



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 08:53 AM GMT

PDB ID : 1FAG
Title : STRUCTURE OF CYTOCHROME P450
Authors : Li, H.Y.; Poulos, T.L.
Deposited on : 1996-08-01
Resolution : 2.70 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

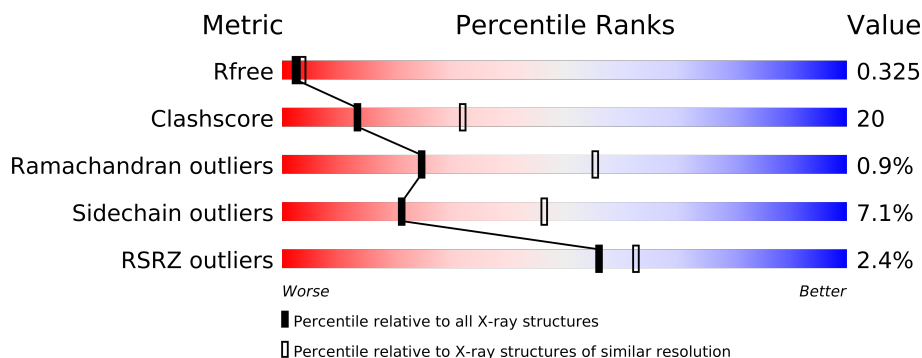
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.70 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}	66092	1557 (2.70-2.70)
Clashscore	79885	1939 (2.70-2.70)
Ramachandran outliers	78287	1905 (2.70-2.70)
Sidechain outliers	78261	1905 (2.70-2.70)
RSRZ outliers	66119	1559 (2.70-2.70)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	471	
1	B	471	
1	C	471	
1	D	471	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	PAM	B	473	-	X
3	PAM	C	473	-	X

2 Entry composition i

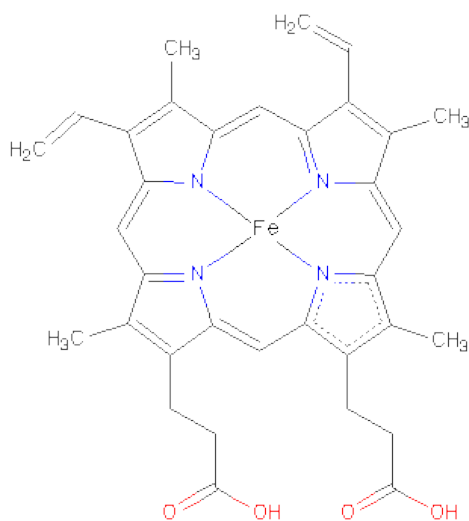
There are 3 unique types of molecules in this entry. The entry contains 14924 atoms, of which 0 are hydrogen and 0 are deuterium.

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

- Molecule 1 is a protein called CYTOCHROME P450 BM-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	455	Total	C	N	O	S	0	0	0
			3670	2345	623	685	17			
1	B	455	Total	C	N	O	S	0	0	0
			3670	2345	623	685	17			
1	C	455	Total	C	N	O	S	0	0	0
			3670	2345	623	685	17			
1	D	455	Total	C	N	O	S	0	0	0
			3670	2345	623	685	17			

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



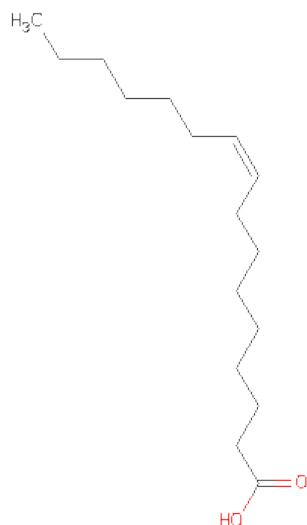
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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

- Molecule 3 is PALMITOLEIC ACID (three-letter code: PAM) (formula: $C_{16}H_{30}O_2$).



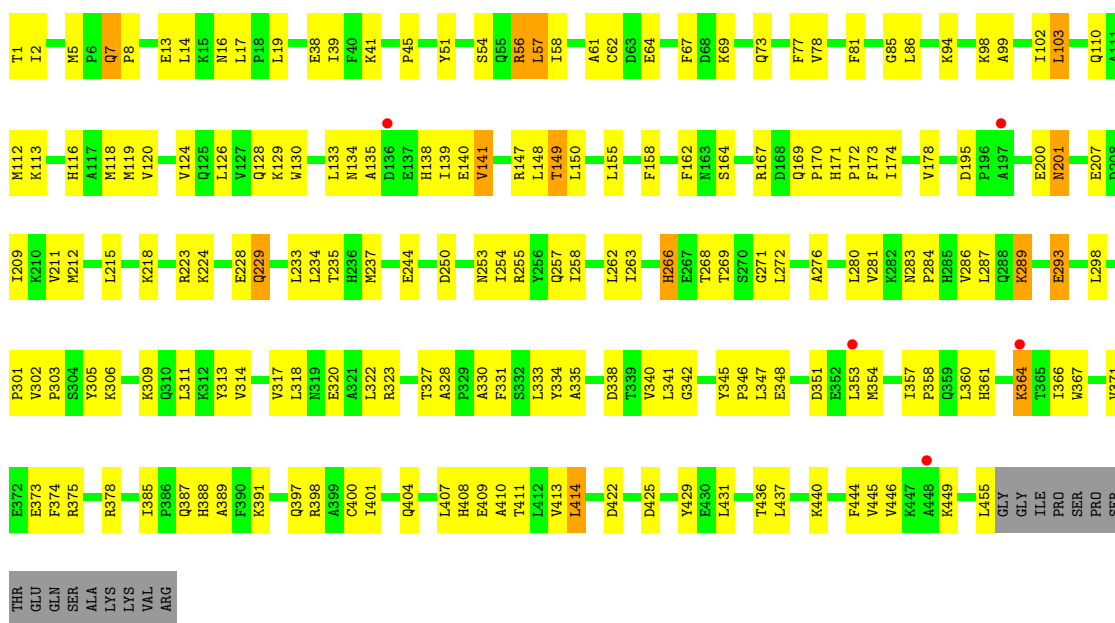
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			18	16	2		
3	B	1	Total	C	O	0	0
			18	16	2		
3	C	1	Total	C	O	0	0
			18	16	2		
3	D	1	Total	C	O	0	0
			18	16	2		

3 Residue-property plots

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

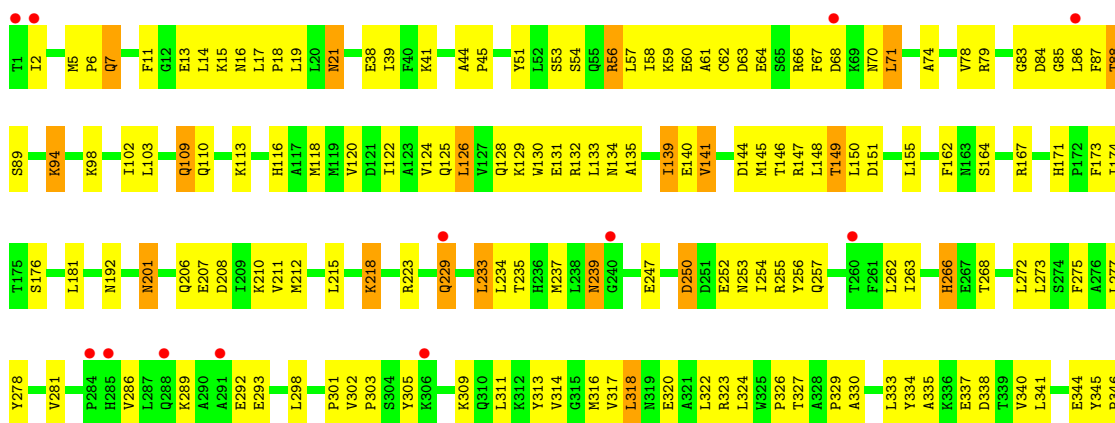
• Molecule 1: CYTOCHROME P450 BM-3

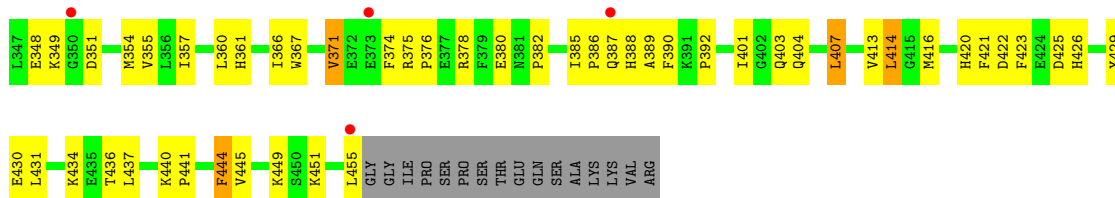
Chain A: 



• Molecule 1: CYTOCHROME P450 BM-3

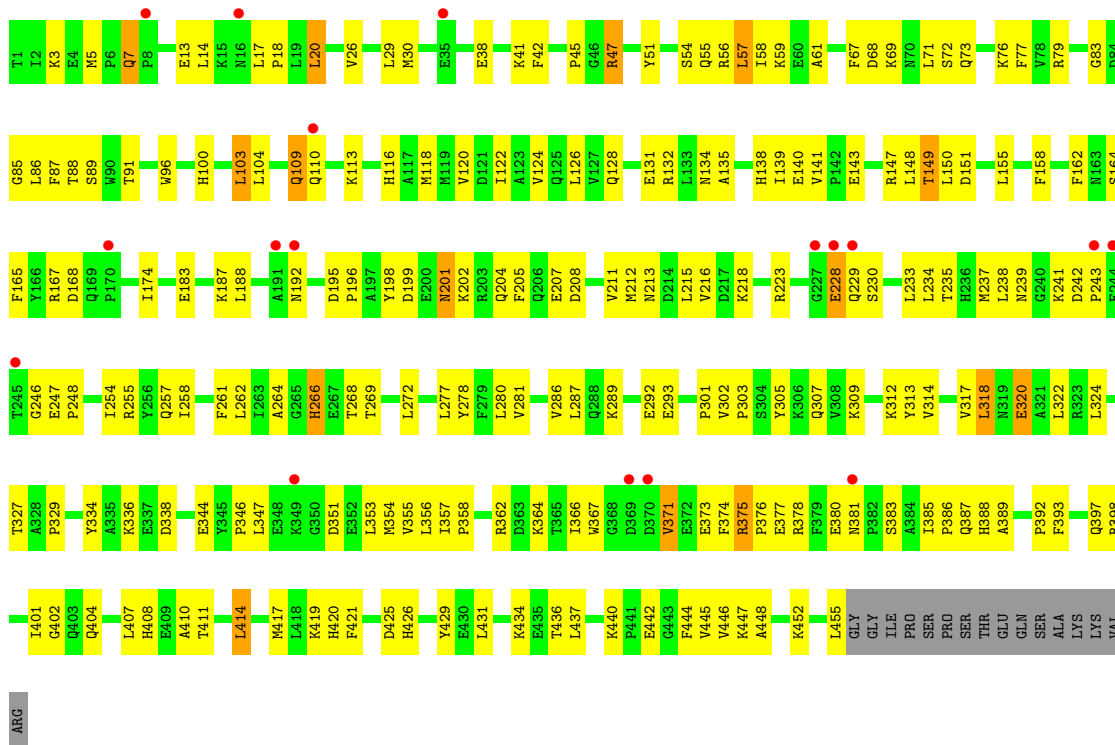
Chain B: 





