Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 12:21 PM GMT

PDB ID	:	3QZ1
Title	:	Crystal Structure of Bovine Steroid of 21-hydroxylase (P450c21)
Authors	:	Zhao, B.; Waterman, M.R.
Deposited on	:	2011-03-04
Resolution	:	3.00 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:

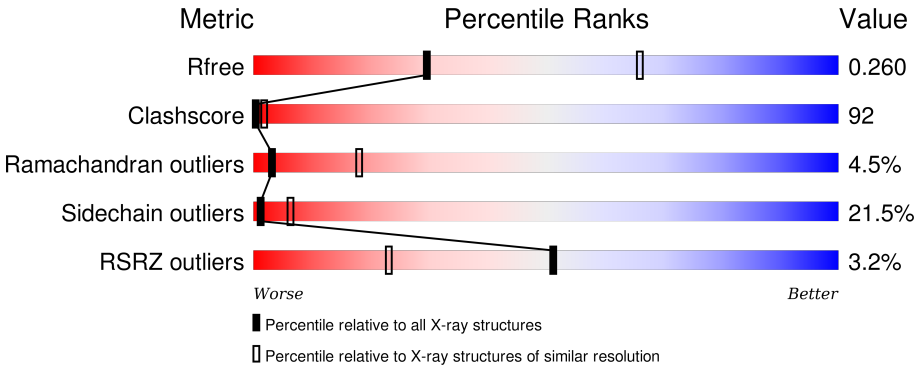
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.00 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	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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	496	% 24% 48% 15% • 10%
1	B	496	4% 24% 50% 14% • 12%
1	C	496	3% 25% 45% 18% • 12%
1	D	496	4% 22% 48% 16% • 13%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	3QZ	A	501	-	-	X	X
3	3QZ	A	502	-	-	-	X
3	3QZ	B	501	-	-	X	X
3	3QZ	B	502	-	-	-	X
3	3QZ	C	501	-	-	X	-
3	3QZ	C	502	-	-	-	X
3	3QZ	D	501	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14525 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.

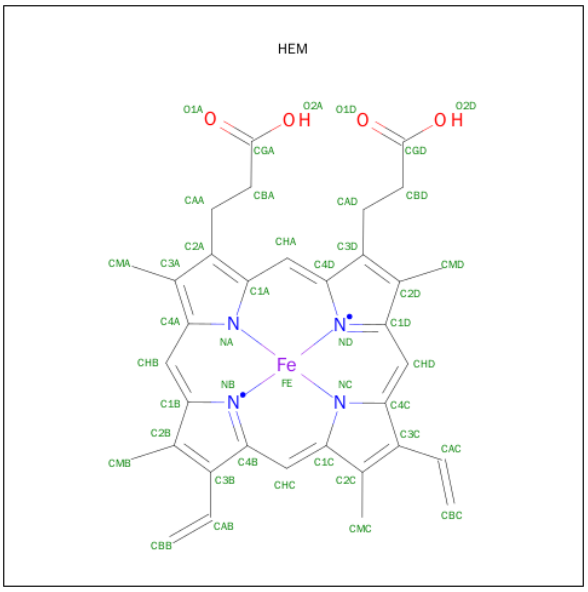
- Molecule 1 is a protein called Steroid 21-hydroxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	445	Total	C	N	O	S	0	0	0
			3571	2294	639	618	20			
1	B	436	Total	C	N	O	S	0	0	0
			3506	2259	621	607	19			
1	C	437	Total	C	N	O	S	0	0	0
			3504	2257	619	609	19			
1	D	434	Total	C	N	O	S	0	0	0
			3483	2245	613	606	19			

There are 8 discrepancies between the modelled and reference sequences:

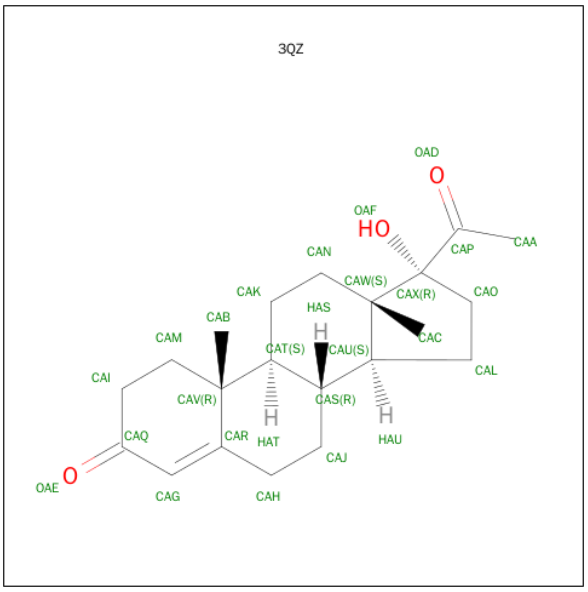
Chain	Residue	Modelled	Actual	Comment	Reference
A	241	ARG	THR	ENGINEERED MUTATION	UNP P00191
A	442	ALA	LEU	ENGINEERED MUTATION	UNP P00191
B	241	ARG	THR	ENGINEERED MUTATION	UNP P00191
B	442	ALA	LEU	ENGINEERED MUTATION	UNP P00191
C	241	ARG	THR	ENGINEERED MUTATION	UNP P00191
C	442	ALA	LEU	ENGINEERED MUTATION	UNP P00191
D	241	ARG	THR	ENGINEERED MUTATION	UNP P00191
D	442	ALA	LEU	ENGINEERED MUTATION	UNP P00191

- 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		
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is (9BETA)-17-HYDROXYPREGN-4-ENE-3,20-DIONE (three-letter code: 3QZ) (formula: $C_{21}H_{30}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 24 21 3	0	0
3	A	1	Total C O 24 21 3	0	0
3	B	1	Total C O 24 21 3	0	0
3	B	1	Total C O 24 21 3	0	0
3	C	1	Total C O 24 21 3	0	0
3	C	1	Total C O 24 21 3	0	0
3	D	1	Total C O 24 21 3	0	0
3	D	1	Total C O 24 21 3	0	0

- Molecule 4 is water.

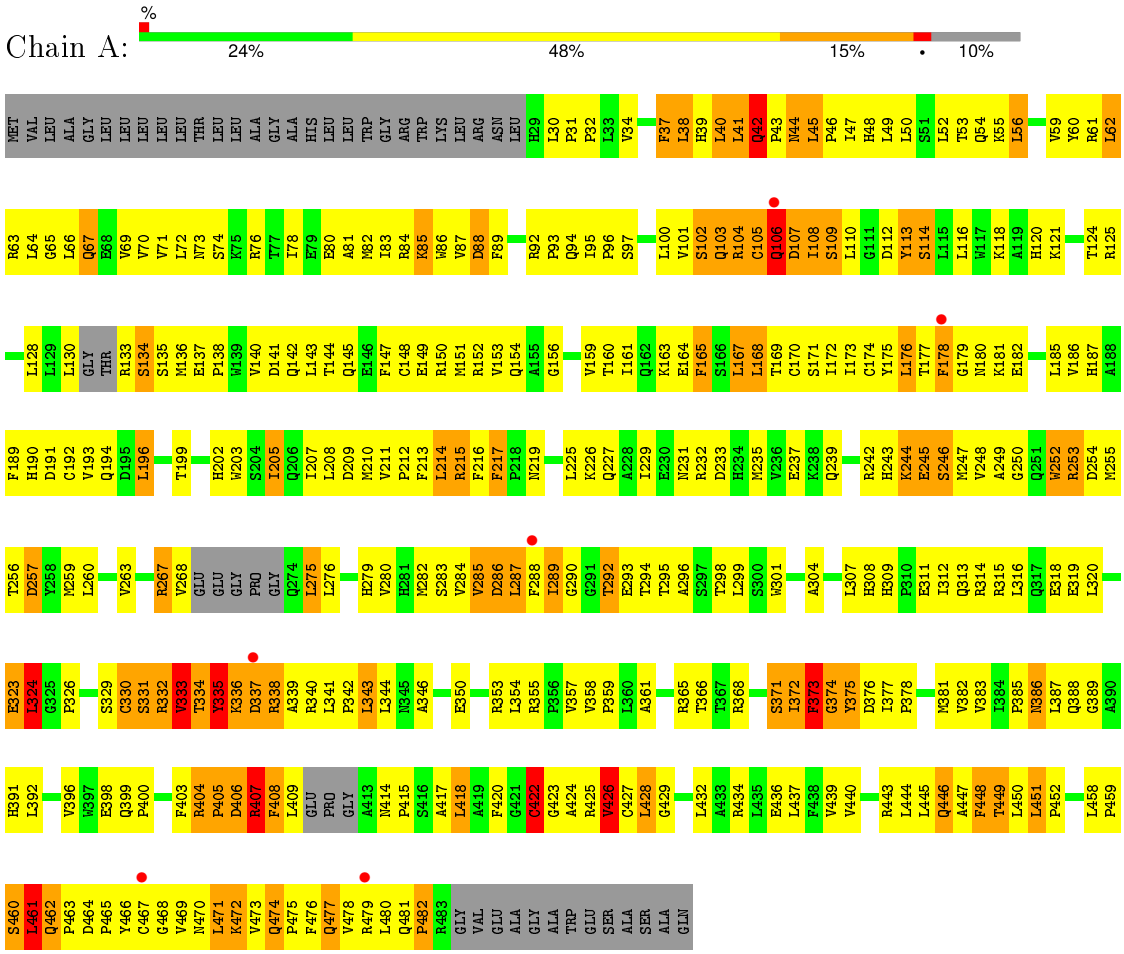
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	22	Total O 22 22	0	0
4	B	28	Total O 28 28	0	0
4	C	22	Total O 22 22	0	0
4	D	25	Total O 25 25	0	0

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.

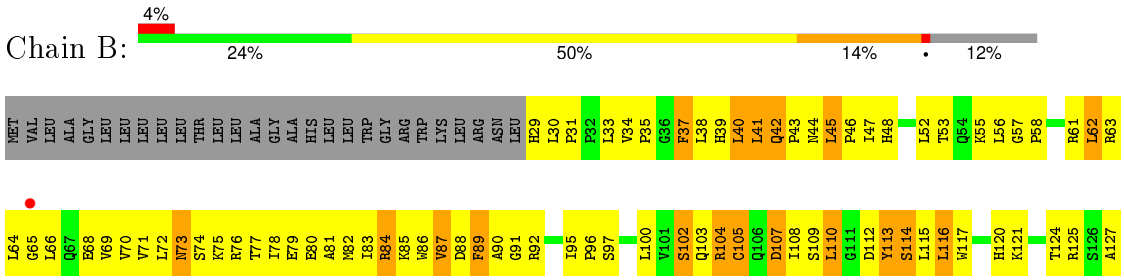
- Molecule 1: Steroid 21-hydroxylase

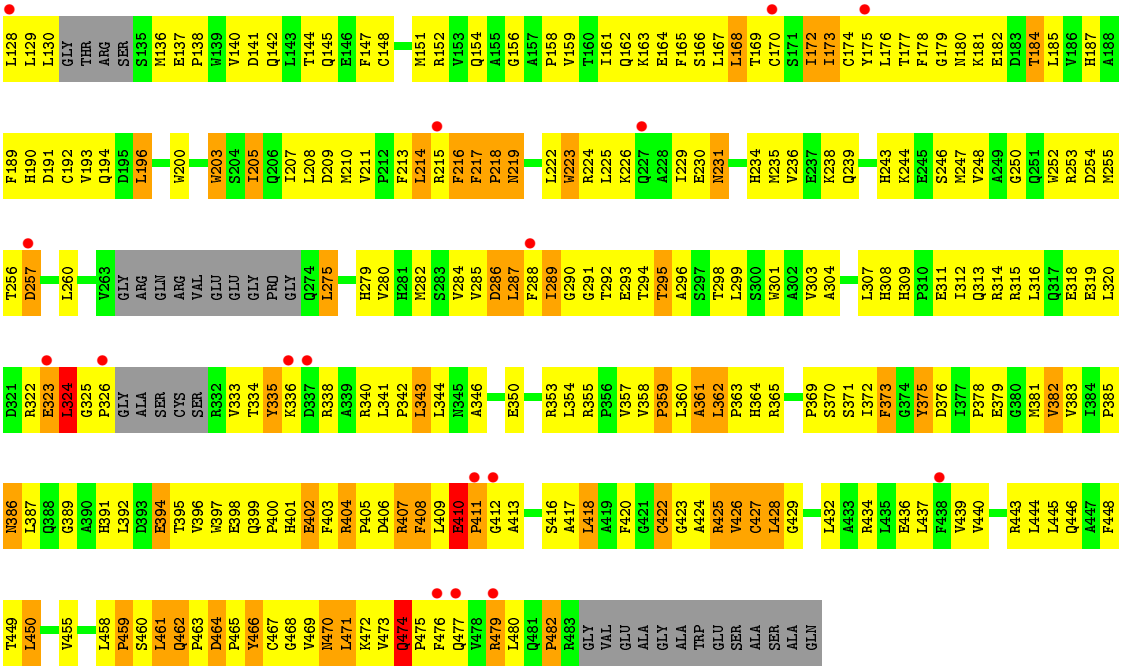
Chain A:



- Molecule 1: Steroid 21-hydroxylase

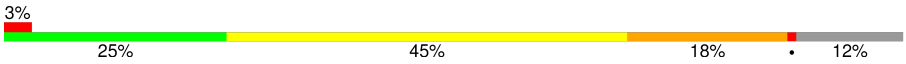
Chain B:

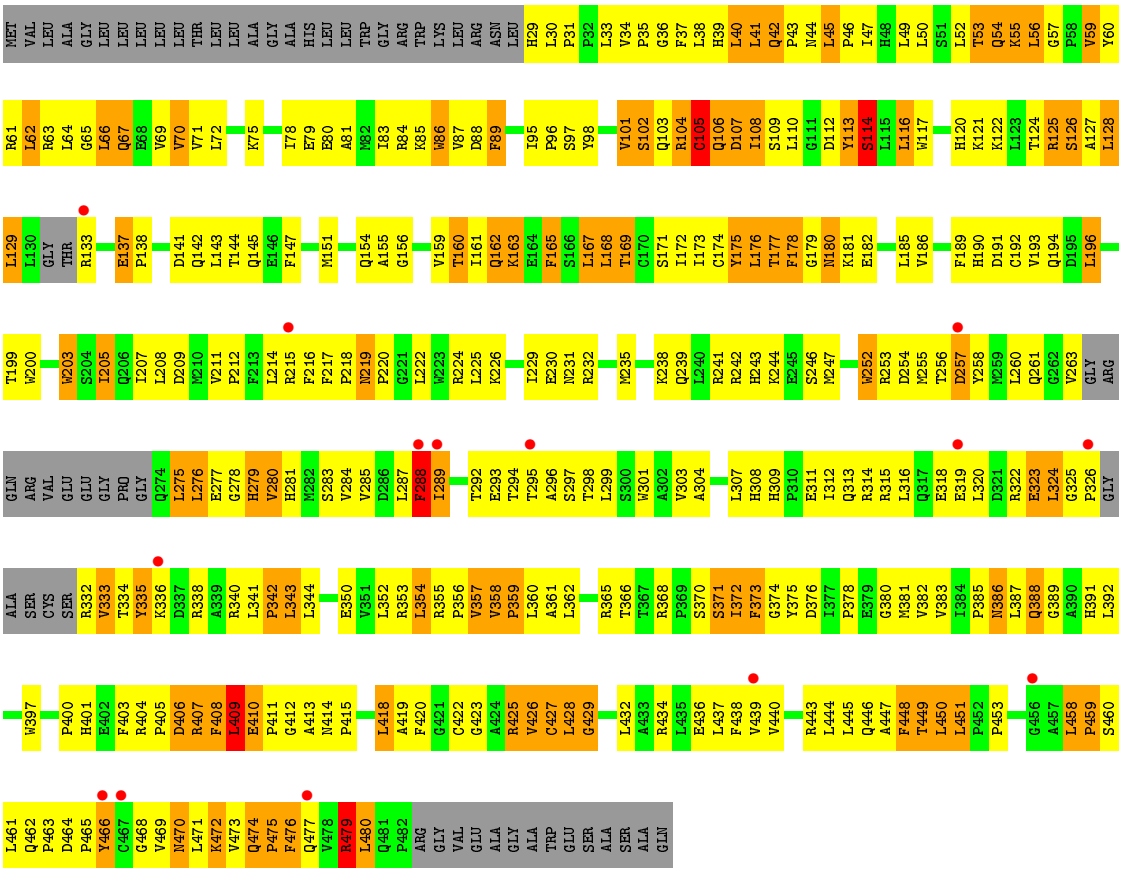




• Molecule 1: Steroid 21-hydroxylase

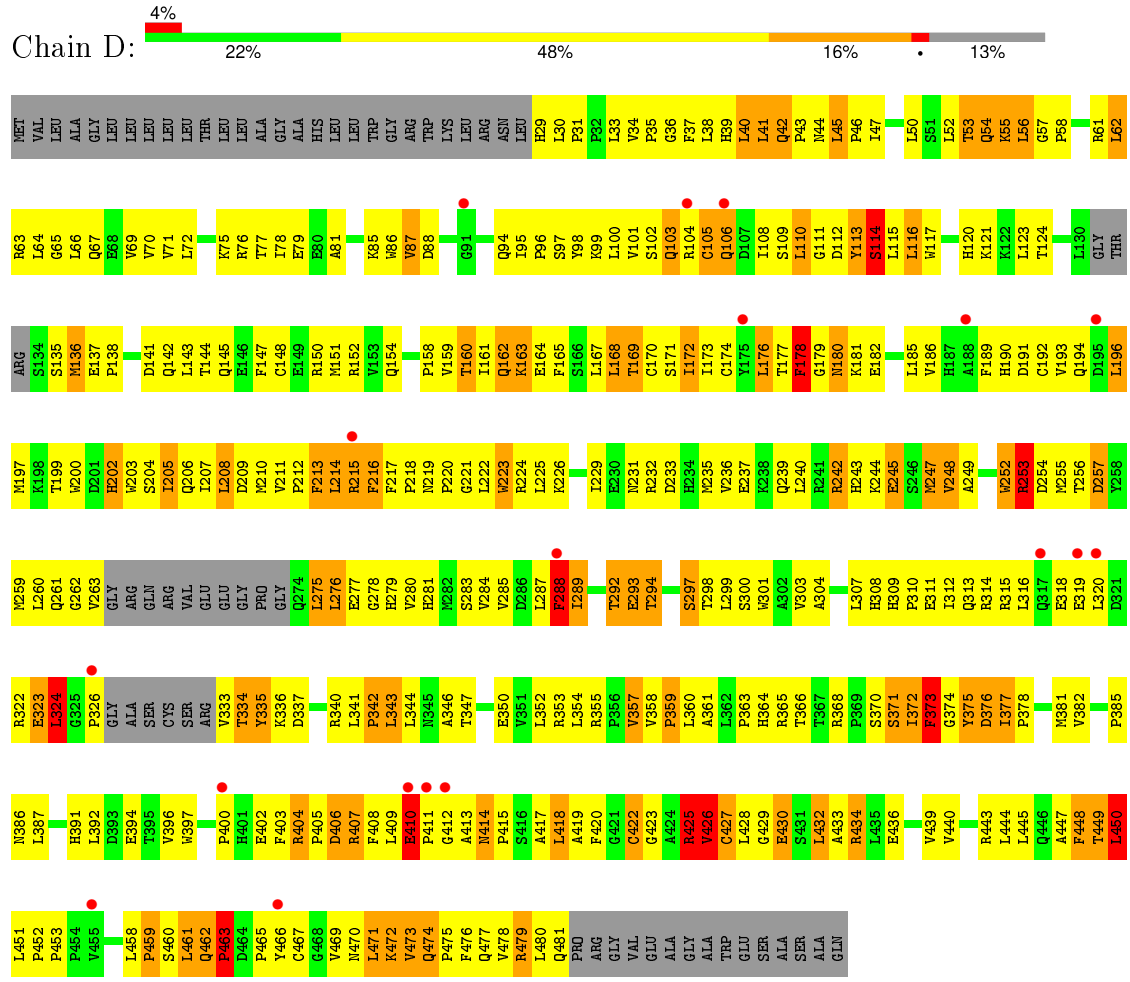
Chain C:





• Molecule 1: Steroid 21-hydroxylase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	67.87Å 168.00Å 111.84Å 90.00° 90.09° 90.00°	Depositor
Resolution (Å)	30.00 – 3.00 29.08 – 3.00	Depositor EDS
% Data completeness (in resolution range)	92.4 (30.00-3.00) 95.1 (29.08-3.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	1.06 (at 3.00Å)	Xtriage
Refinement program	CNS1.3	Depositor
R, R_{free}	0.282 , 0.297 0.252 , 0.260	Depositor DCC
R_{free} test set	4836 reflections (11.25%)	DCC
Wilson B-factor (Å^2)	114.7	Xtriage
Anisotropy	0.084	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 115.7	EDS
Estimated twinning fraction	0.500 for -h,k,-l 0.199 for h,-k,-l	Xtriage
Reported twinning fraction	0.500 for -h,k,-l	Depositor
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.24$	Xtriage
Outliers	0 of 48073 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	14525	wwPDB-VP
Average B, all atoms (Å^2)	119.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% 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: 3QZ, 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	0.49	0/3659	0.69	3/4971 (0.1%)
1	B	0.48	0/3595	0.71	5/4888 (0.1%)
1	C	0.46	1/3592 (0.0%)	0.70	5/4884 (0.1%)
1	D	0.51	1/3571 (0.0%)	0.74	6/4856 (0.1%)
All	All	0.49	2/14417 (0.0%)	0.71	19/19599 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	463	PRO	CA-CB	-6.78	1.40	1.53
1	C	358	VAL	CB-CG1	-5.14	1.42	1.52

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	479	ARG	N-CA-C	10.67	139.81	111.00
1	D	479	ARG	N-CA-C	7.78	132.00	111.00
1	B	479	ARG	N-CA-C	7.52	131.30	111.00
1	A	422	CYS	N-CA-C	-7.07	91.91	111.00
1	D	471	LEU	CA-CB-CG	7.04	131.50	115.30
1	B	335	TYR	N-CA-C	6.79	129.33	111.00
1	C	114	SER	N-CA-C	-6.54	93.35	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	217	PHE	N-CA-C	-6.45	93.59	111.00
1	D	114	SER	N-CA-C	-6.28	94.06	111.00
1	D	425	ARG	NE-CZ-NH2	-6.17	117.21	120.30
1	C	411	PRO	N-CA-CB	6.03	110.54	103.30
1	B	425	ARG	N-CA-C	-6.00	94.79	111.00
1	A	88	ASP	N-CA-C	5.97	127.12	111.00
1	C	480	LEU	N-CA-C	5.89	126.92	111.00
1	C	288	PHE	N-CA-C	5.68	126.33	111.00
1	D	288	PHE	N-CA-C	5.28	125.26	111.00
1	D	410	GLU	N-CA-C	5.20	125.03	111.00
1	B	412	GLY	N-CA-C	-5.13	100.27	113.10
1	A	94	GLN	N-CA-C	-5.12	97.17	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	425	ARG	Sidechain

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	3571	0	3632	699	1
1	B	3506	0	3567	651	3
1	C	3504	0	3555	625	1
1	D	3483	0	3539	719	2
2	A	43	0	30	6	0
2	B	43	0	30	5	0
2	C	43	0	30	13	0
2	D	43	0	30	11	0
3	A	48	0	60	19	0
3	B	48	0	60	20	0
3	C	48	0	60	13	0
3	D	48	0	60	10	0
4	A	22	0	0	16	2
4	B	28	0	0	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	22	0	0	11	1
4	D	25	0	0	13	0
All	All	14525	0	14653	2683	5

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 92.

All (2683) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:463:PRO:CG	1:D:471:LEU:HB3	1.12	1.59
1:D:463:PRO:HG3	1:D:471:LEU:CB	1.17	1.57
1:D:463:PRO:HB3	1:D:471:LEU:CG	1.32	1.54
1:D:106:GLN:HB2	1:D:279:HIS:CE1	1.40	1.53
1:D:463:PRO:CB	1:D:471:LEU:HG	1.31	1.52
1:A:294:THR:CG2	3:A:501:3QZ:HAAA	1.40	1.48
1:A:294:THR:CG2	3:A:501:3QZ:CAA	1.96	1.43
1:A:252:TRP:CE3	1:A:253:ARG:HG3	1.53	1.42
1:A:475:PRO:CB	1:A:477:GLN:HE22	1.34	1.40
1:A:472:LYS:CE	1:A:473:VAL:H	1.35	1.38
1:C:55:LYS:HG2	1:C:56:LEU:CD2	1.54	1.37
1:D:46:PRO:HG3	1:D:466:TYR:CE2	1.56	1.37
1:B:62:LEU:HD23	1:B:63:ARG:N	1.41	1.35
1:A:472:LYS:CE	1:A:473:VAL:N	1.90	1.34
1:C:62:LEU:HD23	1:C:63:ARG:N	1.41	1.34
1:B:288:PHE:CD2	1:B:289:ILE:HD11	1.62	1.33
1:D:106:GLN:CB	1:D:279:HIS:CE1	2.11	1.33
1:B:189:PHE:CE2	1:B:288:PHE:CZ	2.16	1.32
1:A:62:LEU:HD23	1:A:63:ARG:N	1.41	1.32
1:B:178:PHE:HE2	1:B:252:TRP:CZ3	1.47	1.31
1:C:159:VAL:HG12	1:C:476:PHE:CE2	1.65	1.31
1:D:62:LEU:HD23	1:D:63:ARG:N	1.42	1.31
1:D:473:VAL:CG1	1:D:474:GLN:H	1.43	1.31
1:B:178:PHE:CE2	1:B:252:TRP:CZ3	2.18	1.30
1:B:284:VAL:O	1:B:288:PHE:CB	1.79	1.30
1:B:288:PHE:CD2	1:B:289:ILE:CD1	2.15	1.29
1:A:475:PRO:HB2	1:A:477:GLN:NE2	1.46	1.29
1:A:42:GLN:HG2	4:A:613:HOH:O	1.22	1.29
1:D:463:PRO:HB3	1:D:471:LEU:CD1	1.62	1.29
1:D:94:GLN:OE1	1:D:99:LYS:HE2	1.30	1.28
1:B:294:THR:CG2	3:B:501:3QZ:HAAA	1.62	1.28

