Full wwPDB X-ray Structure Validation Report (i)

Nov 5, 2023 – 02:59 AM EST

PDB ID	:	2OZ0
Title	:	Mechanistic and Structural Studies of H373Q Flavocytochrome b2: Effects of Mutating the Active Site Base
Authors	:	Tsai, C.-L.; Gokulan, K.; Sobrado, P.; Sacchettini, J.C.; Fitzpatrick, P.F.
Deposited on	:	2007-02-23
Resolution	:	2.80 Å(reported)

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

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

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

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

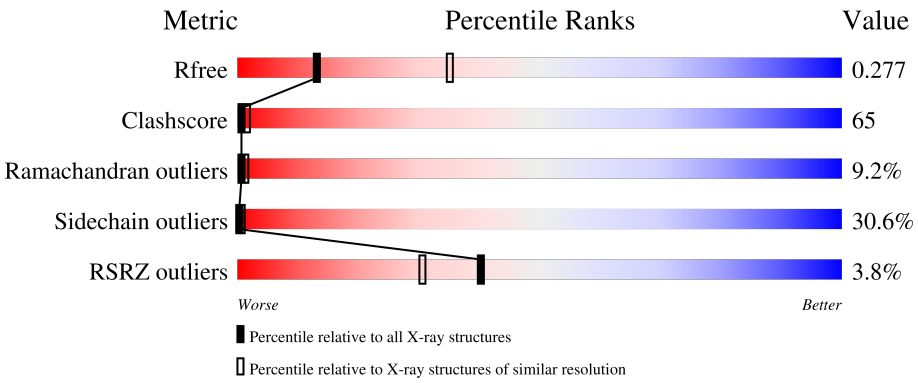
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	511	4%; 16%, 38%, 30%, 13%, •
1	B	511	2%; 11%, 25%, 26%, 16%, 23%

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	FMN	A	569	X	-	X	-
3	FMN	B	570	-	-	X	-
4	PYR	B	571	-	X	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 7042 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

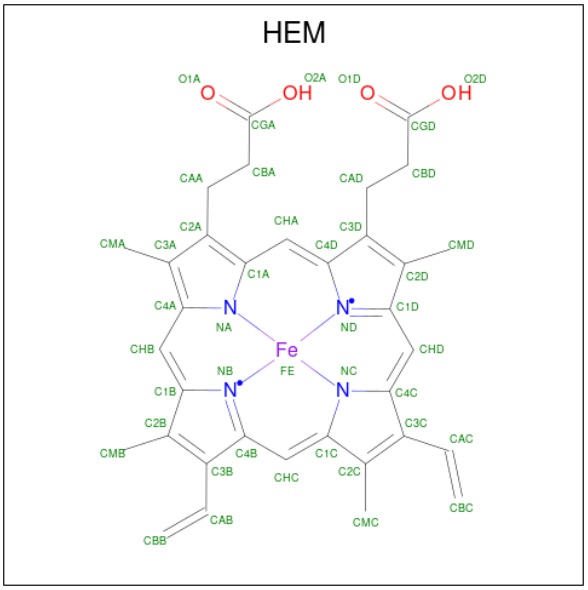
- Molecule 1 is a protein called Cytochrome b2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	492	3833	2441	649	728	15	0	0	0
1	B	396	3081	1953	524	593	11	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

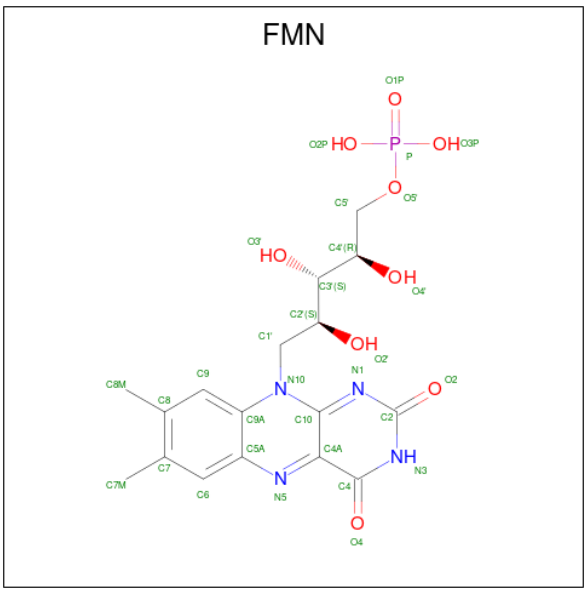
Chain	Residue	Modelled	Actual	Comment	Reference
A	373	GLN	HIS	engineered mutation	UNP P00175
B	373	GLN	HIS	engineered mutation	UNP P00175

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



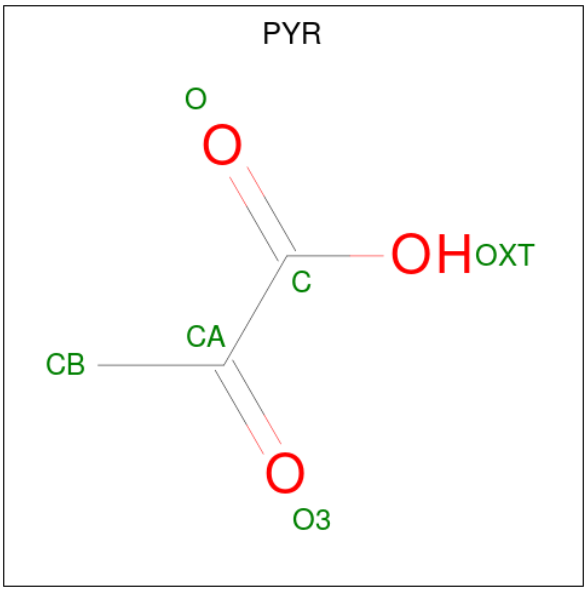
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
2	A	1	43	34	1	4	4	0	0

- Molecule 3 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
3	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 4 is PYRUVIC ACID (three-letter code: PYR) (formula: $C_3H_4O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is water.

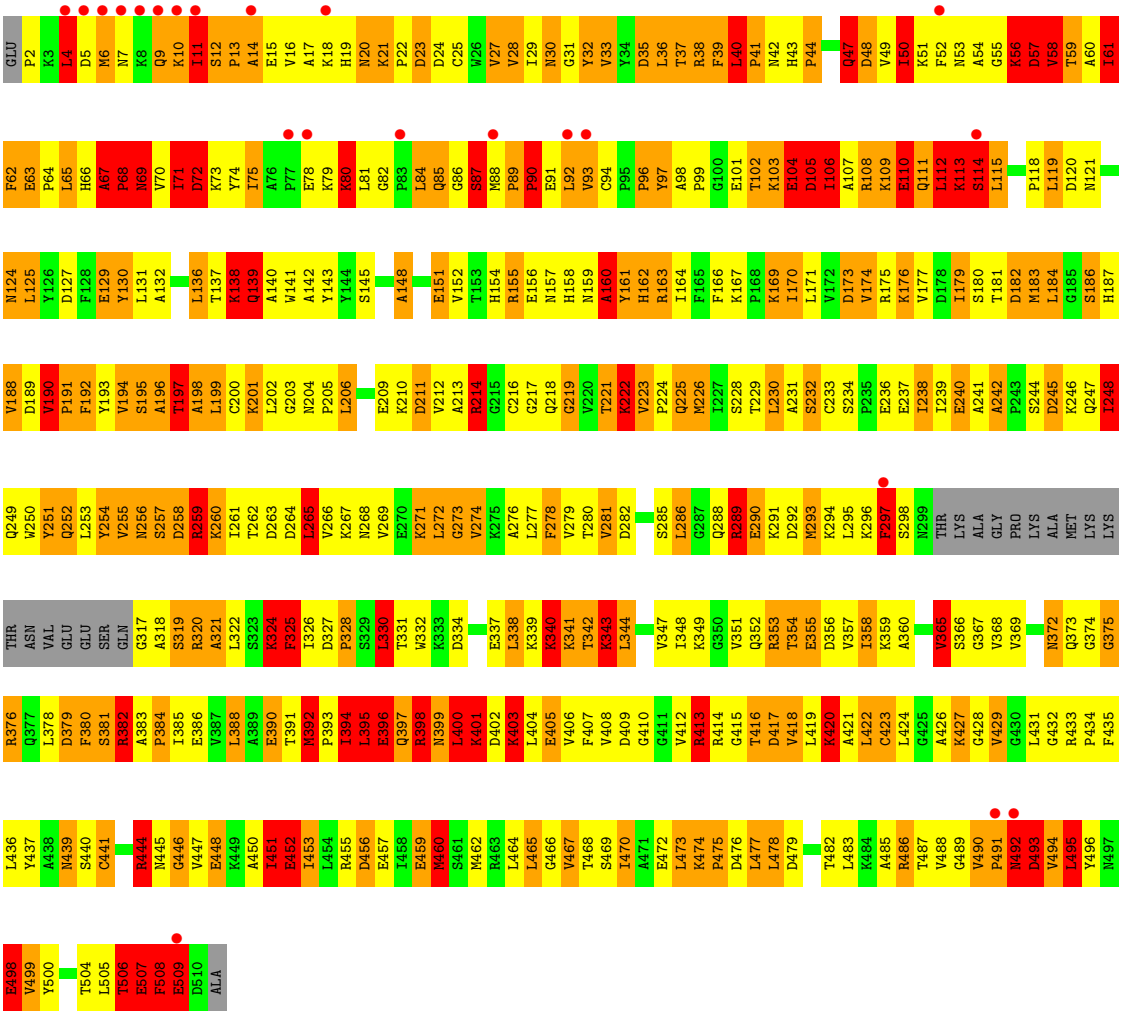
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	7	7	7	0	0
			Total	O		
5	B	10	10	10	0	0

3 Residue-property plots (i)

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

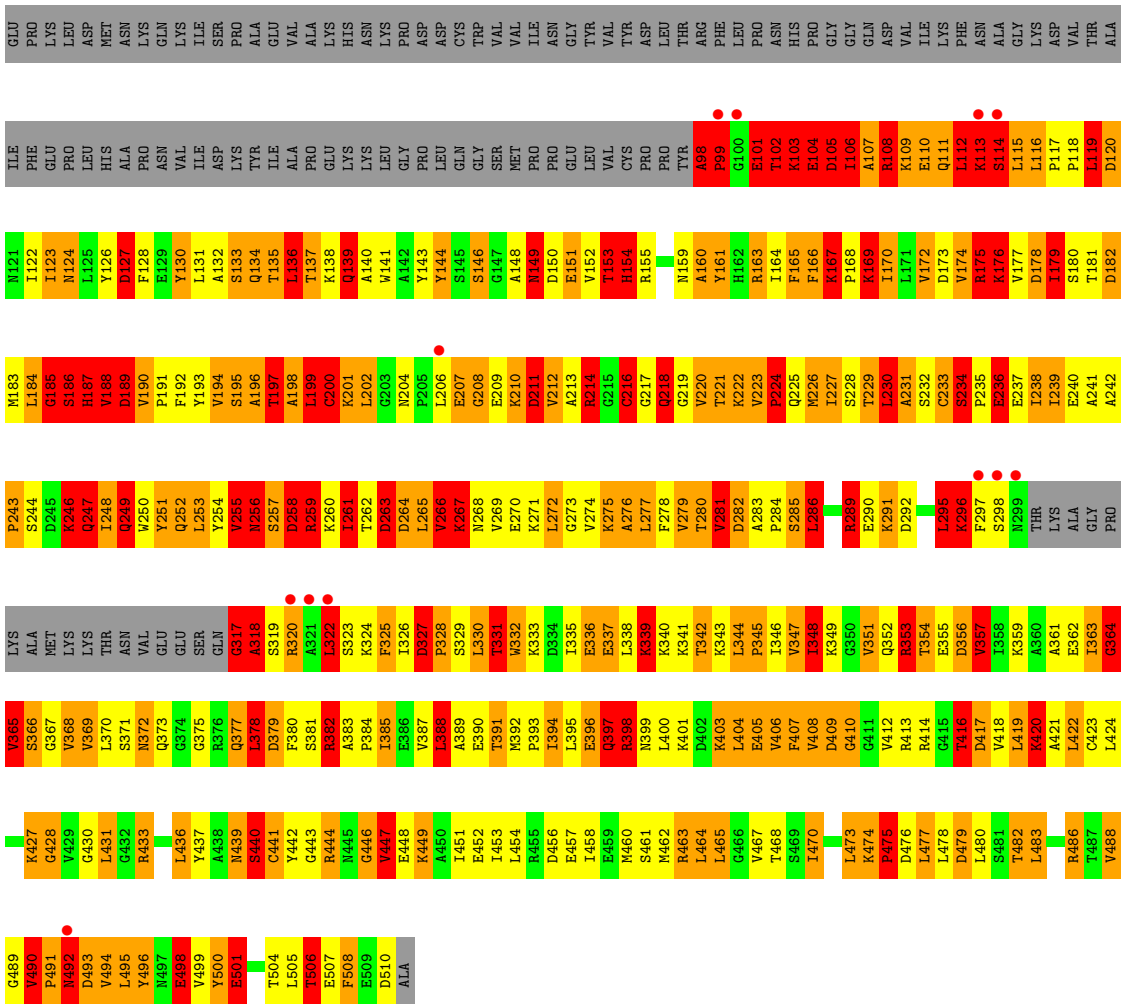
• Molecule 1: Cytochrome b2

Chain A: 4% 16% 38% 30% 13%



• Molecule 1: Cytochrome b2

Chain B: 2% 11% 25% 26% 16% 23%


GLU PRO LYS LEU ASP MET ASN LYS GLN LYS ILE SER PRO ALA GLU VAL ALA LYS HIS ASN LYS PRO ASP ASP CYS TRP VAL VAL ILE ASN GLY TYR VAL TYR ASP LEU THR ARG PHE LEU PRO ASN HIS PRO GLY GLY GLN ASP VAL ILE LYS PHE ASN ALA GLY LYS ASP VAL THR ALA
ILE PHE GLU PRO LEU HIS ALA PRO ASN VAL ILE ASP LYS TYR ILE ALA PRO GLU LYS LYS LEU GLY PRO LEU GLN GLY SER MET PRO PRO GLU LEU VAL CYS PRO PRO TYR A98 P99 G100 E101 T102 K103 E104 D105 I106 A107 R108 K109 E110 Q111 L112 K113 S114 L115 L116 P117 P118 L119 D120
N121 I122 I123 N124 L125 Y126 D127 F128 E129 Y130 L131 A132 S133 Q134 T135 L136 T137 K138 Q139 A140 W141 A142 Y143 Y144 S145 S146 G147 A148 N149 D150 E151 V152 T153 H154 R155 N159 A160 Y161 H162 R163 I164 F165 F166 K167 P168 K169 I170 L171 V172 D173 V174 R175 K176 V177 D178 I179 S180 T181 D182
M183 L184 G185 S186 H187 V188 D189 V190 P191 F192 Y193 V194 S195 A196 T197 A198 L199 C200 K201 L202 G203 N204 P205 L206 E207 G208 E209 K210 D211 V212 A213 R214 G215 C216 G217 Q218 G219 V220 T221 K222 V223 P224 Q225 M226 I227 S228 T229 L230 A231 S232 C233 S234 P235 E236 E237 I238 I239 E240 A241 A242
P243 S244 D245 K246 Q247 I248 Q249 W250 Y251 Q252 L253 Y254 V255 N256 S257 D258 R259 K260 I261 T262 D263 D264 L265 V266 K267 N268 V269 E270 K271 L272 G273 V274 K275 A276 L277 F278 V279 T280 V281 D282 A283 P284 S285 L286 R289 E290 K291 D292 L295 K296 F297 S298 N299 THR LYS ALA GLY PRO
LYS ALA MET LYS LYS THR ASN VAL GLU GLU SER GLN G317 A318 S319 R320 A321 L322 S323 K324 F325 I326 D327 P328 S329 L330 T331 W332 K333 D334 I335 E336 E337 L338 K339 K340 K341 T342 K343 L344 P345 I346 V347 I348 K349 G350 V351 Q352 R353 T354 E355 D356 V357 I358 K359 A360 A361 E362 I363 G364
V365 S366 G367 V368 V369 L370 S371 N372 Q373 G374 G375 R376 Q377 L378 D379 F380 S381 R382 A383 P384 I385 E386 V387 L388 A389 E390 T391 M392 P393 I394 L395 E396 Q397 R398 N399 L400 K401 D402 K403 L404 E405 V406 F407 V408 D409 G410 G411 V412 R413 R414 G415 T416 D417 V418 L419 K420 A421 L422 C423 L424
K427 G428 V429 G430 L431 G432 R433 L436 Y437 A438 N439 S440 C441 Y442 G443 R444 N445 G446 V447 E448 K449 A450 I451 E452 I453 L454 R455 D456 E457 I458 E459 M460 S461 M462 R463 L464 L465 G466 V467 T468 S469 I470 L473 K474 P475 D476 L477 L478 D479 L480 S481 T482 L483 R486 T487 V488
G489 V490 P491 N492 D493 V494 L495 Y496 N497 E498 V499 Y500 E501 T504 L505 T506 E507 F508 E509 D510 ALA

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	163.69Å 163.69Å 112.02Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.80 48.34 – 2.45	Depositor EDS
% Data completeness (in resolution range)	87.6 (50.00-2.80) 64.2 (48.34-2.45)	Depositor EDS
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.50 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.206 , 0.278 0.226 , 0.277	Depositor DCC
R_{free} test set	2123 reflections (5.19%)	wwPDB-VP
Wilson B-factor (Å^2)	62.3	Xtriage
Anisotropy	0.230	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 58.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.017 for -h,-k,l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	7042	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: FMN, PYR, 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	1.94	115/3907 (2.9%)	2.38	216/5291 (4.1%)
1	B	1.85	71/3130 (2.3%)	2.45	202/4230 (4.8%)
All	All	1.90	186/7037 (2.6%)	2.41	418/9521 (4.4%)

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	2	57
1	B	4	64
All	All	6	121

