Full wwPDB X-ray Structure Validation Report (i)

Sep 6, 2023 – 09:29 AM EDT

PDB ID	:	4BLC
Title	:	THE STRUCTURE OF ORTHORHOMBIC CRYSTALS OF BEEF LIVER CATALASE
Authors	:	Ko, T.P.; Day, J.; Malkin, A.; McPherson, A.
Deposited on	:	1998-09-27
Resolution	:	2.30 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 (1)) were used in the production of this report:

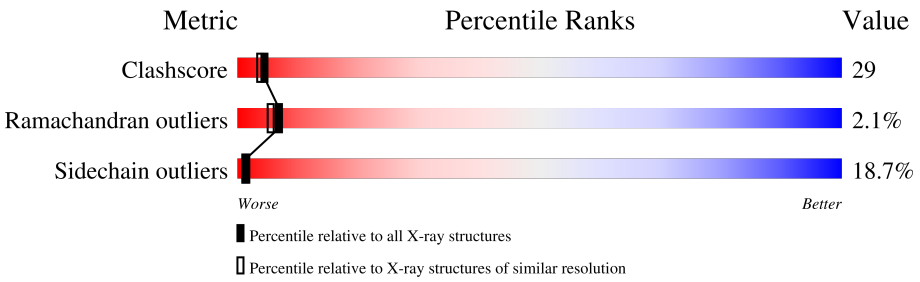
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.30 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))
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	506	56% 36% 6% •
1	B	506	38% 45% 15% ••
1	C	506	44% 41% 13% ••
1	D	506	47% 42% 10% •

2 Entry composition (i)

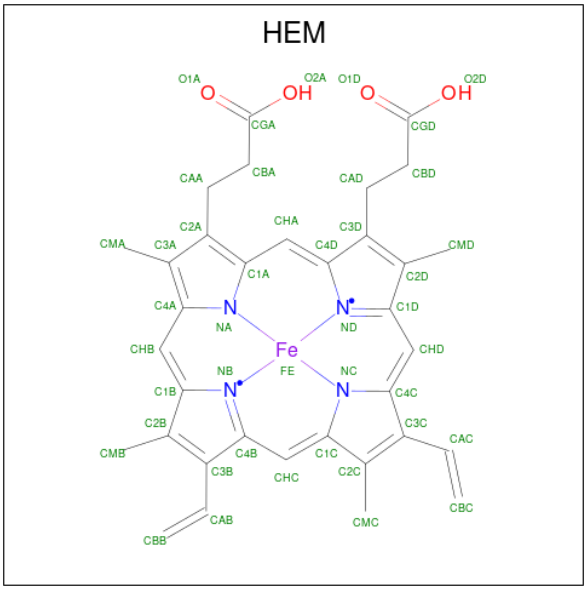
There are 4 unique types of molecules in this entry. The entry contains 16816 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PROTEIN (CATALASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	499	4017	2548	715	740	14	0	0	0
1	B	499	4017	2548	715	740	14	0	0	0
1	C	499	4017	2548	715	740	14	0	0	0
1	D	499	4017	2548	715	740	14	0	0	0

- 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
2	B	1	43	34	1	4	4	0	0

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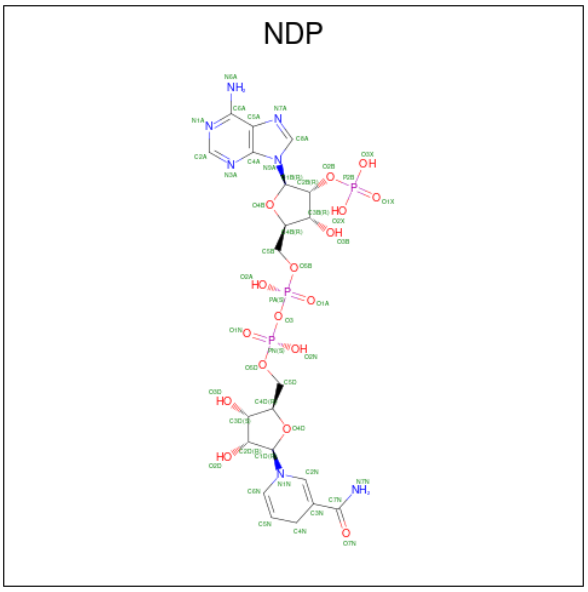
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
2	C	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
2	D	1	43	34	1	4	4	0	0

- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	48	21	7	17	3	0	0
			Total	C	N	O	P		
3	B	1	48	21	7	17	3	0	0
			Total	C	N	O	P		
3	C	1	48	21	7	17	3	0	0
			Total	C	N	O	P		
3	D	1	48	21	7	17	3	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	119	119	119	0	0
			Total	O		
4	B	89	89	89	0	0
			Total	O		
4	C	83	83	83	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	D	93	93	93	0	0

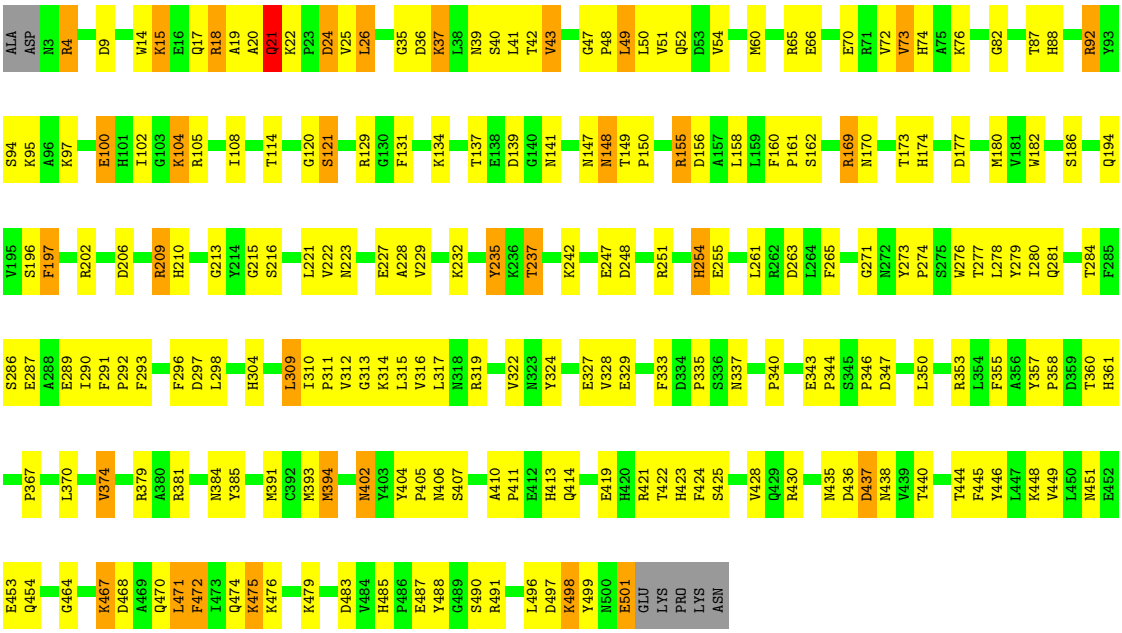
3 Residue-property plots (i)

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. 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. 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.

Note EDS was not executed.

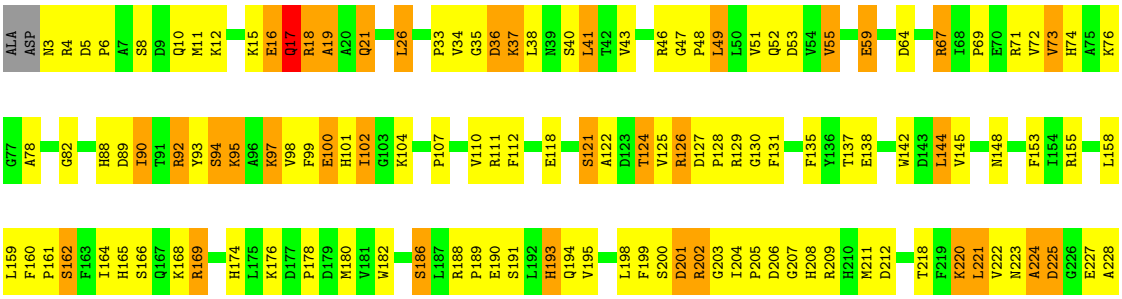
• Molecule 1: PROTEIN (CATALASE)

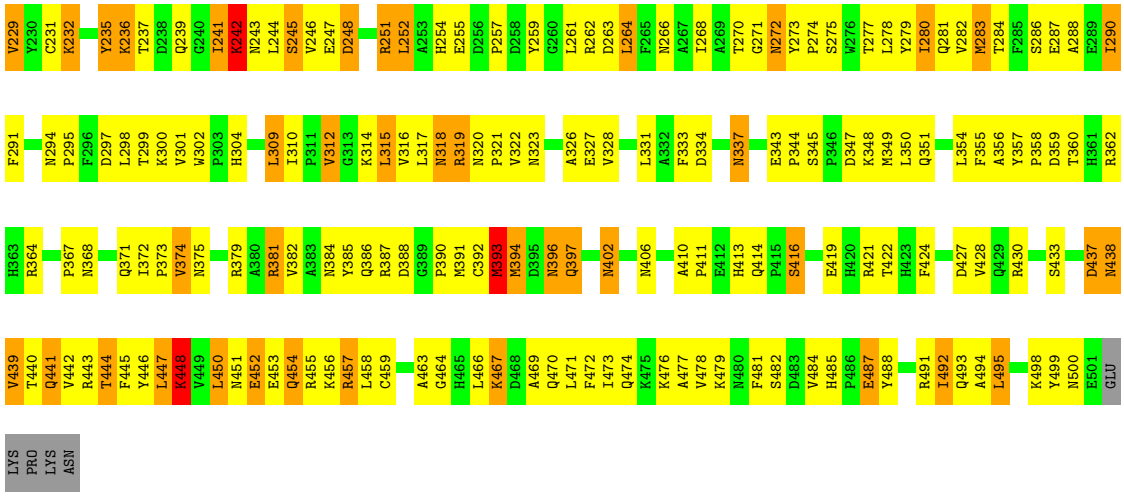
Chain A: 56% 36% 6%



• Molecule 1: PROTEIN (CATALASE)

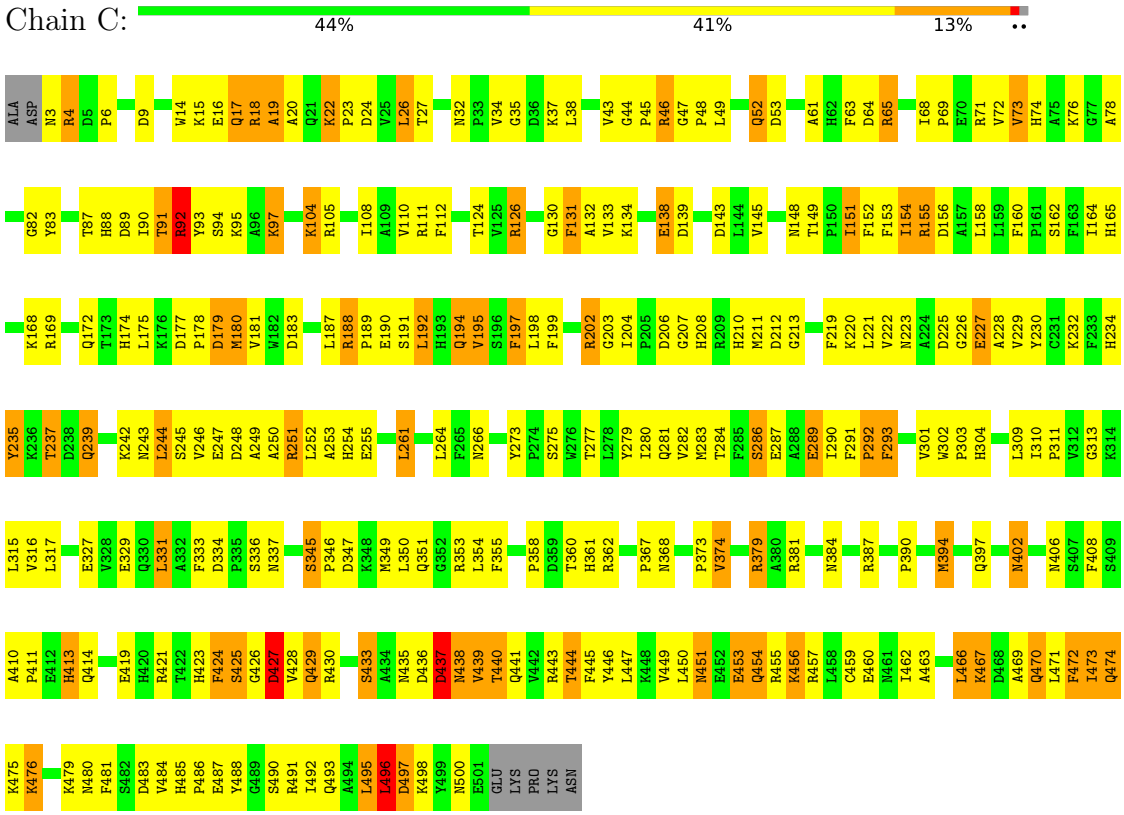
Chain B: 38% 45% 15%





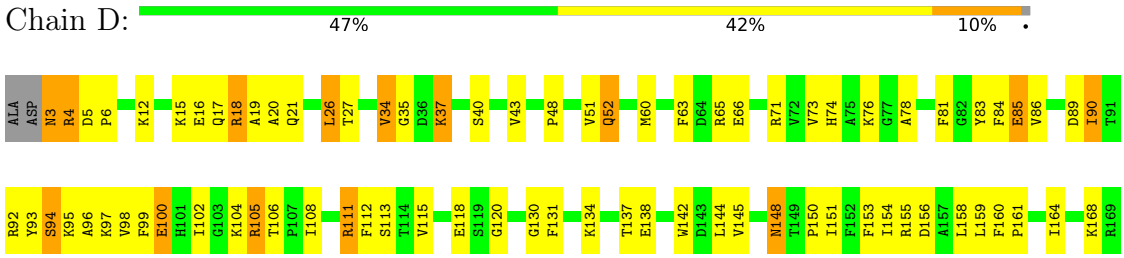
- Molecule 1: PROTEIN (CATALASE)

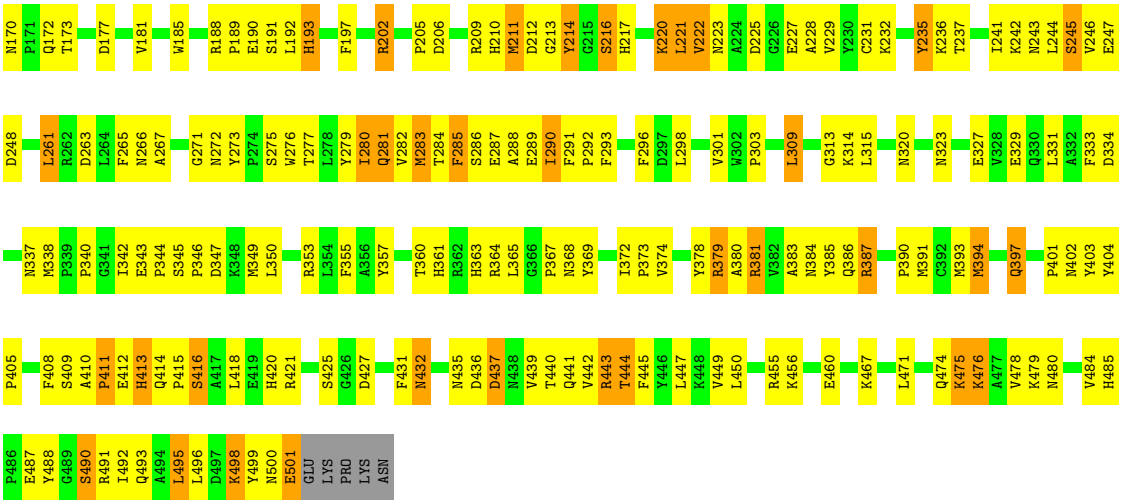
Chain C:



- Molecule 1: PROTEIN (CATALASE)

Chain D:




N170 P171 Q172 T173 D177 V181 W185 R188 P189 E190 S191 L192 H193 F197 R202 P205 D206 R209 H210 M211 D212 G213 Y214 G215 S216 H217 K220 L221 V222 N223 A224 D225 G226 E227 A228 V229 Y230 C231 K232 Y235 K236 T237 I241 K242 N243 L244 S245 V246 E247
D248 L261 R262 D263 L264 F265 N266 A267 G271 N272 Y273 P274 S275 W276 T277 L278 Y279 I280 Q281 V282 M283 T284 F285 S286 E287 A288 E289 I290 F291 P292 F293 F296 D297 L298 V301 W302 P303 L309 G313 K314 L315 N320 N323 E327 V328 E329 Q330 L331 A332 F333 D334
N337 M338 P339 P340 G341 I342 E343 P344 S345 P346 D347 K348 M349 L350 R353 L354 F355 A356 Y357 T360 H361 R362 H363 R364 L365 G366 P367 M368 Y369 I372 P373 V374 Y378 R379 A380 R381 V382 A383 N384 Y385 Q386 R387 P390 M391 C392 M393 M394 Q397 P401 N402 Y403 Y404
P405 F408 S409 A410 P411 E412 H413 Q414 P415 S416 A417 L418 E419 H420 R421 S425 G426 D427 F431 N432 N435 D436 D437 N438 V439 T440 Q441 V442 R443 T444 F445 Y446 L447 K448 V449 L450 R455 K456 E460 K467 L471 Q474 K475 K476 A477 V478 K479 N480 V484 H485
P486 E487 Y488 G489 S490 R491 I492 Q493 A494 L495 L496 D497 K498 Y499 N500 E501 GLU LYS PRO LYS ASN

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	87.80Å 140.60Å 232.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30	Depositor
% Data completeness (in resolution range)	87.5 (20.00-2.30)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.205 , 0.273	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	16816	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

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: HEM, NDP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.41	0/4137	0.62	0/5619
1	B	0.39	0/4137	0.59	0/5619
1	C	0.39	0/4137	0.60	0/5619
1	D	0.41	0/4137	0.60	0/5619
All	All	0.40	0/16548	0.60	0/22476

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4017	0	3839	171	0
1	B	4017	0	3839	305	0
1	C	4017	0	3839	273	0
1	D	4017	0	3839	253	0
2	A	43	0	30	5	0
2	B	43	0	30	0	0
2	C	43	0	30	4	0
2	D	43	0	30	2	0
3	A	48	0	26	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	48	0	26	4	0
3	C	48	0	26	2	0
3	D	48	0	26	1	0
4	A	119	0	0	8	0
4	B	89	0	0	16	0
4	C	83	0	0	8	0
4	D	93	0	0	10	0
All	All	16816	0	15580	917	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 29.

