Full wwPDB X-ray Structure Validation Report (i)

Aug 5, 2026 – 03:47 PM EDT

PDB ID	:	4FM5 / pdb_00004fm5
Title	:	X-ray structure of des-methylflurbiprofen bound to murine COX-2
Authors	:	Xu, S.; Banerjee, S.; Windsor, M.A.; Marnett, L.J.
Deposited on	:	2012-06-15
Resolution	:	2.81 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 (i) 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 (i)) were used in the production of this report:

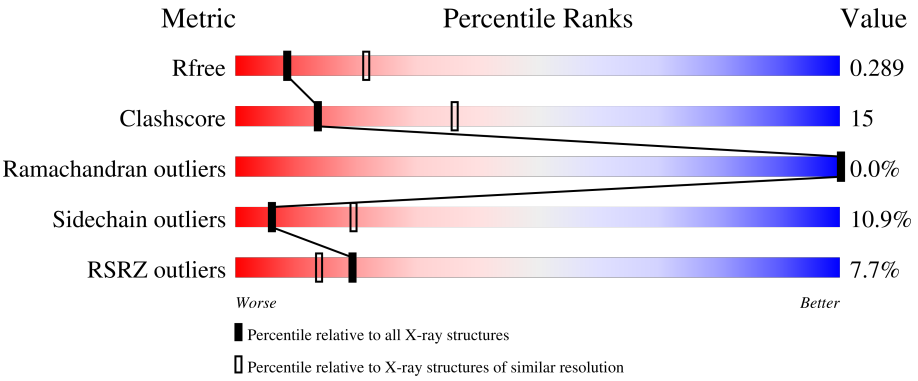
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 (i)

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

The reported resolution of this entry is 2.81 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	4591 (2.84-2.80)
Clashscore	190562	5010 (2.84-2.80)
Ramachandran outliers	187476	4916 (2.84-2.80)
Sidechain outliers	187428	4918 (2.84-2.80)
RSRZ outliers	180081	4594 (2.84-2.80)

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	604	7% 66% 20% 5% 9%
1	B	604	8% 66% 22% • 9%
1	C	604	7% 67% 20% • 9%
1	D	604	6% 64% 21% 5% 9%
2	E	2	100%

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	G	2	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 18554 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 Prostaglandin G/H synthase 2.

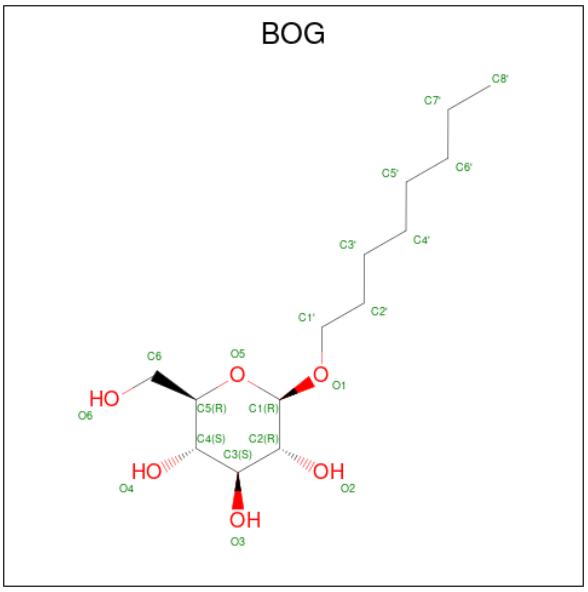
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	552	Total	C	N	O	S	0	0	0
			4474	2885	750	814	25			
1	B	552	Total	C	N	O	S	0	0	0
			4474	2885	750	814	25			
1	C	552	Total	C	N	O	S	0	0	0
			4474	2885	750	814	25			
1	D	552	Total	C	N	O	S	0	0	0
			4474	2885	750	814	25			

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



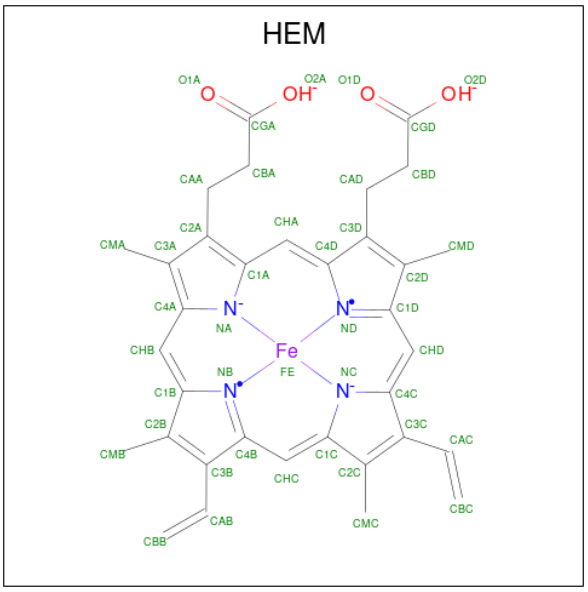
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	H	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is octyl beta-D-glucopyranoside (CCD ID: BOG) (formula: $C_{14}H_{28}O_6$).



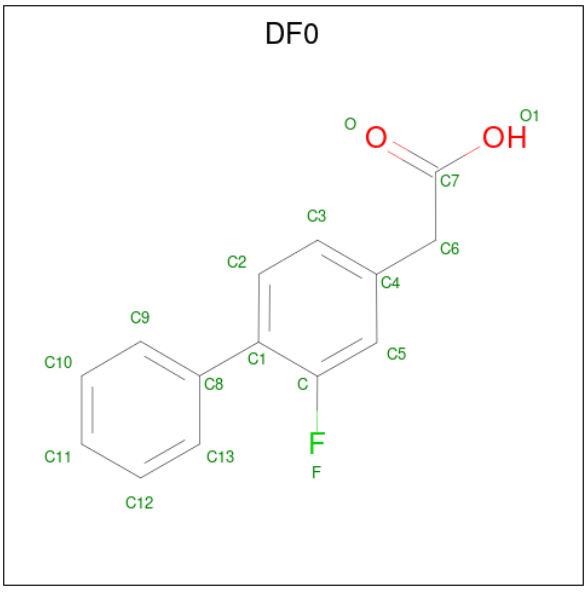
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 20 14 6	0	0
3	A	1	Total C O 20 14 6	0	0
3	B	1	Total C O 20 14 6	0	0
3	C	1	Total C O 20 14 6	0	0
3	C	1	Total C O 20 14 6	0	0
3	D	1	Total C O 20 14 6	0	0

- Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 5 is (2-fluorobiphenyl-4-yl)acetic acid (CCD ID: DF0) (formula: $C_{14}H_{11}FO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	F	O	0	0
			17	14	1	2		
5	B	1	Total	C	F	O	0	0
			17	14	1	2		
5	C	1	Total	C	F	O	0	0
			17	14	1	2		
5	D	1	Total	C	F	O	0	0
			17	14	1	2		

- Molecule 6 is water.

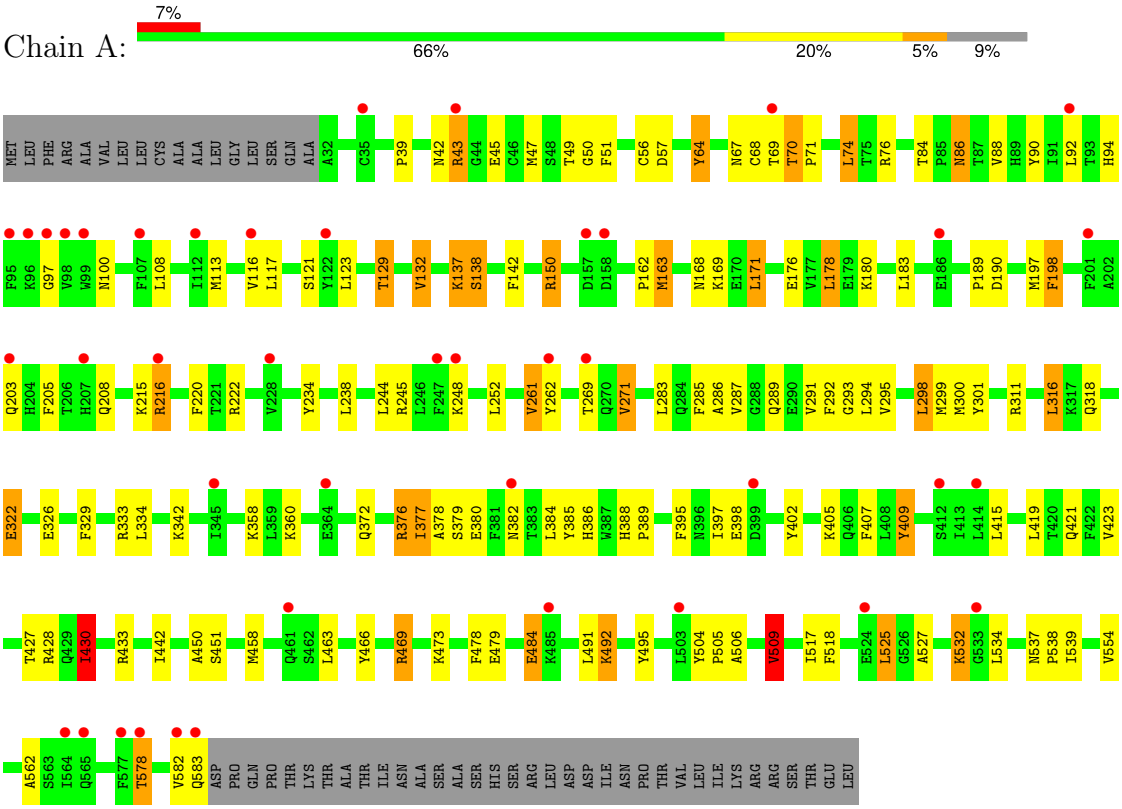
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	63	Total	O	0	0
			63	63		
6	B	39	Total	O	0	0
			39	39		
6	C	37	Total	O	0	0
			37	37		
6	D	47	Total	O	0	0
			47	47		

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.

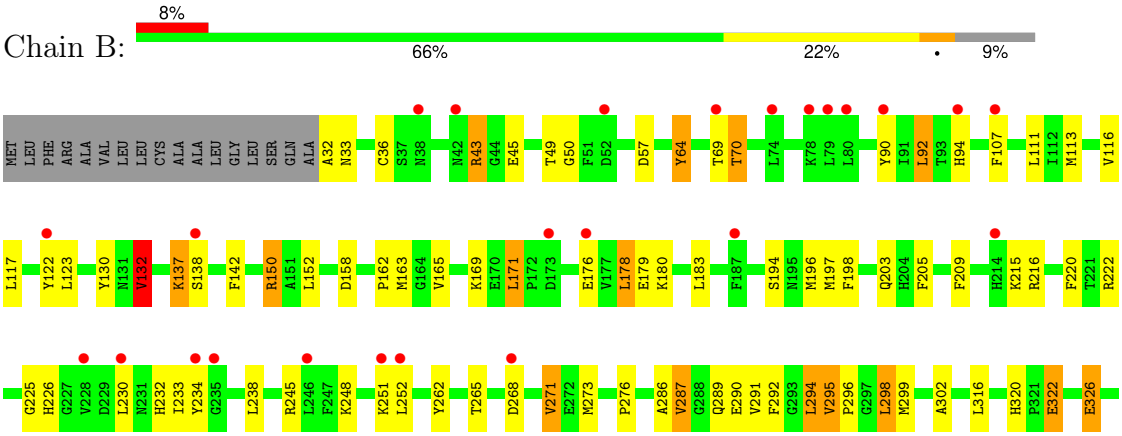
• Molecule 1: Prostaglandin G/H synthase 2

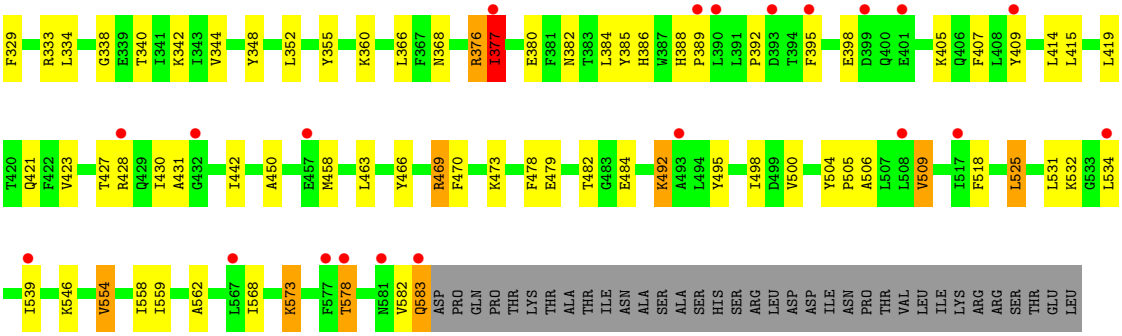
Chain A:



• Molecule 1: Prostaglandin G/H synthase 2

Chain B:

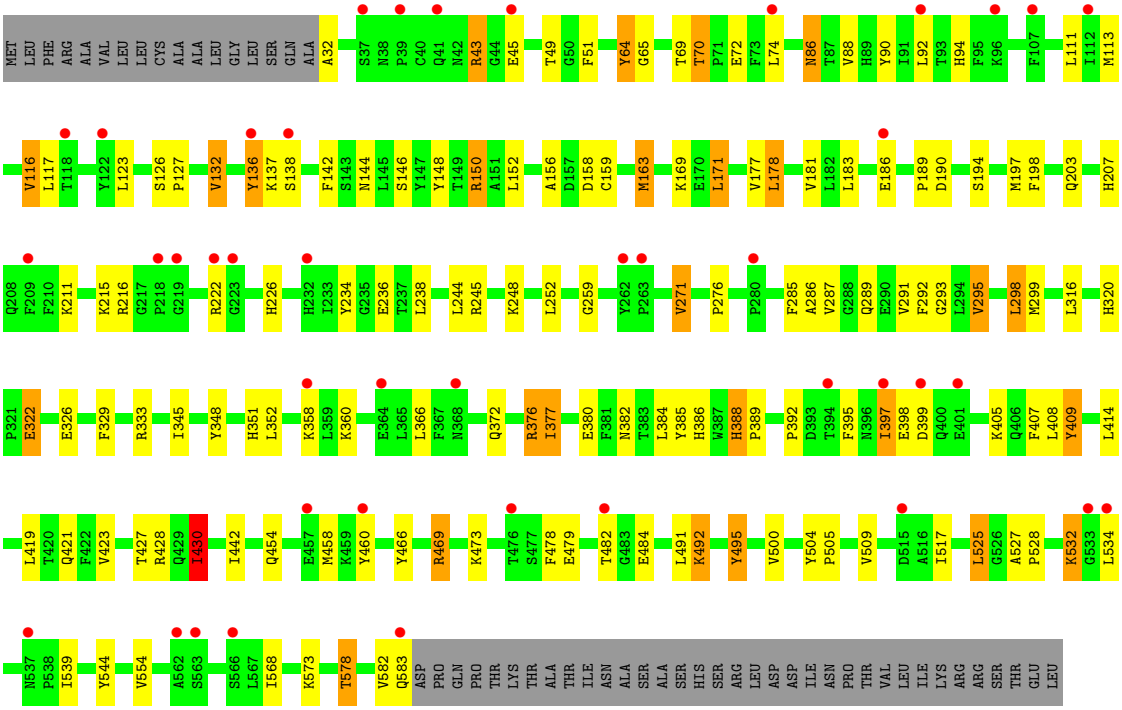




• Molecule 1: Prostaglandin G/H synthase 2

Chain C:

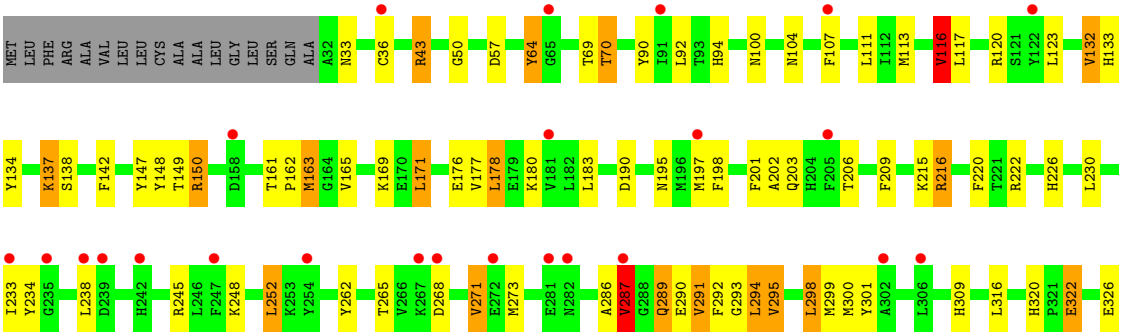


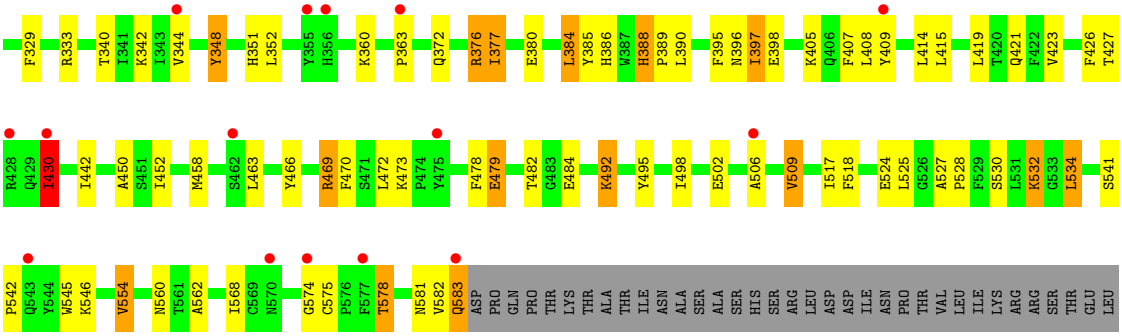


• Molecule 1: Prostaglandin G/H synthase 2

Chain D:

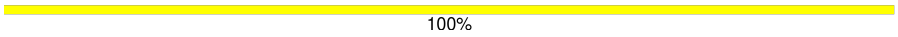






• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:





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

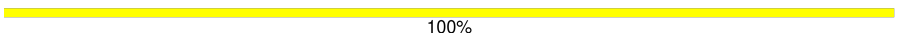
Chain F:





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

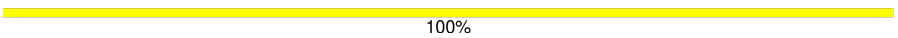
Chain G:





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

Chain H:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	181.63Å 135.70Å 125.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.86 – 2.81 49.86 – 2.81	Depositor EDS
% Data completeness (in resolution range)	98.5 (49.86-2.81) 98.5 (49.86-2.81)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	2.33 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.240 , 0.290 0.240 , 0.289	Depositor DCC
R_{free} test set	3808 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	49.0	Xtriage
Anisotropy	0.282	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 20.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	18554	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 43.74 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.6881e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: DF0, NAG, HEM, BOG

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	0.96	0/4601	1.04	12/6239 (0.2%)
1	B	0.97	2/4601 (0.0%)	1.02	8/6239 (0.1%)
1	C	0.97	4/4601 (0.1%)	1.05	12/6239 (0.2%)
1	D	1.01	6/4601 (0.1%)	1.07	17/6239 (0.3%)
All	All	0.98	12/18404 (0.1%)	1.04	49/24956 (0.2%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	573	LYS	C-O	-9.42	1.12	1.24
1	D	574	GLY	C-O	-9.18	1.11	1.23
1	C	397	ILE	C-O	-8.19	1.14	1.24
1	D	348	TYR	CG-CD2	-6.08	1.26	1.39
1	B	163	MET	C-O	-6.05	1.14	1.23
1	D	147	TYR	CE1-CZ	-5.94	1.24	1.38
1	C	152	LEU	CA-C	-5.83	1.47	1.52
1	D	147	TYR	CG-CD2	-5.78	1.27	1.39
1	D	147	TYR	CG-CD1	-5.68	1.27	1.39
1	D	348	TYR	CE1-CZ	-5.58	1.24	1.38
1	C	351	HIS	CG-CD2	5.55	1.42	1.35
1	B	276	PRO	CA-C	5.02	1.54	1.51

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	163	MET	N-CA-C	-10.58	97.40	110.41
1	D	163	MET	N-CA-C	-10.26	97.29	110.53
1	D	495	TYR	N-CA-C	-9.85	97.25	110.55
1	C	163	MET	N-CA-C	-8.56	98.99	110.55
1	C	430	ILE	CB-CA-C	-8.33	99.79	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	132	VAL	CB-CA-C	-7.81	101.60	112.14
1	A	495	TYR	N-CA-C	-7.78	100.05	110.55
1	C	495	TYR	N-CA-C	-7.08	100.00	110.48
1	B	163	MET	CB-CA-C	-6.97	102.65	111.22
1	D	575	CYS	N-CA-C	-6.92	94.50	109.81
1	A	132	VAL	CB-CA-C	-6.90	102.82	112.14
1	B	495	TYR	N-CA-C	-6.78	100.45	110.48
1	C	132	VAL	CB-CA-C	-6.67	103.13	112.14
1	A	261	VAL	CB-CA-C	-6.66	103.28	111.08
1	D	430	ILE	N-CA-CB	6.46	120.22	110.13
1	D	430	ILE	CB-CA-C	-6.06	102.05	111.26
1	C	388	HIS	CA-C-N	-6.01	113.93	119.82
1	C	388	HIS	C-N-CA	-6.01	113.93	119.82
1	C	442	ILE	CB-CA-C	-5.97	104.22	112.04
1	A	132	VAL	N-CA-CB	5.95	118.64	110.54
1	D	388	HIS	CA-C-N	-5.82	114.12	119.82
1	D	388	HIS	C-N-CA	-5.82	114.12	119.82
1	D	574	GLY	O-C-N	-5.77	115.19	122.70
1	B	132	VAL	CB-CA-C	-5.66	104.50	112.14
1	C	573	LYS	N-CA-C	5.62	120.58	111.37
1	A	377	ILE	CB-CA-C	5.57	119.24	111.34
1	A	509	VAL	N-CA-C	-5.56	107.85	113.47
1	A	42	ASN	N-CA-C	5.53	119.20	111.74
1	D	287	VAL	N-CA-C	5.43	116.58	111.48
1	A	51	PHE	N-CA-C	5.36	117.88	111.71
1	D	148	TYR	N-CA-C	-5.33	102.99	110.50
1	B	377	ILE	CB-CA-C	5.29	118.86	111.34
1	C	345	ILE	N-CA-C	5.18	115.45	110.74
1	D	190	ASP	CA-C-N	5.17	124.97	119.28
1	D	190	ASP	C-N-CA	5.17	124.97	119.28
1	B	558	ILE	CB-CA-C	-5.16	105.18	112.14
1	D	560	ASN	N-CA-C	5.10	119.13	113.01
1	A	430	ILE	N-CA-CB	5.08	118.06	110.13
1	C	51	PHE	N-CA-C	5.08	117.55	111.71
1	D	442	ILE	CB-CA-C	-5.08	105.39	112.04
1	D	177	VAL	CB-CA-C	-5.08	105.47	111.97
1	B	573	LYS	CA-CB-CG	5.06	124.22	114.10
1	D	116	VAL	N-CA-CB	5.04	117.40	110.54
1	B	130	TYR	N-CA-C	5.04	118.23	110.42
1	B	430	ILE	N-CA-CB	-5.02	102.30	110.13
1	C	397	ILE	O-C-N	-5.02	116.30	122.57
1	A	190	ASP	CA-C-N	5.01	124.79	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	190	ASP	C-N-CA	5.01	124.79	119.28
1	C	573	LYS	O-C-N	-5.00	116.15	122.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4474	0	4375	116	0
1	B	4474	0	4375	143	0
1	C	4474	0	4376	125	0
1	D	4474	0	4375	145	0
2	E	28	0	25	1	0
2	F	28	0	25	4	0
2	G	28	0	25	13	0
2	H	28	0	25	2	0
3	A	40	0	56	2	0
3	B	20	0	28	0	0
3	C	40	0	56	1	0
3	D	20	0	28	0	0
4	A	43	0	30	2	0
4	B	43	0	30	2	0
4	C	43	0	30	0	0
4	D	43	0	30	3	0
5	A	17	0	10	1	0
5	B	17	0	10	1	0
5	C	17	0	10	1	0
5	D	17	0	10	1	0
6	A	63	0	0	24	0
6	B	39	0	0	11	0
6	C	37	0	0	9	0
6	D	47	0	0	17	0
All	All	18554	0	17929	530	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 15.

