Full wwPDB X-ray Structure Validation Report ⓘ

Jun 13, 2024 – 12:40 PM EDT

PDB ID	:	1PXX
Title	:	CRYSTAL STRUCTURE OF DICLOFENAC BOUND TO THE CYCLOOXYGENASE ACTIVE SITE OF COX-2
Authors	:	Kiefer, J.R.; Rowlinson, S.W.; Prusakiewicz, J.J.; Pawlitz, J.L.; Kozak, K.R.; Kalgutkar, A.S.; Stallings, W.C.; Marnett, L.J.; Kurumbail, R.G.
Deposited on	:	2003-07-07
Resolution	:	2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

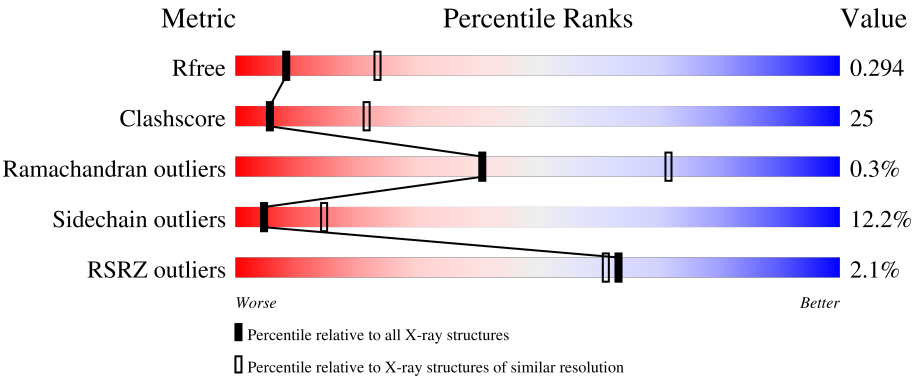
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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

Mol	Chain	Length	Quality of chain
1	A	604	2% 50% 35% 6% 9%
1	B	604	2% 49% 36% 6% 9%
1	C	604	% 50% 36% 6% 9%
1	D	604	2% 50% 36% 6% 9%

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Mol	Chain	Length	Quality of chain
2	E	3	33% 67%
2	F	3	33% 67%
2	G	3	33% 67%
2	H	3	33% 67%

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	E	3	-	-	-	X
2	NAG	F	3	-	-	-	X
2	NAG	G	3	-	-	-	X
2	NAG	H	3	-	-	-	X
3	NAG	A	661	-	-	-	X
3	NAG	C	2661	-	-	X	-
3	NAG	D	3661	-	-	-	X
4	BOG	D	3703	-	-	X	-

2 Entry composition (i)

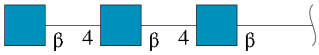
There are 7 unique types of molecules in this entry. The entry contains 18778 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

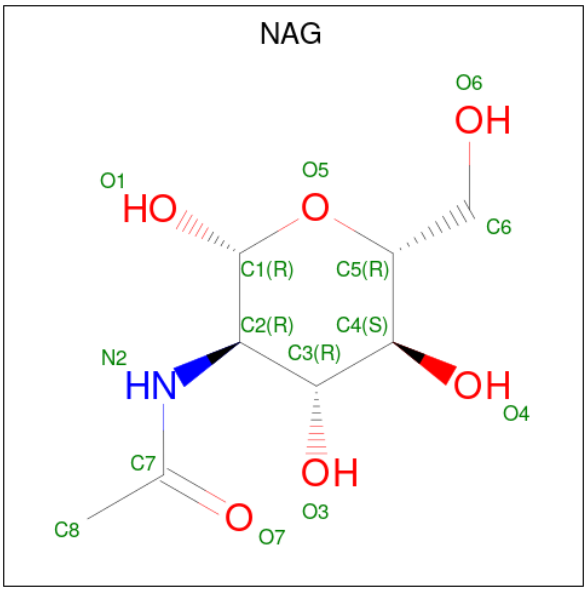
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	552	Total	C	N	O	S	0	0	0
			4472	2885	748	814	25			
1	B	552	Total	C	N	O	S	0	0	0
			4474	2885	750	814	25			
1	C	552	Total	C	N	O	S	0	0	0
			4474	2885	750	814	25			
1	D	552	Total	C	N	O	S	0	0	0
			4474	2885	750	814	25			

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



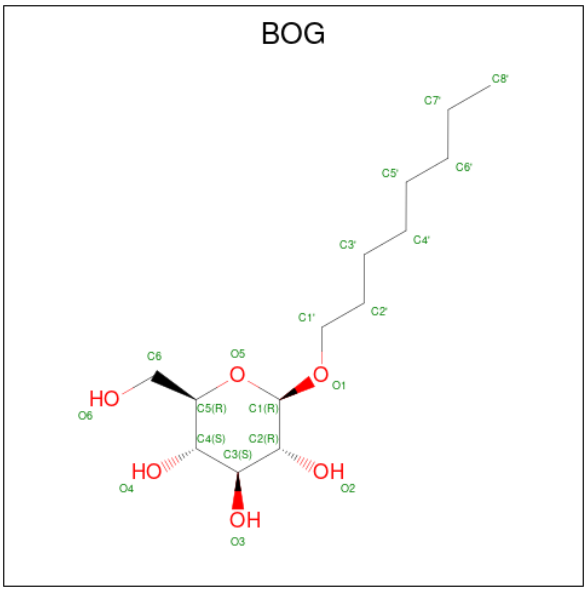
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	3	Total	C	N	O	0	0	0
			42	24	3	15			
2	F	3	Total	C	N	O	0	0	0
			42	24	3	15			
2	G	3	Total	C	N	O	0	0	0
			42	24	3	15			
2	H	3	Total	C	N	O	0	0	0
			42	24	3	15			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



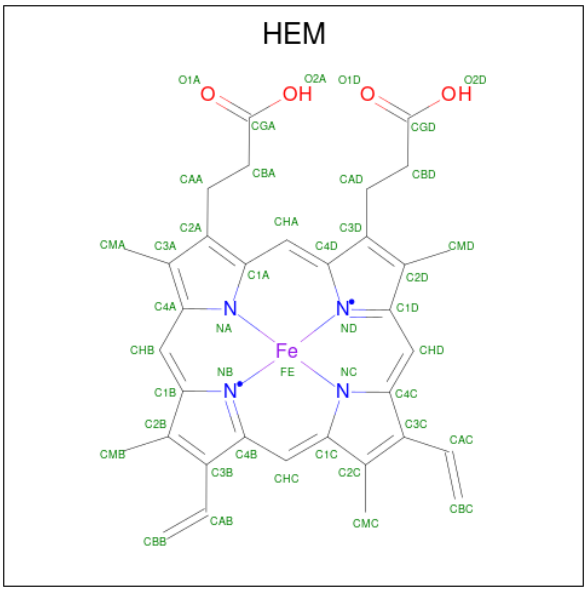
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 14 8 1 5	0	0
3	A	1	Total C N O 14 8 1 5	0	0
3	B	1	Total C N O 14 8 1 5	0	0
3	B	1	Total C N O 14 8 1 5	0	0
3	C	1	Total C N O 14 8 1 5	0	0
3	C	1	Total C N O 14 8 1 5	0	0
3	D	1	Total C N O 14 8 1 5	0	0
3	D	1	Total C N O 14 8 1 5	0	0

- Molecule 4 is octyl beta-D-glucopyranoside (three-letter code: BOG) (formula: $C_{14}H_{28}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 20 14 6	0	0
4	D	1	Total C O 19 13 6	0	0

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

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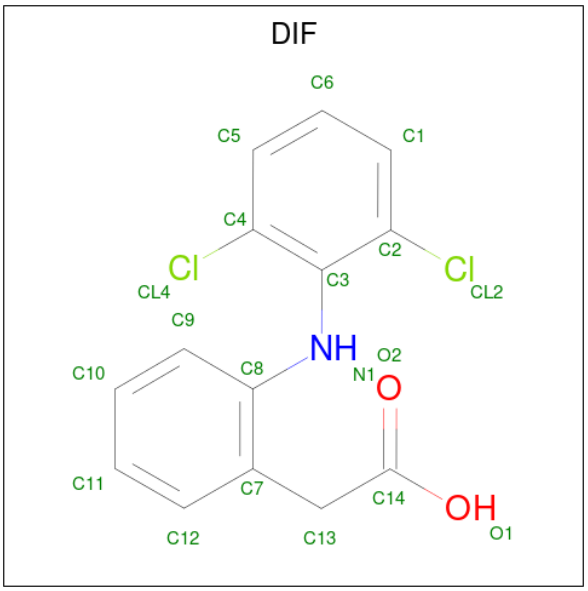
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 6 is 2-[2,6-DICHLOROPHENYL)AMINO]BENZENEACETIC ACID (three-letter code: DIF) (formula: $C_{14}H_{11}Cl_2NO_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	Cl	N	O	0	0
			19	14	2	1	2		
6	B	1	Total	C	Cl	N	O	0	0
			19	14	2	1	2		
6	C	1	Total	C	Cl	N	O	0	0
			19	14	2	1	2		
6	D	1	Total	C	Cl	N	O	0	0
			19	14	2	1	2		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	60	Total	O	0	0
			60	60		
7	B	93	Total	O	0	0
			93	93		

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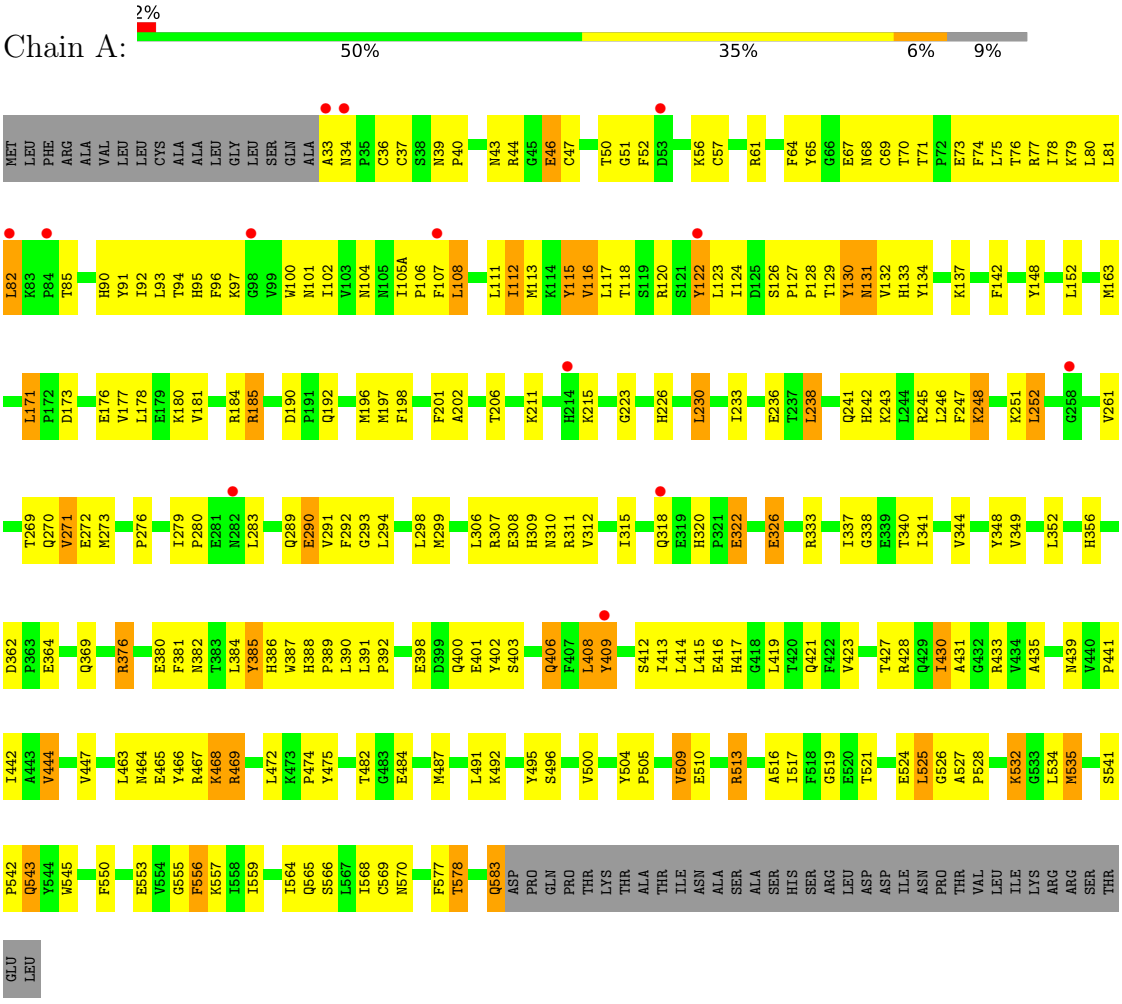
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	69	Total O 69 69	0	0
7	D	95	Total O 95 95	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

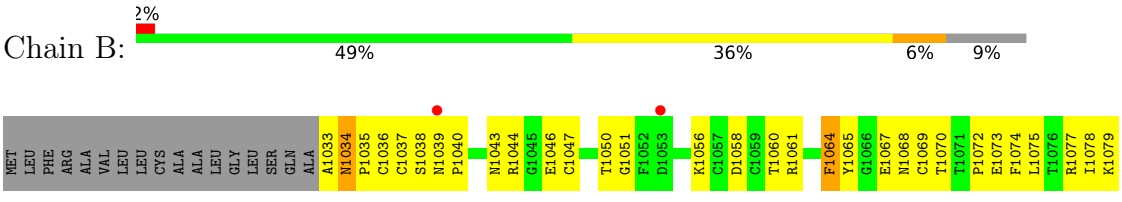
• Molecule 1: Prostaglandin G/H synthase 2

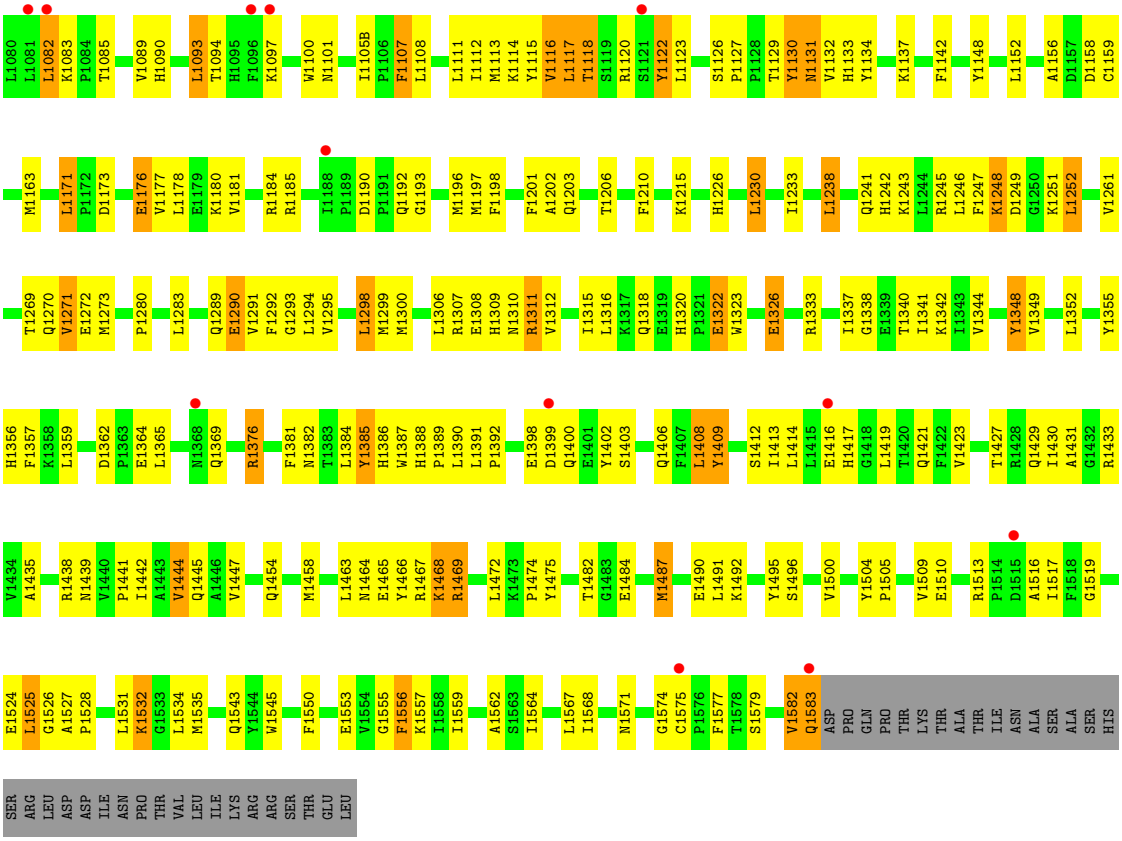
Chain A:



• Molecule 1: Prostaglandin G/H synthase 2

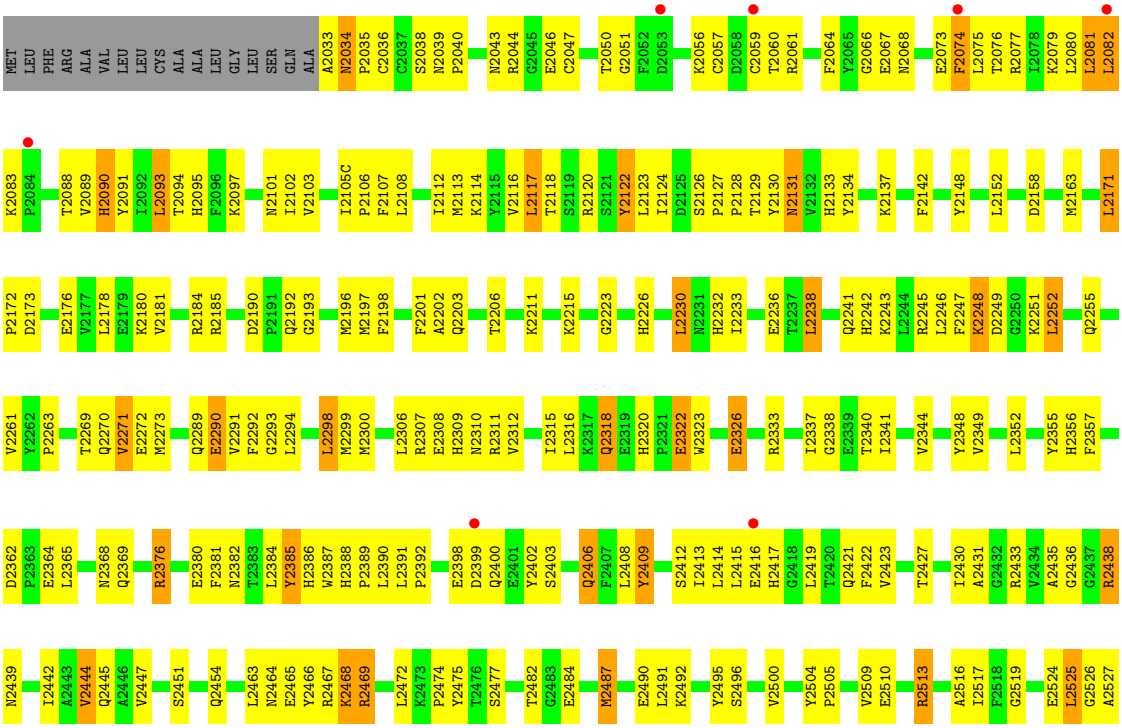
Chain B:

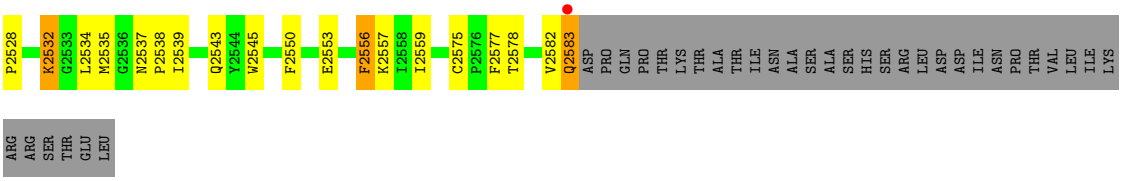




• Molecule 1: Prostaglandin G/H synthase 2

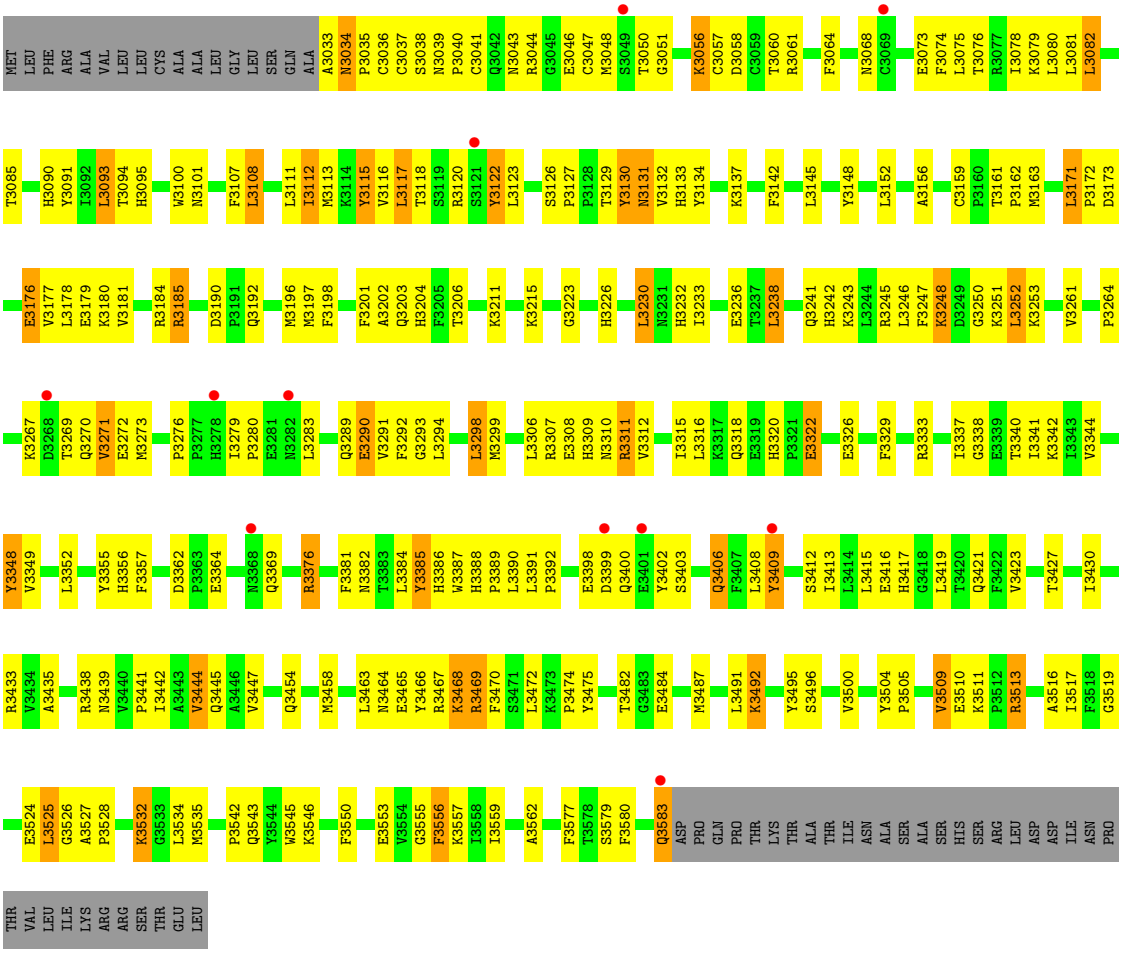
Chain C:





• 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-(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-(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-(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-(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	181.15Å 135.09Å 124.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.90 19.97 – 2.90	Depositor EDS
% Data completeness (in resolution range)	83.6 (20.00-2.90) 83.3 (19.97-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.16	Depositor
$< I/\sigma(I) >$ [1]	6.15 (at 2.88Å)	Xtriage
Refinement program	X-PLOR 98.1	Depositor
R, R_{free}	0.254 , 0.302 0.245 , 0.294	Depositor DCC
R_{free} test set	5475 reflections (9.63%)	wwPDB-VP
Wilson B-factor (Å^2)	21.5	Xtriage
Anisotropy	0.578	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 52.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	18778	wwPDB-VP
Average B, all atoms (Å^2)	23.0	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 64.30 % 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 8.4672e-06. 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DIF, 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	0.47	0/4598	0.66	1/6232 (0.0%)
1	B	0.47	0/4601	0.66	1/6239 (0.0%)
1	C	0.47	0/4601	0.66	1/6239 (0.0%)
1	D	0.47	0/4601	0.66	1/6239 (0.0%)
All	All	0.47	0/18401	0.66	4/24949 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	D	0	1
All	All	0	2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1148	TYR	N-CA-C	-5.71	95.57	111.00
1	D	3148	TYR	N-CA-C	-5.42	96.38	111.00
1	C	2148	TYR	N-CA-C	-5.38	96.47	111.00
1	A	148	TYR	N-CA-C	-5.31	96.67	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	1348	TYR	Sidechain
1	D	3348	TYR	Sidechain

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	4472	0	4366	231	0
1	B	4474	0	4372	234	1
1	C	4474	0	4372	235	1
1	D	4474	0	4372	227	0
2	E	42	0	37	3	0
2	F	42	0	37	1	0
2	G	42	0	37	2	0
2	H	42	0	37	3	0
3	A	28	0	26	5	0
3	B	28	0	26	6	0
3	C	28	0	26	7	0
3	D	28	0	26	4	0
4	A	20	0	28	5	1
4	D	19	0	25	9	1
5	A	43	0	30	4	0
5	B	43	0	30	7	0
5	C	43	0	30	4	0
5	D	43	0	30	4	0
6	A	19	0	10	3	0
6	B	19	0	10	3	0
6	C	19	0	10	4	0
6	D	19	0	10	1	0
7	A	60	0	0	9	0
7	B	93	0	0	9	0
7	C	69	0	0	8	0
7	D	95	0	0	7	0
All	All	18778	0	17947	928	2

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 25.

