Full wwPDB X-ray Structure Validation Report (i)

Aug 22, 2026 – 04:07 am BST

PDB ID	:	2CA0 / pdb_00002ca0
Title	:	Crystal structure of YC-17-bound cytochrome P450 PikC (CYP107L1)
Authors	:	Yermalitskaya, L.I.; Kim, Y.; Sherman, D.H.; Waterman, M.R.; Podust, L.M.
Deposited on	:	2005-12-15
Resolution	:	2.85 Å(reported)

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

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

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

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

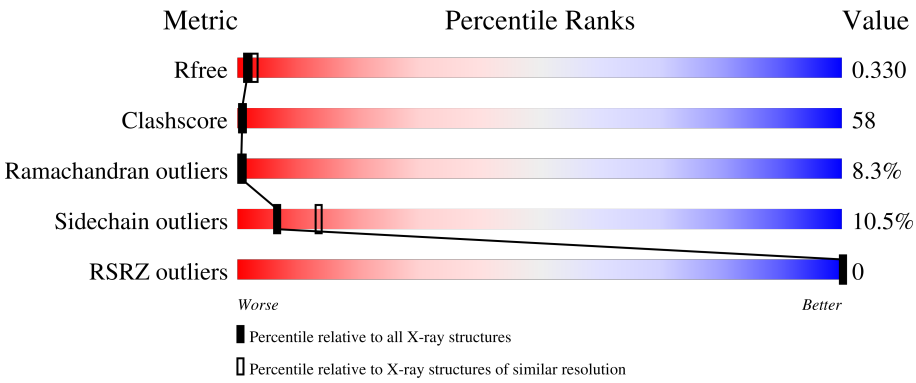
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.85 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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	436	25% 53% 11% • 10%
1	B	436	21% 53% 14% • 10%

2 Entry composition (i)

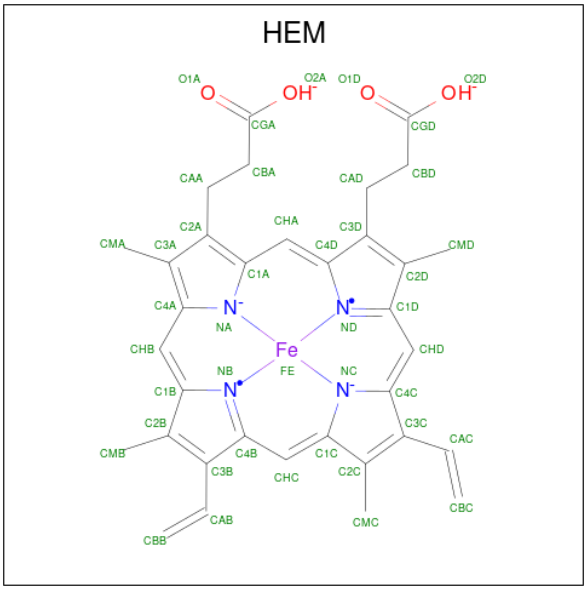
There are 4 unique types of molecules in this entry. The entry contains 6269 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 MONOOXYGENASE.

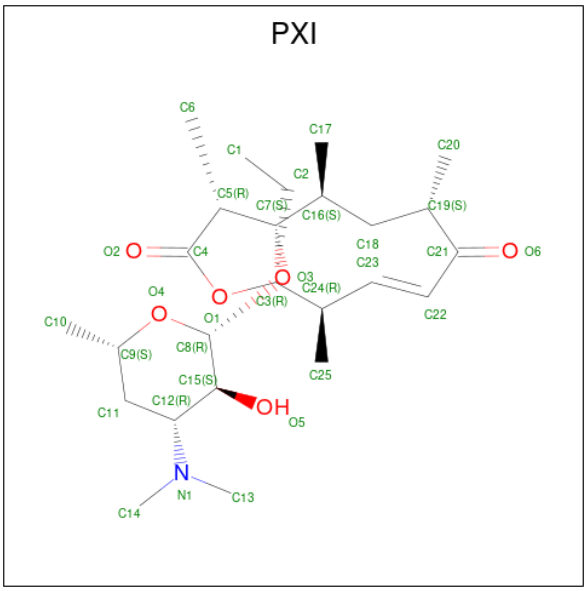
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	393	3028	1910	544	561	13	0	0	0
1	B	393	3028	1910	544	561	13	0	0	0

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 3 is 4-{[4-(DIMETHYLAMINO)-3-HYDROXY-6-METHYLTETRAHYDRO-2H-PYRAN-2-YL]OXY}-12-ETHYL-3,5,7,11-TETRAMETHYLOXACYCLODODEC-9-ENE-2,8-DIONE (CCD ID: PXI) (formula: $C_{25}H_{43}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	32	25	1	6	0	0
			Total	C	N	O		
3	B	1	32	25	1	6	0	0

- Molecule 4 is water.

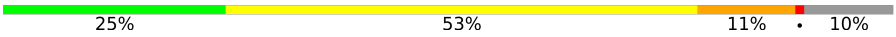
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	33	33	33	0	0
			Total	O		
4	B	30	30	30	0	0

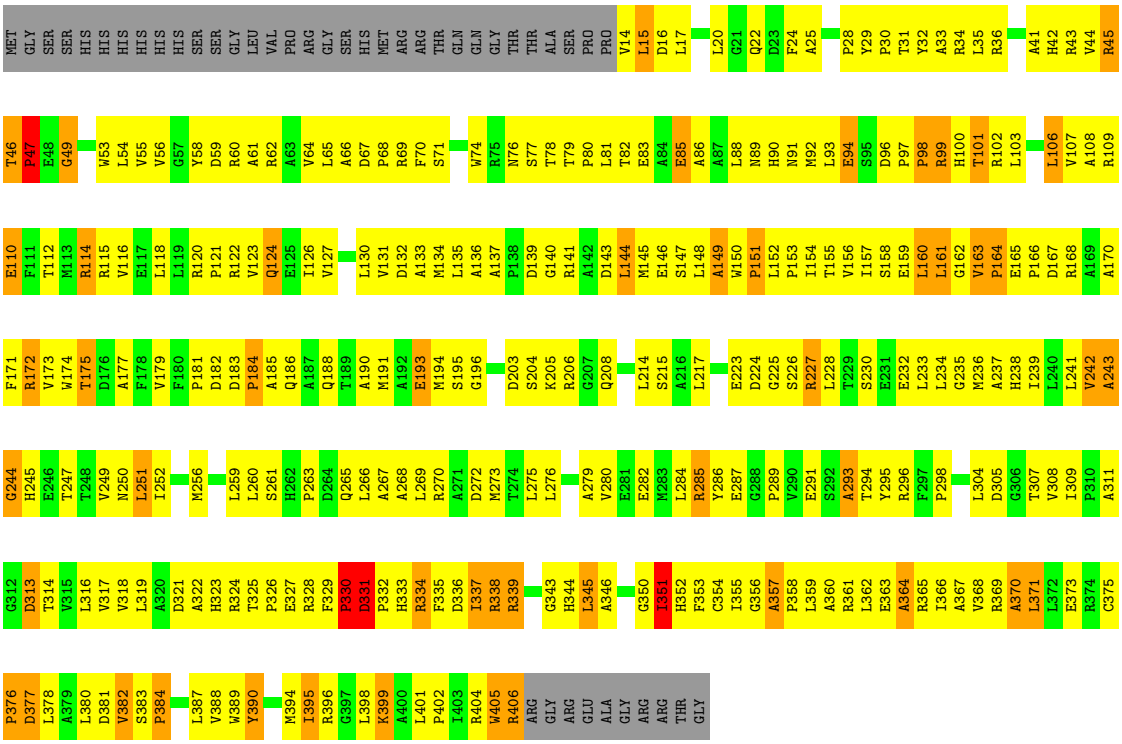
3 Residue-property plots (i)

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

- Molecule 1: CYTOCHROME P450 MONOOXYGENASE

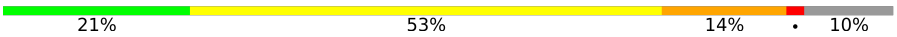
Chain A:

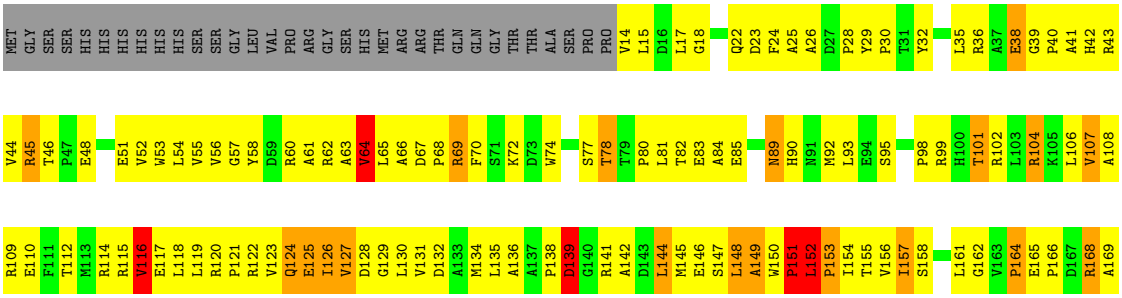


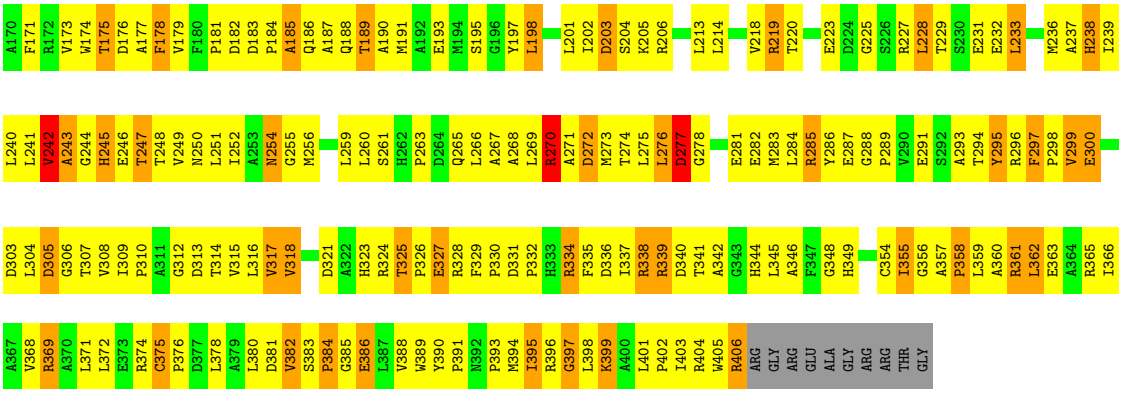


- Molecule 1: CYTOCHROME P450 MONOOXYGENASE

Chain B:






A170 F171 R172 V173 W174 T175 D176 A177 F178 V179 F180 P181 D182 D183 P184 A185 Q186 A187 Q188 T189 A190 M191 A192 E193 M194 S195 G196 Y197 L198 L201 I202 D203 S204 K205 R206 L213 L214 V218 R219 T220 E223 D224 G225 S226 R227 L228 T229 S230 E231 E232 L233 M236 A237 H238 I239
L240 L241 V242 A243 G244 H245 E246 T247 T248 V249 N250 L251 I252 A253 N254 G255 M256 L259 L260 S261 H262 P263 D264 Q265 L266 A267 A268 L269 R270 A271 D272 M273 T274 L275 L276 D277 G278 E281 E282 M283 L284 R285 Y286 E287 G288 P289 V290 E291 S292 A293 T294 Y295 R296 F297 P298 V299 E300
D303 L304 D305 G306 T307 V308 I309 P310 A311 G312 D313 T314 V315 L316 V317 V318 D321 A322 H323 R324 T325 P326 E327 R328 F329 P330 D331 P332 H333 R334 F335 D336 I337 R338 R339 D340 T341 A342 G343 H344 L345 A346 F347 G348 H349 C354 I355 G356 A357 P358 L359 A360 R361 L362 E363 A364 R365 I366
A367 V368 R369 A370 L371 L372 E373 R374 G375 P376 D377 L378 A379 L380 D381 V382 S383 P384 G385 E386 L387 V388 W389 Y390 P391 N392 P393 M394 I395 R396 G397 L398 K399 A400 L401 P402 I403 R404 W405 R406 ARG GLY ARG GLU ALA GLY ARG ARG THR GLY

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	61.09Å 91.97Å 68.90Å 90.00° 89.92° 90.00°	Depositor
Resolution (Å)	32.41 – 2.85 32.41 – 2.85	Depositor EDS
% Data completeness (in resolution range)	92.5 (32.41-2.85) 92.3 (32.41-2.85)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.51 (at 2.86Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.240 , 0.338 0.234 , 0.330	Depositor DCC
R_{free} test set	1675 reflections (10.05%)	wwPDB-VP
Wilson B-factor (Å^2)	31.9	Xtriage
Anisotropy	0.519	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 27.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.22$	Xtriage
Estimated twinning fraction	0.427 for h,-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6269	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.78% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PXI, 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	0.55	0/3098	1.07	22/4229 (0.5%)
1	B	0.54	0/3098	1.11	24/4229 (0.6%)
All	All	0.54	0/6196	1.09	46/8458 (0.5%)

There are no bond length outliers.

