WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Sep 2, 2023 – 11:22 AM EDT

PDB ID	:	3R1B
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)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 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.
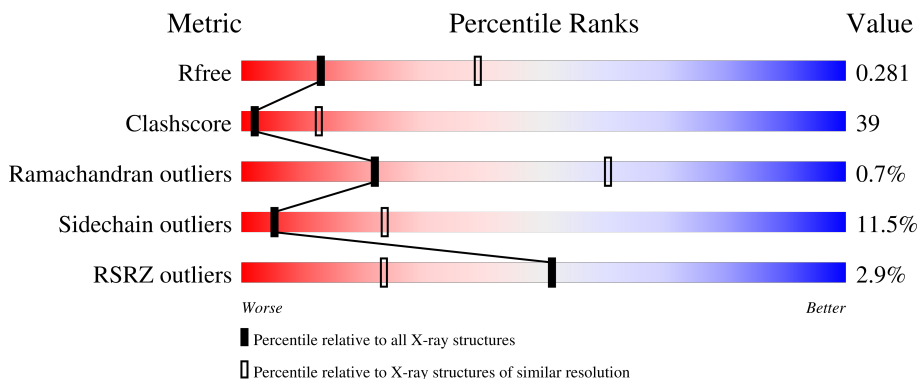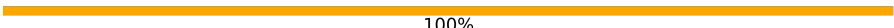

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	.% 58% 34% 6% ·
1	B	476	2% 53% 38% 7% ·
1	C	476	5% 49% 39% 8% ·
1	D	476	3% 42% 46% 9% ·
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	-
5	CM5	A	608	-	-	-	X

2 Entry composition ⓘ

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

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
C	26	SER	ALA	engineered mutation	UNP P00178
C	27	LYS	HIS	engineered mutation	UNP P00178
C	29	LYS	ARG	engineered mutation	UNP P00178
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.
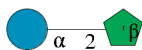
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	E	2	Total 23	C 12	O 11	0	0	0
2	F	2	Total 23	C 12	O 11	0	0	0
2	G	2	Total 23	C 12	O 11	0	0	0

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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 (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).
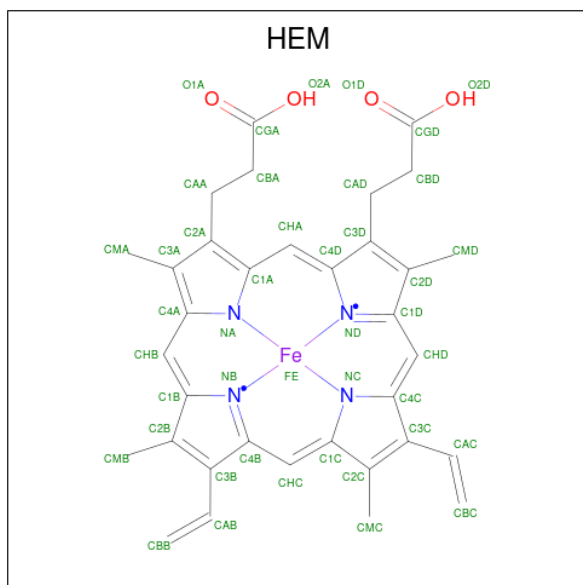
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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

TB2
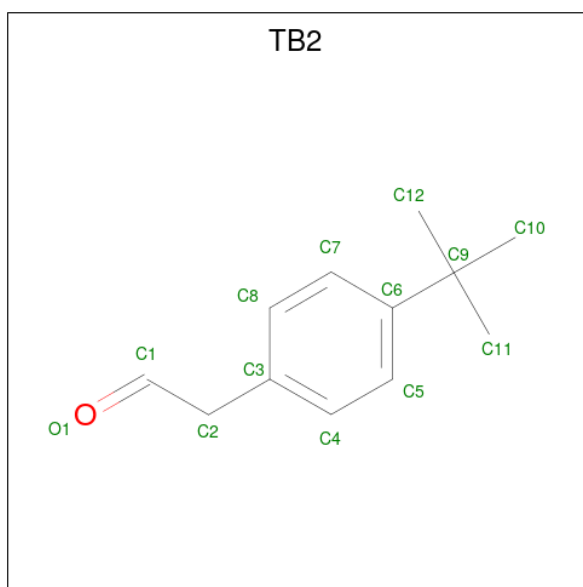
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 13	C 12	O 1	0	0
4	B	1	Total 13	C 12	O 1	0	0
4	C	1	Total 13	C 12	O 1	0	0
4	D	1	Total 13	C 12	O 1	0	0

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

CM5
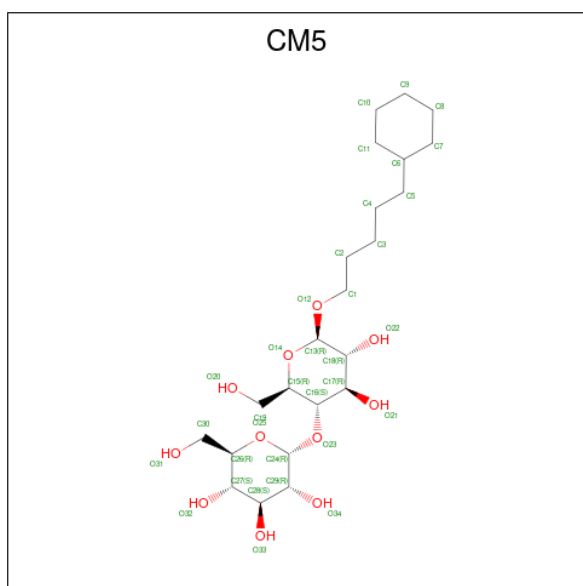
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total 24	C 18	O 6	0	0
5	A	1	Total 34	C 23	O 11	0	0
5	B	1	Total 34	C 23	O 11	0	0
5	B	1	Total 34	C 23	O 11	0	0
5	D	1	Total 34	C 23	O 11	0	0

3 Residue-property plots ⓘ

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

• Molecule 1: Cytochrome P450 2B4

N385 T386 E387 V388 F389 P390 V391 A395 E403 T404 P405 N406 T407 F408 N409 P410 G411 H412 F413 N417 L420 E424 G425 F426 M427 P428 F429 S430 L431 G432 K433 R434 I435 C436 L437 I441 A442 R443 T444 E445 L446 F447 L448 F449 F450 I453 F457 S458 I459 V463

D467 L470 T471 P472 R473 G476 V477 P481 Y484 Q485 I486 R487 F488 L489 H492 HIS HIS HIS

● Molecule 1: Cytochrome P450 2B4
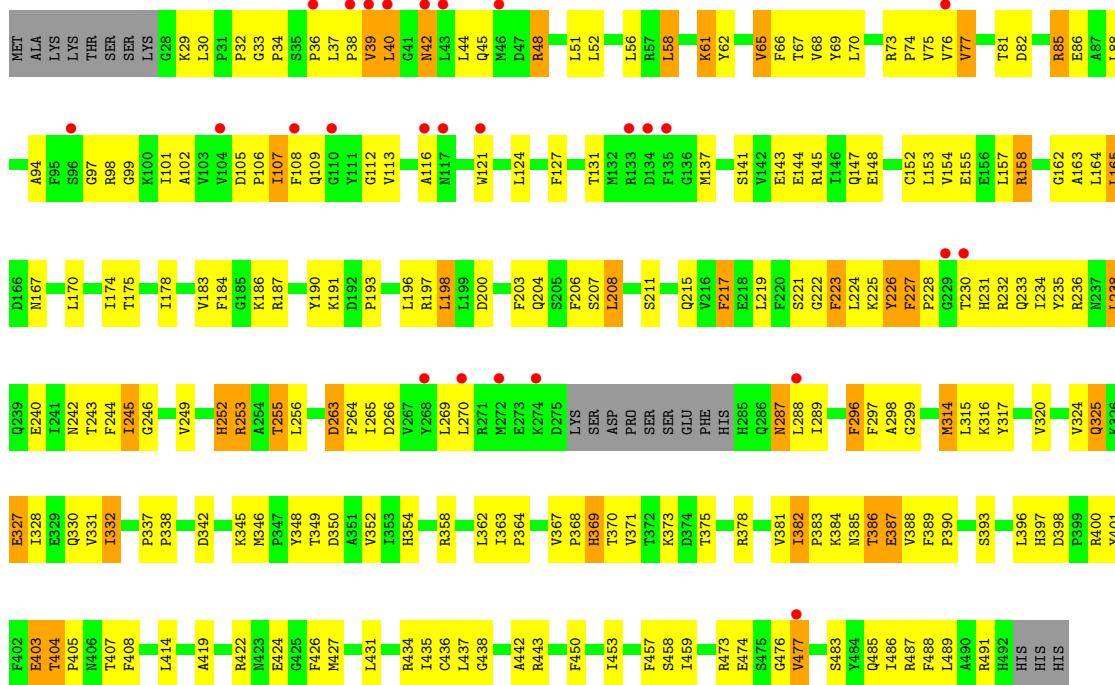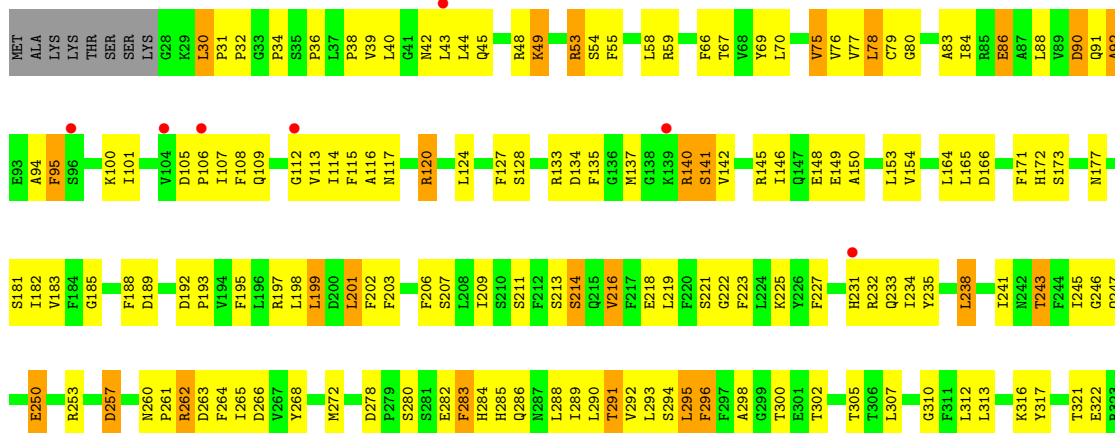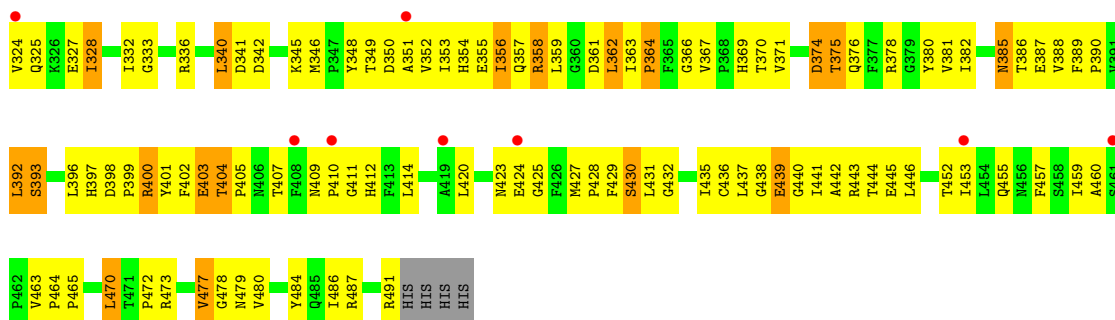
Chain C:

MET ALA LYS LYS THR SER SER LYS G28 K29 L30 P31 P32 G33 P34 S35 P36 L37 P38 V39 L40 G41 N42 L43 L44 Q45 M46 D47 R48 L51 L52 L56 R57 L58 K61 Y62 V65 F66 T67 V68 Y69 L70 R73 P74 V75 V76 V77 T81 D82 R85 E86 A87 L88

A94 F95 S96 G97 R98 G99 K100 I101 A102 V103 V104 D105 P106 I107 F108 Q109 G110 Y111 G112 V113 A116 N117 W121 L124 F127 T131 M132 R133 D134 F135 G136 M137 S141 V142 E143 E144 R145 I146 Q147 E148 C152 V153 V154 E155 E156 L157 R158 G162 A163 L164 L165

D166 N167 L170 I174 T175 I178 V183 F184 G185 K186 R187 Y190 K191 D192 P193 L196 R197 L198 L199 D200 F203 Q204 S205 F206 S207 L208 S211 Q215 V216 F217 E218 L219 F220 S221 G222 F223 L224 K225 Y226 F227 P228 G229 T230 H231 R232 Q233 Y235 R236 N237 L238

