



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 03:13 PM EDT

PDB ID : 6WY7 / pdb_00006wy7
Title : CRYSTAL STRUCTURE OF MYELOPEROXIDASE SUBFORM C (MPO)
COMPLEX WITH Compound-41 A.K.A 7-[1-phenyl-3-({4-phenylbicyclo[2.2.
2]octan-1-yl}amino)propyl]-3H-[1,2,3]triazolo[4,5-b]pyridin-5-amine
Authors : Khan, J.A.
Deposited on : 2020-05-12
Resolution : 2.09 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

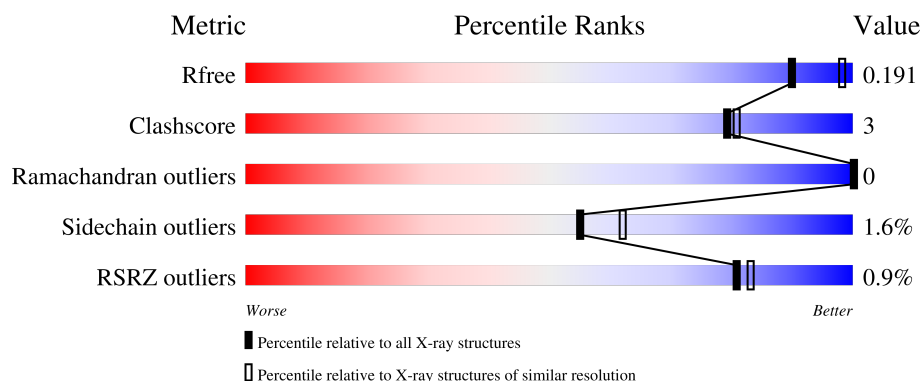
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.09 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}	180053	8172 (2.10-2.06)
Clashscore	190562	8714 (2.10-2.06)
Ramachandran outliers	187476	8641 (2.10-2.06)
Sidechain outliers	187428	8642 (2.10-2.06)
RSRZ outliers	180081	8177 (2.10-2.06)

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	5% 93% 6% ...
1	D	105	% 92% 6% ...
2	B	467	93% 6% ...
2	E	467	93% 6% ...

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Mol	Chain	Length	Quality of chain
3	C	6	
3	F	6	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	HEC	B	601	X	-	-	-
5	HEC	D	201	X	-	-	-

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 10328 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.

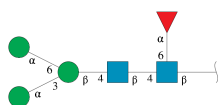
- Molecule 1 is a protein called Myeloperoxidase light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	103	Total	C	N	O	S	0	0	0
			829	525	146	153	5			
1	D	103	Total	C	N	O	S	0	0	0
			828	524	147	152	5			

- Molecule 2 is a protein called Myeloperoxidase heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	465	Total	C	N	O	S	0	0	0
			3701	2335	674	665	27			
2	E	464	Total	C	N	O	S	0	0	0
			3678	2322	668	661	27			

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	6	Total	C	N	O	0	0	0
			71	40	2	29			
3	F	6	Total	C	N	O	0	0	0
			71	40	2	29			

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

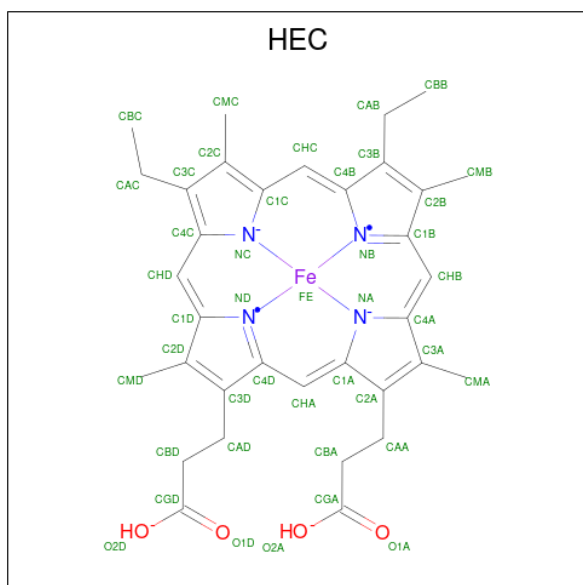
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Cl 1 1	0	0
4	E	1	Total Cl 1 1	0	0

- Molecule 5 is HEME C (CCD ID: HEC) (formula: $\text{C}_{34}\text{H}_{36}\text{FeN}_4\text{O}_4$).



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

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $\text{C}_8\text{H}_{15}\text{NO}_6$).

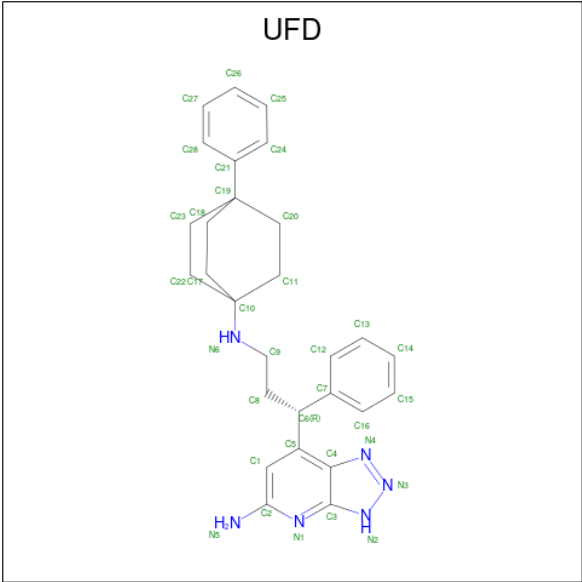


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	N	O	0	0
			14	8	1	5		
6	B	1	Total	C	N	O	0	0
			14	8	1	5		
6	E	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 8 is 7-{(1R)-1-phenyl-3-[(4-phenylbicyclo[2.2.2]octan-1-yl)amino]propyl}-3H-[1,2,3]triazolo[4,5-b]pyridin-5-amine (CCD ID: UFD) (formula: C₂₈H₃₂N₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	N	0	0
			34	28	6		
8	E	1	Total	C	N	0	0
			34	28	6		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	85	Total	O	0	0
			85	85		
9	B	385	Total	O	0	0
			385	385		
9	D	90	Total	O	0	0
			90	90		
9	E	389	Total	O	0	0
			389	389		

Chain C:  50% 50%



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

Chain F:  50% 50%



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	105.00Å 105.00Å 224.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.96 – 2.09 46.96 – 2.09	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.96-2.09) 100.0 (46.96-2.09)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.91 (at 2.08Å)	Xtriage
Refinement program	BUSTER 2.11.7 (17-DEC-2019)	Depositor
R, R_{free}	0.159 , 0.185 0.163 , 0.191	Depositor DCC
R_{free} test set	3777 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	21.8	Xtriage
Anisotropy	0.672	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 49.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10328	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% 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 ⓘ

5.1 Standard geometry ⓘ

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

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	0.73	0/854	0.96	0/1163
1	D	0.70	0/853	0.97	0/1162
2	B	0.71	1/3778 (0.0%)	0.94	1/5128 (0.0%)
2	E	0.71	1/3755 (0.0%)	0.93	1/5100 (0.0%)
All	All	0.71	2/9240 (0.0%)	0.94	2/12553 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	287	MET	SD-CE	-8.11	1.59	1.79
2	E	287	MET	SD-CE	-5.80	1.65	1.79

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	147	PHE	CA-CB-CG	5.55	119.35	113.80
2	B	147	PHE	CA-CB-CG	5.21	119.01	113.80

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	829	0	791	4	0
1	D	828	0	791	3	0
2	B	3701	0	3676	19	0
2	E	3678	0	3644	17	0
3	C	71	0	61	0	0
3	F	71	0	61	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	E	1	0	0	0	0
5	B	43	0	28	2	0
5	D	43	0	28	1	0
6	B	28	0	26	0	0
6	E	14	0	13	0	0
7	B	1	0	0	0	0
7	E	1	0	0	0	0
8	B	34	0	0	0	0
8	E	34	0	0	0	0
9	A	85	0	0	0	0
9	B	385	0	0	0	0
9	D	90	0	0	0	0
9	E	389	0	0	0	0
All	All	10328	0	9119	39	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 3.