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:463:PRO:O	1:A:466:TYR:CE1	1.86	1.28
1:B:214:LEU:HD23	1:B:216:PHE:CD2	1.69	1.27
1:D:105:CYS:HB2	4:D:613:HOH:O	1.35	1.26
1:B:284:VAL:C	1:B:288:PHE:HB2	1.55	1.26
1:B:189:PHE:CE2	1:B:288:PHE:HZ	1.52	1.25
1:A:472:LYS:HE2	1:A:473:VAL:N	1.46	1.25
1:D:418:LEU:HD23	1:D:422:CYS:SG	1.77	1.25
1:C:276:LEU:HD23	1:C:277:GLU:N	1.52	1.24
1:A:177:THR:HB	1:A:288:PHE:CE1	1.70	1.24
1:B:178:PHE:HE2	1:B:252:TRP:CH2	1.53	1.24
1:A:37:PHE:O	1:A:38:LEU:HD23	1.31	1.24
1:D:96:PRO:HG2	1:D:209:ASP:OD1	1.37	1.23
1:D:165:PHE:HE1	1:D:293:GLU:OE2	1.16	1.23
1:B:294:THR:CG2	3:B:501:3QZ:CAA	2.17	1.23
1:D:214:LEU:HD23	1:D:216:PHE:CD1	1.70	1.23
1:D:168:LEU:O	1:D:172:ILE:HD13	1.39	1.22
1:A:449:THR:HB	1:A:480:LEU:O	1.33	1.22
1:A:332:ARG:HA	1:A:332:ARG:NE	1.48	1.22
1:B:288:PHE:C	1:B:289:ILE:HD12	1.60	1.21
1:A:294:THR:HG21	3:A:501:3QZ:CAA	1.60	1.21
1:D:106:GLN:HG2	1:D:279:HIS:NE2	1.56	1.21
1:A:461:LEU:O	1:A:462:GLN:CG	1.88	1.21
1:B:116:LEU:HD23	1:B:116:LEU:C	1.61	1.21
1:B:284:VAL:HG12	1:B:288:PHE:CD1	1.75	1.21
1:D:275:LEU:O	1:D:275:LEU:HD12	1.40	1.20
1:C:179:GLY:N	1:C:254:ASP:OD1	1.73	1.20
1:D:202:HIS:O	1:D:205:ILE:HG22	1.41	1.19
1:B:214:LEU:CD2	1:B:216:PHE:HD2	1.55	1.19
1:A:451:LEU:HG	1:A:452:PRO:HD2	1.24	1.19
1:D:473:VAL:HG12	1:D:474:GLN:N	1.52	1.19
1:D:40:LEU:O	1:D:40:LEU:HD12	1.42	1.18
1:D:55:LYS:HD2	1:D:56:LEU:CD2	1.74	1.18
1:D:461:LEU:HD22	1:D:462:GLN:O	1.41	1.18
1:D:168:LEU:HD23	1:D:292:THR:O	1.39	1.18
1:C:116:LEU:HD23	1:C:116:LEU:C	1.62	1.18
1:D:461:LEU:O	1:D:461:LEU:HD23	1.43	1.17
1:D:116:LEU:HD23	1:D:116:LEU:C	1.62	1.17
1:B:284:VAL:O	1:B:288:PHE:HB2	1.05	1.17
1:A:324:LEU:HD12	1:A:332:ARG:HG2	1.26	1.17
1:A:108:ILE:HG13	1:A:286:ASP:OD2	1.43	1.16
1:B:471:LEU:CD1	1:B:471:LEU:H	1.51	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:463:PRO:CB	1:D:471:LEU:CG	1.99	1.16
1:A:472:LYS:HE3	1:A:473:VAL:HG23	1.28	1.16
1:D:111:GLY:O	1:D:425:ARG:NH2	1.78	1.15
1:C:40:LEU:O	1:C:40:LEU:HD12	1.46	1.15
1:C:358:VAL:CG1	2:C:500:HEM:HMA3	1.77	1.14
1:B:471:LEU:N	1:B:471:LEU:HD12	1.58	1.14
1:A:89:PHE:CZ	1:A:372:ILE:CG1	2.30	1.14
1:B:72:LEU:C	1:B:73:ASN:HD22	1.50	1.14
1:C:412:GLY:O	4:C:604:HOH:O	1.63	1.14
1:D:165:PHE:CE1	1:D:293:GLU:OE2	1.99	1.14
1:D:116:LEU:HD23	1:D:117:TRP:N	1.62	1.13
1:C:219:ASN:OD1	1:C:220:PRO:HD2	1.44	1.13
1:D:52:LEU:O	1:D:56:LEU:HD23	1.46	1.13
1:A:461:LEU:O	1:A:462:GLN:HG2	0.97	1.13
1:B:288:PHE:O	1:B:289:ILE:HD12	1.49	1.13
1:A:283:SER:O	1:A:287:LEU:CD1	1.96	1.13
1:B:41:LEU:N	1:B:41:LEU:HD23	1.56	1.13
1:C:297:SER:HB2	1:C:357:VAL:HG21	1.30	1.13
1:B:116:LEU:HD23	1:B:117:TRP:N	1.62	1.13
1:C:178:PHE:HA	1:C:254:ASP:OD2	1.49	1.13
1:D:46:PRO:CG	1:D:466:TYR:CE2	2.33	1.12
1:A:252:TRP:CZ3	1:A:253:ARG:HD2	1.84	1.12
1:C:55:LYS:CE	1:C:56:LEU:HD21	1.77	1.12
1:B:174:CYS:O	1:B:179:GLY:HA2	1.49	1.12
1:C:448:PHE:HB3	1:C:479:ARG:O	1.49	1.12
1:A:461:LEU:HD23	1:A:461:LEU:O	1.48	1.12
1:B:210:MET:CG	3:B:502:3QZ:HAG	1.78	1.12
1:D:196:LEU:HD23	3:D:501:3QZ:CAI	1.79	1.12
1:A:40:LEU:O	1:A:40:LEU:HD12	1.49	1.12
1:A:252:TRP:HZ3	1:A:253:ARG:HD2	0.95	1.11
1:A:461:LEU:HD23	1:A:461:LEU:C	1.69	1.11
1:D:168:LEU:H	1:D:168:LEU:CD1	1.61	1.11
1:D:65:GLY:O	1:D:66:LEU:HD12	1.49	1.11
1:D:461:LEU:C	1:D:461:LEU:HD23	1.69	1.11
1:B:288:PHE:HD2	1:B:289:ILE:CD1	1.55	1.11
1:B:193:VAL:HG13	1:B:289:ILE:CG2	1.79	1.11
1:D:418:LEU:CD2	1:D:422:CYS:SG	2.38	1.11
1:D:404:ARG:O	1:D:404:ARG:HD2	1.50	1.11
1:B:402:GLU:OE1	1:B:402:GLU:HA	1.49	1.11
1:D:38:LEU:HB3	1:D:41:LEU:HD12	1.18	1.10
1:C:162:GLN:HA	1:C:162:GLN:HE21	1.03	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:181:LYS:HG2	1:C:181:LYS:O	1.50	1.10
1:C:212:PRO:O	1:C:216:PHE:CE2	2.04	1.10
1:D:420:PHE:CZ	2:D:500:HEM:HBB2	1.86	1.10
1:C:62:LEU:HD23	1:C:62:LEU:C	1.67	1.10
1:C:276:LEU:CD2	1:C:278:GLY:H	1.64	1.10
1:A:214:LEU:HD21	1:A:216:PHE:CA	1.81	1.10
1:A:178:PHE:CA	1:A:243:HIS:HE1	1.62	1.10
1:A:196:LEU:HD23	3:A:501:3QZ:HAI	1.31	1.09
1:B:62:LEU:HD23	1:B:62:LEU:C	1.73	1.09
1:C:463:PRO:HG3	1:C:471:LEU:HB3	1.27	1.09
1:B:128:LEU:CG	1:B:287:LEU:HD21	1.80	1.09
1:D:407:ARG:CG	1:D:407:ARG:HH11	1.65	1.09
1:A:459:PRO:HG3	1:A:475:PRO:HB3	1.34	1.09
1:C:447:ALA:HB3	1:C:448:PHE:CE2	1.87	1.09
1:C:212:PRO:O	1:C:216:PHE:HE2	1.33	1.09
1:C:159:VAL:CG1	1:C:476:PHE:CE2	2.35	1.08
1:D:62:LEU:C	1:D:62:LEU:HD23	1.72	1.08
1:A:252:TRP:HZ3	1:A:253:ARG:CD	1.66	1.08
1:C:407:ARG:HH11	1:C:407:ARG:HG3	0.93	1.08
1:D:106:GLN:CB	1:D:279:HIS:NE2	2.15	1.08
1:D:168:LEU:H	1:D:168:LEU:HD12	0.95	1.08
1:B:169:THR:HG22	1:B:173:ILE:HD11	1.34	1.08
1:D:242:ARG:NH1	1:D:242:ARG:HG2	1.56	1.08
1:D:242:ARG:CG	1:D:242:ARG:HH11	1.65	1.08
1:A:193:VAL:HG22	1:A:289:ILE:HG22	1.31	1.08
1:A:171:SER:O	1:A:175:TYR:CE1	2.07	1.08
1:B:409:LEU:O	1:B:409:LEU:HD23	1.49	1.08
1:B:176:LEU:O	1:B:176:LEU:HD23	1.53	1.07
1:A:38:LEU:HB3	1:A:41:LEU:HD21	1.36	1.07
1:A:89:PHE:CZ	1:A:372:ILE:HG12	1.85	1.07
1:C:358:VAL:HG11	2:C:500:HEM:CMA	1.85	1.07
1:C:407:ARG:CG	1:C:407:ARG:HH11	1.66	1.07
1:C:102:SER:OG	1:C:105:CYS:HA	1.55	1.07
1:D:214:LEU:HD21	1:D:216:PHE:HA	1.35	1.07
1:B:128:LEU:HD21	1:B:287:LEU:HD23	1.30	1.07
1:C:167:LEU:HD23	1:C:167:LEU:O	1.54	1.07
1:D:106:GLN:CG	1:D:279:HIS:NE2	2.16	1.07
1:A:283:SER:O	1:A:287:LEU:HD11	1.54	1.07
1:D:372:ILE:O	1:D:373:PHE:HB3	1.53	1.06
1:B:294:THR:HG21	3:B:501:3QZ:HAAA	1.12	1.06
1:D:430:GLU:OE2	4:D:617:HOH:O	1.72	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:472:LYS:HE2	1:A:473:VAL:H	0.96	1.06
1:C:162:GLN:HA	1:C:162:GLN:NE2	1.70	1.06
1:B:418:LEU:N	1:B:418:LEU:HD12	1.58	1.06
1:D:168:LEU:CD2	1:D:292:THR:O	2.04	1.06
1:B:92:ARG:NH1	1:B:363:PRO:O	1.89	1.06
1:A:214:LEU:HD21	1:A:216:PHE:HA	1.34	1.06
1:A:62:LEU:HD23	1:A:62:LEU:C	1.69	1.05
1:B:89:PHE:HE2	1:B:372:ILE:HD11	1.19	1.05
1:A:404:ARG:HH11	1:A:404:ARG:CG	1.69	1.05
1:D:214:LEU:CD2	1:D:216:PHE:HD1	1.67	1.05
1:A:219:ASN:ND2	4:A:621:HOH:O	1.71	1.05
1:A:252:TRP:HB2	1:A:257:ASP:CG	1.77	1.05
1:D:85:LYS:HG3	1:D:88:ASP:OD2	1.54	1.05
1:B:410:GLU:OE2	1:B:411:PRO:HG3	1.53	1.05
1:D:252:TRP:CZ3	1:D:253:ARG:CZ	2.40	1.05
1:C:423:GLY:O	1:C:426:VAL:HG13	1.55	1.05
1:A:287:LEU:H	1:A:287:LEU:HD12	1.12	1.04
1:A:214:LEU:HG	1:A:216:PHE:H	1.21	1.04
1:B:409:LEU:O	1:B:411:PRO:HD3	1.54	1.04
1:C:55:LYS:HE2	1:C:56:LEU:HD21	1.04	1.04
1:C:418:LEU:H	1:C:418:LEU:HD12	0.89	1.04
1:A:161:ILE:O	1:A:165:PHE:HB2	1.56	1.04
1:C:89:PHE:CE2	1:C:372:ILE:CD1	2.41	1.04
1:A:294:THR:HG23	3:A:501:3QZ:CAA	1.81	1.04
1:B:214:LEU:HD21	1:B:216:PHE:HA	1.40	1.04
1:C:418:LEU:N	1:C:418:LEU:HD12	1.62	1.04
1:D:55:LYS:HG3	1:D:56:LEU:CD2	1.88	1.04
1:B:396:VAL:CG1	1:B:397:TRP:CE3	2.42	1.03
1:C:465:PRO:HG2	1:C:471:LEU:HD22	1.40	1.03
1:A:214:LEU:CD2	1:A:216:PHE:CD2	2.41	1.03
1:D:463:PRO:HB2	1:D:471:LEU:HG	1.32	1.03
1:A:460:SER:O	1:A:461:LEU:HB3	1.59	1.03
1:B:460:SER:HA	1:B:472:LYS:HE2	1.39	1.03
1:C:40:LEU:C	1:C:40:LEU:HD12	1.75	1.02
1:B:210:MET:HG2	3:B:502:3QZ:HAG	1.07	1.02
1:D:55:LYS:CD	1:D:56:LEU:HD21	1.88	1.02
1:A:177:THR:HB	1:A:288:PHE:CZ	1.94	1.02
1:D:407:ARG:HG3	1:D:407:ARG:HH11	1.25	1.02
1:A:214:LEU:CG	1:A:216:PHE:H	1.71	1.02
1:A:252:TRP:CE3	1:A:253:ARG:CG	2.43	1.02
1:A:252:TRP:CZ3	1:A:253:ARG:CD	2.41	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:55:LYS:HE2	1:C:56:LEU:CD2	1.89	1.01
1:A:52:LEU:O	1:A:56:LEU:HD23	1.58	1.01
1:C:232:ARG:NH1	3:C:501:3QZ:HAG	1.75	1.01
1:B:285:VAL:HA	1:B:288:PHE:HB3	1.39	1.01
1:D:252:TRP:CE3	1:D:253:ARG:HD2	1.94	1.01
1:A:67:GLN:HA	1:A:67:GLN:OE1	1.60	1.01
1:D:65:GLY:C	1:D:66:LEU:HD12	1.79	1.01
1:B:294:THR:HG21	3:B:501:3QZ:CAA	1.87	1.01
1:A:244:LYS:HG2	1:A:260:LEU:HD21	1.41	1.01
1:A:472:LYS:CA	1:A:472:LYS:HE2	1.90	1.01
1:C:408:PHE:O	1:C:408:PHE:HD1	1.43	1.01
1:D:373:PHE:C	1:D:373:PHE:CD1	2.30	1.01
1:A:332:ARG:O	1:A:333:VAL:HG23	1.61	1.01
1:C:407:ARG:O	1:C:413:ALA:HB1	1.59	1.01
1:A:404:ARG:O	1:A:404:ARG:HG2	1.56	1.01
1:C:294:THR:HG21	3:C:501:3QZ:HAAA	1.41	1.01
1:A:463:PRO:O	1:A:466:TYR:HE1	1.27	1.00
1:B:128:LEU:HD21	1:B:287:LEU:CD2	1.90	1.00
1:C:276:LEU:C	1:C:276:LEU:HD23	1.80	1.00
1:D:196:LEU:CD2	3:D:501:3QZ:HAI	1.90	1.00
1:B:448:PHE:HD1	1:B:479:ARG:O	1.43	1.00
1:C:67:GLN:HA	1:C:67:GLN:OE1	1.59	1.00
1:A:332:ARG:HE	1:A:332:ARG:HA	0.94	1.00
1:C:276:LEU:HD21	1:C:278:GLY:H	1.24	1.00
1:A:178:PHE:CA	1:A:243:HIS:CE1	2.44	1.00
1:A:446:GLN:O	1:A:481:GLN:NE2	1.94	1.00
1:A:332:ARG:C	1:A:333:VAL:HG23	1.82	1.00
1:D:346:ALA:HB1	1:D:405:PRO:O	1.62	1.00
1:D:97:SER:HB2	1:D:209:ASP:OD2	1.60	1.00
1:B:418:LEU:HD12	1:B:418:LEU:H	0.85	1.00
1:A:404:ARG:HH11	1:A:404:ARG:HG3	1.23	1.00
1:D:55:LYS:HD2	1:D:56:LEU:HD21	1.00	0.99
1:B:189:PHE:CZ	1:B:288:PHE:HZ	1.79	0.99
1:A:335:TYR:CD2	1:A:336:LYS:N	2.30	0.99
1:C:472:LYS:C	1:C:472:LYS:HZ3	1.66	0.99
1:D:432:LEU:O	1:D:432:LEU:HD23	1.61	0.99
1:B:288:PHE:HD2	1:B:289:ILE:HD13	1.22	0.99
1:B:396:VAL:HG12	1:B:397:TRP:CE3	1.98	0.99
1:A:472:LYS:NZ	1:A:472:LYS:HB3	1.75	0.99
1:D:38:LEU:HB3	1:D:41:LEU:CD1	1.91	0.99
1:A:214:LEU:CD2	1:A:216:PHE:H	1.75	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:463:PRO:O	1:A:466:TYR:CD1	2.16	0.99
1:B:41:LEU:H	1:B:41:LEU:HD23	1.22	0.99
1:C:358:VAL:HG11	2:C:500:HEM:C3A	1.98	0.99
1:A:178:PHE:HA	1:A:243:HIS:CE1	1.98	0.99
1:C:472:LYS:HE2	1:C:472:LYS:HA	1.44	0.98
1:D:407:ARG:NH1	1:D:407:ARG:HB2	1.77	0.98
1:D:214:LEU:CD2	1:D:216:PHE:H	1.76	0.98
1:B:169:THR:O	1:B:173:ILE:HG12	1.62	0.98
1:B:214:LEU:O	1:B:215:ARG:HG3	1.63	0.98
1:D:211:VAL:O	1:D:211:VAL:HG12	1.61	0.98
1:B:396:VAL:HG11	1:B:397:TRP:CZ3	1.98	0.98
1:A:357:VAL:HG12	1:A:469:VAL:CG1	1.93	0.98
1:B:169:THR:O	1:B:173:ILE:CG1	2.11	0.98
1:A:50:LEU:O	1:A:53:THR:HG23	1.64	0.98
1:B:178:PHE:CE2	1:B:252:TRP:CH2	2.46	0.98
1:D:215:ARG:HB3	1:D:217:PHE:CE1	1.98	0.98
1:A:106:GLN:OE1	1:A:116:LEU:HD13	1.62	0.98
1:D:407:ARG:CB	1:D:407:ARG:HH11	1.76	0.98
1:A:472:LYS:NZ	1:A:473:VAL:N	2.11	0.97
1:C:55:LYS:HG2	1:C:56:LEU:HD22	0.99	0.97
1:A:38:LEU:CB	1:A:41:LEU:HD21	1.93	0.97
1:D:55:LYS:HG3	1:D:56:LEU:HD22	1.45	0.97
1:D:168:LEU:N	1:D:168:LEU:HD12	1.80	0.97
1:D:94:GLN:OE1	1:D:99:LYS:CE	2.12	0.97
1:A:285:VAL:HG12	1:A:286:ASP:OD1	1.62	0.97
1:A:373:PHE:C	1:A:373:PHE:CD1	2.36	0.97
1:B:128:LEU:CD1	1:B:287:LEU:HD21	1.93	0.97
1:A:43:PRO:HB2	1:A:44:ASN:OD1	1.63	0.97
1:D:473:VAL:HG13	1:D:474:GLN:H	1.29	0.97
1:B:189:PHE:CE2	1:B:288:PHE:CE2	2.52	0.96
1:D:448:PHE:N	1:D:448:PHE:HD2	1.63	0.96
1:B:219:ASN:OD1	4:B:626:HOH:O	1.83	0.96
1:D:375:TYR:O	1:D:377:ILE:HD13	1.63	0.96
1:B:350:GLU:HG3	1:B:404:ARG:O	1.65	0.96
1:B:193:VAL:HG22	1:B:289:ILE:HG23	1.48	0.96
1:A:472:LYS:NZ	1:A:473:VAL:O	1.99	0.96
1:C:41:LEU:O	1:C:42:GLN:HB3	1.63	0.96
1:B:33:LEU:HD13	1:B:34:VAL:O	1.64	0.96
1:C:448:PHE:HD2	1:C:448:PHE:N	1.64	0.96
1:D:350:GLU:HG3	1:D:404:ARG:O	1.64	0.96
1:B:418:LEU:H	1:B:418:LEU:CD1	1.78	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:112:ASP:OD2	1:B:365:ARG:NH2	1.97	0.96
1:B:178:PHE:HB2	1:B:243:HIS:CE1	2.01	0.96
1:B:73:ASN:HD22	1:B:73:ASN:N	1.61	0.96
1:B:210:MET:HG2	3:B:502:3QZ:CAG	1.95	0.96
1:B:214:LEU:HD23	1:B:216:PHE:HD2	0.82	0.95
1:D:196:LEU:HD23	3:D:501:3QZ:HAI	0.96	0.95
1:C:55:LYS:CG	1:C:56:LEU:CD2	2.43	0.95
1:A:275:LEU:HD12	1:A:275:LEU:O	1.66	0.95
1:B:284:VAL:CG1	1:B:288:PHE:CD1	2.48	0.95
1:D:214:LEU:HD23	1:D:216:PHE:HD1	0.79	0.95
1:C:232:ARG:HH12	3:C:501:3QZ:HAG	1.27	0.95
1:C:358:VAL:CG1	2:C:500:HEM:CMA	2.41	0.95
1:A:246:SER:O	1:A:252:TRP:NE1	1.99	0.95
1:A:472:LYS:HZ3	1:A:472:LYS:C	1.70	0.95
