



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 19, 2026 – 11:05 AM UTC

PDB ID : 4UYL / pdb_00004uyL
Title : Crystal structure of sterol 14- α 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)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

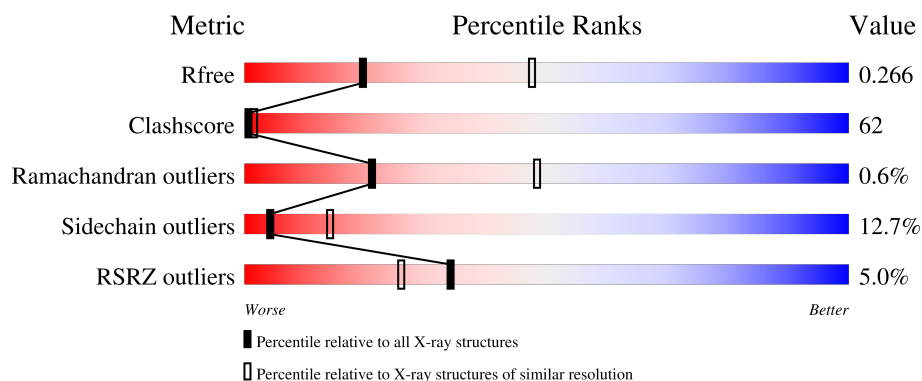
1 Overall quality at a glance

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}	180053	4591 (2.84-2.80)
Clashscore	190562	5010 (2.84-2.80)
Ramachandran outliers	187476	4916 (2.84-2.80)
Sidechain outliers	187428	4918 (2.84-2.80)
RSRZ outliers	180081	4594 (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 $\leq 5\%$. 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	4% 52% 37% 11%
1	B	470	6% 33% 53% 13%

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 [i](#)

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.

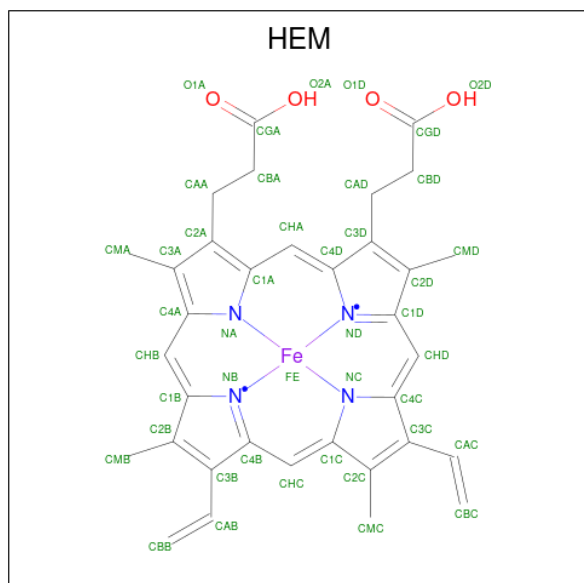
- Molecule 1 is a protein called 14-ALPHA STEROL DEMETHYLASE.

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:

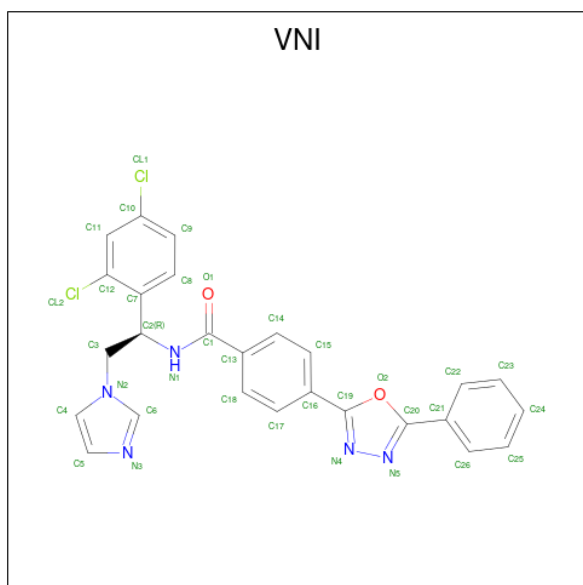
Chain	Residue	Modelled	Actual	Comment	Reference
A	50	LYS	HIS	engineered mutation	UNP Q96W81
A	51	THR	GLU	engineered mutation	UNP Q96W81
A	519	HIS	-	expression tag	UNP Q96W81
B	50	LYS	HIS	engineered mutation	UNP Q96W81
B	51	THR	GLU	engineered mutation	UNP Q96W81
B	519	HIS	-	expression tag	UNP Q96W81

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



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

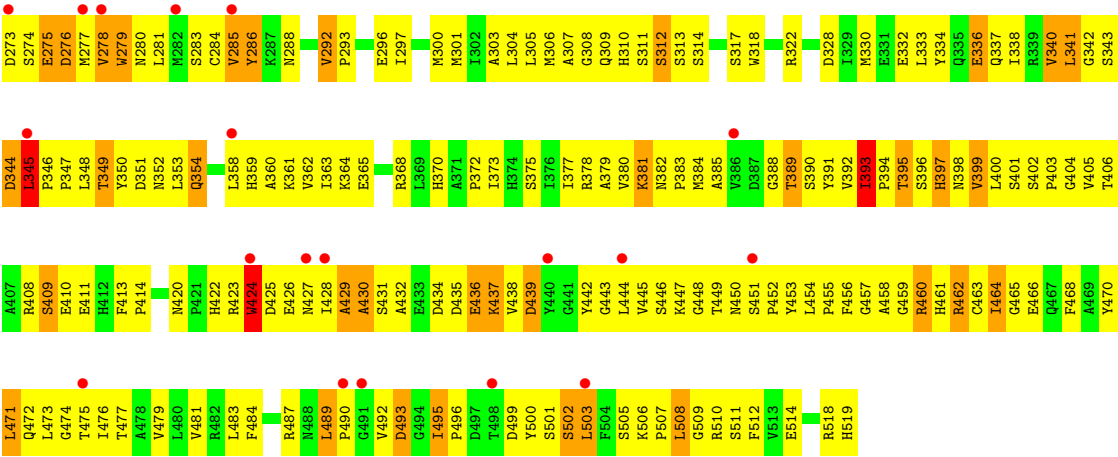
- Molecule 3 is N-[(1R)-1-(2,4-dichlorophenyl)-2-(1H-imidazol-1-yl)ethyl]-4-(5-phenyl-1,3,4-oxadiazol-2-yl)benzamide (CCD ID: VNI) (formula: C₂₆H₁₉Cl₂N₅O₂).



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

- Molecule 4 is water.

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



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 95.69 – 2.81	Depositor EDS
% Data completeness (in resolution range)	99.7 (95.69-2.81) 99.7 (95.69-2.81)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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 , 80.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	0.50	0/3854	0.97	19/5229 (0.4%)
1	B	0.46	2/3854 (0.1%)	1.05	24/5229 (0.5%)
All	All	0.48	2/7708 (0.0%)	1.01	43/10458 (0.4%)

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	430	ALA	CA-C	6.95	1.61	1.52
1	B	345	LEU	C-N	5.10	1.39	1.33