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	390	TYR	CA-C-N	9.86	129.62	119.56
1	A	390	TYR	C-N-CA	9.86	129.62	119.56
1	A	338	ARG	N-CA-C	-8.16	102.92	113.12
1	A	161	LEU	N-CA-C	-7.94	103.49	113.02
1	B	325	THR	CA-C-N	7.69	127.23	119.24
1	B	325	THR	C-N-CA	7.69	127.23	119.24
1	A	163	VAL	N-CA-C	7.55	115.68	107.60
1	B	295	TYR	N-CA-C	7.04	120.52	109.96
1	B	277	ASP	N-CA-C	-6.90	104.39	114.39
1	B	399	LYS	N-CA-C	-6.58	104.73	112.89
1	B	124	GLN	N-CA-C	-6.31	105.40	113.23
1	A	308	VAL	N-CA-C	6.25	115.72	106.85
1	A	399	LYS	N-CA-C	-6.18	105.57	113.23
1	B	397	GLY	N-CA-C	6.15	121.32	110.80
1	A	227	ARG	N-CA-C	-6.09	105.51	113.12
1	B	315	VAL	N-CA-C	6.02	117.15	108.48
1	B	18	GLY	N-CA-C	-5.97	107.26	114.66
1	B	355	ILE	N-CA-C	-5.95	106.94	112.83
1	A	251	LEU	N-CA-C	-5.88	104.87	111.28
1	A	233	LEU	N-CA-C	-5.87	104.78	111.07
1	B	219	ARG	N-CA-C	-5.78	104.89	111.07
1	A	295	TYR	N-CA-C	5.74	119.13	110.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	78	THR	N-CA-C	-5.69	106.50	113.50
1	B	288	GLY	CA-C-N	5.68	125.39	119.82
1	B	288	GLY	C-N-CA	5.68	125.39	119.82
1	B	107	VAL	N-CA-C	5.55	118.33	112.83
1	B	195	SER	N-CA-C	-5.55	106.49	113.20
1	A	46	THR	CA-C-N	5.53	126.75	119.84
1	A	46	THR	C-N-CA	5.53	126.75	119.84
1	A	331	ASP	CA-C-N	5.52	126.74	119.84
1	A	331	ASP	C-N-CA	5.52	126.74	119.84
1	A	79	THR	CA-C-N	5.51	125.41	119.85
1	A	79	THR	C-N-CA	5.51	125.41	119.85
1	A	124	GLN	N-CA-C	-5.50	103.14	111.34
1	B	317	VAL	N-CA-C	-5.46	101.79	109.21
1	B	64	VAL	N-CA-C	-5.43	105.31	110.42
1	B	338	ARG	N-CA-C	-5.33	107.79	114.56
1	A	230	SER	N-CA-C	-5.32	105.60	111.71
1	A	405	TRP	N-CA-C	5.29	118.73	107.67
1	A	172	ARG	N-CA-C	-5.29	105.63	111.71
1	B	395	ILE	N-CA-C	5.17	116.98	108.97
1	B	157	ILE	N-CA-C	5.14	115.75	110.36
1	B	116	VAL	N-CA-C	-5.09	105.75	110.53
1	B	375	CYS	CA-C-N	5.07	126.18	119.84
1	B	375	CYS	C-N-CA	5.07	126.18	119.84
1	A	357	ALA	N-CA-C	-5.01	107.16	113.77

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	3028	0	2986	344	0
1	B	3028	0	2986	367	0
2	A	43	0	30	3	0
2	B	43	0	30	5	0
3	A	32	0	43	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	32	0	43	8	0
4	A	33	0	0	9	0
4	B	30	0	0	9	0
All	All	6269	0	6118	711	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 58.

