



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 18, 2026 – 05:34 AM UTC

PDB ID : 4C1M / pdb_00004c1m
Title : Myeloperoxidase in complex with the reversible inhibitor HX1
Authors : Forbes, L.V.; Sjogren, T.; Auchere, F.; Jenkins, D.W.; Thong, B.; Laughton, D.; Hemsley, P.; Pairaudeau, G.; Eriksson, H.; Unitt, J.F.; Kettle, A.J.
Deposited on : 2013-08-13
Resolution : 2.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

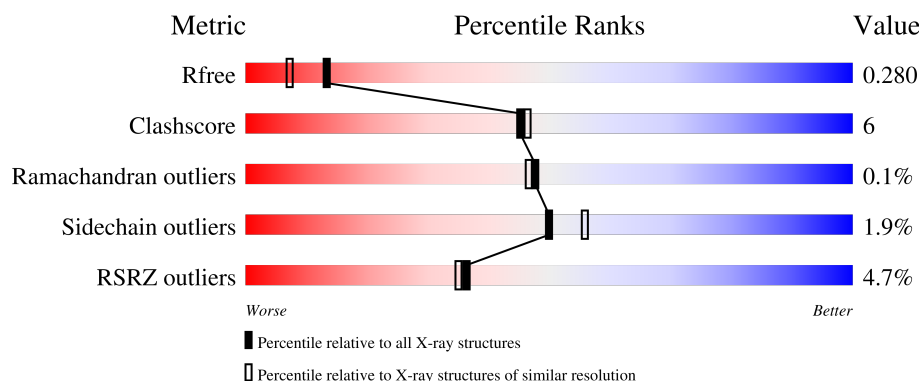
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	108	5% 81% 13% 6%
1	B	108	3% 85% 11% ..
2	C	467	3% 90% 9%
2	D	467	7% 86% 13% .
3	E	6	33% 67%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	F	6	

2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 10168 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.

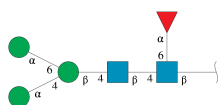
- Molecule 1 is a protein called MYELOPEROXIDASE LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	102	Total	C	N	O	S	0	0	1
			816	516	146	150	4			
1	B	105	Total	C	N	O	S	0	0	1
			838	529	149	155	5			

- Molecule 2 is a protein called MYELOPEROXIDASE HEAVY CHAIN.

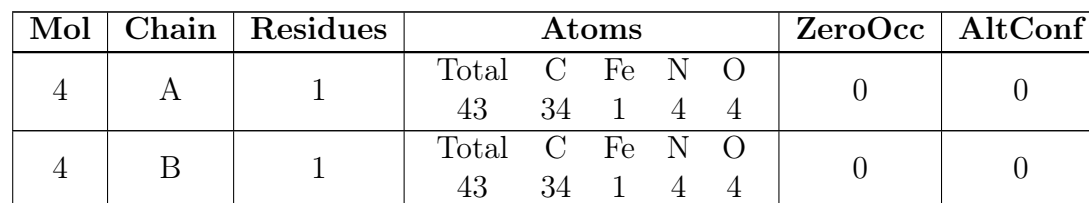
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	467	Total	C	N	O	S	0	0	1
			3733	2351	688	667	27			
2	D	467	Total	C	N	O	S	0	0	1
			3733	2351	688	667	27			

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-4)-[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	E	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 PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C₃₄H₃₂FeN₄O₄).



-

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	F	N	O	0	0
			27	14	6	4	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	F	N	O	0	0
			27	14	6	4	3		

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	C	O	0	0
			6	3	3		
7	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	C	1	Total	Ca	0	0
			1	1		
8	D	1	Total	Ca	0	0
			1	1		

- Molecule 9 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	C	1	Total	Cl	0	0
			1	1		
9	D	1	Total	Cl	0	0
			1	1		

- Molecule 10 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



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

- Molecule 11 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

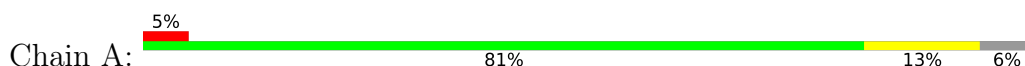
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	103	Total	O	0	0
			103	103		
12	B	108	Total	O	0	0
			108	108		
12	C	254	Total	O	0	0
			254	254		
12	D	199	Total	O	0	0
			199	199		

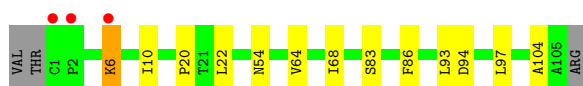
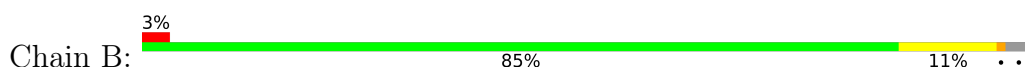
3 Residue-property plots [i](#)

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.

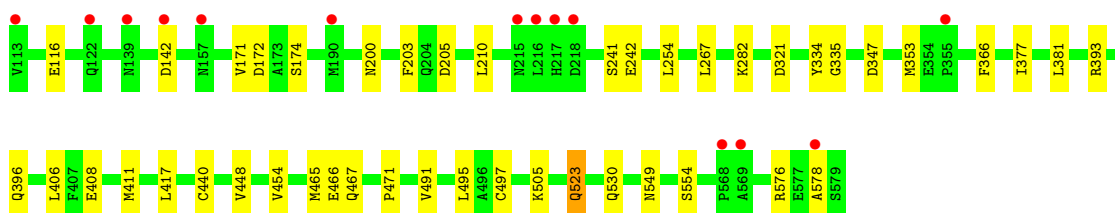
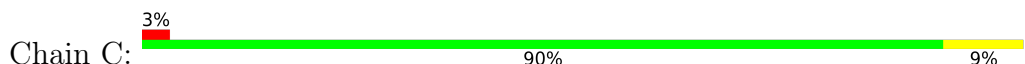
- Molecule 1: MYELOPEROXIDASE LIGHT CHAIN



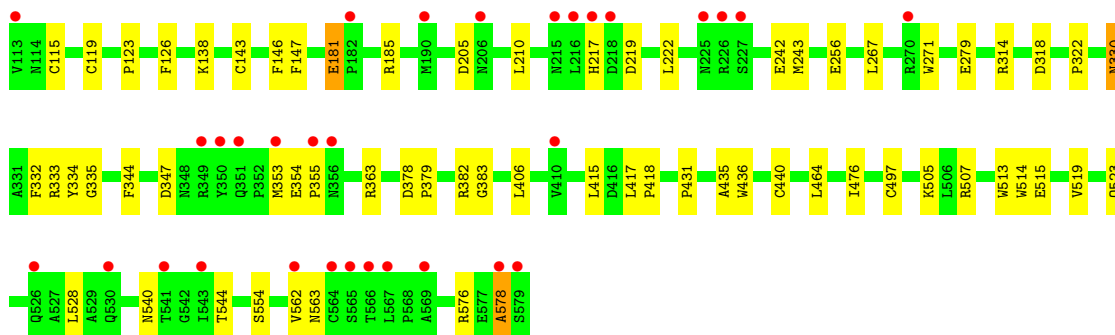
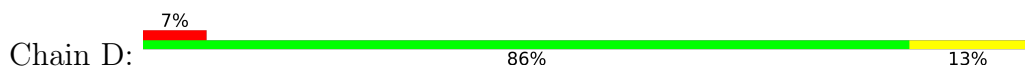
- Molecule 1: MYELOPEROXIDASE LIGHT CHAIN



