Full wwPDB X-ray Structure Validation Report ⓘ

Jan 4, 2024 – 06:24 am GMT

PDB ID	:	4UYL
Title	:	Crystal structure of sterol 14-alpha demethylase (CYP51B) from a pathogenic filamentous fungus Aspergillus fumigatus in complex with VNI
Authors	:	Hargrove, T.Y.; Wawrzak, Z.; Lepesheva, G.I.
Deposited on	:	2014-09-01
Resolution	:	2.81 Å(reported)

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

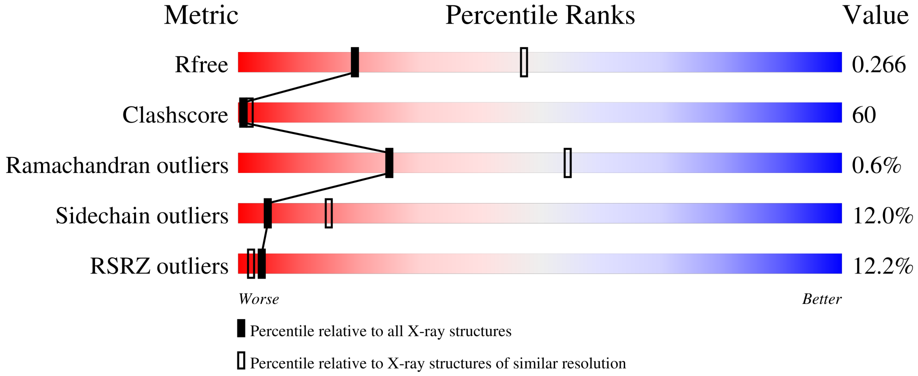
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance ⓘ

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

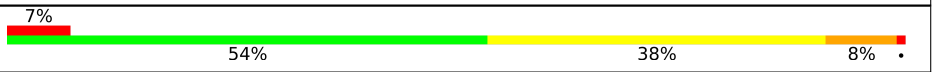
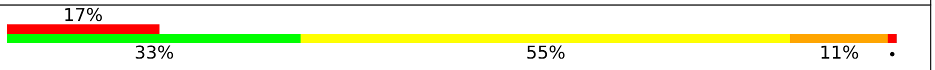
The reported resolution of this entry is 2.81 Å.

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



Metric	**Whole archive (#Entries)**	**Similar resolution (#Entries, resolution range(Å))**
R_{free}	130704	3617 (2.84-2.80)
Clashscore	141614	4060 (2.84-2.80)
Ramachandran outliers	138981	3978 (2.84-2.80)
Sidechain outliers	138945	3980 (2.84-2.80)
RSRZ outliers	127900	3552 (2.84-2.80)

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

Mol	**Chain**	**Length**	**Quality of chain**
1	A	470	
1	B	470	

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
3	VNI	B	590	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7788 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.

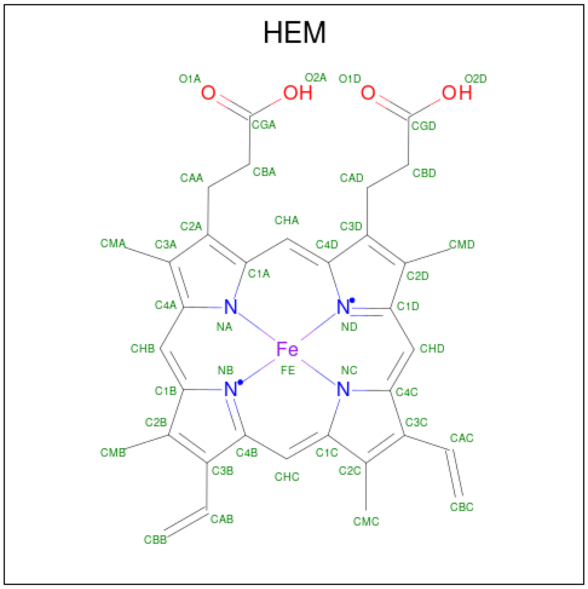
- Molecule 1 is a protein called 14-ALPHA STEROL DEMETHYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	470	Total	C	N	O	S	0	0	0
			3752	2411	639	685	17			
1	B	470	Total	C	N	O	S	0	0	0
			3752	2411	639	685	17			

There are 6 discrepancies between the modelled and reference sequences:

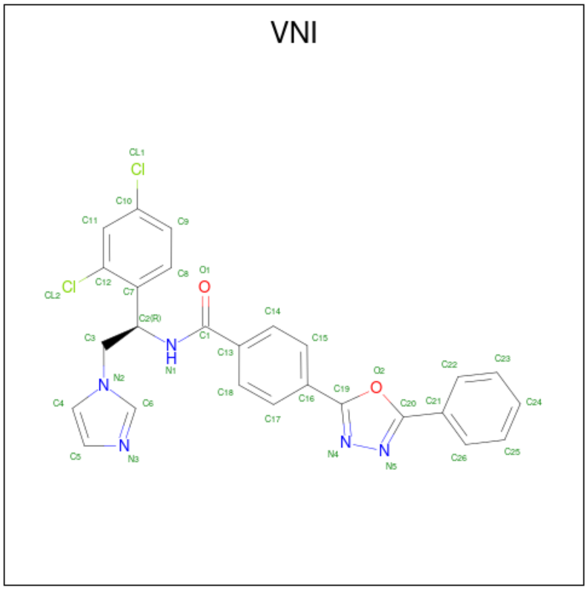
Chain	Residue	Modelled	Actual	Comment	Reference
A	50	LYS	HIS	engineered mutation	UNP Q96W81
A	51	THR	GLU	engineered mutation	UNP Q96W81
A	519	HIS	-	expression tag	UNP Q96W81
B	50	LYS	HIS	engineered mutation	UNP Q96W81
B	51	THR	GLU	engineered mutation	UNP Q96W81
B	519	HIS	-	expression tag	UNP Q96W81

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



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

- Molecule 3 is N-[(1R)-1-(2,4-dichlorophenyl)-2-(1H-imidazol-1-yl)ethyl]-4-(5-phenyl-1,3,4-oxadiazol-2-yl)benzamide (three-letter code: VNI) (formula: $C_{26}H_{19}Cl_2N_5O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C Cl N O 35 26 2 5 2	0	0
3	B	1	Total C Cl N O 35 26 2 5 2	0	0

- Molecule 4 is water.

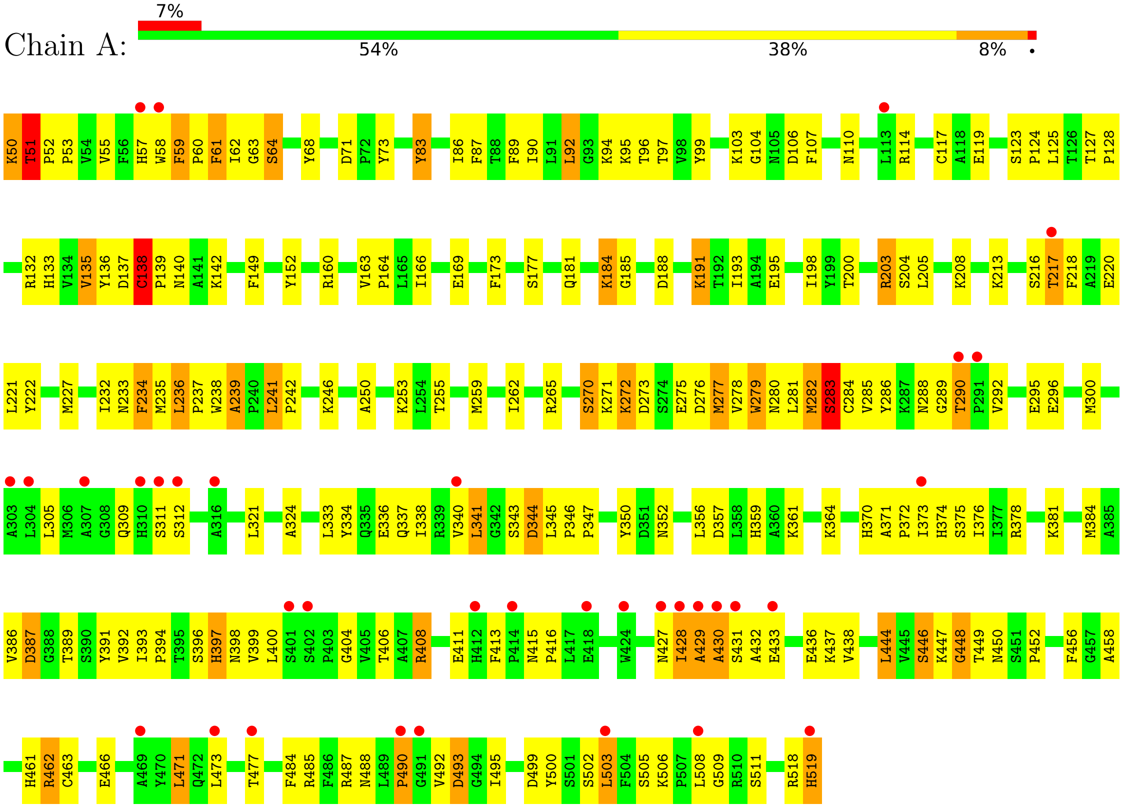
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	85	Total O 85 85	0	0
4	B	43	Total O 43 43	0	0

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.

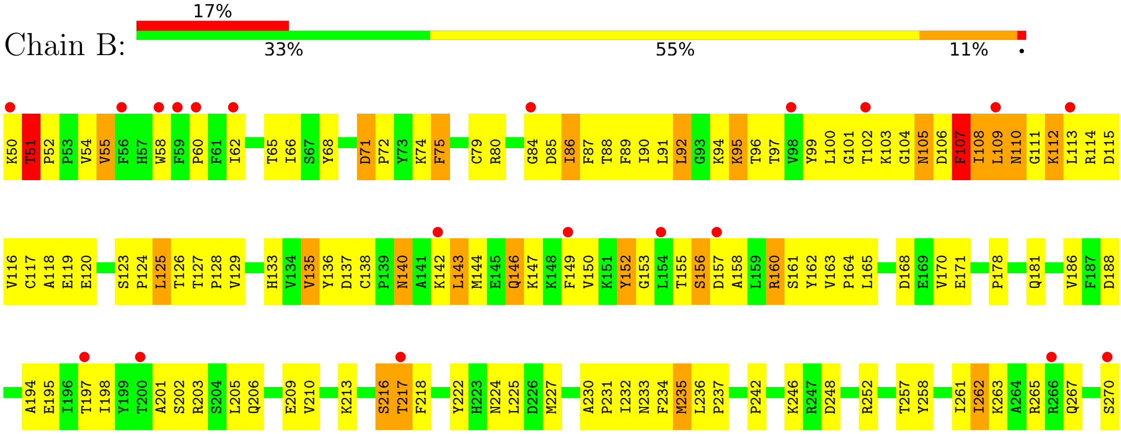
- Molecule 1: 14-ALPHA STEROL DEMETHYLASE

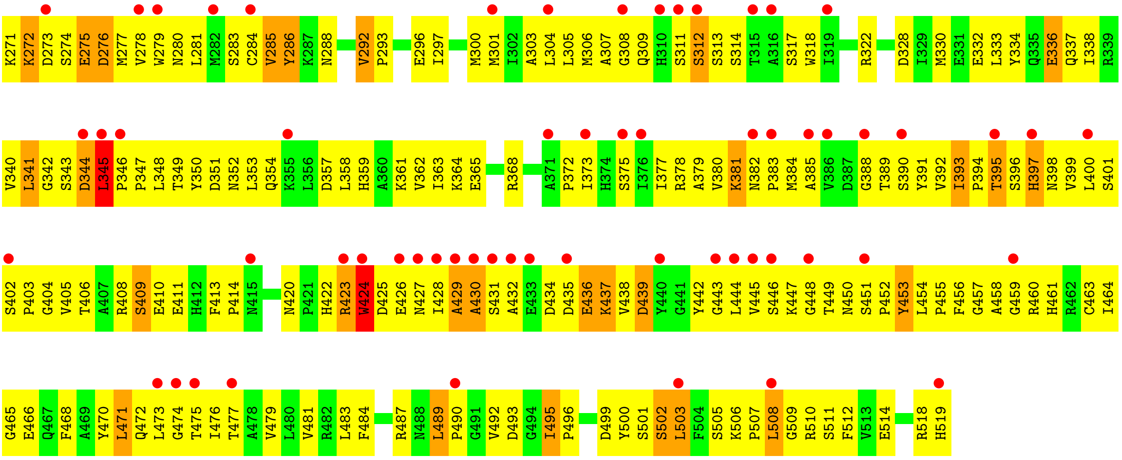
Chain A:



- Molecule 1: 14-ALPHA STEROL DEMETHYLASE

Chain B:




K271 K272 D273 S274 E275 D276 M277 V278 W279 N280 L281 M282 S283 C284 V285 Y286 K287 N288 V292 P293 E296 I297 M300 M301 I302 A303 L304 L305 M306 A307 G308 Q309 H310 S311 S312 S313 S314 T315 A316 S317 W318 I319 R322 D328 I329 M330 E331 E332 L333 Y334 Q335 E336 Q337 I338 R339
V340 L341 G342 S343 D344 L345 P346 P347 L348 T349 Y350 D351 N352 L353 Q354 K355 L356 D357 L358 H359 A360 K361 V362 I363 K364 E365 R368 A371 P372 I373 H374 S375 I376 I377 R378 A379 V380 K381 N382 P383 M384 A385 V386 D387 G388 T389 S390 Y391 V392 I393 P394 T395 S396 H397 N398 V399 L400 S401
S402 P403 G404 V405 T406 A407 R408 S409 E410 E411 H412 F413 P414 N415 N420 P421 H422 R423 W424 D425 E426 N427 I428 A429 A430 S431 A432 E433 D434 D435 E436 K437 V438 D439 Y440 G441 Y442 G443 L444 V445 S446 K447 G448 T449 N450 S451 P452 Y453 L454 P455 F456 G457 A458 G459 R460 H461 R462 C463 I464
G465 E466 Q467 F468 A469 Y470 L471 Q472 L473 G474 T475 I476 T477 A478 V479 L480 V481 R482 L483 F484 R487 N488 L489 P490 G491 V492 D493 G494 I495 P496 D499 Y500 S501 S502 L503 F504 S505 K506 P507 L508 G509 R510 S511 F512 V513 E514 R518 H519

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α, β, γ	110.50Å 110.50Å 90.48Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	95.69 – 2.81 28.76 – 2.81	Depositor EDS
% Data completeness (in resolution range)	99.7 (95.69-2.81) 99.7 (28.76-2.81)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.89 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.237 , 0.279 0.243 , 0.266	Depositor DCC
R_{free} test set	1491 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	85.8	Xtriage
Anisotropy	0.019	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 83.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.007 for -h,-k,l 0.026 for h,-h-k,-l 0.012 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	7788	wwPDB-VP
Average B, all atoms (Å^2)	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.31% 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: VNI, 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	0.36	0/3854	0.63	6/5229 (0.1%)
1	B	0.32	0/3854	0.66	5/5229 (0.1%)
All	All	0.34	0/7708	0.64	11/10458 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	9
1	B	0	3
All	All	0	12

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	448	GLY	N-CA-C	-8.80	91.09	113.10
1	B	430	ALA	N-CA-CB	6.97	119.86	110.10
1	B	107	PHE	CB-CA-C	-6.62	97.16	110.40
1	A	283	SER	N-CA-C	-6.20	94.25	111.00
1	A	448	GLY	N-CA-C	-6.05	97.98	113.10
1	A	138	CYS	C-N-CD	-5.59	108.30	120.60
1	A	282	MET	CB-CA-C	-5.39	99.62	110.40
1	A	239	ALA	C-N-CD	5.27	139.46	128.40
1	B	71	ASP	C-N-CD	5.15	139.22	128.40
1	B	345	LEU	C-N-CD	5.14	139.21	128.40
1	A	430	ALA	N-CA-C	-5.14	97.12	111.00

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	270	SER	Peptide
1	A	272	LYS	Peptide
1	A	273	ASP	Peptide
1	A	279	TRP	Mainchain
1	A	429	ALA	Peptide
1	A	446	SER	Peptide
1	A	484	PHE	Peptide
1	A	490	PRO	Peptide
1	A	509	GLY	Peptide
1	B	105	ASN	Peptide
1	B	424	TRP	Peptide
1	B	429	ALA	Peptide

5.2 Too-close contacts ⓘ

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	3752	0	3719	322	0
1	B	3752	0	3719	581	0
2	A	43	0	30	10	0
2	B	43	0	30	15	0
3	A	35	0	19	2	0
3	B	35	0	19	11	0
4	A	85	0	0	19	0
4	B	43	0	0	8	0
All	All	7788	0	7536	909	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 60.