All (39) 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:E:115:CYS:HG	2:E:125:CYS:HG	0.94	0.90
2:B:153:CYS:HG	2:E:153:CYS:HG	1.15	0.88
2:B:538:CYS:HG	2:B:564:CYS:HG	0.83	0.82
2:B:440:CYS:HG	2:B:497:CYS:HG	1.13	0.81
2:B:115:CYS:HG	2:B:125:CYS:HG	0.90	0.79
2:E:336:HIS:HD1	2:E:421:ASN:HD21	1.31	0.79
2:E:440:CYS:HG	2:E:497:CYS:HG	1.07	0.77
2:B:336:HIS:HD1	2:B:421:ASN:HD21	1.32	0.74
2:B:313:TYR:HD1	2:B:507:ARG:HD3	1.59	0.66
5:D:201:HEC:HBC2	2:E:335:GLY:HA3	1.78	0.66
2:E:313:TYR:HD1	2:E:507:ARG:HD3	1.60	0.66
1:A:3:GLU:H	1:A:3:GLU:CD	2.04	0.63
2:B:313:TYR:CD1	2:B:507:ARG:HD3	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:313:TYR:CD1	2:E:507:ARG:HD3	2.38	0.59
2:B:335:GLY:HA3	5:B:601:HEC:HBC2	1.86	0.58
2:B:535:ARG:HD3	2:B:569:ALA:HA	1.85	0.58
2:B:363:ARG:O	2:B:370:ARG:NH1	2.37	0.57
2:E:153:CYS:SG	2:E:156:SER:HB2	2.45	0.56
2:E:535:ARG:HD3	2:E:569:ALA:HA	1.88	0.55
2:B:153:CYS:SG	2:B:156:SER:HB2	2.47	0.54
2:E:538:CYS:HG	2:E:564:CYS:CB	2.22	0.52
2:B:153:CYS:CB	2:E:153:CYS:HG	2.27	0.48
1:D:83:SER:HB3	2:E:554:SER:O	2.14	0.48
2:B:440:CYS:CB	2:B:497:CYS:HG	2.27	0.47
1:A:83:SER:HB3	2:B:554:SER:O	2.15	0.47
2:E:544:THR:HA	2:E:564:CYS:SG	2.55	0.47
2:B:544:THR:HA	2:B:564:CYS:SG	2.56	0.46
2:B:347:ASP:HA	2:B:353:MET:HE3	1.98	0.45
2:E:347:ASP:HA	2:E:353:MET:HE3	1.98	0.45
2:B:115:CYS:SG	2:B:147:PHE:CD2	3.10	0.45
1:A:38:GLU:HG2	1:A:51:VAL:HG11	1.97	0.45
2:E:115:CYS:SG	2:E:147:PHE:CD2	3.10	0.44
1:D:1:CYS:SG	1:D:14:CYS:SG	3.13	0.43
1:D:38:GLU:HG2	1:D:51:VAL:HG11	2.01	0.42
1:A:90:GLY:HA3	5:B:601:HEC:HBC3	2.02	0.41
2:B:128:LEU:HB2	2:B:144:ILE:HB	2.03	0.41
2:B:411:MET:HE3	2:B:411:MET:HB3	1.96	0.41
2:E:491:VAL:HB	2:E:495:LEU:HB2	2.02	0.40
2:E:544:THR:O	2:E:564:CYS:SG	2.80	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	101/105 (96%)	100 (99%)	1 (1%)	0	100	100
1	D	101/105 (96%)	99 (98%)	2 (2%)	0	100	100
2	B	462/467 (99%)	453 (98%)	9 (2%)	0	100	100
2	E	461/467 (99%)	452 (98%)	9 (2%)	0	100	100
All	All	1125/1144 (98%)	1104 (98%)	21 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	89/90 (99%)	88 (99%)	1 (1%)	65	73
1	D	89/90 (99%)	86 (97%)	3 (3%)	32	34
2	B	402/411 (98%)	395 (98%)	7 (2%)	53	60
2	E	398/411 (97%)	393 (99%)	5 (1%)	61	68
All	All	978/1002 (98%)	962 (98%)	16 (2%)	55	62

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

Mol	Chain	Res	Type
1	A	38	GLU
2	B	115	CYS
2	B	122	GLN
2	B	175	MET
2	B	254	LEU
2	B	348	ASN
2	B	361	LEU
2	B	517	GLU
1	D	1	CYS
1	D	38	GLU
1	D	84	LEU
2	E	115	CYS
2	E	122	GLN

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Mol	Chain	Res	Type
2	E	175	MET
2	E	254	LEU
2	E	361	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	206	ASN
2	B	348	ASN
2	B	473	ASN
2	B	540	ASN
2	B	549	ASN
2	E	206	ASN
2	E	540	ASN
2	E	549	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	B	150	2	3,6,7	0.67	0	1,6,8	1.87	0
2	CSO	E	150	2	3,6,7	0.79	0	1,6,8	2.09	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 (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	E	150	CSO	CB-CA-C	-2.09	105.12	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](#)

12 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAG	C	1	2,3	14,14,15	0.35	0	17,19,21	0.97	2 (11%)
3	NAG	C	2	3	14,14,15	0.37	0	17,19,21	0.70	0
3	BMA	C	3	3	11,11,12	0.28	0	15,15,17	0.42	0
3	MAN	C	4	3	11,11,12	0.34	0	15,15,17	1.04	1 (6%)
3	MAN	C	5	3	11,11,12	0.31	0	15,15,17	0.74	1 (6%)
3	FUC	C	6	3	10,10,11	0.44	0	14,14,16	0.62	0
3	NAG	F	1	2,3	14,14,15	0.31	0	17,19,21	0.98	2 (11%)
3	NAG	F	2	3	14,14,15	0.30	0	17,19,21	0.64	0
3	BMA	F	3	3	11,11,12	0.25	0	15,15,17	0.45	0
3	MAN	F	4	3	11,11,12	0.33	0	15,15,17	0.99	1 (6%)
3	MAN	F	5	3	11,11,12	0.29	0	15,15,17	0.76	1 (6%)
3	FUC	F	6	3	10,10,11	0.34	0	14,14,16	0.61	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	2,3	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	-	0/6/23/26	0/1/1/1
3	BMA	C	3	3	-	0/2/19/22	0/1/1/1
3	MAN	C	4	3	-	0/2/19/22	0/1/1/1
3	MAN	C	5	3	-	0/2/19/22	0/1/1/1
3	FUC	C	6	3	-	-	0/1/1/1
3	NAG	F	1	2,3	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	0/6/23/26	0/1/1/1
3	BMA	F	3	3	-	0/2/19/22	0/1/1/1
3	MAN	F	4	3	-	0/2/19/22	0/1/1/1
3	MAN	F	5	3	-	0/2/19/22	0/1/1/1
3	FUC	F	6	3	-	-	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	C	4	MAN	C1-O5-C5	3.69	117.13	112.19
3	F	4	MAN	C1-O5-C5	3.50	116.88	112.19
3	C	1	NAG	O5-C1-C2	-2.66	107.17	111.29
3	F	1	NAG	O5-C1-C2	-2.64	107.20	111.29
3	F	5	MAN	C1-O5-C5	2.57	115.63	112.19
3	C	5	MAN	C1-O5-C5	2.36	115.34	112.19
3	F	1	NAG	C1-O5-C5	2.17	115.09	112.19
3	C	1	NAG	C1-O5-C5	2.08	114.97	112.19