- Molecule 2: MYELOPEROXIDASE HEAVY CHAIN



- Molecule 2: MYELOPEROXIDASE HEAVY CHAIN



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

Chain E:  33% 67%

NAG1
NAG2
BMA3
MAN4
MAN5
FUC6

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

Chain F:  50% 50%

NAG1
NAG2
BMA3
MAN4
MAN5
FUC6

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	111.28Å 63.44Å 92.38Å 90.00° 97.36° 90.00°	Depositor
Resolution (Å)	50.00 – 2.00 50.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	93.9 (50.00-2.00) 94.0 (50.00-2.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.60 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.222 , 0.278 0.226 , 0.280	Depositor DCC
R_{free} test set	4064 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	13.4	Xtriage
Anisotropy	0.945	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 41.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	10168	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.10% 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: SO4, NIH, NAG, GOL, CA, MAN, CSO, BMA, CL, ACT, FUC, HEM

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	1.13	1/840 (0.1%)	1.06	0/1144
1	B	1.01	1/863 (0.1%)	1.06	0/1176
2	C	1.08	2/3811 (0.1%)	1.06	1/5170 (0.0%)
2	D	0.99	2/3811 (0.1%)	1.02	2/5170 (0.0%)
All	All	1.04	6/9325 (0.1%)	1.05	3/12660 (0.0%)

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	104	ALA	C-N	-7.75	1.22	1.33
1	B	104	ALA	C-N	-6.79	1.23	1.33
2	C	578	ALA	C-N	-6.66	1.24	1.33
2	D	578	ALA	C-N	-6.23	1.24	1.33
2	C	321	ASP	C-N	5.10	1.37	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	467	GLN	N-CA-C	6.12	117.75	111.14
2	D	519	VAL	N-CA-C	-5.92	105.08	110.82
2	D	476	ILE	N-CA-C	5.78	116.43	110.36

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	816	0	779	14	0
1	B	838	0	800	14	0
2	C	3733	0	3727	35	0
2	D	3733	0	3729	44	0
3	E	71	0	61	7	0
3	F	71	0	61	4	0
4	A	43	0	30	10	0
4	B	43	0	30	16	0
5	A	27	0	10	0	0
5	B	27	0	10	1	0
6	B	5	0	0	0	0
6	C	5	0	0	0	0
7	C	6	0	8	0	0
7	D	6	0	8	0	0
8	C	1	0	0	0	0
8	D	1	0	0	0	0
9	C	1	0	0	0	0
9	D	1	0	0	0	0
10	C	8	0	6	0	0
10	D	12	0	9	0	0
11	C	28	0	26	0	0
11	D	28	0	26	0	0
12	A	103	0	0	4	0
12	B	108	0	0	2	0
12	C	254	0	0	12	0
12	D	199	0	0	8	0
All	All	10168	0	9320	111	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 6.

The worst 5 of 111 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)
4:B:605:HEM:HBB1	2:D:243:MET:SD	1.57	1.44
1:A:94:ASP:OD2	4:A:605:HEM:CMD	1.64	1.44
4:A:605:HEM:CMB	2:C:242:GLU:OE2	1.69	1.37
4:B:605:HEM:CBB	2:D:243:MET:SD	2.13	1.35
4:A:605:HEM:HMB1	2:C:242:GLU:OE2	1.17	1.33

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	100/108 (93%)	97 (97%)	3 (3%)	0	100	100
1	B	103/108 (95%)	100 (97%)	3 (3%)	0	100	100
2	C	464/467 (99%)	449 (97%)	15 (3%)	0	100	100
2	D	464/467 (99%)	452 (97%)	11 (2%)	1 (0%)	43	42
All	All	1131/1150 (98%)	1098 (97%)	32 (3%)	1 (0%)	48	46

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	578	ALA

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	87/93 (94%)	87 (100%)	0	100	100
1	B	90/93 (97%)	88 (98%)	2 (2%)	45	50
2	C	410/411 (100%)	403 (98%)	7 (2%)	53	60
2	D	410/411 (100%)	400 (98%)	10 (2%)	43	47
All	All	997/1008 (99%)	978 (98%)	19 (2%)	50	56

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	318	ASP
2	D	544	THR
2	D	562	VAL
2	D	523	GLN
2	C	576	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	530	GLN
2	D	409	GLN
2	D	516	ASN
2	D	467	GLN
2	C	409	GLN

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	C	150	2	3,6,7	0.59	0	1,6,8	0.95	0
2	CSO	D	150	2	3,6,7	0.61	0	1,6,8	1.53	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	C	150	2	-	0/1/5/7	-
2	CSO	D	150	2	-	0/1/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

12 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	NAG	E	1	2,3	14,14,15	0.97	1 (7%)	17,19,21	2.81	6 (35%)
3	NAG	E	2	3	14,14,15	1.30	2 (14%)	17,19,21	1.98	6 (35%)
3	BMA	E	3	3	11,11,12	0.86	0	15,15,17	1.87	4 (26%)
3	MAN	E	4	3	11,11,12	0.72	0	15,15,17	1.46	2 (13%)
3	MAN	E	5	3	11,11,12	0.87	0	15,15,17	1.29	2 (13%)
3	FUC	E	6	3	10,10,11	0.79	0	14,14,16	1.83	4 (28%)
3	NAG	F	1	2,3	14,14,15	0.58	0	17,19,21	1.66	5 (29%)
3	NAG	F	2	3	14,14,15	1.18	2 (14%)	17,19,21	1.75	4 (23%)
3	BMA	F	3	3	11,11,12	1.31	2 (18%)	15,15,17	2.05	6 (40%)
3	MAN	F	4	3	11,11,12	1.02	1 (9%)	15,15,17	2.94	4 (26%)
3	MAN	F	5	3	11,11,12	0.40	0	15,15,17	1.36	3 (20%)
3	FUC	F	6	3	10,10,11	0.73	0	14,14,16	1.33	2 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

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

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	3	BMA	C4-C5	3.14	1.59	1.53
3	E	2	NAG	C2-N2	-3.10	1.41	1.46
3	F	2	NAG	O5-C1	-2.55	1.39	1.43
3	F	2	NAG	C2-N2	-2.42	1.42	1.46
3	E	1	NAG	C1-C2	-2.33	1.49	1.52

The worst 5 of 48 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	4	MAN	C1-O5-C5	8.18	123.15	112.19
3	E	1	NAG	C1-C2-N2	7.01	121.48	110.43
3	E	1	NAG	O5-C1-C2	-6.02	101.97	111.29
3	F	4	MAN	O5-C5-C6	5.27	117.92	107.66
3	E	2	NAG	C1-O5-C5	4.64	118.40	112.19

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	4	MAN	O5-C5-C6-O6
3	E	4	MAN	O5-C5-C6-O6
3	E	4	MAN	C4-C5-C6-O6

