Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 04:48 PM UTC

PDB ID	:	3R1B / pdb_00003r1b
Title	:	Open crystal structure of cytochrome P450 2B4 covalently bound to the mechanism-based inactivator tert-butylphenylacetylene
Authors	:	Gay, S.C.; Zhang, H.; Stout, C.D.; Hollenberg, P.F.; Halpert, J.R.
Deposited on	:	2011-03-09
Resolution	:	3.00 Å(reported)

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

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

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

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

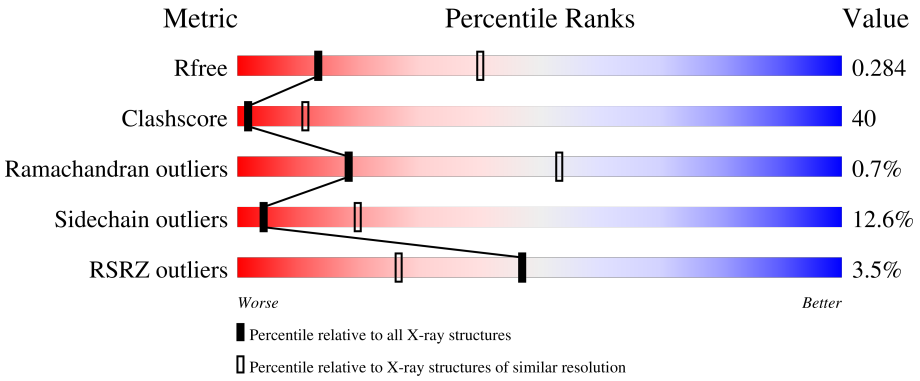
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	476	2% 55% 34% 8%
1	B	476	3% 49% 39% 8%
1	C	476	4% 47% 38% 10%
1	D	476	5% 40% 45% 11%
2	E	2	100%

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GLC	F	1	-	-	X	-
2	FRU	F	2	-	-	X	-
2	GLC	H	1	-	-	X	-
2	FRU	H	2	-	-	X	-
3	HEM	D	500	-	-	X	-
4	TB2	A	501	-	-	X	-
4	TB2	C	501	-	-	X	-
4	TB2	D	501	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 14499 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 Cytochrome P450 2B4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	465	Total 3583	C 2294	N 619	O 659	S 11	2	0	0
1	B	465	Total 3589	C 2308	N 615	O 656	S 10	2	0	0
1	C	456	Total 3406	C 2171	N 589	O 638	S 8	1	0	0
1	D	464	Total 3445	C 2199	N 598	O 640	S 8	0	0	0

There are 132 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	21	ALA	GLU	engineered mutation	UNP P00178
A	?	-	PHE	deletion	UNP P00178
A	?	-	SER	deletion	UNP P00178
A	?	-	LEU	deletion	UNP P00178
A	?	-	LEU	deletion	UNP P00178
A	?	-	LEU	deletion	UNP P00178
A	?	-	LEU	deletion	UNP P00178
A	?	-	LEU	deletion	UNP P00178
A	?	-	ALA	deletion	UNP P00178
A	?	-	PHE	deletion	UNP P00178
A	?	-	LEU	deletion	UNP P00178
A	?	-	ALA	deletion	UNP P00178
A	?	-	GLY	deletion	UNP P00178
A	?	-	LEU	deletion	UNP P00178
A	?	-	LEU	deletion	UNP P00178
A	?	-	LEU	deletion	UNP P00178
A	?	-	LEU	deletion	UNP P00178
A	?	-	LEU	deletion	UNP P00178
A	?	-	PHE	deletion	UNP P00178
A	?	-	ARG	deletion	UNP P00178
A	22	LYS	GLY	engineered mutation	UNP P00178

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Chain	Residue	Modelled	Actual	Comment	Reference
A	23	LYS	HIS	engineered mutation	UNP P00178
A	24	THR	PRO	engineered mutation	UNP P00178
A	25	SER	LYS	engineered mutation	UNP P00178
A	26	SER	ALA	engineered mutation	UNP P00178
A	27	LYS	HIS	engineered mutation	UNP P00178
A	29	LYS	ARG	engineered mutation	UNP P00178
A	221	SER	PRO	conflict	UNP P00178
A	226	TYR	HIS	engineered mutation	UNP P00178
A	492	HIS	-	expression tag	UNP P00178
A	493	HIS	-	expression tag	UNP P00178
A	494	HIS	-	expression tag	UNP P00178
A	495	HIS	-	expression tag	UNP P00178
B	21	ALA	GLU	engineered mutation	UNP P00178
B	?	-	PHE	deletion	UNP P00178
B	?	-	SER	deletion	UNP P00178
B	?	-	LEU	deletion	UNP P00178
B	?	-	LEU	deletion	UNP P00178
B	?	-	LEU	deletion	UNP P00178
B	?	-	LEU	deletion	UNP P00178
B	?	-	LEU	deletion	UNP P00178
B	?	-	ALA	deletion	UNP P00178
B	?	-	PHE	deletion	UNP P00178
B	?	-	LEU	deletion	UNP P00178
B	?	-	ALA	deletion	UNP P00178
B	?	-	GLY	deletion	UNP P00178
B	?	-	LEU	deletion	UNP P00178
B	?	-	LEU	deletion	UNP P00178
B	?	-	LEU	deletion	UNP P00178
B	?	-	LEU	deletion	UNP P00178
B	?	-	LEU	deletion	UNP P00178
B	?	-	PHE	deletion	UNP P00178
B	?	-	ARG	deletion	UNP P00178
B	22	LYS	GLY	engineered mutation	UNP P00178
B	23	LYS	HIS	engineered mutation	UNP P00178
B	24	THR	PRO	engineered mutation	UNP P00178
B	25	SER	LYS	engineered mutation	UNP P00178
B	26	SER	ALA	engineered mutation	UNP P00178
B	27	LYS	HIS	engineered mutation	UNP P00178
B	29	LYS	ARG	engineered mutation	UNP P00178
B	221	SER	PRO	conflict	UNP P00178
B	226	TYR	HIS	engineered mutation	UNP P00178
B	492	HIS	-	expression tag	UNP P00178

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Chain	Residue	Modelled	Actual	Comment	Reference
B	493	HIS	-	expression tag	UNP P00178
B	494	HIS	-	expression tag	UNP P00178
B	495	HIS	-	expression tag	UNP P00178
C	21	ALA	GLU	engineered mutation	UNP P00178
C	?	-	PHE	deletion	UNP P00178
C	?	-	SER	deletion	UNP P00178
C	?	-	LEU	deletion	UNP P00178
C	?	-	LEU	deletion	UNP P00178
C	?	-	LEU	deletion	UNP P00178
C	?	-	LEU	deletion	UNP P00178
C	?	-	LEU	deletion	UNP P00178
C	?	-	ALA	deletion	UNP P00178
C	?	-	PHE	deletion	UNP P00178
C	?	-	LEU	deletion	UNP P00178
C	?	-	ALA	deletion	UNP P00178
C	?	-	GLY	deletion	UNP P00178
C	?	-	LEU	deletion	UNP P00178
C	?	-	LEU	deletion	UNP P00178
C	?	-	LEU	deletion	UNP P00178
C	?	-	LEU	deletion	UNP P00178
C	?	-	LEU	deletion	UNP P00178
C	?	-	PHE	deletion	UNP P00178
C	?	-	ARG	deletion	UNP P00178
C	22	LYS	GLY	engineered mutation	UNP P00178
C	23	LYS	HIS	engineered mutation	UNP P00178
C	24	THR	PRO	engineered mutation	UNP P00178
C	25	SER	LYS	engineered mutation	UNP P00178
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C	221	SER	PRO	conflict	UNP P00178
C	226	TYR	HIS	engineered mutation	UNP P00178
C	492	HIS	-	expression tag	UNP P00178
C	493	HIS	-	expression tag	UNP P00178
C	494	HIS	-	expression tag	UNP P00178
C	495	HIS	-	expression tag	UNP P00178
D	21	ALA	GLU	engineered mutation	UNP P00178
D	?	-	PHE	deletion	UNP P00178
D	?	-	SER	deletion	UNP P00178
D	?	-	LEU	deletion	UNP P00178
D	?	-	LEU	deletion	UNP P00178
D	?	-	LEU	deletion	UNP P00178

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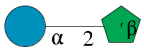
Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	LEU	deletion	UNP P00178
D	?	-	LEU	deletion	UNP P00178
D	?	-	ALA	deletion	UNP P00178
D	?	-	PHE	deletion	UNP P00178
D	?	-	LEU	deletion	UNP P00178
D	?	-	ALA	deletion	UNP P00178
D	?	-	GLY	deletion	UNP P00178
D	?	-	LEU	deletion	UNP P00178
D	?	-	LEU	deletion	UNP P00178
D	?	-	LEU	deletion	UNP P00178
D	?	-	LEU	deletion	UNP P00178
D	?	-	LEU	deletion	UNP P00178
D	?	-	PHE	deletion	UNP P00178
D	?	-	ARG	deletion	UNP P00178
D	22	LYS	GLY	engineered mutation	UNP P00178
D	23	LYS	HIS	engineered mutation	UNP P00178
D	24	THR	PRO	engineered mutation	UNP P00178
D	25	SER	LYS	engineered mutation	UNP P00178
D	26	SER	ALA	engineered mutation	UNP P00178
D	27	LYS	HIS	engineered mutation	UNP P00178
D	29	LYS	ARG	engineered mutation	UNP P00178
D	221	SER	PRO	conflict	UNP P00178
D	226	TYR	HIS	engineered mutation	UNP P00178
D	492	HIS	-	expression tag	UNP P00178
D	493	HIS	-	expression tag	UNP P00178
D	494	HIS	-	expression tag	UNP P00178
D	495	HIS	-	expression tag	UNP P00178

- Molecule 2 is an oligosaccharide called beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	E	2	Total C O 23 12 11	0	0	0
2	F	2	Total C O 23 12 11	0	0	0
2	G	2	Total C O 23 12 11	0	0	0

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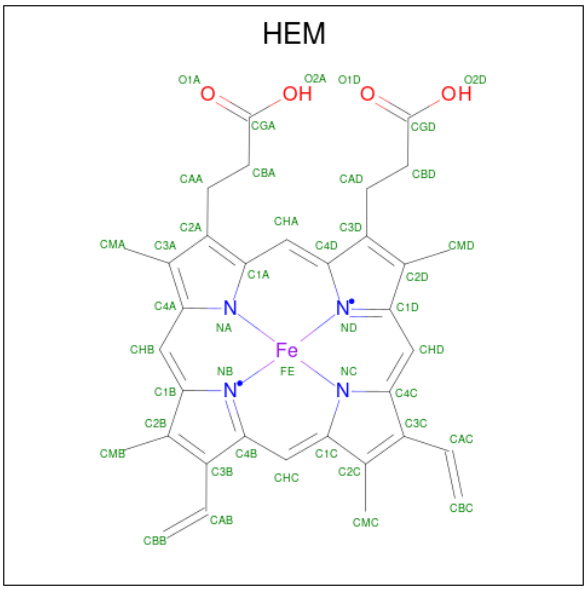
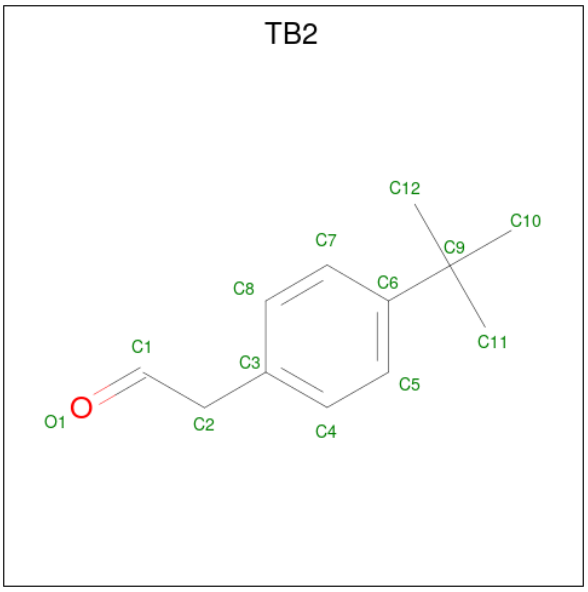
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	H	2	Total C O 23 12 11	0	0	0

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



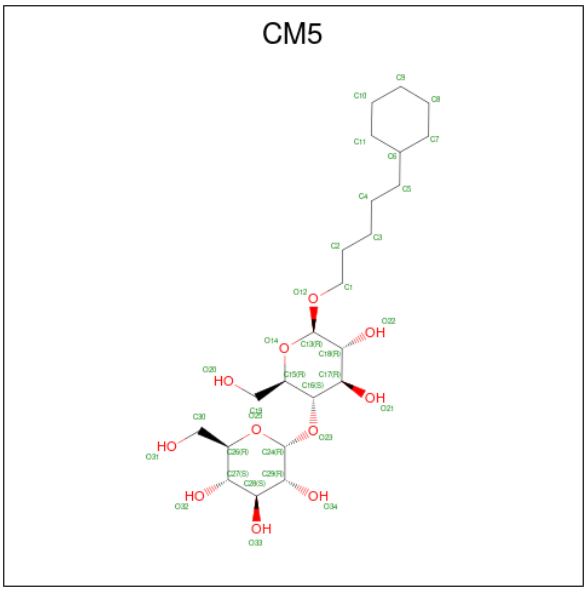
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C Fe N O 43 34 1 4 4	0	0
3	B	1	Total C Fe N O 43 34 1 4 4	0	0
3	C	1	Total C Fe N O 43 34 1 4 4	0	0
3	D	1	Total C Fe N O 43 34 1 4 4	0	0

- Molecule 4 is (4-tert-butylphenyl)acetaldehyde (CCD ID: TB2) (formula: $C_{12}H_{16}O$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 13 12 1	0	0
4	B	1	Total C O 13 12 1	0	0
4	C	1	Total C O 13 12 1	0	0
4	D	1	Total C O 13 12 1	0	0

- Molecule 5 is 5-CYCLOHEXYL-1-PENTYL-BETA-D-MALTOSIDE (CCD ID: CM5) (formula: $C_{23}H_{42}O_{11}$).



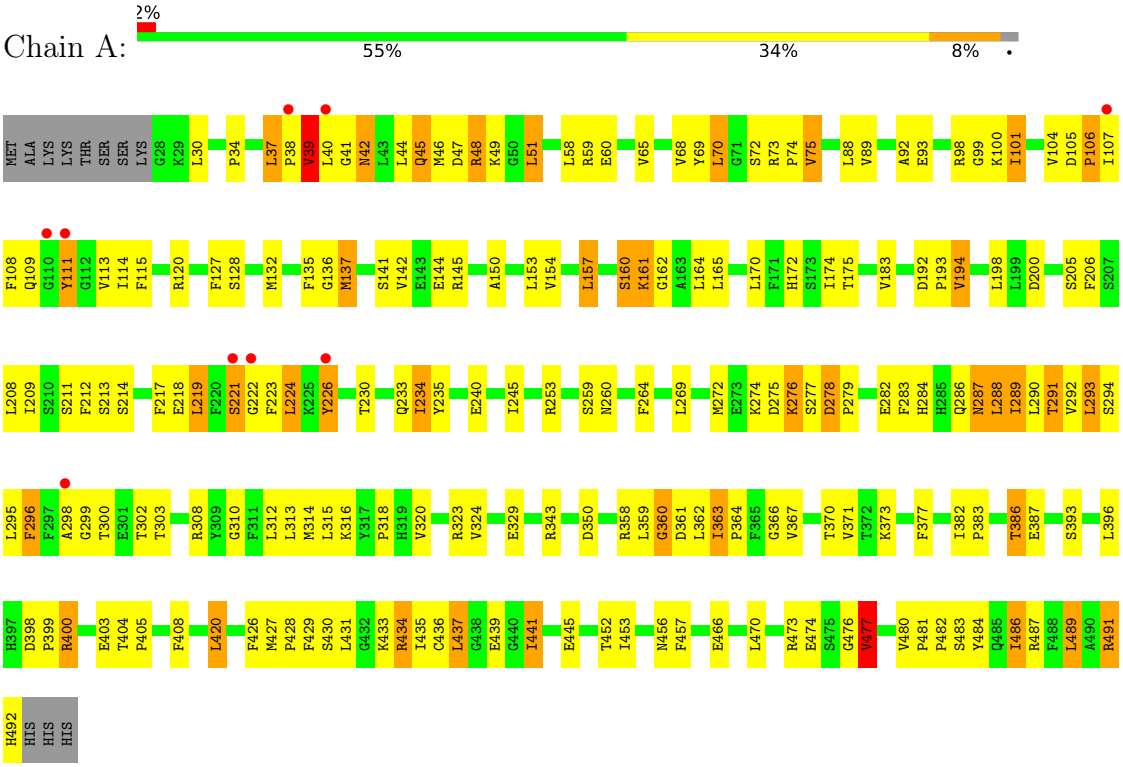
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			24	18	6		
5	A	1	Total	C	O	0	0
			34	23	11		
5	B	1	Total	C	O	0	0
			34	23	11		
5	B	1	Total	C	O	0	0
			34	23	11		
5	D	1	Total	C	O	0	0
			34	23	11		

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.

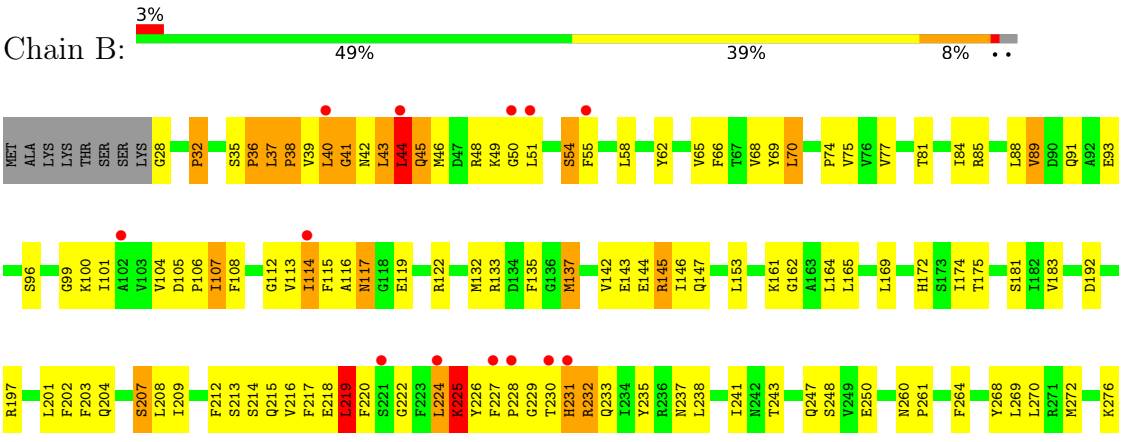
• Molecule 1: Cytochrome P450 2B4

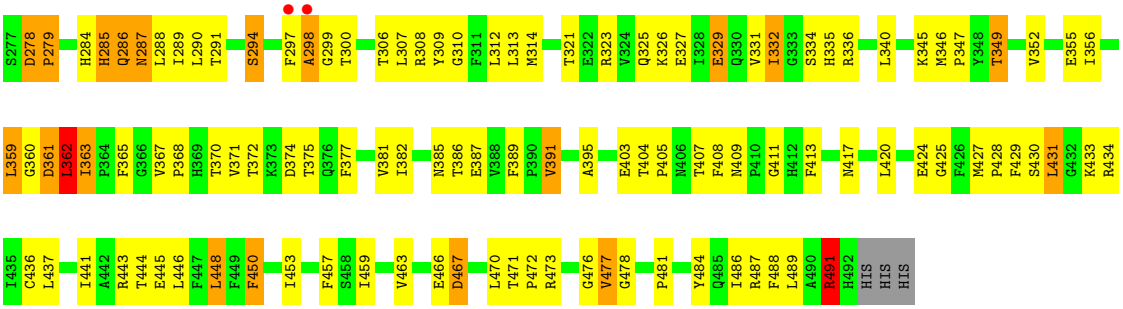
Chain A:



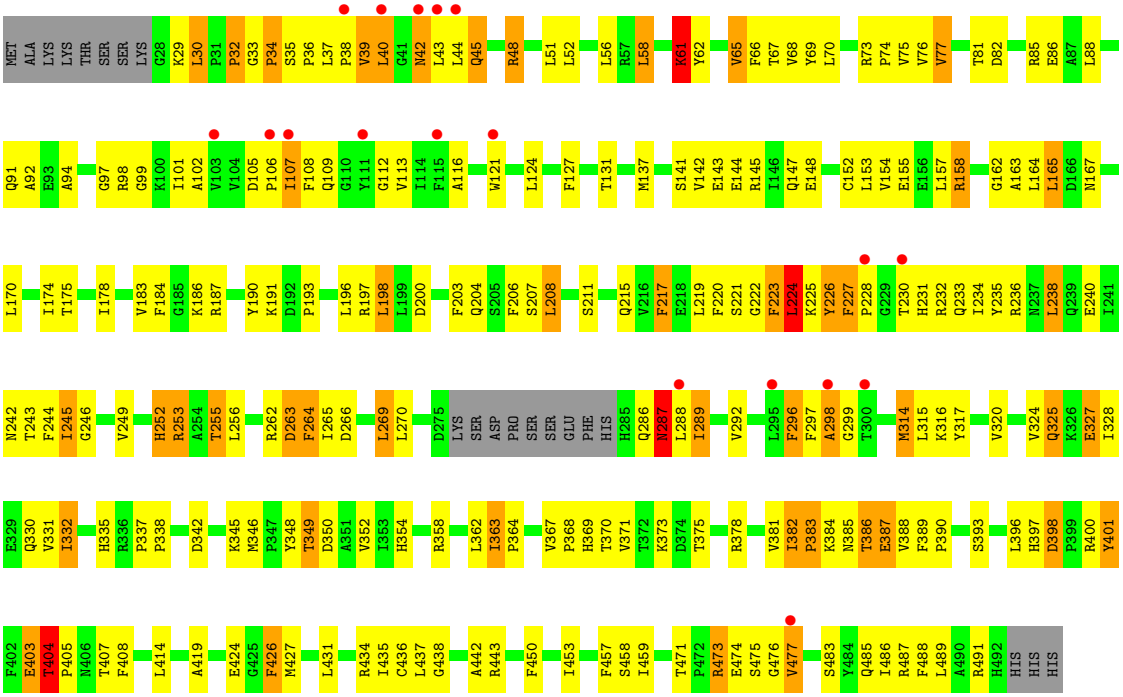
• Molecule 1: Cytochrome P450 2B4

Chain B:

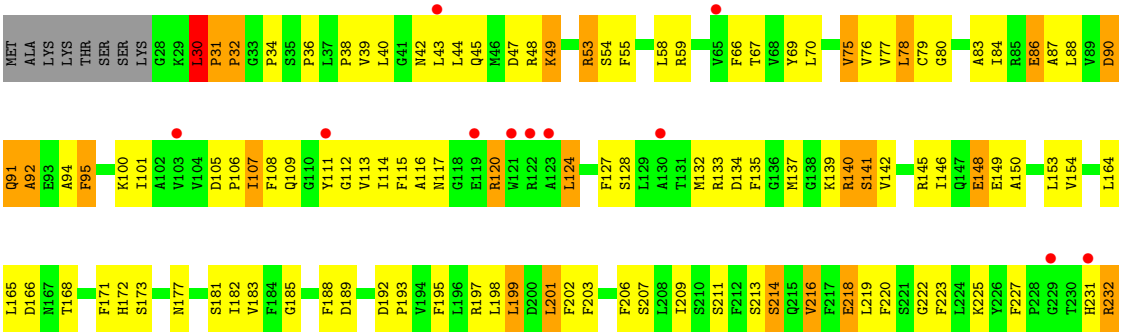


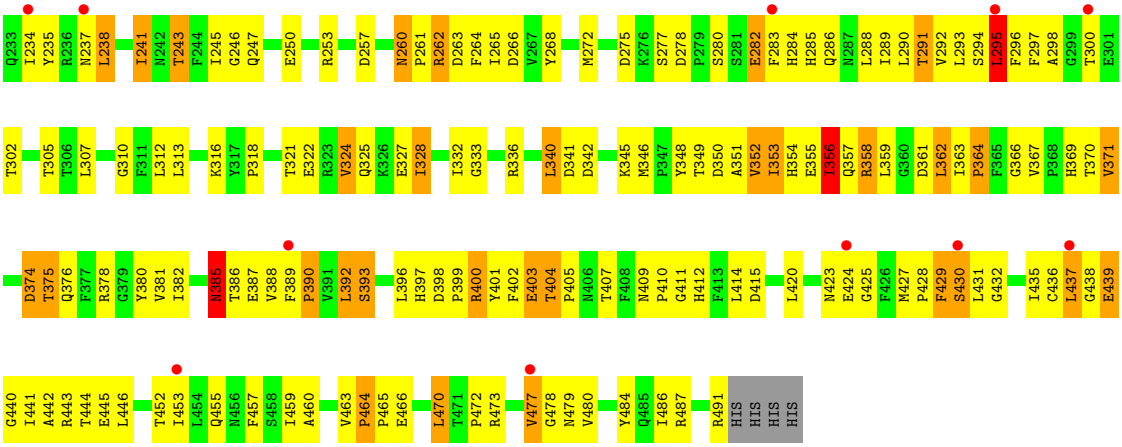


• Molecule 1: Cytochrome P450 2B4



• Molecule 1: Cytochrome P450 2B4





• Molecule 2: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain E:

• Molecule 2: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain F:

• Molecule 2: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain G:

• Molecule 2: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain H:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	193.92Å 153.69Å 129.66Å 90.00° 122.22° 90.00°	Depositor
Resolution (Å)	53.43 – 3.00 53.43 – 3.00	Depositor EDS
% Data completeness (in resolution range)	94.8 (53.43-3.00) 99.3 (53.43-3.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	1.82 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.6.4_486	Depositor
R, R_{free}	0.242 , 0.288 0.244 , 0.284	Depositor DCC
R_{free} test set	3237 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	92.5	Xtriage
Anisotropy	0.236	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 95.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	14499	wwPDB-VP
Average B, all atoms (Å^2)	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.28% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TB2, CM5, HEM, FRU, GLC

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	0.43	3/3672 (0.1%)	0.94	22/4995 (0.4%)
1	B	0.47	2/3679 (0.1%)	1.15	49/5003 (1.0%)
1	C	0.38	0/3484	1.11	37/4749 (0.8%)
1	D	0.44	0/3527	1.15	47/4814 (1.0%)
All	All	0.43	5/14362 (0.0%)	1.09	155/19561 (0.8%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	278	ASP	C-N	-9.04	1.25	1.33
1	A	161	LYS	CA-CB	-8.48	1.41	1.53
1	B	37	LEU	CA-CB	6.91	1.63	1.53
1	B	278	ASP	C-N	-5.94	1.28	1.33
1	A	221	SER	C-N	-5.07	1.27	1.33