All (186) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	289	ARG	CG-CD	12.01	1.81	1.51
1	B	441	CYS	CB-SG	11.82	2.02	1.82
1	A	413	ARG	CG-CD	10.79	1.78	1.51
1	A	266	VAL	CB-CG2	-10.57	1.30	1.52
1	A	421	ALA	CA-CB	-10.42	1.30	1.52
1	B	175	ARG	CG-CD	10.28	1.77	1.51
1	A	390	GLU	CG-CD	10.15	1.67	1.51
1	B	289	ARG	CB-CG	10.06	1.79	1.52
1	B	137	THR	CB-CG2	9.98	1.85	1.52
1	A	161	TYR	CD1-CE1	9.88	1.54	1.39
1	A	343	LYS	CB-CG	9.80	1.79	1.52
1	B	368	VAL	CB-CG1	-9.78	1.32	1.52
1	B	501	GLU	CD-OE1	9.63	1.36	1.25
1	A	274	VAL	CB-CG2	9.33	1.72	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	368	VAL	CB-CG1	-9.27	1.33	1.52
1	A	343	LYS	CD-CE	9.19	1.74	1.51
1	A	509	GLU	C-O	8.84	1.40	1.23
1	A	340	LYS	CE-NZ	8.66	1.70	1.49
1	A	390	GLU	CD-OE2	8.58	1.35	1.25
1	B	500	TYR	CG-CD1	-8.57	1.28	1.39
1	A	340	LYS	CD-CE	8.49	1.72	1.51
1	B	163	ARG	C-O	8.35	1.39	1.23
1	A	248	ILE	CA-CB	-8.31	1.35	1.54
1	B	251	TYR	CD1-CE1	8.29	1.51	1.39
1	A	223	VAL	CB-CG1	-8.22	1.35	1.52
1	B	160	ALA	CA-CB	-8.12	1.35	1.52
1	B	167	LYS	CE-NZ	8.03	1.69	1.49
1	B	216	CYS	CB-SG	-8.00	1.68	1.82
1	A	89	PRO	C-N	-7.85	1.19	1.34
1	B	99	PRO	N-CD	7.71	1.58	1.47
1	A	426	ALA	CA-CB	-7.59	1.36	1.52
1	B	488	VAL	CB-CG2	-7.41	1.37	1.52
1	B	389	ALA	CA-CB	-7.40	1.36	1.52
1	A	470	ILE	CA-CB	-7.33	1.38	1.54
1	A	472	GLU	CG-CD	7.24	1.62	1.51
1	B	351	VAL	CB-CG2	-7.23	1.37	1.52
1	B	369	VAL	CB-CG2	-7.22	1.37	1.52
1	A	195	SER	CB-OG	7.21	1.51	1.42
1	A	194	VAL	CB-CG1	-7.17	1.37	1.52
1	A	193	TYR	CE1-CZ	-7.17	1.29	1.38
1	A	174	VAL	CB-CG2	-7.12	1.37	1.52
1	A	488	VAL	CB-CG1	-7.12	1.37	1.52
1	A	446	GLY	C-O	7.08	1.34	1.23
1	A	286	LEU	CG-CD1	7.07	1.78	1.51
1	A	222	LYS	C-O	7.04	1.36	1.23
1	B	123	ILE	CA-CB	-7.03	1.38	1.54
1	B	499	VAL	CB-CG1	-7.01	1.38	1.52
1	A	417	ASP	CB-CG	6.99	1.66	1.51
1	A	410	GLY	N-CA	-6.96	1.35	1.46
1	A	143	TYR	CG-CD1	-6.94	1.30	1.39
1	B	251	TYR	CG-CD1	6.89	1.48	1.39
1	B	196	ALA	CA-CB	6.88	1.66	1.52
1	B	406	VAL	CA-CB	-6.82	1.40	1.54
1	A	242	ALA	CA-CB	-6.81	1.38	1.52
1	A	142	ALA	CA-CB	-6.76	1.38	1.52
1	B	490	VAL	CB-CG2	-6.73	1.38	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	423	CYS	CB-SG	-6.67	1.71	1.82
1	B	251	TYR	CB-CG	6.66	1.61	1.51
1	A	472	GLU	CD-OE2	6.66	1.32	1.25
1	A	266	VAL	CA-CB	-6.65	1.40	1.54
1	B	406	VAL	CB-CG1	-6.59	1.39	1.52
1	A	444	ARG	CZ-NH2	6.56	1.41	1.33
1	A	407	PHE	C-O	-6.55	1.10	1.23
1	A	161	TYR	CD2-CE2	6.52	1.49	1.39
1	B	447	VAL	CA-CB	-6.51	1.41	1.54
1	A	429	VAL	CB-CG1	-6.48	1.39	1.52
1	A	61	ILE	C-O	-6.46	1.11	1.23
1	B	500	TYR	CD1-CE1	-6.46	1.29	1.39
1	B	498	GLU	CB-CG	-6.43	1.40	1.52
1	B	317	GLY	CA-C	6.43	1.62	1.51
1	A	360	ALA	CA-CB	-6.43	1.39	1.52
1	A	428	GLY	C-O	-6.40	1.13	1.23
1	A	246	LYS	CD-CE	6.38	1.67	1.51
1	B	382	ARG	CB-CG	-6.33	1.35	1.52
1	B	161	TYR	CD1-CE1	-6.29	1.29	1.39
1	B	446	GLY	C-O	6.20	1.33	1.23
1	A	198	ALA	CA-CB	-6.17	1.39	1.52
1	B	498	GLU	CD-OE1	6.11	1.32	1.25
1	A	341	LYS	CD-CE	6.09	1.66	1.51
1	B	161	TYR	CD2-CE2	-6.08	1.30	1.39
1	A	429	VAL	CB-CG2	-6.03	1.40	1.52
1	B	233	CYS	CB-SG	6.01	1.92	1.82
1	B	223	VAL	C-O	6.01	1.34	1.23
1	A	246	LYS	CE-NZ	6.00	1.64	1.49
1	B	98	ALA	C-N	5.98	1.45	1.34
1	A	408	VAL	CB-CG2	-5.89	1.40	1.52
1	A	192	PHE	CD1-CE1	5.89	1.51	1.39
1	B	495	LEU	C-O	-5.87	1.12	1.23
1	A	465	LEU	N-CA	-5.86	1.34	1.46
1	B	407	PHE	C-N	-5.84	1.20	1.34
1	B	501	GLU	CD-OE2	5.83	1.32	1.25
1	A	396	GLU	CD-OE2	-5.83	1.19	1.25
1	A	341	LYS	CG-CD	5.82	1.72	1.52
1	B	463	ARG	CG-CD	5.81	1.66	1.51
1	A	176	LYS	CD-CE	5.80	1.65	1.51
1	B	289	ARG	NE-CZ	5.79	1.40	1.33
1	B	492	ASN	C-O	5.79	1.34	1.23
1	B	166	PHE	CB-CG	-5.78	1.41	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	168	PRO	N-CD	-5.78	1.39	1.47
1	B	200	CYS	CB-SG	-5.78	1.72	1.81
1	B	465	LEU	N-CA	-5.78	1.34	1.46
1	A	267	LYS	CD-CE	5.78	1.65	1.51
1	A	129	GLU	CD-OE2	5.78	1.32	1.25
1	B	190	VAL	C-N	5.78	1.45	1.34
1	A	130	TYR	CB-CG	-5.77	1.43	1.51
1	A	192	PHE	CD2-CE2	5.77	1.50	1.39
1	B	433	ARG	C-N	5.75	1.45	1.34
1	B	406	VAL	C-N	-5.75	1.20	1.34
1	A	418	VAL	CB-CG2	5.72	1.64	1.52
1	A	486	ARG	CB-CG	5.69	1.68	1.52
1	A	452	GLU	CD-OE2	-5.68	1.19	1.25
1	A	420	LYS	CB-CG	5.68	1.67	1.52
1	B	174	VAL	CB-CG2	-5.67	1.41	1.52
1	B	289	ARG	CZ-NH2	5.67	1.40	1.33
1	A	110	GLU	CB-CG	5.67	1.62	1.52
1	A	490	VAL	C-N	5.67	1.45	1.34
1	B	463	ARG	C-O	5.66	1.34	1.23
1	A	193	TYR	CE2-CZ	-5.63	1.31	1.38
1	A	321	ALA	C-O	-5.59	1.12	1.23
1	A	358	ILE	CA-CB	-5.57	1.42	1.54
1	A	390	GLU	C-N	-5.57	1.21	1.34
1	A	396	GLU	CG-CD	5.55	1.60	1.51
1	A	64	PRO	N-CD	5.55	1.55	1.47
1	A	486	ARG	CG-CD	5.55	1.65	1.51
1	B	281	VAL	CB-CG1	-5.53	1.41	1.52
1	B	500	TYR	CE1-CZ	-5.52	1.31	1.38
1	A	163	ARG	CZ-NH1	5.52	1.40	1.33
1	B	369	VAL	CA-CB	-5.51	1.43	1.54
1	B	289	ARG	CZ-NH1	5.51	1.40	1.33
1	A	169	LYS	CB-CG	-5.50	1.37	1.52
1	B	491	PRO	C-N	5.49	1.46	1.34
1	A	351	VAL	C-O	-5.47	1.12	1.23
1	A	418	VAL	CA-CB	-5.47	1.43	1.54
1	A	472	GLU	CD-OE1	5.46	1.31	1.25
1	A	405	GLU	CB-CG	5.43	1.62	1.52
1	A	169	LYS	CG-CD	-5.41	1.34	1.52
1	A	407	PHE	CB-CG	-5.40	1.42	1.51
1	A	225	GLN	CD-NE2	5.39	1.46	1.32
1	A	93	VAL	CA-CB	5.38	1.66	1.54
1	A	238	ILE	CA-CB	-5.36	1.42	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	251	TYR	C-O	5.34	1.33	1.23
1	A	279	VAL	CB-CG1	-5.34	1.41	1.52
1	A	343	LYS	CE-NZ	5.33	1.62	1.49
1	A	219	GLY	C-O	5.33	1.32	1.23
1	A	223	VAL	C-O	5.32	1.33	1.23
1	A	408	VAL	CB-CG1	-5.31	1.41	1.52
1	B	167	LYS	C-O	-5.31	1.13	1.23
1	A	155	ARG	CA-CB	-5.30	1.42	1.53
1	B	405	GLU	CG-CD	5.30	1.59	1.51
1	B	501	GLU	CG-CD	5.30	1.59	1.51
1	A	368	VAL	CB-CG2	-5.30	1.41	1.52
1	A	282	ASP	CB-CG	5.28	1.62	1.51
1	B	282	ASP	CB-CG	5.28	1.62	1.51
1	A	228	SER	C-O	5.27	1.33	1.23
1	A	355	GLU	CG-CD	5.26	1.59	1.51
1	A	485	ALA	CA-CB	-5.26	1.41	1.52
1	B	176	LYS	CE-NZ	5.25	1.62	1.49
1	A	351	VAL	CA-CB	-5.24	1.43	1.54
1	A	498	GLU	CD-OE1	5.24	1.31	1.25
1	A	508	PHE	C-N	5.23	1.46	1.34
1	A	196	ALA	CA-CB	-5.21	1.41	1.52
1	A	57	ASP	C-N	-5.20	1.22	1.34
1	B	317	GLY	C-N	-5.18	1.22	1.34
1	A	277	LEU	CA-CB	-5.17	1.41	1.53
1	B	253	LEU	N-CA	-5.17	1.36	1.46
1	B	251	TYR	CE1-CZ	5.17	1.45	1.38
1	B	467	VAL	CA-CB	-5.16	1.44	1.54
1	A	392	MET	C-N	5.16	1.44	1.34
1	A	129	GLU	CA-CB	-5.15	1.42	1.53
1	B	417	ASP	C-O	5.14	1.33	1.23
1	A	129	GLU	CD-OE1	5.14	1.31	1.25
1	A	197	THR	N-CA	-5.13	1.36	1.46
1	A	190	VAL	CB-CG1	-5.13	1.42	1.52
1	A	470	ILE	CB-CG2	-5.11	1.37	1.52
1	A	327	ASP	C-N	5.10	1.44	1.34
1	A	191	PRO	CG-CD	5.09	1.67	1.50
1	A	496	TYR	CD2-CE2	-5.09	1.31	1.39
1	A	188	VAL	CB-CG1	-5.09	1.42	1.52
1	A	282	ASP	C-O	5.08	1.33	1.23
1	A	129	GLU	N-CA	-5.07	1.36	1.46
1	A	278	PHE	N-CA	-5.03	1.36	1.46
1	A	97	TYR	CD1-CE1	5.03	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	249	GLN	CB-CG	-5.03	1.39	1.52
1	B	165	PHE	CD1-CE1	-5.02	1.29	1.39
1	A	420	LYS	CD-CE	5.02	1.63	1.51
1	A	257	SER	CA-CB	-5.01	1.45	1.52