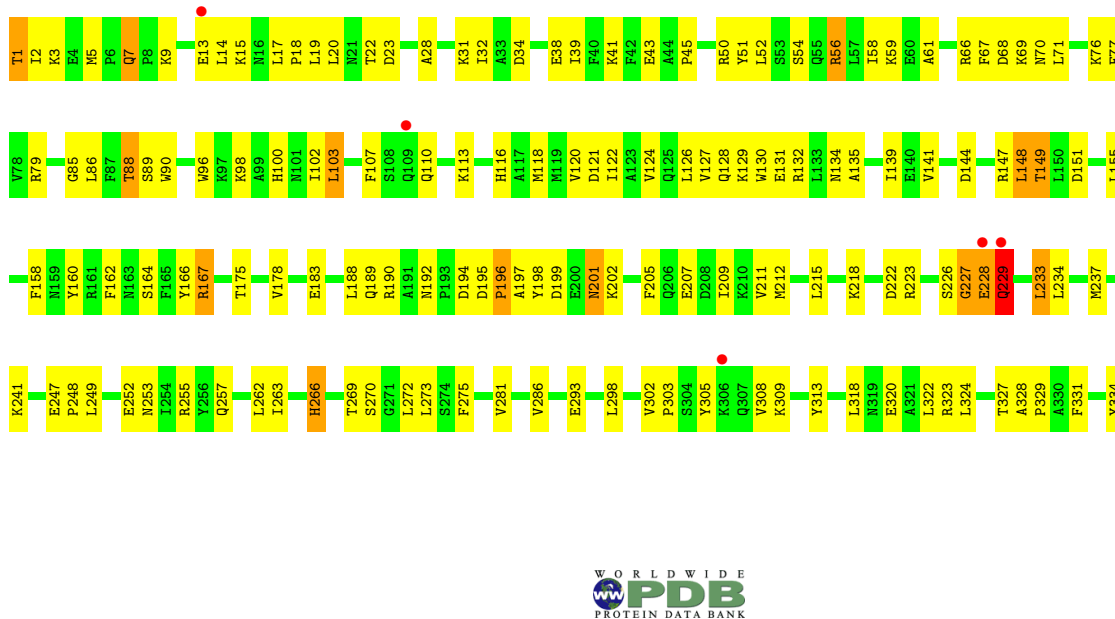
• Molecule 1: CYTOCHROME P450 BM-3

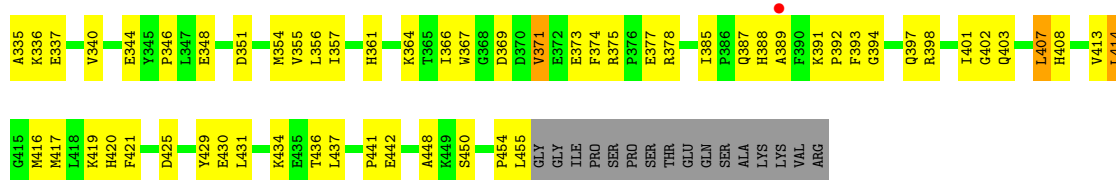
Chain C:



• Molecule 1: CYTOCHROME P450 BM-3

Chain D:





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	106.20Å 165.20Å 223.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.70 19.90 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.4 (10.00-2.70) 99.8 (19.90-2.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 2.59Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.246 , 0.353 0.243 , 0.325	Depositor DCC
R_{free} test set	6122 reflections (11.27%)	DCC
Wilson B-factor (Å ²)	64.0	Xtriage
Anisotropy	0.118	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 52.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 60437 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14924	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, PAM

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	0.48	0/3755	0.69	3/5077 (0.1%)
1	B	0.46	0/3755	0.70	1/5077 (0.0%)
1	C	0.46	0/3755	0.67	0/5077
1	D	0.47	0/3755	0.71	1/5077 (0.0%)
All	All	0.47	0/15020	0.69	5/20308 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	333	LEU	CA-CB-CG	5.64	128.28	115.30
1	A	400	CYS	CA-CB-SG	-5.38	104.31	114.00
1	B	333	LEU	CA-CB-CG	5.22	127.30	115.30
1	D	328	ALA	N-CA-C	-5.10	97.22	111.00
1	A	328	ALA	N-CA-C	-5.09	97.27	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3670	0	3645	127	0
1	B	3670	0	3645	146	0
1	C	3670	0	3645	164	0
1	D	3670	0	3645	164	0
2	A	43	0	30	2	0
2	B	43	0	30	3	0
2	C	43	0	30	5	0
2	D	43	0	30	7	0
3	A	18	0	29	1	0
3	B	18	0	29	2	0
3	C	18	0	29	3	0
3	D	18	0	29	0	0
All	All	14924	0	14816	606	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 20.

All (606) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:241:LYS:HG2	1:C:248:PRO:HG3	1.29	1.14
1:D:241:LYS:HG2	1:D:248:PRO:HG3	1.38	1.03
1:D:5:MET:HG2	1:D:41:LYS:HB2	1.41	1.00
1:A:272:LEU:HD13	1:A:322:LEU:HD13	1.51	0.90
1:C:238:LEU:HD23	1:C:254:ILE:HD13	1.55	0.86
1:C:13:GLU:HG3	1:C:14:LEU:HD22	1.59	0.85
1:B:13:GLU:HG3	1:B:14:LEU:HD22	1.60	0.84
1:A:118:MET:HB3	1:A:155:LEU:HD23	1.59	0.84
1:C:47:ARG:HD3	1:C:73:GLN:HG3	1.60	0.82
1:A:120:VAL:HG11	1:A:302:VAL:HG13	1.62	0.82
1:B:301:PRO:HB3	1:B:455:LEU:HA	1.59	0.81
1:A:171:HIS:HD2	1:A:173:PHE:H	1.30	0.79
1:D:149:THR:HG21	1:D:269:THR:HB	1.64	0.79
1:D:223:ARG:HH21	1:D:234:LEU:HB3	1.47	0.78
1:D:320:GLU:HB3	1:D:374:PHE:CE1	2.19	0.78
1:D:205:PHE:CE2	1:D:209:ILE:HD11	2.20	0.77
1:B:61:ALA:HA	1:B:67:PHE:CD2	2.19	0.77
1:A:364:LYS:H	1:A:364:LYS:HD2	1.49	0.77
1:D:147:ARG:HG3	1:D:164:SER:HB3	1.67	0.76
1:B:380:GLU:O	1:B:382:PRO:HD3	1.84	0.76
1:B:57:LEU:HD12	1:B:341:LEU:HG	1.68	0.76
1:B:422:ASP:HB2	1:B:449:LYS:HB3	1.67	0.75
1:B:85:GLY:HA2	1:B:257:GLN:NE2	2.03	0.73
1:D:272:LEU:HD13	1:D:322:LEU:HD13	1.69	0.73