1:D:196:LEU:HD21	3:D:501:3QZ:OAE	1.64	0.95
1:D:449:THR:O	1:D:450:LEU:HB2	1.67	0.95
1:D:164:GLU:O	1:D:168:LEU:CD1	2.14	0.95
1:D:275:LEU:HD12	1:D:275:LEU:C	1.87	0.95
1:D:463:PRO:CG	1:D:471:LEU:CB	1.96	0.95
1:D:55:LYS:CD	1:D:56:LEU:CD2	2.43	0.95
1:C:472:LYS:CE	1:C:472:LYS:CA	2.43	0.95
1:C:358:VAL:HG11	2:C:500:HEM:HMA3	1.44	0.94
1:B:211:VAL:HG12	1:B:211:VAL:O	1.64	0.94
1:A:475:PRO:CB	1:A:477:GLN:NE2	2.14	0.94
1:B:176:LEU:HD23	1:B:176:LEU:C	1.86	0.94
1:B:178:PHE:CE2	1:B:252:TRP:HZ3	1.76	0.94
1:D:215:ARG:HB3	1:D:217:PHE:HE1	1.31	0.94
1:D:178:PHE:CE1	1:D:242:ARG:NH1	2.35	0.94
1:C:407:ARG:NH1	1:C:407:ARG:HG3	1.58	0.94
1:D:173:ILE:HA	1:D:288:PHE:CE1	2.02	0.94
1:D:463:PRO:CB	1:D:471:LEU:CB	2.40	0.94
1:A:472:LYS:HE2	1:A:472:LYS:C	1.87	0.94
1:B:91:GLY:O	1:B:365:ARG:N	1.98	0.94
1:A:372:ILE:O	1:A:372:ILE:HG22	1.66	0.94
1:B:89:PHE:N	1:B:89:PHE:HD1	1.66	0.94
1:A:301:TRP:CE2	1:A:472:LYS:HG2	2.02	0.94
1:C:358:VAL:HG13	2:C:500:HEM:HMA3	1.47	0.94
1:A:56:LEU:H	1:A:56:LEU:HD22	1.32	0.94
1:B:214:LEU:HD23	1:B:216:PHE:H	1.32	0.94
1:C:89:PHE:CE2	1:C:372:ILE:HD11	2.02	0.94
1:B:34:VAL:HG11	1:B:52:LEU:HD13	1.50	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:GLU:O	1:A:323:GLU:HB2	1.68	0.94
1:B:177:THR:O	1:B:177:THR:HG22	1.64	0.94
1:A:350:GLU:HG3	1:A:404:ARG:O	1.67	0.94
1:D:473:VAL:CG1	1:D:474:GLN:N	2.09	0.94
1:C:358:VAL:HG13	1:C:358:VAL:O	1.65	0.94
1:B:176:LEU:HD11	1:B:287:LEU:HB3	1.49	0.94
1:C:173:ILE:HA	1:C:288:PHE:CE1	2.03	0.94
1:B:214:LEU:CD2	1:B:216:PHE:H	1.80	0.93
1:C:104:ARG:C	1:C:105:CYS:SG	2.46	0.93
1:D:117:TRP:CZ2	1:D:425:ARG:HD3	2.03	0.93
1:B:284:VAL:O	1:B:288:PHE:N	2.01	0.93
1:D:214:LEU:HD23	1:D:216:PHE:H	1.30	0.93
1:D:109:SER:OG	1:D:110:LEU:HD23	1.68	0.93
1:C:37:PHE:O	1:C:38:LEU:HD23	1.67	0.93
1:A:177:THR:CB	1:A:288:PHE:CE1	2.51	0.93
1:C:169:THR:HG21	1:C:190:HIS:HB2	1.50	0.93
1:C:447:ALA:HB3	1:C:448:PHE:HE2	1.24	0.93
1:D:46:PRO:HG3	1:D:466:TYR:HE2	0.89	0.93
1:B:284:VAL:CG1	1:B:288:PHE:HD1	1.82	0.93
1:B:357:VAL:HG12	1:B:469:VAL:HG13	1.49	0.93
1:C:463:PRO:HG3	1:C:471:LEU:CB	1.97	0.93
1:B:248:VAL:HG23	1:B:250:GLY:H	1.33	0.93
1:A:332:ARG:HG3	1:A:337:ASP:OD1	1.67	0.93
1:A:161:ILE:HG22	1:A:165:PHE:HD2	1.33	0.93
1:A:161:ILE:HG22	1:A:165:PHE:CD2	2.04	0.93
1:B:214:LEU:CD2	1:B:216:PHE:CD2	2.40	0.93
1:D:275:LEU:CD1	1:D:275:LEU:C	2.38	0.92
1:B:471:LEU:H	1:B:471:LEU:HD12	0.77	0.92
1:A:103:GLN:N	4:A:610:HOH:O	2.00	0.92
1:D:106:GLN:CG	1:D:279:HIS:CE1	2.52	0.92
1:B:113:TYR:O	1:B:114:SER:HB3	1.67	0.92
1:C:472:LYS:HE2	1:C:473:VAL:H	1.33	0.92
1:C:472:LYS:HE2	1:C:473:VAL:N	1.84	0.92
1:A:42:GLN:CG	4:A:613:HOH:O	1.89	0.92
1:A:178:PHE:N	1:A:243:HIS:CE1	2.38	0.92
1:A:372:ILE:O	1:A:373:PHE:HB3	1.67	0.92
1:B:176:LEU:CD1	1:B:287:LEU:HB3	2.00	0.91
1:A:106:GLN:O	1:A:107:ASP:HB3	1.69	0.91
1:D:448:PHE:HB3	1:D:479:ARG:O	1.71	0.91
1:D:471:LEU:HD13	1:D:472:LYS:N	1.85	0.91
1:A:475:PRO:CG	1:A:477:GLN:NE2	2.33	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:448:PHE:CD2	1:C:448:PHE:N	2.34	0.91
1:C:465:PRO:HG2	1:C:471:LEU:CD2	2.00	0.91
1:C:62:LEU:CD2	1:C:62:LEU:C	2.37	0.91
1:A:462:GLN:HB2	1:A:466:TYR:OH	1.71	0.91
1:C:55:LYS:CG	1:C:56:LEU:HD22	1.96	0.91
1:C:178:PHE:CA	1:C:254:ASP:OD2	2.19	0.91
1:C:167:LEU:CD2	1:C:167:LEU:C	2.39	0.91
1:C:307:LEU:HD13	1:C:458:LEU:HD22	1.52	0.91
1:C:30:LEU:HG	1:C:31:PRO:HD2	1.51	0.91
1:A:313:GLN:HE22	1:A:450:LEU:CD1	1.83	0.90
1:A:335:TYR:HD2	1:A:335:TYR:C	1.74	0.90
1:D:448:PHE:N	1:D:448:PHE:CD2	2.28	0.90
1:C:116:LEU:HD23	1:C:117:TRP:N	1.85	0.90
1:C:472:LYS:CE	1:C:472:LYS:HA	1.92	0.90
1:B:71:VAL:HG12	1:B:73:ASN:HD21	1.37	0.90
1:A:105:CYS:O	1:A:106:GLN:HB2	1.71	0.90
1:D:69:VAL:HG13	1:D:382:VAL:HB	1.52	0.90
1:A:108:ILE:HD13	1:A:124:THR:HG21	1.53	0.90
1:D:55:LYS:CG	1:D:56:LEU:HD22	2.02	0.90
1:D:214:LEU:O	1:D:214:LEU:HG	1.71	0.90
1:B:396:VAL:HG12	1:B:397:TRP:CD2	2.06	0.90
1:C:113:TYR:O	1:C:114:SER:HB3	1.72	0.90
1:C:297:SER:HB2	1:C:357:VAL:CG2	2.01	0.90
1:B:116:LEU:CD2	1:B:116:LEU:C	2.39	0.90
1:A:189:PHE:CZ	1:A:288:PHE:CE2	2.59	0.90
1:C:116:LEU:CD2	1:C:116:LEU:C	2.39	0.90
1:D:473:VAL:HG12	1:D:474:GLN:H	1.10	0.90
1:B:288:PHE:C	1:B:289:ILE:CD1	2.40	0.90
1:A:214:LEU:HD21	1:A:216:PHE:CD2	2.07	0.90
1:D:472:LYS:HD2	1:D:473:VAL:N	1.87	0.89
1:B:128:LEU:HD11	1:B:287:LEU:HD21	1.50	0.89
1:A:214:LEU:HG	1:A:216:PHE:N	1.86	0.89
1:A:101:VAL:HG23	1:A:101:VAL:O	1.72	0.89
1:D:117:TRP:NE1	1:D:425:ARG:NH1	2.21	0.89
1:D:55:LYS:CG	1:D:56:LEU:CD2	2.50	0.89
1:B:62:LEU:C	1:B:62:LEU:CD2	2.38	0.89
1:D:377:ILE:HG23	1:D:378:PRO:HD2	1.54	0.89
1:A:102:SER:OG	4:A:610:HOH:O	1.89	0.89
1:B:248:VAL:HG23	1:B:250:GLY:N	1.86	0.89
1:B:41:LEU:CD2	1:B:41:LEU:N	2.35	0.89
1:B:407:ARG:HH11	1:B:407:ARG:CG	1.86	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:LEU:O	1:A:41:LEU:HG	1.72	0.89
1:A:159:VAL:O	1:A:159:VAL:HG22	1.72	0.89
1:A:38:LEU:HB3	1:A:41:LEU:CD2	2.03	0.89
1:A:56:LEU:HD22	1:A:56:LEU:N	1.87	0.89
1:C:276:LEU:C	1:C:276:LEU:CD2	2.41	0.89
1:D:178:PHE:HE1	1:D:242:ARG:HH12	1.21	0.89
1:D:447:ALA:C	1:D:448:PHE:CD2	2.46	0.89
1:D:461:LEU:C	1:D:461:LEU:CD2	2.37	0.88
1:C:162:GLN:CA	1:C:162:GLN:NE2	2.35	0.88
1:A:472:LYS:NZ	1:A:472:LYS:CB	2.35	0.88
1:D:62:LEU:CD2	1:D:62:LEU:C	2.40	0.88
1:A:89:PHE:CZ	1:A:372:ILE:HG13	2.09	0.88
1:A:294:THR:HG23	3:A:501:3QZ:HAA	1.51	0.88
1:C:56:LEU:CD2	1:C:56:LEU:N	2.36	0.88
1:B:284:VAL:O	1:B:288:PHE:CA	2.21	0.88
1:B:116:LEU:CD2	1:B:117:TRP:N	2.36	0.88
1:A:404:ARG:NH2	1:A:414:ASN:ND2	2.22	0.88
1:B:288:PHE:CE2	1:B:289:ILE:HD11	2.08	0.88
1:D:373:PHE:HD1	1:D:373:PHE:C	1.69	0.88
1:C:425:ARG:O	4:C:606:HOH:O	1.92	0.88
1:B:407:ARG:HH11	1:B:407:ARG:HG3	1.39	0.88
1:A:103:GLN:NE2	1:A:104:ARG:HD3	1.89	0.88
1:C:62:LEU:CD2	1:C:64:LEU:N	2.36	0.88
1:A:62:LEU:C	1:A:62:LEU:CD2	2.40	0.88
1:D:56:LEU:N	1:D:56:LEU:HD22	1.88	0.88
1:C:472:LYS:HE2	1:C:472:LYS:CA	2.02	0.88
1:D:307:LEU:HD13	1:D:458:LEU:HD22	1.56	0.87
1:D:463:PRO:CB	1:D:471:LEU:HB3	2.03	0.87
1:D:185:LEU:HD11	1:D:239:GLN:HE22	1.38	0.87
1:B:189:PHE:HE2	1:B:288:PHE:CZ	1.82	0.87
1:B:128:LEU:HG	1:B:287:LEU:HD21	1.53	0.87
1:C:276:LEU:CD2	1:C:278:GLY:N	2.35	0.87
1:A:263:VAL:HG13	1:A:275:LEU:HD12	1.57	0.87
1:D:423:GLY:O	1:D:426:VAL:HG13	1.73	0.87
1:A:124:THR:HG23	1:A:428:LEU:HD11	1.54	0.87
1:D:463:PRO:HB3	1:D:471:LEU:HD12	1.55	0.87
1:A:189:PHE:CZ	1:A:288:PHE:HE2	1.92	0.87
1:A:313:GLN:NE2	1:A:450:LEU:HD12	1.89	0.87
1:D:232:ARG:NH1	3:D:501:3QZ:OAE	2.06	0.87
1:A:246:SER:O	1:A:252:TRP:CD1	2.28	0.87
1:D:203:TRP:HA	1:D:206:GLN:HB2	1.57	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:116:LEU:CD2	1:D:117:TRP:N	2.37	0.87
1:B:294:THR:CG2	3:B:501:3QZ:HAA	2.04	0.87
1:C:472:LYS:CE	1:C:473:VAL:N	2.37	0.87
1:C:125:ARG:O	1:C:128:LEU:HB2	1.74	0.87
1:D:211:VAL:HG12	1:D:214:LEU:HB2	1.57	0.87
1:D:405:PRO:HD2	1:D:406:ASP:OD1	1.75	0.87
1:C:87:VAL:HG12	1:C:368:ARG:HH12	1.38	0.87
1:A:337:ASP:O	1:A:340:ARG:N	2.08	0.86
1:B:89:PHE:HE2	1:B:372:ILE:CD1	1.88	0.86
1:D:108:ILE:HD11	1:D:124:THR:HG21	1.56	0.86
1:C:418:LEU:H	1:C:418:LEU:CD1	1.81	0.86
1:A:423:GLY:O	1:A:426:VAL:HG13	1.75	0.86
1:D:38:LEU:HD13	1:D:41:LEU:HD11	1.55	0.86
1:A:472:LYS:HA	1:A:472:LYS:HE2	1.58	0.86
1:A:40:LEU:C	1:A:40:LEU:HD12	1.92	0.86
1:B:178:PHE:CD2	1:B:252:TRP:CZ3	2.63	0.86
1:B:89:PHE:CE2	1:B:372:ILE:HD11	2.09	0.86
1:D:373:PHE:HD1	1:D:374:GLY:N	1.74	0.86
1:C:341:LEU:HD13	1:C:344:LEU:HD12	1.56	0.86
1:A:341:LEU:HD13	1:A:344:LEU:HD12	1.57	0.86
1:A:89:PHE:CE1	1:A:372:ILE:HG12	2.08	0.86
1:B:473:VAL:O	1:B:475:PRO:HD3	1.74	0.86
1:B:193:VAL:HG13	1:B:289:ILE:HG22	1.57	0.86
1:A:214:LEU:CD2	1:A:216:PHE:N	2.38	0.86
1:A:337:ASP:O	1:A:339:ALA:N	2.08	0.86
1:D:242:ARG:HG2	1:D:242:ARG:HH11	0.75	0.86
1:A:472:LYS:CA	1:A:472:LYS:CE	2.50	0.86
1:C:38:LEU:HB3	1:C:41:LEU:CD1	2.06	0.86
1:B:193:VAL:CG2	1:B:289:ILE:HG23	2.05	0.86
1:A:177:THR:CB	1:A:288:PHE:CZ	2.57	0.86
1:D:46:PRO:CG	1:D:466:TYR:HE2	1.77	0.85
1:D:472:LYS:HD2	1:D:473:VAL:H	1.38	0.85
1:B:285:VAL:CA	1:B:288:PHE:HB3	2.06	0.85
1:B:89:PHE:CD1	1:B:89:PHE:N	2.41	0.85
1:B:396:VAL:HG11	1:B:397:TRP:CE3	2.09	0.85
1:A:89:PHE:CE2	1:A:372:ILE:HD11	2.11	0.85
1:D:407:ARG:CB	1:D:407:ARG:NH1	2.38	0.85
1:A:42:GLN:OE1	4:A:613:HOH:O	1.94	0.85
1:A:449:THR:CB	1:A:480:LEU:O	2.22	0.85
1:D:105:CYS:CB	4:D:613:HOH:O	2.03	0.85
1:C:333:VAL:O	1:C:333:VAL:HG12	1.75	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:LEU:HD21	1:A:296:ALA:HB2	1.59	0.85
1:A:252:TRP:CZ3	1:A:253:ARG:CG	2.59	0.85
1:B:62:LEU:HD23	1:B:63:ARG:CA	2.07	0.85
1:C:167:LEU:HD23	1:C:167:LEU:C	1.93	0.85
1:B:407:ARG:HG3	1:B:407:ARG:NH1	1.89	0.85
1:C:101:VAL:HG23	1:C:232:ARG:HH22	1.40	0.85
1:A:252:TRP:HE3	1:A:253:ARG:HG3	1.09	0.85
1:A:45:LEU:CD2	1:A:49:LEU:HG	2.07	0.85
1:D:378:PRO:HG2	1:D:381:MET:HB2	1.57	0.85
1:A:42:GLN:OE1	1:A:48:HIS:CG	2.30	0.85
1:A:177:THR:HG21	1:A:288:PHE:CE2	2.12	0.85
1:A:324:LEU:CD1	1:A:332:ARG:HG2	2.05	0.85
1:A:252:TRP:CZ3	1:A:253:ARG:HG3	2.10	0.85
1:C:88:ASP:HB2	1:C:89:PHE:CD1	2.11	0.85
1:A:56:LEU:H	1:A:56:LEU:CD2	1.90	0.84
1:A:332:ARG:HE	1:A:332:ARG:CA	1.86	0.84
1:B:460:SER:CA	1:B:472:LYS:HE2	2.06	0.84
1:C:31:PRO:HG2	1:C:61:ARG:HG3	1.59	0.84
1:C:62:LEU:HD23	1:C:63:ARG:CA	2.08	0.84
1:D:110:LEU:CD2	1:D:110:LEU:N	2.40	0.84
1:A:335:TYR:C	1:A:335:TYR:CD2	2.48	0.84
1:A:243:HIS:CD2	1:A:256:THR:HB	2.12	0.84
1:C:104:ARG:O	1:C:105:CYS:SG	2.36	0.84
1:D:106:GLN:HG2	1:D:116:LEU:HD11	1.58	0.84
1:A:160:THR:OG1	1:A:477:GLN:HG2	1.77	0.84
1:B:168:LEU:HD21	1:B:296:ALA:HB2	1.59	0.84
1:B:408:PHE:HD2	1:B:410:GLU:N	1.76	0.84
1:A:357:VAL:HG12	1:A:469:VAL:HG13	1.58	0.84
1:D:177:THR:HG23	1:D:239:GLN:HG2	1.59	0.84
1:A:169:THR:HG21	1:A:190:HIS:HB2	1.59	0.84
1:B:136:MET:HB3	1:B:175:TYR:CE2	2.13	0.84
1:A:375:TYR:N	1:A:375:TYR:CD2	2.42	0.84
1:D:214:LEU:HD21	1:D:216:PHE:CA	2.07	0.83
1:A:103:GLN:HE22	1:A:104:ARG:HD3	1.43	0.83
1:D:196:LEU:HD11	1:D:229:ILE:HA	1.60	0.83
1:B:448:PHE:CD1	1:B:479:ARG:O	2.32	0.83
1:B:30:LEU:HG	1:B:31:PRO:HD2	1.59	0.83
1:B:176:LEU:HD12	1:B:287:LEU:HD22	1.59	0.83
1:B:214:LEU:O	1:B:217:PHE:CE1	2.31	0.83
1:D:275:LEU:O	1:D:275:LEU:CD1	2.25	0.83
1:C:161:ILE:CD1	1:C:474:GLN:HA	2.08	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:103:GLN:O	1:C:105:CYS:SG	2.36	0.83
1:C:129:LEU:N	1:C:129:LEU:CD1	2.41	0.83
1:C:161:ILE:CG1	1:C:475:PRO:HD2	2.09	0.83
1:D:297:SER:HB2	1:D:357:VAL:HG22	1.58	0.83
1:B:172:ILE:HD13	1:B:172:ILE:N	1.93	0.83
1:A:106:GLN:OE1	1:A:116:LEU:CD1	2.27	0.83
1:B:113:TYR:HD2	1:B:114:SER:H	1.27	0.83
1:A:407:ARG:HH11	1:A:407:ARG:HG3	1.42	0.83
1:C:358:VAL:O	1:C:358:VAL:CG1	2.26	0.83
1:B:193:VAL:HG22	1:B:289:ILE:CG2	2.08	0.82
1:D:215:ARG:CB	1:D:217:PHE:HE1	1.91	0.82
1:A:161:ILE:CG2	1:A:165:PHE:HD2	1.92	0.82
1:A:461:LEU:CD2	1:A:461:LEU:C	2.42	0.82
1:C:472:LYS:HZ3	1:C:472:LYS:CB	1.93	0.82
1:D:252:TRP:HE3	1:D:253:ARG:HD2	1.44	0.82
1:A:104:ARG:O	1:A:105:CYS:SG	2.37	0.82
1:B:61:ARG:NH1	1:B:68:GLU:CD	2.33	0.82
1:D:174:CYS:O	1:D:179:GLY:HA2	1.77	0.82
1:A:472:LYS:HZ2	1:A:472:LYS:HB3	1.40	0.82
1:A:373:PHE:HD1	1:A:373:PHE:C	1.81	0.82
1:C:59:VAL:HG21	1:C:372:ILE:HG21	1.62	0.82
1:C:232:ARG:NH1	3:C:501:3QZ:CAG	2.43	0.82
1:A:113:TYR:HD2	1:A:114:SER:H	1.27	0.82
1:D:461:LEU:O	1:D:462:GLN:HB2	1.77	0.82
1:D:358:VAL:HG12	1:D:361:ALA:HA	1.61	0.82
1:B:459:PRO:CG	1:B:472:LYS:HZ1	1.91	0.82
1:D:168:LEU:N	1:D:168:LEU:CD1	2.31	0.82
1:A:358:VAL:CG1	1:A:361:ALA:HA	2.08	0.82
1:D:463:PRO:HG3	1:D:471:LEU:CA	2.09	0.82
1:A:472:LYS:HE3	1:A:473:VAL:H	1.39	0.82
1:C:447:ALA:CB	1:C:448:PHE:CE2	2.62	0.82