All (530) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:294:LEU:CD2	1:D:295:VAL:CG2	1.79	1.57
1:C:144:ASN:HD21	2:G:1:NAG:C1	0.90	1.55
1:D:294:LEU:HD23	1:D:295:VAL:CG2	1.15	1.55
1:D:294:LEU:CD2	1:D:295:VAL:HG22	1.39	1.47
1:C:144:ASN:ND2	2:G:1:NAG:C1	1.76	1.39
3:A:701:BOG:H8'1	6:A:831:HOH:O	1.27	1.32
1:C:216:ARG:HG3	2:G:2:NAG:C8	1.62	1.29
1:D:430:ILE:HG23	6:D:838:HOH:O	1.27	1.27
1:B:398:GLU:HG3	1:B:421:GLN:NE2	1.60	1.17
1:A:39:PRO:HD3	6:A:823:HOH:O	1.42	1.16
1:A:262:TYR:HE2	1:A:415:LEU:HD23	1.10	1.13
1:B:107:PHE:HB3	6:B:826:HOH:O	1.45	1.13
1:D:294:LEU:HD23	1:D:295:VAL:HG23	1.12	1.11
1:C:216:ARG:CG	2:G:2:NAG:H81	1.81	1.10
1:B:398:GLU:CG	1:B:421:GLN:NE2	2.18	1.07
1:C:276:PRO:HG3	1:C:409:TYR:HD2	1.18	1.05
1:C:276:PRO:HG3	1:C:409:TYR:CD2	1.91	1.04
1:D:527:ALA:HB3	6:D:833:HOH:O	1.58	1.01
1:D:528:PRO:HD3	6:D:833:HOH:O	1.60	1.01
1:D:294:LEU:CD2	1:D:295:VAL:HG23	1.68	1.01
1:C:216:ARG:HG3	2:G:2:NAG:H81	1.01	1.00
1:A:262:TYR:CE2	1:A:415:LEU:HD23	1.96	0.98
1:C:408:LEU:C	1:C:409:TYR:HD1	1.71	0.98
4:D:704:HEM:C1D	6:D:814:HOH:O	2.16	0.97
1:D:554:VAL:HG13	6:D:828:HOH:O	1.64	0.97
1:D:294:LEU:HD21	1:D:295:VAL:CG2	1.91	0.97
1:A:262:TYR:HE2	1:A:415:LEU:CD2	1.78	0.96
1:D:397:ILE:HD11	1:D:426:PHE:CE1	2.01	0.95
1:A:71:PRO:HB2	6:A:838:HOH:O	1.63	0.95
1:B:294:LEU:HD23	1:B:295:VAL:HG23	1.49	0.94
2:F:1:NAG:H61	2:F:2:NAG:C1	1.98	0.93
1:C:216:ARG:NH1	2:G:2:NAG:H83	1.82	0.93
1:D:107:PHE:HB3	6:D:839:HOH:O	1.68	0.93
1:C:123:LEU:O	1:C:469:ARG:NH2	2.02	0.93
1:C:216:ARG:HH11	2:G:2:NAG:C8	1.83	0.91
1:B:398:GLU:HG3	1:B:421:GLN:HE22	1.25	0.91
1:D:294:LEU:HD21	1:D:295:VAL:HG22	1.44	0.91
1:C:276:PRO:CG	1:C:409:TYR:HD2	1.85	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:LEU:O	1:B:469:ARG:NH2	2.06	0.89
1:B:583:GLN:HB3	6:B:833:HOH:O	1.74	0.88
1:D:294:LEU:HA	1:D:409:TYR:CE1	2.09	0.88
1:A:398:GLU:HG3	1:A:421:GLN:NE2	1.89	0.87
1:A:123:LEU:O	1:A:469:ARG:NH2	2.06	0.87
1:B:478:PHE:HD1	1:B:498:ILE:HD13	1.37	0.86
1:D:123:LEU:O	1:D:469:ARG:NH2	2.08	0.86
1:B:392:PRO:HD2	1:B:395:PHE:HE1	1.41	0.85
1:C:197:MET:HE2	1:C:578:THR:HG21	1.55	0.85
1:B:478:PHE:CD1	1:B:498:ILE:HD13	2.10	0.85
1:B:64:TYR:HE1	1:B:70:THR:OG1	1.58	0.85
1:A:262:TYR:CE2	1:A:415:LEU:CD2	2.58	0.85
1:D:294:LEU:HD23	1:D:295:VAL:HG22	0.86	0.84
1:B:197:MET:HE2	1:B:578:THR:HG21	1.59	0.83
1:B:554:VAL:HG13	6:B:837:HOH:O	1.79	0.83
1:D:142:PHE:O	1:D:376:ARG:NH2	2.12	0.82
1:A:43:ARG:HH11	1:A:43:ARG:HG2	1.43	0.82
1:B:398:GLU:CG	1:B:421:GLN:HE21	1.88	0.81
1:C:43:ARG:HG2	1:C:43:ARG:HH11	1.44	0.81
1:A:168:ASN:HB3	6:A:853:HOH:O	1.80	0.81
1:B:478:PHE:HE1	1:B:498:ILE:HA	1.45	0.81
1:B:355:TYR:OH	5:B:705:DF0:O1	1.96	0.81
1:C:216:ARG:HG3	2:G:2:NAG:H82	1.63	0.81
1:A:245:ARG:NH2	1:A:326:GLU:OE2	2.14	0.80
1:B:43:ARG:HG2	1:B:43:ARG:HH11	1.47	0.80
1:B:113:MET:O	1:B:116:VAL:HG22	1.81	0.80
1:D:43:ARG:HG2	1:D:43:ARG:HH11	1.45	0.80
1:B:294:LEU:CD2	1:B:295:VAL:HG23	2.12	0.80
1:C:544:TYR:HA	1:D:137:LYS:NZ	1.97	0.80
1:A:484:GLU:HB3	6:A:851:HOH:O	1.81	0.80
1:C:392:PRO:HD2	1:C:395:PHE:HE1	1.47	0.79
1:C:216:ARG:NH1	2:G:2:NAG:C8	2.45	0.79
1:D:294:LEU:HA	1:D:409:TYR:CD1	2.18	0.79
1:B:216:ARG:NH1	2:F:2:NAG:O7	2.15	0.79
1:C:245:ARG:NH2	1:C:326:GLU:OE2	2.16	0.79
1:B:113:MET:HE3	1:B:117:LEU:HD11	1.65	0.78
1:A:423:VAL:HG13	1:A:578:THR:HG23	1.65	0.77
1:B:64:TYR:CE1	1:B:70:THR:OG1	2.38	0.77
1:B:398:GLU:CD	1:B:421:GLN:HE21	1.93	0.77
1:C:454:GLN:HB3	6:C:821:HOH:O	1.84	0.77
1:D:245:ARG:NH2	1:D:326:GLU:OE2	2.18	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:294:LEU:HB2	1:D:409:TYR:CZ	2.20	0.77
1:C:113:MET:HE3	1:C:117:LEU:HD11	1.67	0.76
1:B:531:LEU:HB2	6:B:816:HOH:O	1.86	0.75
1:C:408:LEU:C	1:C:409:TYR:CD1	2.62	0.75
1:C:216:ARG:CG	2:G:2:NAG:C8	2.51	0.75
1:D:294:LEU:HD22	1:D:295:VAL:HG23	1.68	0.75
1:A:292:PHE:O	1:A:299:MET:HE2	1.86	0.74
1:B:245:ARG:NH2	1:B:326:GLU:OE2	2.20	0.74
1:D:470:PHE:CD1	1:D:525:LEU:HD22	2.22	0.74
1:B:117:LEU:HD23	1:B:366:LEU:HD11	1.69	0.74
1:B:142:PHE:O	1:B:376:ARG:NH2	2.16	0.73
1:D:150:ARG:NH2	1:D:458:MET:O	2.22	0.73
1:B:150:ARG:NH2	1:B:458:MET:O	2.23	0.72
1:C:398:GLU:HG3	1:C:421:GLN:NE2	2.04	0.72
1:D:234:TYR:CE2	1:D:333:ARG:HG3	2.25	0.71
1:C:216:ARG:HH11	2:G:2:NAG:H82	1.55	0.70
2:G:1:NAG:H61	2:G:2:NAG:C1	2.22	0.70
1:D:216:ARG:HG3	2:H:2:NAG:O7	1.91	0.70
1:A:113:MET:O	1:A:116:VAL:HG22	1.91	0.70
1:C:142:PHE:O	1:C:376:ARG:NH2	2.18	0.69
1:A:216:ARG:HG3	2:E:2:NAG:O7	1.93	0.69
1:C:293:GLY:HA2	1:C:299:MET:HE2	1.73	0.69
1:D:203:GLN:HG2	1:D:298:LEU:HD11	1.75	0.69
1:B:294:LEU:HG	1:B:295:VAL:HG22	1.75	0.68
1:A:285:PHE:CE1	6:A:854:HOH:O	2.45	0.68
1:C:189:PRO:HB3	1:C:430:ILE:HD13	1.76	0.68
1:B:271:VAL:HG22	1:B:286:ALA:HB1	1.76	0.68
1:B:294:LEU:CD2	1:B:295:VAL:CG2	2.71	0.68
1:C:276:PRO:CG	1:C:409:TYR:CD2	2.66	0.68
1:D:64:TYR:HE1	1:D:70:THR:OG1	1.76	0.68
1:C:544:TYR:HA	1:D:137:LYS:HZ1	1.59	0.67
1:B:395:PHE:CD2	1:B:407:PHE:CD2	2.83	0.67
1:B:398:GLU:CB	1:B:421:GLN:NE2	2.57	0.67
1:A:68:CYS:SG	6:A:828:HOH:O	2.52	0.67
1:B:294:LEU:HA	1:B:409:TYR:CD1	2.30	0.67
1:D:427:THR:HG22	1:D:583:GLN:HE22	1.59	0.67
1:B:478:PHE:CE1	1:B:498:ILE:HA	2.27	0.67
1:A:203:GLN:HG2	1:A:298:LEU:HD11	1.76	0.67
1:C:458:MET:HE2	6:C:821:HOH:O	1.95	0.66
1:B:478:PHE:CE2	1:B:492:LYS:HA	2.31	0.66
1:D:203:GLN:CG	1:D:298:LEU:HD11	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:113:MET:HE3	1:C:117:LEU:CD1	2.26	0.65
1:C:392:PRO:HD2	1:C:395:PHE:CE1	2.31	0.65
1:B:294:LEU:HA	1:B:409:TYR:CE1	2.31	0.65
1:B:92:LEU:HD23	1:B:355:TYR:CZ	2.31	0.65
1:B:117:LEU:HB3	1:B:366:LEU:HD21	1.79	0.65
1:B:392:PRO:HD2	1:B:395:PHE:CE1	2.28	0.64
1:B:271:VAL:CG2	1:B:286:ALA:HB1	2.26	0.64
1:D:294:LEU:CD2	1:D:295:VAL:HG21	2.17	0.64
1:D:479:GLU:HG3	6:D:809:HOH:O	1.98	0.64
1:C:409:TYR:CD1	1:C:409:TYR:N	2.65	0.64
1:B:414:LEU:HD11	1:B:419:LEU:HD23	1.78	0.64
1:A:216:ARG:HB3	1:A:220:PHE:CD2	2.32	0.64
1:B:470:PHE:CD1	1:B:525:LEU:HD22	2.33	0.64
1:D:195:ASN:HB3	1:D:582:VAL:HG23	1.80	0.64
1:D:64:TYR:CE1	1:D:70:THR:OG1	2.51	0.63
1:D:395:PHE:HD2	1:D:407:PHE:CE2	2.17	0.63
1:A:71:PRO:HG2	6:A:838:HOH:O	1.97	0.63
1:A:163:MET:HE2	1:A:171:LEU:HD21	1.80	0.63
1:B:398:GLU:CG	1:B:421:GLN:HE22	1.95	0.62
1:D:395:PHE:CD2	1:D:407:PHE:CD2	2.87	0.62
1:D:216:ARG:HB3	1:D:220:PHE:CD2	2.34	0.62
1:C:408:LEU:HB3	1:C:409:TYR:CD1	2.33	0.62
1:B:427:THR:OG1	1:B:578:THR:HG22	1.99	0.62
1:D:395:PHE:CD2	1:D:407:PHE:CE2	2.87	0.62
1:C:146:SER:CB	6:C:815:HOH:O	2.46	0.62
1:D:113:MET:HE2	1:D:360:LYS:O	1.99	0.62
1:B:423:VAL:HG13	1:B:578:THR:HG23	1.81	0.62
1:B:342:LYS:HG2	1:B:562:ALA:HB3	1.82	0.62
1:D:450:ALA:HA	6:D:845:HOH:O	2.00	0.62
1:B:423:VAL:CG1	1:B:578:THR:HG23	2.29	0.62
1:C:64:TYR:CE1	1:C:70:THR:OG1	2.52	0.62
1:D:398:GLU:HG3	1:D:421:GLN:NE2	2.14	0.61
1:D:273:MET:CE	1:D:287:VAL:HG22	2.30	0.61
1:B:423:VAL:HG13	1:B:578:THR:CG2	2.30	0.61
1:A:189:PRO:HB3	1:A:430:ILE:HD13	1.83	0.61
1:B:113:MET:HE3	1:B:117:LEU:CD1	2.29	0.61
1:A:203:GLN:CG	1:A:298:LEU:HD11	2.31	0.61
1:A:197:MET:HE2	1:A:578:THR:HG21	1.81	0.60
1:A:285:PHE:CZ	6:A:854:HOH:O	2.53	0.60
1:C:150:ARG:NH2	1:C:458:MET:O	2.34	0.60
1:B:294:LEU:HB2	1:B:409:TYR:CZ	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:463:LEU:HD22	1:B:506:ALA:HB1	1.82	0.60
1:D:352:LEU:C	1:D:352:LEU:HD12	2.26	0.60
1:D:294:LEU:CA	1:D:409:TYR:CE1	2.84	0.60
1:D:427:THR:OG1	1:D:578:THR:HG22	2.00	0.60
1:B:463:LEU:HD22	1:B:506:ALA:CB	2.30	0.59
1:C:245:ARG:HD3	1:C:329:PHE:CD1	2.37	0.59
1:D:463:LEU:HD22	1:D:506:ALA:HB1	1.84	0.59
1:A:245:ARG:HD3	1:A:329:PHE:CD1	2.38	0.59
1:D:344:VAL:HG11	1:D:534:LEU:HD11	1.85	0.59
1:A:451:SER:HB3	6:A:852:HOH:O	2.03	0.59
1:B:245:ARG:HD3	1:B:329:PHE:CE1	2.39	0.58
1:D:463:LEU:HD22	1:D:506:ALA:CB	2.33	0.58
1:A:398:GLU:HG3	1:A:421:GLN:HE22	1.68	0.58
1:B:262:TYR:CE2	1:B:415:LEU:CD2	2.87	0.58
1:A:198:PHE:CD1	1:A:198:PHE:C	2.81	0.58
1:A:150:ARG:NH2	1:A:458:MET:O	2.36	0.58
1:A:427:THR:OG1	1:A:578:THR:HG22	2.03	0.58
1:B:395:PHE:HD2	1:B:407:PHE:CG	2.22	0.58
1:D:198:PHE:CD1	1:D:198:PHE:C	2.81	0.58
1:C:245:ARG:HD3	1:C:329:PHE:CE1	2.39	0.58
1:A:64:TYR:CE1	1:A:70:THR:OG1	2.57	0.57
1:C:203:GLN:HG2	1:C:298:LEU:HD11	1.86	0.57
1:D:271:VAL:HG22	1:D:286:ALA:HB1	1.85	0.57
1:C:88:VAL:HG11	3:C:702:BOG:H1'1	1.86	0.57
1:C:423:VAL:HG13	1:C:578:THR:HG23	1.86	0.57
1:B:292:PHE:O	1:B:299:MET:HE2	2.04	0.56
1:B:209:PHE:HB2	1:B:377:ILE:HG21	1.87	0.56
1:D:33:ASN:HB3	1:D:36:CYS:SG	2.45	0.56
1:B:245:ARG:HD3	1:B:329:PHE:CD1	2.40	0.56
1:B:234:TYR:CE2	1:B:333:ARG:HG3	2.41	0.56
1:A:245:ARG:HD3	1:A:329:PHE:CE1	2.41	0.56
1:D:292:PHE:O	1:D:299:MET:HE2	2.05	0.56
1:B:203:GLN:HG2	1:B:298:LEU:HD11	1.87	0.56
4:B:704:HEM:HMB1	4:B:704:HEM:HBB2	1.87	0.56
1:C:271:VAL:HG22	1:C:286:ALA:HB1	1.86	0.56
1:C:203:GLN:CG	1:C:298:LEU:HD11	2.36	0.55
1:A:57:ASP:OD1	1:A:57:ASP:C	2.48	0.55
1:C:211:LYS:NZ	1:C:236:GLU:OE1	2.38	0.55
1:A:142:PHE:O	1:A:376:ARG:NH2	2.29	0.55
1:D:384:LEU:HD12	1:D:384:LEU:C	2.30	0.55
1:B:117:LEU:HD23	1:B:366:LEU:CD1	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:245:ARG:HD3	1:D:329:PHE:CE1	2.41	0.55
1:A:234:TYR:CE2	1:A:333:ARG:HG3	2.42	0.55
1:D:273:MET:SD	1:D:290:GLU:HA	2.47	0.55
1:B:478:PHE:HE2	1:B:492:LYS:HA	1.72	0.55
1:D:397:ILE:CD1	1:D:426:PHE:CE1	2.85	0.55
1:A:178:LEU:HD22	1:A:183:LEU:HG	1.88	0.54
1:C:395:PHE:CD2	1:C:407:PHE:CD2	2.96	0.54
1:D:90:TYR:CE1	1:D:94:HIS:CE1	2.95	0.54
4:D:704:HEM:HHD	4:D:704:HEM:HBC2	1.89	0.54
1:D:386:HIS:HA	6:D:814:HOH:O	2.05	0.54
1:D:397:ILE:HD11	1:D:426:PHE:CZ	2.43	0.54
1:A:293:GLY:HA2	1:A:299:MET:HE3	1.88	0.54
1:C:352:LEU:C	1:C:352:LEU:HD12	2.33	0.54
1:C:408:LEU:CB	1:C:409:TYR:CD1	2.91	0.53
1:C:478:PHE:CE2	1:C:492:LYS:HA	2.42	0.53
1:B:340:THR:O	1:B:344:VAL:HG23	2.08	0.53
1:B:382:ASN:O	1:B:386:HIS:HD2	1.92	0.53
1:C:207:HIS:CD2	6:C:832:HOH:O	2.62	0.53
1:D:230:LEU:HB3	1:D:233:ILE:HD12	1.89	0.53
1:C:163:MET:HE2	1:C:171:LEU:HD21	1.91	0.53
1:A:76:ARG:HB2	6:A:838:HOH:O	2.08	0.53
1:B:478:PHE:CD1	1:B:498:ILE:CD1	2.90	0.53
1:C:64:TYR:HB2	6:C:818:HOH:O	2.08	0.53
1:D:245:ARG:HD3	1:D:329:PHE:CD1	2.44	0.53
1:B:216:ARG:HG3	2:F:2:NAG:O7	2.08	0.53
1:B:251:LYS:HE2	6:B:824:HOH:O	2.09	0.53
1:C:408:LEU:HB3	1:C:409:TYR:CE1	2.44	0.53
1:D:90:TYR:HE1	1:D:94:HIS:NE2	2.07	0.53
1:B:179:GLU:HA	1:B:183:LEU:HD12	1.91	0.52
1:D:273:MET:HE1	1:D:287:VAL:CG2	2.39	0.52
1:A:450:ALA:HA	6:A:850:HOH:O	2.09	0.52
1:D:294:LEU:HB2	1:D:409:TYR:OH	2.08	0.52
1:D:396:ASN:C	1:D:397:ILE:HD13	2.35	0.52
1:B:384:LEU:HD12	1:B:384:LEU:C	2.35	0.52
1:A:423:VAL:HG13	1:A:578:THR:CG2	2.37	0.52
1:A:525:LEU:N	1:A:525:LEU:HD23	2.25	0.52
1:C:117:LEU:HD23	1:C:366:LEU:HD11	1.92	0.52
1:D:116:VAL:O	1:D:120:ARG:HG2	2.10	0.52
1:D:342:LYS:HG2	1:D:562:ALA:HB3	1.91	0.52
1:A:64:TYR:HD1	1:A:70:THR:O	1.93	0.52
1:A:176:GLU:HG2	1:A:180:LYS:HD2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:262:TYR:CE2	1:D:415:LEU:CD2	2.93	0.52
1:D:478:PHE:CE2	1:D:492:LYS:HA	2.45	0.52
1:A:138:SER:HA	1:B:334:LEU:HD11	1.92	0.51
1:C:113:MET:O	1:C:116:VAL:HG22	2.10	0.51
1:D:398:GLU:OE2	1:D:421:GLN:HG3	2.10	0.51
1:D:427:THR:CG2	1:D:583:GLN:HE22	2.23	0.51
1:A:342:LYS:HG2	1:A:562:ALA:HB3	1.91	0.51
1:A:45:GLU:OE1	1:A:137:LYS:NZ	2.41	0.51
1:B:178:LEU:HD22	1:B:183:LEU:HG	1.91	0.51
1:B:470:PHE:CG	1:B:525:LEU:HD22	2.45	0.51
1:B:265:THR:OG1	1:B:268:ASP:HB3	2.10	0.51
1:D:197:MET:HE3	1:D:301:TYR:OH	2.11	0.51
1:A:261:VAL:C	1:A:262:TYR:HD1	2.18	0.51
1:B:43:ARG:HG2	1:B:43:ARG:NH1	2.21	0.51
1:D:120:ARG:HD2	6:D:833:HOH:O	2.11	0.51
1:D:291:VAL:O	1:D:294:LEU:HB3	2.11	0.51
1:D:386:HIS:CG	6:D:814:HOH:O	2.64	0.51
1:A:491:LEU:HD11	1:A:509:VAL:HG11	1.93	0.50
1:C:382:ASN:O	1:C:386:HIS:HD2	1.93	0.50
1:A:261:VAL:O	1:A:262:TYR:HD1	1.94	0.50
1:C:458:MET:HE3	1:C:460:TYR:CE1	2.46	0.50
1:B:294:LEU:HG	1:B:295:VAL:CG2	2.40	0.50
1:C:244:LEU:CD2	1:C:271:VAL:HG11	2.42	0.50
1:B:33:ASN:HB3	1:B:36:CYS:SG	2.52	0.50
1:B:388:HIS:N	1:B:389:PRO:HD2	2.27	0.50