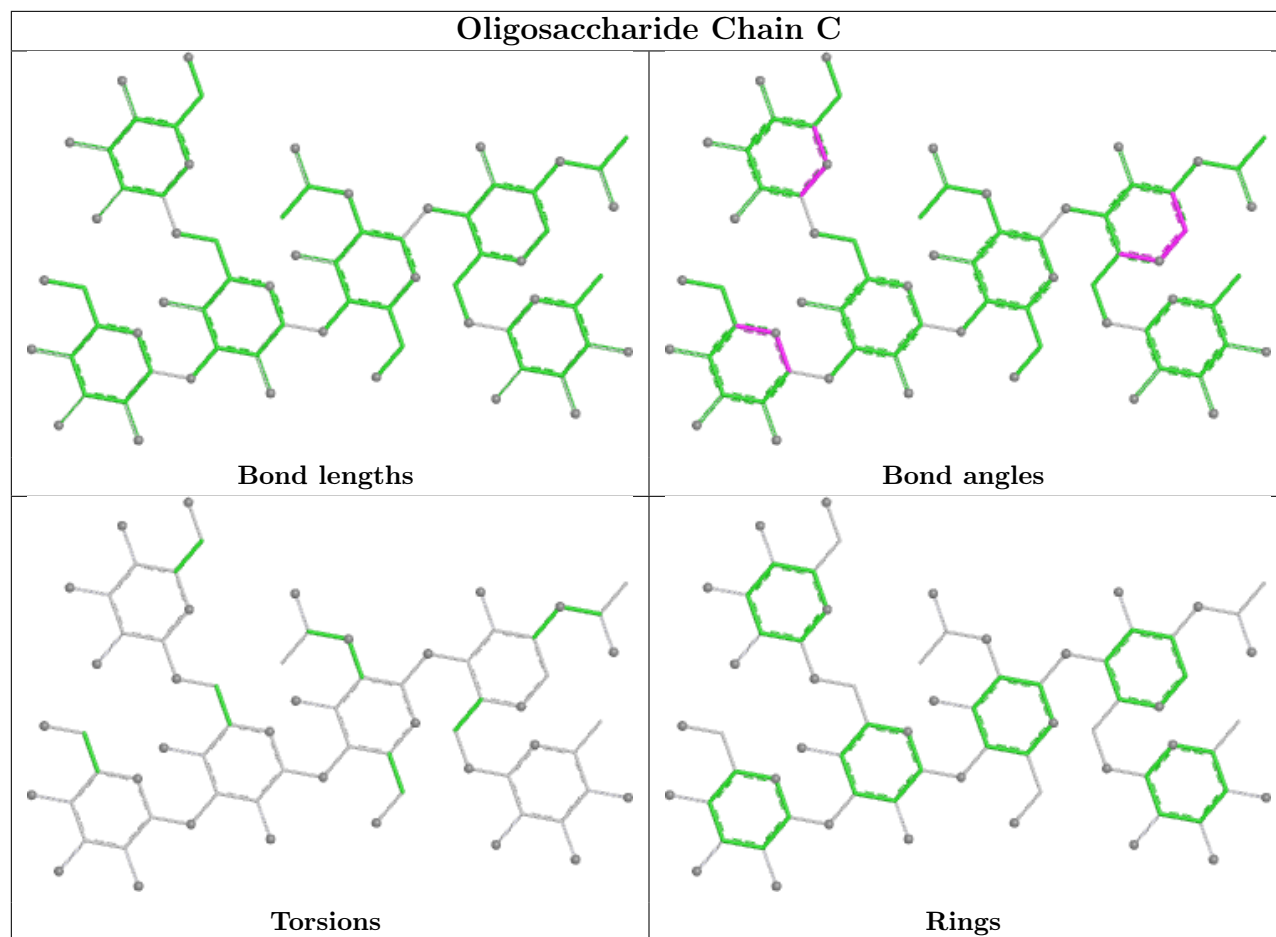
There are no chirality outliers.

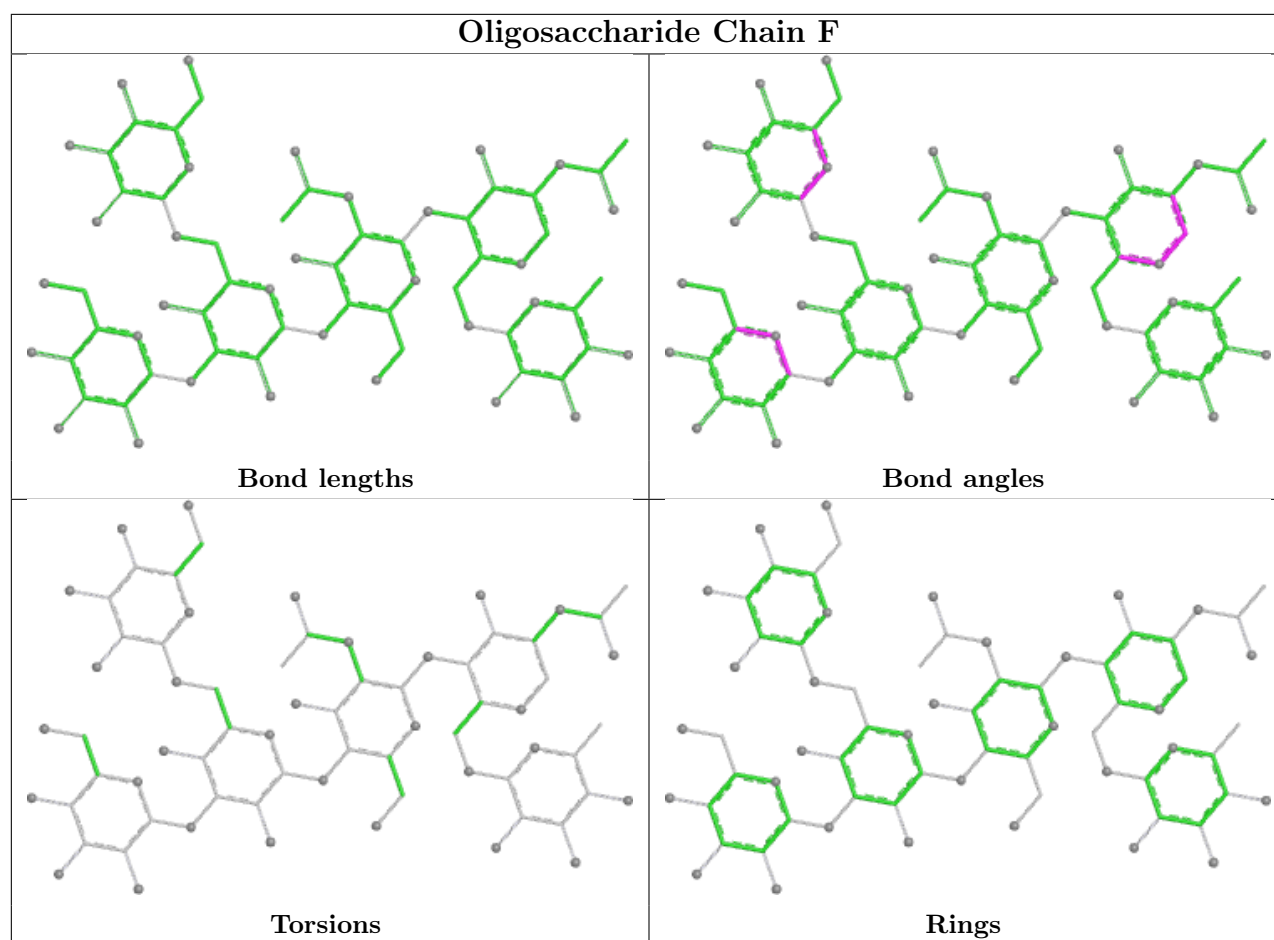
There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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





5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 5 are monoatomic - leaving 7 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	NAG	B	602	2	14,14,15	0.29	0	17,19,21	0.73	1 (5%)
8	UFD	B	606	-	39,39,39	0.67	2 (5%)	50,57,57	1.52	6 (12%)
6	NAG	B	603	2	14,14,15	0.30	0	17,19,21	0.98	1 (5%)
8	UFD	E	604	-	39,39,39	0.54	0	50,57,57	1.44	4 (8%)
5	HEC	D	201	1,2	50,50,50	1.49	10 (20%)	68,82,82	1.91	17 (25%)
6	NAG	E	601	2	14,14,15	0.26	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
5	HEC	B	601	1,2	50,50,50	1.49	10 (20%)	68,82,82	1.87	16 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	B	602	2	-	0/6/23/26	0/1/1/1
8	UFD	B	606	-	-	3/21/42/42	0/7/6/6
6	NAG	B	603	2	-	0/6/23/26	0/1/1/1
8	UFD	E	604	-	-	6/21/42/42	0/7/6/6
5	HEC	D	201	1,2	1/1/3/7	8/14/54/54	-
6	NAG	E	601	2	-	0/6/23/26	0/1/1/1
5	HEC	B	601	1,2	1/1/3/7	8/14/54/54	-