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:201:ASN:HD22	1:A:201:ASN:H	1.37	0.73
1:D:164:SER:HA	1:D:167:ARG:HD3	1.69	0.72
1:C:7:GLN:HB2	1:C:41:LYS:O	1.88	0.72
1:D:120:VAL:HG11	1:D:302:VAL:HG13	1.71	0.72
1:C:86:LEU:HD23	1:C:401:ILE:HG13	1.70	0.71
1:C:51:TYR:CE1	1:C:354:MET:HG2	2.25	0.71
1:D:128:GLN:O	1:D:132:ARG:HG3	1.90	0.71
1:B:103:LEU:HD11	1:B:237:MET:HG2	1.70	0.71
1:D:281:VAL:CG1	1:D:425:ASP:HB2	2.19	0.71
1:C:223:ARG:HH21	1:C:234:LEU:HB3	1.53	0.71
1:A:147:ARG:HG3	1:A:164:SER:HB3	1.72	0.71
1:D:1:THR:O	1:D:344:GLU:HA	1.91	0.70
1:D:131:GLU:HG2	1:D:421:PHE:HZ	1.54	0.70
1:D:201:ASN:HD22	1:D:201:ASN:H	1.39	0.70
1:A:13:GLU:HG3	1:A:14:LEU:HD22	1.73	0.69
1:A:51:TYR:CE2	1:A:354:MET:HG2	2.28	0.69
1:C:198:TYR:HA	1:C:201:ASN:ND2	2.06	0.69
1:C:312:LYS:HG3	1:C:313:TYR:H	1.58	0.69
1:C:367:TRP:HB2	1:C:371:VAL:HG12	1.74	0.69
1:D:252:GLU:HG3	1:D:255:ARG:NH2	2.07	0.69
1:B:281:VAL:CG1	1:B:425:ASP:HB2	2.24	0.68
1:A:281:VAL:CG1	1:A:425:ASP:HB2	2.24	0.68
1:B:367:TRP:HB2	1:B:371:VAL:HG12	1.74	0.68
1:A:56:ARG:HG3	1:A:57:LEU:HD22	1.76	0.67
1:C:286:VAL:HG13	1:C:313:TYR:OH	1.94	0.67
2:B:472:HEM:HBC2	2:B:472:HEM:HMC2	1.77	0.67
1:B:401:ILE:HG12	2:B:472:HEM:HBD2	1.77	0.67
1:C:147:ARG:HG3	1:C:164:SER:HB3	1.76	0.67
1:C:281:VAL:CG1	1:C:425:ASP:HB2	2.25	0.67
1:B:56:ARG:HA	1:B:59:LYS:HE3	1.76	0.67
1:D:58:ILE:HD12	1:D:355:VAL:HG22	1.77	0.67
1:C:100:HIS:HE1	1:C:104:LEU:HD22	1.60	0.66
1:D:7:GLN:HB2	1:D:41:LYS:O	1.94	0.66
1:C:198:TYR:O	1:C:202:LYS:HG3	1.95	0.66
1:C:138:HIS:HA	1:C:447:LYS:HD3	1.77	0.66
1:D:98:LYS:O	1:D:102:ILE:HG13	1.95	0.66
1:B:120:VAL:O	1:B:124:VAL:HG23	1.96	0.66
1:D:5:MET:HB3	1:D:41:LYS:NZ	2.11	0.66
1:D:131:GLU:HG2	1:D:421:PHE:CZ	2.31	0.66
1:C:150:LEU:HD22	1:C:174:ILE:HD11	1.77	0.66
1:D:158:PHE:HE2	1:D:237:MET:HE1	1.61	0.66
1:A:103:LEU:HD11	1:A:237:MET:HG2	1.77	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:122:ILE:HG22	1:B:148:LEU:HD12	1.78	0.66
1:C:87:PHE:CZ	3:C:473:PAM:H10	2.30	0.66
1:D:86:LEU:HD23	1:D:401:ILE:HG13	1.77	0.65
1:B:320:GLU:HB3	1:B:374:PHE:CE1	2.32	0.65
1:D:367:TRP:HB2	1:D:371:VAL:HG12	1.79	0.65
1:C:122:ILE:HG22	1:C:148:LEU:HD12	1.79	0.65
1:B:176:SER:HB3	1:B:208:ASP:HB3	1.79	0.65
1:B:54:SER:O	1:B:58:ILE:HG12	1.97	0.65
1:B:366:ILE:HG21	1:B:389:ALA:HB1	1.78	0.65
1:C:149:THR:HG21	1:C:269:THR:HB	1.78	0.64
1:C:85:GLY:HA2	1:C:257:GLN:NE2	2.12	0.64
1:A:7:GLN:HB2	1:A:41:LYS:O	1.97	0.64
1:C:289:LYS:O	1:C:292:GLU:HG3	1.98	0.63
1:C:56:ARG:HG3	1:C:57:LEU:HD22	1.80	0.63
1:C:397:GLN:HG2	1:C:398:ARG:HG2	1.80	0.63
1:C:419:LYS:HE3	1:C:420:HIS:CD2	2.33	0.63
1:B:329:PRO:HG2	3:B:473:PAM:H52	1.81	0.63
1:A:61:ALA:HA	1:A:67:PHE:CD2	2.33	0.63
1:D:13:GLU:HG3	1:D:14:LEU:HD22	1.81	0.63
1:B:229:GLN:OE1	1:B:229:GLN:HA	1.98	0.63
1:A:224:LYS:HA	1:A:224:LYS:HE2	1.81	0.62
1:D:17:LEU:HB3	1:D:18:PRO:HD3	1.81	0.62
2:D:472:HEM:HMC2	2:D:472:HEM:HBC2	1.80	0.62
1:A:401:ILE:HG12	2:A:472:HEM:HBD2	1.80	0.62
1:C:56:ARG:HA	1:C:59:LYS:HE3	1.80	0.62
1:C:401:ILE:HG12	2:C:472:HEM:HBD2	1.82	0.62
1:B:171:HIS:HD2	1:B:173:PHE:H	1.47	0.62
1:B:275:PHE:CE2	1:B:441:PRO:HD3	2.35	0.62
1:D:364:LYS:HD3	1:D:369:ASP:HA	1.80	0.62
1:C:201:ASN:H	1:C:201:ASN:HD22	1.47	0.62
1:C:96:TRP:CD1	1:C:398:ARG:NH2	2.67	0.62
2:A:472:HEM:HMC2	2:A:472:HEM:HBC2	1.82	0.62
1:D:56:ARG:HA	1:D:59:LYS:HE3	1.82	0.62
1:D:116:HIS:HD2	1:D:408:HIS:NE2	1.98	0.61
1:C:68:ASP:HB2	1:C:336:LYS:HE2	1.82	0.61
1:B:85:GLY:HA2	1:B:257:GLN:HE22	1.63	0.61
1:B:201:ASN:H	1:B:201:ASN:HD22	1.47	0.61
1:D:201:ASN:H	1:D:201:ASN:ND2	1.98	0.61
1:B:17:LEU:HB3	1:B:18:PRO:HD3	1.81	0.61
1:C:38:GLU:OE1	1:C:56:ARG:HD2	2.00	0.61
1:C:103:LEU:HD11	1:C:237:MET:HG2	1.82	0.61
1:D:103:LEU:HD11	1:D:237:MET:HG2	1.83	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:252:GLU:HG3	1:B:255:ARG:NH2	2.16	0.61
1:B:206:GLN:HB3	1:B:210:LYS:NZ	2.16	0.61
1:C:269:THR:O	1:C:272:LEU:HB3	2.01	0.60
1:C:68:ASP:HB3	1:C:334:TYR:CE1	2.36	0.60
1:D:397:GLN:HG3	1:D:398:ARG:HG2	1.81	0.60
1:A:366:ILE:HG21	1:A:389:ALA:HB1	1.81	0.60
1:B:7:GLN:HB2	1:B:41:LYS:O	2.01	0.60
1:B:218:LYS:HE3	1:B:218:LYS:HA	1.83	0.60
1:C:434:LYS:HD3	1:C:440:LYS:HE3	1.82	0.60
1:D:401:ILE:HG12	2:D:472:HEM:HBD2	1.83	0.60
1:C:317:VAL:HG13	1:C:374:PHE:HZ	1.66	0.60
1:D:281:VAL:HG11	1:D:425:ASP:HB2	1.82	0.60
1:C:120:VAL:HG11	1:C:302:VAL:HG13	1.84	0.60
1:C:213:ASN:OD1	1:C:255:ARG:HD2	2.01	0.60
1:D:118:MET:HB3	1:D:155:LEU:HD23	1.82	0.60
1:B:201:ASN:H	1:B:201:ASN:ND2	2.00	0.60
1:D:9:LYS:HE2	1:D:19:LEU:HD21	1.82	0.60
1:A:120:VAL:HG11	1:A:302:VAL:CG1	2.30	0.60
1:C:268:THR:O	1:C:327:THR:HG21	2.02	0.60
1:C:272:LEU:HD22	2:C:472:HEM:HBB1	1.84	0.60
1:B:275:PHE:CE1	1:B:441:PRO:HG3	2.36	0.60
1:A:78:VAL:HG11	3:A:473:PAM:H152	1.82	0.60
1:A:250:ASP:O	1:A:254:ILE:HG13	2.02	0.59
1:A:149:THR:HG21	1:A:269:THR:HB	1.82	0.59
1:A:320:GLU:HB3	1:A:374:PHE:CE1	2.36	0.59
1:B:103:LEU:HD11	1:B:237:MET:CG	2.31	0.59
1:C:216:VAL:HG11	1:C:255:ARG:HG3	1.84	0.59
1:A:301:PRO:HB3	1:A:455:LEU:HA	1.84	0.59
1:B:162:PHE:HE1	1:B:215:LEU:HD21	1.67	0.59
1:C:201:ASN:ND2	1:C:201:ASN:H	2.01	0.59
1:B:5:MET:SD	1:B:39:ILE:HG12	2.42	0.59
1:B:109:GLN:O	1:B:113:LYS:HG3	2.02	0.59
1:B:403:GLN:O	1:B:407:LEU:HD22	2.03	0.59
1:D:5:MET:SD	1:D:50:ARG:HG2	2.43	0.59
1:B:118:MET:HB3	1:B:155:LEU:HD23	1.85	0.58
1:C:199:ASP:HA	1:C:202:LYS:HD2	1.84	0.58
1:B:286:VAL:HG13	1:B:313:TYR:OH	2.03	0.58
1:B:323:ARG:HG2	1:B:361:HIS:HB3	1.84	0.58
1:B:51:TYR:CE2	1:B:354:MET:HG2	2.38	0.58
1:C:207:GLU:O	1:C:211:VAL:HG23	2.03	0.58
1:A:158:PHE:HE1	1:A:237:MET:HE1	1.68	0.58
1:C:327:THR:OG1	2:C:472:HEM:HMB2	2.04	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:54:SER:O	1:A:58:ILE:HG12	2.04	0.58
1:C:54:SER:O	1:C:58:ILE:HG12	2.03	0.58
1:D:366:ILE:HG21	1:D:389:ALA:HB1	1.85	0.58
1:D:110:GLN:HA	1:D:113:LYS:HD2	1.85	0.58
1:C:305:TYR:O	1:C:309:LYS:HG2	2.04	0.57
1:C:5:MET:HG2	1:C:41:LYS:HB2	1.85	0.57
1:C:162:PHE:CE1	1:C:215:LEU:HD21	2.40	0.57
1:D:403:GLN:O	1:D:407:LEU:HD22	2.04	0.57
1:A:422:ASP:HB2	1:A:449:LYS:HB2	1.86	0.57
1:A:98:LYS:O	1:A:102:ILE:HG13	2.05	0.57
1:B:120:VAL:HG11	1:B:302:VAL:HG13	1.86	0.57
1:C:366:ILE:HG21	1:C:389:ALA:HB1	1.84	0.57
1:C:183:GLU:HG2	1:C:205:PHE:CD1	2.40	0.57
1:C:312:LYS:HG3	1:C:313:TYR:N	2.19	0.57
1:A:212:MET:HE2	1:A:263:ILE:HD11	1.87	0.57
1:B:272:LEU:HD13	1:B:322:LEU:HD13	1.87	0.57
1:C:262:LEU:O	1:C:266:HIS:HD2	1.88	0.57
1:D:192:ASN:ND2	1:D:195:ASP:HB2	2.19	0.56
1:C:208:ASP:O	1:C:212:MET:HG3	2.05	0.56
1:C:162:PHE:HE1	1:C:215:LEU:HD21	1.70	0.56
1:B:74:ALA:O	1:B:78:VAL:HG23	2.05	0.56
1:D:122:ILE:HG22	1:D:148:LEU:HD12	1.87	0.56
1:B:54:SER:OG	1:B:57:LEU:HD23	2.05	0.56
1:C:264:ALA:HB2	3:C:473:PAM:H141	1.88	0.56
1:A:5:MET:HG2	1:A:41:LYS:HB2	1.88	0.56
1:B:326:PRO:HG3	1:B:357:ILE:HG22	1.87	0.56
1:A:429:TYR:CE2	1:A:431:LEU:HA	2.41	0.56
1:D:107:PHE:CD2	1:D:401:ILE:HG22	2.41	0.56
1:C:392:PRO:HG2	1:C:393:PHE:CD2	2.41	0.56
1:B:130:TRP:CZ2	1:B:139:ILE:HD12	2.41	0.56
1:A:375:ARG:O	1:A:378:ARG:HG3	2.06	0.55
1:B:223:ARG:HH21	1:B:234:LEU:HB3	1.70	0.55
1:C:286:VAL:HG11	1:C:374:PHE:HE2	1.71	0.55
1:D:51:TYR:CE2	1:D:354:MET:HG2	2.41	0.55
1:A:17:LEU:HD22	1:A:45:PRO:HD2	1.88	0.55
1:B:181:LEU:HD22	1:B:437:LEU:HD12	1.87	0.55
1:B:375:ARG:O	1:B:378:ARG:HG3	2.06	0.55
1:C:131:GLU:HG2	1:C:421:PHE:HZ	1.70	0.55
1:B:235:THR:O	1:B:239:ASN:HB2	2.07	0.55
1:C:116:HIS:HD2	1:C:408:HIS:NE2	2.05	0.55
1:D:158:PHE:CE2	1:D:237:MET:HE1	2.42	0.55
1:B:21:ASN:HD22	1:B:21:ASN:N	2.05	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:16:ASN:HB3	1:B:19:LEU:HD12	1.88	0.55
1:B:420:HIS:O	1:B:451:LYS:HB3	2.07	0.54
1:D:130:TRP:CZ2	1:D:139:ILE:HD12	2.43	0.54
1:D:331:PHE:CD2	1:D:357:ILE:HD11	2.42	0.54
1:B:212:MET:HE2	1:B:263:ILE:HD11	1.88	0.54
1:C:91:THR:OG1	1:C:398:ARG:HD2	2.07	0.54
1:B:140:GLU:HA	1:B:445:VAL:HG12	1.90	0.54
1:B:15:LYS:HB2	1:B:44:ALA:HA	1.90	0.54
1:D:228:GLU:HG3	1:D:229:GLN:H	1.72	0.54
2:C:472:HEM:HBC2	2:C:472:HEM:HMC2	1.90	0.54
1:B:318:LEU:CD1	1:B:414:LEU:HD12	2.37	0.54
1:D:262:LEU:O	1:D:266:HIS:HD2	1.90	0.54
1:D:68:ASP:HB2	1:D:336:LYS:HE3	1.89	0.54
1:B:273:LEU:HD11	1:B:413:VAL:HG11	1.90	0.53
1:C:100:HIS:CE1	1:C:104:LEU:HD22	2.40	0.53
1:C:89:SER:O	1:C:398:ARG:NH1	2.39	0.53
1:A:8:PRO:HB2	1:A:19:LEU:HD11	1.90	0.53
1:D:436:THR:O	1:D:437:LEU:HB2	2.06	0.53
1:A:207:GLU:O	1:A:211:VAL:HG23	2.07	0.53
1:A:323:ARG:HG2	1:A:361:HIS:HB3	1.90	0.53
1:C:158:PHE:HE2	1:C:258:ILE:HG12	1.72	0.53
1:C:277:LEU:HD22	1:C:417:MET:HE1	1.90	0.53
1:C:116:HIS:HE1	1:C:303:PRO:O	1.91	0.53
1:D:66:ARG:O	1:D:336:LYS:HB2	2.08	0.53
1:C:426:HIS:CD2	1:C:446:VAL:HA	2.44	0.53
1:D:28:ALA:O	1:D:32:ILE:HG13	2.09	0.53