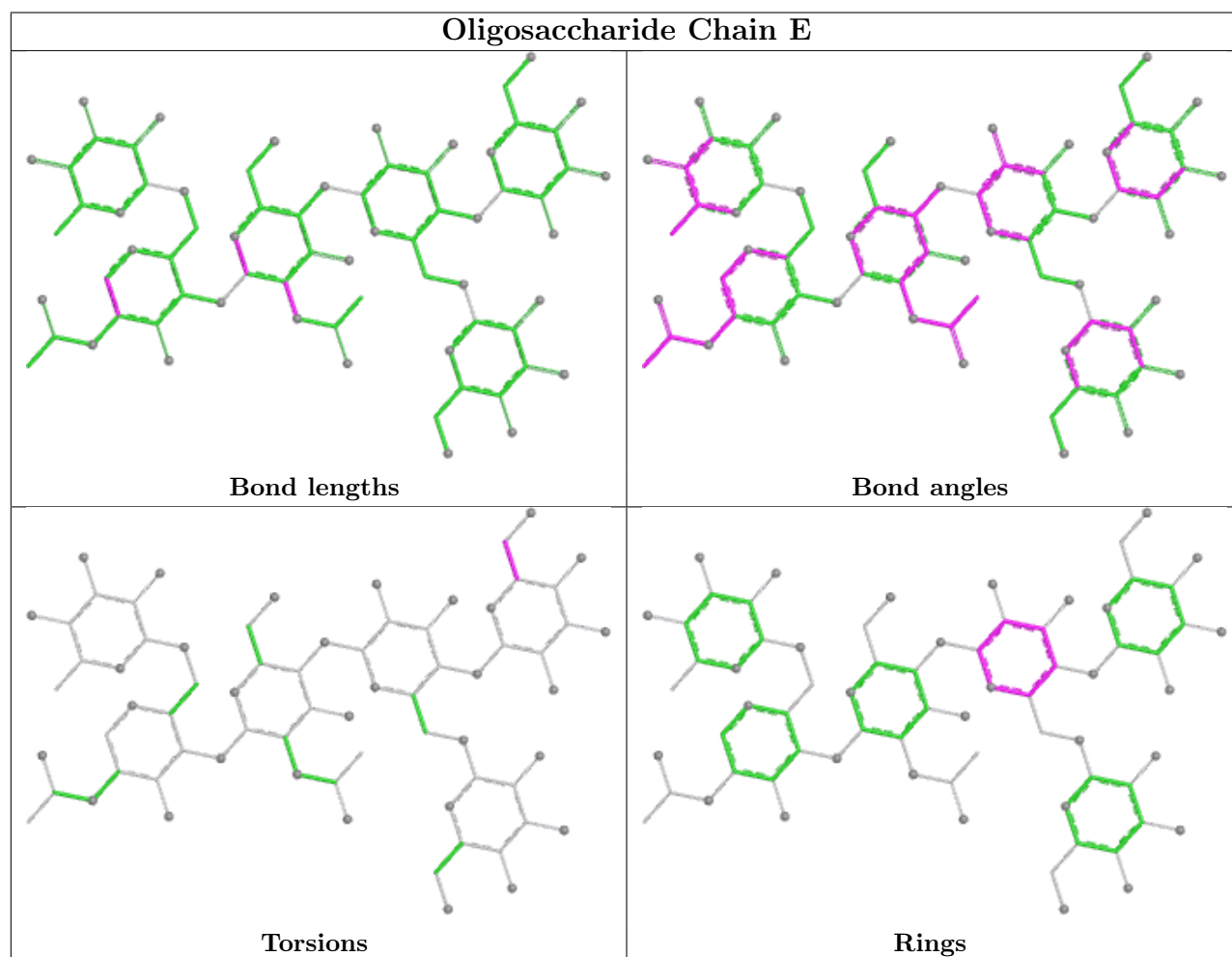
All (1) ring outliers are listed below:

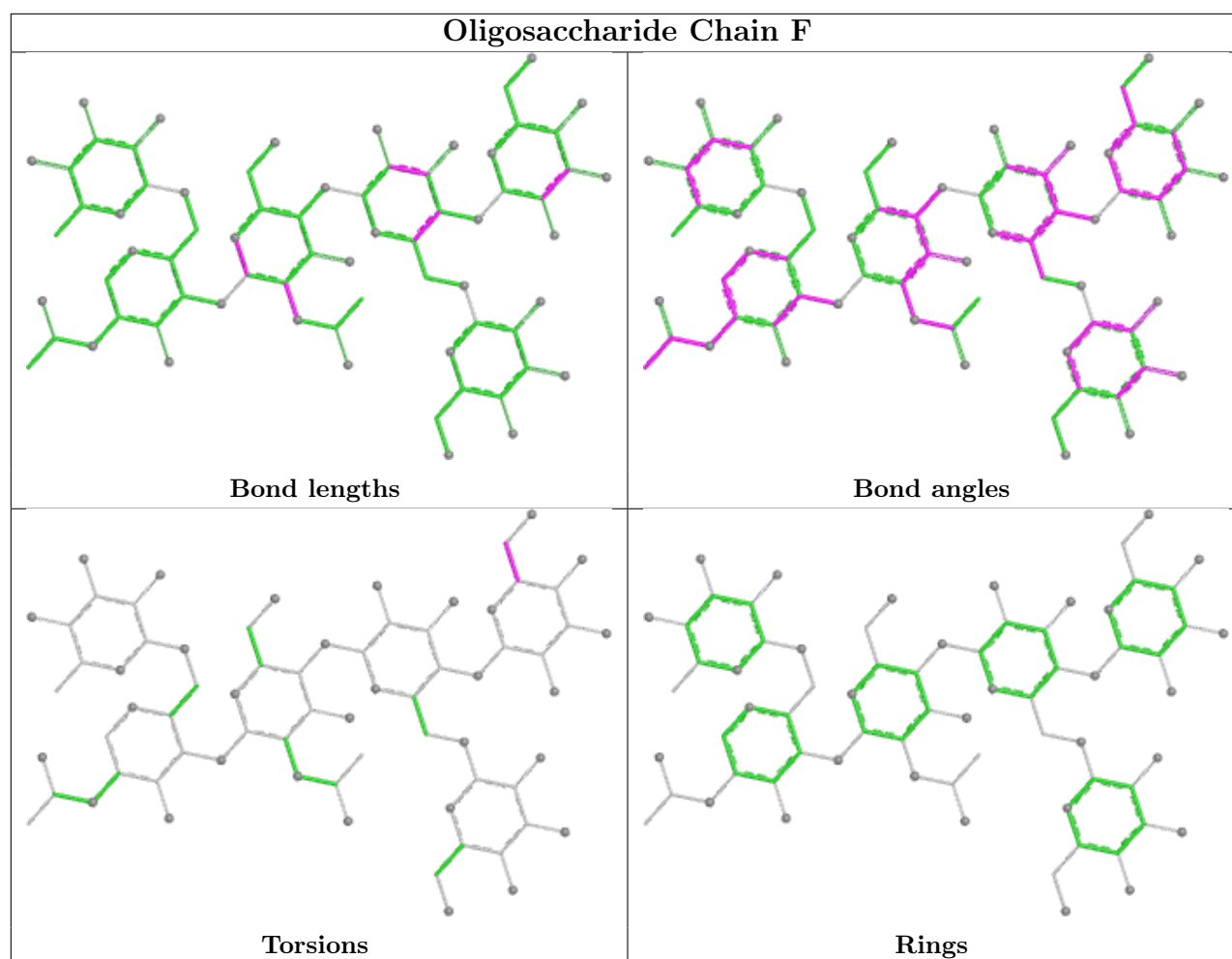
Mol	Chain	Res	Type	Atoms
3	E	3	BMA	C1-C2-C3-C4-C5-O5

