Full wwPDB X-ray Structure Validation Report ⓘ

Dec 15, 2024 – 08:57 PM EST

PDB ID	:	6WY5
Title	:	CRYSTAL STRUCTURE OF MYELOPEROXIDASE SUBFORM C (MPO) COMPLEX WITH Compound-37 A.K.A 7-(1-phenyl-3-(((1S,3S)-3-phenyl-2,3-dihydro-1H-inden-1-yl)amino)propyl)-1H-[1,2,3]triazolo[4,5-b]pyridin-5-amine
Authors	:	Khan, J.A.
Deposited on	:	2020-05-12
Resolution	:	2.90 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 (1)) were used in the production of this report:

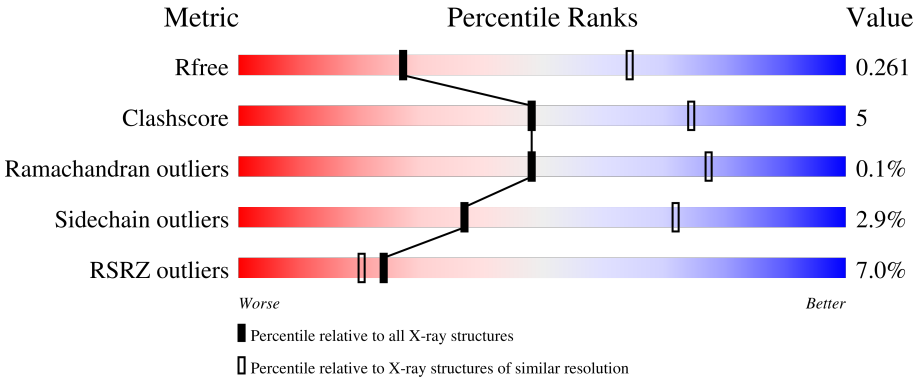
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2335 (2.90-2.90)
Clashscore	180529	2564 (2.90-2.90)
Ramachandran outliers	177936	2514 (2.90-2.90)
Sidechain outliers	177891	2516 (2.90-2.90)
RSRZ outliers	164620	2337 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	105	9% 81% 18%
1	D	105	4% 85% 13%
2	B	467	12% 87% 12%
2	E	467	3% 87% 13%
3	C	2	50% 50%

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Mol	Chain	Length	Quality of chain
3	G	2	100%
4	F	6	17% 83%
4	H	6	17% 83%

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 9075 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	104	Total	C	N	O	S	0	0	0
			805	511	141	148	5			
1	D	104	Total	C	N	O	S	0	0	0
			810	515	141	149	5			

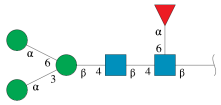
- Molecule 2 is a protein called Myeloperoxidase heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	464	Total	C	N	O	S	7	0	0
			3442	2160	618	638	26			
2	E	465	Total	C	N	O	S	21	0	0
			3645	2303	656	659	27			

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

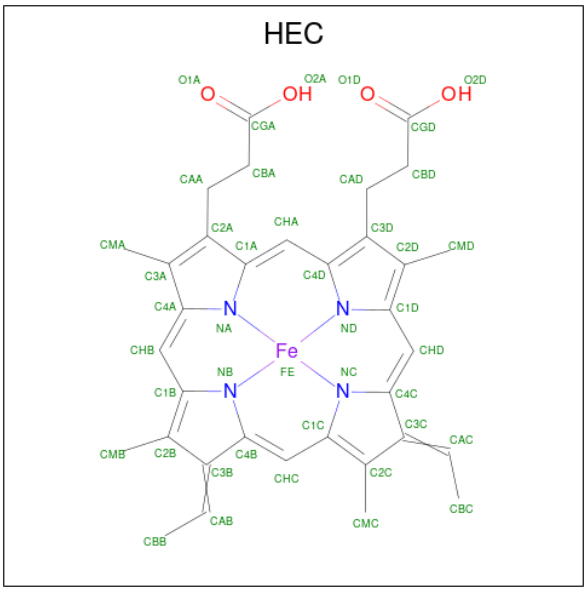
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	G	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 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
4	F	6	Total C N O 71 40 2 29	0	0	0
4	H	6	Total C N O 71 40 2 29	0	0	0

- Molecule 5 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



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

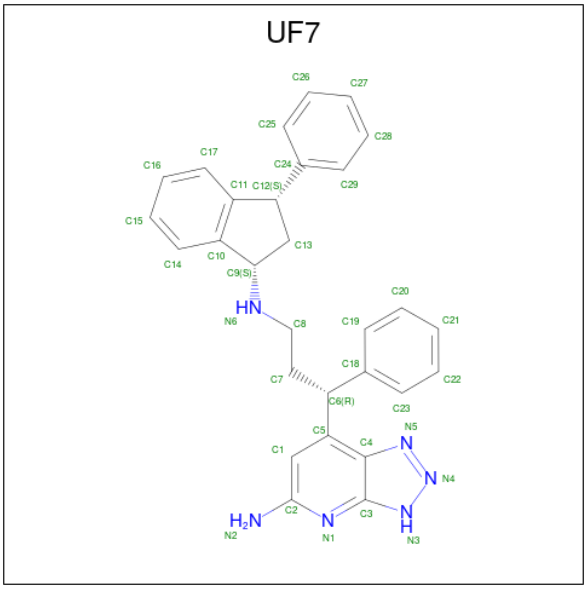
- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

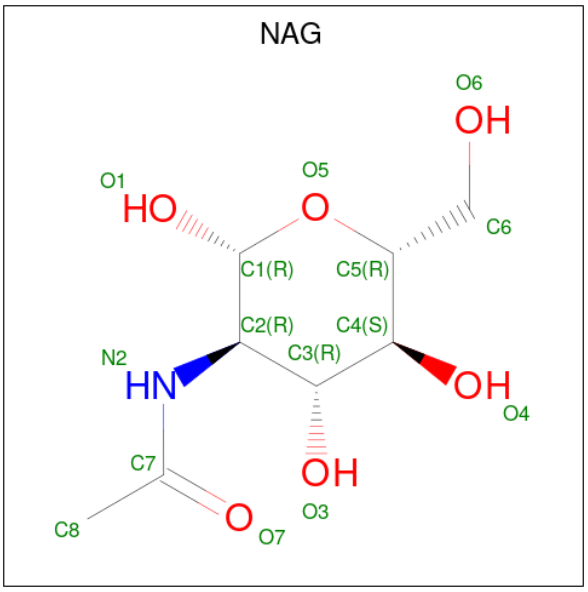
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total Ca 1 1	0	0
7	E	1	Total Ca 1 1	0	0

- Molecule 8 is 7-[(1R)-1-phenyl-3-{[(1S,3S)-3-phenyl-2,3-dihydro-1H-inden-1-yl]amino}propyl]-3H-[1,2,3]triazolo[4,5-b]pyridin-5-amine (three-letter code: UF7) (formula: $C_{29}H_{28}N_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total C N 35 29 6	0	0
8	E	1	Total C N 35 29 6	0	0

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



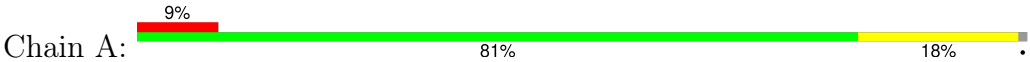
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	E	1	Total	C	N	O	0	0
			14	8	1	5		

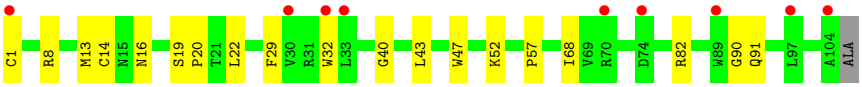
3 Residue-property plots (i)

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

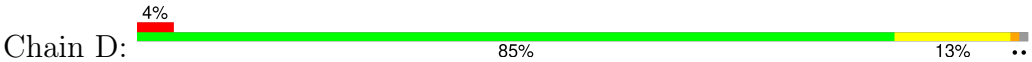
Chain A:





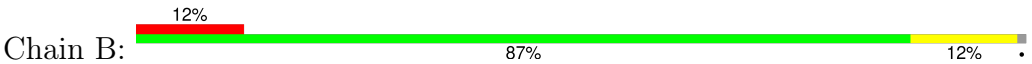
• Molecule 1: Myeloperoxidase light chain

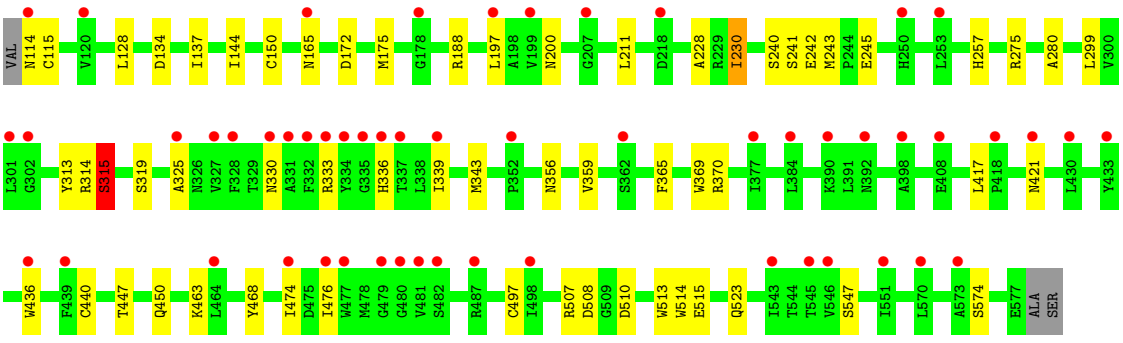
Chain D:



• Molecule 2: Myeloperoxidase heavy chain

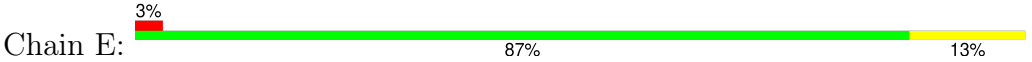
Chain B:

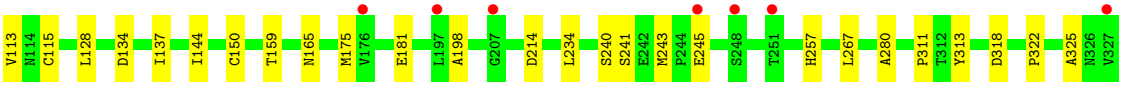


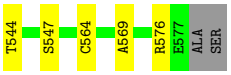


• Molecule 2: Myeloperoxidase heavy chain

Chain E:





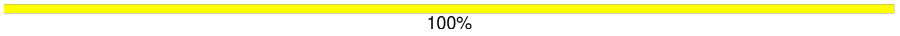


• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:

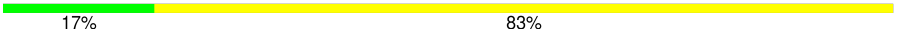
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:



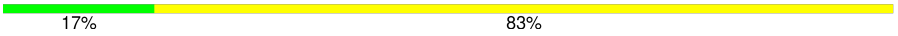
• Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:



• Molecule 4: 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

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	107.90Å 107.90Å 240.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.21 – 2.90 49.21 – 2.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.21-2.90) 99.9 (49.21-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	3.82 (at 2.91Å)	Xtriage
Refinement program	BUSTER 2.11.7 (17-DEC-2019)	Depositor
R, R_{free}	0.222 , 0.245 0.236 , 0.261	Depositor DCC
R_{free} test set	1642 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	74.2	Xtriage
Anisotropy	0.617	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 77.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	9075	wwPDB-VP
Average B, all atoms (Å^2)	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.17% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, CA, MAN, CSO, BMA, FUC, UF7, CL, HEC

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	0.46	0/830	0.66	0/1134
1	D	0.46	0/835	0.65	0/1142
2	B	0.42	0/3517	0.60	0/4799
2	E	0.44	0/3722	0.59	0/5059
All	All	0.43	0/8904	0.61	0/12134

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

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	805	0	742	17	0
1	D	810	0	753	12	0
2	B	3442	0	3150	43	0
2	E	3645	0	3574	32	0
3	C	28	0	25	0	0
3	G	28	0	25	0	0
4	F	71	0	61	0	0
4	H	71	0	61	0	0
5	A	43	0	28	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	43	0	28	2	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	D	1	0	0	0	0
7	B	1	0	0	0	0
7	E	1	0	0	0	0
8	B	35	0	0	1	0
8	E	35	0	0	0	0
9	E	14	0	13	1	0
All	All	9075	0	8460	91	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 (91) 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:B:230:ILE:HG13	2:B:369:TRP:HB3	1.28	1.12
2:E:267:LEU:HG	2:E:576:ARG:HB3	1.46	0.97
2:B:228:ALA:HB3	2:B:230:ILE:HD12	1.60	0.82
2:E:311:PRO:O	2:E:507:ARG:NH2	2.18	0.75
1:A:52:LYS:HE2	1:A:57:PRO:HD3	1.69	0.74
2:B:313:TYR:HD1	2:B:507:ARG:HD3	1.52	0.73
2:B:313:TYR:CD1	2:B:507:ARG:HD3	2.25	0.71
2:B:230:ILE:H	2:B:230:ILE:HD13	1.56	0.70
2:B:230:ILE:CG1	2:B:369:TRP:HB3	2.18	0.64
2:B:314:ARG:O	2:B:315:SER:HB3	1.98	0.63
2:E:333:ARG:HH11	2:E:421:ASN:ND2	1.97	0.62
2:B:333:ARG:HH11	2:B:421:ASN:ND2	1.97	0.60
2:E:313:TYR:CD1	2:E:507:ARG:HD3	2.36	0.60
2:B:356:ASN:HD22	2:B:370:ARG:HH21	1.50	0.60
2:E:267:LEU:CG	2:E:576:ARG:HB3	2.28	0.60
1:D:84:LEU:HD13	2:E:389:ALA:HA	1.84	0.59
2:B:356:ASN:ND2	2:B:370:ARG:HH21	2.00	0.59
2:B:230:ILE:HG13	2:B:369:TRP:CB	2.19	0.58
2:B:230:ILE:O	2:B:230:ILE:HG12	2.03	0.58
2:E:440:CYS:SG	2:E:497:CYS:SG	3.02	0.56
1:A:19:SER:HB3	1:A:22:LEU:HG	1.86	0.56
1:A:8:ARG:NE	2:B:172:ASP:HB3	2.21	0.56
1:D:43:LEU:HD22	1:D:47:TRP:CD1	2.42	0.55
2:E:440:CYS:CB	2:E:497:CYS:HG	2.19	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:LEU:HD22	1:A:47:TRP:CD1	2.42	0.55
2:B:514:TRP:CE2	2:B:515:GLU:HG3	2.42	0.54
1:D:19:SER:HB3	1:D:22:LEU:HG	1.88	0.54
2:B:333:ARG:HH11	2:B:421:ASN:HD22	1.56	0.54
1:D:91:GLN:HB2	5:D:201:HEC:HMC3	1.91	0.53
2:E:333:ARG:HH11	2:E:421:ASN:HD22	1.56	0.53
2:E:538:CYS:SG	2:E:564:CYS:SG	3.08	0.52
2:E:394:GLN:HB3	2:E:460:LEU:HD22	1.92	0.52
2:B:257:HIS:CE1	2:B:280:ALA:HB3	2.45	0.52
2:E:448:VAL:HB	2:E:465:MET:HG3	1.92	0.51
2:B:343:MET:HB3	2:B:359:VAL:HG13	1.92	0.51
2:B:230:ILE:H	2:B:230:ILE:CD1	2.22	0.51
1:A:8:ARG:HE	2:B:172:ASP:HB3	1.76	0.50
1:A:32:TRP:CE2	2:B:325:ALA:HB2	2.47	0.50
2:E:544:THR:O	2:E:564:CYS:SG	2.69	0.50
2:B:440:CYS:CB	2:B:497:CYS:HG	2.25	0.50
2:E:538:CYS:HG	2:E:564:CYS:HG	1.54	0.50
2:B:330:ASN:HA	2:B:333:ARG:HD2	1.93	0.49
2:E:330:ASN:HA	2:E:333:ARG:HD2	1.94	0.49
2:E:340:GLN:OE1	2:E:341:PRO:HD2	2.13	0.48
2:E:243:MET:HG3	2:E:245:GLU:OE2	2.13	0.48
1:D:13:MET:O	1:D:14:CYS:HB2	2.14	0.48
2:E:257:HIS:CE1	2:E:280:ALA:HB3	2.48	0.48
1:A:82:ARG:HH21	2:B:299:LEU:CB	2.27	0.48
2:B:134:ASP:HB3	2:B:137:ILE:O	2.14	0.47
2:E:436:TRP:CD1	2:E:476:ILE:HD13	2.49	0.47
2:B:436:TRP:CD1	2:B:476:ILE:HD13	2.49	0.47
1:A:82:ARG:HH21	2:B:299:LEU:HA	1.80	0.47
2:B:447:THR:H	2:B:450:GLN:HE21	1.63	0.47
1:A:40:GLY:HA2	1:D:20:PRO:HD2	1.96	0.46
1:A:82:ARG:HH21	2:B:299:LEU:CA	2.29	0.46
2:E:128:LEU:HB2	2:E:144:ILE:HB	1.96	0.46
2:E:214:ASP:HB2	2:E:234:LEU:HB2	1.98	0.46
1:A:13:MET:O	1:A:14:CYS:HB2	2.16	0.46
2:E:134:ASP:HB3	2:E:137:ILE:O	2.15	0.46
2:B:128:LEU:HB2	2:B:144:ILE:HB	1.97	0.46
2:B:188:ARG:HA	2:B:197:LEU:HA	1.98	0.46
2:B:440:CYS:SG	2:B:497:CYS:SG	3.12	0.46
1:A:90:GLY:C	5:A:201:HEC:HBC3	2.37	0.45
2:B:523:GLN:NE2	2:B:523:GLN:H	2.14	0.45
2:E:198:ALA:HB1	9:E:601:NAG:H81	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:535:ARG:HE	2:E:569:ALA:HB2	1.82	0.45
1:D:16:ASN:O	1:D:20:PRO:HA	2.17	0.45
1:D:90:GLY:C	5:D:201:HEC:HBC3	2.38	0.44
2:B:507:ARG:HD2	2:B:508:ASP:OD1	2.17	0.44
2:E:523:GLN:NE2	2:E:523:GLN:H	2.15	0.44
2:B:242:GLU:O	2:B:365:PHE:HA	2.17	0.44
1:D:22:LEU:HB3	2:E:322:PRO:HD2	2.00	0.44
2:B:510:ASP:HB3	2:B:513:TRP:HB2	2.00	0.44
2:B:243:MET:HG3	2:B:245:GLU:OE2	2.18	0.43
1:D:29:PHE:CE1	2:E:165:ASN:HB2	2.53	0.43
1:A:16:ASN:O	1:A:20:PRO:HA	2.18	0.43
2:B:336:HIS:HA	2:B:339:ILE:HD12	2.02	0.42
1:A:91:GLN:HB2	5:A:201:HEC:HMC3	2.02	0.42
2:B:200:ASN:HB2	2:B:211:LEU:O	2.20	0.42
1:A:29:PHE:CE1	2:B:165:ASN:HB2	2.55	0.42
2:B:447:THR:H	2:B:450:GLN:NE2	2.18	0.42
2:E:471:PRO:HA	2:E:474:ILE:HG13	2.02	0.41
5:A:201:HEC:O2D	8:B:603:UF7:N2	2.52	0.41
2:E:336:HIS:HA	2:E:339:ILE:HD12	2.02	0.41
1:D:32:TRP:CE2	2:E:325:ALA:HB2	2.55	0.41
1:A:20:PRO:HD2	1:D:40:GLY:HA2	2.01	0.41
2:B:468:TYR:CD2	2:B:474:ILE:HG12	2.56	0.41
1:A:68:ILE:HD12	2:B:463:LYS:HB3	2.03	0.40
2:E:537:ILE:O	2:E:541:THR:OG1	2.24	0.40
2:E:341:PRO:HD3	2:E:399:VAL:HG11	2.02	0.40
2:B:336:HIS:CE1	2:B:417:LEU:HD21	2.57	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	102/105 (97%)	96 (94%)	6 (6%)	0	100 100
1	D	102/105 (97%)	97 (95%)	5 (5%)	0	100 100
2	B	461/467 (99%)	441 (96%)	19 (4%)	1 (0%)	44 73
2	E	462/467 (99%)	448 (97%)	14 (3%)	0	100 100
All	All	1127/1144 (98%)	1082 (96%)	44 (4%)	1 (0%)	48 77