All (711) 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:B:55:VAL:HG11	1:B:64:VAL:HG21	1.41	1.03
1:B:285:ARG:HH11	1:B:285:ARG:HB3	1.25	1.01
1:A:285:ARG:HH21	1:A:286:TYR:HA	1.26	1.00
1:A:152:LEU:HB3	1:A:153:PRO:HD3	1.48	0.95
1:A:45:ARG:HH21	1:A:49:GLY:H	1.02	0.92
1:B:266:LEU:O	1:B:270:ARG:HB2	1.70	0.92
1:A:91:ASN:HD21	1:A:94:GLU:HG3	1.30	0.92
1:B:121:PRO:O	1:B:125:GLU:HG3	1.70	0.92
1:A:167:ASP:HB2	4:A:2015:HOH:O	1.69	0.91
1:A:97:PRO:HA	1:A:98:PRO:O	1.70	0.91
1:A:141:ARG:HB2	1:A:141:ARG:HH11	1.34	0.90
1:B:265:GLN:HE21	1:B:337:ILE:H	1.20	0.89
1:B:162:GLY:HA3	1:B:205:LYS:HZ1	1.33	0.89
1:A:395:ILE:HG22	1:A:396:ARG:H	1.36	0.89
1:B:380:LEU:HD21	1:B:401:LEU:HD11	1.54	0.88
1:B:252:ILE:O	1:B:256:MET:HG2	1.72	0.88
1:A:29:TYR:OH	1:A:287:GLU:HG2	1.72	0.87
1:A:60:ARG:HD2	1:A:304:LEU:HD22	1.56	0.87
1:A:45:ARG:HH21	1:A:49:GLY:N	1.74	0.86
1:A:17:LEU:HB2	1:A:47:PRO:HD3	1.59	0.85
1:A:251:LEU:HD13	1:A:284:LEU:HD23	1.59	0.85
1:B:152:LEU:HB3	1:B:153:PRO:HD3	1.60	0.84
1:A:331:ASP:N	1:A:332:PRO:HD3	1.92	0.83
1:A:395:ILE:HD12	1:A:395:ILE:N	1.94	0.83
1:A:45:ARG:HE	1:A:49:GLY:CA	1.92	0.83
1:B:122:ARG:HA	1:B:125:GLU:OE2	1.78	0.83
1:B:127:VAL:HG22	1:B:152:LEU:HD11	1.60	0.83
1:B:296:ARG:HG3	1:B:296:ARG:HH11	1.41	0.83
1:B:58:TYR:CD2	1:B:328:ARG:HG3	2.14	0.83
1:B:254:ASN:HD22	1:B:287:GLU:HB3	1.44	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:TRP:HE1	1:A:193:GLU:CD	1.86	0.82
1:A:242:VAL:O	1:A:244:GLY:N	2.13	0.82
1:A:350:GLY:O	1:A:352:HIS:N	2.12	0.81
1:A:261:SER:O	1:A:263:PRO:HD3	1.80	0.81
1:A:91:ASN:ND2	1:A:94:GLU:HG3	1.95	0.80
1:B:388:VAL:HG11	1:B:399:LYS:HD2	1.61	0.79
1:B:62:ARG:HH12	1:B:349:HIS:CE1	2.00	0.79
1:A:98:PRO:O	1:A:100:HIS:N	2.16	0.79
1:B:82:THR:HG23	1:B:85:GLU:OE1	1.82	0.78
1:A:398:LEU:HD12	1:A:401:LEU:HB2	1.66	0.78
1:A:331:ASP:H	1:A:332:PRO:HD3	1.47	0.78
1:B:369:ARG:HG3	1:B:369:ARG:HH11	1.48	0.78
1:A:45:ARG:NH2	1:A:49:GLY:H	1.81	0.77
1:A:137:ALA:HA	4:A:2014:HOH:O	1.84	0.77
1:A:285:ARG:C	1:A:285:ARG:HE	1.92	0.77
1:A:15:LEU:HD11	1:A:20:LEU:HD11	1.66	0.77
1:A:285:ARG:HD3	1:A:339:ARG:HD3	1.67	0.77
1:B:179:VAL:HG22	1:B:395:ILE:CD1	2.15	0.77
1:B:273:MET:HE3	1:B:276:LEU:HB2	1.65	0.77
1:B:243:ALA:HA	3:B:1408:PXI:O2	1.84	0.76
1:B:276:LEU:HD13	1:B:276:LEU:O	1.84	0.76
1:B:361:ARG:HB3	1:B:365:ARG:HH12	1.51	0.76
1:A:282:GLU:OE2	1:A:339:ARG:HD2	1.86	0.76
1:B:206:ARG:HB2	1:B:218:VAL:HG11	1.66	0.75
1:B:265:GLN:NE2	1:B:337:ILE:H	1.85	0.75
1:B:162:GLY:HA3	1:B:205:LYS:NZ	2.01	0.75
1:B:361:ARG:HB3	1:B:365:ARG:NH1	2.01	0.75
1:B:62:ARG:NH1	1:B:349:HIS:CE1	2.55	0.75
1:A:250:ASN:HB2	1:A:289:PRO:HB3	1.69	0.75
1:B:214:LEU:O	1:B:218:VAL:HG23	1.86	0.75
1:B:114:ARG:H	1:B:114:ARG:HD3	1.52	0.75
1:B:270:ARG:HH12	1:B:372:LEU:HD22	1.51	0.74
1:B:63:ALA:O	1:B:67:ASP:HB2	1.87	0.74
1:A:141:ARG:HB2	1:A:141:ARG:NH1	2.02	0.73
1:B:249:VAL:HG12	1:B:249:VAL:O	1.88	0.73
1:B:67:ASP:OD1	1:B:69:ARG:HG3	1.88	0.73
1:B:65:LEU:HA	1:B:296:ARG:HE	1.54	0.73
1:A:156:VAL:O	1:A:160:LEU:HD12	1.89	0.73
1:A:188:GLN:HA	1:A:191:MET:HE3	1.71	0.73
1:A:150:TRP:HB3	1:A:151:PRO:HD3	1.68	0.73
1:A:154:ILE:HB	1:A:245:HIS:NE2	2.04	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:ARG:HH11	1:A:45:ARG:HG2	1.54	0.72
1:B:227:ARG:O	1:B:228:LEU:HB2	1.88	0.72
1:A:74:TRP:CD2	1:A:81:LEU:HD21	2.25	0.72
1:B:171:PHE:CE2	1:B:241:LEU:HD22	2.24	0.72
1:A:285:ARG:NH2	1:A:286:TYR:HA	2.04	0.71
1:A:336:ASP:C	1:A:338:ARG:H	1.97	0.71
1:A:148:LEU:O	1:A:151:PRO:HD2	1.89	0.71
1:A:66:ALA:HB2	1:A:350:GLY:HA3	1.73	0.71
1:A:144:LEU:CD2	1:A:256:MET:HG3	2.20	0.71
1:A:382:VAL:HG22	1:A:383:SER:N	2.04	0.71
1:B:115:ARG:HG3	1:B:118:LEU:HD12	1.73	0.70
1:A:127:VAL:HG22	1:A:152:LEU:CD1	2.21	0.70
1:A:336:ASP:OD1	1:A:338:ARG:HB2	1.92	0.70
1:B:25:ALA:HB1	1:B:389:TRP:O	1.91	0.70
1:B:150:TRP:O	1:B:153:PRO:HD2	1.92	0.70
1:A:382:VAL:HG22	1:A:383:SER:H	1.55	0.70
1:B:406:ARG:HH11	1:B:406:ARG:HB2	1.56	0.69
1:A:53:TRP:O	1:A:54:LEU:HD23	1.92	0.69
1:A:259:LEU:HD11	1:A:266:LEU:HA	1.73	0.69
1:B:289:PRO:HA	1:B:396:ARG:HB3	1.75	0.69
1:B:395:ILE:HD11	3:B:1408:PXI:O6	1.93	0.69
1:B:309:ILE:HG13	4:B:2027:HOH:O	1.92	0.69
1:B:66:ALA:HB2	1:B:349:HIS:CD2	2.29	0.68
1:A:165:GLU:HB3	1:A:166:PRO:HD3	1.74	0.68
1:B:56:VAL:HB	1:B:321:ASP:OD1	1.93	0.68
1:B:95:SER:HB3	1:B:99:ARG:HH11	1.58	0.68
1:A:272:ASP:OD2	1:A:275:LEU:HG	1.92	0.68
1:B:306:GLY:O	1:B:308:VAL:HG23	1.93	0.68
1:A:170:ALA:O	1:A:173:VAL:HB	1.94	0.68
1:A:183:ASP:OD1	1:A:185:ALA:HB3	1.94	0.68
1:B:150:TRP:HB3	1:B:151:PRO:HD3	1.76	0.68
1:B:238:HIS:NE2	3:B:1408:PXI:H102	2.08	0.68
1:A:45:ARG:NE	1:A:49:GLY:HA2	2.09	0.68
1:A:122:ARG:C	1:A:124:GLN:H	2.02	0.68
1:A:256:MET:HE2	1:A:371:LEU:HD13	1.76	0.68
1:B:147:SER:O	1:B:151:PRO:HG2	1.94	0.67
1:B:236:MET:O	1:B:239:ILE:HG22	1.95	0.67
1:A:395:ILE:HD12	1:A:395:ILE:H	1.60	0.66
1:A:251:LEU:HD13	1:A:284:LEU:CD2	2.24	0.66
1:A:175:THR:O	1:A:179:VAL:HG23	1.94	0.66
1:A:273:MET:HE1	1:A:369:ARG:HA	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:ARG:HH12	1:B:51:GLU:C	2.03	0.66
1:B:144:LEU:HD21	1:B:256:MET:HG3	1.76	0.66
1:B:269:LEU:O	1:B:271:ALA:N	2.29	0.66
1:A:331:ASP:N	1:A:332:PRO:CD	2.58	0.66
1:A:276:LEU:HD11	1:A:365:ARG:HB3	1.78	0.65
1:A:327:GLU:N	1:A:327:GLU:OE1	2.29	0.65
1:B:74:TRP:CD2	1:B:81:LEU:HD21	2.30	0.65
1:A:149:ALA:O	1:A:249:VAL:HG22	1.97	0.65
1:B:287:GLU:HB2	4:B:2023:HOH:O	1.95	0.65
1:B:14:VAL:HG12	1:B:15:LEU:H	1.62	0.65
1:A:371:LEU:O	1:A:375:CYS:HB2	1.97	0.65
1:B:238:HIS:O	1:B:242:VAL:HG23	1.97	0.65
1:B:329:PHE:O	1:B:332:PRO:HG3	1.96	0.65
1:A:131:VAL:O	1:A:135:LEU:HG	1.96	0.65
1:B:201:LEU:HD12	1:B:204:SER:OG	1.96	0.65
1:B:405:TRP:O	1:B:406:ARG:HG3	1.96	0.65
1:B:295:TYR:HB2	4:B:2025:HOH:O	1.95	0.65
1:B:114:ARG:HD3	1:B:114:ARG:N	2.12	0.65
1:A:174:TRP:CZ2	1:A:193:GLU:HB3	2.32	0.64
1:A:259:LEU:O	1:A:266:LEU:HB2	1.97	0.64
1:B:389:TRP:HA	1:B:397:GLY:O	1.98	0.64
1:A:323:HIS:NE2	1:A:345:LEU:N	2.42	0.64
1:B:41:ALA:HB3	1:B:307:THR:HG21	1.79	0.64
1:B:359:LEU:O	1:B:363:GLU:HG3	1.98	0.64
1:A:61:ALA:HB1	1:A:317:VAL:HG13	1.80	0.64
1:B:291:GLU:N	1:B:394:MET:O	2.31	0.64
1:A:130:LEU:HD21	1:A:151:PRO:HB3	1.80	0.63
1:A:137:ALA:HB3	1:A:405:TRP:HZ2	1.63	0.63
1:A:15:LEU:C	1:A:15:LEU:HD12	2.24	0.63
1:B:250:ASN:O	1:B:254:ASN:HB2	1.99	0.63
1:A:282:GLU:OE1	1:A:285:ARG:HB3	1.99	0.63
1:B:344:HIS:O	1:B:345:LEU:HD23	1.98	0.63
1:B:69:ARG:O	1:B:299:VAL:HG23	1.99	0.63
1:B:36:ARG:HH12	1:B:326:PRO:HD2	1.64	0.62
1:B:124:GLN:OE1	1:B:366:ILE:HG23	1.99	0.62
1:A:120:ARG:HB3	1:A:121:PRO:HD3	1.81	0.62
1:B:164:PRO:O	1:B:168:ARG:HG3	2.00	0.62
1:A:67:ASP:HB3	1:A:70:PHE:CD1	2.35	0.62
1:B:102:ARG:O	1:B:106:LEU:HD13	1.99	0.62
1:B:202:ILE:HG22	1:B:206:ARG:NH1	2.13	0.62
1:B:152:LEU:HB3	1:B:153:PRO:CD	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:MET:HE1	1:A:107:VAL:HG21	1.82	0.61
1:A:183:ASP:O	1:A:185:ALA:N	2.32	0.61
1:A:22:GLN:NE2	1:A:388:VAL:HA	2.15	0.61
1:A:122:ARG:NH2	4:A:2010:HOH:O	2.33	0.61
1:A:273:MET:HE3	1:A:369:ARG:CZ	2.30	0.61
1:B:295:TYR:CE1	1:B:316:LEU:HD21	2.36	0.61
1:A:118:LEU:O	1:A:121:PRO:HD2	2.00	0.61
1:B:344:HIS:HD2	1:B:346:ALA:HB3	1.65	0.61
1:A:238:HIS:NE2	3:A:1408:PXI:H102	2.16	0.61
1:B:304:LEU:O	1:B:305:ASP:C	2.44	0.61
1:B:270:ARG:NH1	1:B:372:LEU:HB3	2.15	0.61
1:B:145:MET:HA	1:B:149:ALA:HB3	1.81	0.61
1:B:238:HIS:HE2	3:B:1408:PXI:H102	1.66	0.61
1:B:35:LEU:HB3	1:B:42:HIS:CD2	2.35	0.61
1:B:57:GLY:N	1:B:321:ASP:OD1	2.33	0.61
1:B:259:LEU:HD23	1:B:266:LEU:HD13	1.81	0.61
1:B:84:ALA:HB3	1:B:188:GLN:NE2	2.15	0.60
1:A:267:ALA:O	1:A:270:ARG:HB2	2.01	0.60
1:B:36:ARG:HH22	1:B:325:THR:HA	1.66	0.60
1:A:150:TRP:NE1	1:A:172:ARG:HB2	2.15	0.60
1:B:285:ARG:HD2	1:B:329:PHE:CE2	2.36	0.60
1:A:24:PHE:HE1	1:A:31:THR:HB	1.67	0.60
1:A:61:ALA:HB1	1:A:317:VAL:CG1	2.31	0.60
1:A:204:SER:O	1:A:208:GLN:HG2	2.01	0.60
1:B:178:PHE:HD2	1:B:178:PHE:N	2.00	0.60
1:B:296:ARG:HG3	1:B:296:ARG:NH1	2.16	0.60
1:A:395:ILE:HG22	1:A:396:ARG:N	2.13	0.60
1:B:261:SER:C	1:B:263:PRO:HD3	2.27	0.60
1:B:242:VAL:O	1:B:243:ALA:C	2.45	0.60
1:A:127:VAL:HG22	1:A:152:LEU:HD11	1.83	0.60
1:A:144:LEU:HD21	1:A:371:LEU:HD11	1.82	0.60
1:B:178:PHE:N	1:B:178:PHE:CD2	2.67	0.60
1:A:141:ARG:NH1	1:A:141:ARG:CB	2.65	0.60
1:A:122:ARG:NE	1:A:126:ILE:HD11	2.16	0.59
1:A:137:ALA:HB3	1:A:405:TRP:CZ2	2.36	0.59
1:B:285:ARG:HB3	1:B:285:ARG:NH1	2.07	0.59
1:B:390:TYR:CD1	1:B:397:GLY:HA3	2.37	0.59
1:B:340:ASP:C	1:B:342:ALA:H	2.10	0.59
1:B:245:HIS:O	1:B:249:VAL:HG23	2.02	0.59
1:B:369:ARG:HG3	1:B:369:ARG:NH1	2.16	0.59
1:B:93:LEU:HD21	1:B:294:THR:HG21	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:265:GLN:HG3	1:B:335:PHE:O	2.02	0.59
1:B:285:ARG:O	1:B:323:HIS:HB3	2.03	0.59
1:B:78:THR:HG23	1:B:312:GLY:HA3	1.85	0.59
1:A:183:ASP:OD2	1:B:138:PRO:HG2	2.03	0.59
1:A:357:ALA:HB3	1:A:358:PRO:HD3	1.85	0.59
1:B:115:ARG:HG3	1:B:118:LEU:CD1	2.31	0.59
1:A:55:VAL:HG11	1:A:64:VAL:HG21	1.85	0.59
1:A:114:ARG:HG3	1:A:114:ARG:HH11	1.68	0.59
1:A:282:GLU:OE1	1:A:282:GLU:HA	2.03	0.59
1:A:17:LEU:HG	1:A:45:ARG:O	2.03	0.59
1:A:45:ARG:HE	1:A:49:GLY:HA2	1.61	0.59
1:B:125:GLU:O	1:B:126:ILE:C	2.45	0.59
1:A:22:GLN:HE22	1:A:388:VAL:HA	1.68	0.58
1:A:170:ALA:HB1	1:A:174:TRP:CH2	2.37	0.58
1:A:251:LEU:HD22	1:A:284:LEU:HD21	1.83	0.58
1:B:119:LEU:O	1:B:123:VAL:HG23	2.03	0.58
1:A:148:LEU:O	1:A:149:ALA:C	2.46	0.58
1:B:114:ARG:O	1:B:117:GLU:HB3	2.03	0.58
1:B:282:GLU:CD	1:B:285:ARG:NH1	2.60	0.58
1:B:251:LEU:HD13	1:B:284:LEU:CD2	2.33	0.58
1:A:71:SER:OG	1:A:76:ASN:ND2	2.35	0.58
1:A:45:ARG:NE	1:A:49:GLY:CA	2.65	0.58
1:A:395:ILE:N	1:A:395:ILE:CD1	2.65	0.58
1:B:151:PRO:O	1:B:152:LEU:C	2.46	0.58
1:B:74:TRP:CE2	1:B:81:LEU:HD21	2.38	0.58
1:A:355:ILE:HG12	1:A:355:ILE:O	2.03	0.58
1:B:395:ILE:HG22	1:B:396:ARG:N	2.18	0.58
1:A:193:GLU:O	1:A:196:GLY:N	2.36	0.57
1:A:336:ASP:O	1:A:338:ARG:N	2.37	0.57
1:A:45:ARG:HE	1:A:49:GLY:C	2.13	0.57
1:A:123:VAL:HG21	1:A:362:LEU:HD23	1.85	0.57
1:A:336:ASP:O	1:A:339:ARG:N	2.37	0.57
1:B:147:SER:O	1:B:151:PRO:HD2	2.04	0.57
1:A:35:LEU:HD22	1:A:42:HIS:CD2	2.39	0.57
1:B:148:LEU:HD23	1:B:371:LEU:HD11	1.85	0.57
1:B:251:LEU:O	1:B:255:GLY:N	2.36	0.57
1:B:406:ARG:HH11	1:B:406:ARG:CB	2.17	0.57
1:A:387:LEU:HB2	4:A:2026:HOH:O	2.03	0.57
1:B:175:THR:O	1:B:179:VAL:HG23	2.04	0.57
1:A:33:ALA:O	1:A:34:ARG:C	2.47	0.57
1:B:148:LEU:CD2	1:B:371:LEU:HD11	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:TRP:HD1	1:A:190:ALA:HB1	1.70	0.57
1:B:169:ALA:O	1:B:173:VAL:HG23	2.05	0.57
1:B:331:ASP:OD1	1:B:334:ARG:HB2	2.05	0.56
1:A:67:ASP:HB3	1:A:70:PHE:HD1	1.70	0.56
1:A:123:VAL:HG12	1:A:123:VAL:O	2.05	0.56
1:A:279:ALA:HA	1:A:337:ILE:HG22	1.86	0.56
1:A:394:MET:HE2	3:A:1408:PXI:H23	1.86	0.56
1:B:147:SER:O	1:B:151:PRO:CG	2.53	0.56
1:B:228:LEU:HA	1:B:232:GLU:OE2	2.04	0.56
1:B:270:ARG:HH11	1:B:270:ARG:HG2	1.69	0.56
1:A:133:ALA:O	1:A:136:ALA:HB3	2.05	0.56
1:A:377:ASP:HB2	1:A:406:ARG:CA	2.36	0.56
1:B:104:ARG:HG3	1:B:104:ARG:HH11	1.70	0.56
1:B:187:ALA:O	1:B:191:MET:HG3	2.05	0.56
1:B:293:ALA:HB1	2:B:1407:HEM:O2A	2.05	0.56
1:B:331:ASP:CG	1:B:334:ARG:HB2	2.30	0.56
1:B:331:ASP:O	1:B:334:ARG:HB3	2.06	0.56
1:B:357:ALA:HB3	1:B:358:PRO:HD3	1.87	0.56
1:A:329:PHE:N	1:A:330:PRO:HD3	2.20	0.56
1:B:273:MET:C	1:B:275:LEU:H	2.12	0.56
1:A:390:TYR:OH	1:A:399:LYS:HA	2.06	0.56
1:B:39:GLY:H	1:B:42:HIS:HE1	1.53	0.56
1:B:285:ARG:HD2	1:B:329:PHE:CD2	2.41	0.56
1:A:354:CYS:HB2	2:A:1407:HEM:C4A	2.40	0.56
1:B:270:ARG:NH1	1:B:270:ARG:HG2	2.21	0.56
1:A:58:TYR:HE1	1:A:343:GLY:O	1.89	0.56
1:B:281:GLU:OE2	1:B:361:ARG:NE	2.39	0.56
1:A:146:GLU:HA	1:A:146:GLU:OE2	2.05	0.56
1:A:296:ARG:HG3	1:A:296:ARG:HH11	1.70	0.56
1:B:127:VAL:HG12	1:B:128:ASP:N	2.19	0.56
1:A:406:ARG:HH11	1:A:406:ARG:HB2	1.70	0.55
1:A:92:MET:HE1	1:A:107:VAL:CG2	2.35	0.55
1:A:144:LEU:HD23	1:A:256:MET:HG3	1.86	0.55
1:A:152:LEU:HB3	1:A:153:PRO:CD	2.31	0.55
1:B:276:LEU:O	1:B:276:LEU:HD22	2.06	0.55
1:A:99:ARG:C	1:A:101:THR:H	2.14	0.55
1:A:405:TRP:O	1:A:406:ARG:HG3	2.07	0.55
1:B:135:LEU:HD21	1:B:375:CYS:SG	2.45	0.55
1:B:231:GLU:HG3	4:B:2018:HOH:O	2.06	0.55
1:B:129:GLY:HA2	1:B:132:ASP:OD2	2.07	0.55
1:B:261:SER:O	1:B:263:PRO:HD3	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:ASP:OD2	1:A:334:ARG:HB2	2.07	0.55
1:B:201:LEU:HD11	1:B:205:LYS:HE2	1.88	0.55
1:A:256:MET:O	1:A:260:LEU:HG	2.07	0.55
1:B:93:LEU:HD23	3:B:1408:PXI:H6C2	1.89	0.55
1:B:344:HIS:CD2	1:B:346:ALA:HB3	2.42	0.55
1:B:35:LEU:O	1:B:38:GLU:HB2	2.07	0.54
1:B:138:PRO:HD2	1:B:139:ASP:OD1	2.08	0.54
1:A:171:PHE:CE2	1:A:241:LEU:HD13	2.43	0.54
1:A:293:ALA:O	1:A:316:LEU:HD22	2.07	0.54
1:B:285:ARG:HH11	1:B:285:ARG:CB	2.11	0.54
1:A:247:THR:O	1:A:289:PRO:HG3	2.07	0.54
1:A:287:GLU:CD	1:A:396:ARG:HH21	2.16	0.54
1:B:142:ALA:O	1:B:403:ILE:HG12	2.06	0.54
1:A:127:VAL:HG22	1:A:152:LEU:HD13	1.88	0.54
1:A:164:PRO:HB2	4:A:2015:HOH:O	2.07	0.54
1:B:236:MET:HA	1:B:239:ILE:HG22	1.89	0.54
1:B:281:GLU:O	1:B:284:LEU:HB2	2.08	0.54
1:B:327:GLU:O	1:B:330:PRO:HD3	2.08	0.54
1:A:171:PHE:HA	1:A:174:TRP:CE3	2.42	0.54
1:A:356:GLY:O	1:A:357:ALA:C	2.51	0.54
1:B:60:ARG:O	1:B:64:VAL:HG23	2.08	0.54
1:B:14:VAL:HG12	1:B:15:LEU:N	2.23	0.54
1:B:17:LEU:HD12	1:B:46:THR:HA	1.90	0.54
1:A:93:LEU:HD23	1:A:239:ILE:HD11	1.90	0.54
1:B:178:PHE:HD2	1:B:178:PHE:H	1.55	0.54
1:B:245:HIS:HB3	1:B:246:GLU:OE1	2.06	0.54
1:B:82:THR:HG21	1:B:188:GLN:OE1	2.08	0.53
1:B:84:ALA:HB3	1:B:188:GLN:HE22	1.73	0.53
1:B:109:ARG:O	1:B:112:THR:HG23	2.08	0.53
1:A:58:TYR:HA	1:A:322:ALA:HB1	1.90	0.53
1:A:112:THR:O	1:A:116:VAL:HG23	2.08	0.53
1:B:151:PRO:O	1:B:154:ILE:HG22	2.09	0.53
1:A:70:PHE:HB2	4:A:2005:HOH:O	2.09	0.53
1:A:149:ALA:HB1	1:A:249:VAL:HG13	1.91	0.53
1:B:259:LEU:HD12	1:B:335:PHE:CE2	2.43	0.53
1:B:406:ARG:CB	1:B:406:ARG:NH1	2.72	0.53
1:A:171:PHE:HA	1:A:174:TRP:HE3	1.72	0.53
1:B:92:MET:HE1	1:B:107:VAL:HG22	1.91	0.53
1:B:281:GLU:O	1:B:284:LEU:N	2.40	0.53
1:A:336:ASP:C	1:A:338:ARG:N	2.64	0.53
1:A:382:VAL:CG2	1:A:383:SER:H	2.21	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:ILE:HG23	1:B:158:SER:N	2.23	0.53
1:A:351:ILE:HG13	1:A:352:HIS:N	2.23	0.53
1:B:227:ARG:O	1:B:227:ARG:HG2	2.09	0.53
1:B:267:ALA:HA	1:B:270:ARG:HB2	1.91	0.53
1:A:91:ASN:CG	1:A:94:GLU:HG3	2.33	0.53
1:B:344:HIS:HD2	1:B:346:ALA:CB	2.22	0.52
1:A:81:LEU:HD12	1:A:86:ALA:HB2	1.90	0.52
1:A:88:LEU:C	1:A:90:HIS:H	2.17	0.52
1:B:298:PRO:HB2	1:B:300:GLU:O	2.10	0.52
1:B:29:TYR:HB2	1:B:30:PRO:HD3	1.91	0.52
1:A:60:ARG:O	1:A:64:VAL:HG23	2.08	0.52
1:B:272:ASP:OD1	1:B:273:MET:N	2.42	0.52
1:B:278:GLY:C	4:B:2022:HOH:O	2.51	0.52
1:A:99:ARG:C	1:A:101:THR:N	2.65	0.52
1:A:144:LEU:HD21	1:A:371:LEU:CD1	2.39	0.52
1:B:344:HIS:C	1:B:345:LEU:HD23	2.35	0.52
1:B:310:PRO:HD2	1:B:313:ASP:OD2	2.10	0.52
1:A:203:ASP:O	1:A:204:SER:C	2.53	0.52
1:A:181:PRO:HA	1:A:186:GLN:OE1	2.09	0.52
1:B:197:TYR:CD2	1:B:198:LEU:HD23	2.45	0.52
1:B:77:SER:HB2	1:B:297:PHE:CD2	2.45	0.51
1:A:325:THR:HG22	1:A:327:GLU:H	1.76	0.51
1:B:269:LEU:O	1:B:270:ARG:C	2.52	0.51
1:A:242:VAL:HG12	1:A:243:ALA:N	2.26	0.51
1:B:101:THR:O	1:B:102:ARG:C	2.52	0.51
1:B:116:VAL:HG21	1:B:358:PRO:HB2	1.92	0.51
1:B:272:ASP:OD1	1:B:274:THR:HG23	2.10	0.51
1:B:243:ALA:O	1:B:247:THR:OG1	2.27	0.51
1:A:139:ASP:CG	1:A:140:GLY:H	2.19	0.51
1:A:330:PRO:O	1:A:331:ASP:HB3	2.11	0.51
1:B:61:ALA:HA	1:B:64:VAL:HG23	1.92	0.51
1:B:299:VAL:O	1:B:300:GLU:CB	2.59	0.51
1:A:150:TRP:CE2	1:A:172:ARG:HD2	2.46	0.51
1:A:256:MET:HE2	1:A:371:LEU:CD1	2.40	0.51
1:B:53:TRP:NE1	1:B:313:ASP:OD2	2.44	0.51
1:A:53:TRP:CD2	1:A:309:ILE:HG12	2.45	0.51
1:A:214:LEU:O	1:A:217:LEU:N	2.43	0.51
1:B:294:THR:HA	1:B:394:MET:HE3	1.93	0.51
1:A:205:LYS:O	1:A:206:ARG:C	2.52	0.51