1:B:32:ALA:HB3	1:B:158:ASP:OD2	2.12	0.50
1:B:427:THR:HG22	1:B:583:GLN:HE22	1.77	0.50
1:A:372:GLN:HB2	1:A:532:LYS:HZ1	1.77	0.49
1:A:395:PHE:HD2	1:A:407:PHE:CE2	2.30	0.49
1:C:259:GLY:HA3	6:C:819:HOH:O	2.12	0.49
1:D:295:VAL:HG23	1:D:298:LEU:HD22	1.94	0.49
1:B:478:PHE:CE1	1:B:498:ILE:CD1	2.95	0.49
1:C:126:SER:HA	1:C:127:PRO:C	2.37	0.49
1:A:47:MET:HE3	1:B:320:HIS:HE1	1.77	0.49
1:A:398:GLU:CG	1:A:421:GLN:NE2	2.70	0.49
1:A:433:ARG:HD3	6:A:834:HOH:O	2.13	0.49
1:C:372:GLN:HB2	1:C:532:LYS:HZ1	1.77	0.49
1:D:252:LEU:HD13	1:D:309:HIS:CD2	2.48	0.49
1:C:427:THR:OG1	1:C:578:THR:HG22	2.13	0.49
1:B:482:THR:HG22	1:B:509:VAL:HG13	1.94	0.49
1:C:384:LEU:C	1:C:384:LEU:HD12	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:352:LEU:HD13	1:B:518:PHE:HE2	1.78	0.49
1:C:177:VAL:O	1:C:181:VAL:HG22	2.13	0.49
1:B:183:LEU:HD22	1:B:442:ILE:HD13	1.95	0.49
1:C:43:ARG:HG2	1:C:43:ARG:NH1	2.21	0.49
1:D:201:PHE:CD1	1:D:348:TYR:CD2	3.01	0.48
1:B:320:HIS:HA	1:B:322:GLU:OE2	2.13	0.48
1:C:113:MET:HE2	1:C:360:LYS:O	2.12	0.48
1:D:472:LEU:HD11	1:D:524:GLU:HB2	1.94	0.48
1:C:65:GLY:N	6:C:818:HOH:O	2.32	0.48
1:C:395:PHE:HD2	1:C:407:PHE:CG	2.31	0.48
1:D:90:TYR:CD1	1:D:94:HIS:CE1	3.02	0.48
1:B:216:ARG:HG3	2:F:2:NAG:H81	1.96	0.48
1:C:285:PHE:HB2	1:C:299:MET:HE3	1.94	0.48
1:A:76:ARG:HG2	6:A:859:HOH:O	2.13	0.48
1:C:234:TYR:CE2	1:C:333:ARG:HG3	2.48	0.48
1:D:271:VAL:CG2	1:D:286:ALA:HB1	2.44	0.48
1:A:378:ALA:O	1:A:379:SER:C	2.55	0.48
1:C:116:VAL:CG2	1:C:117:LEU:N	2.77	0.47
1:C:194:SER:HB3	1:C:198:PHE:HD2	1.79	0.47
1:D:201:PHE:CD1	1:D:348:TYR:HD2	2.32	0.47
4:A:705:HEM:HBC2	4:A:705:HEM:HHD	1.96	0.47
1:C:380:GLU:HG2	1:C:466:TYR:CE1	2.49	0.47
1:A:244:LEU:CD2	1:A:271:VAL:HG11	2.44	0.47
1:A:395:PHE:CD2	1:A:407:PHE:CE2	3.02	0.47
1:C:197:MET:HG3	1:C:578:THR:HG22	1.96	0.47
1:D:202:ALA:O	1:D:206:THR:HG23	2.15	0.47
1:D:388:HIS:N	1:D:389:PRO:HD2	2.30	0.47
1:C:408:LEU:CB	1:C:409:TYR:CE1	2.98	0.47
1:C:276:PRO:HG3	1:C:409:TYR:CE2	2.46	0.47
1:A:423:VAL:CG1	1:A:578:THR:HG23	2.40	0.47
1:B:338:GLY:HA3	1:B:559:ILE:HD13	1.96	0.47
1:B:398:GLU:CB	1:B:421:GLN:HE22	2.22	0.47
1:C:178:LEU:HD22	1:C:183:LEU:HG	1.95	0.47
1:D:265:THR:OG1	1:D:268:ASP:HB3	2.15	0.47
1:A:388:HIS:N	1:A:389:PRO:HD2	2.29	0.47
1:B:427:THR:OG1	1:B:578:THR:CG2	2.62	0.47
1:B:504:TYR:HB3	1:B:505:PRO:HD3	1.96	0.47
1:D:178:LEU:HD22	1:D:183:LEU:HG	1.96	0.47
1:A:76:ARG:CB	6:A:838:HOH:O	2.61	0.47
1:B:57:ASP:OD1	1:B:57:ASP:C	2.58	0.47
1:B:90:TYR:CD1	1:B:90:TYR:C	2.93	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:295:VAL:CG2	1:C:298:LEU:HD22	2.44	0.47
1:D:90:TYR:HE1	1:D:94:HIS:CE1	2.33	0.47
1:C:544:TYR:HA	1:D:137:LYS:HZ3	1.77	0.46
1:A:67:ASN:C	6:A:828:HOH:O	2.57	0.46
1:C:144:ASN:CG	2:G:1:NAG:C1	2.77	0.46
1:A:113:MET:HE2	1:A:360:LYS:O	2.16	0.46
1:D:293:GLY:HA2	1:D:299:MET:HE3	1.97	0.46
1:D:294:LEU:HD21	1:D:295:VAL:HG21	1.90	0.46
1:D:470:PHE:CG	1:D:525:LEU:HD22	2.50	0.46
1:B:395:PHE:CD2	1:B:407:PHE:CG	3.04	0.46
1:C:500:VAL:HG12	1:C:500:VAL:O	2.14	0.46
1:B:226:HIS:HB3	1:B:376:ARG:HA	1.97	0.46
1:B:382:ASN:O	1:B:386:HIS:CD2	2.69	0.46
1:C:527:ALA:HA	5:C:706:DF0:C2	2.45	0.46
1:D:372:GLN:HB2	1:D:532:LYS:HZ1	1.81	0.46
1:D:582:VAL:HB	6:D:838:HOH:O	2.15	0.46
1:A:205:PHE:O	1:A:208:GLN:HG2	2.16	0.46
1:A:395:PHE:HD1	1:A:395:PHE:N	2.14	0.46
1:B:398:GLU:HB2	1:B:421:GLN:NE2	2.31	0.46
1:A:269:THR:OG1	1:A:271:VAL:HG13	2.16	0.46
1:A:395:PHE:N	1:A:395:PHE:CD1	2.83	0.46
1:A:517:ILE:HG23	1:A:518:PHE:CG	2.51	0.46
1:C:90:TYR:HD1	1:C:90:TYR:C	2.24	0.46
1:D:209:PHE:HB2	1:D:377:ILE:HG21	1.97	0.46
1:D:287:VAL:CG2	1:D:289:GLN:O	2.64	0.46
1:D:390:LEU:HD21	1:D:517:ILE:HD11	1.98	0.46
1:A:84:THR:O	1:A:88:VAL:HG23	2.17	0.45
1:A:287:VAL:HG21	1:A:292:PHE:HB2	1.98	0.45
1:D:320:HIS:HA	1:D:322:GLU:OE2	2.16	0.45
1:C:136:TYR:N	1:C:136:TYR:CD1	2.84	0.45
1:D:120:ARG:CZ	6:D:833:HOH:O	2.64	0.45
1:A:162:PRO:HB2	1:A:171:LEU:HD22	1.97	0.45
1:B:287:VAL:HG11	1:B:302:ALA:HB1	1.97	0.45
1:D:161:THR:O	1:D:163:MET:O	2.34	0.45
1:A:322:GLU:HG3	1:B:50:GLY:C	2.42	0.45
1:D:57:ASP:OD1	1:D:57:ASP:C	2.60	0.45
1:A:71:PRO:CB	6:A:838:HOH:O	2.37	0.45
1:B:45:GLU:OE1	1:B:137:LYS:NZ	2.42	0.45
1:A:86:ASN:H	1:A:86:ASN:HD22	1.65	0.45
1:D:133:HIS:C	1:D:134:TYR:CD1	2.95	0.45
1:D:423:VAL:HG13	1:D:578:THR:CG2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:92:LEU:HD23	1:B:355:TYR:CE1	2.51	0.45
1:D:294:LEU:HD23	1:D:294:LEU:C	2.41	0.45
1:A:382:ASN:O	1:A:386:HIS:HD2	1.99	0.45
1:B:194:SER:HB3	1:B:198:PHE:HD2	1.82	0.45
1:C:64:TYR:HD1	1:C:70:THR:O	1.99	0.45
1:C:398:GLU:CG	1:C:421:GLN:NE2	2.76	0.45
1:B:117:LEU:HD23	1:B:366:LEU:CG	2.47	0.45
1:B:273:MET:SD	1:B:290:GLU:HA	2.57	0.45
1:D:64:TYR:CD1	1:D:64:TYR:C	2.95	0.45
1:D:163:MET:HE1	1:D:502:GLU:HG2	1.99	0.45
1:A:395:PHE:CD2	1:A:407:PHE:CD2	3.06	0.44
1:B:113:MET:HE2	1:B:360:LYS:O	2.17	0.44
1:C:183:LEU:HD23	1:C:183:LEU:HA	1.80	0.44
1:C:482:THR:HG22	1:C:509:VAL:CG1	2.46	0.44
1:D:295:VAL:CG2	1:D:298:LEU:HD22	2.46	0.44
1:A:203:GLN:CD	1:A:298:LEU:HD11	2.42	0.44
3:A:701:BOG:C8'	6:A:831:HOH:O	2.11	0.44
1:C:90:TYR:C	1:C:90:TYR:CD1	2.95	0.44
1:D:479:GLU:CG	6:D:809:HOH:O	2.62	0.44
1:B:158:ASP:O	1:B:158:ASP:CG	2.60	0.44
1:C:388:HIS:N	1:C:389:PRO:HD2	2.32	0.44
1:C:500:VAL:O	1:C:500:VAL:CG1	2.65	0.44
1:D:414:LEU:HD11	1:D:419:LEU:HD23	1.98	0.44
1:A:197:MET:HE3	1:A:301:TYR:OH	2.17	0.44
1:C:491:LEU:HD11	1:C:509:VAL:HG11	2.00	0.44
1:A:50:GLY:C	1:B:322:GLU:HG3	2.43	0.44
1:C:198:PHE:HE1	1:C:348:TYR:CE1	2.35	0.44
1:D:64:TYR:C	1:D:64:TYR:HD1	2.25	0.44
1:D:162:PRO:HB2	1:D:171:LEU:HD22	1.98	0.44
1:D:380:GLU:HG2	1:D:466:TYR:CE1	2.53	0.44
1:B:427:THR:CG2	1:B:583:GLN:HE22	2.31	0.44
1:C:320:HIS:HA	1:C:322:GLU:OE2	2.18	0.44
1:A:45:GLU:OE2	1:B:546:LYS:HD2	2.18	0.44
1:B:197:MET:HG3	1:B:578:THR:HG22	1.99	0.44
1:B:320:HIS:CA	1:B:322:GLU:OE2	2.66	0.44
1:C:156:ALA:HB3	1:C:159:CYS:SG	2.58	0.44
1:A:504:TYR:HB3	1:A:505:PRO:HD3	2.00	0.44
1:C:504:TYR:HB3	1:C:505:PRO:HD3	2.00	0.44
1:A:163:MET:HB3	6:A:846:HOH:O	2.18	0.43
1:B:176:GLU:HG2	1:B:180:LYS:HD2	2.00	0.43
1:C:414:LEU:HD11	1:C:419:LEU:HD23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:382:ASN:HB3	6:C:812:HOH:O	2.17	0.43
1:A:90:TYR:HE1	1:A:94:HIS:NE2	2.16	0.43
1:A:198:PHE:C	1:A:198:PHE:HD1	2.24	0.43
1:A:318:GLN:HG3	6:A:822:HOH:O	2.19	0.43
1:C:525:LEU:N	1:C:525:LEU:HD23	2.33	0.43
1:D:198:PHE:CD2	1:D:351:HIS:HD2	2.37	0.43
1:A:129:THR:HG22	1:A:137:LYS:HD2	1.99	0.43
1:A:300:MET:HG3	1:A:419:LEU:HD22	2.00	0.43
1:B:196:MET:HE2	1:B:431:ALA:HB2	2.01	0.43
1:C:482:THR:HG22	1:C:509:VAL:HG12	2.01	0.43
1:D:120:ARG:NH1	6:D:833:HOH:O	2.52	0.43
1:D:294:LEU:HD23	1:D:295:VAL:N	2.34	0.43
1:A:197:MET:HG3	1:A:578:THR:HG22	1.99	0.43
1:B:194:SER:HB3	1:B:198:PHE:CD2	2.53	0.43
1:B:203:GLN:CG	1:B:298:LEU:HD11	2.49	0.43
1:B:230:LEU:HA	1:B:232:HIS:CE1	2.54	0.43
1:D:176:GLU:HG2	1:D:180:LYS:HD2	2.01	0.43
1:D:452:ILE:HG23	6:D:823:HOH:O	2.19	0.43
1:D:541:SER:O	1:D:542:PRO:C	2.62	0.43
1:D:90:TYR:HE1	1:D:94:HIS:CD2	2.37	0.43
1:A:271:VAL:HG22	1:A:286:ALA:HB1	2.01	0.43
1:B:450:ALA:HA	6:B:836:HOH:O	2.18	0.43
4:B:704:HEM:HBC2	4:B:704:HEM:HHD	2.01	0.42
1:C:32:ALA:HB3	1:C:158:ASP:OD2	2.20	0.42
1:C:90:TYR:CE1	1:C:94:HIS:CG	3.07	0.42
1:C:117:LEU:HB3	1:C:366:LEU:HD21	2.02	0.42
1:A:294:LEU:HD22	1:A:409:TYR:CD1	2.54	0.42
1:B:230:LEU:HB3	1:B:233:ILE:HD12	2.01	0.42
1:B:500:VAL:O	1:B:500:VAL:CG1	2.66	0.42
1:A:316:LEU:HD12	1:A:316:LEU:HA	1.83	0.42
1:B:90:TYR:C	1:B:90:TYR:HD1	2.26	0.42
1:B:380:GLU:HG2	1:B:466:TYR:CE1	2.54	0.42
1:D:395:PHE:HD1	1:D:395:PHE:N	2.16	0.42
1:D:395:PHE:N	1:D:395:PHE:CD1	2.87	0.42
1:B:132:VAL:HG22	6:B:806:HOH:O	2.19	0.42
1:B:205:PHE:CE2	1:B:344:VAL:HG21	2.55	0.42
1:B:423:VAL:HG13	1:B:578:THR:HG21	2.01	0.42
1:D:161:THR:C	1:D:163:MET:O	2.63	0.42
1:A:64:TYR:CD1	1:A:70:THR:O	2.73	0.42
1:A:388:HIS:N	1:A:389:PRO:CD	2.83	0.42
1:A:478:PHE:CE2	1:A:492:LYS:HA	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:149:THR:OG1	1:D:150:ARG:N	2.46	0.42
1:D:530:SER:O	1:D:534:LEU:HD22	2.19	0.42
1:A:380:GLU:HG2	1:A:466:TYR:CE1	2.54	0.42
1:B:225:GLY:O	1:B:226:HIS:C	2.62	0.42
1:C:45:GLU:OE2	1:D:546:LYS:HD2	2.20	0.42
1:C:148:TYR:CE1	1:C:377:ILE:HD11	2.55	0.42
1:C:226:HIS:HB3	1:C:376:ARG:HA	2.01	0.42
1:D:120:ARG:NE	5:D:705:DF0:O	2.52	0.42
1:B:132:VAL:HG13	6:B:827:HOH:O	2.19	0.42
1:A:90:TYR:CE1	1:A:94:HIS:CE1	3.08	0.42
1:A:397:ILE:HD13	1:A:402:TYR:CD2	2.55	0.42
1:D:363:PRO:HG2	1:D:545:TRP:CD2	2.54	0.42
1:A:261:VAL:C	1:A:262:TYR:CD1	2.98	0.42
1:A:74:LEU:HD22	1:A:74:LEU:O	2.20	0.41
1:A:293:GLY:HA2	1:A:299:MET:CE	2.49	0.41
1:B:113:MET:O	1:B:117:LEU:HD13	2.20	0.41
1:B:296:PRO:HD3	6:B:802:HOH:O	2.20	0.41
1:C:189:PRO:HB3	1:C:430:ILE:CD1	2.48	0.41
1:C:287:VAL:HG21	1:C:292:PHE:HB2	2.02	0.41
1:D:216:ARG:NH1	2:H:2:NAG:O7	2.53	0.41
1:A:43:ARG:HG2	1:A:43:ARG:NH1	2.20	0.41
1:D:100:ASN:O	1:D:104:ASN:ND2	2.44	0.41
1:A:463:LEU:HD22	1:A:506:ALA:CB	2.50	0.41
1:B:90:TYR:CE1	1:B:94:HIS:CG	3.08	0.41
1:B:478:PHE:CE1	1:B:498:ILE:HD12	2.55	0.41
1:C:492:LYS:O	1:C:495:TYR:O	2.39	0.41
1:D:525:LEU:O	1:D:528:PRO:HD2	2.21	0.41
1:A:90:TYR:CD1	1:A:94:HIS:CE1	3.08	0.41
1:B:294:LEU:CG	1:B:295:VAL:CG2	2.99	0.41
1:C:190:ASP:CG	1:C:517:ILE:HD12	2.46	0.41
1:C:423:VAL:CG1	1:C:578:THR:HG23	2.50	0.41
1:D:226:HIS:HB3	1:D:376:ARG:HA	2.03	0.41
1:D:287:VAL:HG23	1:D:289:GLN:O	2.20	0.41
1:D:287:VAL:HG21	1:D:292:PHE:HB2	2.02	0.41
1:D:517:ILE:HG23	1:D:518:PHE:CG	2.55	0.41
4:A:705:HEM:HBB2	4:A:705:HEM:HMB2	2.02	0.41
1:C:427:THR:OG1	1:C:578:THR:CG2	2.69	0.41
1:D:482:THR:HG22	1:D:509:VAL:HG13	2.02	0.41
1:A:527:ALA:HA	5:A:706:DF0:C2	2.50	0.41
1:B:122:TYR:HB2	6:B:829:HOH:O	2.21	0.41
1:C:198:PHE:CE1	1:C:348:TYR:CE1	3.08	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:423:VAL:HG13	1:D:578:THR:HG21	2.02	0.41
1:D:478:PHE:CD1	1:D:498:ILE:HD13	2.56	0.41
1:B:152:LEU:HD12	1:B:466:TYR:CD1	2.56	0.41
1:B:216:ARG:HG2	1:B:220:PHE:CD2	2.55	0.41
1:C:86:ASN:H	1:C:86:ASN:HD22	1.69	0.41
1:C:271:VAL:CG2	1:C:286:ALA:HB1	2.48	0.41
1:A:245:ARG:HD2	6:A:812:HOH:O	2.20	0.41
1:B:368:ASN:HB3	6:B:825:HOH:O	2.20	0.41
1:C:189:PRO:CB	1:C:430:ILE:HD13	2.48	0.41
1:A:283:LEU:HD21	1:A:415:LEU:HD12	2.03	0.41
1:A:285:PHE:CD1	6:A:854:HOH:O	2.73	0.41
1:A:384:LEU:C	1:A:384:LEU:HD12	2.45	0.41
1:A:525:LEU:N	1:A:525:LEU:CD2	2.83	0.41
1:B:162:PRO:HB2	1:B:171:LEU:HD22	2.02	0.41
1:B:196:MET:CE	1:B:431:ALA:HA	2.51	0.41
1:B:395:PHE:CE2	1:B:407:PHE:CD2	3.09	0.41
1:C:372:GLN:HB2	1:C:532:LYS:NZ	2.36	0.41
1:D:195:ASN:OD1	1:D:195:ASN:C	2.64	0.41
1:A:334:LEU:HD23	1:A:334:LEU:HA	1.83	0.41
1:B:388:HIS:N	1:B:389:PRO:CD	2.84	0.41
1:C:72:GLU:HG2	6:C:828:HOH:O	2.19	0.41
1:C:398:GLU:CD	1:C:421:GLN:NE2	2.79	0.41
4:D:704:HEM:C2D	6:D:814:HOH:O	2.58	0.41
1:C:322:GLU:HG3	1:D:50:GLY:C	2.45	0.40
1:D:273:MET:CE	1:D:287:VAL:CG2	2.96	0.40
1:A:382:ASN:O	1:A:386:HIS:CD2	2.75	0.40
1:A:56:CYS:HB3	6:A:828:HOH:O	2.20	0.40
1:A:97:GLY:HA2	6:A:845:HOH:O	2.21	0.40
1:B:117:LEU:HD23	1:B:366:LEU:HD21	2.02	0.40
1:B:198:PHE:CE1	1:B:348:TYR:CE1	3.09	0.40
1:B:198:PHE:HE1	1:B:348:TYR:CE1	2.39	0.40
1:C:203:GLN:CD	1:C:298:LEU:HD11	2.46	0.40
1:C:525:LEU:O	1:C:528:PRO:HD2	2.22	0.40
1:D:201:PHE:HD1	1:D:348:TYR:CD2	2.39	0.40
1:D:340:THR:O	1:D:344:VAL:HG23	2.22	0.40
1:B:478:PHE:HE1	1:B:498:ILE:HD12	1.86	0.40
1:C:398:GLU:HG3	1:C:421:GLN:HE22	1.79	0.40
1:C:504:TYR:O	1:C:505:PRO:C	2.63	0.40
1:A:537:ASN:CG	1:A:538:PRO:HD2	2.47	0.40
1:D:300:MET:HG3	1:D:419:LEU:HD22	2.03	0.40
1:D:423:VAL:CG1	1:D:578:THR:HG23	2.51	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	550/604 (91%)	527 (96%)	23 (4%)	0	100 100
1	B	550/604 (91%)	526 (96%)	24 (4%)	0	100 100
1	C	550/604 (91%)	523 (95%)	26 (5%)	1 (0%)	43 71
1	D	550/604 (91%)	524 (95%)	26 (5%)	0	100 100
All	All	2200/2416 (91%)	2100 (96%)	99 (4%)	1 (0%)	100 100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	397	ILE

