Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:05 AM GMT

PDB ID	:	3DBG
Title	:	Crystal structure of Cytochrome P450 170A1 (CYP170A1) from Streptomyces coelicolor
Authors	:	Zhao, B.; Vassylyev, D.G.; Waterman, M.R.
Deposited on	:	2008-05-31
Resolution	:	2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

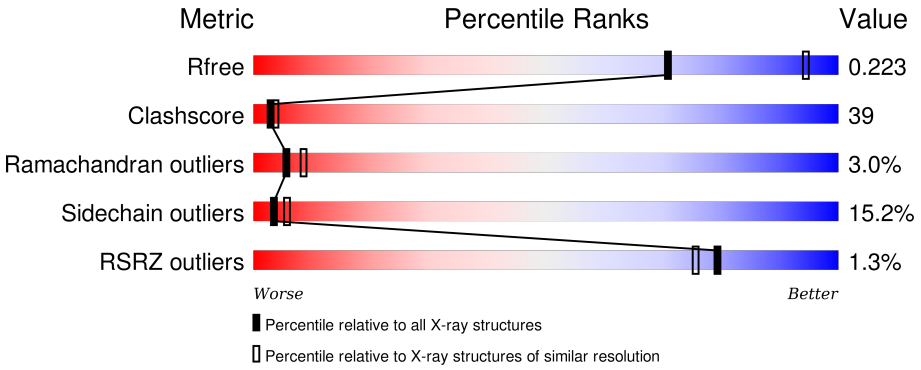
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.60 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	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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	467	% 37% 37% 7% • 19%
1	B	467	% 40% 33% 8% • 19%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6339 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.

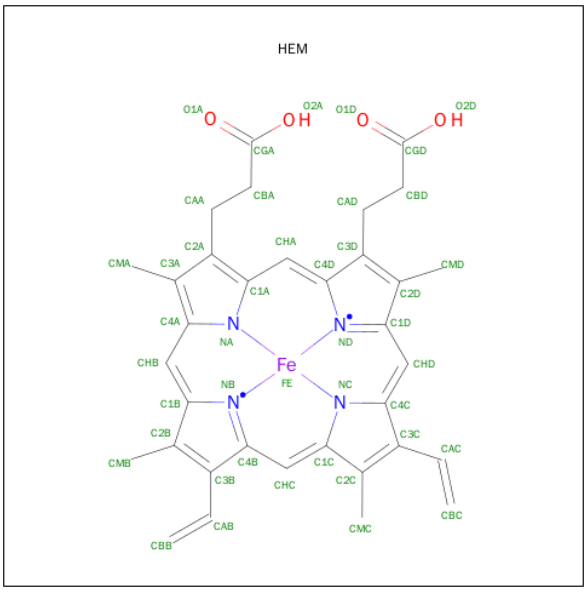
- Molecule 1 is a protein called Putative cytochrome P450.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	379	Total	C	N	O	S	0	0	0
			2944	1856	539	539	10			
1	B	379	Total	C	N	O	S	0	0	0
			2944	1856	539	539	10			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	462	HIS	-	EXPRESSION TAG	UNP Q9K498
A	463	HIS	-	EXPRESSION TAG	UNP Q9K498
A	464	HIS	-	EXPRESSION TAG	UNP Q9K498
A	465	HIS	-	EXPRESSION TAG	UNP Q9K498
A	466	HIS	-	EXPRESSION TAG	UNP Q9K498
A	467	HIS	-	EXPRESSION TAG	UNP Q9K498
B	462	HIS	-	EXPRESSION TAG	UNP Q9K498
B	463	HIS	-	EXPRESSION TAG	UNP Q9K498
B	464	HIS	-	EXPRESSION TAG	UNP Q9K498
B	465	HIS	-	EXPRESSION TAG	UNP Q9K498
B	466	HIS	-	EXPRESSION TAG	UNP Q9K498
B	467	HIS	-	EXPRESSION TAG	UNP Q9K498

- 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		

- Molecule 3 is water.

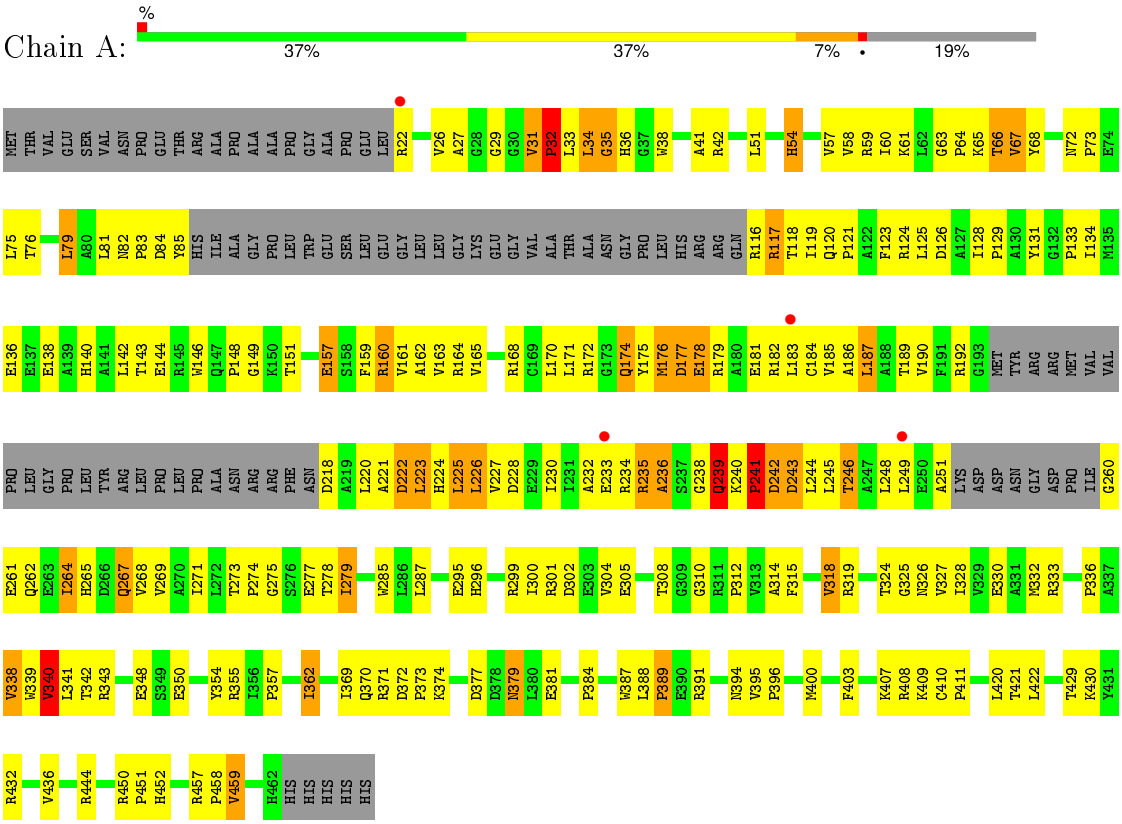
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	178	Total	O	0	0
			178	178		
3	B	187	Total	O	0	0
			187	187		

3 Residue-property plots (i)

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.