Q239 E240 I241 N242 T243 F244 I245 G246 V249 H252 R253 A254 T255 L256 D263 F264 I265 D266 V267 Y268 L269 L270 R271 M272 E273 K274 D275 LYS SER ASP PRO SER SER GLU PHE HIS H285 Q286 N287 L288 I289 F296 F297 A298 G299 M314 L315 K316 Y317 V320 V324 Q325 K326

E327 I328 E329 Q330 V331 I332 P337 P338 D342 K345 M346 P347 Y348 T349 D350 A351 V352 I353 H354 R358 L362 I363 P364 V367 P368 H369 T370 V371 T372 K373 D374 T375 R378 V381 I382 P383 K384 N385 T386 E387 V388 F389 P390 S393 L396 H397 D398 P399 R400 Y401

F402 E403 T404 P405 N406 T407 F408 L414 A419 R422 N423 E424 G425 F426 M427 L431 R434 I435 C436 L437 G438 A442 R443 F450 I453 F457 S458 I459 R473 E474 S475 G476 V477 S483 Y484 Q485 I486 R487 F488 L489 A490 H491 H492 HIS HIS HIS

● Molecule 1: Cytochrome P450 2B4

Chain D:

MET ALA LYS LYS THR SER SER LYS G28 K29 L30 P31 P32 G33 P34 S35 P36 L37 P38 V39 L40 G41 N42 L43 L44 Q45 R48 K49 R53 S54 F55 L58 R59 F66 T67 V68 Y69 L70 V75 V76 V77 L78 C79 G80 A83 I84 R85 E86 A87 L88 V89 D90 Q91 A92

E93 A94 F95 S96 K100 I101 V104 D105 P106 I107 F108 Q109 G112 V113 I114 F115 A116 N117 R120 L124 F127 S128 R133 D134 F135 G136 M137 G138 K139 R140 S141 V142 R145 I146 Q147 E148 E149 A150 L153 V154 L164 L165 D166 F171 H172 S173 N177

S181 I182 V183 F184 G185 F188 D189 D192 P193 V194 F195 L196 R197 L198 L199 D200 L201 F202 P203 F206 S207 L208 I209 S210 S211 F212 S213 S214 Q215 V216 F217 E218 L219 F220 S221 G222 F223 L224 K225 Y226 F227 H231 R232 Q233 I234 Y235 L238 I241 N242 T243 F244 I245 G246 Q247

E250 R253 D257 N260 P261 R262 D263 F264 I265 D266 V267 Y268 M272 D278 P279 S280 S281 E282 F283 H284 H285 Q286 N287 L288 I289 L290 T291 V292 L293 S294 L295 F296 G297 A298 G299 T300 E301 T302 T305 T306 L307 G310 F311 L312 L313 K316 Y317 T321 E322 R323

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

Chain E:

100%

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

Chain F:

100%

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

Chain G:

100%

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

Chain H:

100%

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 53.44 – 3.00	Depositor EDS
% Data completeness (in resolution range)	94.8 (53.43-3.00) 99.3 (53.44-3.00)	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 0.241 , 0.281	Depositor DCC
R_{free} test set	3236 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)	0.31 , 93.8	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.*

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[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, FRU, GLC, CM5, HEM

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$ >5	RMSZ	#$|Z|$ >5
1	A	0.31	1/3672 (0.0%)	0.56	6/4995 (0.1%)
1	B	0.35	0/3679	0.69	14/5003 (0.3%)
1	C	0.31	0/3484	0.67	5/4749 (0.1%)
1	D	0.32	0/3527	0.70	9/4814 (0.2%)
All	All	0.32	1/14362 (0.0%)	0.66	34/19561 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	161	LYS	CA-CB	-5.92	1.41	1.53

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	37	LEU	N-CA-C	-5.98	94.85	111.00
1	D	328	ILE	CB-CA-C	-5.98	99.64	111.60
1	D	378	ARG	N-CA-C	5.97	127.12	111.00
1	B	335	HIS	N-CA-C	5.95	127.07	111.00
1	C	255	THR	N-CA-CB	-5.93	99.03	110.30
1	B	48	ARG	N-CA-C	5.93	127.00	111.00
1	B	38	PRO	CA-N-CD	-5.84	103.32	111.50
1	B	231	HIS	N-CA-C	-5.84	95.24	111.00
1	B	298	ALA	CB-CA-C	-5.82	101.37	110.10
1	C	263	ASP	CB-CA-C	-5.75	98.90	110.40
1	B	48	ARG	CB-CA-C	-5.70	99.00	110.40
1	A	161	LYS	N-CA-CB	-5.68	100.37	110.60
1	D	404	THR	N-CA-C	-5.66	95.73	111.00
1	C	256	LEU	CB-CA-C	-5.65	99.46	110.20
1	A	70	LEU	CB-CA-C	-5.65	99.47	110.20
1	D	477	VAL	CB-CA-C	-5.64	100.69	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	107	ILE	N-CA-C	5.62	126.16	111.00
1	D	232	ARG	N-CA-CB	-5.60	100.52	110.60
1	B	48	ARG	N-CA-CB	-5.59	100.53	110.60
1	A	160	SER	CB-CA-C	5.58	120.70	110.10
1	C	403	GLU	CB-CA-C	5.54	121.49	110.40
1	B	49	LYS	CB-CA-C	-5.48	99.44	110.40
1	D	403	GLU	CB-CA-C	-5.45	99.51	110.40
1	B	334	SER	N-CA-C	5.41	125.61	111.00
1	B	40	LEU	CB-CA-C	-5.38	99.98	110.20
1	A	259	SER	CB-CA-C	5.34	120.25	110.10
1	D	233	GLN	CB-CA-C	-5.32	99.76	110.40
1	B	335	HIS	N-CA-CB	-5.30	101.06	110.60
1	D	92	ALA	CB-CA-C	-5.28	102.18	110.10
1	B	385	ASN	N-CA-C	5.19	125.01	111.00
1	B	225	LYS	N-CA-CB	-5.14	101.35	110.60
1	D	86	GLU	CB-CA-C	5.13	120.67	110.40
1	A	37	LEU	N-CA-C	-5.04	97.38	111.00
1	A	161	LYS	CB-CA-C	-5.03	100.34	110.40

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	226	0
1	B	3589	0	3460	209	0
1	C	3406	0	3187	300	0
1	D	3445	0	3216	382	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	11	0
3	A	43	0	30	17	0
3	B	43	0	30	14	0
3	C	43	0	30	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	43	0	30	25	0
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	1114	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 39.