1:A:38:GLU:HB2	1:A:54:SER:OG	2.09	0.53
1:A:140:GLU:HA	1:A:445:VAL:HG12	1.90	0.53
1:A:280:LEU:HD21	1:A:317:VAL:CG1	2.39	0.53
1:D:237:MET:SD	1:D:257:GLN:HB2	2.49	0.53
1:A:237:MET:HE1	1:A:258:ILE:HG12	1.88	0.53
1:B:162:PHE:CE1	1:B:215:LEU:HD21	2.43	0.53
1:C:131:GLU:HG2	1:C:421:PHE:CZ	2.43	0.53
1:C:305:TYR:CE2	1:C:309:LYS:HE3	2.44	0.53
1:A:357:ILE:N	1:A:358:PRO:HD2	2.24	0.53
1:D:1:THR:HG21	1:D:3:LYS:HE2	1.90	0.53
1:B:59:LYS:HG3	1:B:60:GLU:N	2.23	0.53
1:A:223:ARG:HH21	1:A:234:LEU:HB3	1.72	0.53
1:C:387:GLN:O	1:C:388:HIS:HB2	2.09	0.52
1:C:377:GLU:O	1:C:380:GLU:HB2	2.08	0.52
1:D:5:MET:HB3	1:D:41:LYS:HZ1	1.74	0.52
1:B:334:TYR:HA	1:B:351:ASP:O	2.09	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:96:TRP:NE1	1:C:398:ARG:NH2	2.57	0.52
1:B:120:VAL:HG11	1:B:302:VAL:CG1	2.39	0.52
1:B:164:SER:O	1:B:167:ARG:HG2	2.09	0.52
1:D:305:TYR:O	1:D:309:LYS:HG2	2.09	0.52
1:C:280:LEU:HD22	1:C:287:LEU:HA	1.92	0.52
1:D:9:LYS:CE	1:D:19:LEU:HD21	2.39	0.52
1:A:364:LYS:HD2	1:A:364:LYS:N	2.23	0.52
1:D:198:TYR:O	1:D:202:LYS:HG3	2.09	0.52
1:A:112:MET:HB3	1:A:305:TYR:HE2	1.73	0.52
1:D:31:LYS:O	1:D:34:ASP:HB2	2.10	0.52
1:D:375:ARG:O	1:D:378:ARG:HG3	2.10	0.52
1:D:14:LEU:N	1:D:14:LEU:HD22	2.25	0.52
1:D:212:MET:CE	1:D:263:ILE:HD11	2.39	0.52
1:C:85:GLY:HA2	1:C:257:GLN:HE22	1.74	0.51
1:D:110:GLN:O	1:D:113:LYS:HB2	2.10	0.51
1:A:280:LEU:HD21	1:A:317:VAL:HG11	1.91	0.51
1:D:320:GLU:OE2	1:D:378:ARG:HD2	2.10	0.51
1:A:305:TYR:O	1:A:309:LYS:HG2	2.10	0.51
1:A:150:LEU:HD22	1:A:174:ILE:HD11	1.91	0.51
1:C:61:ALA:HA	1:C:67:PHE:CD2	2.45	0.51
1:C:320:GLU:OE1	1:C:374:PHE:HA	2.10	0.51
1:C:183:GLU:HG3	1:C:187:LYS:HE3	1.91	0.51
1:D:68:ASP:HB3	1:D:334:TYR:CZ	2.45	0.51
1:C:128:GLN:O	1:C:132:ARG:HG3	2.11	0.51
1:A:162:PHE:CE1	1:A:215:LEU:HD21	2.45	0.51
1:A:201:ASN:H	1:A:201:ASN:ND2	2.04	0.51
1:C:281:VAL:HG11	1:C:425:ASP:HB2	1.92	0.51
1:B:421:PHE:HB2	1:B:423:PHE:CZ	2.45	0.51
1:B:62:CYS:HB3	1:B:388:HIS:NE2	2.26	0.51
1:D:385:ILE:H	1:D:385:ILE:HD12	1.75	0.51
1:C:72:SER:O	1:C:76:LYS:HG2	2.11	0.51
1:C:42:PHE:HB3	1:C:51:TYR:HE2	1.76	0.51
1:B:278:TYR:HA	1:B:444:PHE:CZ	2.46	0.51
1:C:71:LEU:O	1:C:76:LYS:HE3	2.11	0.51
1:C:362:ARG:HH11	1:C:362:ARG:HG3	1.76	0.51
1:A:174:ILE:O	1:A:178:VAL:HG22	2.10	0.51
1:B:68:ASP:HB3	1:B:334:TYR:CZ	2.46	0.50
1:A:228:GLU:O	1:A:229:GLN:HB2	2.12	0.50
1:B:98:LYS:O	1:B:102:ILE:HG13	2.10	0.50
1:A:16:ASN:HB3	1:A:19:LEU:HD12	1.93	0.50
1:B:262:LEU:O	1:B:266:HIS:HD2	1.94	0.50
1:D:151:ASP:OD1	1:D:162:PHE:HB2	2.11	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:341:LEU:N	1:A:345:TYR:O	2.43	0.50
1:C:305:TYR:CZ	1:C:309:LYS:HE3	2.47	0.50
1:A:57:LEU:HD12	1:A:341:LEU:HG	1.94	0.50
1:A:367:TRP:HB2	1:A:371:VAL:HG12	1.94	0.50
1:A:62:CYS:HB3	1:A:388:HIS:NE2	2.27	0.50
1:C:139:ILE:HD11	1:C:446:VAL:CG2	2.41	0.50
1:A:323:ARG:CG	1:A:361:HIS:HB3	2.42	0.50
1:B:171:HIS:CD2	1:B:173:PHE:H	2.26	0.50
1:B:206:GLN:O	1:B:210:LYS:HG2	2.11	0.50
1:A:436:THR:O	1:A:437:LEU:HB2	2.12	0.50
1:A:147:ARG:CG	1:A:164:SER:HB3	2.41	0.49
1:D:334:TYR:HA	1:D:351:ASP:O	2.12	0.49
1:D:194:ASP:O	1:D:195:ASP:C	2.49	0.49
1:C:421:PHE:HB3	1:C:448:ALA:HB1	1.94	0.49
1:C:71:LEU:HB3	1:C:76:LYS:HD3	1.94	0.49
1:C:110:GLN:O	1:C:113:LYS:HB2	2.12	0.49
1:C:79:ARG:HG3	1:C:83:GLY:O	2.13	0.49
1:B:58:ILE:HG21	1:B:360:LEU:HD22	1.93	0.49
1:D:103:LEU:HD11	1:D:237:MET:CG	2.43	0.49
1:C:195:ASP:CG	1:C:196:PRO:HD2	2.33	0.49
1:D:120:VAL:O	1:D:124:VAL:HG23	2.12	0.49
1:D:39:ILE:HG13	1:D:52:LEU:HD12	1.93	0.49
1:A:305:TYR:CE1	1:A:309:LYS:HE3	2.47	0.49
1:D:7:GLN:HE22	1:D:43:GLU:HB2	1.78	0.49
1:D:120:VAL:HG11	1:D:302:VAL:CG1	2.42	0.49
1:A:347:LEU:HD13	1:A:353:LEU:HD11	1.95	0.49
1:C:235:THR:O	1:C:239:ASN:HB2	2.13	0.49
1:B:83:GLY:HA3	1:B:256:TYR:CD2	2.48	0.49
1:D:149:THR:OG1	1:D:270:SER:HB3	2.13	0.49
1:B:212:MET:CE	1:B:263:ILE:HD11	2.43	0.49
1:A:305:TYR:CZ	1:A:309:LYS:HE3	2.48	0.49
1:D:323:ARG:HA	1:D:361:HIS:HD1	1.78	0.49
1:B:132:ARG:HD2	1:D:166:TYR:CE2	2.48	0.49
1:C:334:TYR:HA	1:C:351:ASP:O	2.12	0.49
1:A:314:VAL:CG2	1:A:411:THR:HG23	2.42	0.49
1:D:373:GLU:O	1:D:378:ARG:NH2	2.46	0.48
1:A:56:ARG:NH2	1:A:342:GLY:HA3	2.27	0.48
1:A:73:GLN:HG3	1:A:77:PHE:CE2	2.48	0.48
1:C:272:LEU:HD13	1:C:322:LEU:HD13	1.94	0.48
1:D:194:ASP:O	1:D:196:PRO:N	2.46	0.48
1:D:212:MET:HE1	1:D:263:ILE:HD11	1.94	0.48
1:D:79:ARG:HG3	1:D:88:THR:HB	1.94	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:286:VAL:HG13	1:D:313:TYR:OH	2.13	0.48
1:B:340:VAL:HG22	1:B:346:PRO:HA	1.95	0.48
1:B:416:MET:O	1:B:420:HIS:HD2	1.96	0.48
1:D:305:TYR:CE2	1:D:309:LYS:HE3	2.48	0.48
1:B:131:GLU:HG2	1:B:421:PHE:CZ	2.48	0.48
1:A:334:TYR:HA	1:A:351:ASP:O	2.14	0.48
1:B:116:HIS:HE1	1:B:303:PRO:O	1.97	0.48
1:B:305:TYR:O	1:B:309:LYS:HG2	2.13	0.48
1:B:44:ALA:HB1	1:B:45:PRO:HD2	1.95	0.48
1:C:426:HIS:HD2	1:C:446:VAL:HA	1.78	0.48
1:C:109:GLN:O	1:C:113:LYS:HG3	2.13	0.48
1:A:1:THR:HG22	1:A:2:ILE:N	2.29	0.48
1:B:206:GLN:HB3	1:B:210:LYS:HZ2	1.79	0.48
1:A:388:HIS:HD2	1:A:391:LYS:HD2	1.77	0.48
1:B:94:LYS:HD2	1:B:94:LYS:N	2.29	0.48
1:A:330:ALA:HA	1:A:357:ILE:HG13	1.96	0.48
1:D:61:ALA:HA	1:D:67:PHE:CD2	2.49	0.48
1:B:58:ILE:HD12	1:B:355:VAL:HG13	1.96	0.48
1:B:366:ILE:HG23	1:B:386:PRO:HG2	1.96	0.48
1:C:204:GLN:O	1:C:207:GLU:HB3	2.14	0.48
1:B:132:ARG:HD2	1:D:166:TYR:HE2	1.78	0.47
1:D:218:LYS:N	1:D:218:LYS:HD2	2.29	0.47
1:A:130:TRP:CZ2	1:A:139:ILE:HD12	2.49	0.47
1:A:272:LEU:HD13	1:A:322:LEU:CD1	2.34	0.47
1:C:357:ILE:N	1:C:358:PRO:HD2	2.28	0.47
1:B:86:LEU:HD23	1:B:401:ILE:HG13	1.95	0.47
1:C:54:SER:OG	1:C:57:LEU:HD23	2.14	0.47
1:B:413:VAL:HG13	1:B:414:LEU:N	2.29	0.47
1:C:381:ASN:N	1:C:381:ASN:OD1	2.48	0.47
1:A:124:VAL:O	1:A:128:GLN:HG2	2.15	0.47
1:D:196:PRO:HA	1:D:199:ASP:OD1	2.14	0.47
1:D:13:GLU:O	1:D:45:PRO:HG3	2.15	0.47
1:B:318:LEU:O	1:B:322:LEU:HB2	2.14	0.47
1:B:70:ASN:HB2	1:B:334:TYR:HD1	1.80	0.47
1:B:131:GLU:HG2	1:B:421:PHE:HZ	1.79	0.47
1:B:387:GLN:O	1:B:388:HIS:HB2	2.14	0.47
1:D:323:ARG:HG2	1:D:361:HIS:HB3	1.95	0.47
1:B:128:GLN:O	1:B:132:ARG:HG3	2.14	0.47
1:C:436:THR:O	1:C:437:LEU:HB2	2.15	0.47
1:C:17:LEU:HB3	1:C:18:PRO:HD3	1.97	0.47
1:C:5:MET:CG	1:C:41:LYS:HB2	2.45	0.47
1:D:20:LEU:O	1:D:189:GLN:HG2	2.15	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:118:MET:HB3	1:C:155:LEU:HD23	1.96	0.47
1:D:327:THR:OG1	2:D:472:HEM:HMB2	2.14	0.47
1:C:257:GLN:O	1:C:261:PHE:HD1	1.98	0.47
1:D:38:GLU:HG3	1:D:39:ILE:HG22	1.96	0.47
1:C:373:GLU:O	1:C:378:ARG:NH2	2.48	0.47
1:B:429:TYR:CE2	1:B:431:LEU:HA	2.51	0.47
1:A:58:ILE:HG21	1:A:360:LEU:HD22	1.96	0.46
1:A:331:PHE:CD2	1:A:357:ILE:HD11	2.50	0.46
1:D:385:ILE:N	1:D:385:ILE:HD12	2.30	0.46
1:D:192:ASN:O	1:D:198:TYR:HE2	1.98	0.46
1:D:218:LYS:O	1:D:222:ASP:HB2	2.16	0.46
1:B:61:ALA:HA	1:B:67:PHE:CE2	2.50	0.46
1:C:68:ASP:HB3	1:C:334:TYR:CZ	2.50	0.46
1:D:331:PHE:CD2	1:D:394:GLY:HA2	2.50	0.46
1:D:305:TYR:CZ	1:D:309:LYS:HE3	2.50	0.46
1:C:356:LEU:HD23	1:C:356:LEU:HA	1.83	0.46
1:D:127:VAL:HG11	1:D:455:LEU:HD22	1.97	0.46
1:C:42:PHE:CB	1:C:51:TYR:HE2	2.29	0.46
1:D:195:ASP:O	1:D:197:ALA:N	2.49	0.46
2:B:472:HEM:CMC	2:B:472:HEM:HBC2	2.46	0.46
1:D:69:LYS:O	1:D:334:TYR:HE1	1.99	0.46
1:A:38:GLU:HG3	1:A:39:ILE:HG22	1.96	0.46
1:D:308:VAL:HG11	1:D:408:HIS:CE1	2.51	0.46
1:D:89:SER:O	1:D:398:ARG:NH1	2.46	0.46
1:B:147:ARG:HG3	1:B:164:SER:HB3	1.98	0.46
1:B:79:ARG:HH21	1:B:89:SER:HA	1.80	0.46
1:D:318:LEU:CD1	1:D:414:LEU:HD12	2.46	0.46
1:D:413:VAL:HG13	1:D:414:LEU:N	2.29	0.46
1:B:268:THR:O	1:B:327:THR:HG21	2.15	0.46
3:C:473:PAM:H111	3:C:473:PAM:H82	1.76	0.46
1:B:149:THR:HG21	1:B:266:HIS:O	2.16	0.46
1:B:2:ILE:HG23	1:B:344:GLU:O	2.15	0.46
1:C:140:GLU:HB3	1:C:143:GLU:OE1	2.16	0.46
1:B:206:GLN:HB3	1:B:210:LYS:HZ1	1.80	0.46
1:A:116:HIS:CD2	1:A:305:TYR:HA	2.50	0.46
1:B:305:TYR:CE1	1:B:309:LYS:HE3	2.51	0.46
1:A:306:LYS:N	1:A:306:LYS:HD3	2.30	0.46
1:A:86:LEU:HD11	1:A:99:ALA:CB	2.46	0.46
1:D:96:TRP:CZ2	1:D:100:HIS:HD2	2.35	0.45
1:A:162:PHE:HE1	1:A:215:LEU:HD21	1.81	0.45
1:B:141:VAL:CG1	1:B:277:LEU:HD23	2.47	0.45
1:B:250:ASP:O	1:B:254:ILE:HG13	2.16	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:301:PRO:HB2	1:C:455:LEU:HA	1.97	0.45
1:D:5:MET:HB3	1:D:41:LYS:HZ2	1.77	0.45
1:D:327:THR:O	1:D:329:PRO:HD3	2.16	0.45
1:A:340:VAL:HG22	1:A:346:PRO:HA	1.97	0.45
1:C:314:VAL:CG2	1:C:411:THR:HG23	2.46	0.45
1:A:298:LEU:HD21	1:A:311:LEU:HD11	1.98	0.45
1:C:3:LYS:HB3	1:C:3:LYS:NZ	2.31	0.45
1:C:238:LEU:HD23	1:C:254:ILE:CD1	2.37	0.45
1:C:447:LYS:HD2	1:C:448:ALA:H	1.81	0.45
1:A:335:ALA:HB3	1:A:348:GLU:O	2.17	0.45
1:A:385:ILE:N	1:A:385:ILE:HD12	2.32	0.45
1:A:410:ALA:O	1:A:414:LEU:HB2	2.17	0.45
1:C:434:LYS:HB2	1:C:442:GLU:HB2	1.97	0.45
1:B:38:GLU:HB2	1:B:54:SER:OG	2.16	0.45