All (418) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	382	ARG	O-C-N	-25.98	81.14	122.70
1	A	395	LEU	O-C-N	-19.10	92.14	122.70
1	B	317	GLY	C-N-CA	18.27	167.38	121.70
1	A	245	ASP	CB-CG-OD1	-16.45	103.49	118.30
1	A	396	GLU	O-C-N	-16.19	96.79	122.70
1	B	419	LEU	CB-CG-CD2	-15.02	85.47	111.00
1	A	163	ARG	NE-CZ-NH2	-14.63	112.98	120.30
1	A	353	ARG	NE-CZ-NH1	14.27	127.43	120.30
1	B	267	LYS	O-C-N	-14.16	100.04	122.70
1	A	160	ALA	O-C-N	-13.85	100.53	122.70
1	B	473	LEU	O-C-N	-13.59	100.95	122.70
1	A	353	ARG	NE-CZ-NH2	-13.56	113.52	120.30
1	B	463	ARG	NE-CZ-NH1	12.96	126.78	120.30
1	A	89	PRO	C-N-CD	-12.95	92.12	120.60
1	A	509	GLU	CA-C-N	12.70	145.14	117.20
1	A	297	PHE	C-N-CA	12.16	152.10	121.70
1	A	388	LEU	CB-CG-CD1	-11.94	90.70	111.00
1	A	90	PRO	C-N-CA	11.88	151.41	121.70
1	A	492	ASN	C-N-CA	11.88	151.40	121.70
1	A	102	THR	O-C-N	-11.79	103.84	122.70
1	B	163	ARG	NE-CZ-NH1	11.54	126.07	120.30
1	A	72	ASP	CB-CG-OD1	-11.31	108.12	118.30
1	A	486	ARG	NE-CZ-NH1	-11.18	114.71	120.30
1	B	179	ILE	O-C-N	-11.02	105.07	122.70
1	A	321	ALA	O-C-N	-10.88	105.29	122.70
1	A	417	ASP	CB-CG-OD1	10.87	128.09	118.30
1	B	189	ASP	C-N-CA	10.82	148.75	121.70
1	A	392	MET	C-N-CD	10.79	151.05	128.40
1	B	327	ASP	C-N-CD	10.68	150.82	128.40
1	B	495	LEU	CA-CB-CG	-10.65	90.81	115.30
1	B	464	LEU	CB-CG-CD1	10.59	128.99	111.00
1	A	327	ASP	C-N-CD	10.53	150.50	128.40
1	A	376	ARG	NE-CZ-NH1	10.50	125.55	120.30
1	B	135	THR	O-C-N	-10.50	105.91	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	143	TYR	CB-CG-CD1	10.46	127.28	121.00
1	B	398	ARG	NE-CZ-NH1	10.44	125.52	120.30
1	A	382	ARG	CA-C-O	10.33	141.79	120.10
1	A	40	LEU	C-N-CD	10.32	150.06	128.40
1	B	223	VAL	CB-CA-C	-10.28	91.86	111.40
1	B	103	LYS	C-N-CA	9.98	146.65	121.70
1	B	214	ARG	NE-CZ-NH1	9.83	125.21	120.30
1	A	265	LEU	CB-CG-CD2	-9.81	94.31	111.00
1	A	163	ARG	NE-CZ-NH1	9.81	125.20	120.30
1	B	173	ASP	CB-CG-OD1	9.75	127.07	118.30
1	B	105	ASP	O-C-N	-9.63	107.29	122.70
1	A	245	ASP	CB-CG-OD2	9.62	126.96	118.30
1	B	486	ARG	NE-CZ-NH1	9.57	125.09	120.30
1	B	267	LYS	CA-C-O	9.56	140.18	120.10
1	A	141	TRP	CE2-CD2-CG	-9.44	99.75	107.30
1	B	476	ASP	CB-CG-OD1	9.39	126.75	118.30
1	A	320	ARG	CD-NE-CZ	9.34	136.68	123.60
1	B	105	ASP	CA-C-O	9.33	139.70	120.10
1	A	169	LYS	CD-CE-NZ	-9.23	90.47	111.70
1	A	324	LYS	C-N-CA	9.21	144.72	121.70
1	A	115	LEU	O-C-N	9.20	137.42	122.70
1	A	298	SER	C-N-CA	9.16	144.59	121.70
1	B	202	LEU	O-C-N	-9.01	107.88	123.20
1	A	292	ASP	CB-CG-OD1	8.99	126.39	118.30
1	B	259	ARG	NE-CZ-NH1	-8.97	115.82	120.30
1	B	474	LYS	C-N-CD	8.97	147.23	128.40
1	B	127	ASP	CB-CG-OD2	-8.96	110.24	118.30
1	A	155	ARG	NE-CZ-NH2	-8.91	115.84	120.30
1	B	292	ASP	CB-CG-OD1	8.81	126.23	118.30
1	A	57	ASP	N-CA-CB	8.80	126.44	110.60
1	B	344	LEU	CB-CG-CD2	-8.80	96.04	111.00
1	A	258	ASP	CB-CG-OD1	8.79	126.21	118.30
1	B	202	LEU	CA-C-O	8.76	138.49	120.10
1	A	206	LEU	CA-CB-CG	-8.74	95.19	115.30
1	A	182	ASP	CB-CG-OD2	8.69	126.12	118.30
1	B	246	LYS	O-C-N	-8.68	108.82	122.70
1	B	185	GLY	O-C-N	-8.67	108.83	122.70
1	B	256	ASN	C-N-CA	8.66	143.36	121.70
1	B	199	LEU	O-C-N	-8.66	108.84	122.70
1	A	63	GLU	C-N-CD	8.64	146.54	128.40
1	B	327	ASP	CB-CG-OD2	8.62	126.06	118.30
1	B	188	VAL	CA-CB-CG2	8.58	123.77	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	356	ASP	CB-CG-OD1	8.57	126.02	118.30
1	A	456	ASP	CB-CG-OD1	8.54	125.99	118.30
1	A	327	ASP	CB-CG-OD2	8.50	125.95	118.30
1	B	130	TYR	CB-CG-CD2	8.50	126.10	121.00
1	A	444	ARG	NE-CZ-NH2	8.47	124.53	120.30
1	B	214	ARG	CD-NE-CZ	8.44	135.42	123.60
1	A	57	ASP	C-N-CA	8.41	142.73	121.70
1	A	179	ILE	O-C-N	-8.39	109.27	122.70
1	B	379	ASP	CB-CG-OD1	8.39	125.85	118.30
1	A	286	LEU	CA-CB-CG	-8.35	96.10	115.30
1	B	108	ARG	NE-CZ-NH1	8.34	124.47	120.30
1	B	406	VAL	O-C-N	-8.34	109.36	122.70
1	B	317	GLY	CA-C-O	-8.32	105.62	120.60
1	A	264	ASP	CB-CG-OD1	8.30	125.77	118.30
1	A	160	ALA	CA-C-O	8.26	137.45	120.10
1	B	344	LEU	C-N-CD	8.26	145.75	128.40
1	B	465	LEU	CB-CG-CD1	-8.25	96.97	111.00
1	B	433	ARG	CD-NE-CZ	8.23	135.12	123.60
1	B	247	GLN	O-C-N	-8.22	109.54	122.70
1	A	271	LYS	O-C-N	-8.15	109.66	122.70
1	A	5	ASP	CB-CG-OD2	8.15	125.63	118.30
1	A	155	ARG	NE-CZ-NH1	8.13	124.37	120.30
1	A	334	ASP	CB-CG-OD1	8.12	125.61	118.30
1	A	509	GLU	CA-C-O	-8.05	103.19	120.10
1	B	353	ARG	NE-CZ-NH1	-7.99	116.31	120.30
1	A	297	PHE	N-CA-CB	7.92	124.86	110.60
1	A	444	ARG	NE-CZ-NH1	-7.91	116.35	120.30
1	B	264	ASP	CB-CG-OD1	7.91	125.42	118.30
1	A	328	PRO	O-C-N	-7.87	110.10	122.70
1	B	479	ASP	CB-CG-OD2	-7.83	111.25	118.30
1	A	403	LYS	O-C-N	-7.81	110.20	122.70
1	A	344	LEU	CB-CG-CD2	-7.81	97.73	111.00
1	B	464	LEU	CB-CG-CD2	-7.81	97.73	111.00
1	B	491	PRO	C-N-CA	-7.79	102.21	121.70
1	A	115	LEU	CA-C-N	-7.79	100.07	117.20
1	A	68	PRO	C-N-CA	7.79	141.16	121.70
1	A	105	ASP	CB-CG-OD1	7.78	125.30	118.30
1	B	328	PRO	CA-N-CD	-7.73	100.67	111.50
1	A	12	SER	N-CA-C	7.70	131.78	111.00
1	A	452	GLU	CA-CB-CG	7.67	130.28	113.40
1	A	64	PRO	CA-N-CD	-7.66	100.78	111.50
1	B	211	ASP	CB-CG-OD1	7.65	125.19	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	173	ASP	CB-CG-OD2	-7.63	111.43	118.30
1	B	375	GLY	C-N-CA	-7.61	102.67	121.70
1	B	99	PRO	CA-N-CD	-7.61	100.85	111.50
1	A	500	TYR	CB-CG-CD2	7.57	125.54	121.00
1	B	494	VAL	O-C-N	7.57	134.81	122.70
1	A	408	VAL	CG1-CB-CG2	-7.56	98.80	110.90
1	A	490	VAL	O-C-N	7.55	135.44	121.10
1	A	379	ASP	CB-CG-OD1	7.53	125.08	118.30
1	B	99	PRO	O-C-N	-7.53	110.40	123.20
1	A	138	LYS	O-C-N	-7.49	110.72	122.70
1	B	318	ALA	CB-CA-C	7.47	121.31	110.10
1	A	89	PRO	C-N-CA	7.45	153.30	122.00
1	A	317	GLY	O-C-N	7.41	134.56	122.70
1	B	422	LEU	CB-CG-CD1	7.38	123.55	111.00
1	B	486	ARG	NE-CZ-NH2	-7.36	116.62	120.30
1	A	248	ILE	CG1-CB-CG2	-7.35	95.23	111.40
1	B	190	VAL	CA-CB-CG1	7.34	121.91	110.90
1	A	131	LEU	CB-CG-CD1	7.32	123.44	111.00
1	A	490	VAL	CA-CB-CG2	7.30	121.85	110.90
1	B	289	ARG	CB-CG-CD	7.30	130.58	111.60
1	A	58	VAL	CA-CB-CG1	7.29	121.84	110.90
1	B	255	VAL	CA-CB-CG2	7.29	121.83	110.90
1	B	276	ALA	N-CA-C	7.27	130.64	111.00
1	B	499	VAL	CB-CA-C	-7.26	97.60	111.40
1	B	338	LEU	O-C-N	-7.25	111.09	122.70
1	B	494	VAL	CA-C-N	-7.25	101.26	117.20
1	A	114	SER	N-CA-CB	7.20	121.29	110.50
1	A	89	PRO	O-C-N	-7.14	107.53	121.10
1	A	169	LYS	CA-CB-CG	-7.14	97.69	113.40
1	B	281	VAL	CB-CA-C	-7.12	97.88	111.40
1	A	214	ARG	NE-CZ-NH1	-7.12	116.74	120.30
1	B	416	THR	CA-CB-CG2	-7.12	102.44	112.40
1	B	493	ASP	CB-CG-OD1	7.09	124.68	118.30
1	B	146	SER	C-N-CA	7.07	137.14	122.30
1	B	172	VAL	O-C-N	-7.05	111.41	122.70
1	A	356	ASP	CB-CG-OD2	-7.05	111.95	118.30
1	A	41	PRO	CA-N-CD	-7.03	101.66	111.50
1	A	298	SER	N-CA-CB	7.02	121.03	110.50
1	B	463	ARG	NE-CZ-NH2	-7.02	116.79	120.30
1	A	490	VAL	CA-C-N	-6.99	97.52	117.10
1	B	470	ILE	CG1-CB-CG2	-6.99	96.01	111.40
1	B	102	THR	O-C-N	-6.98	111.53	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	71	ILE	C-N-CA	6.97	139.12	121.70
1	A	395	LEU	CA-C-O	6.95	134.70	120.10
1	B	357	VAL	CA-CB-CG1	6.95	121.32	110.90
1	A	509	GLU	O-C-N	-6.91	111.64	122.70
1	A	478	LEU	CA-CB-CG	-6.88	99.47	115.30
1	B	498	GLU	OE1-CD-OE2	6.86	131.53	123.30
1	A	451	ILE	C-N-CA	6.85	138.83	121.70
1	B	427	LYS	CD-CE-NZ	-6.85	95.95	111.70
1	B	318	ALA	C-N-CA	6.84	138.79	121.70
1	A	444	ARG	CG-CD-NE	6.82	126.12	111.80
1	A	413	ARG	CB-CG-CD	6.80	129.29	111.60
1	A	277	LEU	CB-CG-CD1	-6.80	99.45	111.00
1	B	185	GLY	CA-C-N	6.77	132.10	117.20
1	A	265	LEU	CA-CB-CG	-6.77	99.73	115.30
1	A	102	THR	CA-C-O	6.77	134.32	120.10
1	A	321	ALA	CA-C-O	6.76	134.30	120.10
1	A	271	LYS	CA-C-N	6.65	131.82	117.20
1	B	347	VAL	C-N-CA	6.64	138.30	121.70
1	A	211	ASP	C-N-CA	-6.63	105.12	121.70
1	A	330	LEU	CA-CB-CG	6.62	130.53	115.30
1	A	473	LEU	CB-CG-CD1	6.62	122.25	111.00
1	B	259	ARG	NE-CZ-NH2	6.61	123.61	120.30
1	B	234	SER	N-CA-CB	-6.60	100.60	110.50
1	A	330	LEU	CB-CG-CD1	-6.58	99.82	111.00
1	B	480	LEU	CB-CG-CD1	-6.56	99.85	111.00
1	B	492	ASN	O-C-N	-6.55	112.22	122.70
1	B	108	ARG	NE-CZ-NH2	-6.54	117.03	120.30
1	B	144	TYR	CB-CG-CD2	6.54	124.92	121.00
1	A	57	ASP	CA-C-N	6.54	131.58	117.20
1	A	508	PHE	C-N-CA	-6.53	105.38	121.70
1	B	251	TYR	N-CA-CB	6.53	122.35	110.60
1	B	154	HIS	O-C-N	-6.52	112.27	122.70
1	B	230	LEU	CA-CB-CG	6.52	130.30	115.30
1	A	490	VAL	CA-CB-CG1	6.52	120.67	110.90
1	A	112	LEU	C-N-CA	6.50	137.96	121.70
1	B	508	PHE	CB-CG-CD1	6.50	125.35	120.80
1	B	123	ILE	CG1-CB-CG2	-6.49	97.13	111.40
1	A	388	LEU	CA-CB-CG	6.46	130.16	115.30
1	A	509	GLU	CB-CA-C	-6.44	97.52	110.40
1	A	151	GLU	O-C-N	-6.44	112.39	122.70
1	B	460	MET	CG-SD-CE	6.42	110.47	100.20
1	A	221	THR	CA-CB-CG2	-6.41	103.42	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	11	ILE	C-N-CA	6.41	137.73	121.70
1	A	342	THR	CA-CB-CG2	-6.40	103.43	112.40
1	A	173	ASP	N-CA-C	-6.39	93.75	111.00
1	B	279	VAL	O-C-N	-6.38	112.49	122.70
1	A	493	ASP	O-C-N	-6.38	112.50	122.70
1	A	58	VAL	O-C-N	-6.37	112.50	122.70
1	B	105	ASP	CB-CG-OD1	6.35	124.02	118.30
1	B	422	LEU	CA-CB-CG	-6.35	100.69	115.30
1	B	433	ARG	NE-CZ-NH1	6.35	123.47	120.30
1	B	226	MET	O-C-N	6.34	132.85	122.70
1	B	197	THR	N-CA-CB	-6.34	98.25	110.30
1	B	172	VAL	CA-CB-CG1	6.33	120.39	110.90
1	A	183	MET	O-C-N	6.32	132.82	122.70
1	A	365	VAL	N-CA-C	-6.30	93.99	111.00
1	B	134	GLN	O-C-N	-6.30	112.62	122.70
1	B	130	TYR	CB-CG-CD1	-6.28	117.23	121.00
1	A	489	GLY	N-CA-C	-6.26	97.46	113.10
1	A	167	LYS	O-C-N	-6.24	109.24	121.10
1	A	39	PHE	CB-CG-CD1	6.24	125.17	120.80
1	A	396	GLU	CA-C-O	6.21	133.14	120.10
1	B	143	TYR	CB-CG-CD2	-6.20	117.28	121.00
1	A	286	LEU	CB-CG-CD1	6.20	121.54	111.00
1	A	507	GLU	OE1-CD-OE2	-6.19	115.87	123.30
1	B	133	SER	O-C-N	-6.19	112.80	122.70
1	A	417	ASP	CB-CG-OD2	-6.17	112.74	118.30
1	A	493	ASP	N-CA-C	6.17	127.65	111.00
1	B	135	THR	CA-C-O	6.17	133.05	120.10
1	A	58	VAL	CA-CB-CG2	6.15	120.13	110.90
1	B	101	GLU	C-N-CA	6.14	137.05	121.70
1	B	258	ASP	O-C-N	-6.14	112.88	122.70
1	A	495	LEU	CB-CG-CD2	-6.13	100.58	111.00
1	B	365	VAL	C-N-CA	6.13	137.02	121.70
1	B	186	SER	CB-CA-C	-6.12	98.46	110.10
1	A	465	LEU	CB-CG-CD2	6.11	121.39	111.00
1	A	393	PRO	CA-N-CD	-6.11	102.94	111.50
1	A	226	MET	CG-SD-CE	-6.10	90.44	100.20
1	A	119	LEU	CB-CG-CD1	-6.08	100.66	111.00
1	A	254	TYR	C-N-CA	-6.08	106.49	121.70
1	B	456	ASP	CB-CG-OD1	6.08	123.77	118.30
1	B	178	ASP	C-N-CA	6.06	136.84	121.70
1	B	382	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	B	221	THR	CA-CB-CG2	-6.03	103.96	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	261	ILE	CB-CA-C	-6.03	99.55	111.60
1	A	23	ASP	C-N-CA	6.02	136.76	121.70
1	A	183	MET	CA-C-N	-6.02	103.95	117.20
1	B	322	LEU	CA-CB-CG	6.01	129.13	115.30
1	A	322	LEU	CB-CG-CD1	-6.00	100.80	111.00
1	B	98	ALA	N-CA-CB	6.00	118.50	110.10
1	B	475	PRO	CA-N-CD	-6.00	103.10	111.50
1	A	112	LEU	O-C-N	5.99	132.28	122.70
1	A	175	ARG	NE-CZ-NH1	5.99	123.29	120.30
1	B	190	VAL	CG1-CB-CG2	5.98	120.47	110.90
1	B	265	LEU	CB-CG-CD2	5.98	121.16	111.00
1	A	64	PRO	O-C-N	-5.97	113.14	122.70
1	A	161	TYR	CB-CG-CD1	5.97	124.58	121.00
1	B	447	VAL	CB-CA-C	-5.97	100.05	111.40
1	B	112	LEU	C-N-CA	5.97	136.62	121.70
1	A	394	ILE	CA-C-O	5.95	132.60	120.10
1	A	479	ASP	CB-CG-OD1	5.95	123.66	118.30
1	A	422	LEU	CA-CB-CG	-5.93	101.66	115.30
1	A	409	ASP	CB-CG-OD2	-5.92	112.97	118.30
1	B	420	LYS	N-CA-CB	-5.91	99.96	110.60
1	B	508	PHE	CB-CG-CD2	-5.91	116.66	120.80
1	A	348	ILE	CG1-CB-CG2	-5.91	98.41	111.40
1	B	230	LEU	O-C-N	-5.89	113.28	122.70
1	B	473	LEU	CA-C-O	5.88	132.45	120.10
1	B	265	LEU	CA-C-O	5.87	132.43	120.10
1	B	339	LYS	O-C-N	-5.86	113.32	122.70
1	B	496	TYR	N-CA-CB	-5.86	100.05	110.60
1	A	246	LYS	CD-CE-NZ	5.86	125.17	111.70
1	A	223	VAL	CA-CB-CG2	-5.85	102.12	110.90
1	B	187	HIS	CA-CB-CG	5.85	123.55	113.60
1	B	357	VAL	CA-C-N	-5.83	104.38	117.20
1	A	340	LYS	CD-CE-NZ	5.81	125.06	111.70
1	B	238	ILE	C-N-CA	5.81	136.22	121.70
1	B	398	ARG	CD-NE-CZ	5.80	131.72	123.60
1	A	328	PRO	CA-N-CD	-5.78	103.40	111.50
1	B	507	GLU	C-N-CA	5.78	136.16	121.70
1	A	196	ALA	CA-C-N	-5.76	104.52	117.20
1	B	354	THR	CA-CB-CG2	5.75	120.45	112.40
1	B	115	LEU	N-CA-CB	5.75	121.89	110.40
1	A	507	GLU	N-CA-C	5.74	126.51	111.00
1	A	423	CYS	CB-CA-C	-5.74	98.92	110.40
1	B	338	LEU	CA-C-N	5.74	129.82	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	507	GLU	C-N-CA	5.72	136.00	121.70
1	B	104	GLU	CA-CB-CG	5.71	125.97	113.40
1	A	465	LEU	CB-CG-CD1	-5.71	101.29	111.00
1	A	199	LEU	C-N-CA	-5.71	107.43	121.70
1	A	281	VAL	CB-CA-C	-5.71	100.56	111.40
1	B	108	ARG	CD-NE-CZ	5.71	131.59	123.60
1	A	72	ASP	CB-CG-OD2	-5.70	113.17	118.30
1	A	57	ASP	CA-C-O	-5.69	108.15	120.10
1	B	388	LEU	O-C-N	5.69	131.81	122.70
1	A	6	MET	C-N-CA	5.68	135.91	121.70
1	A	57	ASP	CB-CG-OD1	5.68	123.41	118.30
1	B	356	ASP	C-N-CA	-5.67	107.52	121.70
1	B	119	LEU	O-C-N	-5.67	113.63	122.70
1	A	320	ARG	C-N-CA	5.66	135.86	121.70
1	B	420	LYS	CD-CE-NZ	-5.65	98.70	111.70
1	A	48	ASP	N-CA-CB	-5.63	100.47	110.60
1	A	240	GLU	CA-CB-CG	5.63	125.78	113.40
1	B	286	LEU	CB-CA-C	5.61	120.86	110.20
1	A	375	GLY	C-N-CA	-5.60	107.70	121.70
1	A	488	VAL	CG1-CB-CG2	-5.60	101.95	110.90
1	A	491	PRO	CA-C-N	-5.59	104.90	117.20
1	A	397	GLN	O-C-N	-5.58	113.77	122.70
1	B	216	CYS	CA-CB-SG	-5.58	103.95	114.00
1	B	99	PRO	C-N-CA	5.56	133.97	122.30
1	B	136	LEU	CA-CB-CG	5.56	128.08	115.30
1	B	139	GLN	N-CA-CB	-5.55	100.62	110.60
1	B	409	ASP	CB-CG-OD1	5.55	123.29	118.30
1	A	141	TRP	CD1-CG-CD2	-5.54	101.87	106.30
1	B	212	VAL	CA-CB-CG1	5.54	119.21	110.90
1	A	155	ARG	CA-CB-CG	-5.54	101.22	113.40
1	B	342	THR	CA-C-N	-5.54	105.02	117.20
1	B	491	PRO	O-C-N	5.53	131.55	122.70
1	A	420	LYS	CB-CA-C	5.53	121.46	110.40
1	A	476	ASP	CB-CG-OD1	5.52	123.27	118.30
1	B	153	THR	O-C-N	-5.52	113.87	122.70
1	B	317	GLY	N-CA-C	-5.52	99.31	113.10
1	A	23	ASP	CB-CG-OD2	5.51	123.26	118.30
1	A	317	GLY	C-N-CA	5.51	135.47	121.70
1	A	265	LEU	CB-CG-CD1	5.49	120.34	111.00
1	A	49	VAL	CA-CB-CG2	5.48	119.11	110.90
1	B	167	LYS	C-N-CD	5.46	139.88	128.40
1	A	136	LEU	C-N-CA	5.46	135.35	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	189	ASP	CB-CG-OD1	5.46	123.21	118.30
1	B	273	GLY	C-N-CA	5.46	135.35	121.70
1	B	492	ASN	CA-C-O	-5.44	108.67	120.10
1	A	127	ASP	CB-CG-OD2	5.44	123.19	118.30
1	A	69	ASN	C-N-CA	5.42	135.24	121.70
1	B	98	ALA	O-C-N	5.42	131.39	121.10
1	B	253	LEU	CB-CG-CD1	-5.41	101.81	111.00
1	A	278	PHE	N-CA-CB	-5.39	100.90	110.60
1	A	296	LYS	C-N-CA	5.38	135.16	121.70
1	A	500	TYR	CZ-CE2-CD2	-5.38	114.95	119.80
1	B	107	ALA	N-CA-C	-5.37	96.49	111.00
1	A	191	PRO	O-C-N	-5.37	114.11	122.70
1	B	212	VAL	CA-CB-CG2	5.37	118.95	110.90
1	A	214	ARG	CD-NE-CZ	-5.36	116.09	123.60
1	B	427	LYS	C-N-CA	-5.36	111.05	122.30
1	B	389	ALA	C-N-CA	-5.35	108.31	121.70
1	B	255	VAL	CA-CB-CG1	5.35	118.93	110.90
1	A	262	THR	CA-CB-CG2	5.35	119.89	112.40
1	B	272	LEU	CB-CA-C	5.33	120.33	110.20
1	B	480	LEU	CB-CA-C	-5.33	100.07	110.20
1	A	61	ILE	CA-CB-CG1	5.33	121.12	111.00
1	B	169	LYS	CA-CB-CG	5.32	125.10	113.40
1	B	253	LEU	CB-CA-C	-5.32	100.09	110.20
1	A	36	LEU	C-N-CA	5.32	134.99	121.70
1	A	319	SER	CA-C-N	-5.32	105.50	117.20
1	A	467	VAL	C-N-CA	-5.31	108.42	121.70
1	A	398	ARG	CA-CB-CG	5.31	125.07	113.40
1	A	376	ARG	CD-NE-CZ	5.30	131.02	123.60
1	A	65	LEU	CB-CG-CD2	5.29	120.00	111.00
1	A	87	SER	C-N-CA	5.29	134.93	121.70
1	B	178	ASP	N-CA-CB	5.29	120.12	110.60
1	A	173	ASP	CB-CG-OD1	5.28	123.05	118.30
1	B	182	ASP	CB-CG-OD2	-5.28	113.55	118.30
1	B	170	ILE	CA-CB-CG2	5.27	121.45	110.90
1	B	258	ASP	CB-CG-OD1	5.27	123.04	118.30
1	B	408	VAL	CA-CB-CG1	5.27	118.80	110.90
1	A	413	ARG	CB-CA-C	5.27	120.93	110.40
1	A	62	PHE	CB-CG-CD2	-5.26	117.12	120.80
1	A	290	GLU	O-C-N	-5.25	114.30	122.70
1	A	317	GLY	CA-C-O	-5.25	111.15	120.60
1	A	56	LYS	C-N-CA	5.25	134.82	121.70
1	A	97	TYR	N-CA-CB	5.24	120.04	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	400	LEU	CB-CA-C	5.24	120.16	110.20
1	B	102	THR	CA-CB-OG1	5.24	120.00	109.00
1	B	272	LEU	O-C-N	-5.24	114.30	123.20
1	A	398	ARG	O-C-N	-5.24	114.32	122.70
1	A	125	LEU	N-CA-CB	-5.23	99.94	110.40
1	A	473	LEU	N-CA-C	-5.23	96.88	111.00
1	B	417	ASP	N-CA-CB	-5.22	101.20	110.60
1	B	491	PRO	CA-C-N	-5.21	105.73	117.20
1	B	261	ILE	CA-C-N	-5.21	105.74	117.20
1	B	428	GLY	C-N-CA	-5.21	108.68	121.70
1	B	179	ILE	CA-C-O	5.20	131.02	120.10
1	B	218	GLN	N-CA-CB	-5.18	101.27	110.60
1	B	494	VAL	CA-CB-CG2	5.18	118.68	110.90
1	A	396	GLU	CG-CD-OE1	-5.18	107.94	118.30
1	A	289	ARG	NE-CZ-NH1	-5.18	117.71	120.30
1	B	102	THR	OG1-CB-CG2	5.17	121.89	110.00
1	A	184	LEU	CA-C-O	5.17	130.95	120.10
1	A	188	VAL	CB-CA-C	-5.17	101.58	111.40
1	A	420	LYS	CA-CB-CG	5.16	124.76	113.40
1	B	149	ASN	N-CA-CB	5.16	119.90	110.60
1	B	477	LEU	CA-CB-CG	5.16	127.17	115.30
1	B	331	THR	C-N-CA	5.14	134.54	121.70
1	A	499	VAL	CA-CB-CG2	5.12	118.58	110.90
1	B	345	PRO	CA-C-N	-5.12	105.95	117.20
1	A	112	LEU	CA-C-O	-5.11	109.36	120.10
1	B	266	VAL	CA-CB-CG2	5.10	118.55	110.90
1	B	444	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	B	137	THR	CB-CA-C	-5.09	97.85	111.60
1	B	285	SER	C-N-CA	-5.08	108.99	121.70
1	B	226	MET	CA-C-N	-5.08	106.02	117.20
1	B	279	VAL	CA-CB-CG2	5.07	118.51	110.90
1	A	11	ILE	N-CA-C	5.06	124.66	111.00
1	B	440	SER	C-N-CA	-5.06	109.05	121.70
1	A	87	SER	CB-CA-C	5.06	119.71	110.10
1	A	296	LYS	CA-CB-CG	5.05	124.51	113.40
1	B	267	LYS	CA-CB-CG	5.05	124.51	113.40
1	A	369	VAL	C-N-CA	-5.05	109.08	121.70
1	B	98	ALA	C-N-CD	5.04	138.99	128.40
1	A	459	GLU	C-N-CA	5.04	134.31	121.70
1	B	327	ASP	CA-C-N	-5.04	102.99	117.10
1	B	220	VAL	CG1-CB-CG2	5.04	118.96	110.90
1	B	198	ALA	C-N-CA	5.03	134.28	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	35	ASP	C-N-CA	5.03	134.27	121.70
1	A	179	ILE	C-N-CA	-5.01	109.17	121.70
1	A	470	ILE	C-N-CA	-5.01	109.17	121.70
1	B	236	GLU	OE1-CD-OE2	-5.01	117.29	123.30
1	A	67	ALA	CA-C-N	-5.01	103.07	117.10
1	A	114	SER	CB-CA-C	5.01	119.62	110.10

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	11	ILE	CA
1	A	298	SER	CA
1	B	102	THR	CB
1	B	149	ASN	CA
1	B	272	LEU	CA
1	B	507	GLU	CA

All (121) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	10	LYS	Mainchain
1	A	104	GLU	Peptide
1	A	106	ILE	Mainchain,Peptide
1	A	11	ILE	Peptide
1	A	114	SER	Mainchain
1	A	138	LYS	Mainchain
1	A	139	GLN	Mainchain
1	A	148	ALA	Mainchain
1	A	151	GLU	Mainchain
1	A	154	HIS	Sidechain
1	A	160	ALA	Mainchain
1	A	181	THR	Mainchain
1	A	222	LYS	Peptide
1	A	231	ALA	Peptide
1	A	273	GLY	Peptide
1	A	293	MET	Mainchain
1	A	297	PHE	Mainchain,Peptide
1	A	31	GLY	Peptide
1	A	321	ALA	Mainchain
1	A	324	LYS	Peptide
1	A	326	ILE	Mainchain
1	A	380	PHE	Mainchain

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Mol	Chain	Res	Type	Group
1	A	382	ARG	Mainchain
1	A	384	PRO	Mainchain
1	A	395	LEU	Mainchain
1	A	396	GLU	Mainchain
1	A	403	LYS	Peptide
1	A	441	CYS	Mainchain
1	A	445	ASN	Peptide
1	A	452	GLU	Mainchain
1	A	460	MET	Mainchain
1	A	47	GLN	Peptide
1	A	475	PRO	Mainchain
1	A	491	PRO	Mainchain
1	A	492	ASN	Peptide
1	A	493	ASP	Mainchain
1	A	50	ILE	Peptide
1	A	506	THR	Peptide
1	A	507	GLU	Sidechain,Mainchain,Peptide
1	A	508	PHE	Peptide
1	A	509	GLU	Peptide
1	A	56	LYS	Peptide
1	A	57	ASP	Peptide
1	A	58	VAL	Mainchain
1	A	59	THR	Mainchain
1	A	67	ALA	Mainchain
1	A	72	ASP	Sidechain,Mainchain
1	A	80	LYS	Mainchain
1	A	85	GLN	Peptide
1	A	90	PRO	Peptide
1	A	92	LEU	Peptide
1	A	96	PRO	Peptide
1	B	104	GLU	Mainchain
1	B	105	ASP	Sidechain
1	B	106	ILE	Peptide
1	B	111	GLN	Mainchain
1	B	112	LEU	Mainchain
1	B	113	LYS	Peptide
1	B	114	SER	Mainchain
1	B	118	PRO	Mainchain
1	B	119	LEU	Mainchain
1	B	120	ASP	Peptide
1	B	127	ASP	Sidechain
1	B	151	GLU	Mainchain

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Mol	Chain	Res	Type	Group
1	B	153	THR	Mainchain
1	B	154	HIS	Mainchain
1	B	172	VAL	Mainchain
1	B	187	HIS	Mainchain,Peptide
1	B	195	SER	Peptide
1	B	199	LEU	Mainchain
1	B	200	CYS	Mainchain
1	B	208	GLY	Mainchain
1	B	210	LYS	Peptide
1	B	211	ASP	Mainchain
1	B	224	PRO	Mainchain
1	B	229	THR	Mainchain
1	B	231	ALA	Peptide
1	B	242	ALA	Mainchain
1	B	246	LYS	Mainchain
1	B	247	GLN	Mainchain
1	B	255	VAL	Mainchain
1	B	256	ASN	Peptide
1	B	257	SER	Mainchain
1	B	263	ASP	Mainchain
1	B	266	VAL	Mainchain
1	B	267	LYS	Mainchain
1	B	270	GLU	Mainchain
1	B	295	LEU	Mainchain
1	B	296	LYS	Mainchain,Peptide
1	B	317	GLY	Mainchain,Peptide
1	B	324	LYS	Peptide
1	B	327	ASP	Mainchain
1	B	331	THR	Mainchain
1	B	332	TRP	Mainchain
1	B	336	GLU	Mainchain
1	B	339	LYS	Mainchain
1	B	353	ARG	Mainchain
1	B	363	ILE	Mainchain
1	B	364	GLY	Mainchain
1	B	370	LEU	Mainchain
1	B	378	LEU	Mainchain
1	B	380	PHE	Mainchain
1	B	394	ILE	Peptide
1	B	396	GLU	Mainchain
1	B	475	PRO	Mainchain
1	B	492	ASN	Mainchain,Peptide

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Mol	Chain	Res	Type	Group
1	B	493	ASP	Mainchain,Peptide
1	B	506	THR	Mainchain
1	B	98	ALA	Mainchain
1	B	99	PRO	Mainchain,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	3833	0	3888	416	1
1	B	3081	0	3136	511	1
2	A	43	0	30	15	0
3	A	31	0	17	13	0
3	B	31	0	18	15	0
4	B	6	0	0	1	0
5	A	7	0	0	0	0
5	B	10	0	0	1	0
All	All	7042	0	7089	914	1

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 65.