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	283	SER	N-CA-C	-12.19	94.25	111.81
1	B	108	ILE	N-CA-C	-12.06	100.24	111.45
1	B	115	ASP	N-CA-C	10.13	122.08	111.14
1	A	430	ALA	N-CA-C	-9.73	97.12	110.35
1	B	448	GLY	N-CA-C	-9.32	91.09	113.18
1	B	389	THR	N-CA-C	8.73	121.34	108.60
1	A	51	THR	CA-C-N	-7.92	112.23	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	51	THR	C-N-CA	-7.92	112.23	120.38
1	B	118	ALA	N-CA-C	7.74	119.50	111.14
1	B	51	THR	CA-C-N	-7.64	112.51	120.38
1	B	51	THR	C-N-CA	-7.64	112.51	120.38
1	B	460	ARG	N-CA-C	-7.53	98.88	110.10
1	B	370	HIS	N-CA-C	7.14	121.94	111.87
1	B	107	PHE	CB-CA-C	-7.14	97.16	110.01
1	A	502	SER	N-CA-C	-6.86	101.47	110.53
1	B	310	HIS	N-CA-C	6.77	118.74	111.36
1	B	430	ALA	N-CA-CB	6.75	119.86	110.07
1	B	279	TRP	N-CA-C	-6.74	105.61	114.31
1	A	448	GLY	N-CA-C	-6.41	97.98	113.18
1	B	462	ARG	N-CA-C	-6.30	102.21	110.53
1	B	430	ALA	N-CA-C	6.23	117.87	111.14
1	B	493	ASP	N-CA-C	6.18	118.57	108.55
1	A	282	MET	CB-CA-C	-5.91	99.62	109.55
1	B	345	LEU	CA-C-N	-5.79	114.41	120.38
1	B	345	LEU	C-N-CA	-5.79	114.41	120.38
1	B	107	PHE	N-CA-C	5.79	120.34	113.16
1	A	343	SER	N-CA-C	-5.73	105.01	112.23
1	A	59	PHE	CA-C-N	-5.69	114.11	120.14
1	A	59	PHE	C-N-CA	-5.69	114.11	120.14
1	A	86	ILE	N-CA-C	5.67	116.04	108.11
1	B	52	PRO	CA-C-N	-5.65	113.96	119.78
1	B	52	PRO	C-N-CA	-5.65	113.96	119.78
1	B	278	VAL	N-CA-C	-5.64	105.60	112.76
1	A	205	LEU	N-CA-C	5.63	117.50	111.36
1	A	393	ILE	CA-C-N	5.58	125.56	120.03
1	A	393	ILE	C-N-CA	5.58	125.56	120.03
1	A	337	GLN	N-CA-C	-5.50	104.30	111.02
1	A	495	ILE	CA-C-N	-5.35	114.74	120.03
1	A	495	ILE	C-N-CA	-5.35	114.74	120.03
1	B	393	ILE	N-CA-C	5.23	114.66	108.96
1	A	274	SER	N-CA-C	5.18	117.57	108.56
1	A	447	LYS	N-CA-C	-5.14	105.85	111.82
1	B	150	VAL	N-CA-C	-5.10	106.17	111.58

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	270	SER	Peptide

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Mol	Chain	Res	Type	Group
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 [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	3752	0	3719	333	0
1	B	3752	0	3719	598	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	18	0
4	B	43	0	0	8	0
All	All	7788	0	7536	937	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 62.

All (937) 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
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:109:LEU:C	1:B:109:LEU:HD23	1.47	1.26

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:262:ILE:HG23	1:B:281:LEU:CD2	1.71	1.21
1:B:109:LEU:C	1:B:109:LEU:CD2	2.14	1.20
1:B:307:ALA:HA	3:B:590:VNI:CL2	1.79	1.19
1:A:447:LYS:C	1:A:449:THR:HG23	1.69	1.18
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: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: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:384:MET:C	1:B:392:VAL:HG23	1.72	1.12
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:518:ARG:C	1:A:519:HIS:HD1	1.71	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:B:114:ARG:C	1:B:381:LYS:HD2	1.90	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:265:ARG:HH12	1:B:278:VAL:HG13	1.33	0.92
1:B:384:MET:C	1:B:392:VAL:CG2	2.42	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: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: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:100:LEU:C	1:B:104:GLY:HA3	1.98	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:110:ASN:HB3	1:B:447:LYS:HZ3	1.37	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: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:C	1:B:236:LEU:HD23	2.01	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
1:B:242:PRO:O	1:B:246:LYS:HG2	1.75	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:TRP:HB2	1:A:59:PHE:HD1	1.40	0.85
1:B:330:MET:HE3	1:B:484:PHE:O	1.77	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: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:A:279:TRP:C	1:A:283:SER:HB2	2.04	0.83
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:106:ASP:CG	1:B:107:PHE:HD1	1.87	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: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:389:THR:HG22	1:B:390:SER:N	1.87	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