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	493/537 (92%)	435 (88%)	58 (12%)	5 16
1	B	493/537 (92%)	442 (90%)	51 (10%)	7 22
1	C	493/537 (92%)	439 (89%)	54 (11%)	6 19
1	D	493/537 (92%)	441 (90%)	52 (10%)	6 21
All	All	1972/2148 (92%)	1757 (89%)	215 (11%)	6 19

All (215) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	ARG
1	A	49	THR
1	A	64	TYR
1	A	69	THR
1	A	70	THR
1	A	74	LEU
1	A	86	ASN
1	A	92	LEU
1	A	100	ASN
1	A	108	LEU
1	A	117	LEU
1	A	121	SER
1	A	129	THR
1	A	132	VAL
1	A	137	LYS
1	A	138	SER
1	A	150	ARG
1	A	169	LYS
1	A	171	LEU
1	A	178	LEU
1	A	198	PHE
1	A	215	LYS
1	A	216	ARG
1	A	222	ARG
1	A	238	LEU
1	A	248	LYS
1	A	252	LEU
1	A	271	VAL
1	A	289	GLN
1	A	291	VAL
1	A	295	VAL
1	A	298	LEU
1	A	311	ARG
1	A	316	LEU
1	A	322	GLU
1	A	358	LYS
1	A	376	ARG
1	A	377	ILE
1	A	385	TYR
1	A	405	LYS
1	A	409	TYR
1	A	428	ARG

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Mol	Chain	Res	Type
1	A	430	ILE
1	A	442	ILE
1	A	469	ARG
1	A	473	LYS
1	A	479	GLU
1	A	484	GLU
1	A	492	LYS
1	A	509	VAL
1	A	525	LEU
1	A	532	LYS
1	A	534	LEU
1	A	539	ILE
1	A	554	VAL
1	A	578	THR
1	A	582	VAL
1	A	583	GLN
1	B	43	ARG
1	B	49	THR
1	B	64	TYR
1	B	69	THR
1	B	70	THR
1	B	92	LEU
1	B	111	LEU
1	B	132	VAL
1	B	137	LYS
1	B	138	SER
1	B	150	ARG
1	B	165	VAL
1	B	169	LYS
1	B	171	LEU
1	B	178	LEU
1	B	215	LYS
1	B	222	ARG
1	B	238	LEU
1	B	248	LYS
1	B	252	LEU
1	B	271	VAL
1	B	287	VAL
1	B	289	GLN
1	B	291	VAL
1	B	294	LEU
1	B	295	VAL

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Mol	Chain	Res	Type
1	B	298	LEU
1	B	316	LEU
1	B	322	GLU
1	B	326	GLU
1	B	376	ARG
1	B	377	ILE
1	B	385	TYR
1	B	405	LYS
1	B	428	ARG
1	B	469	ARG
1	B	473	LYS
1	B	479	GLU
1	B	484	GLU
1	B	492	LYS
1	B	509	VAL
1	B	525	LEU
1	B	532	LYS
1	B	534	LEU
1	B	539	ILE
1	B	554	VAL
1	B	568	ILE
1	B	573	LYS
1	B	578	THR
1	B	582	VAL
1	B	583	GLN
1	C	43	ARG
1	C	49	THR
1	C	64	TYR
1	C	69	THR
1	C	70	THR
1	C	74	LEU
1	C	86	ASN
1	C	92	LEU
1	C	111	LEU
1	C	116	VAL
1	C	132	VAL
1	C	136	TYR
1	C	137	LYS
1	C	138	SER
1	C	150	ARG
1	C	169	LYS
1	C	171	LEU

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Mol	Chain	Res	Type
1	C	178	LEU
1	C	186	GLU
1	C	215	LYS
1	C	222	ARG
1	C	238	LEU
1	C	248	LYS
1	C	252	LEU
1	C	271	VAL
1	C	289	GLN
1	C	291	VAL
1	C	295	VAL
1	C	298	LEU
1	C	316	LEU
1	C	322	GLU
1	C	358	LYS
1	C	376	ARG
1	C	377	ILE
1	C	385	TYR
1	C	399	ASP
1	C	405	LYS
1	C	409	TYR
1	C	428	ARG
1	C	430	ILE
1	C	469	ARG
1	C	473	LYS
1	C	479	GLU
1	C	484	GLU
1	C	492	LYS
1	C	525	LEU
1	C	532	LYS
1	C	534	LEU
1	C	539	ILE
1	C	554	VAL
1	C	568	ILE
1	C	578	THR
1	C	582	VAL
1	C	583	GLN
1	D	43	ARG
1	D	64	TYR
1	D	69	THR
1	D	70	THR
1	D	92	LEU

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Mol	Chain	Res	Type
1	D	111	LEU
1	D	116	VAL
1	D	117	LEU
1	D	132	VAL
1	D	137	LYS
1	D	138	SER
1	D	150	ARG
1	D	165	VAL
1	D	169	LYS
1	D	171	LEU
1	D	178	LEU
1	D	215	LYS
1	D	216	ARG
1	D	222	ARG
1	D	238	LEU
1	D	248	LYS
1	D	252	LEU
1	D	271	VAL
1	D	287	VAL
1	D	289	GLN
1	D	291	VAL
1	D	294	LEU
1	D	295	VAL
1	D	298	LEU
1	D	316	LEU
1	D	322	GLU
1	D	376	ARG
1	D	377	ILE
1	D	384	LEU
1	D	385	TYR
1	D	397	ILE
1	D	405	LYS
1	D	408	LEU
1	D	430	ILE
1	D	469	ARG
1	D	473	LYS
1	D	479	GLU
1	D	484	GLU
1	D	492	LYS
1	D	509	VAL
1	D	532	LYS
1	D	534	LEU

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Mol	Chain	Res	Type
1	D	554	VAL
1	D	568	ILE
1	D	578	THR
1	D	581	ASN
1	D	583	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	ASN
1	A	86	ASN
1	A	89	HIS
1	A	203	GLN
1	A	406	GLN
1	A	421	GLN
1	A	445	GLN
1	B	86	ASN
1	B	89	HIS
1	B	100	ASN
1	B	204	HIS
1	B	241	GLN
1	B	242	HIS
1	B	421	GLN
1	B	543	GLN
1	B	570	ASN
1	B	571	ASN
1	B	581	ASN
1	B	583	GLN
1	C	67	ASN
1	C	86	ASN
1	C	144	ASN
1	C	214	HIS
1	C	241	GLN
1	C	242	HIS
1	C	327	GLN
1	C	421	GLN
1	C	445	GLN
1	D	86	ASN
1	D	100	ASN
1	D	203	GLN
1	D	214	HIS
1	D	241	GLN

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Mol	Chain	Res	Type
1	D	242	HIS
1	D	255	GLN
1	D	375	ASN
1	D	406	GLN
1	D	421	GLN
1	D	461	GLN
1	D	583	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)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

8 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	E	1	1,2	14,14,15	0.90	1 (7%)	17,19,21	1.81	5 (29%)
2	NAG	E	2	2	14,14,15	0.29	0	17,19,21	0.56	0
2	NAG	F	1	1,2	14,14,15	0.67	0	17,19,21	1.36	2 (11%)
2	NAG	F	2	2	14,14,15	0.29	0	17,19,21	0.57	0
2	NAG	G	1	2	14,14,15	0.29	0	17,19,21	0.56	0
2	NAG	G	2	2	14,14,15	0.29	0	17,19,21	0.56	0
2	NAG	H	1	1,2	14,14,15	0.63	0	17,19,21	1.36	2 (11%)
2	NAG	H	2	2	14,14,15	0.29	0	17,19,21	0.56	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	NAG	E	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	4/6/23/26	0/1/1/1
2	NAG	F	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	F	2	2	-	0/6/23/26	0/1/1/1
2	NAG	G	1	2	-	4/6/23/26	0/1/1/1
2	NAG	G	2	2	-	4/6/23/26	0/1/1/1
2	NAG	H	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	H	2	2	-	3/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1	NAG	O5-C1	-2.76	1.39	1.43

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	1	NAG	C1-C2-N2	-4.12	103.95	110.43
2	H	1	NAG	C1-O5-C5	3.95	117.48	112.19
2	E	1	NAG	C1-O5-C5	3.50	116.88	112.19
2	F	1	NAG	O5-C5-C6	3.11	113.71	107.66
2	H	1	NAG	C1-C2-N2	-2.78	106.06	110.43
2	E	1	NAG	O4-C4-C5	2.43	115.32	109.32
2	E	1	NAG	O5-C1-C2	-2.20	107.89	111.29
2	E	1	NAG	C3-C4-C5	-2.12	106.39	110.23
2	F	1	NAG	C4-C3-C2	-2.00	108.08	111.02

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	2	NAG	C1-C2-N2-C7
2	G	2	NAG	C8-C7-N2-C2
2	G	2	NAG	O7-C7-N2-C2
2	F	1	NAG	O5-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
2	F	1	NAG	C4-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	E	1	NAG	O5-C5-C6-O6
2	E	1	NAG	C4-C5-C6-O6
2	G	1	NAG	O5-C5-C6-O6
2	G	1	NAG	C4-C5-C6-O6
2	G	1	NAG	C8-C7-N2-C2
2	E	2	NAG	C8-C7-N2-C2
2	G	1	NAG	O7-C7-N2-C2
2	E	2	NAG	O7-C7-N2-C2
2	H	2	NAG	C8-C7-N2-C2
2	H	2	NAG	C4-C5-C6-O6
2	G	2	NAG	C3-C2-N2-C7
2	H	2	NAG	O7-C7-N2-C2

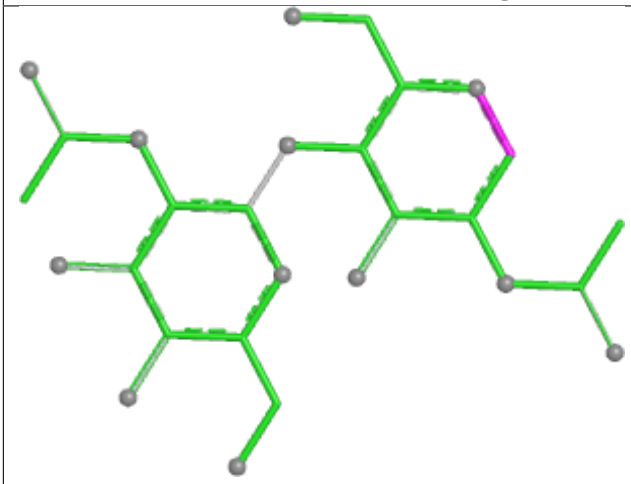
There are no ring outliers.

6 monomers are involved in 20 short contacts:

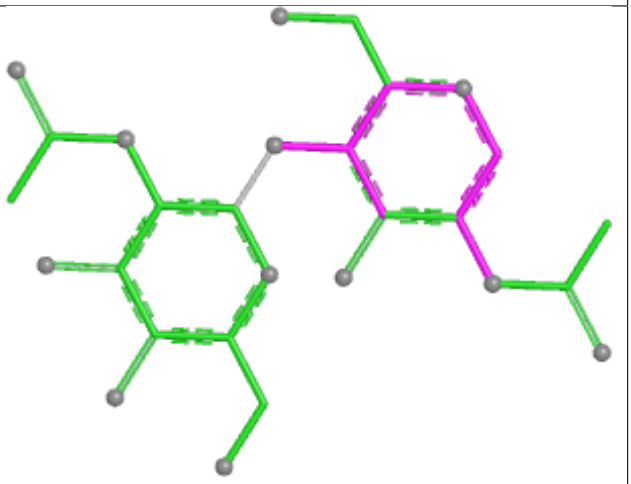
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	1	NAG	4	0
2	E	2	NAG	1	0
2	H	2	NAG	2	0
2	F	1	NAG	1	0
2	F	2	NAG	4	0
2	G	2	NAG	10	0