All (917) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:223:ASN:HD21	1:D:227:GLU:HB3	0.98	1.12
1:A:451:ASN:H	1:A:454:GLN:HE21	1.06	1.01
1:D:223:ASN:ND2	1:D:227:GLU:HB3	1.79	0.98
1:B:169:ARG:HG2	1:B:169:ARG:HH11	1.30	0.95
1:B:457:ARG:HH11	1:B:457:ARG:HB2	1.28	0.95
1:C:251:ARG:HD2	1:C:255:GLU:HG3	1.50	0.93
1:A:92:ARG:HH11	1:A:92:ARG:HB3	1.33	0.93
1:B:457:ARG:HB2	1:B:457:ARG:NH1	1.82	0.92
1:D:291:PHE:HD1	1:D:293:PHE:H	1.17	0.92
1:D:85:GLU:HG2	1:D:105:ARG:HG3	1.52	0.92
1:C:402:ASN:H	1:C:402:ASN:HD22	1.09	0.90
1:B:4:ARG:HH22	1:C:470:GLN:HE21	1.21	0.89
1:C:466:LEU:O	1:C:466:LEU:HD12	1.74	0.88
1:C:485:HIS:CE1	1:C:487:GLU:HB3	2.08	0.87
1:B:100:GLU:HB3	1:B:104:LYS:HG3	1.56	0.86
1:B:129:ARG:HB2	1:B:148:ASN:ND2	1.90	0.85
1:B:406:ASN:HD21	1:B:410:ALA:HB3	1.40	0.85
1:C:438:ASN:N	1:C:438:ASN:HD22	1.71	0.85
1:B:148:ASN:HD22	1:B:211:MET:CE	1.90	0.84
1:C:487:GLU:O	1:C:491:ARG:HG3	1.77	0.84
1:B:223:ASN:HD21	1:B:227:GLU:HB2	1.42	0.82
1:A:353:ARG:HG3	2:A:507:HEM:HBB2	1.62	0.82
1:B:454:GLN:HA	1:B:457:ARG:NH1	1.95	0.81
1:A:43:VAL:O	1:A:47:GLY:HA3	1.78	0.81
1:D:347:ASP:HB3	1:D:350:LEU:HB3	1.63	0.81
1:D:170:ASN:ND2	1:D:172:GLN:H	1.77	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:451:ASN:N	1:A:454:GLN:HE21	1.78	0.81
1:B:495:LEU:HD23	1:B:495:LEU:H	1.46	0.81
1:C:151:ILE:HD12	1:C:194:GLN:HG2	1.62	0.81
1:A:487:GLU:O	1:A:491:ARG:HG3	1.81	0.79
1:A:451:ASN:H	1:A:454:GLN:NE2	1.80	0.79
1:D:221:LEU:HD11	1:D:231:CYS:HB3	1.64	0.79
1:B:223:ASN:ND2	1:B:227:GLU:HB2	1.99	0.78
1:B:178:PRO:HD3	4:B:762:HOH:O	1.83	0.78
1:C:406:ASN:HD21	1:C:410:ALA:HB3	1.47	0.78
1:C:476:LYS:NZ	1:C:476:LYS:HB3	1.98	0.78
1:D:284:THR:OG1	1:D:287:GLU:HG2	1.83	0.78
1:B:241:ILE:HG22	1:B:242:LYS:H	1.47	0.77
1:A:485:HIS:HD2	1:A:487:GLU:H	1.28	0.77
1:B:37:LYS:HE3	1:B:59:GLU:OE2	1.84	0.77
1:D:202:ARG:NH1	1:D:241:ILE:HG21	1.99	0.77
1:B:191:SER:O	1:B:195:VAL:HG23	1.85	0.77
1:D:244:LEU:HD21	1:D:248:ASP:HB2	1.67	0.76
1:C:488:TYR:O	1:C:492:ILE:HG12	1.86	0.76
1:A:35:GLY:HA2	1:C:414:GLN:O	1.86	0.75
1:B:304:HIS:HD2	1:B:309:LEU:HD21	1.51	0.75
1:A:36:ASP:HA	1:C:413:HIS:ND1	2.01	0.75
1:C:110:VAL:HG22	1:C:133:VAL:HG22	1.67	0.75
1:C:210:HIS:HB3	1:C:242:LYS:H	1.52	0.75
1:C:222:VAL:HG22	1:C:228:ALA:HB2	1.68	0.75
1:C:244:LEU:HD13	1:C:248:ASP:HB3	1.69	0.74
1:D:145:VAL:O	2:D:507:HEM:HBC2	1.88	0.74
1:C:78:ALA:HB2	1:C:261:LEU:HD22	1.68	0.74
1:A:223:ASN:ND2	1:A:227:GLU:HB2	2.03	0.73
1:C:191:SER:O	1:C:195:VAL:HG23	1.87	0.73
1:B:182:TRP:O	1:B:186:SER:HB3	1.88	0.72
1:A:223:ASN:HD21	1:A:227:GLU:HB2	1.54	0.72
1:B:122:ALA:HB2	1:B:257:PRO:HB3	1.71	0.72
1:B:89:ASP:HB2	1:B:102:ILE:HD11	1.72	0.72
1:B:414:GLN:HE21	1:B:416:SER:CB	2.03	0.72
1:B:78:ALA:HB2	1:B:261:LEU:HG	1.71	0.72
1:B:6:PRO:HG2	1:B:266:ASN:OD1	1.89	0.71
1:D:78:ALA:HB2	1:D:261:LEU:HG	1.72	0.71
1:D:170:ASN:HD22	1:D:173:THR:H	1.39	0.71
1:B:241:ILE:HG22	1:B:242:LYS:N	2.06	0.71
1:C:72:VAL:HG13	1:C:73:VAL:HG22	1.73	0.71
1:C:491:ARG:O	1:C:495:LEU:HD12	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:ARG:H	1:A:148:ASN:ND2	1.88	0.71
1:B:241:ILE:O	1:B:242:LYS:HB2	1.91	0.70
1:B:281:GLN:OE1	1:B:302:TRP:HB2	1.89	0.70
1:C:183:ASP:O	1:C:187:LEU:HG	1.90	0.70
1:D:137:THR:HA	1:D:379:ARG:HH21	1.56	0.70
1:B:190:GLU:HA	1:B:438:ASN:HB3	1.74	0.70
1:C:301:VAL:HG22	1:C:441:GLN:OE1	1.90	0.70
1:C:189:PRO:O	1:C:192:LEU:HG	1.92	0.70
1:D:286:SER:O	1:D:290:ILE:HD12	1.91	0.70
1:C:289:GLU:HG2	4:C:898:HOH:O	1.92	0.70
1:B:112:PHE:HA	1:B:130:GLY:O	1.91	0.69
1:A:82:GLY:HA3	1:A:316:VAL:O	1.92	0.69
1:B:126:ARG:HE	1:B:199:PHE:HA	1.58	0.69
1:C:402:ASN:HD22	1:C:402:ASN:N	1.84	0.69
1:D:367:PRO:HG2	1:D:390:PRO:HG2	1.72	0.69
1:C:74:HIS:O	1:C:111:ARG:NH2	2.24	0.69
1:D:84:PHE:O	1:D:105:ARG:HA	1.92	0.69
1:A:92:ARG:HH11	1:A:92:ARG:CB	2.04	0.69
1:C:273:TYR:HB3	1:C:317:LEU:O	1.93	0.69
1:D:387:ARG:HG2	1:D:387:ARG:HH11	1.56	0.68
1:A:209:ARG:HG2	1:A:274:PRO:HB3	1.74	0.68
1:A:425:SER:HA	1:B:424:PHE:O	1.93	0.68
1:D:367:PRO:HG2	1:D:390:PRO:CG	2.23	0.68
1:C:232:LYS:HB2	1:C:281:GLN:HB2	1.76	0.68
1:D:221:LEU:HD11	1:D:231:CYS:SG	2.33	0.68
1:C:438:ASN:N	1:C:438:ASN:ND2	2.41	0.68
1:A:51:VAL:HG13	1:B:49:LEU:O	1.93	0.68
4:A:718:HOH:O	1:D:363:HIS:HD2	1.77	0.68
1:B:37:LYS:O	1:C:158:LEU:HD13	1.93	0.68
1:D:364:ARG:HD2	4:D:1022:HOH:O	1.93	0.67
1:C:92:ARG:HG3	1:C:92:ARG:HH11	1.59	0.67
1:B:264:LEU:HD12	1:B:264:LEU:O	1.95	0.67
1:A:94:SER:HB2	1:A:221:LEU:HD22	1.77	0.67
1:B:148:ASN:HD22	1:B:211:MET:HE2	1.59	0.67
1:B:301:VAL:H	1:B:441:GLN:NE2	1.92	0.67
1:C:251:ARG:HG2	1:C:251:ARG:HH11	1.59	0.67
1:B:100:GLU:HB2	1:B:104:LYS:HZ3	1.59	0.67
1:B:301:VAL:H	1:B:441:GLN:HE22	1.41	0.67
1:B:454:GLN:HA	1:B:457:ARG:HH12	1.58	0.66
1:C:471:LEU:HA	1:C:474:GLN:HG3	1.75	0.66
1:B:47:GLY:HA2	1:C:424:PHE:CE1	2.30	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:787:HOH:O	1:C:44:GLY:HA2	1.94	0.66
1:B:414:GLN:HE21	1:B:416:SER:HB2	1.61	0.66
1:D:383:ALA:HB1	1:D:411:PRO:HG3	1.78	0.66
1:D:220:LYS:HE3	1:D:343:GLU:HB2	1.78	0.66
1:B:169:ARG:HH11	1:B:169:ARG:CG	2.06	0.66
1:B:360:THR:HG23	1:C:64:ASP:O	1.95	0.66
1:C:6:PRO:HD2	1:C:266:ASN:OD1	1.95	0.65
1:B:273:TYR:HB3	1:B:317:LEU:O	1.96	0.65
1:D:221:LEU:HD11	1:D:231:CYS:CB	2.26	0.65
1:C:470:GLN:O	1:C:473:ILE:HB	1.96	0.65
1:D:18:ARG:HB3	4:D:841:HOH:O	1.97	0.65
1:A:280:ILE:HG23	1:A:312:VAL:HG21	1.77	0.65
1:D:94:SER:HB2	1:D:221:LEU:HB3	1.79	0.65
1:B:220:LYS:C	1:B:221:LEU:HD23	2.16	0.65
1:A:419:GLU:OE2	1:B:430:ARG:NH1	2.30	0.65
1:D:287:GLU:HA	1:D:290:ILE:HB	1.78	0.65
1:A:170:ASN:HB3	1:A:173:THR:OG1	1.96	0.65
1:D:83:TYR:CE1	1:D:85:GLU:HG3	2.32	0.65
1:B:318:ASN:HD22	1:B:318:ASN:N	1.95	0.64
1:D:223:ASN:HD21	1:D:227:GLU:CB	1.93	0.64
1:A:471:LEU:HA	1:A:474:GLN:HG3	1.79	0.64
1:C:402:ASN:H	1:C:402:ASN:ND2	1.90	0.64
1:B:97:LYS:HB3	1:B:138:GLU:OE1	1.97	0.64
1:D:284:THR:HG23	1:D:287:GLU:OE2	1.98	0.64
1:D:487:GLU:HA	1:D:490:SER:OG	1.97	0.64
1:A:485:HIS:CD2	1:A:487:GLU:H	2.12	0.64
1:C:347:ASP:HB3	1:C:350:LEU:HB3	1.79	0.64
1:A:15:LYS:HD2	4:A:936:HOH:O	1.98	0.64
1:A:95:LYS:HG2	1:A:222:VAL:O	1.98	0.64
1:A:333:PHE:O	1:A:361:HIS:HE1	1.81	0.64
1:C:331:LEU:HD13	1:C:333:PHE:CZ	2.33	0.64
1:A:43:VAL:HG13	1:A:48:PRO:HD2	1.81	0.63
1:C:221:LEU:O	1:C:228:ALA:HA	1.98	0.63
1:C:410:ALA:HB1	1:C:411:PRO:HD2	1.80	0.63
1:D:76:LYS:O	1:D:113:SER:HB2	1.99	0.63
1:D:285:PHE:HD1	1:D:285:PHE:H	1.46	0.63
1:D:347:ASP:HB3	1:D:350:LEU:CB	2.27	0.63
1:A:18:ARG:HG2	4:A:935:HOH:O	1.98	0.63
1:A:498:LYS:HD2	4:A:725:HOH:O	1.97	0.63
1:C:451:ASN:OD1	1:C:454:GLN:HG2	1.99	0.63
1:B:41:LEU:HB3	1:B:53:ASP:HB2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:15:LYS:HD3	1:D:408:PHE:HA	1.80	0.63
1:D:338:MET:CE	1:D:342:ILE:HG22	2.29	0.63
1:B:391:MET:HE2	1:D:365:LEU:O	1.98	0.62
1:C:154:ILE:HG13	1:C:349:MET:CE	2.29	0.62
1:C:445:PHE:O	1:C:450:LEU:HB2	1.99	0.62
1:A:25:VAL:HG13	1:C:414:GLN:HG2	1.80	0.62
1:A:347:ASP:HB3	1:A:350:LEU:HB3	1.80	0.62
1:B:321:PRO:HG2	4:C:996:HOH:O	2.00	0.62
1:B:447:LEU:O	1:B:448:LYS:HB2	1.98	0.62
1:C:4:ARG:HD3	1:C:9:ASP:OD1	2.00	0.62
1:D:63:PHE:O	1:D:66:GLU:HG3	2.00	0.62
1:D:404:TYR:CD1	1:D:405:PRO:HA	2.34	0.62
1:B:466:LEU:CD2	1:B:474:GLN:HG2	2.30	0.62
1:B:229:VAL:HG23	1:B:284:THR:HA	1.81	0.62
1:B:304:HIS:CD2	1:B:309:LEU:HD21	2.32	0.62
1:D:445:PHE:HA	1:D:449:VAL:CG2	2.30	0.62
1:A:451:ASN:N	1:A:454:GLN:NE2	2.43	0.61
1:B:43:VAL:O	1:B:47:GLY:HA3	2.00	0.61
1:B:38:LEU:HG	1:D:413:HIS:CE1	2.35	0.61
1:C:165:HIS:HB3	1:D:402:ASN:ND2	2.15	0.61
1:A:414:GLN:O	1:C:35:GLY:HA2	1.99	0.61
1:D:154:ILE:HG13	1:D:349:MET:CE	2.31	0.61
1:C:358:PRO:O	1:C:362:ARG:HG3	2.00	0.61
1:C:451:ASN:H	1:C:454:GLN:HE21	1.48	0.61
1:D:156:ASP:OD1	1:D:158:LEU:HB2	2.01	0.61
1:B:142:TRP:CZ2	1:B:144:LEU:HD23	2.36	0.61
1:B:318:ASN:N	1:B:318:ASN:ND2	2.49	0.61
1:C:437:ASP:OD2	1:C:440:THR:HB	2.00	0.61
1:D:244:LEU:CD2	1:D:248:ASP:HB2	2.31	0.61
1:C:485:HIS:NE2	1:C:487:GLU:HB3	2.16	0.61
1:B:397:GLN:HG2	4:B:835:HOH:O	2.00	0.61
1:C:138:GLU:HA	1:C:379:ARG:O	2.01	0.61
1:C:251:ARG:HG3	1:C:252:LEU:N	2.16	0.61
1:B:160:PHE:O	1:B:164:ILE:HG12	2.01	0.61
1:A:148:ASN:HD22	1:A:148:ASN:H	1.49	0.60
1:C:26:LEU:HD21	1:C:37:LYS:HD3	1.83	0.60
1:C:425:SER:HB2	1:D:425:SER:OG	2.01	0.60
1:D:170:ASN:ND2	1:D:173:THR:H	1.98	0.60
1:C:213:GLY:HA3	1:C:235:TYR:CE2	2.36	0.60
1:C:329:GLU:OE1	1:C:329:GLU:HA	2.01	0.60
1:A:43:VAL:CG1	1:A:48:PRO:HD2	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:235:TYR:HA	1:C:277:THR:O	2.00	0.60
1:A:197:PHE:HD2	4:A:1043:HOH:O	1.83	0.60
1:B:88:HIS:HB2	1:B:312:VAL:HA	1.82	0.60
1:C:252:LEU:HA	1:C:255:GLU:HB2	1.83	0.60
1:B:323:ASN:O	1:B:327:GLU:HG3	2.01	0.60
1:B:205:PRO:HG3	1:B:211:MET:HE3	1.84	0.60
1:A:160:PHE:HB3	1:A:161:PRO:HD3	1.84	0.60
1:A:206:ASP:O	1:A:210:HIS:HD2	1.85	0.60
1:C:89:ASP:OD1	1:C:91:THR:HB	2.02	0.59
1:C:351:GLN:O	1:C:354:LEU:HB2	2.01	0.59
1:D:150:PRO:HB3	1:D:214:TYR:CD2	2.37	0.59
1:D:338:MET:HE3	1:D:342:ILE:HG22	1.82	0.59
1:A:97:LYS:O	1:A:100:GLU:HB2	2.02	0.59
1:A:150:PRO:HG3	3:A:1102:NDP:H41N	1.83	0.59
1:D:170:ASN:HD22	1:D:172:GLN:H	1.51	0.59
1:D:222:VAL:HG11	1:D:420:HIS:HB2	1.84	0.59
1:C:153:PHE:HZ	1:C:198:LEU:HD22	1.67	0.59
1:C:154:ILE:HG13	1:C:349:MET:HE1	1.84	0.59
1:D:455:ARG:HD2	1:D:491:ARG:HH12	1.67	0.59
1:C:476:LYS:HB3	1:C:476:LYS:HZ3	1.67	0.59
1:B:351:GLN:HE22	1:D:52:GLN:HG3	1.68	0.59
1:C:197:PHE:HB2	4:C:1074:HOH:O	2.03	0.59
1:C:437:ASP:C	1:C:438:ASN:HD22	2.06	0.59
1:B:4:ARG:NH2	1:C:470:GLN:HE21	1.94	0.59
1:D:83:TYR:HE1	1:D:85:GLU:HG3	1.67	0.59
1:B:206:ASP:OD2	1:B:244:LEU:HD21	2.03	0.58
1:C:72:VAL:HG11	2:C:507:HEM:HMA3	1.84	0.58
1:C:374:VAL:HG13	4:C:752:HOH:O	2.03	0.58
1:B:34:VAL:HG13	1:B:55:VAL:HG11	1.84	0.58
1:B:98:VAL:HG13	1:B:99:PHE:CD1	2.38	0.58
1:B:402:ASN:C	1:B:402:ASN:HD22	2.06	0.58
1:D:432:ASN:C	1:D:432:ASN:ND2	2.57	0.58
1:B:495:LEU:H	1:B:495:LEU:CD2	2.17	0.58
1:B:322:VAL:O	1:C:172:GLN:HG3	2.03	0.58
1:A:42:THR:HG22	1:A:49:LEU:HA	1.85	0.58
1:B:232:LYS:O	1:B:280:ILE:HA	2.04	0.58
1:C:188:ARG:HD3	1:C:190:GLU:OE2	2.04	0.58
1:C:284:THR:OG1	1:C:287:GLU:HG3	2.02	0.58
1:C:327:GLU:HA	1:C:374:VAL:HG11	1.86	0.58
1:D:108:ILE:HA	1:D:134:LYS:O	2.04	0.58
1:D:329:GLU:HA	1:D:329:GLU:OE1	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:488:TYR:O	1:D:492:ILE:HD12	2.04	0.58
1:C:446:TYR:CE1	1:C:455:ARG:HG2	2.39	0.57
1:D:280:ILE:HG12	1:D:281:GLN:N	2.19	0.57
1:D:415:PRO:O	1:D:418:LEU:HD12	2.04	0.57
1:A:147:ASN:ND2	2:A:507:HEM:HAC	2.20	0.57
1:B:159:LEU:HD21	1:C:38:LEU:HD22	1.85	0.57
1:C:291:PHE:CD1	1:C:292:PRO:HD2	2.40	0.57
1:A:437:ASP:OD2	1:A:440:THR:HB	2.05	0.57
1:B:82:GLY:HA3	1:B:316:VAL:O	2.04	0.57
1:B:491:ARG:O	1:B:495:LEU:HD23	2.05	0.57
1:C:162:SER:HG	1:D:404:TYR:H	1.48	0.57
1:A:15:LYS:HD3	1:C:408:PHE:HA	1.87	0.57
1:B:223:ASN:C	1:B:225:ASP:H	2.08	0.57
1:D:213:GLY:HA3	1:D:235:TYR:CD2	2.39	0.57
1:C:462:ILE:HD13	1:C:481:PHE:HE2	1.70	0.57
1:D:95:LYS:HG2	1:D:222:VAL:O	2.05	0.57
1:D:212:ASP:HB2	1:D:214:TYR:CE1	2.40	0.57
1:D:220:LYS:NZ	1:D:343:GLU:OE1	2.37	0.57
1:A:52:GLN:HB2	4:C:907:HOH:O	2.03	0.57
1:B:148:ASN:HD22	1:B:211:MET:HE1	1.70	0.57
1:C:287:GLU:HA	1:C:290:ILE:CD1	2.35	0.57
1:D:97:LYS:O	1:D:100:GLU:HB2	2.05	0.57
1:D:108:ILE:HD13	1:D:315:LEU:HD22	1.86	0.57
1:D:217:HIS:CE1	1:D:298:LEU:HD22	2.40	0.57
1:D:237:THR:HA	1:D:276:TRP:CD1	2.39	0.57
1:C:462:ILE:HD13	1:C:481:PHE:CE2	2.40	0.57
1:D:177:ASP:O	1:D:181:VAL:HG23	2.05	0.57
1:D:160:PHE:HB3	1:D:161:PRO:HD3	1.87	0.56
1:B:18:ARG:HD2	1:D:409:SER:O	2.05	0.56
1:B:372:ILE:HB	1:B:375:ASN:HD22	1.70	0.56
1:C:208:HIS:HA	1:C:211:MET:CE	2.35	0.56
1:C:251:ARG:HG2	1:C:251:ARG:NH1	2.20	0.56
1:C:287:GLU:HA	1:C:290:ILE:HD11	1.88	0.56
1:C:462:ILE:HG21	1:C:481:PHE:HE2	1.69	0.56
1:C:178:PRO:HA	1:C:181:VAL:HB	1.87	0.56
1:B:279:TYR:HB3	1:B:309:LEU:HB3	1.87	0.56
1:B:294:ASN:HA	1:C:46:ARG:HH12	1.70	0.56
1:A:446:TYR:OH	1:A:487:GLU:HG2	2.06	0.56
1:B:430:ARG:HH22	1:C:53:ASP:CG	2.08	0.56
1:B:455:ARG:HG3	1:B:455:ARG:HH11	1.71	0.56
1:B:466:LEU:HD23	1:B:466:LEU:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:110:VAL:HG13	1:C:132:ALA:O	2.06	0.56
1:A:284:THR:OG1	1:A:287:GLU:HG3	2.05	0.56
1:C:207:GLY:HA3	4:C:919:HOH:O	2.05	0.56
1:A:335:PRO:HD2	4:A:712:HOH:O	2.05	0.55
1:A:367:PRO:HG3	1:C:65:ARG:HD3	1.89	0.55
1:C:223:ASN:HD21	1:C:227:GLU:HB3	1.72	0.55
1:D:18:ARG:HD3	4:D:887:HOH:O	2.06	0.55
1:D:93:TYR:CE1	1:D:282:VAL:HG11	2.42	0.55
1:A:485:HIS:HD2	1:A:487:GLU:N	2.01	0.55
1:B:126:ARG:HH11	1:B:126:ARG:HB2	1.71	0.55
1:A:232:LYS:HB2	1:A:281:GLN:HB2	1.88	0.55
1:B:382:VAL:HG13	1:B:382:VAL:O	2.05	0.55
1:C:169:ARG:HD3	1:C:174:HIS:CE1	2.41	0.55
1:A:384:ASN:HA	1:C:26:LEU:HD13	1.89	0.55
1:B:160:PHE:CE1	1:B:164:ILE:HD11	2.42	0.55
1:C:97:LYS:O	1:C:104:LYS:NZ	2.39	0.55
1:B:388:ASP:H	1:B:396:ASN:HD21	1.53	0.55
1:B:491:ARG:O	1:B:494:ALA:HB3	2.06	0.55
1:B:334:ASP:O	1:B:337:ASN:HB2	2.07	0.55
1:B:495:LEU:HD23	1:B:495:LEU:N	2.20	0.55
1:A:254:HIS:ND1	1:A:255:GLU:N	2.55	0.55
1:B:38:LEU:HD21	1:D:404:TYR:CD2	2.42	0.55
1:B:283:MET:HB2	1:B:302:TRP:CH2	2.42	0.55
1:B:317:LEU:C	1:B:318:ASN:HD22	2.11	0.55
1:C:443:ARG:C	1:C:445:PHE:H	2.10	0.55
1:D:26:LEU:O	1:D:34:VAL:HG13	2.06	0.54
1:C:206:ASP:HB2	1:C:244:LEU:HD23	1.89	0.54
1:D:211:MET:O	1:D:237:THR:HB	2.08	0.54
1:D:447:LEU:HD11	1:D:485:HIS:CD2	2.42	0.54
1:D:498:LYS:HB3	4:D:1084:HOH:O	2.05	0.54
1:B:208:HIS:O	1:B:211:MET:HG2	2.07	0.54
1:C:169:ARG:HH11	1:C:169:ARG:HG2	1.73	0.54
1:A:485:HIS:CD2	1:A:487:GLU:HB3	2.43	0.54