1:C:419:LYS:HE3	1:C:420:HIS:NE2	2.31	0.45
1:C:324:LEU:HD12	1:C:362:ARG:NH2	2.31	0.45
1:B:289:LYS:O	1:B:292:GLU:HG2	2.16	0.45
1:B:314:VAL:O	1:B:317:VAL:HB	2.16	0.45
1:D:318:LEU:O	1:D:322:LEU:HB2	2.17	0.45
1:A:5:MET:CG	1:A:41:LYS:HB2	2.47	0.45
1:A:309:LYS:NZ	1:A:404:GLN:NE2	2.64	0.45
1:D:71:LEU:HD22	1:D:90:TRP:NE1	2.32	0.45
1:D:429:TYR:CE2	1:D:431:LEU:HA	2.51	0.45
1:A:116:HIS:HE1	1:A:303:PRO:O	1.99	0.45
1:D:249:LEU:HD13	1:D:253:ASN:OD1	2.17	0.45
1:B:281:VAL:HG11	1:B:425:ASP:HB2	1.97	0.45
1:B:233:LEU:O	1:B:237:MET:HG3	2.16	0.45
1:C:58:ILE:HD12	1:C:355:VAL:HG13	1.97	0.45
1:D:116:HIS:HD2	1:D:408:HIS:CE1	2.35	0.45
1:B:421:PHE:HB2	1:B:423:PHE:CE2	2.52	0.45
1:A:69:LYS:HD3	1:A:398:ARG:CZ	2.47	0.45
1:B:11:PHE:CD1	1:B:11:PHE:N	2.85	0.45
1:D:275:PHE:CE2	1:D:441:PRO:HD3	2.52	0.45
1:B:207:GLU:O	1:B:211:VAL:HG23	2.17	0.45
1:D:421:PHE:CE1	1:D:450:SER:HB3	2.52	0.44
1:C:375:ARG:O	1:C:378:ARG:HG3	2.16	0.44
1:B:84:ASP:HB2	1:B:89:SER:HB3	1.99	0.44
1:C:318:LEU:CD1	1:C:414:LEU:HD12	2.48	0.44
1:B:390:PHE:CE2	1:B:392:PRO:HG3	2.52	0.44
1:B:253:ASN:O	1:B:257:GLN:HG2	2.18	0.44
1:C:55:GLN:O	1:C:59:LYS:HG2	2.16	0.44
1:D:392:PRO:HG2	1:D:393:PHE:CD2	2.52	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:207:GLU:O	1:D:211:VAL:HG23	2.18	0.44
1:D:196:PRO:HA	1:D:199:ASP:CG	2.38	0.44
1:D:85:GLY:HA2	1:D:257:GLN:NE2	2.31	0.44
1:C:17:LEU:HD22	1:C:45:PRO:HD2	1.98	0.44
1:D:237:MET:SD	1:D:257:GLN:CB	3.06	0.44
1:B:305:TYR:CZ	1:B:309:LYS:HE3	2.52	0.44
1:D:198:TYR:HA	1:D:201:ASN:ND2	2.32	0.44
1:D:227:GLY:O	1:D:228:GLU:HB2	2.17	0.44
1:A:8:PRO:HB2	1:A:19:LEU:CD1	2.48	0.44
1:C:54:SER:OG	1:C:57:LEU:CD2	2.65	0.44
1:B:298:LEU:HD22	1:B:303:PRO:HG3	1.99	0.44
1:C:5:MET:HG2	1:C:41:LYS:HE3	1.99	0.44
1:C:247:GLU:HA	1:C:248:PRO:HD3	1.70	0.44
1:A:54:SER:OG	1:A:57:LEU:HD23	2.18	0.44
1:C:69:LYS:HD3	1:C:398:ARG:HD3	2.00	0.44
1:B:63:ASP:OD1	1:B:66:ARG:HB2	2.18	0.44
1:C:385:ILE:HA	1:C:386:PRO:HD3	1.85	0.44
1:C:429:TYR:CD2	1:C:444:PHE:CD1	3.06	0.44
1:D:388:HIS:HD2	1:D:391:LYS:HD2	1.82	0.44
1:D:320:GLU:OE1	1:D:374:PHE:HA	2.18	0.43
1:C:402:GLY:HA3	2:C:472:HEM:C3C	2.53	0.43
1:C:303:PRO:HA	1:C:307:GLN:OE1	2.18	0.43
1:A:293:GLU:OE2	1:A:311:LEU:HA	2.18	0.43
1:A:397:GLN:HG3	1:A:398:ARG:HG2	1.99	0.43
1:D:434:LYS:HB2	1:D:442:GLU:HB2	2.00	0.43
1:C:286:VAL:HG11	1:C:374:PHE:CE2	2.53	0.43
1:C:116:HIS:HD2	1:C:408:HIS:CE1	2.35	0.43
1:B:83:GLY:HA3	1:B:256:TYR:CE2	2.53	0.43
1:C:344:GLU:O	1:C:346:PRO:HD3	2.17	0.43
1:B:129:LYS:O	1:B:133:LEU:HD13	2.17	0.43
1:B:5:MET:SD	1:B:6:PRO:HD2	2.59	0.43
1:D:130:TRP:CZ3	1:D:417:MET:HG2	2.53	0.43
1:A:283:ASN:HA	1:A:284:PRO:HD2	1.79	0.43
1:C:198:TYR:HA	1:C:201:ASN:HD22	1.80	0.43
1:D:308:VAL:HG11	1:D:408:HIS:ND1	2.33	0.43
1:A:212:MET:CE	1:A:263:ILE:HD11	2.47	0.43
1:A:218:LYS:HA	1:A:218:LYS:HE2	2.00	0.43
1:B:171:HIS:HD2	1:B:173:PHE:N	2.15	0.43
1:B:275:PHE:O	1:B:278:TYR:HB3	2.19	0.43
1:A:124:VAL:O	1:A:128:GLN:CG	2.67	0.43
1:D:387:GLN:O	1:D:388:HIS:HB2	2.18	0.43
1:A:253:ASN:O	1:A:257:GLN:HG2	2.19	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:122:ILE:O	1:B:125:GLN:HB2	2.18	0.43
1:A:373:GLU:O	1:A:378:ARG:NH2	2.52	0.43
1:D:416:MET:O	1:D:420:HIS:HD2	2.02	0.43
1:D:402:GLY:HA3	2:D:472:HEM:C3C	2.53	0.43
1:C:96:TRP:CZ2	1:C:100:HIS:HD2	2.37	0.43
1:A:67:PHE:CD1	1:A:335:ALA:HA	2.54	0.43
1:A:286:VAL:HG13	1:A:313:TYR:OH	2.18	0.43
1:D:5:MET:HB2	1:D:5:MET:HE2	1.96	0.43
1:D:86:LEU:HB3	2:D:472:HEM:HAD1	2.01	0.43
1:C:322:LEU:HA	1:C:322:LEU:HD12	1.80	0.43
1:D:54:SER:O	1:D:58:ILE:HG12	2.18	0.43
1:D:298:LEU:HB2	1:D:419:LYS:HD2	2.01	0.43
1:D:116:HIS:CD2	1:D:408:HIS:NE2	2.82	0.43
1:C:278:TYR:HA	1:C:444:PHE:CZ	2.54	0.43
1:A:129:LYS:O	1:A:133:LEU:HD13	2.19	0.43
1:C:238:LEU:CD2	1:C:254:ILE:HG21	2.49	0.42
1:D:201:ASN:ND2	1:D:201:ASN:N	2.65	0.42
1:D:116:HIS:HE1	1:D:303:PRO:O	2.02	0.42
1:C:228:GLU:CG	1:C:229:GLN:H	2.32	0.42
1:A:171:HIS:CD2	1:A:173:PHE:H	2.21	0.42
1:B:341:LEU:N	1:B:345:TYR:O	2.52	0.42
1:A:320:GLU:OE1	1:A:374:PHE:HA	2.19	0.42
1:D:393:PHE:CZ	1:D:407:LEU:HD21	2.54	0.42
1:C:140:GLU:HA	1:C:445:VAL:HG12	2.00	0.42
1:C:147:ARG:NH1	1:C:167:ARG:O	2.53	0.42
1:D:356:LEU:HD23	1:D:356:LEU:HA	1.90	0.42
1:D:77:PHE:HE2	1:D:188:LEU:HD23	1.84	0.42
1:A:409:GLU:O	1:A:413:VAL:HG12	2.19	0.42
1:D:160:TYR:CE2	1:D:215:LEU:HD11	2.55	0.42
1:D:272:LEU:HD22	2:D:472:HEM:HBB1	2.00	0.42
1:C:147:ARG:HD2	1:C:165:PHE:CD1	2.54	0.42
1:B:313:TYR:O	1:B:316:MET:HB2	2.19	0.42
1:A:138:HIS:HB2	1:A:446:VAL:O	2.19	0.42
1:B:330:ALA:HB3	3:B:473:PAM:H51	2.02	0.42
1:D:377:GLU:H	1:D:377:GLU:CD	2.22	0.42
1:A:164:SER:O	1:A:167:ARG:HG2	2.20	0.42
1:A:56:ARG:NH2	1:A:342:GLY:CA	2.83	0.42
1:D:96:TRP:CD1	1:D:398:ARG:NH2	2.87	0.42
1:D:70:ASN:HB2	1:D:334:TYR:HD1	1.85	0.42
1:D:129:LYS:HE2	1:D:144:ASP:OD1	2.20	0.42
1:C:242:ASP:HA	1:C:243:PRO:HD3	1.93	0.42
1:C:77:PHE:CE2	1:C:188:LEU:HD23	2.55	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:275:PHE:CZ	1:B:441:PRO:HD3	2.55	0.42
1:D:15:LYS:HB3	1:D:43:GLU:O	2.20	0.42
1:C:29:LEU:HB3	1:C:356:LEU:HD11	2.01	0.42
1:A:271:GLY:HA2	1:A:440:LYS:HG3	2.01	0.42
1:D:183:GLU:OE1	1:D:190:ARG:NH2	2.53	0.42
1:A:57:LEU:HA	1:A:57:LEU:HD13	1.86	0.42
1:C:120:VAL:O	1:C:124:VAL:HG23	2.20	0.42
1:A:149:THR:HG22	1:A:266:HIS:HA	2.02	0.42
1:A:449:LYS:HD3	1:A:449:LYS:HA	1.76	0.42
1:B:141:VAL:HG11	1:B:277:LEU:HD23	2.02	0.42
1:C:410:ALA:O	1:C:414:LEU:HB2	2.20	0.42
1:C:278:TYR:CZ	1:C:431:LEU:HB2	2.55	0.42
1:C:69:LYS:HD3	1:C:398:ARG:NH1	2.35	0.41
1:C:149:THR:HG21	1:C:266:HIS:O	2.20	0.41
1:A:103:LEU:HD11	1:A:237:MET:CG	2.45	0.41
1:B:311:LEU:HB3	1:B:314:VAL:HG22	2.01	0.41
1:A:169:GLN:HA	1:A:170:PRO:HD3	1.86	0.41
1:B:434:LYS:HD3	1:B:440:LYS:HZ2	1.85	0.41
1:B:71:LEU:HD21	1:B:88:THR:O	2.20	0.41
1:C:309:LYS:HA	1:C:309:LYS:HD3	1.89	0.41
1:D:130:TRP:HZ3	1:D:417:MET:HG2	1.85	0.41
1:D:71:LEU:O	1:D:76:LYS:HE3	2.20	0.41
1:B:126:LEU:HD11	1:B:145:MET:CE	2.50	0.41
1:D:335:ALA:HB3	1:D:348:GLU:O	2.19	0.41
1:B:13:GLU:HG3	1:B:14:LEU:CD2	2.42	0.41
1:D:233:LEU:O	1:D:237:MET:HG3	2.21	0.41
1:A:67:PHE:CE1	1:A:335:ALA:HA	2.55	0.41
1:C:318:LEU:HD13	1:C:414:LEU:HD12	2.02	0.41
1:B:150:LEU:HD22	1:B:174:ILE:HD11	2.02	0.41
1:B:58:ILE:HG21	1:B:360:LEU:CD2	2.50	0.41
1:D:273:LEU:HD11	1:D:413:VAL:HG11	2.03	0.41
1:B:71:LEU:HD12	1:B:71:LEU:HA	1.91	0.41
1:A:280:LEU:HB3	1:A:287:LEU:HG	2.03	0.41
1:D:77:PHE:CE2	1:D:188:LEU:HD23	2.56	0.41
1:C:77:PHE:HE2	1:C:188:LEU:HD23	1.84	0.41
1:C:347:LEU:HD13	1:C:353:LEU:HD11	2.03	0.41
1:A:262:LEU:HA	1:A:262:LEU:HD23	1.91	0.41
1:B:110:GLN:O	1:B:113:LYS:HB2	2.21	0.41
1:C:218:LYS:HB2	1:C:218:LYS:HE3	1.93	0.41
2:D:472:HEM:HBC2	2:D:472:HEM:CMC	2.51	0.41
1:B:436:THR:O	1:B:437:LEU:HB2	2.21	0.41
1:A:85:GLY:HA2	1:A:257:GLN:NE2	2.36	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:242:ASP:O	1:C:246:GLY:N	2.49	0.41
1:C:26:VAL:O	1:C:30:MET:HG3	2.21	0.41
1:A:110:GLN:O	1:A:113:LYS:HB2	2.19	0.41
1:D:175:THR:O	1:D:178:VAL:HG22	2.21	0.41
1:D:247:GLU:HA	1:D:248:PRO:HD3	1.76	0.41
1:A:158:PHE:HE1	1:A:237:MET:CE	2.33	0.41
1:D:96:TRP:CZ2	1:D:100:HIS:CD2	3.08	0.41
1:B:146:THR:HG23	1:B:266:HIS:CE1	2.56	0.41
1:B:129:LYS:HE2	1:B:144:ASP:OD2	2.21	0.41
1:A:81:PHE:HB3	1:A:209:ILE:HG12	2.02	0.41
1:B:345:TYR:HA	1:B:346:PRO:HD3	1.88	0.41
1:D:421:PHE:HB3	1:D:448:ALA:HB1	2.02	0.41
1:B:318:LEU:HD11	1:B:414:LEU:HD12	2.02	0.41
1:A:289:LYS:HB3	1:A:313:TYR:CE2	2.55	0.41
1:A:119:MET:SD	1:A:408:HIS:HD2	2.44	0.41
1:A:141:VAL:HG11	1:A:444:PHE:CE2	2.55	0.41
1:C:149:THR:HG22	1:C:266:HIS:HA	2.02	0.40
1:D:344:GLU:O	1:D:346:PRO:HD3	2.21	0.40
1:A:281:VAL:HG13	1:A:425:ASP:HB2	2.02	0.40
1:A:268:THR:O	1:A:327:THR:HG21	2.22	0.40
1:D:22:THR:OG1	1:D:23:ASP:N	2.54	0.40
1:C:183:GLU:O	1:C:187:LYS:HG3	2.21	0.40
1:A:276:ALA:O	1:A:280:LEU:HG	2.21	0.40
1:C:327:THR:O	1:C:329:PRO:HD3	2.21	0.40
1:D:340:VAL:HG22	1:D:346:PRO:HA	2.04	0.40
1:C:320:GLU:HG3	1:C:376:PRO:N	2.36	0.40
1:B:286:VAL:CG1	1:B:376:PRO:HG2	2.52	0.40
1:C:20:LEU:HA	1:C:20:LEU:HD12	1.79	0.40
1:D:147:ARG:NH1	1:D:167:ARG:O	2.54	0.40
1:A:149:THR:HG21	1:A:266:HIS:O	2.22	0.40
1:B:149:THR:HG22	1:B:266:HIS:HA	2.03	0.40
1:B:335:ALA:HB3	1:B:348:GLU:O	2.21	0.40
1:A:244:GLU:O	1:A:244:GLU:HG2	2.21	0.40
1:C:317:VAL:HG13	1:C:374:PHE:CZ	2.53	0.40
1:D:118:MET:O	1:D:121:ASP:HB3	2.20	0.40
1:D:9:LYS:HE2	1:D:19:LEU:CD2	2.49	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	453/471 (96%)	411 (91%)	39 (9%)	3 (1%)	30	62
1	B	453/471 (96%)	397 (88%)	52 (12%)	4 (1%)	25	55
1	C	453/471 (96%)	412 (91%)	38 (8%)	3 (1%)	30	62
1	D	453/471 (96%)	404 (89%)	42 (9%)	7 (2%)	15	38
All	All	1812/1884 (96%)	1624 (90%)	171 (9%)	17 (1%)	25	55

