Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 04:43 AM GMT

PDB ID	:	2NZA
Title	:	Structure and Function Studies of Cytochrome P450 158A1 from Streptomyces coelicolor A3(2)
Authors	:	Zhao, B.; Waterman, M.R.
Deposited on	:	2006-11-22
Resolution	:	2.90 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

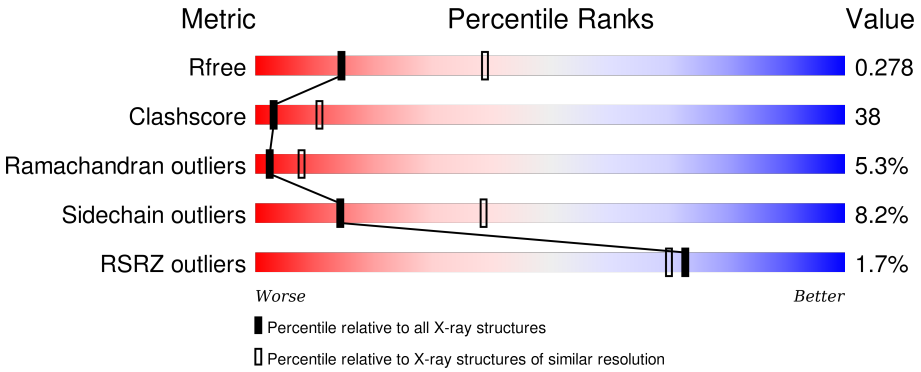
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.90 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	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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	413	43% 46% 7%
1	B	413	2% 42% 44% 8% 6%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6371 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.

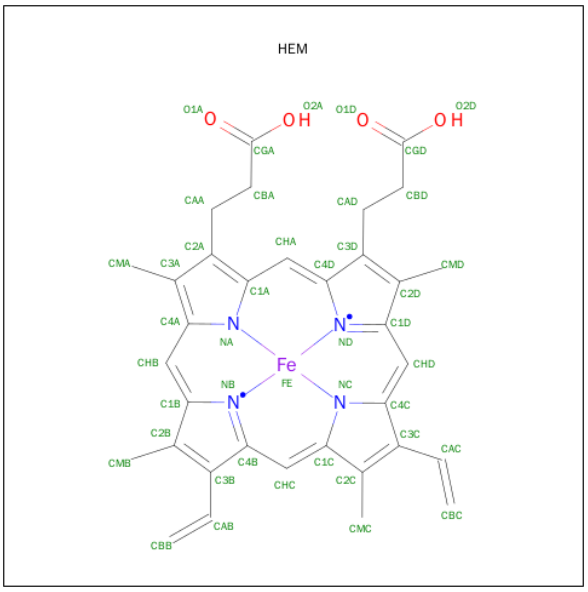
- Molecule 1 is a protein called Cytochrome P450 CYP158A1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	397	Total	C	N	O	S	0	0	0
			3065	1920	581	554	10			
1	B	388	Total	C	N	O	S	0	0	0
			2992	1872	566	544	10			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	408	HIS	-	EXPRESSION TAG	UNP Q9KZF5
A	409	HIS	-	EXPRESSION TAG	UNP Q9KZF5
A	410	HIS	-	EXPRESSION TAG	UNP Q9KZF5
A	411	HIS	-	EXPRESSION TAG	UNP Q9KZF5
A	412	HIS	-	EXPRESSION TAG	UNP Q9KZF5
A	413	HIS	-	EXPRESSION TAG	UNP Q9KZF5
B	408	HIS	-	EXPRESSION TAG	UNP Q9KZF5
B	409	HIS	-	EXPRESSION TAG	UNP Q9KZF5
B	410	HIS	-	EXPRESSION TAG	UNP Q9KZF5
B	411	HIS	-	EXPRESSION TAG	UNP Q9KZF5
B	412	HIS	-	EXPRESSION TAG	UNP Q9KZF5
B	413	HIS	-	EXPRESSION TAG	UNP Q9KZF5

- 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.

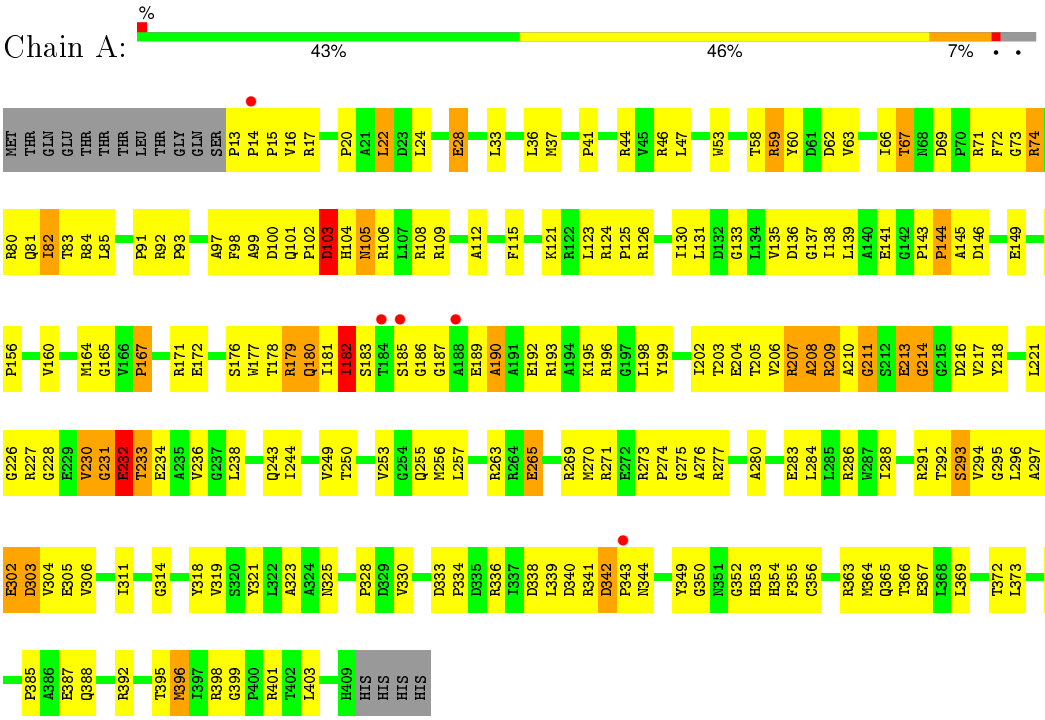
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	117	Total	O	0	0
			117	117		
3	B	111	Total	O	0	0
			111	111		

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.

