Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:16 AM GMT

PDB ID : 2CA0

Title : CRYSTAL STRUCTURE OF YC-17-BOUND CYTOCHROME P450 PIKC (CYP107L1)

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Deposited on : 2005-12-15

Resolution : 2.85 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.85 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.
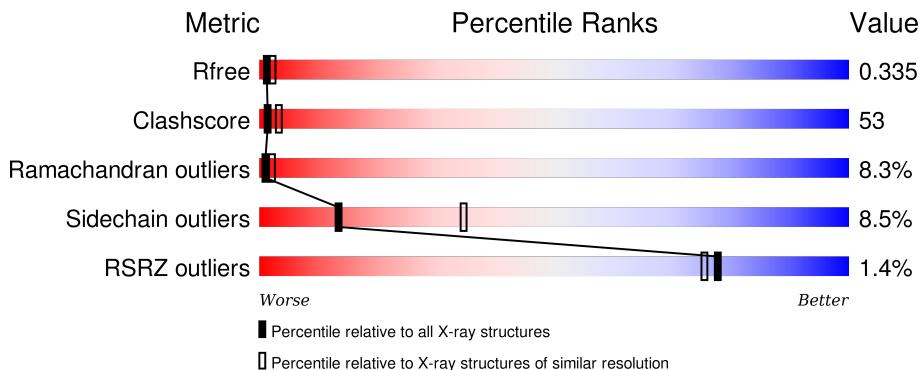
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2228 (2.90-2.82)
Clashscore	102246	2499 (2.90-2.82)
Ramachandran outliers	100387	2439 (2.90-2.82)
Sidechain outliers	100360	2442 (2.90-2.82)
RSRZ outliers	91569	2236 (2.90-2.82)

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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	436	2% 29% 52% 8% 10%
1	B	436	% 24% 55% 10% · 10%
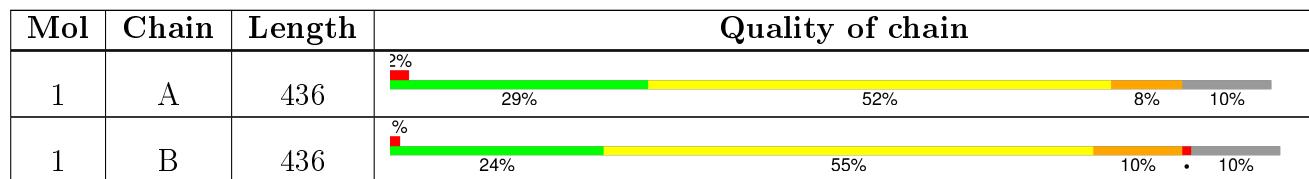
2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6269 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called CYTOCHROME P450 MONOOXYGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	393	Total 3028	C 1910	N 544	O 561	S 13	0	0	0
1	B	393	Total 3028	C 1910	N 544	O 561	S 13	0	0	0

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).
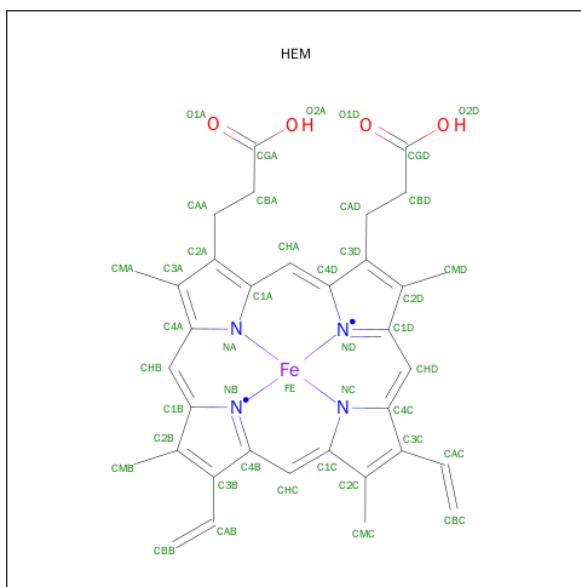
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is 4-{[4-(DIMETHYLAMINO)-3-HYDROXY-6-METHYLTETRAHYDRO-2H-PYRAN-2-YL]OXY}-12-ETHYL-3,5,7,11-TETRAMETHYLOXACYCLODODEC-9-ENE-2,8-DIONE (three-letter code: PXI) (formula: $C_{25}H_{43}NO_6$).
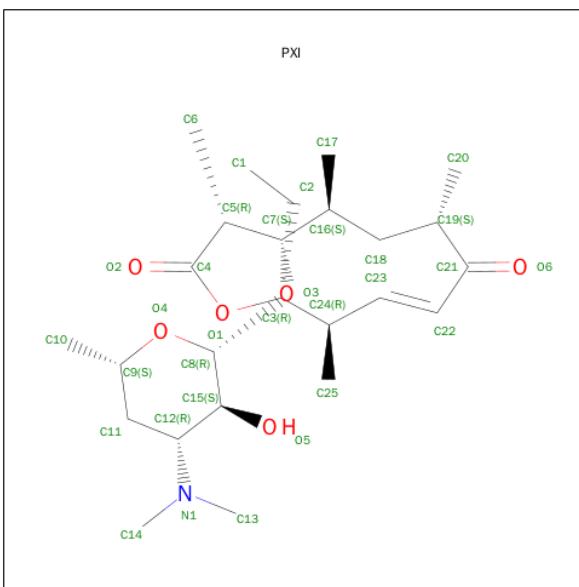
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			32	25	1	6		
3	B	1	Total	C	N	O	0	0
			32	25	1	6		

• Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	33	Total	O	0	0
			33	33		
4	B	30	Total	O	0	0
			30	30		

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 MONOOXYGENASE
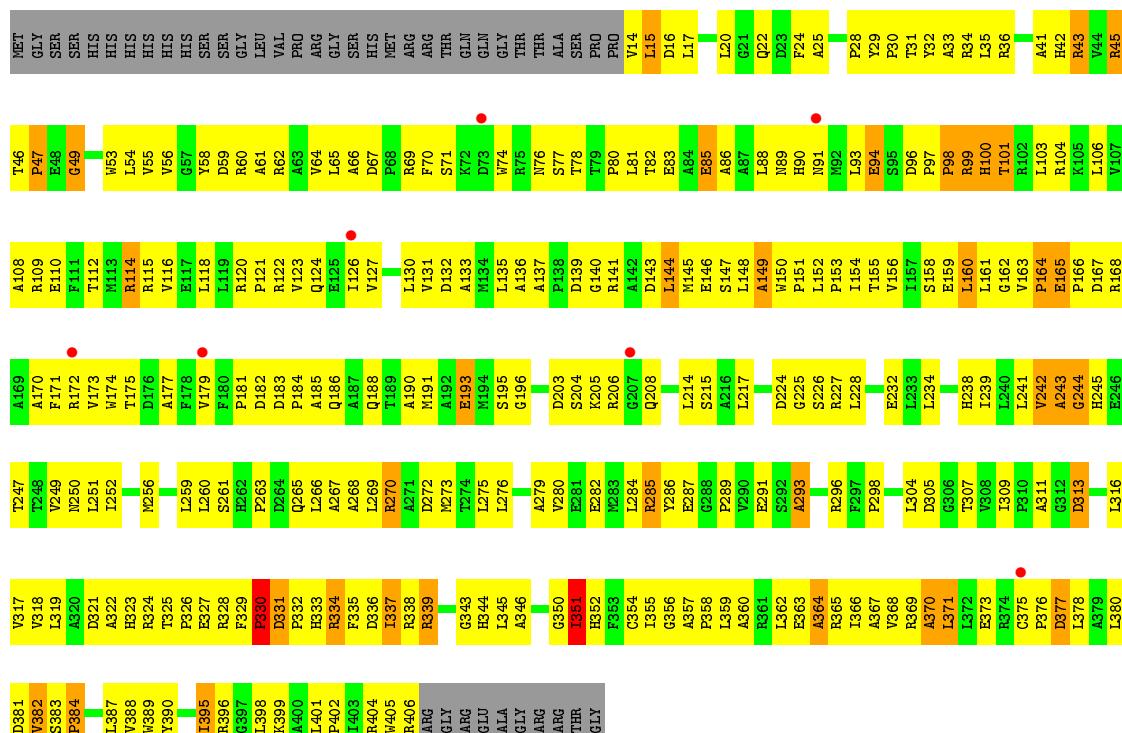
- Molecule 1: CYTOCHROME P450 MONOOXYGENASE
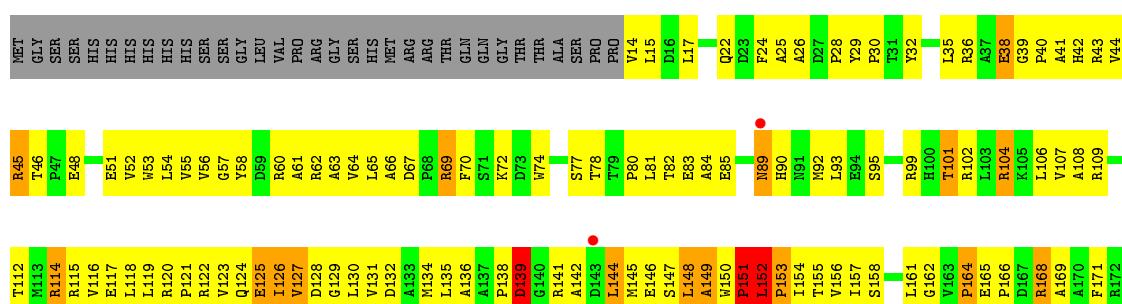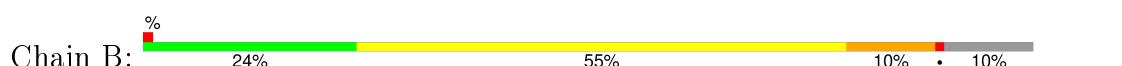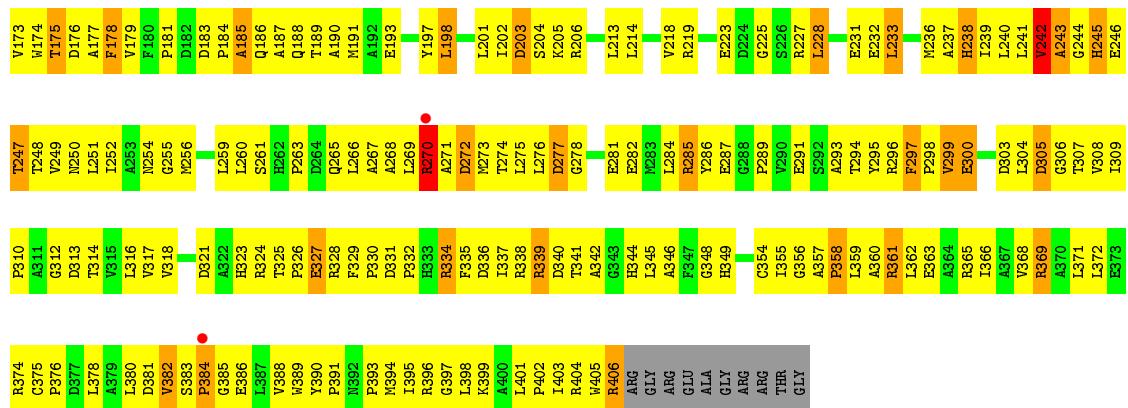
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	61.09Å 91.97Å 68.90Å 90.00° 89.92° 90.00°	Depositor
Resolution (Å)	32.41 – 2.85 45.74 – 2.85	Depositor EDS
% Data completeness (in resolution range)	92.5 (32.41-2.85) 92.2 (45.74-2.85)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.51 (at 2.86Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.240 , 0.338 0.238 , 0.335	Depositor DCC
R_{free} test set	1674 reflections (11.27%)	DCC
Wilson B-factor (Å^2)	31.9	Xtriage
Anisotropy	0.519	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 16.7	EDS
Estimated twinning fraction	0.427 for h,-k,-l	Xtriage
L-test for twinning[2]	$< |L| > = 0.40$, $< L^2 > = 0.22$	Xtriage
Outliers	0 of 16667 reflections	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	6269	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.78% of the height of the origin peak. No significant pseudotranslation is detected.*