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	315	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	81/90 (90%)	80 (99%)	1 (1%)	67 89
1	D	83/90 (92%)	81 (98%)	2 (2%)	44 76
2	B	337/411 (82%)	326 (97%)	11 (3%)	33 68
2	E	389/411 (95%)	377 (97%)	12 (3%)	35 70
All	All	890/1002 (89%)	864 (97%)	26 (3%)	37 72

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	CYS
2	B	114	ASN
2	B	115	CYS
2	B	175	MET
2	B	230	ILE
2	B	240	SER
2	B	241	SER
2	B	275	ARG
2	B	315	SER
2	B	319	SER

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Mol	Chain	Res	Type
2	B	547	SER
2	B	574	SER
1	D	1	CYS
1	D	84	LEU
2	E	113	VAL
2	E	115	CYS
2	E	159	THR
2	E	175	MET
2	E	181	GLU
2	E	240	SER
2	E	241	SER
2	E	318	ASP
2	E	353	MET
2	E	356	ASN
2	E	487	ARG
2	E	547	SER

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

Mol	Chain	Res	Type
1	A	75	GLN
1	A	91	GLN
2	B	114	ASN
2	B	200	ASN
2	B	250	HIS
2	B	356	ASN
2	B	421	ASN
2	B	450	GLN
2	B	523	GLN
1	D	54	ASN
2	E	421	ASN
2	E	523	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	CSO	B	150	2	3,6,7	0.65	0	1,6,8	4.61	1 (100%)
2	CSO	E	150	2	3,6,7	0.71	0	1,6,8	4.52	1 (100%)

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	B	150	2	-	0/1/5/7	-
2	CSO	E	150	2	-	0/1/5/7	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	150	CSO	CB-CA-C	-4.61	98.29	110.80
2	E	150	CSO	CB-CA-C	-4.52	98.51	110.80

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)

16 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	0.32	0	17,19,21	0.58	0
3	NAG	C	2	3	14,14,15	0.32	0	17,19,21	0.96	1 (5%)
4	NAG	F	1	2,4	14,14,15	0.29	0	17,19,21	1.17	2 (11%)
4	NAG	F	2	4	14,14,15	0.33	0	17,19,21	1.00	1 (5%)
4	BMA	F	3	4	11,11,12	0.23	0	15,15,17	1.02	1 (6%)
4	MAN	F	4	4	11,11,12	0.32	0	15,15,17	1.53	2 (13%)
4	MAN	F	5	4	11,11,12	0.29	0	15,15,17	1.10	2 (13%)
4	FUC	F	6	4	10,10,11	0.35	0	14,14,16	0.49	0
3	NAG	G	1	3,2	14,14,15	0.31	0	17,19,21	0.75	1 (5%)
3	NAG	G	2	3	14,14,15	0.29	0	17,19,21	1.11	1 (5%)
4	NAG	H	1	2,4	14,14,15	0.31	0	17,19,21	1.09	1 (5%)
4	NAG	H	2	4	14,14,15	0.35	0	17,19,21	1.01	1 (5%)
4	BMA	H	3	4	11,11,12	0.27	0	15,15,17	0.96	1 (6%)
4	MAN	H	4	4	11,11,12	0.31	0	15,15,17	1.50	2 (13%)
4	MAN	H	5	4	11,11,12	0.33	0	15,15,17	1.28	2 (13%)
4	FUC	H	6	4	10,10,11	0.42	0	14,14,16	0.89	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	-	2/6/23/26	0/1/1/1
3	NAG	C	2	3	-	0/6/23/26	0/1/1/1
4	NAG	F	1	2,4	-	0/6/23/26	0/1/1/1
4	NAG	F	2	4	-	2/6/23/26	0/1/1/1
4	BMA	F	3	4	-	0/2/19/22	0/1/1/1
4	MAN	F	4	4	-	1/2/19/22	0/1/1/1
4	MAN	F	5	4	-	0/2/19/22	0/1/1/1
4	FUC	F	6	4	-	-	0/1/1/1
3	NAG	G	1	3,2	-	2/6/23/26	0/1/1/1
3	NAG	G	2	3	-	0/6/23/26	0/1/1/1
4	NAG	H	1	2,4	-	0/6/23/26	0/1/1/1
4	NAG	H	2	4	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BMA	H	3	4	-	0/2/19/22	0/1/1/1
4	MAN	H	4	4	-	1/2/19/22	0/1/1/1
4	MAN	H	5	4	-	0/2/19/22	0/1/1/1
4	FUC	H	6	4	-	-	0/1/1/1

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	F	4	MAN	C1-O5-C5	4.85	118.69	112.19
4	H	4	MAN	C1-O5-C5	4.81	118.64	112.19
4	H	2	NAG	C1-O5-C5	3.71	117.15	112.19
4	F	2	NAG	C1-O5-C5	3.62	117.04	112.19
4	F	3	BMA	C1-O5-C5	3.55	116.95	112.19
4	H	3	BMA	C1-O5-C5	3.39	116.73	112.19
4	F	1	NAG	O5-C1-C2	-3.20	106.34	111.29
4	H	1	NAG	C1-O5-C5	3.12	116.37	112.19
3	C	2	NAG	C1-O5-C5	3.03	116.25	112.19
3	G	2	NAG	C1-O5-C5	3.01	116.22	112.19
4	H	5	MAN	C1-O5-C5	2.91	116.09	112.19
4	H	5	MAN	C3-C4-C5	2.40	114.59	110.23
4	F	4	MAN	C3-C4-C5	2.40	114.58	110.23
4	H	4	MAN	C3-C4-C5	2.37	114.53	110.23
3	G	1	NAG	C1-C2-N2	-2.31	106.79	110.43
4	F	5	MAN	C1-O5-C5	2.24	115.19	112.19
4	F	1	NAG	C1-C2-N2	2.11	113.76	110.43
4	F	5	MAN	C3-C4-C5	2.09	114.02	110.23

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1	NAG	C4-C5-C6-O6
3	G	1	NAG	C4-C5-C6-O6
3	C	1	NAG	O5-C5-C6-O6
3	G	1	NAG	O5-C5-C6-O6
4	F	4	MAN	O5-C5-C6-O6
4	F	2	NAG	C4-C5-C6-O6
4	F	2	NAG	O5-C5-C6-O6
4	H	2	NAG	C4-C5-C6-O6
4	H	4	MAN	O5-C5-C6-O6

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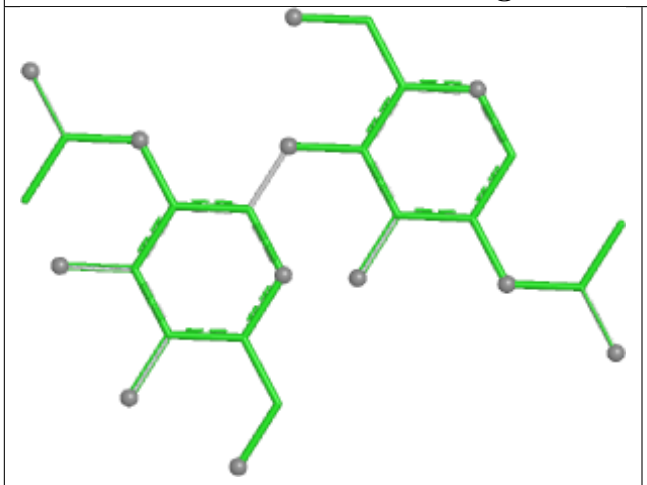
Mol	Chain	Res	Type	Atoms
4	H	2	NAG	O5-C5-C6-O6

There are no ring outliers.

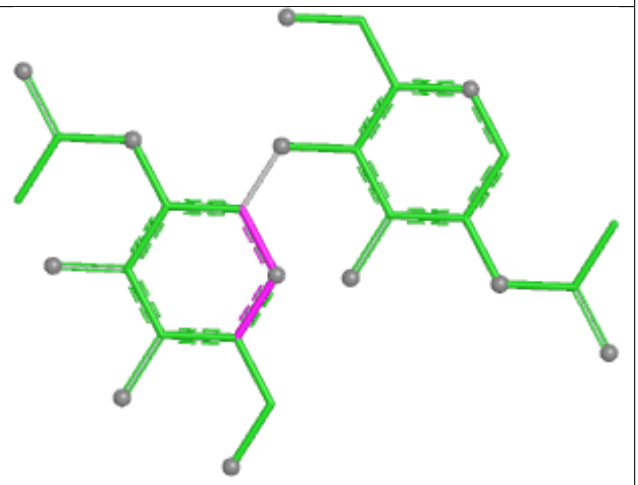
No monomer is involved in short contacts.