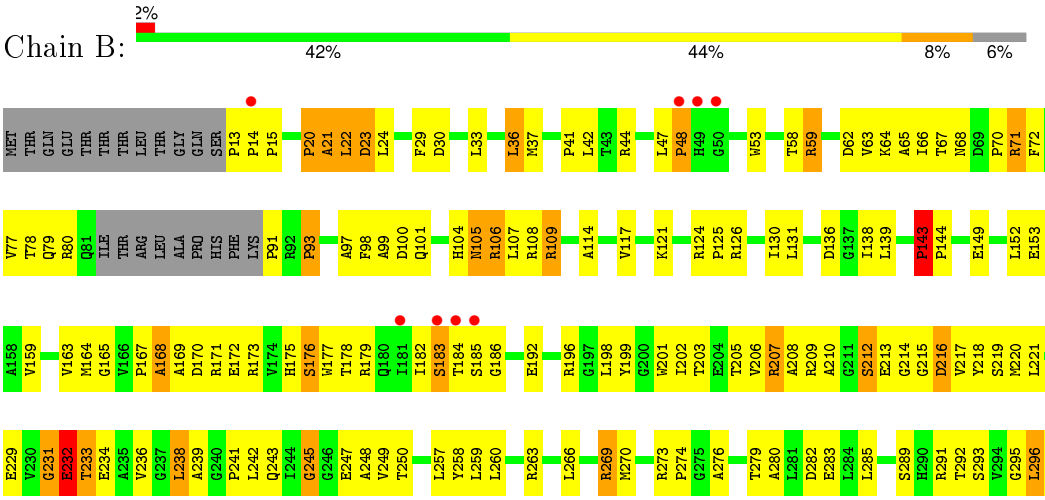
- Molecule 1: Cytochrome P450 CYP158A1

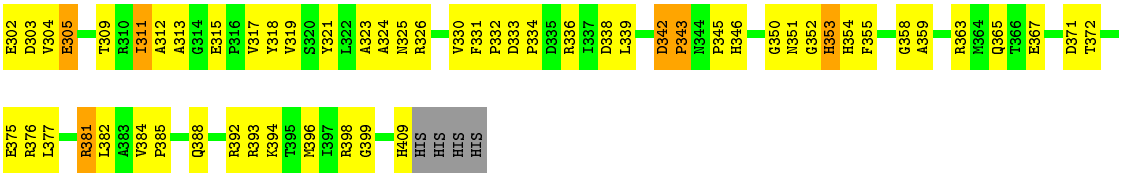
Chain A:



- Molecule 1: Cytochrome P450 CYP158A1

Chain B:




E302
D303
V304
E305
T309
R310
I311
A312
A313
G314
E315
P316
V317
Y318
V319
S320
Y321
L322
A323
A324
N325
R326
V330
F331
P332
D333
P334
D335
R336
I337
D338
L339
D342
P343
N344
P345
H346
G350
N351
G352
H353
H354
F355
G358
A359
R363
M364
Q365
I366
E367
D371
T372
E375
R376
L377
R381
L382
A383
V384
P385
Q388
R392
R393
K394
T395
M396
I397
R398
G399
H409
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	186.61Å 44.35Å 130.62Å 90.00° 98.23° 90.00°	Depositor
Resolution (Å)	10.00 – 2.90 49.72 – 2.80	Depositor EDS
% Data completeness (in resolution range)	85.7 (10.00-2.90) 84.5 (49.72-2.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	4.37 (at 2.81Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.197 , 0.267 0.220 , 0.278	Depositor DCC
R_{free} test set	1010 reflections (4.77%)	DCC
Wilson B-factor (Å^2)	20.3	Xtriage
Anisotropy	0.296	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 41.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	1 of 23648 reflections (0.004%)	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	6371	wwPDB-VP
Average B, all atoms (Å^2)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.37% 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	0.39	0/3136	0.67	1/4271 (0.0%)
1	B	0.36	0/3060	0.67	1/4165 (0.0%)
All	All	0.38	0/6196	0.67	2/8436 (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	B	13	PRO	N-CA-CB	5.43	109.81	103.30
1	A	13	PRO	N-CA-CB	5.38	109.76	103.30

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	3065	0	3047	244	0
1	B	2992	0	2969	226	0
2	A	43	0	30	2	0
2	B	43	0	30	2	0
3	A	117	0	0	21	0
3	B	111	0	0	19	0
All	All	6371	0	6076	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 38.