All (909) 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:108:ILE:CD1	1:B:109:LEU:H	1.38	1.34

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
1:B:222:TYR:CE1	1:B:305:LEU:HD23	1.65	1.31
1:B:427:ASN:ND2	1:B:432:ALA:HB3	1.49	1.27
1:B:384:MET:O	1:B:392:VAL:HG23	1.32	1.25
1:B:384:MET:HB2	1:B:393:ILE:CD1	1.67	1.24
1:B:109:LEU:HD22	1:B:110:ASN:ND2	1.50	1.24
1:B:394:PRO:HD2	1:B:397:HIS:CD2	1.73	1.24
1:B:103:LYS:O	1:B:106:ASP:HB2	1.34	1.23
1:B:109:LEU:CD1	1:B:449:THR:HG21	1.69	1.22
1:B:109:LEU:HG	1:B:458:ALA:O	1.33	1.22
1:B:109:LEU:C	1:B:109:LEU:HD23	1.47	1.22
1:B:262:ILE:HG23	1:B:281:LEU:CD2	1.71	1.21
1:B:307:ALA:HA	3:B:590:VNI:CL2	1.79	1.19
1:B:430:ALA:HB1	1:B:466:GLU:OE2	1.40	1.18
1:A:152:TYR:HB3	1:A:279:TRP:CZ2	1.78	1.18
1:B:307:ALA:CA	3:B:590:VNI:CL2	2.29	1.17
1:B:51:THR:HB	1:B:52:PRO:HD3	1.18	1.16
1:B:108:ILE:HD13	1:B:109:LEU:H	1.00	1.16
1:B:51:THR:HB	1:B:52:PRO:CD	1.75	1.16
1:B:222:TYR:CE1	1:B:305:LEU:CD2	2.27	1.16
1:A:386:VAL:HG23	1:A:391:TYR:O	1.44	1.16
1:B:109:LEU:C	1:B:109:LEU:CD2	2.14	1.16
1:B:222:TYR:CZ	1:B:305:LEU:CD2	2.30	1.14
1:B:109:LEU:HD13	1:B:449:THR:HG21	1.28	1.14
1:A:447:LYS:C	1:A:449:THR:HG23	1.69	1.14
1:B:109:LEU:HD22	1:B:110:ASN:N	1.63	1.13
1:A:492:VAL:HG12	1:B:510:ARG:NH2	1.62	1.13
1:B:109:LEU:CD2	1:B:110:ASN:HD22	1.62	1.12
1:B:51:THR:HA	1:B:391:TYR:CD2	1.84	1.11
1:B:55:VAL:HG21	1:B:89:PHE:HB3	1.25	1.10
1:B:262:ILE:HG23	1:B:281:LEU:HD21	1.20	1.10
1:B:110:ASN:HA	1:B:447:LYS:CE	1.80	1.10
1:B:307:ALA:N	3:B:590:VNI:CL2	2.22	1.09
1:B:109:LEU:CD2	1:B:110:ASN:N	2.15	1.09
1:A:276:ASP:O	1:A:279:TRP:HB3	1.51	1.09
1:B:99:TYR:CE1	1:B:104:GLY:HA2	1.87	1.08
1:B:108:ILE:HD13	1:B:109:LEU:N	1.68	1.08
1:B:384:MET:C	1:B:392:VAL:HG23	1.72	1.07
1:B:393:ILE:HG22	1:B:397:HIS:CE1	1.89	1.07
1:B:108:ILE:CD1	1:B:109:LEU:N	2.18	1.06
1:B:110:ASN:HA	1:B:447:LYS:HE3	1.35	1.06
1:B:394:PRO:HD2	1:B:397:HIS:NE2	1.70	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:205:LEU:HD23	1:B:468:PHE:CZ	1.90	1.06
1:B:114:ARG:O	1:B:381:LYS:HD2	1.57	1.05
1:B:393:ILE:CG2	1:B:397:HIS:CE1	2.40	1.05
1:B:384:MET:HB2	1:B:393:ILE:HD13	1.36	1.04
1:A:492:VAL:CG1	1:B:510:ARG:NH2	2.20	1.04
1:B:410:GLU:HA	1:B:413:PHE:O	1.58	1.04
1:B:153:GLY:HA2	1:B:279:TRP:HE1	1.17	1.03
1:B:262:ILE:CG2	1:B:281:LEU:CD2	2.37	1.02
1:B:389:THR:HG22	1:B:390:SER:H	1.18	1.02
1:B:393:ILE:HD12	1:B:393:ILE:H	1.23	1.02
1:A:428:ILE:HD12	1:A:429:ALA:N	1.75	1.01
1:A:58:TRP:HB2	1:A:59:PHE:CD1	1.95	1.00
1:B:394:PRO:CD	1:B:397:HIS:CD2	2.42	1.00
1:B:427:ASN:ND2	1:B:432:ALA:CB	2.23	1.00
1:B:99:TYR:HD1	1:B:104:GLY:O	1.41	0.99
1:B:66:ILE:HD12	1:B:66:ILE:H	1.20	0.99
1:B:384:MET:HB2	1:B:393:ILE:HD11	1.41	0.99
1:A:138:CYS:HB2	1:A:139:PRO:HD2	1.43	0.99
1:B:108:ILE:HD12	1:B:109:LEU:H	1.28	0.98
1:B:475:THR:O	1:B:479:VAL:HG23	1.63	0.98
1:A:490:PRO:HB2	1:A:492:VAL:HG23	1.44	0.98
1:B:109:LEU:CD1	1:B:449:THR:CG2	2.42	0.98
1:B:265:ARG:NH1	1:B:278:VAL:CG1	2.26	0.98
1:B:393:ILE:CG2	1:B:397:HIS:ND1	2.27	0.98
1:B:393:ILE:HG22	1:B:397:HIS:ND1	1.77	0.98
1:A:337:GLN:O	1:A:341:LEU:HB2	1.65	0.97
1:B:152:TYR:CD1	1:B:153:GLY:N	2.34	0.96
1:B:222:TYR:CZ	1:B:305:LEU:HD22	1.97	0.96
1:A:280:ASN:O	1:A:284:CYS:SG	2.24	0.95
1:B:508:LEU:HD12	1:B:509:GLY:N	1.80	0.95
1:A:518:ARG:C	1:A:519:HIS:HD1	1.71	0.95
1:B:55:VAL:HG21	1:B:89:PHE:CB	1.96	0.95
1:B:265:ARG:NH1	1:B:278:VAL:HG12	1.83	0.94
1:B:262:ILE:CG2	1:B:281:LEU:HD22	1.98	0.94
1:A:372:PRO:HA	1:A:505:SER:OG	1.67	0.94
1:B:472:GLN:O	1:B:476:ILE:HG13	1.68	0.94
1:B:153:GLY:HA2	1:B:279:TRP:NE1	1.81	0.93
1:B:332:GLU:OE2	1:B:422:HIS:CE1	2.22	0.93
1:B:108:ILE:HD12	1:B:108:ILE:H	1.34	0.92
1:A:169:GLU:CG	1:A:203:ARG:HD3	1.99	0.92
1:A:386:VAL:HG21	1:A:391:TYR:HB2	1.51	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:TYR:HB3	1:A:279:TRP:HZ2	1.22	0.92
1:A:58:TRP:CB	1:A:59:PHE:CD1	2.53	0.92
1:B:265:ARG:HH12	1:B:278:VAL:HG13	1.33	0.92
1:B:109:LEU:HD23	1:B:109:LEU:O	1.70	0.91
1:B:99:TYR:CD1	1:B:104:GLY:O	2.23	0.91
1:B:102:THR:CG2	1:B:452:PRO:HB3	2.00	0.91
1:B:341:LEU:HD21	1:B:346:PRO:HG2	1.53	0.91
1:B:114:ARG:C	1:B:381:LYS:HD2	1.90	0.91
1:B:364:LYS:HD3	1:B:470:TYR:OH	1.72	0.90
1:A:336:GLU:O	1:A:340:VAL:HG22	1.71	0.90
1:B:205:LEU:CD2	1:B:468:PHE:CZ	2.55	0.90
1:B:389:THR:HG22	1:B:390:SER:N	1.87	0.90
1:A:337:GLN:O	1:A:341:LEU:CB	2.19	0.90
1:B:429:ALA:HB1	1:B:431:SER:N	1.86	0.89
1:B:394:PRO:CG	1:B:397:HIS:CD2	2.55	0.89
1:B:394:PRO:CD	1:B:397:HIS:NE2	2.35	0.89
1:A:376:ILE:CG2	1:A:378:ARG:HH12	1.84	0.89
1:A:58:TRP:CB	1:A:59:PHE:CE1	2.55	0.89
1:A:386:VAL:CG2	1:A:391:TYR:O	2.21	0.88
1:B:406:THR:HB	1:B:452:PRO:HB2	1.54	0.88
1:B:100:LEU:O	1:B:104:GLY:HA3	1.73	0.88
1:B:307:ALA:HB2	3:B:590:VNI:C11	2.03	0.88
1:A:447:LYS:O	1:A:449:THR:HG23	1.73	0.88
1:B:55:VAL:CG2	1:B:89:PHE:HB3	2.03	0.88
1:B:109:LEU:HD11	1:B:449:THR:CG2	2.02	0.88
1:B:280:ASN:HA	1:B:283:SER:OG	1.72	0.88
1:A:135:VAL:HG12	1:A:136:TYR:N	1.88	0.87
1:B:109:LEU:CG	1:B:458:ALA:O	2.21	0.87
1:A:58:TRP:HB3	1:A:59:PHE:CE1	2.10	0.87
1:A:404:GLY:O	1:A:408:ARG:HG2	1.74	0.87
1:B:384:MET:C	1:B:392:VAL:CG2	2.42	0.86
1:A:51:THR:HB	1:A:52:PRO:CD	2.05	0.86
1:B:453:TYR:O	1:B:454:LEU:HD23	1.75	0.86
1:A:437:LYS:HB3	1:A:444:LEU:HD22	1.57	0.86
1:B:235:MET:O	1:B:236:LEU:HD23	1.76	0.86
1:B:381:LYS:HG3	1:B:382:ASN:OD1	1.75	0.86
1:B:109:LEU:HD11	1:B:449:THR:HG21	1.55	0.85
1:A:169:GLU:HG2	1:A:203:ARG:HD3	1.57	0.85
1:A:387:ASP:O	1:A:389:THR:HG23	1.77	0.85
1:B:137:ASP:HA	4:B:2006:HOH:O	1.77	0.85
1:B:389:THR:CG2	1:B:390:SER:H	1.89	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:242:PRO:O	1:B:246:LYS:HG2	1.75	0.85
1:A:58:TRP:HB2	1:A:59:PHE:HD1	1.40	0.85
1:B:149:PHE:O	1:B:152:TYR:CD1	2.30	0.84
1:B:394:PRO:HG2	1:B:397:HIS:HD2	1.41	0.84
1:A:437:LYS:HB3	1:A:444:LEU:CD2	2.06	0.84
1:B:394:PRO:HG2	1:B:397:HIS:CD2	2.12	0.84
1:B:140:ASN:O	1:B:144:MET:HG2	1.77	0.84
1:B:473:LEU:O	1:B:477:THR:HG23	1.76	0.84
1:B:100:LEU:C	1:B:104:GLY:HA3	1.98	0.84
1:A:279:TRP:O	1:A:283:SER:HB2	1.77	0.84
1:A:492:VAL:HG12	1:B:510:ARG:HH22	1.40	0.84
1:B:430:ALA:CB	1:B:466:GLU:OE2	2.24	0.83
1:B:110:ASN:N	1:B:110:ASN:HD22	1.77	0.82
1:B:336:GLU:O	1:B:340:VAL:HG23	1.79	0.82
1:A:490:PRO:HG2	1:A:492:VAL:HB	1.59	0.82
1:B:213:LYS:O	1:B:218:PHE:HB3	1.78	0.82
1:A:376:ILE:HG22	1:A:378:ARG:NH1	1.94	0.82
1:B:384:MET:O	1:B:392:VAL:CG2	2.23	0.82
1:B:341:LEU:HD23	1:B:342:GLY:O	1.79	0.81
1:B:102:THR:HB	1:B:450:ASN:O	1.81	0.81
1:B:102:THR:HG22	1:B:452:PRO:CA	2.10	0.81
1:A:152:TYR:CB	1:A:279:TRP:CZ2	2.62	0.81
1:B:235:MET:C	1:B:236:LEU:HD23	2.01	0.81
1:B:345:LEU:HD12	1:B:345:LEU:H	1.42	0.81
1:B:117:CYS:HA	1:B:460:ARG:HH22	1.46	0.81
1:A:95:LYS:HD2	1:A:397:HIS:CD2	2.16	0.81
1:B:110:ASN:CA	1:B:447:LYS:CE	2.59	0.80
1:B:153:GLY:CA	1:B:279:TRP:HE1	1.95	0.80
1:B:209:GLU:O	1:B:213:LYS:HG2	1.81	0.80
1:B:265:ARG:NH1	1:B:278:VAL:HG13	1.92	0.80
1:A:152:TYR:CB	1:A:279:TRP:HZ2	1.94	0.80
1:B:103:LYS:O	1:B:106:ASP:CB	2.23	0.80
1:B:108:ILE:HD12	1:B:108:ILE:N	1.96	0.79
1:B:341:LEU:HG	1:B:346:PRO:HG3	1.62	0.79
1:A:95:LYS:HD2	1:A:397:HIS:CG	2.17	0.79
2:A:580:HEM:HMB2	2:A:580:HEM:HBB2	1.64	0.79
1:B:102:THR:HG22	1:B:452:PRO:HA	1.63	0.79
2:A:580:HEM:HBB2	2:A:580:HEM:CMB	2.12	0.79
1:B:439:ASP:OD1	1:B:444:LEU:HA	1.83	0.79
1:A:58:TRP:HB2	1:A:59:PHE:CE1	2.16	0.78
1:A:279:TRP:C	1:A:283:SER:HB2	2.04	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:THR:HG23	1:B:452:PRO:HB3	1.64	0.78
1:A:57:HIS:CD2	4:A:2001:HOH:O	2.36	0.78
1:B:106:ASP:CG	1:B:107:PHE:HD1	1.87	0.78
1:B:152:TYR:CZ	1:B:279:TRP:CD1	2.71	0.77
1:B:280:ASN:HA	1:B:283:SER:CB	2.14	0.77
1:B:381:LYS:CG	1:B:382:ASN:OD1	2.31	0.77
1:A:133:HIS:N	1:A:137:ASP:OD2	2.15	0.77
1:B:384:MET:CB	1:B:393:ILE:CD1	2.57	0.77
1:A:447:LYS:O	1:A:449:THR:N	2.17	0.77
1:B:116:VAL:O	1:B:460:ARG:NH1	2.18	0.77
1:B:349:THR:O	1:B:353:LEU:HG	1.85	0.77
1:B:284:CYS:HA	1:B:292:VAL:HG22	1.65	0.76
1:B:233:ASN:O	1:B:237:PRO:HD3	1.86	0.76
1:A:389:THR:HG1	1:A:391:TYR:HD2	1.33	0.76
1:B:55:VAL:CG2	1:B:89:PHE:CB	2.62	0.76
1:B:110:ASN:CA	1:B:447:LYS:HZ1	1.98	0.76
1:A:518:ARG:O	1:A:519:HIS:ND1	2.16	0.76
1:B:107:PHE:O	1:B:111:GLY:CA	2.34	0.76
1:B:110:ASN:HA	1:B:447:LYS:NZ	2.01	0.76
1:A:490:PRO:CB	1:A:492:VAL:HG23	2.16	0.76
1:B:378:ARG:O	1:B:398:ASN:ND2	2.18	0.76
1:A:490:PRO:HG2	1:A:492:VAL:CB	2.16	0.76
1:A:51:THR:HG22	1:A:52:PRO:HD3	1.67	0.75
1:B:272:LYS:HD2	1:B:272:LYS:O	1.86	0.75
1:A:135:VAL:HG12	1:A:136:TYR:H	1.50	0.75
1:B:110:ASN:CA	1:B:447:LYS:NZ	2.49	0.75
1:A:508:LEU:O	1:A:508:LEU:HD12	1.86	0.75
1:B:109:LEU:HD23	1:B:110:ASN:N	1.93	0.75
1:B:427:ASN:HD21	1:B:432:ALA:HB3	1.47	0.75
1:A:341:LEU:HD12	1:A:346:PRO:HD2	1.67	0.74
1:B:52:PRO:HB2	1:B:88:THR:CG2	2.17	0.74
1:A:63:GLY:HA3	1:A:90:ILE:HG23	1.70	0.74
1:A:138:CYS:CB	1:A:139:PRO:HD2	2.17	0.74
1:A:203:ARG:HG3	1:A:203:ARG:HH11	1.52	0.74
1:B:341:LEU:HD11	1:B:346:PRO:HG2	1.68	0.74
1:A:503:LEU:HD12	3:A:590:VNI:H15	1.67	0.74
1:B:135:VAL:HG12	1:B:136:TYR:N	2.03	0.74
1:B:380:VAL:HG11	1:B:395:THR:O	1.87	0.74
1:A:490:PRO:CB	1:A:492:VAL:H	2.00	0.73
1:B:341:LEU:CD2	1:B:346:PRO:HG2	2.19	0.73
2:B:580:HEM:HBB2	2:B:580:HEM:CMB	2.18	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:306:MET:C	3:B:590:VNI:CL2	2.63	0.73
1:A:503:LEU:HD12	3:A:590:VNI:C15	2.19	0.73
1:B:449:THR:O	1:B:449:THR:HG22	1.88	0.73
1:B:108:ILE:HD12	1:B:109:LEU:N	1.97	0.72
1:A:51:THR:HB	1:A:52:PRO:HD2	1.71	0.72
1:B:163:VAL:HG22	1:B:471:LEU:HD11	1.71	0.72
1:B:52:PRO:HB2	1:B:88:THR:HG21	1.70	0.72
1:B:463:CYS:HB2	2:B:580:HEM:C1A	2.23	0.72
1:B:163:VAL:CG2	1:B:471:LEU:HD11	2.20	0.72
1:B:311:SER:HB2	2:B:580:HEM:CAB	2.19	0.72
1:B:384:MET:CB	1:B:393:ILE:HD13	2.18	0.72
1:B:147:LYS:NZ	2:B:580:HEM:O2D	2.23	0.72
1:A:288:ASN:ND2	1:A:290:THR:OG1	2.23	0.72
1:B:318:TRP:NE1	1:B:507:PRO:HD3	2.05	0.72
1:B:332:GLU:OE2	1:B:422:HIS:HE1	1.69	0.71
1:A:473:LEU:O	1:A:477:THR:HG23	1.89	0.71
2:A:580:HEM:HBD2	2:A:580:HEM:HHA	1.72	0.71
1:B:341:LEU:HG	1:B:346:PRO:CG	2.20	0.71
1:B:406:THR:HB	1:B:452:PRO:CB	2.20	0.71
1:B:455:PRO:O	2:B:580:HEM:HMA1	1.90	0.71
1:A:429:ALA:HB1	1:A:430:ALA:O	1.91	0.71
1:B:489:LEU:HD22	1:B:512:PHE:HB2	1.71	0.71
1:B:393:ILE:HD12	1:B:393:ILE:N	2.03	0.71
1:B:490:PRO:HB2	1:B:492:VAL:O	1.90	0.71
1:A:135:VAL:O	1:A:138:CYS:SG	2.49	0.71
1:B:349:THR:HG23	1:B:352:ASN:ND2	2.04	0.71
1:B:99:TYR:CE1	1:B:104:GLY:CA	2.72	0.71
1:A:500:TYR:O	1:A:502:SER:O	2.09	0.71
1:B:205:LEU:CD2	1:B:468:PHE:CE1	2.74	0.71
1:B:115:ASP:HA	1:B:381:LYS:HG2	1.72	0.70
1:A:433:GLU:OE2	1:A:446:SER:HB2	1.91	0.70
1:B:110:ASN:C	1:B:447:LYS:HZ1	1.93	0.70
1:A:404:GLY:O	1:A:408:ARG:CG	2.38	0.70
1:B:341:LEU:CG	1:B:346:PRO:CG	2.68	0.70
1:B:62:ILE:CG2	1:B:66:ILE:HD11	2.22	0.70
1:A:490:PRO:HB2	1:A:492:VAL:H	1.56	0.70
1:A:276:ASP:C	1:A:279:TRP:HB3	2.12	0.70
1:B:383:PRO:HA	1:B:393:ILE:O	1.92	0.70
1:B:424:TRP:HE1	1:B:427:ASN:HB3	1.57	0.70
1:B:426:GLU:O	1:B:426:GLU:HG2	1.91	0.70
4:A:2040:HOH:O	1:B:492:VAL:HG21	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:580:HEM:HMC2	2:A:580:HEM:HBC2	1.72	0.70
1:B:160:ARG:HG3	1:B:350:TYR:CB	2.22	0.70
1:B:108:ILE:HG22	1:B:399:VAL:HG21	1.72	0.70
1:B:51:THR:HA	1:B:391:TYR:CE2	2.27	0.69
1:B:231:PRO:O	1:B:234:PHE:HB2	1.91	0.69
1:A:490:PRO:CG	1:A:492:VAL:H	2.05	0.69
1:B:283:SER:O	1:B:292:VAL:HG21	1.92	0.69
1:A:490:PRO:HG2	1:A:492:VAL:O	1.92	0.69
1:B:341:LEU:HD21	1:B:343:SER:O	1.92	0.69
1:B:51:THR:HG22	1:B:391:TYR:HD2	1.57	0.69
1:B:330:MET:HE3	1:B:484:PHE:O	1.92	0.68
1:A:376:ILE:CG2	1:A:378:ARG:NH1	2.51	0.68
1:B:152:TYR:OH	1:B:279:TRP:C	2.32	0.68
1:B:51:THR:CB	1:B:52:PRO:CD	2.66	0.68
1:A:374:HIS:NE2	1:A:503:LEU:O	2.27	0.68
1:A:132:ARG:O	1:A:133:HIS:HB2	1.94	0.68
1:B:257:THR:O	1:B:261:ILE:HG13	1.93	0.68
1:B:363:ILE:HD11	1:B:474:GLY:HA2	1.75	0.68
1:B:393:ILE:HG22	1:B:397:HIS:CG	2.29	0.68
1:B:102:THR:CG2	1:B:452:PRO:CB	2.71	0.68
1:B:277:MET:C	1:B:279:TRP:H	1.96	0.68
1:B:281:LEU:O	1:B:284:CYS:SG	2.52	0.68
1:A:222:TYR:CE1	1:A:305:LEU:HD22	2.30	0.67
1:A:92:LEU:HD23	1:A:92:LEU:O	1.94	0.67
1:B:110:ASN:HB3	1:B:447:LYS:HZ3	1.58	0.67
1:B:55:VAL:HG11	1:B:79:CYS:SG	2.35	0.67
1:B:318:TRP:CE2	1:B:507:PRO:HD3	2.29	0.67
1:B:400:LEU:HD23	1:B:401:SER:N	2.09	0.67
1:B:427:ASN:HD22	1:B:432:ALA:HB3	1.55	0.67
1:B:109:LEU:HD22	1:B:110:ASN:HD22	0.67	0.67
1:B:447:LYS:O	1:B:447:LYS:HG2	1.95	0.67
1:B:62:ILE:HG22	1:B:66:ILE:HD11	1.76	0.67
1:A:51:THR:CB	1:A:52:PRO:CD	2.72	0.67
1:A:272:LYS:CE	4:A:2045:HOH:O	2.43	0.67
1:B:364:LYS:HD3	1:B:470:TYR:HH	1.57	0.67
1:B:364:LYS:CD	1:B:470:TYR:OH	2.43	0.67
1:A:138:CYS:HB2	1:A:139:PRO:CD	2.23	0.67
1:B:91:LEU:O	1:B:92:LEU:HD12	1.95	0.67
1:B:508:LEU:HD12	1:B:508:LEU:C	2.14	0.67
1:B:429:ALA:CB	1:B:431:SER:CA	2.73	0.66
1:B:101:GLY:O	1:B:104:GLY:N	2.28	0.66