1:B:24:PHE:O	1:B:28:PRO:HB3	2.10	0.51
1:A:25:ALA:O	1:A:28:PRO:HD3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:PRO:HD2	1:A:313:ASP:O	2.11	0.50
1:A:15:LEU:HD12	1:A:16:ASP:O	2.11	0.50
1:A:276:LEU:CD1	1:A:365:ARG:HB3	2.41	0.50
1:B:388:VAL:CG1	1:B:399:LYS:HD2	2.38	0.50
1:A:145:MET:HA	1:A:149:ALA:HB3	1.94	0.50
1:A:165:GLU:CB	1:A:166:PRO:HD3	2.41	0.50
1:A:225:GLY:HA2	1:A:228:LEU:O	2.11	0.50
1:A:260:LEU:HD21	1:A:378:LEU:HD21	1.93	0.50
1:A:282:GLU:HG3	1:A:335:PHE:CE1	2.46	0.50
1:A:114:ARG:O	1:A:115:ARG:C	2.54	0.50
1:A:252:ILE:O	1:A:256:MET:HG2	2.11	0.50
1:A:364:ALA:O	1:A:367:ALA:HB3	2.11	0.50
1:A:382:VAL:CG2	1:A:383:SER:N	2.73	0.50
1:B:83:GLU:HA	4:B:2004:HOH:O	2.11	0.50
1:B:127:VAL:O	1:B:130:LEU:N	2.44	0.50
1:B:135:LEU:HD11	1:B:374:ARG:HB3	1.94	0.50
1:B:189:THR:O	1:B:193:GLU:HG3	2.11	0.50
1:B:368:VAL:O	1:B:372:LEU:HG	2.11	0.50
1:A:146:GLU:CG	1:A:146:GLU:O	2.60	0.50
1:B:115:ARG:HA	1:B:118:LEU:HG	1.92	0.50
1:B:131:VAL:O	1:B:131:VAL:CG1	2.60	0.50
1:B:244:GLY:HA2	1:B:247:THR:OG1	2.11	0.50
1:B:310:PRO:HG2	1:B:313:ASP:OD1	2.11	0.50
1:A:99:ARG:HG2	1:A:103:LEU:HD11	1.94	0.50
1:B:165:GLU:N	1:B:166:PRO:CD	2.74	0.50
1:B:248:THR:C	1:B:250:ASN:H	2.19	0.50
1:B:127:VAL:O	1:B:128:ASP:C	2.54	0.50
1:B:150:TRP:HA	1:B:249:VAL:HG13	1.93	0.50
1:B:233:LEU:HD12	1:B:233:LEU:C	2.36	0.50
1:A:161:LEU:O	1:A:214:LEU:HB2	2.12	0.49
1:A:336:ASP:O	1:A:339:ARG:HB3	2.12	0.49
1:A:74:TRP:CE2	1:A:81:LEU:HD21	2.47	0.49
1:B:92:MET:HE1	1:B:104:ARG:HA	1.95	0.49
1:A:29:TYR:HH	1:A:287:GLU:HG2	1.73	0.49
1:A:66:ALA:CB	1:A:350:GLY:HA3	2.42	0.49
1:A:139:ASP:CG	1:A:140:GLY:N	2.71	0.49
1:B:247:THR:HB	2:B:1407:HEM:CAB	2.42	0.49
1:B:357:ALA:N	1:B:358:PRO:CD	2.75	0.49
1:A:331:ASP:OD2	1:A:334:ARG:HD2	2.12	0.49
1:B:66:ALA:HB2	1:B:349:HIS:HD2	1.77	0.49
1:B:131:VAL:O	1:B:131:VAL:HG12	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:286:TYR:CD1	1:B:324:ARG:NH2	2.81	0.49
1:B:227:ARG:NH2	4:B:2017:HOH:O	2.45	0.49
1:B:395:ILE:CG2	1:B:396:ARG:N	2.76	0.49
1:A:140:GLY:O	1:A:404:ARG:HA	2.13	0.49
1:B:203:ASP:OD1	1:B:203:ASP:N	2.46	0.49
1:B:243:ALA:HB1	3:B:1408:PXI:H1C2	1.94	0.49
1:A:406:ARG:NH1	1:A:406:ARG:CB	2.75	0.49
1:B:43:ARG:HG3	1:B:53:TRP:CE2	2.47	0.49
1:B:148:LEU:O	1:B:151:PRO:HD2	2.13	0.49
1:B:337:ILE:O	1:B:337:ILE:HG13	2.13	0.49
1:A:15:LEU:O	1:A:15:LEU:HG	2.13	0.49
1:B:132:ASP:O	1:B:136:ALA:N	2.46	0.49
1:B:74:TRP:HD1	1:B:89:ASN:HD22	1.61	0.49
1:B:162:GLY:O	1:B:164:PRO:HD3	2.12	0.49
1:B:247:THR:O	1:B:289:PRO:HG3	2.12	0.49
1:B:277:ASP:HB3	1:B:365:ARG:HE	1.78	0.49
1:A:141:ARG:HH11	1:A:141:ARG:CB	2.15	0.48
1:A:205:LYS:HE2	1:A:214:LEU:HD23	1.95	0.48
1:B:123:VAL:O	1:B:127:VAL:HG23	2.12	0.48
1:B:201:LEU:O	1:B:205:LYS:HG2	2.13	0.48
1:A:114:ARG:HG3	1:A:114:ARG:NH1	2.27	0.48
1:B:149:ALA:O	1:B:249:VAL:HA	2.13	0.48
1:A:122:ARG:C	1:A:124:GLN:N	2.69	0.48
1:A:144:LEU:HD21	1:A:256:MET:HG3	1.92	0.48
1:A:182:ASP:CB	1:A:186:GLN:NE2	2.77	0.48
1:A:45:ARG:HH11	1:A:45:ARG:CG	2.22	0.48
1:A:329:PHE:HB3	1:A:339:ARG:NH1	2.29	0.48
1:B:179:VAL:HG13	1:B:395:ILE:HD12	1.95	0.48
1:B:246:GLU:HG3	3:B:1408:PXI:O6	2.13	0.48
1:A:58:TYR:CE1	1:A:343:GLY:O	2.67	0.48
1:A:108:ALA:O	1:A:110:GLU:N	2.46	0.48
1:B:259:LEU:HD12	1:B:335:PHE:HE2	1.78	0.48
1:A:82:THR:O	1:A:83:GLU:C	2.55	0.48
1:A:97:PRO:HA	1:A:98:PRO:C	2.32	0.48
1:A:282:GLU:CD	1:A:339:ARG:HD2	2.38	0.48
1:B:36:ARG:NH2	1:B:325:THR:HA	2.27	0.48
1:A:69:ARG:O	1:A:298:PRO:HA	2.13	0.48
1:B:177:ALA:O	1:B:181:PRO:HB3	2.14	0.48
1:A:30:PRO:O	1:A:33:ALA:HB3	2.14	0.47
1:A:60:ARG:N	4:A:2003:HOH:O	2.46	0.47
1:B:238:HIS:CD2	3:B:1408:PXI:H102	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:380:LEU:HD21	1:B:401:LEU:CD1	2.36	0.47
1:A:93:LEU:O	1:A:93:LEU:HD12	2.15	0.47
1:B:244:GLY:HA3	2:B:1407:HEM:C2C	2.49	0.47
1:B:295:TYR:CD1	1:B:314:THR:CG2	2.96	0.47
1:B:389:TRP:CE2	1:B:398:LEU:HD21	2.49	0.47
1:A:98:PRO:HA	1:A:101:THR:OG1	2.14	0.47
1:A:239:ILE:O	1:A:243:ALA:HB3	2.14	0.47
1:B:270:ARG:HH22	1:B:372:LEU:HA	1.79	0.47
1:A:147:SER:O	1:A:151:PRO:HG2	2.14	0.47
1:B:144:LEU:HB2	1:B:403:ILE:HD13	1.96	0.47
1:B:369:ARG:NH1	1:B:369:ARG:CG	2.77	0.47
1:A:160:LEU:C	1:A:162:GLY:H	2.23	0.47
1:B:153:PRO:O	1:B:155:THR:N	2.48	0.47
1:B:259:LEU:CD2	1:B:266:LEU:HD13	2.45	0.47
1:A:179:VAL:HG11	1:A:390:TYR:CD1	2.49	0.47
1:B:251:LEU:HD13	1:B:284:LEU:HD21	1.97	0.47
1:A:64:VAL:HG13	1:A:70:PHE:CD1	2.50	0.47
1:A:344:HIS:HD2	1:A:346:ALA:HB3	1.78	0.47
1:B:82:THR:HG1	1:B:85:GLU:H	1.62	0.47
1:B:273:MET:C	1:B:275:LEU:N	2.72	0.47
1:A:24:PHE:O	1:A:28:PRO:CD	2.63	0.47
1:A:174:TRP:NE1	1:A:193:GLU:HB2	2.30	0.47
1:A:177:ALA:O	1:A:181:PRO:HB3	2.14	0.47
1:B:72:LYS:HE3	1:B:294:THR:OG1	2.15	0.47
1:B:270:ARG:HH12	1:B:372:LEU:CD2	2.23	0.47
1:B:303:ASP:C	1:B:303:ASP:OD1	2.57	0.47
1:A:41:ALA:HB3	1:A:307:THR:HG21	1.98	0.46
1:B:147:SER:O	1:B:151:PRO:CD	2.63	0.46
1:A:224:ASP:C	1:A:226:SER:H	2.22	0.46
1:A:324:ARG:HG3	1:A:324:ARG:HH11	1.79	0.46
1:B:144:LEU:HD11	1:B:148:LEU:HD23	1.97	0.46
1:B:148:LEU:O	1:B:150:TRP:N	2.49	0.46
1:B:382:VAL:HG11	1:B:402:PRO:HD2	1.97	0.46
1:A:158:SER:CB	1:A:163:VAL:HB	2.45	0.46
1:A:88:LEU:HD23	1:A:234:LEU:HD21	1.97	0.46
1:A:150:TRP:HE1	1:A:172:ARG:HB2	1.78	0.46
1:A:24:PHE:O	1:A:25:ALA:C	2.58	0.46
1:B:102:ARG:HH12	1:B:232:GLU:CD	2.24	0.46
1:B:249:VAL:O	1:B:249:VAL:CG1	2.60	0.46
1:B:269:LEU:O	1:B:272:ASP:O	2.34	0.46
1:B:270:ARG:O	1:B:270:ARG:HD3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:TRP:CE2	1:A:309:ILE:HG12	2.51	0.46
1:B:228:LEU:HD12	1:B:232:GLU:CB	2.45	0.46
1:B:282:GLU:HA	1:B:282:GLU:OE1	2.14	0.46
1:B:323:HIS:HE1	1:B:346:ALA:HB2	1.80	0.46
1:A:360:ALA:HB1	2:A:1407:HEM:CBB	2.45	0.46
1:B:70:PHE:HB3	1:B:296:ARG:HB3	1.97	0.46
1:B:92:MET:CE	1:B:104:ARG:HA	2.45	0.46
1:A:64:VAL:HG13	1:A:70:PHE:CE1	2.51	0.46
1:A:100:HIS:CD2	1:A:352:HIS:CE1	3.03	0.46
1:A:280:VAL:HG21	1:A:365:ARG:HG3	1.96	0.46
1:B:22:GLN:O	1:B:22:GLN:HG3	2.14	0.46
1:B:197:TYR:HD2	1:B:198:LEU:HD23	1.80	0.46
1:B:269:LEU:HD12	1:B:272:ASP:O	2.15	0.46
1:B:269:LEU:C	1:B:271:ALA:N	2.72	0.46
1:B:381:ASP:O	1:B:382:VAL:HB	2.16	0.46
1:A:91:ASN:OD1	1:A:94:GLU:HG3	2.15	0.46
1:B:291:GLU:HB3	1:B:393:PRO:O	2.16	0.46
1:B:356:GLY:O	1:B:357:ALA:C	2.59	0.46
1:B:388:VAL:HG11	1:B:399:LYS:CD	2.40	0.46
1:A:139:ASP:OD1	1:A:139:ASP:N	2.49	0.46
1:B:388:VAL:HB	1:B:399:LYS:HB2	1.98	0.46
1:A:24:PHE:O	1:A:28:PRO:HB3	2.16	0.45
1:A:91:ASN:HD21	1:A:94:GLU:CG	2.16	0.45
1:A:249:VAL:O	1:A:252:ILE:HB	2.16	0.45
1:B:134:MET:C	1:B:136:ALA:H	2.24	0.45
1:B:287:GLU:HA	4:B:2024:HOH:O	2.15	0.45
1:B:340:ASP:C	1:B:342:ALA:N	2.74	0.45
1:A:45:ARG:CG	1:A:45:ARG:NH1	2.79	0.45
1:B:157:ILE:HD13	4:B:2019:HOH:O	2.15	0.45
1:B:236:MET:O	1:B:237:ALA:C	2.60	0.45
1:B:247:THR:HB	2:B:1407:HEM:C3B	2.51	0.45
1:B:340:ASP:OD2	1:B:342:ALA:CB	2.64	0.45
1:A:123:VAL:O	1:A:366:ILE:HG21	2.16	0.45
1:A:259:LEU:HD21	1:A:269:LEU:HD23	1.97	0.45
1:A:291:GLU:HB2	1:A:395:ILE:O	2.15	0.45
1:A:390:TYR:CE2	1:A:399:LYS:HA	2.52	0.45
1:B:179:VAL:HG11	1:B:390:TYR:CD1	2.52	0.45
1:B:205:LYS:HE3	1:B:214:LEU:HD23	1.98	0.45
1:B:267:ALA:HA	1:B:270:ARG:CB	2.45	0.45
1:A:45:ARG:CZ	1:A:49:GLY:HA2	2.47	0.45
1:B:120:ARG:HB3	1:B:121:PRO:HD3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:383:SER:O	1:B:385:GLY:N	2.49	0.45
1:A:56:VAL:HG12	1:A:318:VAL:HB	1.98	0.45
1:A:62:ARG:HB2	1:A:345:LEU:HD11	1.98	0.45
1:A:78:THR:O	1:A:80:PRO:HD3	2.17	0.45
1:A:24:PHE:HE1	1:A:31:THR:CB	2.29	0.45
1:A:273:MET:HE3	1:A:369:ARG:NH1	2.32	0.45
1:A:328:ARG:HG2	1:A:328:ARG:HH11	1.82	0.45
1:B:74:TRP:CE3	1:B:81:LEU:HD21	2.51	0.45
1:B:380:LEU:HD22	1:B:382:VAL:HG12	1.99	0.45
1:A:14:VAL:N	4:A:2001:HOH:O	2.50	0.45
1:A:224:ASP:OD2	1:A:227:ARG:HG3	2.16	0.45
1:A:367:ALA:O	1:A:368:VAL:C	2.59	0.45
1:B:48:GLU:N	1:B:48:GLU:CD	2.75	0.45
1:A:324:ARG:HG3	1:A:324:ARG:NH1	2.32	0.45
1:A:329:PHE:N	1:A:330:PRO:CD	2.79	0.45
1:B:126:ILE:HD13	1:B:155:THR:CG2	2.46	0.45
1:B:150:TRP:HA	1:B:249:VAL:HG22	1.98	0.45
1:A:20:LEU:HB3	1:A:24:PHE:HB2	1.98	0.45
1:A:32:TYR:HB3	1:A:321:ASP:HB2	1.98	0.45
1:B:77:SER:HB2	1:B:297:PHE:CE2	2.51	0.45
1:B:130:LEU:C	1:B:132:ASP:H	2.25	0.45
1:B:123:VAL:O	1:B:123:VAL:HG12	2.15	0.45
1:B:175:THR:HG23	1:B:246:GLU:OE2	2.17	0.45
1:B:177:ALA:O	1:B:181:PRO:HD3	2.17	0.45
1:B:371:LEU:O	1:B:375:CYS:HB2	2.17	0.45
1:A:61:ALA:O	1:A:62:ARG:C	2.60	0.44
1:A:134:MET:C	1:A:136:ALA:H	2.26	0.44
1:A:150:TRP:HB3	1:A:151:PRO:CD	2.44	0.44
1:A:331:ASP:O	1:A:334:ARG:HB2	2.18	0.44
1:A:150:TRP:CD2	1:A:172:ARG:HD2	2.52	0.44
1:A:376:PRO:C	1:A:378:LEU:H	2.24	0.44
1:B:153:PRO:C	1:B:155:THR:N	2.75	0.44
1:A:90:HIS:ND1	1:A:99:ARG:NH2	2.64	0.44
1:A:193:GLU:O	1:A:194:MET:C	2.61	0.44
1:A:344:HIS:HD2	1:A:346:ALA:CB	2.30	0.44
1:B:174:TRP:O	1:B:176:ASP:N	2.51	0.44
1:B:183:ASP:O	1:B:185:ALA:N	2.47	0.44
1:B:285:ARG:HH12	1:B:286:TYR:HB2	1.83	0.44
1:B:360:ALA:O	1:B:362:LEU:N	2.50	0.44
1:A:148:LEU:O	1:A:151:PRO:CD	2.64	0.44
1:B:155:THR:O	1:B:156:VAL:C	2.60	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:161:LEU:HD23	1:B:213:LEU:HB3	1.99	0.44
1:A:370:ALA:O	1:A:373:GLU:N	2.49	0.44
1:B:296:ARG:NH1	1:B:296:ARG:CG	2.78	0.44
1:B:361:ARG:O	1:B:365:ARG:HG3	2.17	0.44
1:B:380:LEU:HD23	1:B:402:PRO:O	2.17	0.44
1:B:141:ARG:HG2	1:B:404:ARG:HB3	1.99	0.44
1:A:36:ARG:HH12	1:A:326:PRO:HD2	1.83	0.44
1:A:143:ASP:HA	1:A:402:PRO:HA	2.00	0.44
1:A:282:GLU:OE1	1:A:282:GLU:CA	2.66	0.44
1:B:108:ALA:HA	1:B:355:ILE:HD11	1.99	0.44
1:B:284:LEU:O	1:B:346:ALA:HB2	2.17	0.44
1:A:171:PHE:HE2	1:A:241:LEU:HD13	1.80	0.44
1:A:265:GLN:HE21	1:A:336:ASP:HA	1.82	0.44
1:A:333:HIS:CE1	4:A:2023:HOH:O	2.70	0.44
1:B:68:PRO:O	1:B:69:ARG:C	2.60	0.44
1:A:174:TRP:CD1	1:A:190:ALA:HB1	2.51	0.43
1:A:359:LEU:O	1:A:363:GLU:HG3	2.17	0.43
1:A:319:LEU:HD22	1:A:345:LEU:HB2	2.00	0.43
1:B:152:LEU:O	1:B:153:PRO:C	2.60	0.43
1:B:14:VAL:HA	1:B:43:ARG:O	2.18	0.43
1:B:219:ARG:O	1:B:220:THR:C	2.60	0.43
1:A:146:GLU:OE2	1:A:146:GLU:CA	2.64	0.43
1:A:146:GLU:O	1:A:146:GLU:HG3	2.18	0.43
1:A:158:SER:HB3	1:A:163:VAL:HB	2.01	0.43
1:B:45:ARG:HH11	1:B:45:ARG:CB	2.32	0.43
1:B:156:VAL:HG11	1:B:359:LEU:HD11	1.99	0.43
1:B:331:ASP:O	1:B:339:ARG:NH2	2.48	0.43
1:B:153:PRO:O	1:B:154:ILE:C	2.62	0.43
1:B:242:VAL:O	1:B:244:GLY:N	2.52	0.43
1:B:270:ARG:NH1	1:B:372:LEU:HD22	2.26	0.43
1:A:88:LEU:C	1:A:90:HIS:N	2.77	0.43
1:A:161:LEU:HD13	1:A:241:LEU:HG	2.01	0.43
1:A:357:ALA:N	1:A:358:PRO:CD	2.81	0.43
1:B:186:GLN:O	1:B:190:ALA:N	2.42	0.43
1:A:351:ILE:CG1	1:A:352:HIS:N	2.82	0.43
1:A:102:ARG:HH12	1:A:232:GLU:CD	2.27	0.43
1:A:150:TRP:CE2	1:A:172:ARG:HB2	2.53	0.43
1:A:344:HIS:CD2	1:A:346:ALA:HB3	2.52	0.43
1:B:90:HIS:O	1:B:232:GLU:HA	2.19	0.43
1:B:174:TRP:C	1:B:176:ASP:N	2.73	0.43
1:B:227:ARG:O	1:B:227:ARG:CG	2.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:390:TYR:HA	1:B:391:PRO:HD3	1.86	0.43
1:B:44:VAL:HG21	1:B:54:LEU:HD11	2.00	0.43
1:B:55:VAL:HB	1:B:317:VAL:HA	2.01	0.43
1:A:24:PHE:O	1:A:28:PRO:N	2.51	0.42
1:A:96:ASP:HB3	1:A:97:PRO:HD2	2.00	0.42
1:A:194:MET:C	1:A:196:GLY:N	2.76	0.42
1:B:106:LEU:HD23	1:B:228:LEU:HD22	2.01	0.42
1:A:250:ASN:CB	1:A:289:PRO:HB3	2.45	0.42
1:A:279:ALA:HA	1:A:337:ILE:CG2	2.49	0.42
1:A:338:ARG:O	1:A:339:ARG:C	2.62	0.42
1:B:132:ASP:C	1:B:134:MET:N	2.75	0.42
1:B:382:VAL:HG23	1:B:386:GLU:OE1	2.19	0.42
1:A:280:VAL:HG21	1:A:365:ARG:CG	2.49	0.42
1:B:360:ALA:C	1:B:362:LEU:N	2.77	0.42
1:B:389:TRP:O	1:B:390:TYR:C	2.62	0.42
1:A:126:ILE:HD13	1:A:155:THR:CG2	2.49	0.42
1:B:22:GLN:O	1:B:23:ASP:C	2.62	0.42
1:B:110:GLU:CD	1:B:115:ARG:HH21	2.27	0.42
1:B:150:TRP:O	1:B:151:PRO:O	2.38	0.42
1:B:179:VAL:HG22	1:B:395:ILE:HD11	1.99	0.42
1:A:265:GLN:O	1:A:268:ALA:N	2.53	0.42
1:A:325:THR:C	1:A:327:GLU:H	2.27	0.42
1:A:398:LEU:CD1	1:A:401:LEU:HB2	2.44	0.42
1:B:225:GLY:C	1:B:227:ARG:N	2.76	0.42
1:A:149:ALA:O	1:A:153:PRO:HD2	2.20	0.42
1:A:182:ASP:H	1:A:186:GLN:CD	2.27	0.42
1:A:228:LEU:CD1	1:A:232:GLU:HB3	2.49	0.42
1:A:326:PRO:O	1:A:330:PRO:HG3	2.20	0.42
2:B:1407:HEM:HMA2	2:B:1407:HEM:HAA1	1.90	0.42
1:A:194:MET:HE3	1:A:238:HIS:HD2	1.85	0.42
1:B:45:ARG:HH11	1:B:45:ARG:HB3	1.85	0.42
1:B:98:PRO:O	1:B:99:ARG:C	2.62	0.42
1:B:336:ASP:OD1	1:B:338:ARG:HB2	2.19	0.42
1:B:389:TRP:CZ3	1:B:396:ARG:NE	2.88	0.42
1:A:22:GLN:HE22	1:A:389:TRP:H	1.67	0.42
1:A:384:PRO:HA	1:A:387:LEU:CD1	2.50	0.42
1:B:43:ARG:HG2	1:B:43:ARG:HH11	1.85	0.42
1:A:24:PHE:O	1:A:28:PRO:HD3	2.20	0.41
1:A:130:LEU:CD1	1:A:151:PRO:HB2	2.50	0.41
1:A:285:ARG:HD3	1:A:339:ARG:CD	2.46	0.41
1:B:26:ALA:HB2	1:B:389:TRP:CD1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:ARG:O	1:B:122:ARG:HG3	2.19	0.41
1:B:239:ILE:HD12	1:B:239:ILE:HA	1.90	0.41
1:B:255:GLY:C	1:B:283:MET:HE2	2.45	0.41
1:B:304:LEU:O	1:B:307:THR:N	2.53	0.41
1:A:149:ALA:HA	1:A:252:ILE:HG21	2.03	0.41
1:A:370:ALA:O	1:A:371:LEU:C	2.61	0.41
1:B:276:LEU:O	1:B:276:LEU:CD1	2.64	0.41
1:A:377:ASP:HB2	1:A:406:ARG:HA	2.02	0.41
1:B:225:GLY:O	1:B:228:LEU:N	2.35	0.41
1:B:276:LEU:HD13	1:B:276:LEU:C	2.44	0.41
1:A:259:LEU:HG	1:A:266:LEU:HD13	2.03	0.41
1:A:265:GLN:O	1:A:268:ALA:HB3	2.20	0.41
1:B:126:ILE:O	1:B:127:VAL:C	2.63	0.41
1:A:24:PHE:CZ	1:A:28:PRO:HB2	2.55	0.41
1:A:155:THR:HG23	1:A:168:ARG:NH1	2.36	0.41
1:B:348:GLY:O	1:B:349:HIS:HB2	2.19	0.41
1:B:375:CYS:HB3	1:B:378:LEU:HB2	2.02	0.41
1:A:82:THR:H	1:A:85:GLU:HB2	1.86	0.41
1:A:395:ILE:CG2	1:A:396:ARG:H	2.18	0.41
1:B:17:LEU:HD11	1:B:44:VAL:HG21	2.02	0.41
1:B:175:THR:HG23	1:B:246:GLU:CD	2.46	0.41
1:B:282:GLU:OE2	1:B:285:ARG:NH1	2.53	0.41
1:A:127:VAL:CG2	1:A:152:LEU:HD11	2.48	0.41
1:B:225:GLY:HA2	1:B:228:LEU:O	2.21	0.41
1:A:65:LEU:HD12	1:A:345:LEU:HD13	2.02	0.41
1:A:141:ARG:HG2	1:A:381:ASP:OD1	2.21	0.41
1:A:319:LEU:CD2	1:A:345:LEU:HB2	2.50	0.41
1:B:171:PHE:HA	1:B:174:TRP:HE3	1.85	0.41
1:B:179:VAL:HG22	1:B:395:ILE:HD13	1.98	0.41
1:B:181:PRO:O	1:B:182:ASP:C	2.63	0.41
1:B:228:LEU:HD12	1:B:232:GLU:HB3	2.01	0.41
1:B:248:THR:C	1:B:250:ASN:N	2.78	0.41
1:A:14:VAL:HA	1:A:43:ARG:O	2.21	0.41
1:A:67:ASP:O	1:A:68:PRO:C	2.64	0.41
1:A:150:TRP:O	1:A:153:PRO:HD2	2.21	0.41
1:A:156:VAL:HG12	1:A:160:LEU:HD12	2.02	0.41
1:A:158:SER:C	1:A:160:LEU:H	2.28	0.41
1:A:191:MET:O	1:A:195:SER:HB3	2.21	0.41
1:A:236:MET:O	1:A:237:ALA:C	2.63	0.41
1:A:380:LEU:C	1:A:382:VAL:H	2.28	0.41
2:A:1407:HEM:HMA2	2:A:1407:HEM:HAA1	1.81	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:TYR:CE2	1:B:318:VAL:HG11	2.55	0.41
1:B:43:ARG:HH12	1:B:51:GLU:CB	2.34	0.41
1:B:46:THR:HG23	1:B:52:VAL:HG22	2.03	0.41
1:B:74:TRP:CD1	1:B:89:ASN:HD22	2.39	0.41
1:B:282:GLU:CD	1:B:339:ARG:HD2	2.46	0.41
1:A:273:MET:CE	1:A:369:ARG:HG3	2.50	0.41
1:A:294:THR:HA	1:A:394:MET:HE3	2.03	0.41
1:B:254:ASN:HD21	1:B:396:ARG:HG3	1.86	0.41
1:A:234:LEU:O	1:A:235:GLY:C	2.64	0.40
1:A:352:HIS:O	1:A:353:PHE:C	2.64	0.40
1:A:406:ARG:HH11	1:A:406:ARG:CB	2.31	0.40
1:B:260:LEU:HB3	1:B:380:LEU:HG	2.03	0.40
1:A:120:ARG:CB	1:A:121:PRO:HD3	2.50	0.40
1:A:124:GLN:NE2	1:A:124:GLN:HA	2.35	0.40
1:B:150:TRP:O	1:B:151:PRO:C	2.63	0.40
1:B:229:THR:HG23	1:B:232:GLU:CD	2.46	0.40
1:A:45:ARG:HH21	1:A:49:GLY:CA	2.33	0.40
1:A:334:ARG:NE	1:A:334:ARG:HA	2.36	0.40
1:A:361:ARG:O	1:A:362:LEU:C	2.65	0.40
1:B:95:SER:HB2	1:B:99:ARG:HD2	2.04	0.40
1:B:198:LEU:HD13	1:B:237:ALA:HB1	2.03	0.40
1:A:82:THR:HA	1:B:146:GLU:OE1	2.22	0.40
1:A:380:LEU:CD2	1:A:401:LEU:HD11	2.51	0.40
1:B:132:ASP:O	1:B:135:LEU:N	2.54	0.40
1:B:157:ILE:CG2	1:B:158:SER:N	2.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	391/436 (90%)	285 (73%)	77 (20%)	29 (7%)	1 1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	391/436 (90%)	277 (71%)	78 (20%)	36 (9%)	0 0
All	All	782/872 (90%)	562 (72%)	155 (20%)	65 (8%)	0 1