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

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.43	0/3098	0.68	0/4229
1	B	0.41	0/3098	0.71	0/4229
All	All	0.42	0/6196	0.70	0/8458

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	3028	0	2986	314	0
1	B	3028	0	2986	342	0
2	A	43	0	30	3	0
2	B	43	0	30	5	0
3	A	32	0	43	1	0
3	B	32	0	43	7	0
4	A	33	0	0	9	0
4	B	30	0	0	9	0
All	All	6269	0	6118	656	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 53.

All (656) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:55:VAL:HG11	1:B:64:VAL:HG21	1.41	1.03
1:B:285:ARG:HH11	1:B:285:ARG:HB3	1.25	1.01
1:A:285:ARG:HH21	1:A:286:TYR:HA	1.26	1.00
1:A:152:LEU:HB3	1:A:153:PRO:HD3	1.48	0.95
1:B:266:LEU:O	1:B:270:ARG:HB2	1.70	0.92
1:A:45:ARG:HH21	1:A:49:GLY:H	1.02	0.92
1:A:91:ASN:HD21	1:A:94:GLU:HG3	1.30	0.92
1:B:121:PRO:O	1:B:125:GLU:HG3	1.70	0.92
1:A:167:ASP:HB2	4:A:2015:HOH:O	1.69	0.91
1:A:97:PRO:HA	1:A:98:PRO:O	1.70	0.91
1:A:141:ARG:HB2	1:A:141:ARG:HH11	1.34	0.90
1:B:265:GLN:HE21	1:B:337:ILE:H	1.20	0.89
1:A:395:ILE:HG22	1:A:396:ARG:H	1.36	0.89
1:B:380:LEU:HD21	1:B:401:LEU:HD11	1.54	0.88
1:B:252:ILE:O	1:B:256:MET:HG2	1.72	0.88
1:A:29:TYR:OH	1:A:287:GLU:HG2	1.72	0.87
1:A:60:ARG:HD2	1:A:304:LEU:HD22	1.56	0.87
1:A:45:ARG:HH21	1:A:49:GLY:N	1.74	0.86
1:A:17:LEU:HB2	1:A:47:PRO:HD3	1.59	0.85
1:A:251:LEU:HD13	1:A:284:LEU:HD23	1.59	0.85
1:B:152:LEU:HB3	1:B:153:PRO:HD3	1.60	0.84
1:A:331:ASP:N	1:A:332:PRO:HD3	1.92	0.83
1:A:395:ILE:N	1:A:395:ILE:HD12	1.94	0.83
1:A:45:ARG:HE	1:A:49:GLY:CA	1.92	0.83
1:B:122:ARG:HA	1:B:125:GLU:OE2	1.78	0.83
1:B:127:VAL:HG22	1:B:152:LEU:HD11	1.60	0.83
1:B:162:GLY:HA3	1:B:205:LYS:HZ1	1.42	0.83
1:B:296:ARG:HG3	1:B:296:ARG:HH11	1.41	0.83
1:B:254:ASN:HD22	1:B:287:GLU:HB3	1.44	0.83
1:B:58:TYR:CD2	1:B:328:ARG:HG3	2.14	0.83
1:A:242:VAL:O	1:A:244:GLY:N	2.13	0.82
1:A:350:GLY:O	1:A:352:HIS:N	2.12	0.81
1:A:261:SER:O	1:A:263:PRO:HD3	1.80	0.81
1:A:91:ASN:ND2	1:A:94:GLU:HG3	1.95	0.80
1:B:388:VAL:HG11	1:B:399:LYS:HD2	1.61	0.79
1:B:62:ARG:HH12	1:B:349:HIS:CE1	2.00	0.79
1:A:98:PRO:O	1:A:100:HIS:N	2.16	0.79
1:A:174:TRP:HE1	1:A:193:GLU:CD	1.86	0.78
1:B:82:THR:HG23	1:B:85:GLU:OE1	1.82	0.78
1:A:398:LEU:HD12	1:A:401:LEU:HB2	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:ASP:H	1:A:332:PRO:HD3	1.47	0.78
1:B:369:ARG:HH11	1:B:369:ARG:HG3	1.48	0.78
1:A:45:ARG:NH2	1:A:49:GLY:H	1.81	0.77
1:A:137:ALA:HA	4:A:2014:HOH:O	1.84	0.77
1:A:15:LEU:HD11	1:A:20:LEU:HD11	1.66	0.77
1:A:285:ARG:HD3	1:A:339:ARG:HD3	1.67	0.77
1:B:179:VAL:HG22	1:B:395:ILE:CD1	2.15	0.77
1:B:243:ALA:HA	3:B:1408:PXI:O2	1.84	0.76
1:B:276:LEU:O	1:B:276:LEU:HD13	1.84	0.76
1:B:361:ARG:HB3	1:B:365:ARG:HH12	1.51	0.76
1:A:282:GLU:OE2	1:A:339:ARG:HD2	1.86	0.76
1:B:206:ARG:HB2	1:B:218:VAL:HG11	1.66	0.75
1:B:265:GLN:NE2	1:B:337:ILE:H	1.85	0.75
1:B:361:ARG:HB3	1:B:365:ARG:NH1	2.01	0.75
1:B:162:GLY:HA3	1:B:205:LYS:NZ	2.01	0.75
1:B:62:ARG:NH1	1:B:349:HIS:CE1	2.55	0.75
1:B:214:LEU:O	1:B:218:VAL:HG23	1.86	0.75
1:A:250:ASN:HB2	1:A:289:PRO:HB3	1.69	0.75
1:B:114:ARG:HD3	1:B:114:ARG:H	1.52	0.75
1:B:270:ARG:HH12	1:B:372:LEU:HD22	1.51	0.74
1:B:63:ALA:O	1:B:67:ASP:HB2	1.87	0.74
1:A:141:ARG:NH1	1:A:141:ARG:HB2	2.02	0.73
1:B:249:VAL:HG12	1:B:249:VAL:O	1.88	0.73
1:B:67:ASP:OD1	1:B:69:ARG:HG3	1.88	0.73
1:B:65:LEU:HA	1:B:296:ARG:HE	1.54	0.73
1:A:156:VAL:O	1:A:160:LEU:HD12	1.89	0.73
1:A:285:ARG:C	1:A:285:ARG:HE	1.92	0.73
1:A:150:TRP:HB3	1:A:151:PRO:HD3	1.68	0.73
1:A:154:ILE:HB	1:A:245:HIS:NE2	2.04	0.72
1:A:45:ARG:HG2	1:A:45:ARG:HH11	1.54	0.72
1:B:227:ARG:O	1:B:228:LEU:HB2	1.88	0.72
1:A:74:TRP:CD2	1:A:81:LEU:HD21	2.25	0.72
1:A:382:VAL:HG22	1:A:383:SER:N	2.04	0.72
1:B:171:PHE:CE2	1:B:241:LEU:HD22	2.24	0.72
1:A:285:ARG:NH2	1:A:286:TYR:HA	2.04	0.71
1:A:148:LEU:O	1:A:151:PRO:HD2	1.89	0.71
1:A:66:ALA:HB2	1:A:350:GLY:HA3	1.73	0.71
1:A:144:LEU:CD2	1:A:256:MET:HG3	2.20	0.71
1:B:115:ARG:HG3	1:B:118:LEU:HD12	1.73	0.70
1:A:336:ASP:OD1	1:A:338:ARG:HB2	1.92	0.70
1:A:127:VAL:HG22	1:A:152:LEU:CD1	2.21	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:TRP:O	1:B:153:PRO:HD2	1.92	0.70
1:B:25:ALA:HB1	1:B:389:TRP:O	1.91	0.70
1:A:382:VAL:HG22	1:A:383:SER:H	1.55	0.70
1:B:406:ARG:HB2	1:B:406:ARG:HH11	1.56	0.69
1:A:53:TRP:O	1:A:54:LEU:HD23	1.92	0.69
1:A:259:LEU:HD11	1:A:266:LEU:HA	1.73	0.69
1:B:289:PRO:HA	1:B:396:ARG:HB3	1.75	0.69
1:B:395:ILE:HD11	3:B:1408:PXI:O6	1.93	0.69
1:B:309:ILE:HG13	4:B:2027:HOH:O	1.92	0.69
1:B:66:ALA:HB2	1:B:349:HIS:CD2	2.29	0.68
1:B:56:VAL:HB	1:B:321:ASP:OD1	1.93	0.68
1:B:95:SER:HB3	1:B:99:ARG:HH11	1.58	0.68
1:A:165:GLU:HB3	1:A:166:PRO:HD3	1.74	0.68
1:B:306:GLY:O	1:B:308:VAL:HG23	1.93	0.68
1:A:272:ASP:OD2	1:A:275:LEU:HG	1.92	0.68
1:A:336:ASP:C	1:A:338:ARG:H	1.97	0.68
1:A:170:ALA:O	1:A:173:VAL:HB	1.94	0.68
1:A:183:ASP:OD1	1:A:185:ALA:HB3	1.94	0.68
1:B:150:TRP:HB3	1:B:151:PRO:HD3	1.76	0.68
1:B:238:HIS:NE2	3:B:1408:PXI:H102	2.08	0.68
1:A:45:ARG:NE	1:A:49:GLY:HA2	2.09	0.68
1:B:147:SER:O	1:B:151:PRO:HG2	1.94	0.67
1:B:236:MET:O	1:B:239:ILE:HG22	1.95	0.67
1:A:395:ILE:HD12	1:A:395:ILE:H	1.60	0.66
1:A:251:LEU:HD13	1:A:284:LEU:CD2	2.24	0.66
1:A:175:THR:O	1:A:179:VAL:HG23	1.94	0.66
1:B:269:LEU:O	1:B:271:ALA:N	2.29	0.66
1:B:144:LEU:HD21	1:B:256:MET:HG3	1.76	0.66
1:A:331:ASP:N	1:A:332:PRO:CD	2.58	0.66
1:A:327:GLU:OE1	1:A:327:GLU:N	2.29	0.65
1:A:276:LEU:HD11	1:A:365:ARG:HB3	1.78	0.65
1:B:74:TRP:CD2	1:B:81:LEU:HD21	2.30	0.65
1:A:149:ALA:O	1:A:249:VAL:HG22	1.97	0.65
1:B:287:GLU:HB2	4:B:2023:HOH:O	1.95	0.65
1:B:14:VAL:HG12	1:B:15:LEU:H	1.62	0.65
1:A:371:LEU:O	1:A:375:CYS:HB2	1.97	0.65
1:B:238:HIS:O	1:B:242:VAL:HG23	1.97	0.65
1:B:329:PHE:O	1:B:332:PRO:HG3	1.96	0.65
1:B:201:LEU:HD12	1:B:204:SER:OG	1.96	0.65
1:B:405:TRP:O	1:B:406:ARG:HG3	1.96	0.65