7 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	3	BMA	5	0
3	F	4	MAN	3	0
3	E	6	FUC	1	0
3	F	3	BMA	3	0
3	E	4	MAN	3	0
3	F	5	MAN	1	0
3	E	5	MAN	3	0

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





5.6 Ligand geometry [i](#)

Of 21 ligands modelled in this entry, 4 are monoatomic - leaving 17 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	SO4	C	1581	-	4,4,4	0.43	0	6,6,6	0.48	0
7	GOL	C	631	-	5,5,5	0.31	0	5,5,5	0.51	0
10	ACT	D	1582	-	3,3,3	0.89	0	3,3,3	0.45	0
11	NAG	D	2620	2	14,14,15	0.54	0	17,19,21	1.43	2 (11%)
10	ACT	C	1583	-	3,3,3	0.71	0	3,3,3	0.88	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	GOL	D	631	-	5,5,5	0.40	0	5,5,5	0.63	0
11	NAG	C	1630	2	14,14,15	0.72	0	17,19,21	2.12	6 (35%)
4	HEM	B	605	2	50,50,50	2.71	24 (48%)	67,82,82	2.01	21 (31%)
5	NIH	B	606	-	27,28,28	1.22	3 (11%)	34,42,42	1.99	9 (26%)
11	NAG	C	1620	2	14,14,15	0.66	0	17,19,21	1.71	6 (35%)
11	NAG	D	2630	2	14,14,15	0.59	0	17,19,21	1.48	3 (17%)
10	ACT	C	1582	-	3,3,3	0.85	0	3,3,3	0.60	0
10	ACT	D	1581	-	3,3,3	1.07	0	3,3,3	0.17	0
5	NIH	A	606	-	27,28,28	1.24	2 (7%)	34,42,42	1.85	6 (17%)
4	HEM	A	605	2	50,50,50	2.53	25 (50%)	67,82,82	1.85	14 (20%)
10	ACT	D	1583	-	3,3,3	0.97	0	3,3,3	0.65	0
6	SO4	B	1003	-	4,4,4	0.47	0	6,6,6	0.32	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
7	GOL	C	631	-	-	4/4/4/4	-
11	NAG	D	2620	2	-	0/6/23/26	0/1/1/1
7	GOL	D	631	-	-	2/4/4/4	-
11	NAG	C	1630	2	-	0/6/23/26	0/1/1/1
4	HEM	B	605	2	-	4/14/54/54	-
5	NIH	B	606	-	-	1/23/23/23	0/2/2/2
11	NAG	D	2630	2	-	0/6/23/26	0/1/1/1
5	NIH	A	606	-	-	4/23/23/23	0/2/2/2
4	HEM	A	605	2	-	4/14/54/54	-
11	NAG	C	1620	2	-	0/6/23/26	0/1/1/1

The worst 5 of 54 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	605	HEM	FE-ND	5.53	2.11	1.94
4	B	605	HEM	FE-NB	5.49	2.11	1.94
4	A	605	HEM	FE-NC	5.18	2.12	1.95
4	B	605	HEM	FE-NA	5.07	2.11	1.95
4	B	605	HEM	CHB-C1B	4.82	1.48	1.38

The worst 5 of 67 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	606	NIH	C5-C4-N3	-7.15	119.55	126.25
4	B	605	HEM	C3B-C2B-C1B	-7.13	101.06	106.41
4	A	605	HEM	C3B-C2B-C1B	-6.92	101.21	106.41
5	A	606	NIH	C7-C5-C6	-6.26	117.64	122.64
5	A	606	NIH	C5-C4-N3	-6.00	120.63	126.25

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

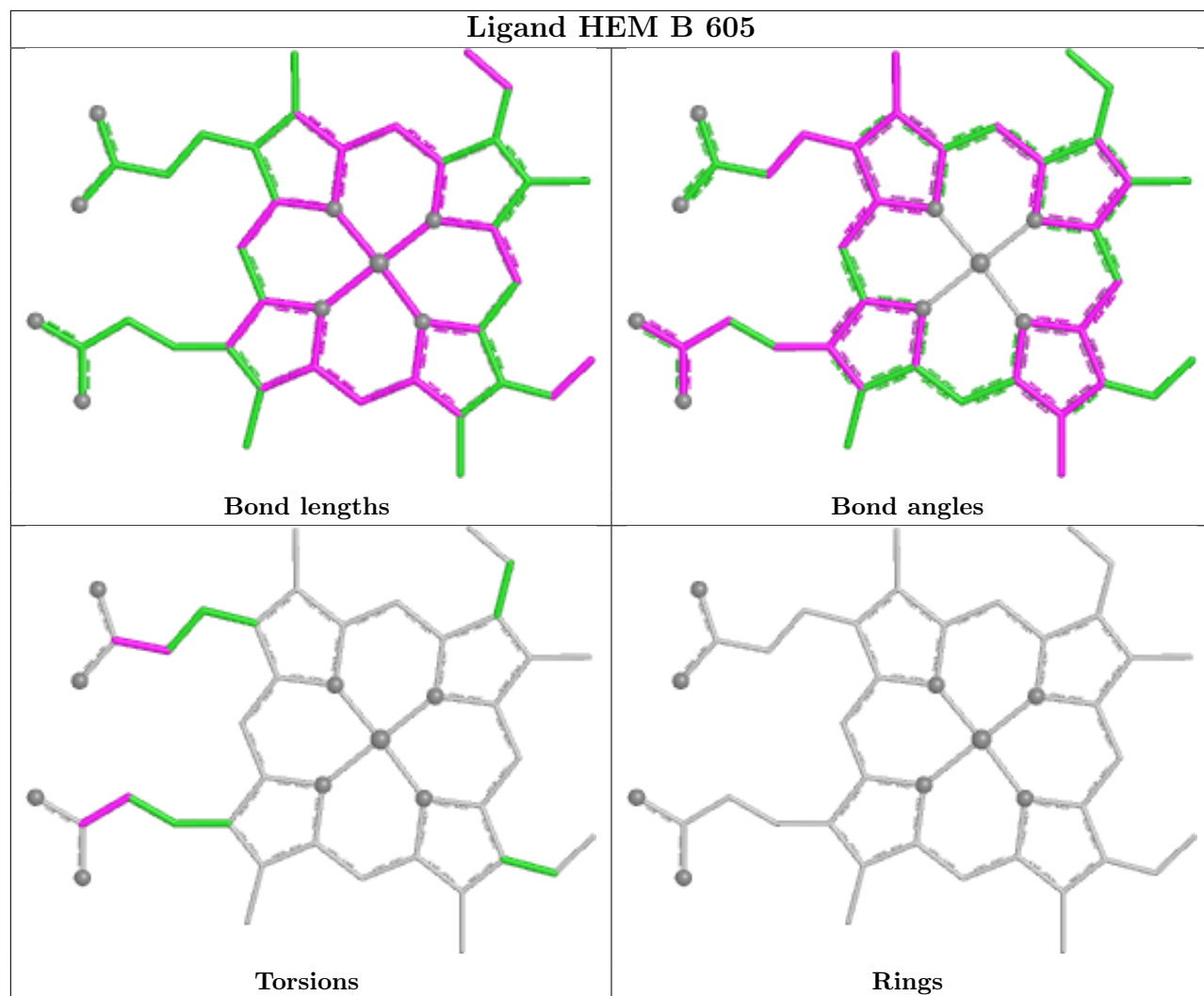
Mol	Chain	Res	Type	Atoms
5	A	606	NIH	C6-C5-C7-N8
5	A	606	NIH	C6-C5-C7-O9
5	B	606	NIH	C6-C5-C7-O9
7	C	631	GOL	O1-C1-C2-C3
7	C	631	GOL	C1-C2-C3-O3

There are no ring outliers.