All (155) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	107	ILE	N-CA-C	15.05	126.16	110.36
1	B	231	HIS	N-CA-C	-13.48	95.24	113.30
1	D	378	ARG	N-CA-C	11.74	127.12	113.38
1	B	37	LEU	N-CA-C	-10.66	94.85	110.20
1	B	335	HIS	N-CA-C	10.63	127.07	112.93
1	B	334	SER	N-CA-C	10.62	125.61	112.87
1	B	332	ILE	N-CA-C	10.55	120.88	111.81
1	B	45	GLN	N-CA-C	10.27	123.75	111.33
1	D	87	ALA	N-CA-C	10.01	124.16	111.24
1	A	89	VAL	N-CA-C	9.72	120.17	111.81
1	B	385	ASN	N-CA-C	9.66	125.01	112.26
1	D	237	ASN	N-CA-C	9.57	121.31	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	328	ILE	CB-CA-C	-9.56	99.64	111.88
1	B	32	PRO	CB-CA-C	-8.72	100.57	111.64
1	A	161	LYS	CB-CA-C	-8.60	100.34	111.86
1	C	92	ALA	N-CA-C	8.48	121.37	111.02
1	C	335	HIS	N-CA-C	8.48	123.97	112.68
1	A	37	LEU	N-CA-C	-8.45	97.38	110.14
1	C	220	PHE	N-CA-C	8.39	120.50	111.36
1	C	255	THR	N-CA-CB	-8.37	99.03	111.25
1	A	276	LYS	N-CA-C	-8.36	100.13	110.41
1	B	371	VAL	CB-CA-C	8.32	120.74	111.59
1	B	279	PRO	N-CA-C	-8.15	106.20	114.68
1	D	403	GLU	N-CA-C	8.15	123.45	111.96
1	C	264	PHE	N-CA-C	8.10	122.59	112.87
1	D	107	ILE	N-CA-C	7.91	117.85	110.42
1	D	218	GLU	N-CA-C	7.79	120.86	111.82
1	B	48	ARG	N-CA-C	7.61	127.00	110.80
1	C	224	LEU	N-CA-C	7.60	119.35	111.14
1	A	161	LYS	N-CA-CB	-7.59	100.37	111.91
1	C	298	ALA	N-CA-C	7.57	119.61	111.36
1	B	40	LEU	N-CA-C	7.50	122.56	112.88
1	B	363	ILE	CA-C-N	7.47	127.49	119.28
1	B	363	ILE	C-N-CA	7.47	127.49	119.28
1	C	256	LEU	CB-CA-C	-7.43	99.46	110.16
1	C	32	PRO	CB-CA-C	-7.42	101.73	111.23
1	C	61	LYS	N-CA-C	7.37	119.10	111.14
1	D	168	THR	N-CA-C	7.36	118.99	110.97
1	A	363	ILE	CA-C-N	7.29	126.82	119.24
1	A	363	ILE	C-N-CA	7.29	126.82	119.24
1	A	278	ASP	O-C-N	7.13	126.86	121.65
1	A	223	PHE	N-CA-C	-7.02	102.26	111.74
1	D	282	GLU	N-CA-C	-7.01	103.64	111.28
1	B	260	ASN	N-CA-CB	-6.92	102.51	111.09
1	B	44	LEU	N-CA-C	-6.82	104.50	114.39
1	D	466	GLU	N-CA-C	6.76	121.13	112.34
1	D	32	PRO	CB-CA-C	-6.72	99.80	110.96
1	B	362	LEU	N-CA-C	6.71	120.92	112.87
1	D	477	VAL	CB-CA-C	-6.66	100.69	110.81
1	D	124	LEU	N-CA-C	6.59	118.12	111.07
1	B	372	THR	N-CA-C	-6.58	105.78	113.88
1	D	403	GLU	CB-CA-C	-6.43	99.51	110.88
1	D	404	THR	N-CA-C	-6.37	95.73	109.81
1	C	263	ASP	CB-CA-C	-6.37	98.90	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	40	LEU	CB-CA-C	-6.36	99.98	110.72
1	D	328	ILE	N-CA-C	6.35	117.03	110.36
1	A	296	PHE	N-CA-C	6.33	118.26	111.36
1	C	287	ASN	N-CA-C	6.33	121.14	113.17
1	A	260	ASN	N-CA-CB	-6.30	101.94	111.21
1	D	139	LYS	N-CA-C	-6.30	104.85	112.54
1	B	40	LEU	N-CA-CB	-6.29	100.98	110.73
1	C	35	SER	N-CA-C	6.27	117.60	109.64
1	B	89	VAL	CB-CA-C	-6.23	103.76	111.92
1	D	464	PRO	CA-C-N	6.22	127.61	119.84
1	D	464	PRO	C-N-CA	6.22	127.61	119.84
1	B	219	LEU	N-CA-C	6.22	118.99	111.40
1	B	38	PRO	CA-N-CD	-6.20	103.32	112.00
1	B	371	VAL	N-CA-C	-6.18	103.31	110.05
1	D	220	PHE	N-CA-C	6.17	117.67	111.07
1	D	91	GLN	N-CA-C	-6.13	103.91	112.25
1	C	383	PRO	CB-CA-C	-6.11	101.48	111.56
1	B	491	ARG	N-CA-C	6.07	119.39	107.98
1	B	225	LYS	N-CA-C	6.06	118.39	111.11
1	C	286	GLN	N-CA-C	6.05	119.77	111.54
1	B	297	PHE	CB-CA-C	-6.03	100.66	110.79
1	C	34	PRO	CB-CA-C	-5.99	103.56	111.23
1	B	450	PHE	N-CA-C	5.98	117.49	110.97
1	D	86	GLU	CB-CA-C	5.95	120.67	110.79
1	D	47	ASP	N-CA-C	-5.95	99.55	109.24
1	C	426	PHE	N-CA-C	5.94	119.14	107.98
1	C	404	THR	N-CA-CB	-5.93	101.61	110.99
1	B	48	ARG	N-CA-CB	-5.89	100.53	110.49
1	C	224	LEU	CB-CA-C	-5.88	101.61	110.90
1	B	89	VAL	N-CA-C	5.87	116.91	111.45
1	B	161	LYS	CB-CA-C	-5.84	103.59	111.89
1	A	89	VAL	CB-CA-C	-5.83	104.84	111.55
1	A	70	LEU	CB-CA-C	-5.82	99.47	109.65
1	B	54	SER	N-CA-C	5.81	117.30	110.97
1	C	473	ARG	N-CA-C	-5.80	101.60	110.30
1	D	31	PRO	CA-C-N	5.79	127.18	120.98
1	D	31	PRO	C-N-CA	5.79	127.18	120.98
1	B	37	LEU	CA-C-N	5.78	126.25	120.52
1	B	37	LEU	C-N-CA	5.78	126.25	120.52
1	B	225	LYS	N-CA-CB	-5.76	101.35	109.94
1	B	48	ARG	CB-CA-C	-5.74	99.00	110.42
1	C	256	LEU	N-CA-C	5.71	118.47	109.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	295	LEU	N-CA-C	-5.71	104.26	111.11
1	D	232	ARG	N-CA-CB	-5.68	100.52	109.78
1	D	124	LEU	CB-CA-C	-5.64	102.03	110.88
1	C	403	GLU	CB-CA-C	5.64	121.49	110.67
1	B	298	ALA	CB-CA-C	-5.61	101.37	110.79
1	B	478	GLY	N-CA-C	-5.61	101.05	111.14
1	D	477	VAL	N-CA-C	5.61	116.66	108.53
1	A	37	LEU	CB-CA-C	5.60	117.28	108.88
1	B	49	LYS	CB-CA-C	-5.60	99.44	109.24
1	C	289	ILE	CB-CA-C	-5.57	104.85	111.81
1	C	262	ARG	CB-CA-C	5.57	120.14	110.79
1	D	277	SER	N-CA-C	-5.54	106.56	113.38
1	D	30	LEU	CA-C-N	5.52	126.06	120.38
1	D	30	LEU	C-N-CA	5.52	126.06	120.38
1	A	72	SER	CB-CA-C	-5.51	100.64	111.06
1	B	391	VAL	N-CA-C	-5.51	101.48	108.93
1	D	464	PRO	O-C-N	5.49	123.84	121.31
1	A	160	SER	CB-CA-C	5.49	120.70	109.67
1	C	475	SER	N-CA-C	5.46	119.90	112.04
1	B	278	ASP	CB-CA-C	5.44	117.40	110.76
1	C	363	ILE	CA-C-N	5.39	124.58	118.97
1	C	363	ILE	C-N-CA	5.39	124.58	118.97
1	D	107	ILE	CB-CA-C	-5.39	104.92	111.87
1	D	356	ILE	N-CA-C	5.36	115.57	110.42
1	C	401	TYR	N-CA-CB	-5.36	103.77	110.90
1	C	404	THR	CA-C-N	5.36	125.69	119.47
1	C	404	THR	C-N-CA	5.36	125.69	119.47
1	C	398	ASP	CA-C-N	5.36	125.18	119.28
1	C	398	ASP	C-N-CA	5.36	125.18	119.28
1	D	390	PRO	N-CA-C	-5.36	101.43	112.47
1	D	371	VAL	CB-CA-C	-5.36	102.50	111.29
1	D	275	ASP	N-CA-C	5.34	117.30	108.49
1	B	335	HIS	N-CA-CB	-5.33	101.06	110.34
1	A	360	GLY	N-CA-C	-5.32	106.20	112.64
1	C	263	ASP	N-CA-CB	-5.32	102.67	110.97
1	B	161	LYS	N-CA-C	-5.31	104.06	111.39
1	B	361	ASP	N-CA-C	5.31	118.72	111.39
1	B	450	PHE	CB-CA-C	-5.30	102.80	110.96
1	A	259	SER	CB-CA-C	5.27	120.25	109.55
1	B	41	GLY	N-CA-C	-5.26	103.28	112.53
1	D	437	LEU	N-CA-C	-5.23	106.74	113.01
1	D	429	PHE	N-CA-C	5.22	119.64	113.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	404	THR	CA-C-N	5.20	126.33	119.84
1	A	404	THR	C-N-CA	5.20	126.33	119.84
1	B	135	PHE	N-CA-C	5.19	119.61	113.12
1	A	160	SER	N-CA-C	-5.19	106.10	112.90
1	B	374	ASP	N-CA-C	-5.19	102.23	109.96
1	D	260	ASN	CA-C-N	5.19	125.59	119.99
1	D	260	ASN	C-N-CA	5.19	125.59	119.99
1	C	43	LEU	N-CA-C	5.18	118.71	111.56
1	D	92	ALA	N-CA-C	5.18	118.38	111.75
1	D	385	ASN	N-CA-C	5.15	119.52	113.23
1	C	223	PHE	N-CA-C	-5.15	106.95	113.18
1	D	297	PHE	CA-C-N	-5.14	113.76	120.44
1	D	297	PHE	C-N-CA	-5.14	113.76	120.44
1	C	43	LEU	N-CA-CB	-5.11	104.13	111.54
1	A	386	THR	N-CA-C	-5.11	100.84	108.96
1	D	318	PRO	N-CA-C	-5.08	107.78	114.03
1	B	162	GLY	N-CA-C	5.04	122.66	114.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3583	0	3434	235	0
1	B	3589	0	3460	221	0
1	C	3406	0	3187	305	0
1	D	3445	0	3216	386	0
2	E	23	0	21	5	0
2	F	23	0	21	9	0
2	G	23	0	21	4	0
2	H	23	0	21	10	0
3	A	43	0	30	17	0
3	B	43	0	30	14	0
3	C	43	0	30	12	0
3	D	43	0	30	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	13	0	15	8	0
4	B	13	0	15	5	0
4	C	13	0	15	6	0
4	D	13	0	15	14	0
5	A	58	0	73	5	0
5	B	68	0	84	5	0
5	D	34	0	42	3	0
All	All	14499	0	13760	1143	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 40.