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

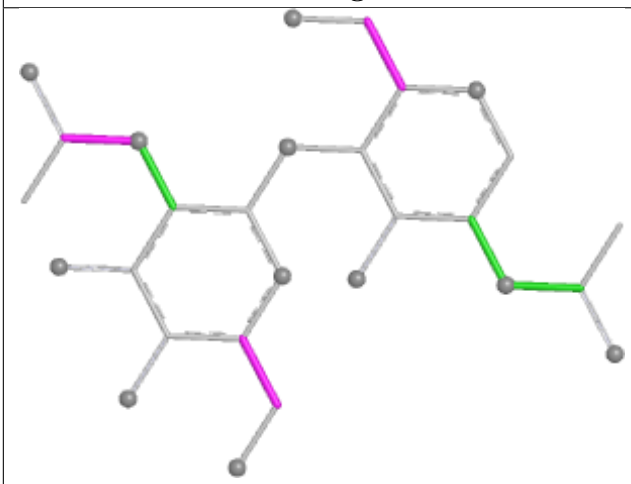
Oligosaccharide Chain E



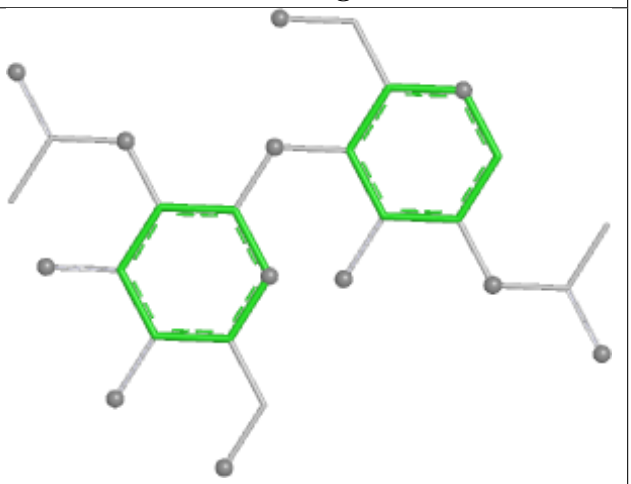
Bond lengths



Bond angles

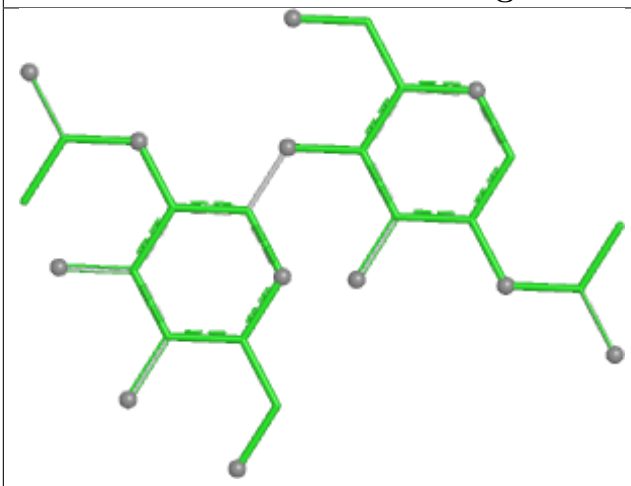


Torsions

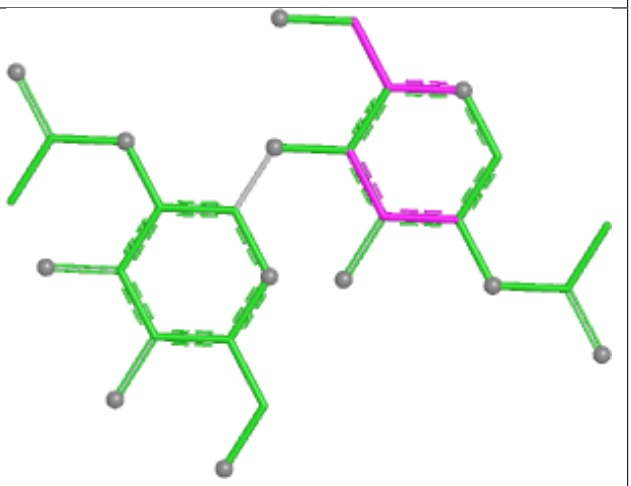


Rings

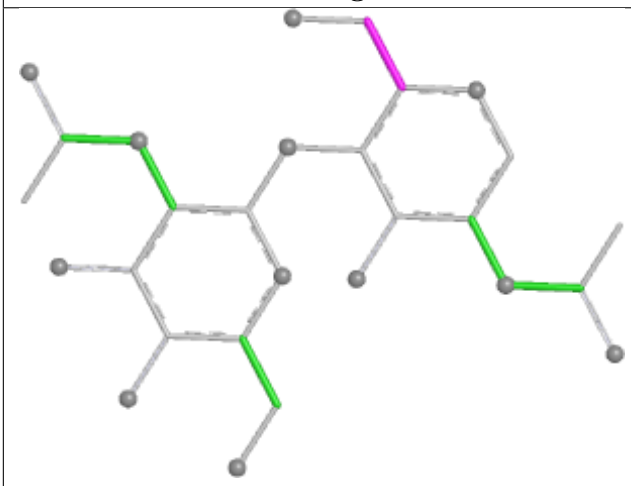
Oligosaccharide Chain F



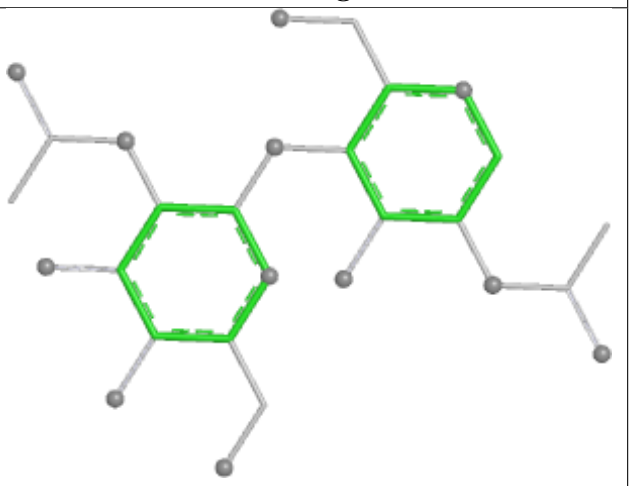
Bond lengths



Bond angles

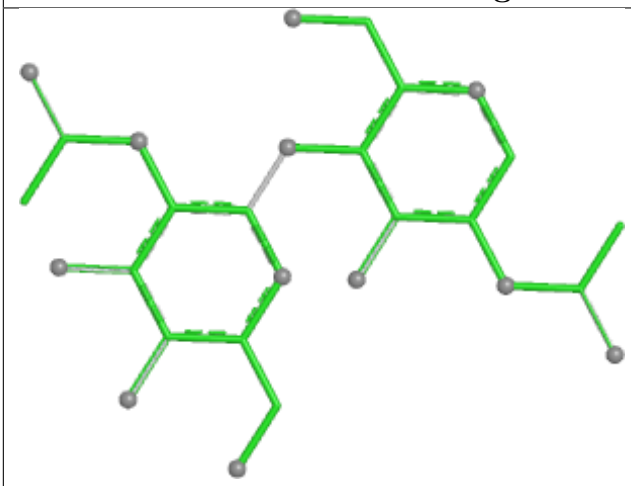


Torsions

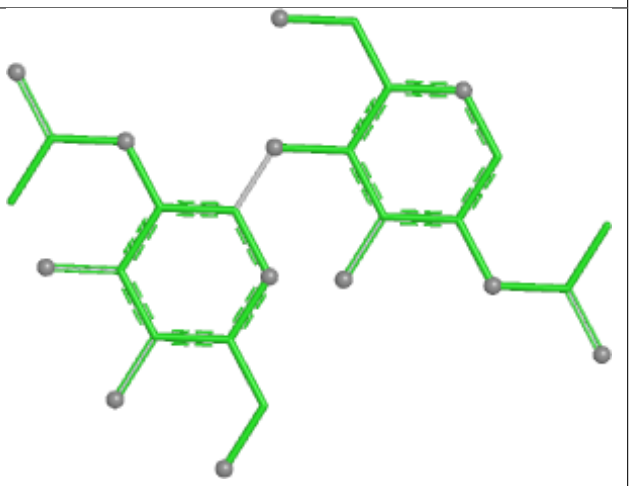


Rings

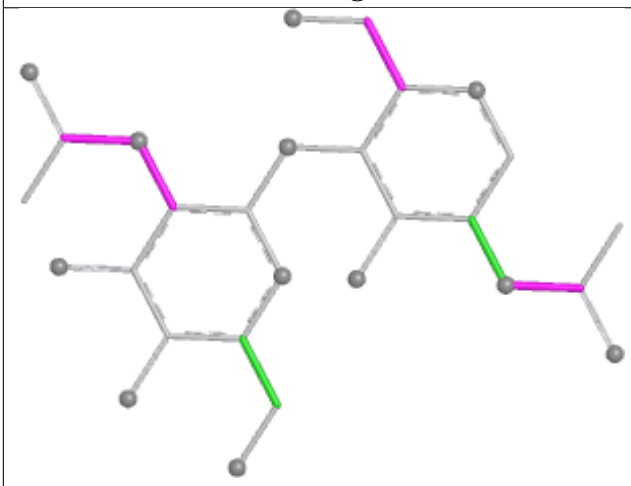
Oligosaccharide Chain G



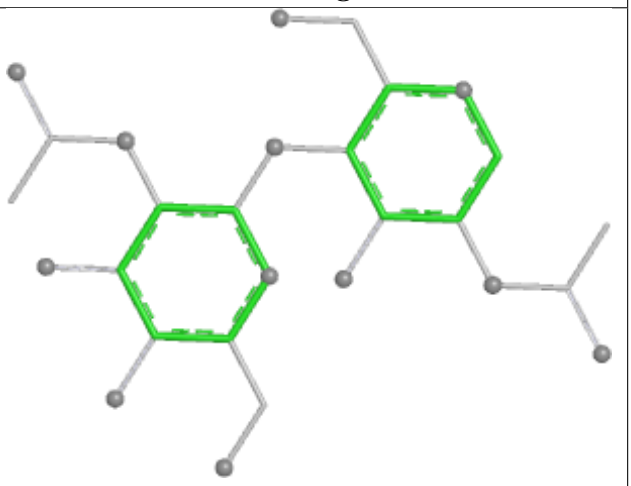
Bond lengths



Bond angles

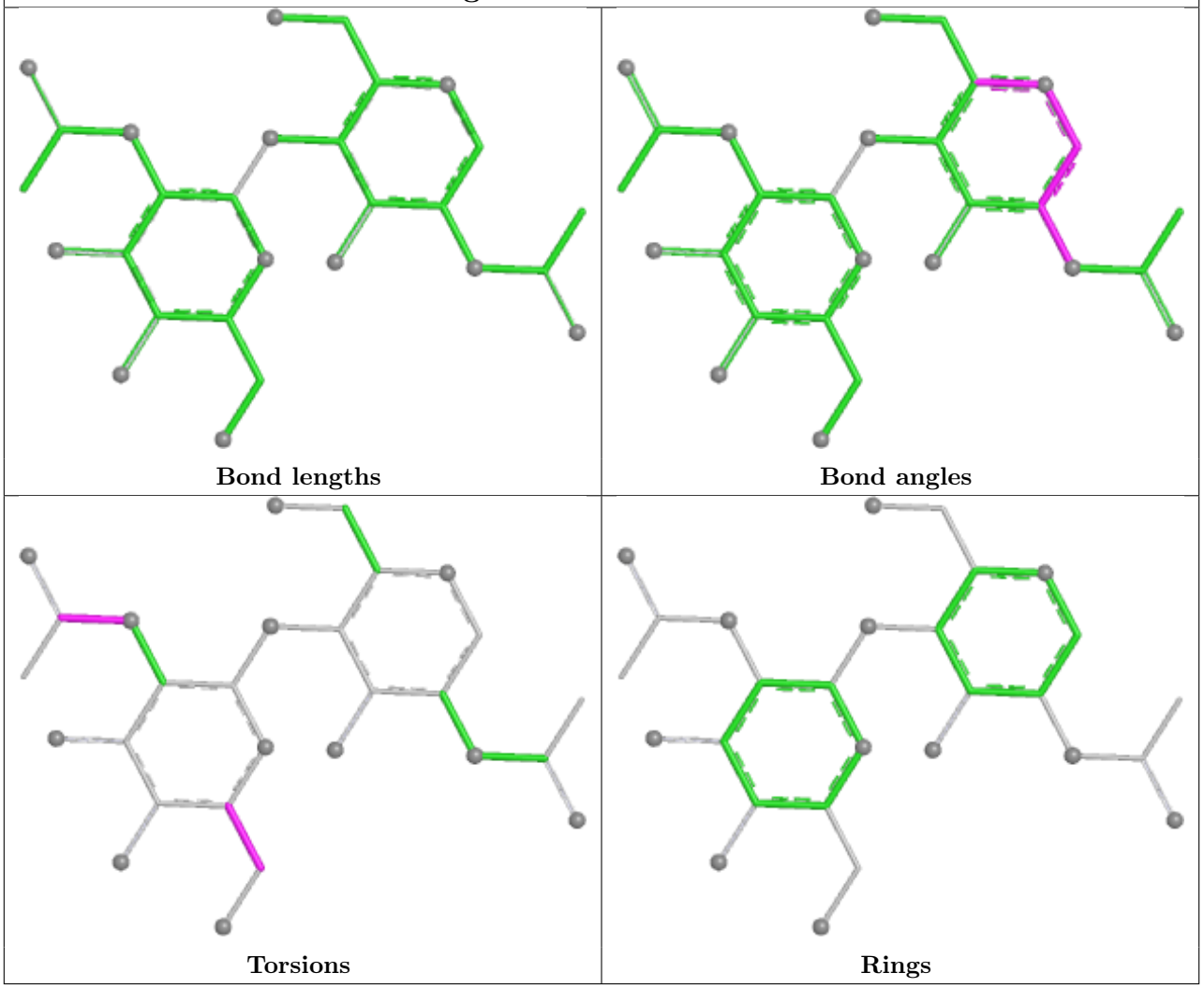


Torsions



Rings

Oligosaccharide Chain H



5.6 Ligand geometry (i)

14 ligands 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	BOG	D	701	-	20,20,20	0.47	0	25,25,25	0.59	0
5	DF0	B	705	-	18,18,18	1.48	1 (5%)	24,24,24	1.33	3 (12%)
5	DF0	D	705	-	18,18,18	1.48	1 (5%)	24,24,24	1.31	2 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	DF0	C	706	-	18,18,18	1.23	1 (5%)	24,24,24	1.27	4 (16%)
4	HEM	C	705	1	50,50,50	2.62	23 (46%)	67,82,82	3.54	35 (52%)
3	BOG	C	702	-	20,20,20	0.76	1 (5%)	25,25,25	1.63	5 (20%)
3	BOG	A	702	-	20,20,20	0.48	0	25,25,25	1.24	4 (16%)
5	DF0	A	706	-	18,18,18	1.31	1 (5%)	24,24,24	1.54	5 (20%)
3	BOG	A	701	-	20,20,20	0.39	0	25,25,25	2.15	6 (24%)
4	HEM	D	704	1	50,50,50	2.74	24 (48%)	67,82,82	3.34	34 (50%)
3	BOG	B	701	-	20,20,20	0.58	0	25,25,25	1.60	7 (28%)
4	HEM	A	705	1	50,50,50	2.60	24 (48%)	67,82,82	3.17	30 (44%)
4	HEM	B	704	1	50,50,50	2.81	24 (48%)	67,82,82	3.30	31 (46%)
3	BOG	C	701	-	20,20,20	0.47	0	25,25,25	0.59	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	BOG	D	701	-	-	7/11/31/31	0/1/1/1
5	DF0	B	705	-	-	0/8/8/8	0/2/2/2
5	DF0	D	705	-	-	0/8/8/8	0/2/2/2
5	DF0	C	706	-	-	0/8/8/8	0/2/2/2
4	HEM	C	705	1	-	6/14/54/54	-
3	BOG	C	702	-	-	4/11/31/31	0/1/1/1
3	BOG	A	702	-	-	6/11/31/31	0/1/1/1
5	DF0	A	706	-	-	0/8/8/8	0/2/2/2
3	BOG	A	701	-	-	6/11/31/31	0/1/1/1
4	HEM	D	704	1	-	4/14/54/54	-
3	BOG	B	701	-	-	7/11/31/31	0/1/1/1
4	HEM	A	705	1	-	2/14/54/54	-
4	HEM	B	704	1	-	5/14/54/54	-
3	BOG	C	701	-	-	9/11/31/31	0/1/1/1

All (100) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	704	HEM	FE-NB	6.43	2.14	1.94
4	B	704	HEM	FE-NB	5.98	2.13	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	705	HEM	FE-NB	5.92	2.13	1.94
4	A	705	HEM	FE-NB	5.51	2.11	1.94
4	B	704	HEM	FE-ND	5.40	2.11	1.94
4	A	705	HEM	FE-ND	5.37	2.11	1.94
5	B	705	DF0	C1-C	5.27	1.48	1.39
5	D	705	DF0	C1-C	5.26	1.48	1.39
4	C	705	HEM	C3B-C2B	5.21	1.47	1.37
4	D	704	HEM	FE-ND	5.21	2.10	1.94
4	D	704	HEM	C3B-C2B	5.05	1.47	1.37
4	C	705	HEM	C3D-C2D	5.00	1.47	1.36
4	B	704	HEM	C3B-C2B	4.99	1.47	1.37
4	B	704	HEM	C1A-NA	4.95	1.48	1.39
5	A	706	DF0	C1-C	4.92	1.47	1.39
4	A	705	HEM	C3B-C2B	4.83	1.47	1.37
4	C	705	HEM	C4A-NA	4.81	1.48	1.39
4	B	704	HEM	CHD-C4C	4.77	1.47	1.38
4	A	705	HEM	C3C-C2C	4.65	1.46	1.37
4	D	704	HEM	C4A-NA	4.65	1.48	1.39
4	D	704	HEM	C4C-NC	4.61	1.48	1.39
4	A	705	HEM	C4A-NA	4.59	1.48	1.39
4	D	704	HEM	C3D-C2D	4.50	1.46	1.36
4	D	704	HEM	C3C-C2C	4.50	1.46	1.37
4	A	705	HEM	C3D-C2D	4.50	1.46	1.36
4	D	704	HEM	C1C-NC	4.48	1.48	1.39
4	B	704	HEM	C4A-NA	4.46	1.48	1.39
4	B	704	HEM	C4C-NC	4.41	1.47	1.39
4	C	705	HEM	FE-ND	4.33	2.08	1.94
4	B	704	HEM	C3D-C2D	4.32	1.46	1.36
5	C	706	DF0	C1-C	4.30	1.46	1.39
4	C	705	HEM	C1C-NC	4.26	1.47	1.39
4	A	705	HEM	C4C-NC	4.25	1.47	1.39
4	A	705	HEM	C1A-NA	4.22	1.47	1.39
4	D	704	HEM	CHD-C4C	4.22	1.46	1.38
4	D	704	HEM	C4D-ND	-4.18	1.33	1.40
4	C	705	HEM	CHD-C4C	4.15	1.46	1.38
4	C	705	HEM	C4D-ND	-4.13	1.33	1.40
4	B	704	HEM	C1C-NC	4.12	1.47	1.39
4	C	705	HEM	C4C-NC	4.01	1.47	1.39
4	B	704	HEM	C3C-C2C	4.00	1.45	1.37
4	B	704	HEM	C4D-ND	-3.97	1.33	1.40
4	A	705	HEM	CHA-C4D	3.97	1.46	1.38
4	B	704	HEM	CHA-C4D	3.81	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	704	HEM	C1A-C2A	3.80	1.52	1.44
4	B	704	HEM	C2A-C3A	3.57	1.48	1.38
4	A	705	HEM	C2A-C3A	3.53	1.48	1.38
4	C	705	HEM	CHB-C1B	3.49	1.45	1.38
4	A	705	HEM	CHD-C4C	3.49	1.45	1.38
4	C	705	HEM	C2A-C3A	3.48	1.48	1.38
4	D	704	HEM	CHC-C1C	3.44	1.45	1.38
4	D	704	HEM	C1A-NA	3.43	1.46	1.39
4	D	704	HEM	CHB-C1B	3.43	1.45	1.38
4	C	705	HEM	CHA-C4D	3.37	1.45	1.38
4	B	704	HEM	CHB-C1B	3.34	1.45	1.38
4	A	705	HEM	C1C-NC	3.23	1.45	1.39
4	D	704	HEM	C2A-C3A	3.20	1.47	1.38
4	D	704	HEM	CHC-C4B	3.19	1.46	1.39
4	C	705	HEM	C1A-NA	3.15	1.45	1.39
4	B	704	HEM	CHC-C1C	3.15	1.44	1.38
4	B	704	HEM	CHA-C1A	3.09	1.46	1.39
4	B	704	HEM	CHD-C1D	3.07	1.46	1.39
4	A	705	HEM	CHB-C1B	3.04	1.44	1.38
4	C	705	HEM	C1A-C2A	3.04	1.50	1.44
4	D	704	HEM	CHB-C4A	3.01	1.46	1.39
4	A	705	HEM	C4D-ND	-3.01	1.35	1.40
4	B	704	HEM	C4A-C3A	2.93	1.50	1.43
4	C	705	HEM	CHB-C4A	2.91	1.45	1.39
4	D	704	HEM	CHA-C4D	2.86	1.44	1.38
4	B	704	HEM	CHB-C4A	2.85	1.45	1.39
4	D	704	HEM	CHD-C1D	2.82	1.45	1.39
4	C	705	HEM	CHC-C4B	2.80	1.45	1.39
4	A	705	HEM	CHA-C1A	2.80	1.45	1.39
4	A	705	HEM	CHD-C1D	2.75	1.45	1.39
4	A	705	HEM	C1A-C2A	2.74	1.50	1.44
4	D	704	HEM	C4A-C3A	2.74	1.49	1.43
4	A	705	HEM	CHB-C4A	2.66	1.45	1.39
4	B	704	HEM	CHC-C4B	2.66	1.45	1.39
4	C	705	HEM	CHD-C1D	2.65	1.45	1.39
4	C	705	HEM	C3C-C4C	2.59	1.50	1.46
4	C	705	HEM	C1B-C2B	2.57	1.49	1.44
4	D	704	HEM	C1A-C2A	2.55	1.49	1.44
4	A	705	HEM	CHC-C4B	2.55	1.45	1.39
4	C	705	HEM	C4A-C3A	2.50	1.49	1.43
4	A	705	HEM	C4A-C3A	2.48	1.48	1.43
4	C	705	HEM	C3C-C2C	2.47	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	705	HEM	C4D-C3D	2.42	1.49	1.45
4	D	704	HEM	C1B-C2B	2.39	1.49	1.44
3	C	702	BOG	O1-C1	2.39	1.44	1.40
4	C	705	HEM	C4D-C3D	2.39	1.49	1.45
4	A	705	HEM	CHC-C1C	2.36	1.43	1.38
4	D	704	HEM	CHA-C1A	2.33	1.44	1.39
4	B	704	HEM	O2D-CGD	-2.32	1.23	1.30
4	B	704	HEM	C1B-NB	-2.29	1.36	1.40
4	B	704	HEM	C1B-C2B	2.29	1.49	1.44
4	D	704	HEM	C3B-C4B	2.15	1.49	1.44
4	C	705	HEM	CHC-C1C	2.15	1.42	1.38
4	A	705	HEM	C4B-NB	-2.08	1.34	1.38
4	A	705	HEM	C1B-C2B	2.06	1.48	1.44
4	D	704	HEM	C4D-C3D	2.04	1.48	1.45

All (166) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	705	HEM	C3B-C4B-NB	10.86	117.27	109.47
4	D	704	HEM	C3B-C4B-NB	10.01	116.66	109.47
4	B	704	HEM	C3B-C2B-C1B	-9.59	99.21	106.41
4	A	705	HEM	C3B-C4B-NB	9.51	116.30	109.47
4	B	704	HEM	C3B-C4B-NB	9.14	116.03	109.47
4	C	705	HEM	C3B-C2B-C1B	-8.79	99.81	106.41
4	A	705	HEM	C3B-C2B-C1B	-8.72	99.86	106.41
4	B	704	HEM	C2B-C1B-NB	8.06	119.10	109.84
4	D	704	HEM	C3B-C2B-C1B	-7.74	100.60	106.41
4	C	705	HEM	C2B-C1B-NB	7.68	118.67	109.84
4	D	704	HEM	C2B-C1B-NB	7.62	118.60	109.84
4	D	704	HEM	C3D-C4D-ND	7.47	118.36	110.17
4	A	705	HEM	C2B-C1B-NB	7.45	118.40	109.84
4	B	704	HEM	C2D-C1D-ND	7.31	118.35	109.90
4	D	704	HEM	C2D-C1D-ND	7.02	118.02	109.90
4	D	704	HEM	C2A-C1A-NA	7.00	117.92	110.15
4	A	705	HEM	C2D-C1D-ND	7.00	118.00	109.90
4	C	705	HEM	C2D-C1D-ND	6.99	117.98	109.90
3	A	701	BOG	O1-C1-C2	-6.78	97.97	108.27
4	B	704	HEM	C2A-C1A-NA	6.54	117.41	110.15
4	C	705	HEM	C4C-NC-C1C	-6.53	95.18	105.82
4	C	705	HEM	C1D-C2D-C3D	-6.26	100.39	106.98
4	C	705	HEM	C2A-C1A-NA	6.19	117.02	110.15
4	B	704	HEM	C1D-C2D-C3D	-6.18	100.47	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	704	HEM	C3D-C4D-ND	6.17	116.94	110.17
4	C	705	HEM	C3C-C2C-C1C	-5.89	101.47	107.05
4	A	705	HEM	C2A-C1A-NA	5.86	116.66	110.15
4	D	704	HEM	C4A-NA-C1A	-5.72	96.50	105.82
4	C	705	HEM	C2C-C1C-NC	5.68	120.14	109.64
4	B	704	HEM	C4A-NA-C1A	-5.67	96.58	105.82
4	C	705	HEM	C3D-C4D-ND	5.65	116.37	110.17
4	A	705	HEM	C1D-C2D-C3D	-5.60	101.09	106.98
4	A	705	HEM	C3D-C4D-ND	5.32	116.01	110.17
3	C	702	BOG	O5-C5-C4	5.30	119.25	109.70
4	D	704	HEM	C1D-C2D-C3D	-5.28	101.43	106.98
4	A	705	HEM	C4A-NA-C1A	-5.19	97.36	105.82
4	A	705	HEM	CHD-C1D-C2D	-5.17	116.86	125.03
4	C	705	HEM	C4A-NA-C1A	-5.10	97.51	105.82
4	D	704	HEM	C3C-C2C-C1C	-4.75	102.55	107.05
4	D	704	HEM	C4C-NC-C1C	-4.49	98.50	105.82
4	B	704	HEM	C3C-C2C-C1C	-4.42	102.87	107.05
4	C	705	HEM	CMC-C2C-C1C	4.37	132.43	124.73
4	B	704	HEM	C3A-C4A-NA	4.35	117.12	110.14
4	D	704	HEM	C4D-ND-C1D	-4.33	100.08	105.21
4	B	704	HEM	CHD-C1D-C2D	-4.30	118.24	125.03
4	C	705	HEM	C1B-NB-C4B	-4.26	100.16	105.21
3	A	701	BOG	O5-C5-C4	4.22	117.30	109.70
4	D	704	HEM	C1B-NB-C4B	-4.13	100.32	105.21
4	D	704	HEM	C3A-C4A-NA	4.12	116.75	110.14
4	D	704	HEM	C2C-C1C-NC	4.08	117.19	109.64
4	C	705	HEM	CHC-C1C-C2C	-4.07	117.02	125.49
4	A	705	HEM	C4C-NC-C1C	-4.04	99.23	105.82
4	A	705	HEM	C3C-C2C-C1C	-3.99	103.27	107.05
4	D	704	HEM	CHD-C1D-C2D	-3.98	118.74	125.03
4	A	705	HEM	C3A-C4A-NA	3.96	116.50	110.14
4	B	704	HEM	C4C-NC-C1C	-3.91	99.44	105.82
4	C	705	HEM	CHD-C1D-C2D	-3.89	118.89	125.03
4	C	705	HEM	C3A-C4A-NA	3.88	116.36	110.14
4	B	704	HEM	C1B-NB-C4B	-3.88	100.62	105.21
4	D	704	HEM	C4B-C3B-C2B	-3.87	103.72	107.28
4	C	705	HEM	CHC-C4B-C3B	-3.86	117.37	125.07
3	A	701	BOG	C1-O5-C5	3.85	121.23	113.72
4	A	705	HEM	C2C-C1C-NC	3.83	116.71	109.64
4	B	704	HEM	C4D-ND-C1D	-3.73	100.79	105.21
4	A	705	HEM	C1B-NB-C4B	-3.69	100.84	105.21
4	B	704	HEM	C2C-C1C-NC	3.68	116.45	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	705	HEM	C4B-C3B-C2B	-3.56	104.00	107.28
4	C	705	HEM	CAC-C3C-C2C	-3.56	116.86	128.43
4	C	705	HEM	CAC-C3C-C4C	3.55	133.29	124.82
4	A	705	HEM	C4D-ND-C1D	-3.50	101.06	105.21
4	C	705	HEM	CHB-C4A-C3A	-3.48	117.32	127.43
4	B	704	HEM	CAA-C2A-C1A	3.47	131.72	124.94
3	B	701	BOG	O5-C5-C4	3.45	115.91	109.70
4	D	704	HEM	C4D-C3D-C2D	-3.43	101.90	106.89
4	A	705	HEM	CHB-C4A-C3A	-3.39	117.60	127.43
4	A	705	HEM	CHC-C1C-C2C	-3.35	118.53	125.49
5	B	705	DF0	O1-C7-O	-3.28	114.90	123.33
4	D	704	HEM	CMC-C2C-C1C	3.27	130.48	124.73
4	C	705	HEM	CBD-CAD-C3D	-3.25	103.55	112.53
4	D	704	HEM	CHB-C4A-C3A	-3.23	118.04	127.43
4	A	705	HEM	CAC-C3C-C4C	3.21	132.49	124.82
4	D	704	HEM	CHC-C1C-C2C	-3.21	118.81	125.49
4	C	705	HEM	CBC-CAC-C3C	-3.21	111.50	127.53
4	A	705	HEM	CHC-C4B-C3B	-3.21	118.67	125.07
4	B	704	HEM	CHB-C4A-C3A	-3.18	118.20	127.43
4	C	705	HEM	CAA-C2A-C1A	3.14	131.08	124.94
4	D	704	HEM	CHA-C1A-C2A	-3.14	118.42	125.30
5	D	705	DF0	O1-C7-O	-3.12	115.31	123.33
4	A	705	HEM	C4B-C3B-C2B	-3.09	104.44	107.28
4	B	704	HEM	CHA-C4D-C3D	-3.05	119.61	125.23
4	B	704	HEM	CMC-C2C-C1C	3.00	130.01	124.73
4	C	705	HEM	CHB-C1B-NB	-2.97	120.70	124.37
4	B	704	HEM	CHC-C1C-C2C	-2.96	119.34	125.49
4	D	704	HEM	CAC-C3C-C4C	2.95	131.87	124.82
3	A	702	BOG	O5-C5-C4	2.95	115.01	109.70
3	A	702	BOG	O1-C1-C2	-2.94	103.80	108.27
3	A	701	BOG	C4-C3-C2	-2.91	105.71	110.83
3	B	701	BOG	C4-C3-C2	-2.91	105.73	110.83
4	B	704	HEM	CHB-C1B-C2B	-2.90	118.69	126.95
4	C	705	HEM	C4D-ND-C1D	-2.90	101.77	105.21
4	A	705	HEM	CMB-C2B-C1B	2.84	129.48	125.03
4	B	704	HEM	CMD-C2D-C1D	2.82	129.44	125.03
4	B	704	HEM	CHC-C4B-C3B	-2.82	119.45	125.07
5	C	706	DF0	C6-C4-C3	-2.81	116.75	120.89
4	D	704	HEM	CHA-C4D-C3D	-2.79	120.08	125.23
4	B	704	HEM	CAC-C3C-C4C	2.77	131.44	124.82
4	C	705	HEM	CMB-C2B-C1B	2.75	129.33	125.03
5	A	706	DF0	O1-C7-O	-2.74	116.28	123.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	702	BOG	C3-C4-C5	2.73	115.18	110.23
4	A	705	HEM	CHA-C1A-C2A	-2.72	119.35	125.30
4	B	704	HEM	CAC-C3C-C2C	-2.69	119.67	128.43
4	D	704	HEM	CHB-C1B-NB	-2.67	121.06	124.37
5	A	706	DF0	F-C-C5	2.67	123.98	118.64
3	C	702	BOG	O1-C1-C2	-2.66	104.23	108.27
3	C	702	BOG	O5-C1-O1	2.65	116.30	110.04
4	D	704	HEM	CHC-C4B-C3B	-2.65	119.79	125.07
3	C	702	BOG	C1-O5-C5	2.64	118.88	113.72
4	B	704	HEM	C1A-C2A-C3A	-2.61	102.83	106.87
3	B	701	BOG	O2-C2-C3	-2.59	104.26	110.38
4	B	704	HEM	C4B-C3B-C2B	-2.59	104.90	107.28
3	B	701	BOG	C1-O5-C5	2.58	118.75	113.72
4	A	705	HEM	C4A-CHB-C1B	-2.57	120.20	126.25
5	A	706	DF0	C8-C1-C	-2.57	118.78	122.86
4	D	704	HEM	CAC-C3C-C2C	-2.56	120.11	128.43
4	C	705	HEM	C4A-CHB-C1B	-2.54	120.28	126.25
5	B	705	DF0	C2-C1-C8	2.53	123.72	118.70
5	C	706	DF0	F-C-C5	2.52	123.68	118.64
4	A	705	HEM	CHB-C1B-C2B	-2.49	119.88	126.95
5	A	706	DF0	C5-C-C1	-2.48	119.62	123.59
4	A	705	HEM	CHB-C1B-NB	-2.47	121.31	124.37
4	B	704	HEM	C4D-C3D-C2D	-2.47	103.29	106.89
4	A	705	HEM	CAA-C2A-C1A	2.44	129.71	124.94
4	D	704	HEM	CHB-C1B-C2B	-2.44	120.01	126.95
3	B	701	BOG	O5-C1-C2	-2.42	105.39	110.37
4	A	705	HEM	CAC-C3C-C2C	-2.41	120.61	128.43
5	A	706	DF0	C6-C4-C3	-2.40	117.35	120.89
4	C	705	HEM	C4D-C3D-C2D	-2.40	103.39	106.89
4	D	704	HEM	C4A-CHB-C1B	-2.39	120.62	126.25
4	D	704	HEM	CMB-C2B-C1B	2.38	128.76	125.03
4	D	704	HEM	CHA-C4D-ND	-2.38	121.42	124.37
5	C	706	DF0	C4-C6-C7	-2.36	106.99	113.71
4	C	705	HEM	CMD-C2D-C1D	2.35	128.70	125.03
3	A	701	BOG	O3-C3-C4	2.34	115.89	110.38
4	C	705	HEM	CHB-C1B-C2B	-2.30	120.40	126.95
5	B	705	DF0	F-C-C5	2.26	123.16	118.64
4	D	704	HEM	CMD-C2D-C1D	2.25	128.55	125.03
5	D	705	DF0	C2-C1-C8	2.24	123.16	118.70
4	C	705	HEM	CHA-C4D-C3D	-2.24	121.09	125.23
5	C	706	DF0	C5-C-C1	-2.24	120.00	123.59
4	A	705	HEM	C4C-CHD-C1D	-2.24	121.26	126.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	701	BOG	C1'-O1-C1	2.22	117.48	113.68
3	A	702	BOG	O5-C1-O1	2.19	115.23	110.04
4	D	704	HEM	C4A-C3A-C2A	-2.19	104.31	106.82
3	A	702	BOG	O5-C1-C2	-2.19	105.88	110.37
3	A	701	BOG	O6-C6-C5	-2.17	103.93	111.33
4	A	705	HEM	C4D-C3D-C2D	-2.16	103.75	106.89
4	D	704	HEM	CAD-C3D-C4D	2.13	128.41	124.70
4	C	705	HEM	CHA-C1A-C2A	-2.12	120.67	125.30
3	B	701	BOG	O4-C4-C5	2.10	114.50	109.32
4	B	704	HEM	CHB-C1B-NB	-2.10	121.77	124.37
4	B	704	HEM	C4A-CHB-C1B	-2.07	121.38	126.25
4	C	705	HEM	C4A-C3A-C2A	-2.06	104.45	106.82
4	B	704	HEM	CHA-C1A-C2A	-2.05	120.81	125.30
4	D	704	HEM	C1A-C2A-C3A	-2.05	103.69	106.87
4	A	705	HEM	CMC-C2C-C1C	2.04	128.33	124.73
4	C	705	HEM	C1C-CHC-C4B	-2.04	121.68	126.02

There are no chirality outliers.