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	201	HEC	CBC-CAC	-4.21	1.33	1.51
5	D	201	HEC	CBB-CAB	-3.68	1.35	1.51
5	B	601	HEC	CBC-CAC	-3.44	1.36	1.51
5	B	601	HEC	CBB-CAB	-3.42	1.37	1.51
5	B	601	HEC	C4B-NB	-2.95	1.35	1.40
5	B	601	HEC	C4B-C3B	2.88	1.49	1.45
8	B	606	UFD	C4-N4	2.75	1.43	1.38
5	D	201	HEC	C1D-C2D	2.60	1.49	1.44
5	B	601	HEC	C1D-C2D	2.59	1.49	1.44
5	D	201	HEC	C1A-C2A	-2.56	1.40	1.45
5	D	201	HEC	C1B-NB	-2.54	1.33	1.38
5	B	601	HEC	C1D-ND	-2.51	1.35	1.40
5	B	601	HEC	C1A-C2A	-2.47	1.40	1.45
5	B	601	HEC	CMD-C2D	2.42	1.55	1.50
5	B	601	HEC	CBA-CAA	2.35	1.60	1.51
5	D	201	HEC	C1D-ND	-2.27	1.36	1.40
5	D	201	HEC	C4B-NB	-2.25	1.36	1.40
5	D	201	HEC	C4B-C3B	2.18	1.48	1.45
5	D	201	HEC	C4C-NC	-2.17	1.35	1.39
5	D	201	HEC	CBA-CGA	2.11	1.55	1.50
8	B	606	UFD	N2-N3	2.09	1.42	1.34
5	B	601	HEC	CHC-C4B	-2.02	1.34	1.38

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	606	UFD	N2-C3-N1	7.54	131.85	125.64
8	E	604	UFD	N2-C3-N1	6.89	131.31	125.64
5	B	601	HEC	CBC-CAC-C3C	6.74	130.68	112.42
5	D	201	HEC	CBC-CAC-C3C	6.43	129.84	112.42
5	B	601	HEC	CBB-CAB-C3B	5.80	128.14	112.42
5	D	201	HEC	CBB-CAB-C3B	5.48	127.27	112.42
5	D	201	HEC	O2D-CGD-O1D	-3.84	113.45	123.33
6	B	603	NAG	C1-O5-C5	3.76	117.22	112.19
8	E	604	UFD	C4-C3-N1	-3.69	122.93	126.55
8	B	606	UFD	C4-C3-N1	-3.65	122.98	126.55
8	E	604	UFD	C3-N2-N3	-3.57	109.20	111.18
5	B	601	HEC	C2B-C1B-NB	3.48	113.92	109.90
5	D	201	HEC	CAC-C3C-C2C	3.38	132.24	126.89
5	B	601	HEC	CAC-C3C-C2C	3.29	132.09	126.89
5	D	201	HEC	O2A-CGA-O1A	-3.23	115.02	123.33
5	B	601	HEC	O2D-CGD-O1D	-3.14	115.27	123.33
5	D	201	HEC	C2B-C1B-NB	3.13	113.53	109.90
5	B	601	HEC	CHB-C1B-C2B	-3.12	120.10	125.03
5	D	201	HEC	CHB-C1B-C2B	-3.08	120.17	125.03
5	B	601	HEC	CHA-C4D-ND	2.93	127.58	124.42
8	B	606	UFD	C3-N2-N3	-2.85	109.59	111.18
5	D	201	HEC	CHA-C4D-ND	2.79	127.43	124.42
5	D	201	HEC	C3B-C4B-NB	2.67	113.10	110.17
5	D	201	HEC	CMD-C2D-C1D	2.64	129.16	125.03
5	D	201	HEC	O2A-CGA-CBA	2.52	121.97	114.00
5	B	601	HEC	CHA-C4D-C3D	-2.39	121.30	124.77
6	B	602	NAG	C1-O5-C5	2.38	115.38	112.19
5	D	201	HEC	C1A-CHA-C4D	-2.37	120.97	126.02
5	D	201	HEC	CHA-C4D-C3D	-2.37	121.32	124.77
8	B	606	UFD	C11-C10-C22	-2.36	106.63	108.84
5	D	201	HEC	CHC-C4B-C3B	-2.36	120.87	125.23
8	E	604	UFD	C8-C6-C5	2.35	117.29	112.69
5	D	201	HEC	C1D-C2D-C3D	-2.29	104.57	106.98
5	B	601	HEC	O2A-CGA-O1A	-2.28	117.47	123.33
5	B	601	HEC	C1D-C2D-C3D	-2.27	104.59	106.98
5	B	601	HEC	C3B-C4B-NB	2.26	112.65	110.17
6	E	601	NAG	C1-O5-C5	2.21	115.15	112.19
5	B	601	HEC	CHC-C4B-C3B	-2.20	121.16	125.23
5	D	201	HEC	O2D-CGD-CBD	2.17	120.85	114.00
8	B	606	UFD	C8-C6-C5	2.17	116.93	112.69
5	B	601	HEC	CMD-C2D-C1D	2.11	128.33	125.03
5	B	601	HEC	O2D-CGD-CBD	2.10	120.64	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	606	UFD	C8-C9-N6	2.07	115.35	111.89
5	B	601	HEC	C2D-C1D-ND	2.06	112.21	109.84
5	D	201	HEC	C4B-C3B-C2B	-2.05	103.90	106.89
5	B	601	HEC	C3C-C4C-NC	2.04	112.42	110.15

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	B	601	HEC	NA
5	D	201	HEC	NA

All (25) torsion outliers are listed below:

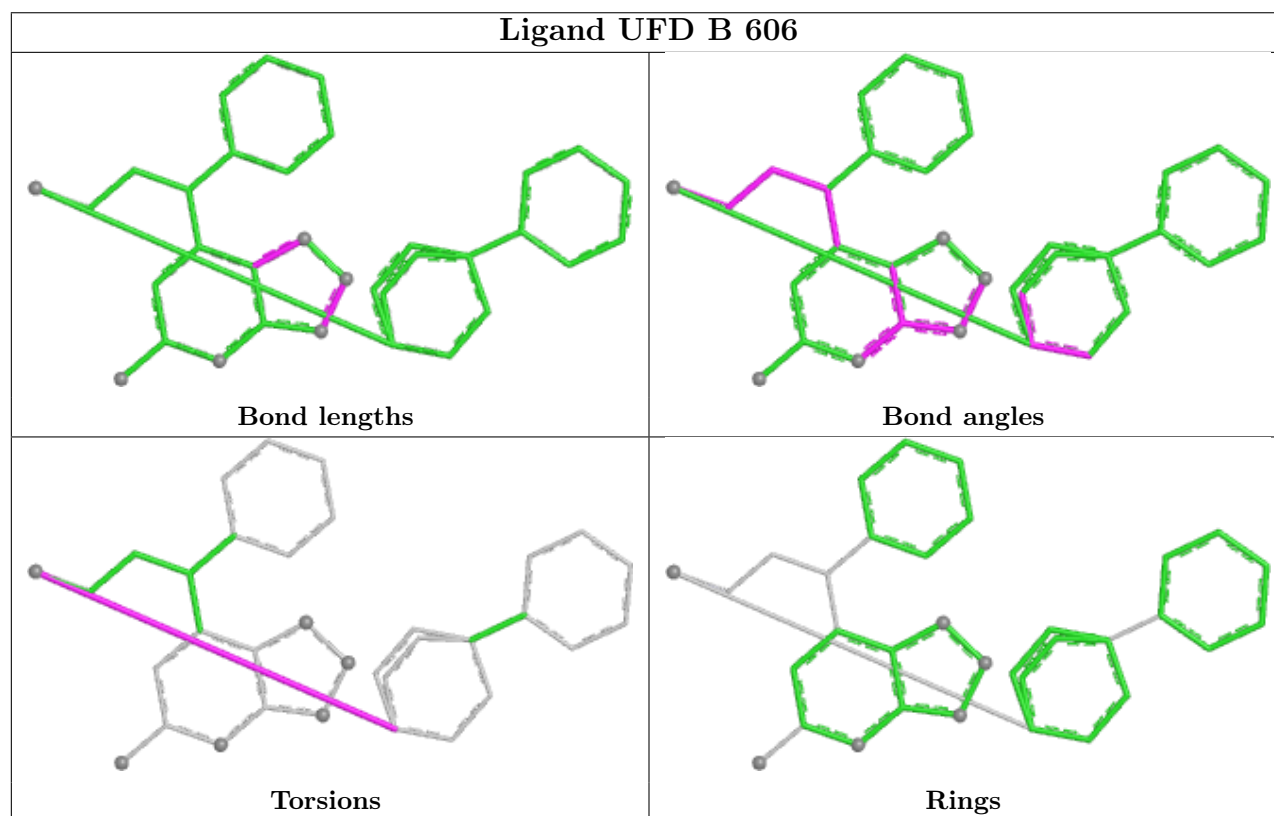
Mol	Chain	Res	Type	Atoms
5	D	201	HEC	C4B-C3B-CAB-CBB
5	D	201	HEC	C2B-C3B-CAB-CBB
5	B	601	HEC	C4B-C3B-CAB-CBB
5	B	601	HEC	C2B-C3B-CAB-CBB
5	B	601	HEC	C4C-C3C-CAC-CBC
5	D	201	HEC	C4C-C3C-CAC-CBC
5	B	601	HEC	C2C-C3C-CAC-CBC
5	D	201	HEC	C2C-C3C-CAC-CBC
8	B	606	UFD	C17-C10-N6-C9
8	E	604	UFD	C18-C19-C21-C28
8	E	604	UFD	C20-C19-C21-C28
8	E	604	UFD	C18-C19-C21-C24
8	E	604	UFD	C20-C19-C21-C24
8	E	604	UFD	C23-C19-C21-C28
8	E	604	UFD	C23-C19-C21-C24
5	B	601	HEC	CAD-CBD-CGD-O2D
5	B	601	HEC	CAD-CBD-CGD-O1D
5	D	201	HEC	CAD-CBD-CGD-O1D
5	D	201	HEC	CAD-CBD-CGD-O2D
8	B	606	UFD	C11-C10-N6-C9
5	B	601	HEC	CAA-CBA-CGA-O2A
5	D	201	HEC	CAA-CBA-CGA-O1A
5	D	201	HEC	CAA-CBA-CGA-O2A
5	B	601	HEC	CAA-CBA-CGA-O1A
8	B	606	UFD	C22-C10-N6-C9