All (1143) 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:30:LEU:HD12	1:D:31:PRO:CD	1.18	1.61
1:A:298:ALA:HB1	4:A:501:TB2:C8	1.39	1.52
1:D:30:LEU:CD1	1:D:31:PRO:HD2	1.39	1.51
1:D:298:ALA:HB2	4:D:501:TB2:C7	1.52	1.37
1:C:233:GLN:NE2	1:C:236:ARG:HD3	1.43	1.34
1:A:293:LEU:HD12	1:A:294:SER:N	1.40	1.33
1:D:402:PHE:HE2	1:D:425:GLY:HA3	1.07	1.17
1:C:238:LEU:O	1:C:238:LEU:HD12	1.46	1.16
1:D:402:PHE:CE2	1:D:425:GLY:HA3	1.81	1.15
1:C:224:LEU:C	1:C:224:LEU:HD13	1.72	1.14
1:D:298:ALA:CB	4:D:501:TB2:C7	2.25	1.14
1:A:298:ALA:HB1	4:A:501:TB2:H8	1.20	1.12
1:C:231:HIS:HA	1:C:234:ILE:HG21	1.28	1.11
1:C:206:PHE:CD1	1:C:208:LEU:HD11	1.86	1.11
1:D:292:VAL:O	1:D:296:PHE:HB2	1.49	1.11
1:B:38:PRO:O	1:B:39:VAL:HG12	1.50	1.11
1:D:420:LEU:HD21	2:H:1:GLC:O4	1.51	1.10
1:C:32:PRO:HB2	1:C:62:TYR:HD1	1.12	1.09
1:A:298:ALA:CB	4:A:501:TB2:C8	2.31	1.08
1:C:231:HIS:HA	1:C:234:ILE:CG2	1.84	1.07
1:C:208:LEU:N	1:C:208:LEU:HD12	1.71	1.06
1:A:224:LEU:O	1:A:224:LEU:HD13	1.54	1.05
1:D:295:LEU:HD13	3:D:500:HEM:CBC	1.87	1.04
1:A:298:ALA:CB	4:A:501:TB2:H8	1.89	1.03
2:H:1:GLC:O5	2:H:2:FRU:H12	1.57	1.03
1:C:58:LEU:HD11	1:C:66:PHE:CZ	1.93	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:224:LEU:HD13	1:C:224:LEU:O	1.59	1.02
1:A:298:ALA:HB1	4:A:501:TB2:C7	1.88	1.02
1:C:208:LEU:HD23	1:C:232:ARG:HG3	1.39	1.02
1:B:225:LYS:H	1:B:225:LYS:HD2	1.24	1.01
1:C:231:HIS:CA	1:C:234:ILE:HG22	1.90	1.01
1:B:232:ARG:HG3	1:B:233:GLN:N	1.71	1.00
1:B:287:ASN:OD1	1:B:287:ASN:O	1.79	1.00
1:D:30:LEU:HD12	1:D:31:PRO:HD3	1.42	1.00
1:C:36:PRO:HB3	1:C:69:TYR:HB2	1.44	0.99
1:A:308:ARG:NH2	1:A:483:SER:HA	1.77	0.98
1:C:231:HIS:CA	1:C:234:ILE:CG2	2.41	0.98
1:D:245:ILE:HG21	1:D:288:LEU:HD13	1.43	0.98
2:F:1:GLC:O5	2:F:2:FRU:H4	1.64	0.98
2:F:1:GLC:C1	2:F:2:FRU:H4	1.94	0.97
1:B:209:ILE:HG22	1:C:207:SER:HA	1.45	0.97
1:A:208:LEU:O	1:D:207:SER:HA	1.65	0.97
1:B:38:PRO:O	1:B:39:VAL:CG1	2.13	0.97
1:D:298:ALA:CB	4:D:501:TB2:C8	2.44	0.96
1:A:491:ARG:O	1:A:492:HIS:HB2	1.66	0.95
1:C:206:PHE:CE1	1:C:208:LEU:HD11	1.99	0.95
1:D:30:LEU:CD1	1:D:31:PRO:CD	2.14	0.95
1:A:293:LEU:HD12	1:A:294:SER:H	1.13	0.95
1:A:293:LEU:CD1	1:A:294:SER:N	2.30	0.94
1:D:358:ARG:NH1	1:D:402:PHE:CD1	2.35	0.94
1:A:290:LEU:HA	1:A:293:LEU:HG	1.47	0.94
1:D:296:PHE:CE1	1:D:300:THR:HG21	2.03	0.94
1:B:367:VAL:HG13	1:C:221:SER:HB2	1.50	0.94
1:C:58:LEU:HD11	1:C:66:PHE:CE2	2.03	0.94
1:B:227:PHE:HD2	1:B:229:GLY:H	1.15	0.93
1:C:32:PRO:HB2	1:C:62:TYR:CD1	2.02	0.93
1:D:42:ASN:HB2	1:D:45:GLN:HE21	1.34	0.93
2:F:1:GLC:C1	2:F:2:FRU:C4	2.47	0.92
1:A:101:ILE:HG21	1:D:219:LEU:O	1.67	0.92
1:C:208:LEU:N	1:C:208:LEU:CD1	2.30	0.92
1:A:206:PHE:CG	1:A:233:GLN:HG2	2.05	0.92
1:B:299:GLY:HA2	3:B:500:HEM:C1C	2.04	0.92
2:H:1:GLC:H3	2:H:2:FRU:O1	1.69	0.92
1:C:207:SER:C	1:C:208:LEU:HD12	1.93	0.92
1:A:224:LEU:HD13	1:A:224:LEU:C	1.93	0.91
1:B:352:VAL:HG23	1:B:408:PHE:HZ	1.34	0.91
1:D:203:PHE:HZ	1:D:300:THR:OG1	1.51	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:288:LEU:HD12	1:D:289:ILE:N	1.84	0.91
1:C:37:LEU:HD22	1:C:42:ASN:HA	1.51	0.91
1:A:278:ASP:OD1	1:A:279:PRO:HD2	1.69	0.91
1:C:231:HIS:C	1:C:234:ILE:HG22	1.94	0.91
1:C:224:LEU:C	1:C:224:LEU:CD1	2.41	0.91
1:C:61:LYS:HG3	1:C:62:TYR:CD2	2.06	0.90
1:C:32:PRO:CB	1:C:62:TYR:HD1	1.85	0.90
1:C:61:LYS:HG3	1:C:62:TYR:HD2	1.35	0.90
1:C:233:GLN:HE21	1:C:236:ARG:HD3	1.12	0.90
1:A:219:LEU:HD13	1:A:219:LEU:C	1.96	0.90
1:D:280:SER:O	1:D:283:PHE:HB3	1.71	0.90
1:B:229:GLY:O	1:B:230:THR:HG22	1.72	0.90
3:A:500:HEM:HBC2	3:A:500:HEM:HHD	1.52	0.89
1:A:295:LEU:HG	3:A:500:HEM:HBC1	1.54	0.89
1:D:460:ALA:HB3	1:D:487:ARG:HB2	1.54	0.89
1:D:436:CYS:SG	3:D:500:HEM:C4A	2.66	0.88
1:A:208:LEU:O	1:D:207:SER:CB	2.21	0.88
1:A:358:ARG:HA	1:A:396:LEU:HD12	1.56	0.88
1:D:296:PHE:CD1	1:D:300:THR:HG21	2.08	0.88
1:A:208:LEU:O	1:D:207:SER:CA	2.22	0.88
1:B:93:GLU:OE1	1:B:433:LYS:HE3	1.72	0.88
1:A:221:SER:HB3	1:D:367:VAL:HG22	1.55	0.88
1:B:38:PRO:C	1:B:39:VAL:HG12	1.99	0.88
1:C:97:GLY:H	1:C:434:ARG:HH21	1.22	0.88
1:D:355:GLU:O	1:D:359:LEU:HD23	1.75	0.87
3:C:500:HEM:HBC2	3:C:500:HEM:HHD	1.56	0.87
1:B:287:ASN:OD1	1:B:287:ASN:C	2.17	0.87
1:D:223:PHE:HB3	1:D:227:PHE:HE1	1.39	0.86
1:A:218:GLU:O	1:A:222:GLY:HA3	1.73	0.86
1:D:298:ALA:HB2	4:D:501:TB2:H7	1.54	0.86
1:D:203:PHE:CZ	1:D:300:THR:OG1	2.24	0.86
3:A:500:HEM:HHC	3:A:500:HEM:HBB2	1.56	0.86
1:C:238:LEU:HD12	1:C:238:LEU:C	2.00	0.85
1:D:290:LEU:HD12	1:D:290:LEU:H	1.42	0.85
3:D:500:HEM:HMB1	3:D:500:HEM:HBB2	1.59	0.85
1:C:66:PHE:CZ	1:C:77:VAL:HG21	2.11	0.84
1:A:477:VAL:HG13	1:A:477:VAL:O	1.77	0.84
1:C:228:PRO:O	1:C:231:HIS:CD2	2.30	0.84
1:C:263:ASP:OD1	1:C:265:ILE:HG12	1.77	0.84
1:D:286:GLN:O	1:D:290:LEU:CD1	2.25	0.84
1:A:298:ALA:CB	4:A:501:TB2:C7	2.55	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:446:LEU:O	1:B:450:PHE:HB2	1.78	0.84
3:B:500:HEM:HBB2	3:B:500:HEM:HHC	1.58	0.84
1:D:302:THR:HG21	3:D:500:HEM:C3B	2.13	0.84
1:B:228:PRO:HB2	1:B:231:HIS:CB	2.07	0.84
1:D:53:ARG:HG3	1:D:53:ARG:HH11	1.43	0.84
1:D:88:LEU:HG	1:D:432:GLY:O	1.78	0.83
3:C:500:HEM:HHC	3:C:500:HEM:HBB2	1.61	0.83
1:D:302:THR:HG21	3:D:500:HEM:C2B	2.14	0.83
1:C:208:LEU:HD23	1:C:232:ARG:CG	2.08	0.83
1:B:477:VAL:HG22	1:B:477:VAL:O	1.80	0.82
2:F:1:GLC:H5	2:F:2:FRU:O3	1.79	0.82
1:A:218:GLU:HA	1:A:222:GLY:HA3	1.62	0.82
1:C:203:PHE:CZ	1:C:296:PHE:HE1	1.98	0.82
1:B:209:ILE:HG22	1:C:207:SER:CA	2.10	0.81
1:B:287:ASN:HA	1:B:290:LEU:HD13	1.62	0.81
1:C:208:LEU:CD2	1:C:232:ARG:HG3	2.10	0.81
1:C:249:VAL:O	1:C:253:ARG:HB3	1.80	0.81
1:D:431:LEU:O	1:D:435:ILE:HG12	1.81	0.80
1:D:392:LEU:H	1:D:392:LEU:HD12	1.46	0.80
2:F:1:GLC:O5	2:F:2:FRU:C4	2.30	0.80
1:D:358:ARG:HH12	1:D:402:PHE:HB3	1.42	0.80
1:D:292:VAL:O	1:D:296:PHE:CB	2.30	0.80
1:C:37:LEU:HD13	1:C:42:ASN:HB3	1.63	0.80
1:A:290:LEU:HD12	1:A:291:THR:N	1.97	0.80
1:C:233:GLN:HE21	1:C:236:ARG:CD	1.93	0.80
1:D:78:LEU:HD21	1:D:390:PRO:HA	1.64	0.80
1:A:292:VAL:O	1:A:296:PHE:CB	2.30	0.79
1:A:218:GLU:O	1:A:222:GLY:CA	2.30	0.79
2:H:1:GLC:C2	2:H:2:FRU:O1	2.30	0.79
2:E:1:GLC:O5	2:E:2:FRU:H11	1.81	0.79
2:H:1:GLC:C3	2:H:2:FRU:O1	2.30	0.79
1:A:39:VAL:O	1:D:106:PRO:HG3	1.83	0.79
1:A:278:ASP:OD1	1:A:279:PRO:CD	2.31	0.78
1:B:46:MET:CB	1:B:50:GLY:HA3	2.13	0.78
1:B:208:LEU:O	1:C:208:LEU:HD13	1.83	0.78
3:D:500:HEM:HBC2	3:D:500:HEM:HHD	1.66	0.78
1:D:342:ASP:HA	1:D:345:LYS:HE2	1.66	0.78
2:E:1:GLC:O5	2:E:2:FRU:C1	2.30	0.78
1:B:225:LYS:HD2	1:B:225:LYS:N	1.99	0.77
1:D:77:VAL:HG12	1:D:389:PHE:HB2	1.66	0.77
1:C:121:TRP:CZ3	1:C:124:LEU:HD12	2.19	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:403:GLU:HG2	1:D:404:THR:HG23	1.66	0.77
1:D:94:ALA:C	1:D:95:PHE:HD2	1.92	0.77
1:D:298:ALA:HA	4:D:501:TB2:H8	1.66	0.77
1:A:218:GLU:CA	1:A:222:GLY:HA3	2.15	0.76
1:B:36:PRO:HB3	1:B:69:TYR:HB2	1.67	0.76
1:A:308:ARG:NH1	1:A:481:PRO:HG2	2.01	0.76
1:D:30:LEU:HD11	1:D:31:PRO:HD2	1.62	0.76
1:D:150:ALA:HB1	1:D:452:THR:HG21	1.67	0.76
1:A:224:LEU:C	1:A:224:LEU:CD1	2.58	0.76
1:C:296:PHE:CD1	1:C:296:PHE:C	2.63	0.76
1:C:476:GLY:O	1:C:477:VAL:HG12	1.86	0.75
1:D:298:ALA:HA	4:D:501:TB2:C8	2.16	0.75
1:D:401:TYR:C	1:D:402:PHE:CD2	2.65	0.75
1:C:371:VAL:HG11	1:C:382:ILE:HG21	1.66	0.75
1:D:245:ILE:CG2	1:D:288:LEU:HD13	2.15	0.75
1:D:430:SER:HB2	3:D:500:HEM:HAA1	1.68	0.75
1:B:225:LYS:HE2	1:C:102:ALA:H	1.51	0.75
1:A:44:LEU:O	1:A:45:GLN:CB	2.35	0.75
1:A:292:VAL:O	1:A:296:PHE:HB2	1.86	0.75
1:A:473:ARG:NH1	1:A:482:PRO:HA	2.01	0.74
1:D:291:THR:O	1:D:295:LEU:HB3	1.87	0.74
1:A:289:ILE:O	1:A:292:VAL:CG1	2.35	0.74
1:C:98:ARG:HE	1:C:99:GLY:H	1.32	0.74
1:C:358:ARG:HA	1:C:396:LEU:HD12	1.70	0.74
1:D:105:ASP:O	1:D:109:GLN:CB	2.35	0.74
1:D:245:ILE:CD1	1:D:292:VAL:HG21	2.16	0.74
1:A:282:GLU:OE1	1:A:282:GLU:C	2.30	0.74
3:B:500:HEM:HMC1	3:B:500:HEM:HBC2	1.69	0.74
1:D:78:LEU:CD2	1:D:390:PRO:HA	2.18	0.74
1:D:282:GLU:C	1:D:282:GLU:OE1	2.30	0.74
1:A:363:ILE:HG22	1:A:366:GLY:HA2	1.68	0.74
1:D:117:ASN:N	1:D:120:ARG:NH2	2.35	0.74
1:C:206:PHE:HD1	1:C:208:LEU:HD11	1.44	0.73
1:C:225:LYS:HG3	1:C:226:TYR:CE2	2.23	0.73
1:C:231:HIS:O	1:C:234:ILE:HG22	1.87	0.73
1:A:308:ARG:HH21	1:A:483:SER:HA	1.48	0.73
1:D:430:SER:HB3	1:D:435:ILE:HD13	1.70	0.73
1:A:219:LEU:HD13	1:A:219:LEU:O	1.88	0.73
1:D:117:ASN:H	1:D:120:ARG:NH2	1.86	0.73
1:D:402:PHE:CE2	1:D:425:GLY:CA	2.67	0.73
1:A:434:ARG:HE	1:A:434:ARG:HA	1.53	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:439:GLU:O	1:D:443:ARG:HG3	1.87	0.73
1:C:167:ASN:HD22	1:C:486:ILE:HG21	1.54	0.73
1:D:36:PRO:HA	1:D:42:ASN:HB3	1.69	0.73
1:D:436:CYS:SG	3:D:500:HEM:C1A	2.78	0.73
1:B:299:GLY:HA3	3:B:500:HEM:C2C	2.24	0.72
1:C:98:ARG:NE	1:C:99:GLY:H	1.86	0.72
1:A:288:LEU:HD13	5:A:605:CM5:H81	1.70	0.72
1:D:223:PHE:O	1:D:227:PHE:HD1	1.72	0.72
1:D:288:LEU:O	1:D:292:VAL:HG22	1.88	0.72
1:B:85:ARG:NE	1:B:424:GLU:HG3	2.05	0.72
1:B:299:GLY:CA	3:B:500:HEM:C2C	2.73	0.72
1:D:243:THR:O	1:D:247:GLN:HG2	1.88	0.72
1:B:232:ARG:CG	1:B:233:GLN:N	2.52	0.72
1:C:223:PHE:O	1:C:227:PHE:HE2	1.72	0.72
1:D:285:HIS:O	1:D:288:LEU:HG	1.89	0.72
1:D:91:GLN:HG3	1:D:94:ALA:HB3	1.72	0.72
1:D:305:THR:HG22	1:D:362:LEU:HD21	1.70	0.72
1:A:289:ILE:O	1:A:292:VAL:HG13	1.90	0.71
1:D:59:ARG:HA	1:D:66:PHE:HE1	1.54	0.71
1:D:164:LEU:HB3	1:D:487:ARG:HG2	1.72	0.71
1:D:298:ALA:CA	4:D:501:TB2:C8	2.68	0.71
1:B:230:THR:O	1:B:230:THR:HG23	1.90	0.71
1:C:287:ASN:C	1:C:287:ASN:HD22	1.98	0.71
1:D:84:ILE:H	1:D:84:ILE:HD12	1.55	0.71
1:A:290:LEU:HA	1:A:293:LEU:CG	2.18	0.71
1:C:29:LYS:C	1:C:30:LEU:HD12	2.14	0.71
2:F:1:GLC:C5	2:F:2:FRU:O3	2.38	0.71
1:B:146:ILE:HD12	1:B:445:GLU:HG2	1.72	0.71
1:C:255:THR:O	1:C:255:THR:HG22	1.88	0.70
1:D:402:PHE:HZ	1:D:425:GLY:C	1.99	0.70
1:C:58:LEU:C	1:C:58:LEU:HD12	2.17	0.70
1:C:231:HIS:CB	1:C:234:ILE:HG22	2.21	0.70
1:D:201:LEU:HB3	1:D:241:ILE:HD11	1.74	0.70
1:C:66:PHE:CZ	1:C:77:VAL:CG2	2.74	0.70
1:D:42:ASN:O	1:D:45:GLN:HG3	1.91	0.70
1:A:100:LYS:O	1:D:225:LYS:HD3	1.91	0.70
1:C:58:LEU:HD11	1:C:66:PHE:CE1	2.27	0.70
1:A:160:SER:O	1:A:161:LYS:CB	2.40	0.70
3:D:500:HEM:HBC2	3:D:500:HEM:CHD	2.21	0.70
1:A:218:GLU:C	1:A:222:GLY:HA3	2.18	0.69
1:C:98:ARG:HE	1:C:98:ARG:HA	1.56	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:206:PHE:HE1	1:C:208:LEU:HD21	1.57	0.69
1:A:206:PHE:CD2	1:A:233:GLN:HG2	2.27	0.69
1:A:299:GLY:HA3	3:A:500:HEM:C2C	2.27	0.69
1:A:293:LEU:HD12	1:A:293:LEU:C	2.14	0.69
1:D:358:ARG:NH1	1:D:402:PHE:HD1	1.88	0.69
1:A:219:LEU:C	1:A:219:LEU:CD1	2.65	0.69
1:C:61:LYS:HZ3	1:C:62:TYR:HE2	1.38	0.69
1:D:113:VAL:HA	1:D:116:ALA:CB	2.22	0.69
1:C:371:VAL:HG21	1:C:382:ILE:CG2	2.23	0.69
1:D:298:ALA:HB2	4:D:501:TB2:C6	2.22	0.69
1:D:182:ILE:HG21	5:D:610:CM5:H111	1.76	0.68
1:D:305:THR:CG2	1:D:362:LEU:HD21	2.24	0.68
1:A:162:GLY:O	1:A:487:ARG:NH1	2.27	0.68
1:D:100:LYS:HD2	1:D:101:ILE:H	1.58	0.68
1:C:225:LYS:HG3	1:C:226:TYR:CD2	2.29	0.68
1:A:296:PHE:C	1:A:296:PHE:CD1	2.72	0.68
1:D:402:PHE:CZ	1:D:425:GLY:C	2.72	0.68
1:A:218:GLU:HA	1:A:222:GLY:CA	2.23	0.68
1:A:278:ASP:OD1	1:A:279:PRO:N	2.27	0.68
1:D:245:ILE:HD13	1:D:292:VAL:HG21	1.76	0.67
1:D:398:ASP:OD1	1:D:398:ASP:C	2.37	0.67
1:D:470:LEU:O	1:D:472:PRO:HD3	1.93	0.67
1:A:299:GLY:HA3	3:A:500:HEM:C3C	2.30	0.67
1:C:30:LEU:HD12	1:C:30:LEU:N	2.10	0.67
2:H:1:GLC:H3	2:H:2:FRU:C1	2.25	0.67
1:A:456:ASN:O	1:A:491:ARG:HG2	1.95	0.67
1:B:285:HIS:HD1	1:B:285:HIS:C	2.03	0.67
1:D:358:ARG:HA	1:D:396:LEU:HD13	1.75	0.67
1:D:437:LEU:HD23	1:D:437:LEU:O	1.93	0.67
1:A:314:MET:HA	1:A:314:MET:HE2	1.75	0.67
1:D:140:ARG:HH22	1:D:148:GLU:CB	2.08	0.67
1:B:142:VAL:O	1:B:146:ILE:HG12	1.95	0.66
1:B:286:GLN:O	1:B:289:ILE:HG22	1.95	0.66
1:B:43:LEU:HD23	1:B:44:LEU:N	2.10	0.66
1:C:143:GLU:O	1:C:147:GLN:HG3	1.96	0.66
1:D:116:ALA:N	1:D:120:ARG:HH22	1.93	0.66
1:D:153:LEU:HD21	1:D:453:ILE:HD11	1.78	0.66
1:C:231:HIS:HB3	1:C:234:ILE:HG22	1.77	0.66
1:B:352:VAL:HG23	1:B:408:PHE:CZ	2.25	0.66
1:A:476:GLY:O	1:A:477:VAL:HG12	1.96	0.66
1:A:41:GLY:HA3	1:A:44:LEU:HB2	1.75	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:ASN:OD1	1:B:43:LEU:N	2.28	0.66
1:C:228:PRO:O	1:C:231:HIS:HD2	1.79	0.66
1:D:30:LEU:HD12	1:D:31:PRO:HD2	0.66	0.66
1:A:290:LEU:CA	1:A:293:LEU:HG	2.25	0.66
1:D:296:PHE:O	1:D:300:THR:HG23	1.96	0.66
1:B:278:ASP:OD2	1:B:279:PRO:N	2.29	0.66
1:D:342:ASP:O	1:D:346:MET:HB2	1.96	0.66
1:A:111:TYR:N	1:A:111:TYR:HD1	1.93	0.65
1:D:59:ARG:HA	1:D:66:PHE:CE1	2.31	0.65
1:D:214:SER:O	1:D:218:GLU:HG3	1.96	0.65
1:A:473:ARG:HH11	1:A:482:PRO:HA	1.61	0.65
1:B:153:LEU:HD21	1:B:453:ILE:HD11	1.79	0.65
1:C:203:PHE:CZ	1:C:296:PHE:CE1	2.82	0.65
1:C:206:PHE:CD1	1:C:208:LEU:CD1	2.73	0.65
1:C:223:PHE:O	1:C:227:PHE:CE2	2.49	0.65
1:C:314:MET:HA	1:C:314:MET:HE3	1.77	0.65
1:D:283:PHE:CD1	1:D:283:PHE:C	2.73	0.65
1:A:235:TYR:CE1	1:D:44:LEU:HB3	2.31	0.65
1:C:219:LEU:HA	1:C:224:LEU:HB2	1.79	0.65
1:C:298:ALA:O	4:C:501:TB2:C1	2.44	0.65
1:D:374:ASP:HA	1:D:382:ILE:O	1.97	0.65
1:D:366:GLY:HA3	1:D:392:LEU:HD11	1.78	0.65
1:D:457:PHE:O	1:D:491:ARG:HD2	1.97	0.65
1:D:222:GLY:O	1:D:225:LYS:HE2	1.97	0.65
1:D:358:ARG:NH1	1:D:402:PHE:HB3	2.12	0.65
1:D:358:ARG:HH12	1:D:402:PHE:CB	2.10	0.65
2:H:1:GLC:C2	2:H:2:FRU:HO1	2.09	0.65
1:A:253:ARG:NH1	1:A:276:LYS:NZ	2.45	0.65
1:B:219:LEU:HD12	1:B:219:LEU:O	1.95	0.65
1:C:371:VAL:HG21	1:C:383:PRO:O	1.96	0.65
1:C:65:VAL:HG21	1:C:378:ARG:HD2	1.79	0.64
1:D:305:THR:CB	1:D:362:LEU:HD11	2.26	0.64
1:A:70:LEU:O	1:A:73:ARG:HG2	1.97	0.64
1:D:398:ASP:OD1	1:D:400:ARG:N	2.30	0.64
2:F:1:GLC:O5	2:F:2:FRU:C3	2.46	0.64
1:A:153:LEU:HD21	1:A:453:ILE:HD11	1.79	0.64
1:B:476:GLY:O	1:B:477:VAL:CG1	2.45	0.64
4:B:501:TB2:H4	1:C:217:PHE:HB2	1.79	0.64
1:C:29:LYS:HA	1:C:381:VAL:HG12	1.79	0.64
1:D:30:LEU:HD12	1:D:31:PRO:N	2.08	0.64
1:D:366:GLY:CA	1:D:392:LEU:HD11	2.26	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:GLU:O	1:A:222:GLY:N	2.31	0.64
1:B:65:VAL:HG21	1:B:377:PHE:HE2	1.63	0.64
1:C:94:ALA:HB1	1:C:375:THR:HG21	1.80	0.64
1:D:31:PRO:HA	1:D:380:TYR:CD2	2.32	0.64
1:D:295:LEU:CD1	3:D:500:HEM:CBC	2.71	0.64
1:C:231:HIS:O	1:C:234:ILE:CG2	2.46	0.64
1:C:381:VAL:HG13	1:C:381:VAL:O	1.98	0.64
1:D:298:ALA:HB1	4:D:501:TB2:C8	2.27	0.64
1:C:48:ARG:HH21	1:C:51:LEU:HD11	1.62	0.64
1:D:48:ARG:C	1:D:49:LYS:HG3	2.23	0.64
1:D:295:LEU:CD1	3:D:500:HEM:CAC	2.76	0.64
1:B:352:VAL:O	1:B:356:ILE:HG13	1.98	0.64
1:C:98:ARG:HE	1:C:99:GLY:N	1.96	0.64
1:C:164:LEU:HD12	1:C:164:LEU:H	1.63	0.64
1:A:135:PHE:O	1:A:137:MET:N	2.31	0.63
1:A:164:LEU:HG	1:A:487:ARG:NH2	2.12	0.63
1:A:290:LEU:O	1:A:293:LEU:HD12	1.97	0.63
1:B:88:LEU:HB2	1:B:431:LEU:CD1	2.28	0.63
1:D:115:PHE:C	1:D:120:ARG:NH2	2.56	0.63
1:A:292:VAL:O	1:A:296:PHE:N	2.29	0.63
1:C:42:ASN:N	1:C:42:ASN:OD1	2.30	0.63
1:C:206:PHE:HD1	1:C:208:LEU:CD1	2.10	0.63
1:A:316:LYS:O	1:A:318:PRO:HD3	1.98	0.63
1:C:226:TYR:CD2	1:C:226:TYR:N	2.65	0.63
1:D:78:LEU:HD22	1:D:78:LEU:H	1.64	0.63
1:D:316:LYS:O	1:D:465:PRO:HB3	1.99	0.63
1:B:36:PRO:HB3	1:B:69:TYR:CB	2.27	0.63
1:D:113:VAL:HA	1:D:116:ALA:HB3	1.77	0.63
1:C:226:TYR:N	1:C:226:TYR:HD2	1.95	0.63
1:A:264:PHE:HB3	5:A:605:CM5:H102	1.81	0.63
1:B:298:ALA:O	4:B:501:TB2:C1	2.46	0.63
1:C:52:LEU:O	1:C:56:LEU:HG	1.98	0.63
1:C:298:ALA:CB	4:C:501:TB2:C4	2.77	0.63
1:C:231:HIS:CB	1:C:234:ILE:CG2	2.77	0.63
1:B:202:PHE:CE1	1:B:241:ILE:HD13	2.34	0.63
1:B:476:GLY:O	1:B:477:VAL:HG13	1.99	0.63
1:C:208:LEU:CG	1:C:232:ARG:HG3	2.28	0.63
1:C:232:ARG:O	1:C:233:GLN:HB3	1.99	0.63
1:C:232:ARG:O	1:C:233:GLN:CB	2.45	0.63
1:C:299:GLY:HA3	3:C:500:HEM:C2C	2.34	0.63
4:D:501:TB2:C4	4:D:501:TB2:O1	2.47	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:THR:O	1:A:295:LEU:HB2	1.98	0.62
1:B:429:PHE:O	1:B:430:SER:HB3	1.97	0.62
1:D:302:THR:HG22	3:D:500:HEM:CBB	2.29	0.62
1:B:269:LEU:HD23	1:B:272:MET:SD	2.39	0.62
1:C:231:HIS:O	1:C:234:ILE:CB	2.47	0.62
1:C:320:VAL:O	1:C:324:VAL:HG23	2.00	0.62
1:D:286:GLN:O	1:D:290:LEU:HD12	1.96	0.62
1:C:127:PHE:O	1:C:131:THR:HG22	2.00	0.62
1:D:402:PHE:HE2	1:D:425:GLY:CA	1.97	0.62
1:B:403:GLU:O	1:B:405:PRO:HD3	1.99	0.62
1:B:43:LEU:HD23	1:B:43:LEU:C	2.25	0.62
1:A:362:LEU:N	1:A:362:LEU:HD12	2.15	0.62
1:D:295:LEU:HD13	3:D:500:HEM:CAC	2.29	0.62
1:C:101:ILE:O	1:C:101:ILE:HG13	1.99	0.62
1:D:327:GLU:OE1	1:D:348:TYR:HB3	1.99	0.62
1:A:69:TYR:O	1:A:70:LEU:HD23	2.01	0.61
1:C:358:ARG:HG3	1:C:396:LEU:HD12	1.82	0.61
1:D:402:PHE:CZ	1:D:425:GLY:O	2.53	0.61
1:C:82:ASP:O	1:C:86:GLU:HG3	2.01	0.61
1:D:145:ARG:NH1	1:D:182:ILE:HA	2.15	0.61
1:D:223:PHE:O	1:D:227:PHE:CD1	2.51	0.61
1:D:375:THR:O	1:D:381:VAL:HA	2.00	0.61
1:D:470:LEU:HD13	1:D:470:LEU:H	1.65	0.61
1:A:308:ARG:HH22	1:A:483:SER:HA	1.60	0.61
1:B:225:LYS:HZ2	1:C:101:ILE:HB	1.65	0.61
1:C:266:ASP:O	1:C:270:LEU:HD23	2.00	0.61
1:C:296:PHE:C	1:C:296:PHE:HD1	2.07	0.61
1:C:154:VAL:HG13	1:C:457:PHE:CE2	2.36	0.61
1:B:164:LEU:HG	1:B:487:ARG:CZ	2.31	0.61
1:B:332:ILE:HG23	1:B:336:ARG:HE	1.64	0.61
1:B:370:THR:HG22	1:B:387:GLU:HG2	1.82	0.61
1:D:173:SER:HB3	1:D:195:PHE:HE2	1.66	0.61
1:D:325:GLN:O	1:D:328:ILE:HB	2.01	0.61
3:B:500:HEM:HBC2	3:B:500:HEM:CMC	2.31	0.60
1:A:290:LEU:O	1:A:293:LEU:CD1	2.49	0.60
1:B:35:SER:O	1:B:42:ASN:HB2	2.01	0.60
1:B:268:TYR:CE2	5:B:606:CM5:H31A	2.36	0.60
3:D:500:HEM:HBB2	3:D:500:HEM:CMB	2.29	0.60
1:B:84:ILE:HD11	1:B:391:VAL:O	1.99	0.60
1:B:477:VAL:O	1:B:477:VAL:CG2	2.49	0.60
1:A:235:TYR:HE1	1:D:44:LEU:HB3	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:346:MET:HB3	1:B:349:THR:OG1	2.02	0.60
1:C:183:VAL:HA	1:C:264:PHE:CB	2.32	0.60
1:D:223:PHE:HB3	1:D:227:PHE:CE1	2.29	0.60
1:D:398:ASP:OD1	1:D:399:PRO:N	2.34	0.60
1:C:265:ILE:HG13	1:C:266:ASP:N	2.16	0.60
1:D:32:PRO:HD3	1:D:380:TYR:CE2	2.37	0.60
1:D:140:ARG:HH22	1:D:148:GLU:HG3	1.67	0.60
1:D:154:VAL:HG13	1:D:457:PHE:HE2	1.67	0.60
1:D:296:PHE:CD1	1:D:300:THR:CG2	2.84	0.60
3:A:500:HEM:HBC2	3:A:500:HEM:CHD	2.26	0.60
1:B:164:LEU:HG	1:B:487:ARG:NE	2.17	0.60
1:B:197:ARG:O	1:B:201:LEU:HD12	2.01	0.60
1:B:214:SER:O	1:B:218:GLU:HG3	2.01	0.60
1:D:78:LEU:HD11	1:D:388:VAL:CG1	2.32	0.60
1:B:38:PRO:C	1:B:39:VAL:CG1	2.68	0.60
1:B:137:MET:HE1	1:B:264:PHE:CD2	2.37	0.60
1:C:231:HIS:HB3	1:C:234:ILE:CG2	2.31	0.60
1:A:288:LEU:C	1:A:288:LEU:HD12	2.27	0.60
1:D:101:ILE:HD11	1:D:112:GLY:O	2.02	0.60
1:A:39:VAL:HG13	1:D:106:PRO:CB	2.32	0.59
1:C:76:VAL:O	1:C:388:VAL:HA	2.02	0.59
1:D:295:LEU:HD13	3:D:500:HEM:HBC1	1.77	0.59
1:A:226:TYR:N	1:A:226:TYR:CD2	2.70	0.59
1:C:231:HIS:O	1:C:234:ILE:HB	2.02	0.59
1:A:206:PHE:CD1	1:A:233:GLN:HG2	2.37	0.59
1:B:212:PHE:O	1:B:216:VAL:HG23	2.02	0.59
1:C:98:ARG:HE	1:C:98:ARG:CA	2.16	0.59
1:C:155:GLU:O	1:C:158:ARG:HG2	2.02	0.59
1:D:442:ALA:O	1:D:446:LEU:HG	2.02	0.59
1:D:188:PHE:HB3	1:D:195:PHE:HB2	1.84	0.59
1:B:224:LEU:O	1:B:224:LEU:HD12	2.02	0.59
1:C:167:ASN:ND2	1:C:486:ILE:HG21	2.17	0.59
1:B:107:ILE:HG13	1:B:108:PHE:N	2.17	0.59
1:C:154:VAL:HG13	1:C:457:PHE:HE2	1.67	0.59
1:C:287:ASN:HD22	1:C:288:LEU:N	2.00	0.59
1:B:225:LYS:H	1:B:225:LYS:CD	2.06	0.59
1:B:332:ILE:HG12	1:B:336:ARG:HH21	1.68	0.59
1:A:308:ARG:HH11	1:A:481:PRO:HG2	1.67	0.59
1:B:227:PHE:HD2	1:B:229:GLY:N	1.93	0.59
1:C:200:ASP:O	1:C:204:GLN:HB3	2.02	0.59
1:D:53:ARG:HH11	1:D:53:ARG:CG	2.15	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:299:GLY:HA2	3:B:500:HEM:C2C	2.37	0.58
1:A:68:VAL:HG12	1:A:75:VAL:HG22	1.85	0.58
1:B:349:THR:HA	1:B:352:VAL:HG12	1.84	0.58
1:C:94:ALA:HB1	1:C:375:THR:CG2	2.33	0.58
1:A:434:ARG:HA	1:A:434:ARG:NE	2.18	0.58
1:D:298:ALA:CB	4:D:501:TB2:C6	2.81	0.58
1:C:370:THR:HA	1:C:386:THR:O	2.03	0.58
1:D:429:PHE:O	1:D:430:SER:CB	2.52	0.58
1:D:127:PHE:HD1	1:D:128:SER:N	2.01	0.58
1:B:113:VAL:HG22	1:B:113:VAL:O	2.04	0.58
1:B:313:LEU:HD21	1:B:408:PHE:CD1	2.38	0.58
1:C:109:GLN:O	1:C:113:VAL:HG23	2.03	0.58
1:D:321:THR:O	1:D:324:VAL:HG22	2.03	0.58
1:B:113:VAL:HG22	1:B:116:ALA:HB2	1.86	0.58
1:B:314:MET:CE	1:B:450:PHE:CZ	2.86	0.58
1:D:116:ALA:N	1:D:120:ARG:NH2	2.51	0.58
1:B:209:ILE:HG22	1:C:207:SER:CB	2.33	0.58
1:C:222:GLY:O	1:C:225:LYS:HE2	2.03	0.58
1:D:76:VAL:O	1:D:388:VAL:HA	2.04	0.58
1:D:358:ARG:HG3	1:D:396:LEU:HB3	1.85	0.58
1:D:398:ASP:OD1	1:D:400:ARG:HG2	2.02	0.58
1:A:111:TYR:N	1:A:111:TYR:CD1	2.66	0.58
1:B:101:ILE:O	1:B:101:ILE:HG13	2.02	0.58
1:C:34:PRO:HD3	1:C:62:TYR:CE2	2.39	0.58
1:C:245:ILE:HG23	1:C:246:GLY:N	2.19	0.58
1:D:305:THR:HB	1:D:362:LEU:HD11	1.84	0.58
1:D:361:ASP:OD2	1:D:393:SER:HB3	2.04	0.58
1:D:245:ILE:HG22	1:D:245:ILE:O	2.03	0.57
1:D:353:ILE:HG22	1:D:354:HIS:N	2.19	0.57
1:D:398:ASP:OD2	1:D:400:ARG:HG3	2.04	0.57
1:B:457:PHE:CD1	1:B:488:PHE:HB3	2.39	0.57
1:D:164:LEU:HB3	1:D:487:ARG:CG	2.33	0.57
1:D:473:ARG:O	1:D:479:ASN:HA	2.05	0.57
1:A:253:ARG:NH1	1:A:276:LYS:HZ1	2.02	0.57
1:B:308:ARG:HG2	1:B:484:TYR:CE1	2.38	0.57
1:D:280:SER:O	1:D:283:PHE:CB	2.49	0.57
1:B:463:VAL:HG13	1:B:467:ASP:HB3	1.86	0.57
1:C:240:GLU:O	1:C:243:THR:HB	2.05	0.57
1:C:245:ILE:HG21	1:C:289:ILE:CB	2.35	0.57
1:D:48:ARG:O	1:D:49:LYS:HG3	2.05	0.57
1:D:95:PHE:N	1:D:95:PHE:CD2	2.72	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:358:ARG:NH1	1:D:402:PHE:CG	2.72	0.57
1:D:145:ARG:HH12	1:D:182:ILE:HA	1.68	0.57
1:D:164:LEU:HD22	1:D:487:ARG:CZ	2.34	0.57
1:A:289:ILE:O	1:A:292:VAL:HG12	2.04	0.57
1:B:112:GLY:O	1:B:113:VAL:HG12	2.05	0.57
3:C:500:HEM:HBC2	3:C:500:HEM:CHD	2.31	0.57
1:D:295:LEU:HD12	1:D:295:LEU:O	2.05	0.57
1:C:98:ARG:NE	1:C:98:ARG:HA	2.20	0.57
1:D:472:PRO:HB2	1:D:479:ASN:HB2	1.86	0.57
1:A:48:ARG:HG3	1:A:49:LYS:N	2.20	0.57
1:C:37:LEU:HD13	1:C:42:ASN:CB	2.34	0.57
1:D:95:PHE:HD2	1:D:95:PHE:N	2.03	0.57
1:C:61:LYS:NZ	1:C:62:TYR:HE2	2.03	0.56
1:C:299:GLY:HA2	3:C:500:HEM:C1C	2.40	0.56
1:D:86:GLU:O	1:D:90:ASP:OD2	2.23	0.56
1:A:157:LEU:HB3	1:A:457:PHE:CZ	2.40	0.56
1:B:429:PHE:HB3	1:B:436:CYS:HB3	1.87	0.56
1:C:227:PHE:N	1:C:228:PRO:HD3	2.20	0.56
1:A:226:TYR:N	1:A:226:TYR:HD2	2.02	0.56
1:C:124:LEU:C	1:C:124:LEU:HD13	2.30	0.56
1:C:226:TYR:C	1:C:228:PRO:HD3	2.31	0.56
1:C:327:GLU:OE1	1:C:346:MET:HB3	2.05	0.56
1:D:117:ASN:H	1:D:120:ARG:HH22	1.54	0.56
1:C:435:ILE:HG12	1:C:436:CYS:N	2.19	0.56
1:D:127:PHE:CD1	1:D:128:SER:N	2.73	0.56
1:D:146:ILE:HD13	1:D:445:GLU:HG2	1.86	0.56
1:B:43:LEU:HD23	1:B:45:GLN:H	1.71	0.56
1:B:243:THR:O	1:B:247:GLN:HG3	2.06	0.56
1:C:231:HIS:O	1:C:234:ILE:N	2.35	0.56
1:A:206:PHE:CD1	1:A:206:PHE:O	2.58	0.56
1:B:226:TYR:CD1	1:C:70:LEU:HD13	2.40	0.56
1:B:345:LYS:C	1:B:347:PRO:HD3	2.31	0.56
1:C:298:ALA:HB2	4:C:501:TB2:C4	2.36	0.56
1:C:342:ASP:O	1:C:346:MET:HG3	2.06	0.56
1:B:314:MET:CE	1:B:450:PHE:HZ	2.19	0.56
1:A:286:GLN:HA	1:A:289:ILE:HG22	1.86	0.56
1:A:362:LEU:N	1:A:362:LEU:CD1	2.69	0.56
1:B:113:VAL:O	1:B:113:VAL:HG13	2.05	0.56
1:C:58:LEU:HA	1:C:61:LYS:CD	2.36	0.56
1:C:68:VAL:HG13	1:C:75:VAL:HG13	1.88	0.56
1:C:154:VAL:O	1:C:158:ARG:HG2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:233:GLN:NE2	1:C:236:ARG:CD	2.40	0.56
1:A:192:ASP:OD1	1:A:194:VAL:HG23	2.04	0.55
1:B:299:GLY:HA3	3:B:500:HEM:C3C	2.41	0.55
1:C:81:THR:O	1:C:85:ARG:HB2	2.07	0.55
1:D:183:VAL:O	1:D:265:ILE:HG12	2.06	0.55
1:D:288:LEU:HD12	1:D:289:ILE:H	1.71	0.55
1:D:358:ARG:NH1	1:D:402:PHE:CB	2.69	0.55
1:B:229:GLY:O	1:B:230:THR:CG2	2.51	0.55
1:B:299:GLY:CA	3:B:500:HEM:C1C	2.85	0.55
1:D:402:PHE:CZ	1:D:425:GLY:HA3	2.38	0.55
1:C:371:VAL:CG2	1:C:383:PRO:O	2.54	0.55
1:D:54:SER:O	1:D:58:LEU:HB2	2.06	0.55
1:D:257:ASP:HB3	1:D:260:ASN:OD1	2.06	0.55
1:A:473:ARG:HG2	1:A:480:VAL:HG13	1.87	0.55
1:D:257:ASP:HB3	1:D:260:ASN:H	1.71	0.55
1:A:217:PHE:CD1	1:A:217:PHE:C	2.82	0.55
1:C:224:LEU:HD13	1:C:225:LYS:N	2.21	0.55
1:B:285:HIS:C	1:B:285:HIS:ND1	2.63	0.55
1:C:48:ARG:HE	1:C:51:LEU:HD21	1.72	0.55
1:D:80:GLY:O	1:D:84:ILE:HD12	2.06	0.55
1:A:226:TYR:HD1	1:D:70:LEU:HD13	1.71	0.55
1:B:105:ASP:CG	1:B:106:PRO:HD2	2.32	0.55
1:C:296:PHE:CD1	1:C:296:PHE:O	2.59	0.55
1:D:420:LEU:HD21	2:H:1:GLC:C4	2.34	0.55
1:A:303:THR:OG1	3:A:500:HEM:CBB	2.55	0.55
1:B:35:SER:O	1:B:42:ASN:CB	2.55	0.55
1:B:105:ASP:OD2	1:B:107:ILE:HG23	2.07	0.55
1:A:474:GLU:OE1	1:A:474:GLU:HA	2.06	0.54
1:B:36:PRO:HA	1:B:42:ASN:HB3	1.89	0.54
1:C:224:LEU:CD1	1:C:225:LYS:N	2.71	0.54
1:D:302:THR:CG2	3:D:500:HEM:CAB	2.84	0.54
1:A:287:ASN:C	1:A:287:ASN:OD1	2.50	0.54
1:A:208:LEU:O	1:D:207:SER:HB2	2.07	0.54
1:B:219:LEU:HD12	1:B:219:LEU:C	2.32	0.54
1:C:58:LEU:HD11	1:C:66:PHE:CD2	2.42	0.54
1:A:51:LEU:O	1:A:51:LEU:HD12	2.08	0.54
1:A:150:ALA:O	1:A:154:VAL:HG23	2.08	0.54
1:A:291:THR:HG21	5:A:605:CM5:H72	1.88	0.54
1:B:225:LYS:N	1:B:225:LYS:CD	2.70	0.54
1:C:144:GLU:OE1	1:C:144:GLU:N	2.37	0.54
1:D:154:VAL:HG13	1:D:457:PHE:CE2	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:610:CM5:O22	5:D:610:CM5:H11	2.08	0.54
1:C:234:ILE:HG23	1:C:235:TYR:N	2.21	0.54
1:B:69:TYR:CE1	1:B:74:PRO:HB3	2.43	0.54
1:B:183:VAL:HA	1:B:264:PHE:HB2	1.88	0.54
1:B:207:SER:HA	1:C:208:LEU:O	2.07	0.54
1:D:140:ARG:HG3	1:D:145:ARG:HE	1.73	0.54
1:D:397:HIS:HA	1:D:405:PRO:CB	2.38	0.54
2:E:1:GLC:C1	2:E:2:FRU:O1	2.52	0.54
1:B:367:VAL:HG13	1:C:221:SER:CB	2.32	0.54
1:D:171:PHE:CD2	1:D:307:LEU:HB3	2.43	0.54
1:B:38:PRO:O	1:B:39:VAL:HG13	2.07	0.53
1:B:231:HIS:O	1:B:235:TYR:CB	2.56	0.53
1:C:40:LEU:H	1:C:40:LEU:HD22	1.73	0.53
1:D:397:HIS:CD2	1:D:405:PRO:HB2	2.43	0.53
1:A:221:SER:HB3	1:D:367:VAL:CG2	2.35	0.53
1:A:293:LEU:CD1	1:A:293:LEU:C	2.75	0.53