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

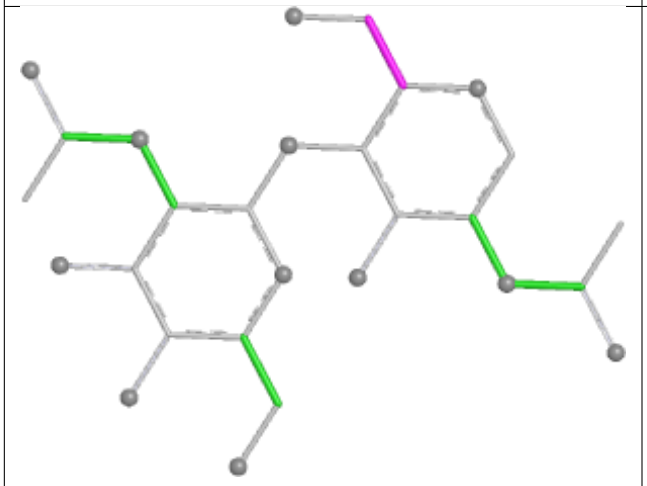
Oligosaccharide Chain C



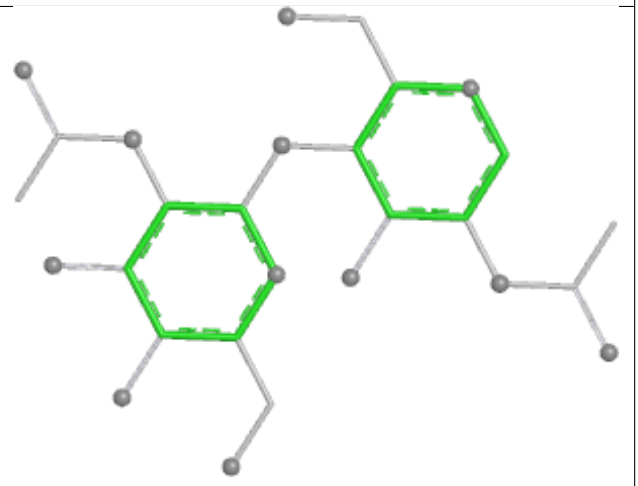
Bond lengths



Bond angles

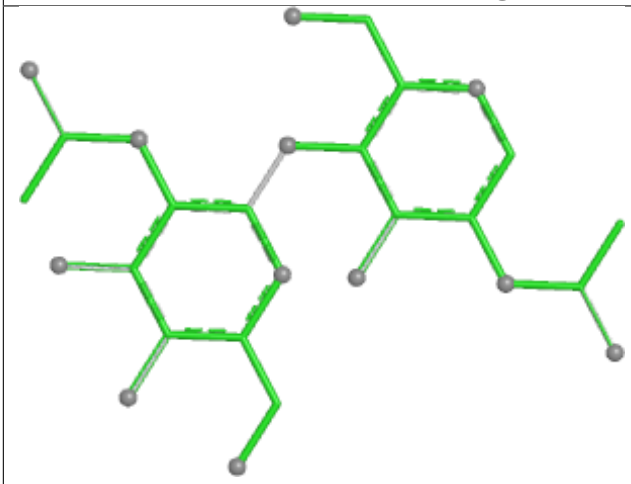


Torsions

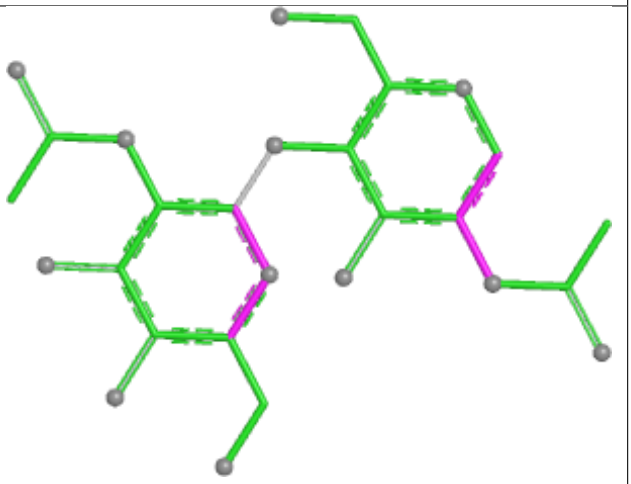


Rings

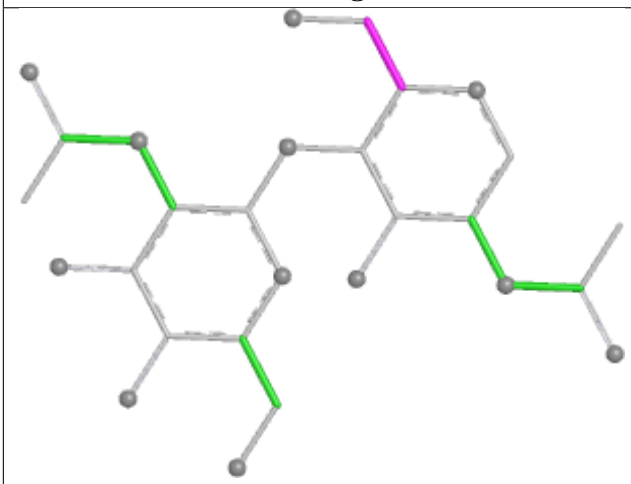
Oligosaccharide Chain G



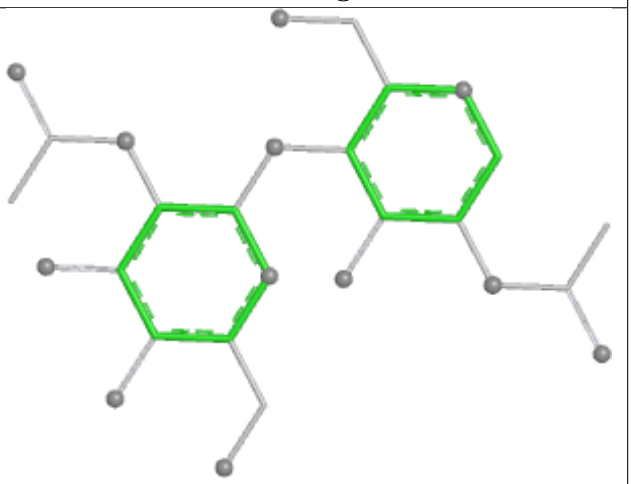
Bond lengths



Bond angles

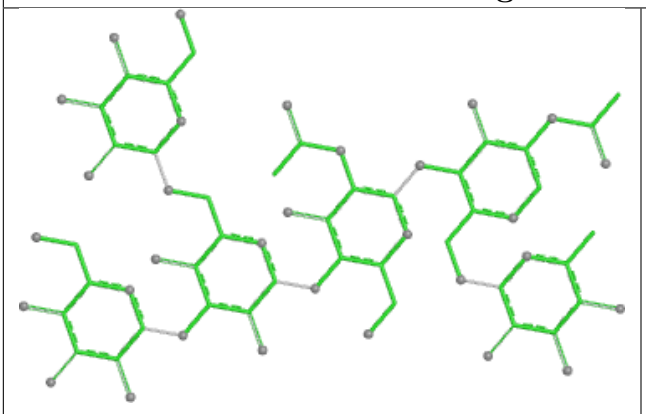


Torsions

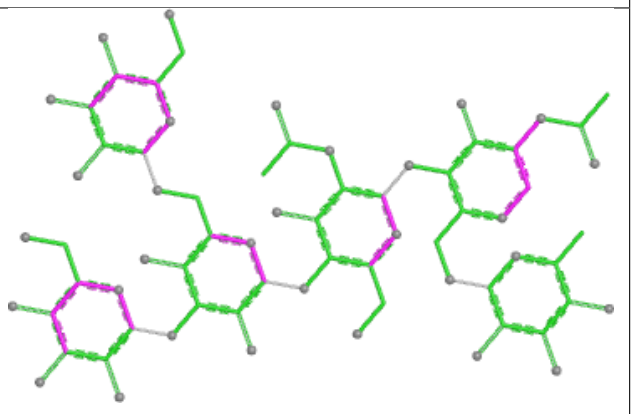


Rings

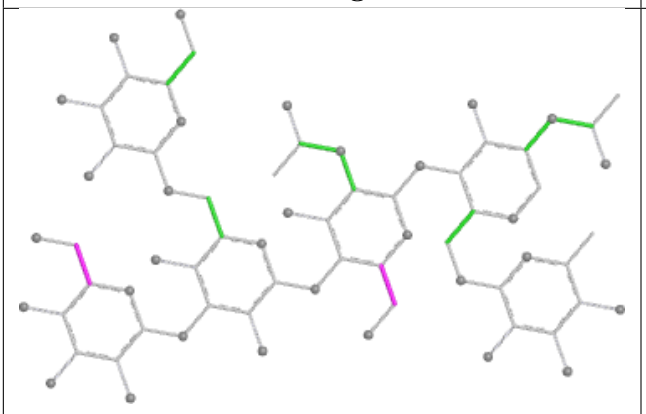
Oligosaccharide Chain F



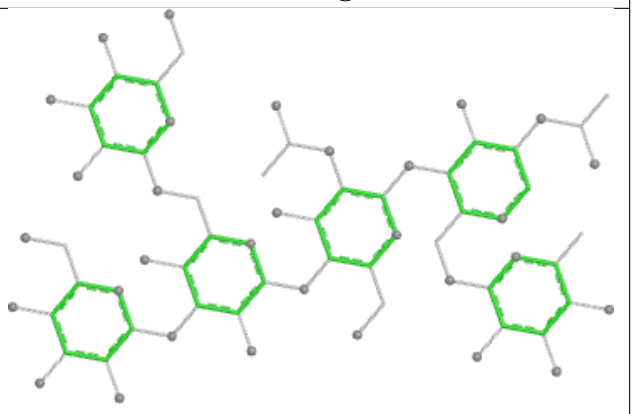
Bond lengths



Bond angles

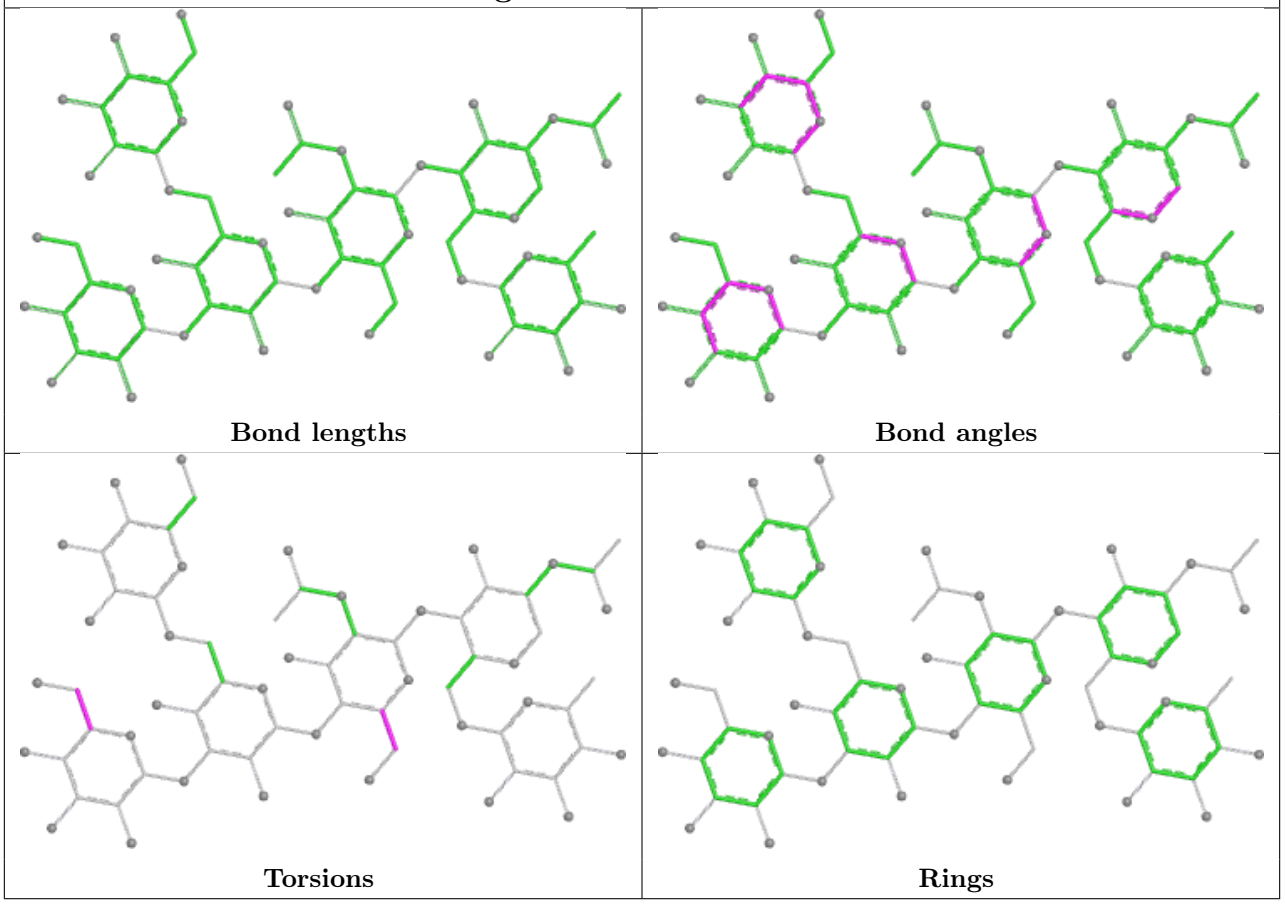


Torsions



Rings

Oligosaccharide Chain H



5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 5 are monoatomic - leaving 5 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	HEC	A	201	2	32,50,50	1.72	5 (15%)	30,82,82	2.30	15 (50%)
8	UF7	E	603	-	37,40,40	1.08	2 (5%)	42,56,56	1.33	4 (9%)
5	HEC	D	201	2	32,50,50	1.49	5 (15%)	30,82,82	2.43	17 (56%)
9	NAG	E	601	2	14,14,15	0.34	0	17,19,21	1.11	2 (11%)
8	UF7	B	603	-	37,40,40	0.83	2 (5%)	42,56,56	0.90	3 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	HEC	A	201	2	-	4/10/54/54	-
8	UF7	E	603	-	-	7/18/30/30	0/6/6/6
5	HEC	D	201	2	-	4/10/54/54	-
9	NAG	E	601	2	-	1/6/23/26	0/1/1/1
8	UF7	B	603	-	-	6/18/30/30	0/6/6/6

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	E	603	UF7	C3-N3	5.24	1.43	1.34
5	A	201	HEC	C2B-C3B	-4.93	1.35	1.40
5	A	201	HEC	CBC-CAC	-4.24	1.33	1.49
5	D	201	HEC	CBC-CAC	-3.85	1.35	1.49
5	A	201	HEC	CBB-CAB	-3.63	1.36	1.49
5	A	201	HEC	C4B-C3B	3.47	1.49	1.43
8	B	603	UF7	C3-N3	3.46	1.40	1.34
5	D	201	HEC	CBB-CAB	-3.32	1.37	1.49
5	D	201	HEC	C3C-C2C	-3.21	1.37	1.40
5	D	201	HEC	C2B-C3B	-2.97	1.37	1.40
5	D	201	HEC	C4B-C3B	2.58	1.47	1.43
8	E	603	UF7	C4-N5	2.42	1.42	1.37
8	B	603	UF7	C4-N5	2.24	1.42	1.37
5	A	201	HEC	C1C-NC	2.20	1.40	1.36

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	201	HEC	CBA-CAA-C2A	-4.72	104.77	112.55
8	E	603	UF7	C10-C11-C12	-4.64	101.32	106.65
5	D	201	HEC	CBD-CAD-C3D	-4.62	104.77	112.54
5	A	201	HEC	CBA-CAA-C2A	-4.42	105.26	112.55
5	A	201	HEC	CMC-C2C-C1C	-4.35	122.08	128.46
5	A	201	HEC	CBD-CAD-C3D	-4.33	105.26	112.54
8	E	603	UF7	C11-C10-C9	-4.25	103.54	110.44
5	D	201	HEC	CMC-C2C-C1C	-3.80	122.89	128.46
5	D	201	HEC	C1D-C2D-C3D	-3.55	104.53	107.00
9	E	601	NAG	C1-O5-C5	3.30	116.60	112.19
5	D	201	HEC	O2D-CGD-O1D	-3.29	114.88	123.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	201	HEC	CMC-C2C-C3C	3.21	129.59	125.82
5	A	201	HEC	C1D-C2D-C3D	-3.16	104.80	107.00
5	D	201	HEC	CMB-C2B-C3B	3.13	129.51	125.82
5	A	201	HEC	C4C-C3C-C2C	-3.13	102.97	106.35
5	D	201	HEC	O2D-CGD-CBD	3.12	123.87	114.00
5	D	201	HEC	CMA-C3A-C2A	3.02	130.63	124.94
5	D	201	HEC	CMD-C2D-C3D	2.99	130.59	124.94
5	A	201	HEC	CMD-C2D-C3D	2.94	130.49	124.94
5	A	201	HEC	O2D-CGD-O1D	-2.90	115.86	123.33
5	A	201	HEC	CMA-C3A-C2A	2.90	130.41	124.94
5	D	201	HEC	C4C-C3C-C2C	-2.89	103.23	106.35
5	A	201	HEC	O2D-CGD-CBD	2.76	122.74	114.00
5	D	201	HEC	CMB-C2B-C1B	-2.74	124.44	128.46
5	D	201	HEC	CMC-C2C-C3C	2.72	129.02	125.82
5	A	201	HEC	CMD-C2D-C1D	-2.62	124.62	128.46
5	D	201	HEC	CAA-CBA-CGA	2.56	120.73	113.83
5	D	201	HEC	CMD-C2D-C1D	-2.55	124.71	128.46
8	E	603	UF7	C7-C6-C18	2.53	119.26	112.48
5	D	201	HEC	O2A-CGA-CBA	2.49	121.87	114.00
5	A	201	HEC	CMB-C2B-C3B	2.46	128.71	125.82
5	A	201	HEC	CMB-C2B-C1B	-2.44	124.88	128.46
5	D	201	HEC	O2A-CGA-O1A	-2.41	117.14	123.33
9	E	601	NAG	O5-C1-C2	-2.39	107.59	111.29
8	B	603	UF7	C18-C6-C5	-2.21	106.01	111.02
5	A	201	HEC	O2A-CGA-O1A	-2.20	117.68	123.33
5	D	201	HEC	C3C-C4C-NC	2.14	114.98	110.94
8	B	603	UF7	N2-C2-N1	-2.11	116.49	118.24
8	B	603	UF7	C13-C9-C10	-2.05	101.65	103.15
8	E	603	UF7	C14-C10-C9	2.04	133.04	129.72
5	A	201	HEC	O2A-CGA-CBA	2.01	120.35	114.00

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	B	603	UF7	C18-C6-C7-C8
8	B	603	UF7	C5-C6-C7-C8
8	B	603	UF7	C6-C7-C8-N6
8	B	603	UF7	C13-C9-N6-C8
8	B	603	UF7	C10-C9-N6-C8
8	E	603	UF7	C6-C7-C8-N6
8	E	603	UF7	C13-C9-N6-C8

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Mol	Chain	Res	Type	Atoms
8	E	603	UF7	C10-C9-N6-C8
8	E	603	UF7	C5-C6-C7-C8
8	E	603	UF7	C7-C8-N6-C9
8	E	603	UF7	C13-C12-C24-C25
5	D	201	HEC	CAD-CBD-CGD-O2D
5	A	201	HEC	CAD-CBD-CGD-O2D
8	B	603	UF7	C7-C8-N6-C9
5	D	201	HEC	CAD-CBD-CGD-O1D
5	A	201	HEC	CAD-CBD-CGD-O1D
5	D	201	HEC	CAA-CBA-CGA-O2A
9	E	601	NAG	O5-C5-C6-O6
5	A	201	HEC	CAA-CBA-CGA-O2A
5	D	201	HEC	CAA-CBA-CGA-O1A
5	A	201	HEC	CAA-CBA-CGA-O1A
8	E	603	UF7	C18-C6-C7-C8

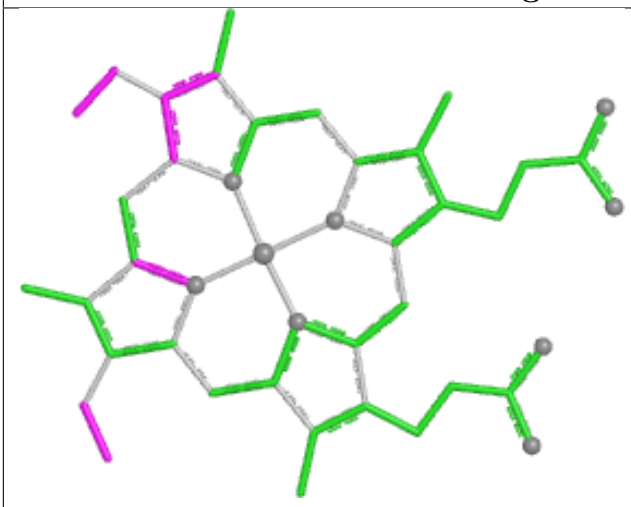
There are no ring outliers.