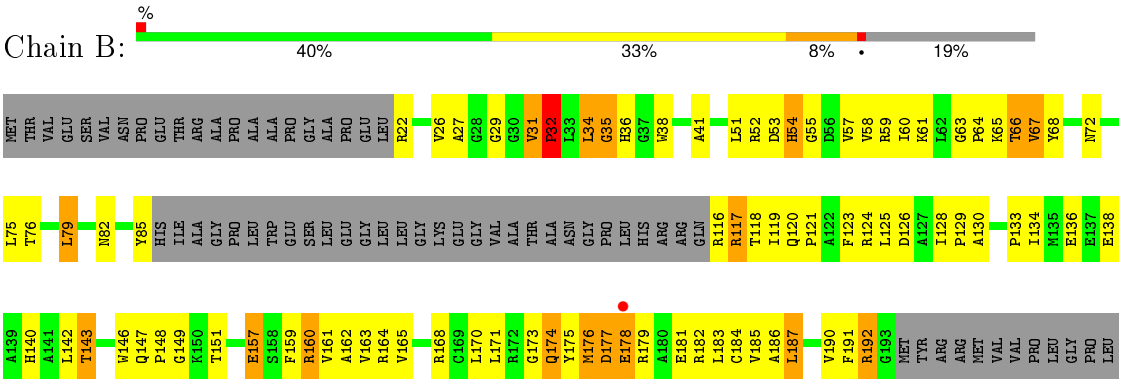
- Molecule 1: Putative cytochrome P450

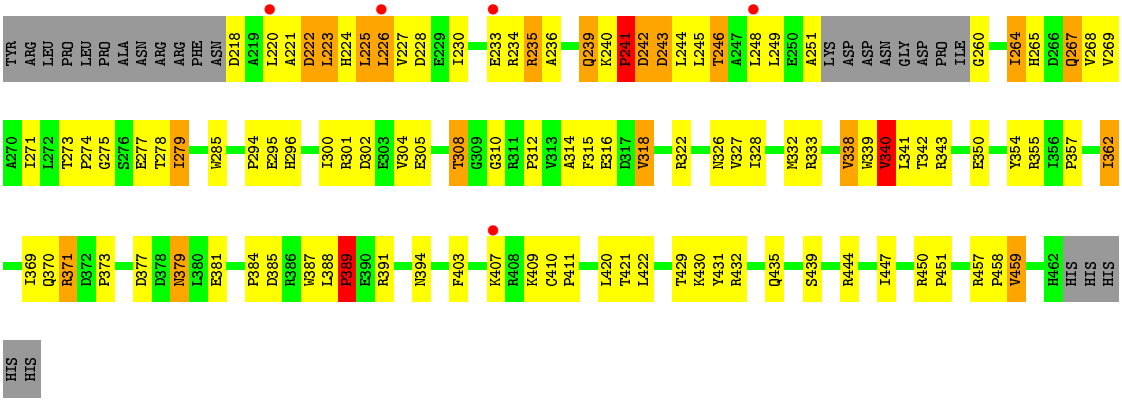
Chain A:



- Molecule 1: Putative cytochrome P450

Chain B:




TYR ARG LEU PRO LEU PRO ALA ASN ARG ARG PHE ASN D218 A219 L220 A221 D222 L223 H224 L225 L226 V227 D228 E229 I230 E233 R234 R235 A236 Q239 K240 P241 D242 D243 L244 L245 T246 A247 L248 L249 E250 A251 LYS ASP ASP ASN GLY ASP PRO ILE G260 I264 H265 D266 Q267 V268 V269
A270 I271 L272 T273 P274 G275 S276 E277 T278 I279 W285 P294 E295 H296 I300 R301 D302 E303 V304 E305 T308 G309 G310 R311 P312 V313 A314 F315 E316 D317 V318 R322 N326 V327 I328 M332 R333 V338 W339 V340 L341 T342 R343 E350 Y354 R355 I356 P357 I362
I369 Q370 R371 D372 P373 D377 D378 N379 L380 E381 P384 D385 R386 W387 L388 P389 E390 R391 N394 F403 K407 R408 K409 C410 P411 L420 T421 L422 T429 K430 Y431 R432 Q435 S439 R444 I447 R450 P451 R457 P458 V459 H462 HIS HIS HIS
HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α, β, γ	103.60Å 103.60Å 140.86Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.00 – 2.60 37.84 – 2.60	Depositor EDS
% Data completeness (in resolution range)	90.5 (40.00-2.60) 95.7 (37.84-2.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.43 (at 2.61Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.208 , 0.230 0.201 , 0.223	Depositor DCC
R_{free} test set	1374 reflections (5.75%)	DCC
Wilson B-factor (Å^2)	38.6	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 77.7	EDS
Estimated twinning fraction	0.499 for h,-h-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 25254 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6339	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.25% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.66	0/3005	0.78	1/4085 (0.0%)
1	B	0.67	0/3005	0.78	1/4085 (0.0%)
All	All	0.67	0/6010	0.78	2/8170 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	340	VAL	CB-CA-C	-5.73	100.50	111.40
1	B	340	VAL	CB-CA-C	-5.20	101.53	111.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-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 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	2944	0	2945	248	0
1	B	2944	0	2945	234	0
2	A	43	0	30	3	0
2	B	43	0	30	3	0
3	A	178	0	0	59	0
3	B	187	0	0	49	0
All	All	6339	0	5950	468	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 39.