All (56) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	701	BOG	C2-C1-O1-C1'
3	A	701	BOG	O5-C1-O1-C1'
3	B	701	BOG	O5-C1-O1-C1'
3	D	701	BOG	O5-C1-O1-C1'
4	C	705	HEM	C1A-C2A-CAA-CBA
3	A	701	BOG	O5-C5-C6-O6
3	A	701	BOG	C4-C5-C6-O6
3	A	702	BOG	O1-C1'-C2'-C3'
3	C	701	BOG	O5-C1-O1-C1'
3	C	701	BOG	O5-C5-C6-O6
3	C	701	BOG	C4-C5-C6-O6
3	B	701	BOG	C2-C1-O1-C1'
3	C	701	BOG	C2-C1-O1-C1'
3	D	701	BOG	C2-C1-O1-C1'
4	B	704	HEM	C2A-CAA-CBA-CGA
4	C	705	HEM	C3A-C2A-CAA-CBA
4	B	704	HEM	C1A-C2A-CAA-CBA
3	C	701	BOG	C3'-C4'-C5'-C6'
3	C	701	BOG	C1'-C2'-C3'-C4'
3	C	702	BOG	C1'-C2'-C3'-C4'
3	B	701	BOG	O1-C1'-C2'-C3'

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Mol	Chain	Res	Type	Atoms
3	A	702	BOG	O5-C1-O1-C1'
3	D	701	BOG	C1'-C2'-C3'-C4'
4	C	705	HEM	C2C-C3C-CAC-CBC
3	B	701	BOG	C4-C5-C6-O6
3	C	701	BOG	C4'-C5'-C6'-C7'
4	C	705	HEM	C2A-CAA-CBA-CGA
3	C	702	BOG	C2'-C3'-C4'-C5'
3	A	702	BOG	C2'-C3'-C4'-C5'
3	B	701	BOG	C5'-C6'-C7'-C8'
3	A	702	BOG	C5'-C6'-C7'-C8'
3	C	701	BOG	C2'-C3'-C4'-C5'
3	A	701	BOG	C3'-C4'-C5'-C6'
3	C	702	BOG	C4'-C5'-C6'-C7'
4	B	704	HEM	C3A-C2A-CAA-CBA
4	D	704	HEM	C4C-C3C-CAC-CBC
3	D	701	BOG	C4-C5-C6-O6
3	D	701	BOG	C3'-C4'-C5'-C6'
3	D	701	BOG	C4'-C5'-C6'-C7'
3	C	702	BOG	C3'-C4'-C5'-C6'
3	D	701	BOG	O5-C5-C6-O6
3	B	701	BOG	C2'-C3'-C4'-C5'
4	B	704	HEM	CAA-CBA-CGA-O1A
3	A	701	BOG	C4'-C5'-C6'-C7'
4	B	704	HEM	CAA-CBA-CGA-O2A
4	D	704	HEM	C4D-C3D-CAD-CBD
3	A	702	BOG	C2-C1-O1-C1'
3	A	702	BOG	C3'-C4'-C5'-C6'
4	A	705	HEM	C4C-C3C-CAC-CBC
3	B	701	BOG	O5-C5-C6-O6
3	C	701	BOG	C2'-C1'-O1-C1
4	D	704	HEM	CAA-CBA-CGA-O1A
4	D	704	HEM	CAA-CBA-CGA-O2A
4	C	705	HEM	CAA-CBA-CGA-O2A
4	C	705	HEM	CAA-CBA-CGA-O1A
4	A	705	HEM	CAD-CBD-CGD-O2D

There are no ring outliers.

9 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	705	DF0	1	0
5	D	705	DF0	1	0

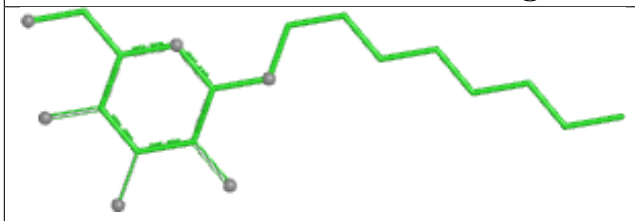
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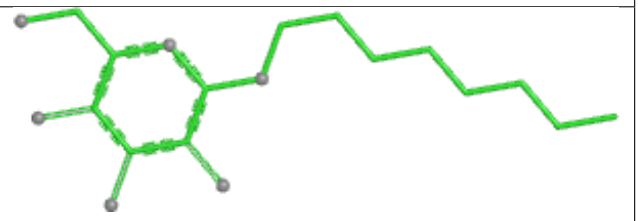
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	706	DF0	1	0
3	C	702	BOG	1	0
5	A	706	DF0	1	0
3	A	701	BOG	2	0
4	D	704	HEM	3	0
4	A	705	HEM	2	0
4	B	704	HEM	2	0

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 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.

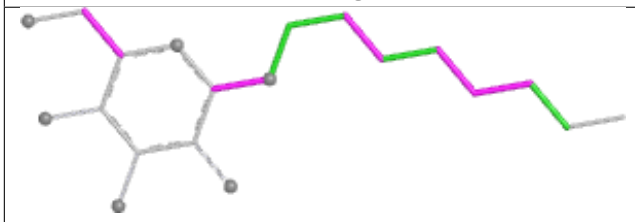
Ligand BOG D 701



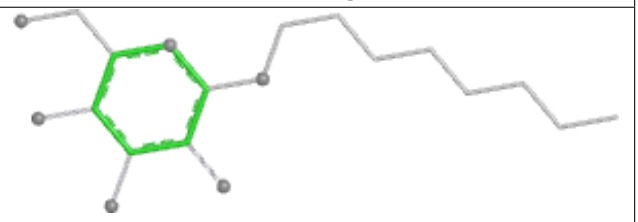
Bond lengths



Bond angles

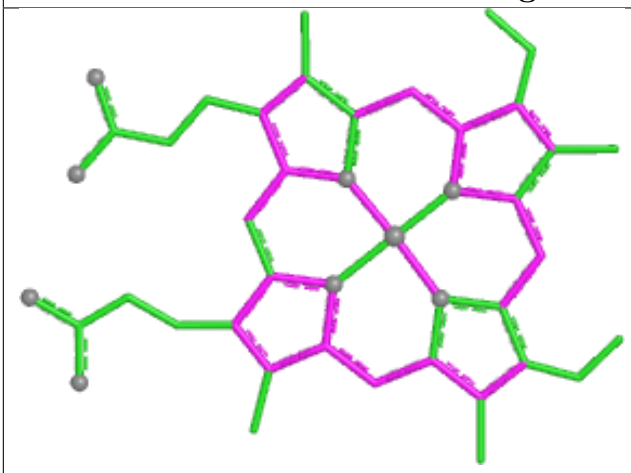


Torsions

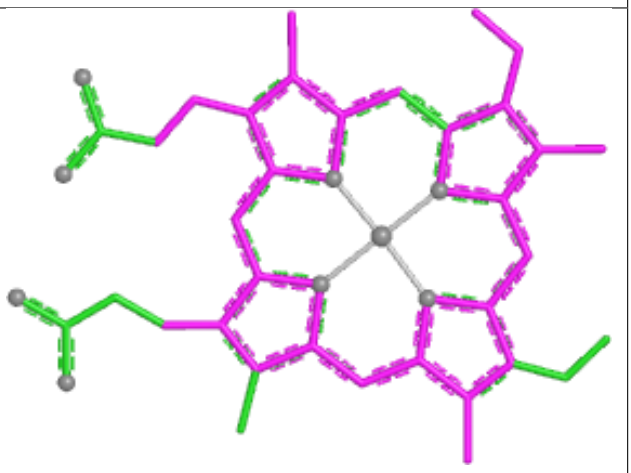


Rings

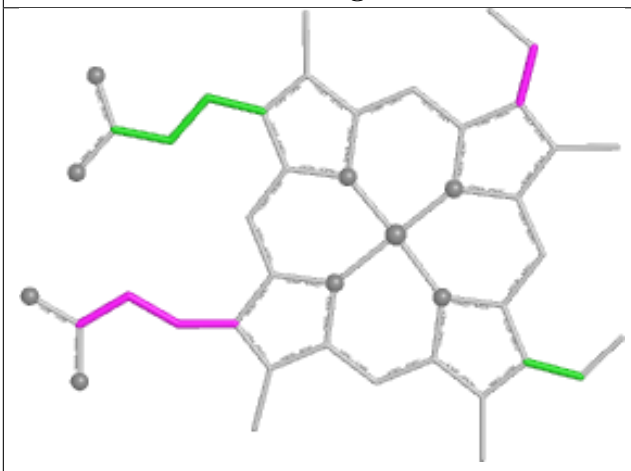
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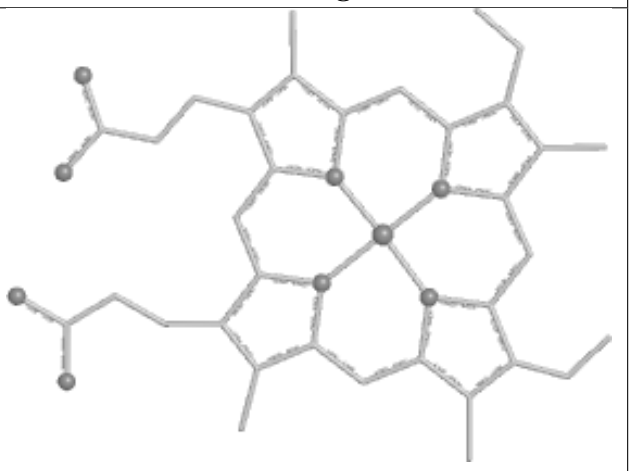
Bond lengths



Bond angles

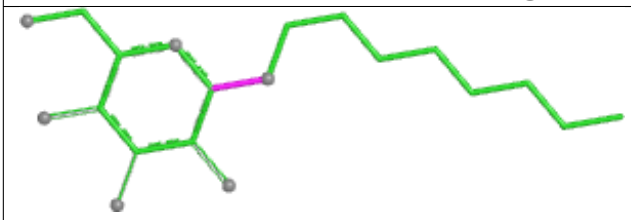


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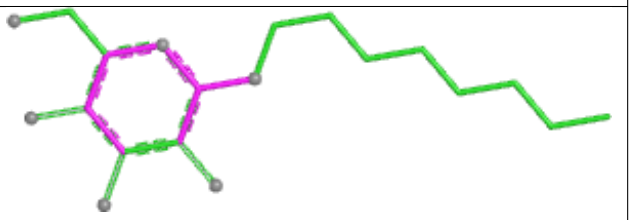


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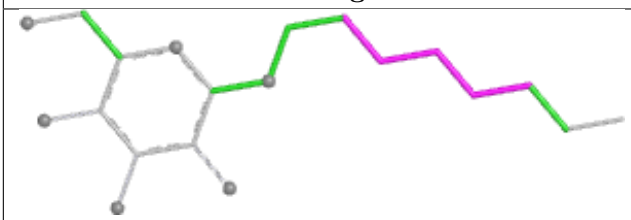
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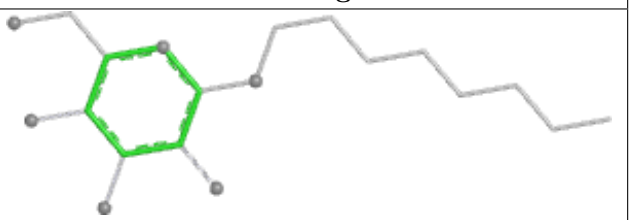
Bond lengths



Bond angles

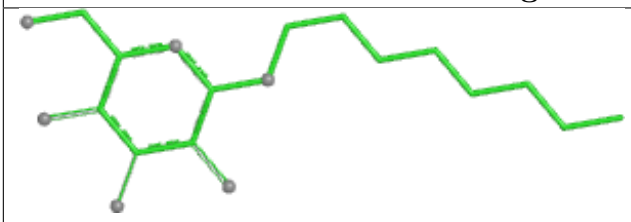


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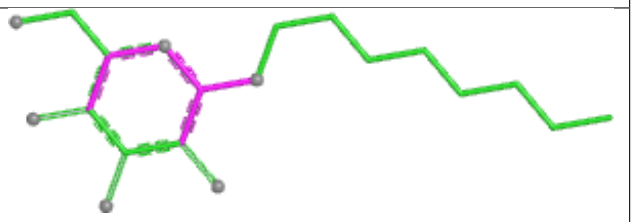


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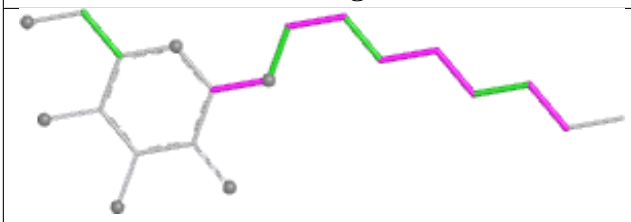
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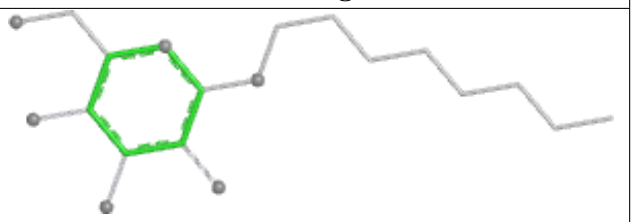
Bond lengths



Bond angles

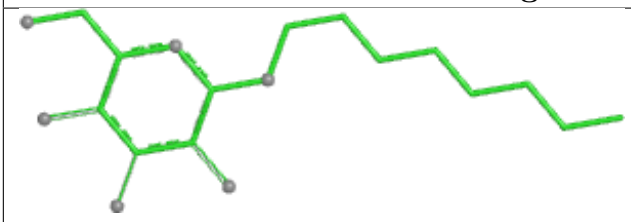


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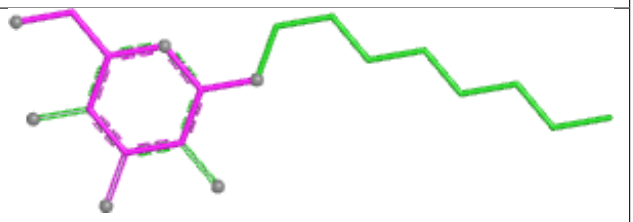


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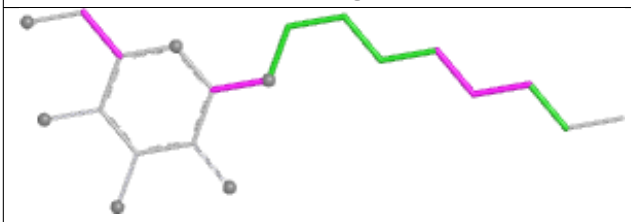
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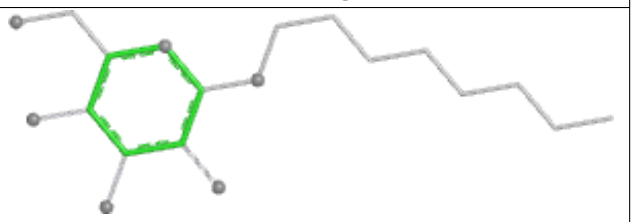
Bond lengths



Bond angles

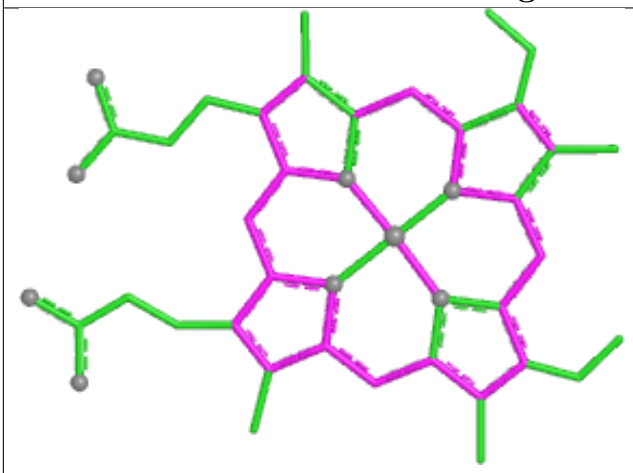


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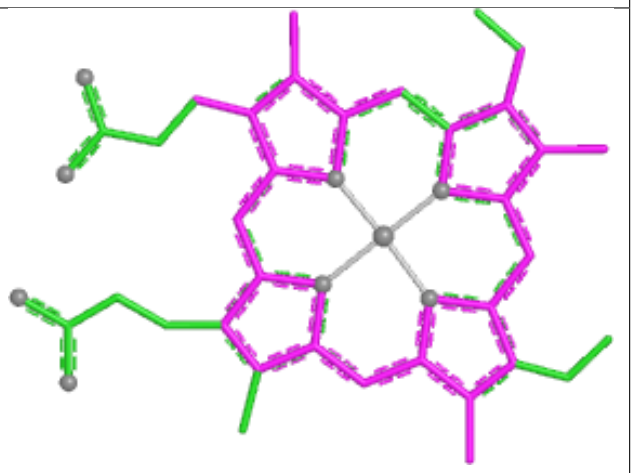


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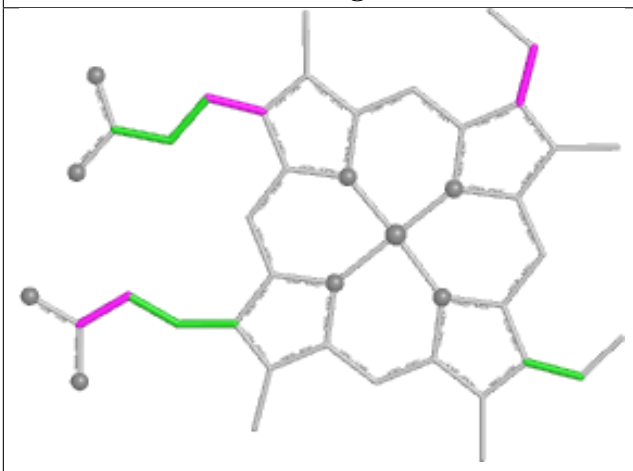
Ligand HEM D 704



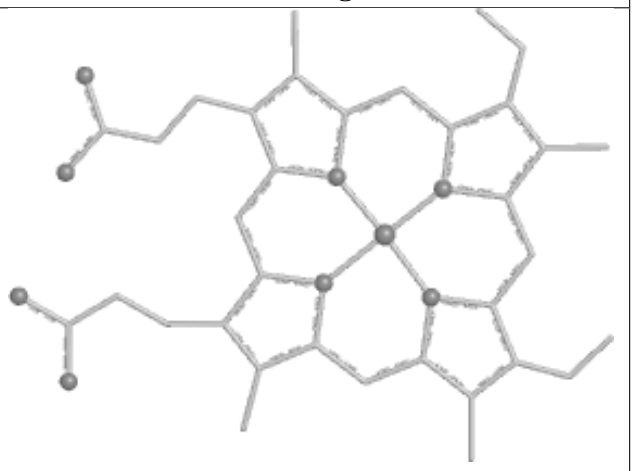
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Bond angles

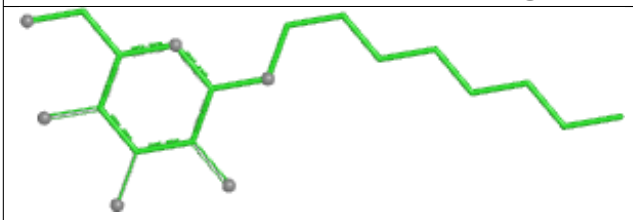


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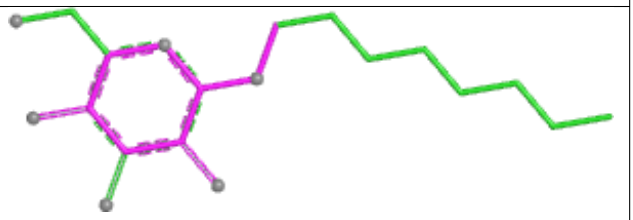


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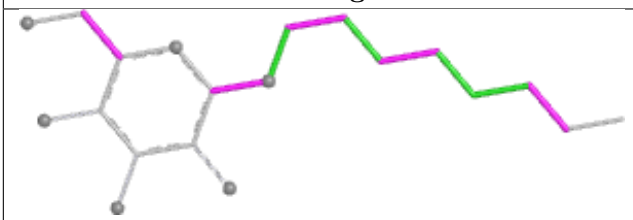
Ligand BOG B 701



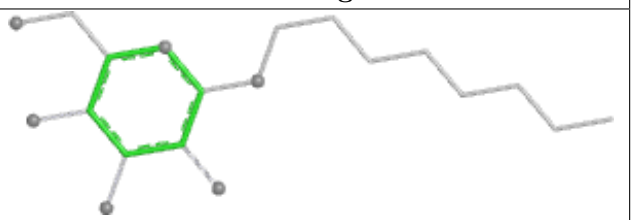
Bond lengths



Bond angles

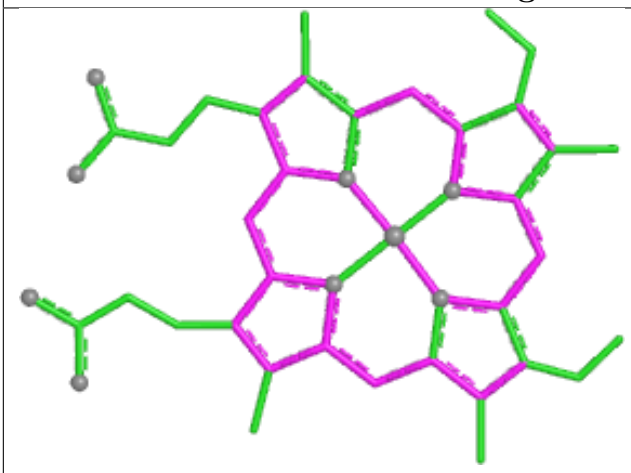


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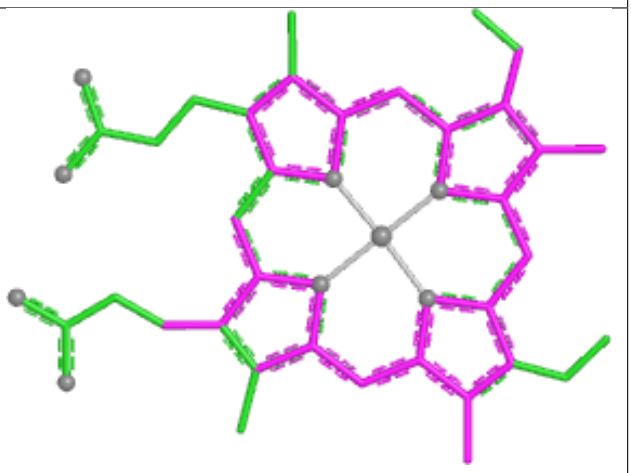