All (928) 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:3294:LEU:HD22	1:D:3409:TYR:HD2	1.03	1.15
1:A:294:LEU:HD22	1:A:409:TYR:CD2	1.80	1.14
1:D:3294:LEU:HD22	1:D:3409:TYR:CD2	1.84	1.12
1:A:294:LEU:HD22	1:A:409:TYR:HD2	1.00	1.11
1:D:3442:ILE:HD13	4:D:3703:BOG:H62	1.34	1.08
1:C:2105(C):ILE:CG2	1:C:2108:LEU:HB2	1.84	1.07
1:C:2294:LEU:HD22	1:C:2409:TYR:HD2	1.13	1.07
1:B:1294:LEU:HD22	1:B:1409:TYR:HD2	1.18	1.07
1:C:2105(C):ILE:HG22	1:C:2108:LEU:HB2	1.32	1.06
1:C:2294:LEU:HD22	1:C:2409:TYR:CD2	1.92	1.03
1:B:1294:LEU:HD22	1:B:1409:TYR:CD2	1.93	1.02
1:D:3113:MET:O	1:D:3116:VAL:HG22	1.59	1.01
1:A:442:ILE:HD13	4:A:703:BOG:H62	1.41	0.99
1:B:1398:GLU:HG3	1:B:1421:GLN:CD	1.88	0.94
1:A:398:GLU:HG3	1:A:421:GLN:CD	1.88	0.93
1:D:3447:VAL:HG13	5:D:3601:HEM:HBA1	1.49	0.93
1:B:1181:VAL:HG12	1:B:1487:MET:HG2	1.52	0.92
1:B:1184:ARG:HB2	1:B:1439:ASN:HA	1.51	0.91
1:A:105(A):ILE:CG2	1:A:108:LEU:HB2	1.99	0.91
1:A:184:ARG:HB2	1:A:439:ASN:HA	1.53	0.91
1:C:2398:GLU:HG3	1:C:2421:GLN:CD	1.89	0.91
1:D:3184:ARG:HB2	1:D:3439:ASN:HA	1.53	0.90
1:C:2039:ASN:HB3	7:C:5138:HOH:O	1.72	0.90
1:C:2447:VAL:HG13	5:C:2601:HEM:HBA2	1.54	0.90
1:B:1447:VAL:HG13	5:B:1601:HEM:HBA1	1.54	0.89
1:C:2181:VAL:HG12	1:C:2487:MET:HG2	1.54	0.88
1:A:294:LEU:CD2	1:A:409:TYR:HD2	1.85	0.88
1:C:2184:ARG:HB2	1:C:2439:ASN:HA	1.53	0.87
1:A:33:ALA:C	1:A:34:ASN:CA	2.43	0.87
1:D:3398:GLU:HG3	1:D:3421:GLN:CD	1.95	0.87
1:B:1105(B):ILE:HD13	1:B:1108:LEU:HD12	1.55	0.86
1:D:3294:LEU:CD2	1:D:3409:TYR:HD2	1.86	0.86
1:D:3075:LEU:CG	1:D:3079:LYS:HE3	2.06	0.85
1:B:1206:THR:HG21	1:B:1385:TYR:CE2	2.13	0.84
1:D:3075:LEU:HG	1:D:3079:LYS:HE3	1.59	0.84
1:B:1034:ASN:HB3	1:B:1037:CYS:SG	2.18	0.84
1:C:2322:GLU:HG2	1:D:3051:GLY:C	1.98	0.84
1:A:293:GLY:HA2	1:A:299:MET:CE	2.08	0.83
1:C:2105(C):ILE:HG22	1:C:2105(C):ILE:O	1.78	0.83
1:B:1387:TRP:HB2	5:B:1601:HEM:HAC	1.61	0.83
1:B:1385:TYR:OH	6:B:1701:DIF:H132	1.78	0.83
1:B:1472:LEU:HD21	1:B:1524:GLU:HG3	1.62	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3206:THR:HG21	1:D:3385:TYR:CE2	2.15	0.82
1:D:3074:PHE:O	1:D:3078:ILE:HD12	1.79	0.81
1:B:1246:LEU:HG	1:B:1248:LYS:HG3	1.62	0.81
1:D:3419:LEU:O	1:D:3423:VAL:HG23	1.80	0.81
1:B:1465:GLU:OE1	1:B:1465:GLU:HA	1.81	0.81
1:C:2123:LEU:O	1:C:2469:ARG:NH2	2.14	0.81
1:D:3293:GLY:HA2	1:D:3299:MET:CE	2.11	0.80
1:A:185:ARG:HH11	4:A:703:BOG:H4'1	1.47	0.80
1:B:1293:GLY:HA2	1:B:1299:MET:CE	2.12	0.80
1:A:123:LEU:O	1:A:469:ARG:NH2	2.15	0.80
1:B:1123:LEU:O	1:B:1469:ARG:NH2	2.15	0.79
1:D:3123:LEU:O	1:D:3469:ARG:NH2	2.15	0.79
1:D:3516:ALA:HB1	7:D:5034:HOH:O	1.83	0.79
1:C:2246:LEU:HG	1:C:2248:LYS:HG3	1.65	0.79
1:D:3181:VAL:HG12	1:D:3487:MET:HG2	1.63	0.79
1:D:3427:THR:HG22	1:D:3583:GLN:HE22	1.47	0.79
1:D:3202:ALA:O	1:D:3206:THR:HG23	1.83	0.79
1:C:2294:LEU:CD2	1:C:2409:TYR:HD2	1.95	0.78
1:C:2198:PHE:CZ	1:C:2352:LEU:HD13	2.19	0.78
1:C:2472:LEU:HD21	1:C:2524:GLU:HG3	1.64	0.78
1:A:427:THR:HG22	1:A:583:GLN:HE22	1.48	0.78
1:C:2293:GLY:HA2	1:C:2299:MET:CE	2.13	0.78
1:B:1294:LEU:CD2	1:B:1409:TYR:HD2	1.96	0.78
1:A:105(A):ILE:HG22	1:A:108:LEU:HB2	1.65	0.77
1:B:1163:MET:CE	1:B:1171:LEU:HD21	2.14	0.77
1:D:3472:LEU:HD21	1:D:3524:GLU:HG3	1.64	0.77
1:C:2051:GLY:O	1:D:3322:GLU:HG2	1.85	0.77
1:B:1427:THR:HG22	1:B:1583:GLN:HE22	1.49	0.77
1:A:181:VAL:HG12	1:A:487:MET:HG2	1.67	0.76
1:B:1131:ASN:HD22	1:B:1131:ASN:C	1.89	0.76
1:A:40:PRO:HA	3:A:661:NAG:H83	1.66	0.76
1:B:1202:ALA:O	1:B:1206:THR:HG23	1.84	0.76
1:D:3039:ASN:N	1:D:3040:PRO:HD3	1.99	0.76
1:D:3162:PRO:HD2	7:D:5121:HOH:O	1.84	0.76
1:A:56:LYS:HG3	1:A:57:CYS:N	2.00	0.76
1:C:2202:ALA:O	1:C:2206:THR:HG23	1.85	0.76
1:A:525:LEU:HD21	7:A:5160:HOH:O	1.86	0.76
1:B:1034:ASN:ND2	1:B:1036:CYS:H	1.82	0.76
1:C:2465:GLU:OE1	1:C:2465:GLU:HA	1.86	0.75
1:B:1034:ASN:HD22	1:B:1036:CYS:H	1.32	0.75
1:A:444:VAL:O	1:A:444:VAL:HG13	1.86	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2131:ASN:HD22	1:C:2131:ASN:C	1.90	0.75
1:A:34:ASN:HD22	1:A:36:CYS:H	1.33	0.75
1:C:2206:THR:HG21	1:C:2385:TYR:CE2	2.21	0.75
1:B:1241:GLN:NE2	1:B:1245:ARG:HH11	1.85	0.75
1:C:2163:MET:HE2	1:C:2171:LEU:HD21	1.68	0.74
1:C:2163:MET:CE	1:C:2171:LEU:HD21	2.18	0.74
1:D:3131:ASN:C	1:D:3131:ASN:HD22	1.91	0.74
1:D:3246:LEU:HG	1:D:3248:LYS:HG3	1.69	0.74
1:C:2113:MET:HA	1:C:2116:VAL:HG13	1.69	0.74
1:D:3230:LEU:HG	1:D:3337:ILE:HG12	1.70	0.74
1:D:3465:GLU:OE1	1:D:3465:GLU:HA	1.87	0.73
1:A:130:TYR:HB3	1:A:134:TYR:O	1.88	0.73
1:D:3403:SER:OG	1:D:3406:GLN:HG3	1.88	0.73
1:A:419:LEU:O	1:A:423:VAL:HG23	1.87	0.73
1:D:3447:VAL:HG13	5:D:3601:HEM:CBA	2.16	0.73
3:B:1661:NAG:O7	3:B:1661:NAG:H3	1.89	0.73
1:A:472:LEU:HD21	1:A:524:GLU:HG3	1.71	0.73
1:D:3464:ASN:HD21	1:D:3475:TYR:H	1.36	0.73
1:A:465:GLU:HA	1:A:465:GLU:OE1	1.88	0.72
1:C:2526:GLY:HA3	6:C:2701:DIF:C10	2.19	0.72
1:C:2419:LEU:O	1:C:2423:VAL:HG23	1.89	0.72
1:A:198:PHE:CZ	1:A:352:LEU:HD13	2.24	0.72
1:B:1113:MET:HE1	1:B:1116:VAL:HG21	1.70	0.72
1:D:3090:HIS:CE1	1:D:3094:THR:HG21	2.24	0.72
1:D:3034:ASN:HD22	1:D:3036:CYS:H	1.36	0.72
1:A:74:PHE:CZ	1:A:78:ILE:HD11	2.25	0.71
1:A:447:VAL:HG13	5:A:704:HEM:HBA1	1.71	0.71
1:B:1292:PHE:O	1:B:1299:MET:HE2	1.90	0.71
1:C:2033:ALA:HB3	1:C:2158:ASP:OD2	1.90	0.71
1:B:1152:LEU:HD12	1:B:1466:TYR:CD1	2.25	0.71
1:C:2322:GLU:HG2	1:D:3051:GLY:O	1.89	0.71
1:B:1464:ASN:HD21	1:B:1475:TYR:H	1.39	0.70
1:A:241:GLN:NE2	1:A:245:ARG:HH11	1.90	0.70
1:A:202:ALA:O	1:A:206:THR:HG23	1.90	0.70
1:D:3241:GLN:NE2	1:D:3245:ARG:HH11	1.89	0.70
1:D:3444:VAL:HG13	1:D:3444:VAL:O	1.90	0.70
1:C:2444:VAL:O	1:C:2444:VAL:HG13	1.91	0.70
3:C:2661:NAG:O7	3:C:2661:NAG:H3	1.90	0.70
1:A:163:MET:HE2	1:A:171:LEU:HD21	1.73	0.70
1:A:34:ASN:ND2	1:A:36:CYS:H	1.89	0.70
1:B:1419:LEU:O	1:B:1423:VAL:HG23	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1444:VAL:O	1:B:1444:VAL:HG13	1.90	0.70
1:A:206:THR:HG21	1:A:385:TYR:CE2	2.27	0.70
1:B:1075:LEU:HD11	1:B:1079:LYS:HE3	1.73	0.69
1:D:3198:PHE:CZ	1:D:3352:LEU:HD13	2.26	0.69
1:D:3252:LEU:HD22	1:D:3309:HIS:CD2	2.27	0.69
1:B:1105(B):ILE:CG2	1:B:1108:LEU:HB2	2.22	0.69
1:C:2198:PHE:CE1	1:C:2352:LEU:HD13	2.28	0.69
1:C:2241:GLN:NE2	1:C:2245:ARG:HH11	1.90	0.69
1:C:2427:THR:HG22	1:C:2583:GLN:HE22	1.57	0.69
1:A:163:MET:CE	1:A:171:LEU:HD21	2.23	0.69
1:C:2504:TYR:HB3	1:C:2505:PRO:HD3	1.75	0.69
1:D:3179:GLU:HG2	4:D:3703:BOG:H1'1	1.73	0.69
1:C:2137:LYS:HE2	1:D:3543:GLN:O	1.93	0.69
1:C:2293:GLY:HA2	1:C:2299:MET:HE2	1.74	0.69
1:B:1039:ASN:N	1:B:1040:PRO:HD3	2.08	0.68
1:A:105(A):ILE:HG22	1:A:108:LEU:H	1.58	0.68
3:D:3661:NAG:O7	3:D:3661:NAG:H3	1.93	0.68
4:D:3703:BOG:O1	4:D:3703:BOG:C2	2.41	0.68
1:A:131:ASN:C	1:A:131:ASN:HD22	1.96	0.68
1:B:1198:PHE:CZ	1:B:1352:LEU:HD13	2.27	0.68
1:A:137:LYS:HE2	1:B:1543:GLN:O	1.93	0.68
1:B:1082:LEU:CD1	1:B:1082:LEU:N	2.57	0.68
1:C:2142:PHE:O	1:C:2376:ARG:NH2	2.27	0.68
1:C:2292:PHE:O	1:C:2299:MET:HE1	1.93	0.68
1:C:2403:SER:OG	1:C:2406:GLN:HG3	1.93	0.68
1:A:403:SER:OG	1:A:406:GLN:HG3	1.93	0.67
1:A:504:TYR:HB3	1:A:505:PRO:HD3	1.75	0.67
1:D:3340:THR:O	1:D:3344:VAL:HG23	1.95	0.67
1:C:2034:ASN:ND2	1:C:2036:CYS:H	1.92	0.67
1:C:2113:MET:HG3	1:C:2117:LEU:HD22	1.75	0.67
1:D:3504:TYR:HB3	1:D:3505:PRO:HD3	1.77	0.67
1:B:1082:LEU:N	1:B:1082:LEU:HD13	2.09	0.67
1:D:3292:PHE:O	1:D:3299:MET:HE2	1.95	0.67
1:A:246:LEU:HG	1:A:248:LYS:HG3	1.76	0.66
1:A:468:LYS:HD2	1:A:474:PRO:HG3	1.76	0.66
1:B:1252:LEU:HD22	1:B:1309:HIS:CD2	2.30	0.66
3:C:2661:NAG:O7	3:C:2661:NAG:C3	2.44	0.66
1:D:3152:LEU:HD12	1:D:3466:TYR:CD1	2.31	0.66
1:C:2051:GLY:C	1:D:3322:GLU:HG2	2.14	0.66
1:C:2464:ASN:HD21	1:C:2475:TYR:H	1.44	0.66
1:D:3362:ASP:OD1	1:D:3364:GLU:HG3	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:THR:O	1:A:344:VAL:HG23	1.95	0.66
1:C:2113:MET:O	1:C:2117:LEU:HD22	1.96	0.66
1:B:1230:LEU:HG	1:B:1337:ILE:HG12	1.77	0.66
1:A:541:SER:HB2	7:B:5184:HOH:O	1.96	0.66
1:A:447:VAL:HG13	5:A:704:HEM:CBA	2.26	0.65
1:B:1403:SER:OG	1:B:1406:GLN:HG3	1.96	0.65
1:A:226:HIS:CE1	1:A:376:ARG:HD2	2.31	0.65
1:B:1163:MET:HE2	1:B:1171:LEU:HD21	1.78	0.65
1:D:3163:MET:CE	1:D:3171:LEU:HD21	2.26	0.65
1:C:2526:GLY:HA3	6:C:2701:DIF:H10	1.78	0.65
4:D:3703:BOG:C2	4:D:3703:BOG:O5	2.45	0.65
1:B:1113:MET:HA	1:B:1116:VAL:HG13	1.78	0.65
1:C:2130:TYR:HB3	1:C:2134:TYR:O	1.95	0.65
1:A:230:LEU:HG	1:A:337:ILE:HG12	1.78	0.65
1:A:247:PHE:C	1:A:248:LYS:HG2	2.17	0.65
1:C:2050:THR:HG21	1:C:2056:LYS:HB3	1.77	0.65
1:D:3041:CYS:SG	1:D:3047:CYS:HB2	2.37	0.65
1:B:1142:PHE:O	1:B:1376:ARG:NH2	2.30	0.64
1:B:1230:LEU:HD13	1:B:1233:ILE:HD12	1.79	0.64
3:B:1661:NAG:O7	3:B:1661:NAG:C3	2.46	0.64
1:A:198:PHE:CE1	1:A:352:LEU:HD13	2.31	0.64
1:B:1090:HIS:CE1	1:B:1094:THR:HG21	2.33	0.64
1:B:1113:MET:HG3	1:B:1117:LEU:HD22	1.78	0.64
1:D:3050:THR:HG21	1:D:3056:LYS:HB3	1.79	0.64
1:C:2068:ASN:ND2	3:C:2661:NAG:H61	2.13	0.64
1:A:526:GLY:HA3	6:A:701:DIF:C10	2.28	0.64
1:B:1040:PRO:HA	3:B:1661:NAG:H83	1.79	0.64
1:B:1043:ASN:O	1:B:1044:ARG:HB2	1.97	0.64
1:D:3163:MET:HE2	1:D:3171:LEU:HD21	1.80	0.64
1:B:1504:TYR:HB3	1:B:1505:PRO:HD3	1.80	0.64
1:D:3427:THR:CG2	1:D:3583:GLN:HE22	2.11	0.64
1:B:1193:GLY:O	1:B:1582:VAL:HG23	1.98	0.63
1:C:2482:THR:HG22	1:C:2509:VAL:HG13	1.79	0.63
1:D:3482:THR:HG22	1:D:3509:VAL:HG13	1.81	0.63
1:C:2043:ASN:O	1:C:2044:ARG:HB2	1.98	0.63
1:D:3468:LYS:HD2	1:D:3474:PRO:HG3	1.81	0.63
1:C:2105(C):ILE:HG22	1:C:2108:LEU:H	1.63	0.63
1:C:2113:MET:HG3	1:C:2117:LEU:CD2	2.29	0.63
1:C:2173:ASP:HB3	1:C:2176:GLU:HB2	1.80	0.63
1:A:521:THR:HG23	7:A:5160:HOH:O	1.97	0.63
1:A:230:LEU:HD13	1:A:233:ILE:HD12	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2075:LEU:HD11	1:C:2079:LYS:HE3	1.80	0.62
1:C:2118:THR:HG21	1:C:2369:GLN:HG2	1.81	0.62
1:D:3090:HIS:HE1	1:D:3094:THR:HG21	1.62	0.62
1:B:1198:PHE:CE1	1:B:1352:LEU:HD13	2.34	0.62
1:A:362:ASP:OD1	1:A:364:GLU:HG3	1.98	0.62
1:D:3198:PHE:CE1	1:D:3352:LEU:HD13	2.35	0.62
1:B:1107:PHE:CD1	1:B:1107:PHE:C	2.72	0.62
1:C:2230:LEU:HD13	1:C:2233:ILE:HD12	1.81	0.62
1:D:3043:ASN:O	1:D:3044:ARG:HB2	1.99	0.62
1:A:243:LYS:HB3	1:A:271:VAL:HG12	1.82	0.62
1:C:2034:ASN:C	1:C:2034:ASN:HD22	2.01	0.62
1:A:543:GLN:OE1	1:A:543:GLN:HA	1.99	0.62
1:C:2131:ASN:ND2	1:C:2134:TYR:H	1.97	0.62
1:B:1430:ILE:HD12	1:B:1582:VAL:HG21	1.80	0.62
1:B:1482:THR:HG22	1:B:1509:VAL:HG13	1.79	0.62
1:B:1577:PHE:HE2	1:B:1583:GLN:HE21	1.46	0.62
1:A:510:GLU:OE1	1:A:519:GLY:HA3	2.00	0.62
1:B:1130:TYR:HB3	1:B:1134:TYR:O	2.00	0.62
1:C:2247:PHE:C	1:C:2248:LYS:HG2	2.19	0.62
1:C:2543:GLN:OE1	1:C:2543:GLN:HA	1.99	0.62
1:A:322:GLU:HG2	1:B:1051:GLY:O	2.00	0.61
1:A:385:TYR:OH	6:A:701:DIF:H132	2.00	0.61
1:A:464:ASN:HD21	1:A:475:TYR:H	1.46	0.61
1:C:2112:ILE:HB	1:C:2357:PHE:CZ	2.35	0.61
1:D:3577:PHE:C	1:D:3577:PHE:CD2	2.73	0.61
1:B:1293:GLY:HA2	1:B:1299:MET:HE3	1.81	0.61
1:C:2243:LYS:HB3	1:C:2271:VAL:HG12	1.81	0.61
1:D:3344:VAL:O	1:D:3349:VAL:HG23	2.00	0.61
1:C:2362:ASP:OD1	1:C:2364:GLU:HG3	2.01	0.61
3:A:661:NAG:O7	3:A:661:NAG:H3	2.01	0.61
1:B:1050:THR:HG21	1:B:1056:LYS:HB3	1.83	0.61
1:C:2468:LYS:HD2	1:C:2474:PRO:HG3	1.82	0.61
1:A:293:GLY:HA2	1:A:299:MET:HE2	1.81	0.61
1:C:2094:THR:O	1:C:2356:HIS:CE1	2.54	0.61
1:A:51:GLY:C	1:B:1322:GLU:HG2	2.21	0.60
1:D:3076:THR:O	1:D:3080:LEU:HG	2.00	0.60
1:B:1152:LEU:HD12	1:B:1466:TYR:CE1	2.36	0.60
1:B:1173:ASP:HB3	1:B:1176:GLU:HB2	1.83	0.60
1:B:1184:ARG:NH1	1:B:1441:PRO:HG3	2.16	0.60
1:B:1574:GLY:O	1:B:1575:CYS:C	2.39	0.60
1:A:261:VAL:O	1:A:307:ARG:NH1	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2198:PHE:CZ	1:C:2352:LEU:CD1	2.84	0.60
2:E:3:NAG:O7	2:E:3:NAG:H3	2.01	0.60
1:B:1251:LYS:HG2	1:B:1310:ASN:CG	2.21	0.60
1:B:1468:LYS:HD2	1:B:1474:PRO:HG3	1.82	0.60
1:D:3130:TYR:HB3	1:D:3134:TYR:O	2.01	0.60
1:C:2550:PHE:CD1	1:C:2556:PHE:CD1	2.89	0.60
1:D:3173:ASP:HB3	1:D:3176:GLU:HB2	1.82	0.60
1:D:3510:GLU:OE1	1:D:3519:GLY:HA3	2.01	0.60
1:B:1137:LYS:HA	7:B:5175:HOH:O	2.01	0.60
1:D:3075:LEU:HA	1:D:3078:ILE:HD13	1.83	0.60
2:E:2:NAG:H4	2:E:3:NAG:N2	2.15	0.60
1:D:3226:HIS:CE1	1:D:3376:ARG:HD2	2.37	0.60
1:C:2040:PRO:HA	3:C:2661:NAG:H83	1.84	0.59
1:D:3342:LYS:HG2	1:D:3562:ALA:HB3	1.84	0.59
1:A:185:ARG:NH1	4:A:703:BOG:H4'1	2.16	0.59
1:B:1073:GLU:O	1:B:1077:ARG:HG3	2.02	0.59
1:A:129:THR:HG22	1:A:137:LYS:HD3	1.84	0.59
1:B:1362:ASP:OD1	1:B:1364:GLU:HG3	2.02	0.59
1:C:2129:THR:HG22	1:C:2137:LYS:HD3	1.83	0.59
1:D:3230:LEU:HD13	1:D:3233:ILE:HD12	1.85	0.59
1:D:3056:LYS:HG3	1:D:3057:CYS:N	2.17	0.59
1:B:1117:LEU:HD12	1:B:1531:LEU:HD22	1.85	0.59
1:B:1381:PHE:O	1:B:1384:LEU:HG	2.02	0.59
1:A:68:ASN:ND2	3:A:661:NAG:H61	2.16	0.59
1:B:1400:GLN:HG3	1:B:1402:TYR:OH	2.03	0.59
1:C:2261:VAL:O	1:C:2307:ARG:NH1	2.35	0.59
3:D:3661:NAG:O7	3:D:3661:NAG:C3	2.51	0.59
1:A:251:LYS:HG2	1:A:310:ASN:CG	2.23	0.59
1:D:3075:LEU:CD2	1:D:3079:LYS:HE3	2.32	0.59
1:D:3577:PHE:HE2	1:D:3583:GLN:HE21	1.51	0.59
1:C:2545:TRP:O	1:D:3061:ARG:NH2	2.36	0.59
1:D:3293:GLY:HA2	1:D:3299:MET:HE3	1.85	0.58
1:A:100:TRP:O	1:A:104:ASN:HB2	2.03	0.58
1:B:1117:LEU:CD1	1:B:1531:LEU:HD22	2.32	0.58
1:B:1034:ASN:HD22	1:B:1034:ASN:C	2.06	0.58
1:C:2251:LYS:HG2	1:C:2310:ASN:CG	2.23	0.58
1:D:3247:PHE:C	1:D:3248:LYS:HG2	2.22	0.58
1:A:131:ASN:ND2	1:A:134:TYR:H	2.00	0.58
1:B:1247:PHE:C	1:B:1248:LYS:HG2	2.24	0.58
1:D:3543:GLN:OE1	1:D:3543:GLN:HA	2.03	0.58
1:A:198:PHE:CZ	1:A:352:LEU:CD1	2.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2091:TYR:O	1:C:2095:HIS:HD2	1.86	0.58
1:B:1113:MET:CE	1:B:1116:VAL:HG21	2.33	0.58
1:B:1190:ASP:OD1	1:B:1517:ILE:HB	2.03	0.58
1:C:2075:LEU:CG	1:C:2079:LYS:HE3	2.34	0.58
1:C:2097:LYS:O	1:C:2097:LYS:HG3	2.02	0.58
1:D:3550:PHE:CD1	1:D:3556:PHE:CD1	2.92	0.58
1:B:1050:THR:HG21	1:B:1056:LYS:CB	2.34	0.57
1:B:1344:VAL:O	1:B:1349:VAL:HG23	2.03	0.57
1:C:2344:VAL:O	1:C:2349:VAL:HG23	2.04	0.57
1:D:3243:LYS:HB3	1:D:3271:VAL:HG12	1.85	0.57
1:A:90:HIS:CD2	1:A:513:ARG:HG2	2.40	0.57
1:C:2333:ARG:O	1:C:2337:ILE:HG13	2.04	0.57
1:B:1050:THR:CG2	1:B:1056:LYS:HB3	2.34	0.57
1:D:3050:THR:CG2	1:D:3056:LYS:HB3	2.34	0.57
1:B:1430:ILE:HD12	1:B:1582:VAL:CG2	2.35	0.57
1:D:3034:ASN:ND2	1:D:3036:CYS:H	2.03	0.57
2:G:2:NAG:H4	2:G:3:NAG:N2	2.19	0.57
1:B:1210:PHE:HB3	5:B:1601:HEM:HBD1	1.87	0.57
1:B:1510:GLU:OE1	1:B:1519:GLY:HA3	2.03	0.57
1:D:3333:ARG:O	1:D:3337:ILE:HG13	2.05	0.57
1:A:73:GLU:O	1:A:77:ARG:HG3	2.04	0.57
1:B:1112:ILE:HB	1:B:1357:PHE:CZ	2.40	0.57
1:D:3391:LEU:HD21	5:D:3601:HEM:HHC	1.85	0.57
1:C:2105(C):ILE:HG21	1:C:2108:LEU:HB2	1.82	0.57
1:A:75:LEU:HD11	1:A:79:LYS:HE3	1.86	0.57
1:D:3252:LEU:HD22	1:D:3309:HIS:CG	2.40	0.57
1:D:3400:GLN:HG3	1:D:3402:TYR:OH	2.04	0.57
1:C:2089:VAL:HG12	1:C:2093:LEU:CD2	2.35	0.57
1:D:3090:HIS:CD2	1:D:3513:ARG:HG2	2.39	0.57
1:D:3116:VAL:CG2	1:D:3117:LEU:N	2.68	0.57
1:A:482:THR:HG22	1:A:509:VAL:HG13	1.87	0.56
1:C:2061:ARG:NH1	1:D:3542:PRO:O	2.35	0.56
1:D:3173:ASP:O	1:D:3177:VAL:HG23	2.05	0.56
1:D:3184:ARG:HB2	1:D:3439:ASN:CA	2.32	0.56
1:A:444:VAL:O	1:A:444:VAL:CG1	2.52	0.56
1:B:1226:HIS:CE1	1:B:1376:ARG:HD2	2.39	0.56
1:B:1243:LYS:HB3	1:B:1271:VAL:HG12	1.86	0.56
1:C:2245:ARG:HH22	1:C:2326:GLU:HG2	1.70	0.56
1:C:2381:PHE:O	1:C:2384:LEU:HG	2.06	0.56
1:C:2543:GLN:O	1:D:3137:LYS:HE2	2.06	0.56
1:D:3387:TRP:O	1:D:3390:LEU:HB2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:3:NAG:O7	2:H:3:NAG:H3	2.05	0.56
1:A:211:LYS:HZ1	1:A:236:GLU:HG3	1.71	0.56
1:C:2447:VAL:HG13	5:C:2601:HEM:CBA	2.32	0.56
1:D:3203:GLN:NE2	1:D:3298:LEU:HD13	2.21	0.56
1:B:1387:TRP:O	1:B:1390:LEU:HB2	2.06	0.56
1:D:3142:PHE:O	1:D:3376:ARG:NH2	2.38	0.56
1:B:1118:THR:HG21	1:B:1369:GLN:HG2	1.88	0.56
1:D:3381:PHE:O	1:D:3384:LEU:HG	2.05	0.56
1:D:3269:THR:O	1:D:3270:GLN:HB2	2.06	0.56
1:A:387:TRP:O	1:A:390:LEU:HB2	2.06	0.56
1:B:1094:THR:O	1:B:1356:HIS:CE1	2.58	0.56
1:B:1116:VAL:CG2	1:B:1117:LEU:N	2.68	0.56
1:D:3152:LEU:HD12	1:D:3466:TYR:CE1	2.41	0.56
1:B:1388:HIS:N	1:B:1389:PRO:CD	2.68	0.56
1:C:2230:LEU:HG	1:C:2337:ILE:HG12	1.88	0.55
1:C:2090:HIS:CE1	1:C:2094:THR:HG21	2.41	0.55
1:C:2400:GLN:HG3	1:C:2402:TYR:OH	2.06	0.55
1:A:105(A):ILE:HD13	1:A:108:LEU:HD12	1.88	0.55
1:B:1543:GLN:OE1	1:B:1543:GLN:HA	2.07	0.55
1:C:2039:ASN:N	1:C:2040:PRO:HD3	2.21	0.55
1:C:2184:ARG:HB2	1:C:2439:ASN:CA	2.32	0.55
1:A:82:LEU:CD1	1:A:82:LEU:N	2.68	0.55
1:B:1398:GLU:HG3	1:B:1421:GLN:OE1	2.06	0.55
1:D:3238:LEU:HD22	1:D:3242:HIS:CE1	2.42	0.55
1:C:2398:GLU:HG3	1:C:2421:GLN:OE1	2.07	0.55
1:A:427:THR:CG2	1:A:583:GLN:HE22	2.18	0.55
1:C:2074:PHE:O	1:C:2077:ARG:HG3	2.06	0.55
1:C:2152:LEU:HD12	1:C:2466:TYR:CD1	2.42	0.55
1:B:1105(B):ILE:CD1	1:B:1108:LEU:HD12	2.32	0.55
1:B:1526:GLY:HA3	6:B:1701:DIF:C10	2.36	0.55
1:D:3145:LEU:HD13	7:D:5194:HOH:O	2.06	0.55
1:A:39:ASN:N	1:A:40:PRO:HD3	2.22	0.55
1:D:3100:TRP:HA	1:D:3100:TRP:CE3	2.42	0.55
1:D:3273:MET:SD	1:D:3290:GLU:HA	2.47	0.55
1:A:535:MET:HB2	7:A:5241:HOH:O	2.05	0.54
1:B:1203:GLN:NE2	1:B:1298:LEU:HD13	2.21	0.54
1:B:1252:LEU:HD22	1:B:1309:HIS:CG	2.41	0.54
1:C:2338:GLY:HA3	1:C:2559:ILE:HD13	1.89	0.54
1:D:3198:PHE:CZ	1:D:3352:LEU:CD1	2.89	0.54
1:C:2075:LEU:CD1	1:C:2079:LYS:HE3	2.38	0.54
1:B:1198:PHE:CZ	1:B:1352:LEU:CD1	2.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1564:ILE:O	1:B:1568:ILE:HD13	2.08	0.54
1:C:2090:HIS:HE1	1:C:2094:THR:HG21	1.73	0.54
1:C:2226:HIS:CE1	1:C:2376:ARG:HD2	2.42	0.54
1:A:543:GLN:O	1:B:1137:LYS:HE2	2.07	0.54
1:D:3269:THR:OG1	1:D:3271:VAL:HG13	2.07	0.54
1:B:1516:ALA:HB1	7:B:5157:HOH:O	2.07	0.54
1:A:322:GLU:HG2	1:B:1051:GLY:C	2.27	0.54
1:A:542:PRO:O	1:B:1061:ARG:NH1	2.33	0.54
1:B:1082:LEU:HD13	1:B:1082:LEU:H	1.72	0.54
1:D:3527:ALA:HB3	1:D:3528:PRO:HD3	1.88	0.54
1:A:568:ILE:HD13	1:A:578:THR:HG21	1.90	0.54
1:B:1105(B):ILE:HG22	1:B:1108:LEU:H	1.72	0.54
1:D:3034:ASN:HB3	1:D:3037:CYS:SG	2.48	0.54
1:A:34:ASN:HD21	1:A:36:CYS:HB2	1.71	0.54
1:C:2388:HIS:N	1:C:2389:PRO:CD	2.71	0.54
1:B:1391:LEU:HD21	5:B:1601:HEM:HHC	1.90	0.53
1:A:196:MET:CE	1:A:392:PRO:HD3	2.38	0.53
1:B:1093:LEU:HB3	1:B:1355:TYR:CD1	2.43	0.53
1:C:2510:GLU:OE1	1:C:2519:GLY:HA3	2.08	0.53
1:B:1129:THR:HG22	1:B:1137:LYS:HD3	1.90	0.53
1:A:173:ASP:HB3	1:A:176:GLU:HB2	1.90	0.53
1:B:1068:ASN:ND2	3:B:1661:NAG:H61	2.21	0.53
1:B:1131:ASN:ND2	1:B:1133:HIS:H	2.06	0.53
1:C:2034:ASN:HD22	1:C:2036:CYS:H	1.56	0.53
1:C:2077:ARG:O	1:C:2081:LEU:HD13	2.08	0.53
1:D:3261:VAL:O	1:D:3307:ARG:NH1	2.41	0.53
2:F:2:NAG:H4	2:F:3:NAG:N2	2.22	0.53
1:B:1131:ASN:ND2	1:B:1134:TYR:H	2.07	0.53
1:B:1342:LYS:HG2	1:B:1562:ALA:HB3	1.89	0.53
1:C:2113:MET:CA	1:C:2116:VAL:HG13	2.39	0.53
1:D:3131:ASN:ND2	1:D:3134:TYR:H	2.07	0.53
1:D:3185:ARG:NH1	4:D:3703:BOG:H4'1	2.23	0.53
1:D:3320:HIS:HA	1:D:3322:GLU:OE2	2.09	0.53
1:A:190:ASP:OD1	1:A:517:ILE:HB	2.08	0.53
1:C:2091:TYR:O	1:C:2095:HIS:CD2	2.62	0.53
1:B:1067:GLU:OE1	3:B:1661:NAG:H61	2.09	0.53
1:A:82:LEU:N	1:A:82:LEU:HD13	2.24	0.53
1:A:142:PHE:O	1:A:376:ARG:NH2	2.41	0.53
1:B:1553:GLU:OE1	1:B:1553:GLU:HA	2.09	0.53
1:C:2398:GLU:HG3	1:C:2421:GLN:CG	2.39	0.52
1:C:2444:VAL:O	1:C:2444:VAL:CG1	2.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3039:ASN:N	1:D:3040:PRO:CD	2.72	0.52
1:A:176:GLU:O	1:A:180:LYS:HG3	2.08	0.52
1:D:3190:ASP:OD1	1:D:3517:ILE:HB	2.09	0.52
1:A:344:VAL:O	1:A:349:VAL:HG23	2.09	0.52
1:A:380:GLU:HG2	1:A:466:TYR:CE1	2.44	0.52
1:C:2387:TRP:O	1:C:2390:LEU:HB2	2.09	0.52
1:C:2059:CYS:HB3	1:C:2064:PHE:O	2.10	0.52
1:A:241:GLN:O	1:A:245:ARG:HG3	2.10	0.52
1:A:398:GLU:HG3	1:A:421:GLN:CG	2.39	0.52
1:D:3108:LEU:O	1:D:3112:ILE:HG12	2.10	0.52
1:D:3444:VAL:O	1:D:3444:VAL:CG1	2.58	0.52
1:C:2090:HIS:CD2	1:C:2513:ARG:NH1	2.77	0.52
1:D:3034:ASN:O	1:D:3037:CYS:HB2	2.10	0.52
1:C:2102:ILE:HG22	1:C:2105(C):ILE:HD12	1.92	0.52
1:C:2128:PRO:HD3	7:C:5118:HOH:O	2.09	0.52
1:C:2131:ASN:ND2	1:C:2133:HIS:H	2.08	0.52
1:C:2380:GLU:HG2	1:C:2466:TYR:CE1	2.45	0.52
1:C:2550:PHE:CD1	1:C:2556:PHE:HD1	2.28	0.52
1:D:3075:LEU:HD21	1:D:3079:LYS:HE3	1.90	0.52
1:A:532:LYS:O	1:A:532:LYS:HD3	2.10	0.51
1:B:1340:THR:O	1:B:1344:VAL:HG23	2.10	0.51
1:C:2340:THR:O	1:C:2344:VAL:HG23	2.10	0.51
1:A:269:THR:O	1:A:270:GLN:HB2	2.09	0.51
1:A:413:ILE:O	1:A:416:GLU:HB3	2.11	0.51
1:B:1184:ARG:HB2	1:B:1439:ASN:CA	2.32	0.51
1:B:1398:GLU:HG3	1:B:1421:GLN:CG	2.40	0.51
1:B:1444:VAL:O	1:B:1444:VAL:CG1	2.58	0.51
1:D:3526:GLY:HA3	6:D:3701:DIF:C10	2.39	0.51
1:D:3058:ASP:OD1	1:D:3060:THR:OG1	2.18	0.51
1:A:90:HIS:HD2	1:A:513:ARG:HG2	1.76	0.51
1:B:1238:LEU:HD22	1:B:1242:HIS:CE1	2.46	0.51
1:D:3241:GLN:HE21	1:D:3245:ARG:HD3	1.75	0.51
1:D:3550:PHE:CD1	1:D:3556:PHE:HD1	2.28	0.51
1:A:75:LEU:CG	1:A:79:LYS:HE3	2.41	0.51
1:A:105(A):ILE:HG22	1:A:105(A):ILE:O	2.11	0.51
1:A:112:ILE:O	1:A:115:TYR:HB3	2.10	0.51
1:B:1131:ASN:C	1:B:1131:ASN:ND2	2.63	0.51
1:C:2442:ILE:O	1:C:2445:GLN:HG2	2.11	0.51
1:D:3137:LYS:HA	7:D:5223:HOH:O	2.10	0.51
1:D:3511:LYS:HG3	7:D:5134:HOH:O	2.10	0.51
1:A:333:ARG:O	1:A:337:ILE:HG13	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1550:PHE:CD1	1:B:1556:PHE:CD1	2.99	0.51
1:D:3251:LYS:HG2	1:D:3310:ASN:CG	2.32	0.51
1:A:122:TYR:CZ	1:A:123:LEU:HD22	2.46	0.51
1:A:292:PHE:O	1:A:299:MET:CE	2.58	0.51
1:A:400:GLN:HG3	1:A:402:TYR:OH	2.11	0.51
1:C:2203:GLN:NE2	1:C:2298:LEU:HD13	2.26	0.51
1:A:464:ASN:HD22	1:A:467:ARG:HD3	1.76	0.50
1:A:527:ALA:HB3	1:A:528:PRO:HD3	1.92	0.50
1:B:1034:ASN:HD21	1:B:1036:CYS:HB2	1.74	0.50
1:B:1307:ARG:HB3	1:B:1571:ASN:OD1	2.10	0.50