All (914) 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:175:ARG:CD	1:B:175:ARG:CG	1.77	1.63
1:A:413:ARG:CD	1:A:413:ARG:CG	1.78	1.61
1:A:343:LYS:CB	1:A:343:LYS:CG	1.79	1.60
1:A:286:LEU:CD1	1:A:286:LEU:CG	1.78	1.59
1:B:106:ILE:CD1	1:B:106:ILE:CG1	1.75	1.59
1:B:289:ARG:CD	1:B:289:ARG:CG	1.82	1.58
1:B:289:ARG:CG	1:B:289:ARG:CB	1.79	1.56
1:B:167:LYS:CE	1:B:167:LYS:NZ	1.69	1.55
1:B:137:THR:CB	1:B:137:THR:CG2	1.85	1.51
1:A:340:LYS:NZ	1:A:340:LYS:CE	1.70	1.49
1:B:347:VAL:HG12	1:B:367:GLY:CA	1.41	1.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:441:CYS:CB	1:B:441:CYS:SG	2.02	1.47
1:B:278:PHE:CE2	1:B:347:VAL:HG21	1.46	1.46
1:B:347:VAL:CG1	1:B:367:GLY:HA3	1.51	1.36
1:B:278:PHE:CD2	1:B:347:VAL:HG23	1.65	1.30
1:B:347:VAL:HG12	1:B:367:GLY:C	1.55	1.26
1:B:228:SER:HA	1:B:252:GLN:NE2	1.50	1.25
1:B:278:PHE:CE2	1:B:347:VAL:CG2	2.19	1.25
1:B:431:LEU:N	1:B:431:LEU:HD12	1.44	1.23
1:B:109:LYS:O	1:B:113:LYS:HB2	1.37	1.23
1:B:229:THR:OG1	1:B:253:LEU:HA	1.31	1.23
1:B:227:ILE:HD12	1:B:250:TRP:O	1.28	1.22
1:B:278:PHE:CD2	1:B:347:VAL:CG2	2.20	1.22
1:B:430:GLY:C	1:B:431:LEU:HD12	1.59	1.20
1:B:361:ALA:CB	1:B:400:LEU:HD23	1.72	1.20
1:A:252:GLN:OE1	3:A:569:FMN:N3	1.74	1.18
1:B:431:LEU:N	1:B:431:LEU:CD1	2.06	1.18
1:B:447:VAL:O	1:B:451:ILE:HD12	1.42	1.17
1:B:233:CYS:HB2	1:B:238:ILE:HD11	1.18	1.14
1:A:2:PRO:HD2	1:A:71:ILE:HD13	1.19	1.14
1:B:227:ILE:CD1	1:B:250:TRP:O	1.95	1.14
1:B:412:VAL:O	1:B:413:ARG:HD3	1.49	1.13
1:A:110:GLU:HA	1:A:113:LYS:HB2	1.21	1.12
2:A:560:HEM:HHC	2:A:560:HEM:HBB2	1.16	1.12
1:B:136:LEU:HD23	1:B:136:LEU:H	1.13	1.12
1:B:196:ALA:HB2	1:B:226:MET:HE3	1.26	1.12
1:B:276:ALA:HB2	1:B:345:PRO:HD2	1.15	1.11
1:B:196:ALA:HB2	1:B:226:MET:CE	1.80	1.11
1:B:347:VAL:CG1	1:B:367:GLY:CA	2.18	1.10
1:A:108:ARG:O	1:A:112:LEU:HD12	1.51	1.10
1:B:234:SER:OG	1:B:237:GLU:HB2	1.51	1.09
1:A:396:GLU:O	1:A:398:ARG:N	1.87	1.08
1:A:256:ASN:HD22	1:A:257:SER:N	1.50	1.08
1:A:102:THR:HB	1:A:104:GLU:HG2	1.32	1.07
1:A:110:GLU:O	1:A:113:LYS:HB3	1.52	1.07
1:B:361:ALA:HB1	1:B:400:LEU:HD23	1.13	1.07
1:A:70:VAL:HG23	1:A:71:ILE:HD12	1.34	1.05
1:A:204:ASN:HD22	1:A:439:ASN:ND2	1.51	1.05
1:B:448:GLU:HA	1:B:451:ILE:CD1	1.86	1.04
1:A:218:GLN:NE2	1:A:444:ARG:HH11	1.55	1.04
1:B:265:LEU:O	1:B:266:VAL:O	1.77	1.03
1:A:33:VAL:HG13	1:A:82:GLY:O	1.58	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:196:ALA:CB	1:B:226:MET:CE	2.36	1.03
1:A:102:THR:O	1:A:103:LYS:C	1.89	1.03
1:B:229:THR:H	1:B:252:GLN:NE2	1.56	1.02
1:B:246:LYS:O	1:B:247:GLN:O	1.77	1.02
1:A:29:ILE:CD1	1:A:58:VAL:HG12	1.91	1.01
2:A:560:HEM:HHC	2:A:560:HEM:CBB	1.91	1.00
1:A:29:ILE:HD11	1:A:58:VAL:HG12	1.38	1.00
1:B:448:GLU:HA	1:B:451:ILE:HD13	1.39	0.99
1:B:276:ALA:CB	1:B:345:PRO:HD2	1.92	0.99
1:B:447:VAL:O	1:B:451:ILE:CD1	2.11	0.98
1:A:2:PRO:CD	1:A:71:ILE:HD13	1.94	0.97
1:B:286:LEU:HD21	1:B:323:SER:HB3	1.43	0.97
1:B:234:SER:OG	1:B:237:GLU:CB	2.12	0.96
1:A:59:THR:HG23	1:A:63:GLU:HG2	1.49	0.95
1:B:104:GLU:C	1:B:106:ILE:H	1.56	0.94
1:B:347:VAL:HG12	1:B:367:GLY:HA3	1.13	0.94
1:A:218:GLN:NE2	1:A:444:ARG:NH1	2.16	0.94
1:A:110:GLU:CA	1:A:113:LYS:HB2	1.98	0.93
1:A:209:GLU:HB3	1:A:238:ILE:HD13	1.51	0.93
1:A:204:ASN:HD22	1:A:439:ASN:HD21	1.13	0.93
1:B:109:LYS:O	1:B:113:LYS:CB	2.16	0.93
1:B:248:ILE:HG13	1:B:249:GLN:N	1.81	0.93
1:B:233:CYS:CB	1:B:238:ILE:HD11	1.99	0.92
1:B:228:SER:HA	1:B:252:GLN:HE22	1.26	0.92
1:B:317:GLY:N	1:B:320:ARG:NH2	2.17	0.92
1:B:322:LEU:HD13	1:B:328:PRO:HG2	1.51	0.92
1:A:196:ALA:H	1:A:226:MET:HE2	1.35	0.92
1:A:218:GLN:HE22	1:A:444:ARG:NH1	1.68	0.92
1:A:204:ASN:ND2	1:A:439:ASN:HD21	1.67	0.91
1:B:248:ILE:HG13	1:B:249:GLN:H	1.34	0.91
1:A:462:MET:HE1	1:A:469:SER:C	1.91	0.91
1:A:413:ARG:NH2	3:A:569:FMN:O3P	2.03	0.91
1:B:201:LYS:HB2	1:B:232:SER:CB	2.00	0.91
1:B:246:LYS:O	1:B:247:GLN:C	2.06	0.90
1:B:108:ARG:HH12	1:B:137:THR:HA	1.35	0.90
2:A:560:HEM:HHD	2:A:560:HEM:HBC2	1.52	0.90
1:B:353:ARG:NH1	1:B:356:ASP:OD1	2.05	0.90
1:B:153:THR:O	1:B:154:HIS:C	2.06	0.90
1:A:67:ALA:C	1:A:70:VAL:HG13	1.92	0.90
1:B:387:VAL:O	1:B:391:THR:HG23	1.72	0.89
1:B:229:THR:OG1	1:B:253:LEU:CA	2.19	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:175:ARG:CG	1:B:175:ARG:HH11	1.84	0.89
1:B:236:GLU:HB3	1:B:272:LEU:HD11	1.53	0.89
1:B:265:LEU:O	1:B:266:VAL:C	2.09	0.88
1:B:267:LYS:O	1:B:268:ASN:C	2.00	0.88
1:B:361:ALA:HB1	1:B:400:LEU:CD2	2.01	0.88
1:A:218:GLN:HE22	1:A:444:ARG:HH11	0.88	0.87
1:B:233:CYS:HB2	1:B:238:ILE:CD1	2.03	0.87
1:A:210:LYS:HG2	1:A:241:ALA:CB	2.04	0.87
1:A:102:THR:O	1:A:103:LYS:O	1.93	0.86
1:A:229:THR:H	1:A:252:GLN:NE2	1.72	0.86
1:B:229:THR:N	1:B:252:GLN:HE22	1.72	0.86
1:A:395:LEU:O	1:A:396:GLU:C	2.01	0.86
1:A:60:ALA:O	1:A:96:PRO:HB3	1.75	0.86
1:B:255:VAL:HG13	1:B:330:LEU:HD11	1.55	0.86
1:A:223:VAL:HG13	1:A:224:PRO:HD2	1.58	0.85
1:B:229:THR:H	1:B:252:GLN:HE22	1.19	0.85
1:B:465:LEU:O	1:B:465:LEU:HD23	1.75	0.85
1:B:278:PHE:HE2	1:B:347:VAL:HG21	1.34	0.85
1:B:136:LEU:H	1:B:136:LEU:CD2	1.90	0.85
1:B:137:THR:HG22	1:B:139:GLN:HB3	1.57	0.85
1:B:228:SER:CA	1:B:252:GLN:HE22	1.90	0.84
1:B:442:TYR:HB2	1:B:446:GLY:HA3	1.58	0.84
1:A:29:ILE:HD11	1:A:58:VAL:CG1	2.07	0.84
1:B:347:VAL:HG11	1:B:367:GLY:HA3	1.56	0.84
1:A:199:LEU:HD21	2:A:560:HEM:HAA1	1.60	0.84
1:A:25:CYS:SG	1:A:54:ALA:HB1	2.18	0.83
1:B:137:THR:CG2	1:B:139:GLN:HB3	2.08	0.83
1:A:160:ALA:O	1:A:161:TYR:C	2.14	0.83
1:A:256:ASN:ND2	1:A:257:SER:N	2.27	0.83
1:B:136:LEU:HD23	1:B:136:LEU:N	1.93	0.82
1:B:394:ILE:HA	1:B:397:GLN:OE1	1.79	0.82
1:A:269:VAL:HA	1:A:272:LEU:HD12	1.60	0.82
1:B:196:ALA:CB	1:B:226:MET:HE3	2.02	0.82
2:A:560:HEM:HBB2	2:A:560:HEM:CHC	2.05	0.82
1:A:229:THR:H	1:A:252:GLN:HE22	1.26	0.82
1:A:179:ILE:HA	1:A:470:ILE:CD1	2.10	0.82
1:A:173:ASP:OD2	1:B:329:SER:HB2	1.78	0.81
1:A:413:ARG:HG3	1:A:413:ARG:HH11	1.44	0.81
1:A:448:GLU:HA	1:A:451:ILE:HG13	1.63	0.81
1:B:179:ILE:HA	1:B:470:ILE:CD1	2.10	0.81
1:B:234:SER:OG	1:B:237:GLU:OE1	1.96	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:GLY:O	1:A:222:LYS:NZ	2.12	0.81
1:B:346:ILE:HG22	1:B:365:VAL:HG11	1.61	0.81
1:B:354:THR:OG1	1:B:391:THR:HG22	1.78	0.81
1:B:276:ALA:HB2	1:B:345:PRO:CD	2.06	0.81
1:A:102:THR:C	1:A:103:LYS:HD3	2.01	0.80
1:A:353:ARG:HH11	1:A:355:GLU:HB2	1.45	0.80
1:A:210:LYS:HG2	1:A:241:ALA:HB2	1.62	0.80
1:B:378:LEU:HD22	1:B:379:ASP:O	1.82	0.80
1:B:132:ALA:O	1:B:136:LEU:HD23	1.82	0.79
1:B:104:GLU:C	1:B:106:ILE:N	2.28	0.79
1:A:54:ALA:O	1:A:56:LYS:NZ	2.15	0.79
1:B:179:ILE:HA	1:B:470:ILE:HD12	1.63	0.79
1:B:196:ALA:CB	1:B:226:MET:HE2	2.12	0.79
1:B:454:LEU:O	1:B:458:ILE:HG12	1.83	0.79
1:B:146:SER:HB3	1:B:291:LYS:HB2	1.65	0.79
1:B:229:THR:OG1	1:B:252:GLN:O	2.00	0.79
1:A:373:GLN:HG3	3:A:569:FMN:H1'1	1.63	0.79
1:A:2:PRO:HG2	1:A:71:ILE:HB	1.64	0.79
1:B:398:ARG:HB2	1:B:400:LEU:HD13	1.63	0.79
1:B:130:TYR:O	1:B:133:SER:OG	2.00	0.79
1:B:175:ARG:HH11	1:B:175:ARG:HG3	1.48	0.78
1:B:175:ARG:NH1	1:B:175:ARG:CB	2.47	0.78
1:B:201:LYS:HB2	1:B:232:SER:HB3	1.65	0.78
1:B:414:ARG:O	1:B:417:ASP:HB2	1.83	0.78
1:B:433:ARG:O	1:B:437:TYR:CD2	2.35	0.78
1:A:286:LEU:CD1	1:A:286:LEU:HG	2.09	0.78
1:A:498:GLU:HG2	1:B:505:LEU:HD11	1.66	0.78
1:B:266:VAL:O	1:B:269:VAL:HG22	1.84	0.78
1:B:322:LEU:HD13	1:B:328:PRO:CG	2.14	0.78
1:A:109:LYS:HE2	1:A:109:LYS:HA	1.65	0.78
1:A:395:LEU:O	1:A:396:GLU:O	2.01	0.78
1:A:53:ASN:ND2	1:A:94:CYS:SG	2.57	0.78
1:A:252:GLN:OE1	3:A:569:FMN:C2	2.32	0.77
1:B:181:THR:O	1:B:188:VAL:HG23	1.84	0.77
1:B:213:ALA:HB2	1:B:225:GLN:HE22	1.49	0.77
1:A:38:ARG:NH2	1:A:75:ILE:HB	1.98	0.77
1:B:433:ARG:HB3	1:B:437:TYR:CE2	2.19	0.77
1:A:372:ASN:C	1:A:372:ASN:HD22	1.87	0.77
1:B:371:SER:HB2	1:B:409:ASP:OD1	1.85	0.77
1:B:228:SER:CA	1:B:252:GLN:NE2	2.39	0.77
1:B:196:ALA:HB3	1:B:226:MET:CE	2.14	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:283:ALA:N	1:B:284:PRO:CD	2.47	0.77
1:B:229:THR:N	1:B:252:GLN:NE2	2.30	0.76
1:A:32:TYR:HE1	1:A:82:GLY:HA2	1.49	0.76
1:A:179:ILE:HA	1:A:470:ILE:HD12	1.67	0.76
1:A:223:VAL:HG13	1:A:224:PRO:CD	2.15	0.76
1:A:204:ASN:ND2	1:A:439:ASN:ND2	2.26	0.76
1:A:256:ASN:HD22	1:A:257:SER:H	1.32	0.76
1:B:228:SER:HA	1:B:252:GLN:HE21	1.50	0.76
1:A:171:LEU:HD12	1:B:332:TRP:CE2	2.20	0.76
1:B:461:SER:O	1:B:465:LEU:HB2	1.85	0.76
1:B:184:LEU:HD22	1:B:250:TRP:CZ2	2.21	0.76
1:A:332:TRP:CZ2	1:A:359:LYS:HD3	2.20	0.76
1:B:275:LYS:HB2	1:B:275:LYS:NZ	2.01	0.75
1:A:347:VAL:HA	1:A:367:GLY:O	1.86	0.75
1:B:196:ALA:O	3:B:570:FMN:C4A	2.34	0.75
1:B:448:GLU:HA	1:B:451:ILE:HD12	1.68	0.75
1:A:41:PRO:HA	1:A:47:GLN:HG3	1.69	0.75
1:B:251:TYR:HB3	1:B:277:LEU:CD2	2.16	0.75
1:B:164:ILE:HB	1:B:420:LYS:HE2	1.69	0.75
1:B:410:GLY:HA2	3:B:570:FMN:P	2.27	0.74
1:B:447:VAL:HG12	1:B:451:ILE:HD11	1.70	0.74
1:A:42:ASN:OD1	1:A:324:LYS:HB2	1.85	0.74
1:B:317:GLY:N	1:B:320:ARG:HH21	1.85	0.74
1:A:110:GLU:HG2	1:A:113:LYS:HD3	1.69	0.74
1:A:392:MET:CE	1:A:395:LEU:HD12	2.17	0.74
1:B:228:SER:OG	3:B:570:FMN:O4	2.05	0.74
1:B:244:SER:OG	1:B:246:LYS:NZ	2.20	0.74
1:B:431:LEU:CD1	1:B:431:LEU:H	2.00	0.74
1:B:447:VAL:O	1:B:447:VAL:HG12	1.84	0.74
1:A:194:VAL:HG22	1:A:435:PHE:CD2	2.22	0.74
1:A:506:THR:OG1	1:B:127:ASP:OD1	2.05	0.74
1:B:325:PHE:HD1	1:B:325:PHE:H	1.35	0.74
1:A:60:ALA:HB2	1:A:94:CYS:O	1.87	0.73
1:A:256:ASN:ND2	1:A:257:SER:H	1.86	0.73
1:A:60:ALA:CB	1:A:94:CYS:O	2.36	0.73
1:A:84:LEU:HD11	1:A:87:SER:HA	1.71	0.73
1:A:256:ASN:ND2	1:A:258:ASP:H	1.85	0.73
1:A:493:ASP:O	1:A:494:VAL:C	2.25	0.73
1:B:361:ALA:CB	1:B:400:LEU:CD2	2.60	0.73
1:A:196:ALA:N	1:A:226:MET:HE2	2.03	0.73
1:B:262:THR:O	1:B:266:VAL:HG23	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:GLU:O	1:A:113:LYS:CB	2.32	0.72
1:B:196:ALA:O	3:B:570:FMN:C10	2.37	0.72
1:A:62:PHE:HZ	1:A:70:VAL:HG21	1.55	0.72
1:A:339:LYS:HD2	1:A:340:LYS:NZ	2.04	0.72
1:A:373:GLN:HG3	3:A:569:FMN:C1'	2.20	0.72
1:B:137:THR:HG22	1:B:139:GLN:H	1.52	0.72
1:B:163:ARG:HH21	1:B:486:ARG:HA	1.53	0.72
1:B:221:THR:HG22	1:B:222:LYS:N	2.05	0.72
1:B:175:ARG:CG	1:B:175:ARG:NH1	2.52	0.71
1:B:278:PHE:HD2	1:B:347:VAL:HG23	1.51	0.71
1:B:331:THR:HG22	1:B:333:LYS:H	1.55	0.71
1:B:252:GLN:HA	1:B:278:PHE:O	1.91	0.71
1:B:212:VAL:HG12	1:B:439:ASN:OD1	1.90	0.71
1:B:388:LEU:HD23	1:B:392:MET:HG2	1.73	0.71
1:B:199:LEU:HB3	1:B:202:LEU:HD12	1.72	0.71
1:A:392:MET:HE1	1:A:395:LEU:HD12	1.73	0.70
1:A:413:ARG:CG	1:A:413:ARG:HH11	2.03	0.70
1:B:201:LYS:HB2	1:B:232:SER:OG	1.90	0.70
1:A:398:ARG:O	1:A:399:ASN:C	2.27	0.70
1:A:182:ASP:HB2	1:A:187:HIS:HA	1.74	0.70
1:B:442:TYR:HB2	1:B:446:GLY:CA	2.22	0.70
1:A:61:ILE:HD11	1:A:94:CYS:HB3	1.73	0.70
1:A:237:GLU:O	1:A:241:ALA:HB2	1.91	0.69
1:B:236:GLU:HA	1:B:239:ILE:HG22	1.74	0.69
1:B:283:ALA:HA	1:B:377:GLN:NE2	2.06	0.69
1:A:498:GLU:HG2	1:B:505:LEU:CD1	2.22	0.69
1:A:413:ARG:HG3	1:A:413:ARG:NH1	2.07	0.69
1:A:56:LYS:C	1:A:58:VAL:HG23	2.13	0.69
1:A:62:PHE:CZ	1:A:70:VAL:HG21	2.28	0.69
1:B:123:ILE:HG22	1:B:123:ILE:O	1.92	0.69
1:B:211:ASP:HB3	1:B:439:ASN:HD21	1.56	0.69
1:A:62:PHE:HZ	1:A:70:VAL:CG2	2.06	0.69
1:B:180:SER:HA	1:B:189:ASP:O	1.93	0.69
1:B:227:ILE:HD11	1:B:250:TRP:H	1.58	0.68
1:B:255:VAL:CG1	1:B:330:LEU:HD11	2.23	0.68
1:B:259:ARG:HG3	1:B:259:ARG:HH11	1.57	0.68
1:A:75:ILE:HD11	1:A:80:LYS:HG2	1.75	0.68
1:B:184:LEU:O	1:B:186:SER:N	2.25	0.68
1:B:161:TYR:CE1	1:B:385:ILE:HD13	2.27	0.68
1:B:180:SER:CB	1:B:189:ASP:O	2.41	0.68
1:B:184:LEU:HD22	1:B:250:TRP:HZ2	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:286:LEU:N	1:B:286:LEU:HD22	2.08	0.68
1:B:98:ALA:HB1	1:B:101:GLU:HG3	1.74	0.68
1:B:236:GLU:HB3	1:B:272:LEU:CD1	2.23	0.68
1:A:171:LEU:HD12	1:B:332:TRP:CD2	2.29	0.68
1:A:148:ALA:O	1:A:379:ASP:OD2	2.11	0.68
1:A:257:SER:HB2	1:A:324:LYS:O	1.94	0.68
1:B:262:THR:O	1:B:264:ASP:N	2.27	0.67
1:A:32:TYR:HE1	1:A:82:GLY:CA	2.07	0.67
1:A:9:GLN:O	1:A:10:LYS:HB3	1.94	0.67
1:B:214:ARG:HG2	1:B:214:ARG:HH11	1.59	0.67
1:B:193:TYR:O	1:B:194:VAL:C	2.29	0.67
1:A:269:VAL:HA	1:A:272:LEU:CD1	2.25	0.67
1:B:108:ARG:NH1	1:B:136:LEU:O	2.27	0.67
1:A:353:ARG:HD3	1:A:355:GLU:OE1	1.94	0.67
1:B:283:ALA:N	1:B:284:PRO:HD2	2.10	0.67
1:B:124:ASN:HD22	1:B:126:TYR:N	1.92	0.67
1:B:491:PRO:C	1:B:492:ASN:O	2.34	0.67
1:A:108:ARG:O	1:A:112:LEU:CD1	2.39	0.67
1:B:259:ARG:HH11	1:B:259:ARG:CG	2.06	0.67
1:B:98:ALA:HB1	1:B:101:GLU:CB	2.25	0.66
1:A:60:ALA:HB1	1:A:96:PRO:CD	2.25	0.66
1:B:214:ARG:HB3	1:B:444:ARG:HD2	1.77	0.66
1:A:14:ALA:O	1:A:17:ALA:HB3	1.96	0.66
1:A:61:ILE:HG23	1:A:97:TYR:HB2	1.78	0.66
1:B:136:LEU:CD2	1:B:136:LEU:N	2.55	0.66
1:B:267:LYS:O	1:B:269:VAL:N	2.28	0.66
1:A:27:VAL:HG22	1:A:56:LYS:O	1.95	0.66
1:A:339:LYS:HD2	1:A:340:LYS:HZ1	1.59	0.66
1:A:4:LEU:HB3	1:A:32:TYR:HE2	1.61	0.66
1:B:102:THR:HB	1:B:104:GLU:HG3	1.77	0.66
1:A:50:ILE:O	1:A:54:ALA:HB2	1.96	0.65
1:A:213:ALA:HB2	1:A:225:GLN:HE22	1.61	0.65
1:B:346:ILE:HB	1:B:365:VAL:HG21	1.77	0.65
1:B:436:LEU:HD11	3:B:570:FMN:HM73	1.78	0.65
1:A:506:THR:HG1	1:B:127:ASP:CG	2.00	0.65
1:A:209:GLU:CB	1:A:238:ILE:HD13	2.26	0.65
1:B:248:ILE:CG1	1:B:249:GLN:N	2.57	0.65
1:B:396:GLU:HG3	1:B:401:LYS:NZ	2.12	0.65
1:B:167:LYS:NZ	1:B:167:LYS:CD	2.60	0.64
1:B:362:GLU:C	1:B:364:GLY:H	2.01	0.64
1:A:394:ILE:O	1:A:395:LEU:C	2.34	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:219:GLY:O	1:B:222:LYS:NZ	2.26	0.64
1:B:347:VAL:CG1	1:B:367:GLY:C	2.50	0.64
1:B:98:ALA:HB1	1:B:101:GLU:CG	2.27	0.64