All (468) 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:301:ARG:HG3	1:B:429:THR:HA	1.39	1.04
1:A:31:VAL:HG12	1:A:32:PRO:HD2	1.37	1.04
1:A:301:ARG:HG3	1:A:429:THR:HA	1.37	1.03
1:B:31:VAL:HG12	1:B:32:PRO:HD2	1.42	1.01
1:A:79:LEU:HD11	1:A:362:ILE:HD11	1.48	0.95
1:A:33:LEU:HD21	1:B:65:LYS:HD2	1.46	0.94
1:B:36:HIS:HD2	1:B:61:LYS:H	1.12	0.94
1:A:29:GLY:H	1:A:36:HIS:CE1	1.86	0.93
1:A:29:GLY:H	1:A:36:HIS:HE1	0.95	0.93
1:B:29:GLY:H	1:B:36:HIS:HE1	0.98	0.92
1:A:36:HIS:HD2	1:A:61:LYS:H	1.16	0.89
1:B:226:LEU:HD23	1:B:230:ILE:HD11	1.53	0.89
1:A:33:LEU:HD22	1:B:65:LYS:H	1.39	0.86
1:A:236:ALA:HB2	3:A:534:HOH:O	1.74	0.86
1:B:27:ALA:HB2	3:B:752:HOH:O	1.74	0.86
1:B:79:LEU:HD11	1:B:362:ILE:HD11	1.56	0.86
1:B:143:THR:HG23	1:B:430:LYS:HD3	1.58	0.85
1:B:29:GLY:H	1:B:36:HIS:CE1	1.90	0.83
1:A:143:THR:HG23	1:A:430:LYS:HD3	1.61	0.83
1:A:278:THR:HG22	2:A:500:HEM:HBB2	1.59	0.82
1:B:244:LEU:C	1:B:244:LEU:HD23	2.01	0.82
1:A:244:LEU:C	1:A:244:LEU:HD23	2.01	0.81
1:B:278:THR:HG22	2:B:500:HEM:HBB2	1.63	0.80
1:B:173:GLY:HA2	3:B:649:HOH:O	1.83	0.79
1:A:179:ARG:HD3	1:A:226:LEU:HD11	1.66	0.77
1:A:319:ARG:HG2	3:A:563:HOH:O	1.83	0.77
1:B:31:VAL:H	1:B:35:GLY:HA2	1.49	0.77
1:A:227:VAL:HG21	1:A:269:VAL:HG22	1.64	0.77
1:A:146:TRP:HE1	1:A:157:GLU:HG2	1.49	0.77
1:B:179:ARG:HD3	1:B:226:LEU:HD11	1.66	0.77
1:B:175:TYR:HB3	1:B:177:ASP:OD1	1.84	0.77
1:B:36:HIS:CD2	1:B:61:LYS:H	2.01	0.76
1:A:168:ARG:HD2	3:A:553:HOH:O	1.86	0.76
1:B:227:VAL:HG21	1:B:269:VAL:HG22	1.66	0.76
1:A:31:VAL:H	1:A:35:GLY:HA2	1.49	0.76
1:A:239:GLN:HG3	3:A:662:HOH:O	1.87	0.75
1:A:277:GLU:HB2	3:A:597:HOH:O	1.86	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:LEU:HD23	1:A:230:ILE:HD11	1.69	0.74
1:A:432:ARG:HB3	1:A:459:VAL:HG22	1.68	0.74
1:A:33:LEU:HD21	1:B:65:LYS:CD	2.18	0.73
1:A:176:MET:HG2	1:A:230:ILE:CD1	2.18	0.73
1:B:308:THR:HG21	3:B:712:HOH:O	1.88	0.73
1:B:76:THR:HG21	1:B:369:ILE:HD11	1.70	0.73
1:A:170:LEU:O	1:A:171:LEU:HD23	1.89	0.72
1:B:388:LEU:HD12	1:B:391:ARG:HH21	1.52	0.72
1:B:226:LEU:CD2	1:B:230:ILE:HD11	2.19	0.72
1:B:146:TRP:HE1	1:B:157:GLU:HG2	1.55	0.71
1:A:235:ARG:HD3	3:A:583:HOH:O	1.89	0.71
1:B:244:LEU:HD21	1:B:248:LEU:CD1	2.20	0.71
1:B:170:LEU:O	1:B:171:LEU:HD23	1.91	0.71
1:B:273:THR:HB	1:B:274:PRO:HD3	1.73	0.70
1:B:432:ARG:HB3	1:B:459:VAL:HG22	1.71	0.70
1:B:29:GLY:N	1:B:36:HIS:HE1	1.82	0.70
1:A:29:GLY:N	1:A:36:HIS:HE1	1.80	0.70
1:B:160:ARG:O	1:B:164:ARG:HG3	1.91	0.70
1:A:31:VAL:CG1	1:A:32:PRO:HD2	2.19	0.70
1:A:223:LEU:O	1:A:227:VAL:HG23	1.92	0.69
1:A:179:ARG:O	1:A:183:LEU:HG	1.92	0.69
1:B:179:ARG:O	1:B:183:LEU:HG	1.92	0.69
1:A:234:ARG:HD3	3:A:577:HOH:O	1.91	0.69
1:A:234:ARG:HD2	1:A:245:LEU:HD22	1.74	0.69
1:A:175:TYR:HB3	1:A:177:ASP:OD1	1.93	0.69
1:A:232:ALA:HA	3:A:583:HOH:O	1.93	0.69
1:A:182:ARG:HA	3:A:533:HOH:O	1.91	0.69
1:A:160:ARG:O	1:A:164:ARG:HG3	1.93	0.68
1:A:244:LEU:HD21	1:A:248:LEU:CD1	2.23	0.68
1:B:223:LEU:O	1:B:227:VAL:HG23	1.93	0.68
1:B:371:ARG:HD3	3:B:654:HOH:O	1.93	0.68
1:A:226:LEU:CD2	1:A:230:ILE:HD11	2.25	0.67
1:A:176:MET:HG2	1:A:230:ILE:HD13	1.76	0.67
1:B:391:ARG:HG2	3:B:614:HOH:O	1.94	0.67
1:B:36:HIS:HD2	1:B:61:LYS:N	1.89	0.67
1:B:170:LEU:O	1:B:243:ASP:HB2	1.95	0.67
1:B:241:PRO:O	1:B:246:THR:HB	1.94	0.67
1:B:176:MET:HG2	1:B:230:ILE:CD1	2.24	0.67
1:A:142:LEU:HD21	1:A:161:VAL:HG21	1.77	0.67
1:A:373:PRO:HG3	1:A:379:ASN:ND2	2.10	0.67
1:B:234:ARG:HD2	1:B:245:LEU:HD22	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:176:MET:HG2	1:B:230:ILE:HD13	1.76	0.66
1:A:336:PRO:HB2	3:A:516:HOH:O	1.96	0.66
1:A:76:THR:HG21	1:A:369:ILE:HD11	1.77	0.66
1:B:373:PRO:HG3	1:B:379:ASN:ND2	2.10	0.66
1:B:68:TYR:OH	1:B:357:PRO:HG2	1.94	0.66
1:A:31:VAL:N	1:A:35:GLY:HA2	2.11	0.66
1:A:241:PRO:O	1:A:246:THR:HB	1.95	0.66
1:A:273:THR:HB	1:A:274:PRO:HD3	1.78	0.65
1:B:389:PRO:HG3	3:B:686:HOH:O	1.96	0.65
1:B:31:VAL:N	1:B:35:GLY:HA2	2.11	0.65
1:A:36:HIS:CD2	1:A:61:LYS:H	2.06	0.65
1:B:179:ARG:HD3	1:B:226:LEU:CD1	2.26	0.65
1:B:300:ILE:HD11	1:B:327:VAL:HG21	1.78	0.64
1:A:142:LEU:HD11	1:A:161:VAL:HG22	1.78	0.64
1:B:157:GLU:O	1:B:161:VAL:HG23	1.97	0.64
1:B:72:ASN:O	1:B:76:THR:HG23	1.98	0.64
1:B:275:GLY:HA3	2:B:500:HEM:HBC2	1.80	0.64
1:B:285:TRP:HB3	3:B:603:HOH:O	1.98	0.64
1:B:161:VAL:O	1:B:165:VAL:HG23	1.98	0.63
1:B:31:VAL:CG1	1:B:32:PRO:HD2	2.25	0.63
1:B:328:ILE:O	1:B:332:MET:HG3	1.99	0.63
1:B:244:LEU:HD21	1:B:248:LEU:HD12	1.80	0.62
1:A:149:GLY:O	1:A:457:ARG:HD3	1.99	0.62
1:A:275:GLY:HA3	2:A:500:HEM:HBC2	1.80	0.62
1:A:179:ARG:HD3	1:A:226:LEU:CD1	2.28	0.62
1:A:116:ARG:HH11	1:A:267:GLN:NE2	1.98	0.62
1:A:388:LEU:HD12	1:A:391:ARG:HH21	1.63	0.62
1:B:326:ASN:OD1	1:B:387:TRP:HB2	2.00	0.62
1:A:285:TRP:CZ3	1:A:451:PRO:HG3	2.34	0.62
1:A:244:LEU:HD21	1:A:248:LEU:HD12	1.81	0.61
1:A:181:GLU:O	1:A:185:VAL:HG23	2.00	0.61
1:B:143:THR:HG23	1:B:430:LYS:CD	2.30	0.61
1:A:170:LEU:O	1:A:243:ASP:HB2	2.00	0.61
1:A:144:GLU:HA	3:A:596:HOH:O	1.98	0.61
1:A:343:ARG:NE	3:A:560:HOH:O	2.32	0.61
1:B:34:LEU:HA	1:B:63:GLY:HA2	1.82	0.61
1:B:391:ARG:HB2	3:B:669:HOH:O	2.00	0.61
1:A:324:THR:HB	3:A:561:HOH:O	2.00	0.61
1:B:226:LEU:HD23	1:B:230:ILE:CD1	2.26	0.61