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
1:B:273:ASP:OD1	1:B:274:SER:N	2.27	0.66
1:A:60:PRO:O	1:A:62:ILE:N	2.29	0.66
1:A:138:CYS:CB	1:A:139:PRO:CD	2.74	0.66
1:B:297:ILE:O	1:B:301:MET:HG2	1.96	0.66
1:A:262:ILE:HG23	1:A:281:LEU:HD21	1.77	0.66
1:A:279:TRP:CD2	1:A:283:SER:OG	2.48	0.66
1:A:429:ALA:CB	1:A:430:ALA:O	2.44	0.66
1:B:429:ALA:CB	1:B:431:SER:N	2.58	0.66
1:B:495:ILE:HG13	1:B:496:PRO:HD2	1.78	0.66
1:A:281:LEU:O	1:A:284:CYS:SG	2.54	0.66
1:A:59:PHE:N	4:A:2001:HOH:O	2.28	0.66
1:B:66:ILE:HD12	1:B:66:ILE:N	2.03	0.66
1:B:135:VAL:HG12	1:B:136:TYR:CG	2.30	0.66
2:B:580:HEM:HMC2	2:B:580:HEM:HBC2	1.78	0.66
1:A:428:ILE:HD12	1:A:428:ILE:C	2.16	0.65
1:B:110:ASN:HB3	1:B:447:LYS:NZ	2.11	0.65
1:A:372:PRO:HA	1:A:505:SER:HG	1.61	0.65
1:B:152:TYR:OH	1:B:283:SER:HB3	1.96	0.65
1:B:341:LEU:HD21	1:B:346:PRO:CG	2.24	0.65
1:B:143:LEU:HA	1:B:146:GLN:HG3	1.77	0.65
1:B:477:THR:O	1:B:481:VAL:HG23	1.96	0.65
4:A:2040:HOH:O	1:B:492:VAL:HG11	1.96	0.65
1:B:100:LEU:O	1:B:104:GLY:CA	2.44	0.65
1:B:393:ILE:HG21	1:B:397:HIS:ND1	2.10	0.65
1:B:91:LEU:N	1:B:94:LYS:O	2.26	0.65
1:B:343:SER:O	1:B:346:PRO:HD2	1.97	0.65
1:B:158:ALA:O	1:B:161:SER:HB3	1.96	0.65
1:A:195:GLU:O	1:A:198:ILE:HG22	1.97	0.64
2:A:580:HEM:HBC2	2:A:580:HEM:CMC	2.26	0.64
1:B:109:LEU:HD13	1:B:110:ASN:HD21	1.62	0.64
1:B:393:ILE:HG22	1:B:394:PRO:HD2	1.77	0.64
1:B:341:LEU:CG	1:B:346:PRO:HG2	2.26	0.64
1:B:99:TYR:CD1	1:B:104:GLY:HA2	2.30	0.64
1:B:394:PRO:HD2	1:B:397:HIS:CE1	2.32	0.64
1:A:270:SER:OG	1:A:271:LYS:N	2.31	0.64
1:A:492:VAL:CG1	1:B:510:ARG:HH21	2.11	0.64
1:A:51:THR:CG2	1:A:52:PRO:HD3	2.28	0.64
1:A:386:VAL:CG2	1:A:391:TYR:HB2	2.26	0.64
1:B:101:GLY:O	1:B:104:GLY:CA	2.46	0.64
1:B:152:TYR:CZ	1:B:283:SER:HB3	2.33	0.64
1:B:372:PRO:HG2	1:B:373:ILE:HD12	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:429:ALA:HB1	1:B:431:SER:CA	2.28	0.64
1:B:109:LEU:CD2	1:B:110:ASN:ND2	2.38	0.64
1:B:110:ASN:ND2	1:B:110:ASN:N	2.44	0.64
1:A:235:MET:C	1:A:237:PRO:HD2	2.18	0.63
1:A:50:LYS:HE2	1:A:50:LYS:HA	1.81	0.63
1:A:490:PRO:HG2	1:A:492:VAL:CA	2.28	0.63
1:B:109:LEU:HD22	1:B:110:ASN:CA	2.27	0.63
1:B:109:LEU:CD2	1:B:110:ASN:CA	2.76	0.63
1:B:105:ASN:O	1:B:108:ILE:CD1	2.46	0.63
1:B:280:ASN:HA	1:B:283:SER:HB3	1.81	0.63
1:B:97:THR:HG1	1:B:397:HIS:CE1	2.15	0.63
1:A:86:ILE:HG13	1:A:99:TYR:CD1	2.33	0.63
1:A:461:HIS:ND1	2:A:580:HEM:O1D	2.20	0.63
1:B:202:SER:O	1:B:206:GLN:HB2	1.99	0.63
1:A:58:TRP:CB	1:A:59:PHE:HE1	2.09	0.63
1:B:280:ASN:CA	1:B:283:SER:OG	2.44	0.63
1:B:307:ALA:HB2	3:B:590:VNI:H11	1.81	0.63
1:A:169:GLU:OE2	1:A:203:ARG:HD2	1.97	0.63
1:B:60:PRO:O	1:B:90:ILE:HD11	1.99	0.63
2:B:580:HEM:HBC2	2:B:580:HEM:CMC	2.29	0.63
1:B:106:ASP:CG	1:B:107:PHE:CD1	2.71	0.62
1:B:152:TYR:HD1	1:B:153:GLY:H	1.45	0.62
1:B:96:THR:HG22	1:B:398:ASN:HB2	1.80	0.62
1:B:230:ALA:O	1:B:233:ASN:HB2	1.99	0.62
1:B:489:LEU:HA	1:B:514:GLU:HG3	1.81	0.62
1:A:204:SER:OG	1:A:205:LEU:N	2.32	0.62
1:A:341:LEU:O	1:A:341:LEU:HD13	1.98	0.62
1:B:60:PRO:O	1:B:90:ILE:CD1	2.47	0.62
1:B:424:TRP:CH2	1:B:453:TYR:HE2	2.17	0.62
2:B:580:HEM:HBB2	2:B:580:HEM:HMB2	1.80	0.62
1:A:333:LEU:HD22	1:A:359:HIS:CD2	2.33	0.62
1:B:72:PRO:HD2	1:B:500:TYR:CG	2.35	0.61
1:A:63:GLY:HA3	1:A:90:ILE:CG2	2.30	0.61
1:B:109:LEU:HD13	1:B:110:ASN:ND2	2.15	0.61
1:A:437:LYS:CB	1:A:444:LEU:HD22	2.28	0.61
1:B:65:THR:OG1	1:B:91:LEU:HD12	2.00	0.61
1:B:54:VAL:O	1:B:54:VAL:HG13	1.98	0.61
1:B:358:LEU:O	1:B:361:LYS:N	2.32	0.61
1:A:334:TYR:CG	1:A:518:ARG:NH1	2.69	0.61
1:A:490:PRO:HB2	1:A:492:VAL:N	2.14	0.61
1:A:344:ASP:OD1	1:A:344:ASP:N	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:205:LEU:HD21	1:B:468:PHE:CE1	2.35	0.61
1:A:208:LYS:NZ	1:A:272:LYS:HD2	2.15	0.61
1:B:402:SER:HB3	1:B:405:VAL:HG23	1.81	0.61
1:B:463:CYS:HB2	2:B:580:HEM:NA	2.16	0.61
1:B:101:GLY:O	1:B:105:ASN:N	2.34	0.60
1:B:375:SER:HB3	1:B:400:LEU:HD11	1.83	0.60
1:B:393:ILE:HG23	1:B:397:HIS:CE1	2.33	0.60
1:B:95:LYS:HZ1	1:B:397:HIS:CD2	2.19	0.60
1:A:138:CYS:HB2	1:A:142:LYS:HB3	1.84	0.60
1:B:107:PHE:O	1:B:111:GLY:N	2.34	0.60
1:B:283:SER:O	1:B:292:VAL:CG2	2.49	0.60
1:A:58:TRP:CB	1:A:59:PHE:HD1	2.02	0.60
1:A:447:LYS:O	1:A:449:THR:CG2	2.48	0.60
1:B:341:LEU:CD1	1:B:346:PRO:HG2	2.30	0.60
1:B:429:ALA:CB	1:B:431:SER:C	2.70	0.60
1:B:95:LYS:HZ1	1:B:397:HIS:CE1	2.19	0.60
1:B:306:MET:HB3	3:B:590:VNI:CL2	2.39	0.60
1:A:340:VAL:HG23	1:A:341:LEU:N	2.17	0.60
1:B:262:ILE:HG22	1:B:281:LEU:HD22	1.83	0.60
1:B:384:MET:N	1:B:392:VAL:CG2	2.65	0.60
1:A:95:LYS:HE3	1:A:396:SER:O	2.01	0.60
1:A:334:TYR:CD2	1:A:518:ARG:NH1	2.70	0.60
1:B:311:SER:HB2	2:B:580:HEM:C3B	2.35	0.60
1:B:152:TYR:CZ	1:B:279:TRP:NE1	2.70	0.59
1:B:341:LEU:HD11	1:B:346:PRO:CG	2.32	0.59
1:B:384:MET:H	1:B:393:ILE:CD1	2.15	0.59
1:B:51:THR:HA	1:B:391:TYR:HD2	1.58	0.59
1:A:284:CYS:HB2	1:A:292:VAL:HG23	1.84	0.59
1:B:110:ASN:CB	1:B:447:LYS:HE2	2.33	0.59
1:B:110:ASN:O	1:B:447:LYS:NZ	2.34	0.59
1:A:265:ARG:NH2	1:A:275:GLU:OE2	2.28	0.59
1:B:110:ASN:HA	1:B:447:LYS:HZ1	1.64	0.59
1:A:346:PRO:HB2	1:A:347:PRO:HD2	1.85	0.59
1:A:450:ASN:CB	4:A:2074:HOH:O	2.51	0.59
1:B:263:LYS:O	1:B:267:GLN:HG2	2.02	0.59
1:A:169:GLU:OE2	1:A:203:ARG:CD	2.50	0.59
1:B:490:PRO:HB2	1:B:493:ASP:OD1	2.03	0.59
1:A:490:PRO:HB3	1:B:512:PHE:HZ	1.66	0.58
1:B:341:LEU:HG	1:B:341:LEU:O	2.01	0.58
1:B:447:LYS:O	1:B:449:THR:N	2.36	0.58
1:A:166:ILE:HG12	1:A:200:THR:HB	1.84	0.58