1:B:146:ILE:CD1	1:B:445:GLU:HG2	2.38	0.53
1:C:424:GLU:OE1	1:C:424:GLU:HA	2.08	0.53
1:D:75:VAL:HG23	1:D:387:GLU:HB2	1.90	0.53
1:C:33:GLY:HA3	1:C:67:THR:O	2.07	0.53
1:D:150:ALA:O	1:D:154:VAL:HG23	2.08	0.53
1:A:290:LEU:HD12	1:A:291:THR:H	1.71	0.53
1:C:36:PRO:HA	1:C:42:ASN:HD21	1.74	0.53
1:D:36:PRO:HG3	1:D:69:TYR:CD2	2.44	0.53
1:D:39:VAL:HG12	1:D:40:LEU:HD22	1.91	0.53
1:C:217:PHE:CD1	1:C:217:PHE:C	2.86	0.53
1:C:362:LEU:C	1:C:364:PRO:HD3	2.34	0.53
1:D:231:HIS:HA	1:D:234:ILE:HB	1.89	0.53
1:D:324:VAL:HG12	1:D:348:TYR:HE2	1.73	0.53
2:E:1:GLC:C5	2:E:2:FRU:H11	2.39	0.53
1:A:296:PHE:O	1:A:300:THR:HB	2.09	0.53
1:A:358:ARG:NH2	1:A:359:LEU:HD21	2.24	0.53
1:B:268:TYR:O	1:B:272:MET:HG3	2.09	0.53
1:C:288:LEU:HD13	1:C:288:LEU:C	2.34	0.53
1:D:53:ARG:HG3	1:D:53:ARG:NH1	2.20	0.53
1:B:308:ARG:HG2	1:B:484:TYR:HE1	1.74	0.53
1:B:314:MET:HE1	1:B:450:PHE:CZ	2.44	0.53
1:B:349:THR:O	1:B:352:VAL:HG12	2.08	0.53
1:D:173:SER:HB3	1:D:195:PHE:CE2	2.44	0.53
1:B:43:LEU:HD23	1:B:45:GLN:N	2.23	0.53
1:D:115:PHE:C	1:D:120:ARG:HH21	2.17	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:LEU:HD12	1:A:294:SER:CA	2.35	0.52
1:C:265:ILE:CG1	1:C:266:ASP:N	2.71	0.52
1:C:434:ARG:NH1	1:C:434:ARG:HA	2.24	0.52
1:D:140:ARG:HH22	1:D:148:GLU:HB2	1.74	0.52
1:D:376:GLN:HA	1:D:380:TYR:O	2.09	0.52
1:A:360:GLY:C	1:A:362:LEU:HD12	2.34	0.52
1:C:153:LEU:O	1:C:157:LEU:HB2	2.09	0.52
1:D:88:LEU:HD12	1:D:88:LEU:O	2.09	0.52
1:D:113:VAL:HA	1:D:116:ALA:HB2	1.91	0.52
1:D:349:THR:HG22	1:D:353:ILE:HD13	1.92	0.52
1:D:473:ARG:N	1:D:480:VAL:O	2.37	0.52
1:B:290:LEU:O	1:B:294:SER:HB2	2.09	0.52
1:A:269:LEU:HD23	1:A:272:MET:CE	2.40	0.52
1:B:326:LYS:HA	1:B:329:GLU:HB2	1.91	0.52
1:D:140:ARG:HH22	1:D:148:GLU:CG	2.21	0.52
1:B:51:LEU:C	1:B:51:LEU:HD23	2.34	0.52
1:C:58:LEU:O	1:C:61:LYS:HG2	2.10	0.52
1:C:107:ILE:HG13	1:C:108:PHE:H	1.75	0.52
1:D:32:PRO:O	1:D:66:PHE:HB2	2.10	0.52
1:D:470:LEU:HD13	1:D:470:LEU:N	2.24	0.52
2:G:1:GLC:O5	2:G:2:FRU:H12	2.08	0.52
1:A:487:ARG:HG2	1:A:489:LEU:CD1	2.40	0.52
1:B:441:ILE:O	1:B:445:GLU:HG3	2.10	0.52
1:C:30:LEU:N	1:C:30:LEU:CD1	2.72	0.52
1:B:42:ASN:CG	1:B:43:LEU:N	2.68	0.52
1:D:292:VAL:HG23	1:D:293:LEU:N	2.25	0.52
1:D:397:HIS:HA	1:D:405:PRO:HB3	1.91	0.52
1:D:402:PHE:CZ	1:D:425:GLY:CA	2.93	0.52
1:D:429:PHE:O	1:D:430:SER:HB3	2.10	0.52
1:C:48:ARG:HD3	1:C:474:GLU:CD	2.35	0.51
1:D:356:ILE:HG22	1:D:357:GLN:N	2.25	0.51
1:D:374:ASP:OD2	1:D:381:VAL:HG22	2.10	0.51
1:A:235:TYR:HE1	1:D:44:LEU:HD13	1.75	0.51
1:B:226:TYR:OH	1:C:387:GLU:OE1	2.28	0.51
1:B:43:LEU:C	1:B:43:LEU:CD2	2.83	0.51
1:B:340:LEU:HD13	1:B:444:THR:HG23	1.93	0.51
1:C:58:LEU:HD12	1:C:58:LEU:O	2.10	0.51
1:D:427:MET:N	1:D:428:PRO:CD	2.72	0.51
1:A:88:LEU:O	1:A:92:ALA:HA	2.11	0.51
1:C:32:PRO:CB	1:C:62:TYR:CD1	2.77	0.51
1:D:285:HIS:O	1:D:285:HIS:HD2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:477:VAL:HG23	1:D:477:VAL:O	2.10	0.51
1:A:387:GLU:OE1	1:D:225:LYS:NZ	2.44	0.51
1:A:473:ARG:HG2	1:A:473:ARG:O	2.11	0.51
1:D:257:ASP:CB	1:D:260:ASN:OD1	2.58	0.51
1:D:268:TYR:CE1	1:D:284:HIS:ND1	2.78	0.51
1:D:353:ILE:O	1:D:356:ILE:HB	2.09	0.51
1:A:40:LEU:HD23	1:A:40:LEU:C	2.36	0.51
1:C:238:LEU:C	1:C:238:LEU:CD1	2.73	0.51
1:D:127:PHE:CD1	1:D:127:PHE:C	2.88	0.51
1:A:441:ILE:HD13	1:A:441:ILE:O	2.11	0.51
1:C:225:LYS:HE3	1:C:226:TYR:HE2	1.75	0.51
1:D:135:PHE:CE1	1:D:261:PRO:HG2	2.45	0.51
1:A:298:ALA:CB	4:A:501:TB2:H7	2.36	0.51
1:A:400:ARG:NH1	1:A:400:ARG:HB3	2.25	0.51
1:C:44:LEU:C	1:C:44:LEU:HD23	2.36	0.51
1:C:426:PHE:CD2	1:C:426:PHE:O	2.63	0.51
1:D:398:ASP:OD1	1:D:400:ARG:CG	2.59	0.51
1:A:217:PHE:CD1	1:A:217:PHE:O	2.64	0.51
1:A:312:LEU:HD13	1:A:484:TYR:CD1	2.46	0.51
1:B:314:MET:HG3	1:B:321:THR:OG1	2.10	0.51
1:B:459:ILE:CG2	1:B:486:ILE:HD11	2.40	0.51
1:C:364:PRO:HA	1:C:393:SER:HB2	1.93	0.51
1:D:305:THR:HG21	1:D:362:LEU:HD11	1.91	0.51
1:D:439:GLU:HG3	1:D:440:GLY:N	2.26	0.51
1:A:288:LEU:HD13	5:A:605:CM5:C8	2.38	0.50
1:A:114:ILE:O	1:A:120:ARG:HG3	2.11	0.50
1:A:367:VAL:HG21	3:A:500:HEM:HAA2	1.91	0.50
1:B:232:ARG:HG3	1:B:233:GLN:H	1.68	0.50
1:D:100:LYS:HE2	1:D:116:ALA:HB1	1.93	0.50
1:A:128:SER:O	1:A:132:MET:HB2	2.11	0.50
1:B:213:SER:HB3	1:C:297:PHE:CB	2.41	0.50
1:B:216:VAL:O	1:B:220:PHE:HD2	1.93	0.50
1:B:404:THR:HB	1:B:407:THR:HB	1.92	0.50
1:D:399:PRO:O	1:D:402:PHE:O	2.30	0.50
1:A:208:LEU:O	1:D:207:SER:HB3	2.09	0.50
1:C:314:MET:SD	1:C:450:PHE:HZ	2.35	0.50
1:C:354:HIS:NE2	2:G:1:GLC:H3	2.27	0.50
1:C:362:LEU:C	1:C:363:ILE:HD12	2.37	0.50
1:D:203:PHE:HZ	1:D:300:THR:HG1	0.69	0.50
1:A:429:PHE:CE1	1:A:439:GLU:HA	2.47	0.50
1:B:219:LEU:O	1:C:101:ILE:HG21	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:361:ASP:CG	1:B:361:ASP:O	2.55	0.50
1:C:435:ILE:HG12	1:C:436:CYS:H	1.76	0.50
1:D:137:MET:HB3	1:D:140:ARG:O	2.12	0.50
1:D:369:HIS:O	1:D:388:VAL:N	2.45	0.50
2:F:1:GLC:O5	2:F:2:FRU:O3	2.30	0.50
1:B:443:ARG:NH2	2:F:2:FRU:H3	2.27	0.50
1:C:320:VAL:HG21	1:C:408:PHE:HE2	1.76	0.50
1:D:78:LEU:HD22	1:D:389:PHE:O	2.12	0.50
1:A:269:LEU:HD23	1:A:272:MET:HE3	1.94	0.50
1:A:310:GLY:O	1:A:314:MET:HG2	2.12	0.50
1:D:310:GLY:HA3	1:D:356:ILE:HD13	1.94	0.50
1:A:298:ALA:O	1:A:302:THR:OG1	2.30	0.49
1:B:427:MET:HE2	1:B:431:LEU:HD21	1.94	0.49
1:D:278:ASP:C	1:D:278:ASP:OD1	2.54	0.49
1:D:296:PHE:HE1	1:D:300:THR:HG21	1.66	0.49
1:A:115:PHE:HE2	1:A:290:LEU:CD1	2.24	0.49
1:A:217:PHE:HD2	1:D:477:VAL:HG11	1.78	0.49
1:A:299:GLY:CA	3:A:500:HEM:C1C	2.95	0.49
1:B:227:PHE:CD2	1:B:228:PRO:HD2	2.47	0.49
1:C:197:ARG:HD3	1:C:240:GLU:OE2	2.13	0.49
1:C:245:ILE:C	1:C:245:ILE:HD13	2.37	0.49
1:C:298:ALA:HB1	4:C:501:TB2:C4	2.42	0.49
1:C:350:ASP:OD2	2:G:1:GLC:O6	2.25	0.49
1:D:189:ASP:HB3	1:D:192:ASP:HB2	1.93	0.49
1:D:283:PHE:C	1:D:283:PHE:HD1	2.18	0.49
1:A:299:GLY:HA2	3:A:500:HEM:C1C	2.47	0.49
1:C:363:ILE:HD12	1:C:363:ILE:N	2.28	0.49
1:B:298:ALA:HB2	4:B:501:TB2:C5	2.43	0.49
1:B:355:GLU:OE1	1:B:413:PHE:HE2	1.95	0.49
1:C:211:SER:O	1:C:215:GLN:HG3	2.12	0.49
1:C:299:GLY:CA	3:C:500:HEM:C2C	2.95	0.49
1:D:282:GLU:OE1	1:D:282:GLU:O	2.30	0.49
1:B:314:MET:HE1	1:B:450:PHE:HZ	1.78	0.49
1:D:305:THR:CG2	1:D:362:LEU:HD11	2.42	0.49
1:A:132:MET:HE2	1:A:142:VAL:CG2	2.43	0.49
1:C:328:ILE:HG12	1:C:346:MET:HE1	1.94	0.49
2:H:1:GLC:H3	2:H:2:FRU:H12	1.95	0.49
1:A:107:ILE:HD12	1:A:108:PHE:N	2.27	0.49
1:C:88:LEU:HD21	1:C:369:HIS:CD2	2.47	0.49
1:C:381:VAL:O	1:C:381:VAL:CG1	2.60	0.49
1:D:283:PHE:HD1	1:D:283:PHE:O	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:227:PHE:HE2	1:B:230:THR:H	1.61	0.49
1:C:315:LEU:HD11	1:C:486:ILE:HD12	1.94	0.49
1:D:165:LEU:HG	1:D:166:ASP:N	2.28	0.49
3:D:500:HEM:CBC	3:D:500:HEM:HHD	2.39	0.49
1:B:313:LEU:HD21	1:B:408:PHE:CE1	2.47	0.49
1:D:172:HIS:CE1	1:D:203:PHE:HB3	2.47	0.49
1:A:303:THR:OG1	3:A:500:HEM:HBB2	2.13	0.49
1:A:101:ILE:CG2	1:D:219:LEU:O	2.50	0.48
1:A:174:ILE:HG13	1:A:175:THR:N	2.28	0.48
1:C:245:ILE:HG13	1:C:289:ILE:HA	1.95	0.48
1:C:434:ARG:HG3	3:C:500:HEM:O1A	2.13	0.48
1:D:381:VAL:C	1:D:382:ILE:HD12	2.38	0.48
1:A:34:PRO:HG3	1:A:58:LEU:HD22	1.95	0.48
1:B:363:ILE:HD12	3:B:500:HEM:HHB	1.95	0.48
1:C:141:SER:O	1:C:145:ARG:HG3	2.13	0.48
1:C:225:LYS:HG3	1:C:226:TYR:HE2	1.72	0.48
1:C:316:LYS:HG2	1:C:317:TYR:CE2	2.48	0.48
1:D:479:ASN:OD1	1:D:479:ASN:O	2.31	0.48
1:A:41:GLY:CA	1:A:44:LEU:HD13	2.43	0.48
1:A:293:LEU:HA	1:A:296:PHE:HB3	1.93	0.48
1:A:299:GLY:CA	3:A:500:HEM:C2C	2.95	0.48
1:B:463:VAL:CG1	1:B:467:ASP:HB3	2.43	0.48
1:C:107:ILE:HG13	1:C:108:PHE:N	2.29	0.48
1:D:302:THR:CG2	3:D:500:HEM:CBB	2.91	0.48
1:A:65:VAL:HG21	1:A:377:PHE:HE2	1.78	0.48
1:A:363:ILE:CG2	1:A:366:GLY:HA2	2.41	0.48
1:C:112:GLY:O	1:C:116:ALA:HB2	2.13	0.48
1:C:384:LYS:O	1:C:385:ASN:HB2	2.13	0.48
1:D:302:THR:CG2	3:D:500:HEM:C3B	2.92	0.48
1:A:127:PHE:CE1	5:A:605:CM5:H111	2.48	0.48
1:A:253:ARG:NH1	1:A:276:LYS:HZ3	2.12	0.48
1:A:426:PHE:CZ	1:A:428:PRO:HG2	2.49	0.48
1:C:208:LEU:CD1	1:C:208:LEU:H	2.20	0.48
1:D:43:LEU:CB	1:D:70:LEU:HD23	2.44	0.48
1:D:234:ILE:HG22	1:D:235:TYR:N	2.27	0.48
1:D:285:HIS:HA	1:D:288:LEU:CD2	2.43	0.48
1:D:321:THR:HG21	1:D:459:ILE:HD11	1.95	0.48
1:D:438:GLY:HA3	3:D:500:HEM:C2C	2.49	0.48
1:A:212:PHE:CD1	1:A:212:PHE:C	2.92	0.48
1:A:362:LEU:CD1	1:A:362:LEU:H	2.25	0.48
1:D:366:GLY:N	1:D:392:LEU:CD1	2.76	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1:GLC:O5	2:E:2:FRU:O1	2.30	0.48
1:A:298:ALA:O	4:A:501:TB2:C1	2.62	0.48
1:C:174:ILE:HG13	1:C:175:THR:N	2.29	0.48
1:A:93:GLU:HG2	1:A:433:LYS:NZ	2.28	0.48
1:B:114:ILE:HG23	1:B:115:PHE:N	2.29	0.48
1:B:427:MET:N	1:B:428:PRO:HD3	2.29	0.48
1:D:145:ARG:HD3	1:D:181:SER:OG	2.14	0.48
1:D:427:MET:N	1:D:428:PRO:HD3	2.29	0.48
1:A:245:ILE:HD13	1:A:289:ILE:HA	1.95	0.48
1:B:226:TYR:OH	1:C:387:GLU:CD	2.57	0.48
1:B:309:TYR:CZ	1:B:360:GLY:HA2	2.49	0.48
1:C:157:LEU:HD11	1:C:488:PHE:CD2	2.49	0.48
1:C:404:THR:HB	1:C:407:THR:HB	1.96	0.48
1:B:32:PRO:O	1:B:66:PHE:HB2	2.14	0.48
1:B:51:LEU:HD11	1:B:365:PHE:CZ	2.48	0.48
1:B:117:ASN:C	1:B:117:ASN:OD1	2.57	0.48
1:C:230:THR:O	1:C:230:THR:OG1	2.30	0.48
1:D:197:ARG:NH1	1:D:201:LEU:HD13	2.29	0.48
1:A:403:GLU:O	1:A:405:PRO:HD3	2.13	0.47
1:A:487:ARG:HG2	1:A:489:LEU:HD11	1.96	0.47
1:B:309:TYR:HB2	1:B:481:PRO:HG3	1.96	0.47
1:D:350:ASP:OD2	2:H:1:GLC:O4	2.32	0.47
1:B:137:MET:HE1	1:B:264:PHE:CE2	2.48	0.47
1:B:313:LEU:HD12	1:B:470:LEU:HD13	1.95	0.47
1:D:132:MET:HE2	1:D:142:VAL:HG23	1.95	0.47
1:D:375:THR:HG22	1:D:376:GLN:H	1.79	0.47
1:D:396:LEU:HD21	1:D:428:PRO:HD3	1.95	0.47
1:A:276:LYS:O	1:A:277:SER:CB	2.60	0.47
1:A:382:ILE:HG22	1:A:386:THR:HB	1.97	0.47
1:B:312:LEU:HB2	1:B:484:TYR:CE1	2.50	0.47
1:C:242:ASN:HA	1:C:245:ILE:HG22	1.97	0.47
1:C:442:ALA:HB1	3:C:500:HEM:CBB	2.45	0.47
1:D:53:ARG:CG	1:D:53:ARG:NH1	2.76	0.47
1:B:261:PRO:HG3	1:B:270:LEU:HD11	1.97	0.47
1:C:331:VAL:HG13	1:C:345:LYS:HE2	1.95	0.47
1:D:76:VAL:HG12	1:D:387:GLU:O	2.14	0.47
1:D:430:SER:HB2	3:D:500:HEM:HMA2	1.96	0.47
1:A:39:VAL:HG13	1:D:106:PRO:HB3	1.97	0.47
1:A:282:GLU:OE1	1:A:283:PHE:N	2.48	0.47
1:A:320:VAL:O	1:A:324:VAL:HG23	2.15	0.47
1:B:37:LEU:O	1:B:41:GLY:O	2.31	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:54:SER:OG	1:B:55:PHE:N	2.48	0.47
1:C:48:ARG:HB3	1:C:48:ARG:NH1	2.30	0.47
1:C:51:LEU:C	1:C:51:LEU:HD12	2.39	0.47
1:C:154:VAL:O	1:C:158:ARG:HD2	2.14	0.47
1:C:208:LEU:HB3	1:C:232:ARG:HG3	1.96	0.47
1:C:263:ASP:OD1	1:C:263:ASP:C	2.58	0.47
1:D:141:SER:OG	1:D:142:VAL:N	2.47	0.47
1:D:173:SER:HA	1:D:199:LEU:HD11	1.97	0.47
1:D:246:GLY:O	1:D:250:GLU:HB2	2.14	0.47
1:D:262:ARG:HG2	1:D:266:ASP:OD2	2.14	0.47
1:D:268:TYR:HE1	1:D:284:HIS:ND1	2.12	0.47
1:D:328:ILE:HD13	1:D:455:GLN:HB2	1.97	0.47
1:A:441:ILE:O	1:A:445:GLU:HG3	2.15	0.47
1:D:94:ALA:C	1:D:95:PHE:CD2	2.83	0.47
1:A:30:LEU:HD21	1:A:383:PRO:HD3	1.97	0.47
1:A:69:TYR:CE2	1:A:74:PRO:HB3	2.50	0.47
1:A:234:ILE:HG22	1:A:235:TYR:N	2.30	0.47
1:C:137:MET:CB	1:C:145:ARG:HH21	2.27	0.47
1:C:39:VAL:CG1	1:C:40:LEU:N	2.78	0.47
1:D:42:ASN:HA	1:D:45:GLN:HG3	1.97	0.47
1:D:268:TYR:O	1:D:272:MET:HG2	2.15	0.47
1:D:298:ALA:HB1	4:D:501:TB2:C7	2.32	0.47
1:A:48:ARG:HD2	1:A:48:ARG:C	2.40	0.46
1:B:314:MET:HE3	1:B:450:PHE:CZ	2.49	0.46
1:B:448:LEU:HD12	1:B:448:LEU:HA	1.72	0.46
1:C:36:PRO:HB3	1:C:69:TYR:CB	2.30	0.46
1:D:327:GLU:HG2	1:D:346:MET:HE3	1.97	0.46
1:D:328:ILE:O	1:D:332:ILE:N	2.40	0.46
1:A:364:PRO:HA	1:A:393:SER:HB2	1.96	0.46
4:D:501:TB2:O1	4:D:501:TB2:H4	2.13	0.46
1:B:291:THR:HG21	5:B:606:CM5:H72	1.97	0.46
1:B:429:PHE:O	1:B:430:SER:CB	2.63	0.46
1:D:302:THR:HG21	3:D:500:HEM:CAB	2.45	0.46
1:D:402:PHE:CD2	1:D:402:PHE:N	2.83	0.46
1:B:28:GLY:O	1:B:381:VAL:HB	2.14	0.46
1:C:245:ILE:HG23	1:C:246:GLY:H	1.80	0.46
1:D:124:LEU:HD22	1:D:291:THR:HG23	1.98	0.46
1:D:165:LEU:HG	1:D:166:ASP:H	1.80	0.46
1:D:288:LEU:HD12	1:D:289:ILE:CG1	2.46	0.46
1:B:225:LYS:HD3	1:C:101:ILE:HA	1.98	0.46
1:B:368:PRO:HD2	1:C:221:SER:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:471:THR:HG22	1:B:472:PRO:HD2	1.98	0.46
1:C:39:VAL:HG13	1:C:40:LEU:N	2.30	0.46
1:D:53:ARG:O	1:D:53:ARG:HD3	2.16	0.46
1:D:88:LEU:HD12	1:D:92:ALA:HA	1.97	0.46
1:D:140:ARG:HA	1:D:140:ARG:HD2	1.46	0.46
1:C:373:LYS:O	1:C:375:THR:HG23	2.16	0.46
1:D:386:THR:HG22	1:D:387:GLU:H	1.80	0.46
1:A:115:PHE:CE2	1:A:290:LEU:CD1	2.98	0.46
1:A:157:LEU:HD12	1:A:157:LEU:HA	1.74	0.46
1:C:255:THR:O	1:C:255:THR:CG2	2.60	0.46
1:D:141:SER:O	1:D:145:ARG:HG3	2.15	0.46
1:D:280:SER:O	1:D:283:PHE:N	2.49	0.46
1:B:314:MET:HE2	1:B:314:MET:HB2	1.65	0.46
1:C:369:HIS:CE1	3:C:500:HEM:O2A	2.68	0.46
1:C:383:PRO:HD2	1:C:386:THR:OG1	2.15	0.46
1:D:370:THR:HG22	1:D:387:GLU:HA	1.98	0.46
1:B:119:GLU:HA	1:B:122:ARG:CZ	2.45	0.46
1:B:362:LEU:N	1:B:362:LEU:CD1	2.79	0.46
1:C:324:VAL:HG13	1:C:349:THR:OG1	2.16	0.46
1:D:140:ARG:HG3	1:D:145:ARG:NE	2.30	0.46
1:D:245:ILE:CG2	1:D:245:ILE:O	2.64	0.46
1:D:410:PRO:C	1:D:412:HIS:H	2.24	0.46
1:A:209:ILE:HA	1:D:206:PHE:O	2.16	0.46
1:A:212:PHE:HE2	1:D:238:LEU:HB2	1.80	0.46
1:B:39:VAL:HG13	1:B:40:LEU:H	1.82	0.45
1:C:203:PHE:HZ	1:C:296:PHE:CE1	2.32	0.45
1:D:423:ASN:OD1	1:D:424:GLU:N	2.49	0.45
1:A:284:HIS:O	1:A:287:ASN:HB3	2.16	0.45
1:A:427:MET:N	1:A:428:PRO:HD3	2.31	0.45
1:B:100:LYS:NZ	1:B:116:ALA:HB1	2.31	0.45
1:B:137:MET:CE	1:B:264:PHE:CD2	3.00	0.45
1:B:226:TYR:HD1	1:C:70:LEU:HD13	1.81	0.45
1:C:141:SER:HB3	1:C:144:GLU:OE1	2.17	0.45
1:D:67:THR:HG23	1:D:75:VAL:O	2.16	0.45
1:D:294:SER:O	1:D:295:LEU:C	2.58	0.45
1:C:227:PHE:N	1:C:227:PHE:CD2	2.83	0.45
1:D:370:THR:HG22	1:D:387:GLU:HG2	1.97	0.45
1:A:40:LEU:HD23	1:A:40:LEU:O	2.17	0.45
1:B:68:VAL:HG12	1:B:70:LEU:HD13	1.98	0.45
1:B:99:GLY:HA2	1:B:370:THR:HG23	1.97	0.45
1:B:225:LYS:HE2	1:C:102:ALA:N	2.25	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:371:VAL:HG23	1:D:385:ASN:H	1.82	0.45
1:A:93:GLU:HG2	1:A:433:LYS:HZ1	1.80	0.45
1:B:269:LEU:HA	1:B:272:MET:SD	2.57	0.45
1:D:140:ARG:NH2	1:D:148:GLU:HG3	2.32	0.45
1:D:410:PRO:O	1:D:412:HIS:N	2.50	0.45
1:A:214:SER:OG	1:D:477:VAL:HG13	2.16	0.45
1:C:208:LEU:HG	1:C:232:ARG:HB3	1.98	0.45
1:D:32:PRO:O	1:D:66:PHE:CB	2.64	0.45
1:D:183:VAL:HA	1:D:264:PHE:HB2	1.98	0.45
1:D:409:ASN:HB2	1:D:412:HIS:CE1	2.52	0.45
1:A:477:VAL:HG23	1:D:227:PHE:HZ	1.82	0.45
1:D:78:LEU:HD22	1:D:78:LEU:N	2.26	0.45
1:B:359:LEU:HD13	1:B:359:LEU:HA	1.84	0.45
1:C:152:CYS:SG	1:C:187:ARG:NH2	2.90	0.45
1:C:330:GLN:O	1:C:330:GLN:HG2	2.17	0.45
1:C:398:ASP:C	1:C:398:ASP:OD1	2.59	0.45
1:D:295:LEU:HD12	1:D:295:LEU:C	2.42	0.45
1:D:302:THR:HG21	3:D:500:HEM:CMB	2.47	0.45
1:A:329:GLU:HA	1:A:329:GLU:OE1	2.16	0.45
1:D:414:LEU:HD12	1:D:414:LEU:N	2.32	0.45
1:D:177:ASN:O	1:D:181:SER:N	2.46	0.45
1:D:264:PHE:CE1	5:D:610:CM5:H112	2.52	0.45
1:B:132:MET:HE3	5:B:607:CM5:H72	1.99	0.44
1:C:252:HIS:HB3	1:C:265:ILE:CD1	2.47	0.44
1:C:298:ALA:HB2	4:C:501:TB2:C5	2.47	0.44
1:C:348:TYR:O	1:C:352:VAL:HG23	2.17	0.44
1:D:213:SER:O	1:D:216:VAL:HG13	2.17	0.44
1:D:108:PHE:O	1:D:112:GLY:HA3	2.18	0.44
1:D:302:THR:HG22	3:D:500:HEM:CAB	2.46	0.44
1:D:409:ASN:HA	1:D:410:PRO:HD3	1.81	0.44
1:A:361:ASP:O	1:A:361:ASP:CG	2.59	0.44
1:A:430:SER:O	1:A:431:LEU:HD23	2.17	0.44
1:C:358:ARG:CG	1:C:396:LEU:HD12	2.46	0.44
1:D:31:PRO:HA	1:D:32:PRO:HD3	1.67	0.44
1:A:288:LEU:O	1:A:292:VAL:HG12	2.18	0.44
1:B:81:THR:HG23	1:B:425:GLY:HA2	1.99	0.44
1:B:132:MET:HE3	5:B:607:CM5:C7	2.47	0.44
1:C:153:LEU:HD21	1:C:453:ILE:HD11	1.99	0.44
1:C:167:ASN:HD22	1:C:486:ILE:CG2	2.28	0.44
1:D:313:LEU:HD13	1:D:356:ILE:HG12	1.98	0.44
1:D:364:PRO:CD	1:D:478:GLY:HA2	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:ARG:HD3	1:B:181:SER:OG	2.17	0.44
1:C:397:HIS:O	1:C:405:PRO:HB3	2.17	0.44
1:D:268:TYR:OH	1:D:284:HIS:CE1	2.71	0.44
1:A:106:PRO:HG2	1:A:235:TYR:OH	2.18	0.44
1:A:292:VAL:HG13	1:A:293:LEU:N	2.33	0.44
1:B:382:ILE:HG22	1:B:386:THR:HB	1.99	0.44
1:C:314:MET:SD	1:C:450:PHE:CZ	3.11	0.44
1:A:367:VAL:CG2	3:A:500:HEM:HAA2	2.48	0.44
1:B:69:TYR:CD1	1:B:74:PRO:HB3	2.52	0.44
1:B:382:ILE:CG2	1:B:386:THR:HB	2.46	0.44
1:C:186:LYS:HE3	1:C:186:LYS:HB2	1.76	0.44
1:C:477:VAL:O	1:C:477:VAL:HG13	2.18	0.44
1:D:133:ARG:HG3	1:D:134:ASP:N	2.33	0.44
1:A:371:VAL:HG22	1:A:373:LYS:O	2.18	0.44
1:A:387:GLU:CD	1:D:225:LYS:NZ	2.76	0.44
1:B:225:LYS:NZ	1:C:101:ILE:HB	2.32	0.44
1:B:409:ASN:ND2	1:B:411:GLY:H	2.15	0.44
1:C:263:ASP:CG	1:C:265:ILE:HG12	2.43	0.44
1:A:109:GLN:O	1:A:113:VAL:HG23	2.17	0.44
1:B:88:LEU:HB2	1:B:431:LEU:HD12	1.99	0.44
1:C:174:ILE:O	1:C:178:ILE:HD13	2.17	0.44
1:C:325:GLN:HG2	1:C:491:ARG:NH2	2.33	0.44
1:C:382:ILE:HD12	1:C:382:ILE:HA	1.72	0.44
1:D:441:ILE:O	1:D:445:GLU:HG3	2.18	0.44
1:A:48:ARG:CG	1:A:49:LYS:N	2.81	0.43
1:A:292:VAL:O	1:A:296:PHE:HB3	2.12	0.43
1:B:284:HIS:O	1:B:285:HIS:C	2.60	0.43
1:C:434:ARG:HG3	3:C:500:HEM:CGA	2.48	0.43
1:D:80:GLY:O	1:D:83:ALA:HB3	2.17	0.43
1:A:98:ARG:HD3	1:A:99:GLY:H	1.83	0.43
1:A:150:ALA:HB1	1:A:452:THR:HG21	1.99	0.43
1:B:310:GLY:O	1:B:314:MET:HE2	2.18	0.43
1:C:51:LEU:HD12	1:C:52:LEU:N	2.32	0.43
1:D:117:ASN:CB	1:D:120:ARG:CZ	2.96	0.43
1:B:36:PRO:C	1:B:37:LEU:O	2.54	0.43
1:D:332:ILE:HG22	1:D:333:GLY:O	2.17	0.43
1:A:46:MET:HE3	1:A:46:MET:HB2	1.91	0.43
1:C:98:ARG:NE	1:C:98:ARG:CA	2.81	0.43
1:D:288:LEU:HD12	1:D:289:ILE:HG13	2.00	0.43
1:A:175:THR:HB	1:A:300:THR:HG23	2.01	0.43
1:A:183:VAL:HA	1:A:264:PHE:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:PHE:CZ	1:B:241:ILE:HD13	2.54	0.43
1:B:436:CYS:HB2	3:B:500:HEM:NA	2.32	0.43
1:D:34:PRO:HB2	1:D:42:ASN:ND2	2.34	0.43
1:D:312:LEU:HB2	1:D:484:TYR:CE1	2.54	0.43
1:D:396:LEU:HD21	1:D:427:MET:H	1.83	0.43
1:D:431:LEU:O	1:D:435:ILE:CG1	2.58	0.43
1:A:37:LEU:N	1:A:42:ASN:OD1	2.50	0.43
1:A:107:ILE:HG23	1:A:235:TYR:OH	2.17	0.43
1:B:367:VAL:CG2	3:B:500:HEM:HAA2	2.49	0.43
1:C:191:LYS:O	1:C:193:PRO:HD3	2.18	0.43
1:C:231:HIS:C	1:C:234:ILE:CG2	2.73	0.43
1:B:100:LYS:HZ1	1:B:116:ALA:HB1	1.83	0.43
1:B:217:PHE:O	1:B:219:LEU:N	2.52	0.43
1:B:309:TYR:HB2	1:B:481:PRO:CG	2.48	0.43
1:D:149:GLU:OE1	1:D:149:GLU:HA	2.19	0.43
1:D:197:ARG:HE	1:D:197:ARG:HA	1.83	0.43
1:D:340:LEU:HD23	1:D:444:THR:HG23	2.00	0.43
1:B:36:PRO:HA	1:B:42:ASN:CB	2.49	0.43
1:C:438:GLY:HA3	3:C:500:HEM:C3C	2.54	0.43
1:A:308:ARG:HH22	1:A:483:SER:CA	2.30	0.43
1:B:93:GLU:HA	1:B:96:SER:HB3	2.00	0.43
1:B:144:GLU:HA	1:B:147:GLN:HE21	1.82	0.43
1:C:367:VAL:HG21	3:C:500:HEM:HAA2	2.01	0.43
1:D:332:ILE:HG12	1:D:336:ARG:NH2	2.33	0.43
1:A:213:SER:HB2	1:D:202:PHE:O	2.19	0.43
1:C:105:ASP:HB3	1:C:106:PRO:HD2	2.00	0.43
1:C:208:LEU:CB	1:C:232:ARG:HG3	2.48	0.43
1:C:269:LEU:N	1:C:269:LEU:HD12	2.34	0.43
1:B:89:VAL:HG23	1:B:431:LEU:HD13	2.01	0.42
1:C:371:VAL:HG21	1:C:382:ILE:HG22	1.98	0.42
1:C:434:ARG:HA	1:C:434:ARG:HH11	1.83	0.42
1:D:197:ARG:HA	1:D:197:ARG:NE	2.34	0.42
1:A:274:LYS:HG3	1:A:275:ASP:N	2.34	0.42
1:A:435:ILE:HG12	1:A:436:CYS:N	2.34	0.42
1:C:98:ARG:HG3	1:C:99:GLY:N	2.34	0.42
1:C:106:PRO:HG2	1:C:107:ILE:H	1.84	0.42
1:C:190:TYR:O	1:C:191:LYS:HD3	2.18	0.42
1:C:225:LYS:CE	1:C:226:TYR:HE2	2.32	0.42
1:C:227:PHE:N	1:C:228:PRO:CD	2.83	0.42
1:D:111:TYR:O	1:D:112:GLY:C	2.60	0.42
1:A:437:LEU:HD22	1:A:437:LEU:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:307:LEU:HD23	1:B:307:LEU:HA	1.85	0.42
1:C:206:PHE:HE1	1:C:208:LEU:HD11	1.73	0.42
1:C:298:ALA:O	4:C:501:TB2:O1	2.37	0.42
1:A:315:LEU:HD11	1:A:486:ILE:HG13	2.00	0.42
1:B:62:TYR:N	1:B:62:TYR:CD2	2.88	0.42
1:C:69:TYR:CE2	1:C:74:PRO:HB3	2.54	0.42
1:D:268:TYR:HH	1:D:284:HIS:CE1	2.37	0.42
1:D:415:ASP:OD1	1:D:415:ASP:C	2.62	0.42
1:A:316:LYS:HD3	1:A:470:LEU:HD11	2.01	0.42
1:A:382:ILE:HA	1:A:383:PRO:HD3	1.86	0.42
1:B:77:VAL:HG22	1:B:389:PHE:HB2	2.01	0.42
1:B:289:ILE:HG23	1:B:290:LEU:HD12	2.02	0.42
1:D:185:GLY:HA2	1:D:263:ASP:HB3	2.01	0.42
1:D:296:PHE:HD1	1:D:300:THR:HG21	1.76	0.42
1:D:351:ALA:HB1	1:D:414:LEU:HD11	2.01	0.42
3:D:500:HEM:HMB1	3:D:500:HEM:CBB	2.42	0.42
1:A:192:ASP:HA	1:A:193:PRO:HD3	1.93	0.42
3:A:500:HEM:HHA	3:A:500:HEM:CBD	2.49	0.42
1:C:388:VAL:O	1:C:390:PRO:HD3	2.19	0.42
1:C:398:ASP:OD1	1:C:400:ARG:CG	2.67	0.42
1:D:120:ARG:HE	1:D:120:ARG:HB2	1.17	0.42
1:D:164:LEU:HA	1:D:486:ILE:O	2.20	0.42
1:D:313:LEU:O	1:D:313:LEU:HD23	2.19	0.42
1:B:143:GLU:O	1:B:147:GLN:HG2	2.19	0.42
1:B:192:ASP:OD1	1:B:192:ASP:C	2.63	0.42
1:D:285:HIS:CD2	1:D:288:LEU:HD11	2.55	0.42
1:A:98:ARG:HH22	3:A:500:HEM:HBD1	1.84	0.42
1:A:371:VAL:HG11	1:A:382:ILE:HG22	2.02	0.42
1:C:105:ASP:HB3	1:C:107:ILE:HG12	2.02	0.42
1:D:397:HIS:O	1:D:405:PRO:HG2	2.20	0.42
1:A:205:SER:HA	1:D:211:SER:HB3	2.02	0.42
1:A:295:LEU:HG	3:A:500:HEM:CBC	2.38	0.42
3:A:500:HEM:HHA	3:A:500:HEM:HBD1	2.02	0.42
4:B:501:TB2:O1	4:B:501:TB2:C8	2.64	0.42
1:B:226:TYR:CD2	1:B:226:TYR:N	2.88	0.42
1:B:430:SER:HB2	3:B:500:HEM:HBA1	2.01	0.42
1:C:163:ALA:O	1:C:165:LEU:HD23	2.20	0.42
1:C:184:PHE:O	1:C:263:ASP:OD2	2.38	0.42
1:C:427:MET:HB2	1:C:431:LEU:HD11	2.02	0.42
1:D:78:LEU:HD23	1:D:78:LEU:O	2.20	0.42
1:D:135:PHE:CD1	1:D:261:PRO:HG2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:ARG:CZ	1:B:133:ARG:HG3	2.50	0.41
1:B:133:ARG:HB2	5:B:607:CM5:O20	2.20	0.41
1:C:38:PRO:O	1:C:40:LEU:HD22	2.20	0.41
1:C:66:PHE:CE2	1:C:77:VAL:CG2	3.03	0.41
1:C:363:ILE:O	1:C:363:ILE:HG22	2.19	0.41
1:D:313:LEU:HD13	1:D:356:ILE:CG1	2.50	0.41
1:D:332:ILE:HG12	1:D:336:ARG:HH22	1.85	0.41
1:D:380:TYR:CD1	1:D:380:TYR:N	2.87	0.41
1:A:48:ARG:HG2	1:A:474:GLU:CG	2.50	0.41
1:A:296:PHE:C	1:A:296:PHE:HD1	2.24	0.41
1:A:313:LEU:HD13	1:A:408:PHE:CD1	2.55	0.41
1:B:91:GLN:NE2	1:B:375:THR:HG23	2.35	0.41
1:C:33:GLY:N	1:C:62:TYR:CD1	2.88	0.41
1:C:44:LEU:O	1:C:45:GLN:C	2.62	0.41
1:C:208:LEU:CD2	1:C:232:ARG:CB	2.99	0.41
1:C:208:LEU:HG	1:C:232:ARG:CB	2.51	0.41
1:C:398:ASP:OD1	1:C:400:ARG:HG2	2.19	0.41
1:D:386:THR:HG22	1:D:387:GLU:N	2.35	0.41
1:B:112:GLY:C	1:B:113:VAL:HG12	2.46	0.41
1:D:91:GLN:HE21	1:D:94:ALA:HB2	1.85	0.41
1:A:68:VAL:CG1	1:A:75:VAL:HG22	2.48	0.41
1:B:39:VAL:HG13	1:B:40:LEU:N	2.35	0.41
1:B:137:MET:CE	1:B:264:PHE:HD2	2.33	0.41
1:B:237:ASN:O	1:B:238:LEU:C	2.63	0.41
1:D:201:LEU:HA	1:D:201:LEU:HD12	1.80	0.41
1:D:285:HIS:O	1:D:285:HIS:CD2	2.72	0.41
1:D:288:LEU:CD1	1:D:289:ILE:HG13	2.50	0.41
1:D:349:THR:O	1:D:352:VAL:HG12	2.20	0.41
1:D:403:GLU:H	1:D:412:HIS:CD2	2.38	0.41
1:D:464:PRO:HA	1:D:465:PRO:HD3	1.90	0.41
1:B:476:GLY:C	1:B:477:VAL:CG1	2.93	0.41
1:C:243:THR:HG22	1:C:244:PHE:N	2.35	0.41
1:D:164:LEU:N	1:D:164:LEU:HD23	2.35	0.41
1:D:401:TYR:O	1:D:402:PHE:CD2	2.74	0.41
1:A:212:PHE:CE2	1:D:238:LEU:HD12	2.56	0.41
1:B:285:HIS:O	1:B:286:GLN:C	2.63	0.41
1:C:73:ARG:HA	1:C:74:PRO:HD3	1.83	0.41
1:C:142:VAL:O	1:C:143:GLU:C	2.62	0.41
1:C:383:PRO:HG2	1:C:386:THR:HG21	2.02	0.41
1:A:290:LEU:O	1:A:291:THR:C	2.64	0.41
1:D:288:LEU:HD12	1:D:289:ILE:CA	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:358:ARG:HD2	1:D:402:PHE:CE1	2.56	0.41
1:A:141:SER:O	1:A:145:ARG:HG3	2.21	0.41
1:A:296:PHE:CD1	1:A:296:PHE:O	2.74	0.41
1:B:84:ILE:HD12	1:B:395:ALA:HB2	2.03	0.41
1:B:174:ILE:HG13	1:B:175:THR:N	2.35	0.41
1:C:401:TYR:CE2	1:C:424:GLU:HB2	2.55	0.41
1:D:192:ASP:OD1	1:D:193:PRO:HD2	2.21	0.41
1:A:41:GLY:HA3	1:A:44:LEU:HD22	2.03	0.41
1:C:234:ILE:CG2	1:C:235:TYR:N	2.84	0.41
1:C:332:ILE:HD11	1:C:342:ASP:HB3	2.02	0.41
1:C:414:LEU:HA	1:C:419:ALA:O	2.21	0.41
1:D:38:PRO:O	1:D:39:VAL:HB	2.21	0.41
1:A:288:LEU:HD12	1:A:288:LEU:O	2.21	0.41
1:B:75:VAL:O	1:B:75:VAL:HG23	2.20	0.41
1:B:172:HIS:CD2	1:B:203:PHE:CD2	3.09	0.41
1:B:222:GLY:HA2	1:C:101:ILE:HG22	2.01	0.41
1:B:232:ARG:CG	1:B:233:GLN:H	2.29	0.41
1:C:58:LEU:C	1:C:58:LEU:CD1	2.87	0.41
1:C:337:PRO:HA	1:C:338:PRO:HD3	1.94	0.41
1:C:368:PRO:HG3	1:C:389:PHE:CE2	2.56	0.41
1:D:59:ARG:CA	1:D:66:PHE:HE1	2.30	0.41
1:A:398:ASP:HA	1:A:399:PRO:HD3	1.85	0.40
1:B:217:PHE:C	1:B:219:LEU:N	2.79	0.40
1:B:476:GLY:C	1:B:477:VAL:HG12	2.46	0.40
4:B:501:TB2:H12B	4:B:501:TB2:H7	1.89	0.40
1:C:198:LEU:HD23	1:C:198:LEU:HA	1.90	0.40
1:C:314:MET:HB3	1:C:459:ILE:HD11	2.03	0.40
1:D:114:ILE:O	1:D:120:ARG:CZ	2.69	0.40
1:D:289:ILE:O	1:D:293:LEU:N	2.43	0.40
2:G:2:FRU:C4	2:G:2:FRU:HO1	2.34	0.40
1:A:34:PRO:HG3	1:A:58:LEU:CD2	2.51	0.40
1:A:104:VAL:C	1:A:105:ASP:OD1	2.65	0.40
1:A:466:GLU:H	1:A:466:GLU:CD	2.29	0.40
1:C:245:ILE:CG2	1:C:246:GLY:N	2.84	0.40
1:D:55:PHE:HE1	1:D:77:VAL:HG11	1.87	0.40
1:A:211:SER:O	1:A:212:PHE:C	2.65	0.40
1:A:477:VAL:CG2	1:D:227:PHE:HZ	2.34	0.40
3:B:500:HEM:HHA	3:B:500:HEM:CBD	2.50	0.40
1:D:108:PHE:O	1:D:112:GLY:N	2.53	0.40
1:D:363:ILE:HA	1:D:364:PRO:HD3	1.76	0.40
1:D:397:HIS:CD2	1:D:405:PRO:O	2.74	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:325:GLN:CD	1:B:491:ARG:HH21	2.30	0.40
1:C:263:ASP:OD1	1:C:263:ASP:N	2.54	0.40
1:C:383:PRO:HB2	1:C:386:THR:OG1	2.21	0.40
1:D:363:ILE:HD11	4:D:501:TB2:H4	2.04	0.40
1:A:40:LEU:O	1:A:44:LEU:HD22	2.21	0.40
1:A:350:ASP:HB3	1:A:420:LEU:HD13	2.03	0.40
1:C:162:GLY:O	1:C:487:ARG:HB3	2.22	0.40
1:D:231:HIS:O	1:D:232:ARG:C	2.63	0.40
1:D:312:LEU:HD22	1:D:484:TYR:CD1	2.57	0.40
1:D:371:VAL:HG23	1:D:385:ASN:N	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	463/476 (97%)	440 (95%)	18 (4%)	5 (1%)	11	43
1	B	463/476 (97%)	426 (92%)	36 (8%)	1 (0%)	43	76
1	C	452/476 (95%)	423 (94%)	27 (6%)	2 (0%)	30	65
1	D	462/476 (97%)	415 (90%)	43 (9%)	4 (1%)	14	48
All	All	1840/1904 (97%)	1704 (93%)	124 (7%)	12 (1%)	18	53