4 monomers are involved in 6 short contacts:

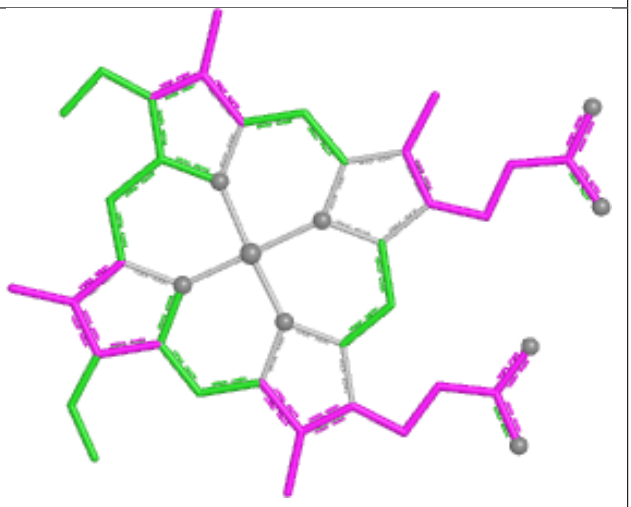
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	201	HEC	3	0
5	D	201	HEC	2	0
9	E	601	NAG	1	0
8	B	603	UF7	1	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