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:289:SER:HB2	1:B:398:ARG:HH21	1.20	1.06
1:A:283:GLU:HG2	1:A:339:LEU:H	1.27	0.99
1:A:182:ILE:HD13	1:A:186:GLY:H	1.28	0.98
1:B:304:VAL:HG12	1:B:305:GLU:H	1.28	0.95
1:B:64:LYS:HD2	1:B:351:ASN:OD1	1.70	0.91
1:A:165:GLY:HA3	1:A:216:ASP:OD1	1.70	0.91
1:B:58:THR:HG23	1:B:323:ALA:HB1	1.53	0.91
1:A:124:ARG:HB3	1:A:125:PRO:HD3	1.52	0.90
1:B:209:ARG:HB3	1:B:219:SER:HA	1.54	0.89
1:A:33:LEU:HD21	1:A:323:ALA:HB2	1.55	0.88
1:A:85:LEU:HD22	1:A:293:SER:HB3	1.56	0.88
1:A:208:ALA:O	1:A:210:ALA:N	2.06	0.87
1:B:33:LEU:HD21	1:B:323:ALA:HB2	1.59	0.84
1:A:392:ARG:HG3	1:A:399:GLY:O	1.78	0.83
1:B:289:SER:CB	1:B:398:ARG:HH21	1.91	0.83
1:B:37:MET:HG2	1:B:58:THR:HG21	1.60	0.81
1:B:289:SER:HB2	1:B:398:ARG:NH2	1.95	0.81
1:A:381:ARG:HD3	3:A:435:HOH:O	1.80	0.81
1:B:351:ASN:ND2	1:B:352:GLY:H	1.79	0.80
1:A:193:ARG:HG2	1:A:196:ARG:NH2	1.95	0.80
1:B:143:PRO:HB2	1:B:144:PRO:HD3	1.60	0.80
1:B:175:HIS:O	1:B:179:ARG:HG3	1.82	0.79
1:B:63:VAL:HG13	1:B:319:VAL:HB	1.64	0.79
1:A:93:PRO:HB2	1:A:233:THR:O	1.82	0.79
1:B:22:LEU:HG	1:B:24:LEU:HD12	1.65	0.79
1:B:202:ILE:O	1:B:206:VAL:HG23	1.83	0.78
1:A:80:ARG:NH1	1:A:314:GLY:O	2.17	0.78
1:B:14:PRO:HA	3:B:452:HOH:O	1.83	0.77
1:A:181:ILE:H	1:A:181:ILE:HD12	1.48	0.76
1:A:41:PRO:HB3	1:A:59:ARG:NH1	2.00	0.76
1:A:291:ARG:NH2	1:A:396:MET:HG3	2.00	0.76
1:A:304:VAL:O	1:A:311:ILE:HG22	1.86	0.76
1:B:342:ASP:HB2	1:B:343:PRO:HD3	1.66	0.75
1:B:342:ASP:CB	1:B:343:PRO:HD3	2.17	0.75
2:B:430:HEM:HHA	2:B:430:HEM:HBA2	1.70	0.74
1:A:338:ASP:HB3	3:A:445:HOH:O	1.86	0.74
1:B:41:PRO:HA	1:B:59:ARG:HD3	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:363:ARG:O	1:B:367:GLU:HG3	1.87	0.73
1:B:304:VAL:HG12	1:B:305:GLU:N	2.02	0.73
1:A:342:ASP:OD2	1:A:343:PRO:HD2	1.88	0.73
1:B:182:ILE:HG23	1:B:186:GLY:O	1.89	0.72
1:A:193:ARG:HG2	1:A:196:ARG:HH21	1.51	0.72
1:B:63:VAL:O	1:B:67:THR:HG22	1.88	0.72
1:A:62:ASP:O	1:A:66:ILE:HG13	1.88	0.72
1:A:210:ALA:HA	1:A:222:GLY:O	1.89	0.71
1:A:182:ILE:HD13	1:A:186:GLY:N	2.04	0.71
1:B:351:ASN:HD22	1:B:352:GLY:H	1.37	0.71
1:A:255:GLN:NE2	1:A:288:ILE:HG23	2.06	0.71
1:B:108:ARG:HG2	1:B:108:ARG:HH11	1.55	0.71
1:B:37:MET:HG2	1:B:58:THR:CG2	2.21	0.70
1:A:291:ARG:HH22	1:A:396:MET:HG3	1.57	0.70
1:A:179:ARG:N	1:A:179:ARG:HD2	2.06	0.70
1:B:303:ASP:HB2	1:B:313:ALA:HB2	1.73	0.69
1:B:342:ASP:OD2	1:B:343:PRO:HD3	1.91	0.69
1:B:205:THR:HG23	1:B:209:ARG:NH1	2.08	0.69
1:A:67:THR:HG22	1:A:298:ARG:NH2	2.08	0.69
1:A:179:ARG:HA	1:A:179:ARG:HH11	1.58	0.69
1:B:205:THR:HG23	1:B:209:ARG:CZ	2.23	0.68
1:B:209:ARG:HA	1:B:212:SER:HB2	1.75	0.68
1:A:67:THR:HG22	1:A:298:ARG:CZ	2.24	0.68
1:A:98:PHE:CE2	1:A:296:LEU:HD23	2.29	0.67
1:A:176:SER:O	1:A:179:ARG:HD3	1.94	0.67
1:A:47:LEU:HD12	1:A:83:THR:O	1.95	0.67
1:A:182:ILE:HG22	1:A:183:SER:H	1.59	0.67
1:A:82:ILE:HD12	1:A:82:ILE:H	1.60	0.67
1:A:207:ARG:HG3	1:A:207:ARG:HH11	1.58	0.67
1:A:181:ILE:N	1:A:181:ILE:HD12	2.10	0.66
1:B:91:PRO:HB3	1:B:98:PHE:CE1	2.29	0.66
1:A:37:MET:HG2	1:A:58:THR:CG2	2.25	0.66
1:A:207:ARG:HG3	1:A:207:ARG:NH1	2.10	0.66
1:A:286:ARG:HH21	1:A:341:ARG:HH21	1.42	0.66
1:B:165:GLY:HA3	1:B:216:ASP:OD2	1.96	0.66
1:B:138:ILE:HG13	1:B:139:LEU:N	2.10	0.66
1:A:230:VAL:O	1:A:231:GLY:O	2.14	0.66
1:B:342:ASP:CG	1:B:343:PRO:HD3	2.16	0.66
1:A:385:PRO:HD2	1:A:388:GLN:HG3	1.78	0.66
1:B:33:LEU:HD23	1:B:33:LEU:O	1.96	0.65
1:B:269:ARG:CG	1:B:269:ARG:HH11	2.09	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:23:ASP:HA	3:B:432:HOH:O	1.97	0.65
1:B:155:PHE:HB3	1:B:156:PRO:HD3	1.77	0.65
1:A:37:MET:HG2	1:A:58:THR:HG21	1.77	0.65
1:A:263:ARG:HB3	1:A:265:GLU:OE2	1.96	0.65
1:A:363:ARG:O	1:A:367:GLU:HG3	1.97	0.65
1:B:351:ASN:ND2	1:B:352:GLY:N	2.45	0.65
1:A:225:VAL:HG13	1:A:231:GLY:HA2	1.78	0.65
1:A:41:PRO:HB3	1:A:59:ARG:HH12	1.62	0.64
1:B:91:PRO:HB3	1:B:98:PHE:CD1	2.32	0.64
1:B:67:THR:HB	3:B:457:HOH:O	1.96	0.64
1:A:342:ASP:HB2	1:A:343:PRO:CD	2.27	0.64
1:B:207:ARG:O	1:B:210:ALA:HB2	1.97	0.64
1:A:135:VAL:HB	1:A:376:ARG:NH1	2.12	0.64
1:B:58:THR:HG23	1:B:323:ALA:CB	2.26	0.64
1:A:221:LEU:O	1:A:225:VAL:HG23	1.98	0.64
1:B:249:VAL:HG11	1:B:365:GLN:HE21	1.62	0.64
1:B:321:TYR:CZ	1:B:350:GLY:HA2	2.33	0.63
1:B:33:LEU:O	1:B:37:MET:HG3	1.97	0.63
1:B:76:GLU:HB3	1:B:299:ILE:HG13	1.80	0.63
1:A:144:PRO:O	1:B:196:ARG:NH1	2.32	0.63
1:A:249:VAL:HG21	1:A:365:GLN:NE2	2.13	0.63
1:A:182:ILE:CD1	1:A:185:SER:HA	2.29	0.62
1:A:342:ASP:HB2	1:A:343:PRO:HD3	1.80	0.62
1:B:47:LEU:HB3	3:B:509:HOH:O	1.99	0.62
1:A:286:ARG:NH2	1:A:341:ARG:NH2	2.48	0.62
1:A:133:GLY:O	1:A:136:ASP:HB2	2.00	0.62
1:B:297:ALA:HB2	1:B:318:TYR:CE2	2.35	0.62
1:A:115:PHE:HB3	3:A:432:HOH:O	2.00	0.62
1:B:124:ARG:HB3	1:B:125:PRO:HD3	1.81	0.62
1:B:375:GLU:HG3	1:B:376:ARG:HG2	1.82	0.62
1:B:44:ARG:HD2	1:B:53:TRP:CZ3	2.36	0.61
1:B:138:ILE:HD11	1:B:377:LEU:HD21	1.82	0.61
1:B:74:ARG:HG2	1:B:97:ALA:O	1.99	0.61
1:B:394:LYS:HE3	3:B:494:HOH:O	2.00	0.61
1:A:231:GLY:O	1:A:232:GLU:O	2.18	0.61
1:A:303:ASP:HA	1:A:311:ILE:O	2.00	0.61
1:A:180:GLN:HE21	1:A:180:GLN:CA	2.14	0.61
1:B:33:LEU:HD23	1:B:37:MET:HG3	1.83	0.61
1:B:159:VAL:O	1:B:163:VAL:HG23	2.01	0.60