1:A:187:LEU:HD11	1:A:220:LEU:HD23	1.83	0.61
1:A:72:ASN:O	1:A:76:THR:HG23	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:LEU:HA	1:A:63:GLY:HA2	1.83	0.60
1:B:186:ALA:O	1:B:190:VAL:HG23	2.00	0.60
1:A:151:THR:HG22	1:A:457:ARG:HG3	1.83	0.60
1:A:161:VAL:O	1:A:165:VAL:HG23	2.00	0.60
1:A:65:LYS:HG3	3:A:544:HOH:O	2.02	0.60
1:A:221:ALA:O	1:A:225:LEU:HB2	2.02	0.60
1:A:157:GLU:O	1:A:161:VAL:HG23	2.01	0.60
1:A:260:GLY:HA3	3:A:604:HOH:O	2.01	0.60
1:A:36:HIS:HD2	1:A:61:LYS:N	1.92	0.59
1:A:227:VAL:HG21	1:A:269:VAL:CG2	2.32	0.59
1:B:149:GLY:O	1:B:457:ARG:HD3	2.01	0.59
1:B:187:LEU:HD11	1:B:220:LEU:HD23	1.84	0.59
1:B:120:GLN:HB3	3:B:670:HOH:O	2.02	0.59
1:A:134:ILE:HG13	3:A:645:HOH:O	2.03	0.58
1:A:84:ASP:HA	3:A:627:HOH:O	2.04	0.58
1:A:68:TYR:OH	1:A:357:PRO:HG2	2.02	0.58
1:A:176:MET:HG2	1:A:230:ILE:HD11	1.86	0.58
1:B:285:TRP:CZ3	1:B:451:PRO:HG3	2.38	0.58
1:B:183:LEU:HD13	1:B:222:ASP:HB3	1.84	0.58
1:B:388:LEU:HB2	3:B:669:HOH:O	2.04	0.58
1:A:83:PRO:HG3	3:A:639:HOH:O	2.02	0.58
1:A:172:ARG:HA	3:A:525:HOH:O	2.04	0.58
1:B:157:GLU:HG3	3:B:626:HOH:O	2.03	0.58
1:B:174:GLN:HB2	1:B:233:GLU:OE2	2.04	0.57
1:B:385:ASP:HB2	3:B:611:HOH:O	2.04	0.57
1:B:26:VAL:HG22	3:B:632:HOH:O	2.04	0.57
1:B:123:PHE:HB3	1:B:411:PRO:O	2.04	0.57
1:A:328:ILE:O	1:A:332:MET:HG3	2.04	0.57
1:B:148:PRO:HA	1:B:458:PRO:O	2.04	0.57
1:B:279:ILE:HG13	1:B:420:LEU:HD21	1.86	0.57
1:A:146:TRP:NE1	1:A:157:GLU:HG2	2.19	0.57
1:B:234:ARG:CZ	1:B:241:PRO:HB3	2.35	0.57
1:B:116:ARG:HB2	3:B:608:HOH:O	2.03	0.57
1:B:226:LEU:O	1:B:230:ILE:HG13	2.05	0.57
1:A:279:ILE:HG13	1:A:420:LEU:HD21	1.85	0.57
1:A:235:ARG:HG3	3:A:567:HOH:O	2.04	0.57
1:A:116:ARG:HA	3:A:506:HOH:O	2.03	0.57
1:B:301:ARG:HH11	1:B:301:ARG:HB3	1.70	0.57
1:B:300:ILE:O	1:B:304:VAL:HG23	2.05	0.57
1:A:230:ILE:O	1:A:233:GLU:HG2	2.04	0.56
1:B:407:LYS:HB2	3:B:697:HOH:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:221:ALA:O	1:B:225:LEU:HB2	2.05	0.56
1:B:142:LEU:HD21	1:B:161:VAL:HG21	1.88	0.56
1:A:391:ARG:O	1:A:394:ASN:HB2	2.05	0.56
1:A:159:PHE:O	1:A:163:VAL:HG23	2.05	0.56
1:A:444:ARG:HH11	1:A:450:ARG:HD2	1.69	0.56
1:B:130:ALA:HB3	3:B:761:HOH:O	2.04	0.56
1:B:260:GLY:N	3:B:745:HOH:O	2.38	0.56
1:A:186:ALA:O	1:A:190:VAL:HG23	2.06	0.56
1:A:301:ARG:HH11	1:A:301:ARG:HB3	1.71	0.56
1:A:143:THR:HG23	1:A:430:LYS:CD	2.33	0.55
1:A:129:PRO:HG2	3:A:631:HOH:O	2.06	0.55
1:A:160:ARG:HG3	1:A:181:GLU:CD	2.27	0.55
1:B:120:GLN:HG2	3:B:604:HOH:O	2.07	0.55
1:B:116:ARG:HH11	1:B:267:GLN:NE2	2.04	0.55
1:A:123:PHE:HB3	1:A:411:PRO:O	2.05	0.55
1:A:64:PRO:HG3	1:B:64:PRO:HG3	1.87	0.55
1:B:244:LEU:HD21	1:B:248:LEU:CG	2.37	0.55
1:B:138:GLU:OE1	1:B:164:ARG:NH1	2.38	0.55
1:A:178:GLU:HG3	1:A:181:GLU:OE2	2.05	0.55
1:B:391:ARG:O	1:B:394:ASN:HB2	2.06	0.55
1:B:244:LEU:O	1:B:244:LEU:HD23	2.07	0.55
1:A:249:LEU:HD12	3:A:577:HOH:O	2.07	0.55
1:B:178:GLU:HG3	1:B:181:GLU:OE2	2.07	0.55
1:B:409:LYS:HE2	3:B:666:HOH:O	2.07	0.55
1:B:391:ARG:NH1	3:B:611:HOH:O	2.38	0.54
1:B:159:PHE:O	1:B:163:VAL:HG23	2.06	0.54
1:A:148:PRO:HA	1:A:458:PRO:O	2.07	0.54
1:A:138:GLU:OE1	1:A:164:ARG:NH1	2.39	0.54
1:B:244:LEU:CD2	1:B:248:LEU:HD12	2.37	0.54
1:A:61:LYS:HG2	1:A:66:THR:HG23	1.89	0.54
1:B:432:ARG:HD3	3:B:668:HOH:O	2.08	0.54
1:A:64:PRO:HG3	1:B:64:PRO:CG	2.38	0.54
1:B:244:LEU:HD21	1:B:248:LEU:HG	1.89	0.54
1:A:244:LEU:CD2	1:A:248:LEU:HD12	2.38	0.54
1:A:183:LEU:HD13	1:A:222:ASP:HB3	1.90	0.54
1:B:388:LEU:HD12	1:B:391:ARG:NH2	2.20	0.54
1:B:234:ARG:HH11	1:B:245:LEU:HB3	1.73	0.54
1:A:326:ASN:OD1	1:A:387:TRP:HB2	2.07	0.54
1:A:226:LEU:HD23	1:A:230:ILE:CD1	2.36	0.53
1:B:248:LEU:CD1	1:B:268:VAL:HG23	2.37	0.53
1:A:234:ARG:CZ	1:A:241:PRO:HB3	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:117:ARG:HB2	3:B:746:HOH:O	2.08	0.53
1:A:355:ARG:O	1:A:357:PRO:HD3	2.09	0.53
1:B:343:ARG:NE	3:B:613:HOH:O	2.40	0.53
1:B:338:VAL:HG21	1:B:341:LEU:HD21	1.89	0.53
1:A:33:LEU:CD2	1:B:64:PRO:HD2	2.39	0.53
1:A:244:LEU:C	1:A:244:LEU:CD2	2.76	0.53
1:A:187:LEU:HD11	1:A:220:LEU:CD2	2.39	0.53
1:B:151:THR:HG22	1:B:457:ARG:HG3	1.91	0.53
1:A:26:VAL:HG21	3:A:593:HOH:O	2.09	0.53
1:A:174:GLN:HB2	1:A:233:GLU:OE2	2.09	0.53
1:B:192:ARG:HD3	3:B:635:HOH:O	2.09	0.53
1:A:301:ARG:HB3	1:A:301:ARG:NH1	2.23	0.52
1:B:444:ARG:HH11	1:B:450:ARG:HD2	1.74	0.52
1:A:125:LEU:H	1:A:125:LEU:HD12	1.74	0.52
1:A:244:LEU:O	1:A:244:LEU:HD23	2.10	0.52
1:B:227:VAL:HG21	1:B:269:VAL:CG2	2.35	0.52
1:A:34:LEU:HD13	1:B:34:LEU:HB2	1.92	0.52
1:B:117:ARG:HG3	3:B:711:HOH:O	2.09	0.52
1:A:300:ILE:O	1:A:304:VAL:HG23	2.09	0.52
1:B:160:ARG:HG3	1:B:181:GLU:CD	2.30	0.52
1:B:277:GLU:HG3	1:B:450:ARG:NH2	2.24	0.52
1:A:60:ILE:HG13	1:A:67:VAL:HG22	1.92	0.52
1:B:142:LEU:HD11	1:B:161:VAL:HG22	1.91	0.52
1:B:136:GLU:HG2	1:B:314:ALA:HA	1.91	0.51
1:B:230:ILE:O	1:B:233:GLU:HG2	2.11	0.51
1:A:407:LYS:HB3	3:A:598:HOH:O	2.10	0.51
1:B:318:VAL:HB	1:B:421:THR:HG21	1.92	0.51
1:B:394:ASN:HA	3:B:641:HOH:O	2.10	0.51
1:B:187:LEU:HD11	1:B:220:LEU:CD2	2.41	0.51
1:B:301:ARG:NH1	1:B:301:ARG:HB3	2.25	0.51
1:A:64:PRO:CG	1:B:64:PRO:HG3	2.41	0.51
1:B:240:LYS:O	1:B:242:ASP:N	2.43	0.51
1:A:407:LYS:O	1:A:409:LYS:N	2.43	0.51
1:A:226:LEU:O	1:A:230:ILE:HG13	2.11	0.51