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
1:A:437:LYS:CB	1:A:444:LEU:CD2	2.79	0.58
1:B:110:ASN:CB	1:B:447:LYS:CE	2.81	0.58
1:B:127:THR:HB	1:B:128:PRO:HD3	1.86	0.58
1:A:488:ASN:HD22	1:A:493:ASP:HB2	1.68	0.58
1:B:361:LYS:NZ	1:B:425:ASP:OD1	2.24	0.58
1:A:492:VAL:HG11	1:B:510:ARG:NH2	2.14	0.58
1:B:393:ILE:CD1	1:B:393:ILE:H	1.96	0.58
1:A:61:PHE:HD1	1:A:62:ILE:N	2.01	0.58
1:B:71:ASP:OD1	1:B:74:LYS:N	2.26	0.58
1:B:149:PHE:O	1:B:152:TYR:CE1	2.57	0.58
1:A:64:SER:HA	4:A:2003:HOH:O	2.04	0.58
1:B:108:ILE:HG12	1:B:401:SER:HB3	1.85	0.58
1:B:194:ALA:O	1:B:309:GLN:NE2	2.36	0.58
1:A:152:TYR:HB3	1:A:279:TRP:CH2	2.37	0.57
1:A:282:MET:C	1:A:284:CYS:H	2.05	0.57
1:A:296:GLU:O	1:A:300:MET:HG3	2.04	0.57
1:A:413:PHE:O	1:A:416:PRO:HG3	2.04	0.57
1:B:277:MET:C	1:B:279:TRP:N	2.58	0.57
1:B:453:TYR:O	1:B:453:TYR:HD1	1.87	0.57
1:A:364:LYS:HE2	1:A:429:ALA:O	2.03	0.57
1:A:406:THR:OG1	1:A:452:PRO:O	2.22	0.57
1:A:488:ASN:ND2	1:A:493:ASP:HB2	2.19	0.57
1:B:107:PHE:HD1	1:B:107:PHE:H	1.49	0.57
1:B:107:PHE:O	1:B:111:GLY:HA3	2.04	0.57
1:A:95:LYS:CD	1:A:397:HIS:CD2	2.88	0.57
1:B:107:PHE:CD1	1:B:107:PHE:N	2.68	0.57
1:A:103:LYS:H	1:A:103:LYS:HD2	1.69	0.57
1:B:129:VAL:HG13	1:B:225:LEU:HG	1.87	0.57
1:B:205:LEU:HD23	1:B:468:PHE:CE1	2.34	0.57
1:B:300:MET:O	1:B:304:LEU:HG	2.04	0.57
1:B:341:LEU:CD2	1:B:346:PRO:CG	2.82	0.57
1:B:409:SER:O	1:B:413:PHE:O	2.22	0.57
1:B:86:ILE:HG22	1:B:99:TYR:CD2	2.39	0.57
1:B:146:GLN:O	1:B:149:PHE:HB2	2.04	0.57
1:A:61:PHE:CD1	1:A:62:ILE:N	2.72	0.57
1:A:279:TRP:CD2	1:A:283:SER:CB	2.88	0.57
1:B:152:TYR:CE2	1:B:279:TRP:CE2	2.92	0.57
1:B:373:ILE:HD12	1:B:373:ILE:N	2.20	0.57
1:B:108:ILE:HG22	1:B:399:VAL:CG2	2.34	0.56
1:A:135:VAL:HG12	1:A:136:TYR:CG	2.41	0.56
1:A:135:VAL:CG1	1:A:136:TYR:N	2.59	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:580:HEM:HMB2	2:A:580:HEM:CBB	2.33	0.56
1:A:191:LYS:NZ	4:A:2040:HOH:O	2.38	0.56
1:B:424:TRP:CH2	1:B:453:TYR:CE2	2.94	0.56
1:B:443:GLY:O	1:B:445:VAL:HG13	2.05	0.56
1:A:281:LEU:C	1:A:284:CYS:SG	2.83	0.56
1:A:71:ASP:OD1	1:A:73:TYR:N	2.39	0.56
1:B:160:ARG:HG3	1:B:350:TYR:CG	2.41	0.56
1:B:102:THR:CG2	1:B:452:PRO:CA	2.82	0.56
1:A:222:TYR:CZ	1:A:305:LEU:HD13	2.41	0.56
1:A:282:MET:C	1:A:284:CYS:N	2.58	0.56
1:A:518:ARG:C	1:A:519:HIS:ND1	2.51	0.56
1:A:218:PHE:CE2	1:A:222:TYR:HE2	2.24	0.55
1:B:341:LEU:CD2	1:B:343:SER:O	2.53	0.55
1:B:384:MET:CB	1:B:393:ILE:HD11	2.26	0.55
1:B:110:ASN:CB	1:B:447:LYS:NZ	2.70	0.55
1:B:489:LEU:HB3	1:B:490:PRO:HD3	1.88	0.55
2:B:580:HEM:HMB2	2:B:580:HEM:CBB	2.35	0.55
1:A:60:PRO:O	1:A:61:PHE:HB3	2.05	0.55
1:A:262:ILE:HG23	1:A:281:LEU:CD2	2.36	0.55
1:A:400:LEU:HD23	1:A:400:LEU:C	2.26	0.55
1:A:288:ASN:OD1	1:A:289:GLY:N	2.40	0.55
1:B:388:GLY:O	1:B:389:THR:OG1	2.19	0.55
1:A:370:HIS:O	1:A:371:ALA:C	2.44	0.55
1:B:118:ALA:H	1:B:460:ARG:NH2	2.04	0.55
1:B:332:GLU:OE2	1:B:422:HIS:NE2	2.40	0.55
1:A:106:ASP:OD1	1:A:110:ASN:ND2	2.34	0.55
1:A:123:SER:N	1:A:124:PRO:HD2	2.22	0.55
1:A:338:ILE:HG23	1:A:343:SER:HA	1.89	0.55
1:B:80:ARG:HA	1:B:84:GLY:O	2.07	0.55
1:A:58:TRP:C	1:A:59:PHE:CD1	2.80	0.54
1:A:490:PRO:CG	1:A:492:VAL:O	2.54	0.54
1:B:100:LEU:N	1:B:100:LEU:HD12	2.22	0.54
1:B:222:TYR:CE1	1:B:305:LEU:HD21	2.36	0.54
1:B:308:GLY:O	1:B:312:SER:OG	2.24	0.54
1:B:394:PRO:HD2	1:B:397:HIS:CG	2.37	0.54
1:A:236:LEU:N	1:A:237:PRO:CD	2.70	0.54
1:B:52:PRO:CB	1:B:88:THR:HG21	2.37	0.54
1:B:436:GLU:HA	1:B:437:LYS:HD3	1.89	0.54
1:B:88:THR:HA	1:B:97:THR:HA	1.88	0.54
1:A:188:ASP:C	1:A:188:ASP:OD1	2.45	0.54
1:A:286:TYR:HB3	4:A:2025:HOH:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:ASN:HD21	1:B:449:THR:HG21	1.71	0.54
1:B:152:TYR:OH	1:B:279:TRP:O	2.25	0.54
1:B:453:TYR:CE1	1:B:455:PRO:CD	2.91	0.54
1:B:110:ASN:ND2	1:B:110:ASN:H	2.06	0.54
1:B:453:TYR:CE1	1:B:455:PRO:HD3	2.42	0.54
1:A:265:ARG:NH1	1:A:278:VAL:HG13	2.23	0.54
1:B:109:LEU:CD1	1:B:449:THR:HG23	2.37	0.54
1:B:307:ALA:HB2	3:B:590:VNI:C12	2.37	0.54
1:B:348:LEU:HD12	1:B:348:LEU:N	2.23	0.54
1:A:184:LYS:HG3	1:A:185:GLY:N	2.21	0.53
1:B:99:TYR:HE1	1:B:104:GLY:HA2	1.63	0.53
1:B:150:VAL:HB	1:B:464:ILE:HD11	1.90	0.53
1:A:58:TRP:HB3	1:A:59:PHE:CD1	2.36	0.53
1:B:490:PRO:HG2	1:B:493:ASP:OD1	2.09	0.53
1:A:235:MET:O	1:A:237:PRO:HD2	2.08	0.53
1:B:109:LEU:HD11	1:B:449:THR:HG23	1.89	0.53
1:B:52:PRO:HB2	1:B:88:THR:HG23	1.90	0.53
1:B:108:ILE:HG12	1:B:401:SER:CB	2.39	0.53
1:B:273:ASP:O	1:B:278:VAL:HG21	2.08	0.53
1:A:59:PHE:CD1	1:A:59:PHE:N	2.76	0.53
1:B:348:LEU:HA	1:B:352:ASN:HD21	1.73	0.53
1:B:490:PRO:CG	1:B:493:ASP:OD1	2.56	0.53
1:A:127:THR:N	1:A:128:PRO:CD	2.71	0.53
1:A:286:TYR:OH	1:A:296:GLU:OE1	2.26	0.53
1:B:271:LYS:HG3	1:B:272:LYS:N	2.24	0.53
1:A:68:TYR:HH	1:A:375:SER:CB	2.21	0.53
1:A:337:GLN:O	1:A:341:LEU:N	2.41	0.53
1:B:424:TRP:CD1	1:B:427:ASN:O	2.61	0.53
1:B:270:SER:OG	1:B:271:LYS:N	2.42	0.53
1:B:460:ARG:O	1:B:461:HIS:HB2	2.07	0.53
4:A:2040:HOH:O	1:B:492:VAL:CG2	2.54	0.52
1:B:501:SER:OG	1:B:502:SER:N	2.42	0.52
1:B:65:THR:HG23	1:B:91:LEU:HD11	1.92	0.52
1:B:389:THR:CG2	1:B:390:SER:N	2.56	0.52
1:A:277:MET:O	1:A:281:LEU:HG	2.08	0.52
1:B:422:HIS:O	1:B:423:ARG:C	2.48	0.52
1:A:372:PRO:HG2	1:A:373:ILE:HD12	1.92	0.52
1:B:314:SER:O	1:B:317:SER:HB2	2.10	0.52
1:B:429:ALA:HB1	1:B:431:SER:C	2.30	0.52
1:A:428:ILE:HD12	1:A:429:ALA:CA	2.38	0.52
1:B:108:ILE:CG2	1:B:399:VAL:HG21	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:THR:HB	1:A:399:VAL:HG12	1.92	0.52
1:A:462:ARG:CG	1:A:462:ARG:HH11	2.21	0.52
1:B:222:TYR:CD1	1:B:305:LEU:CD2	2.89	0.52
1:B:303:ALA:O	3:B:590:VNI:H11	2.09	0.52
1:A:213:LYS:O	1:A:216:SER:O	2.27	0.52
1:B:91:LEU:C	1:B:92:LEU:HG	2.30	0.52
1:B:341:LEU:CD1	1:B:346:PRO:CG	2.88	0.52
1:B:119:GLU:HB3	1:B:136:TYR:HB3	1.91	0.52
1:B:332:GLU:CD	1:B:422:HIS:HE1	2.13	0.52
1:A:53:PRO:HB2	1:A:83:TYR:CD2	2.45	0.51
1:A:99:TYR:CD2	1:A:104:GLY:HA2	2.45	0.51
1:A:490:PRO:CD	1:A:492:VAL:O	2.58	0.51
1:B:115:ASP:HB3	1:B:384:MET:CE	2.40	0.51
1:B:152:TYR:CD1	1:B:152:TYR:C	2.83	0.51
1:A:357:ASP:O	1:A:361:LYS:HG3	2.10	0.51
1:B:293:PRO:HG2	1:B:296:GLU:HG3	1.93	0.51
1:B:163:VAL:N	1:B:164:PRO:HD2	2.25	0.51
1:B:90:ILE:HA	1:B:95:LYS:HA	1.93	0.51
1:B:263:LYS:NZ	4:B:2024:HOH:O	2.40	0.51
1:B:363:ILE:HD11	1:B:474:GLY:CA	2.41	0.51
1:B:109:LEU:HG	1:B:458:ALA:C	2.21	0.51
1:B:117:CYS:O	1:B:379:ALA:HB3	2.10	0.51
1:B:381:LYS:HG3	1:B:382:ASN:N	2.25	0.51
1:B:361:LYS:HE2	1:B:424:TRP:O	2.11	0.51
1:B:384:MET:H	1:B:393:ILE:HD13	1.73	0.51
1:B:106:ASP:OD2	1:B:107:PHE:CD1	2.64	0.51
1:B:280:ASN:O	1:B:283:SER:OG	2.29	0.51
1:B:322:ARG:HD3	1:B:495:ILE:HD13	1.92	0.51
1:B:350:TYR:O	1:B:354:GLN:NE2	2.41	0.51
1:A:279:TRP:CE3	1:A:283:SER:OG	2.63	0.51
1:A:446:SER:OG	1:A:448:GLY:O	2.29	0.51
1:B:106:ASP:OD2	1:B:107:PHE:CE1	2.63	0.51
1:B:341:LEU:CG	1:B:346:PRO:HG3	2.34	0.51
1:A:386:VAL:HG21	1:A:391:TYR:CB	2.33	0.51
1:A:97:THR:OG1	1:A:397:HIS:ND1	2.44	0.51
1:A:234:PHE:HZ	1:A:503:LEU:HG	1.75	0.51
1:A:279:TRP:CE2	1:A:283:SER:CB	2.93	0.51
1:B:222:TYR:OH	1:B:305:LEU:HD22	2.10	0.51
1:A:463:CYS:HA	2:A:580:HEM:C4D	2.46	0.50
1:B:460:ARG:NE	1:B:461:HIS:NE2	2.59	0.50
1:B:213:LYS:O	1:B:218:PHE:CB	2.55	0.50