1:A:342:ASP:CB	1:A:343:PRO:CD	2.79	0.60
1:B:375:GLU:HG3	1:B:376:ARG:N	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:GLY:H	1:A:223:ALA:HA	1.67	0.60
1:A:286:ARG:HH21	1:A:341:ARG:NH2	2.00	0.59
1:A:182:ILE:HD13	1:A:185:SER:HA	1.83	0.59
1:B:153:GLU:HA	1:B:250:THR:CG2	2.32	0.59
1:B:22:LEU:CG	1:B:24:LEU:HD12	2.32	0.59
1:A:224:ALA:CA	1:A:227:ARG:HH21	2.16	0.59
1:B:79:GLN:O	1:B:80:ARG:HG2	2.02	0.58
1:A:180:GLN:HE21	1:A:180:GLN:HA	1.67	0.58
1:A:59:ARG:O	1:A:63:VAL:HG23	2.02	0.58
1:B:259:LEU:O	1:B:263:ARG:HB2	2.04	0.58
1:A:271:ARG:HD3	3:A:440:HOH:O	2.03	0.58
1:A:300:ALA:HB1	3:A:538:HOH:O	2.04	0.58
1:B:342:ASP:OD2	1:B:343:PRO:CD	2.52	0.58
1:B:62:ASP:O	1:B:66:ILE:HG13	2.03	0.58
1:A:249:VAL:O	1:A:253:VAL:HG23	2.03	0.58
1:B:64:LYS:HG3	1:B:64:LYS:O	2.04	0.57
1:B:153:GLU:N	1:B:154:PRO:HD2	2.20	0.57
1:A:131:LEU:O	1:A:135:VAL:HG23	2.04	0.57
1:B:342:ASP:CG	1:B:343:PRO:CD	2.73	0.57
1:B:304:VAL:CG1	1:B:305:GLU:H	2.12	0.57
1:A:63:VAL:O	1:A:67:THR:OG1	2.22	0.57
1:B:208:ALA:O	1:B:209:ARG:HB2	2.02	0.57
1:B:203:THR:O	1:B:207:ARG:HD3	2.05	0.57
1:A:387:GLU:H	1:A:387:GLU:CD	2.08	0.56
1:A:74:ARG:HG3	1:A:74:ARG:O	2.05	0.56
1:A:155:PHE:CD2	1:A:369:LEU:HD21	2.40	0.56
1:A:228:GLY:HA2	3:A:461:HOH:O	2.05	0.56
1:B:311:ILE:O	1:B:311:ILE:HG22	2.06	0.56
1:B:241:PRO:HG2	3:B:522:HOH:O	2.06	0.56
1:A:44:ARG:HG2	1:A:53:TRP:CZ3	2.41	0.56
1:B:22:LEU:HD21	1:B:24:LEU:HB2	1.88	0.56
1:B:105:ASN:O	1:B:106:ARG:C	2.43	0.56
1:B:149:GLU:O	1:B:149:GLU:HG2	2.06	0.56
1:B:338:ASP:O	1:B:339:LEU:HB2	2.06	0.55
1:B:295:GLY:HA3	3:B:513:HOH:O	2.06	0.55
1:A:138:ILE:HD11	1:A:377:LEU:HD11	1.88	0.55
1:A:181:ILE:H	1:A:181:ILE:CD1	2.15	0.55
1:A:385:PRO:HD2	1:A:388:GLN:CG	2.36	0.55
1:A:167:PRO:O	1:A:171:ARG:HG2	2.05	0.55
1:A:85:LEU:HD23	1:A:396:MET:HE2	1.87	0.55
1:B:168:ALA:O	1:B:171:ARG:HG2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:THR:C	1:A:179:ARG:HD2	2.26	0.55
1:B:392:ARG:HG3	1:B:399:GLY:O	2.07	0.55
1:A:171:ARG:HG3	1:A:171:ARG:HH11	1.72	0.55
1:A:28:GLU:OE1	1:A:28:GLU:N	2.40	0.55
1:B:269:ARG:HH11	1:B:269:ARG:HG2	1.70	0.55
1:A:60:TYR:CD2	1:A:330:VAL:HG21	2.42	0.55
1:B:58:THR:CG2	1:B:323:ALA:HB1	2.34	0.55
1:A:208:ALA:C	1:A:210:ALA:H	2.11	0.55
1:A:207:ARG:HH12	1:A:232:GLU:CD	2.10	0.54
1:A:76:GLU:OE1	1:A:80:ARG:HD2	2.07	0.54
1:A:249:VAL:HG21	1:A:365:GLN:HE21	1.71	0.54
1:A:283:GLU:HG2	1:A:339:LEU:N	2.10	0.54
1:A:286:ARG:NH2	1:A:341:ARG:HH21	2.02	0.54
1:A:124:ARG:HB3	1:A:125:PRO:CD	2.33	0.54
1:A:108:ARG:HH11	1:A:108:ARG:HG2	1.73	0.54
1:B:342:ASP:CB	1:B:343:PRO:CD	2.85	0.54
1:A:177:TRP:C	1:A:179:ARG:H	2.10	0.54
1:B:351:ASN:HD22	1:B:352:GLY:N	2.06	0.53
1:A:60:TYR:CG	1:A:330:VAL:HG21	2.43	0.53
1:B:232:GLU:O	1:B:234:GLU:N	2.41	0.53
1:B:153:GLU:OE2	1:B:157:ILE:HD11	2.07	0.53
1:A:99:ALA:HB1	1:A:104:HIS:HA	1.90	0.53
1:B:215:GLY:O	1:B:220:MET:HE2	2.08	0.53
1:B:152:LEU:HD11	1:B:257:LEU:HD12	1.89	0.53
1:B:269:ARG:HH21	1:B:273:ARG:CZ	2.21	0.53
1:A:99:ALA:HB3	1:A:104:HIS:CD2	2.44	0.53
1:B:59:ARG:O	1:B:63:VAL:HG23	2.08	0.53
1:A:143:PRO:HB2	1:A:144:PRO:HD3	1.90	0.52
1:B:372:THR:O	1:B:375:GLU:HG2	2.09	0.52
1:A:205:THR:HG22	1:A:209:ARG:HD2	1.91	0.52
1:A:126:ARG:O	1:A:130:ILE:HG13	2.10	0.52
1:A:181:ILE:C	1:A:182:ILE:HG13	2.29	0.52
1:B:205:THR:HG22	1:B:218:TYR:HB3	1.90	0.52
1:B:182:ILE:HG22	1:B:185:SER:C	2.30	0.52
1:A:91:PRO:HB3	1:A:98:PHE:CE1	2.44	0.52
1:B:165:GLY:HA3	1:B:216:ASP:CG	2.30	0.52
1:B:376:ARG:HD2	3:B:526:HOH:O	2.08	0.52
1:A:100:ASP:O	1:A:103:ASP:HB2	2.09	0.52
1:B:393:ARG:NH2	3:B:448:HOH:O	2.42	0.52
1:A:77:VAL:HG22	1:A:299:ILE:HG12	1.91	0.52
1:B:175:HIS:O	1:B:178:THR:HG22	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:THR:O	1:A:83:THR:HG23	2.08	0.52
1:B:311:ILE:CG2	1:B:311:ILE:O	2.58	0.52
1:A:192:GLU:OE2	1:A:195:LYS:HE2	2.10	0.52
1:A:126:ARG:O	1:A:126:ARG:HD2	2.09	0.52
1:B:42:LEU:HD23	1:B:309:THR:HG21	1.91	0.52
1:A:286:ARG:HG3	1:A:325:ASN:HB3	1.91	0.52
1:A:144:PRO:HB2	1:B:196:ARG:NH1	2.25	0.52
1:A:192:GLU:O	1:A:196:ARG:HG3	2.10	0.51
1:A:77:VAL:CG2	1:A:299:ILE:HG12	2.40	0.51
1:A:149:GLU:HG2	1:A:149:GLU:O	2.11	0.51
1:B:117:VAL:O	1:B:121:LYS:HG3	2.10	0.51
1:B:172:GLU:O	1:B:176:SER:HB2	2.10	0.51
1:A:182:ILE:HG21	1:A:186:GLY:N	2.25	0.51
1:A:105:ASN:ND2	3:A:460:HOH:O	2.42	0.51
1:A:152:LEU:O	1:A:250:THR:HG23	2.10	0.51
1:B:78:THR:HG23	1:B:91:PRO:HG2	1.92	0.51
1:B:231:GLY:O	1:B:232:GLU:O	2.29	0.51
1:B:201:TRP:HZ3	1:B:218:TYR:CE1	2.29	0.51
1:A:232:GLU:C	1:A:234:GLU:H	2.12	0.51
1:B:183:SER:C	1:B:185:SER:H	2.12	0.51
1:A:69:ASP:HB3	1:A:72:PHE:HD1	1.76	0.51
1:A:187:GLY:N	1:A:190:ALA:HB3	2.26	0.51
1:B:77:VAL:HG22	1:B:299:ILE:HD11	1.93	0.51
1:A:16:VAL:HG11	1:A:46:ARG:NH1	2.26	0.51
1:A:206:VAL:HG13	1:A:222:GLY:HA2	1.92	0.50
1:B:192:GLU:O	1:B:196:ARG:HG3	2.12	0.50
1:A:187:GLY:O	1:A:190:ALA:HB3	2.11	0.50
1:B:302:GLU:O	1:B:303:ASP:HB3	2.11	0.50
1:B:291:ARG:HG3	1:B:293:SER:O	2.11	0.50
1:A:178:THR:HG22	1:A:178:THR:O	2.11	0.50
1:A:85:LEU:HD22	1:A:293:SER:CB	2.36	0.50
1:B:303:ASP:CB	1:B:313:ALA:HB2	2.42	0.50
1:B:331:PHE:HE2	1:B:345:PRO:HD2	1.77	0.50
1:A:283:GLU:CG	1:A:339:LEU:H	2.10	0.50