All (1114) 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: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:224:LEU:C	1:C:224:LEU:HD13	1.72	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:58:LEU:HD11	1:C:66:PHE:CZ	1.93	1.03
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: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
1:D:288:LEU:HD12	1:D:289:ILE:N	1.84	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:C:97:GLY:H	1:C:434:ARG:HH21	1.22	0.88
1:C:207:SER:C	1:C:208:LEU:HD12	1.93	0.87
1:D:355:GLU:O	1:D:359:LEU:HD23	1.75	0.87
1:A:224:LEU:HD13	1:A:224:LEU:C	1.93	0.87
3:C:500:HEM:HBC2	3:C:500:HEM:HHD	1.56	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:C:224:LEU:C	1:C:224:LEU:CD1	2.41	0.86
1:D:298:ALA:HB2	4:D:501:TB2:H7	1.54	0.86
1:C:231:HIS:C	1:C:234:ILE:HG22	1.94	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:A:219:LEU:HD13	1:A:219:LEU:C	1.96	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:38:PRO:C	1:B:39:VAL:HG12	1.99	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
1:B:287:ASN:OD1	1:B:287:ASN:C	2.17	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:C:238:LEU:HD12	1:C:238:LEU:C	2.00	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:121:TRP:CZ3	1:C:124:LEU:HD12	2.19	0.77
1:D:403:GLU:HG2	1:D:404:THR:HG23	1.66	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: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: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:C:61:LYS:HZ3	1:C:62:TYR:HE2	1.32	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
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: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:D:94:ALA:C	1:D:95:PHE:HD2	1.92	0.73
1:A:308:ARG:HH21	1:A:483:SER:HA	1.48	0.73
1:C:255:THR:O	1:C:255:THR:HG22	1.88	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:224:LEU:C	1:A:224:LEU:CD1	2.58	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: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
2:F:1:GLC:C5	2:F:2:FRU:O3	2.38	0.71
1:B:314:MET:HE1	1:B:450:PHE:CZ	2.25	0.71
1:C:296:PHE:CD1	1:C:296:PHE:C	2.63	0.71
1:B:146:ILE:HD12	1:B:445:GLU:HG2	1.72	0.71
1:D:401:TYR:C	1:D:402:PHE:CD2	2.65	0.71
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:D:282:GLU:C	1:D:282:GLU:OE1	2.30	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:C:98:ARG:HE	1:C:98:ARG:HA	1.56	0.69
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:282:GLU:OE1	1:A:282:GLU:C	2.30	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:GLY:HA3	3:A:500:HEM:C2C	2.27	0.69
1:D:358:ARG:NH1	1:D:402:PHE:HD1	1.88	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: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:C:29:LYS:C	1:C:30:LEU:HD12	2.14	0.67
1:D:245:ILE:HD13	1:D:292:VAL:HG21	1.76	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:D:358:ARG:HA	1:D:396:LEU:HD13	1.75	0.67
1:C:287:ASN:C	1:C:287:ASN:HD22	1.98	0.67
1:D:437:LEU:HD23	1:D:437:LEU:O	1.93	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
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:D:402:PHE:HZ	1:D:425:GLY:C	1.99	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:TYR:N	1:A:111:TYR:HD1	1.93	0.65
1:C:58:LEU:C	1:C:58:LEU:HD12	2.17	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: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:A:218:GLU:C	1:A:222:GLY:HA3	2.18	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
1:A:219:LEU:C	1:A:219:LEU:CD1	2.65	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:A:293:LEU:HD12	1:A:293:LEU:C	2.14	0.64
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:A:296:PHE:C	1:A:296:PHE:CD1	2.72	0.63
1:C:226:TYR:N	1:C:226:TYR:HD2	1.95	0.63
1:D:402:PHE:CZ	1:D:425:GLY:C	2.72	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
1:D:398:ASP:OD1	1:D:398:ASP:C	2.37	0.63
4:D:501:TB2:C4	4:D:501:TB2:O1	2.47	0.63
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:285:HIS:HD1	1:B:285:HIS:C	2.03	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:C:266:ASP:O	1:C:270:LEU:HD23	2.00	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:D:283:PHE:CD1	1:D:283:PHE:C	2.73	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:231:HIS:HB3	1:C:234:ILE:CG2	2.31	0.60
1:C:287:ASN:HD22	1:C:288:LEU:N	2.00	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:D:48:ARG:C	1:D:49:LYS:HG3	2.23	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: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:D:115:PHE:C	1:D:120:ARG:NH2	2.56	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
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:314:MET:HE1	1:B:450:PHE:CE1	2.37	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:314:MET:HE1	1:B:450:PHE:HZ	1.69	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:C:296:PHE:C	1:C:296:PHE:HD1	2.07	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:B:43:LEU:HD23	1:B:43:LEU:C	2.25	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
1:D:358:ARG:NH1	1:D:402:PHE:CG	2.72	0.57
1:C:435:ILE:HG12	1:C:436:CYS:N	2.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:D:221:SER:HG	1:D:223:PHE:HD2	1.53	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: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: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:253:ARG:NH1	1:A:276:LYS:HZ1	2.04	0.56
1:A:206:PHE:CD1	1:A:206:PHE:O	2.58	0.56
1:B:137:MET:HE1	1:B:264:PHE:CD2	2.41	0.56
1:B:226:TYR:CD1	1:C:70:LEU:HD13	2.40	0.56
1:C:296:PHE:CD1	1:C:296:PHE:O	2.59	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:38:PRO:C	1:B:39:VAL:CG1	2.68	0.55
1:D:257:ASP:HB3	1:D:260:ASN:H	1.71	0.55
1:C:224:LEU:HD13	1:C:225:LYS:N	2.21	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: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:208:LEU:O	1:D:207:SER:HB2	2.07	0.54
1:A:288:LEU:C	1:A:288:LEU:HD12	2.27	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
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:C:265:ILE:CG1	1:C:266:ASP:N	2.71	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:61:LYS:NZ	1:C:62:TYR:HE2	2.03	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:D:328:ILE:HA	1:D:346:MET:HE3	1.91	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: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: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: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: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:A:293:LEU:HD12	1:A:294:SER:CA	2.35	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:124:LEU:C	1:C:124:LEU:HD13	2.30	0.52
1:C:226:TYR:C	1:C:228:PRO:HD3	2.31	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: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: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
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:B:345:LYS:C	1:B:347:PRO:HD3	2.31	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:217:PHE:CD1	1:A:217:PHE:C	2.82	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: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:105:ASP:CG	1:B:106:PRO:HD2	2.32	0.50
1:B:219:LEU:O	1:C:101:ILE:HG21	2.12	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: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:287:ASN:C	1:A:287:ASN:OD1	2.50	0.49
1:A:298:ALA:O	1:A:302:THR:OG1	2.30	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:253:ARG:NH1	1:A:276:LYS:HZ3	2.10	0.49
1:A:299:GLY:HA2	3:A:500:HEM:C1C	2.47	0.49
1:C:363:ILE:N	1:C:363:ILE:HD12	2.28	0.49
1:D:282:GLU:OE1	1:D:282:GLU:O	2.30	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:A:174:ILE:HG13	1:A:175:THR:N	2.28	0.49
1:D:305:THR:CG2	1:D:362:LEU:HD11	2.42	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
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:293:LEU:CD1	1:A:293:LEU:C	2.75	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: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:A:34:PRO:HG3	1:A:58:LEU:HD22	1.95	0.48
1:A:387:GLU:CD	1:D:225:LYS:HZ1	2.17	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:217:PHE:CD1	1:C:217:PHE:C	2.86	0.48
1:C:362:LEU:C	1:C:364:PRO:HD3	2.34	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:B:219:LEU:HD12	1:B:219:LEU:C	2.32	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: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:362:LEU:CD1	1:A:362:LEU:H	2.25	0.48
1:C:288:LEU:HD13	1:C:288:LEU:C	2.34	0.48
1:D:366:GLY:N	1:D:392:LEU:CD1	2.76	0.48
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:132:MET:HE3	5:B:607:CM5:H72	1.95	0.48
1:B:427:MET:N	1:B:428:PRO:HD3	2.29	0.48
1:D:115:PHE:C	1:D:120:ARG:HH21	2.17	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:A:360:GLY:C	1:A:362:LEU:HD12	2.34	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:C:230:THR:O	1:C:230:THR:OG1	2.30	0.48
1:C:328:ILE:HA	1:C:346:MET:HE1	1.96	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:487:ARG:HG2	1:A:489:LEU:HD11	1.96	0.47
1:B:180:CYS:HG	1:B:296:PHE:HZ	1.62	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
2:H:1:GLC:H3	2:H:2:FRU:HO1	1.77	0.47
2:H:1:GLC:O2	2:H:2:FRU:O1	2.33	0.47
1:B:313:LEU:HD12	1:B:470:LEU:HD13	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:43:LEU:C	1:B:43:LEU:CD2	2.83	0.47
1:B:51:LEU:C	1:B:51:LEU:HD23	2.34	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
1:B:42:ASN:CG	1:B:43:LEU:N	2.68	0.47
1:B:54:SER:OG	1:B:55:PHE:N	2.48	0.47
1:C:48:ARG:HD3	1:C:474:GLU:CD	2.35	0.47
1:C:48:ARG:HB3	1:C:48:ARG:NH1	2.30	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:A:40:LEU:HD23	1:A:40:LEU:C	2.36	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:127:PHE:CD1	1:D:127:PHE:C	2.88	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
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:C:44:LEU:C	1:C:44:LEU:HD23	2.36	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:B:137:MET:HE1	1:B:264:PHE:CE2	2.50	0.46
1:C:373:LYS:O	1:C:375:THR:HG23	2.16	0.46
1:D:278:ASP:C	1:D:278:ASP:OD1	2.54	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:269:LEU:HD23	1:A:272:MET:HE3	1.98	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:C:362:LEU:C	1:C:363:ILE:HD12	2.37	0.45
1:D:67:THR:HG23	1:D:75:VAL:O	2.16	0.45
1:D:283:PHE:C	1:D:283:PHE:HD1	2.18	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
1:B:361:ASP:CG	1:B:361:ASP:O	2.55	0.45
1:D:371:VAL:HG23	1:D:385:ASN:H	1.82	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:93:GLU:HG2	1:A:433:LYS:HZ3	1.81	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:245:ILE:C	1:C:245:ILE:HD13	2.37	0.45
1:C:330:GLN:O	1:C:330:GLN:HG2	2.17	0.45
1:D:302:THR:HG21	3:D:500:HEM:CMB	2.47	0.45
2:G:2:FRU:HO1	2:G:2:FRU:C4	2.30	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: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: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: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
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:225:LYS:NZ	1:C:101:ILE:HB	2.32	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:B:409:ASN:ND2	1:B:411:GLY:H	2.15	0.44
1:D:381:VAL:C	1:D:382:ILE:HD12	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:225:LYS:HZ2	1:C:101:ILE:HB	1.83	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:212:PHE:CD1	1:A:212:PHE:C	2.92	0.43
1:C:98:ARG:NE	1:C:98:ARG:CA	2.81	0.43
1:C:287:ASN:C	1:C:287:ASN:ND2	2.69	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
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:B:117:ASN:OD1	1:B:117:ASN:C	2.57	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:B:226:TYR:OH	1:C:387:GLU:CD	2.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:363:ILE:HG22	1:C:363:ILE:O	2.19	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:A:437:LEU:HD22	1:A:437:LEU:O	2.19	0.42
1:B:132:MET:HE3	5:B:607:CM5:C7	2.49	0.42
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:C:263:ASP:OD1	1:C:263:ASP:C	2.58	0.42
1:D:268:TYR:HH	1:D:284:HIS:CE1	2.37	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:C:51:LEU:HD12	1:C:51:LEU:C	2.39	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:B:174:ILE:HG13	1:B:175:THR:N	2.35	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: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:288:LEU:HD12	1:A:288:LEU:O	2.21	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:75:VAL:HG23	1:B:75:VAL:O	2.20	0.41
1:B:285:HIS:C	1:B:285:HIS:ND1	2.63	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: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:A:48:ARG:HD2	1:A:48:ARG:C	2.40	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:C:73:ARG:HA	1:C:74:PRO:HD3	1.83	0.41
1:C:383:PRO:HG2	1:C:386:THR:HG21	2.02	0.41
1:D:288:LEU:HD12	1:D:289:ILE:CA	2.51	0.41
1:D:358:ARG:HD2	1:D:402:PHE:CE1	2.56	0.41
1:D:410:PRO:C	1:D:412:HIS:H	2.24	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: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: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: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:D:294:SER:O	1:D:295:LEU:C	2.58	0.41
1:A:398:ASP:HA	1:A:399:PRO:HD3	1.85	0.40
4:B:501:TB2:H12B	4:B:501:TB2:H7	1.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:404:THR:H	1:C:404:THR:HG1	1.56	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
1:A:34:PRO:HG3	1:A:58:LEU:CD2	2.51	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: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
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:C:398:ASP:OD1	1:C:398:ASP:C	2.59	0.40
1:D:295:LEU:HD12	1:D:295:LEU:C	2.42	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 ⓘ

5.3.1 Protein backbone ⓘ

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%)	14	50
1	B	463/476 (97%)	426 (92%)	36 (8%)	1 (0%)	47	82

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	452/476 (95%)	423 (94%)	27 (6%)	2 (0%)	34	72
1	D	462/476 (97%)	415 (90%)	43 (9%)	4 (1%)	17	55
All	All	1840/1904 (97%)	1704 (93%)	124 (7%)	12 (1%)	22	60

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
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%)	338 (90%)	37 (10%)	8	30
1	B	377/421 (90%)	336 (89%)	41 (11%)	6	25
1	C	343/421 (82%)	299 (87%)	44 (13%)	4	19
1	D	345/421 (82%)	301 (87%)	44 (13%)	4	19
All	All	1440/1684 (86%)	1274 (88%)	166 (12%)	5	24

All (166) 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	101	ILE
1	A	105	ASP
1	A	111	TYR
1	A	137	MET
1	A	144	GLU
1	A	165	LEU
1	A	170	LEU
1	A	198	LEU
1	A	200	ASP
1	A	217	PHE
1	A	224	LEU
1	A	226	TYR
1	A	230	THR
1	A	240	GLU
1	A	287	ASN
1	A	288	LEU
1	A	289	ILE
1	A	293	LEU
1	A	343	ARG
1	A	370	THR
1	A	400	ARG
1	A	420	LEU
1	A	422	ARG
1	A	434	ARG
1	A	441	ILE
1	A	473	ARG
1	A	477	VAL
1	A	486	ILE
1	A	489	LEU
1	A	491	ARG
1	B	44	LEU
1	B	58	LEU
1	B	70	LEU
1	B	107	ILE
1	B	115	PHE
1	B	117	ASN

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Mol	Chain	Res	Type
1	B	145	ARG
1	B	165	LEU
1	B	169	LEU
1	B	172	HIS
1	B	207	SER
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	285	HIS
1	B	286	GLN
1	B	287	ASN
1	B	288	LEU
1	B	294	SER
1	B	323	ARG
1	B	327	GLU
1	B	329	GLU
1	B	349	THR
1	B	359	LEU
1	B	362	LEU
1	B	409	ASN
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	450	PHE
1	B	467	ASP
1	B	473	ARG
1	B	477	VAL
1	B	489	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	85	ARG
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	223	PHE
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	287	ASN
1	C	296	PHE
1	C	314	MET
1	C	325	GLN
1	C	327	GLU
1	C	332	ILE
1	C	369	HIS
1	C	382	ILE
1	C	386	THR
1	C	387	GLU
1	C	403	GLU
1	C	404	THR
1	C	422	ARG
1	C	437	LEU
1	C	443	ARG
1	C	458	SER
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
1	D	75	VAL
1	D	78	LEU

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Mol	Chain	Res	Type
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	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	243	THR
1	D	250	GLU
1	D	253	ARG
1	D	257	ASP
1	D	262	ARG
1	D	283	PHE
1	D	291	THR
1	D	295	LEU
1	D	296	PHE
1	D	317	TYR
1	D	322	GLU
1	D	340	LEU
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 (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	286	GLN
1	B	215	GLN
1	B	233	GLN
1	B	385	ASN
1	B	409	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	237	ASN
1	D	242	ASN
1	D	285	HIS
1	D	479	ASN

5.3.3   RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5   Carbohydrates ⓘ

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	1.24	1 (9%)	15,15,17	2.55	8 (53%)
2	FRU	E	2	2	11,12,12	1.37	3 (27%)	10,18,18	1.78	4 (40%)
2	GLC	F	1	2	11,11,12	1.22	2 (18%)	15,15,17	2.57	7 (46%)
2	FRU	F	2	2	11,12,12	1.28	2 (18%)	10,18,18	1.70	3 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$\|Z\|>2$	Counts	RMSZ	#$\|Z\|>2$
2	GLC	G	1	2	11,11,12	1.27	2 (18%)	15,15,17	2.80	7 (46%)
2	FRU	G	2	2	11,12,12	1.29	1 (9%)	10,18,18	1.73	3 (30%)
2	GLC	H	1	2	11,11,12	1.23	1 (9%)	15,15,17	2.46	7 (46%)
2	FRU	H	2	2	11,12,12	1.28	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 (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	2	FRU	O3-C3	-2.31	1.38	1.42
2	E	2	FRU	O3-C3	-2.28	1.38	1.42
2	H	2	FRU	O3-C3	-2.20	1.38	1.42
2	E	1	GLC	O2-C2	-2.16	1.38	1.43
2	F	2	FRU	O3-C3	-2.13	1.38	1.42
2	E	2	FRU	O4-C4	-2.09	1.38	1.43
2	F	1	GLC	O2-C2	-2.07	1.39	1.43
2	G	1	GLC	O4-C4	-2.06	1.38	1.43
2	G	1	GLC	O2-C2	-2.06	1.39	1.43
2	H	1	GLC	O2-C2	-2.05	1.39	1.43
2	F	1	GLC	O4-C4	-2.04	1.38	1.43
2	F	2	FRU	O4-C4	-2.02	1.38	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	6.13	116.81	107.20
2	F	1	GLC	O5-C5-C6	5.79	116.28	107.20
2	H	1	GLC	O5-C5-C6	5.57	115.94	107.20
2	E	1	GLC	O5-C5-C6	5.30	115.52	107.20
2	G	1	GLC	O3-C3-C2	4.03	117.72	109.99
2	G	1	GLC	O2-C2-C1	3.72	116.76	109.15
2	E	1	GLC	O3-C3-C2	3.67	117.01	109.99
2	H	1	GLC	O2-C2-C1	3.66	116.64	109.15
2	F	1	GLC	O2-C2-C1	3.50	116.31	109.15
2	F	1	GLC	O3-C3-C2	3.36	116.43	109.99
2	G	1	GLC	O4-C4-C5	3.32	117.54	109.30
2	E	1	GLC	O2-C2-C1	3.27	115.84	109.15
2	G	1	GLC	O2-C2-C3	3.25	116.64	110.14
2	G	2	FRU	O5-C5-C6	3.20	117.75	108.85
2	F	1	GLC	O2-C2-C3	3.14	116.42	110.14
2	H	1	GLC	O3-C3-C2	3.03	115.79	109.99
2	E	1	GLC	O2-C2-C3	3.02	116.20	110.14
2	F	1	GLC	O4-C4-C5	2.95	116.62	109.30
2	E	2	FRU	O5-C5-C6	2.92	116.99	108.85
2	H	1	GLC	O2-C2-C3	2.92	115.99	110.14
2	E	1	GLC	O4-C4-C5	2.90	116.49	109.30
2	F	2	FRU	O5-C5-C6	2.87	116.83	108.85
2	H	2	FRU	O5-C5-C6	2.86	116.82	108.85
2	H	1	GLC	O4-C4-C5	2.83	116.33	109.30
2	G	1	GLC	O4-C4-C3	2.73	116.66	110.35
2	H	1	GLC	O4-C4-C3	2.66	116.50	110.35
2	H	1	GLC	O3-C3-C4	2.64	116.46	110.35
2	G	2	FRU	O1-C1-C2	2.63	117.46	111.86
2	G	1	GLC	O3-C3-C4	2.62	116.40	110.35
2	E	1	GLC	O4-C4-C3	2.59	116.34	110.35
2	E	1	GLC	O3-C3-C4	2.59	116.33	110.35
2	F	1	GLC	O4-C4-C3	2.57	116.28	110.35
2	F	1	GLC	O3-C3-C4	2.52	116.17	110.35
2	H	2	FRU	O1-C1-C2	2.51	117.20	111.86
2	E	2	FRU	O2-C2-O5	-2.41	104.85	109.50
2	E	2	FRU	O1-C1-C2	2.34	116.84	111.86
2	H	2	FRU	O4-C4-C5	2.29	117.68	111.05
2	F	2	FRU	O4-C4-C5	2.28	117.64	111.05
2	F	2	FRU	O1-C1-C2	2.17	116.48	111.86
2	E	1	GLC	C1-O5-C5	2.17	115.13	112.19
2	E	2	FRU	O4-C4-C5	2.09	117.09	111.05
2	G	2	FRU	O4-C4-C5	2.02	116.89	111.05