1:B:1495:TYR:O	1:B:1496:SER:HB2	2.11	0.50
1:C:2433:ARG:HD3	7:C:5051:HOH:O	2.11	0.50
1:D:3116:VAL:HG23	1:D:3117:LEU:N	2.25	0.50
1:B:1382:ASN:O	1:B:1386:HIS:HD2	1.93	0.50
1:C:2391:LEU:HD21	5:C:2601:HEM:HHC	1.92	0.50
1:D:3241:GLN:O	1:D:3245:ARG:HG3	2.11	0.50
1:C:2320:HIS:HA	1:C:2322:GLU:OE2	2.11	0.50
1:A:293:GLY:HA2	1:A:299:MET:HE3	1.93	0.50
1:A:382:ASN:O	1:A:386:HIS:HD2	1.95	0.50
2:G:3:NAG:O7	2:G:3:NAG:H3	2.11	0.50
1:A:417:HIS:HB3	1:A:421:GLN:HG2	1.94	0.50
1:B:1181:VAL:CG1	1:B:1487:MET:HG2	2.35	0.50
1:C:2131:ASN:C	1:C:2131:ASN:ND2	2.64	0.50
1:C:2382:ASN:O	1:C:2386:HIS:HD2	1.94	0.50
1:D:3388:HIS:N	1:D:3389:PRO:CD	2.75	0.50
1:A:398:GLU:HG3	1:A:421:GLN:OE1	2.12	0.50
1:C:2500:VAL:HG12	1:C:2500:VAL:O	2.12	0.50
1:B:1241:GLN:HE21	1:B:1245:ARG:HH11	1.60	0.50
1:A:118:THR:HG21	1:A:369:GLN:HG2	1.94	0.50
1:B:1067:GLU:OE1	3:B:1661:NAG:C6	2.59	0.50
1:B:1338:GLY:HA3	1:B:1559:ILE:HD13	1.94	0.50
1:B:1495:TYR:O	1:B:1496:SER:CB	2.59	0.50
1:C:2550:PHE:CE1	1:C:2556:PHE:CE1	3.00	0.50
1:D:3118:THR:HG21	1:D:3369:GLN:HG2	1.94	0.50
1:D:3495:TYR:O	1:D:3496:SER:HB2	2.12	0.50
1:D:3532:LYS:O	1:D:3532:LYS:HD3	2.11	0.50
1:A:105(A):ILE:HG21	1:A:108:LEU:HB2	1.89	0.50
1:A:543:GLN:HB2	7:B:5259:HOH:O	2.11	0.50
1:B:1116:VAL:HG22	1:B:1117:LEU:N	2.27	0.50
1:B:1163:MET:HE3	1:B:1171:LEU:HD21	1.89	0.49
1:C:2269:THR:O	1:C:2270:GLN:HB2	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3033:ALA:O	1:D:3035:PRO:HD3	2.12	0.49
1:A:196:MET:HE1	1:A:392:PRO:HD3	1.93	0.49
1:A:388:HIS:N	1:A:389:PRO:CD	2.74	0.49
1:A:532:LYS:HD3	1:A:532:LYS:C	2.33	0.49
1:B:1308:GLU:OE1	1:B:1311:ARG:NH1	2.44	0.49
1:D:3091:TYR:CD1	1:D:3095:HIS:CD2	3.00	0.49
1:D:3312:VAL:HA	1:D:3315:ILE:HD12	1.94	0.49
1:D:3464:ASN:ND2	1:D:3475:TYR:H	2.09	0.49
1:B:1273:MET:SD	1:B:1290:GLU:HA	2.53	0.49
1:B:1320:HIS:HA	1:B:1322:GLU:OE2	2.12	0.49
1:B:1532:LYS:O	1:B:1532:LYS:HD3	2.12	0.49
1:D:3577:PHE:HE2	1:D:3583:GLN:NE2	2.09	0.49
1:C:2061:ARG:NH2	1:D:3545:TRP:O	2.43	0.49
1:C:2082:LEU:N	1:C:2082:LEU:CD1	2.75	0.49
1:C:2113:MET:HA	1:C:2116:VAL:CG1	2.41	0.49
1:C:2252:LEU:HD22	1:C:2309:HIS:CD2	2.47	0.49
1:D:3082:LEU:N	1:D:3082:LEU:CD1	2.75	0.49
1:D:3398:GLU:HG3	1:D:3421:GLN:OE1	2.12	0.49
1:A:34:ASN:ND2	1:A:36:CYS:HB2	2.27	0.49
1:A:68:ASN:ND2	3:A:661:NAG:C6	2.75	0.49
1:A:184:ARG:HB2	1:A:439:ASN:CA	2.36	0.49
1:B:1114:LYS:HE2	1:B:1365:LEU:O	2.13	0.49
1:B:1112:ILE:O	1:B:1116:VAL:HG13	2.12	0.49
1:B:1246:LEU:O	1:B:1247:PHE:HB2	2.11	0.49
1:B:1269:THR:O	1:B:1270:GLN:HB2	2.12	0.49
1:C:2088:THR:O	1:C:2091:TYR:HB3	2.13	0.49
1:D:3131:ASN:ND2	1:D:3133:HIS:H	2.11	0.49
1:D:3495:TYR:O	1:D:3496:SER:CB	2.60	0.49
1:A:550:PHE:CD1	1:A:556:PHE:CD1	3.00	0.49
1:B:1033:ALA:HB3	1:B:1158:ASP:OD2	2.12	0.49
1:B:1261:VAL:O	1:B:1307:ARG:NH1	2.43	0.49
1:C:2056:LYS:HG3	1:C:2057:CYS:N	2.27	0.49
1:D:3246:LEU:O	1:D:3247:PHE:HB2	2.12	0.49
1:D:3417:HIS:HB3	1:D:3421:GLN:HG2	1.95	0.49
1:D:3442:ILE:HD11	4:D:3703:BOG:H5'1	1.95	0.49
1:B:1108:LEU:O	1:B:1112:ILE:HG12	2.13	0.49
1:C:2060:THR:HG21	1:D:3546:LYS:HB3	1.95	0.49
1:A:131:ASN:HD22	1:A:134:TYR:H	1.60	0.49
1:C:2384:LEU:C	1:C:2384:LEU:HD12	2.33	0.49
1:D:3553:GLU:OE1	1:D:3553:GLU:HA	2.12	0.49
1:A:468:LYS:HD2	1:A:474:PRO:CG	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:525:LEU:O	1:A:528:PRO:HD2	2.13	0.49
1:A:338:GLY:HA3	1:A:559:ILE:HD13	1.95	0.48
2:H:2:NAG:H4	2:H:3:NAG:N2	2.28	0.48
1:A:100:TRP:HA	1:A:100:TRP:CE3	2.48	0.48
1:B:1068:ASN:O	1:B:1069:CYS:HB2	2.13	0.48
1:B:1298:LEU:HD13	7:B:5268:HOH:O	2.11	0.48
1:B:1414:LEU:HD11	1:B:1419:LEU:HD22	1.95	0.48
1:C:2067:GLU:OE1	3:C:2661:NAG:H61	2.12	0.48
1:D:3181:VAL:HG21	1:D:3491:LEU:HD21	1.94	0.48
1:A:545:TRP:O	1:B:1061:ARG:NH2	2.41	0.48
1:B:1468:LYS:HD2	1:B:1474:PRO:CG	2.44	0.48
1:B:1564:ILE:HD12	1:B:1567:LEU:HD23	1.96	0.48
1:C:2413:ILE:O	1:C:2416:GLU:HB3	2.13	0.48
1:A:75:LEU:CD1	1:A:79:LYS:HE3	2.43	0.48
1:A:433:ARG:NH2	1:A:516:ALA:O	2.45	0.48
1:D:3338:GLY:HA3	1:D:3559:ILE:HD13	1.96	0.48
1:C:2211:LYS:HZ1	1:C:2236:GLU:HG3	1.77	0.48
1:D:3413:ILE:O	1:D:3416:GLU:HB3	2.13	0.48
1:B:1417:HIS:HB3	1:B:1421:GLN:HG2	1.95	0.48
1:C:2246:LEU:O	1:C:2247:PHE:HB2	2.13	0.48
1:C:2308:GLU:OE1	1:C:2311:ARG:NH1	2.47	0.48
1:C:2417:HIS:HB3	1:C:2421:GLN:HG2	1.94	0.48
1:B:1070:THR:O	1:B:1072:PRO:HD3	2.14	0.48
1:C:2190:ASP:OD1	1:C:2517:ILE:HB	2.13	0.48
1:A:308:GLU:OE1	1:A:311:ARG:NH1	2.47	0.48
1:B:1034:ASN:O	1:B:1037:CYS:HB2	2.14	0.48
1:B:1064:PHE:CD1	1:B:1064:PHE:N	2.81	0.48
1:D:3532:LYS:HE3	7:D:5260:HOH:O	2.14	0.48
1:B:1173:ASP:O	1:B:1177:VAL:HG23	2.14	0.48
1:A:384:LEU:C	1:A:384:LEU:HD12	2.34	0.48
1:B:1312:VAL:HA	1:B:1315:ILE:HD12	1.96	0.48
1:C:2193:GLY:O	1:C:2582:VAL:HG23	2.14	0.48
1:C:2238:LEU:HD22	1:C:2242:HIS:CE1	2.49	0.48
1:A:238:LEU:HD22	1:A:242:HIS:CE1	2.49	0.47
1:A:423:VAL:HG11	1:A:568:ILE:HG21	1.96	0.47
1:C:2430:ILE:HG13	1:C:2431:ALA:N	2.29	0.47
1:B:1333:ARG:O	1:B:1337:ILE:HG13	2.14	0.47
1:C:2252:LEU:HD22	1:C:2309:HIS:CG	2.49	0.47
1:A:190:ASP:OD2	1:A:192:GLN:HB2	2.14	0.47
1:D:3100:TRP:CD1	1:D:3356:HIS:HB2	2.49	0.47
1:D:3113:MET:CE	1:D:3116:VAL:HG21	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:566:SER:O	1:A:570:ASN:ND2	2.48	0.47
1:B:1206:THR:HG21	1:B:1385:TYR:CD2	2.49	0.47
1:B:1427:THR:CG2	1:B:1583:GLN:HE22	2.21	0.47
1:D:3382:ASN:O	1:D:3386:HIS:HD2	1.97	0.47
1:B:1241:GLN:HE21	1:B:1245:ARG:CD	2.28	0.47
1:A:131:ASN:ND2	1:A:134:TYR:N	2.62	0.47
1:D:3043:ASN:O	1:D:3044:ARG:CB	2.63	0.47
1:D:3075:LEU:CD1	1:D:3079:LYS:HE3	2.45	0.47
1:D:3156:ALA:HB3	1:D:3159:CYS:SG	2.55	0.47
1:D:3176:GLU:O	1:D:3180:LYS:HG3	2.13	0.47
1:D:3184:ARG:NH1	1:D:3441:PRO:HG3	2.28	0.47
1:A:43:ASN:O	1:A:44:ARG:HB2	2.14	0.47
1:B:1294:LEU:CD2	1:B:1409:TYR:CD2	2.80	0.47
1:C:2108:LEU:HD23	1:C:2108:LEU:HA	1.63	0.47
1:C:2122:TYR:CZ	1:C:2123:LEU:HD22	2.49	0.47
1:D:3468:LYS:HD2	1:D:3474:PRO:CG	2.45	0.47
1:A:526:GLY:HA3	6:A:701:DIF:H10	1.97	0.47
1:B:1190:ASP:OD2	1:B:1192:GLN:HB2	2.14	0.47
1:B:1202:ALA:HB2	1:B:1348:TYR:CE1	2.49	0.47
1:C:2436:GLY:HA3	7:C:5051:HOH:O	2.15	0.47
1:D:3532:LYS:HD3	1:D:3532:LYS:C	2.35	0.47
1:D:3550:PHE:CE1	1:D:3556:PHE:CE1	3.03	0.47
1:A:577:PHE:CD2	1:A:577:PHE:C	2.88	0.46
1:B:1241:GLN:HE21	1:B:1245:ARG:HD3	1.79	0.46
1:C:2050:THR:CG2	1:C:2056:LYS:HB3	2.43	0.46
1:A:500:VAL:HG12	1:A:500:VAL:O	2.15	0.46
1:C:2124:ILE:HG21	1:C:2532:LYS:HG3	1.97	0.46
1:B:1298:LEU:HD12	1:B:1298:LEU:HA	1.78	0.46
1:B:1525:LEU:N	1:B:1525:LEU:HD23	2.30	0.46
1:D:3040:PRO:HA	3:D:3661:NAG:H83	1.96	0.46
1:D:3068:ASN:ND2	3:D:3661:NAG:H61	2.31	0.46
1:A:131:ASN:C	1:A:131:ASN:ND2	2.67	0.46
1:A:401:GLU:HG3	7:A:5314:HOH:O	2.15	0.46
1:B:1089:VAL:HG12	1:B:1093:LEU:CD2	2.45	0.46
1:B:1202:ALA:CB	1:B:1348:TYR:OH	2.63	0.46
1:C:2093:LEU:HB3	1:C:2355:TYR:CD1	2.50	0.46
1:C:2525:LEU:O	1:C:2528:PRO:HD2	2.16	0.46
1:D:3129:THR:HG22	1:D:3137:LYS:HD3	1.97	0.46
2:E:2:NAG:H4	2:E:3:NAG:HN2	1.80	0.46
1:A:91:TYR:O	1:A:95:HIS:HD2	1.98	0.46
1:A:113:MET:HA	1:A:116:VAL:HG13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2073:GLU:O	1:C:2076:THR:HB	2.16	0.46
1:A:34:ASN:HB3	1:A:37:CYS:SG	2.56	0.46
1:B:1184:ARG:HH12	1:B:1441:PRO:HG3	1.81	0.46
1:B:1532:LYS:HD3	1:B:1532:LYS:C	2.36	0.46
1:C:2202:ALA:CB	1:C:2348:TYR:OH	2.63	0.46
1:D:3211:LYS:HE2	1:D:3223:GLY:CA	2.46	0.46
1:A:238:LEU:HD23	1:A:238:LEU:HA	1.77	0.46
1:A:252:LEU:HD22	1:A:309:HIS:CG	2.50	0.46
1:A:292:PHE:O	1:A:299:MET:HE2	2.16	0.46
1:A:428:ARG:HG3	7:A:5286:HOH:O	2.15	0.46
1:A:320:HIS:HA	1:A:322:GLU:OE2	2.15	0.46
1:B:1075:LEU:HD11	1:B:1079:LYS:CE	2.44	0.46
1:C:2090:HIS:HD2	1:C:2513:ARG:NH1	2.13	0.46
1:C:2387:TRP:HB2	5:C:2601:HEM:HAC	1.98	0.46
1:C:2464:ASN:HD22	1:C:2467:ARG:HD3	1.81	0.46
1:C:2532:LYS:O	1:C:2532:LYS:HD3	2.15	0.46
1:D:3185:ARG:HH11	4:D:3703:BOG:H4'1	1.81	0.46
1:D:3442:ILE:O	1:D:3445:GLN:HG2	2.15	0.46
1:D:3500:VAL:O	1:D:3500:VAL:HG12	2.16	0.46
1:A:75:LEU:HG	1:A:79:LYS:HE3	1.98	0.46
1:A:77:ARG:O	1:A:81:LEU:HD13	2.16	0.46
1:C:2532:LYS:HD3	1:C:2532:LYS:C	2.36	0.46
1:D:3093:LEU:HB3	1:D:3355:TYR:CD1	2.50	0.46
1:D:3241:GLN:HE21	1:D:3245:ARG:CD	2.29	0.46
1:D:3280:PRO:HG2	1:D:3283:LEU:HB2	1.97	0.46
1:D:3308:GLU:OE1	1:D:3311:ARG:NH1	2.49	0.46
1:A:118:THR:CG2	1:A:369:GLN:HG2	2.46	0.46
1:B:1550:PHE:O	1:B:1555:GLY:HA3	2.16	0.46
1:D:3073:GLU:O	1:D:3076:THR:HB	2.15	0.46
1:D:3550:PHE:O	1:D:3555:GLY:HA3	2.16	0.46
1:C:2468:LYS:HD2	1:C:2474:PRO:CG	2.46	0.45
1:D:3435:ALA:O	1:D:3510:GLU:O	2.33	0.45
1:A:64:PHE:CB	1:A:69:CYS:O	2.64	0.45
1:A:442:ILE:HG23	4:A:703:BOG:H61	1.98	0.45
1:B:1447:VAL:HG13	5:B:1601:HEM:CBA	2.37	0.45
1:D:3202:ALA:HB2	1:D:3348:TYR:CE1	2.52	0.45
1:B:1074:PHE:O	1:B:1077:ARG:HG3	2.16	0.45
1:B:1292:PHE:O	1:B:1299:MET:CE	2.63	0.45
1:B:1419:LEU:HB2	7:B:5247:HOH:O	2.16	0.45
1:B:1454:GLN:O	1:B:1458:MET:HG3	2.15	0.45
1:C:2527:ALA:HB3	1:C:2528:PRO:HD3	1.96	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3126:SER:HA	1:D:3127:PRO:C	2.36	0.45
1:A:173:ASP:O	1:A:177:VAL:HG23	2.16	0.45
1:B:1105(B):ILE:HG22	1:B:1108:LEU:HB2	1.94	0.45
1:B:1442:ILE:O	1:B:1445:GLN:HG2	2.15	0.45
1:C:2068:ASN:ND2	3:C:2661:NAG:C6	2.79	0.45
1:C:2202:ALA:HB2	1:C:2348:TYR:CE1	2.52	0.45
1:C:2433:ARG:NH2	1:C:2516:ALA:O	2.49	0.45
1:A:553:GLU:HA	1:A:553:GLU:OE1	2.17	0.45
1:B:1527:ALA:HB3	1:B:1528:PRO:HD3	1.98	0.45
1:C:2232:HIS:CE1	7:C:5038:HOH:O	2.69	0.45
1:D:3094:THR:O	1:D:3356:HIS:CE1	2.70	0.45
1:D:3132:VAL:HG13	1:D:3133:HIS:CD2	2.51	0.45
1:B:1196:MET:HG2	1:B:1429:GLN:HG2	1.98	0.45
1:B:1413:ILE:O	1:B:1416:GLU:HB3	2.17	0.45
1:C:2197:MET:O	1:C:2201:PHE:HB2	2.17	0.45
1:B:1444:VAL:HG22	1:B:1447:VAL:HG21	1.98	0.45
1:D:3064:PHE:N	1:D:3064:PHE:CD1	2.85	0.45
1:D:3267:LYS:O	1:D:3267:LYS:HG3	2.17	0.45
1:C:2075:LEU:HG	1:C:2079:LYS:HE3	1.98	0.45
1:C:2198:PHE:HZ	1:C:2352:LEU:CD1	2.28	0.45
1:D:3241:GLN:HE21	1:D:3245:ARG:HH11	1.64	0.45
1:D:3398:GLU:HG3	1:D:3421:GLN:CG	2.47	0.45
1:A:294:LEU:CD2	1:A:409:TYR:CD2	2.71	0.45
1:A:391:LEU:HD21	5:A:704:HEM:HHC	1.99	0.45
1:C:2067:GLU:OE1	3:C:2661:NAG:C6	2.64	0.45
1:A:92:ILE:HA	1:A:96:PHE:HE1	1.82	0.45
1:A:252:LEU:HD22	1:A:309:HIS:CD2	2.51	0.45
1:A:381:PHE:O	1:A:384:LEU:HG	2.16	0.45
1:A:542:PRO:HD2	7:B:5184:HOH:O	2.16	0.45
1:C:2034:ASN:ND2	1:C:2034:ASN:C	2.69	0.45
1:D:3091:TYR:CE1	1:D:3095:HIS:CD2	3.05	0.45
1:B:1408:LEU:N	1:B:1408:LEU:HD23	2.32	0.44
1:D:3113:MET:HE3	1:D:3116:VAL:HG21	1.99	0.44
1:A:65:TYR:O	1:A:71:THR:HB	2.17	0.44
1:A:197:MET:O	1:A:201:PHE:HB2	2.16	0.44
1:B:1075:LEU:HD21	1:B:1079:LYS:HE3	2.00	0.44
1:D:3433:ARG:NH2	1:D:3516:ALA:O	2.50	0.44
1:C:2181:VAL:CG1	1:C:2487:MET:HG2	2.39	0.44
1:C:2273:MET:SD	1:C:2290:GLU:HA	2.58	0.44
1:C:2315:ILE:O	1:C:2318:GLN:HB3	2.17	0.44
1:D:3034:ASN:HD22	1:D:3034:ASN:C	2.21	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:TYR:CD1	1:A:122:TYR:C	2.90	0.44
1:C:2090:HIS:HD2	1:C:2513:ARG:CZ	2.30	0.44
1:C:2553:GLU:OE1	1:C:2553:GLU:HA	2.17	0.44
1:D:3415:LEU:HD23	1:D:3415:LEU:HA	1.83	0.44
1:A:246:LEU:O	1:A:247:PHE:HB2	2.18	0.44
1:C:2046:GLU:O	1:C:2057:CYS:HA	2.16	0.44
1:A:102:ILE:HG22	1:A:105(A):ILE:CD1	2.47	0.44
1:B:1156:ALA:HB3	1:B:1159:CYS:SG	2.57	0.44
1:B:1583:GLN:CD	1:B:1583:GLN:H	2.21	0.44
1:C:2118:THR:CG2	1:C:2369:GLN:HG2	2.46	0.44
1:C:2292:PHE:O	1:C:2299:MET:CE	2.65	0.44
1:B:1280:PRO:HG2	1:B:1283:LEU:HB2	1.99	0.44
1:C:2211:LYS:HE2	1:C:2223:GLY:CA	2.48	0.44
1:C:2477:SER:HB2	7:C:5245:HOH:O	2.18	0.44
1:A:152:LEU:HD12	1:A:466:TYR:CD1	2.51	0.44
1:C:2525:LEU:N	1:C:2525:LEU:HD23	2.33	0.44
1:D:3122:TYR:CZ	1:D:3123:LEU:HD22	2.52	0.44
1:D:3203:GLN:HB2	5:D:3601:HEM:HMC3	2.00	0.44
1:B:1464:ASN:HD22	1:B:1467:ARG:HD3	1.82	0.44
6:B:1701:DIF:CL2	6:B:1701:DIF:C9	3.03	0.44
1:C:2076:THR:O	1:C:2080:LEU:HG	2.17	0.44
1:C:2385:TYR:CE1	6:C:2701:DIF:H12	2.53	0.44
1:D:3172:PRO:CG	1:D:3495:TYR:CE2	3.01	0.44
1:D:3211:LYS:HZ1	1:D:3236:GLU:HG3	1.83	0.44
1:D:3454:GLN:O	1:D:3458:MET:HG3	2.18	0.44
1:A:198:PHE:HZ	1:A:352:LEU:CD1	2.29	0.43
1:A:211:LYS:HE2	1:A:223:GLY:CA	2.48	0.43
1:A:500:VAL:O	1:A:500:VAL:CG1	2.66	0.43
1:B:1122:TYR:CD1	1:B:1122:TYR:C	2.91	0.43
1:C:2033:ALA:O	1:C:2035:PRO:HD3	2.18	0.43
1:C:2180:LYS:HD3	1:C:2490:GLU:OE1	2.18	0.43
1:D:3202:ALA:HB2	1:D:3348:TYR:HE1	1.83	0.43
1:C:2196:MET:CE	1:C:2392:PRO:HD3	2.48	0.43
1:C:2435:ALA:O	1:C:2510:GLU:O	2.36	0.43
1:D:3196:MET:CE	1:D:3392:PRO:HD3	2.48	0.43
1:A:400:GLN:HB2	1:A:402:TYR:CE2	2.53	0.43
1:A:464:ASN:ND2	1:A:467:ARG:HD3	2.33	0.43
1:B:1283:LEU:HD23	1:B:1283:LEU:HA	1.88	0.43
1:C:2112:ILE:O	1:C:2116:VAL:HG13	2.18	0.43
1:C:2400:GLN:HB2	1:C:2402:TYR:CE2	2.52	0.43
1:D:3190:ASP:OD2	1:D:3192:GLN:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1196:MET:HE1	1:B:1392:PRO:HD3	1.99	0.43
1:B:1203:GLN:HB2	5:B:1601:HEM:CMC	2.49	0.43
1:C:2131:ASN:HD22	1:C:2134:TYR:H	1.64	0.43
1:C:2255:GLN:NE2	1:C:2263:PRO:O	2.42	0.43
1:C:2398:GLU:HB3	1:C:2399:ASP:H	1.44	0.43
1:A:430:ILE:HG13	1:A:431:ALA:N	2.34	0.43
1:A:435:ALA:O	1:A:510:GLU:O	2.36	0.43
1:A:444:VAL:HG22	1:A:447:VAL:HG21	1.99	0.43
1:B:1400:GLN:HB2	1:B:1402:TYR:CE2	2.54	0.43
1:B:1464:ASN:HD22	1:B:1464:ASN:HA	1.58	0.43
1:C:2152:LEU:HD12	1:C:2466:TYR:CE1	2.53	0.43
1:A:185:ARG:HD3	4:A:703:BOG:H5'2	2.00	0.43
1:A:280:PRO:HG2	1:A:283:LEU:HB2	2.00	0.43
1:B:1245:ARG:HH22	1:B:1326:GLU:HG2	1.83	0.43
1:C:2082:LEU:N	1:C:2082:LEU:HD13	2.33	0.43
1:D:3206:THR:CG2	1:D:3385:TYR:CE2	2.97	0.43
1:A:280:PRO:HG2	1:A:283:LEU:HD12	2.00	0.43
1:A:387:TRP:C	1:A:389:PRO:HD2	2.39	0.43
1:A:495:TYR:O	1:A:496:SER:CB	2.67	0.43
1:B:1398:GLU:HB3	1:B:1399:ASP:H	1.46	0.43
1:C:2172:PRO:CG	1:C:2495:TYR:CE2	3.01	0.43
1:D:3090:HIS:HD2	1:D:3513:ARG:HG2	1.80	0.43
1:D:3444:VAL:HG22	1:D:3447:VAL:HG21	2.00	0.43
1:A:91:TYR:CE1	1:A:95:HIS:CD2	3.07	0.43
1:A:132:VAL:HG13	1:A:133:HIS:CD2	2.54	0.43
1:A:273:MET:SD	1:A:290:GLU:HA	2.58	0.43
1:A:292:PHE:O	1:A:299:MET:HE1	2.19	0.43
1:A:564:ILE:HG22	7:A:5064:HOH:O	2.18	0.43
1:B:1181:VAL:HG21	1:B:1491:LEU:HD21	2.00	0.43
1:B:1435:ALA:O	1:B:1510:GLU:O	2.36	0.43
1:C:2034:ASN:HA	1:C:2035:PRO:HD2	1.89	0.43
1:C:2181:VAL:HG21	1:C:2491:LEU:HD21	2.00	0.43
1:D:3390:LEU:HB2	7:D:5235:HOH:O	2.18	0.43
1:D:3492:LYS:O	1:D:3492:LYS:HG3	2.19	0.43
1:A:105(A):ILE:CB	1:A:108:LEU:HB2	2.47	0.43
1:A:131:ASN:ND2	1:A:133:HIS:H	2.16	0.43
1:A:276:PRO:HG2	1:A:279:ILE:HG12	2.01	0.43
1:A:415:LEU:HD23	1:A:415:LEU:HA	1.85	0.43
1:B:1047:CYS:HB2	7:B:5007:HOH:O	2.19	0.43
1:B:1126:SER:HA	1:B:1127:PRO:C	2.39	0.43
1:C:2131:ASN:ND2	1:C:2134:TYR:N	2.64	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2415:LEU:HD23	1:C:2415:LEU:HA	1.82	0.43
1:C:2500:VAL:O	1:C:2500:VAL:CG1	2.66	0.43
1:D:3112:ILE:O	1:D:3115:TYR:N	2.52	0.43
1:D:3113:MET:HG3	1:D:3117:LEU:HD22	2.00	0.43
1:D:3198:PHE:HZ	1:D:3352:LEU:CD1	2.31	0.43
1:D:3583:GLN:CD	1:D:3583:GLN:H	2.21	0.43
1:C:2039:ASN:N	1:C:2040:PRO:CD	2.81	0.43
1:C:2495:TYR:O	1:C:2496:SER:HB2	2.19	0.43
1:D:3464:ASN:HD22	1:D:3467:ARG:HD3	1.84	0.43
4:D:3703:BOG:O1	4:D:3703:BOG:O5	2.36	0.43
1:B:1090:HIS:HE1	1:B:1094:THR:HG21	1.81	0.42
1:B:1241:GLN:O	1:B:1245:ARG:HG3	2.19	0.42
1:C:2202:ALA:HB2	1:C:2348:TYR:HE1	1.84	0.42
1:C:2414:LEU:HD11	1:C:2419:LEU:HD22	2.01	0.42
1:D:3238:LEU:HD23	1:D:3238:LEU:HA	1.85	0.42
2:H:1:NAG:H61	2:H:2:NAG:O7	2.18	0.42
1:A:91:TYR:CD1	1:A:95:HIS:CD2	3.07	0.42
1:A:565:GLN:O	1:A:569:CYS:HB2	2.19	0.42
1:B:1079:LYS:O	1:B:1083:LYS:HB2	2.19	0.42
1:B:1430:ILE:HG13	1:B:1431:ALA:N	2.34	0.42
1:D:3050:THR:HG21	1:D:3056:LYS:CB	2.48	0.42
1:A:77:ARG:HG3	1:A:77:ARG:H	1.62	0.42
1:B:1320:HIS:HB3	1:B:1323:TRP:CG	2.55	0.42
1:C:2105(C):ILE:CG2	1:C:2108:LEU:CB	2.77	0.42
1:C:2509:VAL:HG13	1:C:2509:VAL:O	2.19	0.42
1:A:105(A):ILE:O	1:A:108:LEU:N	2.51	0.42
1:D:3131:ASN:C	1:D:3131:ASN:ND2	2.65	0.42
1:B:1248:LYS:O	1:B:1249:ASP:HB2	2.18	0.42
1:B:1500:VAL:HG12	1:B:1500:VAL:O	2.18	0.42
1:C:2102:ILE:O	1:C:2103:VAL:C	2.58	0.42
1:A:64:PHE:HB2	1:A:69:CYS:O	2.20	0.42
1:A:126:SER:HA	1:A:127:PRO:C	2.39	0.42
1:A:132:VAL:HB	7:A:5078:HOH:O	2.20	0.42
1:A:525:LEU:N	1:A:525:LEU:HD23	2.34	0.42
1:B:1176:GLU:O	1:B:1180:LYS:HG3	2.20	0.42
1:C:2316:LEU:HD23	1:C:2316:LEU:HA	1.91	0.42
1:D:3298:LEU:HD12	1:D:3298:LEU:HA	1.74	0.42
1:A:61:ARG:NH2	1:B:1545:TRP:O	2.46	0.42
1:A:408:LEU:N	1:A:408:LEU:HD23	2.34	0.42
1:B:1078:ILE:HD12	1:B:1078:ILE:N	2.35	0.42
1:B:1197:MET:O	1:B:1201:PHE:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2454:GLN:HE21	1:C:2454:GLN:HB2	1.64	0.42
1:A:95:HIS:O	1:A:100:TRP:CD1	2.73	0.42
1:A:181:VAL:HG21	1:A:491:LEU:HD21	2.00	0.42
1:A:312:VAL:HA	1:A:315:ILE:HD12	2.02	0.42
1:B:1359:LEU:HD23	1:B:1359:LEU:HA	1.83	0.42
1:D:3113:MET:O	1:D:3117:LEU:HD22	2.20	0.42
1:D:3579:SER:OG	1:D:3580:PHE:N	2.53	0.42
1:A:47:CYS:HB2	7:A:5294:HOH:O	2.19	0.42
1:A:352:LEU:HD12	1:A:352:LEU:HA	1.87	0.42
3:A:661:NAG:O7	3:A:661:NAG:C3	2.66	0.42
1:B:1300:MET:HG2	1:B:1419:LEU:HD11	2.02	0.42
1:C:2113:MET:O	1:C:2117:LEU:CD2	2.67	0.42
1:C:2190:ASP:OD2	1:C:2192:GLN:HB2	2.20	0.42
1:C:2312:VAL:HA	1:C:2315:ILE:HD12	2.01	0.42
1:C:2368:ASN:ND2	7:C:5124:HOH:O	2.52	0.42
1:D:3034:ASN:HA	1:D:3035:PRO:HD2	1.85	0.42
1:A:46:GLU:O	1:A:57:CYS:HA	2.20	0.41
1:A:184:ARG:NH1	1:A:441:PRO:HG3	2.34	0.41
1:A:467:ARG:HA	7:A:5160:HOH:O	2.19	0.41
1:B:1295:VAL:HG11	5:B:1601:HEM:HBB2	2.02	0.41
1:C:2176:GLU:O	1:C:2180:LYS:HG3	2.20	0.41
1:C:2385:TYR:OH	6:C:2701:DIF:H132	2.20	0.41
1:D:3500:VAL:O	1:D:3500:VAL:CG1	2.67	0.41
1:A:73:GLU:O	1:A:76:THR:HB	2.19	0.41
1:A:202:ALA:HB2	1:A:348:TYR:CE1	2.56	0.41
1:A:495:TYR:O	1:A:496:SER:HB2	2.19	0.41
1:B:1464:ASN:ND2	1:B:1467:ARG:HD3	2.35	0.41
1:C:2105(C):ILE:HG22	1:C:2108:LEU:CB	2.23	0.41
1:C:2464:ASN:HD22	1:C:2464:ASN:HA	1.57	0.41
1:C:2575:CYS:O	1:C:2575:CYS:SG	2.78	0.41
1:D:3161:THR:HB	1:D:3162:PRO:HD2	2.02	0.41
1:A:97:LYS:HD2	1:A:356:HIS:CD2	2.54	0.41
1:B:1105(B):ILE:HB	1:B:1108:LEU:HB2	2.02	0.41
1:C:2464:ASN:ND2	1:C:2467:ARG:HD3	2.35	0.41
1:D:3091:TYR:O	1:D:3095:HIS:HD2	2.03	0.41
1:A:124:ILE:HG21	1:A:532:LYS:HG3	2.02	0.41
1:A:309:HIS:HD2	1:A:310:ASN:OD1	2.03	0.41
1:A:447:VAL:HG13	5:A:704:HEM:HBA2	2.02	0.41
1:B:1132:VAL:HG13	1:B:1133:HIS:CD2	2.56	0.41
1:D:3442:ILE:HG23	4:D:3703:BOG:H61	2.03	0.41
1:B:1251:LYS:HG2	1:B:1310:ASN:CB	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2300:MET:CE	1:C:2423:VAL:HG22	2.50	0.41
1:C:2577:PHE:CD2	1:C:2577:PHE:C	2.93	0.41
1:A:44:ARG:HD3	1:A:469:ARG:NE	2.36	0.41
1:A:102:ILE:HG22	1:A:105(A):ILE:HD12	2.03	0.41
1:B:1202:ALA:HB2	1:B:1348:TYR:HE1	1.84	0.41
1:C:2089:VAL:HG12	1:C:2093:LEU:HD22	2.01	0.41
1:C:2114:LYS:HE2	1:C:2365:LEU:O	2.20	0.41
1:A:243:LYS:HE2	1:A:270:GLN:HB3	2.02	0.41
1:A:550:PHE:O	1:A:555:GLY:HA3	2.21	0.41
1:B:1113:MET:CE	1:B:1116:VAL:CG2	2.99	0.41
1:C:2126:SER:HA	1:C:2127:PRO:C	2.39	0.41
1:C:2538:PRO:HG3	1:D:3142:PHE:CE2	2.56	0.41
1:D:3197:MET:O	1:D:3201:PHE:HB2	2.20	0.41
1:D:3398:GLU:HB3	1:D:3399:ASP:H	1.44	0.41
1:D:3470:PHE:CG	1:D:3525:LEU:HD22	2.55	0.41
1:A:34:ASN:HD22	1:A:34:ASN:C	2.23	0.41
1:B:1034:ASN:HD22	1:B:1035:PRO:N	2.19	0.41
1:B:1113:MET:O	1:B:1116:VAL:HG22	2.21	0.41
1:A:50:THR:CG2	1:A:56:LYS:HB3	2.51	0.41
1:A:76:THR:O	1:A:80:LEU:HG	2.20	0.41
1:A:142:PHE:CD2	1:A:142:PHE:C	2.90	0.41
1:A:414:LEU:HD11	1:A:419:LEU:HD22	2.01	0.41
1:A:464:ASN:ND2	1:A:475:TYR:H	2.16	0.41
1:B:1058:ASP:OD1	1:B:1060:THR:OG1	2.33	0.41
1:B:1352:LEU:HA	1:B:1352:LEU:HD12	1.82	0.41
1:B:1433:ARG:NH2	1:B:1516:ALA:O	2.50	0.41
1:C:2047:CYS:HB2	7:C:5307:HOH:O	2.21	0.41
1:C:2066:GLY:O	1:C:2067:GLU:C	2.56	0.41
1:C:2248:LYS:O	1:C:2249:ASP:HB2	2.21	0.41
1:C:2298:LEU:HD12	1:C:2298:LEU:HA	1.74	0.41
1:C:2414:LEU:HA	1:C:2422:PHE:CE1	2.56	0.41
1:D:3048:MET:O	1:D:3050:THR:HG23	2.21	0.41
1:D:3122:TYR:CD1	1:D:3122:TYR:C	2.94	0.41
1:D:3316:LEU:HD23	1:D:3316:LEU:HA	1.82	0.41
1:B:1300:MET:HE1	1:B:1423:VAL:HG22	2.03	0.41
1:B:1316:LEU:HD23	1:B:1316:LEU:HA	1.83	0.41
1:D:3112:ILE:HB	1:D:3357:PHE:CZ	2.56	0.41
1:A:52:PHE:N	1:B:1322:GLU:HG2	2.36	0.40
1:A:245:ARG:HH22	1:A:326:GLU:HG2	1.85	0.40
1:C:2185:ARG:H	1:C:2185:ARG:HG2	1.68	0.40
1:C:2320:HIS:HB3	1:C:2323:TRP:CG	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2537:ASN:OD1	1:C:2539:ILE:HG12	2.20	0.40
1:D:3464:ASN:HD22	1:D:3464:ASN:HA	1.67	0.40
1:A:577:PHE:HE2	1:A:583:GLN:HE21	1.69	0.40
1:B:1075:LEU:CD1	1:B:1079:LYS:HE3	2.46	0.40
1:C:2122:TYR:CD1	1:C:2122:TYR:C	2.94	0.40
1:D:3090:HIS:CE1	1:D:3094:THR:CG2	3.00	0.40
1:D:3387:TRP:C	1:D:3389:PRO:HD2	2.41	0.40
1:A:94:THR:O	1:A:356:HIS:CE1	2.74	0.40
1:A:128:PRO:HG3	1:A:376:ARG:NH1	2.37	0.40
1:B:1050:THR:HG21	1:B:1056:LYS:HB2	2.02	0.40
1:C:2451:SER:HB2	1:C:2504:TYR:CE2	2.56	0.40
1:D:3142:PHE:O	1:D:3142:PHE:CG	2.74	0.40
1:D:3204:HIS:CE1	1:D:3232:HIS:CD2	3.09	0.40
1:D:3250:GLY:HA2	1:D:3329:PHE:HB2	2.04	0.40
1:D:3276:PRO:HG2	1:D:3279:ILE:HG12	2.02	0.40
1:A:269:THR:OG1	1:A:271:VAL:HG13	2.22	0.40
1:B:1113:MET:CA	1:B:1116:VAL:HG13	2.47	0.40
1:B:1198:PHE:HZ	1:B:1352:LEU:CD1	2.33	0.40
1:B:1298:LEU:N	7:B:5268:HOH:O	2.54	0.40
1:C:2064:PHE:CD1	1:C:2064:PHE:N	2.89	0.40
1:C:2142:PHE:CD2	1:C:2142:PHE:C	2.94	0.40
1:C:2292:PHE:C	1:C:2299:MET:HE1	2.40	0.40
1:D:3253:LYS:O	1:D:3264:PRO:HD3	2.21	0.40
1:D:3525:LEU:HD23	1:D:3525:LEU:N	2.36	0.40
1:B:1100:TRP:HA	1:B:1100:TRP:CE3	2.57	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1490:GLU:OE1	4:A:703:BOG:O2[4_555]	2.18	0.02
1:C:2490:GLU:OE1	4:D:3703:BOG:O2[4_456]	2.18	0.02