1:D:451:LEU:HG	1:D:452:PRO:HD2	1.62	0.82
1:C:101:VAL:O	1:C:101:VAL:HG23	1.79	0.82
1:D:65:GLY:C	1:D:66:LEU:CD1	2.46	0.82
1:A:44:ASN:HB2	1:A:47:ILE:HG12	1.59	0.82
1:C:294:THR:CG2	3:C:501:3QZ:HAAA	2.09	0.82
1:D:105:CYS:O	4:D:604:HOH:O	1.96	0.82
1:D:113:TYR:O	1:D:114:SER:HB3	1.79	0.82
1:D:420:PHE:HZ	2:D:500:HEM:HBB2	1.43	0.81
1:A:89:PHE:CD2	1:A:372:ILE:HD11	2.14	0.81
1:A:161:ILE:CG2	1:A:165:PHE:CD2	2.63	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:341:LEU:HD13	1:B:344:LEU:HD12	1.60	0.81
1:D:164:GLU:O	1:D:168:LEU:HD12	1.79	0.81
1:C:174:CYS:O	1:C:179:GLY:HA2	1.81	0.81
1:D:54:GLN:C	1:D:54:GLN:NE2	2.34	0.81
1:A:178:PHE:H	1:A:243:HIS:CE1	1.96	0.81
1:D:46:PRO:CD	1:D:466:TYR:CD2	2.63	0.81
1:C:472:LYS:CE	1:C:473:VAL:H	1.94	0.81
1:A:335:TYR:HD2	1:A:336:LYS:N	1.73	0.81
1:D:373:PHE:O	1:D:373:PHE:CD1	2.33	0.81
1:A:32:PRO:O	1:A:61:ARG:HB2	1.81	0.81
1:C:56:LEU:N	1:C:56:LEU:HD22	1.93	0.81
1:B:360:LEU:O	1:B:361:ALA:HB3	1.78	0.81
1:D:473:VAL:CG1	1:D:474:GLN:OE1	2.29	0.81
1:A:472:LYS:CE	1:A:472:LYS:C	2.47	0.81
1:B:172:ILE:CD1	1:B:172:ILE:N	2.43	0.81
1:B:408:PHE:CD2	1:B:408:PHE:C	2.53	0.81
1:D:177:THR:HB	1:D:288:PHE:CE1	2.16	0.81
1:B:193:VAL:CG1	1:B:289:ILE:CG2	2.59	0.81
1:C:472:LYS:C	1:C:472:LYS:NZ	2.35	0.81
1:A:404:ARG:HG3	1:A:404:ARG:NH1	1.84	0.81
1:B:151:MET:HB3	1:B:479:ARG:HH12	1.44	0.81
1:D:58:PRO:HG3	1:D:76:ARG:HH21	1.43	0.81
1:A:108:ILE:CG1	1:A:286:ASP:OD2	2.29	0.80
1:A:42:GLN:CD	4:A:613:HOH:O	2.14	0.80
1:A:420:PHE:CZ	2:A:500:HEM:HBB2	2.17	0.80
1:D:375:TYR:O	1:D:377:ILE:CD1	2.28	0.80
1:C:159:VAL:CG1	1:C:476:PHE:HE2	1.95	0.80
1:C:89:PHE:CZ	1:C:372:ILE:CD1	2.65	0.80
1:D:471:LEU:HD13	1:D:472:LYS:C	2.00	0.80
1:D:143:LEU:HD21	1:D:181:LYS:HD2	1.63	0.80
1:A:475:PRO:HB2	1:A:477:GLN:HE22	0.64	0.80
1:B:423:GLY:O	1:B:426:VAL:HG13	1.81	0.80
1:A:313:GLN:HE22	1:A:450:LEU:CB	1.95	0.80
1:B:128:LEU:CD2	1:B:287:LEU:CD2	2.60	0.80
1:B:294:THR:HG23	3:B:501:3QZ:HAA	1.62	0.80
1:D:404:ARG:HH12	1:D:407:ARG:HB3	1.46	0.80
1:C:81:ALA:HB2	1:C:372:ILE:HG13	1.63	0.80
1:D:350:GLU:CG	1:D:404:ARG:O	2.29	0.79
1:D:372:ILE:CG2	1:D:372:ILE:O	2.31	0.79
1:C:129:LEU:N	1:C:129:LEU:HD13	1.97	0.79
1:D:463:PRO:CD	1:D:471:LEU:HB3	2.08	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:409:LEU:C	1:B:411:PRO:HD3	2.03	0.79
1:B:90:ALA:HB3	1:B:113:TYR:CD1	2.16	0.79
1:B:338:ARG:HB2	4:B:601:HOH:O	1.82	0.79
1:A:286:ASP:O	1:A:290:GLY:HA3	1.81	0.79
1:C:319:GLU:O	1:C:323:GLU:HB2	1.81	0.79
1:B:386:ASN:ND2	1:B:389:GLY:H	1.81	0.79
1:C:463:PRO:CG	1:C:471:LEU:HB3	2.10	0.79
1:D:214:LEU:CD2	1:D:216:PHE:N	2.45	0.79
1:C:160:THR:CG2	1:C:477:GLN:HB2	2.12	0.79
1:D:106:GLN:HB3	1:D:279:HIS:CD2	2.17	0.79
1:C:464:ASP:N	1:C:465:PRO:HD2	1.98	0.79
1:B:30:LEU:HD11	1:B:378:PRO:HD3	1.65	0.79
1:A:80:GLU:HG3	1:A:84:ARG:HD3	1.63	0.79
1:D:106:GLN:HB2	1:D:279:HIS:ND1	1.94	0.79
1:D:374:GLY:O	1:D:375:TYR:CD2	2.36	0.79
1:A:287:LEU:HD12	1:A:287:LEU:N	1.96	0.79
1:B:288:PHE:CD2	1:B:289:ILE:HD13	2.01	0.79
1:D:447:ALA:HB3	1:D:448:PHE:CE2	2.18	0.79
1:A:285:VAL:CG1	1:A:286:ASP:N	2.45	0.78
1:D:252:TRP:CZ3	1:D:253:ARG:NH1	2.50	0.78
1:B:350:GLU:CG	1:B:404:ARG:O	2.31	0.78
1:B:62:LEU:CD2	1:B:64:LEU:N	2.47	0.78
1:A:214:LEU:O	1:A:215:ARG:HB2	1.83	0.78
1:C:313:GLN:HE21	1:C:445:LEU:HD11	1.46	0.78
1:B:244:LYS:HE2	1:B:260:LEU:HD11	1.65	0.78
1:D:463:PRO:HB3	1:D:471:LEU:HG	0.84	0.78
1:D:324:LEU:HG	1:D:340:ARG:HG3	1.66	0.78
1:B:62:LEU:CD2	1:B:63:ARG:C	2.51	0.78
1:D:214:LEU:HD23	1:D:216:PHE:N	1.99	0.78
1:B:88:ASP:C	1:B:89:PHE:HD1	1.86	0.78
1:C:372:ILE:HG22	1:C:373:PHE:N	1.95	0.78
1:A:472:LYS:NZ	1:A:472:LYS:C	2.36	0.78
1:A:62:LEU:CD2	1:A:63:ARG:N	2.37	0.78
1:D:205:ILE:HD13	1:D:205:ILE:O	1.84	0.78
1:C:472:LYS:NZ	1:C:472:LYS:CB	2.39	0.78
1:A:350:GLU:CG	1:A:404:ARG:O	2.31	0.78
1:C:38:LEU:O	1:C:41:LEU:HD12	1.84	0.78
1:C:308:HIS:CE1	1:C:458:LEU:HB2	2.19	0.78
1:A:404:ARG:HH22	1:A:414:ASN:ND2	1.80	0.78
1:D:62:LEU:HD23	1:D:63:ARG:CA	2.13	0.77
1:B:169:THR:HG22	1:B:173:ILE:CD1	2.12	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:THR:CG2	1:A:239:GLN:HG2	2.15	0.77
1:B:409:LEU:O	1:B:410:GLU:HB3	1.84	0.77
1:B:128:LEU:HD11	1:B:287:LEU:CD2	2.15	0.77
1:B:294:THR:HG22	3:B:501:3QZ:CAA	2.15	0.77
1:C:105:CYS:O	1:C:106:GLN:HB2	1.84	0.77
1:C:88:ASP:HB2	1:C:89:PHE:CE1	2.19	0.77
1:B:214:LEU:HD21	1:B:216:PHE:CA	2.14	0.77
1:C:161:ILE:HD11	1:C:474:GLN:HA	1.66	0.77
1:D:164:GLU:O	1:D:168:LEU:HD11	1.82	0.77
1:B:116:LEU:HD23	1:B:117:TRP:CA	2.15	0.77
1:D:40:LEU:C	1:D:40:LEU:HD12	1.99	0.77
1:C:38:LEU:CB	1:C:41:LEU:CD1	2.63	0.77
1:D:66:LEU:CD1	1:D:66:LEU:N	2.47	0.77
1:B:41:LEU:O	1:B:42:GLN:CB	2.32	0.77
1:C:85:LYS:HG3	1:C:88:ASP:OD2	1.83	0.77
1:A:38:LEU:O	1:A:41:LEU:CD1	2.32	0.77
1:A:372:ILE:O	1:A:372:ILE:CG2	2.32	0.77
1:D:98:TYR:CD1	1:D:110:LEU:CD1	2.67	0.76
1:B:172:ILE:H	1:B:172:ILE:HD13	1.48	0.76
1:C:408:PHE:O	1:C:408:PHE:CD1	2.35	0.76
1:C:423:GLY:O	1:C:426:VAL:CG1	2.32	0.76
1:A:30:LEU:HG	1:A:31:PRO:HD2	1.65	0.76
1:C:178:PHE:N	1:C:254:ASP:CG	2.38	0.76
1:D:98:TYR:CG	1:D:110:LEU:HD12	2.20	0.76
1:D:216:PHE:CD1	1:D:216:PHE:N	2.51	0.76
1:C:472:LYS:NZ	1:C:473:VAL:N	2.33	0.76
1:B:473:VAL:O	1:B:475:PRO:CD	2.32	0.76
1:C:128:LEU:C	1:C:129:LEU:HD12	2.06	0.76
1:B:176:LEU:HA	1:B:255:MET:HB2	1.67	0.76
1:A:373:PHE:CD1	1:A:374:GLY:N	2.52	0.76
1:B:189:PHE:HE2	1:B:288:PHE:CE2	1.97	0.76
1:D:97:SER:CB	1:D:209:ASP:OD2	2.32	0.76
1:C:116:LEU:CD2	1:C:117:TRP:N	2.49	0.76
1:A:463:PRO:HG3	1:A:471:LEU:HB2	1.65	0.76
1:D:53:THR:HG22	1:D:54:GLN:N	2.00	0.76
1:A:451:LEU:CG	1:A:452:PRO:HD2	2.10	0.76
1:C:408:PHE:C	1:C:408:PHE:HD1	1.88	0.76
1:A:178:PHE:CB	1:A:243:HIS:HE1	1.97	0.76
1:B:459:PRO:HG2	1:B:472:LYS:HZ1	1.49	0.76
1:A:332:ARG:CG	1:A:337:ASP:OD1	2.33	0.76
1:D:116:LEU:HD23	1:D:117:TRP:CA	2.15	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:168:LEU:O	1:B:172:ILE:HD13	1.84	0.76
1:C:313:GLN:HE22	1:C:450:LEU:CB	1.99	0.76
1:D:208:LEU:H	1:D:208:LEU:HD23	1.51	0.76
1:A:324:LEU:HD12	1:A:332:ARG:CG	2.13	0.76
1:B:408:PHE:CD2	1:B:408:PHE:O	2.39	0.76
1:D:461:LEU:O	1:D:462:GLN:CB	2.33	0.76
1:C:62:LEU:CD2	1:C:63:ARG:C	2.54	0.76
1:C:407:ARG:O	1:C:413:ALA:CB	2.34	0.76
1:A:196:LEU:HD23	3:A:501:3QZ:CAI	2.13	0.75
1:A:38:LEU:O	1:A:41:LEU:CG	2.34	0.75
1:C:386:ASN:ND2	1:C:389:GLY:H	1.84	0.75
1:C:473:VAL:CG1	1:C:474:GLN:OE1	2.35	0.75
1:A:214:LEU:CG	1:A:216:PHE:N	2.46	0.75
1:A:243:HIS:NE2	1:A:254:ASP:CG	2.40	0.75
1:D:372:ILE:O	1:D:373:PHE:CB	2.34	0.75
1:D:117:TRP:HZ2	1:D:425:ARG:HD3	1.49	0.75
1:D:121:LYS:HD2	1:D:428:LEU:HD21	1.68	0.75
1:A:451:LEU:O	1:A:478:VAL:HG23	1.87	0.75
1:C:116:LEU:HD23	1:C:116:LEU:O	1.85	0.75
1:D:30:LEU:HD12	1:D:31:PRO:HD2	1.68	0.75
1:A:103:GLN:O	4:A:610:HOH:O	2.02	0.75
1:D:121:LYS:HE2	1:D:428:LEU:HD23	1.67	0.75
1:D:117:TRP:HE1	1:D:425:ARG:NH1	1.84	0.75
1:C:463:PRO:HB2	1:C:465:PRO:HD2	1.69	0.75
1:D:98:TYR:CD1	1:D:110:LEU:HD12	2.22	0.75
1:A:43:PRO:CB	1:A:44:ASN:OD1	2.34	0.75
1:D:106:GLN:HB3	1:D:279:HIS:NE2	1.99	0.75
1:B:289:ILE:CD1	1:B:289:ILE:N	2.50	0.75
1:D:111:GLY:O	1:D:425:ARG:CZ	2.35	0.75
1:A:41:LEU:O	1:A:42:GLN:HB3	1.86	0.75
1:A:45:LEU:HD23	1:A:45:LEU:O	1.86	0.75
1:D:212:PRO:C	1:D:214:LEU:H	1.89	0.75
1:A:331:SER:O	1:A:333:VAL:CG2	2.35	0.75
1:D:463:PRO:HG3	1:D:471:LEU:HB2	1.59	0.75
1:D:447:ALA:HB3	1:D:448:PHE:HE2	1.51	0.75
1:A:472:LYS:CE	1:A:473:VAL:HG23	2.14	0.74
1:A:329:SER:HG	1:A:330:CYS:HG	0.76	0.74
1:C:168:LEU:HD21	1:C:296:ALA:HB2	1.68	0.74
1:B:408:PHE:CG	1:B:408:PHE:O	2.39	0.74
1:C:128:LEU:C	1:C:129:LEU:CD1	2.55	0.74
1:B:40:LEU:O	1:B:40:LEU:CD1	2.36	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:ARG:CD	1:A:337:ASP:OD1	2.35	0.74
1:B:72:LEU:C	1:B:73:ASN:ND2	2.35	0.74
1:C:181:LYS:CG	1:C:181:LYS:O	2.29	0.74
1:A:93:PRO:HD3	1:A:365:ARG:HB2	1.67	0.74
1:C:62:LEU:CD2	1:C:63:ARG:N	2.37	0.74
1:D:211:VAL:O	1:D:211:VAL:CG1	2.33	0.74
1:C:301:TRP:CZ2	1:C:472:LYS:HD2	2.22	0.74
1:D:404:ARG:O	1:D:404:ARG:CD	2.32	0.74
1:C:89:PHE:CZ	1:C:372:ILE:HD12	2.22	0.74
1:B:459:PRO:CB	1:B:472:LYS:HZ1	1.98	0.74
1:B:177:THR:O	1:B:177:THR:CG2	2.33	0.74
1:C:159:VAL:HG12	1:C:476:PHE:CZ	2.21	0.74
1:C:59:VAL:O	1:C:59:VAL:HG12	1.86	0.74
1:A:358:VAL:HG12	1:A:361:ALA:HA	1.68	0.74
1:C:159:VAL:HG23	1:C:159:VAL:O	1.86	0.74
1:C:408:PHE:C	1:C:408:PHE:CD1	2.57	0.74
1:C:447:ALA:C	1:C:448:PHE:CD2	2.60	0.74
1:B:461:LEU:HB2	4:B:604:HOH:O	1.86	0.74
1:A:285:VAL:CG1	1:A:286:ASP:OD1	2.35	0.74
1:D:214:LEU:CD2	1:D:216:PHE:HA	2.17	0.74
1:D:432:LEU:C	1:D:432:LEU:CD2	2.56	0.74
1:D:336:LYS:HG3	4:D:614:HOH:O	1.85	0.74
1:B:294:THR:HG22	3:B:501:3QZ:HAAA	1.65	0.74
1:A:50:LEU:O	1:A:53:THR:CG2	2.36	0.74
1:A:106:GLN:HG2	1:A:116:LEU:HD22	1.70	0.74
1:B:104:ARG:O	1:B:105:CYS:SG	2.45	0.74
1:B:62:LEU:HD23	1:B:63:ARG:C	2.08	0.74
1:A:62:LEU:HD23	1:A:63:ARG:CA	2.16	0.74
1:C:420:PHE:CZ	2:C:500:HEM:HBB2	2.23	0.74
1:B:252:TRP:O	1:B:254:ASP:N	2.21	0.74
1:C:102:SER:OG	1:C:105:CYS:CA	2.36	0.74
1:B:459:PRO:HB2	1:B:472:LYS:NZ	2.02	0.74
1:D:466:TYR:C	1:D:467:CYS:SG	2.66	0.73
1:D:177:THR:CG2	1:D:239:GLN:HG2	2.17	0.73
1:B:252:TRP:HB2	1:B:257:ASP:OD2	1.88	0.73
1:B:319:GLU:O	1:B:323:GLU:HB2	1.87	0.73
1:D:95:ILE:HB	1:D:96:PRO:HD2	1.70	0.73
1:B:409:LEU:CD2	1:B:409:LEU:O	2.34	0.73
1:C:30:LEU:HD11	1:C:378:PRO:HD3	1.70	0.73
1:C:151:MET:SD	1:C:163:LYS:HD2	2.29	0.73
1:D:46:PRO:HG3	1:D:466:TYR:CD2	2.19	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:110:LEU:N	1:D:110:LEU:HD23	2.03	0.73
1:D:172:ILE:HD12	1:D:172:ILE:N	2.04	0.73
1:C:297:SER:CB	1:C:357:VAL:CG2	2.67	0.73
1:B:357:VAL:HG12	1:B:469:VAL:CG1	2.19	0.73
1:B:214:LEU:CD2	1:B:216:PHE:N	2.51	0.73
1:B:214:LEU:O	1:B:217:PHE:HE1	1.69	0.73
1:C:276:LEU:CD2	1:C:277:GLU:N	2.44	0.73
1:C:101:VAL:O	1:C:101:VAL:CG2	2.36	0.73
1:C:463:PRO:CG	1:C:471:LEU:CB	2.65	0.73
1:B:73:ASN:ND2	1:B:73:ASN:N	2.33	0.73
1:B:176:LEU:CD1	1:B:287:LEU:HD22	2.19	0.73
1:B:410:GLU:OE2	1:B:411:PRO:CG	2.35	0.73
1:A:196:LEU:CD2	3:A:501:3QZ:HAI	2.17	0.73
1:A:177:THR:CG2	1:A:288:PHE:CZ	2.72	0.73
1:D:81:ALA:HB2	1:D:372:ILE:HG12	1.71	0.73
1:C:307:LEU:HB3	1:C:458:LEU:HD22	1.69	0.73
1:A:159:VAL:O	1:A:159:VAL:CG2	2.37	0.73
1:C:246:SER:HB3	1:C:252:TRP:CZ2	2.24	0.73
1:A:214:LEU:CD2	1:A:216:PHE:CA	2.63	0.73
1:B:285:VAL:HA	1:B:288:PHE:CB	2.15	0.73
1:A:40:LEU:O	1:A:40:LEU:CD1	2.35	0.73
1:A:67:GLN:CA	1:A:67:GLN:OE1	2.36	0.73
1:B:420:PHE:CZ	2:B:500:HEM:HBB2	2.24	0.73
1:B:176:LEU:O	1:B:176:LEU:CD2	2.35	0.72
1:D:205:ILE:CD1	1:D:205:ILE:O	2.37	0.72
1:D:29:HIS:HA	1:D:375:TYR:HD1	1.52	0.72
1:C:294:THR:CG2	3:C:501:3QZ:CAA	2.67	0.72
1:C:29:HIS:O	1:C:376:ASP:HB2	1.88	0.72
1:A:472:LYS:HZ3	1:A:473:VAL:N	1.83	0.72
1:B:37:PHE:CE1	1:B:63:ARG:NE	2.57	0.72
1:B:214:LEU:O	1:B:215:ARG:CG	2.37	0.72
1:D:168:LEU:HD23	1:D:292:THR:C	2.10	0.72
1:B:37:PHE:HE1	1:B:63:ARG:NE	1.87	0.72
1:A:275:LEU:CD1	1:A:275:LEU:O	2.37	0.72
1:C:472:LYS:HZ3	1:C:472:LYS:CA	2.03	0.72
1:D:46:PRO:HD3	1:D:466:TYR:CD2	2.24	0.72
1:A:373:PHE:HD1	1:A:373:PHE:O	1.71	0.72
1:C:472:LYS:HB3	1:C:472:LYS:HZ3	1.54	0.72
1:B:409:LEU:O	1:B:411:PRO:CD	2.36	0.72
1:B:459:PRO:CG	1:B:472:LYS:NZ	2.53	0.72
1:C:378:PRO:HG2	1:C:381:MET:HB2	1.69	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:215:ARG:HH21	1:D:215:ARG:HG2	1.55	0.72
1:C:161:ILE:HG12	1:C:475:PRO:HD2	1.70	0.72
1:C:38:LEU:CB	1:C:41:LEU:HD11	2.20	0.72
1:B:108:ILE:HD12	1:B:428:LEU:HD21	1.72	0.72
1:A:332:ARG:O	1:A:333:VAL:CG2	2.37	0.72
1:A:87:VAL:CG1	1:A:368:ARG:HH21	2.02	0.72
1:D:313:GLN:HE21	1:D:445:LEU:HD11	1.54	0.72