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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:B:306:MET:C	3:B:590:VNI:CL2	2.63	0.78
1:A:57:HIS:CD2	4:A:2001:HOH:O	2.36	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:A:389:THR:HG1	1:A:391:TYR:HD2	1.33	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:B:55:VAL:CG2	1:B:89:PHE:CB	2.62	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:259:MET:HE2	1:A:295:GLU:HA	1.68	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:276:ASP:C	1:A:279:TRP:HB3	2.12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:580:HEM:HBB2	2:B:580:HEM:CMB	2.18	0.73
1:B:152:TYR:OH	1:B:279:TRP:C	2.32	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:HAH	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: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:508:LEU:HD12	1:B:508:LEU:C	2.14	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:A:255:THR:HG22	1:A:259:MET:HE3	1.73	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:A:404:GLY:O	1:A:408:ARG:CG	2.38	0.70
1:B:277:MET:C	1:B:279:TRP:H	1.96	0.70
1:B:341:LEU:CG	1:B:346:PRO:CG	2.68	0.70
1:A:428:ILE:HD12	1:A:428:ILE:C	2.16	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:272:LYS:NZ	4:A:2045:HOH:O	2.24	0.69
1:B:51:THR:HG22	1:B:391:TYR:HD2	1.57	0.69
1:A:376:ILE:CG2	1:A:378:ARG:NH1	2.51	0.68
1:A:235:MET:C	1:A:237:PRO:HD2	2.18	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: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:A:372:PRO:HA	1:A:505:SER:HG	1.59	0.67
1:B:55:VAL:HG11	1:B:79:CYS:SG	2.35	0.67
1:B:106:ASP:CG	1:B:107:PHE:CD1	2.71	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:456:PHE:C	2:B:580:HEM:HMA3	2.20	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: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:A:518:ARG:C	1:A:519:HIS:ND1	2.51	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:429:ALA:CB	1:B:431:SER:C	2.70	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:95:LYS:HZ1	1:B:397:HIS:CE1	2.15	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:152:TYR:HH	1:B:279:TRP:CD1	2.16	0.64
1:B:394:PRO:HD2	1:B:397:HIS:CE1	2.32	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:372:PRO:HG2	1:B:373:ILE:HD12	1.80	0.64
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: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:110:ASN:HB3	1:B:447:LYS:NZ	2.11	0.63
1:A:270:SER:OG	1:A:271:LYS:N	2.31	0.63
1:B:280:ASN:HA	1:B:283:SER:HB3	1.81	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:109:LEU:HG	1:B:458:ALA:C	2.21	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:282:MET:C	1:A:284:CYS:H	2.05	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:400:LEU:HD23	1:A:400:LEU:C	2.26	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:281:LEU:C	1:A:284:CYS:SG	2.83	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:A:227:MET:HE1	1:A:246:LYS:CE	2.31	0.60
1:B:101:GLY:O	1:B:105:ASN:N	2.34	0.60
1:B:110:ASN:CB	1:B:447:LYS:HZ3	2.10	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: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:A:282:MET:C	1:A:284:CYS:N	2.58	0.60
1:B:306:MET:HB3	3:B:590:VNI:CL2	2.39	0.60
1:A:227:MET:HE1	1:A:246:LYS:HE3	1.82	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:A:370:HIS:O	1:A:371:ALA:C	2.44	0.59
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:A:58:TRP:C	1:A:59:PHE:CD1	2.80	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:361:LYS:NZ	1:B:425:ASP:OD1	2.24	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:A:188:ASP:C	1:A:188:ASP:OD1	2.45	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: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:447:LYS:O	1:B:449:THR:OG1	2.21	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:B:422:HIS:O	1:B:423:ARG:C	2.48	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:113:LEU:HD11	1:B:144:MET:HE2	1.87	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
2:A:580:HEM:HMB2	2:A:580:HEM:CBB	2.33	0.56
1:B:277:MET:C	1:B:279:TRP:N	2.58	0.56
1:B:332:GLU:CD	1:B:422:HIS:HE1	2.13	0.56
1:B:429:ALA:HB1	1:B:431:SER:C	2.30	0.56
1:B:152:TYR:CD1	1:B:152:TYR:C	2.83	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: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: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: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:288:ASN:OD1	1:A:289:GLY:N	2.40	0.55
1:B:91:LEU:C	1:B:92:LEU:HG	2.30	0.55
1:B:388:GLY:O	1:B:389:THR:OG1	2.19	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:B:435:ASP:CG	1:B:436:GLU:H	2.14	0.55
1:B:453:TYR:CD1	1:B:453:TYR:C	2.84	0.55
1:A:61:PHE:CD1	1:A:61:PHE:C	2.83	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:B:75:PHE:CD1	1:B:75:PHE:C	2.85	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:113:LEU:HD21	1:B:140:ASN:CG	2.32	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:286:TYR:HB3	4:A:2025:HOH:O	2.08	0.54
1:B:110:ASN:HD21	1:B:449:THR:HG21	1.71	0.54
1:B:453:TYR:CE1	1:B:455:PRO:CD	2.91	0.54
1:B:152:TYR:OH	1:B:279:TRP:O	2.25	0.54
1:B:422:HIS:C	1:B:424:TRP:N	2.64	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: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:263:LYS:NZ	4:B:2024:HOH:O	2.40	0.53
1:B:490:PRO:HG2	1:B:493:ASP:OD1	2.09	0.53
1:A:184:LYS:HG3	1:A:185:GLY:N	2.21	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:115:ASP:HB3	1:B:384:MET:HE3	1.90	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:337:GLN:O	1:A:341:LEU:N	2.41	0.53
1:A:471:LEU:CD1	1:A:471:LEU:C	2.82	0.53
1:B:424:TRP:CD1	1:B:427:ASN:O	2.61	0.53
1:B:460:ARG:O	1:B:461:HIS:HB2	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:277:MET:O	1:A:281:LEU:HG	2.08	0.52
1:A:372:PRO:HG2	1:A:373:ILE:HD12	1.92	0.52
1:B:119:GLU:H	1:B:119:GLU:CD	2.16	0.52
1:B:314:SER:O	1:B:317:SER:HB2	2.10	0.52
1:A:281:LEU:C	1:A:284:CYS:HG	2.17	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
1:A:97:THR:HB	1:A:399:VAL:HG12	1.92	0.52
1:A:133:HIS:H	1:A:137:ASP:CG	2.12	0.52
1:A:235:MET:C	1:A:237:PRO:CD	2.82	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:224:ASN:HA	1:B:227:MET:HE2	1.91	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: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: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:188:ASP:OD1	1:B:188:ASP:C	2.52	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:270:SER:OG	1:B:271:LYS:N	2.42	0.51
1:B:90:ILE:HA	1:B:95:LYS:HA	1.93	0.51
1:B:363:ILE:HD11	1:B:474:GLY:CA	2.41	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:A:499:ASP:OD1	1:A:499:ASP:C	2.53	0.51
1:A:508:LEU:HD12	1:A:508:LEU:C	2.34	0.51
1:B:110:ASN:CB	1:B:447:LYS:NZ	2.70	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:58:TRP:H	1:B:58:TRP:CD1	2.28	0.51
1:B:106:ASP:OD2	1:B:107:PHE:CE1	2.63	0.51
1:B:155:THR:C	1:B:157:ASP:N	2.66	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:277:MET:C	1:A:279:TRP:N	2.67	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:208:LYS:HZ3	1:A:272:LYS:HD2	1.75	0.50
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
1:B:406:THR:OG1	1:B:452:PRO:O	2.29	0.50
1:B:453:TYR:C	1:B:454:LEU:HD23	2.36	0.50
1:A:218:PHE:HE2	1:A:222:TYR:HE2	1.57	0.50
1:A:446:SER:OG	1:A:448:GLY:C	2.54	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:50:LYS:C	1:B:51:THR:OG1	2.54	0.50
1:B:116:VAL:HG23	1:B:460:ARG:NH1	2.26	0.50
1:A:169:GLU:HG3	1:A:203:ARG:HD3	1.91	0.50
1:A:462:ARG:CG	1:A:462:ARG:NH1	2.75	0.50
1:B:54:VAL:O	1:B:54:VAL:CG1	2.60	0.50
1:B:97:THR:OG1	1:B:397:HIS:CE1	2.65	0.50
1:B:437:LYS:HA	1:B:446:SER:HA	1.93	0.50
1:A:471:LEU:C	1:A:471:LEU:HD13	2.37	0.50
1:B:68:TYR:HH	1:B:375:SER:CB	2.25	0.50
1:A:208:LYS:NZ	4:A:2044:HOH:O	2.43	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:372:PRO:HA	1:B:505:SER:OG	2.11	0.49
1:A:282:MET:C	1:A:284:CYS:SG	2.96	0.49
1:A:485:ARG:HD2	4:A:2081:HOH:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:119:GLU:O	1:B:120:GLU:C	2.55	0.48
1:B:435:ASP:CG	1:B:436:GLU:N	2.71	0.48
1:A:386:VAL:HG11	1:A:389:THR:OG1	2.13	0.48
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:B:50:LYS:C	1:B:51:THR:HG1	2.22	0.48
1:A:83:TYR:N	1:A:83:TYR:CD1	2.82	0.48
1:A:490:PRO:HG2	1:A:492:VAL:C	2.38	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:B:109:LEU:HG	1:B:459:GLY:HA3	1.96	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: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:110:ASN:C	1:B:447:LYS:HZ1	2.21	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:492:VAL:HG12	1:B:510:ARG:HH21	1.66	0.48
1:A:117:CYS:SG	1:A:119:GLU:CD	2.97	0.47
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:427:ASN:C	1:B:427:ASN:OD1	2.57	0.47
1:B:232:ILE:HG23	1:B:233:ASN:N	2.29	0.47
1:B:427:ASN:CG	1:B:432:ALA:CB	2.85	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:288:ASN:C	1:B:288:ASN:OD1	2.57	0.47
1:B:86:ILE:O	1:B:86:ILE:HG13	2.11	0.47
1:B:427:ASN:CG	1:B:432:ALA:HB2	2.39	0.47
1:A:123:SER:N	1:A:124:PRO:CD	2.77	0.47
1:B:222:TYR:CZ	1:B:305:LEU:HD21	2.42	0.47
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:430:ALA:O	1:A:431:SER:C	2.58	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:HD13	1:A:471:LEU:O	2.14	0.47
1:A:485:ARG:NH1	4:A:2081:HOH:O	2.43	0.47
1:A:255:THR:CG2	1:A:259:MET:HE3	2.44	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:125:LEU:C	1:A:125:LEU:HD23	2.41	0.46
1:B:347:PRO:O	1:B:352:ASN:ND2	2.48	0.46
1:B:384:MET:C	1:B:392:VAL:HG21	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:110:ASN:CG	1:B:447:LYS:HE2	2.41	0.46
1:B:456:PHE:CA	2:B:580:HEM:HMA3	2.46	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
1:B:125:LEU:HD12	1:B:233:ASN:HB3	1.96	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: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:HG	2.28	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:B:400:LEU:HD23	1:B:400:LEU:C	2.42	0.45
1:B:429:ALA:HB2	1:B:431:SER:C	2.41	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:356:LEU:HB3	1:A:359:HIS:HB2	1.99	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:155:THR:O	1:B:156:SER:C	2.60	0.45
1:B:168:ASP:HA	1:B:171:GLU:HB2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:372:PRO:C	1:A:505:SER:HG	2.25	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:B:110:ASN:C	1:B:447:LYS:NZ	2.75	0.44
1:B:489:LEU:O	1:B:490:PRO:C	2.59	0.44
1:A:288:ASN:ND2	1:A:290:THR:HG1	2.13	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
2:B:580:HEM:HMC2	2:B:580:HEM:CBC	2.47	0.44
1:A:429:ALA:C	1:A:430:ALA:O	2.58	0.44
1:B:51:THR:CA	1:B:391:TYR:CD2	2.78	0.44
1:A:107:PHE:CZ	1:A:384:MET:HE2	2.53	0.44
1:A:149:PHE:O	1:A:279:TRP:NE1	2.45	0.44
1:A:448:GLY:N	1:A:449:THR:HG23	2.26	0.44
1:B:216:SER:C	1:B:218:PHE:H	2.23	0.44
1:A:224:ASN:HA	1:A:227:MET:HE2	1.99	0.44
1:B:86:ILE:CG2	1:B:99:TYR:CD2	3.01	0.44
1:B:465:GLY:O	1:B:466:GLU:C	2.59	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:B:235:MET:HE3	1:B:235:MET:HB3	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:VAL:O	1:A:392:VAL:HG13	2.16	0.43
1:B:99:TYR:CD1	1:B:104:GLY:C	2.95	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:A:266:ARG:C	1:A:268:ALA:N	2.75	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:B:109:LEU:C	1:B:111:GLY:H	2.25	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:110:ASN:CA	1:B:447:LYS:HZ1	2.30	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:155:THR:C	1:B:157:ASP:H	2.26	0.43
1:B:162:TYR:O	1:B:165:LEU:HB2	2.18	0.43
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:461:HIS:O	1:B:462:ARG:C	2.61	0.43
1:A:52:PRO:O	1:A:53:PRO:C	2.59	0.43
1:A:58:TRP:C	1:A:59:PHE:HD1	2.24	0.43
1:A:87:PHE:CD1	1:A:87:PHE:N	2.86	0.43
1:B:116:VAL:HG13	1:B:384:MET:HE1	1.99	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:105:ASN:O	1:B:106:ASP:C	2.61	0.43
1:B:138:CYS:SG	1:B:142:LYS:HB3	2.59	0.43
1:A:321:LEU:O	1:A:324:ALA:HB3	2.19	0.43
1:A:490:PRO:CG	1:A:492:VAL:N	2.78	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:358:LEU:O	1:B:359:HIS:C	2.62	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: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: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:272:LYS:O	1:A:273:ASP:CG	2.63	0.42
1:A:321:LEU:HB3	1:A:495:ILE:HD11	2.00	0.42
1:A:388:GLY:C	1:A:389:THR:CG2	2.91	0.42
1:A:395:THR:C	1:A:397:HIS:H	2.27	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:A:271:LYS:CG	1:A:272:LYS:N	2.83	0.42
1:B:110:ASN:HB3	1:B:447:LYS:HE2	2.01	0.42
1:B:113:LEU:CD2	1:B:140:ASN:CG	2.92	0.42
1:B:368:ARG:HD3	1:B:424:TRP:CH2	2.54	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:359:HIS:O	1:B:360:ALA:C	2.62	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:91:LEU:C	1:B:92:LEU:CG	2.93	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:OH	1:B:279:TRP:CD1	2.73	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:428:ILE:C	1:A:428:ILE:CD1	2.80	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:400:LEU:C	1:A:400:LEU:CD2	2.92	0.41
1:B:227:MET:HE1	1:B:246:LYS:HB2	2.02	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:338:ILE:O	1:B:342:GLY:HA2	2.20	0.41
1:B:365:GLU:OE2	1:B:423:ARG:HD2	2.20	0.41
1:A:340:VAL:CG2	1:A:341:LEU:N	2.84	0.41
1:A:447:LYS:O	1:A:449:THR:CB	2.69	0.41
1:B:471:LEU:O	1:B:475:THR:OG1	2.30	0.41
1:B:149:PHE:HE2	1:B:286:TYR:CE1	2.39	0.41
1:B:170:VAL:O	1:B:170:VAL:HG12	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:229:PHE:CE2	1:A:306:MET:HE3	2.56	0.41
1:A:288:ASN:CG	1:A:290:THR:OG1	2.64	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:268:ALA:O	1:B:269:GLY:C	2.63	0.41
1:B:285:VAL:O	1:B:286:TYR:CD1	2.74	0.41
1:B:450:ASN:CG	1:B:451:SER:N	2.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:388:GLY:C	1:A:389:THR:HG23	2.46	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:420:ASN:HB3	1:B:423:ARG:HB3	2.03	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:A:337:GLN:C	1:A:341:LEU:HB2	2.39	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:332:GLU:CD	1:B:422:HIS:CE1	2.92	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
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 [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	468/470 (100%)	445 (95%)	20 (4%)	3 (1%)	21	48
1	B	468/470 (100%)	442 (94%)	23 (5%)	3 (1%)	21	48
All	All	936/940 (100%)	887 (95%)	43 (5%)	6 (1%)	21	48