1:A:179:ILE:HD11	1:A:455:ARG:HG3	1.80	0.64
1:B:153:THR:HG21	1:B:381:SER:HB3	1.79	0.64
1:B:209:GLU:CD	1:B:231:ALA:HB1	2.18	0.64
1:B:184:LEU:CD2	1:B:250:TRP:CZ2	2.81	0.64
1:B:392:MET:N	1:B:393:PRO:HD2	2.12	0.64
1:B:197:THR:OG1	1:B:436:LEU:HG	1.98	0.63
1:B:236:GLU:HA	1:B:239:ILE:CG2	2.28	0.63
1:A:148:ALA:HB2	1:A:376:ARG:O	1.98	0.63
1:B:105:ASP:O	1:B:109:LYS:HB2	1.98	0.63
1:A:19:HIS:O	1:A:21:LYS:N	2.31	0.63
1:A:382:ARG:O	1:A:383:ALA:C	2.13	0.63
1:A:212:VAL:HG12	1:A:439:ASN:OD1	1.99	0.63
1:B:174:VAL:HG21	1:B:463:ARG:HB3	1.80	0.63
1:A:196:ALA:O	3:A:569:FMN:O2'	2.08	0.63
1:A:105:ASP:HA	1:A:108:ARG:HB2	1.80	0.63
1:B:102:THR:O	1:B:104:GLU:N	2.31	0.63
1:B:174:VAL:HG23	1:B:174:VAL:O	1.98	0.63
1:B:234:SER:OG	1:B:237:GLU:HB3	1.98	0.63
1:B:239:ILE:CD1	1:B:274:VAL:HG13	2.29	0.63
1:A:173:ASP:OD2	1:B:329:SER:CB	2.45	0.62
1:A:179:ILE:HA	1:A:470:ILE:HD11	1.81	0.62
1:A:179:ILE:CA	1:A:470:ILE:HD12	2.29	0.62
1:B:439:ASN:HD22	1:B:443:GLY:HA2	1.64	0.62
1:A:201:LYS:HB2	1:A:232:SER:CB	2.30	0.62
1:B:382:ARG:NH2	1:B:390:GLU:OE2	2.33	0.62
1:B:111:GLN:HB3	1:B:135:THR:HG22	1.82	0.62
1:A:462:MET:CE	1:A:469:SER:C	2.66	0.62
1:B:152:VAL:O	1:B:153:THR:C	2.36	0.62
1:B:195:SER:O	1:B:197:THR:HG22	1.98	0.62
1:B:239:ILE:HD11	1:B:274:VAL:HG13	1.82	0.62
1:B:286:LEU:CD2	1:B:323:SER:HB3	2.25	0.62
1:B:430:GLY:CA	1:B:431:LEU:HD12	2.28	0.62
1:B:198:ALA:HB2	3:B:570:FMN:O4	2.00	0.62
1:B:262:THR:C	1:B:264:ASP:N	2.47	0.62
1:B:491:PRO:O	1:B:492:ASN:O	2.16	0.62
1:A:257:SER:CB	1:A:324:LYS:O	2.48	0.61
1:B:371:SER:CB	1:B:409:ASP:OD1	2.48	0.61
1:B:175:ARG:NH1	1:B:175:ARG:HB3	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:268:ASN:O	1:B:268:ASN:ND2	2.33	0.61
1:A:265:LEU:HD22	1:A:265:LEU:O	2.00	0.61
1:A:372:ASN:C	1:A:372:ASN:ND2	2.54	0.61
1:B:153:THR:HG23	1:B:381:SER:O	2.00	0.61
1:B:282:ASP:OD2	1:B:373:GLN:HG3	2.01	0.61
1:B:392:MET:HE1	1:B:406:VAL:HG21	1.81	0.61
1:A:177:VAL:HG12	1:A:468:THR:HA	1.83	0.61
1:A:242:ALA:HB1	1:A:247:GLN:OE1	2.00	0.61
1:B:354:THR:HG21	1:B:394:ILE:CD1	2.31	0.61
1:A:4:LEU:HD22	1:A:80:LYS:HD2	1.83	0.61
1:A:60:ALA:HB1	1:A:96:PRO:HD3	1.82	0.61
1:A:164:ILE:O	1:A:420:LYS:CE	2.49	0.61
1:B:175:ARG:HH11	1:B:175:ARG:CB	2.10	0.61
1:B:494:VAL:O	1:B:498:GLU:HB2	2.01	0.61
1:A:171:LEU:HD12	1:B:332:TRP:CZ2	2.36	0.61
1:A:223:VAL:CG1	1:A:224:PRO:CD	2.78	0.61
1:B:182:ASP:HA	1:B:188:VAL:HG23	1.81	0.61
1:B:451:ILE:HD12	1:B:451:ILE:H	1.66	0.61
1:B:123:ILE:O	1:B:123:ILE:CG2	2.43	0.60
1:B:201:LYS:HD3	1:B:232:SER:HB3	1.81	0.60
1:B:412:VAL:O	1:B:413:ARG:CD	2.39	0.60
1:B:261:ILE:HG22	1:B:261:ILE:O	2.00	0.60
1:A:19:HIS:O	1:A:24:ASP:O	2.19	0.60
1:A:110:GLU:C	1:A:113:LYS:CB	2.69	0.60
1:A:163:ARG:NH2	1:A:486:ARG:HA	2.16	0.60
1:A:29:ILE:CD1	1:A:58:VAL:CG1	2.72	0.60
1:A:70:VAL:HG23	1:A:71:ILE:CD1	2.23	0.60
1:A:38:ARG:NH1	1:A:39:PHE:HB3	2.17	0.60
1:A:59:THR:HG23	1:A:63:GLU:CG	2.29	0.60
1:A:67:ALA:O	1:A:70:VAL:HG13	2.01	0.60
1:B:175:ARG:O	1:B:463:ARG:NH2	2.34	0.60
1:A:84:LEU:HG	1:A:86:GLY:O	2.01	0.59
1:A:27:VAL:HG13	1:A:28:VAL:N	2.17	0.59
1:A:160:ALA:O	1:A:162:HIS:N	2.34	0.59
1:A:394:ILE:O	1:A:395:LEU:O	2.20	0.59
1:A:462:MET:HE1	1:A:470:ILE:N	2.16	0.59
1:B:163:ARG:NH2	1:B:486:ARG:HG3	2.17	0.59
1:B:388:LEU:CD2	1:B:392:MET:HG2	2.32	0.59
1:A:349:LYS:NZ	3:A:569:FMN:O2'	2.34	0.59
1:A:234:SER:O	1:A:238:ILE:HG13	2.03	0.59
1:A:10:LYS:HG2	1:A:11:ILE:N	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:LYS:HA	1:A:112:LEU:HD13	1.84	0.59
1:B:447:VAL:O	1:B:447:VAL:CG1	2.50	0.59
1:A:179:ILE:CA	1:A:470:ILE:CD1	2.81	0.59
1:B:213:ALA:CB	1:B:225:GLN:HE22	2.15	0.59
1:A:124:ASN:HD22	1:A:124:ASN:C	2.06	0.58
1:A:506:THR:OG1	1:B:127:ASP:CG	2.40	0.58
1:A:247:GLN:C	1:A:248:ILE:HG22	2.18	0.58
1:A:263:ASP:OD2	1:A:341:LYS:HD2	2.02	0.58
1:B:207:GLU:HG3	1:B:214:ARG:HH22	1.68	0.58
1:A:413:ARG:HH22	3:A:569:FMN:P	2.26	0.58
1:A:433:ARG:HG3	3:A:569:FMN:O1P	2.03	0.58
1:A:252:GLN:OE1	3:A:569:FMN:O2	2.21	0.58
1:B:132:ALA:O	1:B:136:LEU:CD2	2.51	0.58
1:B:286:LEU:HD22	1:B:286:LEU:H	1.68	0.58
1:A:29:ILE:HD13	1:A:59:THR:OG1	2.03	0.58
1:A:42:ASN:OD1	1:A:324:LYS:N	2.29	0.58
1:B:330:LEU:HD23	1:B:331:THR:H	1.69	0.58
1:B:399:ASN:ND2	5:B:587:HOH:O	2.36	0.57
1:A:396:GLU:O	1:A:397:GLN:C	2.27	0.57
1:B:440:SER:O	1:B:441:CYS:HB3	2.04	0.57
1:A:179:ILE:C	1:A:470:ILE:HD12	2.25	0.57
1:B:365:VAL:HG13	1:B:366:SER:H	1.69	0.57
1:B:275:LYS:O	1:B:276:ALA:HB2	2.04	0.57
1:B:258:ASP:HB3	1:B:261:ILE:HG13	1.86	0.57
1:B:262:THR:O	1:B:263:ASP:C	2.38	0.57
1:A:136:LEU:HD21	1:A:440:SER:HB3	1.85	0.57
1:A:182:ASP:CB	1:A:187:HIS:HA	2.35	0.57
1:B:337:GLU:C	1:B:341:LYS:HE2	2.25	0.57
1:A:29:ILE:CG1	1:A:58:VAL:HG12	2.35	0.56
1:A:69:ASN:O	1:A:73:LYS:HB2	2.05	0.56
1:A:223:VAL:CG1	1:A:224:PRO:HD2	2.34	0.56
1:B:163:ARG:NH2	1:B:486:ARG:CB	2.68	0.56
1:A:265:LEU:HD22	1:A:265:LEU:C	2.25	0.56
1:A:211:ASP:O	1:A:212:VAL:C	2.36	0.56
1:A:392:MET:HE3	1:A:395:LEU:HD12	1.86	0.56
1:B:176:LYS:HB2	1:B:176:LYS:NZ	2.21	0.56
1:B:221:THR:CG2	1:B:222:LYS:N	2.68	0.56
1:A:110:GLU:C	1:A:113:LYS:HB2	2.26	0.56
1:B:325:PHE:CD1	1:B:325:PHE:N	2.74	0.56
1:B:392:MET:N	1:B:393:PRO:CD	2.67	0.56
1:A:29:ILE:HG12	1:A:58:VAL:CG1	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:LEU:HD23	1:A:341:LYS:HE3	1.86	0.56
1:A:456:ASP:O	1:A:460:MET:HB2	2.06	0.56
2:A:560:HEM:HBA2	2:A:560:HEM:HHA	1.87	0.56
1:B:225:GLN:O	1:B:250:TRP:HB2	2.06	0.56
1:A:177:VAL:HG12	1:A:468:THR:HG22	1.88	0.56
1:A:36:LEU:HA	1:A:38:ARG:HH11	1.70	0.56
1:A:57:ASP:O	1:A:93:VAL:HA	2.06	0.56
1:A:272:LEU:HD12	1:A:272:LEU:H	1.71	0.56
1:B:318:ALA:O	1:B:320:ARG:N	2.33	0.56
1:A:473:LEU:O	1:A:474:LYS:HG2	2.06	0.55
1:A:157:ASN:HD22	1:A:384:PRO:HD2	1.71	0.55
1:B:137:THR:CG2	1:B:137:THR:CA	2.77	0.55
1:B:362:GLU:O	1:B:364:GLY:N	2.39	0.55
1:A:431:LEU:HB2	1:A:435:PHE:HE2	1.72	0.55
1:B:433:ARG:CB	1:B:437:TYR:CE2	2.88	0.55
1:B:201:LYS:CD	1:B:232:SER:HB3	2.37	0.55
1:A:268:ASN:O	1:A:269:VAL:C	2.42	0.55
1:B:207:GLU:HG3	1:B:214:ARG:NH2	2.22	0.55
1:A:58:VAL:O	1:A:59:THR:C	2.43	0.55
1:B:210:LYS:HD3	1:B:237:GLU:HG2	1.87	0.55
1:B:431:LEU:H	1:B:431:LEU:HD13	1.71	0.55
1:B:137:THR:O	1:B:139:GLN:N	2.39	0.55
1:B:196:ALA:HB2	1:B:226:MET:HE2	1.72	0.55
1:A:25:CYS:SG	1:A:54:ALA:CB	2.92	0.55
1:A:203:GLY:HA3	1:A:440:SER:OG	2.07	0.55
1:A:256:ASN:HD22	1:A:258:ASP:H	1.55	0.55
1:A:29:ILE:CG1	1:A:58:VAL:CG1	2.84	0.54
1:A:229:THR:HG22	1:A:230:LEU:HD13	1.88	0.54
1:B:196:ALA:HB2	1:B:226:MET:HB3	1.89	0.54
1:A:32:TYR:CE1	1:A:82:GLY:CA	2.88	0.54
1:A:106:ILE:O	1:A:107:ALA:C	2.45	0.54
1:A:204:ASN:C	1:A:206:LEU:H	2.09	0.54
1:A:447:VAL:O	1:A:450:ALA:HB3	2.07	0.54
1:B:152:VAL:O	1:B:153:THR:O	2.26	0.54
1:B:183:MET:HE2	1:B:428:GLY:HA3	1.89	0.54
1:B:124:ASN:HD22	1:B:126:TYR:H	1.53	0.54
1:B:137:THR:C	1:B:139:GLN:N	2.59	0.54
1:B:254:TYR:O	1:B:255:VAL:C	2.43	0.54
1:B:351:VAL:HG12	1:B:352:GLN:N	2.22	0.54
1:A:38:ARG:HD3	1:A:39:PHE:H	1.73	0.54
1:A:157:ASN:HD22	1:A:384:PRO:CD	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:THR:HG22	1:A:197:THR:O	2.05	0.54
1:B:223:VAL:O	1:B:224:PRO:O	2.26	0.54
1:A:402:ASP:O	1:A:404:LEU:N	2.40	0.54
1:B:184:LEU:N	1:B:405:GLU:OE1	2.26	0.54
1:B:258:ASP:O	1:B:260:LYS:N	2.41	0.54
1:B:362:GLU:C	1:B:364:GLY:N	2.60	0.54
1:B:275:LYS:HB2	1:B:275:LYS:HZ3	1.72	0.54
1:B:400:LEU:O	1:B:403:LYS:HB2	2.07	0.54
1:B:252:GLN:NE2	1:B:252:GLN:O	2.41	0.54
1:B:477:LEU:O	1:B:478:LEU:HD23	2.08	0.54
1:A:179:ILE:C	1:A:470:ILE:CD1	2.76	0.54
1:B:333:LYS:HA	1:B:336:GLU:HG2	1.90	0.54
1:B:388:LEU:CD2	1:B:392:MET:CG	2.86	0.54
1:A:57:ASP:C	1:A:58:VAL:HG23	2.28	0.54
1:B:318:ALA:C	1:B:320:ARG:H	2.05	0.54
1:B:354:THR:HG21	1:B:394:ILE:HD13	1.89	0.54
1:B:111:GLN:O	1:B:112:LEU:C	2.46	0.53
1:A:226:MET:HE1	1:A:349:LYS:HD2	1.90	0.53
1:A:4:LEU:HB3	1:A:32:TYR:CE2	2.42	0.53
1:A:155:ARG:CZ	1:B:491:PRO:HB2	2.39	0.53
1:A:354:THR:OG1	1:A:391:THR:HG23	2.08	0.53
1:B:449:LYS:O	1:B:452:GLU:HB2	2.09	0.53
1:A:98:ALA:O	1:A:99:PRO:C	2.46	0.53
1:B:361:ALA:HB2	1:B:404:LEU:HD23	1.89	0.53
1:B:361:ALA:HB3	1:B:400:LEU:HD23	1.80	0.53
1:A:163:ARG:NH2	1:B:488:VAL:O	2.38	0.53
1:A:372:ASN:ND2	1:A:375:GLY:H	2.07	0.53
1:B:137:THR:O	1:B:140:ALA:N	2.42	0.53
1:A:222:LYS:C	1:A:223:VAL:HG23	2.29	0.53
1:A:406:VAL:O	1:A:406:VAL:HG12	2.06	0.53
1:B:180:SER:CA	1:B:189:ASP:O	2.57	0.53
1:B:259:ARG:O	1:B:263:ASP:HB2	2.09	0.53
1:B:108:ARG:HG2	1:B:108:ARG:HH11	1.73	0.53
1:A:487:THR:O	1:B:490:VAL:HG13	2.09	0.53
1:B:132:ALA:HA	1:B:136:LEU:HD21	1.90	0.53
1:A:256:ASN:HA	1:A:325:PHE:O	2.07	0.53
1:B:227:ILE:CD1	1:B:250:TRP:C	2.76	0.53
1:B:222:LYS:HE2	1:B:244:SER:HB2	1.90	0.52
1:B:260:LYS:O	1:B:263:ASP:N	2.42	0.52
1:B:286:LEU:HD21	1:B:323:SER:CB	2.29	0.52
1:B:347:VAL:HG12	1:B:368:VAL:N	2.19	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:ILE:O	1:A:420:LYS:HE3	2.09	0.52
1:B:387:VAL:O	1:B:388:LEU:C	2.46	0.52
1:A:372:ASN:ND2	1:A:372:ASN:O	2.43	0.52
1:B:349:LYS:NZ	3:B:570:FMN:O2	2.39	0.52
1:A:110:GLU:HA	1:A:113:LYS:CB	2.15	0.52
1:A:166:PHE:CE2	1:A:416:THR:HG22	2.43	0.52
1:A:352:GLN:OE1	1:A:381:SER:OG	2.17	0.52
1:A:474:LYS:O	1:A:477:LEU:HB2	2.10	0.52
1:B:190:VAL:HG13	1:B:192:PHE:H	1.74	0.52
1:B:254:TYR:CE1	1:B:280:THR:HB	2.45	0.52
1:B:369:VAL:HG22	1:B:407:PHE:HB2	1.91	0.52
1:B:433:ARG:HG2	3:B:570:FMN:HM83	1.92	0.52
1:B:337:GLU:HG3	1:B:341:LYS:NZ	2.24	0.52
1:B:433:ARG:HG2	3:B:570:FMN:C8M	2.39	0.52
2:A:560:HEM:HHA	2:A:560:HEM:CBA	2.40	0.52
1:B:101:GLU:OE2	1:B:137:THR:HG23	2.09	0.52
1:B:259:ARG:CG	1:B:259:ARG:NH1	2.73	0.52
1:A:188:VAL:HG12	1:A:189:ASP:N	2.23	0.52
1:A:431:LEU:HB2	1:A:435:PHE:CE2	2.44	0.52
1:B:175:ARG:HB3	1:B:175:ARG:CZ	2.39	0.52
1:B:332:TRP:CZ2	1:B:359:LYS:HD3	2.44	0.52
1:B:124:ASN:ND2	1:B:127:ASP:H	2.08	0.52
1:B:396:GLU:CG	1:B:401:LYS:NZ	2.73	0.52
1:B:137:THR:HG21	1:B:139:GLN:HB3	1.89	0.52
1:A:38:ARG:CZ	1:A:39:PHE:HB3	2.40	0.52
1:A:251:TYR:CE1	1:A:265:LEU:HD13	2.45	0.52
1:B:137:THR:C	1:B:139:GLN:H	2.11	0.52
1:B:212:VAL:HG22	1:B:225:GLN:OE1	2.10	0.52
1:A:35:ASP:OD1	1:A:37:THR:HG22	2.11	0.51
1:B:109:LYS:NZ	1:B:112:LEU:HD13	2.25	0.51
1:A:450:ALA:O	1:A:451:ILE:C	2.47	0.51
1:B:366:SER:O	1:B:404:LEU:HD13	2.11	0.51
1:A:402:ASP:C	1:A:404:LEU:H	2.14	0.51
1:B:163:ARG:CZ	1:B:486:ARG:HB2	2.40	0.51
1:B:183:MET:CE	1:B:428:GLY:HA3	2.41	0.51
1:B:337:GLU:O	1:B:340:LYS:HB2	2.10	0.51
1:A:110:GLU:HG2	1:A:113:LYS:CD	2.39	0.51
1:A:171:LEU:CD1	1:B:332:TRP:CD2	2.94	0.51
1:A:183:MET:O	1:A:184:LEU:C	2.49	0.51
1:B:333:LYS:C	1:B:335:ILE:H	2.12	0.51
1:B:505:LEU:O	1:B:506:THR:O	2.28	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:333:LYS:O	1:B:335:ILE:N	2.44	0.51
1:B:103:LYS:HA	1:B:105:ASP:OD1	2.11	0.51
1:B:227:ILE:HD11	1:B:250:TRP:N	2.24	0.51
1:B:281:VAL:HG11	1:B:348:ILE:HG23	1.91	0.51
1:B:405:GLU:HB3	1:B:407:PHE:CE2	2.46	0.51
1:B:190:VAL:HG13	1:B:192:PHE:CD2	2.46	0.51
1:B:282:ASP:C	1:B:284:PRO:HD2	2.31	0.51
1:B:353:ARG:NH1	1:B:356:ASP:CG	2.64	0.51
1:B:409:ASP:OD2	3:B:570:FMN:O3'	2.10	0.51
1:B:433:ARG:O	1:B:437:TYR:HD2	1.91	0.50
1:B:236:GLU:O	1:B:240:GLU:HB2	2.10	0.50
1:B:281:VAL:HG11	1:B:348:ILE:CG2	2.40	0.50
1:A:132:ALA:HA	1:A:441:CYS:SG	2.52	0.50
1:B:229:THR:HG21	1:B:254:TYR:H	1.76	0.50
1:B:409:ASP:O	1:B:410:GLY:O	2.29	0.50
1:A:22:PRO:HB2	1:A:51:LYS:HG2	1.93	0.50
1:A:198:ALA:O	1:A:199:LEU:HB2	2.12	0.50
1:A:405:GLU:OE1	1:A:427:LYS:HG2	2.12	0.50
1:B:108:ARG:HH22	1:B:138:LYS:HG3	1.77	0.50
1:A:57:ASP:CA	1:A:58:VAL:HG23	2.42	0.50
1:A:158:HIS:O	1:A:159:ASN:C	2.50	0.50
1:B:470:ILE:HG22	1:B:470:ILE:O	2.08	0.50
1:A:233:CYS:HB3	1:A:237:GLU:OE1	2.12	0.50
1:A:278:PHE:HA	1:A:347:VAL:O	2.11	0.50
1:A:412:VAL:HG12	1:A:431:LEU:HD21	1.93	0.50
1:B:98:ALA:HB1	1:B:101:GLU:HB2	1.94	0.50
1:B:396:GLU:HG3	1:B:401:LYS:HZ2	1.77	0.50
1:B:412:VAL:HG13	1:B:417:ASP:HB3	1.94	0.50
1:A:210:LYS:HG2	1:A:241:ALA:HB1	1.93	0.49
1:B:108:ARG:HH12	1:B:137:THR:CA	2.17	0.49
1:A:255:VAL:HG11	1:A:330:LEU:HD21	1.94	0.49
1:B:332:TRP:CE2	1:B:359:LYS:HD3	2.47	0.49
1:B:482:THR:O	1:B:483:LEU:C	2.49	0.49
1:A:113:LYS:C	1:A:115:LEU:N	2.63	0.49
1:B:163:ARG:NH2	1:B:486:ARG:HB2	2.26	0.49
1:B:233:CYS:CB	1:B:238:ILE:CD1	2.77	0.49
1:A:174:VAL:HG23	1:A:174:VAL:O	2.11	0.49
1:A:239:ILE:HG23	1:A:249:GLN:HE22	1.76	0.49
1:A:286:LEU:CD1	1:A:286:LEU:CD2	2.80	0.49
1:B:108:ARG:NH2	1:B:138:LYS:HG3	2.26	0.49
1:B:116:LEU:HD12	1:B:442:TYR:CZ	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:180:SER:O	1:B:181:THR:HB	2.12	0.49
1:B:144:TYR:OH	1:B:200:CYS:HA	2.13	0.49
1:B:281:VAL:CG1	1:B:348:ILE:HG23	2.42	0.49
1:B:447:VAL:HG12	1:B:451:ILE:CD1	2.41	0.49
1:A:28:VAL:O	1:A:57:ASP:OD1	2.30	0.49
1:A:192:PHE:CD1	1:A:192:PHE:C	2.85	0.49
1:A:402:ASP:C	1:A:404:LEU:N	2.66	0.49
1:A:29:ILE:HG12	1:A:58:VAL:HG11	1.93	0.49
1:A:226:MET:CE	1:A:349:LYS:HD2	2.43	0.49
1:A:494:VAL:O	1:A:495:LEU:C	2.49	0.49
1:A:509:GLU:HG2	1:B:115:LEU:O	2.13	0.49
1:A:13:PRO:HA	1:A:88:MET:HG2	1.95	0.49
1:A:110:GLU:CA	1:A:113:LYS:CB	2.82	0.49
1:B:256:ASN:HD22	1:B:258:ASP:H	1.60	0.49
1:B:396:GLU:HG3	1:B:401:LYS:HZ3	1.77	0.49
1:A:66:HIS:HE1	2:A:560:HEM:C1D	2.31	0.49
1:A:118:PRO:O	1:A:121:ASN:HB2	2.13	0.49
1:B:282:ASP:CG	1:B:373:GLN:HG3	2.34	0.49
1:B:322:LEU:CD1	1:B:328:PRO:HG2	2.35	0.49
1:B:253:LEU:O	1:B:279:VAL:HA	2.12	0.48
1:B:352:GLN:HG3	1:B:371:SER:O	2.11	0.48
1:B:500:TYR:CG	1:B:501:GLU:N	2.81	0.48
1:B:207:GLU:O	1:B:210:LYS:HB2	2.14	0.48