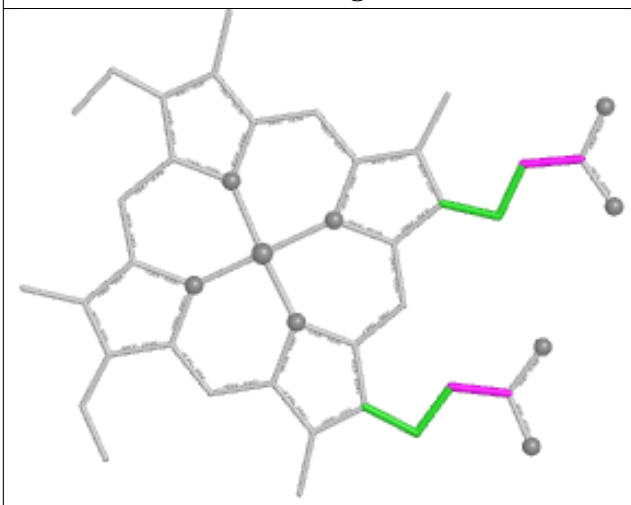
Ligand HEC A 201



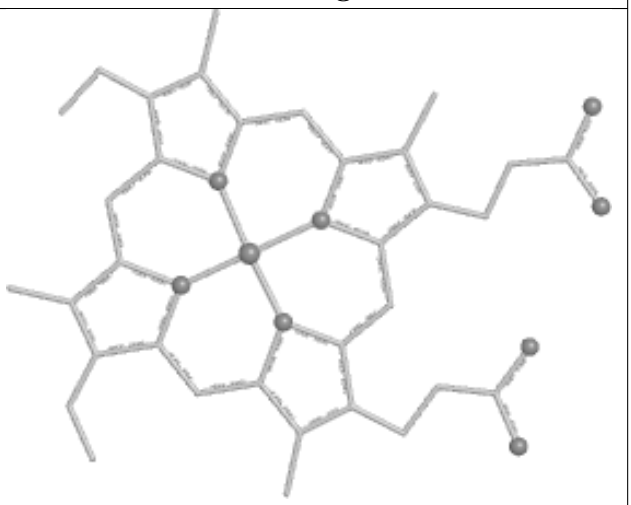
Bond lengths



Bond angles

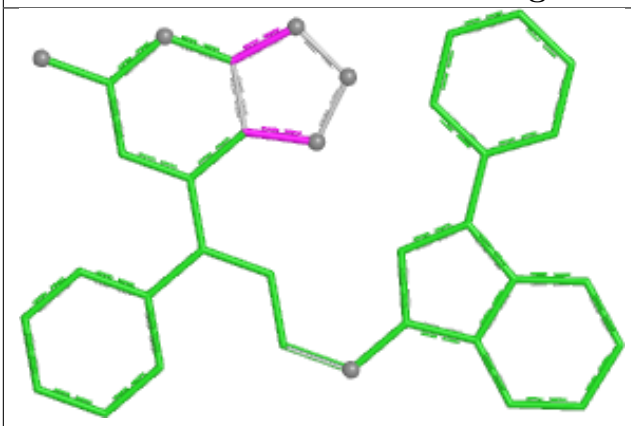


Torsions

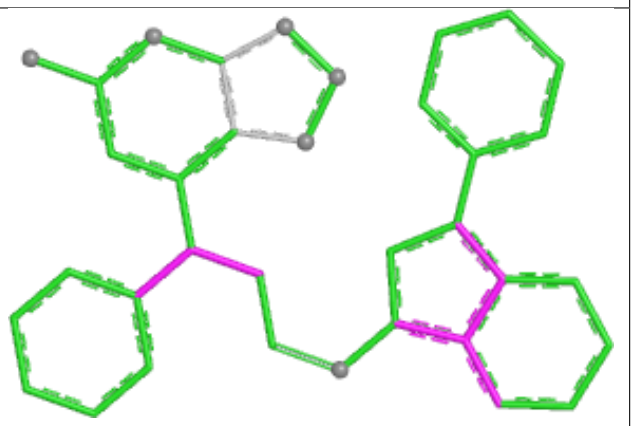


Rings

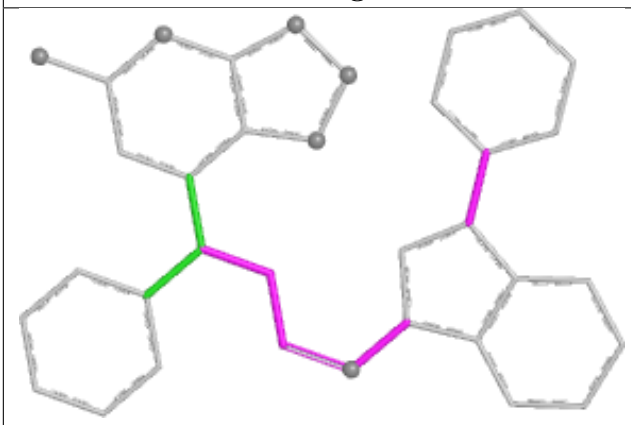
Ligand UF7 E 603



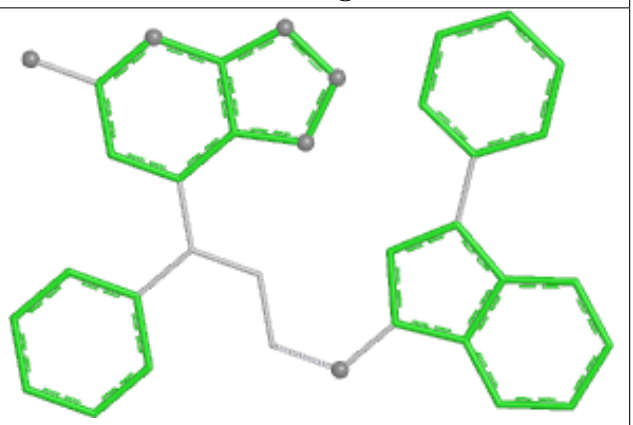
Bond lengths



Bond angles

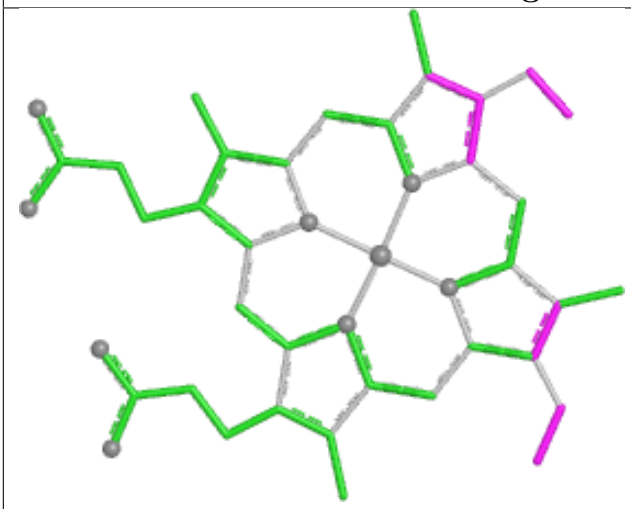


Torsions

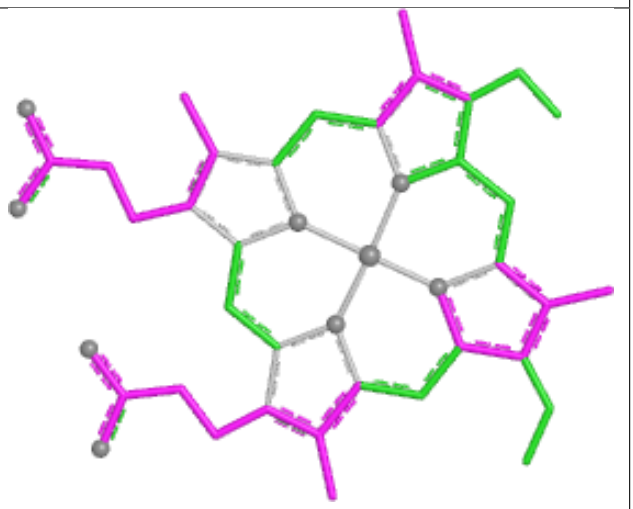


Rings

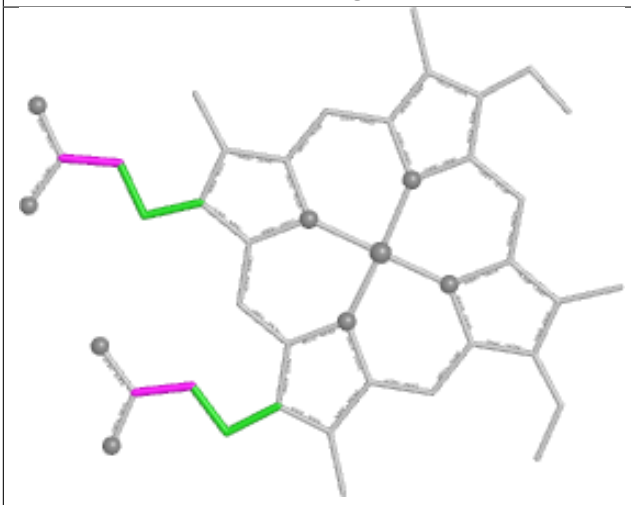
Ligand HEC D 201



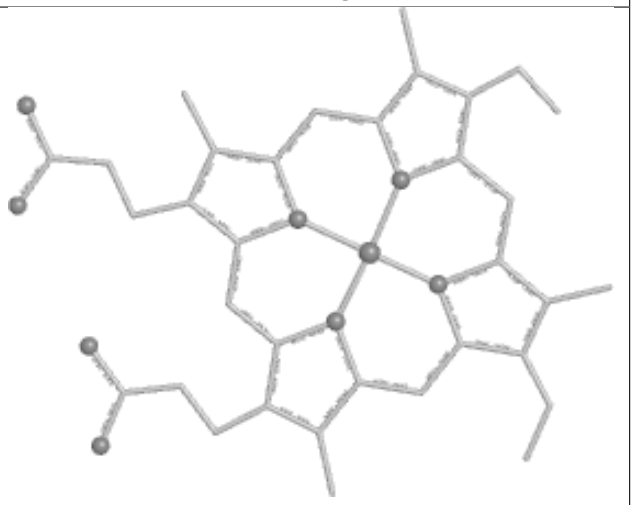
Bond lengths



Bond angles

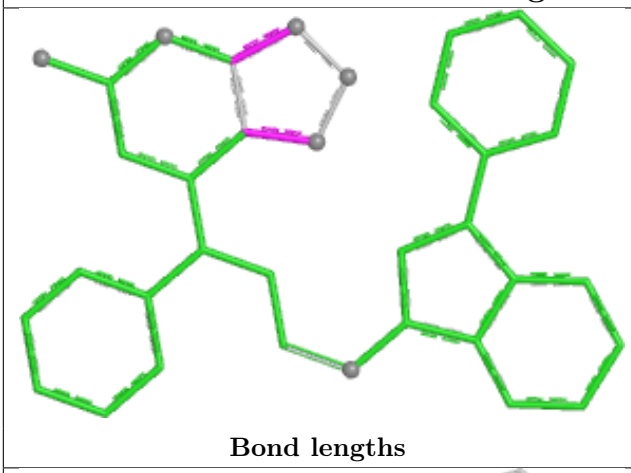


Torsions

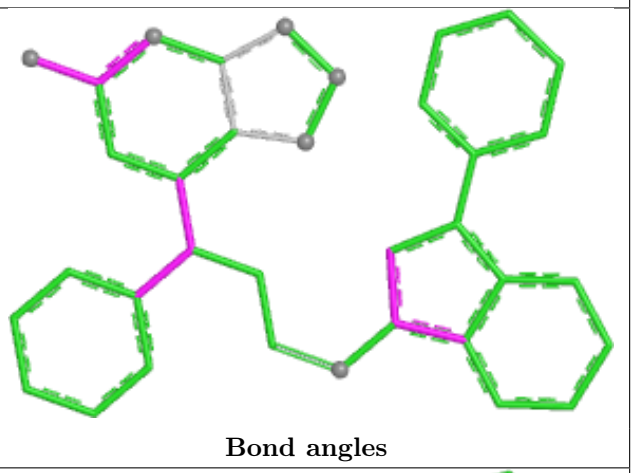


Rings

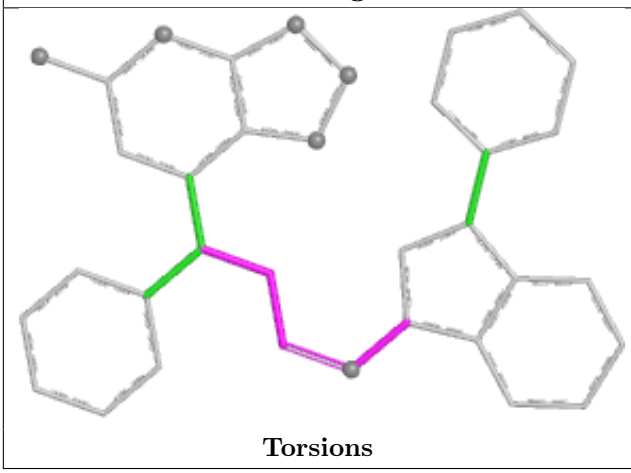
Ligand UF7 B 603



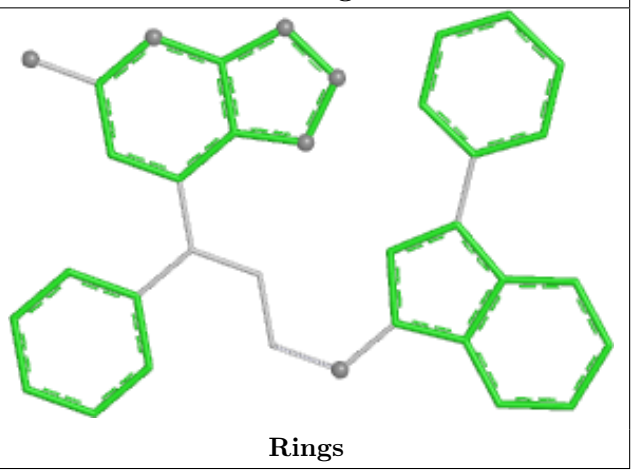
Bond lengths



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, 95^{th} 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	104/105 (99%)	0.48	9 (8%) 17 15	56, 89, 146, 153	0
1	D	104/105 (99%)	-0.03	4 (3%) 44 38	58, 79, 100, 109	0
2	B	463/467 (99%)	0.63	54 (11%) 10 9	42, 110, 172, 184	3 (0%)
2	E	464/467 (99%)	-0.03	12 (2%) 57 51	46, 88, 113, 139	7 (1%)
All	All	1135/1144 (99%)	0.28	79 (6%) 24 20	42, 94, 148, 184	10 (0%)

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	331	ALA	6.9
1	A	32	TRP	5.6
2	B	481	VAL	5.4
2	B	327	VAL	4.6
2	B	476	ILE	4.6
2	E	331	ALA	4.2
2	B	482	SER	4.1
2	B	392	ASN	4.0
2	B	337	THR	3.9
2	B	334	TYR	3.9
2	E	421	ASN	3.8
2	E	248	SER	3.8
2	B	332	PHE	3.6
1	D	30	VAL	3.6
2	B	218	ASP	3.5
2	E	207	GLY	3.5
2	B	336	HIS	3.5
2	B	253	LEU	3.4
2	B	178	GLY	3.3
2	B	430	LEU	3.2
2	B	302	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	35	ALA	3.2
2	B	474	ILE	3.1
2	B	199	VAL	3.1
2	B	477	TRP	3.1