1:B:241:ILE:CG2	1:B:242:LYS:H	2.20	0.54
1:B:294:ASN:HB3	1:B:297:ASP:HB2	1.89	0.54
1:B:439:VAL:O	1:B:442:VAL:N	2.38	0.54
1:C:195:VAL:O	1:C:199:PHE:HD1	1.91	0.54
1:A:72:VAL:HG13	1:A:73:VAL:HG22	1.90	0.54
1:B:4:ARG:HH22	1:C:470:GLN:NE2	1.99	0.54
1:C:91:THR:HG22	1:C:92:ARG:N	2.21	0.54
1:C:112:PHE:HA	1:C:130:GLY:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:LYS:HB3	1:B:224:ALA:HB2	1.89	0.54
1:C:94:SER:HA	1:C:222:VAL:O	2.07	0.54
1:D:285:PHE:N	1:D:285:PHE:CD1	2.75	0.54
1:A:148:ASN:HD22	1:A:148:ASN:N	2.05	0.54
1:B:160:PHE:N	1:B:161:PRO:HD2	2.23	0.54
1:B:464:GLY:O	1:B:467:LYS:HE3	2.07	0.54
1:B:76:LYS:HD3	1:B:121:SER:O	2.07	0.54
1:B:101:HIS:O	1:B:104:LYS:HB2	2.07	0.54
1:B:221:LEU:HD23	1:B:221:LEU:N	2.23	0.54
1:C:22:LYS:HD3	1:C:23:PRO:HD2	1.90	0.54
1:C:444:THR:HG21	4:C:801:HOH:O	2.07	0.54
1:C:206:ASP:HB3	1:C:242:LYS:HG2	1.89	0.53
1:C:453:GLU:O	1:C:456:LYS:HB3	2.08	0.53
1:C:281:GLN:OE1	1:C:302:TRP:HB2	2.09	0.53
1:D:73:VAL:O	1:D:74:HIS:HB2	2.08	0.53
1:B:357:TYR:HB2	1:B:358:PRO:HD3	1.91	0.53
1:C:310:ILE:N	1:C:310:ILE:HD12	2.24	0.53
1:C:406:ASN:ND2	1:C:410:ALA:HB3	2.19	0.53
1:D:437:ASP:HA	4:D:827:HOH:O	2.07	0.53
1:A:73:VAL:O	1:A:74:HIS:HB2	2.09	0.53
1:B:138:GLU:H	1:B:138:GLU:CD	2.12	0.53
1:B:169:ARG:CG	1:B:169:ARG:NH1	2.69	0.53
1:C:446:TYR:O	1:C:455:ARG:HD3	2.08	0.53
1:C:466:LEU:HD12	1:C:469:ALA:HB3	1.91	0.53
1:C:493:GLN:HA	1:C:496:LEU:HD23	1.90	0.53
1:A:141:ASN:O	1:A:337:ASN:HB3	2.09	0.53
1:B:153:PHE:CE2	1:B:194:GLN:HG3	2.43	0.53
4:B:998:HOH:O	1:D:386:GLN:HA	2.08	0.53
1:C:88:HIS:ND1	1:C:311:PRO:HB2	2.24	0.53
1:D:439:VAL:HG23	1:D:440:THR:N	2.24	0.53
1:D:445:PHE:HA	1:D:449:VAL:HG23	1.89	0.53
1:D:471:LEU:O	1:D:475:LYS:HG3	2.09	0.53
1:A:280:ILE:HG23	1:A:312:VAL:CG2	2.37	0.53
1:B:456:LYS:HB2	1:B:491:ARG:NH2	2.23	0.53
1:D:34:VAL:HG21	1:D:37:LYS:HB2	1.89	0.53
1:A:424:PHE:CE2	1:D:48:PRO:HD3	2.43	0.53
1:B:4:ARG:HD2	1:B:8:SER:HB2	1.90	0.53
1:B:322:VAL:C	1:C:172:GLN:HG3	2.29	0.53
1:D:432:ASN:C	1:D:432:ASN:HD22	2.12	0.53
1:B:235:TYR:N	1:B:235:TYR:CD1	2.77	0.52
1:C:245:SER:OG	1:C:248:ASP:HB2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:6:PRO:HD2	1:D:266:ASN:OD1	2.09	0.52
1:C:108:ILE:HD13	1:C:315:LEU:HD22	1.91	0.52
1:C:145:VAL:CG1	1:C:353:ARG:HH22	2.22	0.52
1:B:485:HIS:CE1	1:B:487:GLU:HB3	2.44	0.52
1:B:201:ASP:O	1:B:243:ASN:ND2	2.42	0.52
1:C:440:THR:HG22	1:C:441:GLN:N	2.25	0.52
1:D:327:GLU:O	1:D:331:LEU:HG	2.09	0.52
1:A:215:GLY:O	1:A:216:SER:HB2	2.08	0.52
1:D:164:ILE:HG22	1:D:168:LYS:HD2	1.91	0.52
1:A:402:ASN:C	1:A:402:ASN:HD22	2.12	0.52
1:B:327:GLU:O	1:B:374:VAL:HG11	2.10	0.52
1:D:401:PRO:HA	4:D:995:HOH:O	2.09	0.52
1:B:64:ASP:HB3	1:C:360:THR:HB	1.91	0.52
1:B:368:ASN:O	1:B:371:GLN:HB2	2.09	0.52
1:B:100:GLU:HB2	1:B:104:LYS:NZ	2.24	0.52
1:B:110:VAL:HG11	1:B:131:PHE:HE1	1.74	0.52
1:C:49:LEU:HG	1:D:51:VAL:HG21	1.92	0.52
1:B:36:ASP:HB3	1:C:430:ARG:HD2	1.92	0.52
1:B:164:ILE:O	1:B:168:LYS:HG3	2.09	0.52
1:B:280:ILE:CD1	1:B:282:VAL:HG22	2.40	0.52
1:C:462:ILE:HG21	1:C:481:PHE:CE2	2.45	0.52
1:A:36:ASP:OD2	1:A:39:ASN:HB2	2.09	0.51
1:C:479:LYS:HG3	1:C:480:ASN:N	2.23	0.51
1:D:232:LYS:HB2	1:D:281:GLN:HG3	1.90	0.51
1:D:478:VAL:HG21	1:D:493:GLN:OE1	2.10	0.51
1:C:449:VAL:HG21	3:C:1302:NDP:O4D	2.10	0.51
1:D:12:LYS:O	1:D:16:GLU:HG3	2.10	0.51
1:C:19:ALA:O	1:C:20:ALA:HB3	2.09	0.51
1:C:239:GLN:HE22	1:C:275:SER:H	1.56	0.51
1:C:291:PHE:CG	1:C:292:PRO:HD2	2.45	0.51
1:C:463:ALA:O	1:C:467:LYS:HB3	2.10	0.51
1:A:37:LYS:NZ	1:D:158:LEU:HD22	2.24	0.51
1:A:424:PHE:CD2	1:D:48:PRO:HD3	2.46	0.51
1:B:205:PRO:HA	1:B:243:ASN:HA	1.92	0.51
1:C:73:VAL:O	1:C:74:HIS:HB2	2.09	0.51
1:A:446:TYR:OH	1:A:491:ARG:HD2	2.11	0.51
1:D:447:LEU:HD11	1:D:485:HIS:HD2	1.75	0.51
1:A:92:ARG:H	1:A:92:ARG:NH1	2.08	0.51
1:A:385:TYR:HE1	1:C:26:LEU:HD22	1.75	0.51
1:C:303:PRO:HA	3:C:1302:NDP:O2N	2.11	0.51
1:D:277:THR:HB	1:D:279:TYR:CE1	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:GLU:HG2	1:C:387:ARG:O	2.10	0.51
1:B:37:LYS:C	1:C:158:LEU:HD13	2.31	0.51
1:D:267:ALA:O	1:D:272:ASN:HB3	2.10	0.51
1:A:472:PHE:HA	1:A:475:LYS:HD3	1.93	0.51
1:B:444:THR:O	1:B:448:LYS:HB3	2.10	0.51
1:C:394:MET:HE3	1:C:394:MET:HA	1.93	0.51
1:A:276:TRP:HB2	1:A:315:LEU:HD12	1.92	0.51
1:B:331:LEU:HD13	1:B:333:PHE:CZ	2.46	0.51
1:B:495:LEU:CD2	1:B:495:LEU:N	2.74	0.51
1:C:34:VAL:HG21	1:C:37:LYS:HB2	1.92	0.51
1:A:88:HIS:CD2	1:A:311:PRO:HG2	2.46	0.50
1:A:139:ASP:O	1:C:32:ASN:HA	2.11	0.50
1:A:213:GLY:HA3	1:A:235:TYR:CE2	2.46	0.50
1:A:411:PRO:HA	1:C:24:ASP:O	2.10	0.50
1:B:198:LEU:O	1:B:203:GLY:HA3	2.10	0.50
1:D:188:ARG:HB3	1:D:190:GLU:OE1	2.11	0.50
1:D:202:ARG:HB3	4:D:1019:HOH:O	2.11	0.50
1:B:221:LEU:HD21	1:B:231:CYS:SG	2.51	0.50
1:C:449:VAL:O	1:C:449:VAL:HG12	2.11	0.50
1:D:74:HIS:O	1:D:111:ARG:NH2	2.44	0.50
1:D:443:ARG:NE	1:D:484:VAL:O	2.44	0.50
1:B:11:MET:HB3	1:D:408:PHE:CE2	2.47	0.50
1:D:213:GLY:HA3	1:D:235:TYR:CE2	2.46	0.50
1:B:248:ASP:O	1:B:251:ARG:HB3	2.11	0.50
1:B:450:LEU:HD22	1:B:454:GLN:HG3	1.92	0.50
4:B:787:HOH:O	1:C:45:PRO:HD3	2.12	0.50
1:C:225:ASP:HB2	4:C:895:HOH:O	2.10	0.50
1:C:61:ALA:O	1:C:65:ARG:HG3	2.11	0.50
1:C:124:THR:O	1:C:249:ALA:HB1	2.12	0.50
1:D:296:PHE:CE1	1:D:346:PRO:HD2	2.45	0.50
1:B:155:ARG:HD2	4:B:1005:HOH:O	2.12	0.50
1:C:487:GLU:HA	1:C:490:SER:HB3	1.94	0.50
1:D:60:MET:CE	1:D:63:PHE:HD2	2.24	0.50
1:D:282:VAL:HG12	1:D:283:MET:N	2.26	0.50
1:A:445:PHE:HA	1:A:449:VAL:CG2	2.42	0.50
1:B:386:GLN:C	1:B:387:ARG:HG2	2.32	0.50
1:B:430:ARG:NH2	1:C:53:ASP:OD2	2.44	0.50
1:D:153:PHE:HE2	1:D:185:TRP:CZ2	2.30	0.50
1:D:284:THR:HG23	1:D:287:GLU:CD	2.32	0.50
1:B:301:VAL:CG2	1:B:441:GLN:HE22	2.25	0.50
1:B:466:LEU:HD21	1:B:474:GLN:HA	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:367:PRO:CG	1:D:390:PRO:HG2	2.42	0.50
1:C:177:ASP:OD1	1:C:179:ASP:HB2	2.12	0.49
1:A:182:TRP:O	1:A:186:SER:HB3	2.12	0.49
1:C:451:ASN:H	1:C:454:GLN:NE2	2.09	0.49
1:D:441:GLN:HA	1:D:444:THR:CG2	2.42	0.49
1:B:207:GLY:HA3	4:B:763:HOH:O	2.11	0.49
1:B:301:VAL:HG22	1:B:441:GLN:HE22	1.77	0.49
1:C:287:GLU:O	1:C:290:ILE:HG12	2.12	0.49
1:C:466:LEU:CD1	1:C:469:ALA:HB3	2.42	0.49
1:D:205:PRO:HA	1:D:243:ASN:HA	1.94	0.49
1:D:279:TYR:C	1:D:280:ILE:HG22	2.32	0.49
1:D:440:THR:O	1:D:444:THR:HG22	2.11	0.49
1:B:442:VAL:O	1:B:445:PHE:HB3	2.13	0.49
1:C:26:LEU:HD12	1:C:27:THR:N	2.28	0.49
1:C:334:ASP:OD1	1:C:361:HIS:ND1	2.45	0.49
1:A:87:THR:HG23	1:A:313:GLY:HA2	1.95	0.49
1:A:357:TYR:HB2	1:A:358:PRO:HD3	1.95	0.49
1:D:106:THR:O	1:D:108:ILE:HG23	2.12	0.49
1:A:108:ILE:HA	1:A:134:LYS:O	2.12	0.49
1:A:120:GLY:H	1:D:120:GLY:H	1.60	0.49
1:B:148:ASN:CB	1:B:211:MET:HE2	2.42	0.49
1:B:169:ARG:HG2	1:B:169:ARG:NH1	2.09	0.49
1:D:112:PHE:HA	1:D:130:GLY:O	2.13	0.49
1:B:40:SER:O	1:C:430:ARG:HA	2.12	0.49
1:B:41:LEU:CB	1:B:53:ASP:HB2	2.43	0.49
1:B:51:VAL:HG23	1:B:52:GLN:N	2.27	0.49
1:B:492:ILE:HG22	1:B:493:GLN:N	2.28	0.49
1:B:97:LYS:HD2	1:B:138:GLU:HB2	1.95	0.49
1:B:128:PRO:O	1:B:129:ARG:HD2	2.12	0.49
1:C:88:HIS:CE1	1:C:311:PRO:HB2	2.47	0.49
1:C:155:ARG:HD2	1:C:433:SER:HB2	1.94	0.49
1:B:275:SER:HA	1:B:315:LEU:O	2.13	0.49
1:B:391:MET:HE2	1:D:365:LEU:C	2.32	0.49
1:B:406:ASN:ND2	1:B:410:ALA:HB3	2.20	0.49
1:C:223:ASN:HD21	1:C:227:GLU:CB	2.26	0.49
1:C:293:PHE:CD1	1:C:293:PHE:N	2.72	0.49
1:C:423:HIS:HA	1:D:427:ASP:HA	1.94	0.49
1:D:357:TYR:O	1:D:360:THR:HG22	2.13	0.49
1:D:439:VAL:HG23	1:D:440:THR:H	1.78	0.49
1:D:442:VAL:O	1:D:445:PHE:HB3	2.13	0.49
1:D:442:VAL:CG1	1:D:484:VAL:HG11	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:86:VAL:HG23	1:D:104:LYS:O	2.12	0.48
1:A:54:VAL:HG11	1:C:336:SER:HB2	1.95	0.48
1:B:11:MET:HE1	1:C:180:MET:HG2	1.95	0.48
1:B:241:ILE:CG2	1:B:242:LYS:N	2.76	0.48
1:B:328:VAL:O	1:B:331:LEU:HB2	2.12	0.48
1:B:367:PRO:HG2	1:B:390:PRO:CG	2.43	0.48
1:B:456:LYS:HB2	1:B:491:ARG:HH22	1.78	0.48
1:C:126:ARG:CZ	1:C:126:ARG:HB2	2.42	0.48
1:C:208:HIS:HA	1:C:211:MET:HE1	1.95	0.48
1:D:471:LEU:O	1:D:474:GLN:HB2	2.13	0.48
1:C:197:PHE:HD1	1:C:197:PHE:O	1.95	0.48
1:B:127:ASP:O	1:B:129:ARG:NH1	2.45	0.48
1:C:402:ASN:N	1:C:402:ASN:ND2	2.55	0.48
1:D:85:GLU:O	1:D:313:GLY:HA3	2.13	0.48
1:B:440:THR:O	1:B:444:THR:HG23	2.14	0.48
1:D:244:LEU:HD23	1:D:245:SER:N	2.29	0.48
1:B:402:ASN:C	1:B:402:ASN:ND2	2.66	0.48
1:B:439:VAL:O	1:B:442:VAL:HG23	2.14	0.48
1:A:37:LYS:O	1:D:158:LEU:HD22	2.13	0.48
1:B:17:GLN:HG2	4:B:1026:HOH:O	2.14	0.48
1:B:201:ASP:HB3	1:B:243:ASN:HD22	1.79	0.48
1:B:205:PRO:HB3	4:B:1001:HOH:O	2.13	0.48
1:B:452:GLU:HB2	1:B:455:ARG:NH2	2.28	0.48
1:B:463:ALA:O	1:B:467:LYS:HG2	2.14	0.48
1:C:476:LYS:HB3	1:C:476:LYS:HZ2	1.78	0.48
1:D:338:MET:HE2	1:D:342:ILE:C	2.33	0.48
1:D:397:GLN:HE21	1:D:397:GLN:HB2	1.54	0.48
1:D:491:ARG:O	1:D:495:LEU:HD12	2.14	0.48
1:A:18:ARG:HG2	1:A:18:ARG:HH11	1.77	0.48
1:A:97:LYS:HG2	1:A:100:GLU:OE1	2.13	0.48
1:A:324:TYR:CE1	1:A:328:VAL:HG11	2.49	0.48
1:A:419:GLU:CD	1:A:419:GLU:H	2.17	0.48
1:B:100:GLU:CB	1:B:104:LYS:HG3	2.38	0.48
1:B:326:ALA:O	1:B:374:VAL:HG21	2.12	0.48
1:D:86:VAL:HB	1:D:102:ILE:HA	1.95	0.48
1:B:206:ASP:HB2	1:B:244:LEU:HG	1.95	0.48
1:D:81:PHE:HZ	1:D:327:GLU:HB3	1.79	0.48
1:D:387:ARG:HG2	1:D:387:ARG:NH1	2.27	0.48
1:B:319:ARG:HD2	1:B:319:ARG:O	2.14	0.48
1:C:310:ILE:HD12	1:C:310:ILE:H	1.79	0.48
1:A:248:ASP:O	1:A:251:ARG:N	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:396:ASN:HB3	1:D:323:ASN:ND2	2.28	0.47
1:B:472:PHE:CE2	1:B:473:ILE:HG13	2.49	0.47
1:C:94:SER:OG	1:C:221:LEU:HD22	2.14	0.47
1:C:345:SER:O	1:C:347:ASP:N	2.47	0.47
1:D:154:ILE:HG13	1:D:349:MET:HE2	1.95	0.47
1:D:235:TYR:N	1:D:235:TYR:CD1	2.81	0.47
1:D:291:PHE:CE1	1:D:293:PHE:HB2	2.49	0.47
1:C:202:ARG:HA	1:C:243:ASN:ND2	2.28	0.47
1:A:464:GLY:O	1:A:467:LYS:HD3	2.14	0.47
1:B:125:VAL:HG22	1:B:126:ARG:N	2.28	0.47
1:B:297:ASP:HB3	1:B:300:LYS:HG3	1.95	0.47
1:C:126:ARG:O	1:C:126:ARG:HG3	2.13	0.47
1:C:439:VAL:HG12	1:C:484:VAL:HA	1.95	0.47
1:C:480:ASN:O	1:C:484:VAL:HG23	2.15	0.47
1:D:298:LEU:HD23	1:D:349:MET:HG3	1.96	0.47
1:A:42:THR:O	1:D:431:PHE:HE1	1.97	0.47
1:A:402:ASN:C	1:A:402:ASN:ND2	2.68	0.47
1:B:176:LYS:HG2	4:B:800:HOH:O	2.13	0.47
1:D:212:ASP:OD1	1:D:237:THR:HG22	2.14	0.47
1:D:265:PHE:CD1	1:D:320:ASN:ND2	2.83	0.47
1:B:229:VAL:CG2	1:B:284:THR:HA	2.43	0.47
1:B:351:GLN:O	1:B:354:LEU:HB2	2.14	0.47
1:A:60:MET:HB3	1:D:355:PHE:HE2	1.79	0.47
1:A:357:TYR:O	1:A:360:THR:HG22	2.14	0.47
1:B:135:PHE:HB2	1:B:142:TRP:HB3	1.95	0.47
1:C:444:THR:HG22	1:C:444:THR:O	2.14	0.47
1:D:19:ALA:N	4:D:841:HOH:O	2.47	0.47
1:D:65:ARG:HH11	1:D:65:ARG:HG3	1.79	0.47
1:D:74:HIS:CE1	1:D:115:VAL:HG22	2.49	0.47
1:D:279:TYR:O	1:D:280:ILE:HG22	2.14	0.47
1:A:147:ASN:CG	2:A:507:HEM:HAC	2.34	0.47
1:B:264:LEU:HD12	1:B:264:LEU:C	2.34	0.47
1:B:270:THR:O	1:B:272:ASN:N	2.48	0.47
1:C:151:ILE:CD1	1:C:194:GLN:HG2	2.41	0.47
1:A:271:GLY:HA2	1:A:273:TYR:CE1	2.50	0.47
1:A:277:THR:OG1	1:A:314:LYS:NZ	2.48	0.47
1:B:46:ARG:HD2	4:B:1056:HOH:O	2.15	0.47
1:B:235:TYR:HA	1:B:277:THR:O	2.15	0.47
1:D:500:ASN:C	1:D:501:GLU:HG3	2.34	0.47
1:A:177:ASP:HB3	1:A:180:MET:HB2	1.97	0.47
1:D:443:ARG:HG3	1:D:484:VAL:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:PHE:CE2	1:D:173:THR:HG22	2.50	0.47
1:A:467:LYS:HG2	1:A:468:ASP:N	2.30	0.47
1:B:71:ARG:HG3	1:B:71:ARG:HH11	1.80	0.47
1:B:95:LYS:HG3	1:B:222:VAL:O	2.15	0.47
1:D:148:ASN:C	1:D:148:ASN:ND2	2.68	0.47
1:D:214:TYR:N	1:D:214:TYR:CD1	2.83	0.47
1:D:245:SER:HB3	1:D:248:ASP:OD2	2.15	0.47
1:A:381:ARG:HG2	1:A:381:ARG:HH11	1.80	0.46
1:B:5:ASP:HB2	1:B:6:PRO:HD2	1.96	0.46
1:B:485:HIS:CE1	1:B:487:GLU:HG2	2.50	0.46
1:A:50:LEU:HD12	1:B:48:PRO:HB2	1.98	0.46
1:B:145:VAL:HG22	1:B:333:PHE:HB3	1.97	0.46
1:C:349:MET:HE3	2:C:507:HEM:HBB1	1.98	0.46
1:D:154:ILE:HG13	1:D:349:MET:HE1	1.96	0.46
1:D:210:HIS:HB3	1:D:242:LYS:H	1.81	0.46
1:A:155:ARG:NH2	1:A:438:ASN:OD1	2.49	0.46
1:B:19:ALA:HB3	1:B:21:GLN:HG3	1.97	0.46
1:B:268:ILE:HB	1:B:320:ASN:HD21	1.80	0.46
1:C:219:PHE:O	1:C:230:TYR:HA	2.15	0.46
1:C:367:PRO:HG2	1:C:390:PRO:CG	2.46	0.46
1:C:446:TYR:OH	1:C:488:TYR:HA	2.15	0.46
1:D:142:TRP:HA	1:D:337:ASN:O	2.14	0.46
1:D:476:LYS:O	1:D:480:ASN:OD1	2.34	0.46
1:B:155:ARG:NH2	1:B:438:ASN:OD1	2.46	0.46
1:A:51:VAL:HG11	1:B:49:LEU:HD13	1.98	0.46
1:B:254:HIS:ND1	1:C:254:HIS:ND1	2.64	0.46
1:B:359:ASP:O	1:B:362:ARG:HB2	2.16	0.46
1:C:156:ASP:OD1	1:C:158:LEU:HB2	2.15	0.46
1:C:283:MET:HE2	1:C:291:PHE:CD1	2.51	0.46
1:B:280:ILE:O	1:B:280:ILE:HG13	2.15	0.46
1:B:419:GLU:CD	1:B:419:GLU:H	2.19	0.46
1:C:244:LEU:HD11	1:C:252:LEU:HD12	1.98	0.46
1:C:250:ALA:O	1:C:253:ALA:HB3	2.16	0.46
1:C:428:VAL:O	1:C:429:GLN:HB3	2.15	0.46
1:C:459:CYS:SG	1:C:492:ILE:HD13	2.54	0.46
1:D:71:ARG:HG3	4:D:1078:HOH:O	2.15	0.46
1:D:118:GLU:OE1	1:D:118:GLU:N	2.44	0.46
1:D:209:ARG:HB2	4:D:1020:HOH:O	2.15	0.46
1:B:33:PRO:HD2	1:D:340:PRO:HD3	1.98	0.46
1:C:239:GLN:CD	1:C:239:GLN:H	2.19	0.46
1:C:446:TYR:O	1:C:447:LEU:HD23	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:369:TYR:O	1:D:372:ILE:HG13	2.16	0.46
1:D:455:ARG:HD2	1:D:491:ARG:NH1	2.29	0.46
1:A:42:THR:HG22	1:A:48:PRO:O	2.16	0.46
1:B:35:GLY:O	1:D:413:HIS:HB3	2.16	0.46
1:B:209:ARG:HG2	1:B:274:PRO:CG	2.46	0.46
1:D:189:PRO:C	1:D:191:SER:H	2.19	0.46
1:D:284:THR:O	1:D:288:ALA:N	2.48	0.46
1:D:492:ILE:HA	1:D:495:LEU:HD12	1.98	0.46
1:B:393:MET:HB3	1:B:394:MET:H	1.55	0.46
1:D:96:ALA:HB3	1:D:99:PHE:CD2	2.51	0.46
1:D:217:HIS:HE1	1:D:298:LEU:HD22	1.81	0.46
1:B:202:ARG:HG2	1:B:202:ARG:HH11	1.80	0.45
1:C:92:ARG:HH11	1:C:92:ARG:CG	2.27	0.45
1:C:212:ASP:OD1	1:C:237:THR:HG22	2.16	0.45