1:A:131:VAL:O	1:A:135:LEU:HG	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:295:TYR:HB2	4:B:2025:HOH:O	1.95	0.65
1:B:114:ARG:N	1:B:114:ARG:HD3	2.12	0.65
1:A:174:TRP:CZ2	1:A:193:GLU:HB3	2.32	0.64
1:A:259:LEU:O	1:A:266:LEU:HB2	1.97	0.64
1:B:389:TRP:HA	1:B:397:GLY:O	1.98	0.64
1:A:323:HIS:NE2	1:A:345:LEU:N	2.42	0.64
1:B:359:LEU:O	1:B:363:GLU:HG3	1.98	0.64
1:B:41:ALA:HB3	1:B:307:THR:HG21	1.79	0.64
1:B:291:GLU:N	1:B:394:MET:O	2.31	0.64
1:A:61:ALA:HB1	1:A:317:VAL:HG13	1.80	0.64
1:A:130:LEU:HD21	1:A:151:PRO:HB3	1.80	0.63
1:A:137:ALA:HB3	1:A:405:TRP:HZ2	1.63	0.63
1:B:250:ASN:O	1:B:254:ASN:HB2	1.99	0.63
1:A:122:ARG:C	1:A:124:GLN:H	2.02	0.63
1:B:344:HIS:O	1:B:345:LEU:HD23	1.98	0.63
1:A:282:GLU:OE1	1:A:285:ARG:HB3	1.99	0.63
1:B:69:ARG:O	1:B:299:VAL:HG23	1.99	0.63
1:B:124:GLN:OE1	1:B:366:ILE:HG23	1.99	0.62
1:B:36:ARG:HH12	1:B:326:PRO:HD2	1.64	0.62
1:A:120:ARG:HB3	1:A:121:PRO:HD3	1.81	0.62
1:B:164:PRO:O	1:B:168:ARG:HG3	2.00	0.62
1:A:67:ASP:HB3	1:A:70:PHE:CD1	2.35	0.62
1:B:202:ILE:HG22	1:B:206:ARG:NH1	2.13	0.62
1:B:102:ARG:O	1:B:106:LEU:HD13	1.99	0.62
1:B:152:LEU:HB3	1:B:153:PRO:CD	2.29	0.62
1:A:183:ASP:O	1:A:185:ALA:N	2.32	0.61
1:B:295:TYR:CE1	1:B:316:LEU:HD21	2.36	0.61
1:A:122:ARG:NH2	4:A:2010:HOH:O	2.33	0.61
1:A:22:GLN:NE2	1:A:388:VAL:HA	2.15	0.61
1:A:118:LEU:O	1:A:121:PRO:HD2	2.00	0.61
1:B:344:HIS:HD2	1:B:346:ALA:HB3	1.65	0.61
1:B:43:ARG:HH12	1:B:51:GLU:C	2.03	0.61
1:A:238:HIS:NE2	3:A:1408:PXI:H102	2.16	0.61
1:B:270:ARG:NH1	1:B:372:LEU:HB3	2.15	0.61
1:B:145:MET:HA	1:B:149:ALA:HB3	1.81	0.61
1:B:259:LEU:HD23	1:B:266:LEU:HD13	1.81	0.61
1:B:57:GLY:N	1:B:321:ASP:OD1	2.33	0.61
1:B:35:LEU:HB3	1:B:42:HIS:CD2	2.35	0.61
1:B:84:ALA:HB3	1:B:188:GLN:NE2	2.15	0.60
1:B:36:ARG:HH22	1:B:325:THR:HA	1.66	0.60
1:A:267:ALA:O	1:A:270:ARG:HB2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:285:ARG:HD2	1:B:329:PHE:CE2	2.36	0.60
1:A:150:TRP:NE1	1:A:172:ARG:HB2	2.15	0.60
1:B:296:ARG:NH1	1:B:296:ARG:HG3	2.16	0.60
1:A:24:PHE:HE1	1:A:31:THR:HB	1.67	0.60
1:A:61:ALA:HB1	1:A:317:VAL:CG1	2.31	0.60
1:A:204:SER:O	1:A:208:GLN:HG2	2.01	0.60
1:B:178:PHE:HD2	1:B:178:PHE:N	2.00	0.60
1:A:395:ILE:HG22	1:A:396:ARG:N	2.13	0.60
1:A:127:VAL:HG22	1:A:152:LEU:HD11	1.83	0.60
1:A:144:LEU:HD21	1:A:371:LEU:HD11	1.82	0.60
1:B:178:PHE:CD2	1:B:178:PHE:N	2.67	0.60
1:A:141:ARG:CB	1:A:141:ARG:NH1	2.65	0.60
1:B:285:ARG:HB3	1:B:285:ARG:NH1	2.07	0.59
1:B:390:TYR:CD1	1:B:397:GLY:HA3	2.37	0.59
1:A:137:ALA:HB3	1:A:405:TRP:CZ2	2.36	0.59
1:A:122:ARG:NE	1:A:126:ILE:HD11	2.16	0.59
1:B:245:HIS:O	1:B:249:VAL:HG23	2.02	0.59
1:B:369:ARG:HG3	1:B:369:ARG:NH1	2.16	0.59
1:B:285:ARG:O	1:B:323:HIS:HB3	2.03	0.59
1:B:265:GLN:HG3	1:B:335:PHE:O	2.02	0.59
1:B:93:LEU:HD21	1:B:294:THR:HG21	1.83	0.59
1:B:78:THR:HG23	1:B:312:GLY:HA3	1.85	0.59
1:B:115:ARG:HG3	1:B:118:LEU:CD1	2.31	0.59
1:A:183:ASP:OD2	1:B:138:PRO:HG2	2.03	0.59
1:A:357:ALA:HB3	1:A:358:PRO:HD3	1.85	0.59
1:A:282:GLU:HA	1:A:282:GLU:OE1	2.03	0.59
1:A:55:VAL:HG11	1:A:64:VAL:HG21	1.85	0.59
1:A:114:ARG:HG3	1:A:114:ARG:HH11	1.68	0.59
1:A:45:ARG:HE	1:A:49:GLY:HA2	1.61	0.59
1:A:17:LEU:HG	1:A:45:ARG:O	2.03	0.59
1:B:119:LEU:O	1:B:123:VAL:HG23	2.03	0.58
1:A:251:LEU:HD22	1:A:284:LEU:HD21	1.83	0.58
1:A:170:ALA:HB1	1:A:174:TRP:CH2	2.37	0.58
1:A:22:GLN:HE22	1:A:388:VAL:HA	1.68	0.58
1:B:114:ARG:O	1:B:117:GLU:HB3	2.03	0.58
1:A:15:LEU:HD12	1:A:15:LEU:C	2.24	0.58
1:B:251:LEU:HD13	1:B:284:LEU:CD2	2.33	0.58
1:A:71:SER:OG	1:A:76:ASN:ND2	2.35	0.58
1:A:45:ARG:NE	1:A:49:GLY:CA	2.65	0.58
1:B:395:ILE:HG22	1:B:396:ARG:N	2.18	0.58
1:A:395:ILE:N	1:A:395:ILE:CD1	2.65	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:TRP:CE2	1:B:81:LEU:HD21	2.38	0.58
1:A:355:ILE:HG12	1:A:355:ILE:O	2.03	0.58
1:A:336:ASP:O	1:A:338:ARG:N	2.37	0.57
1:A:193:GLU:O	1:A:196:GLY:N	2.36	0.57
1:A:336:ASP:O	1:A:339:ARG:N	2.37	0.57
1:B:147:SER:O	1:B:151:PRO:HD2	2.04	0.57
1:A:123:VAL:HG21	1:A:362:LEU:HD23	1.85	0.57
1:B:251:LEU:O	1:B:255:GLY:N	2.36	0.57
1:B:148:LEU:HD23	1:B:371:LEU:HD11	1.85	0.57
1:B:406:ARG:CB	1:B:406:ARG:HH11	2.17	0.57
1:A:35:LEU:HD22	1:A:42:HIS:CD2	2.39	0.57
1:B:175:THR:O	1:B:179:VAL:HG23	2.04	0.57
1:A:387:LEU:HB2	4:A:2026:HOH:O	2.03	0.57
1:B:148:LEU:CD2	1:B:371:LEU:HD11	2.34	0.57
1:A:174:TRP:HD1	1:A:190:ALA:HB1	1.70	0.57
1:B:169:ALA:O	1:B:173:VAL:HG23	2.05	0.57
1:B:331:ASP:OD1	1:B:334:ARG:HB2	2.05	0.56
1:B:270:ARG:HH11	1:B:270:ARG:HG2	1.69	0.56
1:B:147:SER:O	1:B:151:PRO:CG	2.53	0.56
1:A:67:ASP:HB3	1:A:70:PHE:HD1	1.70	0.56
1:B:228:LEU:HA	1:B:232:GLU:OE2	2.04	0.56
1:A:123:VAL:O	1:A:123:VAL:HG12	2.05	0.56
1:A:279:ALA:HA	1:A:337:ILE:HG22	1.86	0.56
1:B:127:VAL:HG12	1:B:128:ASP:N	2.19	0.56
1:B:293:ALA:HB1	2:B:1407:HEM:O2A	2.05	0.56
1:A:377:ASP:HB2	1:A:406:ARG:CA	2.36	0.56
1:B:304:LEU:O	1:B:305:ASP:C	2.44	0.56
1:B:331:ASP:O	1:B:334:ARG:HB3	2.06	0.56
1:A:133:ALA:O	1:A:136:ALA:HB3	2.05	0.56
1:B:357:ALA:HB3	1:B:358:PRO:HD3	1.87	0.56
1:B:187:ALA:O	1:B:191:MET:HG3	2.05	0.56
1:B:104:ARG:HG3	1:B:104:ARG:HH11	1.70	0.56
1:A:329:PHE:N	1:A:330:PRO:HD3	2.20	0.56
1:A:390:TYR:OH	1:A:399:LYS:HA	2.06	0.56
1:B:285:ARG:HD2	1:B:329:PHE:CD2	2.41	0.56
1:B:39:GLY:H	1:B:42:HIS:HE1	1.53	0.56
1:B:270:ARG:HG2	1:B:270:ARG:NH1	2.21	0.56
1:A:354:CYS:HB2	2:A:1407:HEM:C4A	2.40	0.56
1:B:281:GLU:OE2	1:B:361:ARG:NE	2.39	0.56
1:A:58:TYR:HE1	1:A:343:GLY:O	1.89	0.56
1:A:146:GLU:OE2	1:A:146:GLU:HA	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:ARG:HH11	1:A:296:ARG:HG3	1.70	0.56
1:A:406:ARG:HB2	1:A:406:ARG:HH11	1.70	0.55
1:B:261:SER:C	1:B:263:PRO:HD3	2.27	0.55
1:A:144:LEU:HD23	1:A:256:MET:HG3	1.86	0.55
1:A:152:LEU:HB3	1:A:153:PRO:CD	2.31	0.55
1:B:276:LEU:O	1:B:276:LEU:HD22	2.06	0.55
1:B:242:VAL:O	1:B:243:ALA:C	2.45	0.55
1:B:135:LEU:HD21	1:B:375:CYS:SG	2.45	0.55
1:A:405:TRP:O	1:A:406:ARG:HG3	2.07	0.55
1:B:231:GLU:HG3	4:B:2018:HOH:O	2.06	0.55