1:A:244:LEU:HD21	1:A:248:LEU:HG	1.93	0.51
1:A:171:LEU:C	3:A:515:HOH:O	2.49	0.51
1:B:146:TRP:NE1	1:B:157:GLU:HG2	2.23	0.51
1:B:240:LYS:N	1:B:241:PRO:CD	2.74	0.51
1:B:274:PRO:HB2	3:B:743:HOH:O	2.10	0.51
1:B:117:ARG:O	1:B:121:PRO:HD3	2.10	0.51
1:A:408:ARG:HG2	3:A:571:HOH:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:LEU:HB3	1:B:64:PRO:HD2	1.94	0.50
1:B:403:PHE:HD2	1:B:410:CYS:HB3	1.76	0.50
1:A:42:ARG:HD2	3:B:631:HOH:O	2.10	0.50
1:A:248:LEU:CD1	1:A:268:VAL:HG23	2.41	0.50
1:B:128:ILE:HG13	1:B:129:PRO:HD3	1.92	0.50
1:B:181:GLU:O	1:B:185:VAL:HG23	2.12	0.50
1:A:117:ARG:O	1:A:121:PRO:HD3	2.12	0.50
1:A:60:ILE:CG1	1:A:67:VAL:HG22	2.41	0.50
1:A:79:LEU:CD1	1:A:362:ILE:HD11	2.31	0.50
1:A:244:LEU:HD21	1:A:248:LEU:CG	2.41	0.50
1:A:224:HIS:ND1	1:A:265:HIS:HE1	2.09	0.50
1:B:57:VAL:HG22	1:B:354:TYR:CD1	2.46	0.50
1:A:116:ARG:HB2	3:A:509:HOH:O	2.12	0.49
1:B:22:ARG:NH1	1:B:355:ARG:HG3	2.27	0.49
1:A:238:GLY:C	1:A:241:PRO:HD2	2.33	0.49
1:A:240:LYS:O	1:A:242:ASP:N	2.45	0.49
1:A:159:PHE:CE2	1:A:184:CYS:HB3	2.47	0.49
1:A:136:GLU:HG2	1:A:314:ALA:HA	1.92	0.49
1:B:60:ILE:CG1	1:B:67:VAL:HG22	2.43	0.49
1:A:343:ARG:HA	3:A:503:HOH:O	2.12	0.49
1:B:128:ILE:CG1	1:B:129:PRO:HD3	2.42	0.49
1:B:52:ARG:HB3	3:B:769:HOH:O	2.12	0.49
1:B:183:LEU:CD1	1:B:222:ASP:HB3	2.42	0.49
1:B:224:HIS:ND1	1:B:265:HIS:HE1	2.10	0.49
1:B:159:PHE:CE2	1:B:184:CYS:HB3	2.48	0.49
1:A:338:VAL:HG21	1:A:341:LEU:HD21	1.93	0.49
1:A:33:LEU:HD22	1:B:65:LYS:N	2.18	0.48
1:A:295:GLU:HG2	1:A:296:HIS:N	2.28	0.48
1:A:444:ARG:HD2	3:A:547:HOH:O	2.14	0.48
1:B:355:ARG:O	1:B:357:PRO:HD3	2.13	0.48
1:A:391:ARG:HA	1:A:394:ASN:HD22	1.79	0.48
1:B:187:LEU:HD21	1:B:220:LEU:HD21	1.94	0.48
1:A:296:HIS:O	1:A:300:ILE:HG13	2.13	0.48
1:A:234:ARG:HH11	1:A:245:LEU:HB3	1.77	0.48
1:A:240:LYS:N	1:A:241:PRO:CD	2.76	0.48
1:B:407:LYS:O	1:B:409:LYS:N	2.45	0.48
1:A:403:PHE:HD2	1:A:410:CYS:HB3	1.79	0.48
1:A:124:ARG:NH1	3:A:638:HOH:O	2.46	0.48
1:B:230:ILE:O	1:B:233:GLU:CG	2.62	0.48
1:B:244:LEU:C	1:B:244:LEU:CD2	2.76	0.48
1:B:234:ARG:NH2	1:B:241:PRO:HB3	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:LEU:O	1:B:129:PRO:HD3	2.13	0.48
1:A:245:LEU:C	1:A:245:LEU:HD23	2.34	0.48
1:B:147:GLN:NE2	3:B:730:HOH:O	2.44	0.48
1:B:391:ARG:HA	1:B:394:ASN:HD22	1.77	0.48
1:B:118:THR:HG23	3:B:625:HOH:O	2.13	0.48
1:B:118:THR:O	1:B:121:PRO:HD2	2.13	0.48
1:A:159:PHE:HE2	1:A:184:CYS:HB3	1.78	0.48
1:A:57:VAL:HG22	1:A:354:TYR:CD1	2.48	0.48
1:B:82:ASN:HB3	1:B:85:TYR:CD1	2.49	0.48
1:B:339:TRP:CD2	1:B:340:VAL:HG22	2.48	0.48
1:A:42:ARG:NH1	3:A:668:HOH:O	2.45	0.47
1:A:249:LEU:CD1	3:A:577:HOH:O	2.62	0.47
1:B:60:ILE:HG13	1:B:67:VAL:HG22	1.95	0.47
1:B:79:LEU:CD1	1:B:362:ILE:HD11	2.36	0.47
1:A:430:LYS:NZ	3:A:596:HOH:O	2.47	0.47
1:A:432:ARG:CB	1:A:459:VAL:HG22	2.40	0.47
1:B:245:LEU:C	1:B:245:LEU:HD23	2.33	0.47
1:B:159:PHE:HE2	1:B:184:CYS:HB3	1.78	0.47
1:A:54:HIS:CB	1:A:58:VAL:HG11	2.44	0.47
1:B:176:MET:CE	3:B:688:HOH:O	2.62	0.47
1:A:38:TRP:HE3	3:A:650:HOH:O	1.98	0.47
1:B:76:THR:HG21	1:B:369:ILE:CD1	2.42	0.47
1:A:369:ILE:HG13	3:A:606:HOH:O	2.13	0.47
1:A:301:ARG:HD2	3:A:508:HOH:O	2.15	0.47
1:B:119:ILE:HG23	1:B:123:PHE:CE1	2.50	0.47
1:A:131:TYR:HA	3:A:645:HOH:O	2.14	0.46
1:B:75:LEU:O	1:B:79:LEU:HB2	2.15	0.46
1:A:34:LEU:C	3:A:538:HOH:O	2.54	0.46
1:A:230:ILE:O	1:A:233:GLU:CG	2.63	0.46
1:A:187:LEU:HD21	1:A:220:LEU:HD21	1.97	0.46
1:A:128:ILE:CG1	1:A:129:PRO:HD3	2.46	0.46
1:B:182:ARG:HG2	3:B:750:HOH:O	2.16	0.46
1:A:444:ARG:NH1	1:A:450:ARG:HD2	2.30	0.46
1:A:260:GLY:N	3:A:574:HOH:O	2.47	0.46
1:B:61:LYS:HG2	1:B:66:THR:HG23	1.98	0.46
1:B:315:PHE:O	1:B:318:VAL:HG22	2.16	0.46
1:A:218:ASP:N	3:A:644:HOH:O	2.48	0.46
1:B:176:MET:HG2	1:B:230:ILE:HD11	1.97	0.46
1:A:234:ARG:NH2	1:A:241:PRO:HB3	2.30	0.46
1:B:173:GLY:HA3	3:B:693:HOH:O	2.15	0.46
1:B:240:LYS:N	1:B:241:PRO:HD2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:LEU:O	1:A:129:PRO:HD3	2.16	0.46
1:A:120:GLN:O	1:A:124:ARG:HG3	2.16	0.46
1:A:333:ARG:HG2	1:A:370:GLN:HB3	1.98	0.46
1:A:403:PHE:CD2	1:A:410:CYS:HB3	2.50	0.46
1:B:181:GLU:HB3	3:B:731:HOH:O	2.16	0.45
1:A:31:VAL:O	1:A:35:GLY:HA2	2.17	0.45
1:A:174:GLN:HG3	1:A:233:GLU:CD	2.37	0.45
1:B:116:ARG:HA	3:B:590:HOH:O	2.15	0.45
1:A:119:ILE:HG23	1:A:123:PHE:CE1	2.52	0.45
1:B:218:ASP:N	3:B:586:HOH:O	2.49	0.45
1:B:409:LYS:CG	1:B:410:CYS:N	2.79	0.45
1:A:82:ASN:HB3	1:A:85:TYR:CD1	2.51	0.45
1:B:125:LEU:HD12	1:B:125:LEU:H	1.82	0.45
1:A:244:LEU:HD11	1:A:271:ILE:HD12	1.97	0.45
1:B:295:GLU:HG2	1:B:296:HIS:N	2.31	0.45
1:B:430:LYS:HE2	1:B:431:TYR:CZ	2.52	0.45
1:A:325:GLY:N	3:A:561:HOH:O	2.49	0.45
1:B:403:PHE:CD2	1:B:410:CYS:HB3	2.51	0.45
1:A:374:LYS:HD2	3:A:667:HOH:O	2.16	0.45
1:A:315:PHE:CD2	3:A:563:HOH:O	2.69	0.45
1:B:409:LYS:HG2	3:B:666:HOH:O	2.15	0.45
1:A:118:THR:O	1:A:121:PRO:HD2	2.17	0.45
1:A:54:HIS:HB3	1:A:58:VAL:HG11	1.98	0.45
1:A:330:GLU:OE2	1:A:330:GLU:HA	2.17	0.45
1:A:176:MET:CE	3:A:515:HOH:O	2.65	0.45
1:B:218:ASP:N	3:B:650:HOH:O	2.49	0.45
1:A:244:LEU:HD11	1:A:271:ILE:CD1	2.47	0.44
1:A:234:ARG:NH2	1:A:243:ASP:OD1	2.50	0.44
1:A:241:PRO:O	1:A:246:THR:CB	2.64	0.44
1:B:318:VAL:HB	1:B:421:THR:CG2	2.47	0.44