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	549/604 (91%)	516 (94%)	31 (6%)	2 (0%)	34 66
1	B	550/604 (91%)	513 (93%)	36 (6%)	1 (0%)	47 78
1	C	550/604 (91%)	510 (93%)	37 (7%)	3 (0%)	29 61
1	D	550/604 (91%)	510 (93%)	40 (7%)	0	100 100
All	All	2199/2416 (91%)	2049 (93%)	144 (6%)	6 (0%)	41 71

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	67	GLU
1	C	2106	PRO
1	C	2074	PHE
1	C	2438	ARG
1	A	106	PRO
1	B	1582	VAL

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	492/537 (92%)	432 (88%)	60 (12%)	5 15
1	B	493/537 (92%)	430 (87%)	63 (13%)	4 13
1	C	493/537 (92%)	439 (89%)	54 (11%)	6 19
1	D	493/537 (92%)	430 (87%)	63 (13%)	4 13
All	All	1971/2148 (92%)	1731 (88%)	240 (12%)	5 15

All (240) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	GLU
1	A	70	THR

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Mol	Chain	Res	Type
1	A	82	LEU
1	A	85	THR
1	A	93	LEU
1	A	101	ASN
1	A	107	PHE
1	A	108	LEU
1	A	111	LEU
1	A	112	ILE
1	A	115	TYR
1	A	116	VAL
1	A	117	LEU
1	A	120	ARG
1	A	122	TYR
1	A	130	TYR
1	A	131	ASN
1	A	171	LEU
1	A	178	LEU
1	A	185	ARG
1	A	215	LYS
1	A	230	LEU
1	A	238	LEU
1	A	248	LYS
1	A	252	LEU
1	A	271	VAL
1	A	272	GLU
1	A	289	GLN
1	A	290	GLU
1	A	291	VAL
1	A	298	LEU
1	A	306	LEU
1	A	318	GLN
1	A	322	GLU
1	A	326	GLU
1	A	341	ILE
1	A	376	ARG
1	A	385	TYR
1	A	406	GLN
1	A	408	LEU
1	A	409	TYR
1	A	412	SER
1	A	430	ILE
1	A	444	VAL

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Mol	Chain	Res	Type
1	A	463	LEU
1	A	468	LYS
1	A	469	ARG
1	A	484	GLU
1	A	492	LYS
1	A	509	VAL
1	A	513	ARG
1	A	525	LEU
1	A	532	LYS
1	A	534	LEU
1	A	535	MET
1	A	543	GLN
1	A	556	PHE
1	A	557	LYS
1	A	578	THR
1	A	583	GLN
1	B	1034	ASN
1	B	1038	SER
1	B	1046	GLU
1	B	1064	PHE
1	B	1065	TYR
1	B	1082	LEU
1	B	1085	THR
1	B	1093	LEU
1	B	1097	LYS
1	B	1101	ASN
1	B	1107	PHE
1	B	1111	LEU
1	B	1115	TYR
1	B	1116	VAL
1	B	1117	LEU
1	B	1118	THR
1	B	1120	ARG
1	B	1122	TYR
1	B	1130	TYR
1	B	1131	ASN
1	B	1171	LEU
1	B	1176	GLU
1	B	1178	LEU
1	B	1185	ARG
1	B	1215	LYS
1	B	1230	LEU

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Mol	Chain	Res	Type
1	B	1238	LEU
1	B	1248	LYS
1	B	1252	LEU
1	B	1271	VAL
1	B	1272	GLU
1	B	1289	GLN
1	B	1290	GLU
1	B	1291	VAL
1	B	1298	LEU
1	B	1306	LEU
1	B	1311	ARG
1	B	1318	GLN
1	B	1322	GLU
1	B	1326	GLU
1	B	1341	ILE
1	B	1376	ARG
1	B	1385	TYR
1	B	1408	LEU
1	B	1409	TYR
1	B	1412	SER
1	B	1438	ARG
1	B	1444	VAL
1	B	1463	LEU
1	B	1468	LYS
1	B	1469	ARG
1	B	1484	GLU
1	B	1487	MET
1	B	1492	LYS
1	B	1513	ARG
1	B	1525	LEU
1	B	1532	LYS
1	B	1534	LEU
1	B	1535	MET
1	B	1556	PHE
1	B	1557	LYS
1	B	1579	SER
1	B	1583	GLN
1	C	2034	ASN
1	C	2038	SER
1	C	2081	LEU
1	C	2082	LEU
1	C	2083	LYS