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
1:A:218:PHE:HE2	1:A:222:TYR:HE2	1.57	0.50
1:B:105:ASN:O	1:B:108:ILE:HD11	2.11	0.50
1:B:258:TYR:O	1:B:262:ILE:HG13	2.11	0.50
1:B:116:VAL:HG23	1:B:460:ARG:NH1	2.26	0.50
1:B:435:ASP:CG	1:B:436:GLU:H	2.14	0.50
1:B:453:TYR:CD1	1:B:453:TYR:C	2.84	0.50
1:A:169:GLU:HG3	1:A:203:ARG:HD3	1.91	0.50
1:A:208:LYS:NZ	4:A:2044:HOH:O	2.43	0.50
1:A:272:LYS:NZ	4:A:2045:HOH:O	2.24	0.50
1:A:462:ARG:CG	1:A:462:ARG:NH1	2.75	0.50
1:A:61:PHE:CD1	1:A:61:PHE:C	2.83	0.50
1:B:54:VAL:O	1:B:54:VAL:CG1	2.60	0.50
1:B:330:MET:CE	1:B:484:PHE:O	2.60	0.50
1:B:437:LYS:HA	1:B:446:SER:HA	1.93	0.50
1:B:68:TYR:HH	1:B:375:SER:CB	2.25	0.50
1:B:75:PHE:CD1	1:B:75:PHE:C	2.85	0.50
1:B:91:LEU:HG	1:B:92:LEU:HG	1.94	0.50
1:B:133:HIS:HB3	1:B:296:GLU:OE2	2.10	0.49
1:B:380:VAL:HG13	4:B:2034:HOH:O	2.11	0.49
1:A:55:VAL:HG21	1:A:89:PHE:HB2	1.93	0.49
1:B:108:ILE:CG2	1:B:399:VAL:CG2	2.91	0.49
1:B:113:LEU:HD21	1:B:140:ASN:CG	2.32	0.49
1:B:447:LYS:HG2	1:B:449:THR:HG1	1.76	0.49
1:B:97:THR:OG1	1:B:397:HIS:CE1	2.65	0.49
1:B:372:PRO:HA	1:B:505:SER:OG	2.11	0.49
1:B:422:HIS:C	1:B:424:TRP:N	2.64	0.49
1:A:485:ARG:HD2	4:A:2081:HOH:O	2.13	0.49
1:B:135:VAL:HG12	1:B:136:TYR:CD1	2.47	0.49
1:B:186:VAL:HG13	1:B:489:LEU:HD13	1.95	0.49
1:A:456:PHE:CE2	1:A:466:GLU:HG3	2.48	0.49
1:A:462:ARG:HH11	1:A:462:ARG:HG2	1.78	0.49
1:B:68:TYR:CE1	1:B:72:PRO:HB3	2.47	0.49
1:B:140:ASN:ND2	1:B:144:MET:SD	2.86	0.49
1:B:343:SER:OG	1:B:344:ASP:N	2.44	0.49
1:B:429:ALA:HB1	1:B:431:SER:O	2.13	0.49
1:A:394:PRO:HD2	1:A:397:HIS:CD2	2.47	0.49
1:B:51:THR:CG2	1:B:391:TYR:HD2	2.25	0.49
1:B:115:ASP:HA	1:B:381:LYS:CG	2.43	0.49
1:B:135:VAL:HG12	1:B:136:TYR:H	1.75	0.49
1:A:265:ARG:NH1	1:A:277:MET:SD	2.86	0.49
1:A:386:VAL:HG11	1:A:389:THR:OG1	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:155:THR:O	1:B:157:ASP:N	2.46	0.48
1:A:280:ASN:O	1:A:284:CYS:CB	2.60	0.48
1:A:83:TYR:N	1:A:83:TYR:CD1	2.82	0.48
1:B:152:TYR:CE1	1:B:279:TRP:NE1	2.82	0.48
1:B:160:ARG:CG	1:B:350:TYR:CB	2.89	0.48
1:B:210:VAL:HG23	4:B:2019:HOH:O	2.12	0.48
1:A:471:LEU:CD1	1:A:471:LEU:C	2.82	0.48
1:B:109:LEU:HG	1:B:459:GLY:HA3	1.96	0.48
1:B:155:THR:C	1:B:157:ASP:N	2.66	0.48
1:B:368:ARG:NH2	1:B:423:ARG:NH1	2.61	0.48
1:B:216:SER:OG	1:B:217:THR:N	2.46	0.48
1:B:227:MET:HE3	1:B:246:LYS:HB2	1.95	0.48
1:B:66:ILE:H	1:B:66:ILE:CD1	1.96	0.48
1:B:109:LEU:CD2	1:B:110:ASN:HA	2.42	0.48
1:B:490:PRO:O	1:B:493:ASP:OD2	2.32	0.48
1:A:203:ARG:HG3	1:A:203:ARG:NH1	2.26	0.48
1:A:227:MET:HE3	1:A:246:LYS:HB2	1.96	0.48
1:A:279:TRP:CE2	1:A:283:SER:HB3	2.48	0.48
1:A:429:ALA:HB1	1:A:432:ALA:HB2	1.96	0.48
1:A:450:ASN:HB2	4:A:2074:HOH:O	2.14	0.48
4:A:2040:HOH:O	1:B:492:VAL:CG1	2.57	0.48
1:B:307:ALA:CB	3:B:590:VNI:CL2	2.98	0.48
1:A:221:LEU:HD22	1:A:250:ALA:HA	1.96	0.48
1:A:415:ASN:N	1:A:416:PRO:HD3	2.29	0.48
1:B:55:VAL:CG1	1:B:79:CYS:SG	3.02	0.48
1:A:284:CYS:HB2	1:A:292:VAL:CG2	2.44	0.48
1:A:492:VAL:HG12	1:B:510:ARG:HH21	1.66	0.48
1:B:188:ASP:OD1	1:B:188:ASP:C	2.52	0.48
1:A:386:VAL:HG12	1:A:387:ASP:N	2.29	0.47
1:B:343:SER:OG	1:B:344:ASP:OD1	2.32	0.47
1:B:396:SER:O	1:B:397:HIS:CD2	2.67	0.47
1:B:232:ILE:HG23	1:B:233:ASN:N	2.29	0.47
1:B:479:VAL:HG12	1:B:483:LEU:HD12	1.96	0.47
1:B:201:ALA:O	1:B:205:LEU:HB2	2.13	0.47
1:B:86:ILE:O	1:B:86:ILE:HG13	2.11	0.47
1:B:119:GLU:H	1:B:119:GLU:CD	2.16	0.47
1:A:123:SER:N	1:A:124:PRO:CD	2.77	0.47
1:A:281:LEU:C	1:A:284:CYS:HG	2.17	0.47
1:B:222:TYR:CZ	1:B:305:LEU:HD21	2.42	0.47
1:A:133:HIS:H	1:A:137:ASP:CG	2.12	0.47
1:A:235:MET:C	1:A:237:PRO:CD	2.82	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:ASN:O	1:A:237:PRO:HD3	2.14	0.47
1:A:280:ASN:O	1:A:284:CYS:HB3	2.15	0.47
1:A:386:VAL:HG12	1:A:387:ASP:H	1.79	0.47
1:A:433:GLU:OE2	1:A:437:LYS:HE2	2.14	0.47
1:B:51:THR:HG22	1:B:391:TYR:CD2	2.44	0.47
1:B:123:SER:N	1:B:124:PRO:HD2	2.29	0.47
1:B:227:MET:CE	1:B:246:LYS:HB2	2.45	0.47
1:B:345:LEU:H	1:B:345:LEU:CD1	2.14	0.47
1:A:471:LEU:O	1:A:471:LEU:HD13	2.14	0.47
1:A:485:ARG:NH1	4:A:2081:HOH:O	2.43	0.47
1:B:112:LYS:O	1:B:115:ASP:N	2.48	0.47
1:B:422:HIS:O	1:B:424:TRP:N	2.47	0.47
1:A:92:LEU:O	1:A:92:LEU:CD2	2.63	0.47
1:A:334:TYR:CE1	1:A:338:ILE:HD11	2.50	0.47
1:B:377:ILE:CG2	1:B:398:ASN:HB3	2.44	0.47
1:B:401:SER:O	1:B:403:PRO:CD	2.62	0.47
1:A:86:ILE:CG1	1:A:99:TYR:CD1	2.98	0.46
1:B:328:ASP:O	1:B:332:GLU:HB2	2.15	0.46
1:A:490:PRO:HB3	1:B:512:PHE:CZ	2.47	0.46
1:B:202:SER:HA	1:B:206:GLN:HB2	1.98	0.46
1:B:449:THR:CG2	1:B:449:THR:O	2.59	0.46
1:A:499:ASP:OD1	1:A:499:ASP:C	2.53	0.46
1:A:508:LEU:HD12	1:A:508:LEU:C	2.34	0.46
1:B:347:PRO:O	1:B:352:ASN:ND2	2.48	0.46
1:A:135:VAL:CG1	1:A:136:TYR:H	2.16	0.46
1:B:155:THR:O	1:B:158:ALA:N	2.47	0.46
1:B:178:PRO:HA	1:B:181:GLN:HG2	1.96	0.46
1:A:279:TRP:CZ3	1:A:283:SER:OG	2.67	0.46
1:B:149:PHE:HZ	1:B:285:VAL:O	1.98	0.46
1:B:149:PHE:CE2	1:B:286:TYR:CE1	3.03	0.46
2:B:580:HEM:HBA1	2:B:580:HEM:HHA	1.97	0.46
1:A:86:ILE:HG13	1:A:99:TYR:HD1	1.81	0.46
1:A:203:ARG:NH1	1:A:203:ARG:CG	2.78	0.46
1:A:279:TRP:CZ2	1:A:283:SER:OG	2.64	0.46
1:A:436:GLU:O	1:A:448:GLY:N	2.49	0.46
1:B:113:LEU:CD2	1:B:140:ASN:OD1	2.64	0.46
1:B:434:ASP:HA	4:B:2039:HOH:O	2.16	0.46
1:A:96:THR:HG22	1:A:398:ASN:HB2	1.98	0.46
1:B:50:LYS:C	1:B:51:THR:OG1	2.54	0.46
1:B:109:LEU:HD21	1:B:447:LYS:HE3	1.98	0.46
1:B:361:LYS:CE	1:B:424:TRP:O	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:LEU:HD12	1:B:233:ASN:HB3	1.96	0.46
1:B:453:TYR:C	1:B:454:LEU:HD23	2.36	0.46
1:A:53:PRO:HB2	1:A:83:TYR:HD2	1.82	0.45
1:A:217:THR:O	1:A:217:THR:OG1	2.33	0.45
1:B:110:ASN:HB3	1:B:447:LYS:CE	2.45	0.45
1:A:341:LEU:HA	1:A:341:LEU:HD22	1.74	0.45
1:B:333:LEU:HD22	1:B:359:HIS:CE1	2.51	0.45
1:B:377:ILE:HG23	1:B:398:ASN:HB3	1.98	0.45
1:A:446:SER:OG	1:A:448:GLY:C	2.54	0.45
1:B:195:GLU:O	1:B:198:ILE:HG22	2.16	0.45
1:A:238:TRP:CZ3	1:A:239:ALA:HB2	2.51	0.45
1:A:241:LEU:N	1:A:241:LEU:HD23	2.31	0.45
1:A:372:PRO:CA	1:A:505:SER:OG	2.53	0.45
1:B:345:LEU:HD12	1:B:345:LEU:N	2.21	0.45
1:B:205:LEU:HD21	1:B:468:PHE:CZ	2.42	0.45
1:A:132:ARG:HA	1:A:137:ASP:OD2	2.16	0.45
1:A:272:LYS:HE2	4:A:2045:HOH:O	2.13	0.45
1:A:277:MET:C	1:A:279:TRP:N	2.67	0.45
1:A:356:LEU:HB3	1:A:359:HIS:HB2	1.99	0.45
1:A:471:LEU:C	1:A:471:LEU:HD13	2.37	0.45
1:B:453:TYR:O	1:B:453:TYR:CD1	2.68	0.45
1:A:364:LYS:HE3	1:A:429:ALA:H	1.82	0.45
1:B:168:ASP:HA	1:B:171:GLU:HB2	1.97	0.45
1:B:334:TYR:CD2	1:B:518:ARG:NH1	2.85	0.45
1:B:453:TYR:CD1	1:B:455:PRO:HD3	2.52	0.45
1:A:55:VAL:HG11	1:A:89:PHE:HB3	1.98	0.45
1:B:58:TRP:CD1	1:B:58:TRP:N	2.84	0.45
1:B:147:LYS:NZ	1:B:461:HIS:HA	2.32	0.45
1:B:414:PRO:O	1:B:423:ARG:NH2	2.50	0.45
1:A:232:ILE:HD11	1:A:236:LEU:HD12	1.99	0.45
1:B:136:TYR:OH	2:B:580:HEM:O1D	2.21	0.45
1:A:53:PRO:CG	1:A:83:TYR:HD2	2.29	0.44
1:A:92:LEU:O	1:A:92:LEU:CG	2.62	0.44
1:B:135:VAL:CG1	1:B:136:TYR:N	2.71	0.44
1:B:344:ASP:N	1:B:344:ASP:OD1	2.50	0.44
1:B:346:PRO:HA	1:B:347:PRO:HD3	1.84	0.44
1:A:311:SER:OG	1:A:312:SER:N	2.50	0.44
1:A:282:MET:C	1:A:284:CYS:SG	2.96	0.44
1:A:456:PHE:CZ	1:A:466:GLU:HG3	2.53	0.44
1:B:138:CYS:CB	1:B:142:LYS:HE2	2.47	0.44
1:B:427:ASN:HD21	1:B:432:ALA:CB	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:580:HEM:HMC2	2:B:580:HEM:CBC	2.47	0.44
1:B:51:THR:CA	1:B:391:TYR:CD2	2.78	0.44
1:B:224:ASN:HA	1:B:227:MET:HE2	1.98	0.44
1:A:149:PHE:O	1:A:279:TRP:NE1	2.45	0.44
1:A:392:VAL:O	1:A:392:VAL:HG13	2.16	0.44
1:A:448:GLY:N	1:A:449:THR:HG23	2.26	0.44
1:A:208:LYS:HZ3	1:A:272:LYS:HD2	1.82	0.44
1:B:435:ASP:CG	1:B:436:GLU:N	2.71	0.44
1:B:86:ILE:CG2	1:B:99:TYR:CD2	3.01	0.44
1:B:119:GLU:O	1:B:120:GLU:C	2.55	0.44
1:B:490:PRO:CB	1:B:493:ASP:OD1	2.65	0.44
2:A:580:HEM:HMC2	2:A:580:HEM:CBC	2.44	0.44
1:B:277:MET:O	1:B:279:TRP:N	2.50	0.44
1:B:396:SER:O	1:B:397:HIS:HD2	2.01	0.44
1:A:160:ARG:HG2	1:A:350:TYR:CB	2.47	0.44
1:A:309:GLN:OE1	1:A:309:GLN:HA	2.18	0.44
1:B:99:TYR:CD1	1:B:104:GLY:CA	3.00	0.44
1:B:109:LEU:CD2	1:B:447:LYS:HE3	2.48	0.44
1:B:160:ARG:HG3	1:B:350:TYR:HB3	1.99	0.44
1:A:208:LYS:HZ2	1:A:272:LYS:HD2	1.82	0.43
1:A:490:PRO:HG2	1:A:492:VAL:C	2.38	0.43
1:B:108:ILE:CD1	1:B:108:ILE:N	2.70	0.43
1:B:114:ARG:O	1:B:381:LYS:CD	2.48	0.43
1:A:238:TRP:CE3	1:A:239:ALA:N	2.86	0.43
1:B:146:GLN:NE2	1:B:300:MET:SD	2.91	0.43
1:B:186:VAL:HG12	1:B:512:PHE:CD2	2.53	0.43
1:B:222:TYR:CE2	1:B:305:LEU:CD2	2.94	0.43
1:B:378:ARG:HB2	1:B:399:VAL:HG22	1.99	0.43
1:A:255:THR:HG22	1:A:259:MET:HE3	1.99	0.43
1:A:288:ASN:ND2	1:A:290:THR:HG1	2.14	0.43
1:B:454:LEU:HB3	1:B:457:GLY:HA2	2.00	0.43
1:A:181:GLN:OE1	1:A:181:GLN:HA	2.18	0.43
1:A:282:MET:O	1:A:284:CYS:N	2.40	0.43
1:B:113:LEU:HD21	1:B:140:ASN:OD1	2.18	0.43
1:B:341:LEU:HD11	1:B:346:PRO:CB	2.48	0.43
1:B:414:PRO:HG2	4:B:2036:HOH:O	2.17	0.43
1:A:55:VAL:HG21	1:A:89:PHE:CB	2.48	0.43
1:A:345:LEU:HD12	1:A:345:LEU:HA	1.75	0.43
1:B:52:PRO:CB	1:B:88:THR:CG2	2.95	0.43
1:B:88:THR:HA	1:B:96:THR:O	2.19	0.43
1:B:162:TYR:O	1:B:165:LEU:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:109:LEU:HD22	1:B:110:ASN:H	1.72	0.43
1:B:125:LEU:CD1	1:B:233:ASN:HB3	2.48	0.43
1:B:232:ILE:O	1:B:235:MET:N	2.49	0.43
1:B:385:ALA:N	4:B:2035:HOH:O	2.51	0.43
1:B:427:ASN:C	1:B:427:ASN:OD1	2.57	0.43
1:A:87:PHE:CD1	1:A:87:PHE:N	2.86	0.43
1:A:117:CYS:SG	1:A:119:GLU:CD	2.97	0.43
1:B:197:THR:HG21	1:B:313:SER:HA	2.00	0.43
1:B:348:LEU:HB3	1:B:353:LEU:HD21	2.01	0.43
1:A:394:PRO:O	1:A:397:HIS:HB2	2.18	0.43
1:B:68:TYR:OH	1:B:375:SER:CB	2.66	0.43
1:B:138:CYS:SG	1:B:142:LYS:HB3	2.59	0.43
1:B:427:ASN:CG	1:B:432:ALA:CB	2.85	0.43
1:A:321:LEU:O	1:A:324:ALA:HB3	2.19	0.43
1:A:372:PRO:CA	1:A:505:SER:HG	2.30	0.43
1:A:490:PRO:CG	1:A:492:VAL:N	2.78	0.43
1:B:55:VAL:CG2	1:B:89:PHE:CA	2.97	0.43
1:B:89:PHE:N	1:B:96:THR:O	2.52	0.43
1:B:152:TYR:CD2	1:B:279:TRP:CZ2	3.07	0.43
1:B:276:ASP:O	1:B:280:ASN:HB2	2.19	0.43
1:B:288:ASN:OD1	1:B:288:ASN:C	2.57	0.43
1:B:384:MET:H	1:B:393:ILE:HD12	1.83	0.43
1:B:437:LYS:CD	1:B:437:LYS:N	2.82	0.43
1:A:132:ARG:CA	1:A:137:ASP:OD2	2.66	0.42
1:B:364:LYS:NZ	1:B:453:TYR:CZ	2.74	0.42
1:B:146:GLN:HA	1:B:149:PHE:HB2	2.01	0.42
1:B:427:ASN:CG	1:B:432:ALA:HB2	2.39	0.42
1:B:456:PHE:HA	2:B:580:HEM:HMA1	2.00	0.42
1:A:232:ILE:HG23	1:A:233:ASN:OD1	2.19	0.42
1:A:234:PHE:HD1	1:A:234:PHE:HA	1.73	0.42
1:A:270:SER:N	4:A:2057:HOH:O	2.52	0.42
1:A:279:TRP:O	1:A:283:SER:N	2.49	0.42
1:A:376:ILE:HG23	1:A:378:ARG:HH12	1.78	0.42
1:A:107:PHE:CZ	1:A:384:MET:HE2	2.54	0.42
1:A:241:LEU:HB3	1:A:242:PRO:HD2	2.02	0.42
1:A:272:LYS:HE3	1:A:272:LYS:HB2	1.81	0.42
1:A:321:LEU:HB3	1:A:495:ILE:HD11	2.00	0.42
1:B:65:THR:HA	1:B:91:LEU:CD1	2.49	0.42
1:B:373:ILE:HD12	1:B:373:ILE:H	1.83	0.42
1:B:447:LYS:C	1:B:449:THR:HG1	2.15	0.42
1:A:271:LYS:CG	1:A:272:LYS:N	2.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:430:ALA:O	1:A:431:SER:C	2.58	0.42
1:B:110:ASN:HB3	1:B:447:LYS:HE2	2.01	0.42
1:B:368:ARG:HD3	1:B:424:TRP:CH2	2.54	0.42
1:B:384:MET:C	1:B:392:VAL:HG21	2.34	0.42
1:A:235:MET:O	1:A:235:MET:SD	2.78	0.42
1:B:55:VAL:CG2	1:B:89:PHE:HA	2.50	0.42
1:B:117:CYS:O	1:B:379:ALA:CB	2.67	0.42
1:B:248:ASP:O	1:B:252:ARG:HG3	2.19	0.42
1:B:361:LYS:HD3	1:B:424:TRP:O	2.19	0.42
1:B:365:GLU:OE1	1:B:368:ARG:NE	2.29	0.42
1:B:375:SER:O	1:B:503:LEU:HD21	2.19	0.42
1:B:404:GLY:O	1:B:408:ARG:HG2	2.19	0.42
1:B:499:ASP:O	1:B:505:SER:HA	2.18	0.42
1:A:58:TRP:HB3	1:A:59:PHE:HE1	1.71	0.42
1:A:411:GLU:N	1:A:411:GLU:OE1	2.52	0.42
1:B:222:TYR:CD1	1:B:305:LEU:HD21	2.52	0.42
1:B:352:ASN:OD1	1:B:353:LEU:N	2.53	0.42
1:A:438:VAL:N	1:A:444:LEU:HD23	2.34	0.42
1:A:447:LYS:O	1:A:449:THR:OG1	2.22	0.42
1:B:460:ARG:O	1:B:461:HIS:CB	2.68	0.42
1:A:433:GLU:N	1:A:433:GLU:OE1	2.52	0.42
1:B:107:PHE:CE2	1:B:384:MET:SD	3.12	0.42
1:B:275:GLU:O	1:B:279:TRP:HB3	2.20	0.42
1:B:428:ILE:HD12	1:B:429:ALA:H	1.83	0.42
1:B:117:CYS:SG	1:B:119:GLU:OE1	2.78	0.42
1:B:118:ALA:H	1:B:460:ARG:HH22	1.66	0.42
1:B:152:TYR:CE1	1:B:279:TRP:CD1	3.08	0.42
1:B:202:SER:HA	1:B:206:GLN:HG3	2.01	0.42
1:A:125:LEU:C	1:A:125:LEU:HD23	2.41	0.41
1:B:217:THR:O	1:B:217:THR:OG1	2.36	0.41
1:A:446:SER:OG	1:A:448:GLY:N	2.53	0.41
1:A:490:PRO:CD	1:A:492:VAL:H	2.32	0.41
1:B:87:PHE:CE1	1:B:100:LEU:HD11	2.55	0.41
1:B:377:ILE:HD13	3:B:590:VNI:H26	2.00	0.41
1:A:218:PHE:CE2	1:A:222:TYR:CE2	3.07	0.41
1:A:288:ASN:CG	1:A:290:THR:HG1	2.23	0.41
1:B:160:ARG:CG	1:B:350:TYR:HB3	2.51	0.41
1:B:334:TYR:O	1:B:338:ILE:HG12	2.20	0.41
1:A:456:PHE:CD2	1:A:466:GLU:HG3	2.56	0.41
1:B:110:ASN:CG	1:B:447:LYS:HE2	2.41	0.41
1:B:338:ILE:O	1:B:342:GLY:HA2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:365:GLU:OE2	1:B:423:ARG:HD2	2.20	0.41
1:A:259:MET:CE	1:A:295:GLU:HA	2.51	0.41
1:A:340:VAL:CG2	1:A:341:LEU:N	2.84	0.41
1:A:384:MET:HE2	1:A:384:MET:HB3	1.93	0.41
1:A:447:LYS:O	1:A:449:THR:CB	2.69	0.41
1:A:58:TRP:C	1:A:59:PHE:HD1	2.24	0.41
1:B:149:PHE:HE2	1:B:286:TYR:CE1	2.39	0.41
1:B:170:VAL:HG12	1:B:170:VAL:O	2.20	0.41
1:B:270:SER:N	4:B:2025:HOH:O	2.49	0.41
1:B:453:TYR:CD1	1:B:455:PRO:CD	3.03	0.41
1:A:340:VAL:HG23	1:A:341:LEU:H	1.84	0.41
1:B:405:VAL:O	1:B:408:ARG:O	2.39	0.41
1:B:150:VAL:CG1	1:B:464:ILE:HD11	2.51	0.41
1:B:285:VAL:O	1:B:286:TYR:CD1	2.74	0.41
1:A:191:LYS:CE	4:A:2040:HOH:O	2.68	0.40
1:A:193:ILE:HD13	1:A:193:ILE:HA	1.94	0.40
1:A:279:TRP:CH2	1:A:283:SER:OG	2.70	0.40
1:A:53:PRO:CB	1:A:83:TYR:HD2	2.34	0.40
1:A:94:LYS:HG3	1:A:95:LYS:N	2.35	0.40
1:A:163:VAL:N	1:A:164:PRO:HD2	2.36	0.40
1:A:449:THR:HB	1:A:458:ALA:CB	2.51	0.40
1:B:358:LEU:O	1:B:361:LYS:HB2	2.21	0.40
1:B:358:LEU:O	1:B:362:VAL:N	2.45	0.40
1:B:384:MET:N	1:B:393:ILE:CD1	2.83	0.40
1:B:400:LEU:HD23	1:B:400:LEU:C	2.42	0.40
1:B:420:ASN:HB3	1:B:423:ARG:HB3	2.03	0.40
1:B:429:ALA:HB2	1:B:431:SER:C	2.41	0.40
1:B:489:LEU:O	1:B:490:PRO:C	2.59	0.40
1:A:336:GLU:O	1:A:340:VAL:CG2	2.54	0.40
1:A:393:ILE:HA	1:A:394:PRO:HD3	1.68	0.40
1:B:105:ASN:O	1:B:108:ILE:HG13	2.20	0.40
1:B:465:GLY:O	1:B:466:GLU:C	2.59	0.40
1:A:447:LYS:O	1:A:447:LYS:HG3	2.21	0.40
1:B:80:ARG:NH2	1:B:411:GLU:OE2	2.52	0.40
1:B:107:PHE:HE2	1:B:384:MET:SD	2.45	0.40
1:B:152:TYR:CE2	1:B:283:SER:HB3	2.57	0.40
1:B:155:THR:O	1:B:156:SER:C	2.60	0.40
1:B:341:LEU:CD1	1:B:346:PRO:HB2	2.52	0.40
1:B:345:LEU:N	1:B:346:PRO:HD2	2.37	0.40
1:B:351:ASP:O	1:B:354:GLN:HG2	2.22	0.40
1:A:59:PHE:HD1	1:A:59:PHE:N	2.17	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:PHE:O	1:A:177:SER:HB3	2.21	0.40
1:A:236:LEU:HD23	1:A:238:TRP:CH2	2.55	0.40
1:A:284:CYS:O	1:A:285:VAL:CG2	2.70	0.40
1:A:463:CYS:HB2	2:A:580:HEM:NA	2.35	0.40
1:B:275:GLU:OE1	1:B:278:VAL:HG13	2.21	0.40
1:B:451:SER:OG	1:B:452:PRO:CD	2.69	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	468/470 (100%)	445 (95%)	20 (4%)	3 (1%)	25	54
1	B	468/470 (100%)	442 (94%)	23 (5%)	3 (1%)	25	54
All	All	936/940 (100%)	887 (95%)	43 (5%)	6 (1%)	25	54