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%)	367 (89%)	44 (11%)	6	20
1	B	411/411 (100%)	351 (85%)	60 (15%)	3	10
All	All	822/822 (100%)	718 (87%)	104 (13%)	4	14

All (104) 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	88	THR

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Mol	Chain	Res	Type
1	A	95	LYS
1	A	114	ARG
1	A	138	CYS
1	A	140	ASN
1	A	184	LYS
1	A	191	LYS
1	A	217	THR
1	A	220	GLU
1	A	232	ILE
1	A	234	PHE
1	A	241	LEU
1	A	253	LYS
1	A	266	ARG
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	364	LYS
1	A	373	ILE
1	A	381	LYS
1	A	386	VAL
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
1	A	487	ARG
1	A	492	VAL
1	A	493	ASP
1	A	503	LEU
1	A	511	SER
1	A	513	VAL
1	B	51	THR
1	B	55	VAL
1	B	66	ILE
1	B	75	PHE
1	B	86	ILE

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Mol	Chain	Res	Type
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	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	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	340	VAL
1	B	341	LEU
1	B	344	ASP
1	B	345	LEU
1	B	349	THR
1	B	354	GLN
1	B	381	LYS
1	B	393	ILE
1	B	395	THR
1	B	397	HIS
1	B	399	VAL
1	B	409	SER
1	B	424	TRP
1	B	436	GLU
1	B	437	LYS
1	B	438	VAL

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Mol	Chain	Res	Type
1	B	439	ASP
1	B	442	TYR
1	B	464	ILE
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	133	HIS
1	A	183	HIS
1	A	427	ASN
1	A	450	ASN
1	A	472	GLN
1	B	110	ASN
1	B	280	ASN
1	B	397	HIS
1	B	422	HIS
1	B	427	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	580	3,1	50,50,50	1.91	13 (26%)	67,82,82	1.95	18 (26%)
2	HEM	A	580	3,1	50,50,50	2.11	21 (42%)	67,82,82	2.12	20 (29%)
3	VNI	B	590	2	39,39,39	1.71	5 (12%)	53,54,54	2.11	11 (20%)
3	VNI	A	590	2	39,39,39	1.70	9 (23%)	53,54,54	1.88	16 (30%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	B	580	3,1	-	1/14/54/54	-
2	HEM	A	580	3,1	-	5/14/54/54	-
3	VNI	B	590	2	-	6/24/24/24	0/5/5/5
3	VNI	A	590	2	-	7/24/24/24	0/5/5/5

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	590	VNI	C12-C7	7.21	1.48	1.39
2	A	580	HEM	C1B-NB	-5.11	1.31	1.40
3	A	590	VNI	C12-C7	5.03	1.45	1.39
2	B	580	HEM	C4D-ND	-4.83	1.31	1.40
2	B	580	HEM	C1B-NB	-4.39	1.32	1.40
2	A	580	HEM	C3C-C4C	-4.32	1.38	1.46
3	A	590	VNI	C7-C2	-4.16	1.45	1.52
2	B	580	HEM	FE-ND	-4.01	1.82	1.94
2	A	580	HEM	C4D-ND	-3.92	1.33	1.40
2	B	580	HEM	FE-NB	3.90	2.06	1.94
2	A	580	HEM	FE-ND	-3.79	1.83	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	590	VNI	C7-C2	-3.76	1.46	1.52
2	A	580	HEM	C4B-NB	-3.58	1.31	1.38
2	A	580	HEM	C1D-ND	-3.56	1.31	1.38
2	B	580	HEM	C1C-C2C	-3.53	1.38	1.45
2	A	580	HEM	C1C-C2C	-3.31	1.38	1.45
2	B	580	HEM	C4B-NB	-3.27	1.32	1.38
2	A	580	HEM	C1B-C2B	-3.24	1.37	1.44
2	B	580	HEM	C3C-C4C	-3.18	1.40	1.46
2	A	580	HEM	C4C-NC	-3.10	1.33	1.39
2	B	580	HEM	C1C-NC	-3.08	1.33	1.39
2	A	580	HEM	C1C-NC	-3.01	1.33	1.39
3	A	590	VNI	C19-N4	2.97	1.33	1.29
2	A	580	HEM	C1A-C2A	-2.89	1.38	1.44
2	A	580	HEM	FE-NB	2.84	2.03	1.94
3	B	590	VNI	C19-N4	2.81	1.33	1.29
2	B	580	HEM	FE-NC	2.78	2.04	1.95
2	A	580	HEM	C4A-NA	-2.73	1.34	1.39
3	A	590	VNI	C20-N5	2.62	1.33	1.29
3	B	590	VNI	C20-N5	2.56	1.33	1.29
3	A	590	VNI	C8-C7	-2.54	1.36	1.39
2	B	580	HEM	C1D-ND	-2.52	1.33	1.38
3	A	590	VNI	C3-C2	-2.50	1.50	1.53
3	A	590	VNI	C2-N1	-2.46	1.43	1.46
2	A	580	HEM	FE-NC	2.42	2.03	1.95
2	A	580	HEM	C2A-C3A	-2.39	1.32	1.38
3	A	590	VNI	C11-C12	-2.36	1.34	1.38
2	A	580	HEM	C3D-C2D	-2.35	1.31	1.36
2	A	580	HEM	O2D-CGD	-2.30	1.23	1.30
3	B	590	VNI	C4-N2	-2.29	1.31	1.37
2	A	580	HEM	C4A-C3A	-2.26	1.37	1.43
2	A	580	HEM	CHB-C4A	-2.19	1.34	1.39
2	B	580	HEM	C1A-C2A	-2.16	1.40	1.44
2	A	580	HEM	O2A-CGA	-2.13	1.23	1.30
2	B	580	HEM	C4C-NC	-2.11	1.35	1.39
2	B	580	HEM	O2A-CGA	-2.07	1.24	1.30
2	A	580	HEM	C1A-NA	-2.04	1.35	1.39
3	A	590	VNI	C11-C10	-2.01	1.35	1.38