1:B:129:GLY:HA2	1:B:132:ASP:OD2	2.07	0.55
1:B:261:SER:O	1:B:263:PRO:HD3	2.07	0.55
1:A:331:ASP:OD2	1:A:334:ARG:HB2	2.07	0.55
1:B:201:LEU:HD11	1:B:205:LYS:HE2	1.88	0.55
1:A:256:MET:O	1:A:260:LEU:HG	2.07	0.55
1:B:93:LEU:HD23	3:B:1408:PXI:H6C2	1.89	0.55
1:B:340:ASP:C	1:B:342:ALA:H	2.10	0.55
1:B:282:GLU:CD	1:B:285:ARG:NH1	2.60	0.55
1:B:344:HIS:CD2	1:B:346:ALA:HB3	2.42	0.55
1:B:138:PRO:HD2	1:B:139:ASP:OD1	2.08	0.54
1:B:35:LEU:O	1:B:38:GLU:HB2	2.07	0.54
1:A:171:PHE:CE2	1:A:241:LEU:HD13	2.43	0.54
1:B:285:ARG:HH11	1:B:285:ARG:CB	2.11	0.54
1:A:293:ALA:O	1:A:316:LEU:HD22	2.07	0.54
1:A:247:THR:O	1:A:289:PRO:HG3	2.07	0.54
1:B:142:ALA:O	1:B:403:ILE:HG12	2.06	0.54
1:B:281:GLU:O	1:B:284:LEU:HB2	2.08	0.54
1:A:127:VAL:HG22	1:A:152:LEU:HD13	1.88	0.54
1:B:125:GLU:O	1:B:126:ILE:C	2.45	0.54
1:A:164:PRO:HB2	4:A:2015:HOH:O	2.07	0.54
1:B:236:MET:HA	1:B:239:ILE:HG22	1.89	0.54
1:B:327:GLU:O	1:B:330:PRO:HD3	2.08	0.54
1:A:171:PHE:HA	1:A:174:TRP:CE3	2.42	0.54
1:B:60:ARG:O	1:B:64:VAL:HG23	2.08	0.54
1:A:148:LEU:O	1:A:149:ALA:C	2.46	0.54
1:B:14:VAL:HG12	1:B:15:LEU:N	2.23	0.54
1:B:17:LEU:HD12	1:B:46:THR:HA	1.90	0.54
1:B:245:HIS:HB3	1:B:246:GLU:OE1	2.06	0.54
1:A:93:LEU:HD23	1:A:239:ILE:HD11	1.90	0.54
1:B:178:PHE:H	1:B:178:PHE:HD2	1.55	0.54
1:B:84:ALA:HB3	1:B:188:GLN:HE22	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:82:THR:HG21	1:B:188:GLN:OE1	2.08	0.53
1:B:109:ARG:O	1:B:112:THR:HG23	2.08	0.53
1:B:151:PRO:O	1:B:152:LEU:C	2.46	0.53
1:B:157:ILE:HG23	1:B:158:SER:N	2.23	0.53
1:B:151:PRO:O	1:B:154:ILE:HG22	2.09	0.53
1:A:58:TYR:HA	1:A:322:ALA:HB1	1.90	0.53
1:A:112:THR:O	1:A:116:VAL:HG23	2.08	0.53
1:A:149:ALA:HB1	1:A:249:VAL:HG13	1.91	0.53
1:B:259:LEU:HD12	1:B:335:PHE:CE2	2.43	0.53
1:A:70:PHE:HB2	4:A:2005:HOH:O	2.09	0.53
1:B:406:ARG:CB	1:B:406:ARG:NH1	2.72	0.53
1:B:281:GLU:O	1:B:284:LEU:N	2.40	0.53
1:A:171:PHE:HA	1:A:174:TRP:HE3	1.72	0.53
1:A:382:VAL:CG2	1:A:383:SER:H	2.21	0.53
1:B:267:ALA:HA	1:B:270:ARG:HB2	1.91	0.53
1:A:351:ILE:HG13	1:A:352:HIS:N	2.23	0.53
1:B:227:ARG:HG2	1:B:227:ARG:O	2.09	0.53
1:A:45:ARG:HE	1:A:49:GLY:C	2.13	0.53
1:B:344:HIS:HD2	1:B:346:ALA:CB	2.22	0.52
1:B:298:PRO:HB2	1:B:300:GLU:O	2.10	0.52
1:A:81:LEU:HD12	1:A:86:ALA:HB2	1.90	0.52
1:B:92:MET:HE1	1:B:104:ARG:HA	1.92	0.52
1:A:33:ALA:O	1:A:34:ARG:C	2.47	0.52
1:B:29:TYR:HB2	1:B:30:PRO:HD3	1.91	0.52
1:B:272:ASP:OD1	1:B:273:MET:N	2.42	0.52
1:A:60:ARG:O	1:A:64:VAL:HG23	2.08	0.52
1:A:144:LEU:HD21	1:A:371:LEU:CD1	2.39	0.52
1:B:310:PRO:HD2	1:B:313:ASP:OD2	2.10	0.52
1:B:273:MET:C	1:B:275:LEU:H	2.12	0.52
1:B:331:ASP:CG	1:B:334:ARG:HB2	2.30	0.52
1:B:92:MET:HE1	1:B:107:VAL:HG22	1.92	0.52
1:B:197:TYR:CD2	1:B:198:LEU:HD23	2.45	0.52
1:A:181:PRO:HA	1:A:186:GLN:OE1	2.09	0.52
1:B:77:SER:HB2	1:B:297:PHE:CD2	2.45	0.51
1:A:325:THR:HG22	1:A:327:GLU:H	1.76	0.51
1:B:272:ASP:OD1	1:B:274:THR:HG23	2.10	0.51
1:A:99:ARG:C	1:A:101:THR:H	2.14	0.51
1:A:242:VAL:HG12	1:A:243:ALA:N	2.26	0.51
1:B:116:VAL:HG21	1:B:358:PRO:HB2	1.92	0.51
1:B:61:ALA:HA	1:B:64:VAL:HG23	1.92	0.51
1:A:330:PRO:O	1:A:331:ASP:HB3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:299:VAL:O	1:B:300:GLU:CB	2.59	0.51
1:A:150:TRP:CE2	1:A:172:ARG:HD2	2.46	0.51
1:B:53:TRP:NE1	1:B:313:ASP:OD2	2.44	0.51
1:A:214:LEU:O	1:A:217:LEU:N	2.43	0.51
1:A:53:TRP:CD2	1:A:309:ILE:HG12	2.45	0.51
1:B:24:PHE:O	1:B:28:PRO:HB3	2.10	0.51
1:A:25:ALA:O	1:A:28:PRO:HD3	2.11	0.50
1:A:298:PRO:HD2	1:A:313:ASP:O	2.11	0.50
1:B:388:VAL:CG1	1:B:399:LYS:HD2	2.38	0.50
1:A:15:LEU:HD12	1:A:16:ASP:O	2.11	0.50
1:A:276:LEU:CD1	1:A:365:ARG:HB3	2.41	0.50
1:A:282:GLU:HG3	1:A:335:PHE:CE1	2.46	0.50
1:A:145:MET:HA	1:A:149:ALA:HB3	1.94	0.50
1:A:260:LEU:HD21	1:A:378:LEU:HD21	1.93	0.50
1:B:243:ALA:O	1:B:247:THR:OG1	2.27	0.50
1:A:165:GLU:CB	1:A:166:PRO:HD3	2.41	0.50
1:A:225:GLY:HA2	1:A:228:LEU:O	2.11	0.50
1:A:252:ILE:O	1:A:256:MET:HG2	2.11	0.50
1:B:368:VAL:O	1:B:372:LEU:HG	2.11	0.50
1:B:127:VAL:O	1:B:130:LEU:N	2.44	0.50
1:B:135:LEU:HD11	1:B:374:ARG:HB3	1.94	0.50
1:A:382:VAL:CG2	1:A:383:SER:N	2.73	0.50
1:B:189:THR:O	1:B:193:GLU:HG3	2.11	0.50
1:B:83:GLU:HA	4:B:2004:HOH:O	2.11	0.50
1:A:364:ALA:O	1:A:367:ALA:HB3	2.11	0.50
1:B:244:GLY:HA2	1:B:247:THR:OG1	2.11	0.50
1:B:115:ARG:HA	1:B:118:LEU:HG	1.92	0.50
1:B:310:PRO:HG2	1:B:313:ASP:OD1	2.11	0.50
1:A:146:GLU:CG	1:A:146:GLU:O	2.60	0.50
1:B:131:VAL:CG1	1:B:131:VAL:O	2.60	0.50
1:A:99:ARG:C	1:A:101:THR:N	2.65	0.50
1:A:99:ARG:HG2	1:A:103:LEU:HD11	1.94	0.50
1:B:165:GLU:N	1:B:166:PRO:CD	2.74	0.50
1:B:150:TRP:HA	1:B:249:VAL:HG13	1.93	0.50
1:A:336:ASP:O	1:A:339:ARG:HB3	2.12	0.49
1:B:273:MET:HE3	1:B:276:LEU:HB2	1.94	0.49
1:A:161:LEU:O	1:A:214:LEU:HB2	2.12	0.49
1:A:287:GLU:CD	1:A:396:ARG:HH21	2.16	0.49
1:A:74:TRP:CE2	1:A:81:LEU:HD21	2.47	0.49
1:B:247:THR:HB	2:B:1407:HEM:CAB	2.42	0.49
1:A:66:ALA:CB	1:A:350:GLY:HA3	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:357:ALA:N	1:B:358:PRO:CD	2.75	0.49
1:A:331:ASP:OD2	1:A:334:ARG:HD2	2.12	0.49
1:B:286:TYR:CD1	1:B:324:ARG:NH2	2.81	0.49
1:B:66:ALA:HB2	1:B:349:HIS:HD2	1.77	0.49
1:A:356:GLY:O	1:A:357:ALA:C	2.51	0.49
1:B:131:VAL:HG12	1:B:131:VAL:O	2.12	0.49
1:B:395:ILE:CG2	1:B:396:ARG:N	2.76	0.49
1:B:227:ARG:NH2	4:B:2017:HOH:O	2.45	0.49
1:B:243:ALA:HB1	3:B:1408:PXI:H1C2	1.94	0.49
1:B:203:ASP:N	1:B:203:ASP:OD1	2.46	0.49
1:A:140:GLY:O	1:A:404:ARG:HA	2.13	0.49
1:B:337:ILE:HG13	1:B:337:ILE:O	2.13	0.49
1:B:148:LEU:O	1:B:151:PRO:HD2	2.13	0.49
1:A:406:ARG:NH1	1:A:406:ARG:CB	2.75	0.49
1:B:43:ARG:HG3	1:B:53:TRP:CE2	2.47	0.49
1:B:132:ASP:O	1:B:136:ALA:N	2.46	0.49
1:A:15:LEU:HG	1:A:15:LEU:O	2.13	0.49
1:B:277:ASP:HB3	1:B:365:ARG:HE	1.78	0.49
1:B:247:THR:O	1:B:289:PRO:HG3	2.12	0.49
1:B:162:GLY:O	1:B:164:PRO:HD3	2.12	0.49
1:B:74:TRP:HD1	1:B:89:ASN:HD22	1.61	0.49
1:B:123:VAL:O	1:B:127:VAL:HG23	2.12	0.48
1:A:141:ARG:CB	1:A:141:ARG:HH11	2.15	0.48