1:A:363:ARG:HD3	3:A:450:HOH:O	2.12	0.50
1:A:195:LYS:HE3	3:A:491:HOH:O	2.12	0.50
1:A:177:TRP:O	1:A:180:GLN:OE1	2.30	0.50
1:B:330:VAL:O	1:B:332:PRO:HD3	2.11	0.50
1:A:224:ALA:N	1:A:227:ARG:HH21	2.10	0.49
1:A:28:GLU:O	1:A:398:ARG:NH2	2.42	0.49
1:B:224:ALA:HB1	1:B:229:GLU:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:VAL:HG13	1:A:319:VAL:HB	1.95	0.49
1:B:203:THR:OG1	1:B:236:VAL:HG21	2.12	0.49
1:A:305:GLU:HG3	1:A:305:GLU:O	2.12	0.49
1:A:328:PRO:HG3	1:A:334:PRO:HG3	1.94	0.49
1:B:354:HIS:O	2:B:430:HEM:HBA1	2.11	0.49
1:B:21:ALA:O	1:B:22:LEU:HB2	2.12	0.49
1:B:168:ALA:HA	1:B:171:ARG:HE	1.78	0.49
1:B:22:LEU:CD2	1:B:24:LEU:HB2	2.42	0.49
1:A:224:ALA:HA	1:A:227:ARG:HH21	1.78	0.49
1:B:225:VAL:HB	3:B:466:HOH:O	2.12	0.49
1:A:199:TYR:HB3	1:A:236:VAL:HG11	1.94	0.49
1:A:67:THR:HG21	1:A:321:TYR:OH	2.12	0.49
1:A:14:PRO:HB3	3:A:525:HOH:O	2.12	0.49
1:B:63:VAL:O	1:B:67:THR:CG2	2.60	0.49
1:A:225:VAL:HG13	1:A:232:GLU:N	2.28	0.49
1:B:105:ASN:O	1:B:107:LEU:N	2.46	0.49
1:B:108:ARG:HG2	1:B:108:ARG:NH1	2.23	0.49
1:A:209:ARG:HD3	1:A:218:TYR:C	2.33	0.49
1:A:77:VAL:O	1:A:77:VAL:HG12	2.12	0.49
1:A:349:TYR:CE2	2:A:430:HEM:HBB2	2.48	0.49
1:A:283:GLU:HG2	1:A:338:ASP:H	1.78	0.48
1:B:283:GLU:HG2	1:B:339:LEU:H	1.77	0.48
1:A:273:ARG:NH1	3:A:446:HOH:O	2.27	0.48
1:A:192:GLU:HG3	1:A:196:ARG:NE	2.28	0.48
1:B:109:ARG:O	1:B:109:ARG:HD2	2.13	0.48
1:B:333:ASP:N	1:B:334:PRO:CD	2.76	0.48
1:B:67:THR:HG21	1:B:351:ASN:OD1	2.13	0.48
1:B:29:PHE:CE2	1:B:33:LEU:HD22	2.47	0.48
1:A:302:GLU:O	1:A:302:GLU:HG3	2.12	0.48
1:A:341:ARG:O	1:A:342:ASP:O	2.32	0.48
1:A:193:ARG:CG	1:A:196:ARG:HH21	2.24	0.48
1:A:225:VAL:HG13	1:A:232:GLU:H	1.77	0.48
1:A:292:THR:HG22	1:A:398:ARG:HG2	1.95	0.48
1:A:198:LEU:HD21	1:A:243:GLN:HG2	1.96	0.48
1:A:180:GLN:NE2	1:A:180:GLN:CA	2.76	0.48
1:B:199:TYR:HB3	1:B:236:VAL:HG11	1.95	0.48
1:A:20:PRO:HB2	1:A:22:LEU:HD23	1.96	0.48
1:A:256:MET:HB3	1:A:284:LEU:HD13	1.95	0.48
1:B:229:GLU:HA	3:B:502:HOH:O	2.13	0.48
1:B:257:LEU:O	1:B:258:TYR:C	2.51	0.47
1:B:213:GLU:CD	1:B:214:GLY:N	2.68	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:203:THR:HG23	1:B:232:GLU:OE2	2.15	0.47
1:B:312:ALA:HB3	1:B:315:GLU:HG3	1.97	0.47
1:A:203:THR:OG1	1:A:236:VAL:HG21	2.15	0.47
1:A:92:ARG:HG2	1:A:93:PRO:HD2	1.95	0.47
1:B:198:LEU:O	1:B:202:ILE:HG13	2.13	0.47
1:B:242:LEU:O	1:B:243:GLN:C	2.53	0.47
1:A:99:ALA:HB1	1:A:104:HIS:CA	2.44	0.47
1:A:33:LEU:HD23	1:A:37:MET:HG3	1.95	0.47
1:A:176:SER:C	1:A:179:ARG:HD3	2.35	0.47
1:A:74:ARG:HG2	1:A:97:ALA:O	2.15	0.47
1:A:155:PHE:HD2	1:A:369:LEU:HD21	1.79	0.47
1:B:241:PRO:O	1:B:245:GLY:N	2.44	0.47
1:A:202:ILE:O	1:A:206:VAL:HG23	2.15	0.47
1:B:108:ARG:HD2	3:B:482:HOH:O	2.15	0.47
1:B:220:MET:N	3:B:498:HOH:O	2.47	0.47
1:A:182:ILE:HD12	1:A:185:SER:HA	1.97	0.47
1:A:124:ARG:CB	1:A:125:PRO:HD3	2.35	0.47
1:B:212:SER:OG	1:B:213:GLU:N	2.44	0.47
1:A:85:LEU:HD23	1:A:396:MET:CE	2.44	0.47
1:A:236:VAL:HG12	1:A:236:VAL:O	2.14	0.47
1:B:184:THR:O	1:B:185:SER:HB2	2.14	0.47
1:B:155:PHE:CZ	1:B:159:VAL:HG21	2.49	0.47
1:B:375:GLU:CG	1:B:376:ARG:N	2.77	0.47
1:B:99:ALA:HB3	1:B:104:HIS:HD2	1.79	0.47
1:B:367:GLU:O	1:B:371:ASP:HB2	2.15	0.47
1:B:274:PRO:C	1:B:276:ALA:H	2.17	0.47
1:A:137:GLY:O	1:A:141:GLU:HG3	2.15	0.47
1:B:269:ARG:CG	1:B:269:ARG:NH1	2.70	0.47
1:B:203:THR:HG22	1:B:207:ARG:HE	1.80	0.47
1:A:154:PRO:HD3	3:A:540:HOH:O	2.14	0.47
1:B:93:PRO:O	1:B:234:GLU:HA	2.15	0.47
1:B:33:LEU:HD23	1:B:33:LEU:C	2.35	0.46
1:A:124:ARG:HD2	1:A:364:MET:HG2	1.96	0.46
1:A:232:GLU:C	1:A:233:THR:HG23	2.35	0.46
1:A:296:LEU:N	1:A:296:LEU:HD12	2.29	0.46
1:A:207:ARG:C	1:A:208:ALA:O	2.53	0.46
1:B:59:ARG:HD2	1:B:59:ARG:N	2.30	0.46
1:B:201:TRP:CZ3	1:B:218:TYR:CE1	3.04	0.46
1:A:155:PHE:HB3	1:A:156:PRO:HD3	1.98	0.46
1:A:256:MET:HB3	1:A:284:LEU:CD1	2.45	0.46
1:A:280:ALA:HA	1:A:339:LEU:HA	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:280:ALA:HA	1:B:339:LEU:HA	1.98	0.46
1:A:153:GLU:H	1:A:154:PRO:HD2	1.79	0.46
1:B:97:ALA:HB1	1:B:296:LEU:CD2	2.46	0.46
1:B:167:PRO:O	1:B:170:ASP:N	2.43	0.46
1:B:14:PRO:HG2	1:B:44:ARG:NE	2.31	0.46
1:A:99:ALA:HB3	1:A:104:HIS:HD2	1.81	0.46
1:A:123:LEU:HD23	1:A:364:MET:CE	2.46	0.46
1:B:303:ASP:HB2	1:B:313:ALA:CB	2.43	0.46
1:B:136:ASP:OD1	1:B:376:ARG:NH2	2.45	0.46
1:A:209:ARG:N	3:A:464:HOH:O	2.49	0.46
1:A:207:ARG:CG	1:A:207:ARG:HH11	2.24	0.45
1:B:15:PRO:HD2	3:B:452:HOH:O	2.15	0.45
1:A:321:TYR:CZ	1:A:350:GLY:HA2	2.51	0.45
1:A:178:THR:O	1:A:179:ARG:NH1	2.49	0.45
1:A:297:ALA:HB2	1:A:318:TYR:CE2	2.50	0.45
1:B:247:GLU:HG3	1:B:248:ALA:N	2.31	0.45
1:B:208:ALA:N	3:B:495:HOH:O	2.50	0.45
1:B:212:SER:OG	1:B:219:SER:HB3	2.17	0.45
1:B:97:ALA:O	1:B:354:HIS:CE1	2.68	0.45
1:A:270:MET:O	1:A:277:ARG:NH1	2.49	0.45
1:B:208:ALA:HB2	3:B:495:HOH:O	2.16	0.45
1:A:153:GLU:N	1:A:154:PRO:HD2	2.32	0.45
1:B:259:LEU:O	1:B:266:LEU:HD12	2.16	0.45
1:A:226:GLY:HA2	3:A:545:HOH:O	2.17	0.45
1:A:28:GLU:OE1	1:A:28:GLU:CA	2.64	0.45
1:B:71:ARG:NH1	1:B:304:VAL:HG13	2.32	0.45
1:A:123:LEU:O	1:A:124:ARG:C	2.55	0.45
1:B:167:PRO:O	1:B:169:ALA:N	2.49	0.45
1:A:373:LEU:HA	1:A:373:LEU:HD23	1.79	0.45
1:B:78:THR:HG23	1:B:91:PRO:CG	2.46	0.44