1:B:54:HIS:CB	1:B:58:VAL:HG11	2.47	0.44
1:A:179:ARG:NH2	1:A:222:ASP:OD1	2.51	0.44
1:B:459:VAL:HG21	3:B:668:HOH:O	2.16	0.44
1:A:34:LEU:HD13	1:B:34:LEU:CB	2.47	0.44
1:B:118:THR:HG23	1:B:251:ALA:HB2	1.99	0.44
1:A:82:ASN:HB3	1:A:85:TYR:CE1	2.53	0.44
1:A:131:TYR:HE2	3:A:670:HOH:O	2.00	0.44
1:A:34:LEU:HD11	3:A:650:HOH:O	2.17	0.44
1:B:333:ARG:HA	1:B:370:GLN:NE2	2.32	0.44
1:A:27:ALA:HA	1:A:59:ARG:O	2.18	0.44
1:B:430:LYS:HE2	1:B:431:TYR:CE2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:ARG:NH2	1:B:243:ASP:OD1	2.51	0.44
1:A:409:LYS:CG	1:A:410:CYS:N	2.80	0.44
1:B:134:ILE:HG21	1:B:168:ARG:HB3	2.00	0.44
1:B:227:VAL:HG11	1:B:269:VAL:HG23	1.98	0.44
1:A:300:ILE:HD11	1:A:327:VAL:HG21	1.98	0.44
1:A:118:THR:HG23	1:A:251:ALA:HB2	2.00	0.44
1:B:82:ASN:HB3	1:B:85:TYR:CE1	2.52	0.44
1:B:248:LEU:HD12	1:B:268:VAL:HG23	2.00	0.44
1:B:245:LEU:CD2	1:B:249:LEU:HD11	2.47	0.44
1:A:116:ARG:N	3:A:602:HOH:O	2.51	0.44
1:B:191:PHE:HB3	1:B:447:ILE:HD11	1.99	0.44
1:B:27:ALA:HA	1:B:59:ARG:O	2.18	0.44
1:A:315:PHE:O	1:A:318:VAL:HG22	2.18	0.44
1:A:22:ARG:NH1	1:A:355:ARG:HG3	2.32	0.44
1:A:119:ILE:HG23	1:A:123:PHE:HE1	1.83	0.44
1:A:118:THR:CG2	1:A:251:ALA:HB2	2.48	0.44
1:B:333:ARG:HG2	1:B:370:GLN:HB3	2.00	0.44
1:A:33:LEU:CD1	1:B:65:LYS:HB2	2.48	0.44
1:A:171:LEU:HA	1:A:234:ARG:HH12	1.82	0.44
1:B:371:ARG:HB2	3:B:654:HOH:O	2.18	0.44
1:A:140:HIS:CD2	3:A:573:HOH:O	2.71	0.44
1:B:322:ARG:HD3	3:B:733:HOH:O	2.18	0.44
1:A:395:VAL:HA	1:A:396:PRO:HD3	1.85	0.43
1:A:277:GLU:HG3	1:A:450:ARG:NH2	2.33	0.43
1:A:41:ALA:HB2	1:B:38:TRP:CE3	2.53	0.43
1:B:31:VAL:O	1:B:35:GLY:HA2	2.17	0.43
1:B:245:LEU:O	1:B:245:LEU:HD23	2.18	0.43
1:B:432:ARG:CB	1:B:459:VAL:HG22	2.45	0.43
1:B:235:ARG:HD3	3:B:615:HOH:O	2.18	0.43
1:B:435:GLN:HE21	1:B:439:SER:CB	2.32	0.43
1:B:222:ASP:O	1:B:226:LEU:HB2	2.19	0.43
1:A:372:ASP:HA	1:A:373:PRO:HD3	1.93	0.43
1:A:261:GLU:HG2	3:A:586:HOH:O	2.17	0.43
1:B:244:LEU:HD11	1:B:271:ILE:HD12	2.01	0.43
1:A:333:ARG:HA	1:A:370:GLN:NE2	2.34	0.43
1:A:189:THR:HG21	3:A:568:HOH:O	2.17	0.43
1:A:179:ARG:HD2	3:A:675:HOH:O	2.19	0.43
1:A:318:VAL:HG22	3:A:563:HOH:O	2.18	0.43
1:B:444:ARG:NH1	3:B:651:HOH:O	2.50	0.43
1:A:296:HIS:CE1	1:A:384:PRO:HD2	2.54	0.43
1:A:330:GLU:OE1	1:A:333:ARG:NH1	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:248:LEU:HD13	1:B:264:ILE:HG22	2.01	0.42
1:B:385:ASP:CB	3:B:611:HOH:O	2.63	0.42
1:A:287:LEU:HD23	1:A:287:LEU:HA	1.93	0.42
1:A:172:ARG:NH2	3:A:645:HOH:O	2.51	0.42
1:A:260:GLY:CA	3:A:604:HOH:O	2.65	0.42
1:B:53:ASP:O	1:B:55:GLY:N	2.52	0.42
1:B:118:THR:CG2	1:B:251:ALA:HB2	2.49	0.42
1:A:387:TRP:CH2	1:A:400:MET:HG2	2.54	0.42
1:B:140:HIS:CE1	1:B:312:PRO:HB3	2.54	0.42
1:B:296:HIS:O	1:B:300:ILE:HG13	2.19	0.42
1:B:326:ASN:HB3	1:B:384:PRO:O	2.20	0.42
1:A:75:LEU:O	1:A:79:LEU:HB2	2.19	0.42
1:B:162:ALA:HB1	1:B:279:ILE:HG22	2.02	0.42
1:B:54:HIS:HB3	1:B:58:VAL:HG11	2.00	0.42
1:B:124:ARG:HD3	3:B:655:HOH:O	2.19	0.42
1:A:339:TRP:CD2	1:A:340:VAL:HG22	2.54	0.42
1:B:61:LYS:HD2	3:B:642:HOH:O	2.19	0.42
2:A:500:HEM:HBA1	2:A:500:HEM:HMA1	2.01	0.42
2:B:500:HEM:HMA1	2:B:500:HEM:HBA1	2.02	0.42
1:A:222:ASP:O	1:A:226:LEU:HB2	2.19	0.42
1:A:183:LEU:CD1	1:A:222:ASP:HB3	2.49	0.42
1:A:151:THR:CG2	1:A:436:VAL:HG21	2.48	0.42
1:A:116:ARG:N	3:A:509:HOH:O	2.52	0.42
1:B:316:GLU:HG2	3:B:724:HOH:O	2.20	0.42
1:B:53:ASP:C	1:B:55:GLY:N	2.73	0.42
1:B:241:PRO:O	1:B:246:THR:CB	2.64	0.42
1:A:262:GLN:NE2	3:A:615:HOH:O	2.52	0.42
1:A:248:LEU:HD13	1:A:264:ILE:HG22	2.02	0.42
1:A:162:ALA:HB1	1:A:279:ILE:HG22	2.02	0.42
1:B:444:ARG:NH1	1:B:450:ARG:HD2	2.34	0.42
1:A:234:ARG:HG2	3:A:577:HOH:O	2.20	0.41
1:A:76:THR:HG21	1:A:369:ILE:CD1	2.47	0.41
1:B:301:ARG:HG3	1:B:429:THR:CA	2.28	0.41
1:A:33:LEU:HD23	1:B:64:PRO:HD2	2.02	0.41
1:B:179:ARG:NH2	1:B:222:ASP:OD1	2.53	0.41
1:A:240:LYS:N	1:A:241:PRO:HD2	2.36	0.41
1:A:444:ARG:HB2	1:A:452:HIS:CD2	2.56	0.41
1:B:385:ASP:O	1:B:388:LEU:HG	2.20	0.41
1:A:295:GLU:HG2	1:A:296:HIS:H	1.84	0.41
1:A:296:HIS:HA	1:A:299:ARG:HB2	2.01	0.41
1:A:41:ALA:HB3	1:B:41:ALA:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:PRO:HG2	3:A:633:HOH:O	2.20	0.41
1:A:81:LEU:HA	1:A:81:LEU:HD23	1.81	0.41
1:B:244:LEU:HD11	1:B:271:ILE:CD1	2.51	0.41
1:A:234:ARG:CD	1:A:245:LEU:HD22	2.49	0.41
1:A:72:ASN:HA	1:A:73:PRO:HD3	1.90	0.41
1:B:242:ASP:O	1:B:242:ASP:CG	2.59	0.41
1:A:34:LEU:HD22	1:B:63:GLY:CA	2.51	0.41
1:B:117:ARG:HG2	1:B:120:GLN:HB2	2.02	0.41
1:B:119:ILE:HG23	1:B:123:PHE:HE1	1.85	0.41
1:A:128:ILE:N	1:A:129:PRO:CD	2.84	0.41
1:B:294:PRO:HB3	3:B:620:HOH:O	2.20	0.41
1:A:301:ARG:HG3	1:A:429:THR:CA	2.27	0.41
1:A:134:ILE:HG21	1:A:168:ARG:HB3	2.03	0.41
1:A:68:TYR:CZ	1:A:357:PRO:HD2	2.55	0.41
1:A:318:VAL:HB	1:A:421:THR:HG21	2.02	0.41
1:B:53:ASP:C	1:B:55:GLY:H	2.24	0.41
1:A:410:CYS:HA	1:A:411:PRO:HD3	1.94	0.40
1:B:296:HIS:CE1	1:B:384:PRO:HD2	2.55	0.40
1:A:403:PHE:HD2	1:A:410:CYS:CB	2.35	0.40
1:A:403:PHE:HB3	1:A:410:CYS:HB3	2.03	0.40
1:B:435:GLN:HE21	1:B:439:SER:HB3	1.86	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	371/467 (79%)	337 (91%)	23 (6%)	11 (3%)	5 8
1	B	371/467 (79%)	338 (91%)	22 (6%)	11 (3%)	5 8
All	All	742/934 (79%)	675 (91%)	45 (6%)	22 (3%)	5 8