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	39	VAL
1	A	45	GLN
1	D	430	SER
1	A	136	GLY
1	B	36	PRO

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Mol	Chain	Res	Type
1	C	45	GLN
1	D	341	ASP
1	D	364	PRO
1	D	411	GLY
1	A	477	VAL
1	A	106	PRO
1	C	477	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	375/421 (89%)	333 (89%)	42 (11%)	6	24
1	B	377/421 (90%)	329 (87%)	48 (13%)	4	20
1	C	343/421 (82%)	296 (86%)	47 (14%)	3	17
1	D	345/421 (82%)	301 (87%)	44 (13%)	4	19
All	All	1440/1684 (86%)	1259 (87%)	181 (13%)	4	20

All (181) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	PRO
1	A	39	VAL
1	A	42	ASN
1	A	47	ASP
1	A	48	ARG
1	A	51	LEU
1	A	59	ARG
1	A	60	GLU
1	A	75	VAL
1	A	101	ILE
1	A	111	TYR
1	A	137	MET
1	A	144	GLU
1	A	157	LEU

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Mol	Chain	Res	Type
1	A	165	LEU
1	A	170	LEU
1	A	172	HIS
1	A	194	VAL
1	A	198	LEU
1	A	200	ASP
1	A	219	LEU
1	A	224	LEU
1	A	226	TYR
1	A	230	THR
1	A	234	ILE
1	A	240	GLU
1	A	287	ASN
1	A	288	LEU
1	A	289	ILE
1	A	291	THR
1	A	293	LEU
1	A	343	ARG
1	A	370	THR
1	A	400	ARG
1	A	420	LEU
1	A	434	ARG
1	A	437	LEU
1	A	441	ILE
1	A	477	VAL
1	A	486	ILE
1	A	489	LEU
1	A	491	ARG
1	B	43	LEU
1	B	44	LEU
1	B	58	LEU
1	B	70	LEU
1	B	104	VAL
1	B	107	ILE
1	B	114	ILE
1	B	117	ASN
1	B	137	MET
1	B	145	ARG
1	B	165	LEU
1	B	169	LEU
1	B	204	GLN
1	B	207	SER

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Mol	Chain	Res	Type
1	B	215	GLN
1	B	219	LEU
1	B	224	LEU
1	B	225	LYS
1	B	232	ARG
1	B	248	SER
1	B	250	GLU
1	B	276	LYS
1	B	285	HIS
1	B	286	GLN
1	B	287	ASN
1	B	288	LEU
1	B	294	SER
1	B	300	THR
1	B	306	THR
1	B	323	ARG
1	B	327	GLU
1	B	329	GLU
1	B	331	VAL
1	B	349	THR
1	B	359	LEU
1	B	362	LEU
1	B	417	ASN
1	B	420	LEU
1	B	431	LEU
1	B	434	ARG
1	B	437	LEU
1	B	448	LEU
1	B	466	GLU
1	B	467	ASP
1	B	473	ARG
1	B	477	VAL
1	B	489	LEU
1	B	491	ARG
1	C	30	LEU
1	C	39	VAL
1	C	40	LEU
1	C	42	ASN
1	C	48	ARG
1	C	58	LEU
1	C	61	LYS
1	C	65	VAL

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Mol	Chain	Res	Type
1	C	77	VAL
1	C	91	GLN
1	C	148	GLU
1	C	158	ARG
1	C	165	LEU
1	C	170	LEU
1	C	196	LEU
1	C	198	LEU
1	C	208	LEU
1	C	217	PHE
1	C	224	LEU
1	C	226	TYR
1	C	227	PHE
1	C	238	LEU
1	C	245	ILE
1	C	252	HIS
1	C	253	ARG
1	C	269	LEU
1	C	287	ASN
1	C	292	VAL
1	C	296	PHE
1	C	314	MET
1	C	325	GLN
1	C	327	GLU
1	C	332	ILE
1	C	349	THR
1	C	382	ILE
1	C	386	THR
1	C	387	GLU
1	C	403	GLU
1	C	404	THR
1	C	437	LEU
1	C	443	ARG
1	C	458	SER
1	C	471	THR
1	C	473	ARG
1	C	483	SER
1	C	485	GLN
1	C	489	LEU
1	D	30	LEU
1	D	49	LYS
1	D	53	ARG

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Mol	Chain	Res	Type
1	D	75	VAL
1	D	78	LEU
1	D	79	CYS
1	D	90	ASP
1	D	95	PHE
1	D	107	ILE
1	D	120	ARG
1	D	140	ARG
1	D	141	SER
1	D	148	GLU
1	D	198	LEU
1	D	199	LEU
1	D	201	LEU
1	D	209	ILE
1	D	214	SER
1	D	216	VAL
1	D	238	LEU
1	D	241	ILE
1	D	243	THR
1	D	253	ARG
1	D	262	ARG
1	D	291	THR
1	D	295	LEU
1	D	322	GLU
1	D	324	VAL
1	D	340	LEU
1	D	352	VAL
1	D	353	ILE
1	D	356	ILE
1	D	358	ARG
1	D	362	LEU
1	D	374	ASP
1	D	375	THR
1	D	385	ASN
1	D	392	LEU
1	D	393	SER
1	D	400	ARG
1	D	407	THR
1	D	439	GLU
1	D	463	VAL
1	D	470	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22)

such sidechains are listed below:

Mol	Chain	Res	Type
1	B	147	GLN
1	B	215	GLN
1	B	233	GLN
1	B	287	ASN
1	B	385	ASN
1	B	406	ASN
1	B	409	ASN
1	B	455	GLN
1	B	456	ASN
1	B	479	ASN
1	C	215	GLN
1	C	231	HIS
1	C	287	ASN
1	D	42	ASN
1	D	45	GLN
1	D	91	GLN
1	D	233	GLN
1	D	237	ASN
1	D	242	ASN
1	D	285	HIS
1	D	455	GLN
1	D	479	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

8 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	GLC	E	1	2	11,11,12	1.21	1 (9%)	15,15,17	2.29	8 (53%)
2	FRU	E	2	2	11,12,12	1.38	2 (18%)	10,18,18	1.78	4 (40%)
2	GLC	F	1	2	11,11,12	1.19	1 (9%)	15,15,17	2.28	7 (46%)
2	FRU	F	2	2	11,12,12	1.28	1 (9%)	10,18,18	1.70	3 (30%)
2	GLC	G	1	2	11,11,12	1.23	1 (9%)	15,15,17	2.52	7 (46%)
2	FRU	G	2	2	11,12,12	1.30	1 (9%)	10,18,18	1.73	3 (30%)
2	GLC	H	1	2	11,11,12	1.20	1 (9%)	15,15,17	2.19	7 (46%)
2	FRU	H	2	2	11,12,12	1.29	1 (9%)	10,18,18	1.73	3 (30%)

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	GLC	E	1	2	-	0/2/19/22	0/1/1/1
2	FRU	E	2	2	-	1/5/24/24	0/1/1/1
2	GLC	F	1	2	-	0/2/19/22	0/1/1/1
2	FRU	F	2	2	-	1/5/24/24	0/1/1/1
2	GLC	G	1	2	-	2/2/19/22	0/1/1/1
2	FRU	G	2	2	-	4/5/24/24	0/1/1/1
2	GLC	H	1	2	-	0/2/19/22	0/1/1/1
2	FRU	H	2	2	-	2/5/24/24	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	2	FRU	O3-C3	-2.34	1.38	1.42
2	E	2	FRU	O3-C3	-2.30	1.38	1.42
2	H	2	FRU	O3-C3	-2.22	1.38	1.42
2	E	1	GLC	O2-C2	-2.18	1.38	1.43
2	F	2	FRU	O3-C3	-2.15	1.38	1.42
2	F	1	GLC	O2-C2	-2.09	1.39	1.43
2	G	1	GLC	O2-C2	-2.07	1.39	1.43
2	H	1	GLC	O2-C2	-2.07	1.39	1.43
2	E	2	FRU	O2-C2	2.01	1.44	1.40

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	1	GLC	O5-C5-C6	4.70	116.81	107.66
2	F	1	GLC	O5-C5-C6	4.43	116.28	107.66
2	H	1	GLC	O5-C5-C6	4.25	115.94	107.66
2	E	1	GLC	O5-C5-C6	4.03	115.52	107.66
2	G	1	GLC	O3-C3-C2	3.76	117.72	110.05
2	E	1	GLC	O3-C3-C2	3.41	117.01	110.05
2	G	1	GLC	O4-C4-C5	3.34	117.54	109.32
2	G	1	GLC	O2-C2-C1	3.29	116.76	109.22
2	G	2	FRU	O5-C5-C6	3.25	117.75	108.89
2	H	1	GLC	O2-C2-C1	3.24	116.64	109.22
2	G	1	GLC	O2-C2-C3	3.13	116.64	110.15
2	F	1	GLC	O3-C3-C2	3.12	116.43	110.05
2	F	1	GLC	O2-C2-C1	3.10	116.31	109.22
2	F	1	GLC	O2-C2-C3	3.03	116.42	110.15
2	E	2	FRU	O5-C5-C6	2.97	116.99	108.89
2	F	1	GLC	O4-C4-C5	2.96	116.62	109.32
2	E	1	GLC	O2-C2-C3	2.92	116.20	110.15
2	F	2	FRU	O5-C5-C6	2.91	116.83	108.89
2	H	2	FRU	O5-C5-C6	2.91	116.82	108.89
2	E	1	GLC	O4-C4-C5	2.91	116.49	109.32
2	E	1	GLC	O2-C2-C1	2.89	115.84	109.22
2	H	1	GLC	O4-C4-C5	2.85	116.33	109.32
2	H	1	GLC	O2-C2-C3	2.82	115.99	110.15
2	H	1	GLC	O3-C3-C2	2.81	115.79	110.05
2	G	1	GLC	O4-C4-C3	2.67	116.66	110.38
2	G	2	FRU	O1-C1-C2	2.61	117.46	111.67
2	H	1	GLC	O4-C4-C3	2.60	116.50	110.38
2	H	1	GLC	O3-C3-C4	2.58	116.46	110.38
2	G	1	GLC	O3-C3-C4	2.56	116.40	110.38
2	E	1	GLC	O4-C4-C3	2.53	116.34	110.38
2	E	1	GLC	O3-C3-C4	2.53	116.33	110.38
2	F	1	GLC	O4-C4-C3	2.50	116.28	110.38
2	H	2	FRU	O1-C1-C2	2.50	117.20	111.67
2	F	1	GLC	O3-C3-C4	2.46	116.17	110.38
2	E	2	FRU	O1-C1-C2	2.34	116.84	111.67
2	E	2	FRU	O2-C2-O5	-2.33	104.85	109.33
2	H	2	FRU	O4-C4-C5	2.30	117.68	111.08
2	F	2	FRU	O4-C4-C5	2.28	117.64	111.08
2	E	1	GLC	C1-O5-C5	2.20	115.13	112.19
2	F	2	FRU	O1-C1-C2	2.17	116.48	111.67
2	E	2	FRU	O4-C4-C5	2.09	117.09	111.08
2	G	2	FRU	O4-C4-C5	2.02	116.89	111.08

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	2	FRU	O1-C1-C2-O2
2	G	2	FRU	C4-C5-C6-O6
2	G	2	FRU	O5-C5-C6-O6
2	G	1	GLC	O5-C5-C6-O6
2	G	1	GLC	C4-C5-C6-O6
2	H	2	FRU	C4-C5-C6-O6
2	G	2	FRU	O1-C1-C2-O5
2	E	2	FRU	C4-C5-C6-O6
2	F	2	FRU	O1-C1-C2-C3
2	H	2	FRU	O1-C1-C2-C3

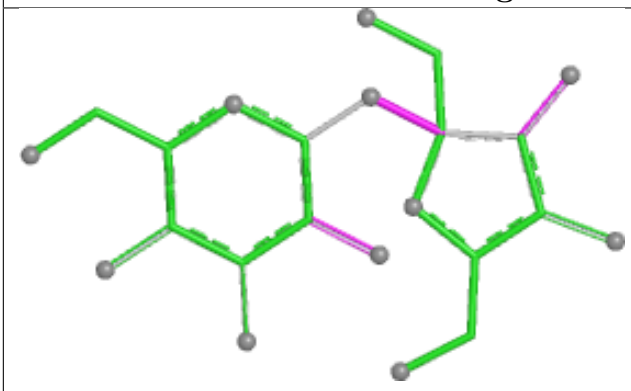
There are no ring outliers.