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 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	2	FRU	2	0
2	H	1	GLC	11	0
2	E	1	GLC	5	0
2	G	1	GLC	3	0
2	F	2	FRU	9	0
2	H	2	FRU	8	0
2	E	2	FRU	5	0
2	F	1	GLC	8	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
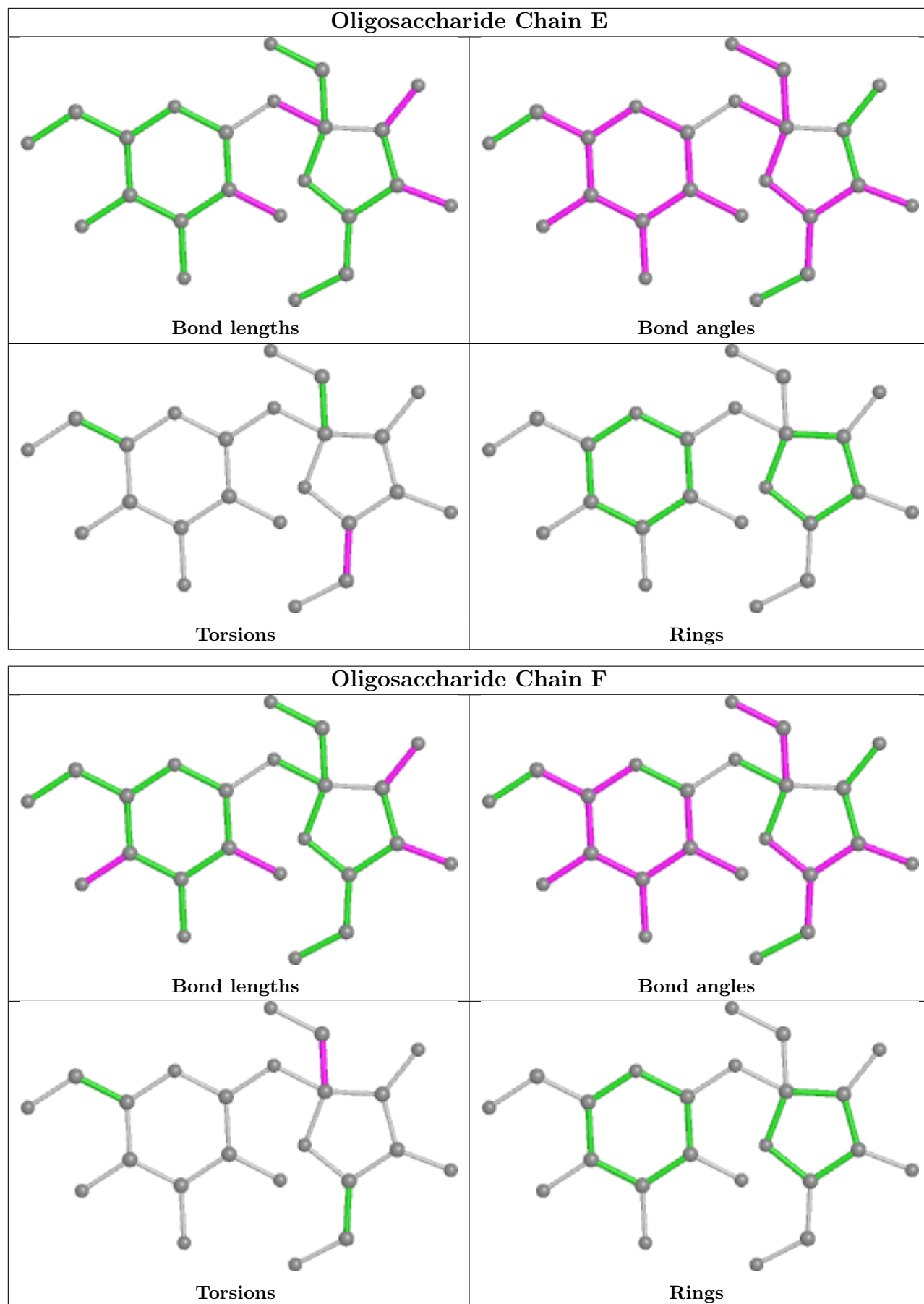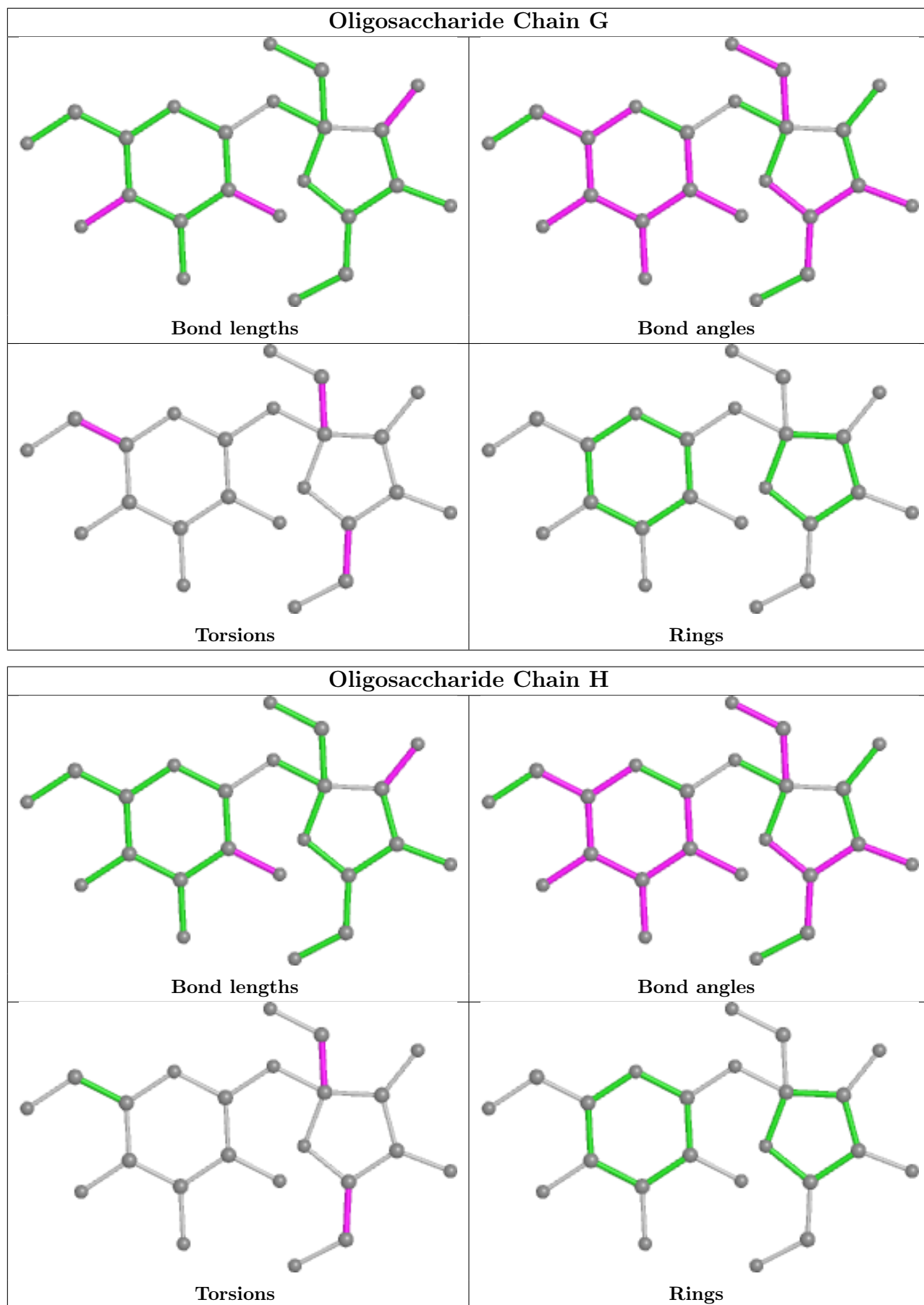
5.6 Ligand geometry ⓘ

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	A	501	1	13,13,13	0.60	0	18,18,18	0.95	1 (5%)
4	TB2	D	501	1	13,13,13	0.69	0	18,18,18	2.00	1 (5%)
3	HEM	D	500	1	41,50,50	1.97	6 (14%)	45,82,82	1.59	6 (13%)
4	TB2	C	501	1	13,13,13	0.60	0	18,18,18	0.97	1 (5%)
5	CM5	B	607	-	36,36,36	0.41	0	49,49,49	0.79	1 (2%)
5	CM5	D	610	-	36,36,36	0.39	0	49,49,49	0.75	1 (2%)
5	CM5	A	605	-	25,25,36	0.44	0	32,32,49	0.81	1 (3%)
3	HEM	B	500	1	41,50,50	1.94	6 (14%)	45,82,82	1.75	7 (15%)
3	HEM	C	500	1	41,50,50	1.97	6 (14%)	45,82,82	1.70	6 (13%)
5	CM5	A	608	-	36,36,36	0.44	0	49,49,49	1.19	4 (8%)
3	HEM	A	500	1	41,50,50	1.98	6 (14%)	45,82,82	1.82	8 (17%)
4	TB2	B	501	1	13,13,13	0.60	0	18,18,18	0.88	1 (5%)
5	CM5	B	606	-	36,36,36	0.41	0	49,49,49	0.98	3 (6%)