All (65) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	98	PRO
1	A	99	ARG
1	A	149	ALA
1	A	242	VAL
1	A	243	ALA
1	A	351	ILE
1	A	376	PRO
1	B	38	GLU
1	B	127	VAL
1	B	149	ALA
1	B	151	PRO
1	B	152	LEU
1	B	228	LEU
1	B	243	ALA
1	B	270	ARG
1	B	300	GLU
1	B	384	PRO
1	A	109	ARG
1	A	114	ARG
1	A	311	ALA
1	A	337	ILE
1	A	339	ARG
1	A	370	ALA
1	B	126	ILE
1	B	148	LEU
1	B	305	ASP
1	B	327	GLU
1	B	382	VAL
1	A	47	PRO
1	A	144	LEU
1	A	184	PRO
1	A	305	ASP
1	A	377	ASP
1	B	125	GLU
1	B	139	ASP
1	B	175	THR

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Mol	Chain	Res	Type
1	B	245	HIS
1	B	341	THR
1	B	354	CYS
1	B	361	ARG
1	A	85	GLU
1	A	193	GLU
1	A	293	ALA
1	A	364	ALA
1	A	382	VAL
1	B	69	ARG
1	B	168	ARG
1	B	358	PRO
1	B	376	PRO
1	A	106	LEU
1	A	244	GLY
1	A	371	LEU
1	B	40	PRO
1	B	80	PRO
1	B	144	LEU
1	B	164	PRO
1	B	268	ALA
1	A	330	PRO
1	B	153	PRO
1	B	185	ALA
1	B	242	VAL
1	B	299	VAL
1	A	49	GLY
1	B	184	PRO
1	A	331	ASP