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	135	ALA
1	D	135	ALA
1	D	196	PRO
1	B	135	ALA
1	A	135	ALA
1	A	229	GLN
1	D	141	VAL
1	D	229	GLN
1	A	141	VAL
1	B	426	HIS
1	D	454	PRO
1	D	227	GLY
1	B	141	VAL
1	D	371	VAL
1	B	371	VAL
1	C	141	VAL
1	C	371	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	399/412 (97%)	373 (94%)	26 (6%)	24	51
1	B	399/412 (97%)	363 (91%)	36 (9%)	14	31
1	C	399/412 (97%)	370 (93%)	29 (7%)	20	44
1	D	399/412 (97%)	376 (94%)	23 (6%)	28	57
All	All	1596/1648 (97%)	1482 (93%)	114 (7%)	21	46

All (114) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	56	ARG
1	A	57	LEU
1	A	64	GLU
1	A	94	LYS
1	A	103	LEU
1	A	126	LEU
1	A	134	ASN
1	A	148	LEU
1	A	149	THR
1	A	172	PRO
1	A	195	ASP
1	A	200	GLU
1	A	201	ASN
1	A	233	LEU
1	A	235	THR
1	A	255	ARG
1	A	266	HIS
1	A	289	LYS
1	A	293	GLU
1	A	318	LEU
1	A	338	ASP
1	A	364	LYS
1	A	387	GLN
1	A	407	LEU
1	A	414	LEU
1	B	7	GLN
1	B	21	ASN
1	B	53	SER
1	B	56	ARG
1	B	64	GLU
1	B	71	LEU
1	B	87	PHE