1:A:87:VAL:HG11	1:A:368:ARG:HH21	1.55	0.72
1:B:63:ARG:NH2	4:B:617:HOH:O	1.77	0.72
1:D:208:LEU:HD13	1:D:214:LEU:HD22	1.70	0.72
1:C:41:LEU:O	1:C:42:GLN:CB	2.38	0.72
1:D:407:ARG:HG3	1:D:407:ARG:NH1	1.96	0.72
1:D:193:VAL:HG22	1:D:289:ILE:HG22	1.71	0.71
1:C:53:THR:CG2	1:C:54:GLN:N	2.52	0.71
1:B:40:LEU:O	1:B:40:LEU:HD13	1.89	0.71
1:A:286:ASP:O	1:A:290:GLY:CA	2.38	0.71
1:B:285:VAL:O	1:B:289:ILE:N	2.21	0.71
1:D:196:LEU:CD2	3:D:501:3QZ:OAE	2.37	0.71
1:C:105:CYS:HB2	1:C:106:GLN:NE2	2.04	0.71
1:C:276:LEU:HD23	1:C:277:GLU:CA	2.20	0.71
1:D:432:LEU:O	1:D:432:LEU:CD2	2.36	0.71
1:D:432:LEU:C	1:D:432:LEU:HD23	2.10	0.71
1:A:461:LEU:O	1:A:461:LEU:CD2	2.36	0.71
1:B:196:LEU:HD23	3:B:501:3QZ:HAI	1.71	0.71
1:D:214:LEU:CD2	1:D:216:PHE:CD1	2.54	0.71
1:C:67:GLN:OE1	1:C:67:GLN:CA	2.36	0.71
1:B:88:ASP:C	1:B:89:PHE:CD1	2.64	0.71
1:D:62:LEU:CD2	1:D:63:ARG:N	2.38	0.71
1:B:88:ASP:HB3	1:B:89:PHE:CE1	2.26	0.71
1:D:242:ARG:NH1	1:D:242:ARG:CG	2.34	0.71
1:C:69:VAL:HG13	1:C:382:VAL:HB	1.73	0.71
1:B:127:ALA:HB1	1:B:255:MET:HG2	1.70	0.71
1:A:337:ASP:O	1:A:340:ARG:HG2	1.89	0.71
1:D:123:LEU:HD11	1:D:262:GLY:O	1.91	0.71
1:A:332:ARG:C	1:A:333:VAL:CG2	2.53	0.71
1:C:161:ILE:HD11	1:C:475:PRO:HD2	1.73	0.71
1:A:309:HIS:HE1	1:A:403:PHE:HB3	1.54	0.71
1:B:211:VAL:CG1	1:B:211:VAL:O	2.35	0.71
1:B:402:GLU:OE1	1:B:402:GLU:CA	2.33	0.71
1:B:407:ARG:CG	1:B:407:ARG:NH1	2.51	0.71
1:B:128:LEU:CG	1:B:287:LEU:CD2	2.66	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:VAL:HG11	1:A:52:LEU:CD1	2.21	0.70
1:C:449:THR:OG1	1:C:480:LEU:O	2.08	0.70
1:D:109:SER:C	1:D:110:LEU:HD22	2.11	0.70
1:B:410:GLU:HG2	1:B:410:GLU:O	1.90	0.70
1:B:418:LEU:N	1:B:418:LEU:CD1	2.36	0.70
1:D:168:LEU:HD22	1:D:292:THR:HB	1.74	0.70
1:D:172:ILE:CD1	1:D:172:ILE:N	2.54	0.70
1:D:262:GLY:O	1:D:263:VAL:HG23	1.91	0.70
1:B:394:GLU:C	1:B:394:GLU:OE1	2.29	0.70
1:A:110:LEU:HD11	3:A:501:3QZ:HAH	1.73	0.70
1:A:375:TYR:N	1:A:375:TYR:HD2	1.90	0.70
1:D:150:ARG:HD2	1:D:163:LYS:HE3	1.72	0.70
1:B:33:LEU:CD1	1:B:34:VAL:O	2.38	0.70
1:A:82:MET:HB3	1:A:422:CYS:O	1.91	0.70
1:D:466:TYR:O	1:D:467:CYS:SG	2.50	0.70
1:D:361:ALA:HB1	2:D:500:HEM:HAA2	1.73	0.70
1:A:420:PHE:CE1	2:A:500:HEM:HBB2	2.26	0.70
1:B:81:ALA:HB2	1:B:372:ILE:HG23	1.72	0.70
1:C:143:LEU:HD13	1:C:171:SER:HA	1.73	0.70
1:C:177:THR:HB	1:C:288:PHE:CE1	2.27	0.70
1:C:307:LEU:CD1	1:C:458:LEU:HD22	2.22	0.70
1:A:50:LEU:C	1:A:53:THR:HG23	2.11	0.70
1:D:121:LYS:CE	1:D:428:LEU:HD23	2.21	0.70
1:C:307:LEU:HB3	1:C:458:LEU:CD2	2.21	0.70
1:C:37:PHE:N	4:C:601:HOH:O	2.20	0.70
1:A:332:ARG:CA	1:A:332:ARG:NE	2.38	0.70
1:C:161:ILE:HD11	1:C:474:GLN:CA	2.21	0.70
1:A:313:GLN:HE22	1:A:450:LEU:HD12	1.50	0.70
1:D:101:VAL:HG12	1:D:229:ILE:HD12	1.71	0.70
1:C:31:PRO:HA	1:C:375:TYR:CD1	2.26	0.70
1:B:74:SER:OG	1:B:77:THR:OG1	2.08	0.70
1:D:109:SER:OG	1:D:110:LEU:CD2	2.39	0.69
1:B:128:LEU:CD2	1:B:287:LEU:HD21	2.21	0.69
1:D:359:PRO:O	1:D:387:LEU:HB2	1.92	0.69
1:A:275:LEU:CD1	1:A:275:LEU:C	2.59	0.69
1:C:40:LEU:C	1:C:40:LEU:CD1	2.52	0.69
1:C:447:ALA:HB3	1:C:448:PHE:CD2	2.27	0.69
1:D:377:ILE:CG2	1:D:378:PRO:HD2	2.22	0.69
1:A:160:THR:CG2	1:A:164:GLU:OE1	2.41	0.69
1:A:64:LEU:HD22	3:A:502:3QZ:CAB	2.21	0.69
1:C:165:PHE:O	1:C:168:LEU:CD1	2.39	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:214:LEU:HD23	1:B:216:PHE:N	2.08	0.69
1:A:128:LEU:HD21	1:A:287:LEU:HD23	1.74	0.69
1:B:244:LYS:HG2	1:B:260:LEU:HD21	1.74	0.69
1:D:319:GLU:O	1:D:323:GLU:HB2	1.91	0.69
1:B:69:VAL:HG22	1:B:382:VAL:CG2	2.22	0.69
1:B:426:VAL:O	1:B:427:CYS:HB2	1.91	0.69
1:A:283:SER:O	1:A:287:LEU:HD12	1.93	0.69
1:C:307:LEU:HB3	1:C:458:LEU:HD13	1.74	0.69
1:C:426:VAL:O	1:C:427:CYS:HB2	1.92	0.69
1:B:340:ARG:HH21	1:C:340:ARG:HH21	1.38	0.69
1:C:313:GLN:NE2	1:C:450:LEU:HB2	2.08	0.69
1:C:309:HIS:HD1	1:C:403:PHE:HD2	1.39	0.69
1:A:43:PRO:C	1:A:44:ASN:OD1	2.30	0.69
1:D:459:PRO:HB3	1:D:473:VAL:HB	1.75	0.69
1:C:161:ILE:CD1	1:C:475:PRO:HD2	2.23	0.69
1:C:342:PRO:HG2	1:C:343:LEU:H	1.58	0.69
1:A:475:PRO:HG3	4:A:605:HOH:O	1.92	0.69
1:C:45:LEU:HD21	1:C:64:LEU:HD21	1.75	0.69
1:B:174:CYS:O	1:B:179:GLY:CA	2.34	0.69
1:B:180:ASN:ND2	1:B:185:LEU:HD13	2.08	0.69
1:B:307:LEU:HD21	1:B:477:GLN:HG3	1.73	0.69
1:B:459:PRO:HB2	1:B:472:LYS:HZ1	1.55	0.69
1:D:104:ARG:O	1:D:105:CYS:HB2	1.92	0.69
1:D:425:ARG:O	1:D:426:VAL:C	2.30	0.69
1:B:216:PHE:CD2	1:B:216:PHE:N	2.53	0.69
1:A:185:LEU:HD11	1:A:239:GLN:HE22	1.58	0.69
1:B:301:TRP:CE3	1:B:472:LYS:HD3	2.28	0.69
1:C:357:VAL:HG12	1:C:358:VAL:N	2.08	0.69
1:B:136:MET:SD	1:B:175:TYR:CD2	2.86	0.69
1:C:101:VAL:HG21	3:C:501:3QZ:HAG	1.75	0.69
1:D:212:PRO:O	1:D:216:PHE:HE1	1.77	0.68
1:D:376:ASP:O	1:D:377:ILE:HD12	1.94	0.68
1:C:418:LEU:HD13	1:C:418:LEU:O	1.94	0.68
1:C:276:LEU:HD23	1:C:278:GLY:H	1.54	0.68
1:D:471:LEU:HD13	1:D:472:LYS:CA	2.22	0.68
1:B:151:MET:HB3	1:B:479:ARG:NH1	2.08	0.68
1:A:78:ILE:HD11	1:A:385:PRO:HB2	1.74	0.68
1:A:294:THR:HG21	3:A:501:3QZ:HAAA	0.69	0.68
1:C:46:PRO:HB2	1:C:388:GLN:HG2	1.74	0.68
1:A:177:THR:HG21	1:A:288:PHE:CZ	2.27	0.68
1:C:408:PHE:O	1:C:409:LEU:HB2	1.91	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:301:TRP:CE2	1:C:472:LYS:HD2	2.28	0.68
1:A:461:LEU:C	1:A:462:GLN:HG2	2.04	0.68
1:A:472:LYS:HZ3	1:A:472:LYS:HB3	1.58	0.68
1:C:34:VAL:HG11	1:C:52:LEU:HD13	1.75	0.68
1:C:313:GLN:HE21	1:C:445:LEU:CD1	2.07	0.68
1:C:62:LEU:HD23	1:C:63:ARG:C	2.12	0.68
1:B:128:LEU:HD13	1:B:428:LEU:O	1.94	0.68
1:A:41:LEU:O	1:A:42:GLN:CB	2.42	0.68
1:D:350:GLU:HG3	1:D:404:ARG:C	2.14	0.68
1:A:313:GLN:NE2	1:A:450:LEU:CB	2.56	0.68
1:C:161:ILE:HD11	1:C:475:PRO:CD	2.24	0.68
1:D:447:ALA:O	1:D:481:GLN:HB3	1.93	0.68
1:D:462:GLN:CD	1:D:466:TYR:OH	2.32	0.68
1:C:167:LEU:CD2	1:C:167:LEU:O	2.37	0.68
1:C:159:VAL:HG13	1:C:476:PHE:CE2	2.29	0.68
1:A:280:VAL:O	1:A:284:VAL:HG23	1.94	0.68
1:D:252:TRP:HB2	1:D:257:ASP:CG	2.14	0.68
1:C:147:PHE:O	1:C:151:MET:HG2	1.94	0.68
1:A:44:ASN:N	1:A:44:ASN:OD1	2.26	0.67
1:A:284:VAL:HG12	1:A:288:PHE:HB2	1.75	0.67
1:B:360:LEU:O	1:B:361:ALA:CB	2.42	0.67
1:C:472:LYS:NZ	1:C:472:LYS:CA	2.57	0.67
1:C:38:LEU:CB	1:C:41:LEU:HD12	2.24	0.67
1:B:396:VAL:CG1	1:B:397:TRP:CD2	2.74	0.67
1:B:31:PRO:HG2	1:B:61:ARG:HG3	1.76	0.67
1:D:106:GLN:CG	1:D:116:LEU:HD11	2.23	0.67
1:A:252:TRP:HB2	1:A:257:ASP:CB	2.25	0.67
1:A:45:LEU:N	1:A:46:PRO:HD2	2.09	0.67
1:D:473:VAL:HG13	1:D:474:GLN:OE1	1.94	0.67
1:D:108:ILE:CD1	1:D:124:THR:HG21	2.24	0.67
1:C:470:ASN:OD1	1:C:470:ASN:C	2.33	0.67
1:C:472:LYS:NZ	1:C:473:VAL:O	2.27	0.67
1:A:168:LEU:CD2	1:A:292:THR:O	2.43	0.67
1:A:130:LEU:HD13	1:A:134:SER:O	1.95	0.67
1:D:117:TRP:CZ2	1:D:425:ARG:CD	2.77	0.67
1:C:42:GLN:HG3	1:C:43:PRO:HD2	1.76	0.67
1:C:46:PRO:HG3	1:C:466:TYR:CZ	2.30	0.67
1:D:56:LEU:N	1:D:56:LEU:CD2	2.57	0.67
1:B:192:CYS:O	1:B:196:LEU:HB2	1.95	0.67
1:C:161:ILE:HD13	1:C:474:GLN:HA	1.77	0.67
1:D:214:LEU:CD2	1:D:216:PHE:CA	2.72	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:459:PRO:HD3	1:D:475:PRO:HB3	1.77	0.67
1:A:464:ASP:N	1:A:465:PRO:HD2	2.10	0.67
1:C:297:SER:CB	1:C:357:VAL:HG21	2.17	0.67
1:B:252:TRP:HB2	1:B:257:ASP:CG	2.15	0.67
1:D:62:LEU:CD2	1:D:64:LEU:N	2.58	0.67
1:A:37:PHE:C	1:A:38:LEU:HD23	2.11	0.67
1:A:38:LEU:O	1:A:41:LEU:HD11	1.95	0.67
1:B:104:ARG:C	1:B:105:CYS:SG	2.73	0.67
1:A:309:HIS:CE1	1:A:403:PHE:HB3	2.29	0.67
1:C:178:PHE:C	1:C:254:ASP:OD1	2.32	0.67
1:C:244:LYS:HG2	1:C:260:LEU:HD21	1.77	0.67
1:D:203:TRP:HA	1:D:206:GLN:CB	2.23	0.67
1:C:386:ASN:HD21	1:C:389:GLY:H	1.40	0.67
1:B:313:GLN:HE21	1:B:445:LEU:HD12	1.60	0.67
1:D:38:LEU:CD1	1:D:41:LEU:HD11	2.25	0.67
1:A:177:THR:HG22	1:A:239:GLN:HG2	1.76	0.67
1:D:168:LEU:HD22	1:D:292:THR:CB	2.25	0.66
1:D:404:ARG:NH1	1:D:407:ARG:HB3	2.09	0.66
1:C:387:LEU:HD22	1:C:418:LEU:HD13	1.77	0.66
1:C:89:PHE:CD1	1:C:89:PHE:N	2.61	0.66
1:B:301:TRP:CZ3	1:B:472:LYS:HD3	2.30	0.66
1:B:169:THR:O	1:B:173:ILE:CD1	2.43	0.66
1:B:178:PHE:H	1:B:254:ASP:HB2	1.61	0.66
1:D:418:LEU:HD22	1:D:422:CYS:SG	2.35	0.66
1:A:449:THR:O	1:A:450:LEU:HB2	1.96	0.66
1:C:101:VAL:HG23	1:C:232:ARG:NH2	2.10	0.66
1:A:357:VAL:CG1	1:A:469:VAL:CG1	2.69	0.66
1:D:117:TRP:CE2	1:D:425:ARG:CZ	2.79	0.66
1:C:276:LEU:HD21	1:C:278:GLY:N	2.05	0.66
1:C:473:VAL:HG13	1:C:474:GLN:OE1	1.94	0.66
1:A:214:LEU:HD21	1:A:216:PHE:N	2.04	0.66
1:B:409:LEU:C	1:B:411:PRO:CD	2.63	0.66
1:D:248:VAL:HG23	1:D:249:ALA:N	2.09	0.66
1:A:423:GLY:O	1:A:426:VAL:N	2.27	0.66
1:C:178:PHE:CA	1:C:254:ASP:CG	2.63	0.66
1:D:211:VAL:O	1:D:214:LEU:HB3	1.96	0.66
1:C:474:GLN:CD	1:C:474:GLN:O	2.33	0.66
1:A:178:PHE:N	1:A:243:HIS:HE1	1.83	0.66
1:A:243:HIS:NE2	1:A:254:ASP:OD1	2.29	0.66
1:A:338:ARG:O	1:A:338:ARG:HG2	1.94	0.66
1:D:192:CYS:O	1:D:196:LEU:HB2	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:471:LEU:HD13	1:D:472:LYS:O	1.96	0.66
1:D:56:LEU:HD22	1:D:56:LEU:H	1.60	0.66
1:C:219:ASN:CG	1:C:220:PRO:HD2	2.15	0.66
1:C:89:PHE:CE2	1:C:372:ILE:HD13	2.31	0.66
1:C:192:CYS:O	1:C:196:LEU:HB2	1.96	0.66
1:C:196:LEU:HD11	1:C:229:ILE:HA	1.77	0.66
1:B:246:SER:HB3	1:B:252:TRP:CH2	2.31	0.66
1:A:174:CYS:O	1:A:179:GLY:HA2	1.96	0.66
1:B:357:VAL:O	1:B:470:ASN:HB3	1.95	0.66
1:A:459:PRO:O	1:A:460:SER:CB	2.44	0.66
1:A:472:LYS:HE3	1:A:473:VAL:CG2	2.17	0.66
1:A:40:LEU:C	1:A:40:LEU:CD1	2.63	0.66
1:B:200:TRP:HD1	1:B:225:LEU:HD11	1.61	0.66
1:A:374:GLY:C	1:A:375:TYR:CD2	2.69	0.66
1:C:219:ASN:OD1	1:C:220:PRO:CD	2.34	0.66
1:C:203:TRP:O	1:C:207:ILE:HG13	1.96	0.66
1:D:176:LEU:HG	1:D:255:MET:SD	2.36	0.66
1:D:44:ASN:HB3	1:D:47:ILE:HG12	1.77	0.65
1:A:285:VAL:HG12	1:A:286:ASP:N	2.11	0.65
1:B:180:ASN:OD1	1:B:182:GLU:HB2	1.95	0.65
1:C:276:LEU:HD23	1:C:278:GLY:N	2.08	0.65
1:C:307:LEU:HB3	1:C:458:LEU:CD1	2.25	0.65
1:D:72:LEU:HD11	1:D:372:ILE:HD11	1.77	0.65
1:D:462:GLN:HG2	1:D:463:PRO:HD2	1.78	0.65
1:B:176:LEU:CD2	1:B:176:LEU:C	2.62	0.65
1:A:354:LEU:O	1:A:355:ARG:HD2	1.96	0.65
1:A:87:VAL:CB	1:A:368:ARG:HH21	2.10	0.65
1:D:392:LEU:HA	1:D:400:PRO:HB2	1.77	0.65
1:A:245:GLU:OE1	1:A:246:SER:N	2.29	0.65
1:B:121:LYS:HD2	1:B:428:LEU:HD22	1.77	0.65
1:C:444:LEU:HD22	1:C:450:LEU:HD11	1.79	0.65
1:A:192:CYS:O	1:A:196:LEU:HB2	1.96	0.65
1:B:189:PHE:CZ	1:B:288:PHE:CZ	2.66	0.65
1:A:313:GLN:HE22	1:A:450:LEU:HB3	1.62	0.65
1:B:161:ILE:HD12	1:B:161:ILE:H	1.61	0.65
1:D:169:THR:HG21	1:D:190:HIS:HB2	1.78	0.65
1:C:277:GLU:O	1:C:280:VAL:HB	1.96	0.65
1:C:38:LEU:HB3	1:C:41:LEU:HD11	1.77	0.65
1:C:464:ASP:N	1:C:465:PRO:CD	2.60	0.65
1:A:69:VAL:HG13	1:A:382:VAL:HB	1.78	0.65
1:A:333:VAL:HA	4:A:622:HOH:O	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:420:PHE:CE1	2:D:500:HEM:HBB2	2.30	0.65
1:A:294:THR:CG2	3:A:501:3QZ:HAAB	2.16	0.65
1:B:89:PHE:CE2	1:B:372:ILE:CD1	2.77	0.65
1:D:376:ASP:N	1:D:376:ASP:OD1	2.28	0.65
1:D:448:PHE:HD1	1:D:479:ARG:HB3	1.62	0.65
1:C:324:LEU:HG	1:C:340:ARG:HG3	1.76	0.65
1:A:97:SER:HB2	1:A:209:ASP:OD1	1.95	0.65
1:B:284:VAL:HG12	1:B:288:PHE:CG	2.30	0.65
1:D:33:LEU:HD22	1:D:34:VAL:H	1.61	0.65
1:D:52:LEU:O	1:D:56:LEU:CD2	2.37	0.65
1:A:404:ARG:HH11	1:A:404:ARG:HG2	1.58	0.65
1:D:172:ILE:CD1	1:D:172:ILE:H	2.10	0.64
1:D:121:LYS:CE	1:D:428:LEU:CD2	2.75	0.64
1:C:420:PHE:CE1	2:C:500:HEM:HBB2	2.30	0.64
1:A:38:LEU:N	4:A:601:HOH:O	2.22	0.64
1:D:426:VAL:HG23	1:D:427:CYS:H	1.62	0.64
1:A:108:ILE:CD1	1:A:124:THR:HG21	2.26	0.64
1:A:429:GLY:HA3	2:A:500:HEM:HBC2	1.78	0.64
1:A:52:LEU:N	1:A:52:LEU:HD23	2.12	0.64
1:D:252:TRP:CE3	1:D:253:ARG:CD	2.78	0.64
1:B:289:ILE:HD12	1:B:289:ILE:N	2.02	0.64
1:B:31:PRO:HG2	1:B:61:ARG:CG	2.28	0.64
1:C:358:VAL:HG11	2:C:500:HEM:C4A	2.33	0.64
1:D:208:LEU:N	1:D:208:LEU:CD2	2.60	0.64