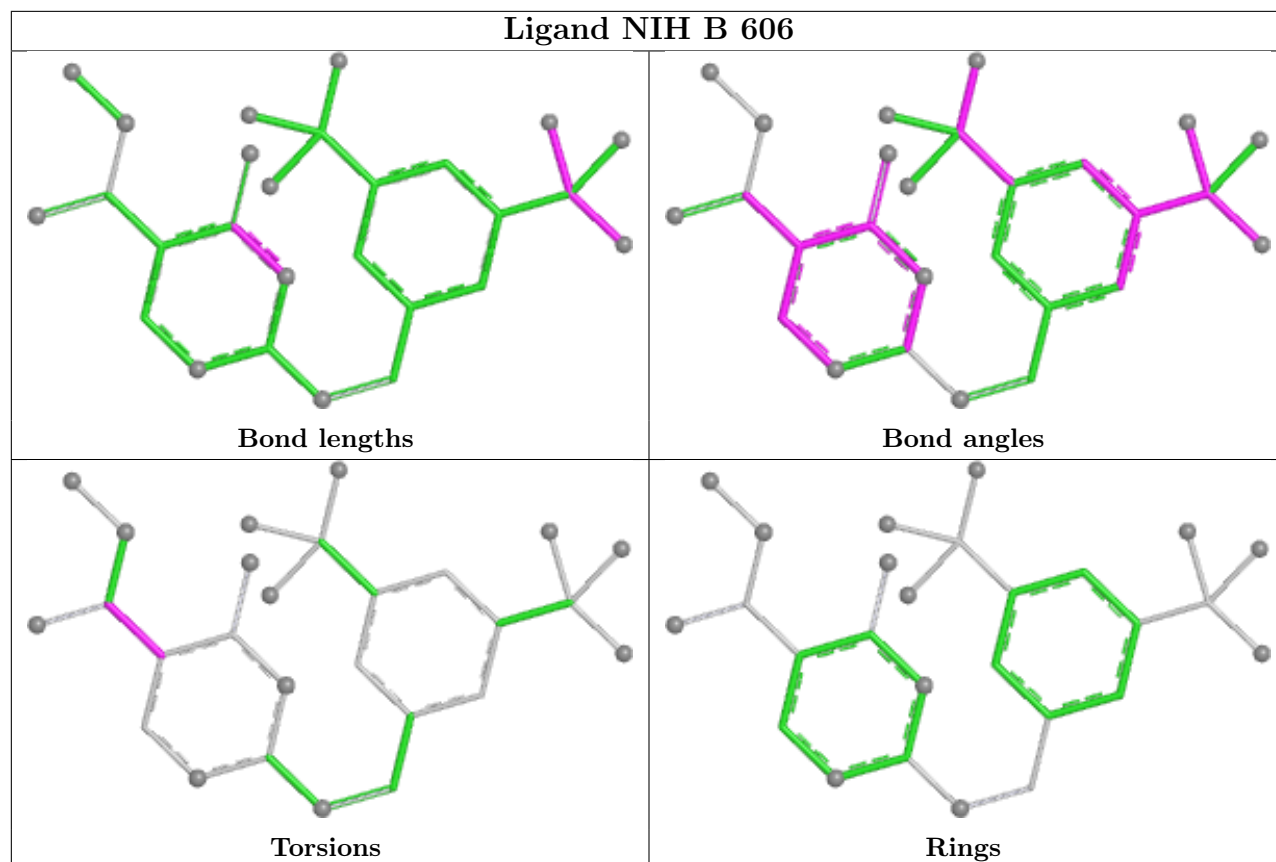
3 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	605	HEM	16	0
5	B	606	NIH	1	0
4	A	605	HEM	10	0

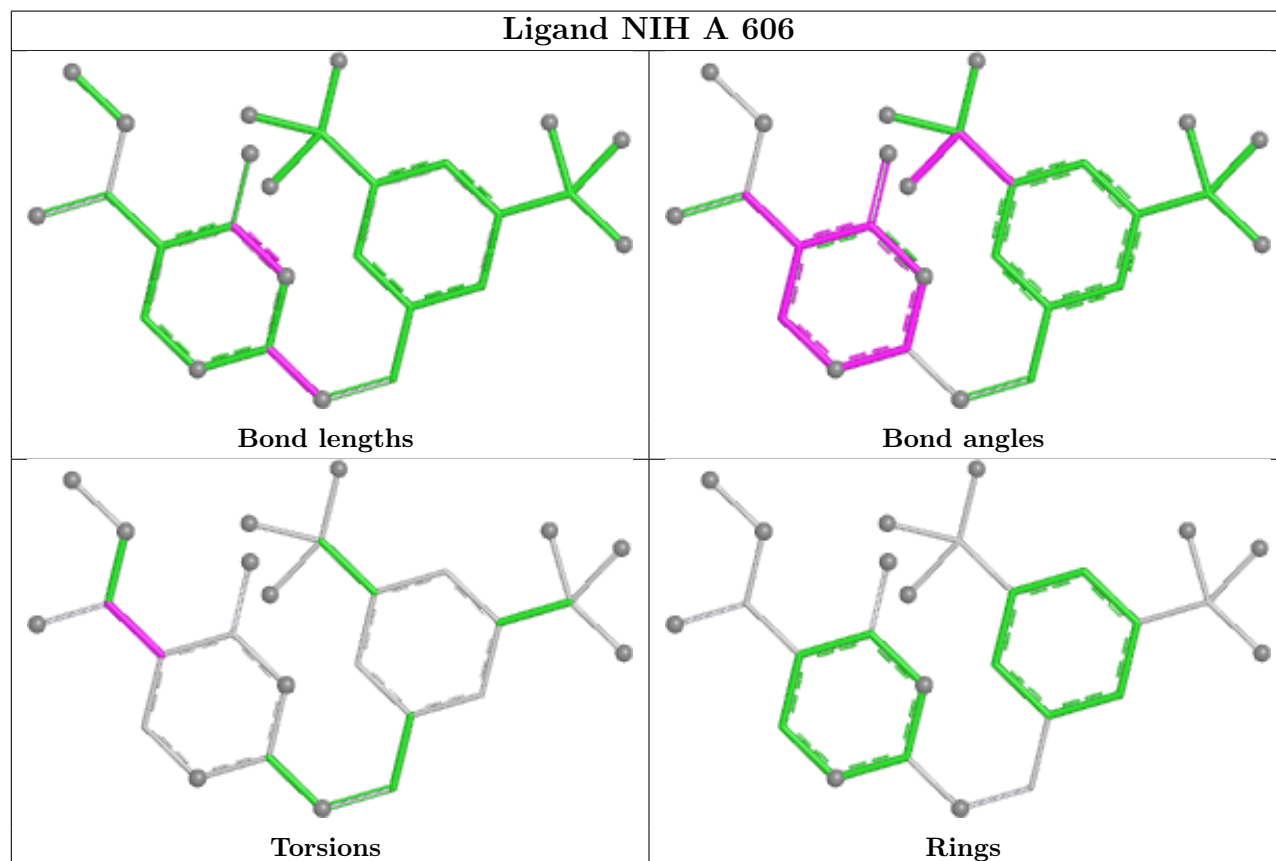
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