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	313/355 (88%)	281 (90%)	32 (10%)	7 15
1	B	313/355 (88%)	279 (89%)	34 (11%)	6 12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	626/710 (88%)	560 (90%)	66 (10%)	6 13

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	LEU
1	A	44	VAL
1	A	45	ARG
1	A	46	THR
1	A	47	PRO
1	A	59	ASP
1	A	77	SER
1	A	89	ASN
1	A	94	GLU
1	A	101	THR
1	A	106	LEU
1	A	110	GLU
1	A	132	ASP
1	A	151	PRO
1	A	157	ILE
1	A	159	GLU
1	A	160	LEU
1	A	164	PRO
1	A	175	THR
1	A	184	PRO
1	A	215	SER
1	A	223	GLU
1	A	285	ARG
1	A	313	ASP
1	A	314	THR
1	A	330	PRO
1	A	334	ARG
1	A	345	LEU
1	A	351	ILE
1	A	384	PRO
1	A	395	ILE
1	A	406	ARG
1	B	45	ARG
1	B	64	VAL
1	B	89	ASN
1	B	101	THR
1	B	104	ARG

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Mol	Chain	Res	Type
1	B	116	VAL
1	B	139	ASP
1	B	151	PRO
1	B	152	LEU
1	B	178	PHE
1	B	189	THR
1	B	198	LEU
1	B	203	ASP
1	B	223	GLU
1	B	233	LEU
1	B	238	HIS
1	B	240	LEU
1	B	242	VAL
1	B	247	THR
1	B	254	ASN
1	B	270	ARG
1	B	272	ASP
1	B	276	LEU
1	B	277	ASP
1	B	285	ARG
1	B	297	PHE
1	B	318	VAL
1	B	334	ARG
1	B	339	ARG
1	B	362	LEU
1	B	369	ARG
1	B	384	PRO
1	B	386	GLU
1	B	406	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	76	ASN
1	A	89	ASN
1	A	100	HIS
1	A	333	HIS
1	A	344	HIS
1	A	349	HIS
1	B	89	ASN
1	B	188	GLN

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Mol	Chain	Res	Type
1	B	254	ASN
1	B	262	HIS
1	B	265	GLN
1	B	344	HIS
1	B	349	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

4 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	$\#\|Z\| > 2$
2	HEM	B	1407	-	50,50,50	1.48	4 (8%)	66,82,82	1.32	6 (9%)
2	HEM	A	1407	-	50,50,50	1.41	9 (18%)	66,82,82	1.45	9 (13%)
3	PXI	B	1408	-	33,33,33	1.94	6 (18%)	40,47,47	2.04	9 (22%)
3	PXI	A	1408	-	33,33,33	2.07	7 (21%)	40,47,47	1.85	10 (25%)

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	HEM	B	1407	-	-	8/14/54/54	-
2	HEM	A	1407	-	-	10/14/54/54	-
3	PXI	B	1408	-	-	19/43/59/59	0/1/2/2
3	PXI	A	1408	-	-	14/43/59/59	0/1/2/2

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1408	PXI	C16-C7	6.32	1.64	1.53
3	A	1408	PXI	C19-C21	5.87	1.61	1.51
3	A	1408	PXI	C16-C7	5.44	1.63	1.53
3	B	1408	PXI	C19-C21	4.07	1.58	1.51
3	B	1408	PXI	C24-C3	3.98	1.63	1.53
3	A	1408	PXI	C15-C12	3.78	1.61	1.53
2	B	1407	HEM	CBC-CAC	3.76	1.48	1.30
3	A	1408	PXI	C24-C3	3.69	1.62	1.53
2	B	1407	HEM	CAB-C3B	-3.61	1.37	1.47
2	A	1407	HEM	CBB-CAB	3.28	1.46	1.30
2	A	1407	HEM	CAB-C3B	-3.16	1.38	1.47
2	B	1407	HEM	CBB-CAB	3.05	1.45	1.30
2	A	1407	HEM	CAC-C3C	-3.02	1.39	1.47
3	B	1408	PXI	C11-C9	2.95	1.57	1.51
2	A	1407	HEM	C4D-C3D	2.95	1.50	1.45
3	B	1408	PXI	C15-C12	2.91	1.59	1.53
2	A	1407	HEM	C2A-C3A	-2.88	1.31	1.38
2	B	1407	HEM	FE-NA	2.63	2.04	1.95
2	A	1407	HEM	CMD-C2D	2.58	1.56	1.50
2	A	1407	HEM	CBC-CAC	2.56	1.43	1.30
3	A	1408	PXI	O3-C7	2.35	1.50	1.43
2	A	1407	HEM	FE-NC	2.25	2.02	1.95
3	A	1408	PXI	O4-C9	2.20	1.48	1.44
3	A	1408	PXI	O3-C8	2.17	1.47	1.41
3	B	1408	PXI	O4-C9	2.09	1.48	1.44
2	A	1407	HEM	O2A-CGA	-2.01	1.24	1.30

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1408	PXI	C3-O1-C4	7.97	129.85	117.89
3	A	1408	PXI	C3-O1-C4	7.11	128.56	117.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1407	HEM	CAA-C2A-C1A	5.23	135.18	124.89
3	B	1408	PXI	O3-C7-C5	-4.96	102.51	111.14
2	B	1407	HEM	CBD-CAD-C3D	4.43	124.94	112.63
2	A	1407	HEM	CAD-C3D-C4D	4.19	131.99	124.66
2	A	1407	HEM	CAA-C2A-C3A	-3.78	118.41	127.07
3	A	1408	PXI	O3-C7-C5	-3.53	104.99	111.14
2	B	1407	HEM	CAA-C2A-C1A	3.46	131.69	124.89
2	B	1407	HEM	CAA-C2A-C3A	-3.29	119.52	127.07
3	A	1408	PXI	O1-C3-C2	3.23	112.09	106.92
2	B	1407	HEM	CMA-C3A-C4A	3.22	130.28	125.37
2	A	1407	HEM	CAD-C3D-C2D	-3.06	122.18	127.88
3	B	1408	PXI	O1-C3-C2	3.00	111.72	106.92
3	B	1408	PXI	C10-C9-C11	-2.98	108.72	113.40
3	B	1408	PXI	C6-C5-C7	-2.84	106.48	112.92
3	A	1408	PXI	C10-C9-C11	-2.81	108.99	113.40
3	B	1408	PXI	C7-C5-C4	2.77	115.68	110.01
3	A	1408	PXI	C7-C5-C4	2.73	115.59	110.01
2	A	1407	HEM	C4A-C3A-C2A	2.70	109.98	106.83
2	A	1407	HEM	CHD-C1D-C2D	-2.66	120.82	124.98
2	B	1407	HEM	CBA-CAA-C2A	2.64	119.95	112.63
2	B	1407	HEM	CAD-C3D-C4D	2.55	129.11	124.66
3	B	1408	PXI	C25-C24-C23	-2.34	104.33	109.99
3	A	1408	PXI	C19-C21-C22	2.30	124.06	118.29
2	A	1407	HEM	CHD-C4C-NC	-2.26	121.99	124.44
2	A	1407	HEM	CAC-C3C-C4C	2.17	130.13	124.90
3	A	1408	PXI	C17-C16-C7	2.14	114.65	111.15
3	B	1408	PXI	C11-C12-C15	-2.12	106.91	109.97
3	A	1408	PXI	C9-C11-C12	-2.10	106.79	110.46
2	A	1407	HEM	CBD-CAD-C3D	2.09	118.44	112.63
3	A	1408	PXI	C25-C24-C23	-2.07	105.00	109.99
3	A	1408	PXI	C6-C5-C7	-2.06	108.24	112.92
3	B	1408	PXI	C13-N1-C12	-2.00	107.09	113.11

There are no chirality outliers.