1:B:351:VAL:HG12	1:B:352:GLN:H	1.78	0.48
1:A:385:ILE:HG23	1:A:386:GLU:H	1.78	0.48
1:B:159:ASN:O	1:B:160:ALA:C	2.49	0.48
1:B:194:VAL:HG12	1:B:195:SER:N	2.28	0.48
1:B:236:GLU:CA	1:B:239:ILE:HG22	2.42	0.48
1:B:275:LYS:HB2	1:B:275:LYS:HZ2	1.76	0.48
1:B:394:ILE:HG23	1:B:397:GLN:HE22	1.77	0.48
1:A:223:VAL:HA	1:A:224:PRO:HD3	1.51	0.48
1:B:161:TYR:O	1:B:420:LYS:HE2	2.13	0.48
1:A:198:ALA:H	3:A:569:FMN:C6	2.26	0.48
1:A:417:ASP:O	1:A:418:VAL:C	2.52	0.48
1:A:111:GLN:O	1:A:115:LEU:HB3	2.14	0.48
1:A:198:ALA:H	3:A:569:FMN:H6	1.79	0.48
1:A:260:LYS:O	1:A:261:ILE:C	2.49	0.48
1:A:124:ASN:C	1:A:124:ASN:ND2	2.64	0.48
1:A:383:ALA:HB1	1:A:385:ILE:HG22	1.96	0.48
1:B:164:ILE:HB	1:B:420:LYS:CE	2.43	0.48
1:B:262:THR:C	1:B:264:ASP:H	2.16	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:LYS:HE3	1:A:244:SER:OG	2.14	0.48
1:A:229:THR:HG22	1:A:229:THR:O	2.13	0.48
1:A:256:ASN:HD22	1:A:257:SER:CA	2.24	0.47
1:A:194:VAL:HG22	1:A:435:PHE:CG	2.49	0.47
1:A:252:GLN:HG2	1:A:253:LEU:N	2.28	0.47
1:A:402:ASP:O	1:A:403:LYS:C	2.49	0.47
1:B:295:LEU:HA	1:B:297:PHE:O	2.13	0.47
1:B:405:GLU:HB3	1:B:407:PHE:HE2	1.78	0.47
1:B:436:LEU:CD1	3:B:570:FMN:HM73	2.43	0.47
1:B:454:LEU:O	1:B:454:LEU:HG	2.13	0.47
1:A:89:PRO:HA	1:A:90:PRO:HD2	1.24	0.47
1:B:179:ILE:CA	1:B:470:ILE:CD1	2.86	0.47
1:B:216:CYS:HB3	1:B:223:VAL:O	2.14	0.47
1:A:196:ALA:HB2	1:A:226:MET:HG2	1.97	0.47
1:A:344:LEU:HA	1:A:344:LEU:HD23	1.53	0.47
1:B:148:ALA:O	1:B:149:ASN:C	2.51	0.47
1:B:184:LEU:HD13	1:B:405:GLU:OE1	2.13	0.47
1:B:368:VAL:HG12	1:B:369:VAL:N	2.27	0.47
1:A:107:ALA:O	1:A:111:GLN:HB2	2.14	0.47
1:A:353:ARG:O	1:A:354:THR:C	2.51	0.47
1:B:127:ASP:O	1:B:128:PHE:C	2.50	0.47
1:B:177:VAL:HG11	1:B:462:MET:HG2	1.96	0.47
1:B:333:LYS:C	1:B:335:ILE:N	2.67	0.47
1:A:67:ALA:HA	1:A:68:PRO:HD3	1.74	0.47
1:B:106:ILE:HA	1:B:109:LYS:HB2	1.96	0.47
1:B:149:ASN:HB3	1:B:290:GLU:OE2	2.15	0.47
1:B:369:VAL:HG12	1:B:371:SER:HB2	1.97	0.47
1:B:446:GLY:O	1:B:447:VAL:C	2.51	0.47
1:B:475:PRO:C	1:B:477:LEU:N	2.68	0.47
1:B:116:LEU:HA	1:B:117:PRO:HD3	1.79	0.47
1:B:243:PRO:O	1:B:244:SER:C	2.50	0.47
1:B:317:GLY:N	1:B:320:ARG:HH22	2.07	0.47
1:B:410:GLY:HA2	3:B:570:FMN:O5'	2.15	0.47
1:B:439:ASN:ND2	1:B:443:GLY:HA2	2.28	0.47
1:A:68:PRO:O	1:A:70:VAL:HG22	2.14	0.47
1:B:107:ALA:O	1:B:109:LYS:N	2.47	0.47
1:B:166:PHE:CE2	1:B:416:THR:HG22	2.50	0.47
1:A:47:GLN:HE21	1:A:47:GLN:HB3	1.59	0.47
1:A:473:LEU:C	1:A:474:LYS:CG	2.84	0.47
1:B:216:CYS:CB	1:B:223:VAL:O	2.63	0.47
1:A:36:LEU:O	1:A:38:ARG:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:ALA:O	1:A:70:VAL:CG1	2.63	0.46
1:A:199:LEU:HA	1:A:232:SER:OG	2.15	0.46
1:A:466:GLY:O	1:A:467:VAL:HG13	2.15	0.46
1:B:104:GLU:C	1:B:107:ALA:H	2.18	0.46
1:B:392:MET:CE	1:B:406:VAL:HG21	2.45	0.46
1:B:410:GLY:CA	3:B:570:FMN:O5'	2.63	0.46
1:A:27:VAL:CG2	1:A:56:LYS:H	2.29	0.46
1:B:137:THR:CG2	1:B:139:GLN:H	2.26	0.46
1:B:496:TYR:O	1:B:496:TYR:CD1	2.69	0.46
1:A:453:ILE:O	1:A:457:GLU:HG3	2.15	0.46
1:B:179:ILE:C	1:B:470:ILE:CD1	2.84	0.46
1:B:207:GLU:CG	1:B:214:ARG:HH22	2.28	0.46
1:B:337:GLU:HB3	1:B:341:LYS:HE3	1.96	0.46
1:A:60:ALA:C	1:A:96:PRO:HB3	2.35	0.46
1:A:62:PHE:CE1	1:A:66:HIS:CD2	3.04	0.46
1:A:164:ILE:O	1:A:420:LYS:HE2	2.15	0.46
1:A:473:LEU:O	1:A:474:LYS:CG	2.64	0.46
1:B:228:SER:C	1:B:252:GLN:HE22	2.18	0.46
2:A:560:HEM:HHD	2:A:560:HEM:CBC	2.34	0.46
1:B:282:ASP:OD1	1:B:373:GLN:HG3	2.16	0.46
1:A:382:ARG:O	1:A:384:PRO:CD	2.64	0.46
1:B:184:LEU:O	1:B:185:GLY:C	2.54	0.46
1:B:254:TYR:OH	4:B:571:PYR:O3	2.29	0.46
1:B:344:LEU:HD23	1:B:344:LEU:HA	1.18	0.46
1:A:115:LEU:HD12	1:A:115:LEU:HA	1.83	0.46
1:A:229:THR:O	1:A:229:THR:CG2	2.61	0.46
1:B:251:TYR:O	1:B:278:PHE:N	2.31	0.46
1:B:440:SER:O	1:B:441:CYS:CB	2.59	0.46
1:A:280:THR:HA	1:A:349:LYS:HB3	1.98	0.45
1:A:331:THR:O	1:A:332:TRP:C	2.53	0.45
1:A:398:ARG:O	1:A:400:LEU:HG	2.16	0.45
1:A:414:ARG:HH21	1:B:150:ASP:CG	2.18	0.45
1:B:416:THR:O	1:B:420:LYS:HB2	2.15	0.45
1:B:422:LEU:C	1:B:424:LEU:H	2.15	0.45
1:A:6:MET:HB2	1:A:32:TYR:OH	2.16	0.45
1:A:43:HIS:HA	1:A:44:PRO:HD2	1.44	0.45
1:B:163:ARG:NH2	1:B:486:ARG:HA	2.28	0.45
1:B:252:GLN:HG2	1:B:253:LEU:N	2.31	0.45
1:B:230:LEU:O	1:B:231:ALA:C	2.53	0.45
1:A:182:ASP:HB2	1:A:186:SER:O	2.17	0.45
1:A:206:LEU:HA	1:A:206:LEU:HD12	1.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:283:ALA:HA	1:B:377:GLN:HE21	1.80	0.45
1:A:4:LEU:HD22	1:A:80:LYS:CD	2.46	0.45
1:A:204:ASN:HA	1:A:205:PRO:HD3	1.55	0.45
1:A:432:GLY:O	1:A:433:ARG:C	2.54	0.45
1:A:57:ASP:N	1:A:58:VAL:HG23	2.30	0.45
1:A:66:HIS:CE1	2:A:560:HEM:C1D	3.04	0.45
1:A:212:VAL:O	1:A:213:ALA:C	2.55	0.45
1:A:439:ASN:O	1:A:440:SER:C	2.53	0.45
1:B:109:LYS:HZ2	1:B:112:LEU:HD13	1.81	0.45
1:B:422:LEU:HA	1:B:422:LEU:HD23	1.58	0.45
1:B:439:ASN:O	1:B:441:CYS:N	2.49	0.45
1:B:163:ARG:NH2	1:B:486:ARG:CG	2.79	0.45
1:B:371:SER:HG	1:B:409:ASP:CG	2.19	0.45
1:B:433:ARG:CB	1:B:437:TYR:HE2	2.29	0.45
1:B:475:PRO:C	1:B:477:LEU:H	2.20	0.45
1:A:36:LEU:HD12	1:A:38:ARG:HH12	1.82	0.45
1:A:67:ALA:C	1:A:70:VAL:CG1	2.77	0.45
1:B:174:VAL:CG2	1:B:463:ARG:HB3	2.46	0.45
1:A:166:PHE:HE2	1:A:416:THR:HG22	1.80	0.45
1:B:110:GLU:O	1:B:113:LYS:O	2.34	0.45
1:B:188:VAL:O	1:B:189:ASP:O	2.35	0.45
1:B:219:GLY:C	1:B:221:THR:N	2.69	0.45
1:B:222:LYS:HE2	1:B:244:SER:CB	2.47	0.45
1:B:214:ARG:HH11	1:B:444:ARG:HD3	1.82	0.45
1:B:214:ARG:HD3	1:B:241:ALA:HB1	1.99	0.45
1:B:113:LYS:O	1:B:114:SER:C	2.54	0.44
1:B:175:ARG:CG	1:B:175:ARG:NE	2.69	0.44
1:B:463:ARG:C	1:B:465:LEU:H	2.19	0.44
1:B:175:ARG:CG	1:B:175:ARG:CZ	2.95	0.44
1:A:347:VAL:HG22	1:A:367:GLY:C	2.37	0.44
1:A:508:PHE:HA	1:B:115:LEU:O	2.17	0.44
1:B:218:GLN:HE21	1:B:218:GLN:HB2	1.22	0.44
1:B:251:TYR:HB3	1:B:277:LEU:HD21	1.98	0.44
1:B:353:ARG:NH2	1:B:355:GLU:HG2	2.32	0.44
1:B:413:ARG:NH2	3:B:570:FMN:O1P	2.50	0.44
1:A:271:LYS:C	1:A:273:GLY:H	2.21	0.44
1:B:296:LYS:HE2	1:B:296:LYS:HB3	1.50	0.44
1:A:57:ASP:HB3	1:A:93:VAL:HG23	1.99	0.44
1:A:196:ALA:O	3:A:569:FMN:C10	2.66	0.44
1:B:108:ARG:NH1	1:B:108:ARG:HG2	2.32	0.44
1:B:353:ARG:HH11	1:B:356:ASP:CG	2.21	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:413:ARG:NH1	3:B:570:FMN:O1P	2.50	0.44
1:A:38:ARG:HH21	1:A:75:ILE:HB	1.77	0.44
1:A:55:GLY:O	1:A:56:LYS:HG3	2.17	0.44
1:A:490:VAL:O	1:A:492:ASN:HB2	2.18	0.44
1:B:137:THR:HG22	1:B:139:GLN:N	2.25	0.44
1:B:463:ARG:C	1:B:465:LEU:N	2.70	0.44
1:B:505:LEU:C	1:B:506:THR:O	2.55	0.44
1:A:155:ARG:NH2	1:B:491:PRO:HB2	2.32	0.44
1:A:226:MET:HA	1:A:250:TRP:HB2	1.99	0.44
1:A:416:THR:O	1:A:419:LEU:HB2	2.18	0.44
1:B:159:ASN:O	1:B:161:TYR:N	2.51	0.44
1:B:226:MET:HE3	1:B:226:MET:HB3	1.63	0.44
1:B:227:ILE:HD13	1:B:250:TRP:O	2.04	0.44
1:A:61:ILE:HG23	1:A:97:TYR:CB	2.47	0.43
1:A:268:ASN:ND2	1:A:272:LEU:HD11	2.33	0.43
1:B:285:SER:HA	1:B:322:LEU:HA	2.00	0.43
1:B:383:ALA:HA	1:B:384:PRO:HD3	1.75	0.43
1:A:200:CYS:C	1:A:202:LEU:N	2.71	0.43
1:A:347:VAL:HG22	1:A:367:GLY:O	2.18	0.43
1:A:453:ILE:HG23	1:A:453:ILE:HD13	1.62	0.43
1:B:98:ALA:O	1:B:101:GLU:HG2	2.19	0.43
1:B:137:THR:O	1:B:138:LYS:C	2.57	0.43
1:B:222:LYS:HE3	1:B:222:LYS:HB3	1.60	0.43
1:B:351:VAL:CG1	1:B:352:GLN:N	2.81	0.43
1:A:43:HIS:CD2	2:A:560:HEM:NB	2.87	0.43
1:B:422:LEU:C	1:B:424:LEU:N	2.65	0.43
1:A:60:ALA:O	1:A:96:PRO:CB	2.59	0.43
1:A:400:LEU:O	1:A:401:LYS:C	2.57	0.43
1:A:473:LEU:HD23	1:A:473:LEU:HA	1.55	0.43
1:A:487:THR:H	1:B:489:GLY:HA2	1.84	0.43
1:A:16:VAL:C	1:A:18:LYS:N	2.72	0.43
1:A:40:LEU:O	1:A:47:GLN:HG3	2.17	0.43
1:A:401:LYS:HD2	1:A:402:ASP:OD1	2.19	0.43
1:A:495:LEU:HD12	1:A:495:LEU:HA	1.84	0.43
1:B:151:GLU:N	1:B:379:ASP:OD2	2.52	0.43
1:B:249:GLN:O	1:B:250:TRP:CD1	2.71	0.43
1:B:439:ASN:O	1:B:443:GLY:HA2	2.18	0.43
1:A:339:LYS:O	1:A:339:LYS:HG2	2.18	0.43
1:B:101:GLU:O	1:B:103:LYS:N	2.51	0.43
1:A:55:GLY:C	1:A:56:LYS:HG3	2.39	0.43
1:A:163:ARG:HH21	1:A:486:ARG:HA	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:VAL:HG22	1:A:225:GLN:OE1	2.19	0.43
1:A:238:ILE:O	1:A:238:ILE:HG22	2.19	0.43
1:A:250:TRP:CD1	1:A:276:ALA:HB3	2.54	0.43
1:B:194:VAL:HG12	1:B:195:SER:H	1.82	0.43
1:A:162:HIS:N	1:A:162:HIS:ND1	2.66	0.43
1:A:286:LEU:HD21	1:A:289:ARG:HH22	1.84	0.43
1:A:474:LYS:HA	1:A:475:PRO:HD3	1.72	0.43
1:B:220:VAL:O	1:B:220:VAL:HG12	2.19	0.43
1:A:16:VAL:C	1:A:18:LYS:H	2.21	0.43
1:A:218:GLN:HE21	1:A:218:GLN:HB3	1.52	0.43
1:A:355:GLU:O	1:A:358:ILE:N	2.51	0.43
1:B:152:VAL:N	1:B:379:ASP:OD1	2.51	0.43
1:B:188:VAL:O	1:B:189:ASP:C	2.56	0.43
1:A:14:ALA:HA	1:A:17:ALA:HB2	2.01	0.42
1:A:29:ILE:O	1:A:30:ASN:C	2.58	0.42
1:A:38:ARG:HD3	1:A:39:PHE:N	2.34	0.42
1:A:103:LYS:HD3	1:A:103:LYS:N	2.33	0.42
1:A:478:LEU:HD23	1:A:478:LEU:HA	1.31	0.42
1:B:249:GLN:HB3	1:B:274:VAL:HG12	2.01	0.42
1:B:283:ALA:N	1:B:284:PRO:HD3	2.32	0.42
1:A:372:ASN:HD22	1:A:374:GLY:H	1.67	0.42
1:B:109:LYS:HA	1:B:109:LYS:HD3	1.68	0.42
1:B:204:ASN:HB3	1:B:208:GLY:H	1.85	0.42
1:A:43:HIS:CD2	2:A:560:HEM:C4B	3.07	0.42
1:A:253:LEU:HA	1:A:253:LEU:HD12	1.72	0.42
1:B:154:HIS:O	1:B:154:HIS:ND1	2.52	0.42
1:B:165:PHE:O	1:B:479:ASP:N	2.48	0.42
1:B:239:ILE:CD1	1:B:274:VAL:CG1	2.97	0.42
1:A:268:ASN:O	1:A:272:LEU:HD12	2.18	0.42
1:B:195:SER:OG	1:B:196:ALA:N	2.53	0.42
1:B:137:THR:CG2	1:B:137:THR:HB	2.23	0.42
1:A:230:LEU:HG	2:A:560:HEM:HMA3	2.01	0.42
1:A:365:VAL:HG13	1:A:366:SER:N	2.33	0.42
1:B:419:LEU:HA	1:B:419:LEU:HD23	1.83	0.42
1:A:179:ILE:HD13	1:A:459:GLU:HG3	2.01	0.42
1:A:179:ILE:O	1:A:470:ILE:CD1	2.67	0.42
1:A:210:LYS:HB2	1:A:210:LYS:HE3	1.47	0.42
1:A:414:ARG:O	1:A:415:GLY:C	2.55	0.42
1:B:183:MET:HE2	1:B:428:GLY:CA	2.48	0.42
1:B:195:SER:O	1:B:197:THR:CG2	2.67	0.42
1:A:27:VAL:HG22	1:A:56:LYS:H	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:VAL:HG23	1:A:33:VAL:HG12	2.01	0.42
1:A:239:ILE:HD12	1:A:272:LEU:HB2	2.01	0.42
1:A:415:GLY:O	1:A:416:THR:C	2.57	0.42
1:B:235:PRO:O	1:B:239:ILE:HG22	2.19	0.42
1:A:398:ARG:O	1:A:400:LEU:N	2.53	0.42
1:B:163:ARG:HH22	1:B:486:ARG:HG3	1.82	0.42
1:B:176:LYS:HB2	1:B:176:LYS:HZ2	1.85	0.42
1:B:286:LEU:CD2	1:B:323:SER:CB	2.96	0.42
1:B:286:LEU:HD11	1:B:326:ILE:HD11	2.02	0.42
1:A:41:PRO:HA	1:A:47:GLN:CG	2.44	0.42
1:A:104:GLU:C	1:A:106:ILE:N	2.73	0.42
1:A:219:GLY:HA3	1:A:448:GLU:OE2	2.20	0.42
1:A:278:PHE:CE2	1:A:347:VAL:HG11	2.55	0.42
1:B:213:ALA:HB2	1:B:225:GLN:NE2	2.27	0.42
1:A:118:PRO:O	1:A:119:LEU:C	2.57	0.41
1:A:188:VAL:HG12	1:A:190:VAL:H	1.85	0.41
1:B:104:GLU:O	1:B:106:ILE:N	2.52	0.41
1:A:74:TYR:CD1	2:A:560:HEM:CMB	3.04	0.41
1:A:112:LEU:HD12	1:A:112:LEU:H	1.84	0.41
1:A:281:VAL:O	1:A:281:VAL:HG23	2.20	0.41
1:A:293:MET:O	1:A:295:LEU:N	2.53	0.41
1:B:98:ALA:CB	1:B:101:GLU:HG3	2.47	0.41
1:B:276:ALA:HB1	1:B:345:PRO:O	2.20	0.41
1:A:170:ILE:HB	1:B:356:ASP:OD2	2.20	0.41
1:A:180:SER:HB2	1:A:188:VAL:O	2.21	0.41
1:A:272:LEU:CD1	1:A:272:LEU:H	2.32	0.41
1:B:265:LEU:HA	1:B:268:ASN:HB3	2.03	0.41
1:A:43:HIS:O	1:A:43:HIS:ND1	2.54	0.41
1:A:119:LEU:HD12	1:A:119:LEU:HA	1.70	0.41
1:A:137:THR:O	1:A:138:LYS:C	2.58	0.41
1:A:132:ALA:HB2	1:A:437:TYR:HB3	2.02	0.41
1:A:191:PRO:HD2	1:A:192:PHE:CD2	2.56	0.41
1:A:197:THR:HG21	1:A:436:LEU:HD21	2.03	0.41
1:B:110:GLU:HA	1:B:113:LYS:HB3	2.03	0.41
1:B:244:SER:O	1:B:247:GLN:HB3	2.20	0.41
1:B:495:LEU:HA	1:B:495:LEU:HD12	1.04	0.41
1:A:129:GLU:O	1:A:130:TYR:C	2.59	0.41
1:A:412:VAL:HG12	1:A:412:VAL:O	2.17	0.41
1:A:433:ARG:O	1:A:434:PRO:C	2.59	0.41
1:B:177:VAL:CG1	1:B:462:MET:HG2	2.51	0.41
1:B:217:GLY:HA3	1:B:247:GLN:OE1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:227:ILE:HD13	1:B:251:TYR:HD2	1.85	0.41
1:B:346:ILE:CG2	1:B:365:VAL:HG11	2.42	0.41
1:A:66:HIS:HE1	2:A:560:HEM:CHD	2.33	0.41
1:A:152:VAL:N	1:A:379:ASP:OD1	2.53	0.41
1:A:239:ILE:HD13	1:A:239:ILE:HG21	1.81	0.41
1:A:357:VAL:O	1:A:357:VAL:HG12	2.18	0.41
1:A:422:LEU:O	1:A:423:CYS:C	2.56	0.41
1:B:490:VAL:HA	1:B:491:PRO:HD3	1.83	0.41
1:A:257:SER:OG	1:A:324:LYS:O	2.37	0.41
1:A:259:ARG:CG	1:A:259:ARG:HH11	2.32	0.41
1:B:295:LEU:HD23	1:B:296:LYS:H	1.84	0.41
1:B:418:VAL:O	1:B:421:ALA:HB3	2.20	0.41
1:A:201:LYS:O	1:A:205:PRO:HA	2.21	0.41
1:A:214:ARG:HB3	1:A:444:ARG:HB3	2.03	0.41
1:A:258:ASP:O	1:A:260:LYS:N	2.53	0.41
1:A:290:GLU:HG2	1:A:293:MET:HE1	2.02	0.41
1:B:347:VAL:CG1	1:B:367:GLY:N	2.79	0.41
1:B:356:ASP:O	1:B:357:VAL:C	2.54	0.41
1:B:414:ARG:HA	1:B:457:GLU:OE1	2.20	0.41
1:B:443:GLY:O	1:B:447:VAL:HG23	2.21	0.41
1:A:210:LYS:HD3	1:A:237:GLU:HB3	2.03	0.41
1:A:382:ARG:O	1:A:384:PRO:HD3	2.21	0.41
1:A:453:ILE:HG21	1:A:453:ILE:HD12	1.58	0.41
1:B:190:VAL:CG1	1:B:192:PHE:H	2.34	0.41
1:B:229:THR:OG1	1:B:252:GLN:C	2.58	0.41
1:B:278:PHE:HA	1:B:347:VAL:O	2.21	0.41
1:B:332:TRP:CH2	1:B:359:LYS:HB3	2.56	0.41
1:A:256:ASN:HD22	1:A:258:ASP:N	2.16	0.40
1:B:199:LEU:O	1:B:202:LEU:HB2	2.21	0.40
1:A:132:ALA:CA	1:A:441:CYS:SG	3.09	0.40
1:A:139:GLN:HG3	1:A:140:ALA:N	2.37	0.40
1:A:259:ARG:HH11	1:A:259:ARG:HG3	1.86	0.40
1:B:457:GLU:O	1:B:458:ILE:C	2.56	0.40
1:A:179:ILE:CA	1:A:470:ILE:HD11	2.48	0.40
1:B:347:VAL:HA	1:B:367:GLY:O	2.22	0.40
1:A:462:MET:HE1	1:A:469:SER:CA	2.49	0.40
1:B:108:ARG:NH1	1:B:137:THR:HA	2.18	0.40
1:B:133:SER:HB3	1:B:141:TRP:CH2	2.56	0.40
1:B:354:THR:OG1	1:B:391:THR:CG2	2.61	0.40
1:B:449:LYS:HD2	1:B:453:ILE:HG13	2.01	0.40
1:A:106:ILE:HA	1:A:109:LYS:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:422:LEU:C	1:A:424:LEU:N	2.72	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:ARG:NH2	1:B:169:LYS:CG[6_555]	2.19	0.01