1:B:201:LEU:O	1:B:205:LYS:HG2	2.13	0.48
1:A:205:LYS:HE2	1:A:214:LEU:HD23	1.95	0.48
1:B:149:ALA:O	1:B:249:VAL:HA	2.13	0.48
1:A:114:ARG:HG3	1:A:114:ARG:NH1	2.27	0.48
1:A:144:LEU:HD21	1:A:256:MET:HG3	1.92	0.48
1:A:182:ASP:CB	1:A:186:GLN:NE2	2.77	0.48
1:A:336:ASP:C	1:A:338:ARG:N	2.64	0.48
1:A:329:PHE:HB3	1:A:339:ARG:NH1	2.29	0.48
1:A:45:ARG:CG	1:A:45:ARG:HH11	2.22	0.48
1:B:179:VAL:HG13	1:B:395:ILE:HD12	1.95	0.48
1:A:88:LEU:C	1:A:90:HIS:H	2.17	0.48
1:B:246:GLU:HG3	3:B:1408:PXI:O6	2.13	0.48
1:B:259:LEU:HD12	1:B:335:PHE:HE2	1.78	0.48
1:A:58:TYR:CE1	1:A:343:GLY:O	2.67	0.48
1:A:108:ALA:O	1:A:110:GLU:N	2.46	0.48
1:A:91:ASN:CG	1:A:94:GLU:HG3	2.33	0.48
1:B:36:ARG:NH2	1:B:325:THR:HA	2.27	0.48
1:A:69:ARG:O	1:A:298:PRO:HA	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:177:ALA:O	1:B:181:PRO:HB3	2.14	0.48
1:B:238:HIS:CD2	3:B:1408:PXI:H102	2.49	0.47
1:B:380:LEU:HD21	1:B:401:LEU:CD1	2.36	0.47
1:A:60:ARG:N	4:A:2003:HOH:O	2.46	0.47
1:A:30:PRO:O	1:A:33:ALA:HB3	2.14	0.47
1:B:244:GLY:HA3	2:B:1407:HEM:C2C	2.49	0.47
1:B:389:TRP:CE2	1:B:398:LEU:HD21	2.49	0.47
1:A:93:LEU:HD12	1:A:93:LEU:O	2.15	0.47
1:B:295:TYR:CD1	1:B:314:THR:CG2	2.96	0.47
1:B:270:ARG:HH22	1:B:372:LEU:HA	1.79	0.47
1:A:98:PRO:HA	1:A:101:THR:OG1	2.14	0.47
1:A:239:ILE:O	1:A:243:ALA:HB3	2.14	0.47
1:A:147:SER:O	1:A:151:PRO:HG2	2.14	0.47
1:B:144:LEU:HB2	1:B:403:ILE:HD13	1.96	0.47
1:B:369:ARG:NH1	1:B:369:ARG:CG	2.77	0.47
1:B:344:HIS:C	1:B:345:LEU:HD23	2.35	0.47
1:B:259:LEU:CD2	1:B:266:LEU:HD13	2.45	0.47
1:B:153:PRO:O	1:B:155:THR:N	2.48	0.47
1:B:278:GLY:C	4:B:2022:HOH:O	2.51	0.47
1:B:251:LEU:HD13	1:B:284:LEU:HD21	1.97	0.47
1:A:179:VAL:HG11	1:A:390:TYR:CD1	2.49	0.47
1:A:64:VAL:HG13	1:A:70:PHE:CD1	2.50	0.47
1:A:203:ASP:O	1:A:204:SER:C	2.53	0.47
1:A:344:HIS:HD2	1:A:346:ALA:HB3	1.78	0.47
1:B:273:MET:CE	1:B:276:LEU:HB2	2.45	0.47
1:A:174:TRP:NE1	1:A:193:GLU:HB2	2.30	0.47
1:A:24:PHE:O	1:A:28:PRO:CD	2.63	0.47
1:A:177:ALA:O	1:A:181:PRO:HB3	2.14	0.47
1:B:270:ARG:HH12	1:B:372:LEU:CD2	2.23	0.47
1:B:72:LYS:HE3	1:B:294:THR:OG1	2.15	0.47
1:B:269:LEU:O	1:B:270:ARG:C	2.52	0.46
1:B:147:SER:O	1:B:151:PRO:CD	2.63	0.46
1:A:41:ALA:HB3	1:A:307:THR:HG21	1.98	0.46
1:B:123:VAL:O	1:B:123:VAL:HG12	2.15	0.46
1:B:144:LEU:HD11	1:B:148:LEU:HD23	1.97	0.46
1:B:148:LEU:O	1:B:150:TRP:N	2.49	0.46
1:B:382:VAL:HG11	1:B:402:PRO:HD2	1.97	0.46
1:B:101:THR:O	1:B:102:ARG:C	2.52	0.46
1:A:139:ASP:CG	1:A:140:GLY:H	2.19	0.46
1:A:324:ARG:HG3	1:A:324:ARG:HH11	1.79	0.46
1:A:158:SER:CB	1:A:163:VAL:HB	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:TRP:HE1	1:A:172:ARG:HB2	1.78	0.46
1:A:88:LEU:HD23	1:A:234:LEU:HD21	1.97	0.46
1:B:269:LEU:O	1:B:272:ASP:O	2.34	0.46
1:B:270:ARG:HD3	1:B:270:ARG:O	2.16	0.46
1:B:249:VAL:O	1:B:249:VAL:CG1	2.60	0.46
1:B:282:GLU:HA	1:B:282:GLU:OE1	2.14	0.46
1:B:323:HIS:HE1	1:B:346:ALA:HB2	1.80	0.46
1:B:228:LEU:HD12	1:B:232:GLU:CB	2.45	0.46
1:A:53:TRP:CE2	1:A:309:ILE:HG12	2.51	0.46
1:B:70:PHE:HB3	1:B:296:ARG:HB3	1.97	0.46
1:A:205:LYS:O	1:A:206:ARG:C	2.52	0.46
1:A:360:ALA:HB1	2:A:1407:HEM:CBB	2.45	0.46
1:B:233:LEU:C	1:B:233:LEU:HD12	2.36	0.46
1:B:269:LEU:HD12	1:B:272:ASP:O	2.15	0.46
1:A:100:HIS:CD2	1:A:352:HIS:CE1	3.03	0.46
1:B:381:ASP:O	1:B:382:VAL:HB	2.16	0.46
1:A:64:VAL:HG13	1:A:70:PHE:CE1	2.51	0.46
1:B:197:TYR:HD2	1:B:198:LEU:HD23	1.80	0.46
1:A:280:VAL:HG21	1:A:365:ARG:HG3	1.96	0.46
1:B:22:GLN:O	1:B:22:GLN:HG3	2.14	0.46
1:A:91:ASN:OD1	1:A:94:GLU:HG3	2.15	0.46
1:B:388:VAL:HG11	1:B:399:LYS:CD	2.40	0.46
1:B:291:GLU:HB3	1:B:393:PRO:O	2.16	0.46
1:B:388:VAL:HB	1:B:399:LYS:HB2	1.98	0.46
1:A:139:ASP:N	1:A:139:ASP:OD1	2.49	0.46
1:A:249:VAL:O	1:A:252:ILE:HB	2.16	0.45
1:A:91:ASN:HD21	1:A:94:GLU:CG	2.16	0.45
1:B:287:GLU:HA	4:B:2024:HOH:O	2.15	0.45
1:A:24:PHE:O	1:A:28:PRO:HB3	2.16	0.45
1:A:45:ARG:CG	1:A:45:ARG:NH1	2.79	0.45
1:B:247:THR:HB	2:B:1407:HEM:C3B	2.51	0.45
1:B:248:THR:C	1:B:250:ASN:H	2.19	0.45
1:A:114:ARG:O	1:A:115:ARG:C	2.54	0.45
1:B:92:MET:CE	1:B:104:ARG:HA	2.45	0.45
1:B:340:ASP:OD2	1:B:342:ALA:CB	2.64	0.45
1:B:157:ILE:HD13	4:B:2019:HOH:O	2.15	0.45
1:B:267:ALA:HA	1:B:270:ARG:CB	2.45	0.45
1:B:179:VAL:HG11	1:B:390:TYR:CD1	2.52	0.45
1:A:291:GLU:HB2	1:A:395:ILE:O	2.15	0.45
1:B:205:LYS:HE3	1:B:214:LEU:HD23	1.98	0.45
1:B:82:THR:HG1	1:B:85:GLU:H	1.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:LEU:HD21	1:A:269:LEU:HD23	1.97	0.45
1:A:390:TYR:CE2	1:A:399:LYS:HA	2.52	0.45
1:A:123:VAL:O	1:A:366:ILE:HG21	2.16	0.45
1:A:45:ARG:CZ	1:A:49:GLY:HA2	2.47	0.45
1:B:120:ARG:HB3	1:B:121:PRO:HD3	1.98	0.45
1:B:383:SER:O	1:B:385:GLY:N	2.49	0.45
1:A:62:ARG:HB2	1:A:345:LEU:HD11	1.98	0.45
1:A:56:VAL:HG12	1:A:318:VAL:HB	1.98	0.45
1:A:78:THR:O	1:A:80:PRO:HD3	2.17	0.45
1:B:127:VAL:O	1:B:128:ASP:C	2.54	0.45
1:B:380:LEU:HD22	1:B:382:VAL:HG12	1.99	0.45
1:A:24:PHE:HE1	1:A:31:THR:CB	2.29	0.45
1:B:74:TRP:CE3	1:B:81:LEU:HD21	2.51	0.45
1:A:328:ARG:HG2	1:A:328:ARG:HH11	1.82	0.45
1:A:224:ASP:OD2	1:A:227:ARG:HG3	2.16	0.45
1:A:14:VAL:N	4:A:2001:HOH:O	2.50	0.45
1:A:329:PHE:N	1:A:330:PRO:CD	2.79	0.45
1:B:126:ILE:HD13	1:B:155:THR:CG2	2.46	0.45
1:B:150:TRP:HA	1:B:249:VAL:HG22	1.98	0.45
1:A:324:ARG:HG3	1:A:324:ARG:NH1	2.32	0.45
1:A:20:LEU:HB3	1:A:24:PHE:HB2	1.98	0.45
1:B:77:SER:HB2	1:B:297:PHE:CE2	2.51	0.45
1:A:139:ASP:CG	1:A:140:GLY:N	2.71	0.45
1:A:32:TYR:HB3	1:A:321:ASP:HB2	1.98	0.45
1:B:175:THR:HG23	1:B:246:GLU:OE2	2.17	0.45
1:B:371:LEU:O	1:B:375:CYS:HB2	2.17	0.45
1:B:177:ALA:O	1:B:181:PRO:HD3	2.17	0.45
1:A:331:ASP:O	1:A:334:ARG:HB2	2.18	0.44
1:A:150:TRP:HB3	1:A:151:PRO:CD	2.44	0.44
1:A:150:TRP:CD2	1:A:172:ARG:HD2	2.52	0.44
1:B:285:ARG:HH12	1:B:286:TYR:HB2	1.83	0.44
1:A:90:HIS:ND1	1:A:99:ARG:NH2	2.64	0.44
1:B:174:TRP:O	1:B:176:ASP:N	2.51	0.44
1:A:344:HIS:HD2	1:A:346:ALA:CB	2.30	0.44
1:B:183:ASP:O	1:B:185:ALA:N	2.47	0.44