1	A	1	CYS	3.0
2	E	477	TRP	3.0
1	D	32	TRP	2.9
2	B	165	ASN	2.9
1	A	30	VAL	2.7
2	B	546	VAL	2.7
2	B	328	PHE	2.7
2	E	245	GLU	2.7
1	A	33	LEU	2.6
2	B	335	GLY	2.6
2	B	433	TYR	2.6
2	B	120	VAL	2.5
1	A	89	TRP	2.5
2	B	352	PRO	2.5
2	B	479	GLY	2.5
2	E	327	VAL	2.5
2	E	432	GLY	2.5
2	B	197	LEU	2.5
2	B	301	LEU	2.5
2	B	362	SER	2.4
2	B	325	ALA	2.4
2	E	251	THR	2.4
2	B	543	ILE	2.4
2	B	418	PRO	2.3
1	D	80	GLN	2.3
1	A	74	ASP	2.3
2	B	487	ARG	2.3
2	B	330	ASN	2.3
2	B	545	THR	2.3
2	B	114	ASN	2.2
2	B	436	TRP	2.2
2	B	570	LEU	2.2
2	B	421	ASN	2.2
1	A	70	ARG	2.2
2	B	207	GLY	2.2
2	E	176	VAL	2.2
2	B	498	ILE	2.1
2	B	377	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	104	ALA	2.1
2	B	398	ALA	2.1
2	B	408	GLU	2.1
2	B	339	ILE	2.1
2	B	250	HIS	2.1
2	B	333	ARG	2.1
2	B	384	LEU	2.0
2	B	390	LYS	2.0
1	A	97	LEU	2.0
2	B	439	PHE	2.0
2	B	464	LEU	2.0
2	E	197	LEU	2.0
2	B	573	ALA	2.0
2	E	425	SER	2.0
2	B	551	ILE	2.0
2	B	480	GLY	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, 95^{th} 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	E	150	7/8	0.91	0.13	74,75,77,77	0
2	CSO	B	150	7/8	0.94	0.07	72,74,75,75	0

6.3 Carbohydrates (i)

SUGAR-RSR INFOmissingINFO

6.4 Ligands (i)

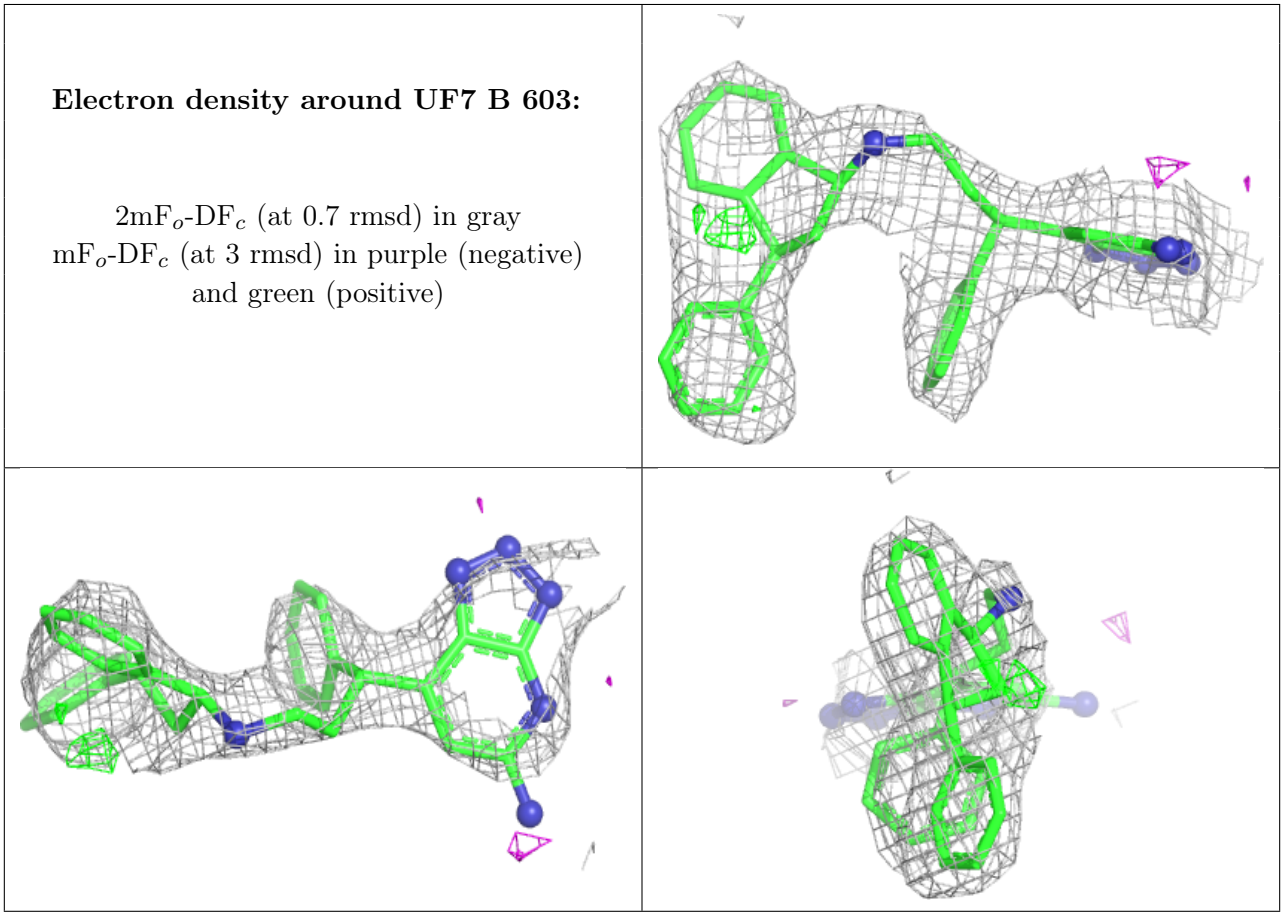
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
9	NAG	E	601	14/15	0.67	0.11	98,101,102,103	0
8	UF7	B	603	35/35	0.83	0.18	109,111,112,112	0
6	CL	B	602	1/1	0.85	0.21	112,112,112,112	0
8	UF7	E	603	35/35	0.88	0.14	76,79,89,89	0
6	CL	A	202	1/1	0.95	0.15	69,69,69,69	0
5	HEC	A	201	43/43	0.95	0.11	104,109,112,113	0
6	CL	D	202	1/1	0.95	0.18	63,63,63,63	0
5	HEC	D	201	43/43	0.98	0.07	69,73,79,84	0
7	CA	B	601	1/1	0.99	0.03	94,94,94,94	0
7	CA	E	602	1/1	1.00	0.02	62,62,62,62	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.