1:A:337:ASP:OD2	1:A:337:ASP:N	2.30	0.64
1:C:473:VAL:HG12	1:C:474:GLN:OE1	1.97	0.64
1:A:353:ARG:NH2	1:A:404:ARG:HD3	2.12	0.64
1:B:473:VAL:CG1	1:B:474:GLN:N	2.60	0.64
1:D:357:VAL:HG13	1:D:469:VAL:HG13	1.77	0.64
1:C:171:SER:HB3	1:C:175:TYR:OH	1.97	0.64
1:D:44:ASN:OD1	1:D:462:GLN:NE2	2.31	0.64
1:B:286:ASP:O	1:B:290:GLY:N	2.31	0.64
1:A:89:PHE:CE2	1:A:372:ILE:CG1	2.81	0.64
1:B:41:LEU:H	1:B:41:LEU:CD2	1.93	0.64
1:A:404:ARG:NH1	1:A:406:ASP:O	2.31	0.64
1:B:141:ASP:HA	1:B:439:VAL:HG11	1.80	0.64
1:B:324:LEU:HD22	1:C:336:LYS:HE2	1.78	0.64
1:A:205:ILE:HG13	1:A:225:LEU:HD13	1.78	0.64
1:B:285:VAL:CA	1:B:288:PHE:CB	2.74	0.64
1:D:62:LEU:CD2	1:D:63:ARG:C	2.66	0.64
1:A:333:VAL:HG11	1:A:443:ARG:NH1	2.12	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:372:ILE:HG23	1:D:372:ILE:O	1.98	0.64
1:B:112:ASP:CG	1:B:365:ARG:NH2	2.50	0.64
1:D:110:LEU:N	1:D:110:LEU:HD22	2.13	0.64
1:D:38:LEU:CB	1:D:41:LEU:CD1	2.74	0.64
1:C:263:VAL:HG13	1:C:275:LEU:O	1.98	0.64
1:C:275:LEU:HD12	1:C:275:LEU:O	1.96	0.64
1:C:162:GLN:HE22	1:C:165:PHE:HB3	1.60	0.64
1:A:211:VAL:O	1:A:214:LEU:HB3	1.98	0.64
1:A:214:LEU:HD23	1:A:216:PHE:CD2	2.32	0.64
1:A:406:ASP:OD1	1:A:406:ASP:N	2.31	0.64
1:D:168:LEU:CD2	1:D:292:THR:C	2.66	0.64
1:C:38:LEU:HB3	1:C:41:LEU:HD12	1.76	0.64
1:C:62:LEU:HD21	1:C:64:LEU:N	2.12	0.64
1:C:279:HIS:ND1	4:C:608:HOH:O	2.29	0.64
1:D:430:GLU:OE1	1:D:434:ARG:NH1	2.29	0.64
1:A:477:GLN:OE1	1:A:477:GLN:N	2.31	0.64
1:B:40:LEU:C	1:B:40:LEU:CD1	2.66	0.64
1:B:172:ILE:O	1:B:176:LEU:HB3	1.98	0.64
1:D:53:THR:CG2	1:D:54:GLN:N	2.60	0.64
1:C:472:LYS:CE	1:C:472:LYS:C	2.66	0.64
1:A:214:LEU:CD2	1:A:216:PHE:HA	2.19	0.64
1:A:104:ARG:C	1:A:105:CYS:SG	2.74	0.64
1:D:202:HIS:O	1:D:206:GLN:N	2.30	0.63
1:A:74:SER:O	1:A:78:ILE:HG22	1.98	0.63
1:A:86:TRP:CH2	1:A:424:ALA:HA	2.34	0.63
1:A:193:VAL:CG2	1:A:289:ILE:HG22	2.18	0.63
1:D:30:LEU:CD1	1:D:31:PRO:HD2	2.28	0.63
1:A:42:GLN:OE1	1:A:48:HIS:ND1	2.32	0.63
1:D:196:LEU:HD21	1:D:232:ARG:HD3	1.80	0.63
1:C:226:LYS:O	1:C:229:ILE:HG22	1.99	0.63
1:B:136:MET:HE1	4:B:602:HOH:O	1.97	0.63
1:B:30:LEU:CG	1:B:31:PRO:HD2	2.27	0.63
1:C:38:LEU:N	4:C:601:HOH:O	2.29	0.63
1:A:116:LEU:HD11	1:A:279:HIS:NE2	2.14	0.63
1:C:137:GLU:H	1:C:138:PRO:HD2	1.63	0.63
1:B:354:LEU:O	1:B:355:ARG:HD2	1.98	0.63
1:B:62:LEU:CD2	1:B:63:ARG:N	2.37	0.63
1:D:215:ARG:HB3	1:D:217:PHE:CD1	2.33	0.63
1:C:472:LYS:HE2	1:C:472:LYS:C	2.18	0.63
1:A:178:PHE:HD2	1:A:243:HIS:CE1	2.17	0.63
1:D:173:ILE:HD12	1:D:186:VAL:HG13	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:185:LEU:HD11	1:D:239:GLN:NE2	2.13	0.63
1:D:288:PHE:HB3	1:D:289:ILE:HD13	1.80	0.63
1:C:37:PHE:CA	4:C:601:HOH:O	2.45	0.63
1:A:335:TYR:CD2	1:A:336:LYS:CA	2.81	0.63
1:D:158:PRO:HD2	1:D:477:GLN:O	1.98	0.63
1:A:34:VAL:HG11	1:A:52:LEU:HD13	1.79	0.63
1:B:464:ASP:N	1:B:465:PRO:CD	2.61	0.63
1:C:239:GLN:HG3	1:C:243:HIS:CE1	2.34	0.63
1:A:331:SER:O	1:A:333:VAL:HG23	1.99	0.63
1:C:459:PRO:O	1:C:460:SER:HB3	1.99	0.63
1:D:370:SER:OG	1:D:371:SER:N	2.31	0.63
1:A:116:LEU:HD21	1:A:279:HIS:NE2	2.13	0.63
1:A:38:LEU:CD2	1:A:65:GLY:O	2.47	0.63
1:B:69:VAL:HG22	1:B:382:VAL:HG23	1.80	0.63
1:A:248:VAL:HG23	1:A:249:ALA:N	2.14	0.63
1:B:284:VAL:HG12	1:B:288:PHE:HD1	1.30	0.63
1:C:159:VAL:CG1	1:C:476:PHE:CZ	2.81	0.63
1:D:54:GLN:CD	1:D:55:LYS:N	2.52	0.63
1:A:475:PRO:HG2	1:A:477:GLN:NE2	2.14	0.62
1:D:37:PHE:O	1:D:38:LEU:HD23	1.99	0.62
1:D:56:LEU:CD2	1:D:56:LEU:H	2.11	0.62
1:D:215:ARG:CB	1:D:217:PHE:CE1	2.73	0.62
1:D:410:GLU:HB3	1:D:411:PRO:C	2.20	0.62
1:A:214:LEU:HD21	1:A:216:PHE:CG	2.33	0.62
1:D:117:TRP:CE2	1:D:425:ARG:NH1	2.67	0.62
1:B:176:LEU:HD11	1:B:287:LEU:CB	2.27	0.62
1:D:66:LEU:O	1:D:67:GLN:NE2	2.31	0.62
1:A:89:PHE:CE2	1:A:372:ILE:CD1	2.80	0.62
1:C:307:LEU:CB	1:C:458:LEU:HD22	2.28	0.62
1:B:461:LEU:O	1:B:462:GLN:HB3	1.98	0.62
1:A:477:GLN:CD	1:A:477:GLN:N	2.51	0.62
1:C:429:GLY:HA3	2:C:500:HEM:HBC2	1.82	0.62
1:D:406:ASP:N	1:D:406:ASP:OD1	2.31	0.62
1:C:238:LYS:HE2	1:C:238:LYS:HA	1.80	0.62
1:D:204:SER:OG	1:D:221:GLY:HA3	1.98	0.62
1:A:462:GLN:CB	1:A:466:TYR:OH	2.46	0.62
1:B:193:VAL:HG13	1:B:289:ILE:HG21	1.77	0.62
1:A:64:LEU:HD12	1:A:69:VAL:HB	1.81	0.62
1:C:391:HIS:NE2	1:C:418:LEU:HD12	2.14	0.62
1:B:61:ARG:NH1	1:B:68:GLU:OE1	2.32	0.62
1:B:97:SER:HB2	1:B:209:ASP:OD2	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:214:LEU:C	1:B:215:ARG:HG3	2.19	0.62
1:B:61:ARG:NH1	1:B:68:GLU:OE2	2.32	0.62
1:A:463:PRO:HB2	1:A:465:PRO:HD2	1.80	0.62
1:B:243:HIS:O	1:B:247:MET:HB2	2.00	0.62
1:B:88:ASP:CB	1:B:89:PHE:CE1	2.82	0.62
1:D:232:ARG:HH11	3:D:501:3QZ:CAQ	2.09	0.62
1:A:85:LYS:HE3	1:A:371:SER:O	1.99	0.62
1:C:406:ASP:OD1	1:C:406:ASP:N	2.31	0.62
1:D:46:PRO:CD	1:D:466:TYR:CE2	2.82	0.62
1:D:109:SER:C	1:D:110:LEU:CD2	2.67	0.62
1:C:474:GLN:N	1:C:474:GLN:OE1	2.33	0.62
1:D:313:GLN:CD	1:D:449:THR:O	2.37	0.62
1:C:165:PHE:O	1:C:168:LEU:HD11	1.99	0.62
1:B:357:VAL:CG1	1:B:469:VAL:CG1	2.77	0.62
1:A:71:VAL:O	1:A:72:LEU:HD23	1.99	0.62
1:A:396:VAL:HG13	1:A:415:PRO:HG2	1.80	0.62
1:B:112:ASP:OD2	1:B:365:ARG:CZ	2.47	0.62
1:C:425:ARG:C	4:C:606:HOH:O	2.36	0.61
1:C:241:ARG:HA	1:C:244:LYS:HB2	1.80	0.61
1:A:332:ARG:NH1	1:A:337:ASP:OD1	2.32	0.61
1:B:41:LEU:O	1:B:42:GLN:HB3	1.99	0.61
1:B:301:TRP:CD2	1:B:472:LYS:HD3	2.35	0.61
1:A:423:GLY:H	1:A:426:VAL:CG1	2.12	0.61
1:C:161:ILE:CD1	1:C:474:GLN:CA	2.78	0.61
1:C:214:LEU:H	1:C:214:LEU:HD23	1.65	0.61
1:B:473:VAL:HG12	1:B:474:GLN:N	2.14	0.61
1:A:106:GLN:O	1:A:107:ASP:CB	2.43	0.61
1:D:55:LYS:HG3	1:D:56:LEU:HD23	1.81	0.61
1:C:162:GLN:O	1:C:162:GLN:NE2	2.33	0.61
1:D:353:ARG:HH12	1:D:400:PRO:HA	1.65	0.61
1:A:423:GLY:C	1:A:426:VAL:H	2.04	0.61
1:C:53:THR:O	1:C:57:GLY:N	2.31	0.61
1:A:298:THR:OG1	1:A:357:VAL:CG2	2.48	0.61
1:D:447:ALA:C	1:D:481:GLN:HB3	2.20	0.61
1:B:136:MET:SD	1:B:175:TYR:HD2	2.24	0.61
1:B:61:ARG:HH11	1:B:68:GLU:CD	2.02	0.61
1:D:62:LEU:HD23	1:D:63:ARG:C	2.21	0.61
1:D:72:LEU:CD1	1:D:372:ILE:CD1	2.78	0.61
1:B:151:MET:HE1	1:B:163:LYS:HG3	1.83	0.61
1:C:392:LEU:HD23	1:C:401:HIS:NE2	2.16	0.61
1:D:53:THR:O	1:D:57:GLY:N	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:211:VAL:HG12	1:B:214:LEU:HB2	1.83	0.61
1:D:202:HIS:O	1:D:205:ILE:CG2	2.33	0.61
1:B:304:ALA:CB	1:B:472:LYS:HE3	2.31	0.61
1:D:161:ILE:HD12	1:D:161:ILE:H	1.66	0.61
1:D:461:LEU:CD2	1:D:462:GLN:O	2.33	0.61
1:A:38:LEU:HB2	1:A:41:LEU:HD21	1.81	0.61
1:D:448:PHE:CD1	1:D:479:ARG:O	2.53	0.61
1:D:104:ARG:O	1:D:105:CYS:CB	2.48	0.61
1:A:46:PRO:HB2	1:A:388:GLN:HG2	1.83	0.61
1:D:212:PRO:C	1:D:214:LEU:N	2.54	0.61
1:C:307:LEU:CB	1:C:458:LEU:HD13	2.31	0.61
1:A:358:VAL:HG11	1:A:361:ALA:HA	1.81	0.61
1:D:341:LEU:HD13	1:D:344:LEU:HD12	1.82	0.61
1:B:185:LEU:HD11	1:B:239:GLN:NE2	2.15	0.61
1:B:470:ASN:OD1	1:B:470:ASN:C	2.39	0.61
1:C:275:LEU:HD12	1:C:275:LEU:C	2.19	0.61
1:C:447:ALA:C	1:C:448:PHE:HD2	2.03	0.61
1:A:147:PHE:O	1:A:151:MET:HG2	2.01	0.60
1:C:45:LEU:N	1:C:46:PRO:HD2	2.15	0.60
1:B:205:ILE:HD13	1:B:205:ILE:O	2.01	0.60
1:D:463:PRO:CB	1:D:471:LEU:HD12	2.27	0.60
1:D:470:ASN:OD1	1:D:471:LEU:N	2.35	0.60
1:C:56:LEU:HD23	1:C:56:LEU:N	2.16	0.60
1:B:286:ASP:OD2	1:B:286:ASP:N	2.32	0.60
1:C:177:THR:CG2	1:C:239:GLN:HG2	2.32	0.60
1:C:472:LYS:HB3	1:C:472:LYS:NZ	2.13	0.60
1:D:196:LEU:CD2	3:D:501:3QZ:CAI	2.67	0.60
1:A:212:PRO:C	1:A:214:LEU:H	2.03	0.60
1:B:459:PRO:HG2	1:B:472:LYS:NZ	2.14	0.60
1:D:135:SER:O	1:D:138:PRO:HD2	2.00	0.60
1:B:169:THR:O	1:B:173:ILE:HD11	2.01	0.60
1:D:216:PHE:HD1	1:D:216:PHE:N	1.95	0.60
1:A:334:THR:HG23	1:A:335:TYR:N	2.15	0.60
1:C:104:ARG:O	1:C:105:CYS:CB	2.49	0.60
1:A:199:THR:O	1:A:225:LEU:HD12	2.00	0.60
1:D:463:PRO:CB	1:D:471:LEU:CD1	2.55	0.60
1:A:64:LEU:HD22	3:A:502:3QZ:HABA	1.83	0.60
1:D:36:GLY:O	1:D:63:ARG:HD3	2.01	0.60
1:D:81:ALA:HB2	1:D:372:ILE:CG1	2.31	0.60
1:D:72:LEU:HD21	1:D:372:ILE:HD12	1.84	0.60
1:C:196:LEU:HD21	1:C:232:ARG:HD3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:97:SER:HB2	1:C:209:ASP:OD1	2.01	0.60
1:D:98:TYR:CG	1:D:110:LEU:CD1	2.85	0.60
1:B:280:VAL:O	1:B:284:VAL:HG23	2.02	0.60
1:C:391:HIS:NE2	1:C:418:LEU:CD1	2.65	0.60
1:A:423:GLY:H	1:A:426:VAL:HG13	1.67	0.60
1:A:147:PHE:CE2	1:A:163:LYS:HB3	2.37	0.60
1:A:38:LEU:HD21	1:A:66:LEU:HD12	1.82	0.60
1:D:212:PRO:O	1:D:216:PHE:CE1	2.55	0.60
1:A:243:HIS:NE2	1:A:254:ASP:OD2	2.35	0.60
1:A:161:ILE:O	1:A:165:PHE:CB	2.43	0.60
1:C:31:PRO:HB3	1:C:375:TYR:HD1	1.65	0.60
1:C:108:ILE:HD11	1:C:121:LYS:HD2	1.83	0.60
1:A:34:VAL:HG21	1:A:62:LEU:HG	1.83	0.60
1:A:49:LEU:O	1:A:60:TYR:OH	2.19	0.60
1:B:216:PHE:HD2	1:B:216:PHE:N	1.97	0.60
1:D:214:LEU:O	1:D:215:ARG:HB2	2.02	0.60
1:A:171:SER:O	1:A:175:TYR:CD1	2.54	0.60
1:A:104:ARG:O	1:A:105:CYS:CB	2.50	0.60
1:D:205:ILE:CG2	1:D:206:GLN:N	2.64	0.60
1:C:40:LEU:O	1:C:40:LEU:CD1	2.37	0.60
1:A:178:PHE:CD2	1:A:243:HIS:CE1	2.90	0.60
1:C:418:LEU:O	1:C:418:LEU:CD1	2.49	0.60
1:D:410:GLU:H	1:D:412:GLY:H	1.50	0.60
1:D:50:LEU:O	1:D:53:THR:HB	2.00	0.60
1:C:243:HIS:HD1	1:C:256:THR:HG21	1.67	0.60
1:A:331:SER:O	1:A:333:VAL:HG22	2.02	0.60
1:D:248:VAL:CG2	1:D:249:ALA:N	2.65	0.60
1:D:279:HIS:ND1	4:D:604:HOH:O	2.25	0.59
1:A:214:LEU:O	1:A:215:ARG:CB	2.50	0.59
1:C:124:THR:HG23	1:C:428:LEU:HD11	1.85	0.59
1:D:252:TRP:CZ3	1:D:253:ARG:NE	2.69	0.59
1:D:374:GLY:O	1:D:375:TYR:CB	2.49	0.59
1:B:78:ILE:HD11	1:B:385:PRO:HB2	1.84	0.59
1:B:324:LEU:HD13	1:C:336:LYS:HG2	1.84	0.59
1:C:83:ILE:HG13	1:C:422:CYS:SG	2.42	0.59
1:D:276:LEU:HG	1:D:277:GLU:N	2.15	0.59
1:B:469:VAL:HG22	3:B:501:3QZ:HAAB	1.85	0.59
1:C:177:THR:HG23	1:C:239:GLN:HG2	1.84	0.59
1:B:88:ASP:HB3	1:B:89:PHE:HE1	1.66	0.59
1:B:386:ASN:C	1:B:386:ASN:HD22	2.06	0.59
1:D:304:ALA:HA	1:D:307:LEU:HD12	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:301:TRP:CZ3	1:D:460:SER:HA	2.37	0.59
1:D:173:ILE:HA	1:D:288:PHE:HE1	1.65	0.59
1:D:425:ARG:HB3	2:D:500:HEM:O2D	2.03	0.59
1:A:160:THR:HG22	1:A:164:GLU:OE1	2.02	0.59
1:D:55:LYS:CD	1:D:56:LEU:HD22	2.23	0.59
1:B:205:ILE:HG13	1:B:225:LEU:HD12	1.83	0.59
1:D:211:VAL:O	1:D:214:LEU:CB	2.50	0.59
1:B:346:ALA:HB2	1:B:408:PHE:CD1	2.37	0.59
1:B:399:GLN:OE1	1:B:404:ARG:NH1	2.34	0.59
1:C:30:LEU:HD12	1:C:376:ASP:O	2.03	0.59
1:C:303:VAL:HG13	1:C:450:LEU:HD21	1.82	0.59
1:B:96:PRO:HG2	1:B:209:ASP:OD1	2.01	0.59
1:B:178:PHE:H	1:B:254:ASP:CB	2.14	0.59
1:B:463:PRO:HB2	1:B:465:PRO:HD2	1.83	0.59
1:A:324:LEU:HG	1:A:340:ARG:HG3	1.84	0.59
1:C:418:LEU:N	1:C:418:LEU:CD1	2.38	0.59
1:B:308:HIS:CE1	1:B:458:LEU:HB2	2.38	0.59
1:B:387:LEU:HD22	1:B:418:LEU:HD13	1.83	0.59
1:B:320:LEU:HA	1:B:341:LEU:CD2	2.33	0.59
1:A:44:ASN:O	1:A:47:ILE:HG12	2.03	0.59
1:A:168:LEU:HD21	1:A:292:THR:O	2.03	0.59
1:C:49:LEU:HD13	1:C:71:VAL:HG11	1.84	0.59
1:D:472:LYS:CD	1:D:473:VAL:H	2.13	0.59
1:B:216:PHE:HD2	1:B:216:PHE:H	1.49	0.59
1:D:205:ILE:CD1	1:D:205:ILE:C	2.70	0.59
1:A:89:PHE:CZ	1:A:372:ILE:CD1	2.85	0.59
1:B:85:LYS:O	1:B:87:VAL:N	2.35	0.59
1:D:196:LEU:CD2	3:D:501:3QZ:CAQ	2.80	0.59
1:D:463:PRO:CG	1:D:471:LEU:HB2	2.20	0.59
1:A:60:TYR:HE1	1:A:73:ASN:ND2	2.00	0.59
1:C:162:GLN:HE22	1:C:165:PHE:CB	2.16	0.59
1:C:294:THR:HG21	3:C:501:3QZ:CAA	2.22	0.59
1:B:420:PHE:HZ	2:B:500:HEM:HBB2	1.67	0.59
1:A:408:PHE:O	1:A:408:PHE:HD1	1.86	0.59
1:D:280:VAL:O	1:D:284:VAL:HG23	2.03	0.59
1:C:304:ALA:HA	1:C:307:LEU:HD12	1.84	0.59
1:B:91:GLY:C	1:B:365:ARG:HB3	2.23	0.59
1:A:97:SER:HB2	1:A:209:ASP:CG	2.24	0.59
1:C:193:VAL:HG22	1:C:289:ILE:HG22	1.84	0.58
1:D:97:SER:HB2	1:D:209:ASP:CG	2.23	0.58
1:D:252:TRP:CH2	1:D:253:ARG:NH1	2.70	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:215:ARG:HD3	1:D:217:PHE:CE1	2.38	0.58