1:A:188:GLN:HA	1:A:191:MET:HE3	1.99	0.44
1:B:360:ALA:O	1:B:362:LEU:N	2.50	0.44
1:A:148:LEU:O	1:A:151:PRO:CD	2.64	0.44
1:B:161:LEU:HD23	1:B:213:LEU:HB3	1.99	0.44
1:B:361:ARG:O	1:B:365:ARG:HG3	2.17	0.44
1:B:380:LEU:HD23	1:B:402:PRO:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:296:ARG:NH1	1:B:296:ARG:CG	2.78	0.44
1:A:370:ALA:O	1:A:373:GLU:N	2.49	0.44
1:B:141:ARG:HG2	1:B:404:ARG:HB3	1.99	0.44
1:A:36:ARG:HH12	1:A:326:PRO:HD2	1.83	0.44
1:B:284:LEU:O	1:B:346:ALA:HB2	2.17	0.44
1:A:282:GLU:CA	1:A:282:GLU:OE1	2.66	0.44
1:A:122:ARG:C	1:A:124:GLN:N	2.69	0.44
1:B:108:ALA:HA	1:B:355:ILE:HD11	1.99	0.44
1:A:143:ASP:HA	1:A:402:PRO:HA	2.00	0.44
1:A:265:GLN:HE21	1:A:336:ASP:HA	1.82	0.44
1:A:171:PHE:HE2	1:A:241:LEU:HD13	1.80	0.44
1:A:333:HIS:CE1	4:A:2023:HOH:O	2.70	0.44
1:A:174:TRP:CD1	1:A:190:ALA:HB1	2.51	0.43
1:A:359:LEU:O	1:A:363:GLU:HG3	2.17	0.43
1:A:319:LEU:HD22	1:A:345:LEU:HB2	2.00	0.43
1:B:14:VAL:HA	1:B:43:ARG:O	2.18	0.43
1:A:282:GLU:CD	1:A:339:ARG:HD2	2.38	0.43
1:B:156:VAL:HG11	1:B:359:LEU:HD11	1.99	0.43
1:B:331:ASP:O	1:B:339:ARG:NH2	2.48	0.43
1:A:146:GLU:HG3	1:A:146:GLU:O	2.18	0.43
1:A:146:GLU:OE2	1:A:146:GLU:CA	2.64	0.43
1:A:158:SER:HB3	1:A:163:VAL:HB	2.01	0.43
1:B:45:ARG:HH11	1:B:45:ARG:CB	2.32	0.43
1:B:242:VAL:O	1:B:244:GLY:N	2.52	0.43
1:A:82:THR:O	1:A:83:GLU:C	2.55	0.43
1:B:270:ARG:NH1	1:B:372:LEU:HD22	2.26	0.43
1:A:161:LEU:HD13	1:A:241:LEU:HG	2.01	0.43
1:A:357:ALA:N	1:A:358:PRO:CD	2.81	0.43
1:B:186:GLN:O	1:B:190:ALA:N	2.42	0.43
1:A:351:ILE:CG1	1:A:352:HIS:N	2.82	0.43
1:A:150:TRP:CE2	1:A:172:ARG:HB2	2.53	0.43
1:B:390:TYR:HA	1:B:391:PRO:HD3	1.86	0.43
1:B:227:ARG:CG	1:B:227:ARG:O	2.67	0.43
1:B:90:HIS:O	1:B:232:GLU:HA	2.19	0.43
1:A:344:HIS:CD2	1:A:346:ALA:HB3	2.52	0.43
1:B:55:VAL:HB	1:B:317:VAL:HA	2.01	0.43
1:B:44:VAL:HG21	1:B:54:LEU:HD11	2.00	0.43
1:A:96:ASP:HB3	1:A:97:PRO:HD2	2.00	0.42
1:B:348:GLY:O	1:B:349:HIS:HB2	2.19	0.42
1:A:24:PHE:O	1:A:28:PRO:N	2.51	0.42
1:B:106:LEU:HD23	1:B:228:LEU:HD22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:382:VAL:HG23	1:B:386:GLU:OE1	2.19	0.42
1:A:250:ASN:CB	1:A:289:PRO:HB3	2.45	0.42
1:A:160:LEU:C	1:A:162:GLY:H	2.23	0.42
1:A:279:ALA:HA	1:A:337:ILE:CG2	2.49	0.42
1:B:273:MET:C	1:B:275:LEU:N	2.72	0.42
1:A:280:VAL:HG21	1:A:365:ARG:CG	2.49	0.42
1:B:150:TRP:O	1:B:151:PRO:O	2.38	0.42
1:B:179:VAL:HG22	1:B:395:ILE:HD11	1.99	0.42
1:A:126:ILE:HD13	1:A:155:THR:CG2	2.49	0.42
1:A:265:GLN:O	1:A:268:ALA:N	2.53	0.42
1:A:398:LEU:CD1	1:A:401:LEU:HB2	2.44	0.42
1:A:149:ALA:O	1:A:153:PRO:HD2	2.20	0.42
1:A:228:LEU:CD1	1:A:232:GLU:HB3	2.49	0.42
1:A:326:PRO:O	1:A:330:PRO:HG3	2.20	0.42
2:B:1407:HEM:HMA2	2:B:1407:HEM:HAA1	1.90	0.42
1:B:303:ASP:OD1	1:B:303:ASP:C	2.57	0.42
1:B:389:TRP:CZ3	1:B:396:ARG:NE	2.88	0.42
1:A:224:ASP:C	1:A:226:SER:H	2.22	0.42
1:B:45:ARG:HB3	1:B:45:ARG:HH11	1.85	0.42
1:B:336:ASP:OD1	1:B:338:ARG:HB2	2.19	0.42
1:B:43:ARG:HH11	1:B:43:ARG:HG2	1.85	0.42
1:A:22:GLN:HE22	1:A:389:TRP:H	1.67	0.42
1:A:384:PRO:HA	1:A:387:LEU:CD1	2.50	0.42
1:A:285:ARG:HD3	1:A:339:ARG:CD	2.46	0.41
1:A:130:LEU:CD1	1:A:151:PRO:HB2	2.50	0.41
1:B:122:ARG:O	1:B:122:ARG:HG3	2.19	0.41
1:B:26:ALA:HB2	1:B:389:TRP:CD1	2.55	0.41
1:A:24:PHE:O	1:A:28:PRO:HD3	2.20	0.41
1:B:239:ILE:HA	1:B:239:ILE:HD12	1.90	0.41
1:B:304:LEU:O	1:B:307:THR:N	2.53	0.41
1:A:149:ALA:HA	1:A:252:ILE:HG21	2.03	0.41
1:B:276:LEU:CD1	1:B:276:LEU:O	2.64	0.41
1:A:377:ASP:HB2	1:A:406:ARG:HA	2.02	0.41
1:A:24:PHE:O	1:A:25:ALA:C	2.58	0.41
1:B:102:ARG:HH12	1:B:232:GLU:CD	2.24	0.41
1:B:225:GLY:O	1:B:228:LEU:N	2.35	0.41
1:A:265:GLN:O	1:A:268:ALA:HB3	2.20	0.41
1:A:259:LEU:HG	1:A:266:LEU:HD13	2.03	0.41
1:B:375:CYS:HB3	1:B:378:LEU:HB2	2.02	0.41
1:A:24:PHE:CZ	1:A:28:PRO:HB2	2.55	0.41
1:A:155:THR:HG23	1:A:168:ARG:NH1	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:282:GLU:OE2	1:B:285:ARG:NH1	2.53	0.41
1:B:269:LEU:C	1:B:271:ALA:N	2.72	0.41
1:B:134:MET:C	1:B:136:ALA:H	2.24	0.41
1:A:395:ILE:CG2	1:A:396:ARG:H	2.18	0.41
1:B:17:LEU:HD11	1:B:44:VAL:HG21	2.02	0.41
1:A:82:THR:H	1:A:85:GLU:HB2	1.86	0.41
1:A:127:VAL:CG2	1:A:152:LEU:HD11	2.48	0.41
1:B:225:GLY:HA2	1:B:228:LEU:O	2.21	0.41
1:B:174:TRP:C	1:B:176:ASP:N	2.73	0.41
1:B:356:GLY:O	1:B:357:ALA:C	2.59	0.41
1:B:179:VAL:HG22	1:B:395:ILE:HD13	1.98	0.41
1:A:141:ARG:HG2	1:A:381:ASP:OD1	2.21	0.41
1:B:228:LEU:HD12	1:B:232:GLU:HB3	2.01	0.41
1:B:171:PHE:HA	1:B:174:TRP:HE3	1.85	0.41
1:A:319:LEU:CD2	1:A:345:LEU:HB2	2.50	0.41
1:A:65:LEU:HD12	1:A:345:LEU:HD13	2.02	0.41
1:A:150:TRP:O	1:A:153:PRO:HD2	2.21	0.41
1:A:156:VAL:HG12	1:A:160:LEU:HD12	2.02	0.41
1:B:236:MET:O	1:B:237:ALA:C	2.60	0.41
1:B:43:ARG:HH12	1:B:51:GLU:CB	2.34	0.41
2:A:1407:HEM:HMA2	2:A:1407:HEM:HAA1	1.81	0.41
1:B:46:THR:HG23	1:B:52:VAL:HG22	2.03	0.41
1:A:14:VAL:HA	1:A:43:ARG:O	2.21	0.41
1:A:191:MET:O	1:A:195:SER:HB3	2.21	0.41
1:B:48:GLU:CD	1:B:48:GLU:N	2.75	0.41
1:B:32:TYR:CE2	1:B:318:VAL:HG11	2.55	0.41
1:B:254:ASN:HD21	1:B:396:ARG:HG3	1.86	0.41
1:B:340:ASP:C	1:B:342:ALA:N	2.74	0.41
1:A:273:MET:CE	1:A:369:ARG:HG3	2.50	0.41
1:B:260:LEU:HB3	1:B:380:LEU:HG	2.03	0.40
1:A:406:ARG:CB	1:A:406:ARG:HH11	2.31	0.40
1:A:124:GLN:NE2	1:A:124:GLN:HA	2.35	0.40
1:A:120:ARG:CB	1:A:121:PRO:HD3	2.50	0.40
1:A:334:ARG:HA	1:A:334:ARG:NE	2.36	0.40
1:A:45:ARG:HH21	1:A:49:GLY:CA	2.33	0.40
1:B:95:SER:HB2	1:B:99:ARG:HD2	2.04	0.40
1:B:198:LEU:HD13	1:B:237:ALA:HB1	2.03	0.40
1:A:367:ALA:O	1:A:368:VAL:C	2.59	0.40
1:B:132:ASP:O	1:B:135:LEU:N	2.54	0.40
1:A:380:LEU:CD2	1:A:401:LEU:HD11	2.51	0.40
1:B:157:ILE:CG2	1:B:158:SER:N	2.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:THR:HA	1:B:146:GLU:OE1	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	391/436 (90%)	285 (73%)	77 (20%)	29 (7%)	1 3
1	B	391/436 (90%)	277 (71%)	78 (20%)	36 (9%)	1 1
All	All	782/872 (90%)	562 (72%)	155 (20%)	65 (8%)	1 2