1:C:459:CYS:SG	1:C:492:ILE:CD1	3.04	0.45
1:D:153:PHE:CE2	1:D:185:TRP:CZ2	3.05	0.45
1:B:16:GLU:C	1:B:18:ARG:H	2.19	0.45
1:B:73:VAL:HG11	1:B:164:ILE:HD12	1.98	0.45
1:B:281:GLN:HB2	1:B:302:TRP:CE3	2.51	0.45
1:C:82:GLY:HA3	1:C:316:VAL:O	2.16	0.45
1:D:202:ARG:HH11	1:D:241:ILE:HG21	1.78	0.45
1:B:381:ARG:CG	1:B:381:ARG:HH11	2.29	0.45
1:C:90:ILE:O	1:C:93:TYR:HB2	2.16	0.45
1:D:334:ASP:OD1	1:D:361:HIS:ND1	2.49	0.45
1:D:410:ALA:HB1	1:D:411:PRO:HD2	1.98	0.45
1:A:304:HIS:HB2	3:A:1102:NDP:O2A	2.17	0.45
1:B:273:TYR:HA	1:B:274:PRO:HD3	1.78	0.45
1:B:316:VAL:HG12	1:B:318:ASN:ND2	2.31	0.45
1:D:3:ASN:HB2	1:D:4:ARG:H	1.62	0.45
1:A:4:ARG:HD3	1:A:9:ASP:OD1	2.16	0.45
1:B:67:ARG:HB2	4:B:753:HOH:O	2.15	0.45
1:B:452:GLU:OE2	1:B:491:ARG:NH2	2.50	0.45
1:C:220:LYS:HA	1:C:229:VAL:O	2.17	0.45
1:C:446:TYR:HE2	1:C:485:HIS:ND1	2.15	0.45
1:D:475:LYS:HG3	1:D:475:LYS:H	1.53	0.45
1:B:16:GLU:O	1:B:18:ARG:N	2.49	0.45
1:B:223:ASN:HD21	1:B:227:GLU:CD	2.20	0.45
1:C:251:ARG:HG3	1:C:252:LEU:H	1.80	0.45
1:A:280:ILE:O	1:A:280:ILE:HG13	2.14	0.45
1:B:287:GLU:O	1:B:290:ILE:N	2.44	0.45
1:B:451:ASN:OD1	1:B:451:ASN:O	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:480:ASN:O	1:C:483:ASP:HB2	2.16	0.45
1:D:98:VAL:HG13	1:D:99:PHE:CD1	2.52	0.45
1:D:343:GLU:HB3	1:D:344:PRO:HD2	1.99	0.45
1:A:39:ASN:OD1	1:D:432:ASN:HA	2.17	0.45
1:A:329:GLU:HA	1:A:329:GLU:OE1	2.16	0.45
1:B:110:VAL:HG11	1:B:131:PHE:CE1	2.52	0.45
1:C:179:ASP:O	1:C:183:ASP:HB2	2.17	0.45
1:C:280:ILE:HG13	1:C:280:ILE:O	2.17	0.45
1:D:63:PHE:HA	1:D:66:GLU:HG3	1.98	0.45
1:D:71:ARG:HG3	1:D:71:ARG:HH11	1.82	0.45
1:D:228:ALA:HB2	1:D:420:HIS:CE1	2.52	0.45
1:D:271:GLY:HA2	1:D:273:TYR:CE1	2.52	0.45
1:A:156:ASP:OD1	1:A:158:LEU:HB2	2.17	0.45
1:A:24:ASP:OD1	1:A:24:ASP:N	2.50	0.45
1:A:470:GLN:HG3	1:D:4:ARG:NH2	2.32	0.45
1:B:38:LEU:HG	1:D:413:HIS:HE1	1.81	0.45
1:B:90:ILE:O	1:B:93:TYR:HB2	2.17	0.45
1:B:92:ARG:H	1:B:92:ARG:HG3	1.43	0.45
1:B:155:ARG:NH1	1:B:299:THR:OG1	2.50	0.45
1:B:280:ILE:HD12	1:B:282:VAL:HG22	1.99	0.45
1:B:345:SER:C	1:B:347:ASP:H	2.19	0.45
1:C:126:ARG:HA	1:C:204:ILE:HG12	1.98	0.45
1:C:148:ASN:HA	1:C:212:ASP:O	2.16	0.45
1:D:331:LEU:HD23	1:D:331:LEU:HA	1.81	0.45
1:A:498:LYS:O	1:A:501:GLU:N	2.49	0.44
1:A:499:TYR:C	1:A:501:GLU:H	2.21	0.44
1:B:364:ARG:HD3	4:B:961:HOH:O	2.17	0.44
1:C:73:VAL:HB	1:C:74:HIS:HD2	1.81	0.44
1:D:291:PHE:CD1	1:D:292:PRO:HD2	2.52	0.44
1:B:166:SER:HA	1:B:180:MET:HE3	1.99	0.44
1:B:298:LEU:HD23	1:B:349:MET:HE2	1.99	0.44
1:C:14:TRP:O	1:C:18:ARG:HB2	2.17	0.44
1:C:52:GLN:HE21	1:C:52:GLN:HB3	1.52	0.44
1:A:422:THR:O	1:B:428:VAL:HG22	2.16	0.44
1:B:218:THR:O	1:B:345:SER:HB3	2.18	0.44
1:B:278:LEU:O	1:B:312:VAL:HG13	2.17	0.44
1:B:283:MET:SD	1:B:288:ALA:HA	2.58	0.44
1:D:206:ASP:HB3	1:D:242:LYS:HG2	1.99	0.44
1:A:273:TYR:HA	1:A:274:PRO:HD3	1.86	0.44
1:A:273:TYR:HB3	1:A:317:LEU:O	2.17	0.44
1:A:428:VAL:HG23	1:B:424:PHE:HD1	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:445:PHE:HB2	3:A:1102:NDP:O2D	2.17	0.44
1:B:477:ALA:O	1:B:481:PHE:CD2	2.70	0.44
1:C:73:VAL:HG11	1:C:164:ILE:HD12	2.00	0.44
1:C:154:ILE:H	1:C:154:ILE:HG12	1.68	0.44
1:C:155:ARG:NH2	1:C:190:GLU:HB3	2.32	0.44
1:C:446:TYR:CE2	1:C:485:HIS:ND1	2.86	0.44
1:C:481:PHE:N	1:C:481:PHE:HD1	2.16	0.44
1:A:76:LYS:HD3	1:A:121:SER:O	2.17	0.44
1:A:278:LEU:HD23	1:A:312:VAL:HB	1.99	0.44
1:A:291:PHE:HD2	1:A:293:PHE:O	2.00	0.44
1:B:202:ARG:HD3	3:B:1202:NDP:C6A	2.48	0.44
1:C:481:PHE:N	1:C:481:PHE:CD1	2.85	0.44
1:D:5:ASP:N	1:D:5:ASP:OD1	2.50	0.44
1:D:90:ILE:HD11	1:D:99:PHE:CG	2.52	0.44
1:A:235:TYR:CD1	1:A:235:TYR:N	2.85	0.44
1:A:322:VAL:O	1:D:172:GLN:HB2	2.17	0.44
1:B:237:THR:OG1	1:B:239:GLN:NE2	2.51	0.44
1:B:252:LEU:HD23	1:B:259:TYR:CD2	2.53	0.44
1:C:17:GLN:HE21	1:C:17:GLN:HB3	1.61	0.44
1:D:150:PRO:HB3	1:D:214:TYR:HD2	1.80	0.44
1:D:284:THR:O	1:D:288:ALA:HB2	2.18	0.44
1:A:37:LYS:HZ2	1:D:158:LEU:HD22	1.82	0.44
1:B:16:GLU:O	1:B:19:ALA:N	2.46	0.44
1:B:36:ASP:OD1	1:B:36:ASP:C	2.56	0.44
1:B:162:SER:O	1:B:165:HIS:HB2	2.18	0.44
1:B:245:SER:O	1:B:248:ASP:N	2.51	0.44
1:B:283:MET:CE	1:B:295:PRO:HB3	2.48	0.44
1:C:143:ASP:HB2	1:C:334:ASP:O	2.18	0.44
1:D:281:GLN:HG2	1:D:309:LEU:HD12	2.00	0.44
1:A:216:SER:HB3	1:A:298:LEU:HD11	1.99	0.44
1:B:69:PRO:HD3	1:C:69:PRO:HG3	2.00	0.44
1:B:251:ARG:NH1	1:B:251:ARG:HG2	2.33	0.44
1:D:220:LYS:HB3	1:D:343:GLU:HB2	2.00	0.44
1:A:221:LEU:O	1:A:228:ALA:HA	2.17	0.44
1:B:245:SER:O	1:B:246:VAL:C	2.55	0.44
1:C:110:VAL:HG11	1:C:131:PHE:CE1	2.53	0.44
1:C:110:VAL:HG11	1:C:131:PHE:HE1	1.83	0.44
1:C:168:LYS:HB3	1:C:169:ARG:H	1.71	0.44
1:D:228:ALA:HB1	1:D:285:PHE:HZ	1.82	0.44
1:B:18:ARG:HH11	1:B:18:ARG:CG	2.30	0.43
1:B:55:VAL:CG2	1:C:430:ARG:NH2	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:470:GLN:CB	1:C:473:ILE:HD12	2.48	0.43
1:A:155:ARG:NH1	1:A:297:ASP:OD2	2.51	0.43
1:B:382:VAL:O	1:B:382:VAL:CG1	2.66	0.43
1:B:467:LYS:HD3	1:B:499:TYR:CD1	2.54	0.43
1:C:419:GLU:CD	1:C:419:GLU:H	2.22	0.43
1:D:151:ILE:HD13	1:D:193:HIS:CD2	2.53	0.43
1:D:291:PHE:HE1	1:D:293:PHE:HB2	1.83	0.43
1:A:74:HIS:HA	1:A:114:THR:O	2.18	0.43
1:A:343:GLU:HB3	1:A:344:PRO:CD	2.48	0.43
1:B:26:LEU:HD22	1:D:385:TYR:HE1	1.83	0.43
1:B:37:LYS:O	1:C:158:LEU:HB3	2.19	0.43
1:C:154:ILE:CD1	1:C:160:PHE:HA	2.48	0.43
1:D:301:VAL:O	1:D:303:PRO:HD3	2.18	0.43
1:D:391:MET:C	1:D:393:MET:HE2	2.38	0.43
1:D:442:VAL:HB	1:D:484:VAL:HG13	2.00	0.43
1:A:436:ASP:O	1:A:437:ASP:O	2.36	0.43
1:B:142:TRP:HA	1:B:337:ASN:O	2.19	0.43
1:A:343:GLU:HB3	1:A:344:PRO:HD2	2.00	0.43
1:A:496:LEU:O	1:A:497:ASP:C	2.57	0.43
1:C:337:ASN:HD22	1:C:337:ASN:HA	1.70	0.43
1:B:218:THR:OG1	1:B:232:LYS:HE3	2.19	0.43
1:B:358:PRO:HD3	4:B:965:HOH:O	2.19	0.43
1:C:15:LYS:O	1:C:15:LYS:HG2	2.19	0.43
1:C:232:LYS:O	1:C:280:ILE:HA	2.18	0.43
1:D:85:GLU:OE2	1:D:105:ARG:NH1	2.52	0.43
1:A:50:LEU:C	1:A:52:GLN:N	2.71	0.43
1:A:451:ASN:OD1	1:A:451:ASN:C	2.57	0.43
1:B:220:LYS:HB3	1:B:343:GLU:HB2	2.01	0.43
1:C:43:VAL:O	1:C:47:GLY:HA3	2.18	0.43
1:C:291:PHE:HD2	1:C:293:PHE:O	2.01	0.43
1:D:210:HIS:CG	1:D:242:LYS:HB3	2.54	0.43
1:D:381:ARG:HH11	1:D:381:ARG:HG2	1.84	0.43
1:B:414:GLN:O	1:D:35:GLY:HA2	2.18	0.43
1:C:169:ARG:HG2	1:C:169:ARG:NH1	2.33	0.43
1:C:426:GLY:O	1:C:427:ASP:O	2.37	0.43
1:C:445:PHE:HD1	1:C:449:VAL:HB	1.83	0.43
1:A:100:GLU:HB3	1:A:104:LYS:HE3	2.01	0.43
1:A:445:PHE:HA	1:A:449:VAL:HG23	2.01	0.43
1:B:11:MET:HE3	1:B:11:MET:HB2	1.92	0.43
1:B:51:VAL:CG2	1:B:52:GLN:N	2.82	0.43
1:B:193:HIS:HB2	4:B:941:HOH:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:236:LYS:H	1:B:236:LYS:HG2	1.45	0.43
1:C:466:LEU:HD12	1:C:466:LEU:C	2.38	0.43
1:C:496:LEU:O	1:C:500:ASN:OD1	2.37	0.43
1:C:282:VAL:HG12	1:C:283:MET:N	2.33	0.43
1:D:241:ILE:O	1:D:241:ILE:HG22	2.19	0.43
1:B:26:LEU:O	1:B:34:VAL:HG23	2.19	0.42
1:B:212:ASP:OD1	1:B:236:LYS:HA	2.19	0.42
1:B:437:ASP:HA	4:B:1007:HOH:O	2.18	0.42
1:D:170:ASN:HD22	1:D:172:GLN:N	2.16	0.42
1:A:279:TYR:HA	1:A:310:ILE:O	2.20	0.42
1:B:386:GLN:O	1:B:387:ARG:HG2	2.19	0.42
1:B:466:LEU:HD23	1:B:474:GLN:HG2	2.01	0.42
1:C:202:ARG:O	1:C:204:ILE:N	2.53	0.42
1:C:239:GLN:CD	1:C:239:GLN:N	2.73	0.42
1:A:235:TYR:HA	1:A:277:THR:O	2.20	0.42
1:A:281:GLN:HG3	1:A:309:LEU:HD13	2.02	0.42
1:A:501:GLU:OE1	1:A:501:GLU:HA	2.19	0.42
1:C:191:SER:C	1:C:195:VAL:HG23	2.39	0.42
1:D:189:PRO:C	1:D:191:SER:N	2.71	0.42
1:A:160:PHE:CD1	2:A:507:HEM:HAB	2.55	0.42
1:A:391:MET:HE2	1:C:368:ASN:HB2	2.01	0.42
1:C:22:LYS:CD	1:C:23:PRO:HD2	2.50	0.42
1:D:60:MET:CE	1:D:63:PHE:CD2	3.01	0.42
1:D:220:LYS:HZ3	1:D:420:HIS:HD2	1.67	0.42
1:A:18:ARG:H	1:A:18:ARG:HG3	1.58	0.42
1:A:169:ARG:HD2	1:A:174:HIS:CE1	2.55	0.42
1:B:262:ARG:HB3	1:C:175:LEU:HD11	2.00	0.42
1:C:108:ILE:HA	1:C:134:LYS:O	2.20	0.42
1:C:286:SER:O	1:C:289:GLU:N	2.53	0.42
1:C:433:SER:C	1:C:435:ASN:H	2.22	0.42
1:D:220:LYS:HB2	1:D:344:PRO:O	2.20	0.42
1:A:139:ASP:HB3	1:A:340:PRO:HD2	2.02	0.42
1:A:209:ARG:CG	1:A:274:PRO:HB3	2.46	0.42
1:A:430:ARG:HA	1:D:40:SER:O	2.19	0.42
1:B:74:HIS:O	1:B:111:ARG:NH2	2.53	0.42
1:B:95:LYS:HG3	1:B:95:LYS:H	1.50	0.42
1:D:279:TYR:C	1:D:280:ILE:CG2	2.87	0.42
1:D:442:VAL:HB	1:D:484:VAL:CG1	2.49	0.42
1:D:415:PRO:HA	1:D:418:LEU:CD1	2.50	0.42
1:A:393:MET:O	1:A:394:MET:HB2	2.19	0.42
1:B:169:ARG:HD3	1:B:174:HIS:CE1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:347:ASP:HB3	1:B:350:LEU:HB3	2.01	0.42
1:B:355:PHE:CD2	1:B:356:ALA:N	2.88	0.42
1:C:290:ILE:O	1:C:291:PHE:C	2.57	0.42
1:D:76:LYS:O	1:D:113:SER:CB	2.67	0.42
1:D:95:LYS:O	1:D:96:ALA:C	2.58	0.42
1:D:217:HIS:HD1	1:D:347:ASP:CG	2.22	0.42
1:C:43:VAL:CG1	1:C:48:PRO:HD2	2.50	0.42
1:C:472:PHE:HA	1:C:475:LYS:HG3	2.02	0.42
1:D:20:ALA:O	1:D:21:GLN:C	2.58	0.42
1:B:122:ALA:CB	1:B:257:PRO:HB3	2.44	0.41
1:B:279:TYR:HA	1:B:310:ILE:O	2.20	0.41
1:B:414:GLN:HG2	1:B:416:SER:OG	2.20	0.41
1:A:406:ASN:HD21	1:A:410:ALA:HB3	1.85	0.41
1:B:126:ARG:HA	1:B:204:ILE:HG12	2.02	0.41
1:B:231:CYS:HA	1:B:281:GLN:O	2.20	0.41
1:B:268:ILE:HB	1:B:320:ASN:ND2	2.35	0.41
1:C:180:MET:HB3	1:D:403:TYR:CE1	2.55	0.41
1:A:72:VAL:CG1	2:A:507:HEM:HMA1	2.50	0.41
1:A:223:ASN:OD1	1:A:223:ASN:C	2.59	0.41
1:A:296:PHE:CD1	1:A:346:PRO:HD2	2.55	0.41
1:B:26:LEU:HD13	1:D:384:ASN:HA	2.00	0.41
1:D:221:LEU:HD21	1:D:231:CYS:SG	2.60	0.41
1:D:391:MET:O	1:D:393:MET:HE2	2.19	0.41
1:A:350:LEU:O	1:A:353:ARG:HB2	2.21	0.41
1:A:374:VAL:HB	4:A:929:HOH:O	2.20	0.41
1:D:104:LYS:NZ	1:D:138:GLU:OE1	2.54	0.41
1:A:20:ALA:O	1:A:21:GLN:C	2.59	0.41
1:B:94:SER:HB3	1:B:221:LEU:HD13	2.02	0.41
1:B:158:LEU:O	1:C:37:LYS:NZ	2.54	0.41
1:B:304:HIS:HB2	3:B:1202:NDP:O2A	2.21	0.41
1:C:71:ARG:HG3	1:C:71:ARG:HH11	1.86	0.41
1:C:87:THR:OG1	1:C:313:GLY:HA2	2.19	0.41
1:C:284:THR:HG23	1:C:287:GLU:OE2	2.20	0.41
1:D:170:ASN:ND2	1:D:172:GLN:N	2.58	0.41
1:D:296:PHE:CD1	1:D:346:PRO:HD2	2.55	0.41
1:A:173:THR:O	1:A:174:HIS:HB3	2.20	0.41
1:B:16:GLU:C	1:B:18:ARG:N	2.73	0.41
1:B:223:ASN:C	1:B:225:ASP:N	2.74	0.41
1:C:83:TYR:CD1	1:C:83:TYR:C	2.94	0.41
1:C:90:ILE:O	1:C:91:THR:C	2.59	0.41
1:D:148:ASN:C	1:D:148:ASN:HD22	2.23	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:189:PRO:O	1:D:192:LEU:HG	2.21	0.41
1:A:26:LEU:CD1	1:C:384:ASN:HA	2.50	0.41
1:B:393:MET:HG3	1:D:373:PRO:HD3	2.03	0.41
1:B:430:ARG:NH2	1:C:53:ASP:CG	2.73	0.41
1:C:72:VAL:HG12	2:C:507:HEM:HAA2	2.03	0.41
1:C:126:ARG:HD3	1:C:198:LEU:HG	2.02	0.41
1:C:496:LEU:O	1:C:498:LYS:N	2.53	0.41
1:A:423:HIS:HA	1:B:427:ASP:HA	2.03	0.41
1:A:444:THR:HG21	4:A:972:HOH:O	2.21	0.41
1:B:221:LEU:O	1:B:228:ALA:HA	2.21	0.41
1:B:439:VAL:HG12	1:B:484:VAL:HG22	2.02	0.41
1:C:63:PHE:CD1	1:C:63:PHE:C	2.94	0.41
1:C:460:GLU:HG2	1:C:495:LEU:HD21	2.03	0.41
1:A:14:TRP:O	1:A:17:GLN:HB3	2.21	0.41
1:A:39:ASN:C	1:D:158:LEU:HD12	2.40	0.41
1:A:237:THR:HA	1:A:276:TRP:CD1	2.56	0.41
1:A:404:TYR:CD1	1:A:405:PRO:HA	2.56	0.41
1:B:107:PRO:HD2	1:B:379:ARG:HE	1.85	0.41
1:B:188:ARG:HA	1:B:189:PRO:HD2	1.91	0.41
1:B:290:ILE:O	1:B:291:PHE:C	2.59	0.41
1:B:301:VAL:HB	3:B:1202:NDP:N7N	2.36	0.41
1:B:410:ALA:HB1	1:B:411:PRO:HD2	2.02	0.41
1:C:152:PHE:HA	1:C:194:GLN:HG3	2.02	0.41
1:C:232:LYS:HG3	1:C:302:TRP:CE3	2.56	0.41
1:D:93:TYR:CZ	1:D:282:VAL:HG21	2.56	0.41
1:D:440:THR:HG22	1:D:441:GLN:N	2.35	0.41
1:B:209:ARG:HG2	1:B:274:PRO:HB3	2.03	0.41
1:B:327:GLU:O	1:B:331:LEU:HG	2.21	0.41
1:B:343:GLU:HB3	1:B:344:PRO:HD2	2.02	0.41
1:C:347:ASP:O	1:C:350:LEU:HB3	2.21	0.41
1:D:93:TYR:CE1	1:D:282:VAL:HG21	2.56	0.41
1:D:450:LEU:HD21	3:D:1402:NDP:N6A	2.36	0.41
1:D:496:LEU:HD23	1:D:496:LEU:HA	1.94	0.41
1:A:430:ARG:HG2	1:A:430:ARG:HH11	1.86	0.40
1:B:10:GLN:HE21	1:C:172:GLN:NE2	2.19	0.40
1:B:118:GLU:O	1:B:121:SER:HB3	2.21	0.40
1:B:381:ARG:HH11	1:B:381:ARG:HB2	1.86	0.40
1:B:445:PHE:HD1	3:B:1202:NDP:HO2N	1.70	0.40
1:C:72:VAL:CG1	2:C:507:HEM:HMA3	2.50	0.40
1:C:172:GLN:HE21	1:C:172:GLN:HB3	1.69	0.40
1:C:234:HIS:O	1:C:279:TYR:N	2.43	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:442:VAL:HG12	1:D:484:VAL:HG11	2.03	0.40
1:A:355:PHE:O	1:A:358:PRO:HD2	2.21	0.40
1:B:469:ALA:HB1	1:B:473:ILE:HG21	2.04	0.40
1:C:89:ASP:CG	1:C:91:THR:HB	2.41	0.40
1:C:310:ILE:HA	1:C:311:PRO:HD3	1.96	0.40
1:D:160:PHE:CD1	2:D:507:HEM:HAB	2.56	0.40
1:D:220:LYS:HE3	1:D:343:GLU:CB	2.48	0.40
1:D:331:LEU:HD13	1:D:333:PHE:CZ	2.56	0.40
1:D:378:TYR:C	1:D:380:ALA:H	2.24	0.40
1:A:291:PHE:HA	1:A:292:PRO:HD3	1.88	0.40
1:A:370:LEU:HA	1:A:370:LEU:HD23	1.89	0.40
1:B:188:ARG:HB3	1:B:190:GLU:OE2	2.21	0.40
1:B:439:VAL:HG23	1:B:440:THR:H	1.86	0.40
1:B:446:TYR:CZ	1:B:455:ARG:HD2	2.56	0.40
1:C:264:LEU:O	1:C:264:LEU:HD12	2.21	0.40
1:D:145:VAL:CG1	1:D:353:ARG:NH2	2.85	0.40
1:A:155:ARG:HD3	1:A:297:ASP:OD1	2.21	0.40
1:B:55:VAL:HG21	1:C:430:ARG:NH2	2.36	0.40
1:B:384:ASN:HB2	1:B:385:TYR:H	1.66	0.40
1:C:384:ASN:OD1	1:C:397:GLN:NE2	2.55	0.40
1:D:488:TYR:CE1	1:D:492:ILE:HD11	2.56	0.40
1:A:428:VAL:HG23	1:B:424:PHE:CD1	2.56	0.40
1:B:205:PRO:O	1:B:244:LEU:HD12	2.22	0.40
1:B:447:LEU:O	1:B:448:LYS:HE2	2.21	0.40
1:C:22:LYS:HD3	1:C:23:PRO:CD	2.50	0.40
1:D:189:PRO:HG3	1:D:480:ASN:ND2	2.37	0.40
1:D:228:ALA:HB1	1:D:285:PHE:CZ	2.56	0.40
1:D:345:SER:C	1:D:347:ASP:H	2.25	0.40
1:D:414:GLN:O	1:D:416:SER:N	2.53	0.40
1:D:499:TYR:O	1:D:501:GLU:HG3	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	497/506 (98%)	442 (89%)	50 (10%)	5 (1%)	15	17
1	B	497/506 (98%)	423 (85%)	58 (12%)	16 (3%)	4	2
1	C	497/506 (98%)	417 (84%)	65 (13%)	15 (3%)	4	2
1	D	497/506 (98%)	442 (89%)	49 (10%)	6 (1%)	13	14
All	All	1988/2024 (98%)	1724 (87%)	222 (11%)	42 (2%)	7	5