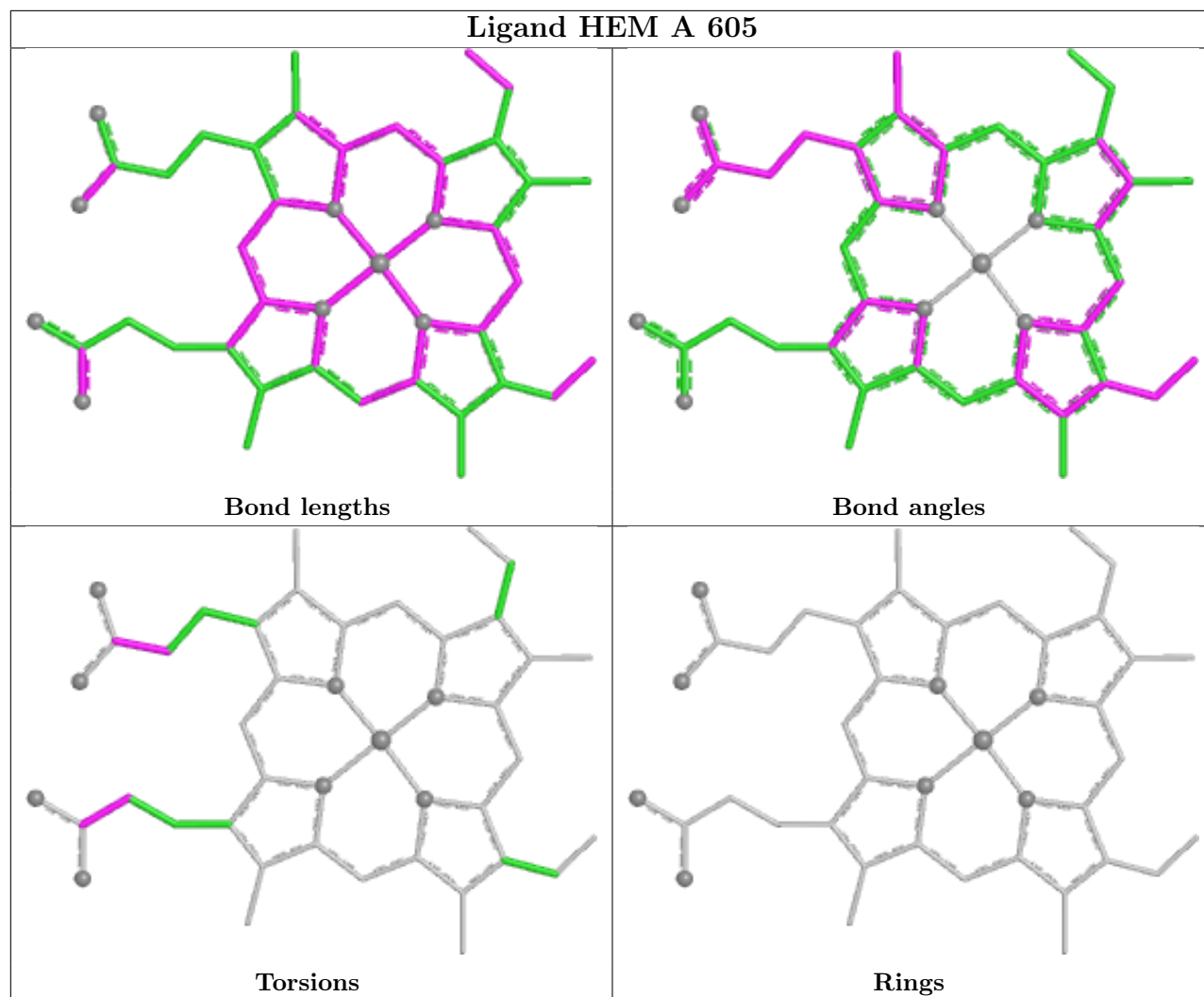


Ligand NIH B 606



Ligand NIH A 606





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	102/108 (94%)	0.22	5 (4%) 35 34	4, 8, 21, 44	0
1	B	105/108 (97%)	0.23	3 (2%) 53 52	6, 11, 26, 35	0
2	C	466/467 (99%)	0.23	14 (3%) 52 51	3, 10, 24, 37	0
2	D	466/467 (99%)	0.52	31 (6%) 24 22	4, 15, 32, 42	0
All	All	1139/1150 (99%)	0.35	53 (4%) 36 35	3, 12, 29, 44	0

The worst 5 of 53 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	105	ALA	9.9
2	C	113	VAL	5.6
2	D	578	ALA	4.9
2	C	578	ALA	4.8
2	C	217	HIS	4.5

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	CSO	D	150	7/8	0.94	0.10	8,10,16,19	0
2	CSO	C	150	7/8	0.96	0.08	5,6,10,12	0

6.3 Carbohydrates ⓘ

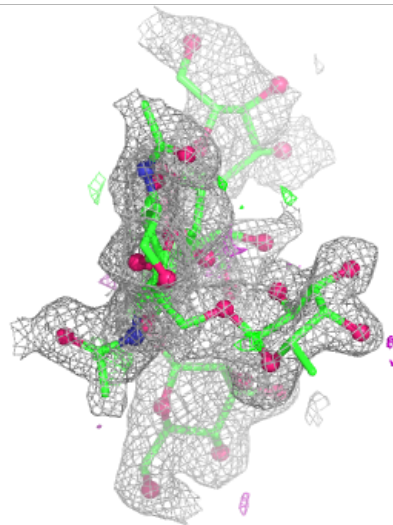
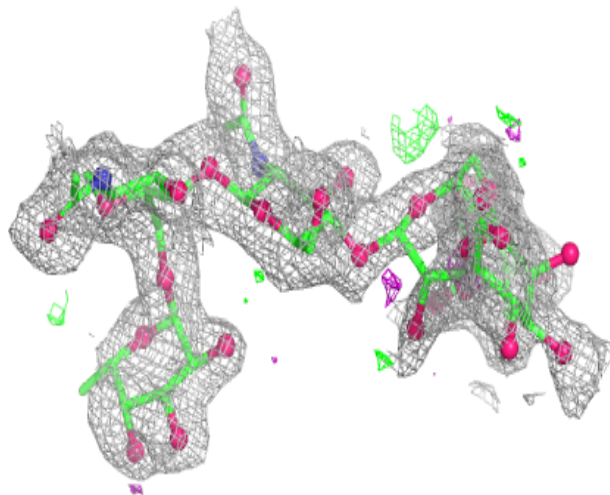
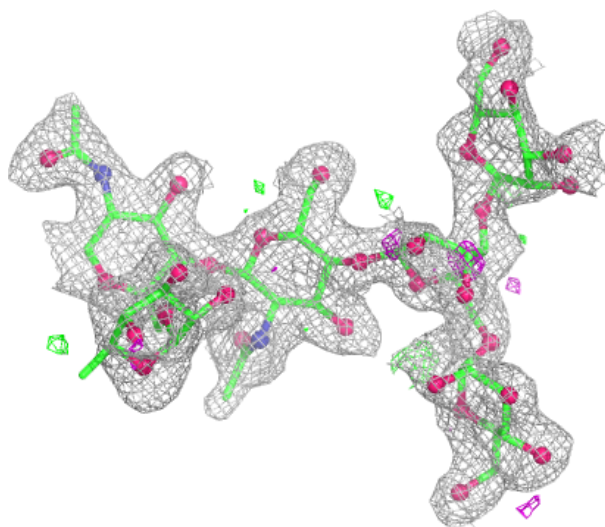
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