All (65) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	98	PRO
1	A	99	ARG
1	A	149	ALA
1	A	242	VAL
1	A	243	ALA
1	A	351	ILE
1	A	376	PRO
1	B	38	GLU
1	B	127	VAL
1	B	149	ALA
1	B	151	PRO
1	B	152	LEU
1	B	228	LEU
1	B	243	ALA
1	B	270	ARG
1	B	300	GLU
1	B	384	PRO

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Mol	Chain	Res	Type
1	A	109	ARG
1	A	114	ARG
1	A	311	ALA
1	A	337	ILE
1	A	339	ARG
1	A	370	ALA
1	B	126	ILE
1	B	148	LEU
1	B	305	ASP
1	B	327	GLU
1	B	382	VAL
1	A	47	PRO
1	A	144	LEU
1	A	184	PRO
1	A	305	ASP
1	A	377	ASP
1	B	125	GLU
1	B	139	ASP
1	B	175	THR
1	B	245	HIS
1	B	341	THR
1	B	354	CYS
1	B	361	ARG
1	A	85	GLU
1	A	193	GLU
1	A	293	ALA
1	A	364	ALA
1	A	382	VAL
1	B	69	ARG
1	B	168	ARG
1	B	358	PRO
1	B	376	PRO
1	A	106	LEU
1	A	244	GLY
1	A	371	LEU
1	B	40	PRO
1	B	80	PRO
1	B	144	LEU
1	B	164	PRO
1	B	268	ALA
1	A	330	PRO
1	B	153	PRO