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	488/511 (96%)	381 (78%)	67 (14%)	40 (8%)	1 2
1	B	392/511 (77%)	273 (70%)	78 (20%)	41 (10%)	0 1
All	All	880/1022 (86%)	654 (74%)	145 (16%)	81 (9%)	1 1

All (81) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	11	ILE
1	A	20	ASN
1	A	37	THR
1	A	48	ASP
1	A	58	VAL
1	A	69	ASN
1	A	72	ASP
1	A	106	ILE
1	A	113	LYS
1	A	114	SER
1	A	259	ARG

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Mol	Chain	Res	Type
1	A	319	SER
1	A	380	PHE
1	B	99	PRO
1	B	102	THR
1	B	103	LYS
1	B	105	ASP
1	B	119	LEU
1	B	167	LYS
1	B	185	GLY
1	B	243	PRO
1	B	298	SER
1	B	318	ALA
1	B	319	SER
1	B	395	LEU
1	B	508	PHE
1	A	7	ASN
1	A	13	PRO
1	A	14	ALA
1	A	44	PRO
1	A	80	LYS
1	A	105	ASP
1	A	318	ALA
1	A	325	PHE
1	A	399	ASN
1	A	401	LYS
1	B	120	ASP
1	B	149	ASN
1	B	189	ASP
1	B	218	GLN
1	B	224	PRO
1	B	255	VAL
1	B	258	ASP
1	B	364	GLY
1	B	372	ASN
1	B	410	GLY
1	B	440	SER
1	B	473	LEU
1	A	4	LEU
1	A	52	PHE
1	A	68	PRO
1	A	138	LYS
1	B	108	ARG

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Mol	Chain	Res	Type
1	B	114	SER
1	B	154	HIS
1	B	191	PRO
1	B	363	ILE
1	A	23	ASP
1	A	104	GLU
1	A	493	ASP
1	A	498	GLU
1	B	113	LYS
1	B	211	ASP
1	B	263	ASP
1	B	377	GLN
1	A	71	ILE
1	A	294	LYS
1	A	446	GLY
1	B	397	GLN
1	B	506	THR
1	A	274	VAL
1	A	403	LYS
1	A	508	PHE
1	A	40	LEU
1	B	266	VAL
1	B	194	VAL
1	A	494	VAL
1	B	365	VAL
1	B	348	ILE
1	B	447	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	424/440 (96%)	298 (70%)	126 (30%)	0 1
1	B	340/440 (77%)	232 (68%)	108 (32%)	0 0
All	All	764/880 (87%)	530 (69%)	234 (31%)	0 1

All (234) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	11	ILE
1	A	12	SER
1	A	15	GLU
1	A	20	ASN
1	A	21	LYS
1	A	27	VAL
1	A	28	VAL
1	A	30	ASN
1	A	32	TYR
1	A	33	VAL
1	A	38	ARG
1	A	40	LEU
1	A	47	GLN
1	A	50	ILE
1	A	57	ASP
1	A	58	VAL
1	A	61	ILE
1	A	65	LEU
1	A	69	ASN
1	A	72	ASP
1	A	75	ILE
1	A	78	GLU
1	A	79	LYS
1	A	81	LEU
1	A	84	LEU
1	A	85	GLN
1	A	87	SER
1	A	91	GLU
1	A	92	LEU
1	A	101	GLU
1	A	103	LYS
1	A	104	GLU
1	A	105	ASP
1	A	106	ILE
1	A	108	ARG
1	A	109	LYS
1	A	110	GLU
1	A	111	GLN
1	A	112	LEU
1	A	113	LYS
1	A	120	ASP

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Mol	Chain	Res	Type
1	A	124	ASN
1	A	125	LEU
1	A	139	GLN
1	A	145	SER
1	A	156	GLU
1	A	162	HIS
1	A	169	LYS
1	A	170	ILE
1	A	176	LYS
1	A	186	SER
1	A	190	VAL
1	A	195	SER
1	A	197	THR
1	A	201	LYS
1	A	214	ARG
1	A	216	CYS
1	A	221	THR
1	A	222	LYS
1	A	230	LEU
1	A	232	SER
1	A	236	GLU
1	A	240	GLU
1	A	245	ASP
1	A	248	ILE
1	A	252	GLN
1	A	254	TYR
1	A	255	VAL
1	A	256	ASN
1	A	259	ARG
1	A	260	LYS
1	A	265	LEU
1	A	272	LEU
1	A	285	SER
1	A	288	GLN
1	A	289	ARG
1	A	291	LYS
1	A	297	PHE
1	A	320	ARG
1	A	325	PHE
1	A	328	PRO
1	A	330	LEU
1	A	337	GLU

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Mol	Chain	Res	Type
1	A	338	LEU
1	A	340	LYS
1	A	342	THR
1	A	343	LYS
1	A	354	THR
1	A	365	VAL
1	A	372	ASN
1	A	378	LEU
1	A	381	SER
1	A	388	LEU
1	A	390	GLU
1	A	392	MET
1	A	394	ILE
1	A	396	GLU
1	A	398	ARG
1	A	400	LEU
1	A	401	LYS
1	A	413	ARG
1	A	416	THR
1	A	420	LYS
1	A	427	LYS
1	A	429	VAL
1	A	439	ASN
1	A	444	ARG
1	A	448	GLU
1	A	451	ILE
1	A	452	GLU
1	A	453	ILE
1	A	460	MET
1	A	464	LEU
1	A	465	LEU
1	A	474	LYS
1	A	477	LEU
1	A	482	THR
1	A	483	LEU
1	A	493	ASP
1	A	495	LEU
1	A	499	VAL
1	A	504	THR
1	A	505	LEU
1	A	506	THR
1	A	507	GLU

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Mol	Chain	Res	Type
1	B	99	PRO
1	B	101	GLU
1	B	102	THR
1	B	103	LYS
1	B	104	GLU
1	B	105	ASP
1	B	106	ILE
1	B	108	ARG
1	B	109	LYS
1	B	110	GLU
1	B	112	LEU
1	B	116	LEU
1	B	122	ILE
1	B	124	ASN
1	B	131	LEU
1	B	134	GLN
1	B	136	LEU
1	B	139	GLN
1	B	149	ASN
1	B	155	ARG
1	B	169	LYS
1	B	170	ILE
1	B	175	ARG
1	B	176	LYS
1	B	178	ASP
1	B	179	ILE
1	B	184	LEU
1	B	186	SER
1	B	187	HIS
1	B	188	VAL
1	B	197	THR
1	B	201	LYS
1	B	206	LEU
1	B	207	GLU
1	B	214	ARG
1	B	216	CYS
1	B	222	LYS
1	B	227	ILE
1	B	230	LEU
1	B	234	SER
1	B	236	GLU
1	B	239	ILE

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Mol	Chain	Res	Type
1	B	246	LYS
1	B	247	GLN
1	B	248	ILE
1	B	249	GLN
1	B	252	GLN
1	B	255	VAL
1	B	256	ASN
1	B	257	SER
1	B	258	ASP
1	B	259	ARG
1	B	261	ILE
1	B	263	ASP
1	B	271	LYS
1	B	275	LYS
1	B	277	LEU
1	B	280	THR
1	B	281	VAL
1	B	286	LEU
1	B	289	ARG
1	B	291	LYS
1	B	295	LEU
1	B	296	LYS
1	B	320	ARG
1	B	322	LEU
1	B	325	PHE
1	B	327	ASP
1	B	330	LEU
1	B	337	GLU
1	B	339	LYS
1	B	342	THR
1	B	343	LYS
1	B	348	ILE
1	B	353	ARG
1	B	357	VAL
1	B	365	VAL
1	B	366	SER
1	B	372	ASN
1	B	378	LEU
1	B	382	ARG
1	B	385	ILE
1	B	388	LEU
1	B	391	THR

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Mol	Chain	Res	Type
1	B	397	GLN
1	B	398	ARG
1	B	403	LYS
1	B	404	LEU
1	B	408	VAL
1	B	416	THR
1	B	420	LYS
1	B	423	CYS
1	B	427	LYS
1	B	431	LEU
1	B	436	LEU
1	B	439	ASN
1	B	440	SER
1	B	449	LYS
1	B	464	LEU
1	B	468	THR
1	B	474	LYS
1	B	482	THR
1	B	483	LEU
1	B	490	VAL
1	B	498	GLU
1	B	501	GLU
1	B	504	THR
1	B	510	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	ASN
1	A	47	GLN
1	A	53	ASN
1	A	124	ASN
1	A	139	GLN
1	A	157	ASN
1	A	218	GLN
1	A	225	GLN
1	A	249	GLN
1	A	252	GLN
1	A	256	ASN
1	A	268	ASN
1	A	372	ASN
1	A	439	ASN

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Mol	Chain	Res	Type
1	A	497	ASN
1	B	124	ASN
1	B	157	ASN
1	B	218	GLN
1	B	225	GLN
1	B	249	GLN
1	B	252	GLN
1	B	256	ASN
1	B	268	ASN
1	B	372	ASN
1	B	373	GLN
1	B	439	ASN
1	B	445	ASN
1	B	497	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	FMN	B	570	-	33,33,33	1.06	1 (3%)	48,50,50	2.27	15 (31%)
2	HEM	A	560	1	41,50,50	2.53	13 (31%)	45,82,82	3.05	18 (40%)
4	PYR	B	571	-	5,5,5	3.27	3 (60%)	3,6,6	0.76	0
3	FMN	A	569	-	33,33,33	0.96	1 (3%)	48,50,50	2.38	16 (33%)

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	FMN	B	570	-	-	4/18/18/18	0/3/3/3
2	HEM	A	560	1	-	8/12/54/54	-
4	PYR	B	571	-	-	4/4/4/4	-
3	FMN	A	569	-	1/1/4/4	3/18/18/18	0/3/3/3

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	560	HEM	C3D-C2D	7.41	1.52	1.36
2	A	560	HEM	C3C-C2C	-5.92	1.32	1.40
4	B	571	PYR	CA-C	-5.10	1.36	1.54
2	A	560	HEM	CAA-C2A	5.07	1.59	1.52
4	B	571	PYR	O-C	4.42	1.34	1.22
2	A	560	HEM	FE-ND	4.13	2.17	1.96
2	A	560	HEM	CBA-CGA	3.92	1.59	1.50
2	A	560	HEM	CAB-C3B	3.81	1.57	1.47
2	A	560	HEM	CBD-CGD	3.09	1.57	1.50
2	A	560	HEM	CBB-CAB	3.06	1.45	1.30
2	A	560	HEM	CAD-C3D	2.90	1.58	1.51
2	A	560	HEM	O1D-CGD	2.63	1.30	1.22
4	B	571	PYR	O3-CA	2.50	1.28	1.23
3	A	569	FMN	C9A-N10	-2.28	1.37	1.41
2	A	560	HEM	CHC-C4B	-2.22	1.34	1.41
2	A	560	HEM	C4A-NA	2.16	1.40	1.36
2	A	560	HEM	C3C-CAC	2.12	1.52	1.47
3	B	570	FMN	P-O5'	-2.02	1.53	1.60

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	569	FMN	P-O5'-C5'	7.21	138.14	118.30
2	A	560	HEM	C4C-CHD-C1D	6.49	131.12	122.56
2	A	560	HEM	CHC-C4B-NB	6.46	131.44	124.43
3	B	570	FMN	O5'-P-O1P	6.05	123.43	106.47
2	A	560	HEM	CAA-CBA-CGA	5.98	130.53	113.76
2	A	560	HEM	C4A-C3A-C2A	5.98	111.15	107.00
2	A	560	HEM	CAD-CBD-CGD	5.48	125.41	113.60
3	B	570	FMN	C4'-C3'-C2'	5.33	124.44	113.36
2	A	560	HEM	C3D-C4D-ND	5.29	116.06	110.17
2	A	560	HEM	C4D-C3D-C2D	-5.19	99.34	106.90
3	A	569	FMN	C4'-C3'-C2'	4.99	123.75	113.36
3	A	569	FMN	O2'-C2'-C1'	4.89	121.64	109.80
3	B	570	FMN	P-O5'-C5'	4.67	131.17	118.30
2	A	560	HEM	CHA-C4D-ND	-4.50	118.82	124.38
2	A	560	HEM	O2A-CGA-O1A	-4.34	112.48	123.30
2	A	560	HEM	CHB-C1B-NB	4.34	129.74	124.38
2	A	560	HEM	C3B-C2B-C1B	4.32	109.69	106.49
3	A	569	FMN	O3'-C3'-C2'	-4.08	98.95	108.81
3	A	569	FMN	O3'-C3'-C4'	4.06	118.63	108.81
2	A	560	HEM	CAD-C3D-C4D	3.95	131.56	124.66
2	A	560	HEM	CHC-C4B-C3B	-3.85	118.68	124.57
3	A	569	FMN	O4'-C4'-C5'	3.75	118.35	109.92
3	B	570	FMN	O3P-P-O5'	3.72	116.64	106.73
3	B	570	FMN	O4'-C4'-C3'	3.66	118.00	109.10
2	A	560	HEM	O2A-CGA-CBA	3.66	125.79	114.03
3	A	569	FMN	O2-C2-N1	3.65	127.88	121.83
3	B	570	FMN	O2'-C2'-C1'	3.60	118.52	109.80
3	A	569	FMN	C5'-C4'-C3'	-3.56	105.34	112.20
3	A	569	FMN	C1'-C2'-C3'	3.50	119.57	109.79
3	B	570	FMN	O4'-C4'-C5'	3.40	117.56	109.92
3	A	569	FMN	O2'-C2'-C3'	3.39	117.34	109.10
3	B	570	FMN	C9A-C5A-N5	-3.30	118.85	122.43
2	A	560	HEM	C2B-C1B-NB	-3.27	105.97	109.84
3	B	570	FMN	O2P-P-O1P	-3.22	98.09	110.68
3	A	569	FMN	C9A-C5A-N5	-3.15	119.01	122.43
3	B	570	FMN	O3'-C3'-C2'	-3.12	101.27	108.81
2	A	560	HEM	CMB-C2B-C1B	-2.98	120.50	125.04
3	A	569	FMN	C6-C5A-N5	2.88	123.54	118.51
2	A	560	HEM	C1B-NB-C4B	2.83	108.00	105.07
3	A	569	FMN	C10-N1-C2	2.72	122.33	116.90
3	B	570	FMN	O2'-C2'-C3'	2.59	115.40	109.10
3	A	569	FMN	C7M-C7-C6	2.43	123.99	119.49
3	B	570	FMN	O3'-C3'-C4'	2.42	114.66	108.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	570	FMN	C7M-C7-C6	2.37	123.88	119.49
3	A	569	FMN	N3-C2-N1	-2.33	114.81	119.38
3	B	570	FMN	C6-C7-C8	-2.27	116.41	119.67
3	B	570	FMN	O3P-P-O2P	-2.24	99.08	107.64
2	A	560	HEM	CMA-C3A-C2A	-2.22	120.76	124.94
3	A	569	FMN	C4-C4A-N5	2.06	121.16	118.23

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	569	FMN	C2'

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	560	HEM	C1A-C2A-CAA-CBA
2	A	560	HEM	C3D-CAD-CBD-CGD
4	B	571	PYR	O-C-CA-O3
4	B	571	PYR	OXT-C-CA-O3
3	A	569	FMN	O2'-C2'-C3'-C4'
3	A	569	FMN	O2'-C2'-C3'-O3'
3	B	570	FMN	O2'-C2'-C3'-C4'
3	B	570	FMN	C2'-C3'-C4'-O4'
3	A	569	FMN	C4'-C5'-O5'-P
3	B	570	FMN	C4'-C5'-O5'-P
2	A	560	HEM	C2A-CAA-CBA-CGA
2	A	560	HEM	C4B-C3B-CAB-CBB
4	B	571	PYR	O-C-CA-CB
3	B	570	FMN	O4'-C4'-C5'-O5'
4	B	571	PYR	OXT-C-CA-CB
2	A	560	HEM	CAA-CBA-CGA-O2A
2	A	560	HEM	CAA-CBA-CGA-O1A
2	A	560	HEM	CAD-CBD-CGD-O1D
2	A	560	HEM	CAD-CBD-CGD-O2D

There are no ring outliers.