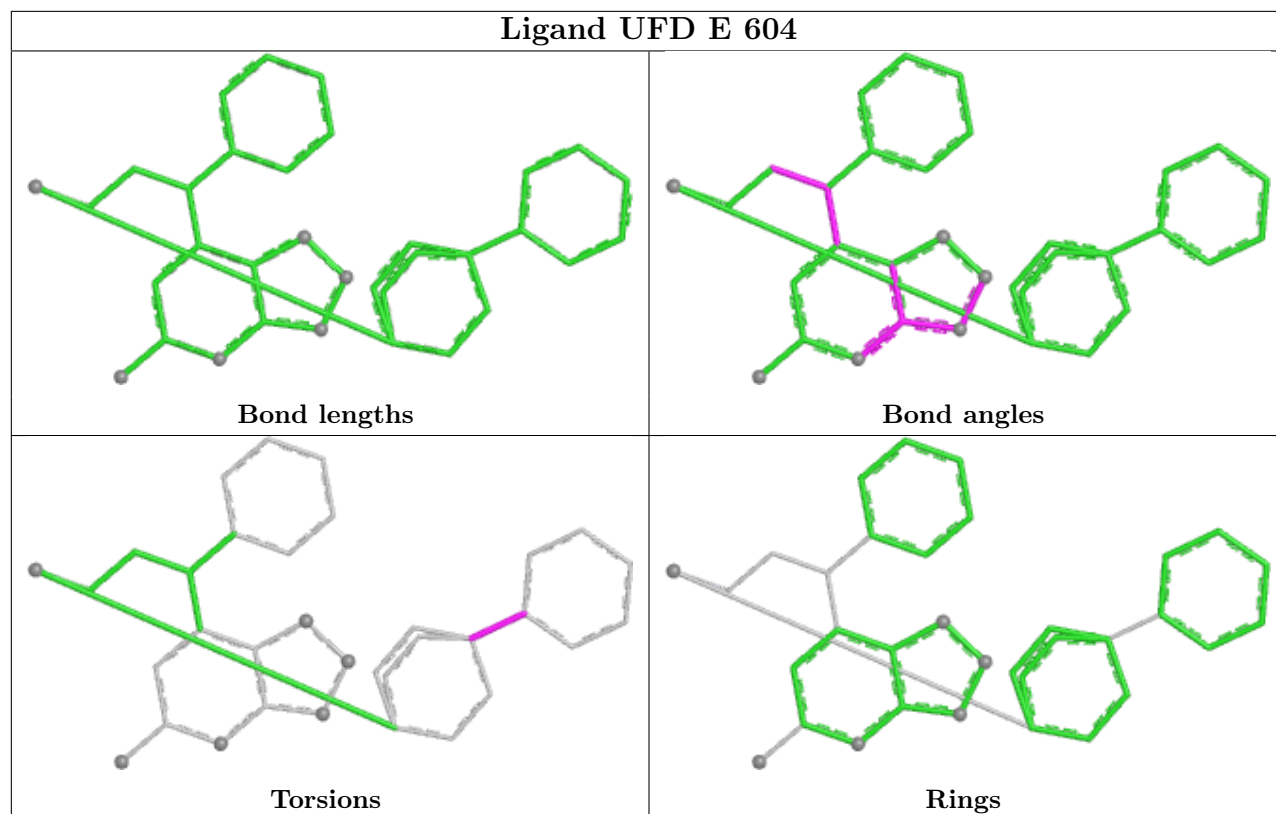
There are no ring outliers.

2 monomers are involved in 3 short contacts:

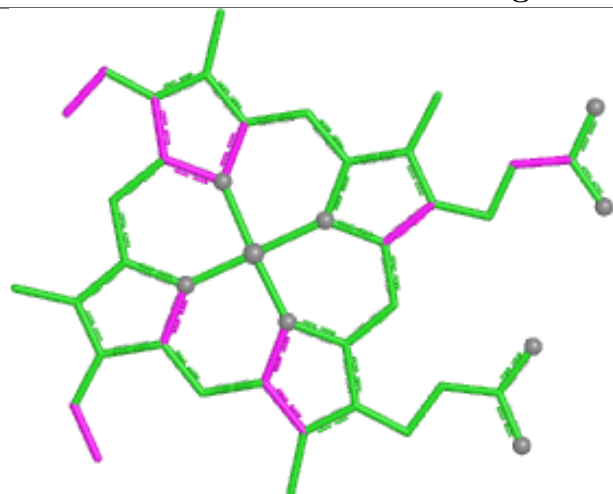
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	201	HEC	1	0
5	B	601	HEC	2	0