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	32	PRO
1	A	177	ASP
1	B	32	PRO
1	B	177	ASP
1	A	35	GLY
1	A	236	ALA
1	A	239	GLN
1	A	377	ASP
1	B	35	GLY
1	B	236	ALA
1	B	239	GLN
1	B	241	PRO
1	B	377	ASP
1	A	241	PRO
1	A	310	GLY
1	A	379	ASN
1	B	54	HIS
1	B	310	GLY
1	B	379	ASN
1	B	389	PRO
1	A	389	PRO
1	A	54	HIS

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	303/378 (80%)	257 (85%)	46 (15%)	3	6
1	B	303/378 (80%)	257 (85%)	46 (15%)	3	6
All	All	606/756 (80%)	514 (85%)	92 (15%)	3	6

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	VAL

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Mol	Chain	Res	Type
1	A	32	PRO
1	A	34	LEU
1	A	51	LEU
1	A	66	THR
1	A	67	VAL
1	A	79	LEU
1	A	117	ARG
1	A	126	ASP
1	A	133	PRO
1	A	157	GLU
1	A	160	ARG
1	A	174	GLN
1	A	176	MET
1	A	178	GLU
1	A	187	LEU
1	A	192	ARG
1	A	222	ASP
1	A	223	LEU
1	A	225	LEU
1	A	226	LEU
1	A	228	ASP
1	A	235	ARG
1	A	239	GLN
1	A	241	PRO
1	A	242	ASP
1	A	243	ASP
1	A	246	THR
1	A	264	ILE
1	A	267	GLN
1	A	279	ILE
1	A	302	ASP
1	A	305	GLU
1	A	308	THR
1	A	318	VAL
1	A	338	VAL
1	A	340	VAL
1	A	342	THR
1	A	348	GLU
1	A	350	GLU
1	A	362	ILE
1	A	371	ARG
1	A	381	GLU