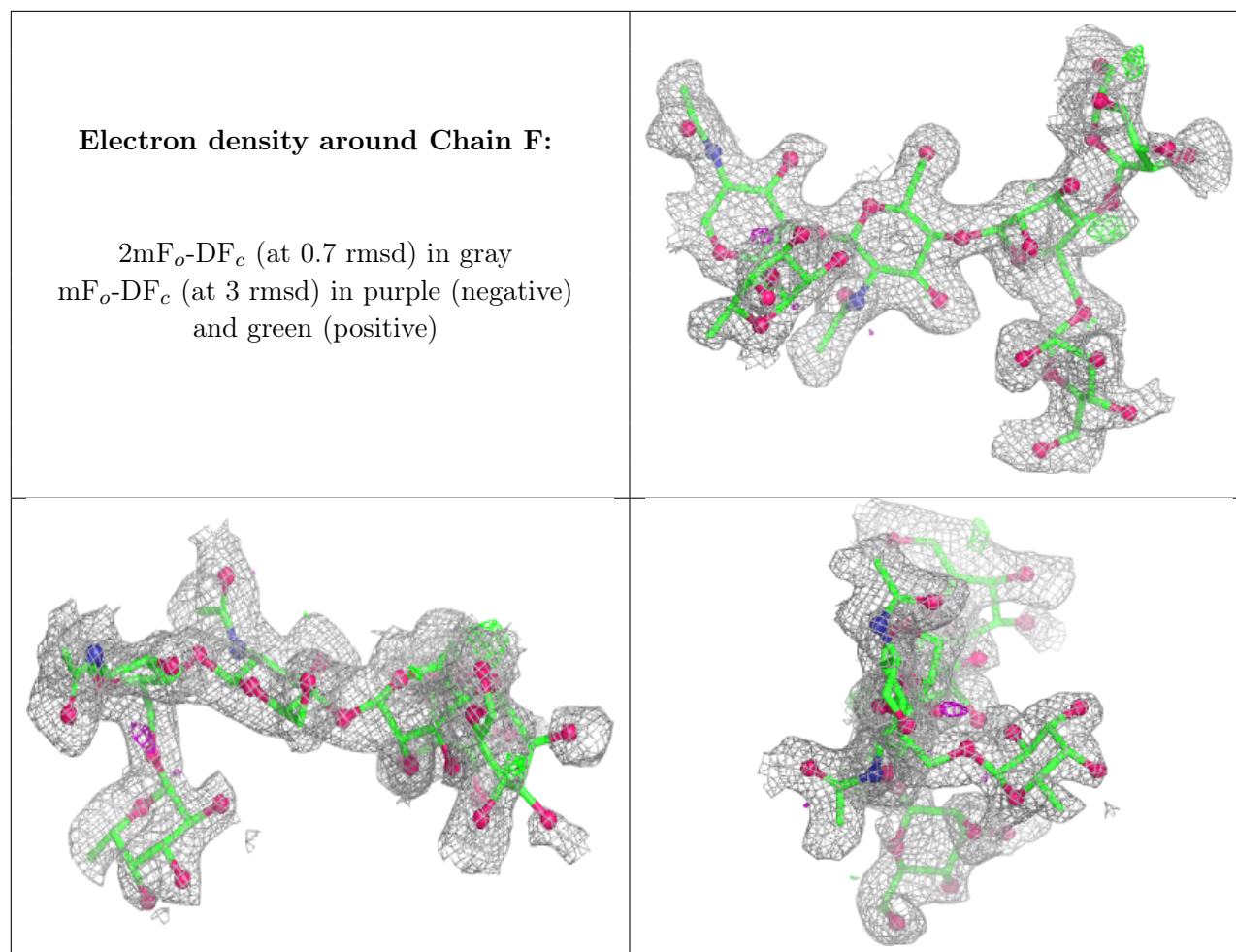
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MAN	F	4	11/12	0.70	0.21	36,43,46,46	0
3	BMA	F	3	11/12	0.74	0.17	24,27,36,41	0
3	MAN	E	4	11/12	0.74	0.17	36,42,46,48	0
3	MAN	F	5	11/12	0.77	0.15	21,24,25,29	0
3	BMA	E	3	11/12	0.79	0.17	19,23,28,32	0
3	FUC	E	6	10/11	0.81	0.14	17,20,21,22	0
3	FUC	F	6	10/11	0.81	0.15	23,25,28,30	0
3	MAN	E	5	11/12	0.87	0.10	24,25,27,28	0
3	NAG	F	1	14/15	0.93	0.08	10,12,13,17	0
3	NAG	F	2	14/15	0.93	0.08	9,11,13,17	0
3	NAG	E	2	14/15	0.93	0.08	8,10,12,15	0
3	NAG	E	1	14/15	0.94	0.09	10,11,14,15	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 E:

$2mF_o-DF_c$ (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
10	ACT	D	1582	4/4	0.58	0.24	39,39,40,40	0
6	SO4	B	1003	5/5	0.61	0.20	29,29,31,31	5
7	GOL	D	631	6/6	0.72	0.20	32,34,36,37	0
5	NIH	B	606	27/27	0.74	0.20	10,12,13,14	27
10	ACT	D	1581	4/4	0.76	0.18	22,27,27,28	0
10	ACT	D	1583	4/4	0.76	0.17	34,34,34,36	0
7	GOL	C	631	6/6	0.79	0.20	35,39,41,46	0
11	NAG	D	2630	14/15	0.79	0.14	31,34,36,37	0
5	NIH	A	606	27/27	0.80	0.15	4,6,7,8	27
11	NAG	C	1630	14/15	0.83	0.13	19,21,24,25	0
10	ACT	C	1582	4/4	0.83	0.16	35,37,38,38	0

Continued on next page...

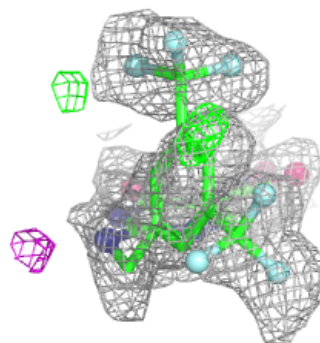
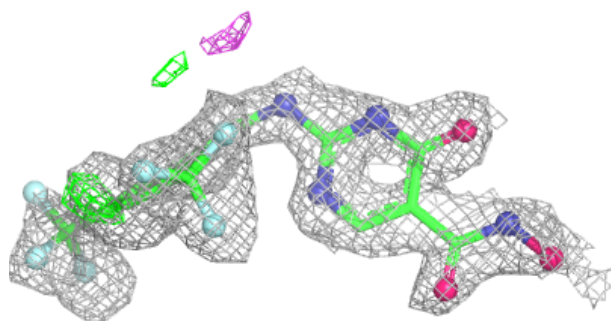
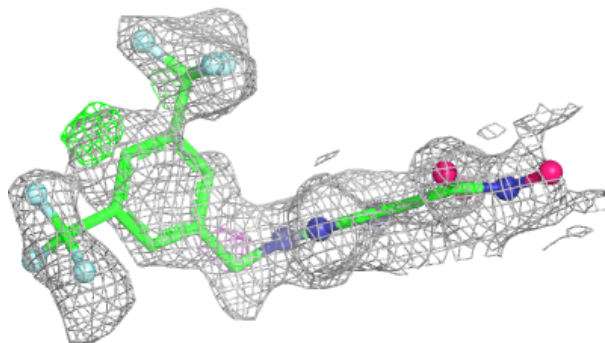
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
11	NAG	D	2620	14/15	0.89	0.11	22,23,25,27	0
10	ACT	C	1583	4/4	0.91	0.10	25,26,27,27	0
11	NAG	C	1620	14/15	0.93	0.07	15,17,19,20	0
6	SO4	C	1581	5/5	0.95	0.08	34,34,36,37	0
4	HEM	B	605	43/43	0.96	0.10	5,7,9,12	0
4	HEM	A	605	43/43	0.96	0.08	4,5,7,10	0
9	CL	D	1580	1/1	0.99	0.02	6,6,6,6	0
8	CA	C	1579	1/1	0.99	0.04	4,4,4,4	0
8	CA	D	1579	1/1	1.00	0.01	7,7,7,7	0
9	CL	C	1580	1/1	1.00	0.02	4,4,4,4	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.