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

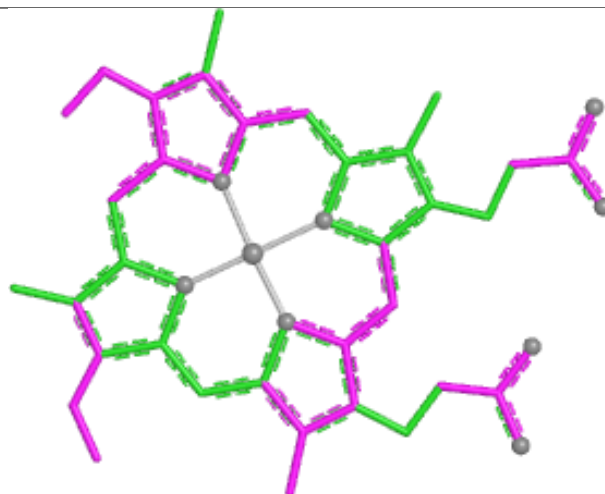




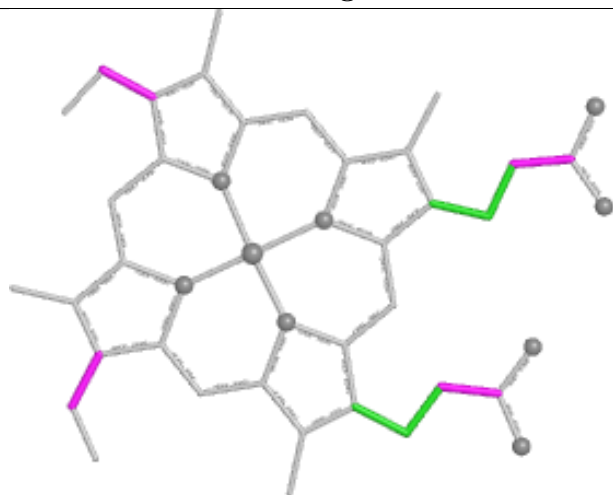
Ligand HEC D 201



Bond lengths



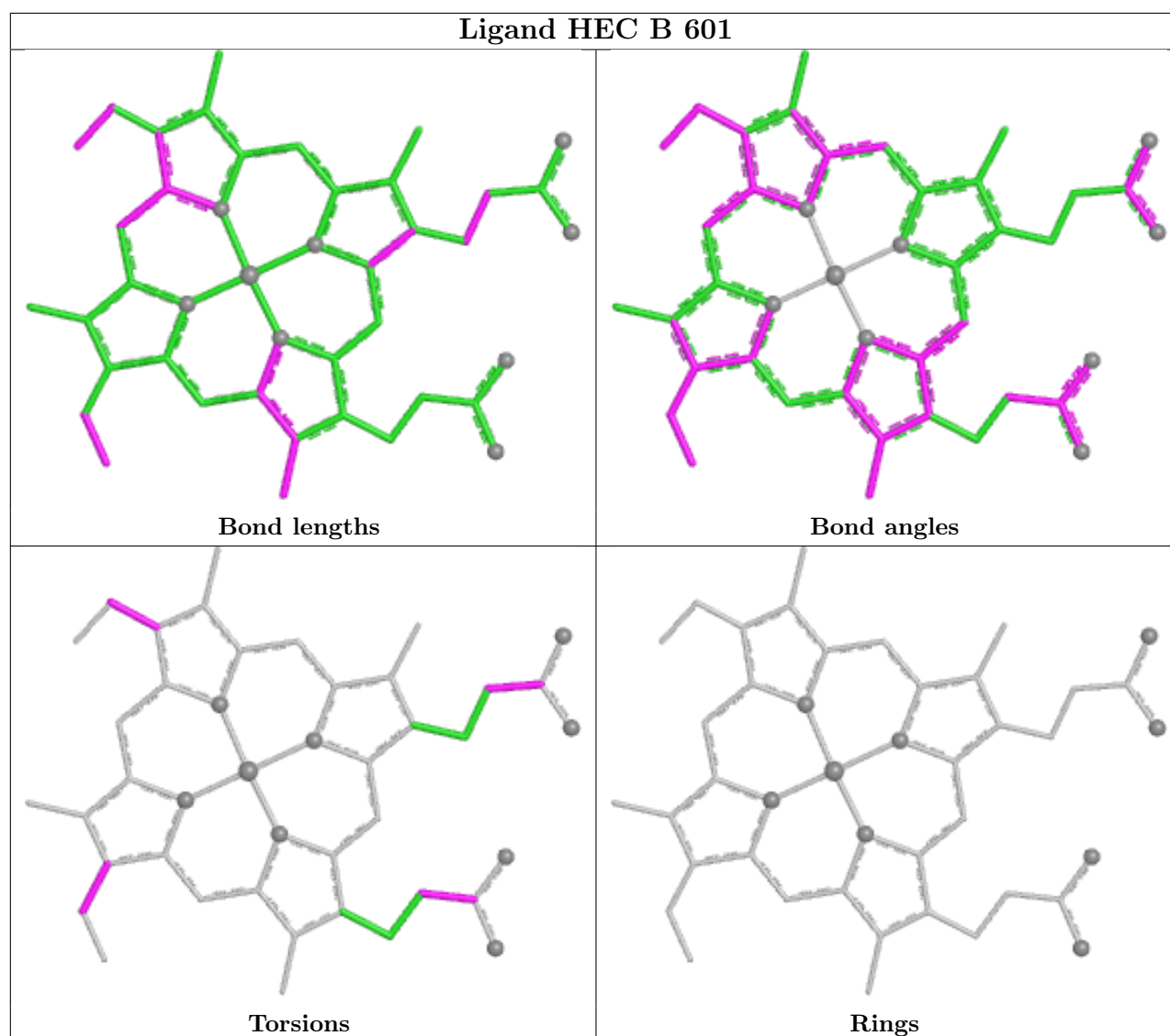
Bond angles



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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	-0.39	5 (4%) 35 36	15, 21, 40, 63	0
1	D	103/105 (98%)	-0.44	1 (0%) 79 82	14, 20, 38, 50	0
2	B	464/467 (99%)	-0.48	2 (0%) 88 90	14, 22, 37, 50	0
2	E	463/467 (99%)	-0.48	2 (0%) 88 90	14, 21, 35, 46	0
All	All	1133/1144 (99%)	-0.47	10 (0%) 81 83	14, 22, 37, 63	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	355	PRO	3.0
1	A	2	PRO	2.8
1	D	1	CYS	2.8
2	E	216	LEU	2.4
1	A	3	GLU	2.3
2	E	569	ALA	2.3
2	B	155	GLY	2.2
1	A	4	GLN	2.2
1	A	1	CYS	2.1
1	A	80	GLN	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	E	150	7/8	0.96	0.07	19,21,26,27	0
2	CSO	B	150	7/8	0.98	0.04	19,20,25,25	0

6.3 Carbohydrates ⓘ

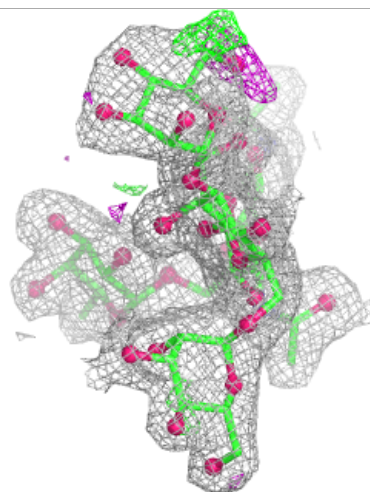
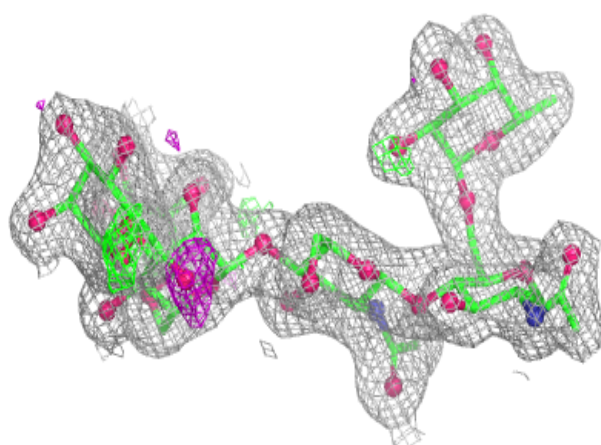
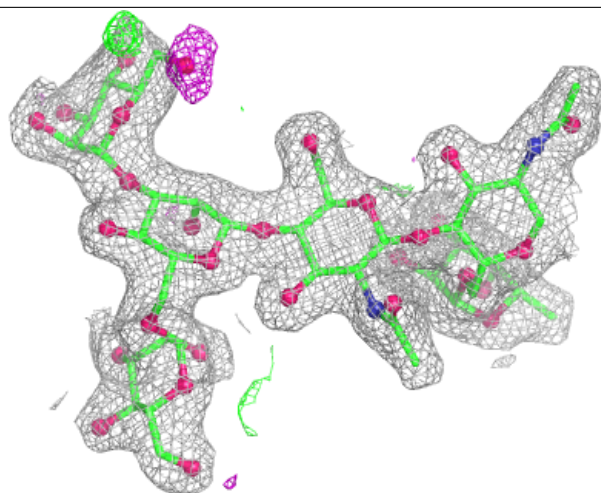
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