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	590	VNI	C20-O2-C19	5.97	108.40	102.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	580	HEM	CHC-C4B-NB	5.87	130.74	124.42
2	B	580	HEM	CHC-C4B-NB	5.60	130.45	124.42
2	B	580	HEM	CHD-C1D-ND	5.58	130.42	124.42
3	B	590	VNI	O2-C19-N4	-5.49	107.39	112.34
3	B	590	VNI	O2-C19-C16	5.35	128.05	118.73
2	A	580	HEM	CHB-C1B-NB	5.26	130.87	124.37
3	A	590	VNI	C20-O2-C19	5.21	107.66	102.64
3	B	590	VNI	O2-C20-C21	4.96	127.36	118.73
2	A	580	HEM	CHD-C1D-ND	4.94	129.74	124.42
2	A	580	HEM	C3B-C4B-NB	-4.59	106.17	109.47
3	B	590	VNI	C7-C12-CL2	4.56	125.08	120.41
2	B	580	HEM	CHA-C4D-ND	4.40	129.81	124.37
2	A	580	HEM	CHD-C4C-NC	4.34	129.18	124.45
3	B	590	VNI	O2-C20-N5	-4.16	108.58	112.34
2	A	580	HEM	C1B-NB-C4B	4.09	110.05	105.21
2	B	580	HEM	O2D-CGD-CBD	3.91	126.35	114.00
3	A	590	VNI	O2-C19-N4	-3.88	108.83	112.34
2	B	580	HEM	CHD-C1D-C2D	-3.87	118.92	125.03
3	B	590	VNI	C11-C12-C7	-3.72	118.45	122.46
2	A	580	HEM	CAD-C3D-C4D	3.71	131.17	124.70
2	A	580	HEM	CHD-C1D-C2D	-3.60	119.34	125.03
2	A	580	HEM	CHA-C4D-ND	3.53	128.74	124.37
2	B	580	HEM	CBA-CAA-C2A	-3.29	103.44	112.53
2	B	580	HEM	C1B-NB-C4B	3.26	109.07	105.21
3	A	590	VNI	O2-C20-N5	-3.20	109.45	112.34
2	B	580	HEM	CAD-CBD-CGD	-3.14	105.34	113.67
2	A	580	HEM	C1A-CHA-C4D	-3.13	118.89	126.25
3	A	590	VNI	C12-C7-C2	-3.08	117.69	121.82
2	B	580	HEM	C3B-C4B-NB	-3.07	107.26	109.47
3	A	590	VNI	O2-C19-C16	3.01	123.97	118.73
3	A	590	VNI	C11-C10-CL1	-2.97	115.44	119.17
3	A	590	VNI	O2-C20-C21	2.93	123.84	118.73
2	B	580	HEM	C1A-CHA-C4D	-2.90	119.42	126.25
2	B	580	HEM	CHB-C1B-NB	2.90	127.95	124.37
2	A	580	HEM	CHB-C1B-C2B	-2.84	118.87	126.95
3	B	590	VNI	C21-C20-N5	-2.80	124.01	128.36
2	B	580	HEM	CHA-C4D-C3D	-2.79	120.08	125.23
3	A	590	VNI	C7-C2-N1	-2.76	106.00	111.44
3	A	590	VNI	C26-C21-C22	2.75	122.06	118.57
2	B	580	HEM	C4C-CHD-C1D	-2.69	120.30	126.02
2	B	580	HEM	O2D-CGD-O1D	-2.65	116.53	123.33
3	A	590	VNI	C3-N2-C6	-2.64	123.25	126.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	580	HEM	CHD-C4C-NC	2.63	127.32	124.45
2	A	580	HEM	C4C-CHD-C1D	-2.63	120.44	126.02
2	A	580	HEM	C4A-CHB-C1B	-2.62	120.10	126.25
2	A	580	HEM	CHA-C1A-NA	2.61	128.59	123.86
2	A	580	HEM	CAD-C3D-C2D	-2.54	123.11	127.87
3	B	590	VNI	C16-C19-N4	-2.45	124.56	128.36
2	A	580	HEM	CHA-C4D-C3D	-2.40	120.80	125.23
3	A	590	VNI	C7-C12-CL2	2.37	122.84	120.41
3	B	590	VNI	C19-N4-N5	2.34	108.55	106.33
2	A	580	HEM	O2D-CGD-O1D	-2.33	117.34	123.33
3	A	590	VNI	C23-C22-C21	-2.27	118.13	120.36
3	A	590	VNI	C17-C16-C15	2.17	121.32	118.57
2	A	580	HEM	O2D-CGD-CBD	2.17	120.84	114.00
2	B	580	HEM	CHA-C1A-NA	2.12	127.71	123.86
3	A	590	VNI	C17-C16-C19	-2.09	117.39	120.56
3	A	590	VNI	C9-C10-CL1	2.09	122.44	119.36
2	A	580	HEM	C1C-CHC-C4B	-2.08	121.60	126.02
3	A	590	VNI	C14-C15-C16	-2.05	118.61	120.80
2	A	580	HEM	CAA-CBA-CGA	-2.04	108.25	113.67
2	B	580	HEM	CHB-C1B-C2B	-2.02	121.22	126.95
3	B	590	VNI	C8-C7-C12	2.01	118.84	116.82
2	B	580	HEM	CMB-C2B-C1B	2.00	128.17	125.03

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	590	VNI	C7-C2-N1-C1
3	A	590	VNI	C17-C16-C19-O2
2	A	580	HEM	C2D-C3D-CAD-CBD
2	A	580	HEM	C4D-C3D-CAD-CBD
3	A	590	VNI	C15-C16-C19-O2
3	B	590	VNI	O2-C20-C21-C22
3	A	590	VNI	C17-C16-C19-N4
3	B	590	VNI	O2-C20-C21-C26
3	A	590	VNI	C15-C16-C19-N4
3	B	590	VNI	N5-C20-C21-C22
3	B	590	VNI	N5-C20-C21-C26
3	A	590	VNI	C7-C2-N1-C1
2	A	580	HEM	CAA-CBA-CGA-O1A
2	A	580	HEM	CAA-CBA-CGA-O2A
3	B	590	VNI	C17-C16-C19-O2