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Mol	Chain	Res	Type
1	B	185	ALA
1	B	242	VAL
1	B	299	VAL
1	A	49	GLY
1	B	184	PRO
1	A	331	ASP

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	313/355 (88%)	288 (92%)	25 (8%)	15	38
1	B	313/355 (88%)	285 (91%)	28 (9%)	12	32
All	All	626/710 (88%)	573 (92%)	53 (8%)	13	34

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	LEU
1	A	43	ARG
1	A	45	ARG
1	A	46	THR
1	A	59	ASP
1	A	77	SER
1	A	89	ASN
1	A	94	GLU
1	A	100	HIS
1	A	101	THR
1	A	104	ARG
1	A	132	ASP
1	A	159	GLU
1	A	160	LEU
1	A	164	PRO
1	A	165	GLU
1	A	215	SER

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Mol	Chain	Res	Type
1	A	270	ARG
1	A	285	ARG
1	A	313	ASP
1	A	330	PRO
1	A	334	ARG
1	A	351	ILE
1	A	384	PRO
1	A	395	ILE
1	B	45	ARG
1	B	89	ASN
1	B	101	THR
1	B	104	ARG
1	B	114	ARG
1	B	139	ASP
1	B	151	PRO
1	B	152	LEU
1	B	178	PHE
1	B	198	LEU
1	B	203	ASP
1	B	219	ARG
1	B	223	GLU
1	B	233	LEU
1	B	238	HIS
1	B	240	LEU
1	B	242	VAL
1	B	247	THR
1	B	270	ARG
1	B	272	ASP
1	B	277	ASP
1	B	285	ARG
1	B	297	PHE
1	B	334	ARG
1	B	339	ARG
1	B	369	ARG
1	B	384	PRO
1	B	406	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	76	ASN

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Mol	Chain	Res	Type
1	A	100	HIS
1	A	124	GLN
1	A	238	HIS
1	A	344	HIS
1	B	89	ASN
1	B	188	GLN
1	B	254	ASN
1	B	265	GLN
1	B	344	HIS
1	B	349	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$\|Z\|>2$	Counts	RMSZ	#$\|Z\|>2$
2	HEM	A	1407	1	30,50,50	2.91	11 (36%)	24,82,82	2.81	9 (37%)
3	PXI	A	1408	-	31,33,33	1.67	5 (16%)	37,47,47	1.90	10 (27%)
2	HEM	B	1407	1	30,50,50	2.62	12 (40%)	24,82,82	2.57	12 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$\|Z\|>2$	Counts	RMSZ	#$\|Z\|>2$
3	PXI	B	1408	-	31,33,33	1.64	4 (12%)	37,47,47	2.09	11 (29%)

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	1407	1	-	0/10/54/54	0/0/8/8
3	PXI	A	1408	-	-	0/43/59/59	0/1/2/2
2	HEM	B	1407	1	-	0/10/54/54	0/0/8/8
3	PXI	B	1408	-	-	0/43/59/59	0/1/2/2

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1407	HEM	C3B-CAB	-7.32	1.37	1.51
2	A	1407	HEM	C3B-C4B	-6.88	1.45	1.51
2	A	1407	HEM	C3B-CAB	-6.66	1.38	1.51
2	A	1407	HEM	C3C-CAC	-6.46	1.39	1.51
2	B	1407	HEM	C2D-C3D	-5.47	1.38	1.54
2	A	1407	HEM	C2D-C3D	-5.29	1.38	1.54
2	B	1407	HEM	C3D-C4D	-4.96	1.45	1.51
2	B	1407	HEM	C3C-CAC	-4.80	1.42	1.51
2	B	1407	HEM	C3B-C4B	-3.51	1.48	1.51
2	A	1407	HEM	C2C-C1C	-3.36	1.46	1.52
2	B	1407	HEM	C2D-C1D	-2.80	1.42	1.51
2	B	1407	HEM	C2C-C1C	-2.30	1.48	1.52
2	A	1407	HEM	C2A-C3A	-2.20	1.31	1.37
2	A	1407	HEM	C2B-C1B	-2.04	1.45	1.51
3	B	1408	PXI	O4-C9	2.13	1.48	1.44
2	B	1407	HEM	CHC-C1C	2.18	1.41	1.36
3	A	1408	PXI	O4-C9	2.23	1.48	1.44
3	A	1408	PXI	O3-C8	2.27	1.47	1.41
2	A	1407	HEM	CBC-CAC	2.36	1.43	1.29
2	B	1407	HEM	C1C-NC	2.39	1.38	1.36
3	A	1408	PXI	O3-C7	2.44	1.50	1.43
2	B	1407	HEM	C4C-NC	2.62	1.39	1.36
2	B	1407	HEM	CBB-CAB	2.79	1.45	1.29
3	B	1408	PXI	C11-C9	2.80	1.57	1.51
3	B	1408	PXI	C15-C12	2.86	1.59	1.53
2	A	1407	HEM	CBB-CAB	2.98	1.46	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1407	HEM	CBC-CAC	3.40	1.48	1.29
2	A	1407	HEM	C1C-NC	3.49	1.40	1.36
3	A	1408	PXI	C15-C12	3.71	1.61	1.53
3	A	1408	PXI	C16-C7	5.10	1.63	1.53
2	A	1407	HEM	C4C-NC	5.50	1.42	1.36
3	B	1408	PXI	C16-C7	5.92	1.64	1.53

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1408	PXI	O3-C7-C5	-4.59	102.51	111.10
2	A	1407	HEM	CAA-C2A-C3A	-3.71	118.41	129.00
2	B	1407	HEM	CAA-C2A-C3A	-3.32	119.52	129.00
3	A	1408	PXI	O3-C7-C5	-3.27	104.99	111.10
3	B	1408	PXI	C6-C5-C7	-2.92	106.48	112.97
3	B	1408	PXI	C10-C9-C11	-2.79	108.72	113.38
3	A	1408	PXI	C10-C9-C11	-2.63	108.99	113.38
3	B	1408	PXI	C25-C24-C23	-2.35	104.33	110.07
3	B	1408	PXI	C11-C12-C15	-2.14	106.91	110.03
3	A	1408	PXI	C6-C5-C7	-2.13	108.24	112.97
3	B	1408	PXI	C13-N1-C12	-2.08	107.09	113.09
3	A	1408	PXI	C25-C24-C23	-2.07	105.00	110.07
2	B	1407	HEM	C3C-CAC-CBC	2.02	127.55	124.46
3	A	1408	PXI	O3-C8-O4	2.13	116.06	110.68
3	B	1408	PXI	O3-C8-O4	2.17	116.19	110.68
3	A	1408	PXI	C23-C22-C21	2.18	126.09	123.22
2	B	1407	HEM	C3B-C4B-CHC	2.29	126.39	123.16
2	A	1407	HEM	C3C-CAC-CBC	2.33	128.04	124.46
2	B	1407	HEM	C2D-C3D-C4D	2.40	105.57	101.50
2	B	1407	HEM	CMD-C2D-C3D	2.54	125.59	114.35
2	A	1407	HEM	C2D-C3D-C4D	2.55	105.83	101.50
2	A	1407	HEM	CMD-C2D-C3D	2.84	126.91	114.35
3	A	1408	PXI	C7-C5-C4	2.93	115.59	109.86
3	B	1408	PXI	O3-C7-C16	2.95	113.30	108.46
3	B	1408	PXI	C7-C5-C4	2.97	115.68	109.86
3	A	1408	PXI	O3-C7-C16	2.98	113.35	108.46
3	B	1408	PXI	O1-C3-C2	3.02	111.72	106.59
2	A	1407	HEM	CAD-C3D-C2D	3.12	122.18	113.22
3	A	1408	PXI	O1-C3-C2	3.23	112.09	106.59
2	B	1407	HEM	CMB-C2B-C3B	3.79	126.00	116.53
2	B	1407	HEM	CBD-CAD-C3D	3.91	124.94	113.55
2	B	1407	HEM	CMC-C2C-C3C	3.99	126.50	116.53

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Full wwPDB X-ray Structure Validation Report

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1407	HEM	CBA-CAA-C2A	4.14	119.95	112.53
2	B	1407	HEM	CAD-C3D-C2D	4.21	125.31	113.22
2	B	1407	HEM	CAA-C2A-C1A	4.31	131.69	127.01
2	A	1407	HEM	CMB-C2B-C3B	4.68	128.21	116.53
2	B	1407	HEM	CAD-C3D-C4D	4.72	129.11	112.47
2	A	1407	HEM	CMC-C2C-C3C	4.77	128.43	116.53
2	A	1407	HEM	CAD-C3D-C4D	5.53	131.99	112.47
3	A	1408	PXI	C3-O1-C4	6.91	128.56	117.92
2	A	1407	HEM	CAA-C2A-C1A	7.53	135.18	127.01
3	B	1408	PXI	C3-O1-C4	7.75	129.85	117.92

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1407	HEM	3	0
3	A	1408	PXI	1	0
2	B	1407	HEM	5	0
3	B	1408	PXI	7	0

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)

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(Å²)	Q<0.9
1	A	393/436 (90%)	0.33	7 (1%)	71	68	4, 23, 37, 48	0
1	B	393/436 (90%)	0.36	4 (1%)	84	81	5, 22, 39, 46	0
All	All	786/872 (90%)	0.35	11 (1%)	78	75	4, 23, 38, 48	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	126	ILE	3.2
1	B	89	ASN	3.1
1	B	384	PRO	2.6
1	A	207	GLY	2.4
1	A	91	ASN	2.4
1	A	172	ARG	2.3
1	A	375	CYS	2.3
1	A	179	VAL	2.2
1	B	270	ARG	2.1
1	B	143	ASP	2.1
1	A	73	ASP	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	RSCC	RSR	LLDF	B-factors($Å^2$)	Q<0.9
3	PXI	A	1408	32/32	0.82	0.29	1.17	27,31,32,35	0
3	PXI	B	1408	32/32	0.89	0.28	0.86	28,31,33,34	0
2	HEM	B	1407	43/43	0.94	0.19	-0.60	3,6,12,19	0
2	HEM	A	1407	43/43	0.94	0.20	-0.74	3,4,12,15	0

6.5 Other polymers (i)

There are no such residues in this entry.