4 monomers are involved in 44 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	570	FMN	15	0
2	A	560	HEM	15	0

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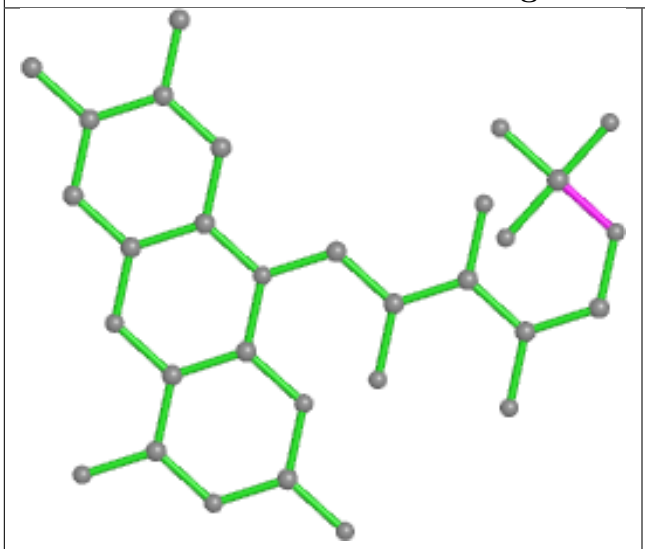
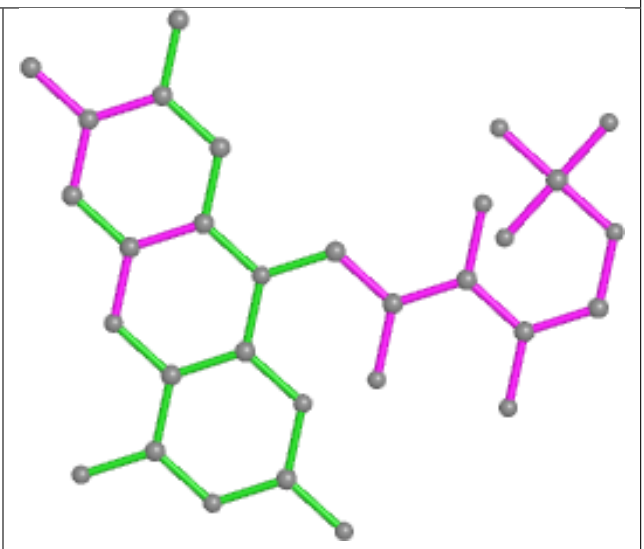
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	571	PYR	1	0
3	A	569	FMN	13	0

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.

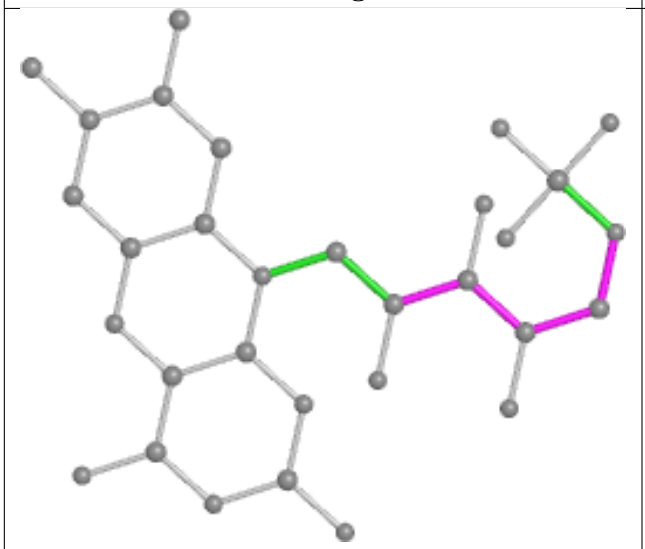
Ligand FMN B 570



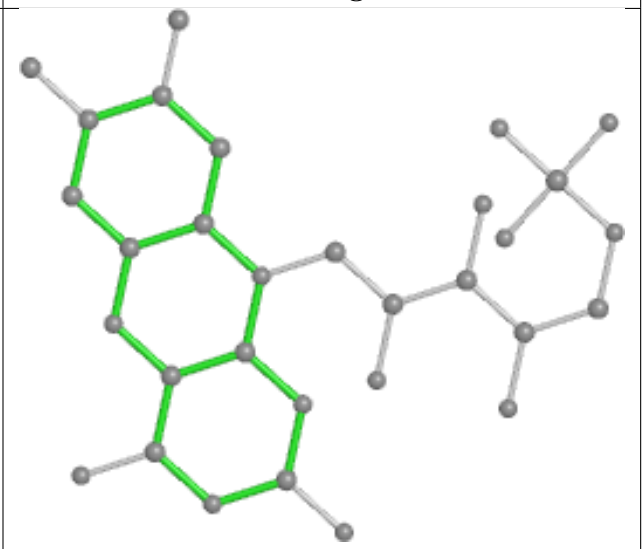
Bond lengths



Bond angles

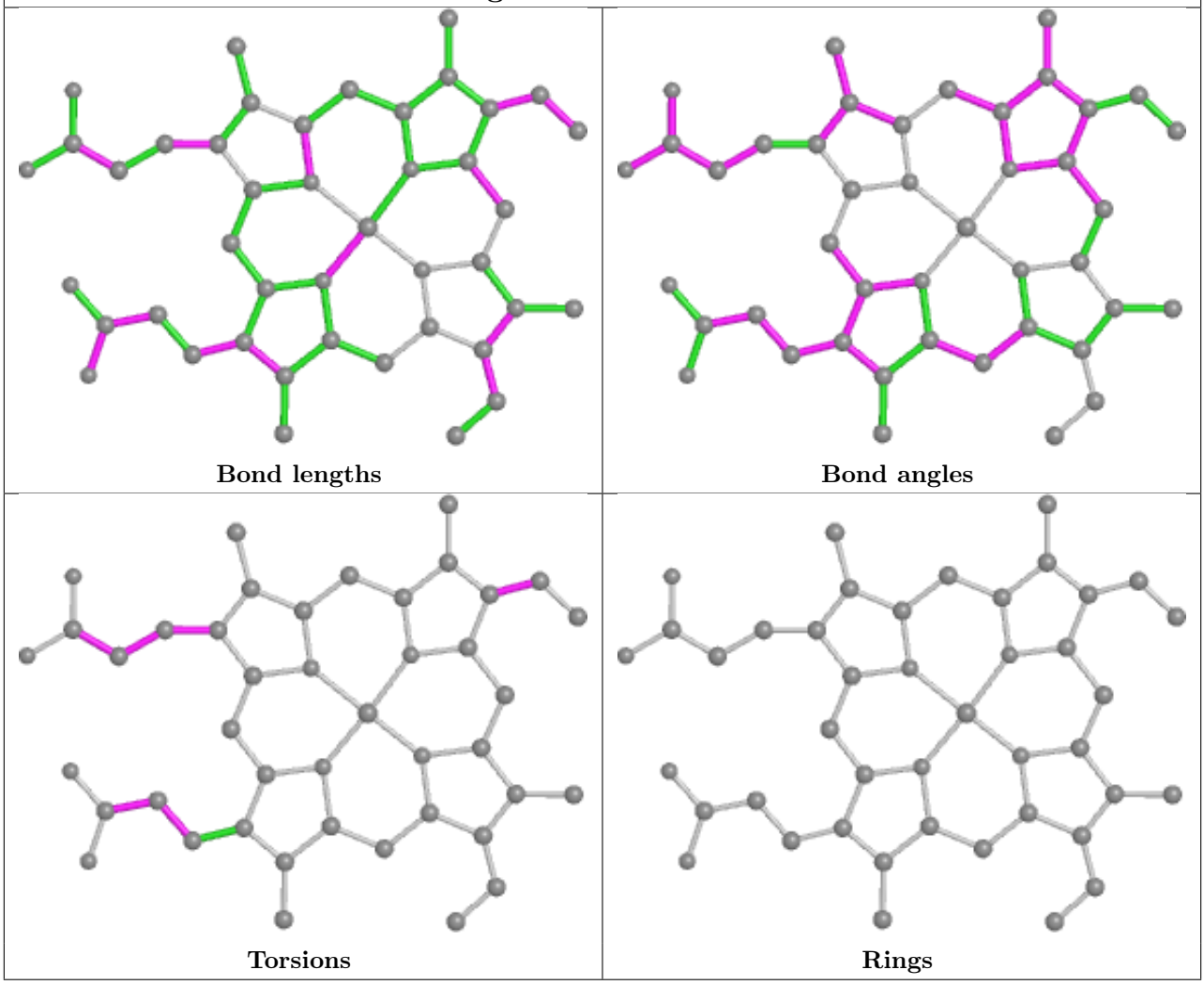


Torsions

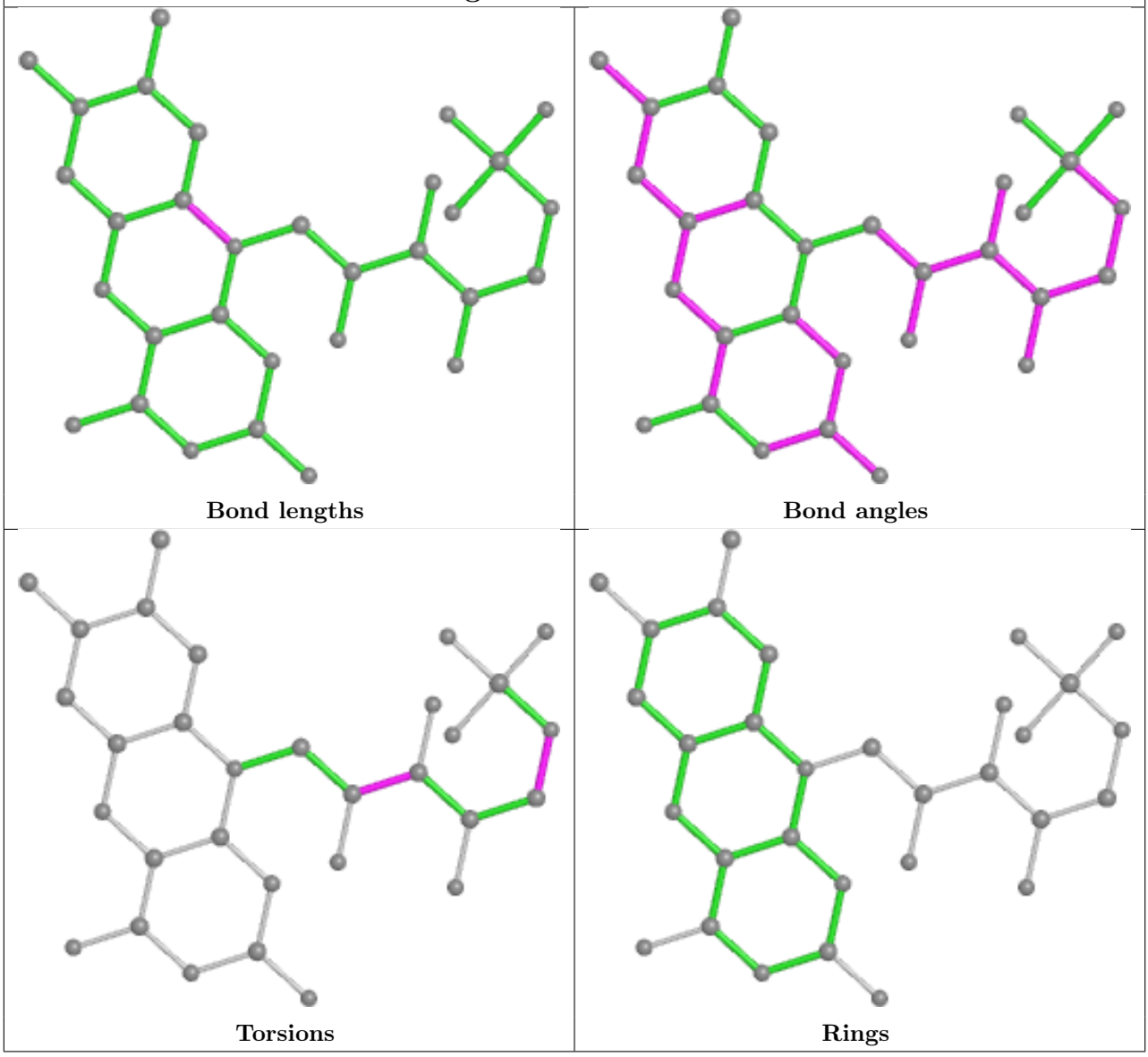


Rings

Ligand HEM A 560



Ligand FMN A 569



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	89:PRO	C	90:PRO	N	1.19

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	492/511 (96%)	-0.21	22 (4%)	33	23	19, 52, 147, 183	0
1	B	396/511 (77%)	-0.28	12 (3%)	50	40	18, 65, 107, 171	0
All	All	888/1022 (86%)	-0.24	34 (3%)	40	30	18, 58, 138, 183	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	7	ASN	8.5
1	A	9	GLN	8.3
1	A	6	MET	6.7
1	B	99	PRO	6.4
1	A	5	ASP	5.9
1	A	11	ILE	4.8
1	A	8	LYS	4.1
1	A	88	MET	3.8
1	A	18	LYS	3.7
1	B	100	GLY	3.6
1	B	320	ARG	3.5
1	A	93	VAL	3.4
1	B	299	ASN	3.4
1	A	78	GLU	3.3
1	A	83	PRO	3.2
1	A	509	GLU	3.1
1	A	4	LEU	2.9
1	A	10	LYS	2.8
1	B	492	ASN	2.8
1	B	298	SER	2.7
1	B	321	ALA	2.7
1	B	297	PHE	2.7
1	A	77	PRO	2.7
1	A	297	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	492	ASN	2.5
1	B	322	LEU	2.5
1	A	52	PHE	2.4
1	B	114	SER	2.3
1	A	14	ALA	2.3
1	B	113	LYS	2.2
1	B	206	LEU	2.1
1	A	114	SER	2.1
1	A	491	PRO	2.0
1	A	92	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

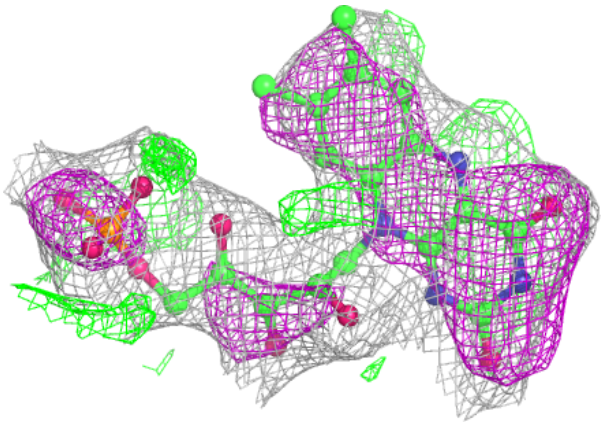
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

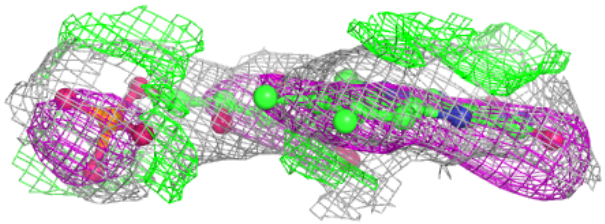
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	PYR	B	571	6/6	0.80	0.44	120,125,128,133	0
3	FMN	B	570	31/31	0.87	0.18	16,21,24,26	0
3	FMN	A	569	31/31	0.88	0.17	10,14,17,18	0
2	HEM	A	560	43/43	0.97	0.21	90,98,116,122	0

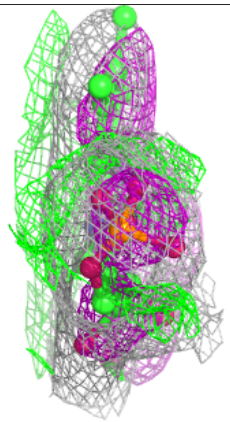
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FMN B 570:

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

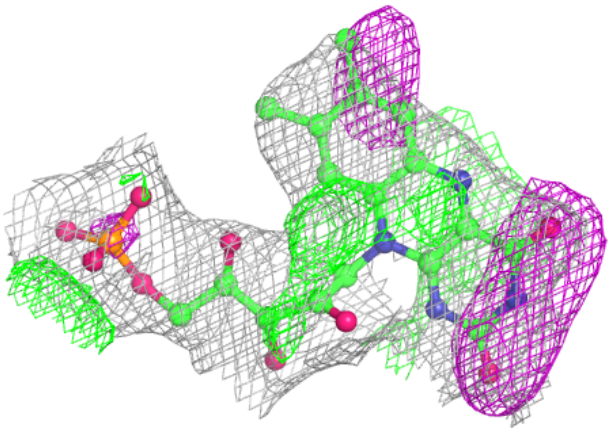


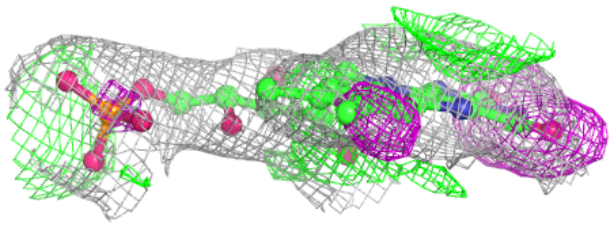


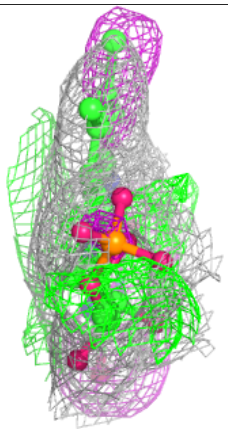


Electron density around FMN A 569:

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

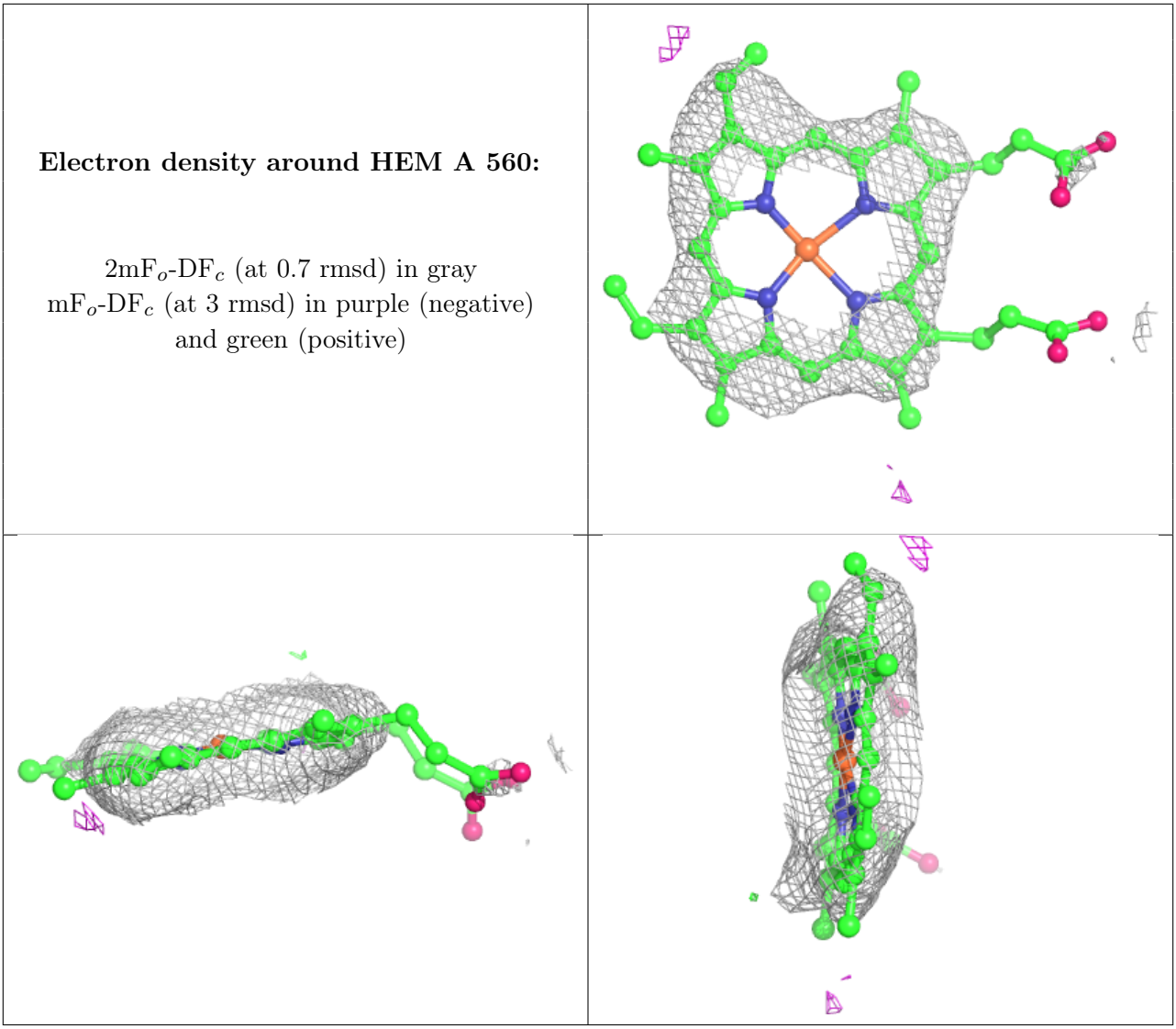






Electron density around HEM A 560:

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



6.5 Other polymers (i)

There are no such residues in this entry.