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	19	ALA
1	A	437	ASP
1	B	124	THR
1	B	242	LYS
1	B	394	MET
1	B	448	LYS
1	C	292	PRO
1	C	427	ASP
1	B	100	GLU
1	B	271	GLY
1	B	348	LYS
1	B	437	ASP
1	C	440	THR
1	C	444	THR
1	C	496	LEU
1	C	497	ASP
1	D	411	PRO
1	D	413	HIS
1	A	21	GLN
1	A	121	SER
1	B	17	GLN
1	B	224	ALA
1	B	241	ILE
1	B	393	MET
1	B	470	GLN
1	C	92	ARG
1	C	226	GLY
1	C	346	PRO
1	C	437	ASP
1	D	437	ASP

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Mol	Chain	Res	Type
1	B	452	GLU
1	C	19	ALA
1	C	203	GLY
1	D	394	MET
1	C	192	LEU
1	D	216	SER
1	A	100	GLU
1	B	19	ALA
1	D	100	GLU
1	C	486	PRO
1	B	373	PRO
1	C	373	PRO

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	431/437 (99%)	365 (85%)	66 (15%)	2 2
1	B	431/437 (99%)	332 (77%)	99 (23%)	1 0
1	C	431/437 (99%)	349 (81%)	82 (19%)	1 1
1	D	431/437 (99%)	356 (83%)	75 (17%)	2 2
All	All	1724/1748 (99%)	1402 (81%)	322 (19%)	1 1