All (51) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1407	HEM	C1A-C2A-CAA-CBA
2	A	1407	HEM	C2B-C3B-CAB-CBB
2	A	1407	HEM	C4B-C3B-CAB-CBB
2	B	1407	HEM	C2C-C3C-CAC-CBC
3	A	1408	PXI	C11-C12-N1-C13

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Mol	Chain	Res	Type	Atoms
3	A	1408	PXI	C11-C12-N1-C14
3	A	1408	PXI	C7-C16-C18-C19
3	A	1408	PXI	C16-C18-C19-C20
3	A	1408	PXI	C16-C18-C19-C21
3	B	1408	PXI	C23-C24-C3-O1
3	B	1408	PXI	C18-C16-C7-O3
3	B	1408	PXI	C11-C12-N1-C13
3	B	1408	PXI	C11-C12-N1-C14
3	B	1408	PXI	C7-C16-C18-C19
3	A	1408	PXI	O4-C8-O3-C7
3	B	1408	PXI	O4-C8-O3-C7
2	A	1407	HEM	C4D-C3D-CAD-CBD
2	B	1407	HEM	C4D-C3D-CAD-CBD
3	A	1408	PXI	C22-C23-C24-C25
3	B	1408	PXI	C22-C23-C24-C25
2	A	1407	HEM	C2D-C3D-CAD-CBD
2	B	1407	HEM	C2D-C3D-CAD-CBD
3	A	1408	PXI	C15-C12-N1-C13
3	B	1408	PXI	C4-C5-C7-C16
3	B	1408	PXI	C15-C12-N1-C13
3	A	1408	PXI	O6-C21-C22-C23
3	B	1408	PXI	O6-C21-C22-C23
2	B	1407	HEM	C4C-C3C-CAC-CBC
3	B	1408	PXI	C6-C5-C7-O3
3	B	1408	PXI	C17-C16-C18-C19
3	A	1408	PXI	C19-C21-C22-C23
3	B	1408	PXI	C19-C21-C22-C23
3	B	1408	PXI	C16-C18-C19-C21
3	B	1408	PXI	C25-C24-C3-O1
2	A	1407	HEM	C3A-C2A-CAA-CBA
3	B	1408	PXI	C23-C24-C3-C2
3	B	1408	PXI	C17-C16-C7-O3
3	A	1408	PXI	C25-C24-C3-O1
3	B	1408	PXI	C25-C24-C3-C2
3	B	1408	PXI	C17-C16-C7-C5
3	A	1408	PXI	C17-C16-C18-C19
3	A	1408	PXI	C15-C12-N1-C14
2	A	1407	HEM	CAD-CBD-CGD-O2D
2	A	1407	HEM	CAA-CBA-CGA-O2A
2	A	1407	HEM	CAD-CBD-CGD-O1D
3	A	1408	PXI	C5-C4-O1-C3
2	B	1407	HEM	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
2	A	1407	HEM	CAA-CBA-CGA-O1A
2	B	1407	HEM	CAA-CBA-CGA-O2A
2	B	1407	HEM	CAD-CBD-CGD-O1D
2	B	1407	HEM	CAA-CBA-CGA-O1A

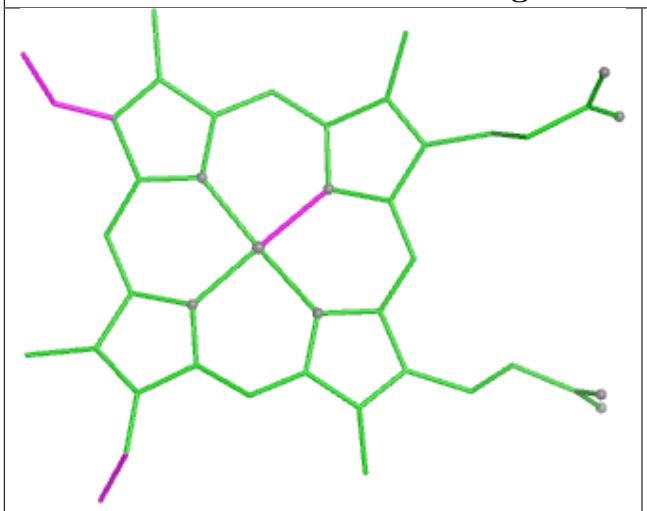
There are no ring outliers.

4 monomers are involved in 18 short contacts:

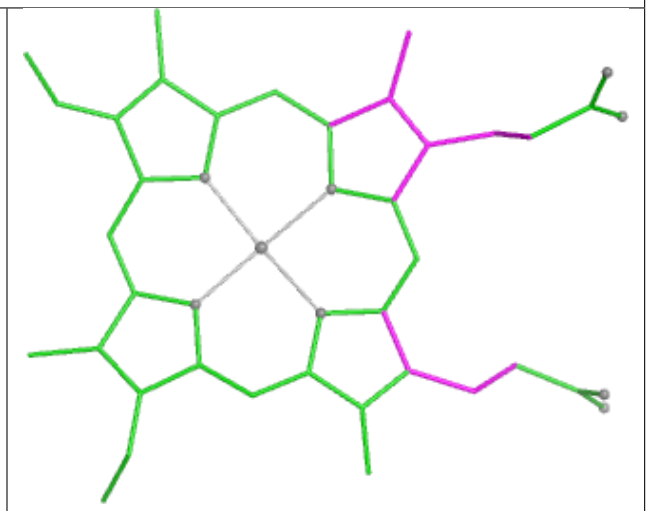
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1407	HEM	5	0
2	A	1407	HEM	3	0
3	B	1408	PXI	8	0
3	A	1408	PXI	2	0

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.