1:A:138:ILE:HG13	1:A:139:LEU:N	2.31	0.44
1:A:214:GLY:C	1:A:216:ASP:H	2.19	0.44
1:B:107:LEU:O	1:B:238:LEU:HD11	2.17	0.44
1:A:295:GLY:O	1:A:318:TYR:HE2	2.00	0.44
1:B:22:LEU:CD1	1:B:24:LEU:HD12	2.47	0.44
1:A:341:ARG:HB3	1:A:344:ASN:HB2	1.99	0.44
1:A:265:GLU:H	1:A:265:GLU:HG3	1.43	0.44
1:A:143:PRO:O	1:A:145:ALA:N	2.49	0.44
1:B:291:ARG:HD3	1:B:293:SER:O	2.17	0.44
1:B:20:PRO:O	1:B:21:ALA:O	2.36	0.44
1:A:82:ILE:HD12	1:A:82:ILE:N	2.30	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:385:PRO:HD2	1:B:388:GLN:HG3	1.99	0.44
1:A:181:ILE:N	1:A:181:ILE:CD1	2.79	0.44
1:A:152:LEU:HD11	1:A:257:LEU:HD12	1.99	0.44
1:B:72:PHE:HB3	1:B:298:ARG:HB3	2.00	0.44
1:B:153:GLU:HA	1:B:250:THR:HG23	1.99	0.44
1:B:105:ASN:O	1:B:108:ARG:N	2.50	0.44
1:A:203:THR:CG2	1:A:207:ARG:NH1	2.81	0.44
1:B:215:GLY:O	1:B:216:ASP:C	2.55	0.44
1:A:69:ASP:HB3	1:A:72:PHE:CD1	2.53	0.44
1:A:189:GLU:HA	3:A:488:HOH:O	2.16	0.44
1:A:69:ASP:OD2	1:A:71:ARG:NH2	2.51	0.44
1:B:232:GLU:O	1:B:233:THR:HB	2.18	0.43
1:A:198:LEU:O	1:A:202:ILE:HG13	2.18	0.43
1:B:215:GLY:O	1:B:217:VAL:N	2.51	0.43
1:B:239:ALA:HA	1:B:242:LEU:HD12	2.00	0.43
1:A:156:PRO:O	1:A:160:VAL:HG23	2.18	0.43
1:B:283:GLU:HA	1:B:283:GLU:OE1	2.18	0.43
1:A:209:ARG:HH11	1:A:209:ARG:HG3	1.83	0.43
1:A:146:ASP:HA	1:A:403:LEU:O	2.17	0.43
1:A:60:TYR:HB3	3:A:437:HOH:O	2.17	0.43
1:B:37:MET:CG	1:B:58:THR:HG21	2.41	0.43
1:B:296:LEU:CD1	1:B:296:LEU:N	2.81	0.43
1:A:203:THR:HG23	1:A:207:ARG:NH1	2.33	0.43
1:A:192:GLU:HG3	1:A:196:ARG:HE	1.83	0.43
1:A:302:GLU:O	1:A:303:ASP:O	2.37	0.43
1:A:115:PHE:CD1	1:A:115:PHE:N	2.86	0.43
1:B:67:THR:HG21	1:B:351:ASN:HB3	2.00	0.43
1:B:209:ARG:HD3	1:B:219:SER:OG	2.18	0.43
1:A:37:MET:HG2	1:A:58:THR:HG23	1.97	0.43
1:B:321:TYR:O	1:B:325:ASN:N	2.51	0.43
1:A:171:ARG:NH1	1:A:171:ARG:HG3	2.33	0.43
1:A:108:ARG:HH11	1:A:112:ALA:HB2	1.82	0.43
1:B:36:LEU:HD12	1:B:36:LEU:HA	1.90	0.43
1:A:15:PRO:HG2	1:A:17:ARG:CZ	2.48	0.43
1:B:153:GLU:OE1	1:B:179:ARG:NH2	2.52	0.43
1:A:83:THR:O	1:A:83:THR:CG2	2.65	0.43
1:B:109:ARG:C	1:B:109:ARG:HD2	2.39	0.43
1:A:81:GLN:HA	1:A:81:GLN:OE1	2.18	0.43
1:B:249:VAL:HG11	1:B:365:GLN:NE2	2.32	0.43
1:B:168:ALA:HA	1:B:171:ARG:NE	2.33	0.43
1:A:214:GLY:C	1:A:216:ASP:N	2.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:THR:HG23	1:A:323:ALA:HB1	2.01	0.43
1:B:321:TYR:HA	1:B:324:ALA:HB3	1.99	0.43
1:B:333:ASP:OD1	1:B:336:ARG:HD3	2.19	0.43
1:A:164:MET:HA	1:A:217:VAL:HB	2.00	0.43
1:B:326:ARG:HB3	3:B:489:HOH:O	2.18	0.43
1:B:170:ASP:CG	1:B:173:ARG:HH11	2.23	0.42
1:B:114:ALA:HB2	1:B:220:MET:HE1	2.01	0.42
1:A:403:LEU:HD23	1:A:403:LEU:HA	1.90	0.42
1:B:63:VAL:C	1:B:65:ALA:H	2.22	0.42
1:B:212:SER:CB	1:B:219:SER:HB3	2.50	0.42
1:A:349:TYR:HE2	2:A:430:HEM:HBB2	1.82	0.42
1:B:358:GLY:O	1:B:359:ALA:C	2.57	0.42
1:A:291:ARG:HD2	3:A:473:HOH:O	2.19	0.42
1:B:131:LEU:HD21	1:B:372:THR:HB	2.01	0.42
1:B:143:PRO:CG	1:B:409:HIS:HB2	2.49	0.42
1:B:221:LEU:O	1:B:225:VAL:HG23	2.18	0.42
1:B:212:SER:HB3	1:B:219:SER:HB3	2.02	0.42
1:B:47:LEU:O	1:B:48:PRO:O	2.38	0.42
1:A:244:ILE:O	1:A:244:ILE:HG22	2.20	0.42
1:A:274:PRO:O	1:A:275:GLY:C	2.56	0.42
1:B:22:LEU:HD13	1:B:292:THR:HA	2.01	0.42
1:B:173:ARG:HH12	1:B:201:TRP:HE1	1.67	0.41
1:A:177:TRP:C	1:A:179:ARG:N	2.73	0.41
1:A:47:LEU:HD12	1:A:84:ARG:HA	2.02	0.41
1:A:105:ASN:HA	3:A:460:HOH:O	2.20	0.41
1:A:106:ARG:HA	1:A:109:ARG:HH21	1.84	0.41
1:A:355:PHE:CD2	1:A:356:CYS:N	2.88	0.41
1:A:131:LEU:HD21	1:A:372:THR:HB	2.03	0.41
1:B:259:LEU:HD22	1:B:263:ARG:HD2	2.02	0.41
1:B:167:PRO:CG	1:B:209:ARG:NH2	2.83	0.41
1:B:381:ARG:HD3	3:B:503:HOH:O	2.21	0.41
1:A:190:ALA:C	1:A:192:GLU:H	2.24	0.41
1:B:342:ASP:OD1	1:B:342:ASP:N	2.54	0.41
1:B:164:MET:CE	1:B:239:ALA:HB1	2.51	0.41
1:A:336:ARG:NH2	1:A:338:ASP:OD2	2.53	0.41
1:A:338:ASP:C	1:A:340:ASP:H	2.24	0.41
1:A:230:VAL:O	1:A:231:GLY:C	2.59	0.41
1:B:101:GLN:OE1	1:B:104:HIS:HB3	2.19	0.41
1:A:297:ALA:HB2	1:A:318:TYR:CZ	2.55	0.41
1:A:146:ASP:OD1	1:A:146:ASP:C	2.59	0.41
1:B:164:MET:O	1:B:216:ASP:OD2	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:ARG:HG2	1:A:93:PRO:CD	2.50	0.41
1:B:198:LEU:HD23	1:B:202:ILE:HG13	2.02	0.41
1:A:333:ASP:N	1:A:334:PRO:CD	2.84	0.41
1:B:384:VAL:HB	1:B:385:PRO:CD	2.51	0.41
1:A:353:HIS:HB3	3:A:436:HOH:O	2.20	0.41
1:A:352:GLY:C	1:A:354:HIS:H	2.24	0.41
1:A:283:GLU:HA	1:A:283:GLU:OE1	2.20	0.41
1:A:186:GLY:O	1:B:79:GLN:OE1	2.39	0.40
1:B:22:LEU:HD12	1:B:30:ASP:OD1	2.21	0.40
1:A:73:GLY:HA3	3:A:526:HOH:O	2.21	0.40
1:A:401:ARG:NH2	3:A:531:HOH:O	2.52	0.40
1:B:126:ARG:O	1:B:130:ILE:HG13	2.21	0.40
1:B:353:HIS:CD2	1:B:353:HIS:N	2.88	0.40
1:B:319:VAL:HG21	3:B:457:HOH:O	2.22	0.40
1:B:353:HIS:C	1:B:355:PHE:H	2.24	0.40
1:B:279:THR:O	1:B:282:ASP:HB2	2.22	0.40
1:B:177:TRP:C	1:B:179:ARG:H	2.25	0.40
1:A:101:GLN:OE1	1:A:105:ASN:HB2	2.22	0.40
1:B:285:LEU:HD23	1:B:285:LEU:HA	1.90	0.40
1:A:123:LEU:HD23	1:A:364:MET:HE1	2.04	0.40
1:B:14:PRO:O	1:B:15:PRO:C	2.60	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	395/413 (96%)	335 (85%)	41 (10%)	19 (5%)	3 10
1	B	384/413 (93%)	305 (79%)	57 (15%)	22 (6%)	2 6
All	All	779/826 (94%)	640 (82%)	98 (13%)	41 (5%)	2 8