8 monomers are involved in 28 short contacts:

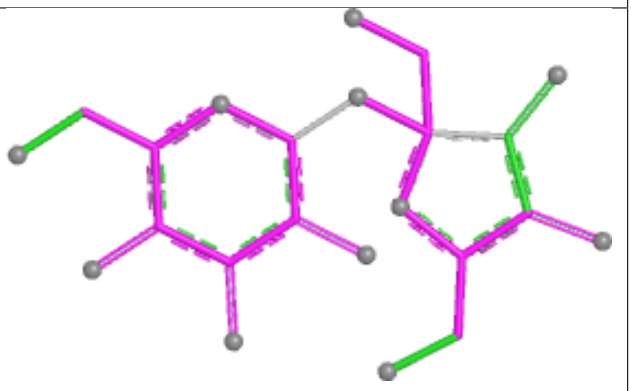
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	1	GLC	8	0
2	G	2	FRU	2	0
2	H	1	GLC	10	0
2	G	1	GLC	3	0
2	F	2	FRU	9	0
2	E	1	GLC	5	0
2	H	2	FRU	7	0
2	E	2	FRU	5	0

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

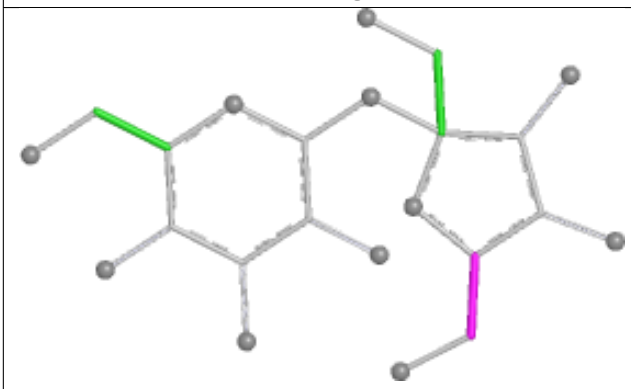
Oligosaccharide Chain E



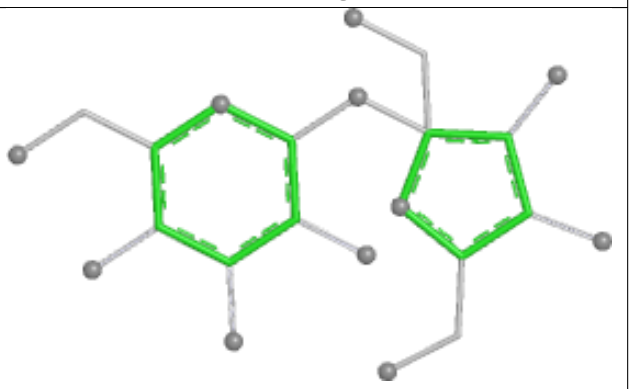
Bond lengths



Bond angles

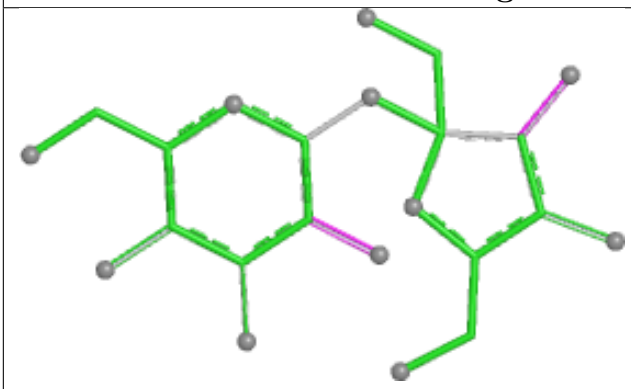


Torsions

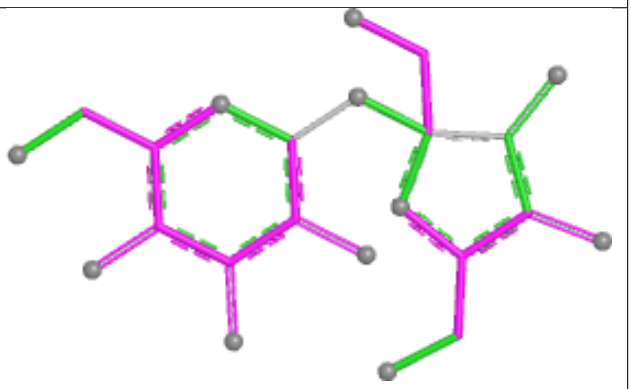


Rings

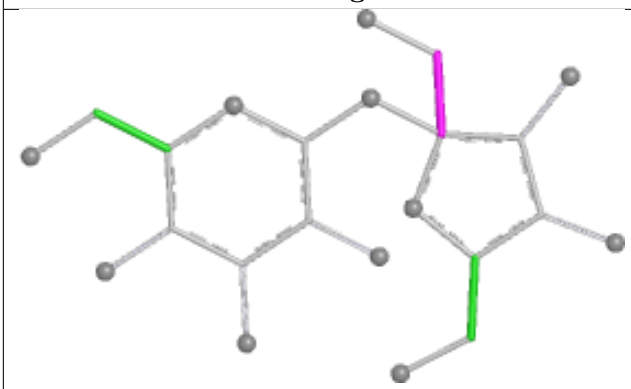
Oligosaccharide Chain F



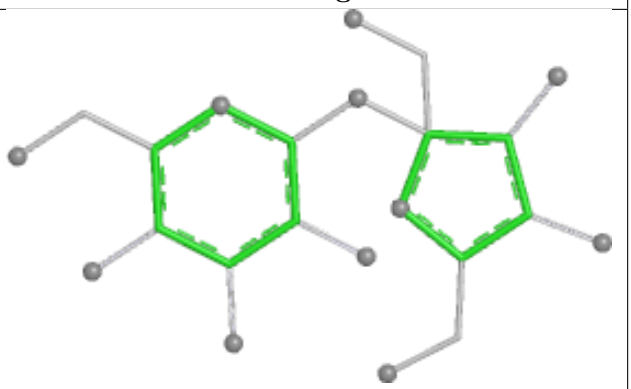
Bond lengths



Bond angles

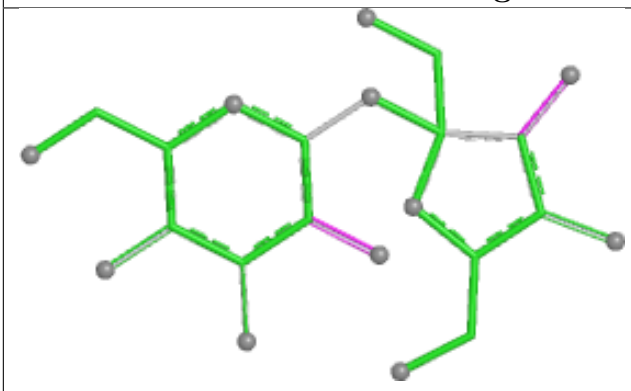


Torsions

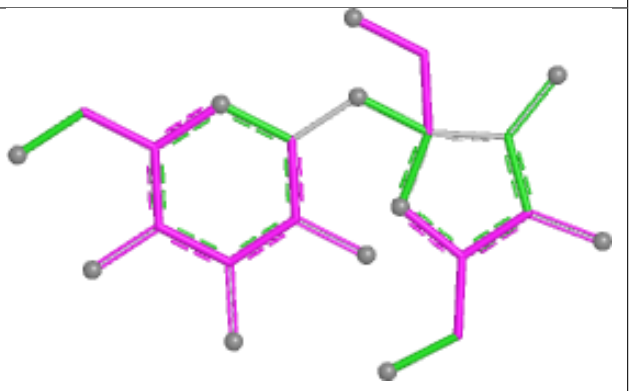


Rings

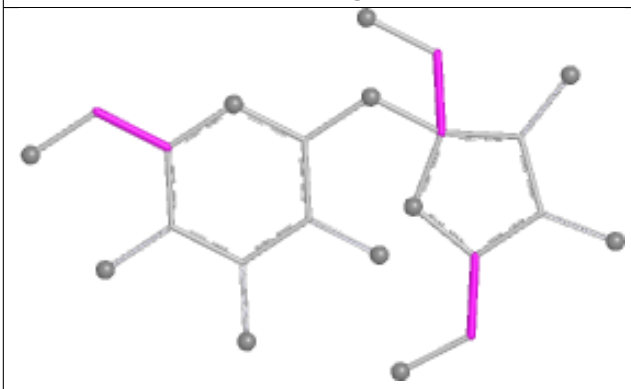
Oligosaccharide Chain G



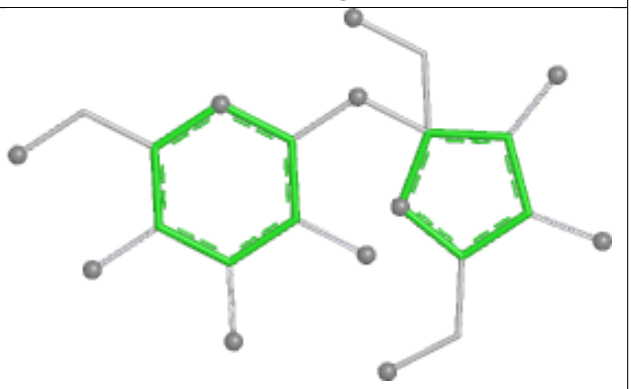
Bond lengths



Bond angles

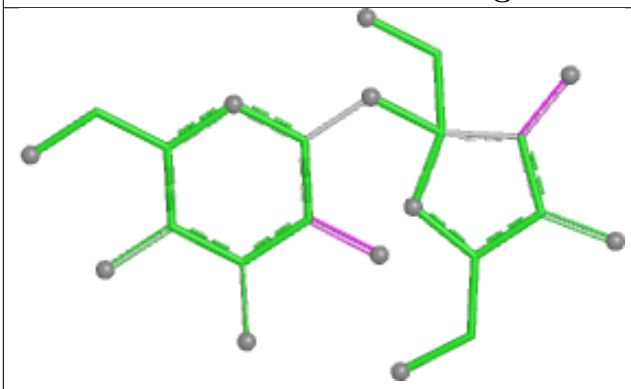


Torsions

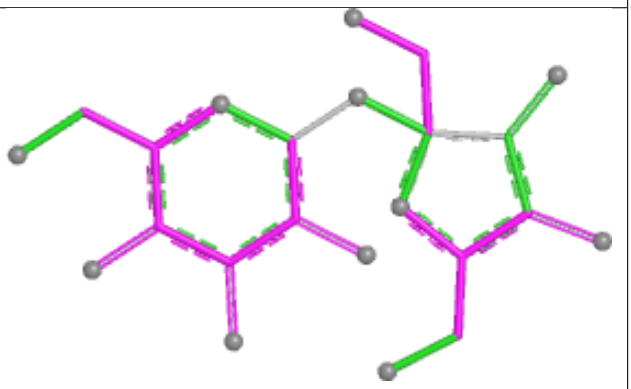


Rings

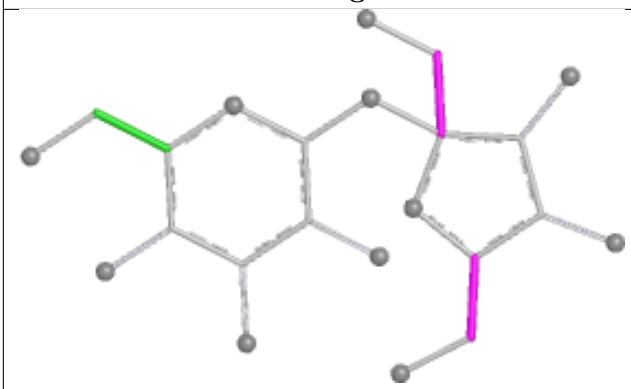
Oligosaccharide Chain H



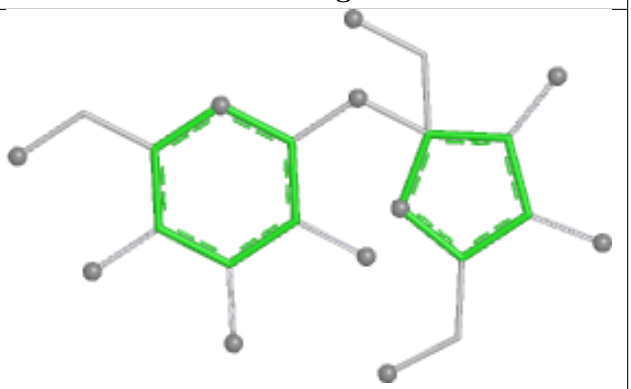
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

13 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	$\#\|Z\| > 2$
4	TB2	B	501	1	12,13,13	0.59	0	18,18,18	0.82	0
5	CM5	A	608	-	36,36,36	0.44	0	49,49,49	1.18	4 (8%)
5	CM5	B	606	-	36,36,36	0.41	0	49,49,49	0.99	3 (6%)
5	CM5	D	610	-	36,36,36	0.40	0	49,49,49	0.75	1 (2%)
5	CM5	A	605	-	25,25,36	0.44	0	32,32,49	0.79	1 (3%)
5	CM5	B	607	-	36,36,36	0.41	0	49,49,49	0.78	1 (2%)
3	HEM	C	500	1	50,50,50	1.89	8 (16%)	67,82,82	1.35	4 (5%)
4	TB2	C	501	1	12,13,13	0.60	0	18,18,18	0.92	0
4	TB2	D	501	1	12,13,13	0.69	0	18,18,18	1.81	1 (5%)
4	TB2	A	501	1	12,13,13	0.60	0	18,18,18	0.89	0
3	HEM	A	500	1	50,50,50	1.90	8 (16%)	67,82,82	1.42	7 (10%)
3	HEM	D	500	1	50,50,50	1.87	9 (18%)	67,82,82	1.25	3 (4%)
3	HEM	B	500	1	50,50,50	1.85	10 (20%)	67,82,82	1.36	7 (10%)

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
4	TB2	B	501	1	-	6/9/9/9	0/1/1/1
5	CM5	A	608	-	-	9/17/65/65	0/3/3/3
5	CM5	B	606	-	-	9/17/65/65	0/3/3/3
5	CM5	D	610	-	-	8/17/65/65	0/3/3/3
5	CM5	A	605	-	-	8/13/41/65	0/2/2/3
5	CM5	B	607	-	-	9/17/65/65	0/3/3/3
3	HEM	C	500	1	-	2/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	TB2	C	501	1	-	6/9/9/9	0/1/1/1
4	TB2	D	501	1	-	0/9/9/9	0/1/1/1
4	TB2	A	501	1	-	0/9/9/9	0/1/1/1
3	HEM	A	500	1	-	8/14/54/54	-
3	HEM	D	500	1	-	3/14/54/54	-
3	HEM	B	500	1	-	6/14/54/54	-

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	500	HEM	C3D-C2D	8.01	1.54	1.36
3	D	500	HEM	C3D-C2D	7.90	1.53	1.36
3	B	500	HEM	C3D-C2D	7.80	1.53	1.36
3	A	500	HEM	C3D-C2D	7.77	1.53	1.36
3	A	500	HEM	FE-ND	4.77	2.09	1.94
3	A	500	HEM	FE-NB	4.68	2.09	1.94
3	B	500	HEM	FE-ND	4.58	2.09	1.94
3	C	500	HEM	FE-ND	4.51	2.08	1.94
3	D	500	HEM	FE-ND	4.51	2.08	1.94
3	C	500	HEM	FE-NB	3.99	2.07	1.94
3	D	500	HEM	FE-NB	3.95	2.07	1.94
3	B	500	HEM	FE-NB	3.86	2.06	1.94
3	C	500	HEM	FE-NA	3.39	2.06	1.95
3	D	500	HEM	FE-NA	3.24	2.05	1.95
3	A	500	HEM	FE-NA	3.22	2.05	1.95
3	C	500	HEM	FE-NC	3.05	2.05	1.95
3	D	500	HEM	CAB-C3B	2.93	1.55	1.47
3	D	500	HEM	FE-NC	2.87	2.04	1.95
3	B	500	HEM	CAB-C3B	2.86	1.55	1.47
3	C	500	HEM	CAC-C3C	2.86	1.55	1.47
3	B	500	HEM	CAC-C3C	2.85	1.55	1.47
3	A	500	HEM	CAB-C3B	2.85	1.55	1.47
3	B	500	HEM	FE-NC	2.83	2.04	1.95
3	C	500	HEM	CAB-C3B	2.80	1.54	1.47
3	D	500	HEM	CAC-C3C	2.77	1.54	1.47
3	B	500	HEM	FE-NA	2.75	2.04	1.95
3	A	500	HEM	CAC-C3C	2.74	1.54	1.47
3	A	500	HEM	FE-NC	2.67	2.04	1.95
3	B	500	HEM	CMC-C2C	2.13	1.55	1.50
3	D	500	HEM	CMD-C2D	2.07	1.55	1.50
3	D	500	HEM	C2A-C3A	-2.06	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	500	HEM	CMD-C2D	2.01	1.54	1.50
3	B	500	HEM	CMA-C3A	2.01	1.54	1.50
3	C	500	HEM	CMC-C2C	2.00	1.54	1.50
3	B	500	HEM	CMD-C2D	2.00	1.54	1.50

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	501	TB2	O1-C1-C2	-6.92	104.91	126.34
3	A	500	HEM	C4D-ND-C1D	5.42	111.63	105.21
3	C	500	HEM	C4D-ND-C1D	5.41	111.61	105.21
3	B	500	HEM	C4D-ND-C1D	5.27	111.45	105.21
3	D	500	HEM	C4D-ND-C1D	5.15	111.30	105.21
5	A	608	CM5	O25-C26-C27	4.14	117.17	109.70
5	A	608	CM5	C24-O25-C26	3.87	121.27	113.72
3	A	500	HEM	CAD-C3D-C4D	3.23	130.32	124.70
3	B	500	HEM	CAD-C3D-C4D	2.93	129.80	124.70
5	B	606	CM5	C18-C17-C16	2.89	116.24	109.68
3	B	500	HEM	C3B-C2B-C1B	2.67	108.42	106.41
3	C	500	HEM	C3B-C4B-NB	-2.67	107.55	109.47
3	A	500	HEM	C3B-C2B-C1B	2.64	108.39	106.41
3	B	500	HEM	C3B-C4B-NB	-2.64	107.57	109.47
3	C	500	HEM	C3B-C2B-C1B	2.55	108.33	106.41
3	B	500	HEM	C1B-NB-C4B	2.49	108.16	105.21
3	A	500	HEM	CAD-CBD-CGD	-2.39	107.34	113.67
5	A	605	CM5	C13-C18-C17	2.36	114.97	110.01
3	A	500	HEM	C3B-C4B-NB	-2.34	107.79	109.47
3	C	500	HEM	C1B-NB-C4B	2.33	107.97	105.21
3	A	500	HEM	C1B-NB-C4B	2.26	107.88	105.21
3	D	500	HEM	C2A-C1A-NA	-2.26	107.65	110.15
3	B	500	HEM	CAD-CBD-CGD	-2.22	107.77	113.67
3	D	500	HEM	C3B-C2B-C1B	2.21	108.07	106.41
5	D	610	CM5	O14-C15-C16	2.19	114.24	109.72
5	A	608	CM5	C24-O23-C16	-2.15	112.89	117.98
5	A	608	CM5	C28-C27-C26	2.08	114.00	110.23
5	B	606	CM5	C13-O14-C15	-2.07	109.67	113.72
3	A	500	HEM	CAA-CBA-CGA	-2.07	108.18	113.67
5	B	607	CM5	C1-O12-C13	-2.04	110.20	113.68
5	B	606	CM5	C13-C18-C17	2.04	114.30	110.01
3	B	500	HEM	C2A-C1A-NA	-2.02	107.91	110.15

There are no chirality outliers.

All (74) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	605	CM5	O14-C13-O12-C1
5	B	606	CM5	C18-C13-O12-C1
5	B	606	CM5	O14-C13-O12-C1
5	D	610	CM5	O14-C13-O12-C1
3	A	500	HEM	C2D-C3D-CAD-CBD
3	B	500	HEM	C2D-C3D-CAD-CBD
3	A	500	HEM	C4D-C3D-CAD-CBD
3	B	500	HEM	C4D-C3D-CAD-CBD
5	A	608	CM5	C27-C26-C30-O31
3	D	500	HEM	C3D-CAD-CBD-CGD
5	A	608	CM5	O14-C13-O12-C1
5	A	605	CM5	C18-C13-O12-C1
5	A	608	CM5	C18-C13-O12-C1
5	D	610	CM5	C18-C13-O12-C1
5	A	608	CM5	O25-C26-C30-O31
5	B	606	CM5	C15-C16-O23-C24
5	D	610	CM5	O25-C26-C30-O31
5	B	606	CM5	C3-C4-C5-C6
5	B	606	CM5	C17-C16-O23-C24
5	B	607	CM5	O14-C15-C19-O20
5	A	605	CM5	O14-C15-C19-O20
5	A	605	CM5	C16-C15-C19-O20
5	B	607	CM5	C15-C16-O23-C24
5	A	608	CM5	C2-C3-C4-C5
5	B	607	CM5	C17-C16-O23-C24
5	A	605	CM5	C2-C3-C4-C5
5	D	610	CM5	C1-C2-C3-C4
5	D	610	CM5	O14-C15-C19-O20
3	A	500	HEM	C4B-C3B-CAB-CBB
5	B	606	CM5	O12-C1-C2-C3
5	B	606	CM5	O25-C26-C30-O31
3	A	500	HEM	C3A-C2A-CAA-CBA
5	A	605	CM5	C4-C5-C6-C7
5	A	605	CM5	C4-C5-C6-C11
5	A	608	CM5	C2-C1-O12-C13
5	D	610	CM5	O25-C24-O23-C16
5	A	608	CM5	C3-C4-C5-C6
5	B	607	CM5	C16-C15-C19-O20
3	A	500	HEM	C4C-C3C-CAC-CBC
3	B	500	HEM	C4B-C3B-CAB-CBB
3	C	500	HEM	C4B-C3B-CAB-CBB
3	C	500	HEM	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
3	D	500	HEM	C4C-C3C-CAC-CBC
5	A	608	CM5	C17-C16-O23-C24
5	B	606	CM5	C2-C3-C4-C5
3	A	500	HEM	C1A-C2A-CAA-CBA
5	B	607	CM5	O14-C13-O12-C1
3	B	500	HEM	C3D-CAD-CBD-CGD
5	B	607	CM5	C18-C13-O12-C1
5	A	608	CM5	C15-C16-O23-C24
5	D	610	CM5	C29-C24-O23-C16
5	D	610	CM5	C27-C26-C30-O31
3	B	500	HEM	CAD-CBD-CGD-O2D
3	A	500	HEM	CAD-CBD-CGD-O2D
3	B	500	HEM	CAD-CBD-CGD-O1D
4	C	501	TB2	C5-C6-C9-C11
4	B	501	TB2	C5-C6-C9-C11
4	C	501	TB2	C7-C6-C9-C11
5	B	607	CM5	C1-C2-C3-C4
4	B	501	TB2	C7-C6-C9-C11
5	B	607	CM5	C2-C3-C4-C5
5	B	606	CM5	O25-C24-O23-C16
3	A	500	HEM	CAD-CBD-CGD-O1D
4	C	501	TB2	C7-C6-C9-C12
4	C	501	TB2	C5-C6-C9-C12
4	C	501	TB2	C5-C6-C9-C10
4	C	501	TB2	C7-C6-C9-C10
4	B	501	TB2	C5-C6-C9-C10
4	B	501	TB2	C5-C6-C9-C12
4	B	501	TB2	C7-C6-C9-C12
5	B	607	CM5	C2-C1-O12-C13
4	B	501	TB2	C7-C6-C9-C10
3	D	500	HEM	C2B-C3B-CAB-CBB
5	A	605	CM5	C17-C16-O23-C24

There are no ring outliers.

12 monomers are involved in 114 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	501	TB2	5	0
5	B	606	CM5	2	0
5	D	610	CM5	3	0
5	A	605	CM5	5	0
5	B	607	CM5	3	0

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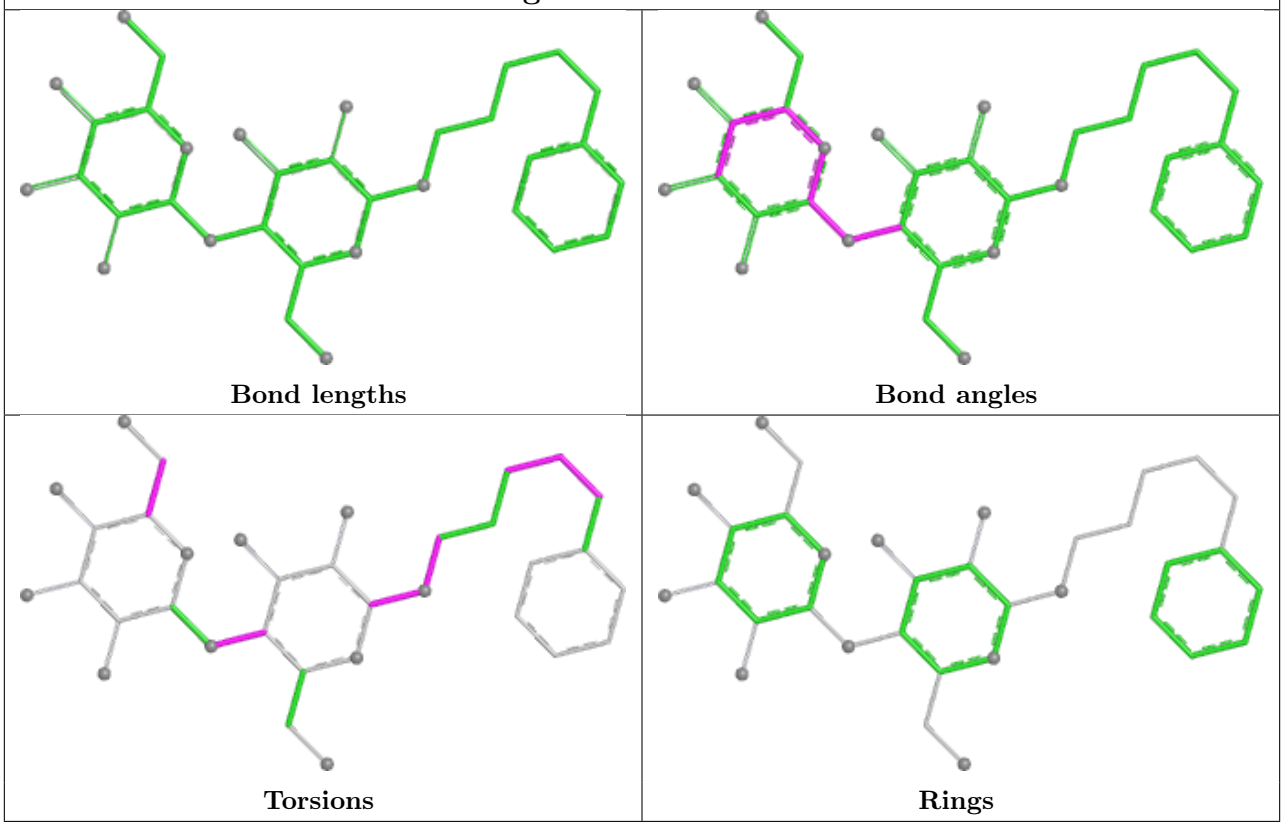
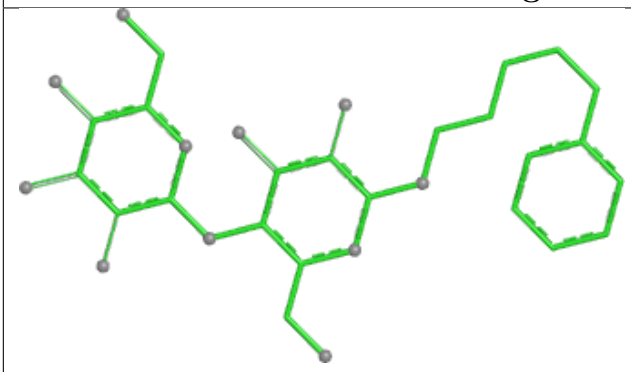
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	500	HEM	12	0
4	C	501	TB2	6	0
4	D	501	TB2	14	0
4	A	501	TB2	8	0
3	A	500	HEM	17	0
3	D	500	HEM	25	0
3	B	500	HEM	14	0

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.