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Mol	Chain	Res	Type
1	C	2090	HIS
1	C	2093	LEU
1	C	2101	ASN
1	C	2107	PHE
1	C	2117	LEU
1	C	2120	ARG
1	C	2122	TYR
1	C	2131	ASN
1	C	2171	LEU
1	C	2178	LEU
1	C	2215	LYS
1	C	2230	LEU
1	C	2238	LEU
1	C	2248	LYS
1	C	2252	LEU
1	C	2271	VAL
1	C	2272	GLU
1	C	2289	GLN
1	C	2290	GLU
1	C	2291	VAL
1	C	2298	LEU
1	C	2306	LEU
1	C	2318	GLN
1	C	2322	GLU
1	C	2326	GLU
1	C	2341	ILE
1	C	2376	ARG
1	C	2385	TYR
1	C	2406	GLN
1	C	2408	LEU
1	C	2409	TYR
1	C	2412	SER
1	C	2438	ARG
1	C	2444	VAL
1	C	2463	LEU
1	C	2468	LYS
1	C	2469	ARG
1	C	2484	GLU
1	C	2487	MET
1	C	2492	LYS
1	C	2513	ARG
1	C	2525	LEU

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Mol	Chain	Res	Type
1	C	2532	LYS
1	C	2534	LEU
1	C	2535	MET
1	C	2556	PHE
1	C	2557	LYS
1	C	2578	THR
1	C	2583	GLN
1	D	3034	ASN
1	D	3038	SER
1	D	3046	GLU
1	D	3056	LYS
1	D	3081	LEU
1	D	3082	LEU
1	D	3085	THR
1	D	3093	LEU
1	D	3101	ASN
1	D	3107	PHE
1	D	3108	LEU
1	D	3111	LEU
1	D	3112	ILE
1	D	3115	TYR
1	D	3117	LEU
1	D	3120	ARG
1	D	3122	TYR
1	D	3130	TYR
1	D	3131	ASN
1	D	3171	LEU
1	D	3176	GLU
1	D	3178	LEU
1	D	3185	ARG
1	D	3215	LYS
1	D	3230	LEU
1	D	3238	LEU
1	D	3248	LYS
1	D	3252	LEU
1	D	3271	VAL
1	D	3272	GLU
1	D	3289	GLN
1	D	3290	GLU
1	D	3291	VAL
1	D	3298	LEU
1	D	3306	LEU

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Mol	Chain	Res	Type
1	D	3311	ARG
1	D	3318	GLN
1	D	3322	GLU
1	D	3326	GLU
1	D	3341	ILE
1	D	3376	ARG
1	D	3385	TYR
1	D	3406	GLN
1	D	3408	LEU
1	D	3409	TYR
1	D	3412	SER
1	D	3430	ILE
1	D	3438	ARG
1	D	3444	VAL
1	D	3463	LEU
1	D	3468	LYS
1	D	3469	ARG
1	D	3484	GLU
1	D	3492	LYS
1	D	3509	VAL
1	D	3513	ARG
1	D	3525	LEU
1	D	3532	LYS
1	D	3534	LEU
1	D	3535	MET
1	D	3556	PHE
1	D	3557	LYS
1	D	3583	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	90	HIS
1	A	95	HIS
1	A	131	ASN
1	A	203	GLN
1	A	204	HIS
1	A	241	GLN
1	A	242	HIS
1	A	356	HIS
1	A	370	GLN
1	A	386	HIS

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Mol	Chain	Res	Type
1	A	421	GLN
1	A	454	GLN
1	A	464	ASN
1	A	570	ASN
1	A	583	GLN
1	B	1034	ASN
1	B	1090	HIS
1	B	1095	HIS
1	B	1131	ASN
1	B	1203	GLN
1	B	1204	HIS
1	B	1241	GLN
1	B	1242	HIS
1	B	1370	GLN
1	B	1386	HIS
1	B	1454	GLN
1	B	1464	ASN
1	B	1583	GLN
1	C	2034	ASN
1	C	2090	HIS
1	C	2095	HIS
1	C	2131	ASN
1	C	2203	GLN
1	C	2204	HIS
1	C	2241	GLN
1	C	2242	HIS
1	C	2356	HIS
1	C	2370	GLN
1	C	2386	HIS
1	C	2454	GLN
1	C	2464	ASN
1	C	2583	GLN
1	D	3034	ASN
1	D	3090	HIS
1	D	3095	HIS
1	D	3131	ASN
1	D	3203	GLN
1	D	3204	HIS
1	D	3241	GLN
1	D	3242	HIS
1	D	3327	GLN
1	D	3356	HIS

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Mol	Chain	Res	Type
1	D	3370	GLN
1	D	3386	HIS
1	D	3454	GLN
1	D	3464	ASN
1	D	3583	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)

12 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAG	E	1	1,2	14,14,15	0.47	0	17,19,21	0.65	0
2	NAG	E	2	2	14,14,15	0.81	0	17,19,21	0.77	1 (5%)
2	NAG	E	3	2	14,14,15	0.83	0	17,19,21	0.82	1 (5%)
2	NAG	F	1	1,2	14,14,15	0.53	0	17,19,21	0.70	1 (5%)
2	NAG	F	2	2	14,14,15	0.77	0	17,19,21	0.80	1 (5%)
2	NAG	F	3	2	14,14,15	0.96	1 (7%)	17,19,21	0.78	1 (5%)
2	NAG	G	1	1,2	14,14,15	0.46	0	17,19,21	0.67	0
2	NAG	G	2	2	14,14,15	0.69	0	17,19,21	0.78	1 (5%)
2	NAG	G	3	2	14,14,15	0.91	1 (7%)	17,19,21	0.66	0
2	NAG	H	1	1,2	14,14,15	0.58	0	17,19,21	0.66	0
2	NAG	H	2	2	14,14,15	0.85	0	17,19,21	0.82	1 (5%)
2	NAG	H	3	2	14,14,15	0.93	1 (7%)	17,19,21	0.85	1 (5%)

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	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	NAG	E	3	2	-	1/6/23/26	0/1/1/1
2	NAG	F	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	2/6/23/26	0/1/1/1
2	NAG	F	3	2	-	1/6/23/26	0/1/1/1
2	NAG	G	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	G	2	2	-	2/6/23/26	0/1/1/1
2	NAG	G	3	2	-	1/6/23/26	0/1/1/1
2	NAG	H	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	H	2	2	-	1/6/23/26	0/1/1/1
2	NAG	H	3	2	-	1/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	3	NAG	C1-C2	2.54	1.56	1.52
2	G	3	NAG	C1-C2	2.51	1.56	1.52
2	H	3	NAG	C1-C2	2.22	1.55	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	3	NAG	C1-O5-C5	2.60	115.72	112.19
2	G	2	NAG	C4-C3-C2	-2.25	107.72	111.02
2	F	2	NAG	C4-C3-C2	-2.21	107.78	111.02
2	H	3	NAG	C1-O5-C5	2.14	115.10	112.19
2	H	2	NAG	O5-C1-C2	-2.13	107.93	111.29
2	E	2	NAG	O5-C1-C2	-2.09	107.98	111.29
2	E	3	NAG	C1-O5-C5	2.05	114.97	112.19
2	F	1	NAG	C2-N2-C7	-2.01	120.05	122.90

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	2	NAG	C1-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
2	E	3	NAG	C3-C2-N2-C7
2	G	3	NAG	C3-C2-N2-C7
2	H	3	NAG	C3-C2-N2-C7
2	F	2	NAG	C1-C2-N2-C7
2	G	2	NAG	C4-C5-C6-O6
2	E	2	NAG	C1-C2-N2-C7
2	F	3	NAG	C3-C2-N2-C7
2	G	2	NAG	C3-C2-N2-C7
2	E	2	NAG	C3-C2-N2-C7
2	F	2	NAG	C3-C2-N2-C7

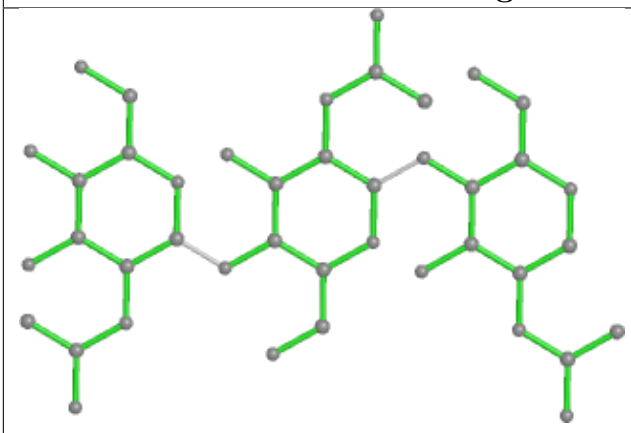
There are no ring outliers.

9 monomers are involved in 9 short contacts:

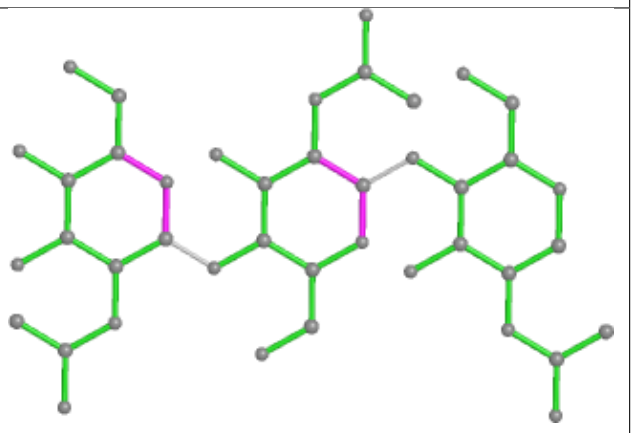
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	2	NAG	1	0
2	F	3	NAG	1	0
2	H	2	NAG	2	0
2	E	2	NAG	2	0
2	H	1	NAG	1	0
2	E	3	NAG	3	0
2	F	2	NAG	1	0
2	H	3	NAG	2	0
2	G	3	NAG	2	0

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

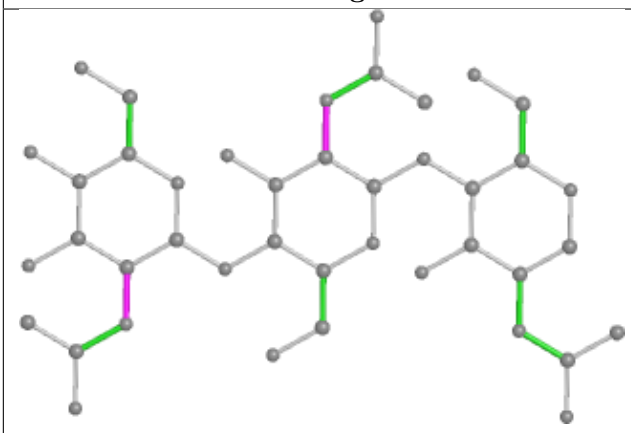
Oligosaccharide Chain E



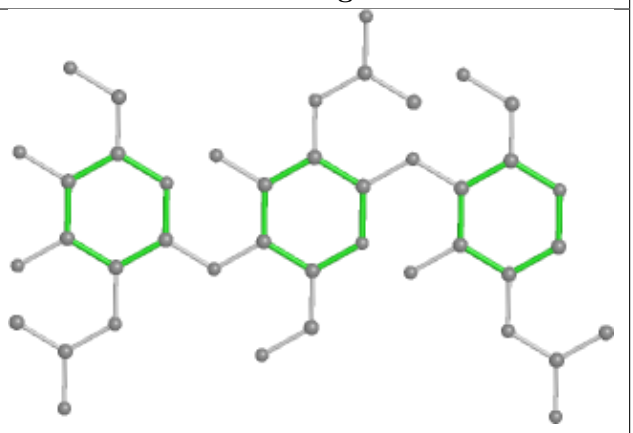
Bond lengths



Bond angles

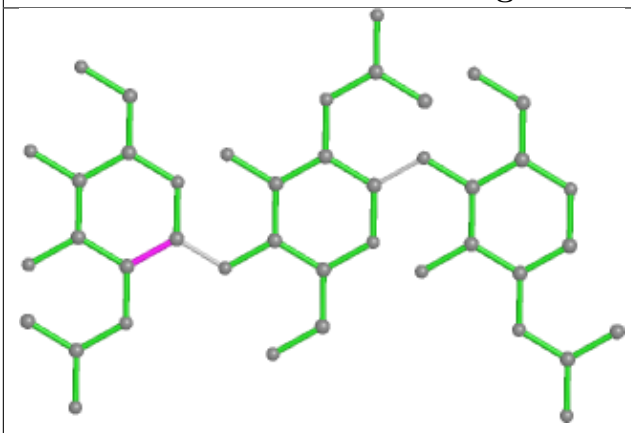


Torsions

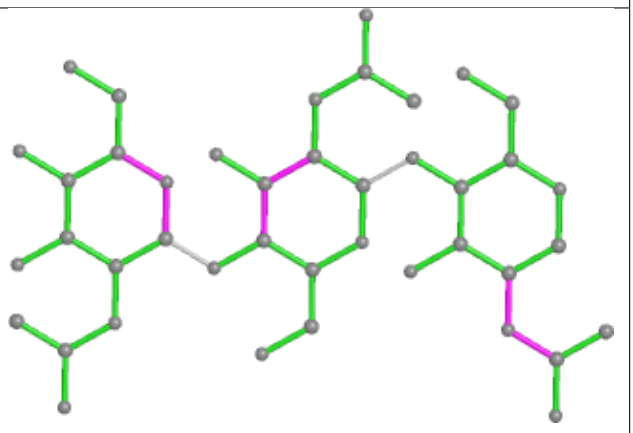


Rings

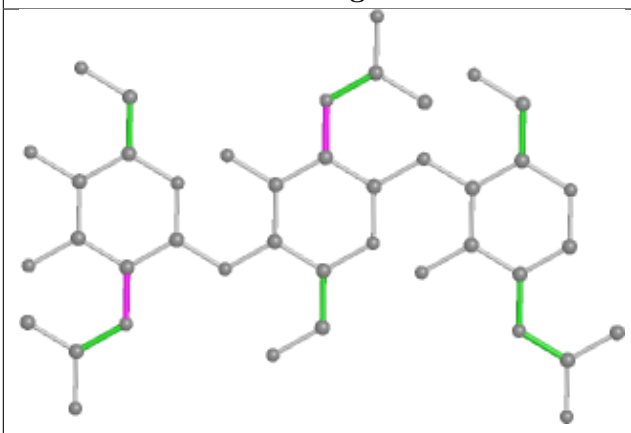
Oligosaccharide Chain F



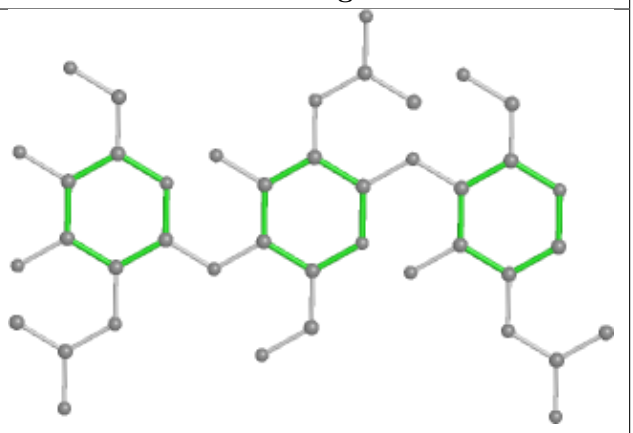
Bond lengths



Bond angles

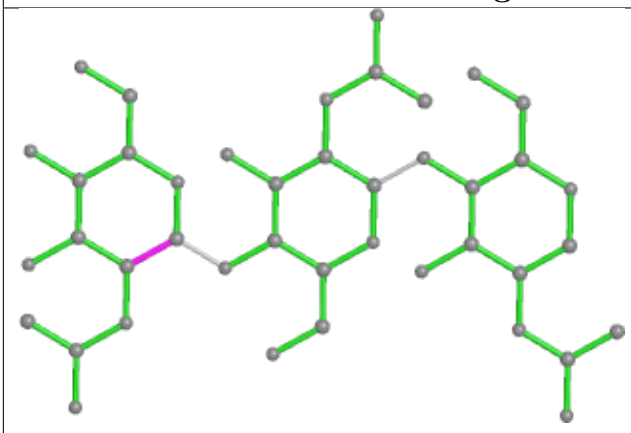


Torsions

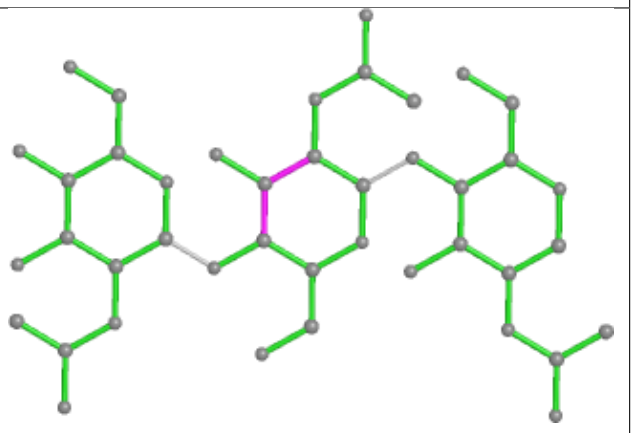


Rings

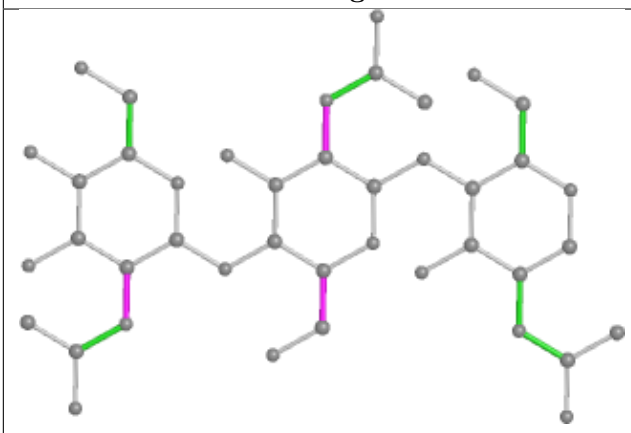
Oligosaccharide Chain G



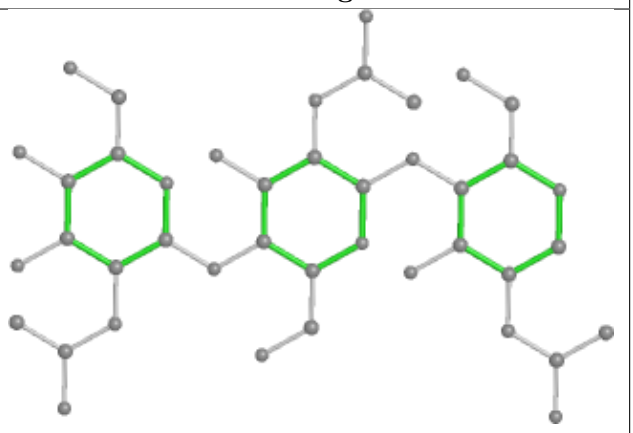
Bond lengths



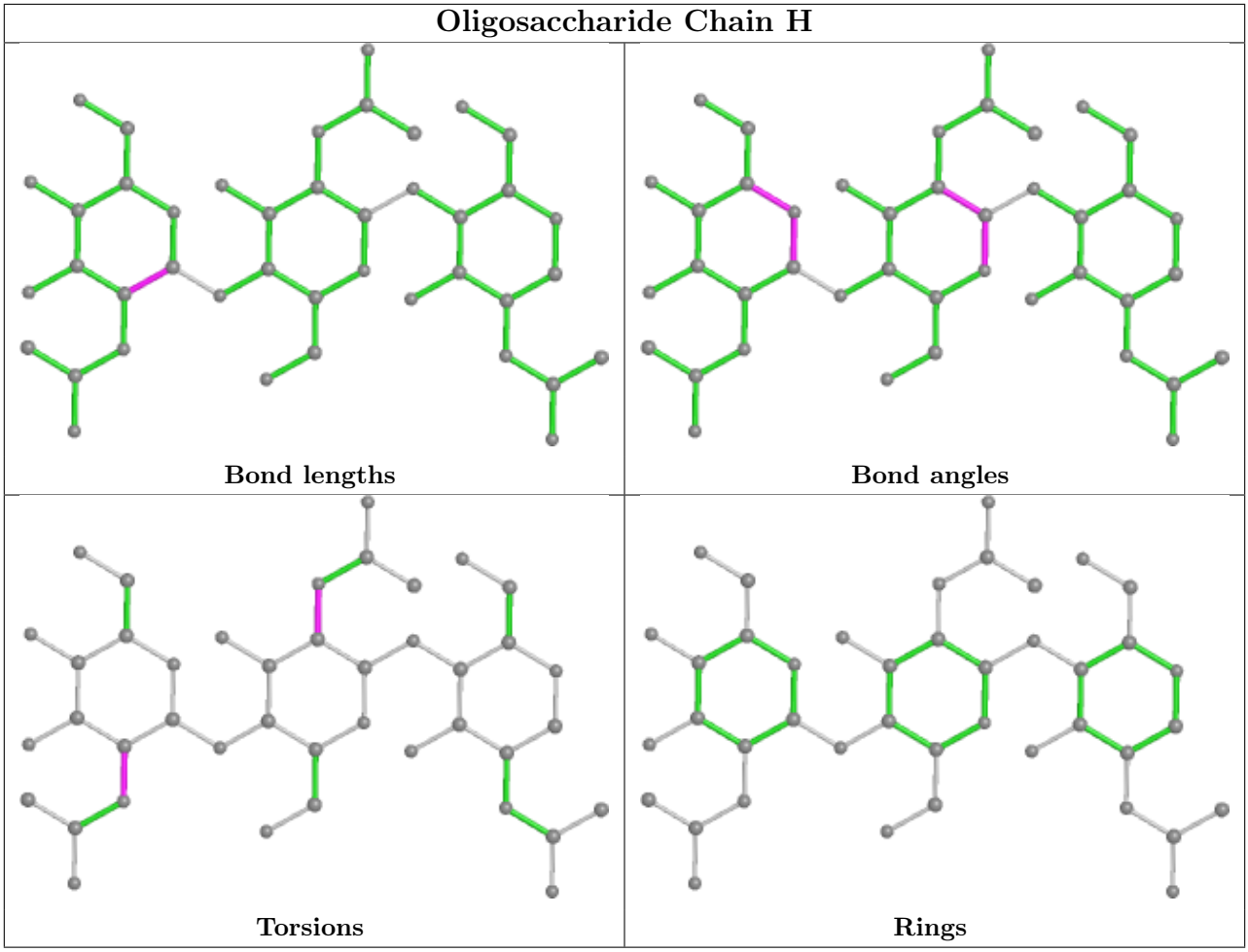
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

18 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	$\#\|Z\| > 2$
5	HEM	A	704	1	41,50,50	1.51	6 (14%)	45,82,82	1.10	1 (2%)
3	NAG	A	661	1	14,14,15	0.54	0	17,19,21	0.63	0
4	BOG	A	703	-	20,20,20	0.72	1 (5%)	25,25,25	0.64	0
3	NAG	C	2681	1	14,14,15	0.48	0	17,19,21	1.02	2 (11%)
5	HEM	D	3601	1	41,50,50	1.41	6 (14%)	45,82,82	1.08	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	HEM	B	1601	1	41,50,50	1.42	4 (9%)	45,82,82	1.10	1 (2%)
6	DIF	A	701	-	20,20,20	1.45	3 (15%)	27,27,27	2.30	7 (25%)
3	NAG	B	1681	1	14,14,15	0.46	0	17,19,21	0.80	0
6	DIF	B	1701	-	20,20,20	1.36	3 (15%)	27,27,27	1.96	6 (22%)
3	NAG	B	1661	1	14,14,15	0.48	0	17,19,21	0.68	0
6	DIF	C	2701	-	20,20,20	1.48	3 (15%)	27,27,27	1.77	7 (25%)
4	BOG	D	3703	-	17,17,20	0.37	0	18,18,25	0.84	1 (5%)
3	NAG	C	2661	1	14,14,15	0.59	0	17,19,21	0.62	0
3	NAG	D	3661	1	14,14,15	0.71	0	17,19,21	0.81	1 (5%)
3	NAG	A	681	1	14,14,15	0.58	0	17,19,21	0.75	0
6	DIF	D	3701	-	20,20,20	1.43	3 (15%)	27,27,27	2.05	7 (25%)
3	NAG	D	3681	1	14,14,15	0.47	0	17,19,21	0.86	0
5	HEM	C	2601	1	41,50,50	1.57	5 (12%)	45,82,82	1.06	2 (4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	HEM	A	704	1	-	4/12/54/54	-
3	NAG	A	661	1	-	1/6/23/26	0/1/1/1
4	BOG	A	703	-	-	6/11/31/31	0/1/1/1
3	NAG	C	2681	1	-	1/6/23/26	0/1/1/1
5	HEM	D	3601	1	-	4/12/54/54	-
5	HEM	B	1601	1	-	6/12/54/54	-
6	DIF	A	701	-	-	0/8/8/8	0/2/2/2
3	NAG	B	1681	1	-	2/6/23/26	0/1/1/1
6	DIF	B	1701	-	-	0/8/8/8	0/2/2/2
3	NAG	B	1661	1	-	1/6/23/26	0/1/1/1
6	DIF	C	2701	-	-	0/8/8/8	0/2/2/2
4	BOG	D	3703	-	-	5/18/18/31	-
3	NAG	C	2661	1	-	1/6/23/26	0/1/1/1
3	NAG	D	3661	1	-	1/6/23/26	0/1/1/1
3	NAG	A	681	1	-	2/6/23/26	0/1/1/1
6	DIF	D	3701	-	-	0/8/8/8	0/2/2/2
3	NAG	D	3681	1	-	2/6/23/26	0/1/1/1
5	HEM	C	2601	1	-	4/12/54/54	-

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	2601	HEM	C3C-CAC	-4.26	1.39	1.47
5	B	1601	HEM	C3C-CAC	-4.16	1.39	1.47
6	B	1701	DIF	O2-C14	4.15	1.35	1.22
5	D	3601	HEM	C3C-CAC	-4.09	1.39	1.47
5	C	2601	HEM	C3C-C2C	-4.08	1.34	1.40
5	A	704	HEM	C3C-CAC	-4.06	1.39	1.47
6	C	2701	DIF	O2-C14	4.01	1.35	1.22
5	C	2601	HEM	CBB-CAB	3.92	1.49	1.30
6	A	701	DIF	O2-C14	3.90	1.35	1.22
6	D	3701	DIF	O2-C14	3.77	1.34	1.22
5	D	3601	HEM	CBB-CAB	3.65	1.48	1.30
5	A	704	HEM	C3C-C2C	-3.57	1.35	1.40
5	B	1601	HEM	C3C-C2C	-3.55	1.35	1.40
5	A	704	HEM	CBB-CAB	3.39	1.47	1.30
5	B	1601	HEM	CBB-CAB	3.37	1.47	1.30
5	C	2601	HEM	CAB-C3B	-3.28	1.38	1.47
5	B	1601	HEM	CAB-C3B	-3.23	1.38	1.47
6	C	2701	DIF	C3-C4	3.10	1.44	1.40
5	A	704	HEM	CBC-CAC	3.02	1.49	1.29
6	D	3701	DIF	C3-C4	2.95	1.44	1.40
5	D	3601	HEM	CAB-C3B	-2.94	1.39	1.47
5	D	3601	HEM	C3C-C2C	-2.88	1.36	1.40
5	A	704	HEM	CAB-C3B	-2.65	1.40	1.47
5	C	2601	HEM	CBC-CAC	2.64	1.46	1.29
6	A	701	DIF	C3-C4	2.59	1.44	1.40
6	C	2701	DIF	O1-C14	-2.38	1.22	1.30
6	B	1701	DIF	C3-C4	2.35	1.43	1.40
5	D	3601	HEM	CBC-CAC	2.33	1.44	1.29
6	B	1701	DIF	O1-C14	-2.32	1.22	1.30
4	A	703	BOG	O1-C1	2.27	1.44	1.40
6	A	701	DIF	O1-C14	-2.22	1.23	1.30
6	D	3701	DIF	O1-C14	-2.14	1.23	1.30
5	A	704	HEM	CBD-CGD	2.07	1.55	1.50
5	D	3601	HEM	CBD-CGD	2.02	1.55	1.50