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	A	501	1	-	0/9/9/9	0/1/1/1
4	TB2	D	501	1	-	0/9/9/9	0/1/1/1
3	HEM	D	500	1	-	1/12/54/54	-
4	TB2	C	501	1	-	6/9/9/9	0/1/1/1
5	CM5	B	607	-	-	9/17/65/65	0/3/3/3
5	CM5	D	610	-	-	8/17/65/65	0/3/3/3
5	CM5	A	605	-	-	7/13/41/65	0/2/2/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEM	B	500	1	-	6/12/54/54	-
3	HEM	C	500	1	-	2/12/54/54	-
5	CM5	A	608	-	-	10/17/65/65	0/3/3/3
3	HEM	A	500	1	-	7/12/54/54	-
4	TB2	B	501	1	-	6/9/9/9	0/1/1/1
5	CM5	B	606	-	-	9/17/65/65	0/3/3/3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	500	HEM	C3D-C2D	8.13	1.54	1.36
3	D	500	HEM	C3D-C2D	8.02	1.53	1.36
3	B	500	HEM	C3D-C2D	7.92	1.53	1.36
3	A	500	HEM	C3D-C2D	7.89	1.53	1.36
3	A	500	HEM	C3C-C2C	-4.90	1.33	1.40
3	D	500	HEM	C3C-C2C	-4.72	1.33	1.40
3	C	500	HEM	C3C-C2C	-4.66	1.33	1.40
3	B	500	HEM	C3C-C2C	-4.25	1.34	1.40
3	C	500	HEM	C3C-CAC	3.51	1.55	1.47
3	B	500	HEM	C3C-CAC	3.51	1.55	1.47
3	D	500	HEM	C3C-CAC	3.40	1.54	1.47
3	A	500	HEM	C3C-CAC	3.36	1.54	1.47
3	D	500	HEM	CAB-C3B	2.85	1.55	1.47
3	B	500	HEM	CAB-C3B	2.78	1.55	1.47
3	A	500	HEM	CAB-C3B	2.77	1.55	1.47
3	C	500	HEM	CAB-C3B	2.72	1.54	1.47
3	A	500	HEM	FE-ND	2.57	2.09	1.96
3	A	500	HEM	FE-NB	2.51	2.09	1.96
3	B	500	HEM	FE-ND	2.46	2.09	1.96
3	C	500	HEM	FE-ND	2.41	2.08	1.96
3	D	500	HEM	FE-ND	2.41	2.08	1.96
3	C	500	HEM	FE-NB	2.09	2.07	1.96
3	D	500	HEM	FE-NB	2.06	2.07	1.96
3	B	500	HEM	FE-NB	2.00	2.06	1.96

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	501	TB2	O1-C1-C2	-7.78	104.91	126.64
3	A	500	HEM	C4D-ND-C1D	6.35	111.63	105.07
3	C	500	HEM	C4D-ND-C1D	6.33	111.61	105.07

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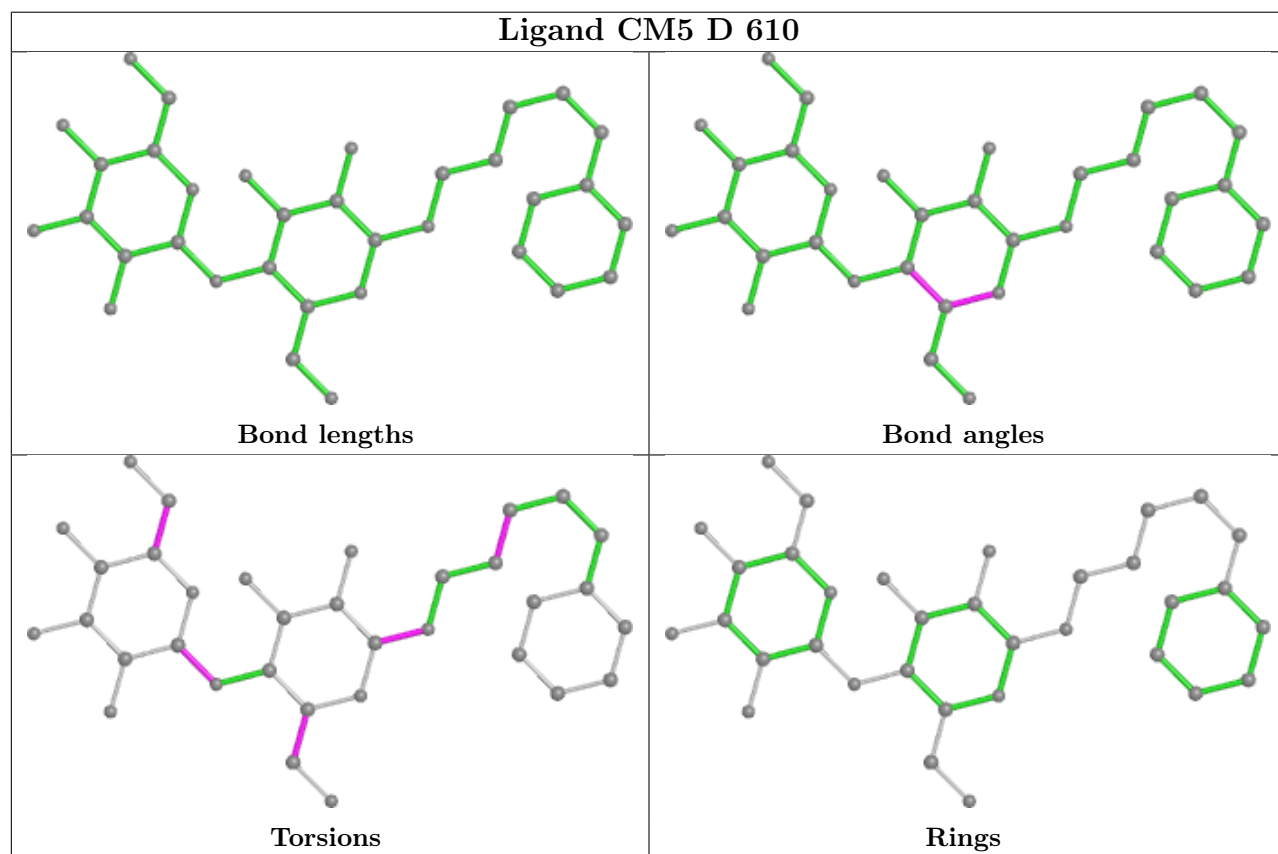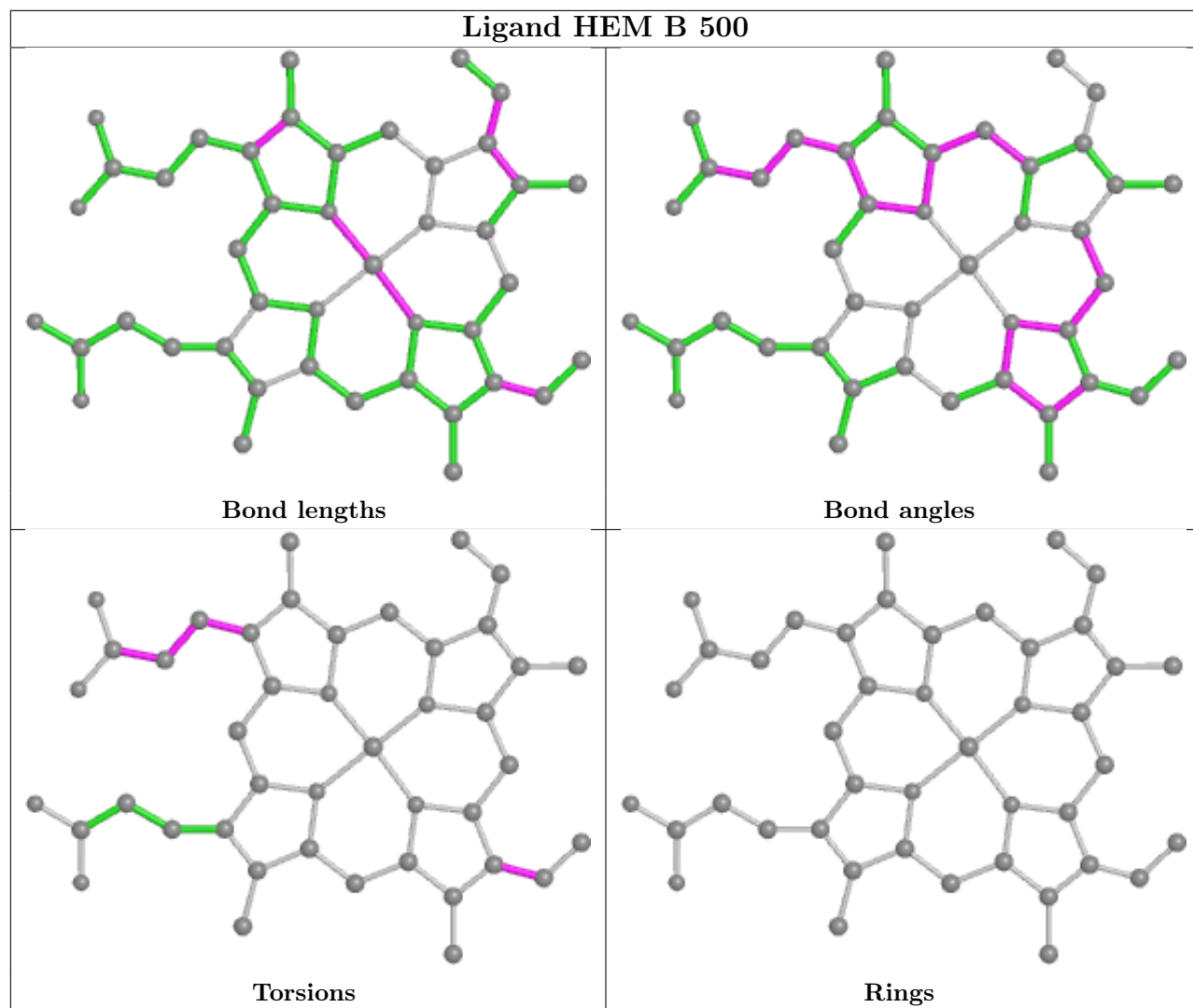| Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	500	HEM	C4D-ND-C1D	6.17	111.45	105.07
3	D	500	HEM	C4D-ND-C1D	6.03	111.30	105.07
5	A	608	CM5	O25-C26-C27	4.12	117.17	109.69
5	A	608	CM5	C24-O25-C26	3.86	121.27	113.69
3	D	500	HEM	C4C-CHD-C1D	3.37	127.00	122.56
3	A	500	HEM	C4C-CHD-C1D	3.27	126.88	122.56
3	A	500	HEM	CAD-C3D-C4D	3.24	130.32	124.66
3	C	500	HEM	C4B-CHC-C1C	3.03	126.56	122.56
3	B	500	HEM	C1B-NB-C4B	2.98	108.16	105.07
3	B	500	HEM	CAD-C3D-C4D	2.94	129.80	124.66
3	A	500	HEM	CAD-CBD-CGD	-2.91	107.34	113.60
5	B	606	CM5	C18-C17-C16	2.87	116.24	109.68
3	A	500	HEM	C4B-CHC-C1C	2.87	126.35	122.56
3	C	500	HEM	C1B-NB-C4B	2.80	107.97	105.07
3	B	500	HEM	C4C-CHD-C1D	2.74	126.17	122.56
3	A	500	HEM	C1B-NB-C4B	2.72	107.88	105.07
3	B	500	HEM	CAD-CBD-CGD	-2.71	107.77	113.60
3	C	500	HEM	C4C-CHD-C1D	2.65	126.05	122.56
3	B	500	HEM	C3B-C2B-C1B	2.61	108.42	106.49
3	B	500	HEM	C4B-CHC-C1C	2.61	126.00	122.56
3	A	500	HEM	C3B-C2B-C1B	2.57	108.39	106.49
3	C	500	HEM	C3B-C2B-C1B	2.48	108.33	106.49
3	D	500	HEM	C1B-NB-C4B	2.40	107.55	105.07
5	A	605	CM5	C13-C18-C17	2.39	114.97	110.00
3	C	500	HEM	CAD-CBD-CGD	-2.33	108.59	113.60
4	A	501	TB2	O1-C1-C2	-2.28	120.26	126.64
3	A	500	HEM	CMA-C3A-C4A	-2.27	124.98	128.46
5	B	607	CM5	C1-O12-C13	-2.20	110.20	113.84
3	D	500	HEM	C3B-C2B-C1B	2.14	108.07	106.49
4	C	501	TB2	O1-C1-C2	-2.14	120.66	126.64
5	D	610	CM5	O14-C15-C16	2.13	114.24	109.75
3	D	500	HEM	CAD-CBD-CGD	-2.11	109.06	113.60
5	A	608	CM5	C28-C27-C26	2.11	114.00	110.24
3	D	500	HEM	C2C-C3C-C4C	2.11	108.37	106.90
4	B	501	TB2	O1-C1-C2	-2.08	120.82	126.64
5	B	606	CM5	C13-C18-C17	2.07	114.30	110.00
5	A	608	CM5	C24-O23-C16	-2.05	112.89	117.96
5	B	606	CM5	C13-O14-C15	-2.04	109.67	113.69

There are no chirality outliers.