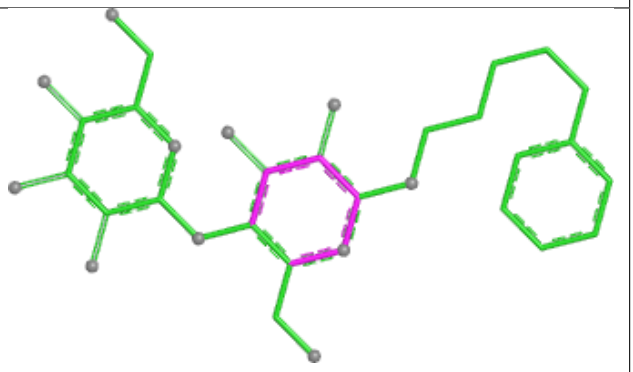
Ligand CM5 A 608



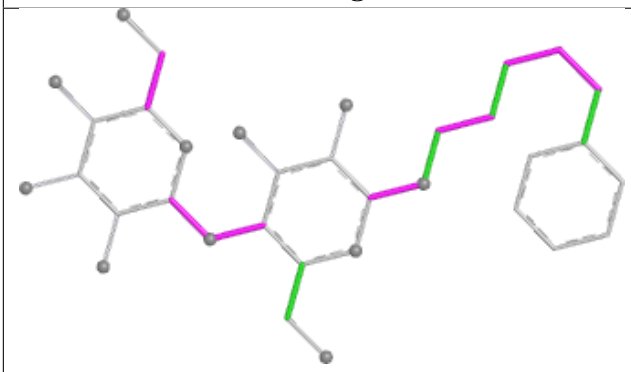
Ligand CM5 B 606



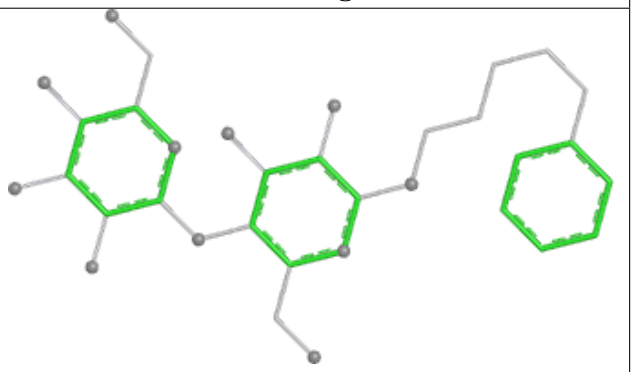
Bond lengths



Bond angles

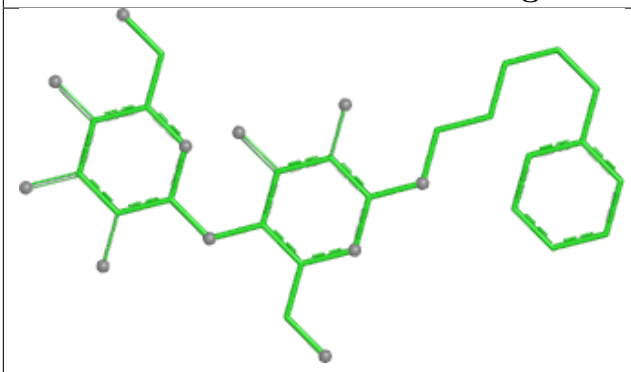


Torsions

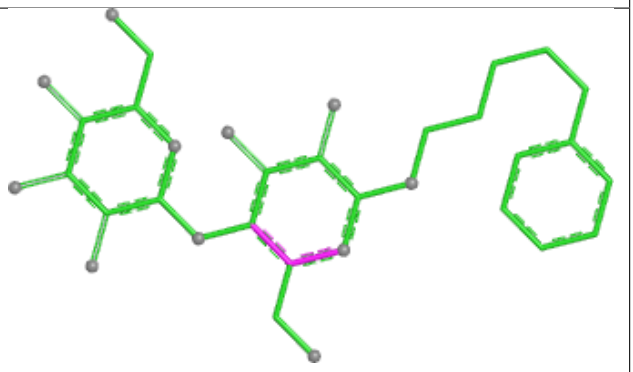


Rings

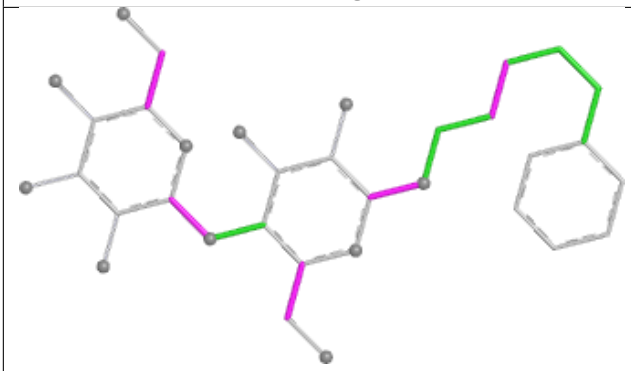
Ligand CM5 D 610



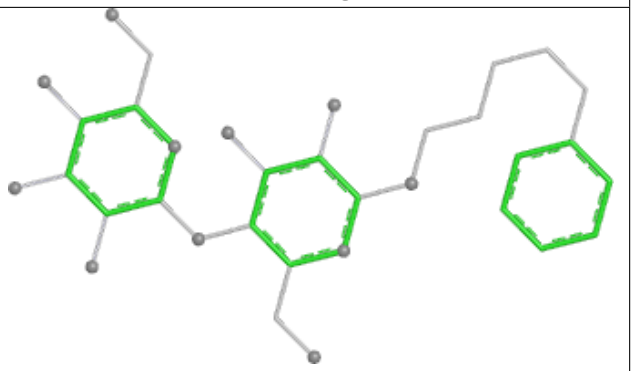
Bond lengths



Bond angles

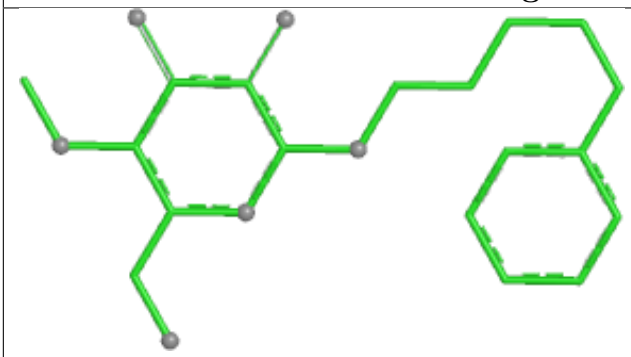


Torsions

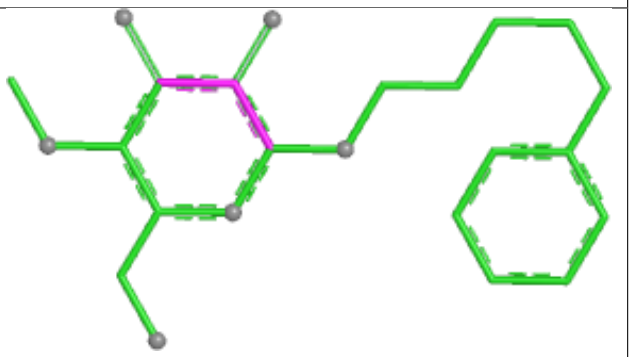


Rings

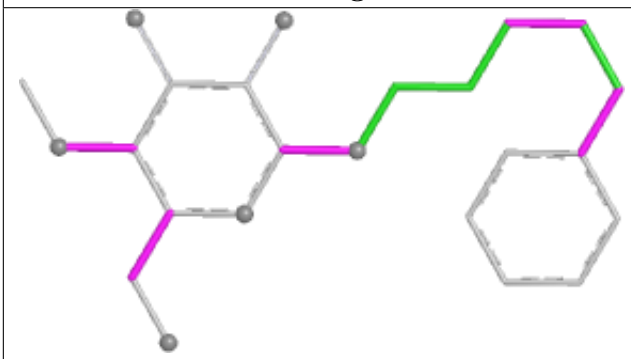
Ligand CM5 A 605



Bond lengths



Bond angles



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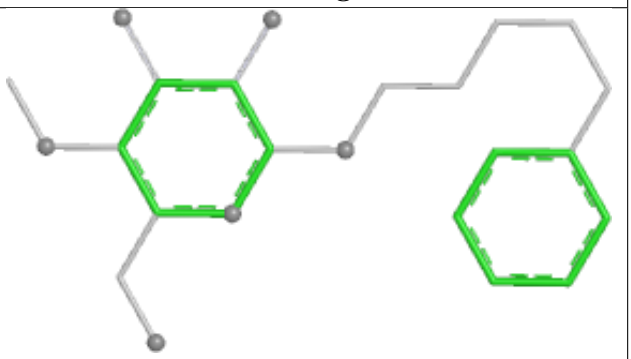
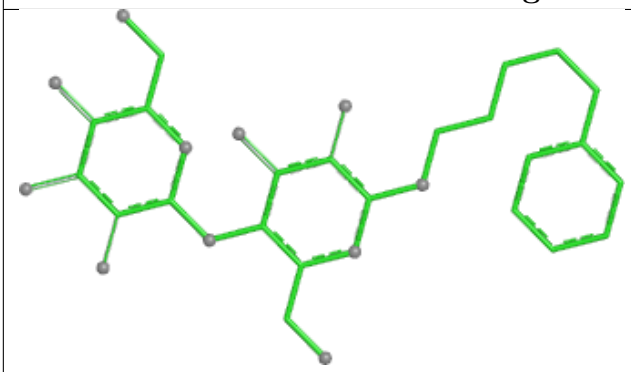
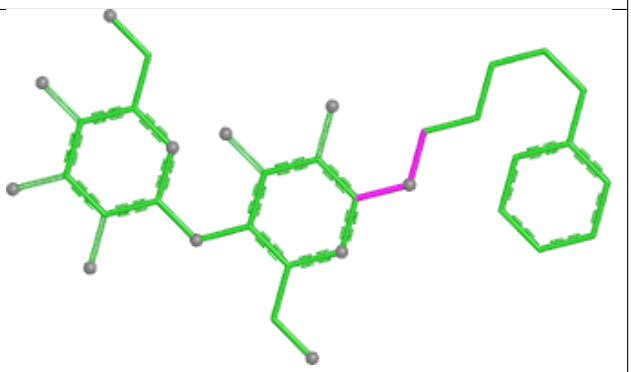


Rings

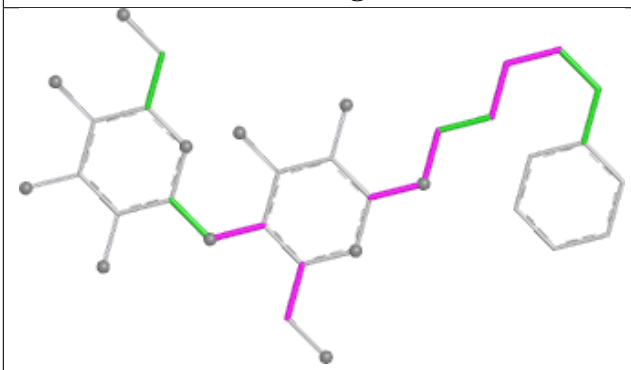
Ligand CM5 B 607



Bond lengths



Bond angles



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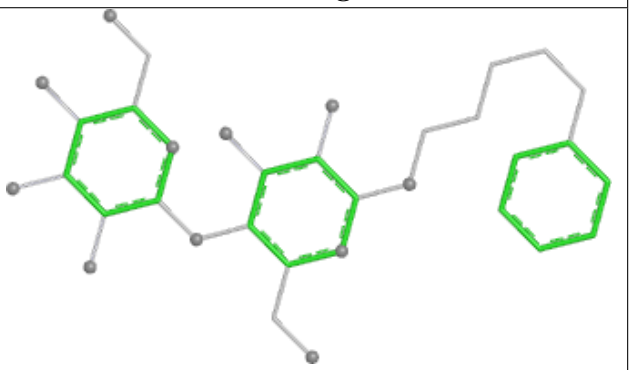
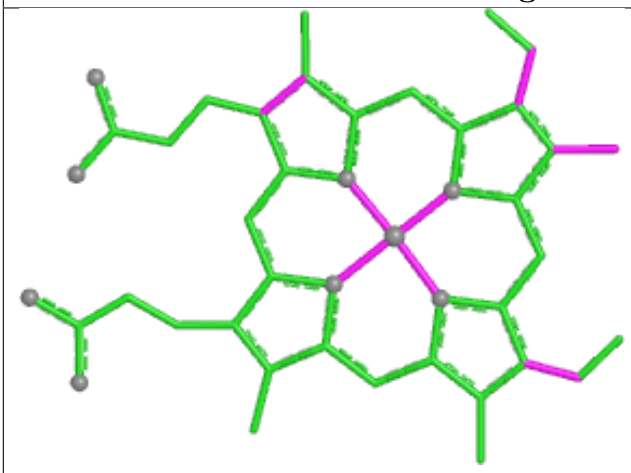
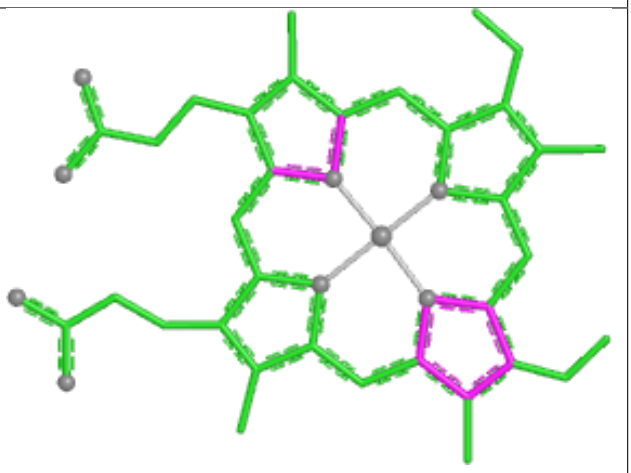


Rings

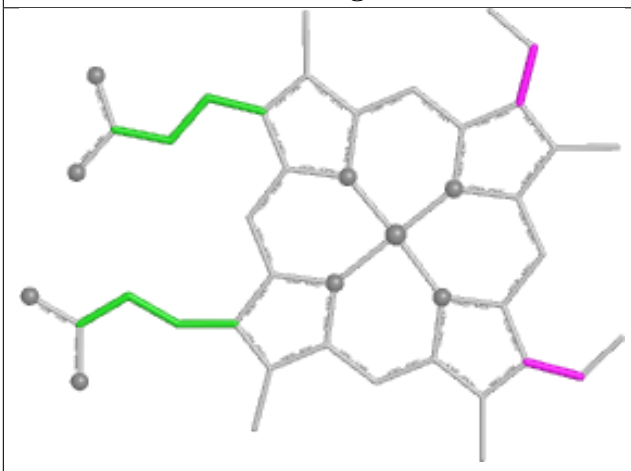
Ligand HEM C 500



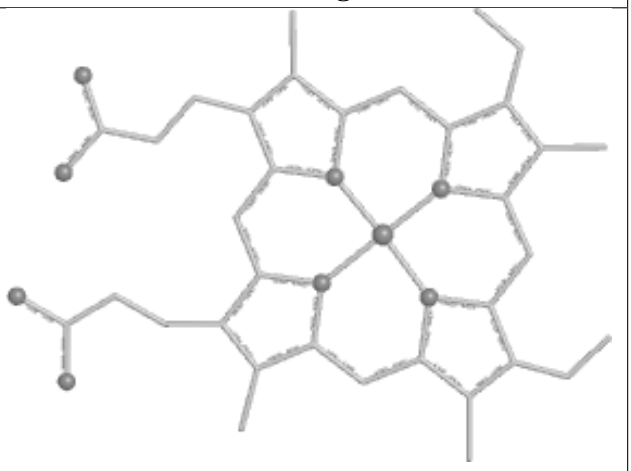
Bond lengths



Bond angles

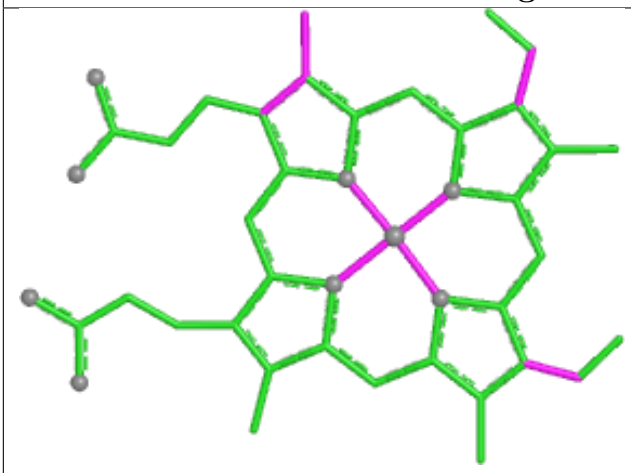


Torsions

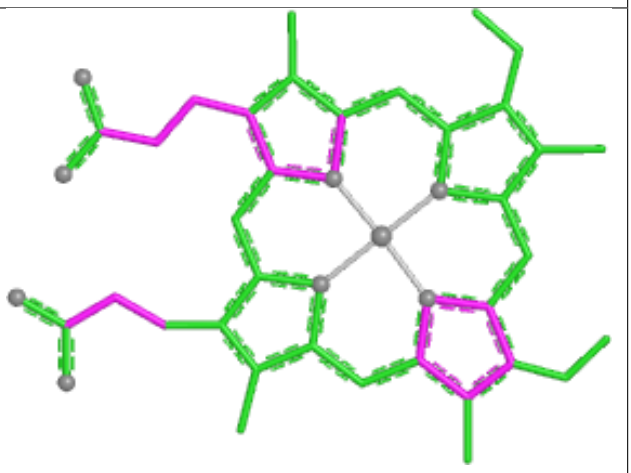


Rings

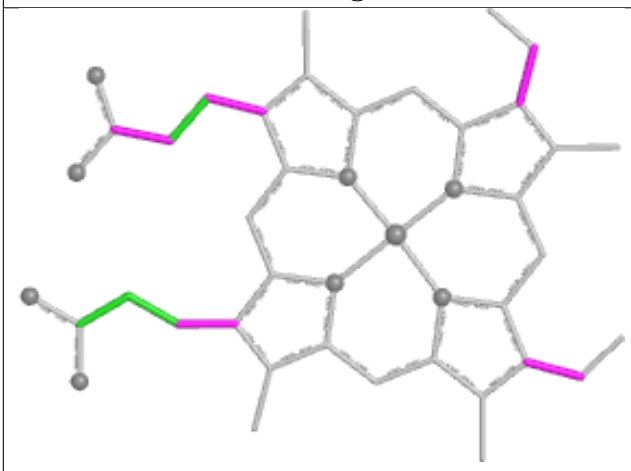
Ligand HEM A 500



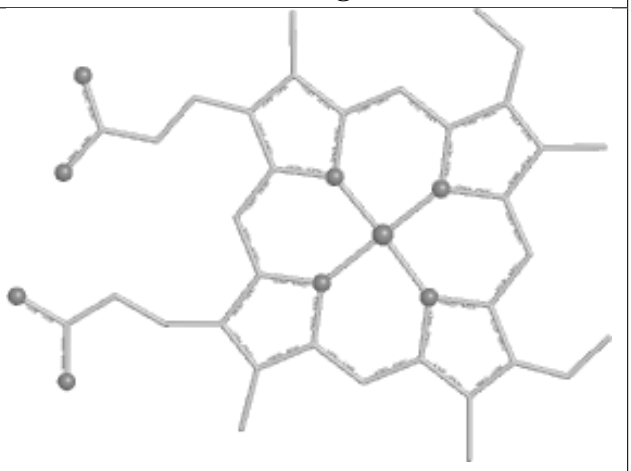
Bond lengths



Bond angles

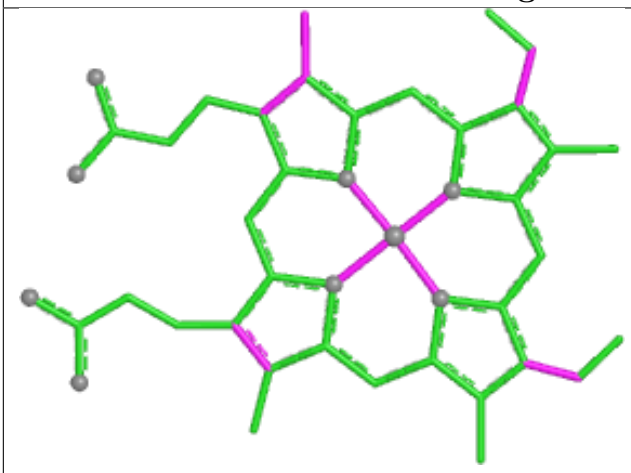


Torsions

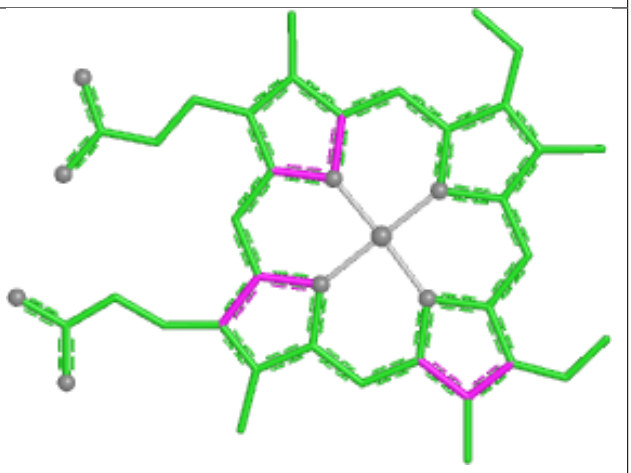


Rings

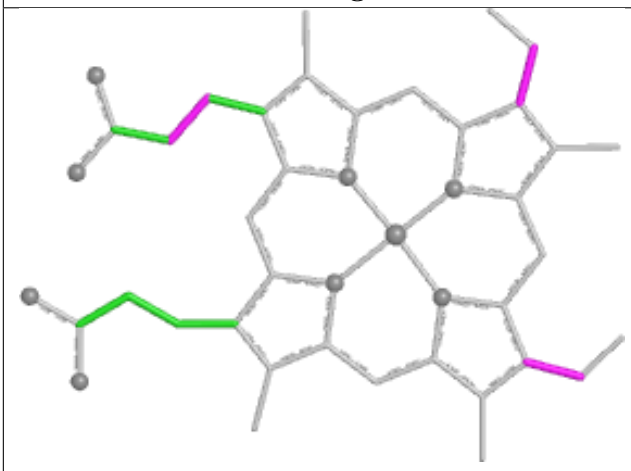
Ligand HEM D 500



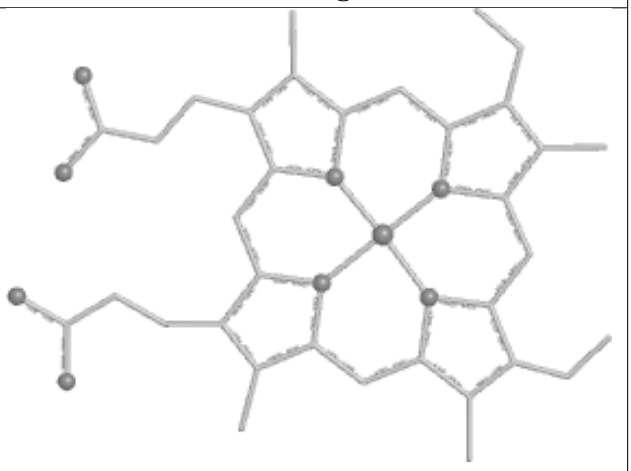
Bond lengths



Bond angles

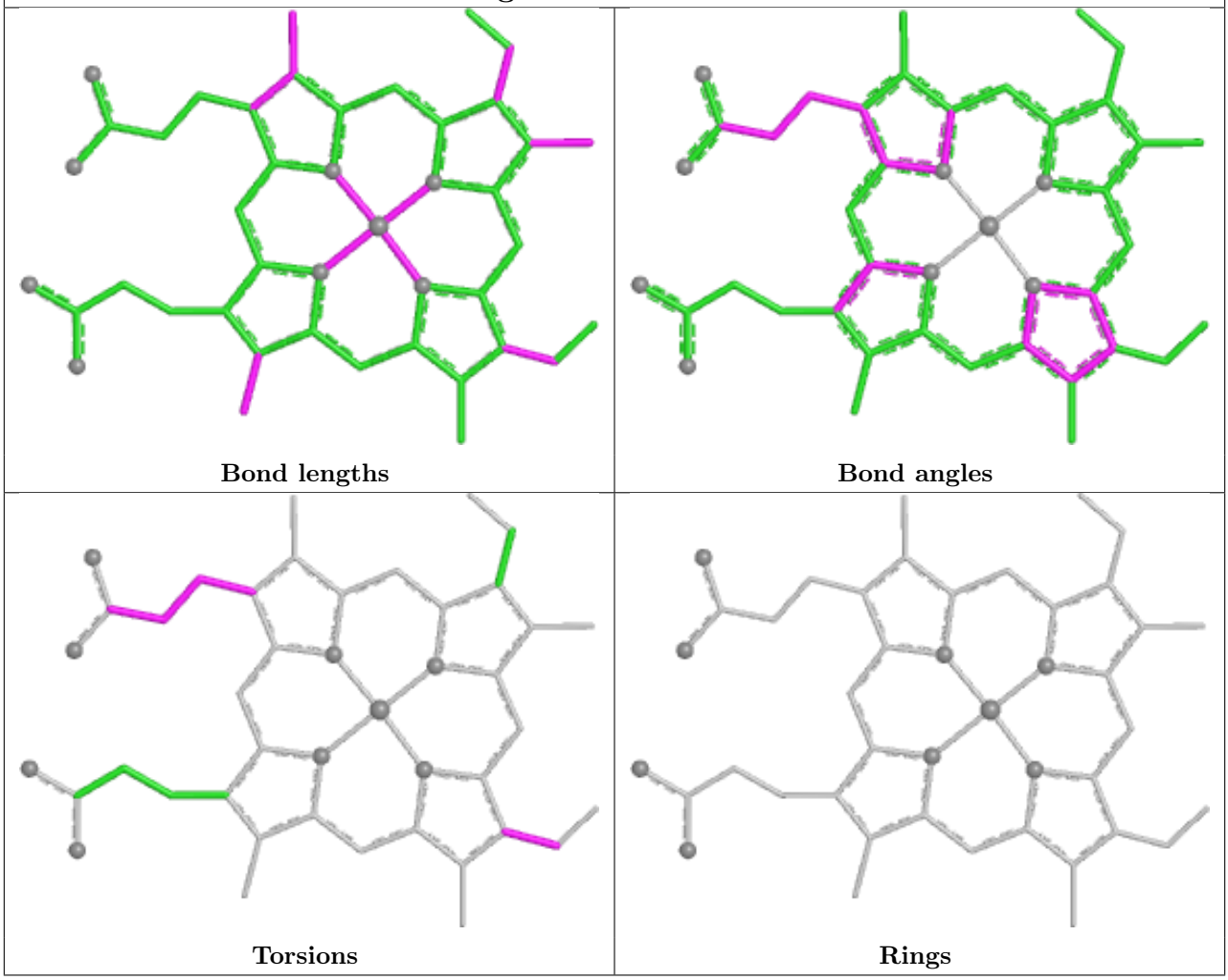


Torsions



Rings

Ligand HEM B 500



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	465/476 (97%)	-0.12	9 (1%)	66	43	49, 78, 130, 196	1 (0%)
1	B	465/476 (97%)	0.09	15 (3%)	50	29	54, 88, 160, 184	2 (0%)
1	C	456/476 (95%)	0.22	18 (3%)	43	24	56, 97, 181, 211	1 (0%)
1	D	464/476 (97%)	0.46	22 (4%)	36	19	60, 127, 166, 206	0
All	All	1850/1904 (97%)	0.16	64 (3%)	47	27	49, 95, 166, 211	4 (0%)

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	221	SER	6.1
1	B	50	GLY	5.3
1	A	221	SER	5.3
1	B	55	PHE	5.2
1	C	115	PHE	4.6
1	B	51	LEU	4.6
1	B	231	HIS	4.4
1	C	230	THR	4.0
1	D	231	HIS	3.9
1	A	40	LEU	3.9
1	D	43	LEU	3.5
1	B	298	ALA	3.4
1	D	130	ALA	3.3
1	B	102	ALA	3.3
1	C	107	ILE	3.3
1	B	40	LEU	3.3
1	D	477	VAL	3.1
1	A	110	GLY	3.1
1	C	44	LEU	3.1
1	D	437	LEU	3.1
1	D	229	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	300	THR	3.0
1	C	40	LEU	3.0
1	B	228	PRO	3.0
1	C	103	VAL	3.0
1	C	477	VAL	2.9
1	B	44	LEU	2.9
1	B	227	PHE	2.7
1	B	224	LEU	2.7
1	D	103	VAL	2.7
1	D	119	GLU	2.7
1	B	230	THR	2.7
1	A	107	ILE	2.6
1	A	111	TYR	2.6
1	C	228	PRO	2.6
1	D	111	TYR	2.6
1	C	111	TYR	2.5
1	C	43	LEU	2.4
1	A	38	PRO	2.4
1	A	298	ALA	2.4
1	B	297	PHE	2.3
1	C	288	LEU	2.3
1	C	300	THR	2.3
1	D	283	PHE	2.3
1	D	430	SER	2.3
1	C	42	ASN	2.3
1	C	106	PRO	2.2
1	B	114	ILE	2.2
1	D	121	TRP	2.2
1	C	38	PRO	2.2
1	D	234	ILE	2.1
1	D	453	ILE	2.1
1	C	295	LEU	2.1
1	D	424	GLU	2.1
1	A	222	GLY	2.1
1	D	122	ARG	2.1
1	D	123	ALA	2.1
1	C	121	TRP	2.0
1	A	226	TYR	2.0
1	D	237	ASN	2.0
1	C	298	ALA	2.0
1	D	389	PHE	2.0
1	D	65	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	295	LEU	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)

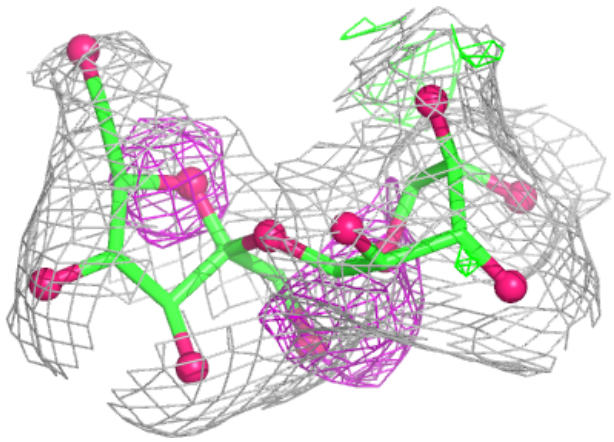
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

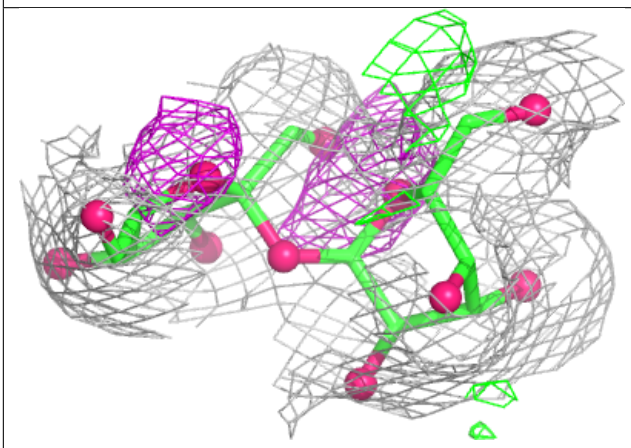
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FRU	G	2	12/12	0.68	0.11	91,108,111,120	0
2	FRU	H	2	12/12	0.73	0.08	141,148,151,154	0
2	GLC	H	1	11/12	0.75	0.11	140,144,153,155	0
2	GLC	F	1	11/12	0.75	0.14	78,90,98,100	0
2	GLC	G	1	11/12	0.76	0.14	82,92,101,102	0
2	FRU	F	2	12/12	0.79	0.10	85,89,94,95	0
2	GLC	E	1	11/12	0.80	0.11	54,76,86,98	0
2	FRU	E	2	12/12	0.81	0.12	66,87,93,93	0

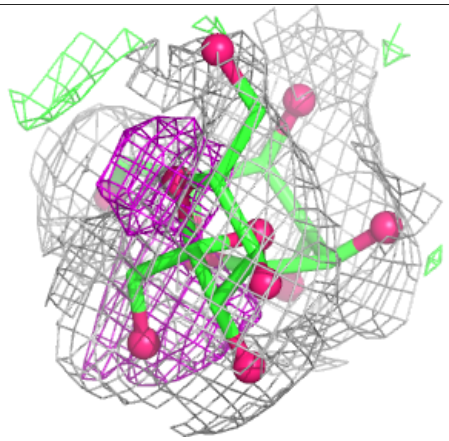
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain E:

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

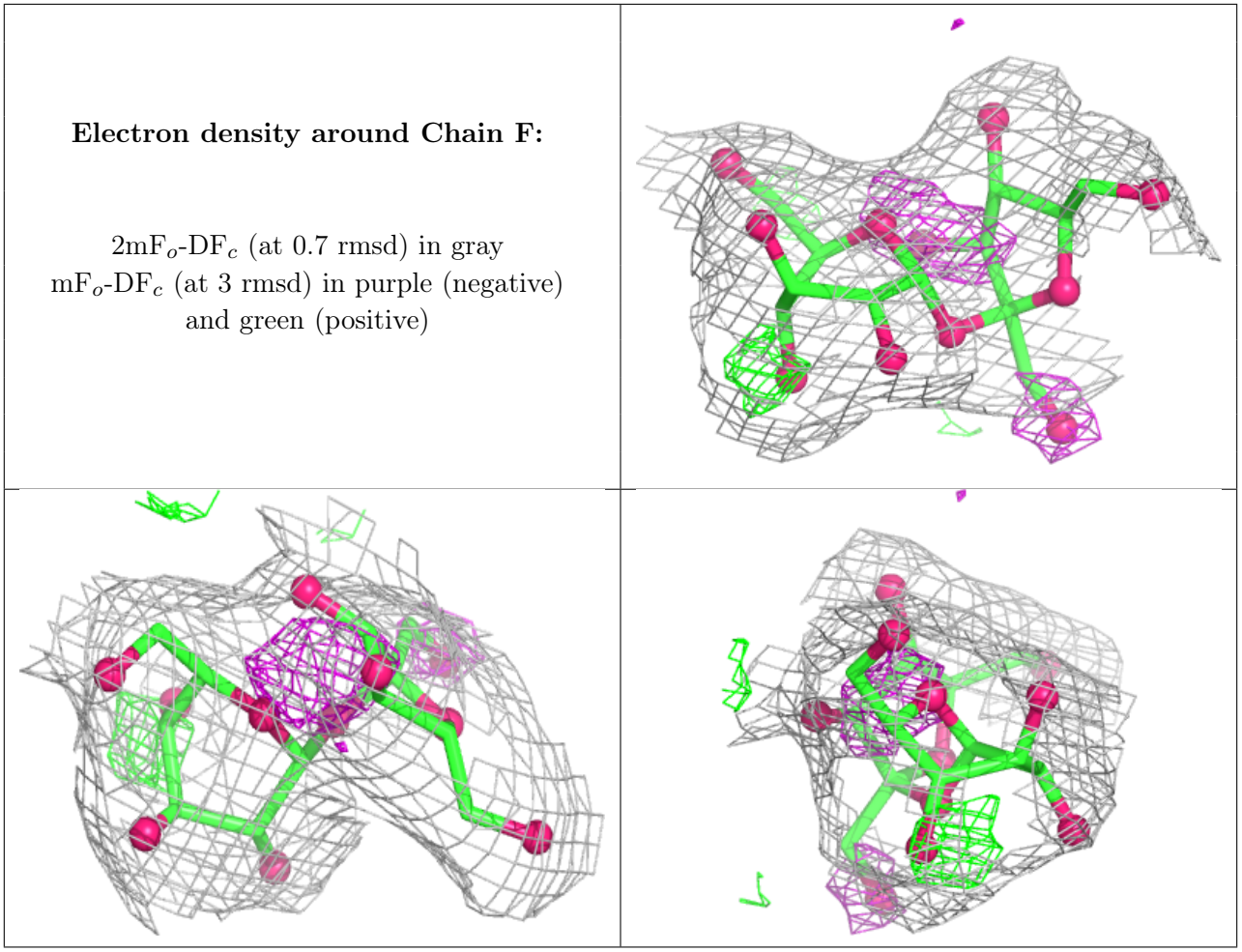






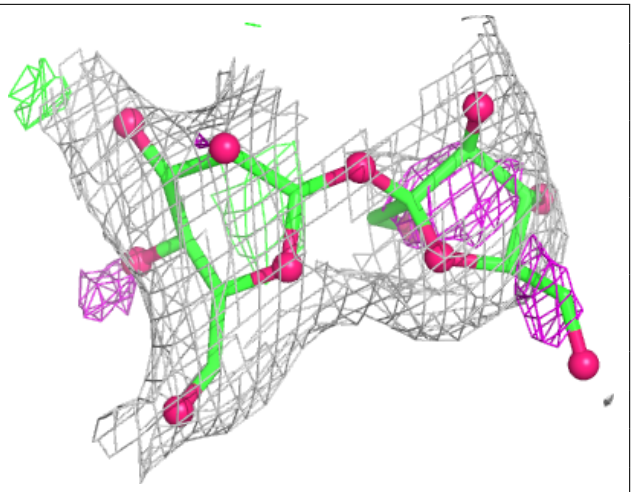
Electron density around Chain F:

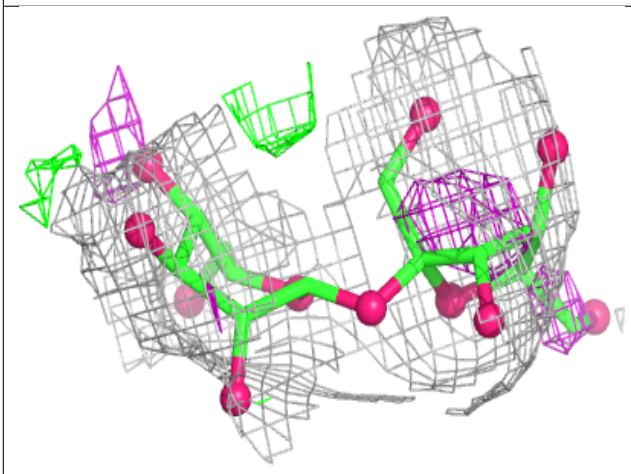
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

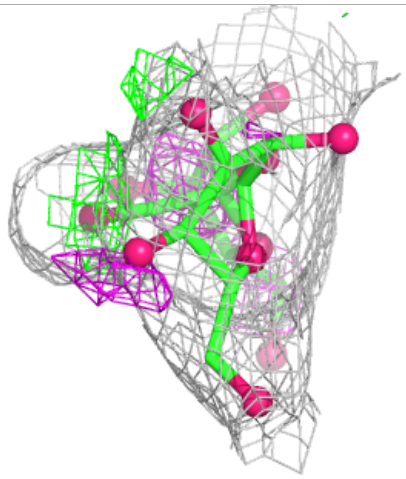


Electron density around Chain G:

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

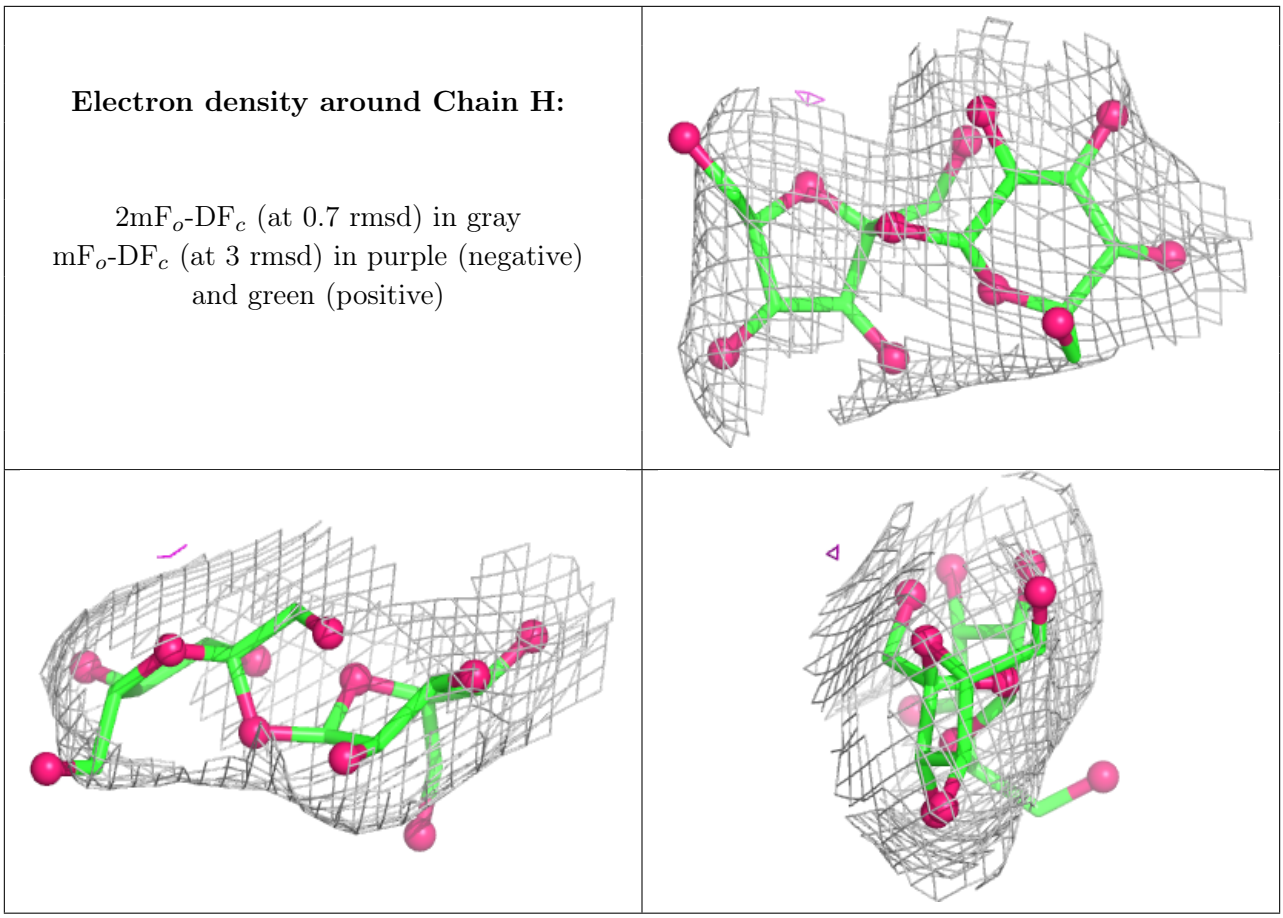






Electron density around Chain H:

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



6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	CM5	A	608	34/34	0.82	0.15	61,125,148,155	0
5	CM5	B	607	34/34	0.83	0.16	59,122,134,136	0
5	CM5	A	605	24/34	0.86	0.15	65,96,109,115	0
5	CM5	D	610	34/34	0.86	0.14	89,144,167,172	0
4	TB2	D	501	13/13	0.88	0.19	98,106,114,116	0
5	CM5	B	606	34/34	0.90	0.11	68,114,133,137	0
3	HEM	D	500	43/43	0.93	0.15	94,103,118,127	0
4	TB2	B	501	13/13	0.93	0.14	53,65,74,76	0
4	TB2	A	501	13/13	0.95	0.11	50,61,66,68	0
4	TB2	C	501	13/13	0.95	0.12	71,79,85,88	0
3	HEM	C	500	43/43	0.97	0.11	66,83,95,108	0
3	HEM	B	500	43/43	0.98	0.10	46,60,72,85	0

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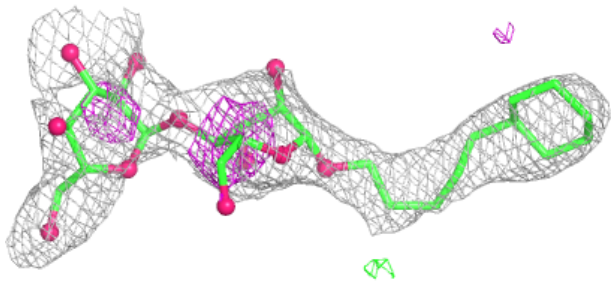
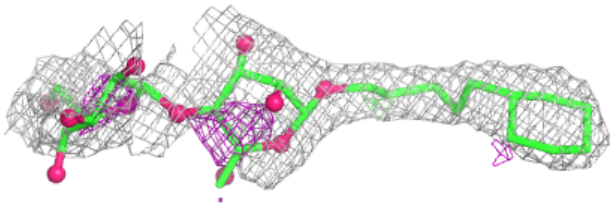
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	HEM	A	500	43/43	0.98	0.09	40,54,64,71	0

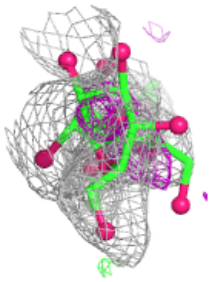
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CM5 A 608:

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

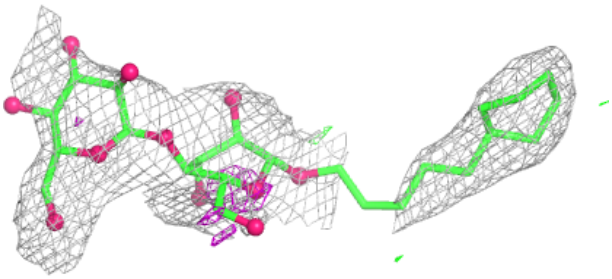


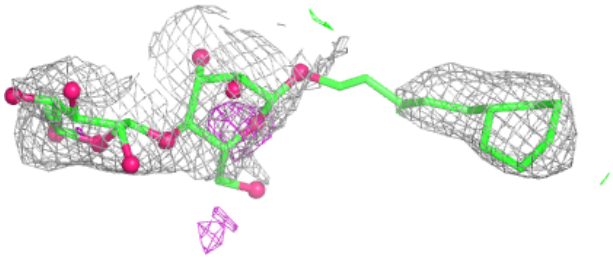


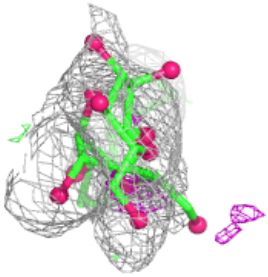


Electron density around CM5 B 607:

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

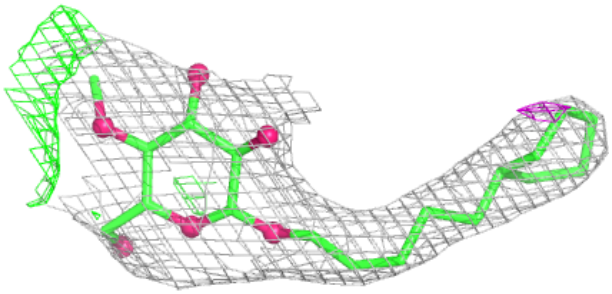


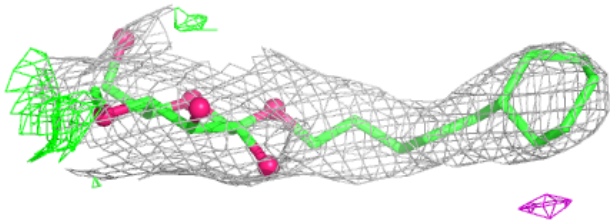


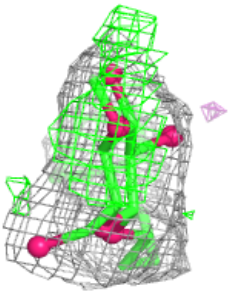


Electron density around CM5 A 605:

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

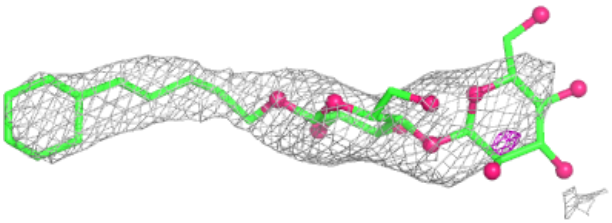


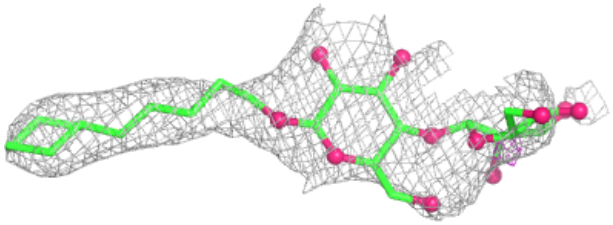


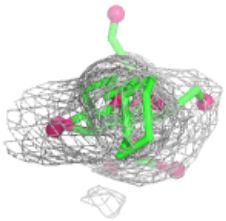


Electron density around CM5 D 610:

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

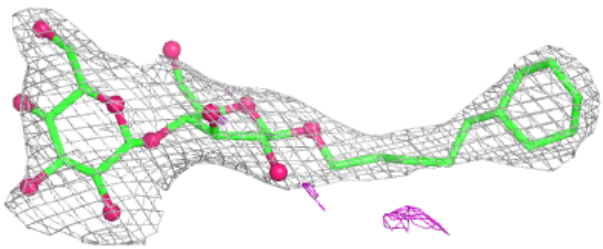


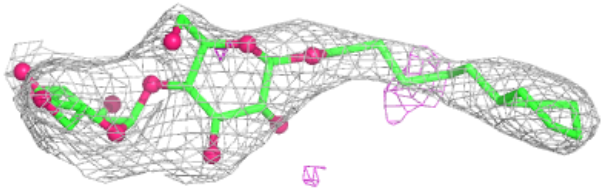


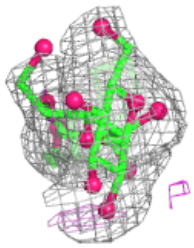


Electron density around CM5 B 606:

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

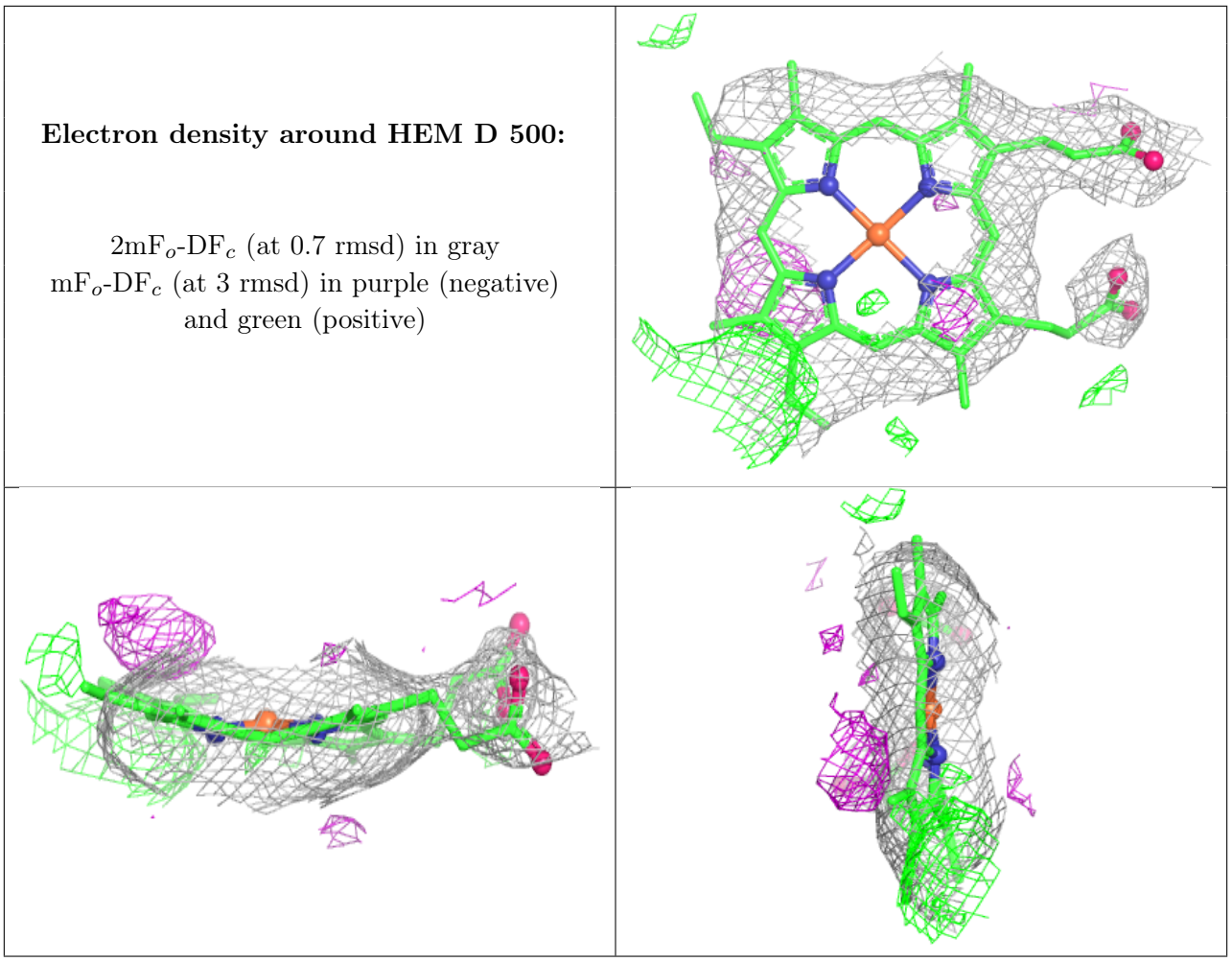






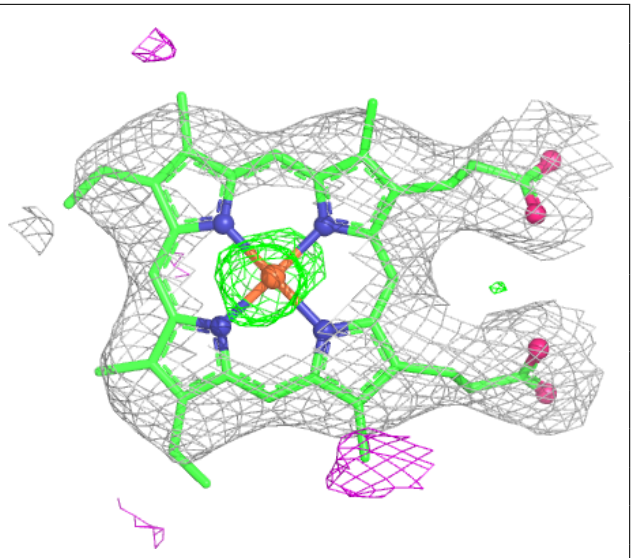
Electron density around HEM D 500:

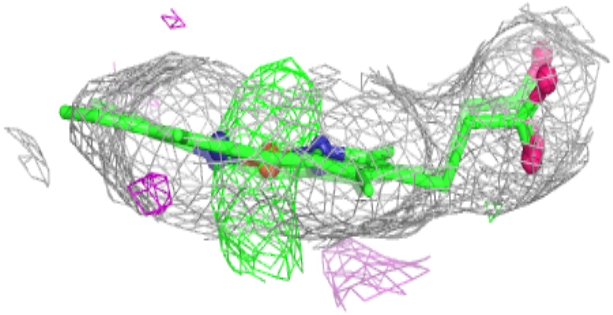
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

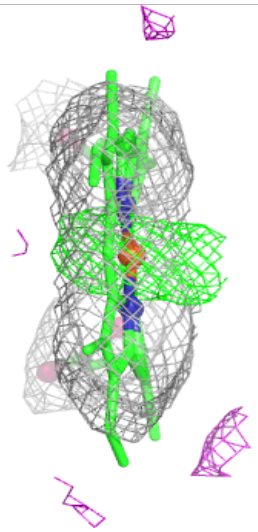


Electron density around HEM C 500:

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

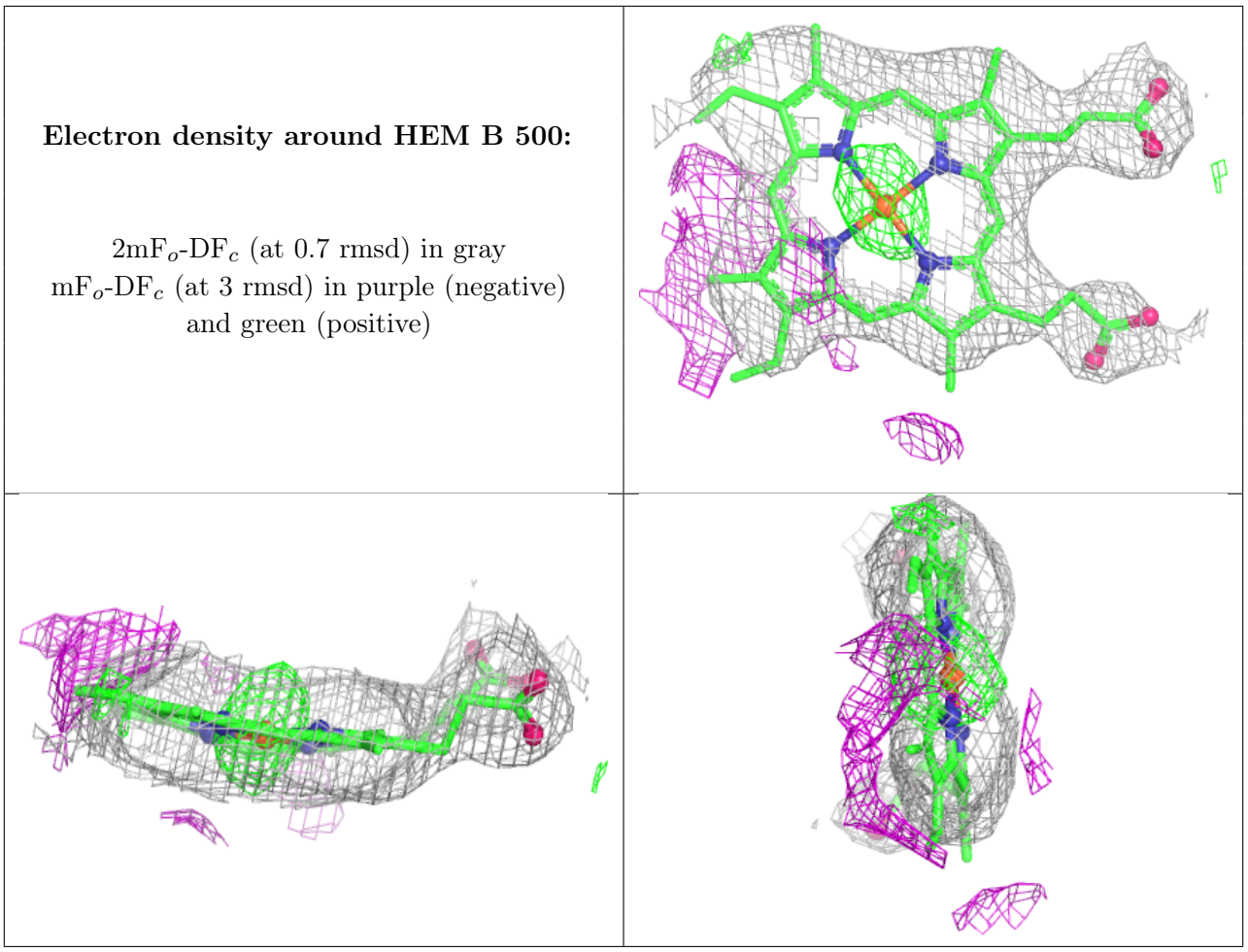






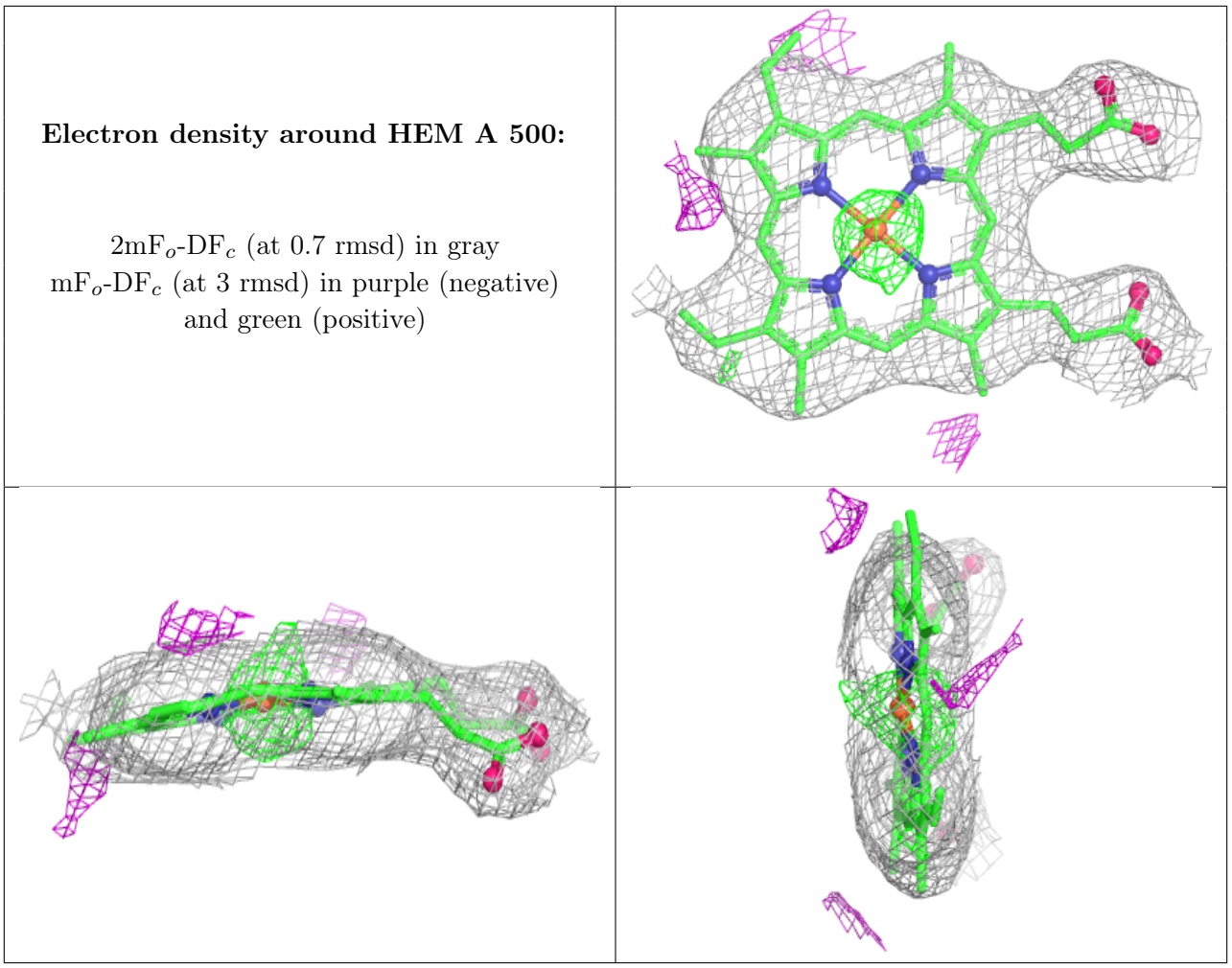
Electron density around HEM B 500:

$2mF_o$-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 500:

$2mF_o$-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.