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Mol	Chain	Res	Type
1	B	88	THR
1	B	94	LYS
1	B	109	GLN
1	B	126	LEU
1	B	134	ASN
1	B	139	ILE
1	B	149	THR
1	B	151	ASP
1	B	192	ASN
1	B	201	ASN
1	B	218	LYS
1	B	229	GLN
1	B	233	LEU
1	B	239	ASN
1	B	247	GLU
1	B	250	ASP
1	B	266	HIS
1	B	293	GLU
1	B	318	LEU
1	B	324	LEU
1	B	337	GLU
1	B	338	ASP
1	B	349	LYS
1	B	385	ILE
1	B	404	GLN
1	B	407	LEU
1	B	414	LEU
1	B	430	GLU
1	B	444	PHE
1	C	7	GLN
1	C	20	LEU
1	C	47	ARG
1	C	57	LEU
1	C	88	THR
1	C	103	LEU
1	C	109	GLN
1	C	126	LEU
1	C	134	ASN
1	C	149	THR
1	C	151	ASP
1	C	168	ASP
1	C	192	ASN

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Mol	Chain	Res	Type
1	C	201	ASN
1	C	228	GLU
1	C	230	SER
1	C	233	LEU
1	C	266	HIS
1	C	293	GLU
1	C	318	LEU
1	C	320	GLU
1	C	338	ASP
1	C	364	LYS
1	C	375	ARG
1	C	383	SER
1	C	404	GLN
1	C	407	LEU
1	C	414	LEU
1	C	452	LYS
1	D	1	THR
1	D	2	ILE
1	D	7	GLN
1	D	56	ARG
1	D	88	THR
1	D	103	LEU
1	D	126	LEU
1	D	134	ASN
1	D	148	LEU
1	D	149	THR
1	D	167	ARG
1	D	201	ASN
1	D	226	SER
1	D	228	GLU
1	D	229	GLN
1	D	233	LEU
1	D	266	HIS
1	D	293	GLU
1	D	324	LEU
1	D	337	GLU
1	D	407	LEU
1	D	414	LEU
1	D	430	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	100	HIS
1	A	109	GLN
1	A	116	HIS
1	A	134	ASN
1	A	171	HIS
1	A	192	ASN
1	A	201	ASN
1	A	204	GLN
1	A	239	ASN
1	A	403	GLN
1	A	404	GLN
1	A	408	HIS
1	A	426	HIS
1	B	7	GLN
1	B	21	ASN
1	B	27	GLN
1	B	100	HIS
1	B	116	HIS
1	B	171	HIS
1	B	201	ASN
1	B	239	ASN
1	B	266	HIS
1	B	307	GLN
1	B	310	GLN
1	B	403	GLN
1	C	7	GLN
1	C	21	ASN
1	C	27	GLN
1	C	100	HIS
1	C	116	HIS
1	C	171	HIS
1	C	192	ASN
1	C	201	ASN
1	C	204	GLN
1	C	239	ASN
1	C	310	GLN
1	C	403	GLN
1	C	426	HIS
1	D	7	GLN
1	D	92	HIS
1	D	100	HIS
1	D	116	HIS