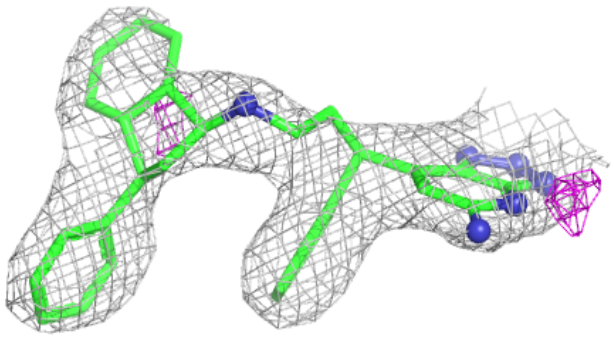
Electron density around UF7 B 603:

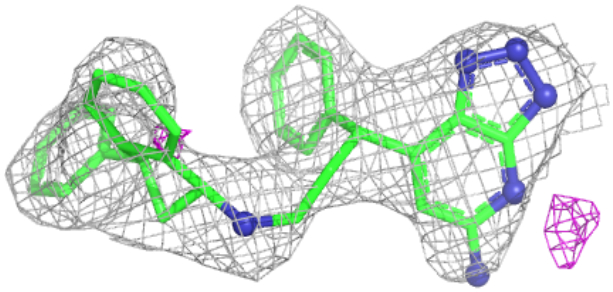
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

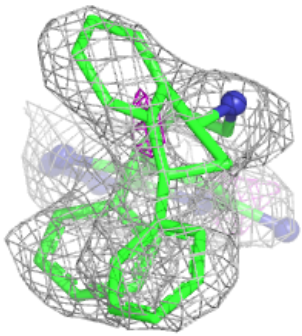


Electron density around UF7 E 603:

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

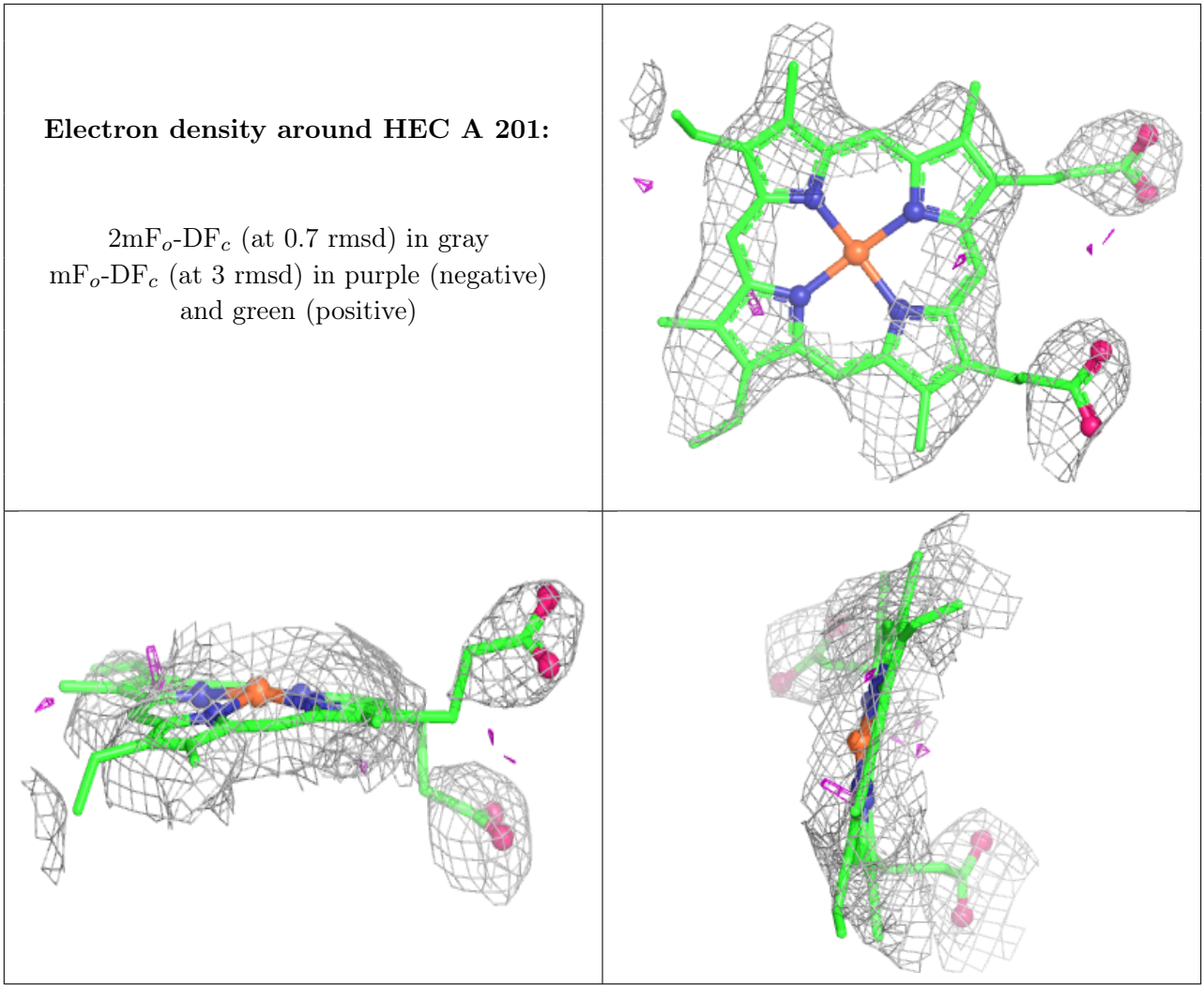






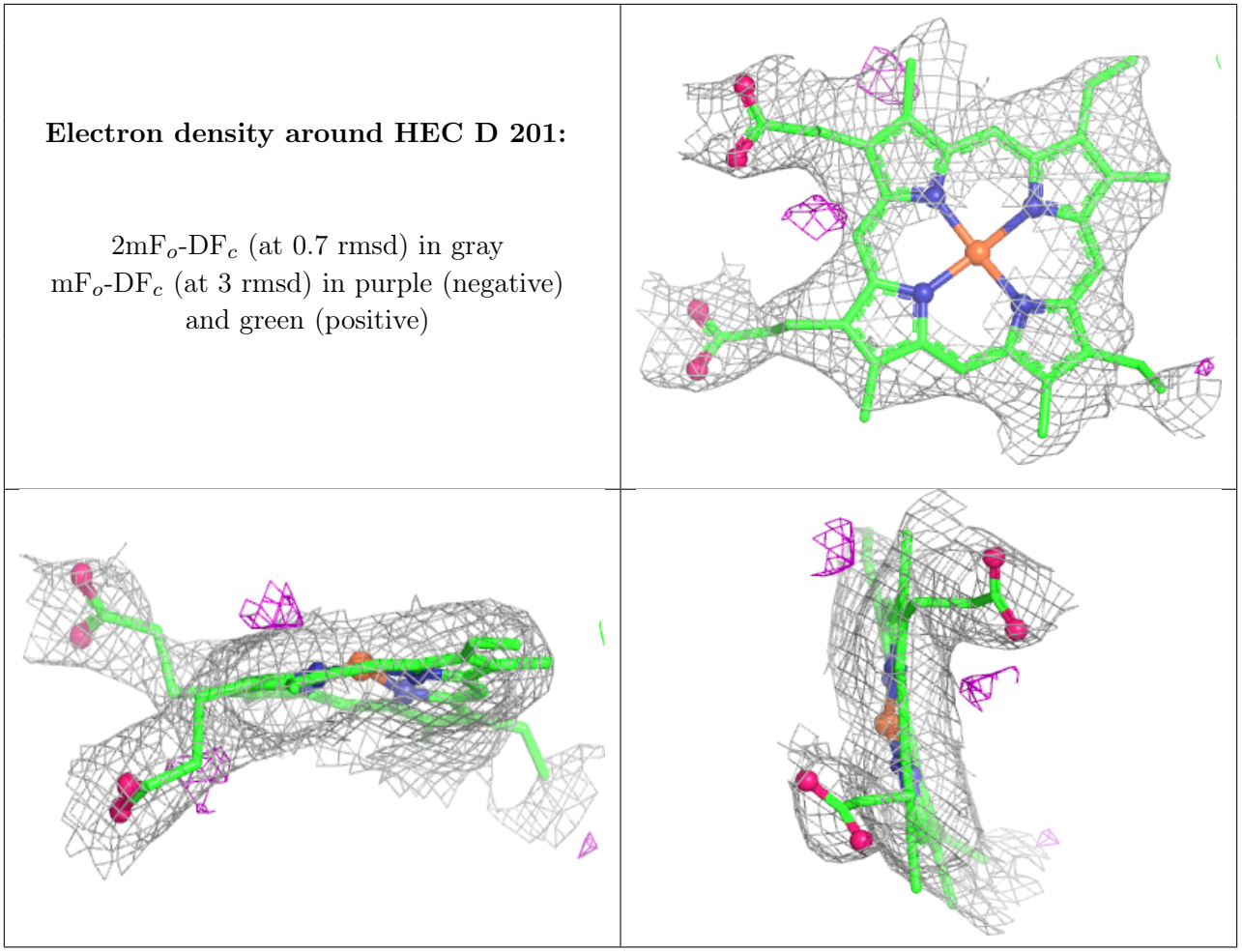
Electron density around HEC A 201:

$2mF_o$-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 D 201:

$2mF_o$-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.