All (322) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ARG
1	A	15	LYS
1	A	18	ARG
1	A	21	GLN
1	A	22	LYS
1	A	24	ASP
1	A	26	LEU
1	A	37	LYS
1	A	40	SER

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Mol	Chain	Res	Type
1	A	41	LEU
1	A	43	VAL
1	A	49	LEU
1	A	65	ARG
1	A	70	GLU
1	A	73	VAL
1	A	92	ARG
1	A	102	ILE
1	A	104	LYS
1	A	105	ARG
1	A	131	PHE
1	A	137	THR
1	A	148	ASN
1	A	149	THR
1	A	155	ARG
1	A	162	SER
1	A	169	ARG
1	A	194	GLN
1	A	196	SER
1	A	197	PHE
1	A	202	ARG
1	A	209	ARG
1	A	229	VAL
1	A	235	TYR
1	A	237	THR
1	A	242	LYS
1	A	247	GLU
1	A	254	HIS
1	A	261	LEU
1	A	263	ASP
1	A	286	SER
1	A	289	GLU
1	A	290	ILE
1	A	309	LEU
1	A	319	ARG
1	A	327	GLU
1	A	374	VAL
1	A	379	ARG
1	A	394	MET
1	A	402	ASN
1	A	407	SER
1	A	413	HIS

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Mol	Chain	Res	Type
1	A	421	ARG
1	A	435	ASN
1	A	448	LYS
1	A	453	GLU
1	A	467	LYS
1	A	471	LEU
1	A	472	PHE
1	A	475	LYS
1	A	476	LYS
1	A	479	LYS
1	A	483	ASP
1	A	488	TYR
1	A	490	SER
1	A	498	LYS
1	A	501	GLU
1	B	3	ASN
1	B	12	LYS
1	B	16	GLU
1	B	17	GLN
1	B	18	ARG
1	B	21	GLN
1	B	26	LEU
1	B	36	ASP
1	B	37	LYS
1	B	41	LEU
1	B	49	LEU
1	B	55	VAL
1	B	59	GLU
1	B	67	ARG
1	B	72	VAL
1	B	73	VAL
1	B	90	ILE
1	B	92	ARG
1	B	94	SER
1	B	95	LYS
1	B	97	LYS
1	B	102	ILE
1	B	121	SER
1	B	124	THR
1	B	126	ARG
1	B	137	THR
1	B	144	LEU

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Mol	Chain	Res	Type
1	B	162	SER
1	B	169	ARG
1	B	186	SER
1	B	193	HIS
1	B	200	SER
1	B	201	ASP
1	B	202	ARG
1	B	220	LYS
1	B	221	LEU
1	B	225	ASP
1	B	229	VAL
1	B	232	LYS
1	B	235	TYR
1	B	236	LYS
1	B	242	LYS
1	B	245	SER
1	B	247	GLU
1	B	248	ASP
1	B	251	ARG
1	B	252	LEU
1	B	255	GLU
1	B	263	ASP
1	B	264	LEU
1	B	272	ASN
1	B	280	ILE
1	B	283	MET
1	B	286	SER
1	B	290	ILE
1	B	309	LEU
1	B	312	VAL
1	B	314	LYS
1	B	315	LEU
1	B	318	ASN
1	B	319	ARG
1	B	337	ASN
1	B	374	VAL
1	B	381	ARG
1	B	392	CYS
1	B	393	MET
1	B	396	ASN
1	B	397	GLN
1	B	402	ASN

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Mol	Chain	Res	Type
1	B	413	HIS
1	B	416	SER
1	B	421	ARG
1	B	422	THR
1	B	433	SER
1	B	438	ASN
1	B	439	VAL
1	B	441	GLN
1	B	443	ARG
1	B	444	THR
1	B	447	LEU
1	B	448	LYS
1	B	450	LEU
1	B	453	GLU
1	B	454	GLN
1	B	457	ARG
1	B	458	LEU
1	B	459	CYS
1	B	467	LYS
1	B	471	LEU
1	B	476	LYS
1	B	478	VAL
1	B	479	LYS
1	B	482	SER
1	B	487	GLU
1	B	488	TYR
1	B	492	ILE
1	B	495	LEU
1	B	498	LYS
1	B	500	ASN
1	C	3	ASN
1	C	4	ARG
1	C	16	GLU
1	C	17	GLN
1	C	18	ARG
1	C	22	LYS
1	C	26	LEU
1	C	46	ARG
1	C	52	GLN
1	C	65	ARG
1	C	68	ILE
1	C	73	VAL

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Mol	Chain	Res	Type
1	C	76	LYS
1	C	91	THR
1	C	92	ARG
1	C	95	LYS
1	C	97	LYS
1	C	104	LYS
1	C	105	ARG
1	C	126	ARG
1	C	131	PHE
1	C	138	GLU
1	C	139	ASP
1	C	149	THR
1	C	151	ILE
1	C	154	ILE
1	C	155	ARG
1	C	179	ASP
1	C	180	MET
1	C	188	ARG
1	C	194	GLN
1	C	195	VAL
1	C	197	PHE
1	C	202	ARG
1	C	227	GLU
1	C	235	TYR
1	C	237	THR
1	C	239	GLN
1	C	244	LEU
1	C	246	VAL
1	C	247	GLU
1	C	251	ARG
1	C	261	LEU
1	C	286	SER
1	C	289	GLU
1	C	293	PHE
1	C	304	HIS
1	C	309	LEU
1	C	331	LEU
1	C	345	SER
1	C	355	PHE
1	C	374	VAL
1	C	379	ARG
1	C	381	ARG

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Mol	Chain	Res	Type
1	C	394	MET
1	C	402	ASN
1	C	413	HIS
1	C	421	ARG
1	C	424	PHE
1	C	425	SER
1	C	427	ASP
1	C	429	GLN
1	C	433	SER
1	C	436	ASP
1	C	437	ASP
1	C	438	ASN
1	C	439	VAL
1	C	451	ASN
1	C	453	GLU
1	C	454	GLN
1	C	456	LYS
1	C	457	ARG
1	C	466	LEU
1	C	467	LYS
1	C	470	GLN
1	C	472	PHE
1	C	473	ILE
1	C	474	GLN
1	C	476	LYS
1	C	495	LEU
1	C	496	LEU
1	C	497	ASP
1	D	3	ASN
1	D	4	ARG
1	D	15	LYS
1	D	17	GLN
1	D	18	ARG
1	D	26	LEU
1	D	27	THR
1	D	34	VAL
1	D	37	LYS
1	D	43	VAL
1	D	52	GLN
1	D	85	GLU
1	D	89	ASP
1	D	90	ILE

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Mol	Chain	Res	Type
1	D	92	ARG
1	D	94	SER
1	D	105	ARG
1	D	111	ARG
1	D	131	PHE
1	D	144	LEU
1	D	148	ASN
1	D	155	ARG
1	D	159	LEU
1	D	193	HIS
1	D	197	PHE
1	D	202	ARG
1	D	211	MET
1	D	214	TYR
1	D	216	SER
1	D	220	LYS
1	D	221	LEU
1	D	222	VAL
1	D	225	ASP
1	D	229	VAL
1	D	235	TYR
1	D	236	LYS
1	D	245	SER
1	D	246	VAL
1	D	247	GLU
1	D	261	LEU
1	D	263	ASP
1	D	275	SER
1	D	280	ILE
1	D	281	GLN
1	D	283	MET
1	D	285	PHE
1	D	289	GLU
1	D	290	ILE
1	D	309	LEU
1	D	314	LYS
1	D	368	ASN
1	D	374	VAL
1	D	379	ARG
1	D	381	ARG
1	D	387	ARG
1	D	394	MET

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Mol	Chain	Res	Type
1	D	397	GLN
1	D	412	GLU
1	D	416	SER
1	D	421	ARG
1	D	432	ASN
1	D	435	ASN
1	D	436	ASP
1	D	443	ARG
1	D	444	THR
1	D	456	LYS
1	D	460	GLU
1	D	467	LYS
1	D	475	LYS
1	D	476	LYS
1	D	479	LYS
1	D	490	SER
1	D	495	LEU
1	D	498	LYS
1	D	501	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	GLN
1	A	32	ASN
1	A	148	ASN
1	A	167	GLN
1	A	210	HIS
1	A	320	ASN
1	A	337	ASN
1	A	402	ASN
1	A	420	HIS
1	A	429	GLN
1	A	454	GLN
1	A	485	HIS
1	A	500	ASN
1	B	32	ASN
1	B	148	ASN
1	B	167	GLN
1	B	193	HIS
1	B	208	HIS
1	B	243	ASN

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Mol	Chain	Res	Type
1	B	272	ASN
1	B	318	ASN
1	B	320	ASN
1	B	337	ASN
1	B	396	ASN
1	B	402	ASN
1	B	414	GLN
1	B	435	ASN
1	B	441	GLN
1	C	3	ASN
1	C	17	GLN
1	C	52	GLN
1	C	88	HIS
1	C	172	GLN
1	C	243	ASN
1	C	337	ASN
1	C	402	ASN
1	C	432	ASN
1	C	435	ASN
1	C	438	ASN
1	C	454	GLN
1	C	461	ASN
1	C	470	GLN
1	C	480	ASN
1	D	32	ASN
1	D	52	GLN
1	D	148	ASN
1	D	170	ASN
1	D	193	HIS
1	D	254	HIS
1	D	363	HIS
1	D	368	ASN
1	D	413	HIS
1	D	420	HIS
1	D	432	ASN
1	D	500	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)

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	HEM	C	507	1	41,50,50	1.37	5 (12%)	45,82,82	1.08	1 (2%)
3	NDP	D	1402	-	45,52,52	1.55	9 (20%)	53,80,80	1.42	7 (13%)
2	HEM	B	507	1	41,50,50	1.27	5 (12%)	45,82,82	1.04	3 (6%)
2	HEM	A	507	1	41,50,50	1.41	6 (14%)	45,82,82	0.99	2 (4%)
3	NDP	B	1202	-	45,52,52	1.55	7 (15%)	53,80,80	1.81	10 (18%)
3	NDP	C	1302	-	45,52,52	1.55	7 (15%)	53,80,80	1.78	10 (18%)
3	NDP	A	1102	-	45,52,52	1.53	7 (15%)	53,80,80	1.53	8 (15%)
2	HEM	D	507	1	41,50,50	1.29	6 (14%)	45,82,82	1.25	5 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	C	507	1	-	4/12/54/54	-
3	NDP	D	1402	-	-	11/30/77/77	0/5/5/5
2	HEM	B	507	1	-	6/12/54/54	-
2	HEM	A	507	1	-	3/12/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NDP	B	1202	-	-	10/30/77/77	0/5/5/5
3	NDP	C	1302	-	-	7/30/77/77	0/5/5/5
3	NDP	A	1102	-	-	6/30/77/77	0/5/5/5
2	HEM	D	507	1	-	4/12/54/54	-

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1302	NDP	C6N-C5N	4.91	1.42	1.33
3	D	1402	NDP	C6N-C5N	4.71	1.41	1.33
3	A	1102	NDP	C6N-C5N	4.69	1.41	1.33
3	B	1202	NDP	C6N-C5N	4.61	1.41	1.33
2	A	507	HEM	C3C-CAC	-4.15	1.39	1.47
3	D	1402	NDP	P2B-O1X	4.03	1.63	1.50
3	C	1302	NDP	P2B-O1X	3.78	1.62	1.50
3	A	1102	NDP	P2B-O1X	3.75	1.62	1.50
3	B	1202	NDP	C4N-C3N	-3.66	1.42	1.49
3	C	1302	NDP	C4N-C3N	-3.59	1.42	1.49
2	C	507	HEM	CBB-CAB	3.56	1.47	1.30
3	B	1202	NDP	P2B-O1X	3.50	1.61	1.50
3	A	1102	NDP	C7N-C3N	3.45	1.56	1.48
2	A	507	HEM	CAB-C3B	-3.16	1.38	1.47
2	D	507	HEM	CBB-CAB	3.14	1.45	1.30
3	A	1102	NDP	C4N-C3N	-3.11	1.43	1.49
3	D	1402	NDP	C7N-C3N	3.11	1.55	1.48
3	D	1402	NDP	C4N-C3N	-3.10	1.43	1.49
2	D	507	HEM	C3C-CAC	-3.05	1.41	1.47
2	B	507	HEM	CBB-CAB	3.05	1.45	1.30
3	B	1202	NDP	C7N-C3N	3.04	1.55	1.48
2	C	507	HEM	C3C-CAC	-2.96	1.41	1.47
2	B	507	HEM	C3C-CAC	-2.88	1.41	1.47
3	C	1302	NDP	C7N-C3N	2.85	1.54	1.48
3	D	1402	NDP	C6N-N1N	2.75	1.44	1.37
2	B	507	HEM	CBC-CAC	2.72	1.47	1.29
2	D	507	HEM	CBC-CAC	2.71	1.47	1.29
3	C	1302	NDP	C6N-N1N	2.67	1.44	1.37
2	C	507	HEM	CBC-CAC	2.65	1.46	1.29
2	A	507	HEM	CHA-C4D	2.65	1.41	1.35
3	A	1102	NDP	C6N-N1N	2.61	1.43	1.37
3	B	1202	NDP	C4N-C5N	-2.61	1.42	1.48
3	C	1302	NDP	C4N-C5N	-2.55	1.42	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	507	HEM	CBB-CAB	2.49	1.42	1.30
2	A	507	HEM	CBC-CAC	2.44	1.45	1.29
3	A	1102	NDP	O4B-C1B	2.39	1.44	1.41
3	C	1302	NDP	C2N-C3N	2.39	1.41	1.34
3	B	1202	NDP	C2N-C3N	2.38	1.41	1.34
2	A	507	HEM	C3C-C2C	-2.32	1.37	1.40
2	C	507	HEM	CAB-C3B	-2.26	1.41	1.47
3	A	1102	NDP	C2A-N3A	2.24	1.35	1.32
3	D	1402	NDP	C4N-C5N	-2.24	1.43	1.48
2	D	507	HEM	CAB-C3B	-2.23	1.41	1.47
3	D	1402	NDP	C2N-C3N	2.21	1.41	1.34
2	D	507	HEM	C1A-NA	2.20	1.40	1.36
3	D	1402	NDP	O4B-C1B	2.19	1.44	1.41
3	D	1402	NDP	C2A-N3A	2.18	1.35	1.32
3	B	1202	NDP	C6N-N1N	2.16	1.42	1.37
2	D	507	HEM	C4A-NA	2.09	1.40	1.36
2	C	507	HEM	C2C-C1C	2.09	1.47	1.42
2	B	507	HEM	CAA-C2A	2.07	1.55	1.52
2	B	507	HEM	CAB-C3B	-2.04	1.41	1.47