All (71) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	500	HEM	C1A-C2A-CAA-CBA
3	A	500	HEM	C3A-C2A-CAA-CBA
5	A	605	CM5	O14-C13-O12-C1
5	A	608	CM5	C18-C13-O12-C1
5	A	608	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	605	CM5	C18-C13-O12-C1
5	D	610	CM5	C18-C13-O12-C1
5	B	606	CM5	C3-C4-C5-C6
5	A	608	CM5	O25-C26-C30-O31
5	D	610	CM5	O25-C26-C30-O31
5	B	606	CM5	C15-C16-O23-C24
5	B	606	CM5	C17-C16-O23-C24
5	A	605	CM5	O14-C15-C19-O20
5	B	607	CM5	O14-C15-C19-O20
5	A	605	CM5	C16-C15-C19-O20
5	A	608	CM5	C2-C3-C4-C5
5	B	607	CM5	C15-C16-O23-C24
5	A	605	CM5	C2-C3-C4-C5
5	A	608	CM5	C2-C1-O12-C13
5	B	607	CM5	C17-C16-O23-C24
5	D	610	CM5	C1-C2-C3-C4
3	A	500	HEM	C4B-C3B-CAB-CBB
5	B	606	CM5	O12-C1-C2-C3
5	D	610	CM5	O14-C15-C19-O20
5	A	605	CM5	C4-C5-C6-C11
5	B	606	CM5	O25-C26-C30-O31
5	A	605	CM5	C4-C5-C6-C7
5	A	608	CM5	C3-C4-C5-C6
5	B	607	CM5	C2-C1-O12-C13
5	D	610	CM5	O25-C24-O23-C16
5	B	607	CM5	C16-C15-C19-O20
3	B	500	HEM	C4B-C3B-CAB-CBB
3	C	500	HEM	C4B-C3B-CAB-CBB
5	B	607	CM5	O14-C13-O12-C1

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

There are no ring outliers.

12 monomers are involved in 114 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	501	TB2	8	0
4	D	501	TB2	14	0
3	D	500	HEM	25	0
4	C	501	TB2	6	0
5	B	607	CM5	3	0
5	D	610	CM5	3	0
5	A	605	CM5	5	0
3	B	500	HEM	14	0
3	C	500	HEM	12	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	500	HEM	17	0
4	B	501	TB2	5	0
5	B	606	CM5	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand HEM D 500

Bond lengths

Bond angles

Torsions

Rings

Ligand CM5 B 607

Bond lengths

Bond angles

Torsions

Rings

Ligand CM5 D 610

Bond lengths

Bond angles

Torsions

Rings

Ligand CM5 A 605

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM B 500

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM C 500

Bond lengths

Bond angles

Torsions

Rings

Ligand CM5 A 608

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM A 500

Bond lengths

Bond angles

Torsions

Rings

Ligand CM5 B 606

Bond lengths

Bond angles

Torsions

Rings

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	465/476 (97%)	-0.21	4 (0%)	84	63	49, 79, 130, 196	2 (0%)
1	B	465/476 (97%)	-0.13	8 (1%)	70	41	54, 88, 160, 184	2 (0%)
1	C	456/476 (95%)	0.07	26 (5%)	23	8	56, 97, 181, 211	1 (0%)
1	D	464/476 (97%)	0.06	15 (3%)	47	20	60, 127, 166, 206	0
All	All	1850/1904 (97%)	-0.05	53 (2%)	51	23	49, 95, 166, 211	5 (0%)