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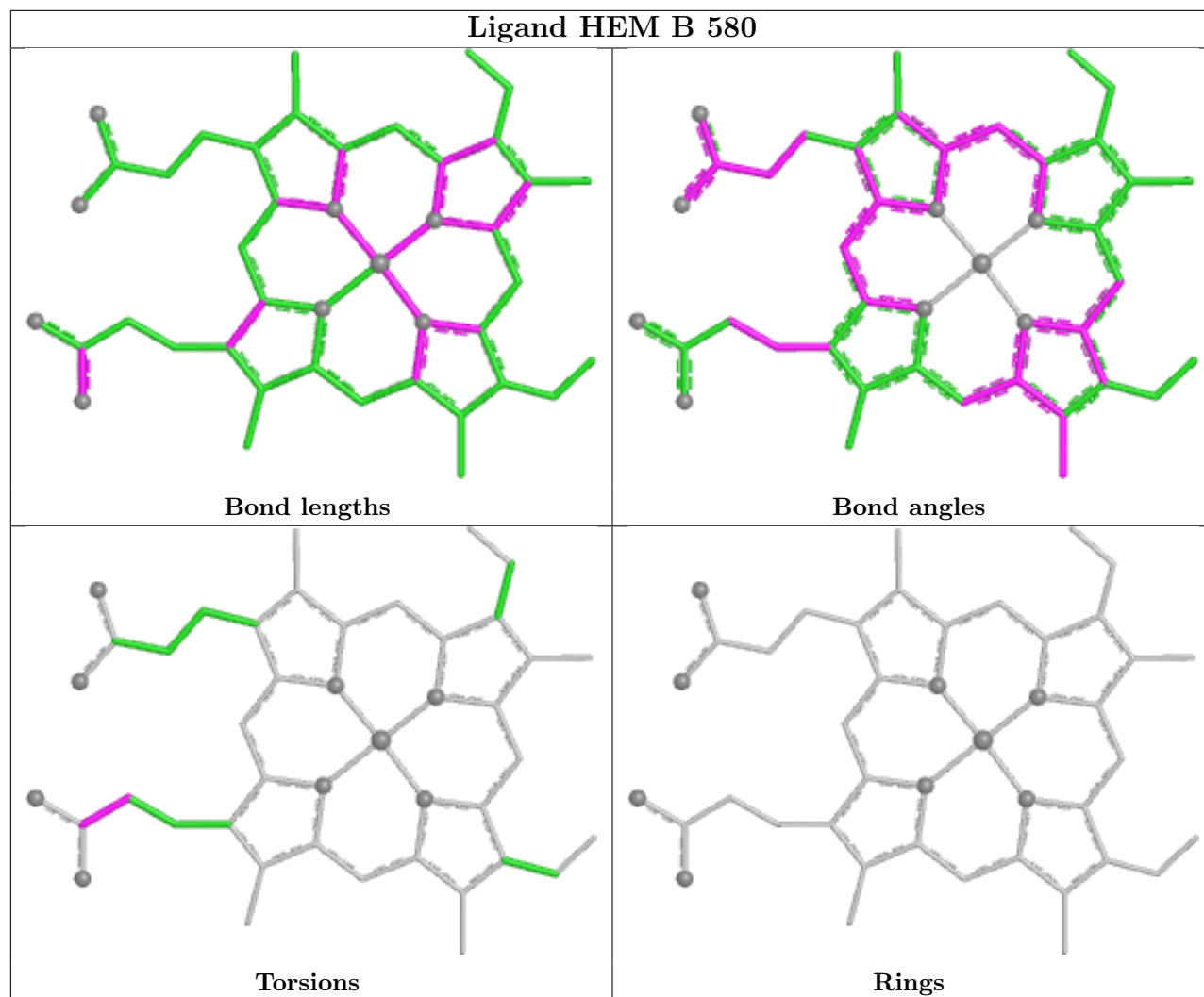
Mol	Chain	Res	Type	Atoms
3	A	590	VNI	C3-C2-C7-C8
3	A	590	VNI	C3-C2-C7-C12
2	A	580	HEM	CAD-CBD-CGD-O2D
2	B	580	HEM	CAA-CBA-CGA-O2A

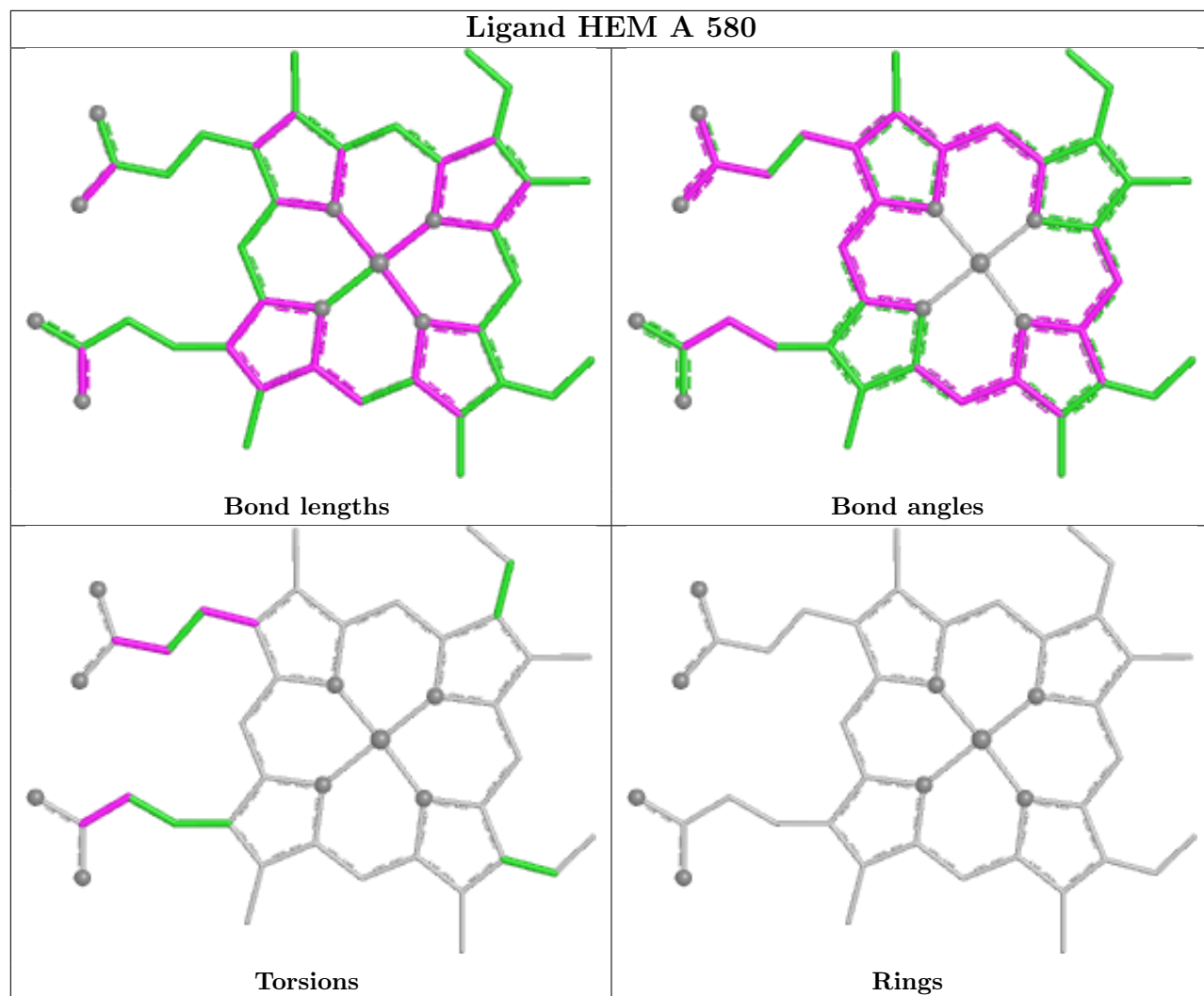
There are no ring outliers.