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	1302	NDP	O4D-C1D-N1N	6.07	119.91	108.06
3	B	1202	NDP	N3A-C2A-N1A	-5.63	119.88	128.68
3	B	1202	NDP	O4D-C1D-N1N	5.39	118.60	108.06
3	C	1302	NDP	N3A-C2A-N1A	-4.95	120.94	128.68
3	D	1402	NDP	N3A-C2A-N1A	-4.36	121.86	128.68
3	A	1102	NDP	N3A-C2A-N1A	-4.32	121.93	128.68
3	A	1102	NDP	O4D-C1D-N1N	4.02	115.91	108.06
3	D	1402	NDP	O4D-C1D-N1N	3.90	115.68	108.06
3	B	1202	NDP	C3D-C2D-C1D	3.85	108.75	101.43
3	B	1202	NDP	C1B-N9A-C4A	-3.82	119.93	126.64
3	A	1102	NDP	C3B-C2B-C1B	3.80	110.03	102.89
3	C	1302	NDP	C3D-C2D-C1D	3.63	108.31	101.43
3	A	1102	NDP	C3D-C2D-C1D	3.48	108.03	101.43
3	C	1302	NDP	C3B-C2B-C1B	3.27	109.03	102.89
3	C	1302	NDP	O3X-P2B-O2X	3.13	119.58	107.64
3	B	1202	NDP	PN-O3-PA	3.09	143.42	132.83
3	A	1102	NDP	O3X-P2B-O2X	3.06	119.35	107.64
3	D	1402	NDP	O3X-P2B-O2X	3.04	119.26	107.64
3	A	1102	NDP	C4A-C5A-N7A	2.96	112.49	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	507	HEM	C4B-C3B-C2B	-2.80	104.89	107.11
3	B	1202	NDP	O3X-P2B-O2X	2.74	118.10	107.64
3	D	1402	NDP	C1B-N9A-C4A	-2.73	121.84	126.64
2	A	507	HEM	CBA-CAA-C2A	-2.65	108.10	112.62
3	C	1302	NDP	C4A-C5A-N7A	2.60	112.11	109.40
3	D	1402	NDP	C4A-C5A-N7A	2.57	112.08	109.40
3	C	1302	NDP	O4B-C4B-C3B	2.55	110.16	105.11
2	A	507	HEM	CMB-C2B-C1B	2.53	128.88	125.04
3	D	1402	NDP	C3D-C2D-C1D	2.46	106.10	101.43
2	D	507	HEM	CBA-CAA-C2A	-2.44	108.45	112.62
3	D	1402	NDP	C3B-C2B-C1B	2.43	107.47	102.89
3	B	1202	NDP	O5D-C5D-C4D	2.42	117.31	108.99
3	B	1202	NDP	C2A-N1A-C6A	2.35	122.78	118.75
3	B	1202	NDP	C4A-C5A-N7A	2.33	111.83	109.40
3	C	1302	NDP	C1B-N9A-C4A	-2.31	122.58	126.64
2	B	507	HEM	C3D-C4D-ND	2.27	112.69	110.17
2	D	507	HEM	CMC-C2C-C3C	2.25	128.89	124.68
3	B	1202	NDP	C5D-C4D-C3D	-2.23	106.81	115.18
3	A	1102	NDP	O2B-C2B-C1B	-2.22	102.10	110.10
2	B	507	HEM	C4B-C3B-C2B	-2.19	105.37	107.11
2	B	507	HEM	CHA-C4D-C3D	-2.17	121.25	125.33
2	D	507	HEM	C3B-C2B-C1B	2.13	108.07	106.49
2	D	507	HEM	C3D-C4D-ND	2.11	112.52	110.17
2	C	507	HEM	C4A-C3A-C2A	2.07	108.44	107.00
3	A	1102	NDP	C5A-C6A-N6A	2.01	123.41	120.35
3	C	1302	NDP	O4B-C4B-C5B	-2.01	102.75	109.37
3	C	1302	NDP	C2A-N1A-C6A	2.01	122.19	118.75

There are no chirality outliers.

All (51) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	507	HEM	C2B-C3B-CAB-CBB
2	A	507	HEM	C4B-C3B-CAB-CBB
2	B	507	HEM	C2B-C3B-CAB-CBB
2	D	507	HEM	C2B-C3B-CAB-CBB
2	D	507	HEM	C4B-C3B-CAB-CBB
3	A	1102	NDP	C5D-O5D-PN-O1N
3	A	1102	NDP	C5D-O5D-PN-O2N
3	B	1202	NDP	C5D-O5D-PN-O1N
3	B	1202	NDP	C5D-O5D-PN-O2N
3	B	1202	NDP	O4D-C1D-N1N-C6N

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Mol	Chain	Res	Type	Atoms
3	C	1302	NDP	C5D-O5D-PN-O2N
3	C	1302	NDP	O4D-C1D-N1N-C6N
3	D	1402	NDP	C5D-O5D-PN-O2N
3	D	1402	NDP	O4D-C1D-N1N-C6N
3	A	1102	NDP	O4D-C1D-N1N-C6N
2	C	507	HEM	C2B-C3B-CAB-CBB
2	B	507	HEM	C4B-C3B-CAB-CBB
3	D	1402	NDP	O4B-C4B-C5B-O5B
3	B	1202	NDP	C4D-C5D-O5D-PN
3	D	1402	NDP	C4D-C5D-O5D-PN
3	B	1202	NDP	C2B-O2B-P2B-O3X
3	C	1302	NDP	C5D-O5D-PN-O3
3	D	1402	NDP	C2B-O2B-P2B-O3X
3	D	1402	NDP	C5D-O5D-PN-O3
3	C	1302	NDP	C5D-O5D-PN-O1N
3	A	1102	NDP	C4D-C5D-O5D-PN
2	B	507	HEM	C4D-C3D-CAD-CBD
3	B	1202	NDP	O4B-C4B-C5B-O5B
2	B	507	HEM	C2D-C3D-CAD-CBD
2	D	507	HEM	CAD-CBD-CGD-O1D
2	B	507	HEM	CAD-CBD-CGD-O1D
2	D	507	HEM	CAD-CBD-CGD-O2D
2	B	507	HEM	CAD-CBD-CGD-O2D
3	B	1202	NDP	PN-O3-PA-O1A
3	C	1302	NDP	PN-O3-PA-O2A
2	C	507	HEM	CAD-CBD-CGD-O2D
2	C	507	HEM	CAD-CBD-CGD-O1D
2	C	507	HEM	C4B-C3B-CAB-CBB
3	A	1102	NDP	C5D-O5D-PN-O3
3	B	1202	NDP	C2B-O2B-P2B-O2X
3	B	1202	NDP	C5D-O5D-PN-O3
3	D	1402	NDP	C2B-O2B-P2B-O2X
3	A	1102	NDP	O4B-C4B-C5B-O5B
3	D	1402	NDP	C3B-C4B-C5B-O5B
3	B	1202	NDP	PN-O3-PA-O2A
3	D	1402	NDP	PA-O3-PN-O2N
3	C	1302	NDP	C4D-C5D-O5D-PN
3	D	1402	NDP	C5D-O5D-PN-O1N
3	D	1402	NDP	C2N-C3N-C7N-N7N
3	C	1302	NDP	O4B-C4B-C5B-O5B
2	A	507	HEM	CAA-CBA-CGA-O2A

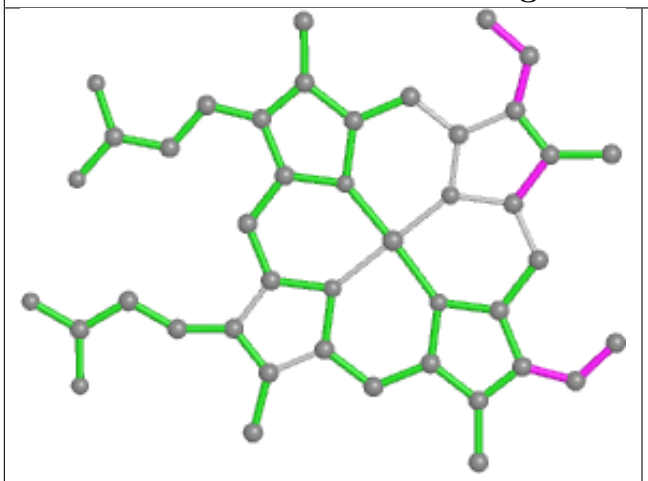
There are no ring outliers.

7 monomers are involved in 21 short contacts:

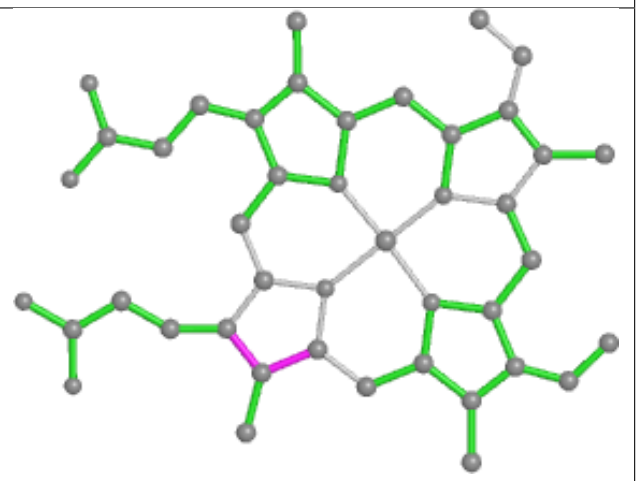
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	507	HEM	4	0
3	D	1402	NDP	1	0
2	A	507	HEM	5	0
3	B	1202	NDP	4	0
3	C	1302	NDP	2	0
3	A	1102	NDP	3	0
2	D	507	HEM	2	0

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

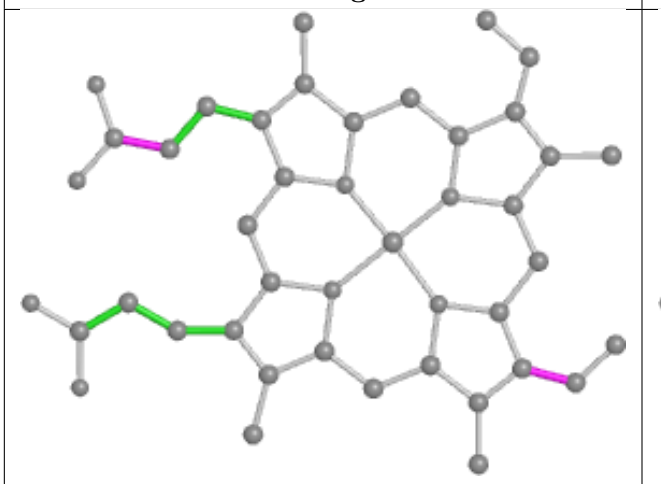
Ligand HEM C 507



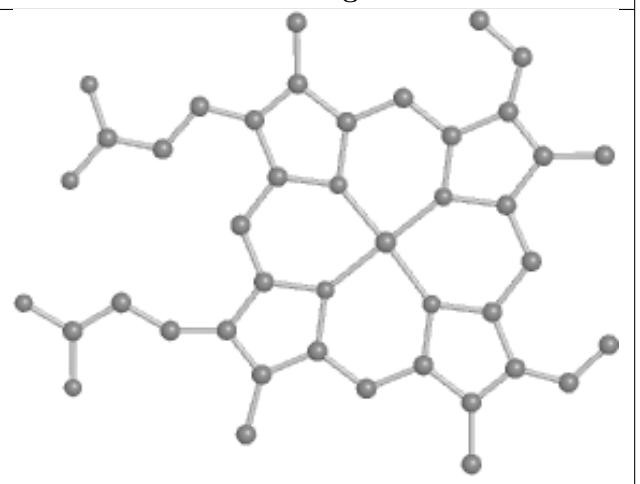
Bond lengths



Bond angles

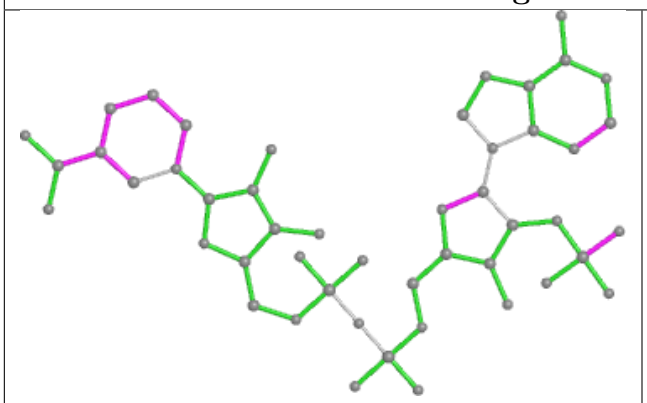


Torsions



Rings

Ligand NDP D 1402



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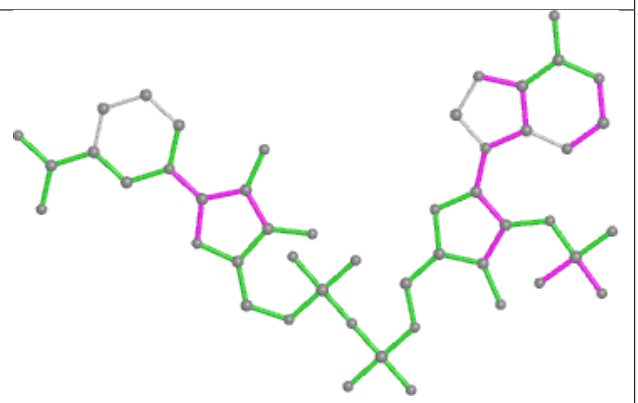

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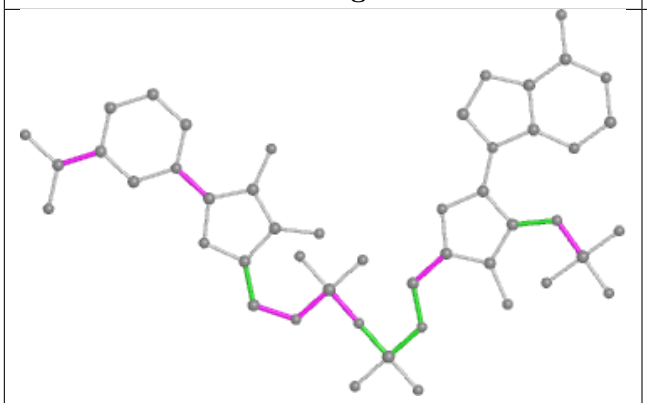

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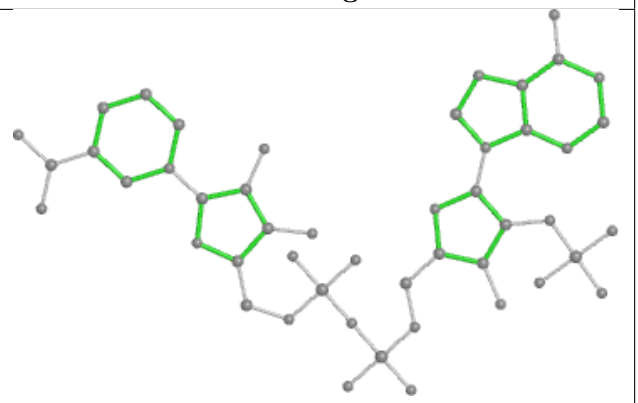
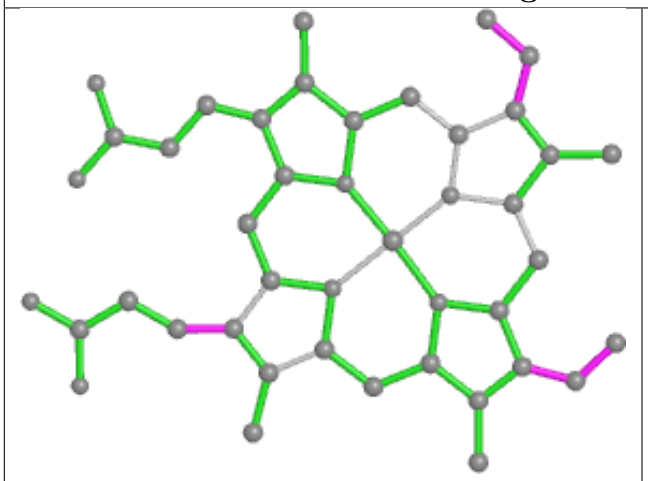


Rings

Ligand HEM B 507



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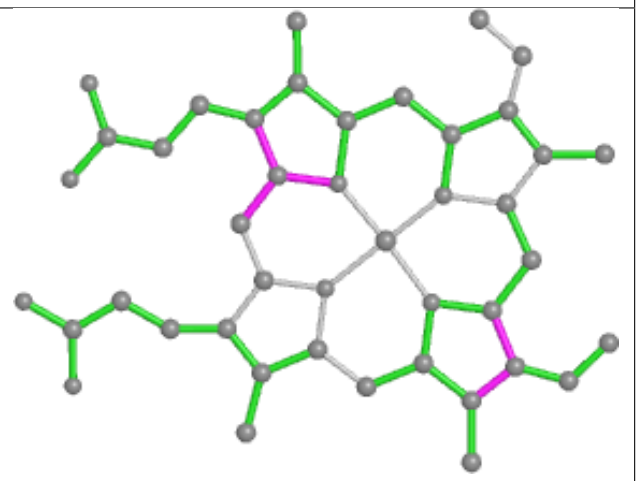

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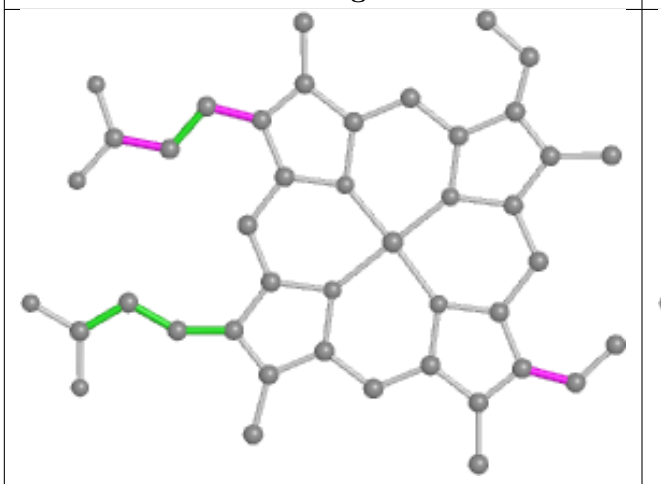