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	50	GLY	10.7
1	A	38	PRO	6.6
1	C	39	VAL	6.3
1	A	39	VAL	6.0
1	C	43	LEU	5.2
1	C	134	ASP	5.0
1	B	231	HIS	4.2
1	C	230	THR	4.2
1	B	28	GLY	3.9
1	C	229	GLY	3.9
1	A	221	SER	3.7
1	C	46	MET	3.6
1	D	351	ALA	3.4
1	D	104	VAL	3.3
1	C	42	ASN	3.3
1	C	38	PRO	3.3
1	D	139	LYS	3.3
1	B	221	SER	3.2
1	D	408	PHE	3.1
1	B	55	PHE	3.1
1	C	270	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	104	VAL	3.0
1	C	40	LEU	2.9
1	C	121	TRP	2.9
1	C	116	ALA	2.8
1	B	51	LEU	2.8
1	C	108	PHE	2.8
1	D	453	ILE	2.8
1	D	324	VAL	2.7
1	C	288	LEU	2.7
1	D	424	GLU	2.6
1	D	461	SER	2.6
1	C	135	PHE	2.6
1	C	477	VAL	2.6
1	D	410	PRO	2.6
1	D	112	GLY	2.5
1	B	42	ASN	2.4
1	A	37	LEU	2.4
1	D	96	SER	2.3
1	D	106	PRO	2.3
1	C	268	TYR	2.3
1	C	110	GLY	2.3
1	C	272	MET	2.3
1	C	117	ASN	2.3
1	C	274	LYS	2.3
1	C	96	SER	2.2
1	C	76	VAL	2.2
1	D	43	LEU	2.2
1	B	228	PRO	2.1
1	C	36	PRO	2.1
1	D	419	ALA	2.1
1	D	231	HIS	2.1
1	C	133	ARG	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FRU	G	2	12/12	0.80	0.23	91,108,111,120	0
2	FRU	E	2	12/12	0.86	0.18	66,87,93,93	0
2	GLC	E	1	11/12	0.86	0.15	54,76,86,98	0
2	GLC	H	1	11/12	0.88	0.25	140,144,153,155	0
2	GLC	G	1	11/12	0.90	0.17	82,92,101,102	0
2	GLC	F	1	11/12	0.92	0.14	78,90,98,100	0
2	FRU	H	2	12/12	0.92	0.11	141,148,151,154	0
2	FRU	F	2	12/12	0.93	0.15	85,89,94,95	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:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative) and green (positive)
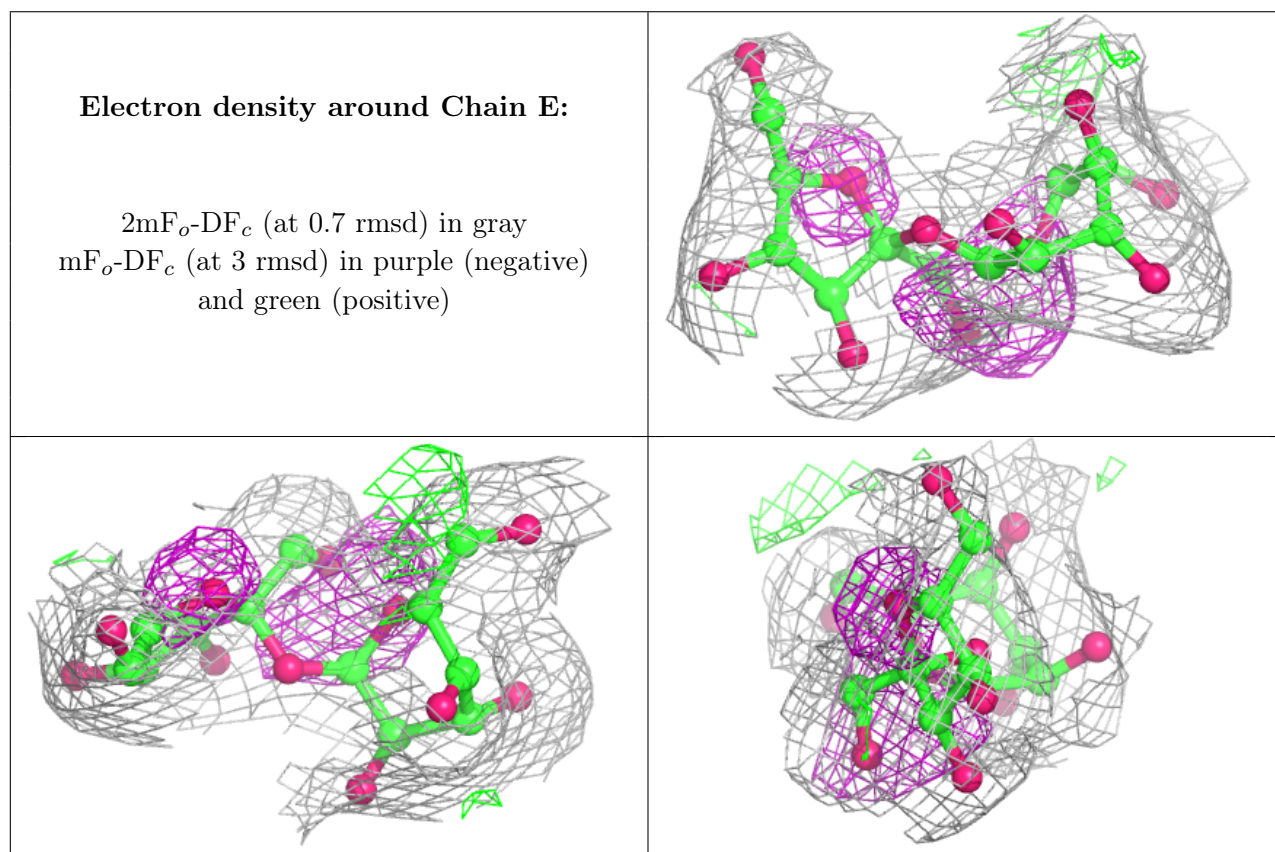
Electron density around Chain F:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
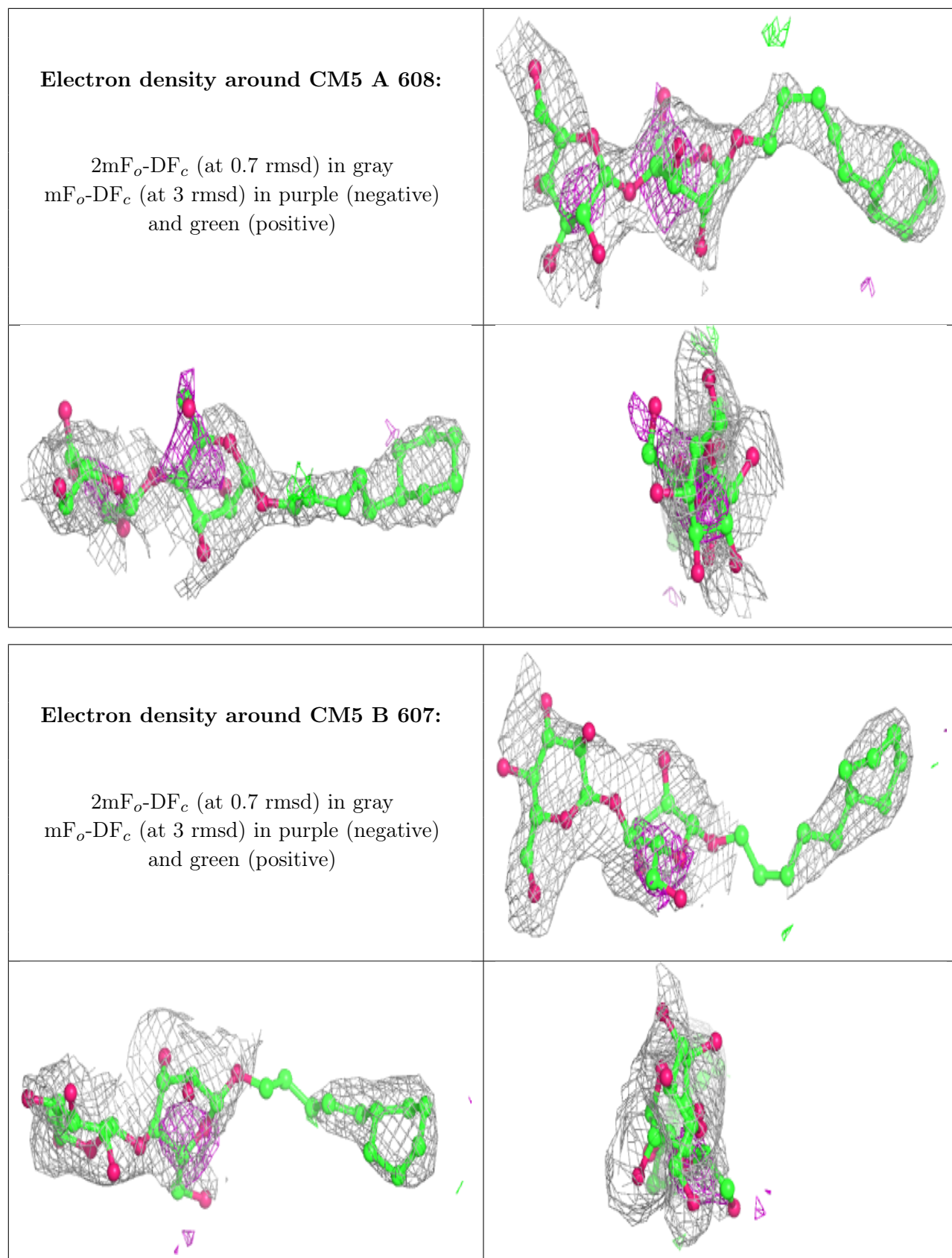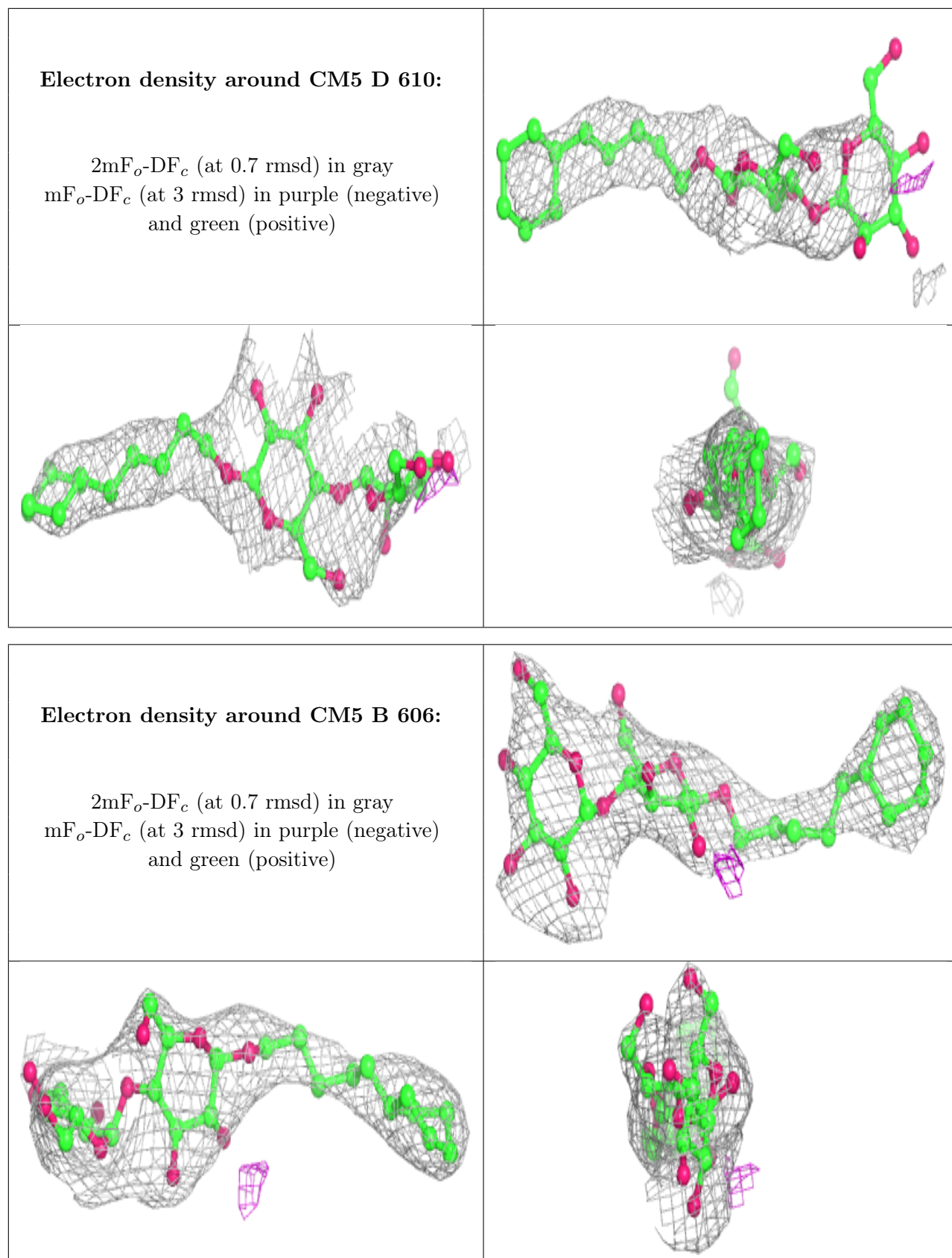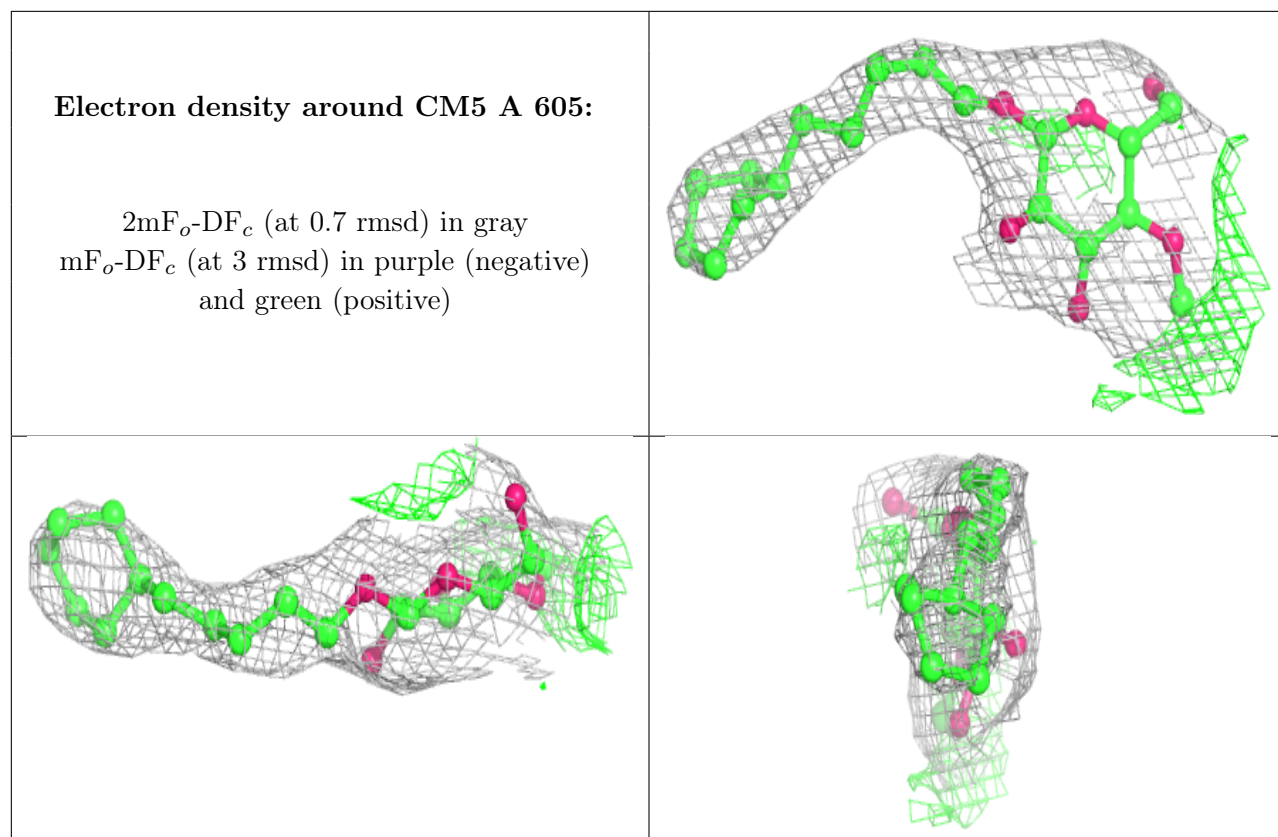and green (positive)
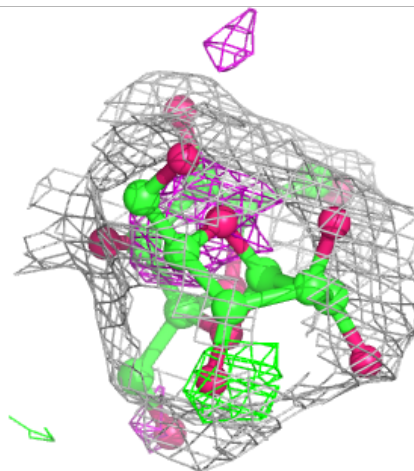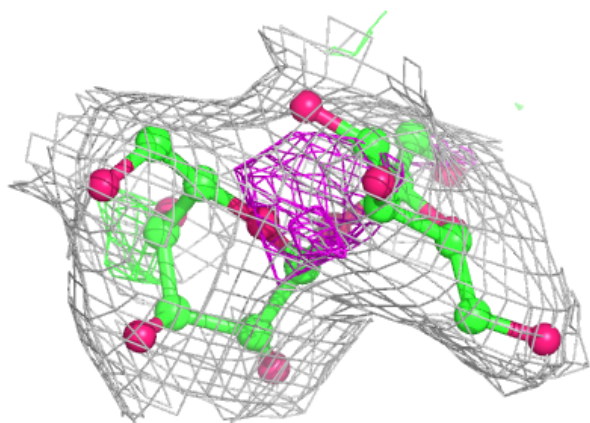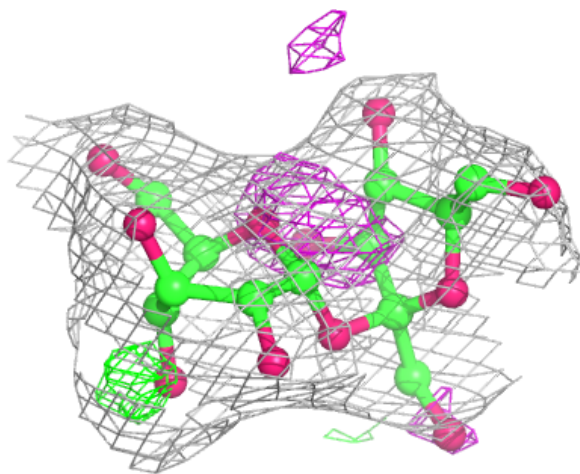
Electron density around Chain G:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
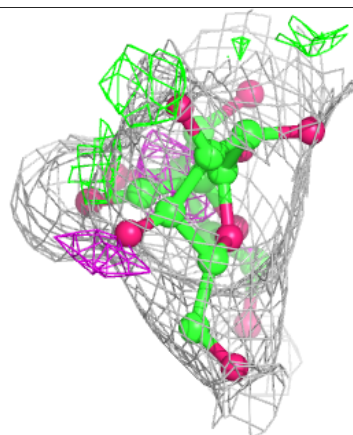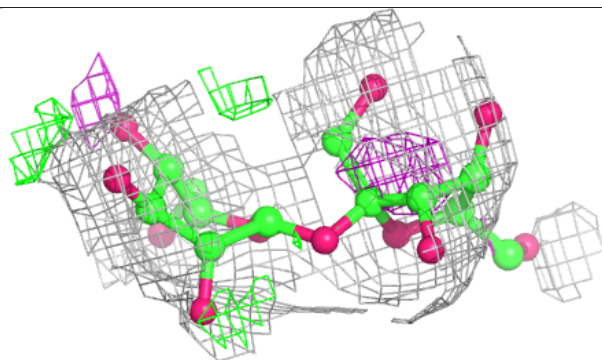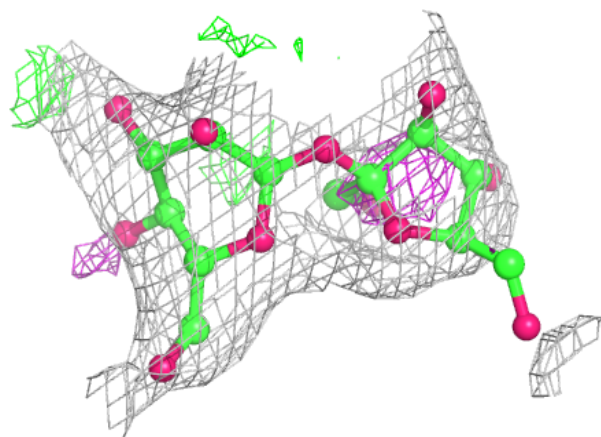
Electron density around Chain H:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
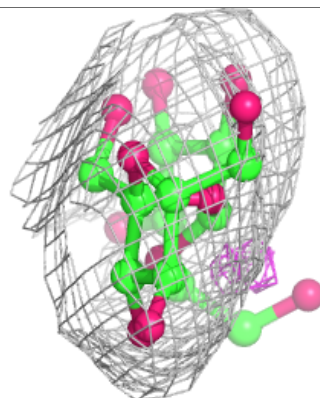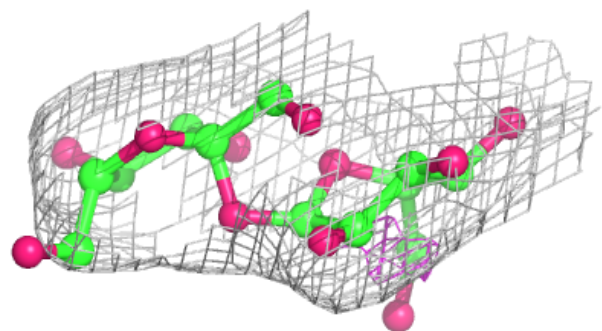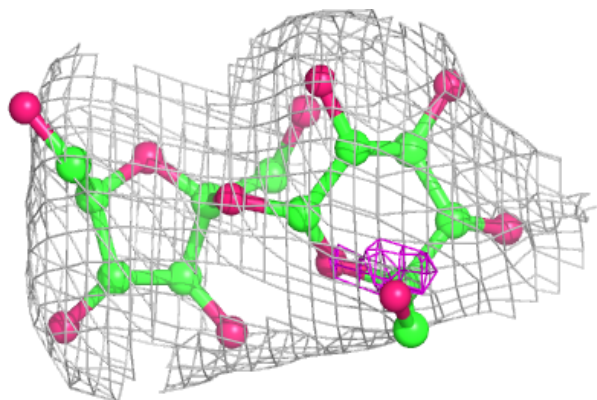
6.4 Ligands ⓘ