1:A:31:PRO:HG2	1:A:61:ARG:HG3	1.85	0.58
1:A:391:HIS:CD2	1:A:417:ALA:HB1	2.38	0.58
1:C:56:LEU:HD23	1:C:56:LEU:H	1.68	0.58
1:D:387:LEU:HD22	1:D:418:LEU:O	2.03	0.58
1:C:106:GLN:O	1:C:107:ASP:HB3	2.03	0.58
1:B:313:GLN:HE22	1:B:450:LEU:HB2	1.68	0.58
1:A:461:LEU:O	1:A:462:GLN:CB	2.52	0.58
1:C:357:VAL:O	1:C:359:PRO:HD3	2.03	0.58
1:B:86:TRP:CZ2	1:B:424:ALA:HA	2.39	0.58
1:D:215:ARG:CD	1:D:217:PHE:HE1	2.16	0.58
1:D:376:ASP:C	1:D:377:ILE:CD1	2.72	0.58
1:D:236:VAL:O	1:D:240:LEU:HB2	2.03	0.58
1:B:203:TRP:O	1:B:207:ILE:HG13	2.03	0.58
1:A:285:VAL:HG13	1:A:286:ASP:N	2.18	0.58
1:A:286:ASP:OD1	1:A:286:ASP:N	2.33	0.58
1:C:169:THR:HG21	1:C:190:HIS:CB	2.30	0.58
1:C:160:THR:HG22	1:C:477:GLN:HB2	1.84	0.58
1:D:252:TRP:HB2	1:D:257:ASP:CB	2.33	0.58
1:D:252:TRP:HZ3	1:D:253:ARG:CZ	2.13	0.58
1:C:54:GLN:HG2	1:C:55:LYS:N	2.19	0.58
1:D:208:LEU:HD23	1:D:208:LEU:N	2.16	0.58
1:A:143:LEU:HD13	1:A:171:SER:HA	1.84	0.58
1:C:101:VAL:HG21	1:C:232:ARG:HH12	1.68	0.58
1:D:394:GLU:O	1:D:394:GLU:HG2	2.03	0.58
1:A:284:VAL:HG12	1:A:288:PHE:CB	2.32	0.58
1:A:313:GLN:NE2	1:A:450:LEU:CD1	2.51	0.58
1:C:101:VAL:CG2	1:C:232:ARG:HH12	2.16	0.58
1:B:214:LEU:CD2	1:B:216:PHE:CA	2.82	0.58
1:B:473:VAL:CG1	1:B:474:GLN:OE1	2.52	0.58
1:A:447:ALA:O	1:A:481:GLN:HB3	2.04	0.58
1:B:40:LEU:O	1:B:40:LEU:HD12	2.04	0.58
1:C:38:LEU:HB2	1:C:41:LEU:CD1	2.33	0.58
1:B:449:THR:O	1:B:450:LEU:HB2	2.03	0.58
1:D:453:PRO:HB3	1:D:476:PHE:O	2.04	0.58
1:A:164:GLU:HA	1:A:167:LEU:HB2	1.85	0.58
1:A:475:PRO:CG	1:A:477:GLN:HE21	2.17	0.58
1:A:180:ASN:OD1	1:A:182:GLU:HB2	2.03	0.58
1:B:459:PRO:CB	1:B:472:LYS:NZ	2.63	0.58
1:B:113:TYR:CD2	1:B:114:SER:N	2.68	0.58
1:B:284:VAL:C	1:B:288:PHE:CB	2.47	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:159:VAL:HG13	1:C:476:PHE:HE2	1.66	0.57
1:C:159:VAL:O	1:C:159:VAL:CG2	2.52	0.57
1:A:49:LEU:CA	1:A:60:TYR:OH	2.52	0.57
1:C:263:VAL:HG11	1:C:277:GLU:HA	1.85	0.57
1:C:477:GLN:HB3	1:C:479:ARG:HD2	1.85	0.57
1:C:85:LYS:CG	1:C:88:ASP:OD2	2.52	0.57
1:B:320:LEU:HA	1:B:341:LEU:HD21	1.85	0.57
1:B:96:PRO:CG	1:B:209:ASP:HA	2.33	0.57
1:D:46:PRO:CG	1:D:466:TYR:CD2	2.78	0.57
1:C:165:PHE:O	1:C:168:LEU:HD12	2.04	0.57
1:C:374:GLY:C	1:C:375:TYR:HD2	2.07	0.57
1:C:44:ASN:C	1:C:46:PRO:HD2	2.25	0.57
1:D:181:LYS:HB3	1:D:181:LYS:NZ	2.19	0.57
1:B:210:MET:HG3	3:B:502:3QZ:HAG	1.81	0.57
1:B:110:LEU:HD11	3:B:501:3QZ:HAH	1.85	0.57
1:C:288:PHE:HB3	1:C:289:ILE:HD13	1.86	0.57
1:D:141:ASP:HA	1:D:439:VAL:CG1	2.34	0.57
1:C:112:ASP:HB2	1:C:365:ARG:NH2	2.20	0.57
1:D:160:THR:OG1	1:D:477:GLN:HB2	2.04	0.57
1:B:193:VAL:CG1	1:B:289:ILE:HG23	2.33	0.57
1:A:45:LEU:C	1:A:45:LEU:CD2	2.72	0.57
1:D:359:PRO:HG2	1:D:360:LEU:H	1.68	0.57
1:A:315:ARG:HH11	1:A:343:LEU:HD21	1.70	0.57
1:D:75:LYS:HA	1:D:78:ILE:HG22	1.87	0.57
1:B:37:PHE:CD1	1:B:63:ARG:HD3	2.39	0.57
1:A:40:LEU:HB2	1:A:64:LEU:O	2.04	0.57
1:C:59:VAL:HG21	1:C:372:ILE:CG2	2.32	0.57
1:D:340:ARG:HA	1:D:340:ARG:NE	2.19	0.57
1:C:185:LEU:HD11	1:C:239:GLN:HE22	1.69	0.57
1:A:275:LEU:HD13	1:A:275:LEU:C	2.25	0.57
1:A:89:PHE:CE2	1:A:372:ILE:HG13	2.39	0.57
1:C:373:PHE:CD1	1:C:373:PHE:C	2.78	0.57
1:C:80:GLU:HG3	1:C:84:ARG:HD3	1.86	0.57
1:C:232:ARG:HH11	3:C:501:3QZ:CAG	2.18	0.57
1:C:113:TYR:O	1:C:114:SER:CB	2.47	0.57
1:A:407:ARG:HH11	1:A:407:ARG:CG	2.11	0.57
1:A:103:GLN:NE2	1:A:104:ARG:CD	2.64	0.57
1:D:121:LYS:HE2	1:D:428:LEU:CD2	2.33	0.57
1:A:59:VAL:HG13	1:A:72:LEU:HD23	1.86	0.57
1:D:377:ILE:CD1	1:D:377:ILE:N	2.67	0.57
1:B:168:LEU:HD12	1:B:168:LEU:N	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:212:PRO:O	1:D:214:LEU:N	2.38	0.57
1:B:43:PRO:O	1:B:44:ASN:HB2	2.05	0.57
1:D:374:GLY:O	1:D:375:TYR:CG	2.58	0.57
1:C:232:ARG:NH1	3:C:501:3QZ:OAE	2.38	0.57
1:A:316:LEU:HD23	1:A:343:LEU:HB3	1.87	0.57
1:B:324:LEU:HB2	1:B:340:ARG:HB3	1.86	0.57
1:B:102:SER:OG	1:B:105:CYS:HA	2.05	0.57
1:C:137:GLU:N	1:C:138:PRO:HD2	2.19	0.57
1:A:226:LYS:O	1:A:229:ILE:HG22	2.05	0.57
1:C:53:THR:HG22	1:C:54:GLN:N	2.19	0.56
1:B:426:VAL:O	1:B:427:CYS:CB	2.53	0.56
1:C:161:ILE:CD1	1:C:474:GLN:CB	2.83	0.56
1:C:333:VAL:O	1:C:333:VAL:CG1	2.48	0.56
1:B:136:MET:SD	1:B:175:TYR:CE2	2.98	0.56
1:D:358:VAL:CG1	1:D:361:ALA:HA	2.34	0.56
1:A:252:TRP:H	1:A:257:ASP:HB3	1.70	0.56
1:A:62:LEU:CD2	1:A:63:ARG:C	2.74	0.56
1:D:54:GLN:C	1:D:54:GLN:CD	2.63	0.56
1:A:37:PHE:O	1:A:38:LEU:CD2	2.27	0.56
1:A:87:VAL:HB	1:A:368:ARG:HH21	1.69	0.56
1:D:176:LEU:HD11	1:D:287:LEU:HD23	1.87	0.56
1:D:116:LEU:O	1:D:116:LEU:HD23	2.03	0.56
1:B:40:LEU:HD21	3:B:502:3QZ:HALA	1.87	0.56
1:B:275:LEU:HD22	1:B:279:HIS:HD2	1.70	0.56
1:B:178:PHE:HB2	1:B:243:HIS:NE2	2.19	0.56
1:A:180:ASN:ND2	1:A:185:LEU:HD13	2.19	0.56
1:D:216:PHE:HD1	1:D:216:PHE:H	1.54	0.56
1:D:196:LEU:HD23	3:D:501:3QZ:CAQ	2.34	0.56
1:D:72:LEU:CD1	1:D:372:ILE:HD11	2.35	0.56
1:C:324:LEU:HG	1:C:340:ARG:CG	2.35	0.56
1:D:141:ASP:HA	1:D:439:VAL:HG11	1.86	0.56
1:B:117:TRP:CH2	1:B:425:ARG:HG2	2.39	0.56
1:B:92:ARG:HE	1:B:425:ARG:HE	1.53	0.56
1:C:116:LEU:O	1:C:120:HIS:N	2.38	0.56
1:B:394:GLU:HA	1:B:397:TRP:O	2.04	0.56
1:A:423:GLY:C	1:A:425:ARG:N	2.56	0.56
1:A:459:PRO:O	1:A:460:SER:HB2	2.06	0.56
1:B:108:ILE:HD13	1:B:124:THR:HG21	1.88	0.56
1:C:357:VAL:HG13	1:C:469:VAL:HG13	1.87	0.56
1:D:66:LEU:C	1:D:67:GLN:HE21	2.09	0.56
1:A:287:LEU:H	1:A:287:LEU:CD1	1.95	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:72:LEU:CD2	1:D:372:ILE:HD12	2.36	0.56
1:A:30:LEU:HD11	1:A:378:PRO:HD3	1.86	0.56
1:D:342:PRO:HG2	1:D:343:LEU:H	1.69	0.56
1:D:203:TRP:CA	1:D:206:GLN:HB2	2.34	0.56
1:B:219:ASN:ND2	4:B:616:HOH:O	1.99	0.56
1:D:313:GLN:HE22	1:D:450:LEU:HB2	1.71	0.56
1:A:168:LEU:HD21	1:A:296:ALA:CB	2.35	0.56
1:B:97:SER:HB2	1:B:209:ASP:OD1	2.05	0.56
1:D:120:HIS:O	1:D:124:THR:HG22	2.05	0.56
1:C:44:ASN:HB3	1:C:47:ILE:HG12	1.88	0.56
1:B:189:PHE:O	1:B:193:VAL:HG23	2.06	0.56
1:C:116:LEU:HD23	1:C:117:TRP:CA	2.36	0.56
1:A:243:HIS:CD2	1:A:254:ASP:OD2	2.59	0.56
1:B:472:LYS:HG3	1:B:473:VAL:N	2.19	0.56
1:D:313:GLN:HE22	1:D:450:LEU:HD13	1.71	0.56
1:C:112:ASP:HB2	1:C:365:ARG:HH22	1.70	0.56
1:D:304:ALA:HB1	1:D:459:PRO:HG2	1.88	0.56
1:A:464:ASP:N	1:A:465:PRO:CD	2.69	0.56
1:B:85:LYS:O	1:B:87:VAL:HG23	2.06	0.56
1:D:372:ILE:O	1:D:372:ILE:HG22	2.03	0.56
1:A:311:GLU:HG3	1:A:312:ILE:H	1.71	0.56
1:D:168:LEU:HD21	1:D:292:THR:O	2.02	0.56
1:C:60:TYR:HE2	1:C:62:LEU:HB2	1.69	0.56
1:A:34:VAL:HG22	1:A:62:LEU:HA	1.87	0.56
1:C:386:ASN:HD22	1:C:386:ASN:C	2.08	0.56
1:D:347:THR:HA	1:D:405:PRO:HB3	1.87	0.56
1:D:448:PHE:CD1	1:D:479:ARG:HB3	2.40	0.56
1:D:425:ARG:HD2	2:D:500:HEM:O2D	2.07	0.55
1:B:225:LEU:O	1:B:229:ILE:HB	2.06	0.55
1:B:469:VAL:HG12	1:B:470:ASN:N	2.21	0.55
1:D:252:TRP:C	1:D:254:ASP:H	2.09	0.55
1:C:175:TYR:O	1:C:255:MET:HE2	2.05	0.55
1:D:263:VAL:HG13	1:D:275:LEU:O	2.06	0.55
1:C:160:THR:HG21	1:C:477:GLN:HB2	1.88	0.55
1:C:232:ARG:HD2	1:C:285:VAL:CG1	2.37	0.55
1:B:450:LEU:HD23	1:B:479:ARG:HG2	1.89	0.55
1:A:460:SER:OG	1:A:461:LEU:N	2.38	0.55
1:C:85:LYS:CB	1:C:88:ASP:OD2	2.54	0.55
1:B:90:ALA:HB3	1:B:113:TYR:CE1	2.40	0.55
1:C:341:LEU:HD13	1:C:344:LEU:CD1	2.33	0.55
1:B:141:ASP:HA	1:B:439:VAL:CG1	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:LEU:HD21	1:B:63:ARG:C	2.26	0.55
1:B:181:LYS:HB3	1:B:181:LYS:NZ	2.22	0.55
1:D:34:VAL:HG22	1:D:62:LEU:HA	1.87	0.55
1:C:275:LEU:CD1	1:C:275:LEU:C	2.75	0.55
1:A:189:PHE:CE2	1:A:288:PHE:CE2	2.95	0.55
1:B:304:ALA:HA	1:B:307:LEU:HD12	1.88	0.55
1:D:479:ARG:HH11	1:D:479:ARG:HB2	1.69	0.55
1:C:128:LEU:O	1:C:129:LEU:HD12	2.04	0.55
1:B:80:GLU:HA	1:B:84:ARG:HG3	1.87	0.55
1:D:420:PHE:CG	1:D:430:GLU:HG3	2.41	0.55
1:A:55:LYS:HB2	1:A:56:LEU:HD22	1.87	0.55
1:D:75:LYS:O	1:D:79:GLU:HB2	2.05	0.55
1:B:311:GLU:HG3	1:B:312:ILE:H	1.72	0.55
1:D:106:GLN:CB	1:D:279:HIS:CD2	2.80	0.55
1:C:62:LEU:HD21	1:C:63:ARG:C	2.26	0.55
1:B:165:PHE:CD2	1:B:296:ALA:HB1	2.41	0.55
1:C:128:LEU:C	1:C:129:LEU:HD13	2.24	0.55
1:A:147:PHE:HE2	1:A:163:LYS:HB3	1.72	0.55
1:C:444:LEU:CD2	1:C:450:LEU:HD11	2.37	0.55
1:D:323:GLU:HG2	1:D:340:ARG:O	2.07	0.55
1:B:96:PRO:HG2	1:B:209:ASP:HA	1.88	0.55
1:A:425:ARG:HB3	2:A:500:HEM:O2D	2.06	0.55
1:A:176:LEU:HA	1:A:255:MET:HB2	1.89	0.55
1:A:404:ARG:O	1:A:404:ARG:CG	2.43	0.55
1:C:85:LYS:HG2	1:C:89:PHE:HE1	1.72	0.55
1:B:30:LEU:HD23	1:B:61:ARG:CZ	2.37	0.55
1:D:106:GLN:HG2	1:D:279:HIS:CE1	2.27	0.55
1:C:120:HIS:O	1:C:124:THR:HG22	2.07	0.55
1:A:71:VAL:HG12	1:A:72:LEU:H	1.71	0.55
1:B:42:GLN:OE1	1:B:48:HIS:CG	2.60	0.55
1:D:252:TRP:O	1:D:254:ASP:N	2.40	0.55
1:B:346:ALA:HB2	1:B:408:PHE:HD1	1.71	0.55
1:A:168:LEU:HD22	1:A:292:THR:O	2.07	0.55
1:C:127:ALA:HA	1:C:258:TYR:HD1	1.72	0.55
1:D:248:VAL:HG23	1:D:249:ALA:H	1.72	0.55
1:C:88:ASP:CB	1:C:89:PHE:CE1	2.90	0.55
1:C:315:ARG:HH11	1:C:343:LEU:HD21	1.72	0.55
1:B:443:ARG:HA	1:B:446:GLN:HB3	1.89	0.55
1:A:304:ALA:HA	1:A:307:LEU:HD12	1.88	0.54
1:C:167:LEU:HD22	1:C:167:LEU:C	2.25	0.54
1:C:85:LYS:HE3	1:C:371:SER:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:425:ARG:HB3	2:D:500:HEM:CGD	2.36	0.54
1:C:178:PHE:N	1:C:243:HIS:NE2	2.55	0.54
1:D:200:TRP:O	1:D:205:ILE:HG21	2.07	0.54
1:B:406:ASP:C	1:B:408:PHE:H	2.10	0.54
1:C:88:ASP:HB2	1:C:89:PHE:HD1	1.71	0.54
1:C:205:ILE:O	1:C:205:ILE:HD13	2.06	0.54
1:C:122:LYS:O	1:C:126:SER:OG	2.24	0.54
1:D:168:LEU:HD13	1:D:169:THR:H	1.71	0.54
1:A:301:TRP:CH2	1:A:472:LYS:HD2	2.43	0.54
1:B:117:TRP:CZ2	1:B:425:ARG:NH1	2.75	0.54
1:C:278:GLY:O	1:C:281:HIS:N	2.41	0.54
1:B:459:PRO:CB	1:B:473:VAL:HB	2.38	0.54
1:A:113:TYR:OH	1:A:118:LYS:HE2	2.07	0.54
1:A:45:LEU:CD2	1:A:45:LEU:O	2.55	0.54
1:D:147:PHE:HE2	1:D:163:LYS:HD2	1.71	0.54
1:C:451:LEU:N	1:C:451:LEU:CD1	2.70	0.54
1:D:168:LEU:O	1:D:172:ILE:CD1	2.33	0.54
1:D:173:ILE:HG12	1:D:288:PHE:CZ	2.43	0.54
1:D:231:ASN:HB3	1:D:235:MET:CE	2.38	0.54
1:D:429:GLY:HA2	2:D:500:HEM:HBC2	1.90	0.54
1:C:55:LYS:CD	1:C:56:LEU:HD21	2.37	0.54
1:B:89:PHE:CE2	1:B:372:ILE:CG1	2.91	0.54
1:C:307:LEU:CG	1:C:458:LEU:HD22	2.37	0.54
1:C:386:ASN:HD22	1:C:387:LEU:N	2.06	0.54
1:B:97:SER:HB2	1:B:209:ASP:CG	2.27	0.54
1:C:200:TRP:HD1	1:C:225:LEU:HD11	1.71	0.54
1:C:451:LEU:N	1:C:451:LEU:HD13	2.22	0.54
1:D:38:LEU:HD13	1:D:41:LEU:CD1	2.35	0.54
1:B:88:ASP:CB	1:B:89:PHE:HE1	2.20	0.54
1:C:161:ILE:O	1:C:165:PHE:HD2	1.90	0.54
1:D:448:PHE:CB	1:D:479:ARG:O	2.51	0.54
1:D:311:GLU:HG3	1:D:312:ILE:H	1.72	0.54
1:C:461:LEU:O	1:C:461:LEU:HG	2.07	0.54
1:B:70:VAL:HG13	1:B:383:VAL:HA	1.90	0.54
1:D:169:THR:O	1:D:173:ILE:HG13	2.07	0.54
1:D:420:PHE:CB	1:D:430:GLU:HG3	2.38	0.54
1:D:203:TRP:O	1:D:206:GLN:N	2.41	0.54
1:D:211:VAL:HG12	1:D:214:LEU:CB	2.35	0.54
1:D:294:THR:O	1:D:357:VAL:HG21	2.07	0.54
1:B:386:ASN:ND2	1:B:389:GLY:N	2.54	0.54
1:D:137:GLU:N	1:D:138:PRO:HD2	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:145:GLN:HE21	1:D:443:ARG:HD3	1.71	0.54
1:D:440:VAL:O	1:D:444:LEU:HB2	2.07	0.54
1:D:231:ASN:HB3	1:D:235:MET:HE1	1.89	0.54
1:A:189:PHE:O	1:A:193:VAL:HG23	2.08	0.54
1:A:333:VAL:HG11	1:A:443:ARG:HH12	1.71	0.54
1:C:283:SER:O	1:C:287:LEU:HD13	2.08	0.54
1:D:322:ARG:HA	1:D:322:ARG:NE	2.23	0.54
1:A:137:GLU:N	1:A:138:PRO:HD2	2.23	0.54
1:D:301:TRP:HZ3	1:D:460:SER:HA	1.73	0.54
1:C:463:PRO:CG	1:C:471:LEU:HB2	2.37	0.54
1:B:128:LEU:HD11	1:B:287:LEU:CG	2.38	0.54
1:C:189:PHE:O	1:C:193:VAL:HG23	2.08	0.54
1:D:376:ASP:C	1:D:377:ILE:HD13	2.28	0.54
1:C:226:LYS:HA	1:C:229:ILE:HG22	1.89	0.54
1:A:470:ASN:OD1	1:A:470:ASN:C	2.46	0.54
1:A:49:LEU:HA	1:A:60:TYR:OH	2.08	0.54
1:C:177:THR:O	1:C:179:GLY:N	2.40	0.54
1:B:89:PHE:CE2	1:B:372:