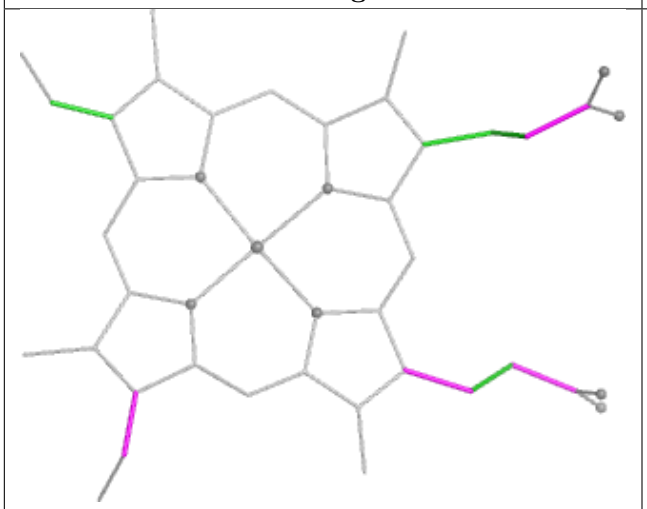
Ligand HEM B 1407



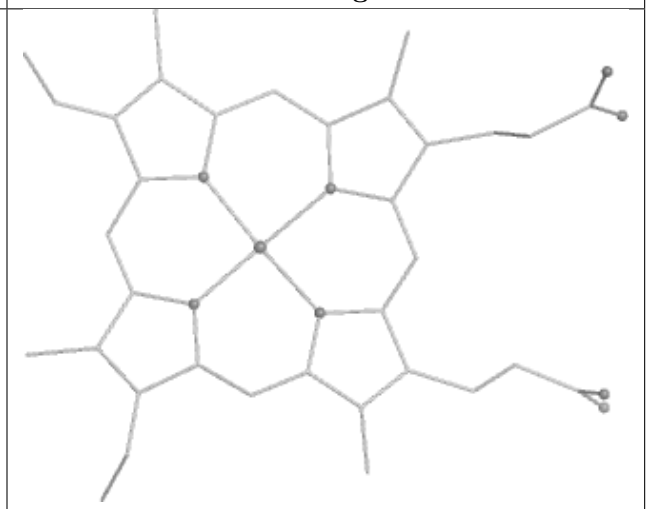
Bond lengths



Bond angles

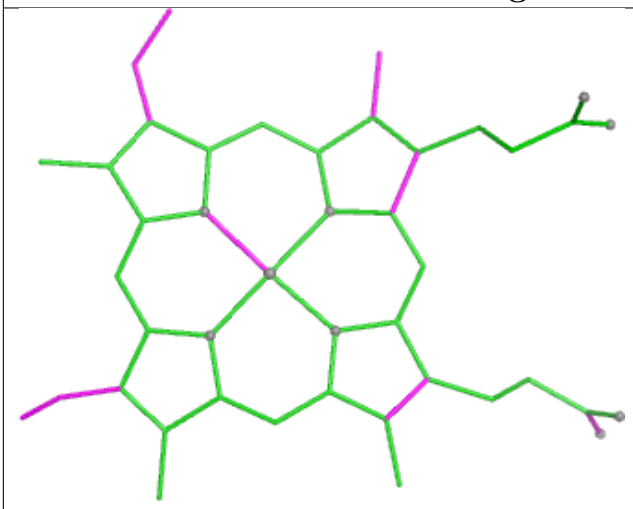


Torsions

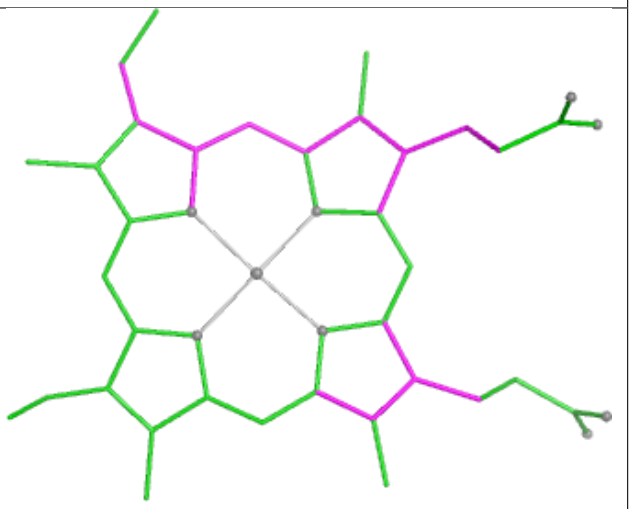


Rings

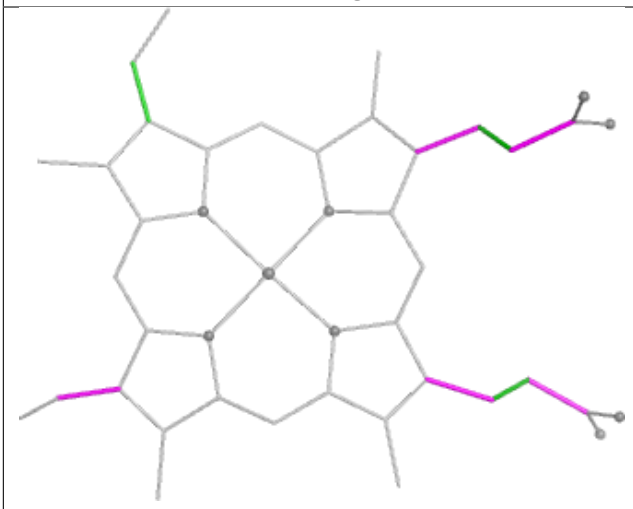
Ligand HEM A 1407



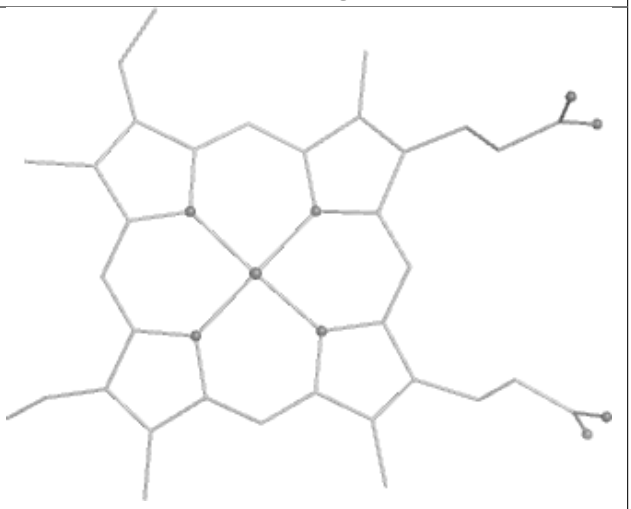
Bond lengths



Bond angles

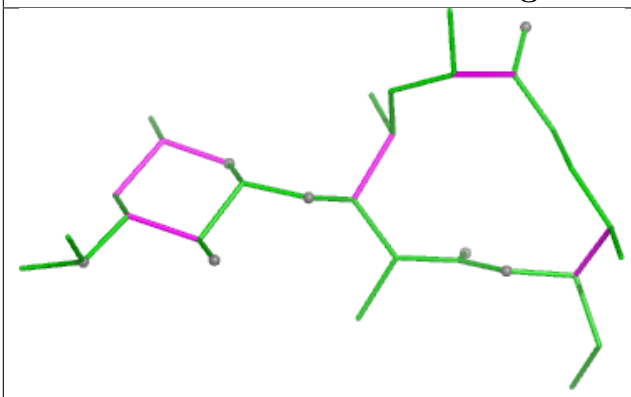


Torsions

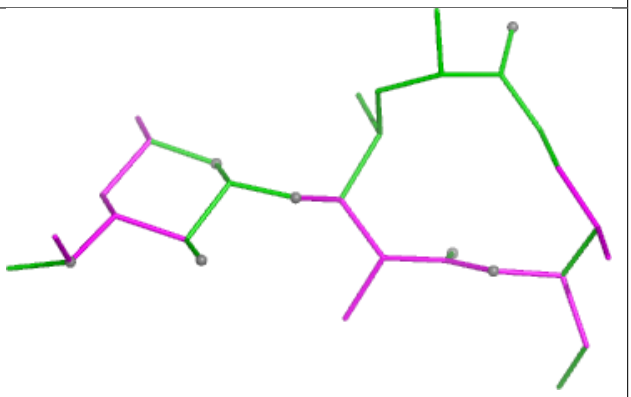


Rings

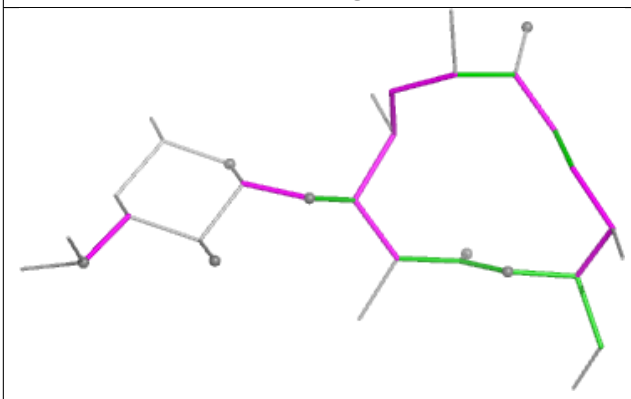
Ligand PXI B 1408



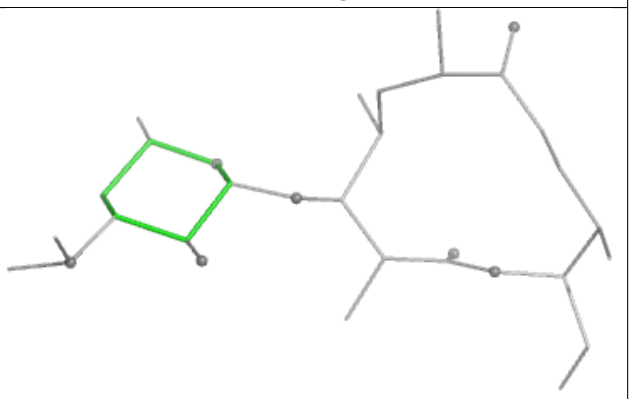
Bond lengths



Bond angles

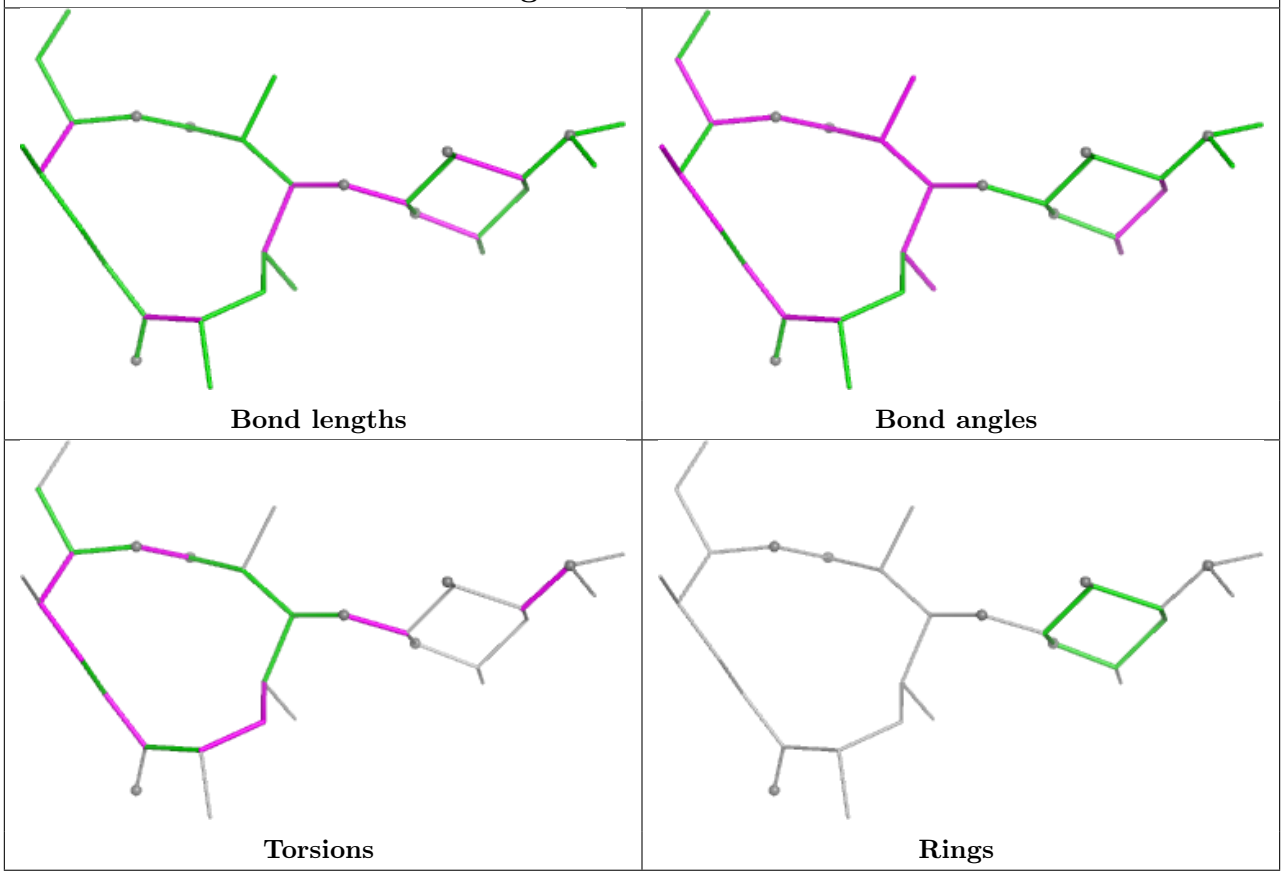


Torsions



Rings

Ligand PXI A 1408



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	393/436 (90%)	-1.37	0	100	100	4, 23, 37, 48	0
1	B	393/436 (90%)	-1.38	0	100	100	5, 22, 39, 46	0
All	All	786/872 (90%)	-1.37	0	100	100	4, 23, 38, 48	0

There are no RSRZ outliers to report.

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)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

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

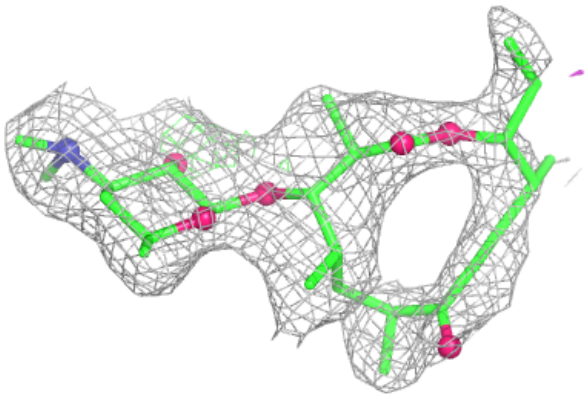
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	PXI	A	1408	32/32	0.98	0.06	27,31,32,35	0
2	HEM	B	1407	43/43	0.99	0.03	3,6,12,19	0
2	HEM	A	1407	43/43	0.99	0.04	3,4,12,15	0
3	PXI	B	1408	32/32	0.99	0.04	28,31,33,34	0

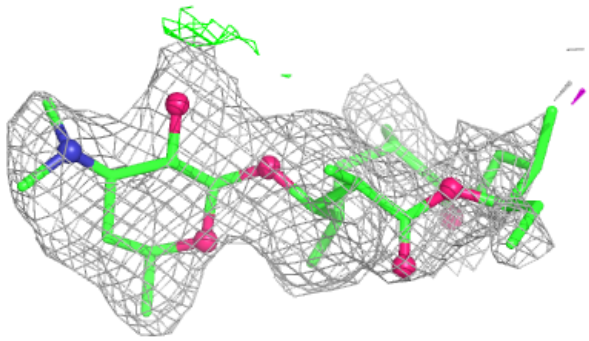
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

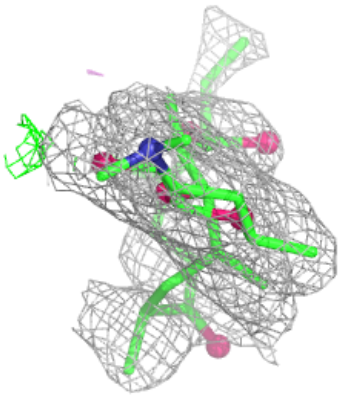
as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around PXI A 1408:

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

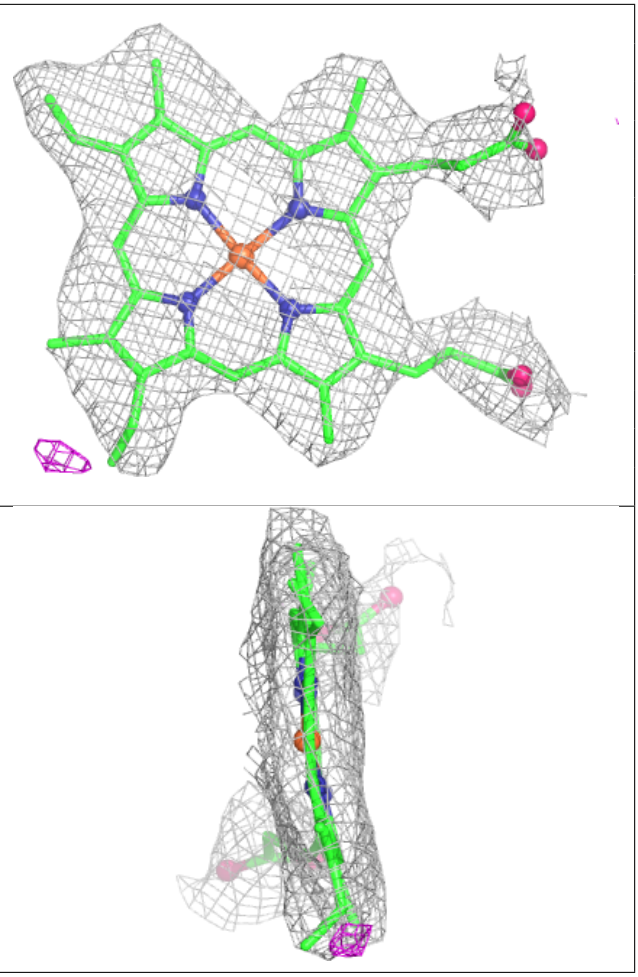






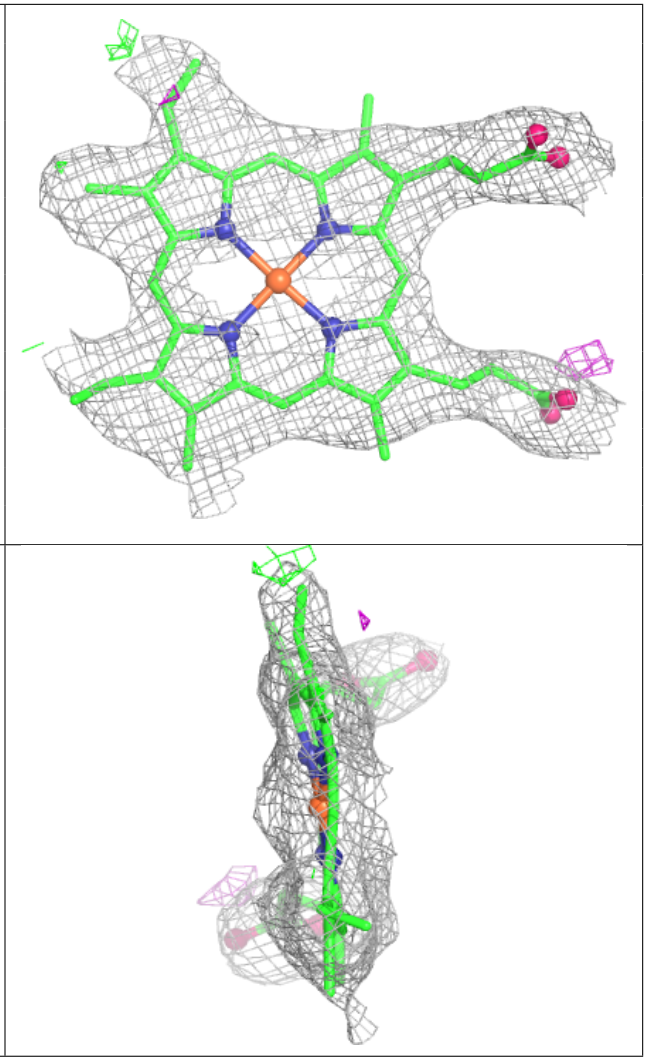
Electron density around HEM B 1407:

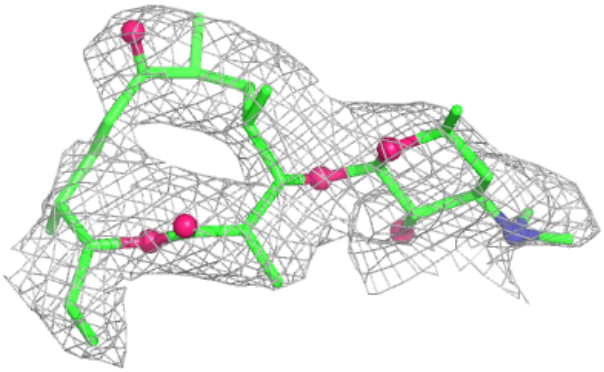
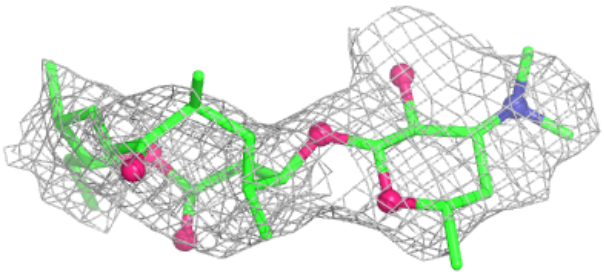
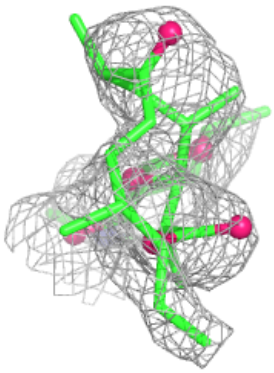
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM A 1407:

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



Electron density around PXI B 1408: 2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)	
	

6.5 Other polymers (i)

There are no such residues in this entry.