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	51	THR
1	B	51	THR
1	B	156	SER
1	A	135	VAL
1	B	135	VAL
1	A	236	LEU

5.3.2 Protein sidechains ⓘ

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	411/411 (100%)	372 (90%)	39 (10%)	8	24
1	B	411/411 (100%)	351 (85%)	60 (15%)	3	9
All	All	822/822 (100%)	723 (88%)	99 (12%)	5	15

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	LYS
1	A	51	THR
1	A	59	PHE
1	A	61	PHE
1	A	64	SER
1	A	83	TYR
1	A	92	LEU
1	A	114	ARG
1	A	138	CYS
1	A	140	ASN
1	A	184	LYS
1	A	191	LYS
1	A	203	ARG
1	A	217	THR
1	A	220	GLU
1	A	234	PHE
1	A	241	LEU
1	A	253	LYS
1	A	277	MET
1	A	283	SER
1	A	290	THR
1	A	341	LEU
1	A	344	ASP
1	A	352	ASN
1	A	381	LYS
1	A	387	ASP
1	A	397	HIS
1	A	408	ARG
1	A	427	ASN
1	A	428	ILE
1	A	444	LEU
1	A	462	ARG
1	A	471	LEU

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Mol	Chain	Res	Type
1	A	487	ARG
1	A	493	ASP
1	A	503	LEU
1	A	506	LYS
1	A	511	SER
1	A	519	HIS
1	B	51	THR
1	B	55	VAL
1	B	75	PHE
1	B	85	ASP
1	B	86	ILE
1	B	92	LEU
1	B	95	LYS
1	B	107	PHE
1	B	108	ILE
1	B	109	LEU
1	B	110	ASN
1	B	112	LYS
1	B	125	LEU
1	B	126	THR
1	B	140	ASN
1	B	143	LEU
1	B	146	GLN
1	B	152	TYR
1	B	160	ARG
1	B	203	ARG
1	B	216	SER
1	B	217	THR
1	B	235	MET
1	B	262	ILE
1	B	272	LYS
1	B	275	GLU
1	B	276	ASP
1	B	285	VAL
1	B	286	TYR
1	B	292	VAL
1	B	312	SER
1	B	336	GLU
1	B	337	GLN
1	B	341	LEU
1	B	344	ASP
1	B	345	LEU

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Mol	Chain	Res	Type
1	B	357	ASP
1	B	381	LYS
1	B	393	ILE
1	B	395	THR
1	B	397	HIS
1	B	409	SER
1	B	423	ARG
1	B	424	TRP
1	B	436	GLU
1	B	437	LYS
1	B	438	VAL
1	B	439	ASP
1	B	442	TYR
1	B	453	TYR
1	B	471	LEU
1	B	487	ARG
1	B	489	LEU
1	B	495	ILE
1	B	502	SER
1	B	503	LEU
1	B	506	LYS
1	B	508	LEU
1	B	511	SER
1	B	519	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	359	HIS
1	A	450	ASN
1	A	472	GLN
1	A	488	ASN
1	B	110	ASN
1	B	181	GLN
1	B	280	ASN
1	B	397	HIS
1	B	422	HIS
1	B	427	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides 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	$\#\|Z\| > 2$
3	VNI	A	590	2	31,39,39	1.78	7 (22%)	39,54,54	1.59	6 (15%)
3	VNI	B	590	2	31,39,39	1.90	4 (12%)	39,54,54	1.37	5 (12%)
2	HEM	A	580	3,1	41,50,50	1.89	12 (29%)	45,82,82	2.22	13 (28%)
2	HEM	B	580	3,1	41,50,50	1.69	8 (19%)	45,82,82	2.29	12 (26%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	VNI	A	590	2	-	3/16/24/24	0/5/5/5
3	VNI	B	590	2	-	1/16/24/24	0/5/5/5
2	HEM	A	580	3,1	-	5/12/54/54	-
2	HEM	B	580	3,1	-	1/12/54/54	-

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	590	VNI	C12-C7	7.07	1.48	1.39
2	A	580	HEM	C1B-NB	-5.16	1.31	1.40
3	A	590	VNI	C12-C7	4.94	1.45	1.39
2	B	580	HEM	C4D-ND	-4.88	1.31	1.40
2	B	580	HEM	C1B-NB	-4.44	1.32	1.40
3	A	590	VNI	C7-C2	-3.98	1.45	1.52
2	A	580	HEM	C4D-ND	-3.97	1.33	1.40
3	B	590	VNI	C7-C2	-3.59	1.46	1.52
2	A	580	HEM	C1B-C2B	-3.42	1.37	1.44
2	A	580	HEM	C4B-NB	-3.39	1.31	1.38
2	A	580	HEM	C1D-ND	-3.37	1.31	1.38
3	B	590	VNI	C4-N2	-3.25	1.31	1.37
2	A	580	HEM	C3C-C2C	-3.19	1.35	1.40
2	B	580	HEM	C4B-NB	-3.09	1.32	1.38
3	A	590	VNI	C3-N2	-2.95	1.45	1.48
2	B	580	HEM	FE-ND	-2.89	1.82	1.96
2	A	580	HEM	FE-ND	-2.76	1.83	1.96
3	B	590	VNI	C3-N2	-2.73	1.45	1.48
3	A	590	VNI	C4-N2	-2.71	1.32	1.37
2	B	580	HEM	C3C-C2C	-2.45	1.37	1.40
2	B	580	HEM	C1D-ND	-2.38	1.33	1.38
3	A	590	VNI	C11-C12	-2.35	1.34	1.38
2	A	580	HEM	C4A-CHB	-2.34	1.34	1.41
2	A	580	HEM	C3D-C2D	-2.33	1.31	1.36
3	A	590	VNI	C8-C7	-2.31	1.36	1.39
3	A	590	VNI	C2-N1	-2.27	1.43	1.46
2	A	580	HEM	O2D-CGD	-2.24	1.23	1.30
2	A	580	HEM	CAA-C2A	-2.13	1.48	1.52
2	A	580	HEM	O2A-CGA	-2.07	1.23	1.30
2	B	580	HEM	FE-NB	2.03	2.06	1.96
2	B	580	HEM	O2A-CGA	-2.01	1.24	1.30