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	701	DIF	C7-C8-N1	5.52	122.98	118.60
6	A	701	DIF	C4-C3-N1	-5.36	115.08	122.04
6	D	3701	DIF	C4-C3-N1	-5.17	115.33	122.04
6	A	701	DIF	C2-C3-N1	5.08	128.64	122.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	1701	DIF	C7-C8-N1	5.00	122.57	118.60
6	B	1701	DIF	C4-C3-N1	-4.65	116.01	122.04
6	D	3701	DIF	C2-C3-N1	4.48	127.85	122.04
6	A	701	DIF	C3-C2-CL2	4.26	124.15	119.27
6	D	3701	DIF	C3-C2-CL2	4.08	123.94	119.27
6	C	2701	DIF	C4-C3-N1	-3.87	117.02	122.04
6	D	3701	DIF	C7-C8-N1	3.83	121.64	118.60
6	C	2701	DIF	C7-C8-N1	3.61	121.47	118.60
5	A	704	HEM	CBA-CAA-C2A	-3.56	106.55	112.62
6	A	701	DIF	O2-C14-C13	-3.46	113.16	123.04
6	B	1701	DIF	C2-C3-N1	3.41	126.47	122.04
5	B	1601	HEM	CBA-CAA-C2A	-3.40	106.83	112.62
6	B	1701	DIF	C3-C2-CL2	3.34	123.10	119.27
6	D	3701	DIF	O2-C14-C13	-3.34	113.51	123.04
6	C	2701	DIF	C2-C3-N1	3.26	126.27	122.04
6	C	2701	DIF	O2-C14-C13	-3.14	114.09	123.04
6	B	1701	DIF	O2-C14-C13	-3.09	114.23	123.04
6	C	2701	DIF	C3-C2-CL2	3.07	122.78	119.27
6	C	2701	DIF	C3-C4-CL4	2.81	122.49	119.27
6	D	3701	DIF	O1-C14-C13	2.67	124.15	114.02
6	A	701	DIF	O1-C14-C13	2.64	124.04	114.02
5	C	2601	HEM	CBA-CAA-C2A	-2.57	108.23	112.62
6	B	1701	DIF	O1-C14-C13	2.55	123.69	114.02
6	C	2701	DIF	O1-C14-C13	2.47	123.40	114.02
3	D	3661	NAG	C1-O5-C5	2.36	115.39	112.19
4	D	3703	BOG	C2-C3-C4	-2.24	107.56	112.41
5	D	3601	HEM	CMA-C3A-C4A	-2.23	125.04	128.46
3	C	2681	NAG	C2-N2-C7	-2.20	119.77	122.90
6	D	3701	DIF	C3-C4-CL4	2.17	121.76	119.27
6	A	701	DIF	C1-C2-CL2	-2.16	114.08	118.41
5	C	2601	HEM	C4B-CHC-C1C	2.12	125.35	122.56
3	C	2681	NAG	C6-C5-C4	2.09	117.90	113.00
5	D	3601	HEM	C4C-CHD-C1D	2.06	125.28	122.56

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1661	NAG	C3-C2-N2-C7
3	C	2661	NAG	C3-C2-N2-C7
3	D	3661	NAG	C3-C2-N2-C7
5	B	1601	HEM	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
5	B	1601	HEM	C4B-C3B-CAB-CBB
4	D	3703	BOG	O5-C5-C6-O6
4	D	3703	BOG	C4-C5-C6-O6
4	A	703	BOG	C4-C5-C6-O6
4	A	703	BOG	O5-C1-O1-C1'
4	A	703	BOG	C3'-C4'-C5'-C6'
4	A	703	BOG	C2-C1-O1-C1'
4	D	3703	BOG	C3'-C4'-C5'-C6'
4	A	703	BOG	O5-C5-C6-O6
5	A	704	HEM	C2B-C3B-CAB-CBB
5	C	2601	HEM	C2B-C3B-CAB-CBB
5	A	704	HEM	C4B-C3B-CAB-CBB
5	C	2601	HEM	C4B-C3B-CAB-CBB
3	D	3681	NAG	C4-C5-C6-O6
3	A	661	NAG	C3-C2-N2-C7
4	A	703	BOG	C2'-C1'-O1-C1
3	D	3681	NAG	O5-C5-C6-O6
3	A	681	NAG	C4-C5-C6-O6
3	B	1681	NAG	C4-C5-C6-O6
5	A	704	HEM	CAA-CBA-CGA-O1A
5	C	2601	HEM	CAA-CBA-CGA-O1A
5	B	1601	HEM	CAA-CBA-CGA-O1A
5	A	704	HEM	CAA-CBA-CGA-O2A
5	D	3601	HEM	CAA-CBA-CGA-O1A
5	C	2601	HEM	CAA-CBA-CGA-O2A
5	D	3601	HEM	CAD-CBD-CGD-O2D
5	D	3601	HEM	CAD-CBD-CGD-O1D
5	B	1601	HEM	CAA-CBA-CGA-O2A
3	B	1681	NAG	O5-C5-C6-O6
4	D	3703	BOG	C2-C3-C4-O4
5	D	3601	HEM	CAA-CBA-CGA-O2A
5	B	1601	HEM	CAD-CBD-CGD-O2D
3	C	2681	NAG	C4-C5-C6-O6
3	A	681	NAG	O5-C5-C6-O6
5	B	1601	HEM	CAD-CBD-CGD-O1D
4	D	3703	BOG	O1-C1'-C2'-C3'

There are no ring outliers.

14 monomers are involved in 68 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	704	HEM	4	0

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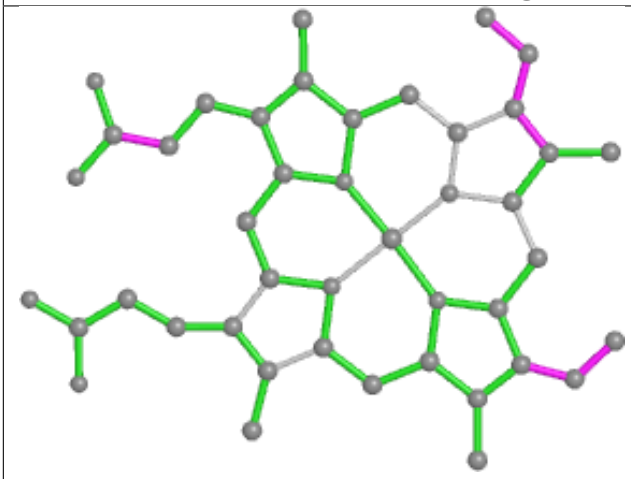
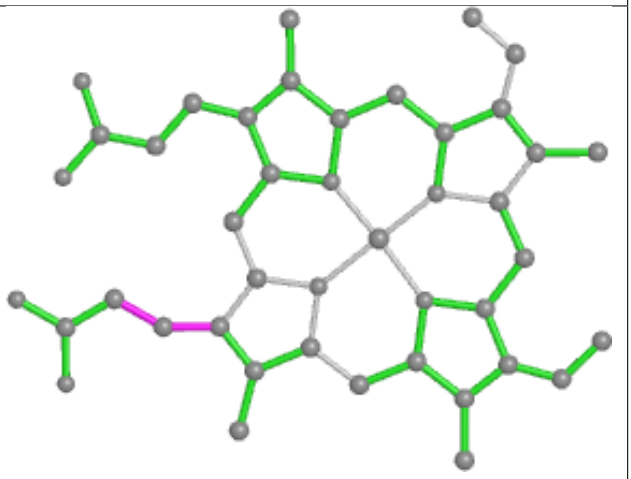
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	661	NAG	5	0
4	A	703	BOG	5	1
5	D	3601	HEM	4	0
5	B	1601	HEM	7	0
6	A	701	DIF	3	0
6	B	1701	DIF	3	0
3	B	1661	NAG	6	0
6	C	2701	DIF	4	0
4	D	3703	BOG	9	1
3	C	2661	NAG	7	0
3	D	3661	NAG	4	0
6	D	3701	DIF	1	0
5	C	2601	HEM	4	0

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.

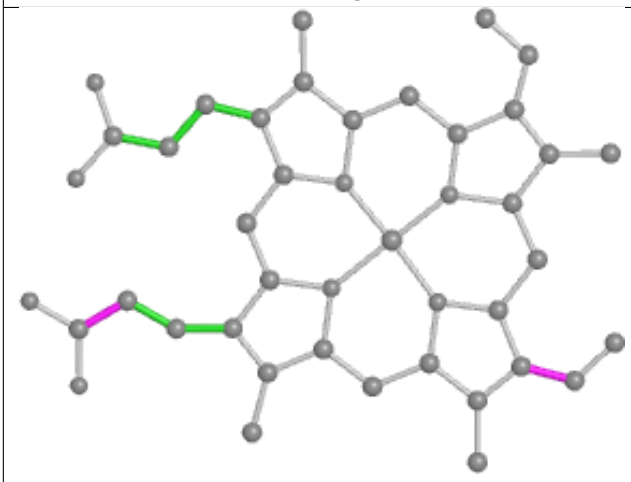
Ligand HEM A 704



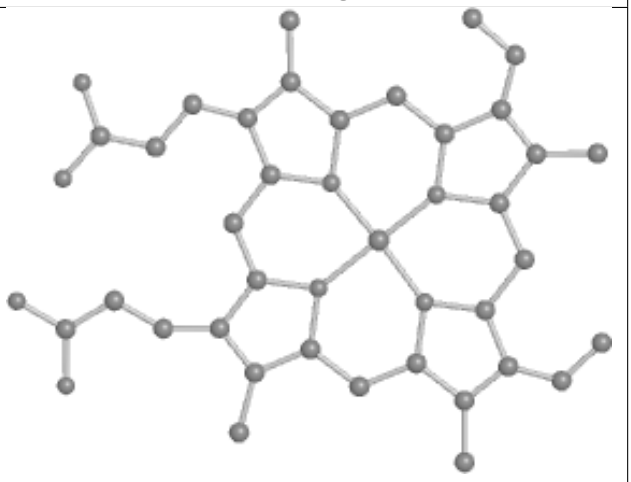
Bond lengths



Bond angles

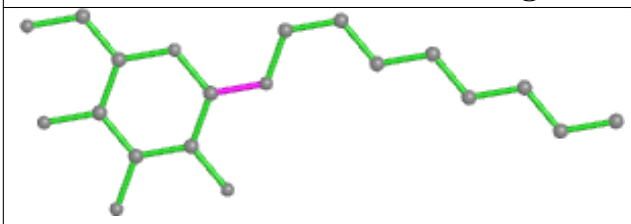


Torsions



Rings

Ligand BOG A 703



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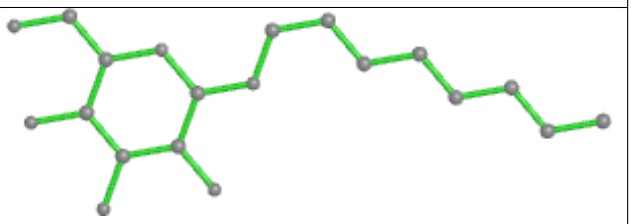

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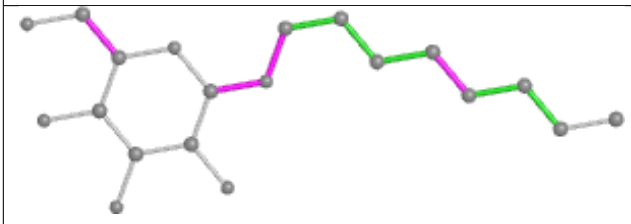

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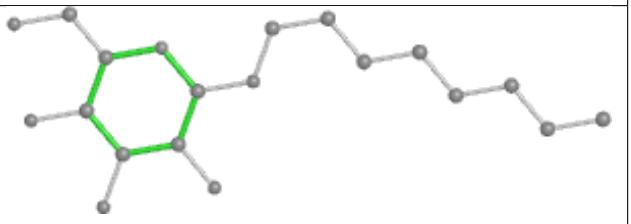
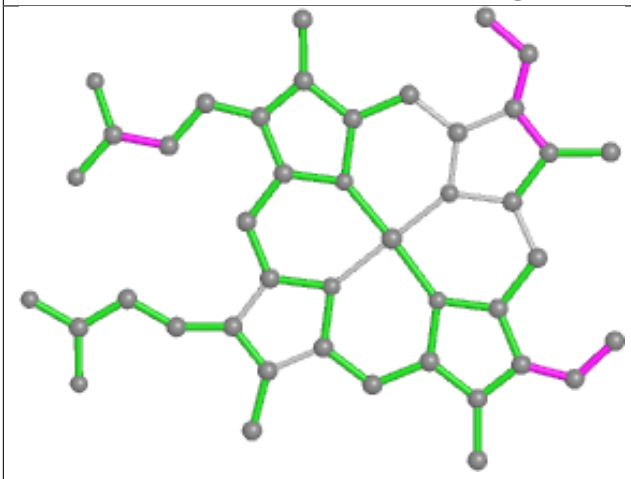


Rings

Ligand HEM D 3601



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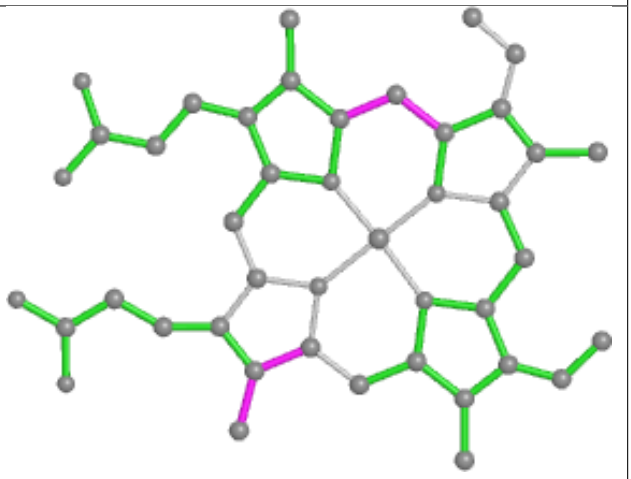

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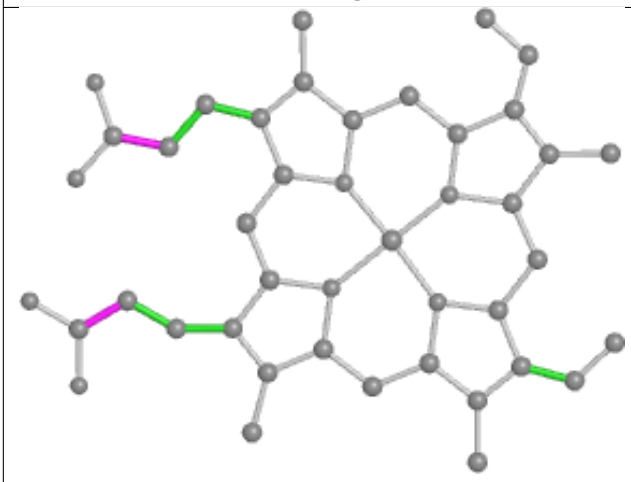

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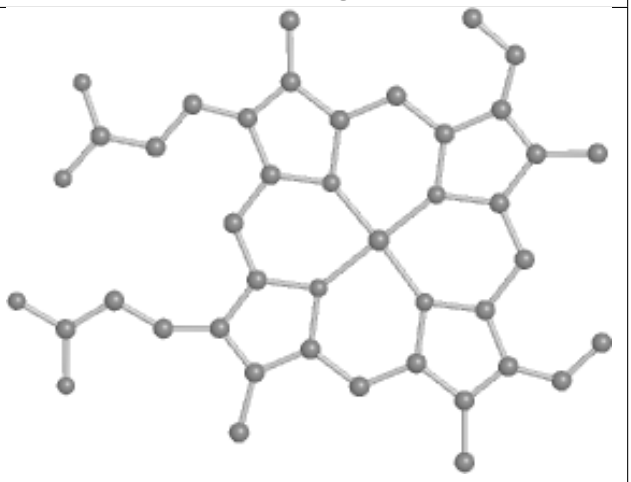
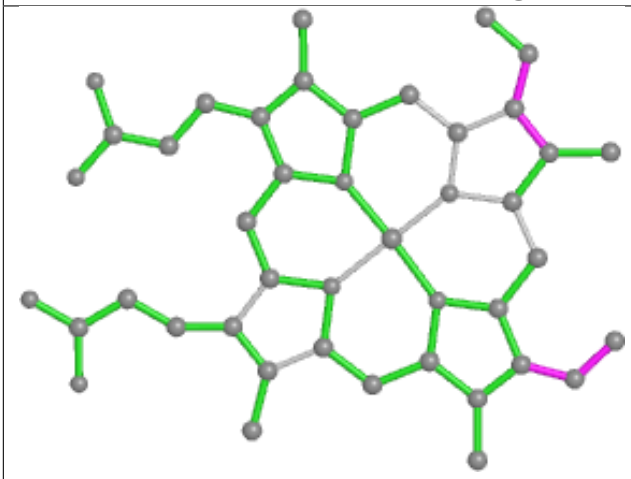


Rings

Ligand HEM B 1601



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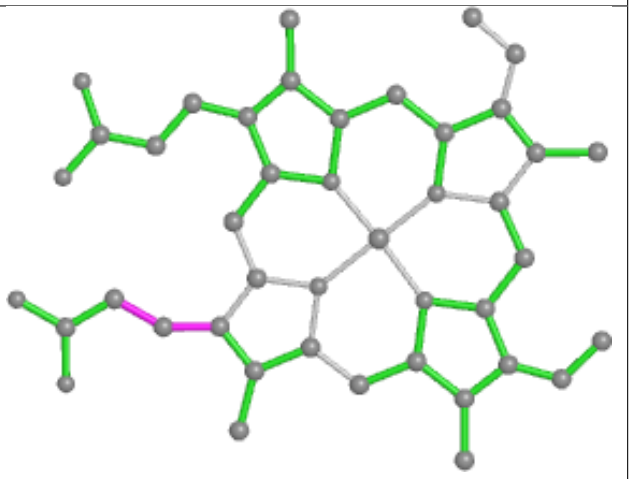
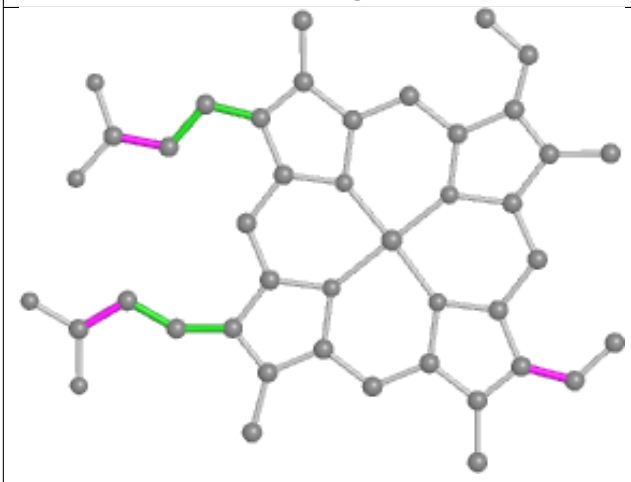
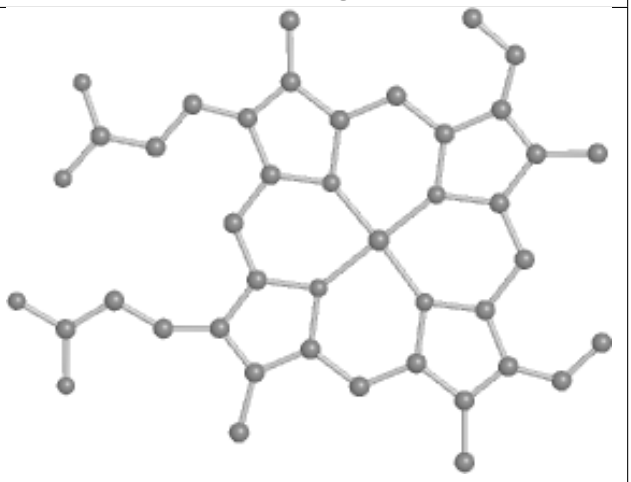


Bond angles

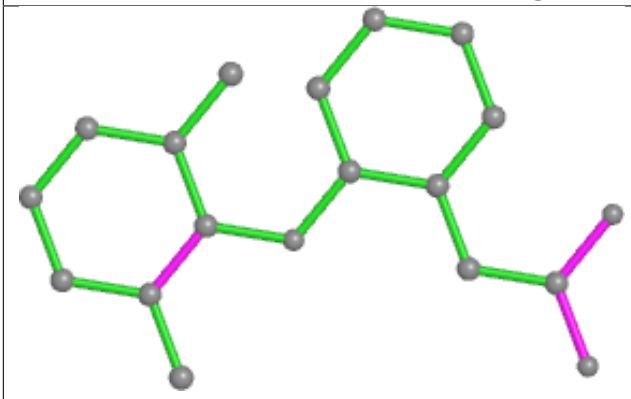


Torsions

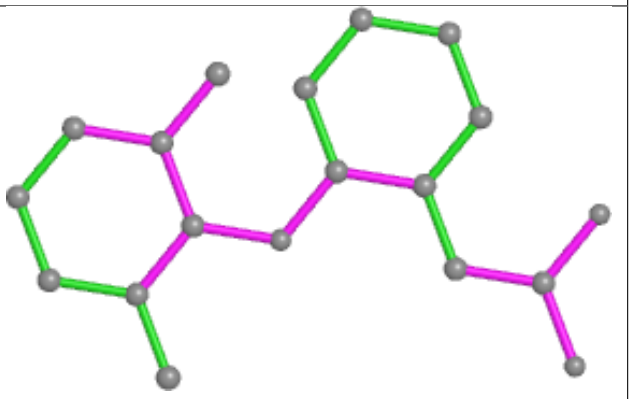


Rings

Ligand DIF A 701



Bond lengths



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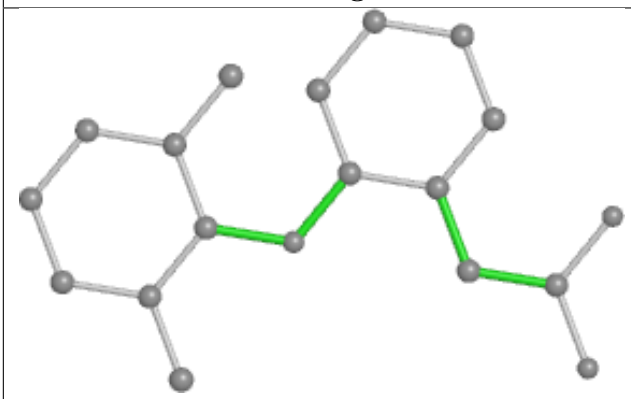

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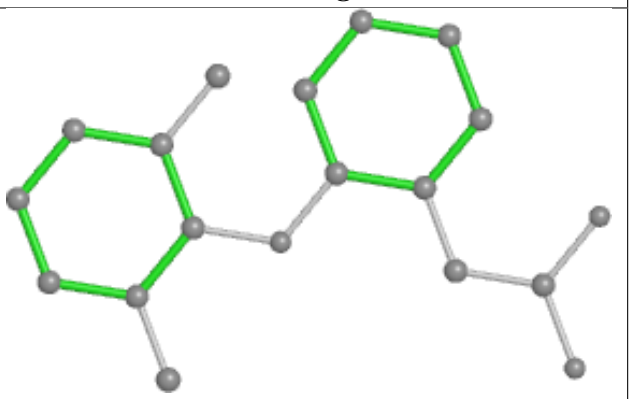

Rings

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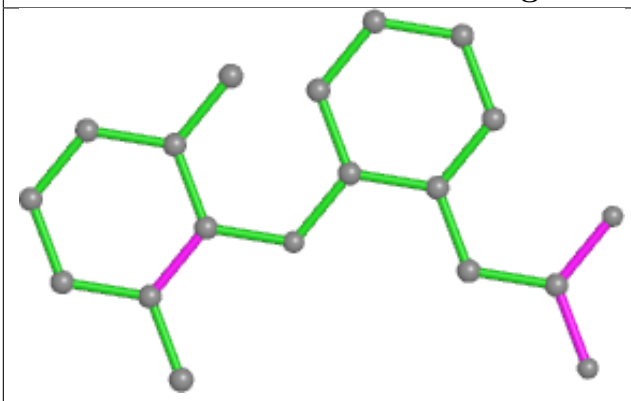

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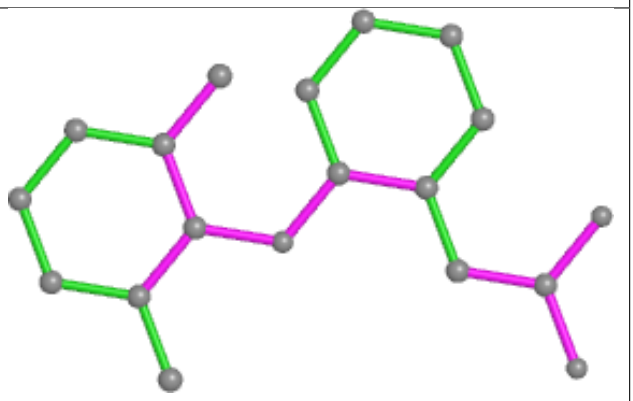

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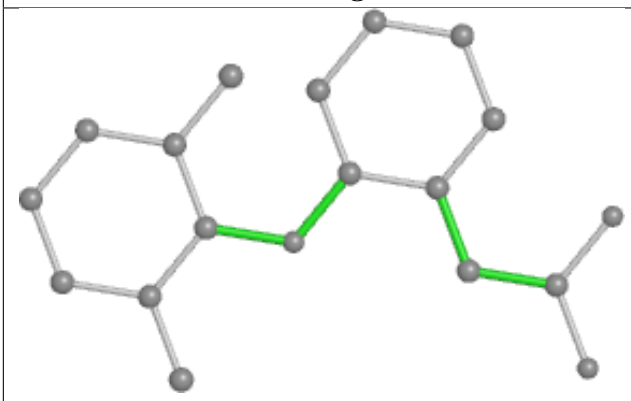

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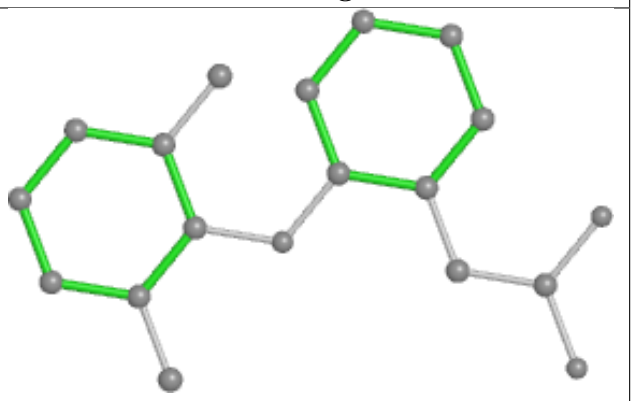
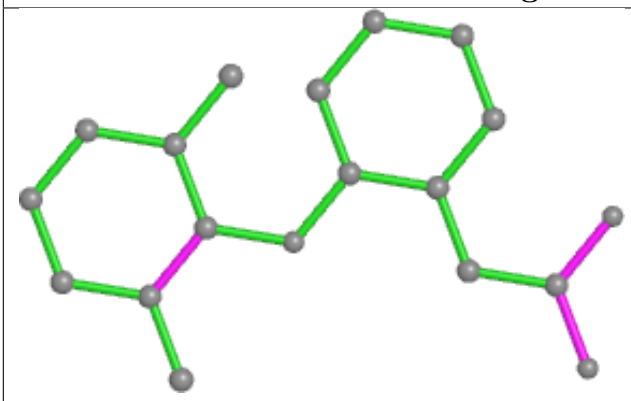
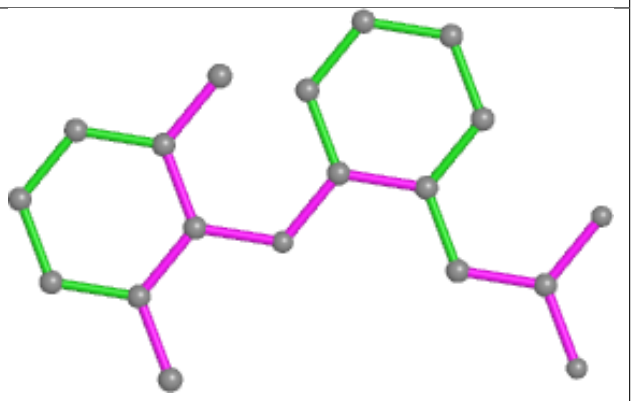