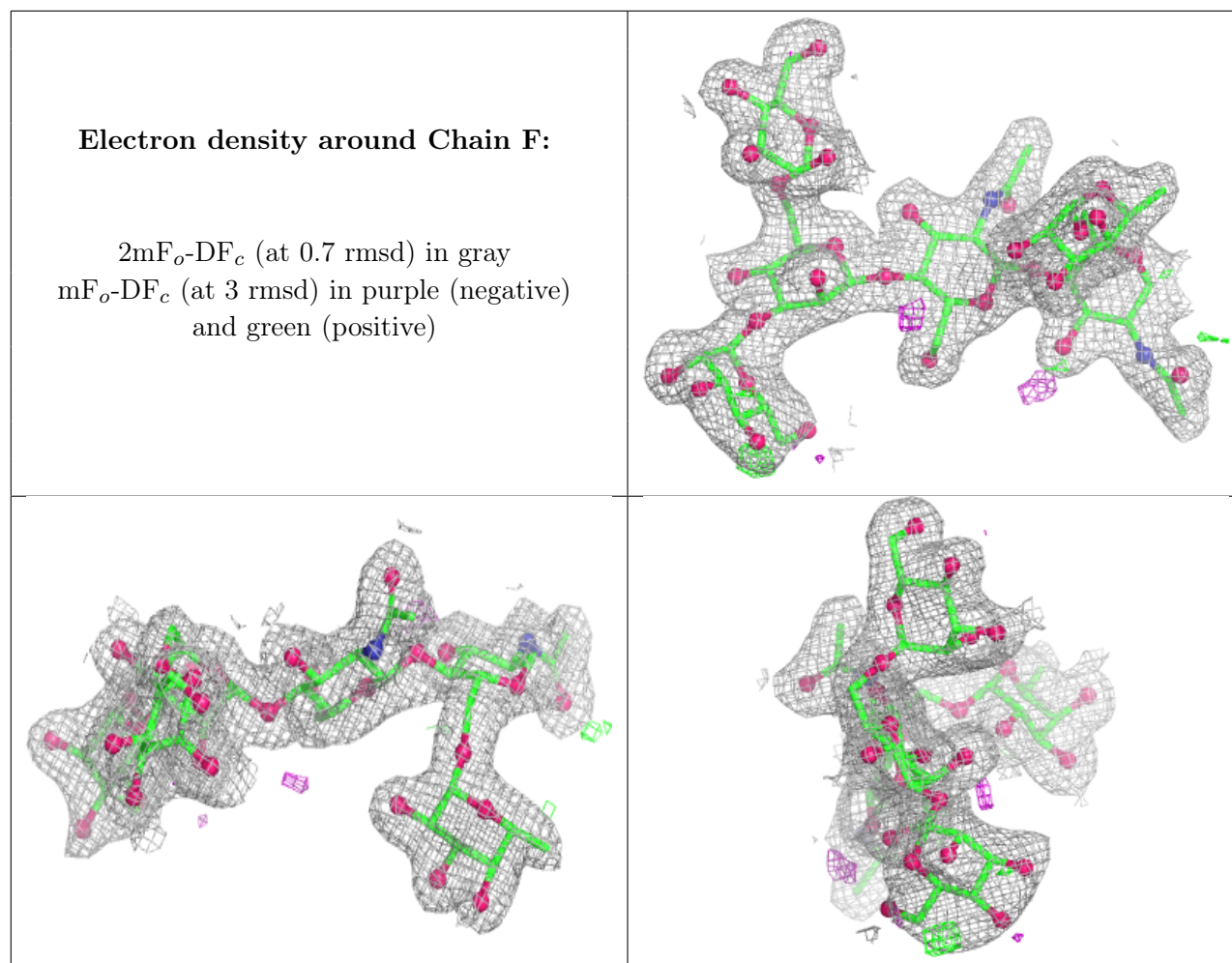
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	C	1	14/15	-	-	20,21,23,23	0
3	NAG	C	2	14/15	-	-	18,20,21,22	0
3	BMA	C	3	11/12	-	-	23,24,27,31	0
3	MAN	C	4	11/12	-	-	35,38,40,42	0
3	MAN	C	5	11/12	-	-	25,26,27,28	0
3	FUC	C	6	10/11	-	-	22,23,23,23	0
3	MAN	F	4	11/12	0.75	0.12	38,41,44,44	0
3	MAN	F	5	11/12	0.95	0.05	25,26,26,27	0
3	FUC	F	6	10/11	0.95	0.06	22,23,24,25	0
3	BMA	F	3	11/12	0.96	0.05	25,26,29,33	0
3	NAG	F	1	14/15	0.96	0.06	19,21,23,23	0
3	NAG	F	2	14/15	0.98	0.04	19,20,21,23	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 C:

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





6.4 Ligands [i](#)

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

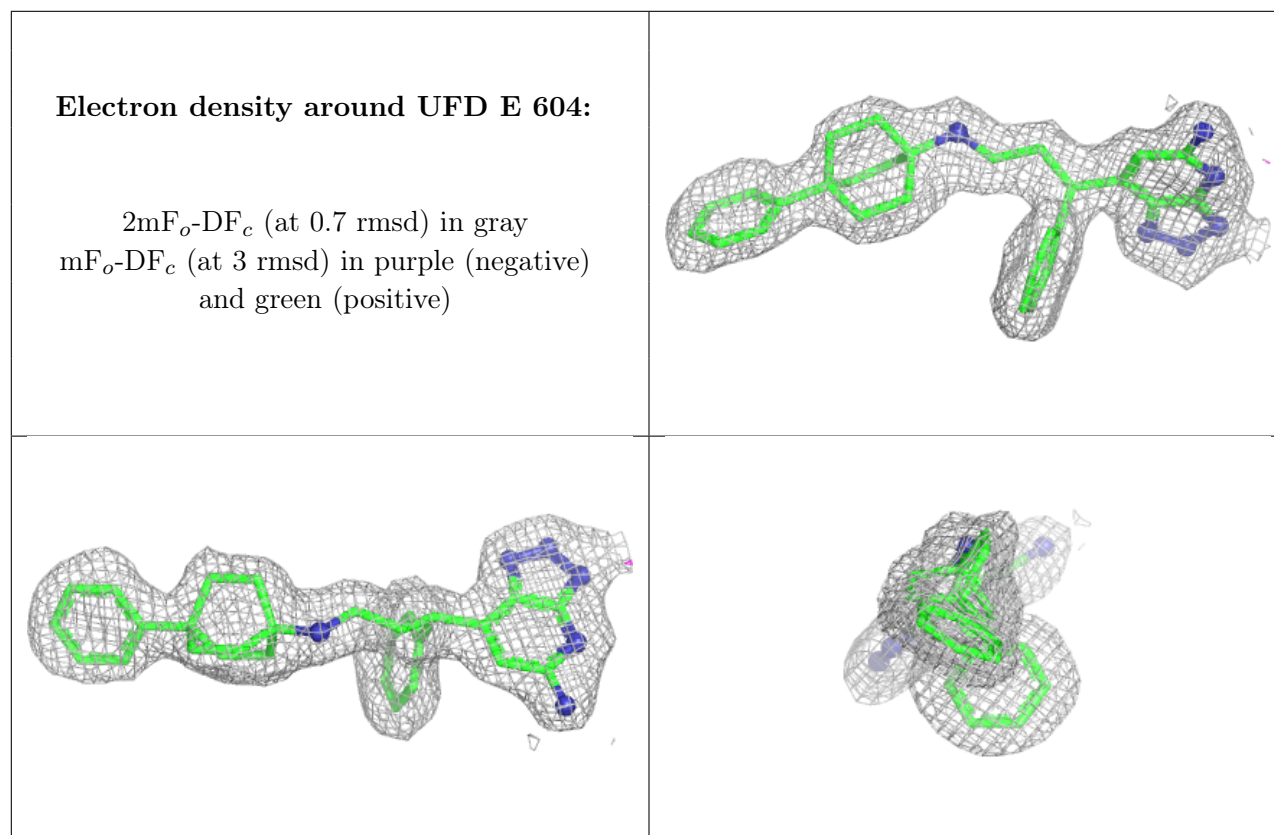
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	NAG	B	603	14/15	0.82	0.12	41,43,44,44	0
6	NAG	B	602	14/15	0.89	0.08	31,35,37,37	0
6	NAG	E	601	14/15	0.93	0.06	34,36,38,39	0
8	UFD	E	604	34/34	0.93	0.08	22,24,27,28	0
8	UFD	B	606	34/34	0.94	0.07	21,22,23,23	0
4	CL	E	603	1/1	0.97	0.19	35,35,35,35	0
4	CL	B	605	1/1	0.97	0.24	42,42,42,42	0
5	HEC	D	201	43/43	0.98	0.05	15,18,22,27	0
5	HEC	B	601	43/43	0.98	0.05	16,18,21,25	0
7	CA	E	602	1/1	0.99	0.02	16,16,16,16	0