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	580	HEM	CHC-C4B-NB	5.81	130.74	124.43
2	B	580	HEM	CHC-C4B-NB	5.54	130.45	124.43
2	B	580	HEM	CHD-C1D-ND	5.52	130.42	124.43
2	B	580	HEM	CBA-CAA-C2A	-5.38	103.44	112.62
2	A	580	HEM	CHB-C1B-NB	5.25	130.87	124.38
2	A	580	HEM	CHD-C1D-ND	4.88	129.74	124.43
2	A	580	HEM	C1B-NB-C4B	4.82	110.05	105.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	590	VNI	C7-C12-CL2	4.51	125.08	120.41
2	B	580	HEM	CHA-C4D-ND	4.39	129.81	124.38
2	B	580	HEM	CHD-C1D-C2D	-3.88	118.92	124.98
2	B	580	HEM	C1B-NB-C4B	3.87	109.07	105.07
3	A	590	VNI	C26-C21-C22	3.85	122.06	118.65
2	B	580	HEM	CAD-CBD-CGD	-3.84	105.34	113.60
2	B	580	HEM	O2D-CGD-CBD	3.83	126.35	114.03
2	A	580	HEM	CAD-C3D-C4D	3.72	131.17	124.66
2	A	580	HEM	CHD-C1D-C2D	-3.61	119.34	124.98
2	A	580	HEM	CHA-C4D-ND	3.52	128.74	124.38
3	B	590	VNI	C11-C12-C7	-3.32	118.45	122.41
2	A	580	HEM	CBA-CAA-C2A	-3.16	107.22	112.62
3	A	590	VNI	C12-C7-C2	-3.14	117.69	121.71
3	A	590	VNI	C15-C16-C17	3.01	121.32	118.65
3	A	590	VNI	C11-C10-CL1	-2.97	115.44	119.15
2	B	580	HEM	CHB-C1B-NB	2.89	127.95	124.38
2	A	580	HEM	CHB-C1B-C2B	-2.84	118.87	126.72
2	B	580	HEM	CHA-C4D-C3D	-2.80	120.08	125.33
2	B	580	HEM	O2D-CGD-O1D	-2.72	116.53	123.30
3	A	590	VNI	C7-C2-N1	-2.71	106.00	111.47
2	A	580	HEM	CAD-C3D-C2D	-2.56	123.11	127.88
2	A	580	HEM	CHA-C4D-C3D	-2.41	120.80	125.33
2	A	580	HEM	O2D-CGD-O1D	-2.39	117.34	123.30
3	A	590	VNI	C7-C12-CL2	2.35	122.84	120.41
3	B	590	VNI	C3-C2-N1	-2.29	106.46	110.45
3	B	590	VNI	C26-C21-C22	2.14	120.55	118.65
2	A	580	HEM	O2D-CGD-CBD	2.12	120.84	114.03
2	B	580	HEM	CMB-C2B-C1B	2.05	128.17	125.04
3	B	590	VNI	C8-C7-C12	2.04	118.84	116.81

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	590	VNI	C7-C2-N1-C1
2	A	580	HEM	C2D-C3D-CAD-CBD
2	A	580	HEM	C4D-C3D-CAD-CBD
3	A	590	VNI	C3-C2-C7-C12
3	A	590	VNI	C3-C2-C7-C8
2	A	580	HEM	CAA-CBA-CGA-O1A
2	A	580	HEM	CAA-CBA-CGA-O2A
3	A	590	VNI	C7-C2-N1-C1

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Mol	Chain	Res	Type	Atoms
2	B	580	HEM	CAA-CBA-CGA-O2A
2	A	580	HEM	CAD-CBD-CGD-O2D

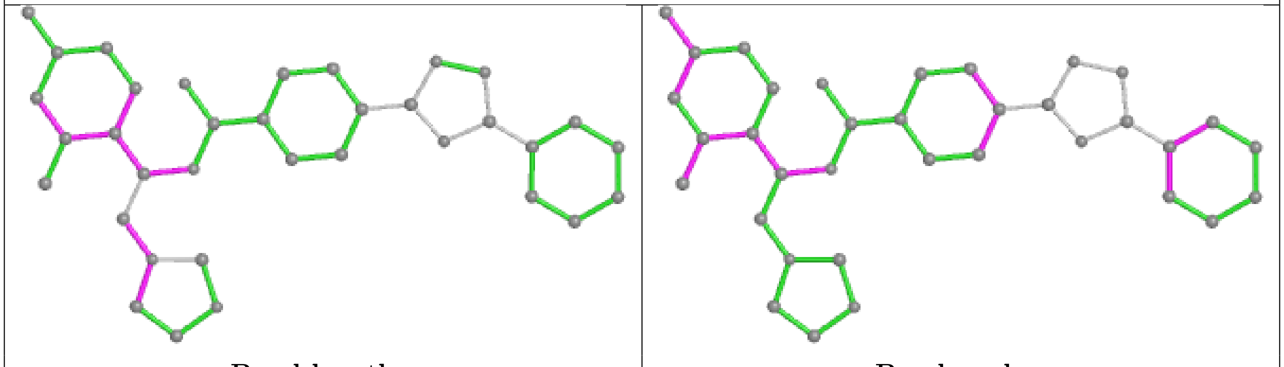
There are no ring outliers.

4 monomers are involved in 38 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	590	VNI	2	0
3	B	590	VNI	11	0
2	A	580	HEM	10	0
2	B	580	HEM	15	0

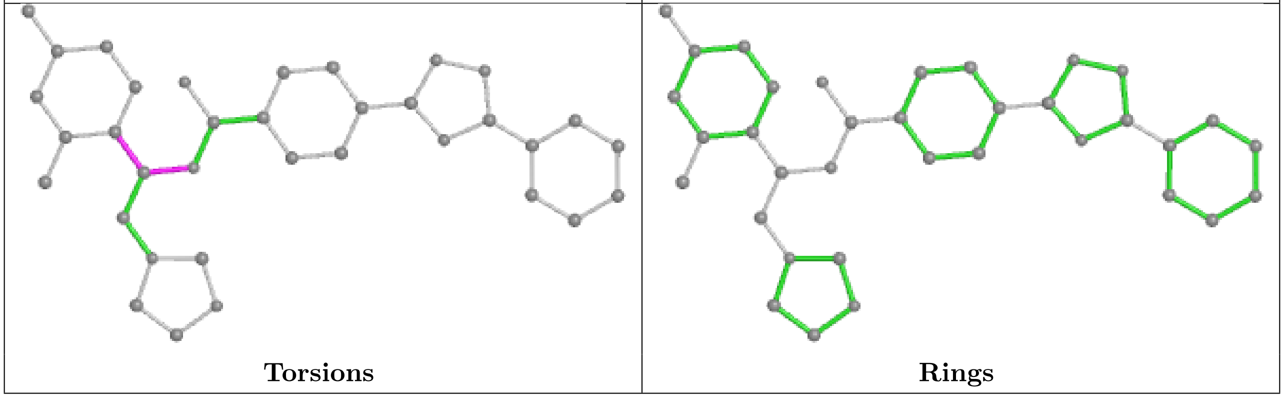
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 VNI A 590



Bond lengths

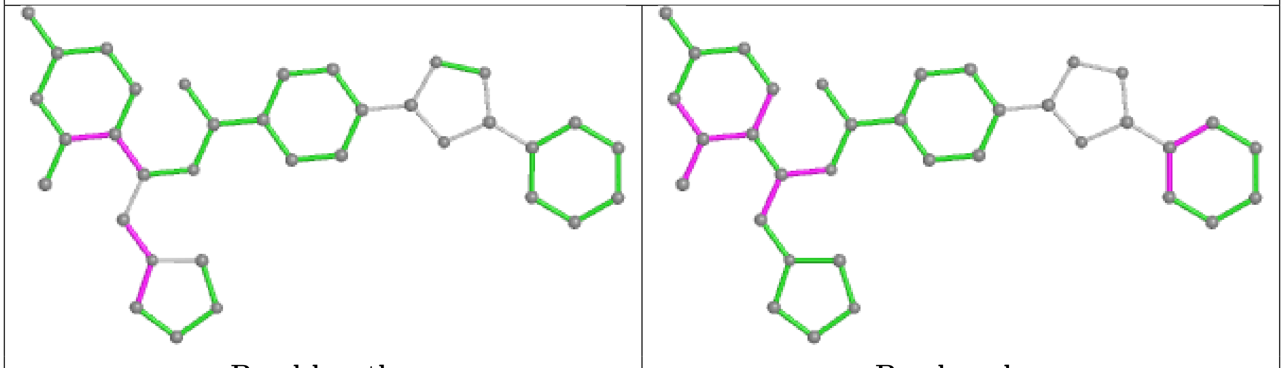
Bond angles



Torsions

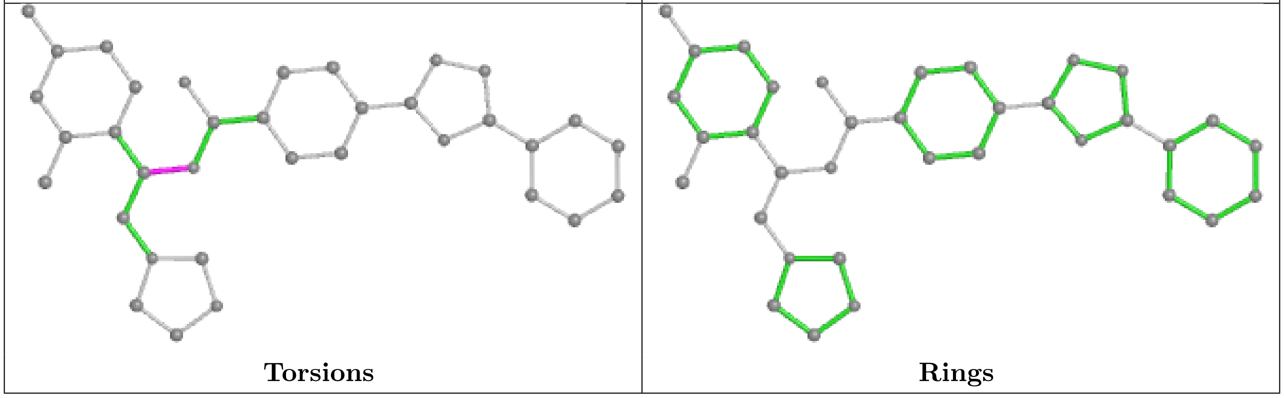
Rings

Ligand VNI B 590



Bond lengths

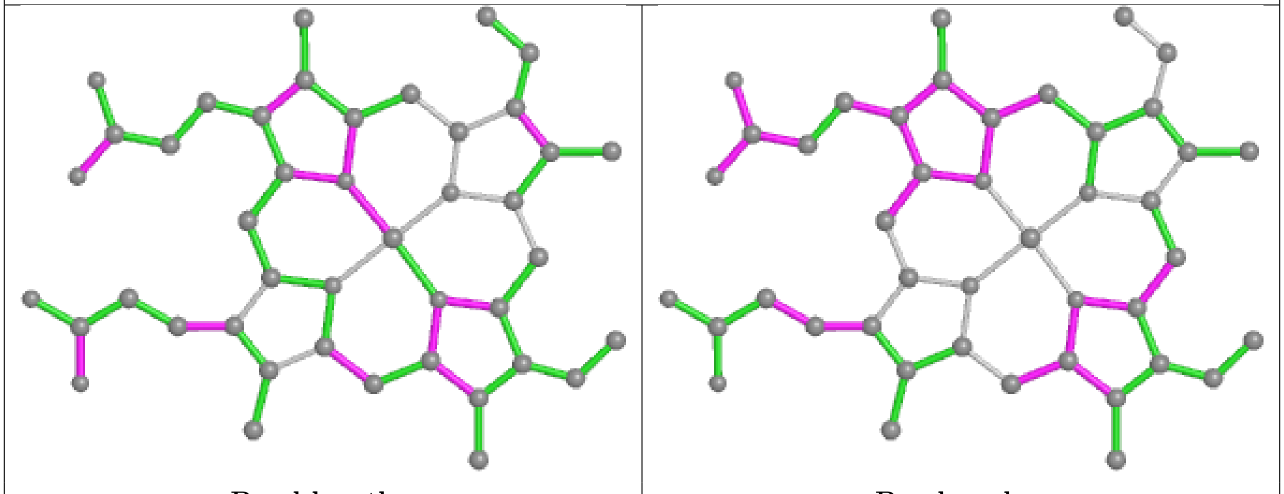
Bond angles



Torsions

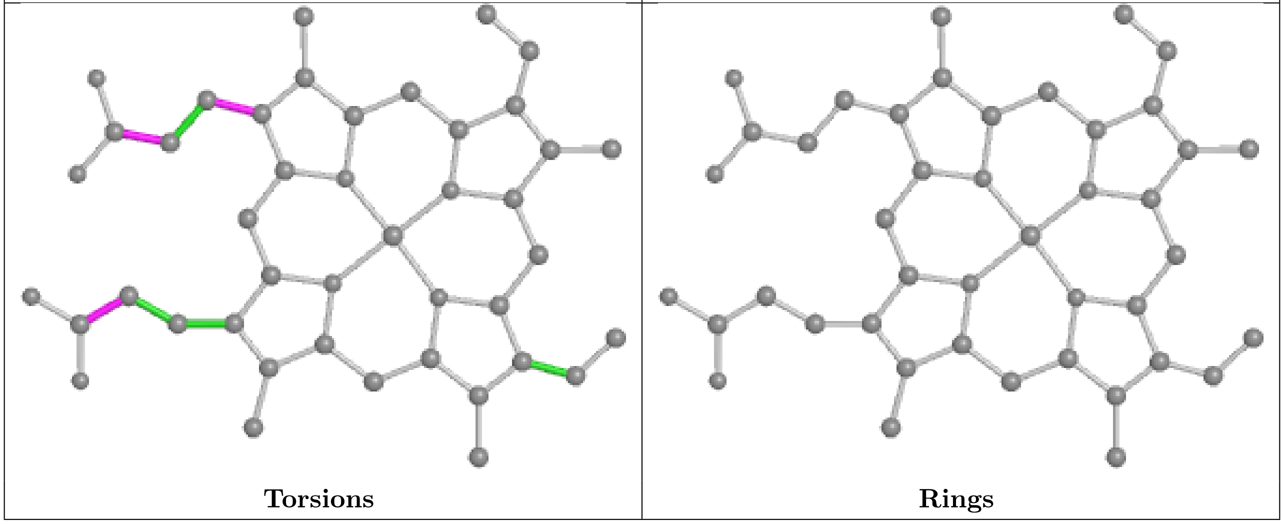
Rings

Ligand HEM A 580



Bond lengths

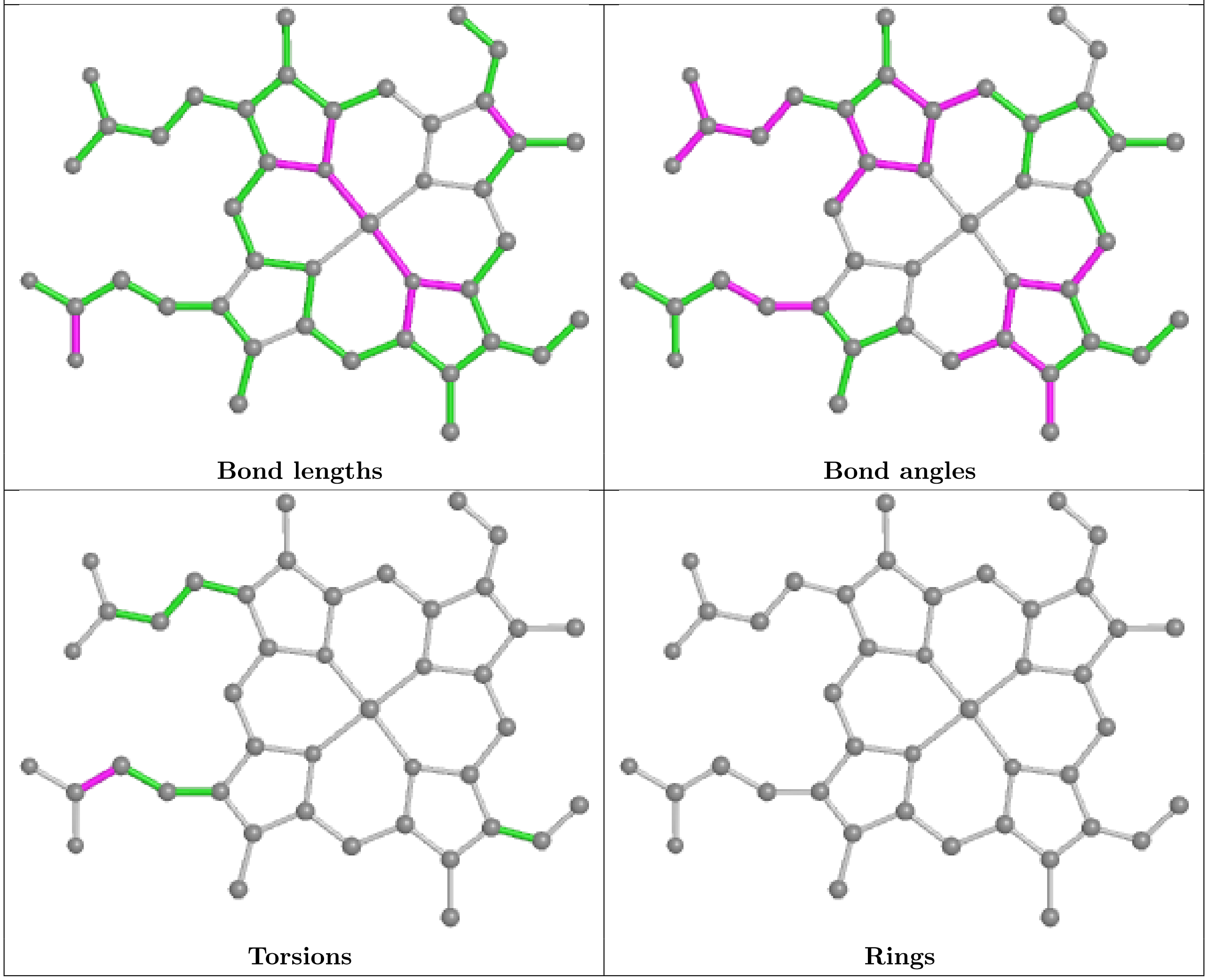
Bond angles



Torsions

Rings

Ligand HEM B 580



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	470/470 (100%)	0.35	35 (7%) 14 8	48, 78, 121, 184	0
1	B	470/470 (100%)	0.80	80 (17%) 1 1	64, 100, 152, 235	0
All	All	940/940 (100%)	0.58	115 (12%) 4 2	48, 89, 143, 235	0