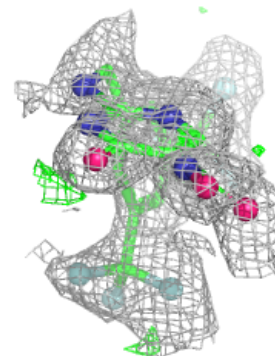
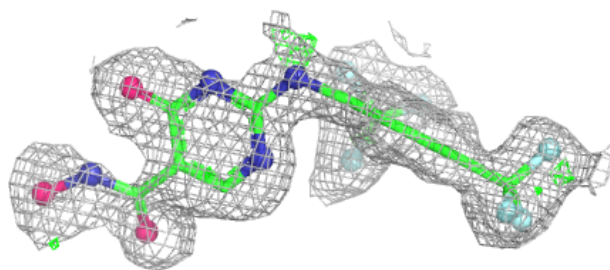
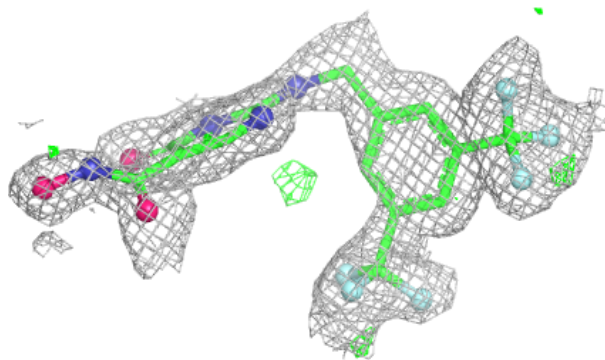
Electron density around NIH B 606:

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



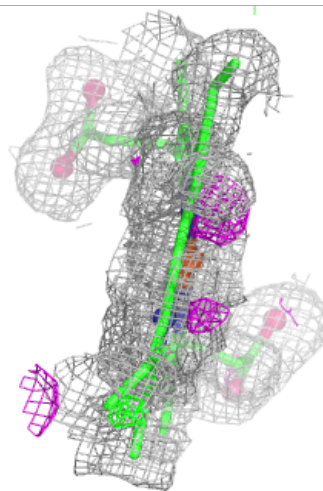
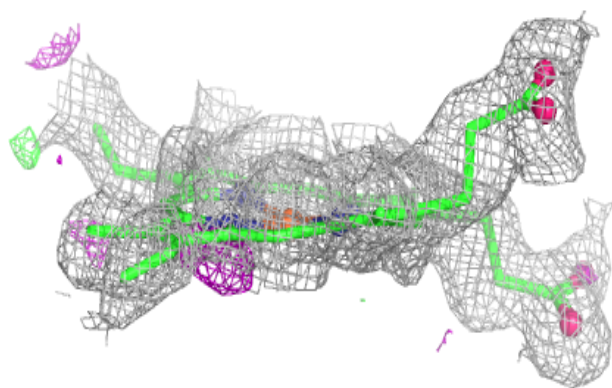
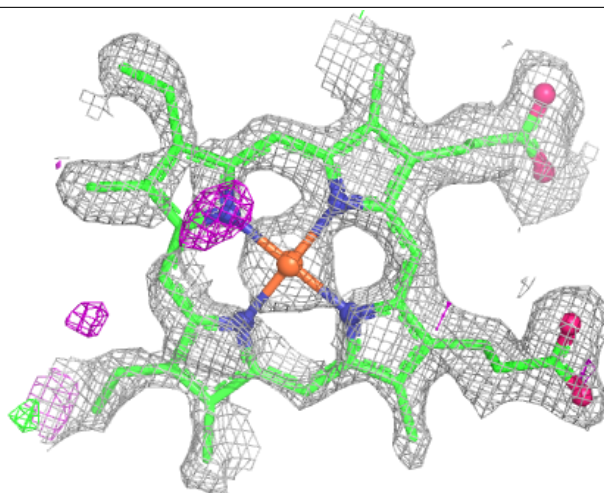
Electron density around NIH A 606:

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



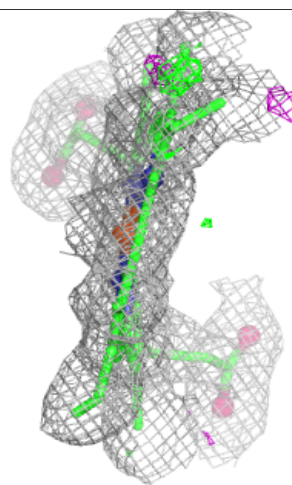
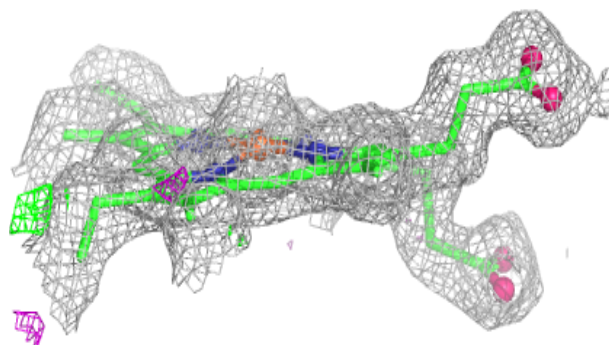
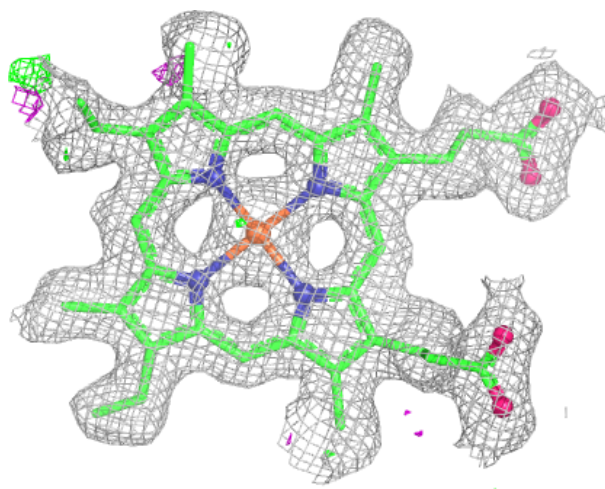
Electron density around HEM B 605:

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



Electron density around HEM A 605:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.