All (41) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	182	ILE
1	A	208	ALA
1	A	209	ARG
1	A	213	GLU
1	A	231	GLY
1	A	232	GLU
1	A	276	ALA
1	A	303	ASP
1	A	342	ASP
1	B	21	ALA
1	B	48	PRO
1	B	168	ALA
1	B	232	GLU
1	B	342	ASP
1	A	211	GLY
1	A	214	GLY
1	B	22	LEU
1	B	71	ARG
1	B	143	PRO
1	B	216	ASP
1	B	231	GLY
1	B	245	GLY
1	A	190	ALA
1	B	106	ARG
1	B	176	SER
1	A	103	ASP
1	A	302	GLU
1	B	105	ASN
1	B	183	SER
1	B	212	SER
1	B	233	THR
1	B	343	PRO
1	A	167	PRO
1	A	230	VAL
1	A	293	SER
1	B	346	HIS
1	B	93	PRO
1	A	144	PRO
1	A	306	VAL
1	B	20	PRO
1	B	70	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	310/329 (94%)	282 (91%)	28 (9%)	12 34
1	B	303/329 (92%)	281 (93%)	22 (7%)	17 45
All	All	613/658 (93%)	563 (92%)	50 (8%)	14 39

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	LEU
1	A	24	LEU
1	A	28	GLU
1	A	36	LEU
1	A	59	ARG
1	A	67	THR
1	A	74	ARG
1	A	82	ILE
1	A	102	PRO
1	A	103	ASP
1	A	105	ASN
1	A	121	LYS
1	A	172	GLU
1	A	179	ARG
1	A	180	GLN
1	A	182	ILE
1	A	204	GLU
1	A	207	ARG
1	A	213	GLU
1	A	232	GLU
1	A	233	THR
1	A	238	LEU
1	A	265	GLU
1	A	269	ARG
1	A	294	VAL
1	A	366	THR
1	A	395	THR