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	CM5	A	608	34/34	0.76	0.43	61,125,148,155	0
5	CM5	B	607	34/34	0.77	0.32	59,122,134,136	0
5	CM5	D	610	34/34	0.79	0.34	89,144,167,172	0
4	TB2	D	501	13/13	0.86	0.51	98,106,114,116	0
5	CM5	B	606	34/34	0.88	0.24	68,114,133,137	0
5	CM5	A	605	24/34	0.89	0.30	65,96,109,115	0
3	HEM	D	500	43/43	0.93	0.29	94,103,118,127	0
4	TB2	B	501	13/13	0.95	0.30	53,65,74,76	0
4	TB2	C	501	13/13	0.96	0.33	71,79,85,88	0
3	HEM	C	500	43/43	0.97	0.27	66,83,95,108	0
4	TB2	A	501	13/13	0.97	0.29	50,61,66,68	0
3	HEM	B	500	43/43	0.98	0.28	46,60,72,85	0
3	HEM	A	500	43/43	0.98	0.27	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.
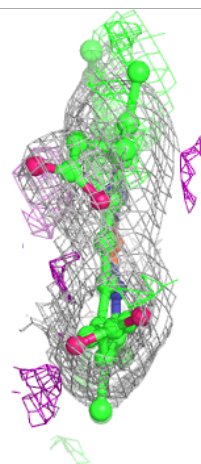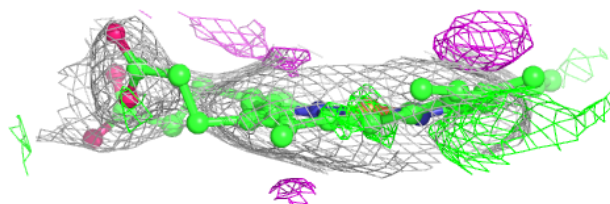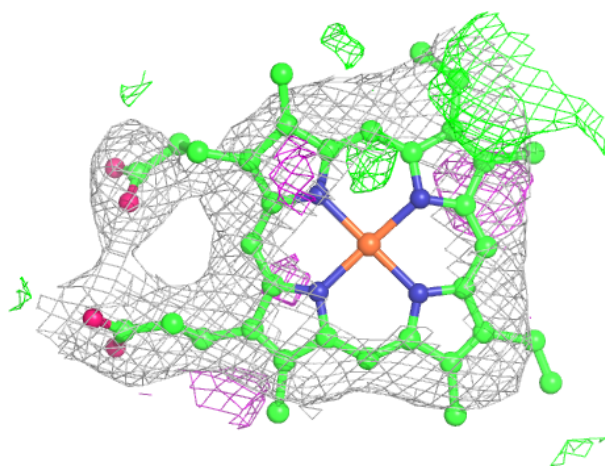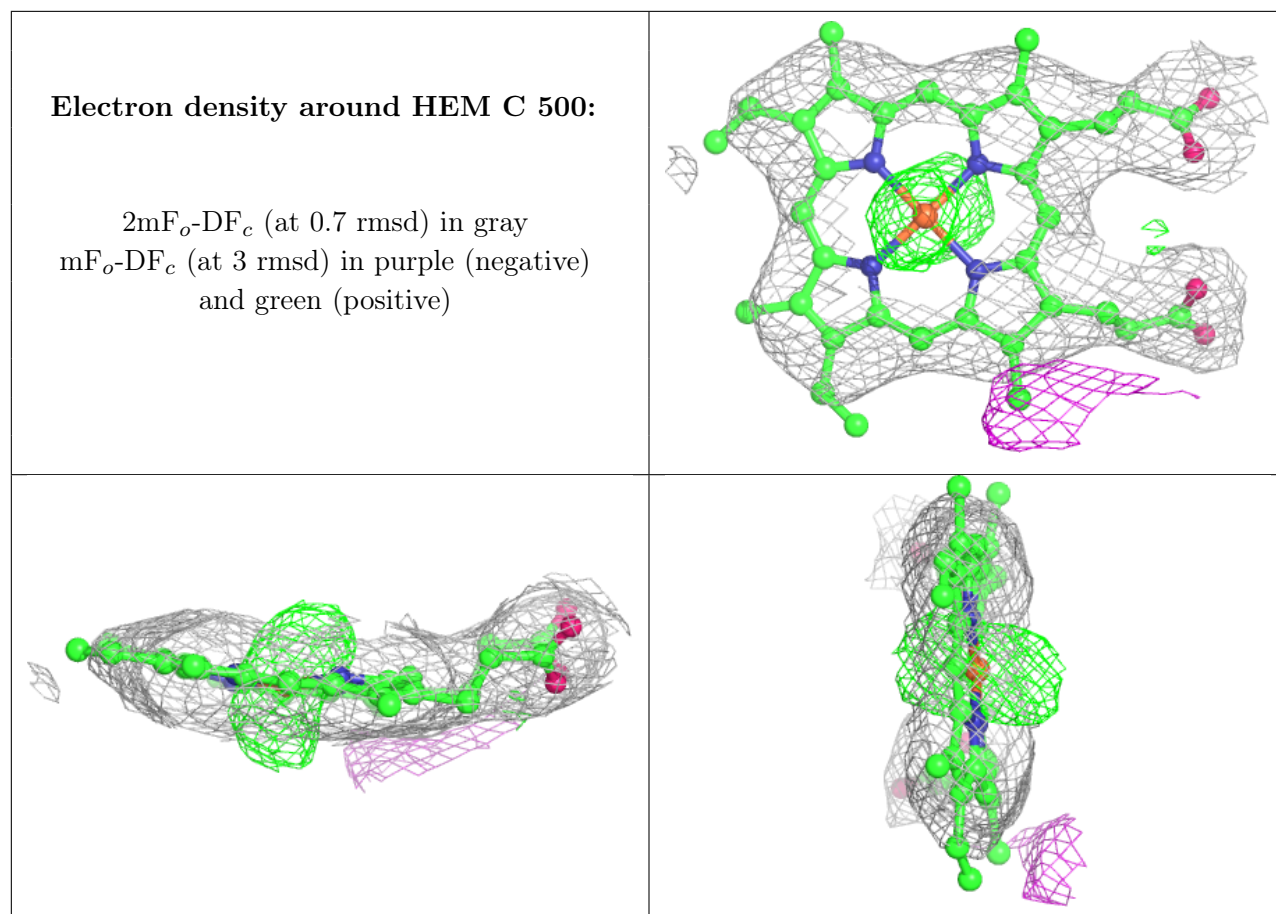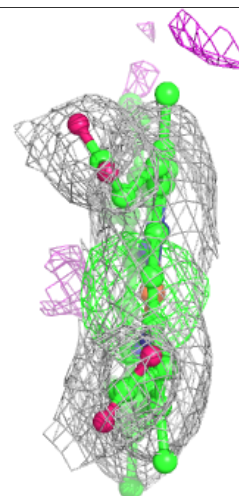
Electron density around CM5 A 608:

$2mF_o-DF_c$ (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)
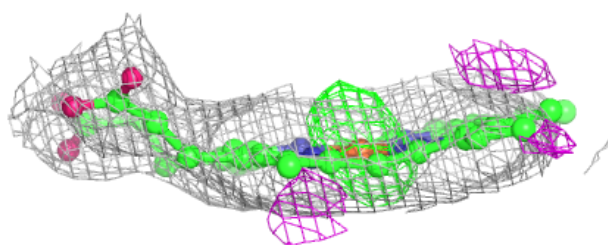
Electron density around CM5 D 610:

$2mF_o$-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 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)

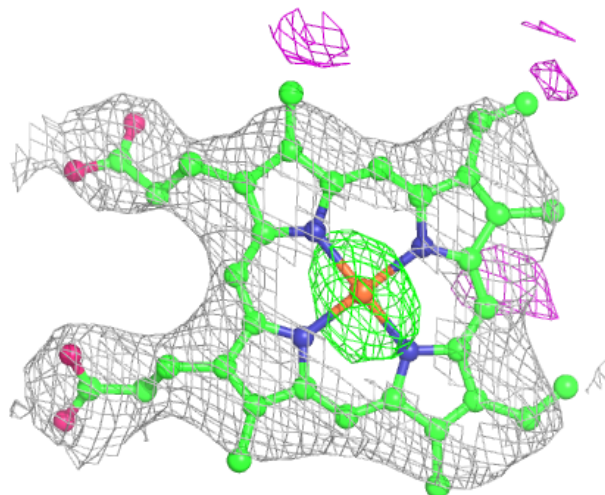**Electron density around HEM D 500:**

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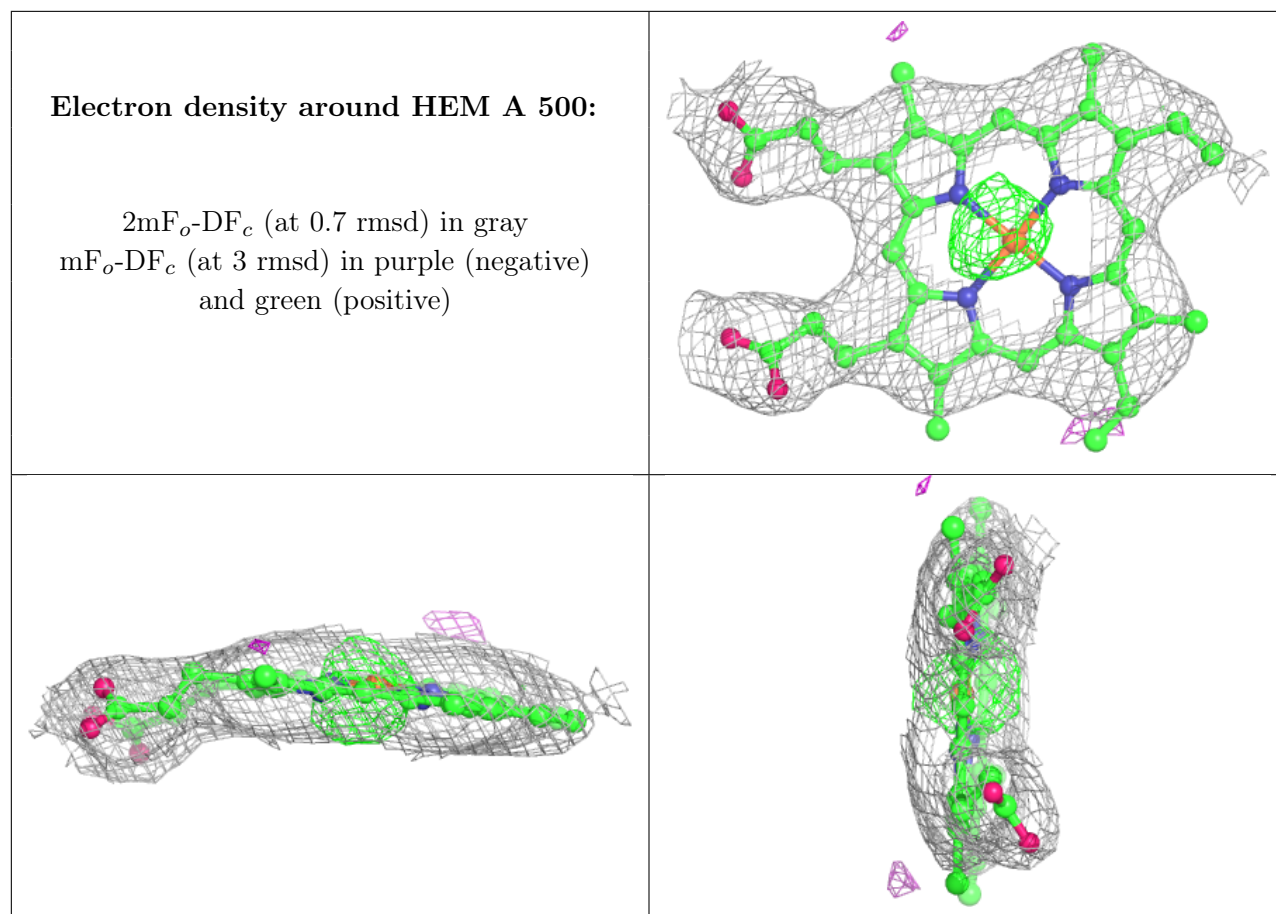mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

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:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.