4 monomers are involved in 38 short contacts:

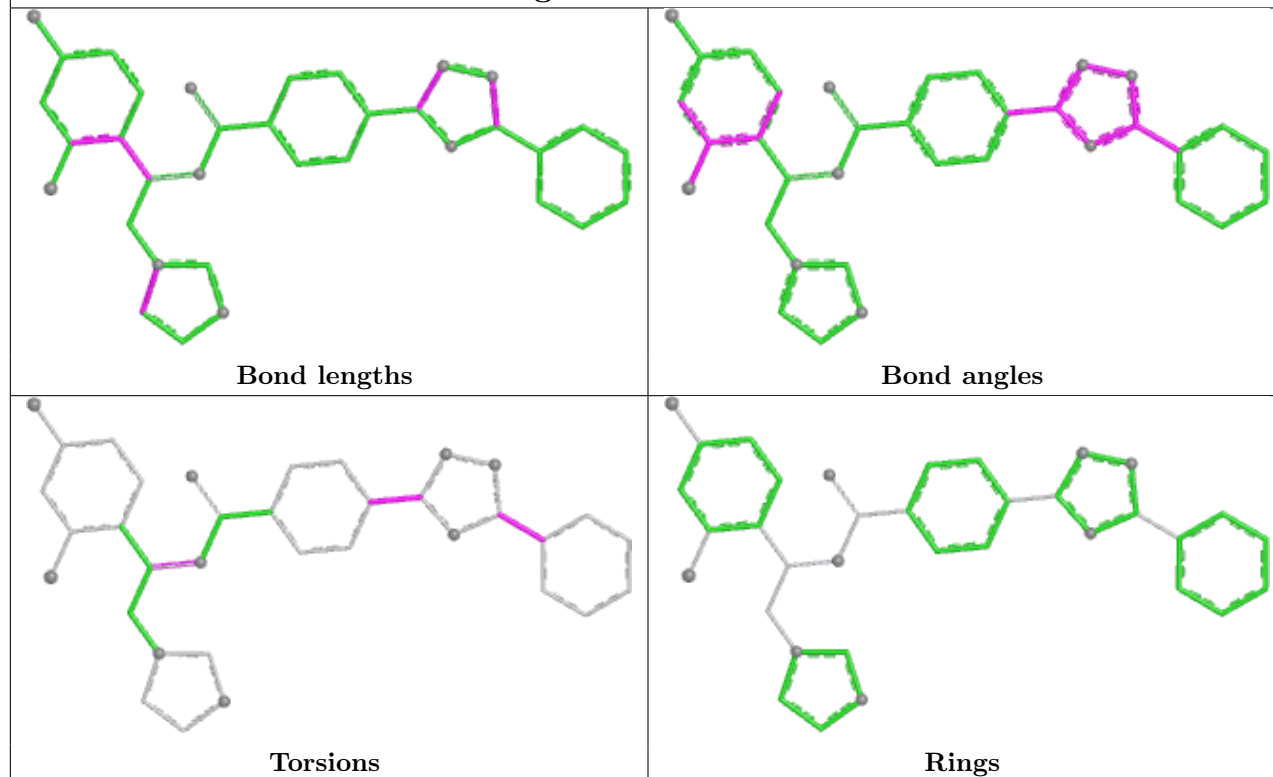
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	580	HEM	15	0
2	A	580	HEM	10	0
3	B	590	VNI	11	0
3	A	590	VNI	2	0

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 than 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.

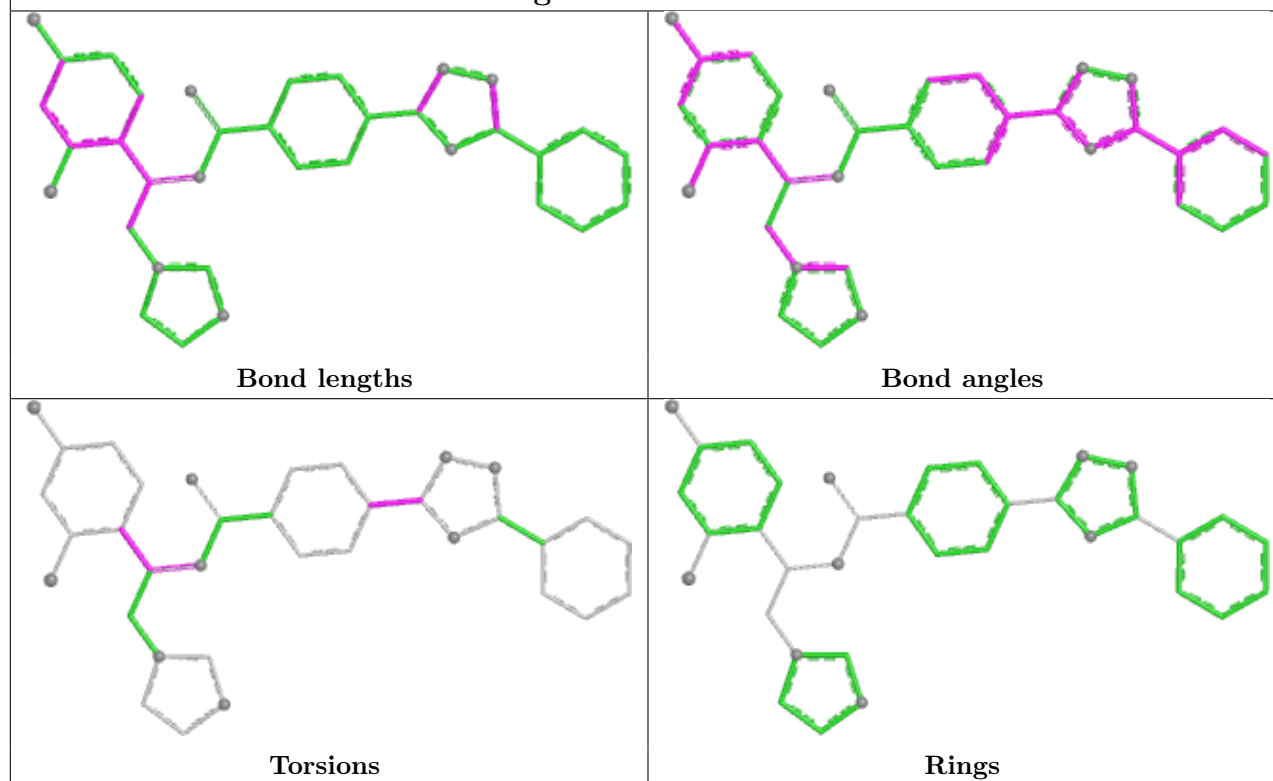




Ligand VNI B 590



Ligand VNI A 590



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, 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	470/470 (100%)	0.21	19 (4%) 42 33	48, 78, 121, 184	0
1	B	470/470 (100%)	0.56	28 (5%) 27 20	64, 100, 152, 235	0
All	All	940/940 (100%)	0.39	47 (5%) 34 26	48, 89, 143, 235	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	503	LEU	4.5
1	B	491	GLY	3.9
1	A	217	THR	3.6
1	B	278	VAL	3.5
1	A	427	ASN	3.5
1	B	198	ILE	3.5
1	B	154	LEU	3.4
1	B	285	VAL	3.3
1	A	430	ALA	3.2
1	B	358	LEU	3.2
1	B	427	ASN	3.2
1	B	490	PRO	3.2
1	A	431	SER	3.1
1	B	222	TYR	3.0
1	B	345	LEU	3.0
1	B	102	THR	2.9
1	A	277	MET	2.8
1	B	157	ASP	2.8
1	B	277	MET	2.8
1	B	428	ILE	2.7
1	A	57	HIS	2.7
1	A	428	ILE	2.7
1	B	424	TRP	2.6
1	B	444	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	273	ASP	2.6
1	A	502	SER	2.5
1	A	278	VAL	2.5
1	A	77	PHE	2.5
1	B	386	VAL	2.4
1	B	105	ASN	2.3
1	A	508	LEU	2.3
1	B	475	THR	2.3
1	A	222	TYR	2.3
1	A	489	LEU	2.2
1	B	498	THR	2.2
1	B	218	PHE	2.2
1	B	109	LEU	2.2
1	A	340	VAL	2.1
1	B	503	LEU	2.1
1	A	99	TYR	2.1
1	B	440	TYR	2.1
1	B	451	SER	2.1
1	A	418	GLU	2.1
1	A	509	GLY	2.0
1	A	303	ALA	2.0
1	B	143	LEU	2.0
1	B	282	MET	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

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.