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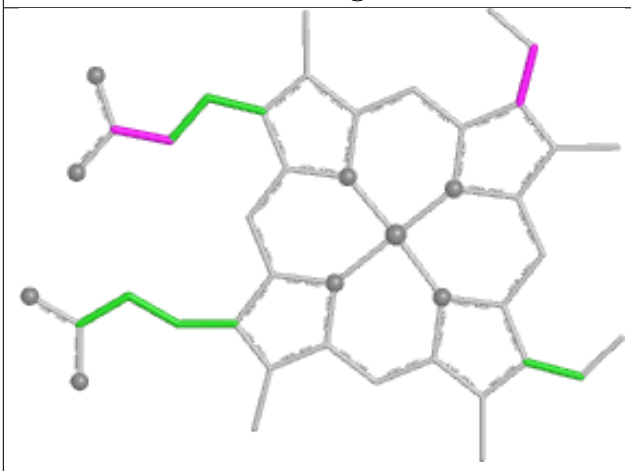
Ligand HEM A 705



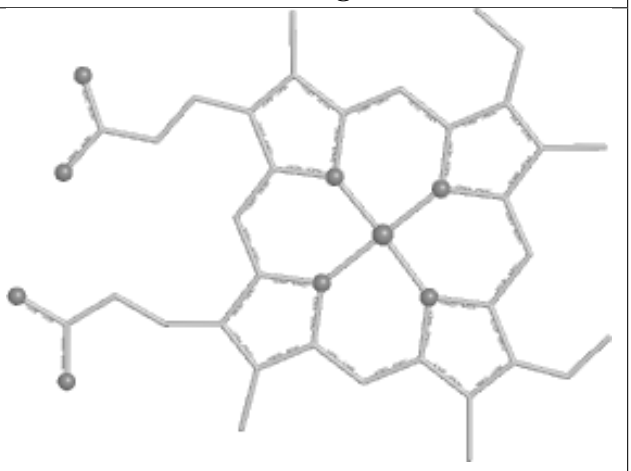
Bond lengths



Bond angles

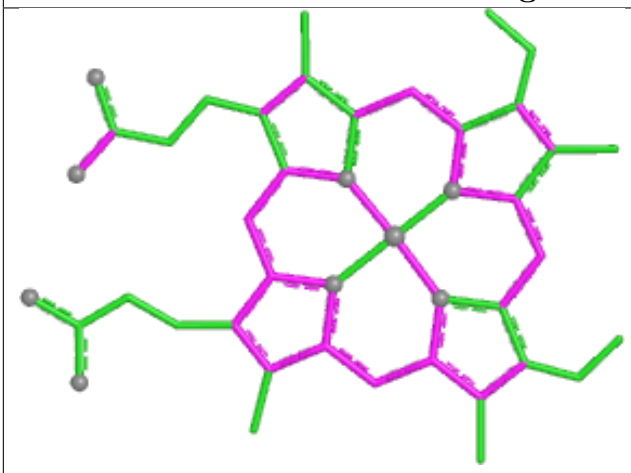


Torsions

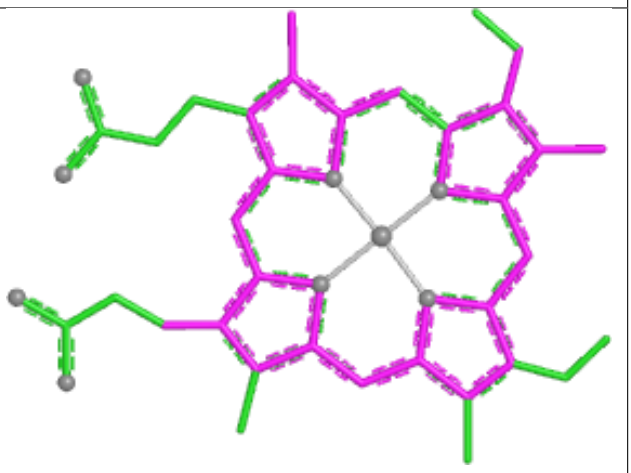


Rings

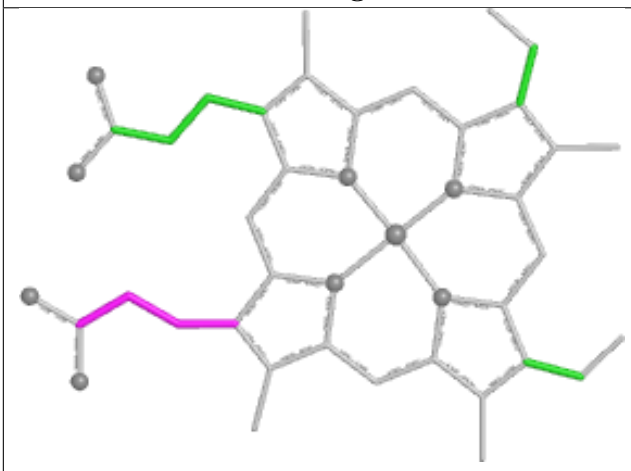
Ligand HEM B 704



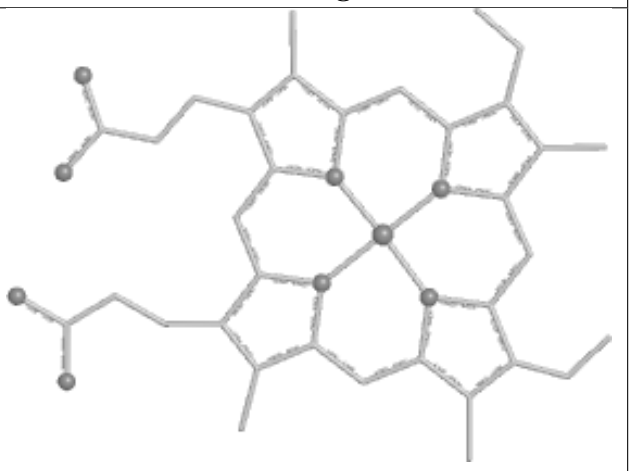
Bond lengths



Bond angles

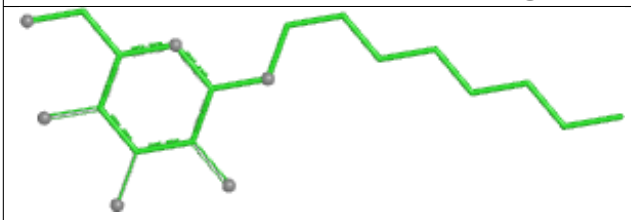


Torsions

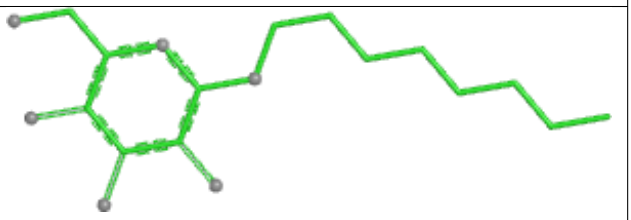


Rings

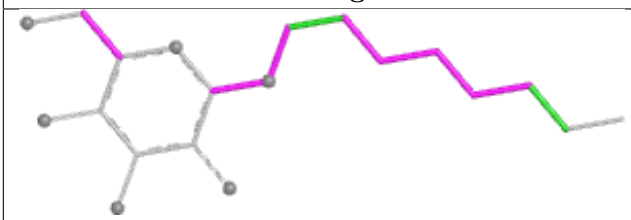
Ligand BOG C 701



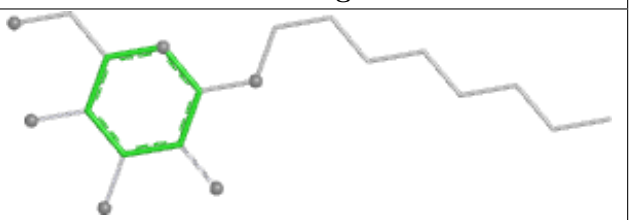
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

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	552/604 (91%)	0.52	42 (7%)	20	14	24, 44, 67, 110	0
1	B	552/604 (91%)	0.47	46 (8%)	17	12	27, 43, 68, 90	0
1	C	552/604 (91%)	0.49	42 (7%)	20	14	26, 43, 66, 110	0
1	D	552/604 (91%)	0.43	39 (7%)	22	16	24, 42, 67, 101	0
All	All	2208/2416 (91%)	0.48	169 (7%)	19	14	24, 43, 67, 110	0

All (169) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	563	SER	6.2
1	C	45	GLU	5.7
1	D	242	HIS	5.5
1	B	234	TYR	5.3
1	D	233	ILE	5.1
1	D	268	ASP	5.1
1	B	401	GLU	5.1
1	D	462	SER	4.9
1	B	428	ARG	4.8
1	A	107	PHE	4.6
1	B	176	GLU	4.6
1	C	399	ASP	4.4
1	B	583	GLN	4.3
1	A	122	TYR	4.3
1	D	254	TYR	4.3
1	C	41	GLN	4.3
1	B	493	ALA	4.3
1	D	287	VAL	4.2
1	B	107	PHE	4.1
1	D	235	GLY	4.0
1	C	583	GLN	3.9

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Mol	Chain	Res	Type	RSRZ
1	C	74	LEU	3.8
1	C	263	PRO	3.8
1	B	252	LEU	3.8
1	D	306	LEU	3.7
1	D	272	GLU	3.6
1	D	281	GLU	3.6
1	B	90	TYR	3.6
1	A	583	GLN	3.6
1	C	37	SER	3.5
1	C	222	ARG	3.4
1	C	107	PHE	3.4
1	A	158	ASP	3.4
1	A	577	PHE	3.4
1	D	107	PHE	3.4
1	D	344	VAL	3.4
1	D	267	LYS	3.4
1	B	230	LEU	3.3
1	A	186	GLU	3.3
1	A	364	GLU	3.2
1	B	38	ASN	3.2
1	A	565	GLN	3.2
1	B	251	LYS	3.2
1	C	39	PRO	3.2
1	D	543	GLN	3.1
1	A	524	GLU	3.1
1	A	564	ILE	3.1
1	B	409	TYR	3.0
1	D	122	TYR	3.0
1	A	582	VAL	3.0
1	C	232	HIS	3.0
1	A	157	ASP	3.0
1	A	578	THR	3.0
1	D	583	GLN	2.9
1	C	566	SER	2.9
1	A	201	PHE	2.9
1	B	432	GLY	2.8
1	C	368	ASN	2.8
1	C	562	ALA	2.8
1	B	138	SER	2.8
1	C	122	TYR	2.8
1	D	197	MET	2.8
1	C	186	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	262	TYR	2.8
1	B	173	ASP	2.8
1	B	577	PHE	2.7
1	C	118	THR	2.7
1	B	578	THR	2.7
1	B	393	ASP	2.7
1	D	91	ILE	2.6
1	D	506	ALA	2.6
1	B	69	THR	2.6
1	B	539	ILE	2.6
1	B	52	ASP	2.6
1	C	138	SER	2.6
1	B	74	LEU	2.6
1	B	508	LEU	2.6
1	A	228	VAL	2.5
1	B	246	LEU	2.5
1	C	397	ILE	2.5
1	D	282	ASN	2.5
1	A	412	SER	2.5
1	C	280	PRO	2.5
1	C	96	LYS	2.5
1	A	35	CYS	2.5
1	B	122	TYR	2.4
1	B	214	HIS	2.4
1	A	503	LEU	2.4
1	B	534	LEU	2.4
1	C	112	ILE	2.4
1	C	136	TYR	2.4
1	D	239	ASP	2.4
1	D	574	GLY	2.4
1	C	364	GLU	2.4
1	D	570	ASN	2.4
1	B	78	LYS	2.4
1	C	218	PRO	2.4
1	C	92	LEU	2.3
1	D	355	TYR	2.3
1	D	475	TYR	2.3
1	A	96	LYS	2.3
1	D	363	PRO	2.3
1	A	98	VAL	2.3
1	A	382	ASN	2.3
1	D	205	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	485	LYS	2.3
1	D	577	PHE	2.3
1	B	268	ASP	2.3
1	B	94	HIS	2.3
1	B	228	VAL	2.3
1	A	247	PHE	2.3
1	A	345	ILE	2.3
1	B	377	ILE	2.3
1	B	567	LEU	2.2
1	D	356	HIS	2.2
1	A	99	TRP	2.2
1	A	248	LYS	2.2
1	D	430	ILE	2.2
1	A	43	ARG	2.2
1	C	515	ASP	2.2
1	B	80	LEU	2.2
1	C	457	GLU	2.2
1	D	302	ALA	2.2
1	A	203	GLN	2.2
1	D	428	ARG	2.2
1	B	399	ASP	2.2
1	D	247	PHE	2.2
1	C	534	LEU	2.2
1	B	457	GLU	2.2
1	C	401	GLU	2.2
1	B	517	ILE	2.2
1	A	207	HIS	2.2
1	A	269	THR	2.2
1	C	476	THR	2.2
1	B	79	LEU	2.2
1	B	42	ASN	2.1
1	B	389	PRO	2.1
1	A	97	GLY	2.1
1	B	390	LEU	2.1
1	A	216	ARG	2.1
1	C	358	LYS	2.1
1	A	399	ASP	2.1
1	A	69	THR	2.1
1	A	95	PHE	2.1
1	B	187	PHE	2.1
1	C	209	PHE	2.1
1	A	112	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	116	VAL	2.1
1	A	92	LEU	2.1
1	D	238	LEU	2.1
1	B	395	PHE	2.1
1	A	262	TYR	2.1
1	C	223	GLY	2.1
1	D	65	GLY	2.1
1	D	409	TYR	2.1
1	D	36	CYS	2.0
1	D	181	VAL	2.0
1	A	414	LEU	2.0
1	C	537	ASN	2.0
1	B	235	GLY	2.0
1	C	460	TYR	2.0
1	A	461	GLN	2.0
1	B	581	ASN	2.0
1	A	533	GLY	2.0
1	C	219	GLY	2.0
1	C	533	GLY	2.0
1	C	394	THR	2.0
1	C	482	THR	2.0
1	D	158	ASP	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	NAG	H	2	14/15	0.73	0.14	50,59,63,64	0
2	NAG	E	2	14/15	0.75	0.14	62,71,78,82	0
2	NAG	G	2	14/15	0.76	0.12	47,57,64,65	0
2	NAG	F	2	14/15	0.76	0.17	38,43,47,48	0
2	NAG	F	1	14/15	0.89	0.11	34,38,40,43	0
2	NAG	G	1	14/15	0.90	0.10	28,35,37,39	0

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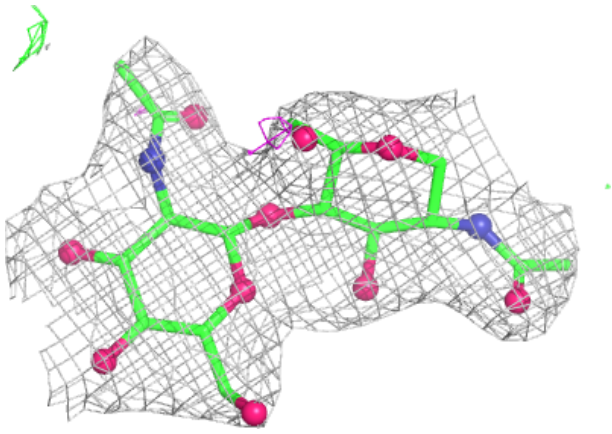
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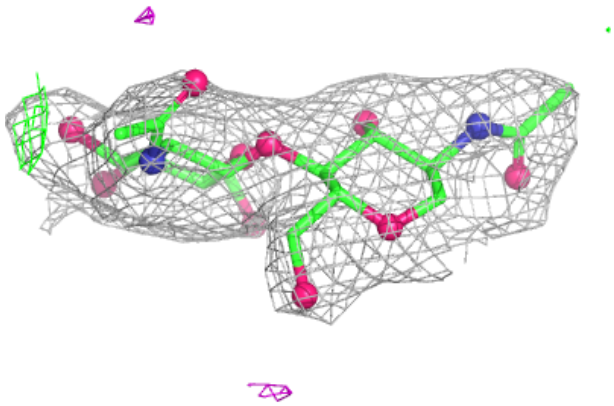
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	E	1	14/15	0.92	0.10	36,39,44,47	0
2	NAG	H	1	14/15	0.93	0.09	32,38,41,41	0

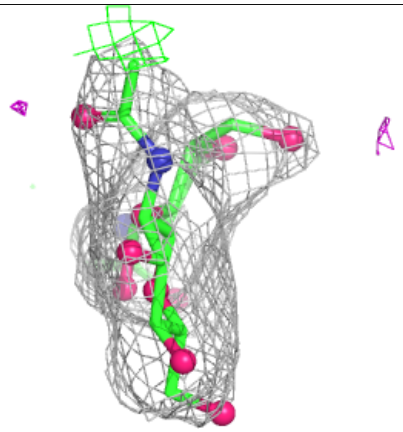
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

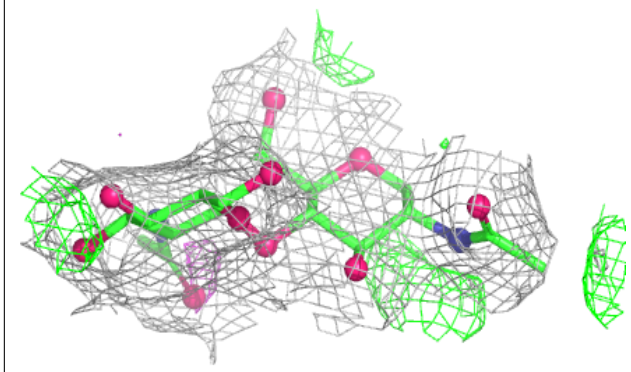


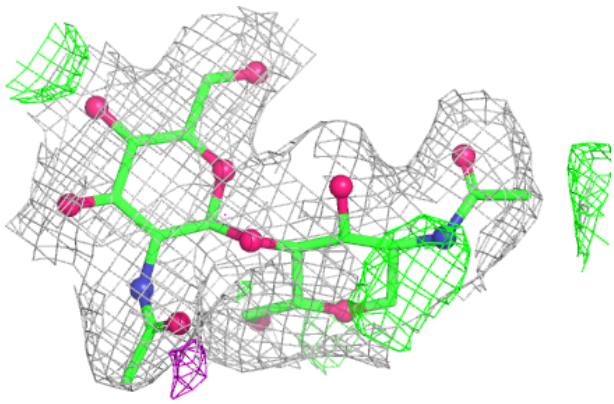


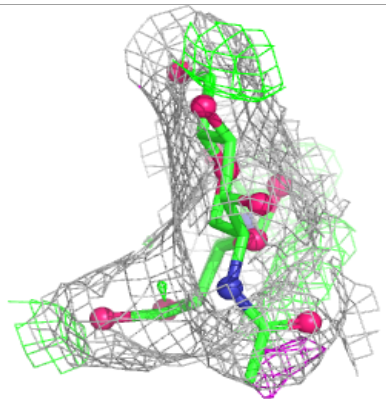


Electron density around Chain F:

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

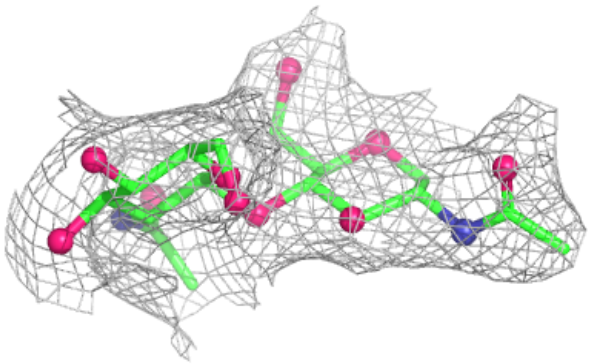


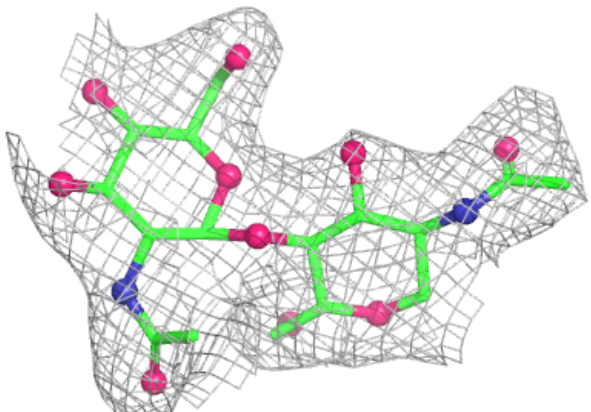


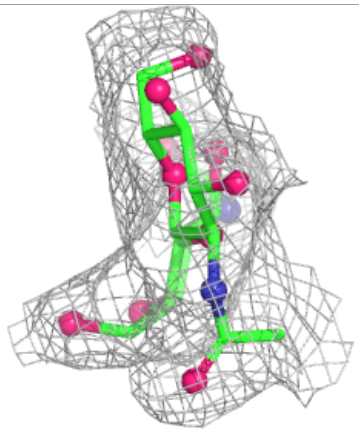


Electron density around Chain G:

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

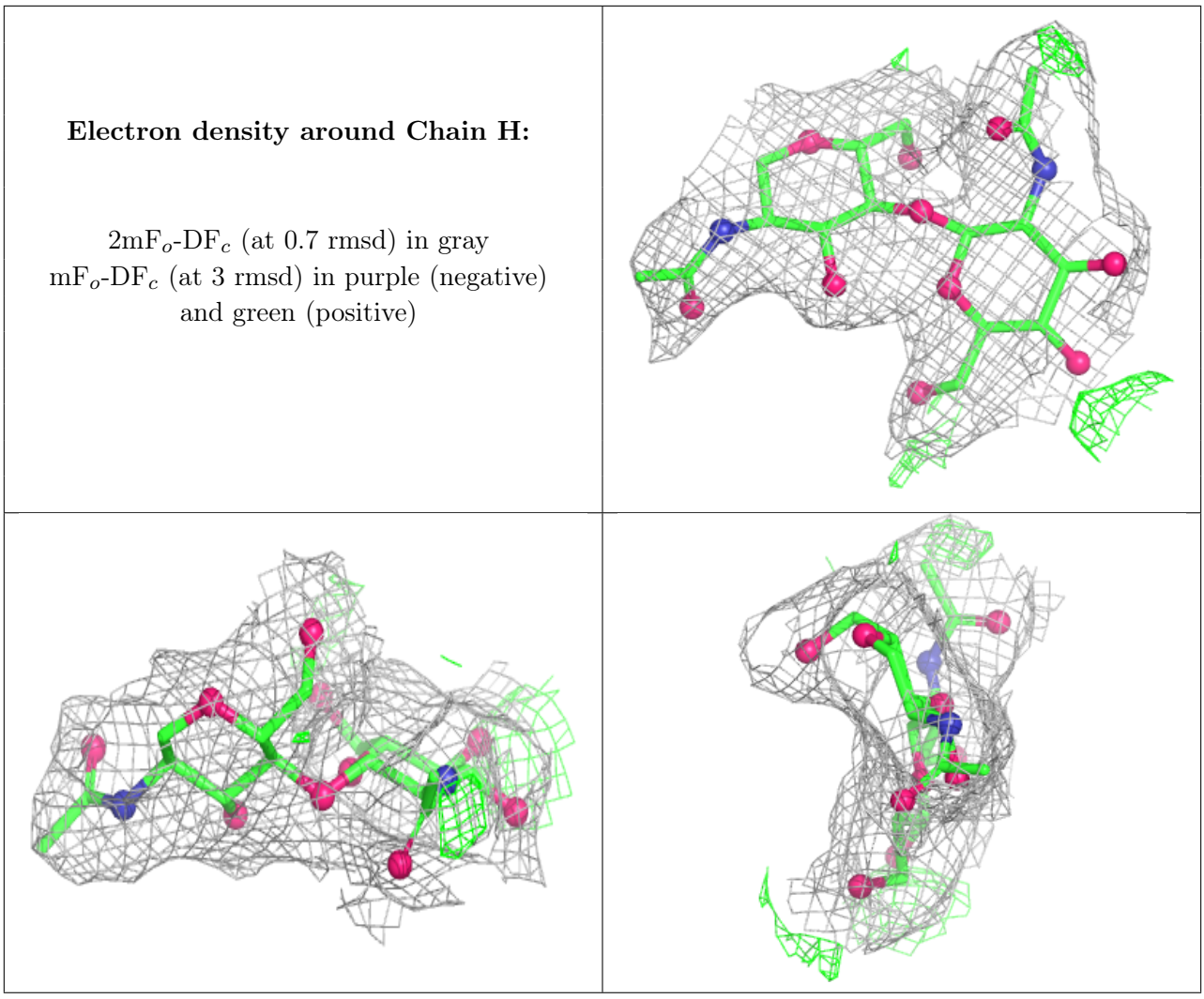






Electron density around Chain H:

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



6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
5	DF0	D	705	17/17	0.84	0.15	34,37,44,45	0
3	BOG	C	701	20/20	0.85	0.14	47,53,59,62	0
5	DF0	B	705	17/17	0.88	0.13	37,46,52,53	0
3	BOG	A	702	20/20	0.88	0.20	58,66,73,74	0
3	BOG	C	702	20/20	0.90	0.14	54,62,67,69	0
3	BOG	A	701	20/20	0.91	0.13	53,58,70,70	0
5	DF0	C	706	17/17	0.91	0.11	41,43,48,48	0
3	BOG	D	701	20/20	0.91	0.11	40,45,50,50	0
5	DF0	A	706	17/17	0.92	0.10	47,49,54,54	0

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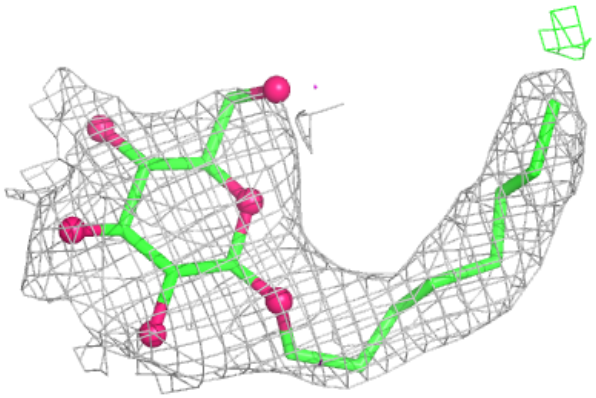
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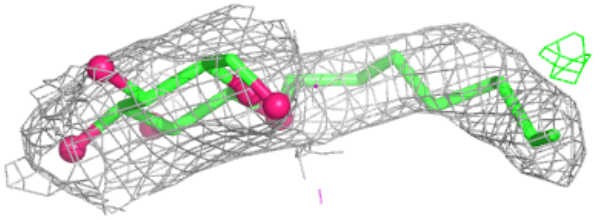
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	BOG	B	701	20/20	0.92	0.13	55,61,68,69	0
4	HEM	A	705	43/43	0.94	0.13	30,47,69,92	0
4	HEM	D	704	43/43	0.94	0.14	35,47,78,93	0
4	HEM	C	705	43/43	0.95	0.13	37,44,58,60	0
4	HEM	B	704	43/43	0.95	0.10	33,44,59,67	0

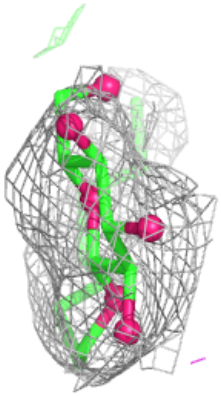
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around BOG C 701:

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

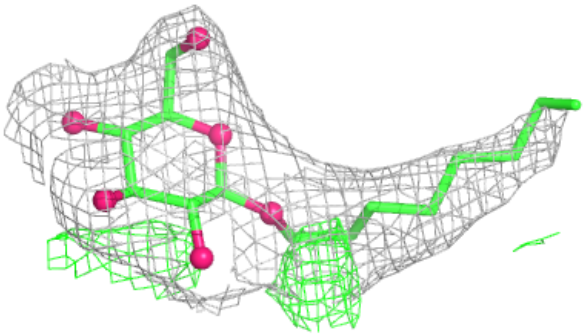


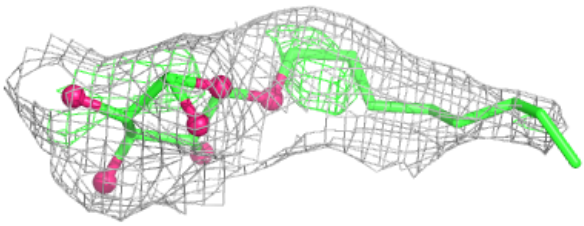


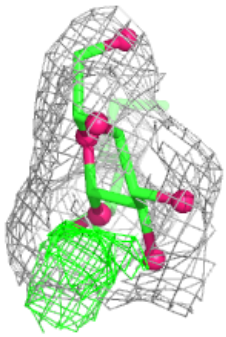


Electron density around BOG A 702:

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

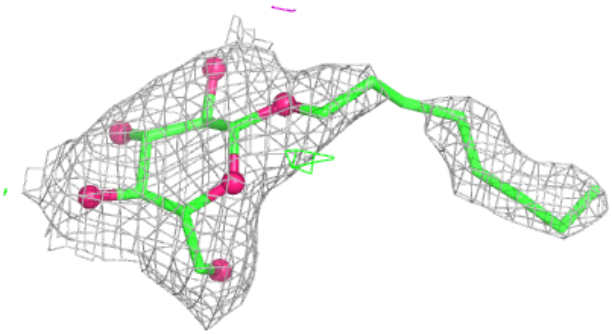


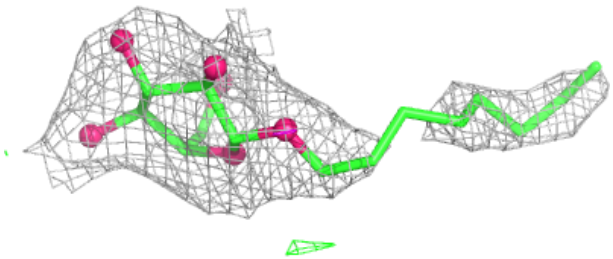


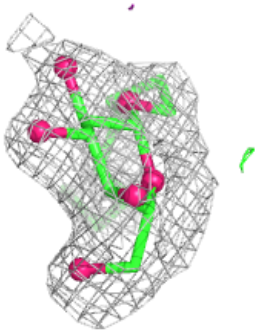


Electron density around BOG C 702:

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

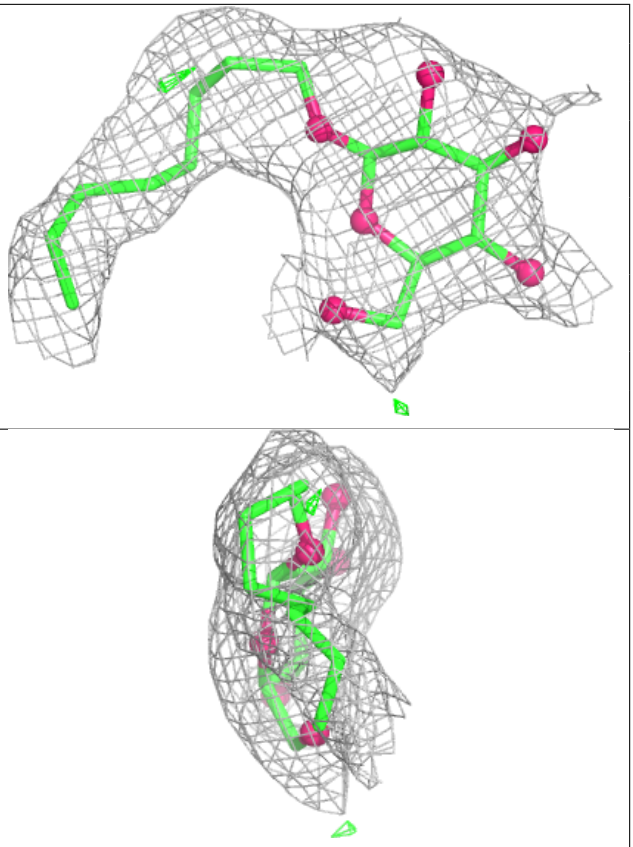






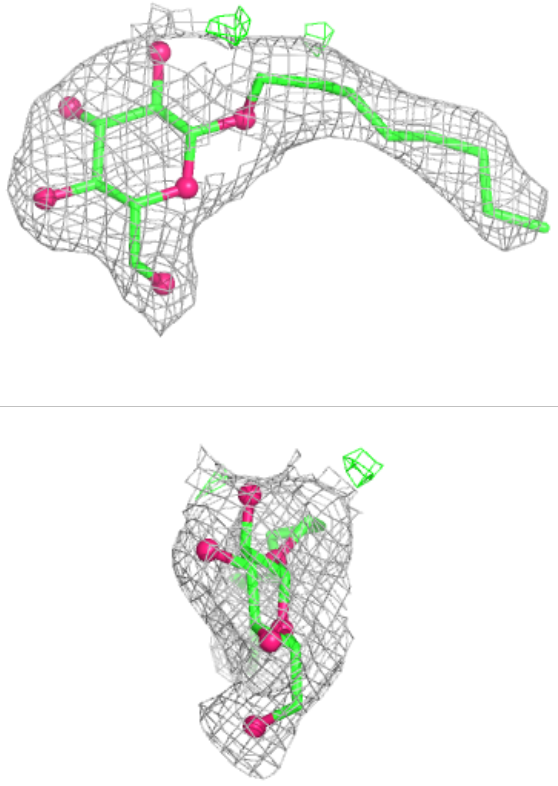
Electron density around BOG A 701:

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



Electron density around BOG D 701:

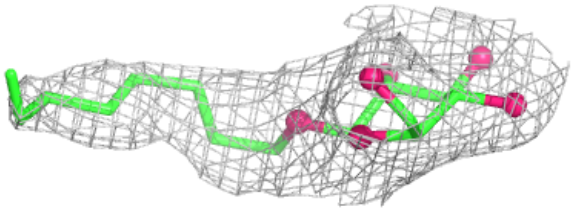
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

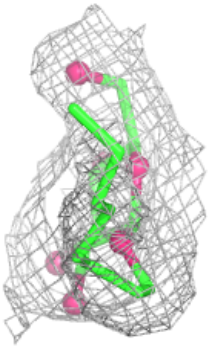


Electron density around BOG B 701:

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

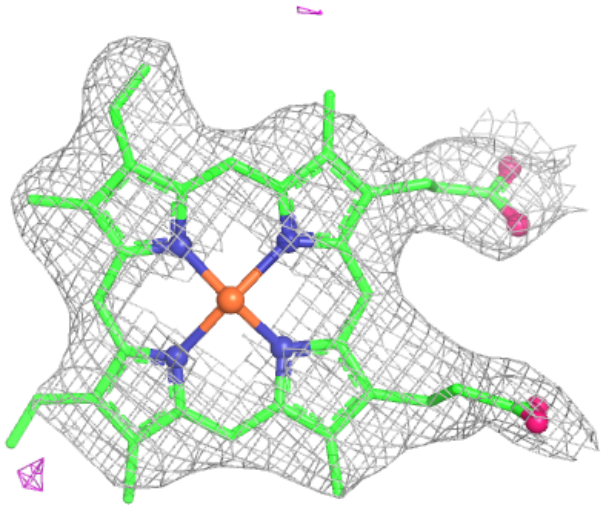


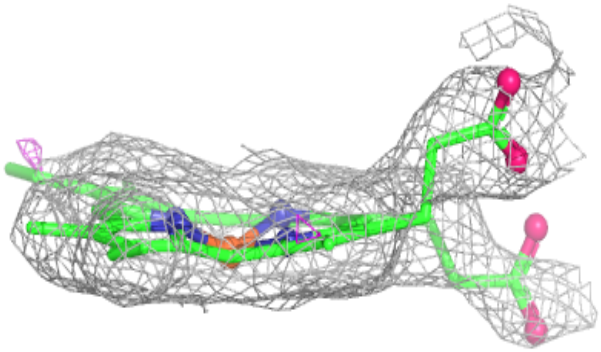


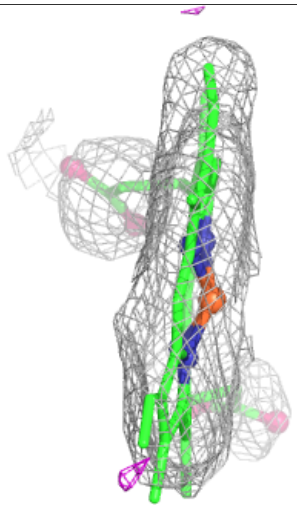


Electron density around HEM A 705:

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

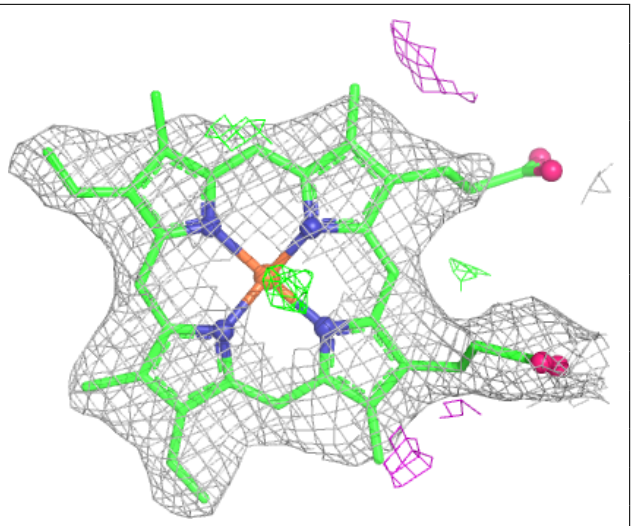


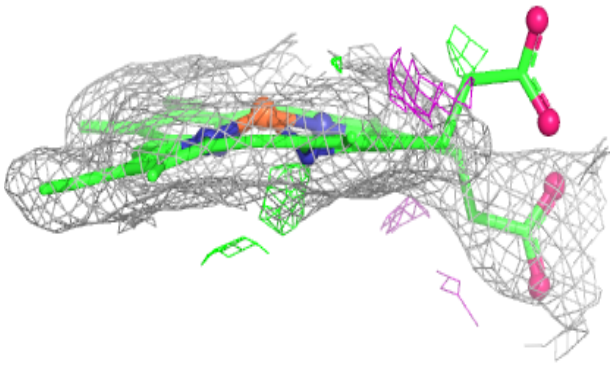


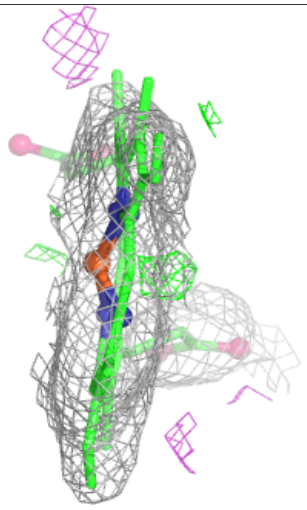


Electron density around HEM D 704:

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

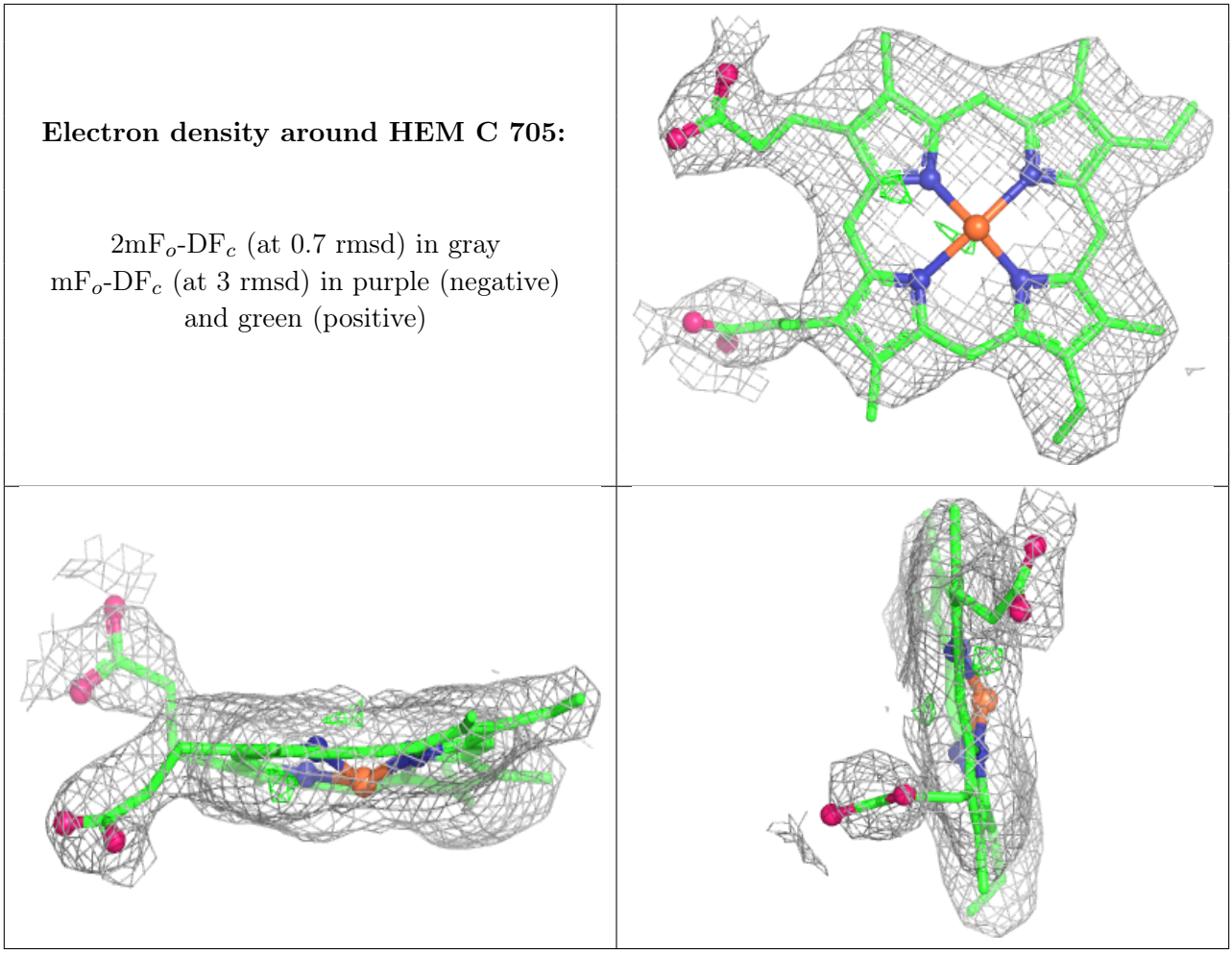






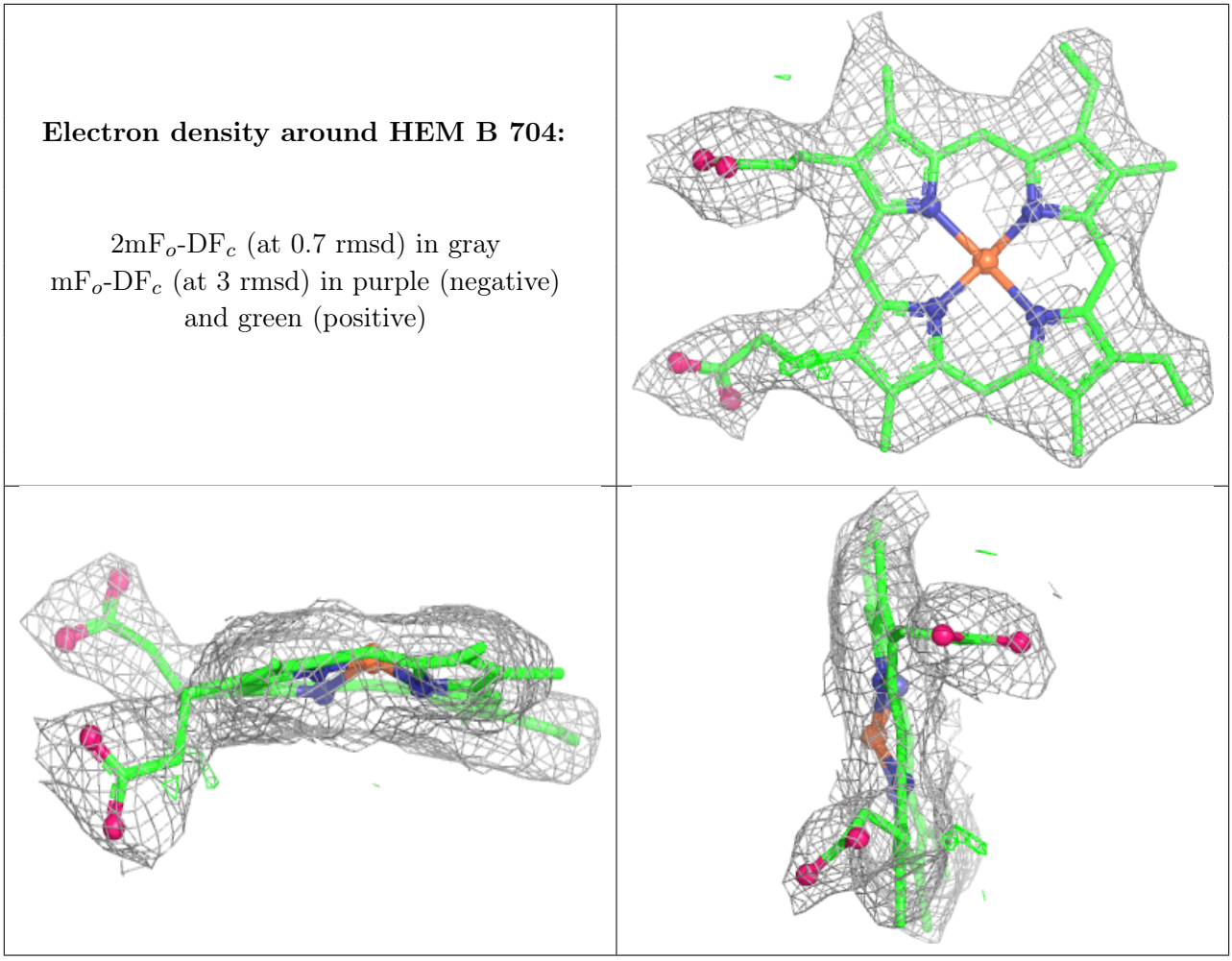
Electron density around HEM C 705:

$2mF_o$-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 704:

$2mF_o$-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.