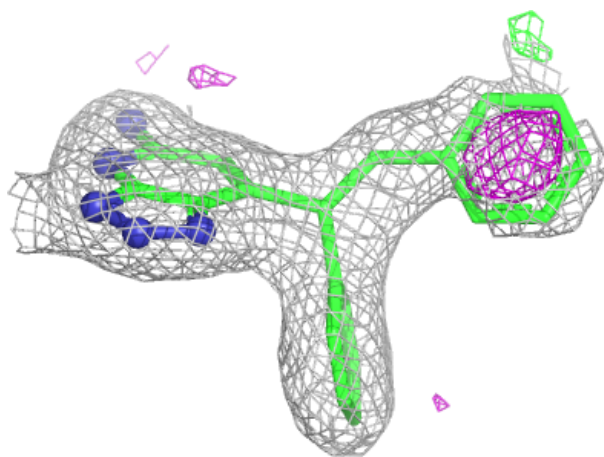
Electron density around UEY B 605:

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



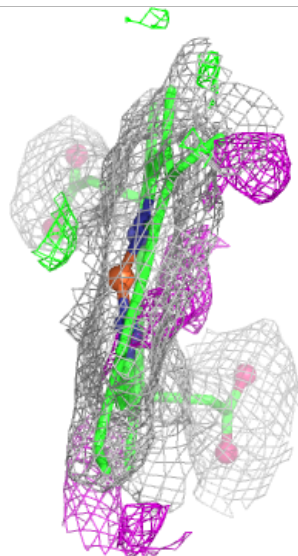
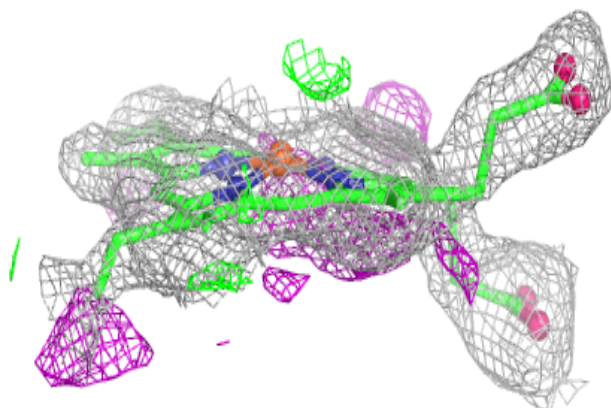
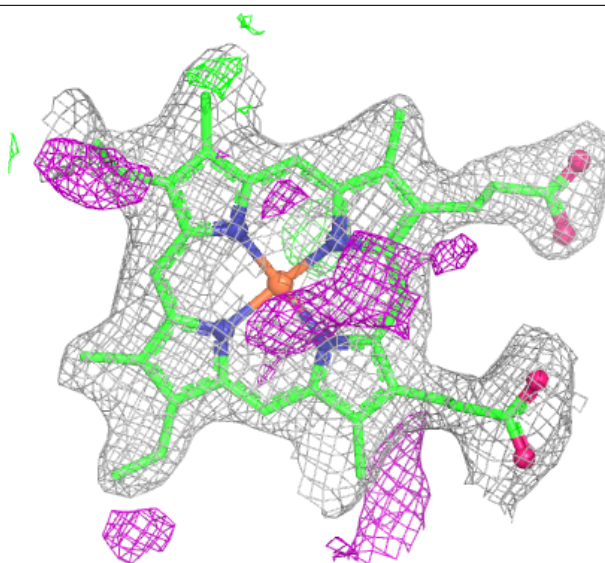
Electron density around UEY E 608:

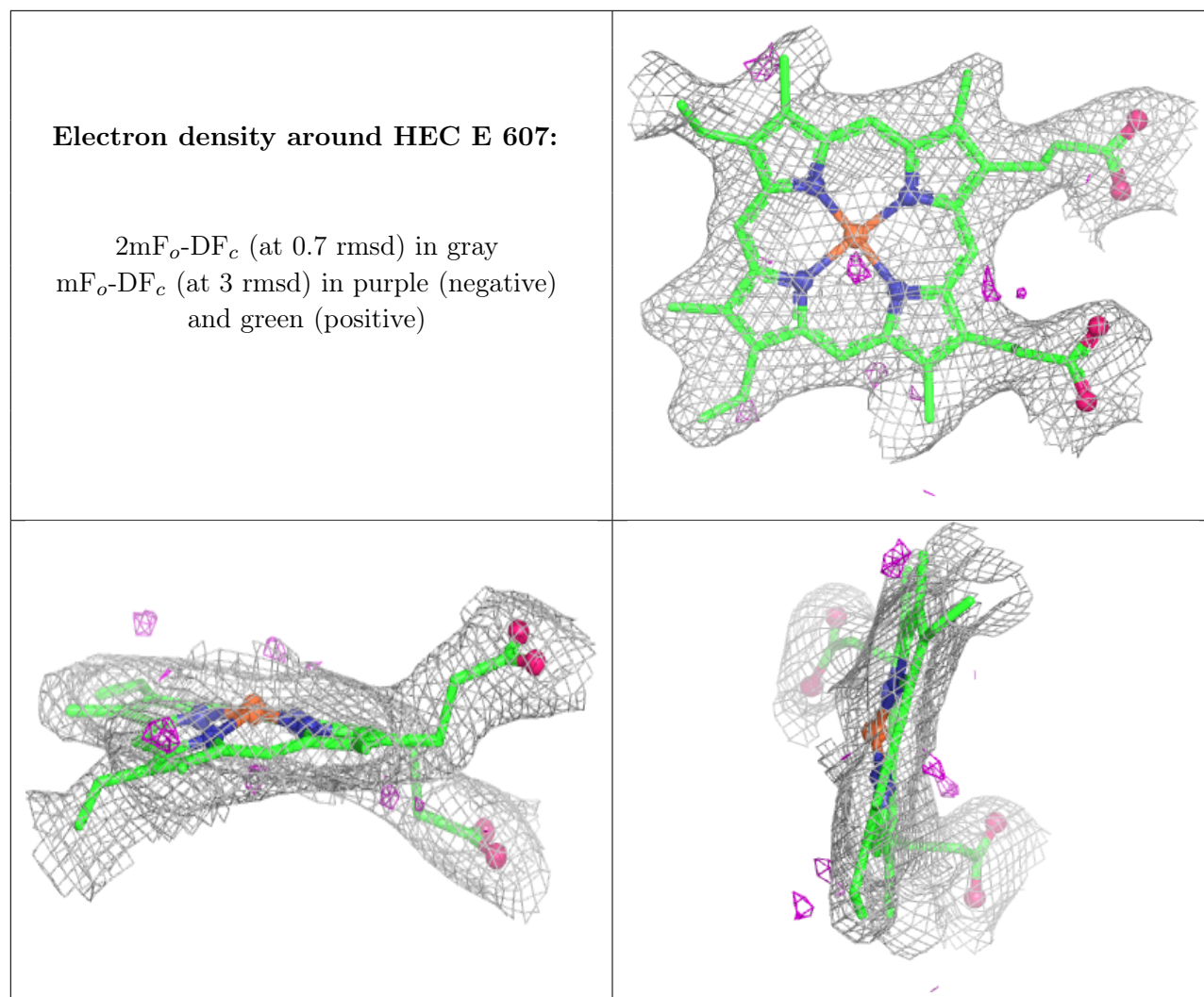
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEC B 604:

$2mF_o-DF_c$ (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.