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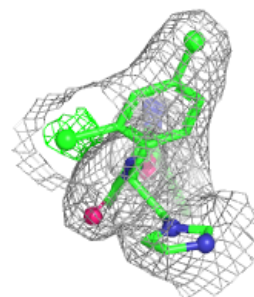
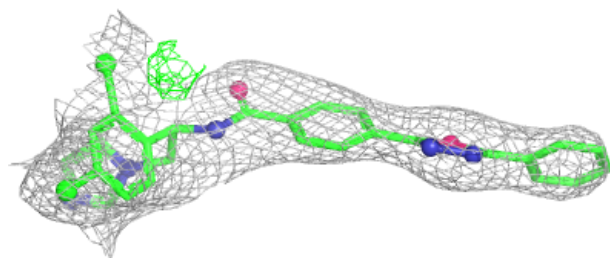
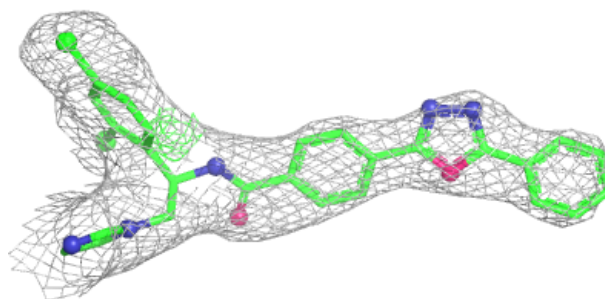
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	VNI	B	590	35/35	0.92	0.10	63,93,105,106	0
3	VNI	A	590	35/35	0.94	0.10	56,86,101,104	0
2	HEM	B	580	43/43	0.96	0.10	68,89,99,107	0
2	HEM	A	580	43/43	0.98	0.08	52,65,80,83	0

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.

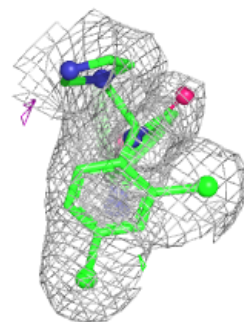
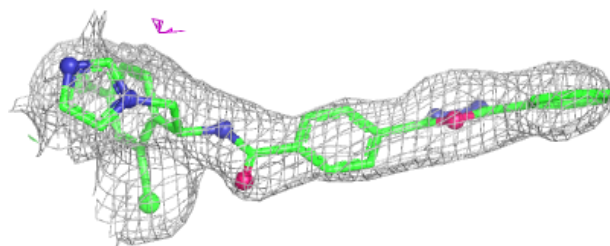
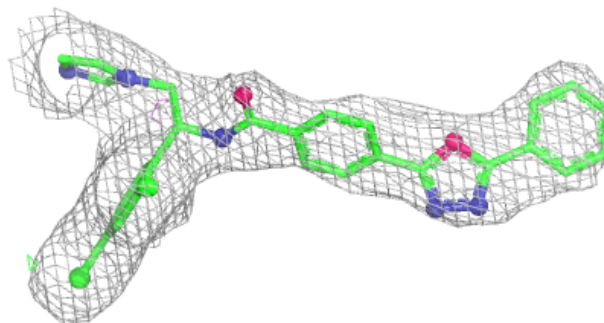
Electron density around VNI B 590:

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



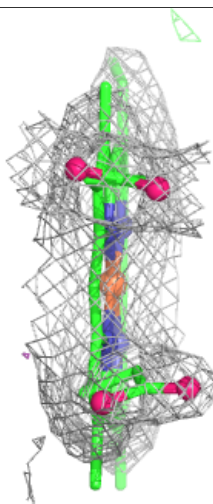
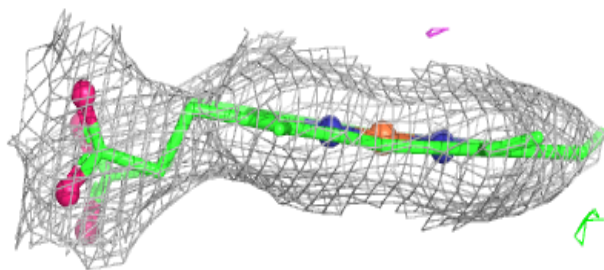
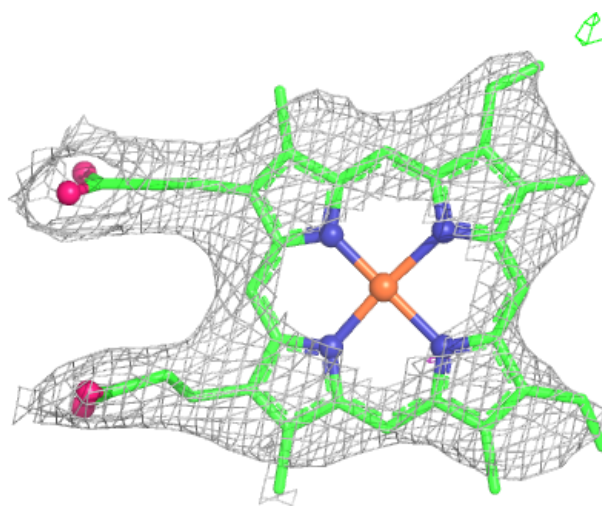
Electron density around VNI A 590:

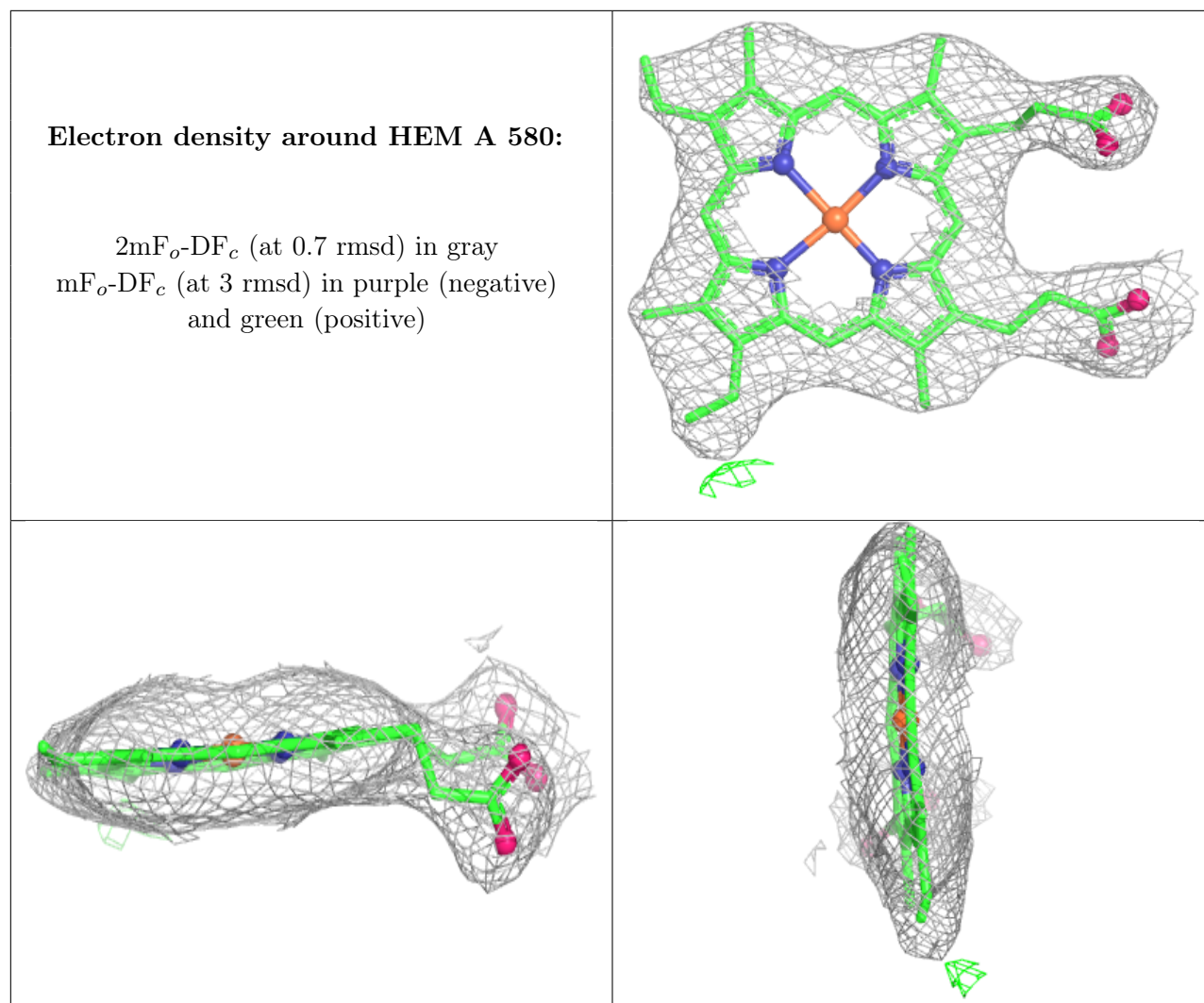
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM 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.