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Mol	Chain	Res	Type
1	D	134	ASN
1	D	201	ASN
1	D	388	HIS
1	D	403	GLN
1	D	420	HIS
1	D	426	HIS

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	A	472	1	49,50,50	2.26	11 (22%)	46,82,82	1.37	7 (15%)
3	PAM	A	473	-	17,17,17	0.60	0	17,17,17	0.83	0
2	HEM	B	472	1	49,50,50	2.74	12 (24%)	46,82,82	1.27	6 (13%)
3	PAM	B	473	-	17,17,17	0.61	0	17,17,17	0.68	0
2	HEM	C	472	1	49,50,50	2.12	9 (18%)	46,82,82	1.35	5 (10%)
3	PAM	C	473	-	17,17,17	0.64	0	17,17,17	0.56	0
2	HEM	D	472	1	49,50,50	2.25	8 (16%)	46,82,82	1.39	7 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PAM	D	473	-	17,17,17	0.58	0	17,17,17	0.72	0

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	A	472	1	-	0/14/114/114	0/0/8/8
3	PAM	A	473	-	-	0/15/15/15	0/0/0/0
2	HEM	B	472	1	-	0/14/114/114	0/0/8/8
3	PAM	B	473	-	-	0/15/15/15	0/0/0/0
2	HEM	C	472	1	-	0/14/114/114	0/0/8/8
3	PAM	C	473	-	-	0/15/15/15	0/0/0/0
2	HEM	D	472	1	-	0/14/114/114	0/0/8/8
3	PAM	D	473	-	-	0/15/15/15	0/0/0/0

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	472	HEM	C2B-C1B	12.86	1.47	1.44
2	D	472	HEM	C2B-C1B	10.33	1.47	1.44
2	C	472	HEM	C2B-C1B	8.87	1.46	1.44
2	A	472	HEM	C2B-C1B	7.75	1.46	1.44
2	A	472	HEM	C3D-C2D	-6.71	1.32	1.43
2	B	472	HEM	C3D-C2D	-6.13	1.33	1.43
2	D	472	HEM	C3D-C2D	-5.62	1.33	1.43
2	B	472	HEM	C3D-C4D	-5.52	1.43	1.44
2	A	472	HEM	C2D-C1D	-4.88	1.43	1.44
2	C	472	HEM	C3D-C2D	-4.87	1.35	1.43
2	C	472	HEM	C4A-C3A	4.62	1.45	1.40
2	A	472	HEM	C4A-C3A	4.57	1.45	1.40
2	D	472	HEM	C4A-C3A	4.49	1.45	1.40
2	C	472	HEM	C2D-C1D	4.43	1.45	1.44
2	A	472	HEM	C3D-C4D	-4.16	1.43	1.44
2	B	472	HEM	C4A-C3A	4.07	1.45	1.40
2	B	472	HEM	C3C-C2C	-4.01	1.36	1.43
2	B	472	HEM	C3B-C2B	-3.87	1.37	1.43
2	D	472	HEM	C3C-C2C	-3.77	1.37	1.43
2	D	472	HEM	C3B-C2B	-3.73	1.37	1.43
2	A	472	HEM	C3B-C4B	3.55	1.48	1.44
2	A	472	HEM	C3C-C2C	-3.25	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	472	HEM	C3B-C4B	3.21	1.48	1.44
2	A	472	HEM	CHC-C1C	3.20	1.42	1.36
2	D	472	HEM	C3B-C4B	3.09	1.48	1.44
2	C	472	HEM	CHC-C1C	3.07	1.42	1.36
2	A	472	HEM	C3B-C2B	-3.03	1.38	1.43
2	C	472	HEM	C3B-C2B	-3.03	1.38	1.43
2	B	472	HEM	CHB-C1B	2.74	1.39	1.35
2	C	472	HEM	CHB-C1B	2.72	1.39	1.35
2	C	472	HEM	C3C-C2C	-2.72	1.39	1.43
2	B	472	HEM	C4C-NC	2.55	1.41	1.38
2	B	472	HEM	CHD-C4C	2.49	1.40	1.36
2	D	472	HEM	CHD-C4C	2.34	1.40	1.36
2	A	472	HEM	CMC-C2C	2.31	1.54	1.47
2	B	472	HEM	CMB-C2B	2.30	1.54	1.47
2	C	472	HEM	CMB-C2B	2.24	1.54	1.47
2	B	472	HEM	C2D-C1D	-2.23	1.44	1.44
2	D	472	HEM	CMB-C2B	2.02	1.53	1.47
2	A	472	HEM	CHA-C4D	2.01	1.38	1.35

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	472	HEM	C3B-C4B-NB	-3.73	111.33	114.00
2	C	472	HEM	C3A-C4A-NA	3.63	112.15	109.41
2	D	472	HEM	C3B-C4B-NB	-3.45	111.53	114.00
2	A	472	HEM	CBD-CAD-C3D	-3.38	106.99	114.37
2	C	472	HEM	C3B-C4B-NB	-3.27	111.66	114.00
2	B	472	HEM	CHC-C4B-NB	-2.98	122.11	124.58
2	C	472	HEM	C4A-NA-C1A	-2.86	103.00	106.76
2	B	472	HEM	C3A-C4A-NA	2.78	111.51	109.41
2	D	472	HEM	CBD-CAD-C3D	-2.78	108.31	114.37
2	D	472	HEM	C4A-NA-C1A	-2.77	103.12	106.76
2	C	472	HEM	CBD-CAD-C3D	-2.76	108.36	114.37
2	C	472	HEM	C1A-CHA-C4D	-2.70	123.92	127.47
2	B	472	HEM	CBD-CAD-C3D	-2.69	108.50	114.37
2	D	472	HEM	CHC-C4B-NB	-2.66	122.38	124.58
2	B	472	HEM	C1A-CHA-C4D	-2.55	124.11	127.47
2	A	472	HEM	C4A-NA-C1A	-2.53	103.43	106.76
2	B	472	HEM	C3B-C4B-NB	-2.50	112.21	114.00
2	D	472	HEM	C2A-C1A-NA	2.46	113.15	109.73
2	B	472	HEM	C4A-NA-C1A	-2.45	103.54	106.76
2	A	472	HEM	CHC-C4B-NB	-2.44	122.55	124.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	472	HEM	C3A-C4A-NA	2.41	111.23	109.41
2	A	472	HEM	C1A-CHA-C4D	-2.30	124.45	127.47
2	D	472	HEM	C1B-NB-C4B	-2.10	103.02	105.16
2	A	472	HEM	C3A-C4A-NA	2.06	110.97	109.41
2	A	472	HEM	C1B-NB-C4B	-2.04	103.08	105.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	455/471 (96%)	-0.18	5 (1%) 77 82	18, 45, 84, 100	0
1	B	455/471 (96%)	0.08	16 (3%) 42 47	26, 54, 89, 100	0
1	C	455/471 (96%)	0.09	17 (3%) 39 44	25, 56, 89, 100	0
1	D	455/471 (96%)	-0.07	6 (1%) 74 79	22, 50, 90, 100	0
All	All	1820/1884 (96%)	-0.02	44 (2%) 56 62	18, 52, 89, 100	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	228	GLU	5.0
1	B	229	GLN	4.6
1	D	229	GLN	4.6
1	C	191	ALA	4.3
1	C	229	GLN	3.6
1	B	240	GLY	3.4
1	B	350	GLY	3.4
1	D	109	GLN	3.4
1	B	288	GLN	3.4
1	C	227	GLY	3.3
1	C	16	ASN	3.1
1	C	370	ASP	3.0
1	A	136	ASP	3.0
1	A	448	ALA	2.8
1	D	228	GLU	2.8
1	D	306	LYS	2.8
1	C	245	THR	2.8
1	C	349	LYS	2.7
1	C	192	ASN	2.7
1	B	455	LEU	2.7
1	C	170	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	369	ASP	2.5
1	B	284	PRO	2.4
1	B	291	ALA	2.4
1	B	285	HIS	2.4
1	B	68	ASP	2.4
1	B	2	ILE	2.3
1	C	35	GLU	2.3
1	A	197	ALA	2.3
1	B	387	GLN	2.3
1	A	353	LEU	2.3
1	B	1	THR	2.3
1	B	86	LEU	2.3
1	D	389	ALA	2.3
1	B	373	GLU	2.3
1	C	381	ASN	2.3
1	C	243	PRO	2.2
1	A	364	LYS	2.1
1	D	13	GLU	2.1
1	C	244	GLU	2.1
1	B	260	THR	2.0
1	C	110	GLN	2.0
1	B	306	LYS	2.0
1	C	8	PRO	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	PAM	C	473	18/18	0.32	4.27	58,69,96,99	0
3	PAM	B	473	18/18	0.27	2.03	45,52,77,80	0
3	PAM	A	473	18/18	0.23	1.79	28,48,80,83	0
3	PAM	D	473	18/18	0.22	1.72	31,49,64,66	0
2	HEM	A	472	43/43	0.14	-0.35	15,30,46,51	0
2	HEM	C	472	43/43	0.15	-0.65	19,38,52,56	0
2	HEM	B	472	43/43	0.14	-0.68	19,29,54,68	0
2	HEM	D	472	43/43	0.10	-1.65	15,30,44,68	0

6.5 Other polymers ⓘ

There are no such residues in this entry.