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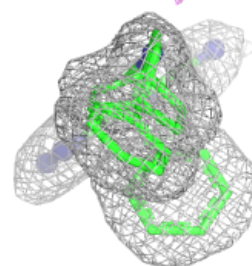
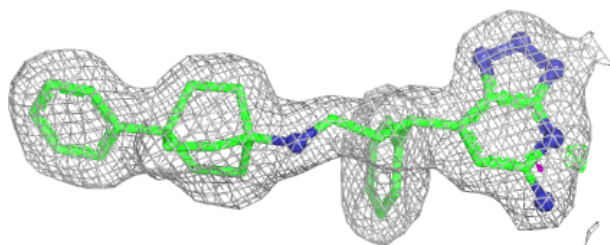
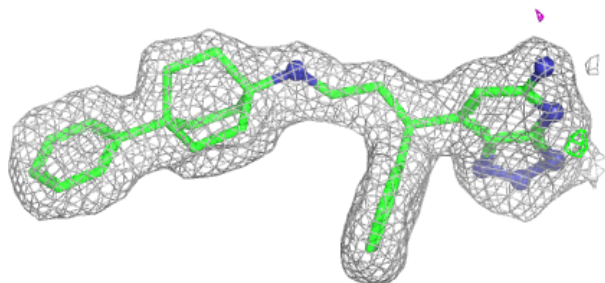
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	CA	B	604	1/1	1.00	0.02	17,17,17,17	0
4	CL	A	201	1/1	1.00	0.02	16,16,16,16	0

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.



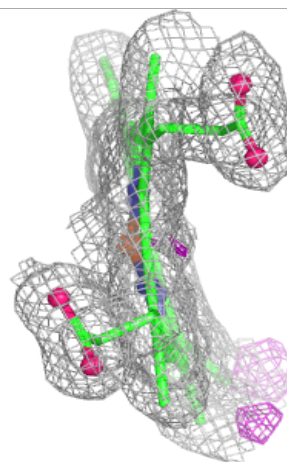
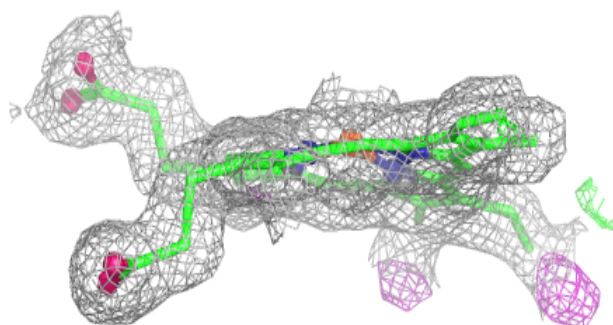
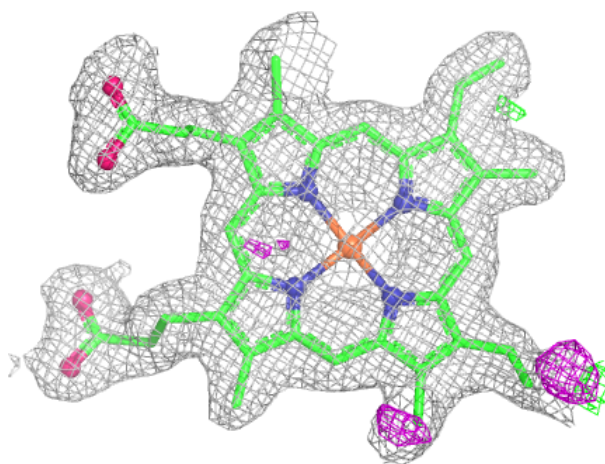
Electron density around UFD B 606:

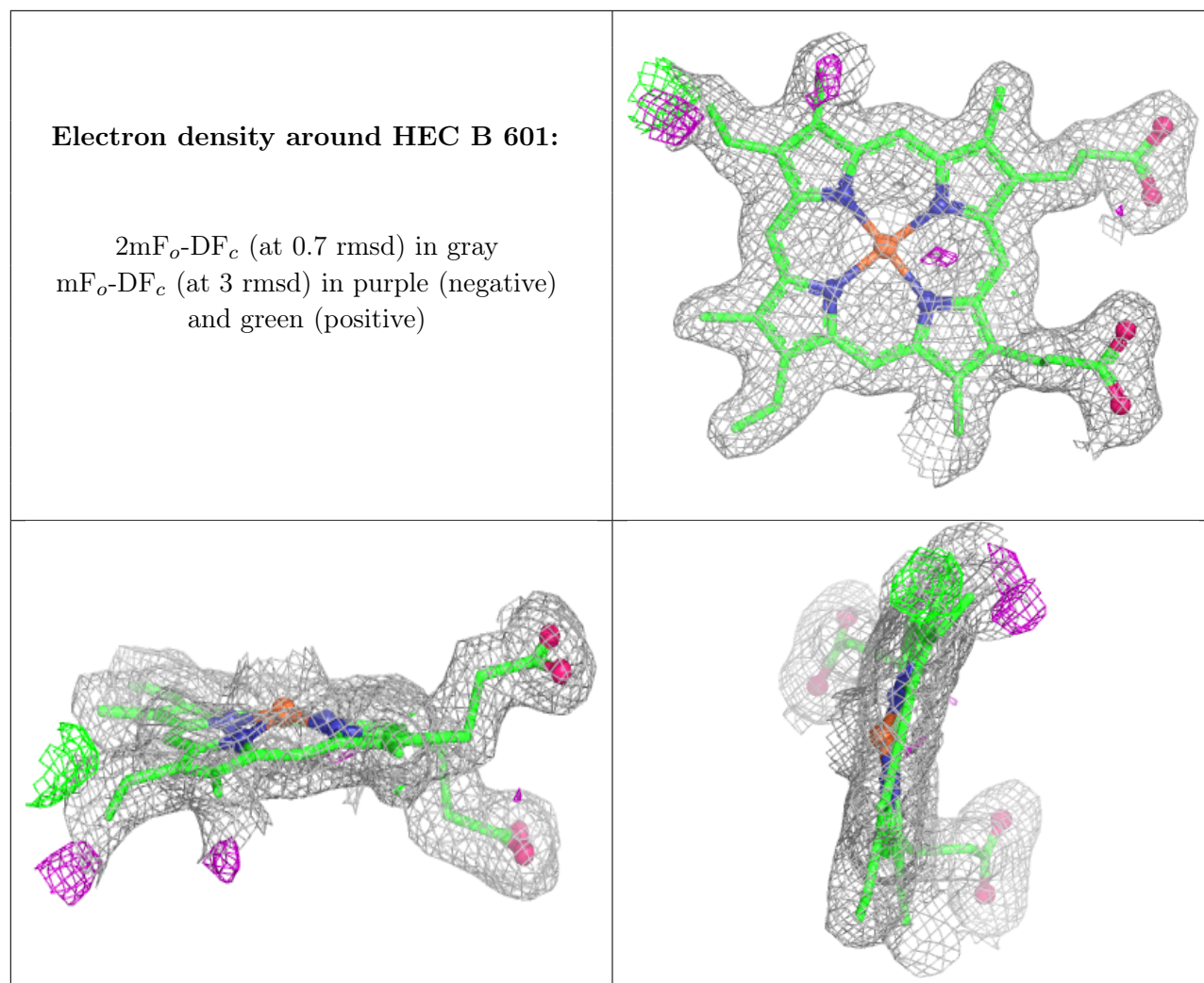
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 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.