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Mol	Chain	Res	Type
1	A	389	PRO
1	A	422	LEU
1	A	459	VAL
1	B	31	VAL
1	B	32	PRO
1	B	34	LEU
1	B	51	LEU
1	B	66	THR
1	B	67	VAL
1	B	79	LEU
1	B	117	ARG
1	B	126	ASP
1	B	133	PRO
1	B	143	THR
1	B	157	GLU
1	B	160	ARG
1	B	174	GLN
1	B	176	MET
1	B	178	GLU
1	B	187	LEU
1	B	192	ARG
1	B	222	ASP
1	B	223	LEU
1	B	225	LEU
1	B	226	LEU
1	B	228	ASP
1	B	235	ARG
1	B	239	GLN
1	B	241	PRO
1	B	242	ASP
1	B	243	ASP
1	B	246	THR
1	B	264	ILE
1	B	267	GLN
1	B	279	ILE
1	B	302	ASP
1	B	305	GLU
1	B	308	THR
1	B	318	VAL
1	B	338	VAL
1	B	340	VAL
1	B	342	THR

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Mol	Chain	Res	Type
1	B	350	GLU
1	B	362	ILE
1	B	371	ARG
1	B	381	GLU
1	B	389	PRO
1	B	422	LEU
1	B	459	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	HIS
1	A	265	HIS
1	A	267	GLN
1	A	288	GLN
1	A	296	HIS
1	A	323	HIS
1	A	379	ASN
1	A	394	ASN
1	A	419	GLN
1	A	435	GLN
1	B	36	HIS
1	B	265	HIS
1	B	267	GLN
1	B	288	GLN
1	B	296	HIS
1	B	323	HIS
1	B	379	ASN
1	B	394	ASN
1	B	419	GLN
1	B	435	GLN
1	B	452	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)

2 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	500	1	30,50,50	2.93	14 (46%)	24,82,82	3.23	12 (50%)
2	HEM	B	500	1	30,50,50	2.94	14 (46%)	24,82,82	3.25	12 (50%)

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	500	1	-	0/10/54/54	0/0/8/8
2	HEM	B	500	1	-	0/10/54/54	0/0/8/8

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	HEM	C3B-C4B	-7.37	1.45	1.51
2	B	500	HEM	C3B-C4B	-6.95	1.45	1.51
2	B	500	HEM	C2D-C3D	-4.99	1.39	1.54
2	A	500	HEM	C2D-C3D	-4.83	1.40	1.54
2	A	500	HEM	C3D-C4D	-3.11	1.47	1.51
2	B	500	HEM	C3D-C4D	-2.88	1.47	1.51
2	A	500	HEM	FE-ND	2.06	2.08	1.97
2	B	500	HEM	FE-NB	2.19	2.09	1.97
2	A	500	HEM	C3C-CAC	2.36	1.55	1.51
2	B	500	HEM	FE-ND	2.47	2.10	1.97
2	B	500	HEM	CHD-C4C	2.49	1.42	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	HEM	C3C-CAC	2.70	1.56	1.51
2	A	500	HEM	CHD-C4C	2.72	1.42	1.36
2	A	500	HEM	FE-NB	2.77	2.12	1.97
2	B	500	HEM	CHC-C1C	2.89	1.43	1.36
2	A	500	HEM	CHC-C1C	2.93	1.43	1.36
2	A	500	HEM	CBB-CAB	3.77	1.51	1.29
2	B	500	HEM	CBB-CAB	3.84	1.51	1.29
2	A	500	HEM	FE-NC	3.89	2.11	1.95
2	B	500	HEM	FE-NC	3.93	2.11	1.95
2	A	500	HEM	CBC-CAC	3.98	1.52	1.29
2	B	500	HEM	CAA-C2A	4.04	1.58	1.52
2	A	500	HEM	CAA-C2A	4.06	1.59	1.52
2	B	500	HEM	CBC-CAC	4.16	1.53	1.29
2	A	500	HEM	C1C-NC	4.90	1.42	1.36
2	B	500	HEM	C1C-NC	5.31	1.42	1.36
2	A	500	HEM	C4C-NC	5.35	1.42	1.36
2	B	500	HEM	C4C-NC	5.51	1.42	1.36

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	500	HEM	C3B-CAB-CBB	-7.06	113.62	124.46
2	B	500	HEM	C3B-CAB-CBB	-6.92	113.84	124.46
2	B	500	HEM	C3C-CAC-CBC	-5.94	115.35	124.46
2	A	500	HEM	C3C-CAC-CBC	-5.71	115.70	124.46
2	B	500	HEM	CAA-C2A-C1A	-5.09	121.48	127.01
2	A	500	HEM	CAA-C2A-C1A	-5.05	121.52	127.01
2	B	500	HEM	CMA-C3A-C4A	-2.65	123.98	128.36
2	A	500	HEM	CMA-C3A-C4A	-2.43	124.35	128.36
2	A	500	HEM	CMD-C2D-C3D	2.85	126.95	114.35
2	B	500	HEM	CMD-C2D-C3D	2.89	127.13	114.35
2	A	500	HEM	C2D-C3D-C4D	2.91	106.43	101.50
2	A	500	HEM	C3B-C4B-CHC	2.95	127.32	123.16
2	B	500	HEM	C2D-C3D-C4D	3.02	106.62	101.50
2	B	500	HEM	C3B-C4B-CHC	3.22	127.70	123.16
2	B	500	HEM	CAD-C3D-C4D	3.96	126.44	112.47
2	A	500	HEM	CAD-C3D-C4D	4.00	126.57	112.47
2	A	500	HEM	CMB-C2B-C3B	4.19	126.99	116.53
2	B	500	HEM	CMB-C2B-C3B	4.28	127.21	116.53
2	B	500	HEM	CBA-CAA-C2A	4.30	120.24	112.53
2	A	500	HEM	CBA-CAA-C2A	4.57	120.73	112.53
2	B	500	HEM	CAD-C3D-C2D	4.78	126.95	113.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	500	HEM	CAD-C3D-C2D	4.79	126.98	113.22
2	B	500	HEM	CMC-C2C-C3C	4.79	128.50	116.53
2	A	500	HEM	CMC-C2C-C3C	4.82	128.57	116.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	HEM	3	0
2	B	500	HEM	3	0

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, 95^{th} 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	379/467 (81%)	-0.07	4 (1%)	82 79	11, 44, 68, 78	0
1	B	379/467 (81%)	0.00	6 (1%)	74 69	6, 44, 68, 77	0
All	All	758/934 (81%)	-0.03	10 (1%)	79 75	6, 44, 68, 78	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	220	LEU	4.2
1	B	407	LYS	3.9
1	B	178	GLU	3.5
1	A	233	GLU	3.3
1	B	233	GLU	2.8
1	A	22	ARG	2.6
1	B	248	LEU	2.5
1	A	183	LEU	2.4
1	B	226	LEU	2.3
1	A	249	LEU	2.2

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, 95^{th} 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
2	HEM	A	500	43/43	0.96	0.20	0.45	25,46,54,58	0
2	HEM	B	500	43/43	0.96	0.19	-0.07	32,42,50,55	0

6.5 Other polymers

There are no such residues in this entry.