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Mol	Chain	Res	Type
1	A	396	MET
1	B	23	ASP
1	B	36	LEU
1	B	59	ARG
1	B	68	ASN
1	B	76	GLU
1	B	100	ASP
1	B	109	ARG
1	B	143	PRO
1	B	207	ARG
1	B	232	GLU
1	B	238	LEU
1	B	260	LEU
1	B	269	ARG
1	B	270	MET
1	B	296	LEU
1	B	305	GLU
1	B	311	ILE
1	B	317	VAL
1	B	353	HIS
1	B	381	ARG
1	B	382	LEU
1	B	396	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	ASN
1	A	105	ASN
1	A	180	GLN
1	A	255	GLN
1	A	351	ASN
1	A	365	GLN
1	B	79	GLN
1	B	81	GLN
1	B	105	ASN
1	B	243	GLN
1	B	290	HIS
1	B	307	HIS
1	B	365	GLN

5.3.3 RNA

There are no RNA molecules 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

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	430	1	30,50,50	2.64	8 (26%)	24,82,82	2.93	12 (50%)
2	HEM	B	430	1,3	30,50,50	2.54	9 (30%)	24,82,82	3.02	11 (45%)

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	430	1	-	0/10/54/54	0/0/8/8
2	HEM	B	430	1,3	-	0/10/54/54	0/0/8/8

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	430	HEM	C3B-C4B	-8.42	1.44	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	430	HEM	C3B-C4B	-7.06	1.45	1.51
2	B	430	HEM	C2D-C3D	-6.45	1.35	1.54
2	A	430	HEM	C2D-C3D	-6.21	1.35	1.54
2	A	430	HEM	C3D-C4D	-4.56	1.45	1.51
2	B	430	HEM	C3D-C4D	-4.13	1.46	1.51
2	A	430	HEM	C2C-C1C	-2.30	1.48	1.52
2	B	430	HEM	C2C-C1C	-2.21	1.48	1.52
2	B	430	HEM	C1C-NC	2.27	1.38	1.36
2	A	430	HEM	C4C-NC	2.30	1.38	1.36
2	B	430	HEM	C3C-CAC	2.42	1.55	1.51
2	A	430	HEM	C3C-CAC	2.69	1.56	1.51
2	B	430	HEM	CAA-C2A	3.00	1.57	1.52
2	A	430	HEM	CBB-CAB	4.18	1.53	1.29
2	B	430	HEM	CBC-CAC	4.28	1.54	1.29
2	A	430	HEM	CBC-CAC	4.33	1.54	1.29
2	B	430	HEM	CBB-CAB	4.39	1.54	1.29

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	430	HEM	C3B-CAB-CBB	-6.81	114.02	124.46
2	A	430	HEM	C3B-CAB-CBB	-6.65	114.26	124.46
2	B	430	HEM	C3C-CAC-CBC	-5.51	116.01	124.46
2	A	430	HEM	C3C-CAC-CBC	-3.99	118.33	124.46
2	A	430	HEM	CAA-C2A-C1A	-3.02	123.73	127.01
2	B	430	HEM	CMA-C3A-C4A	-2.59	124.09	128.36
2	A	430	HEM	CMA-C3A-C4A	-2.46	124.29	128.36
2	A	430	HEM	C3B-C4B-CHC	2.22	126.28	123.16
2	B	430	HEM	C3B-C4B-CHC	2.55	126.75	123.16
2	A	430	HEM	CBA-CAA-C2A	2.63	117.25	112.53
2	B	430	HEM	CMD-C2D-C3D	3.09	128.00	114.35
2	B	430	HEM	C2D-C3D-C4D	3.11	106.77	101.50
2	A	430	HEM	CMD-C2D-C3D	3.15	128.28	114.35
2	B	430	HEM	CBA-CAA-C2A	3.21	118.29	112.53
2	A	430	HEM	C2D-C3D-C4D	3.25	107.01	101.50
2	A	430	HEM	CAD-C3D-C4D	3.75	125.70	112.47
2	B	430	HEM	CAD-C3D-C4D	3.99	126.56	112.47
2	B	430	HEM	CMB-C2B-C3B	4.67	128.18	116.53
2	B	430	HEM	CAD-C3D-C2D	4.68	126.67	113.22
2	A	430	HEM	CMB-C2B-C3B	4.75	128.40	116.53
2	A	430	HEM	CAD-C3D-C2D	4.89	127.29	113.22
2	B	430	HEM	CMC-C2C-C3C	5.15	129.40	116.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	430	HEM	CMC-C2C-C3C	5.49	130.25	116.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	430	HEM	2	0
2	B	430	HEM	2	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	397/413 (96%)	-0.31	5 (1%)	79 78	2, 8, 34, 73	0
1	B	388/413 (93%)	-0.06	8 (2%)	67 62	2, 14, 48, 66	0
All	All	785/826 (95%)	-0.18	13 (1%)	73 70	2, 10, 45, 73	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	184	THR	4.2
1	B	14	PRO	4.2
1	A	185	SER	4.2
1	B	183	SER	4.1
1	B	184	THR	4.1
1	B	185	SER	3.8
1	A	188	ALA	3.4
1	B	181	ILE	3.3
1	A	14	PRO	3.0
1	A	343	PRO	2.8
1	B	50	GLY	2.8
1	B	49	HIS	2.6
1	B	48	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, 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	B	430	43/43	0.95	0.18	0.53	10,13,16,21	0
2	HEM	A	430	43/43	0.96	0.15	-0.09	1,6,7,8	0

6.5 Other polymers

There are no such residues in this entry.