Rings

Ligand DIF C 2701



Bond lengths



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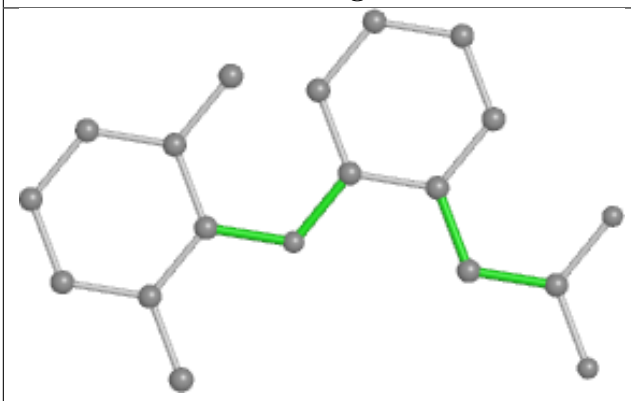

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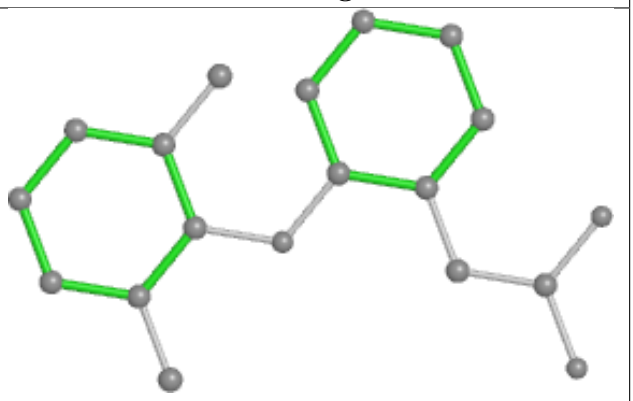
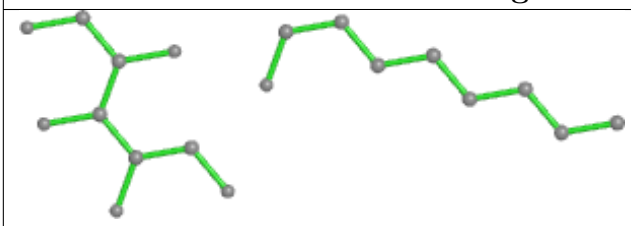


Rings

Ligand BOG D 3703



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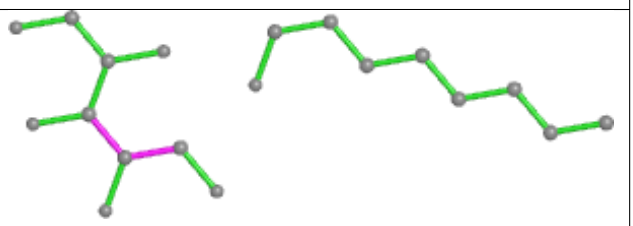
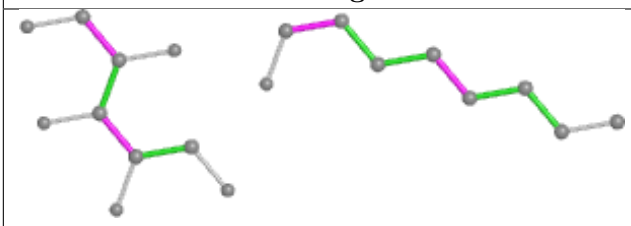


Bond angles



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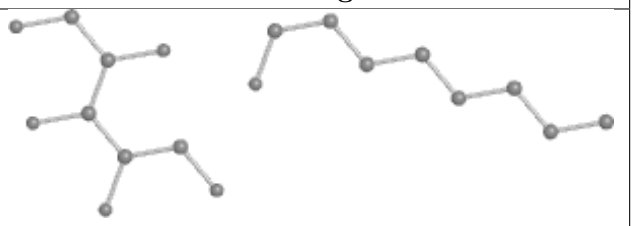
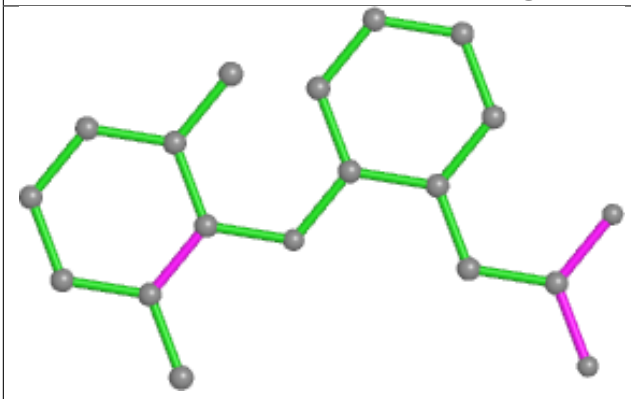


Rings

Ligand DIF D 3701



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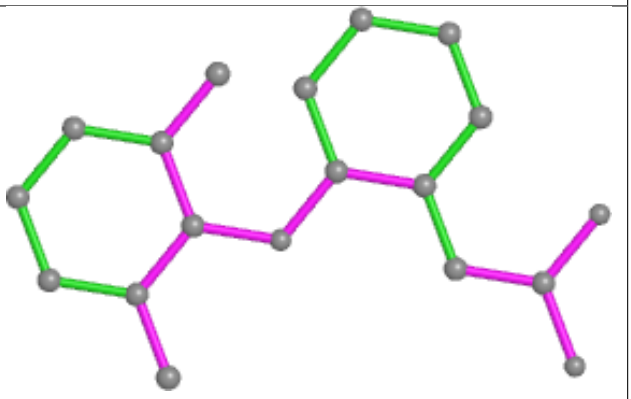
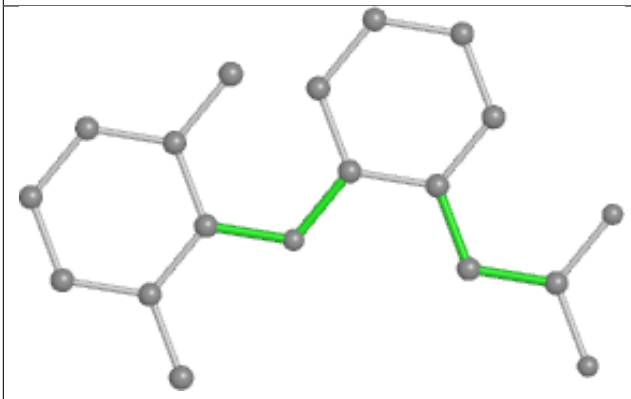
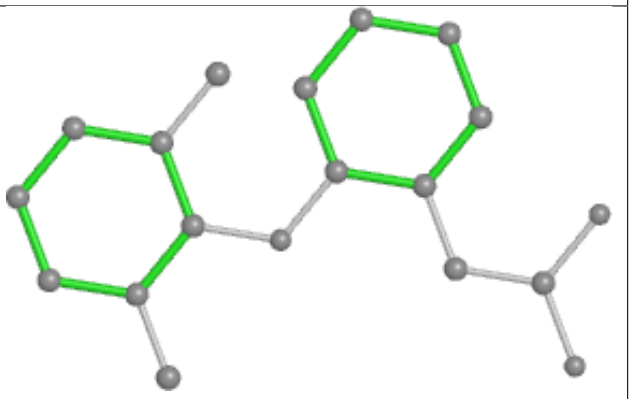


Bond angles

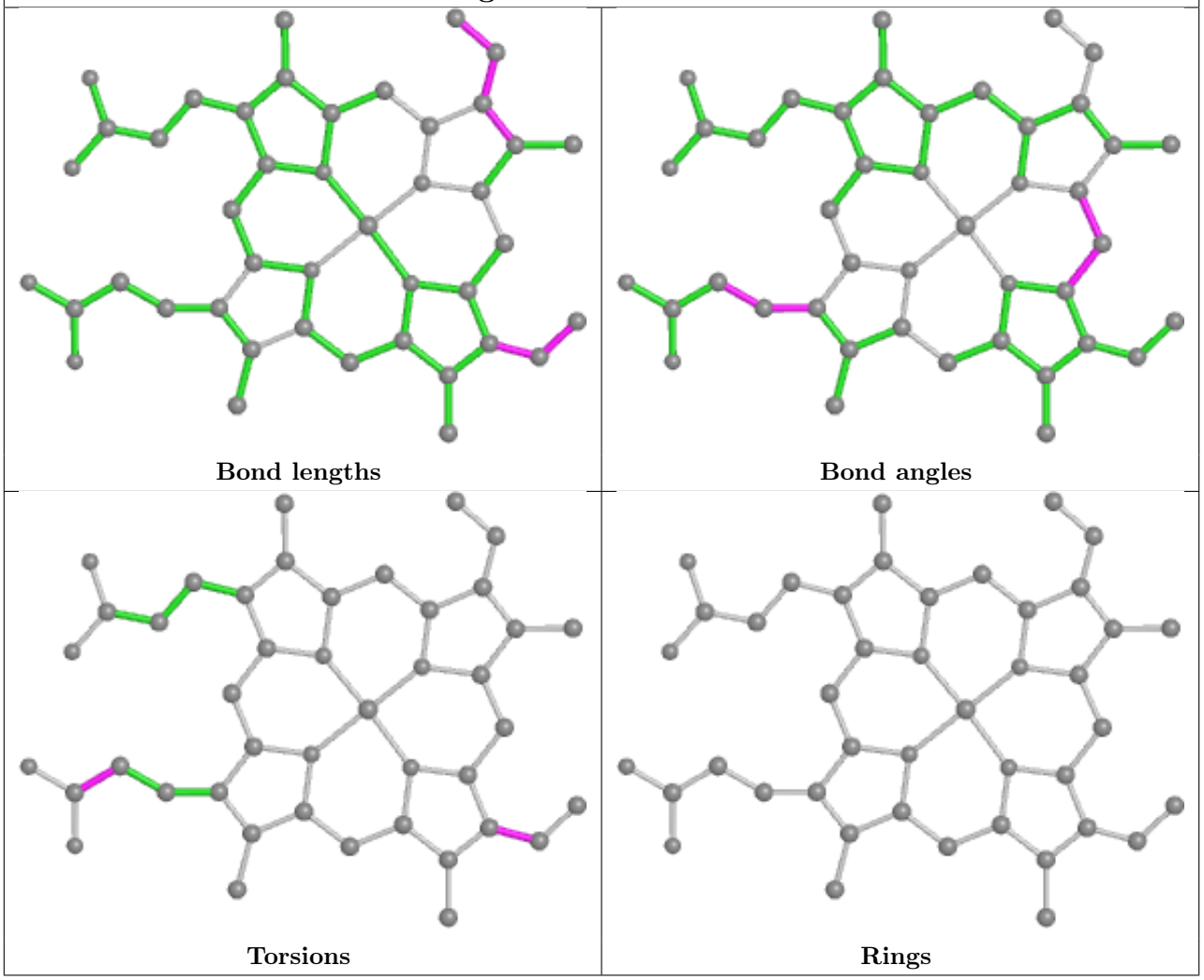


Torsions



Rings

Ligand HEM C 2601



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	552/604 (91%)	0.07	13 (2%)	59	56	5, 21, 42, 53	0
1	B	552/604 (91%)	0.11	14 (2%)	57	55	5, 21, 42, 58	0
1	C	552/604 (91%)	0.03	8 (1%)	75	75	3, 21, 41, 62	0
1	D	552/604 (91%)	0.16	11 (1%)	65	63	5, 21, 42, 55	0
All	All	2208/2416 (91%)	0.09	46 (2%)	63	61	3, 21, 42, 62	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1583	GLN	5.4
1	C	2583	GLN	4.7
1	D	3368	ASN	3.3
1	D	3401	GLU	2.9
1	A	82	LEU	2.8
1	C	2082	LEU	2.8
1	B	1399	ASP	2.8
1	B	1121	SER	2.7
1	B	1081	LEU	2.6
1	B	1188	ILE	2.6
1	D	3121	SER	2.6
1	D	3399	ASP	2.5
1	D	3069	CYS	2.5
1	C	2399	ASP	2.5
1	D	3409	TYR	2.4
1	D	3282	ASN	2.4
1	B	1368	ASN	2.4
1	B	1575	CYS	2.4
1	A	33	ALA	2.4
1	D	3049	SER	2.4
1	A	53	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	3268	ASP	2.4
1	A	98	GLY	2.3
1	A	258	GLY	2.3
1	B	1096	PHE	2.3
1	B	1053	ASP	2.3
1	A	409	TYR	2.3
1	B	1082	LEU	2.3
1	D	3278	HIS	2.3
1	A	282	ASN	2.2
1	A	84	PRO	2.2
1	C	2059	CYS	2.2
1	D	3583	GLN	2.2
1	A	107	PHE	2.1
1	C	2053	ASP	2.1
1	C	2074	PHE	2.1
1	B	1097	LYS	2.1
1	C	2084	PRO	2.1
1	B	1416	GLU	2.1
1	C	2416	GLU	2.1
1	A	122	TYR	2.1
1	A	214	HIS	2.1
1	A	34	ASN	2.1
1	B	1515	ASP	2.0
1	A	318	GLN	2.0
1	B	1039	ASN	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	3	14/15	0.34	0.51	51,66,71,72	0
2	NAG	G	3	14/15	0.37	0.66	66,71,73,74	0
2	NAG	F	3	14/15	0.42	0.61	41,65,67,69	0

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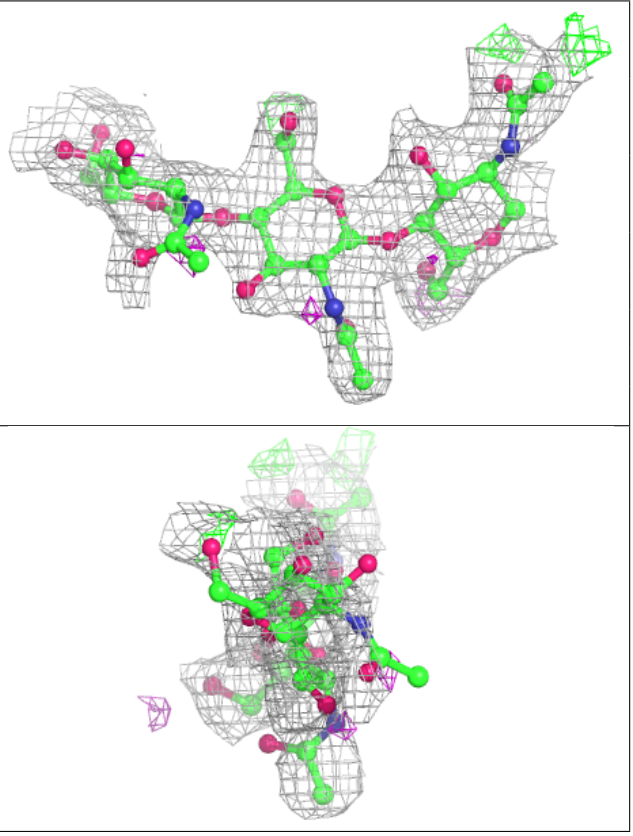
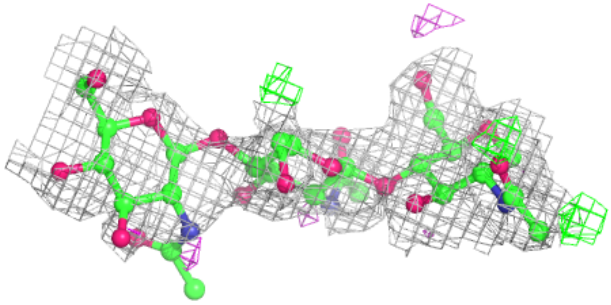
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	E	3	14/15	0.56	0.53	58,64,72,73	0
2	NAG	E	2	14/15	0.74	0.38	44,51,56,57	0
2	NAG	G	2	14/15	0.75	0.34	50,55,62,65	0
2	NAG	F	2	14/15	0.81	0.31	51,57,61,61	0
2	NAG	H	2	14/15	0.82	0.31	44,50,55,59	0
2	NAG	F	1	14/15	0.85	0.23	17,25,39,43	0
2	NAG	E	1	14/15	0.86	0.20	18,26,30,38	0
2	NAG	H	1	14/15	0.88	0.22	18,23,26,36	0
2	NAG	G	1	14/15	0.91	0.18	22,27,40,46	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:

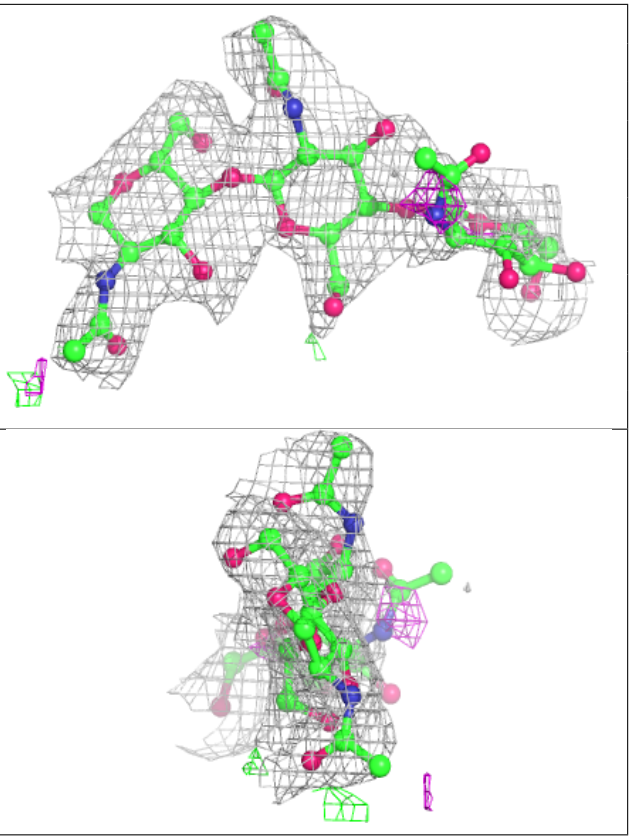
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





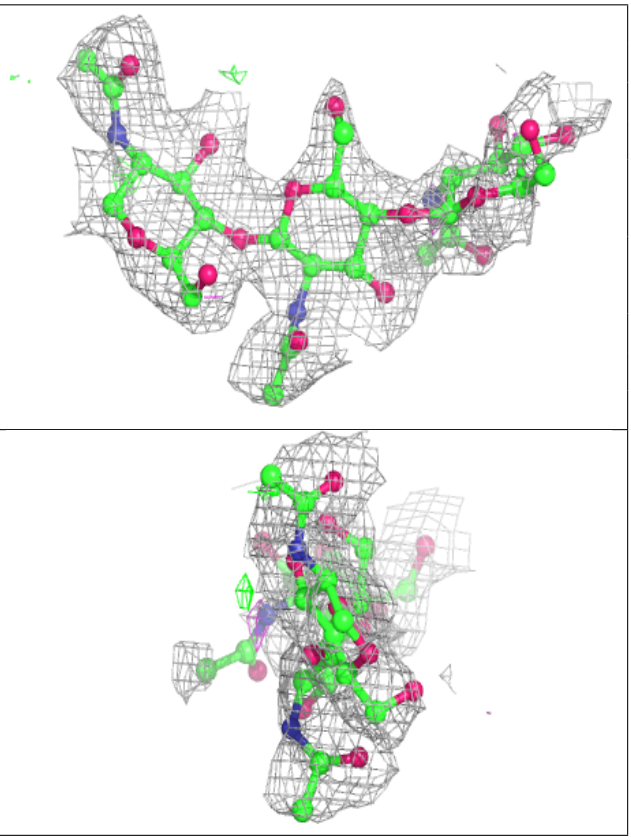
Electron density around Chain F:

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



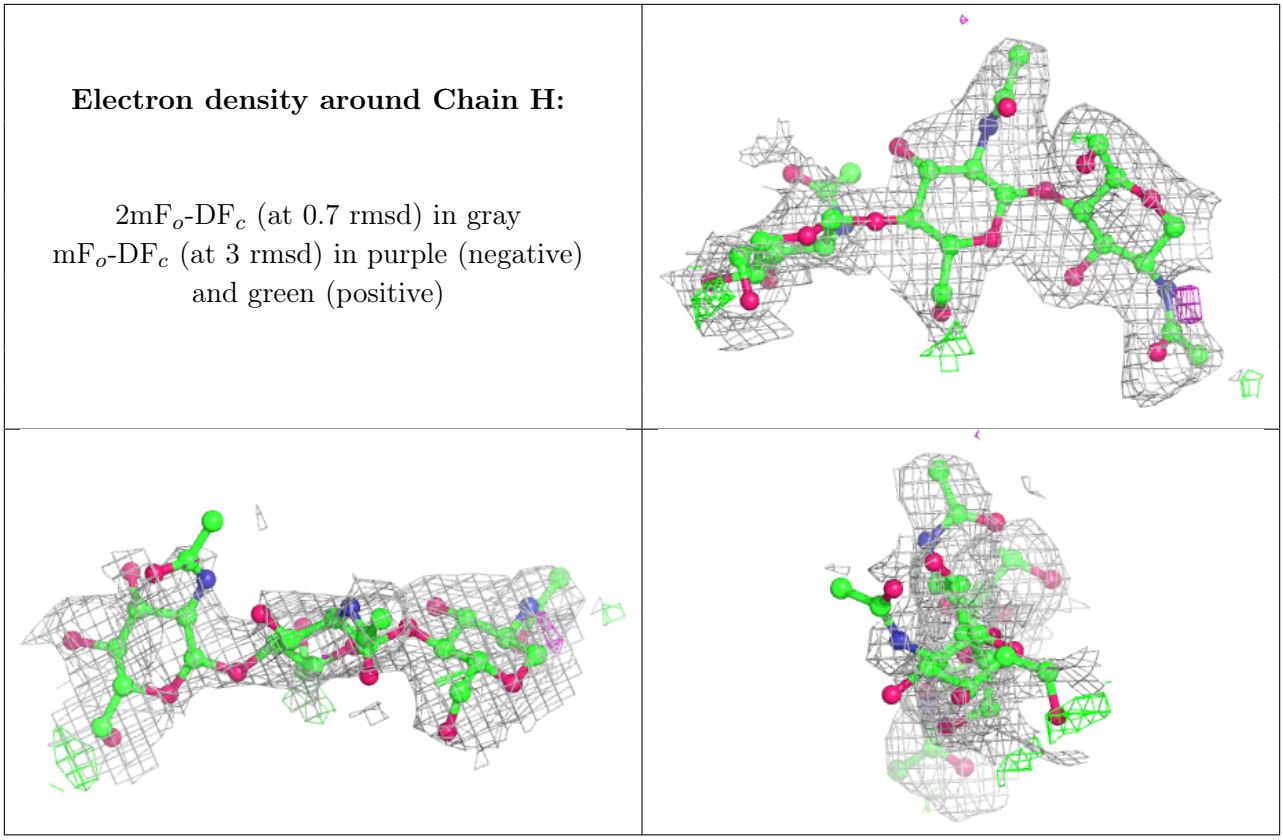
Electron density around Chain G:

$2mF_o$-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
3	NAG	B	1661	14/15	0.68	0.35	55,58,61,62	0
3	NAG	C	2661	14/15	0.77	0.32	45,54,61,63	0
3	NAG	B	1681	14/15	0.78	0.38	46,48,56,56	0
3	NAG	D	3661	14/15	0.79	0.46	51,55,59,61	0
3	NAG	A	661	14/15	0.80	0.42	55,57,61,61	0
3	NAG	C	2681	14/15	0.82	0.34	44,46,56,57	0
3	NAG	A	681	14/15	0.84	0.27	44,48,51,52	0
3	NAG	D	3681	14/15	0.84	0.36	47,51,59,62	0
6	DIF	B	1701	19/19	0.88	0.23	13,31,51,52	0
6	DIF	D	3701	19/19	0.88	0.20	17,38,44,55	0
4	BOG	D	3703	19/20	0.89	0.23	19,22,30,30	0
6	DIF	A	701	19/19	0.89	0.24	28,30,46,48	0
5	HEM	D	3601	43/43	0.90	0.21	13,21,41,43	0
6	DIF	C	2701	19/19	0.90	0.24	9,29,57,58	0

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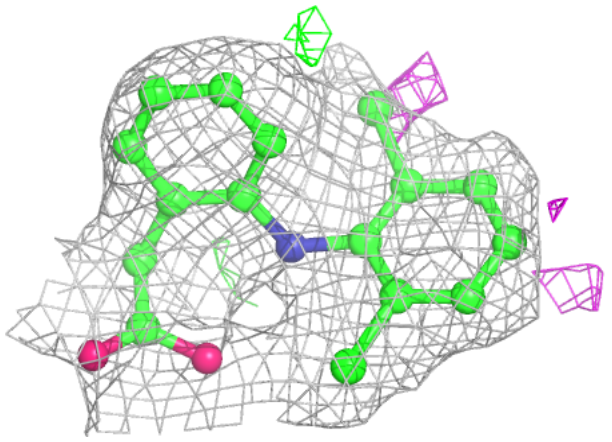
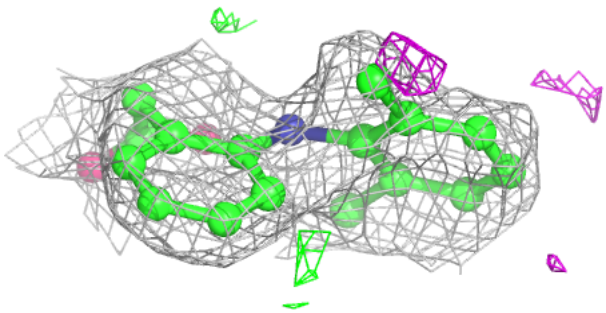
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	BOG	A	703	20/20	0.90	0.23	17,20,24,25	0
5	HEM	B	1601	43/43	0.91	0.21	4,22,48,54	0
5	HEM	A	704	43/43	0.94	0.17	2,15,36,43	0
5	HEM	C	2601	43/43	0.95	0.15	8,20,35,40	0

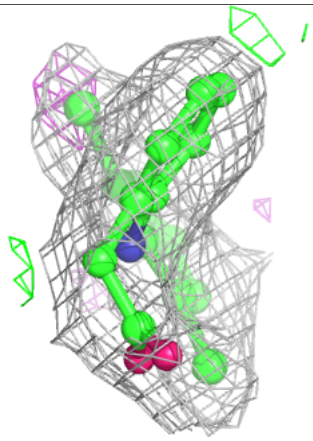
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around DIF B 1701:

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

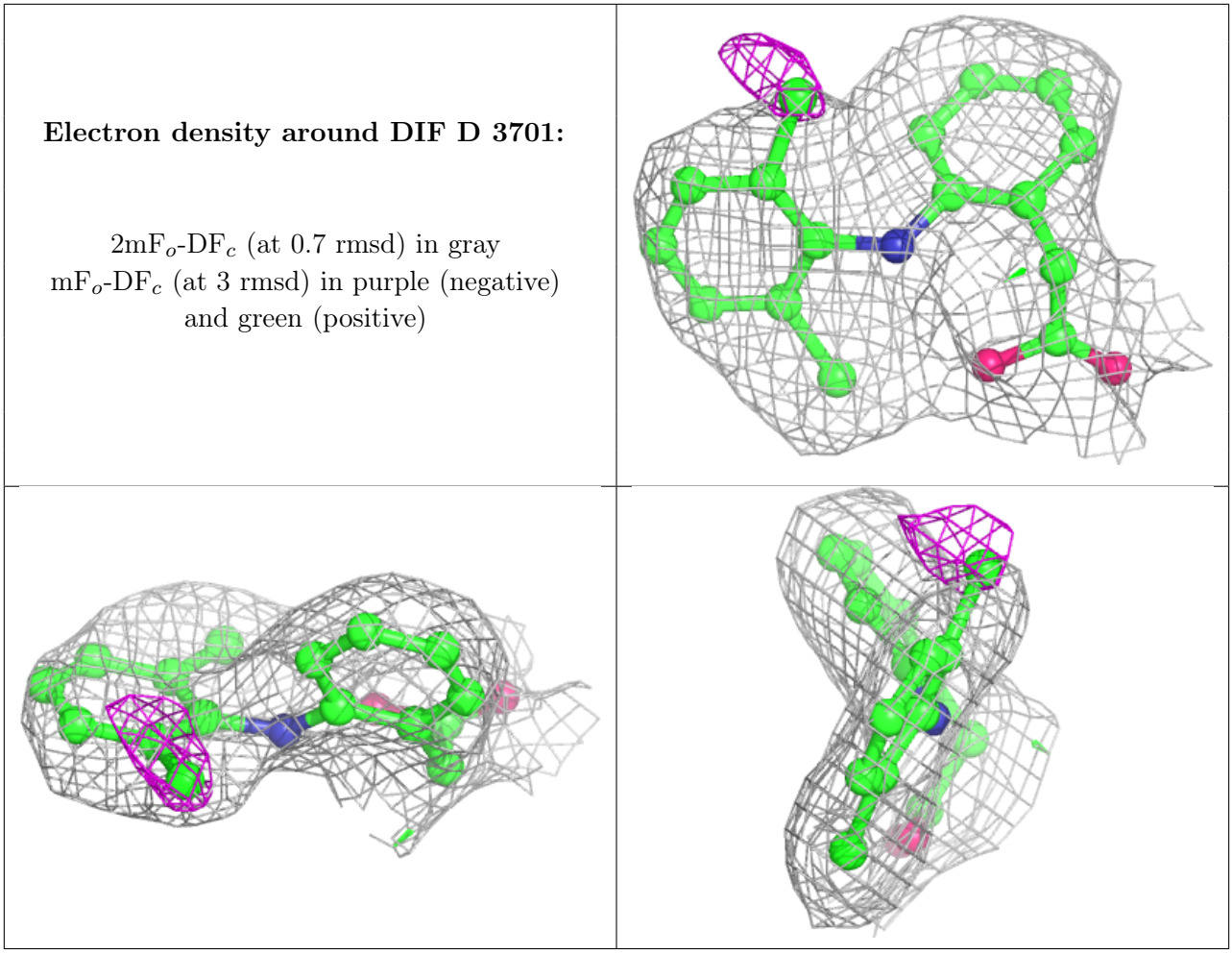






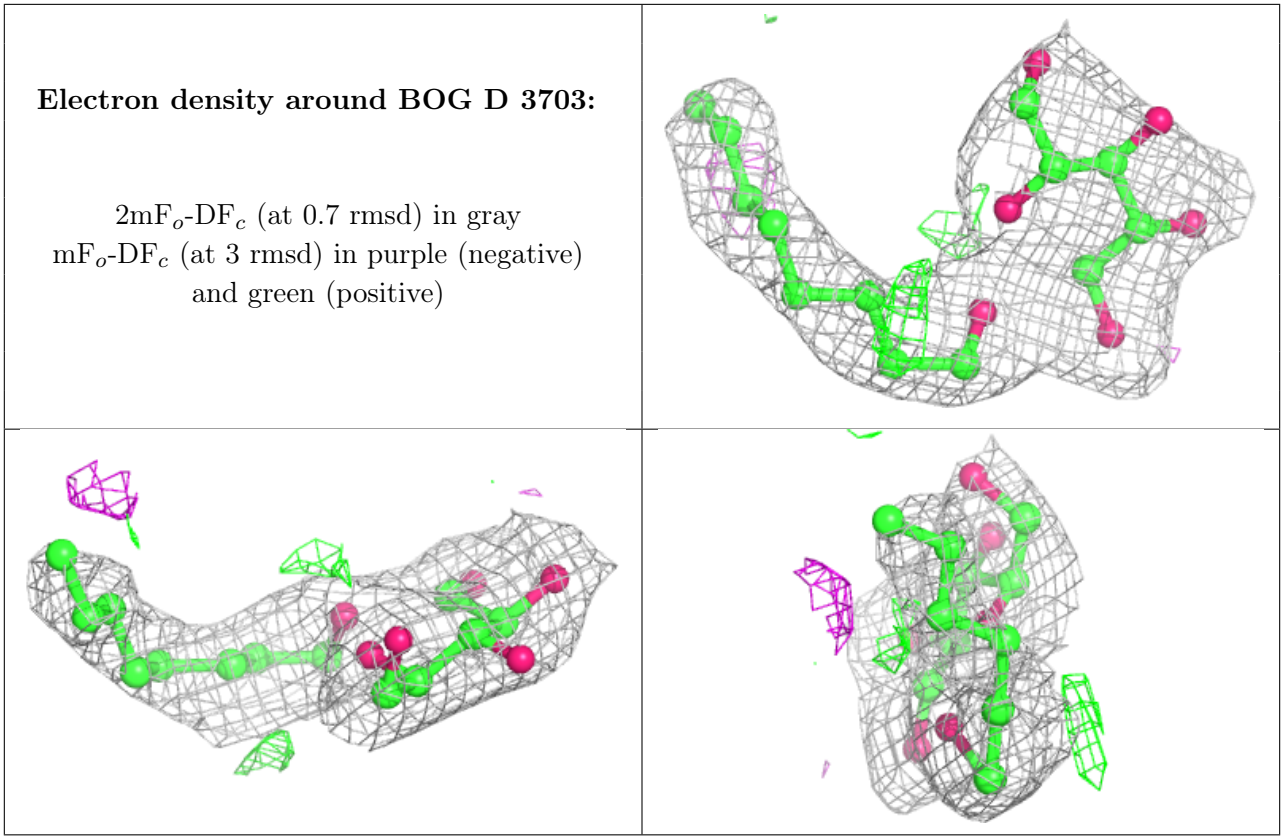
Electron density around DIF D 3701:

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



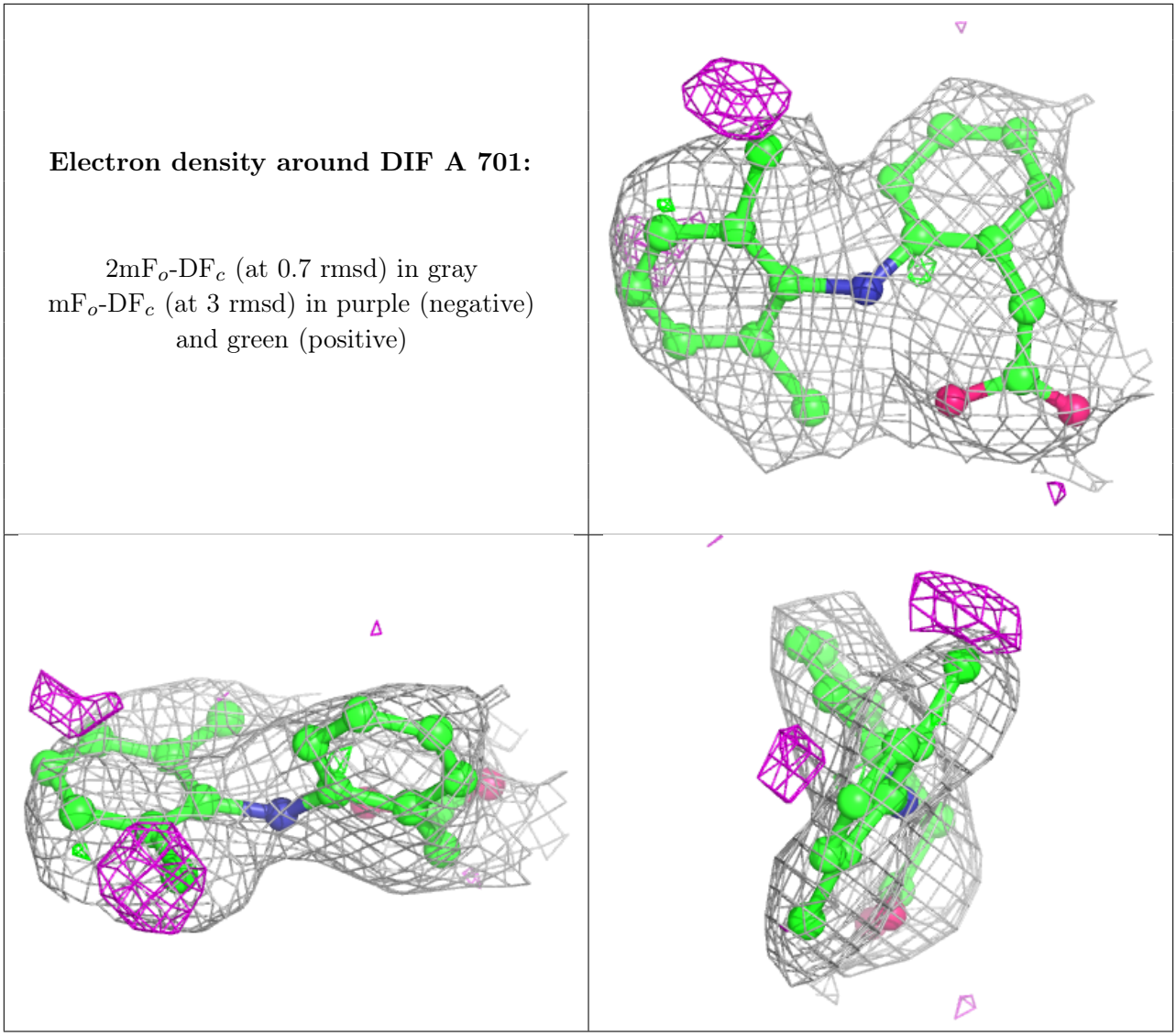
Electron density around BOG D 3703:

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



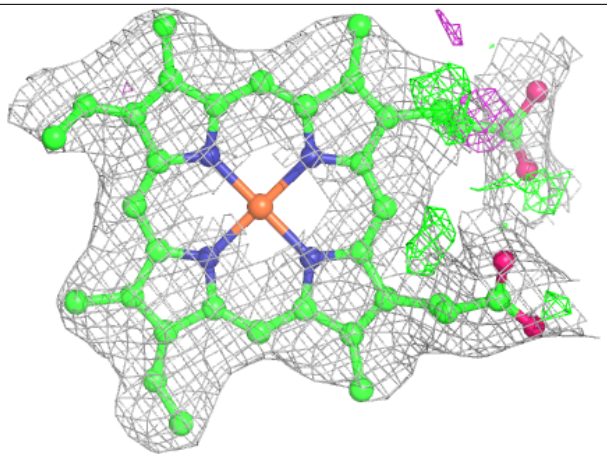
Electron density around DIF A 701:

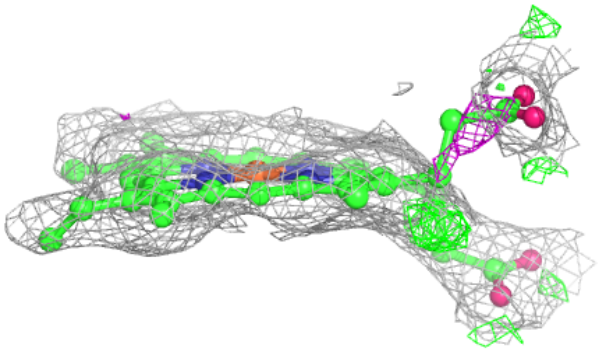
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

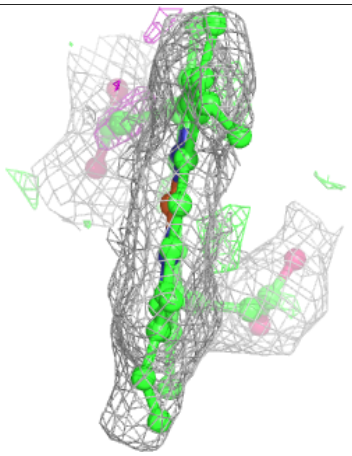


Electron density around HEM D 3601:

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

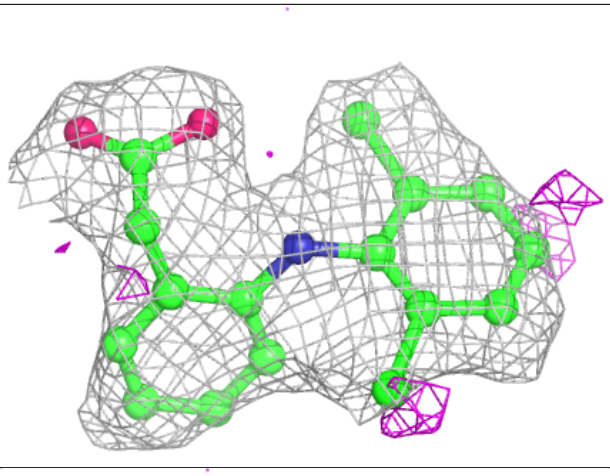


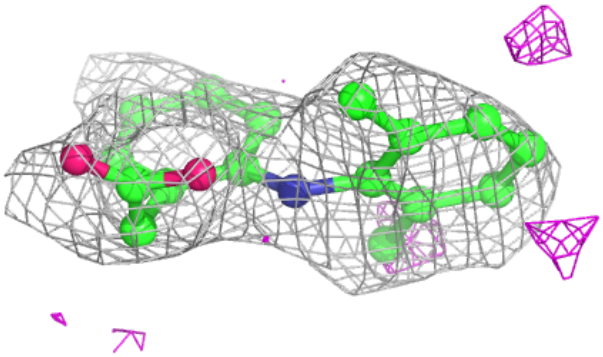


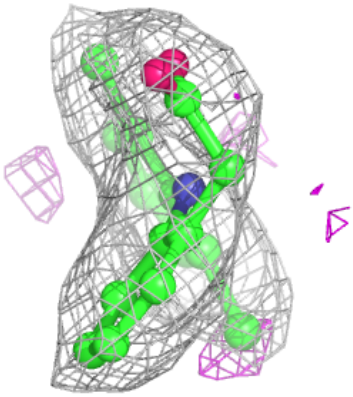


Electron density around DIF C 2701:

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

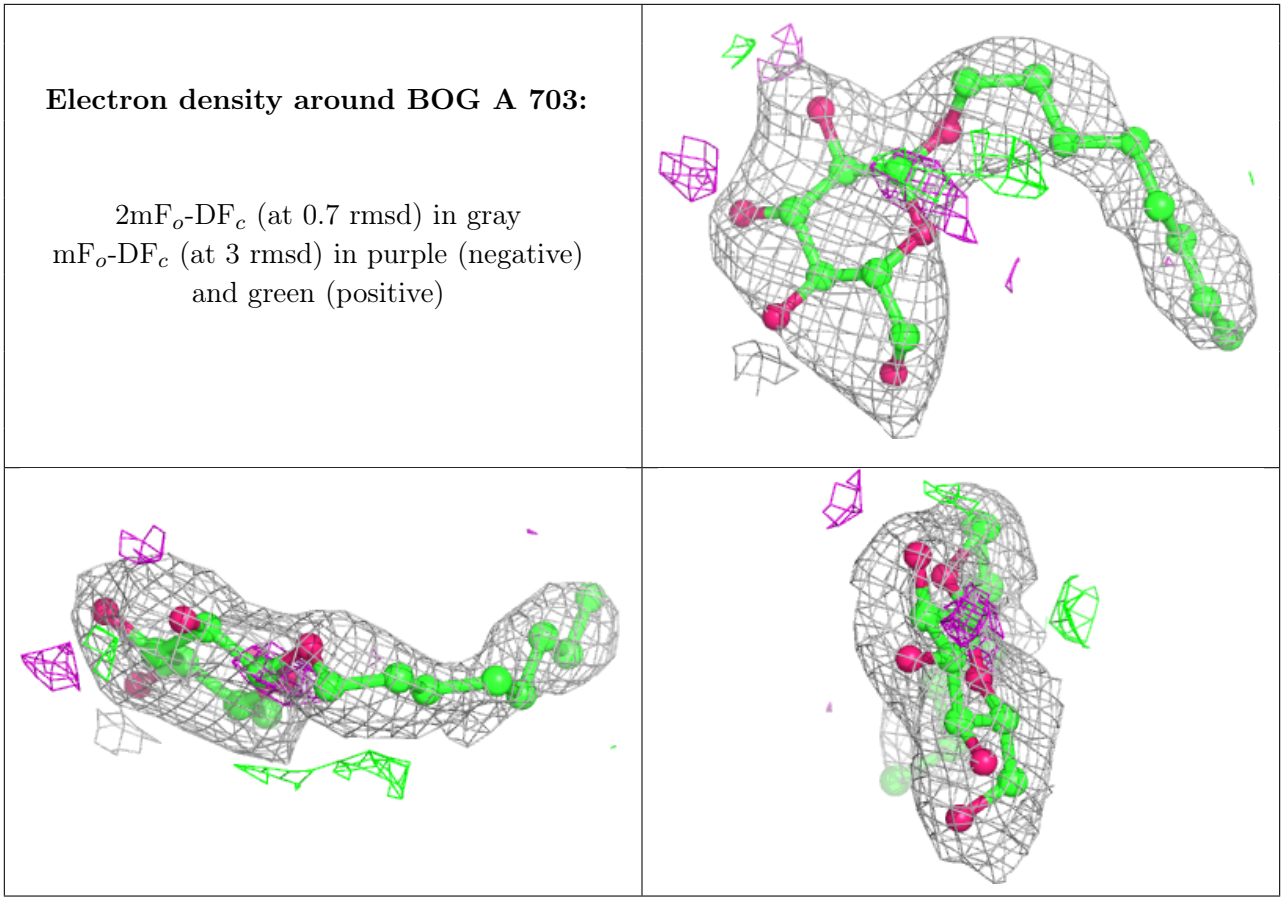






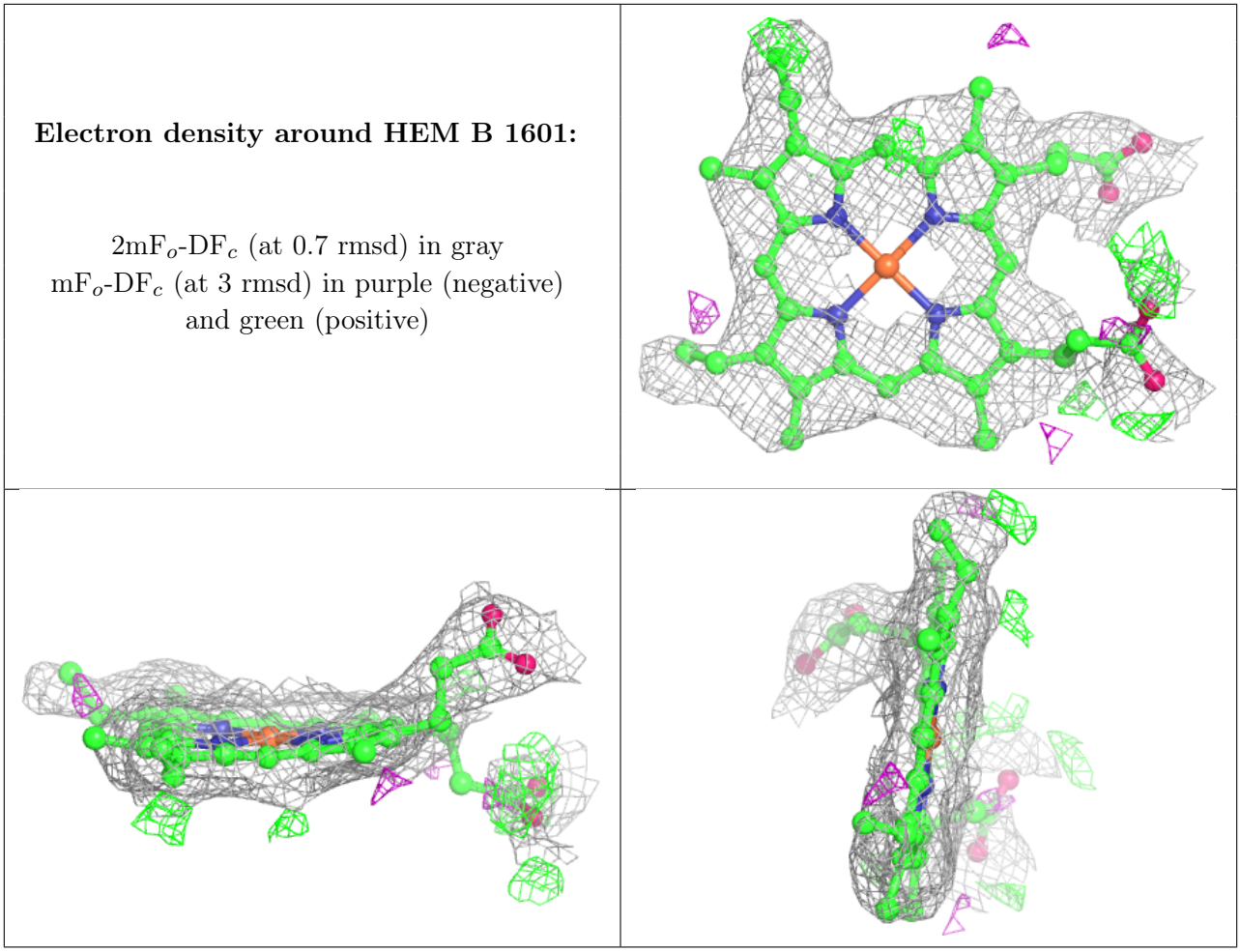
Electron density around BOG A 703:

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



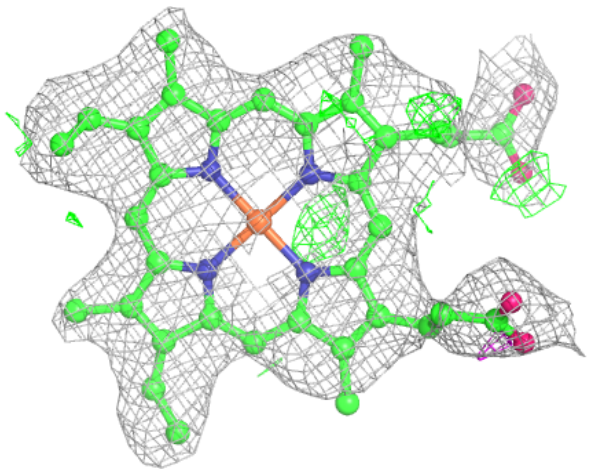
Electron density around HEM B 1601:

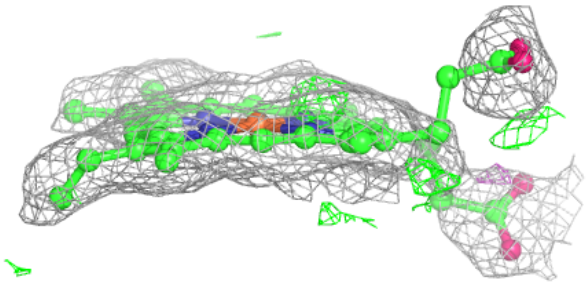
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

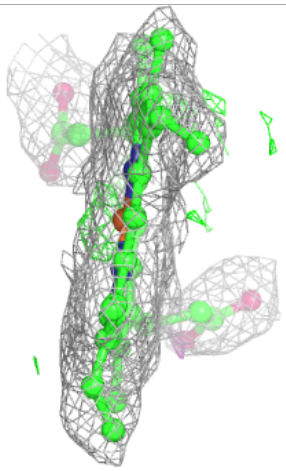


Electron density around HEM A 704:

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

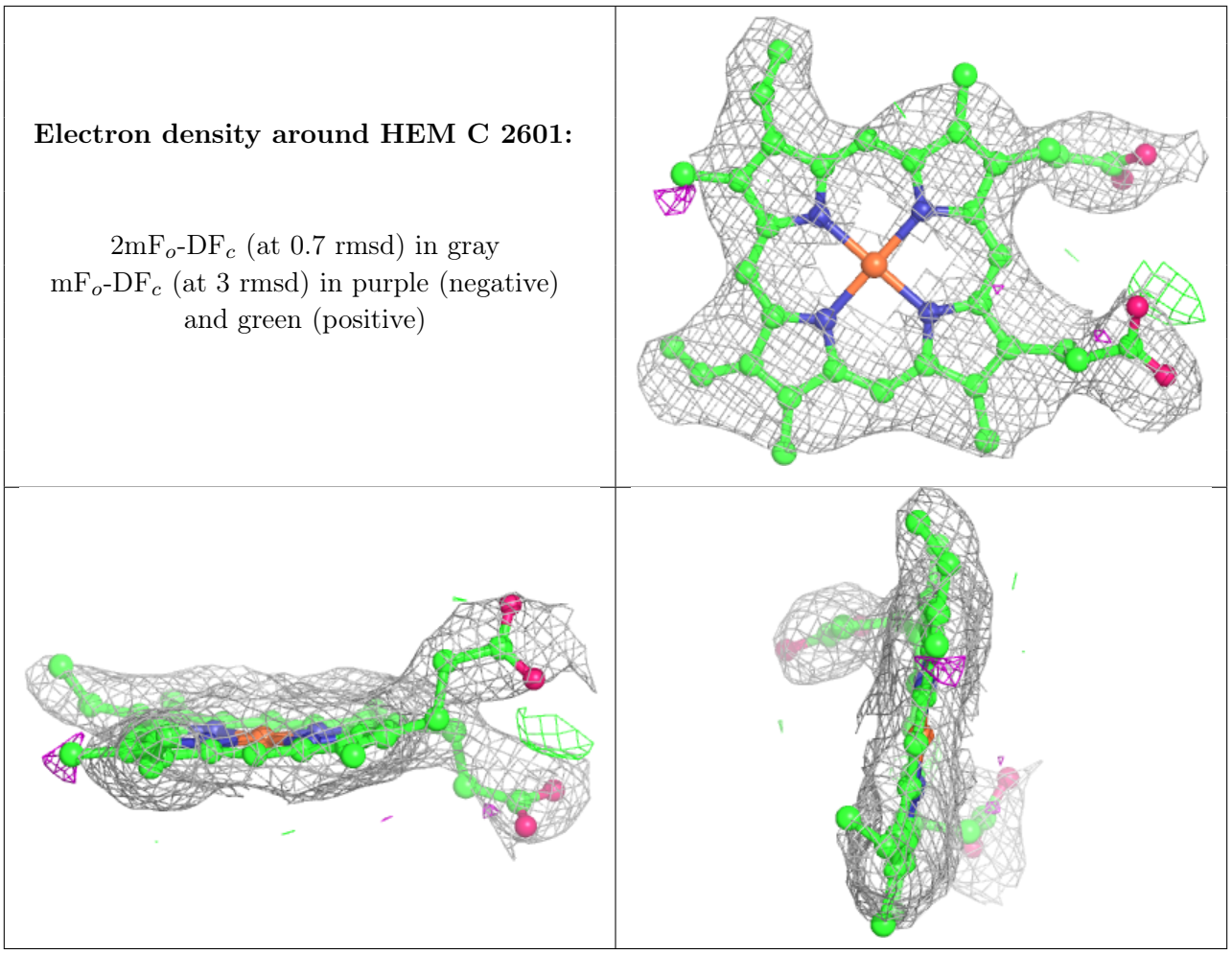






Electron density around HEM C 2601:

$2mF_o$-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.