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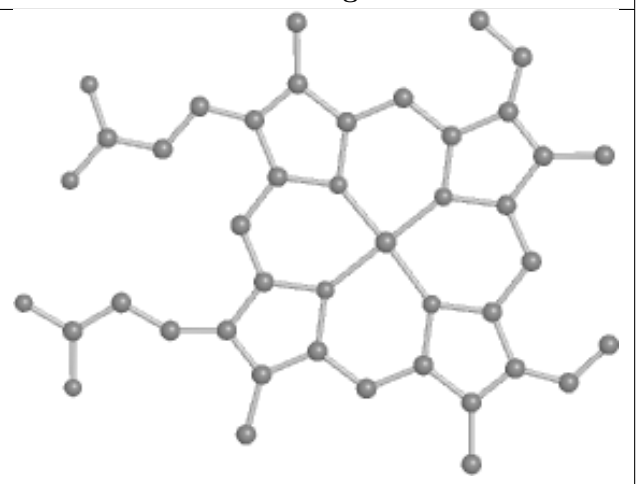
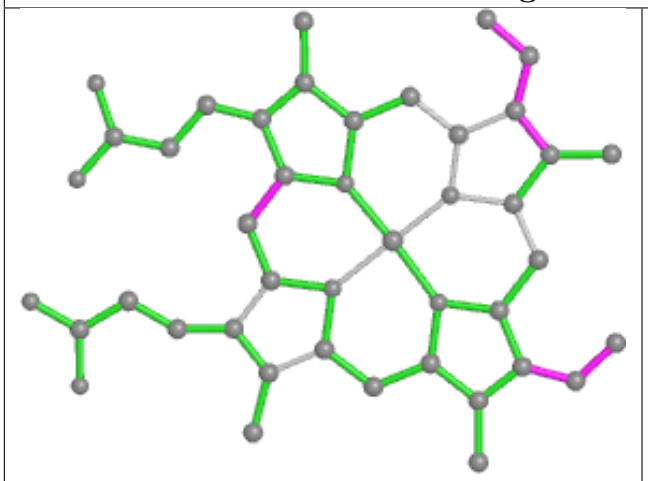


Rings

Ligand HEM A 507



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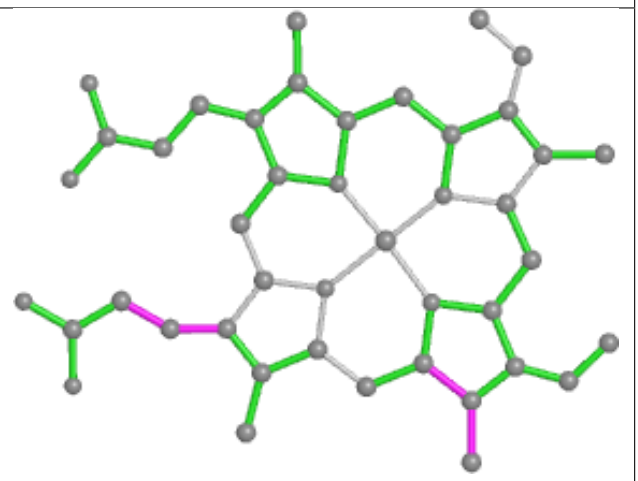

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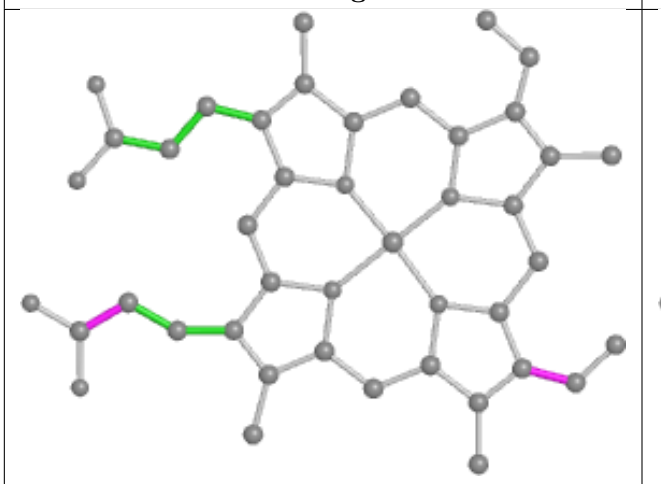

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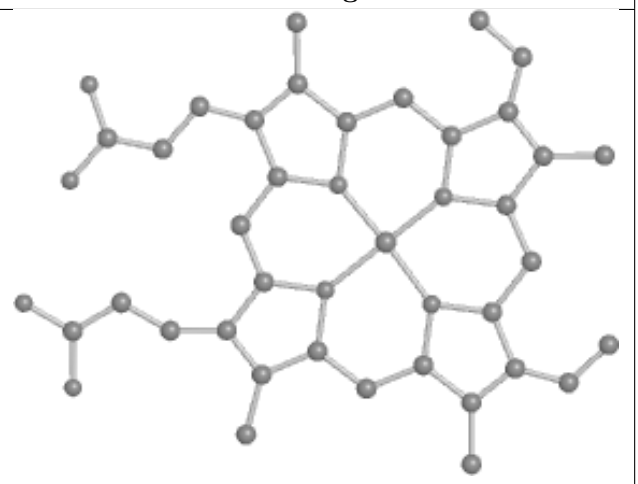
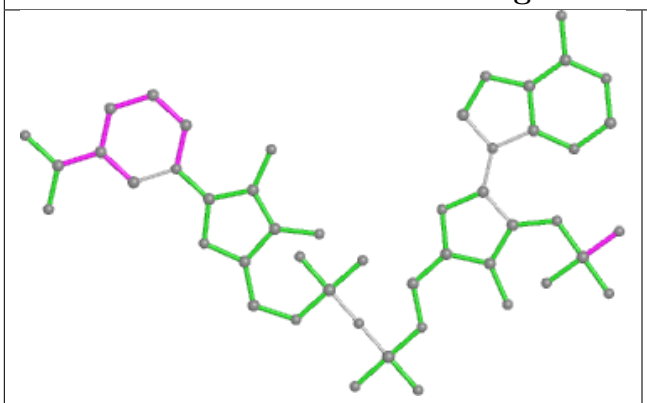


Rings

Ligand NDP B 1202



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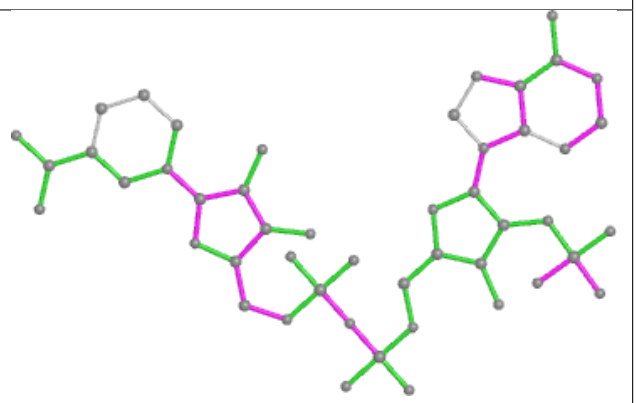
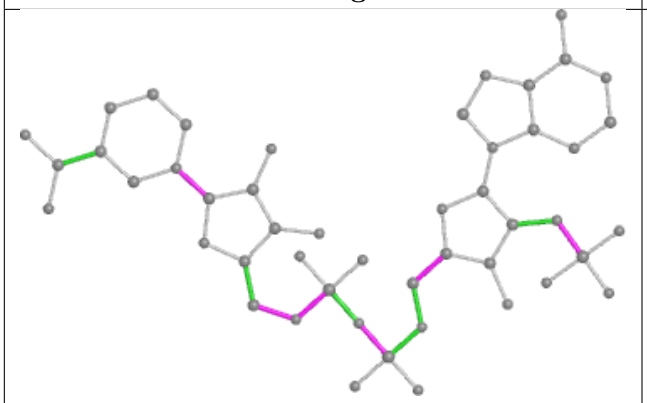


Bond angles



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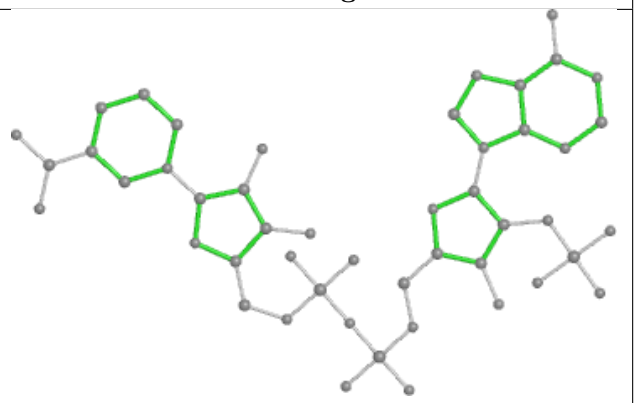
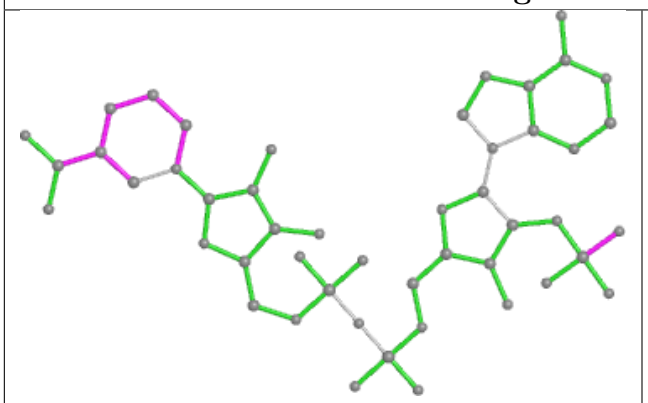
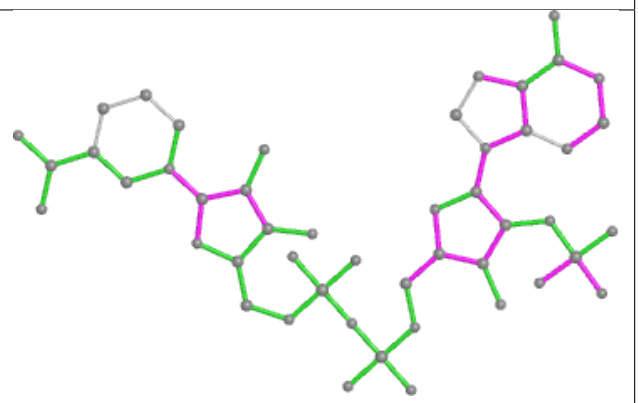


Rings

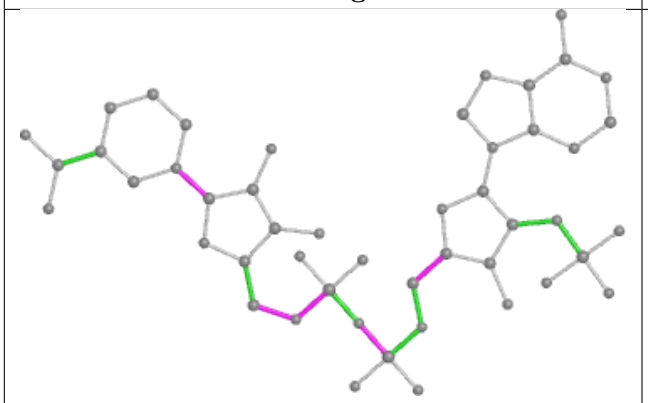
Ligand NDP C 1302



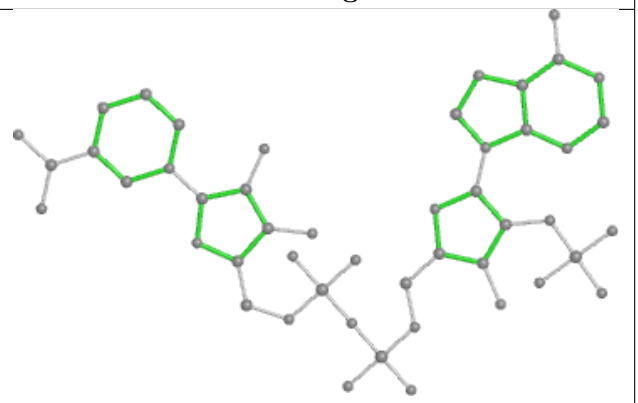
Bond lengths



Bond angles

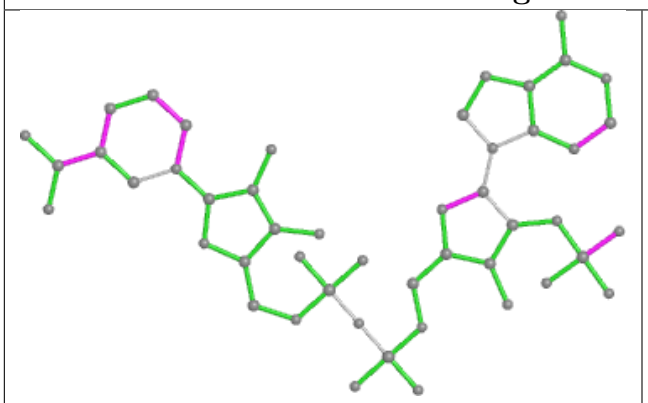


Torsions



Rings

Ligand NDP A 1102



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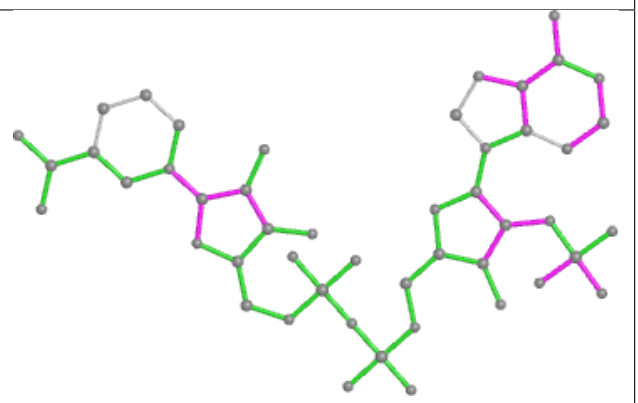
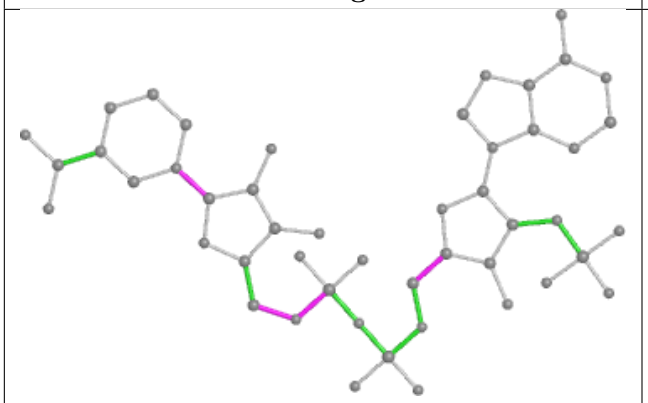
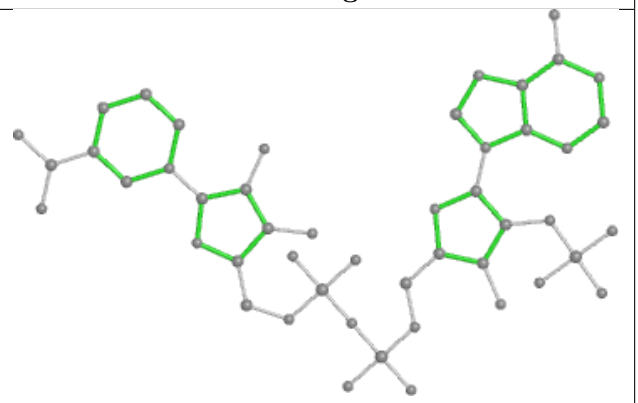


Bond angles

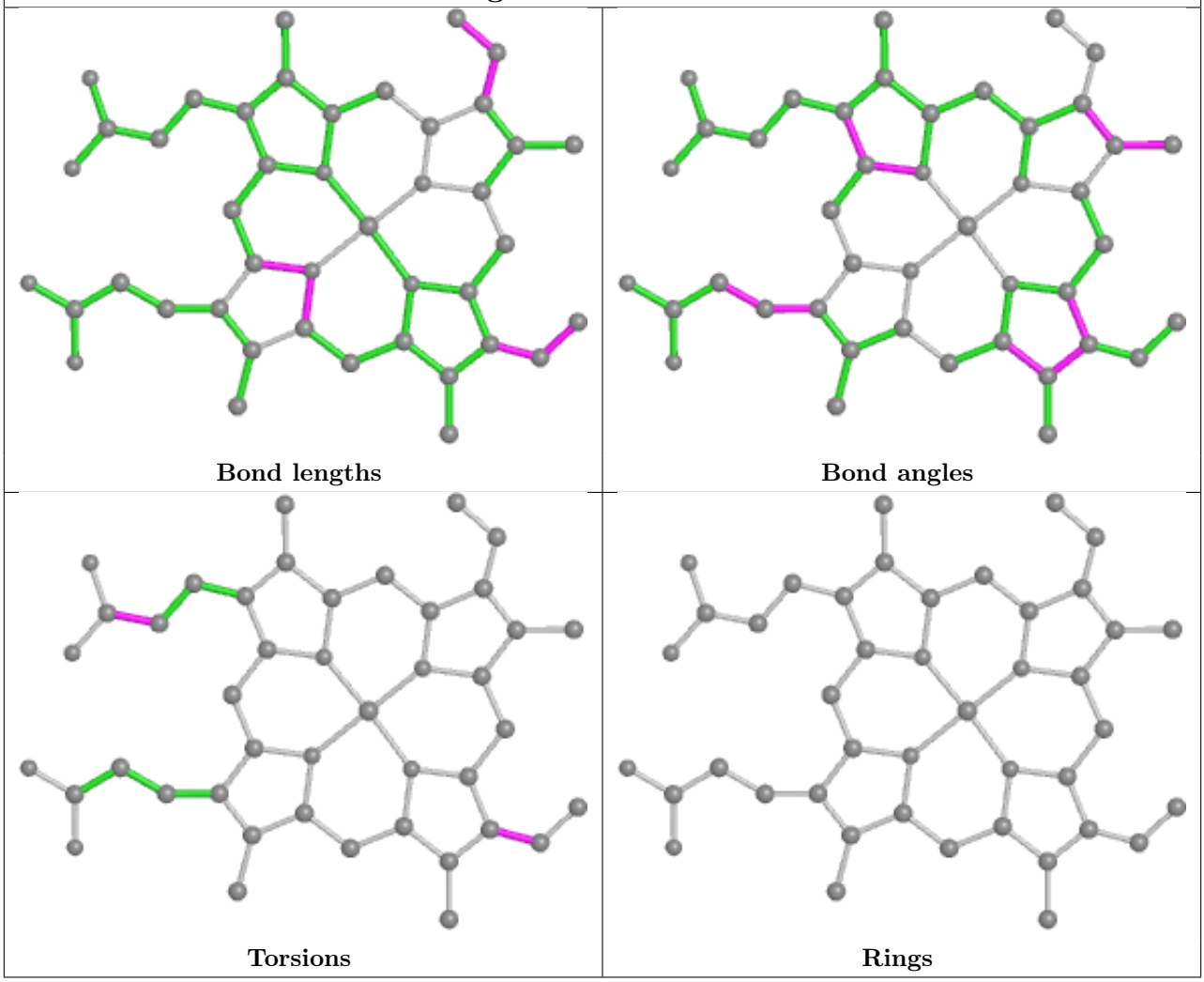


Torsions



Rings

Ligand HEM D 507



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.