All (115) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	427	ASN	11.1
1	B	428	ILE	8.8
1	A	428	ILE	8.3
1	B	429	ALA	7.7
1	A	427	ASN	7.4
1	B	432	ALA	6.9
1	B	60	PRO	6.5
1	B	430	ALA	5.5
1	B	444	LEU	4.9
1	B	440	TYR	4.9
1	A	431	SER	4.6
1	B	431	SER	4.2
1	B	59	PHE	4.1
1	B	345	LEU	4.1
1	B	448	GLY	3.9
1	B	56	PHE	3.8
1	B	433	GLU	3.8
1	A	303	ALA	3.7
1	B	113	LEU	3.6
1	B	312	SER	3.5
1	B	157	ASP	3.5
1	A	113	LEU	3.5
1	B	424	TRP	3.5
1	A	402	SER	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	386	VAL	3.4
1	A	58	TRP	3.4
1	B	50	LYS	3.3
1	A	57	HIS	3.3
1	B	519	HIS	3.2
1	B	344	ASP	3.1
1	B	315	THR	3.1
1	A	291	PRO	3.1
1	A	418	GLU	3.0
1	B	383	PRO	3.0
1	A	503	LEU	3.0
1	B	373	ILE	3.0
1	A	304	LEU	3.0
1	B	316	ALA	2.9
1	B	382	ASN	2.9
1	B	270	SER	2.9
1	B	397	HIS	2.9
1	B	308	GLY	2.9
1	B	445	VAL	2.9
1	B	273	ASP	2.9
1	A	519	HIS	2.9
1	B	426	GLU	2.8
1	B	304	LEU	2.8
1	B	311	SER	2.8
1	A	290	THR	2.8
1	B	490	PRO	2.8
1	B	284	CYS	2.7
1	B	58	TRP	2.7
1	B	355	LYS	2.7
1	B	319	ILE	2.7
1	B	282	MET	2.7
1	B	375	SER	2.6
1	A	430	ALA	2.6
1	A	401	SER	2.6
1	B	385	ALA	2.5
1	A	217	THR	2.5
1	A	508	LEU	2.5
1	B	102	THR	2.5
1	B	84	GLY	2.5
1	B	395	THR	2.5
1	B	475	THR	2.5
1	B	371	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	443	GLY	2.4
1	B	400	LEU	2.4
1	B	200	THR	2.4
1	B	346	PRO	2.4
1	B	390	SER	2.4
1	B	197	THR	2.4
1	B	310	HIS	2.3
1	A	312	SER	2.3
1	B	98	VAL	2.3
1	B	266	ARG	2.3
1	A	311	SER	2.3
1	A	340	VAL	2.3
1	B	301	MET	2.3
1	A	414	PRO	2.3
1	A	473	LEU	2.3
1	B	474	GLY	2.3
1	B	279	TRP	2.3
1	A	316	ALA	2.3
1	A	477	THR	2.3
1	B	415	ASN	2.3
1	B	388	GLY	2.3
1	B	435	ASP	2.2
1	B	459	GLY	2.2
1	B	402	SER	2.2
1	B	423	ARG	2.2
1	A	307	ALA	2.2
1	B	154	LEU	2.2
1	B	62	ILE	2.2
1	B	473	LEU	2.2
1	A	490	PRO	2.2
1	A	491	GLY	2.2
1	B	109	LEU	2.2
1	A	412	HIS	2.2
1	B	217	THR	2.2
1	B	446	SER	2.2
1	A	429	ALA	2.2
1	A	433	GLU	2.2
1	B	451	SER	2.1
1	B	149	PHE	2.1
1	B	503	LEU	2.1
1	A	424	TRP	2.1
1	B	477	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	278	VAL	2.1
1	A	373	ILE	2.1
1	A	469	ALA	2.1
1	A	310	HIS	2.0
1	B	376	ILE	2.0
1	B	508	LEU	2.0
1	B	142	LYS	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

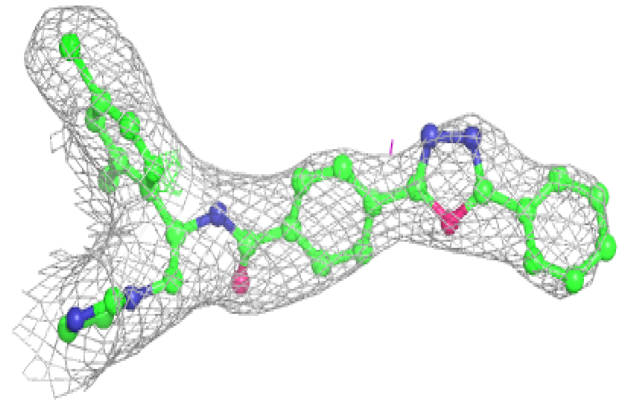
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

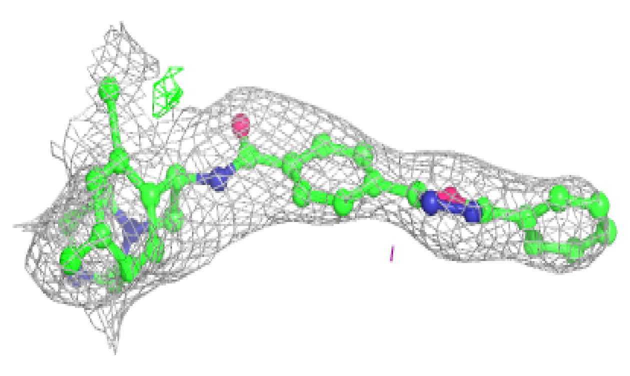
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	VNI	B	590	35/35	0.93	0.26	63,93,105,106	0
3	VNI	A	590	35/35	0.94	0.28	56,86,101,104	0
2	HEM	A	580	43/43	0.97	0.27	52,65,80,83	0
2	HEM	B	580	43/43	0.97	0.21	68,89,99,107	0

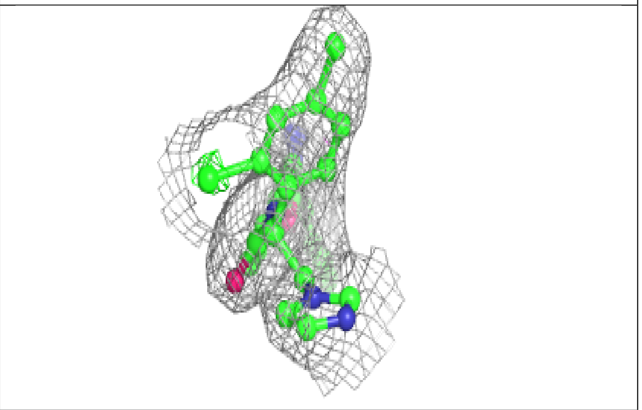
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around VNI B 590:

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

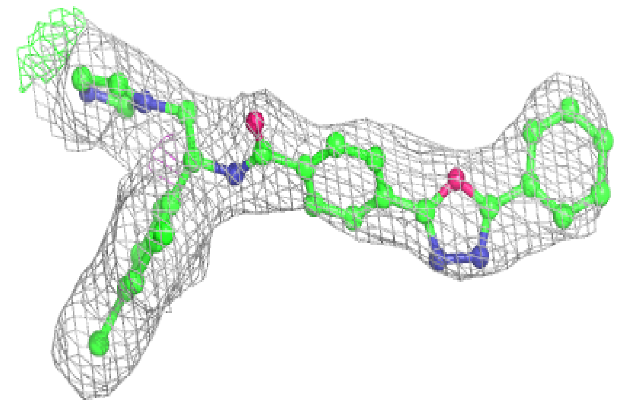


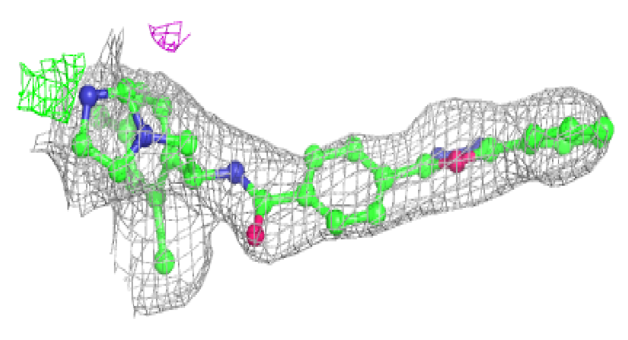


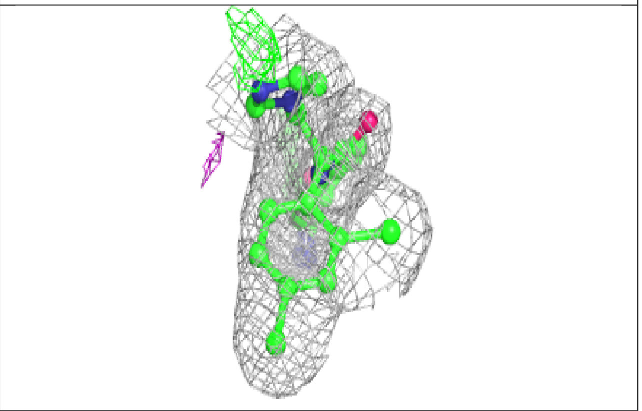


Electron density around VNI A 590:

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

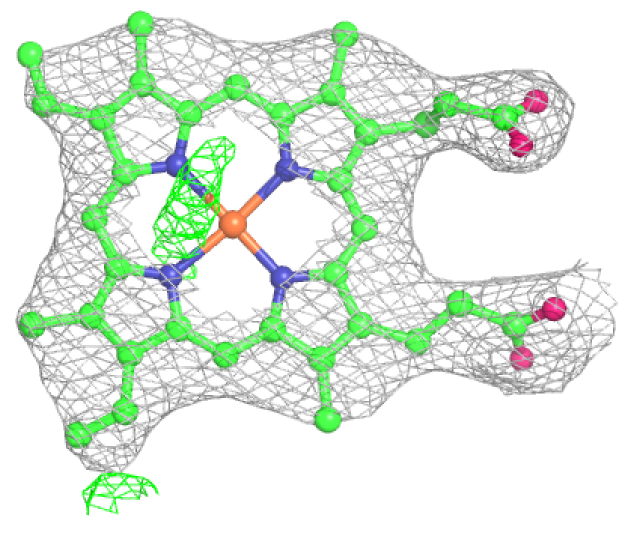


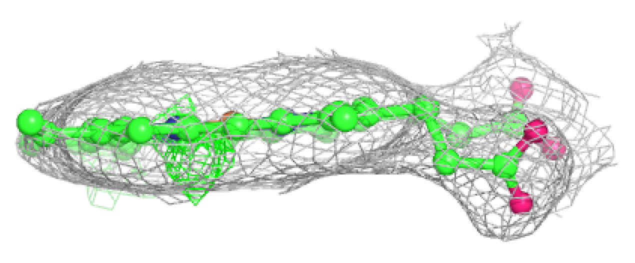


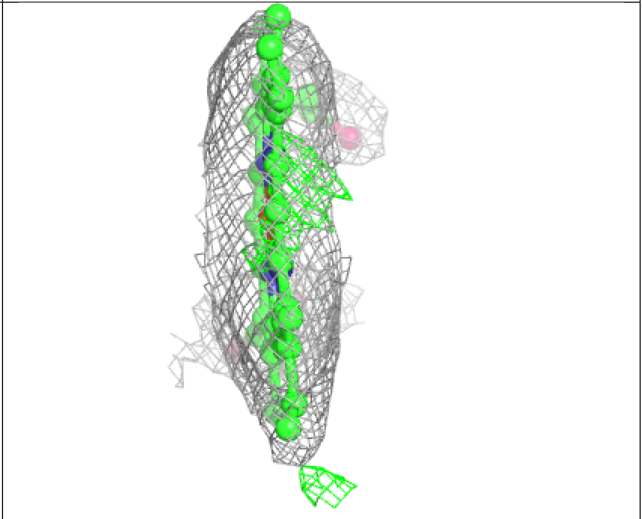


Electron density around HEM A 580:

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

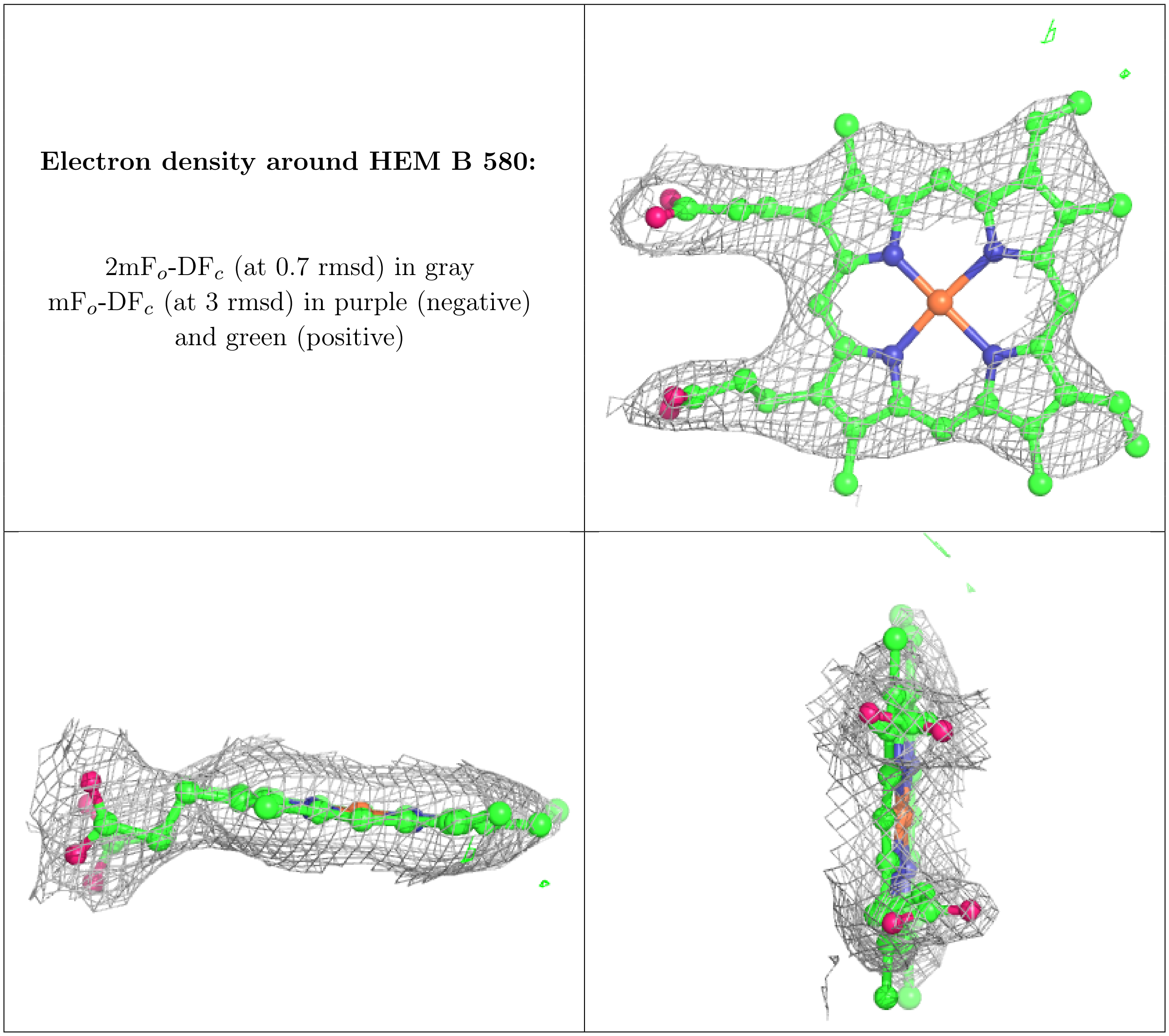






Electron density around HEM B 580:

$2mF_o$-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

There are no such residues in this entry.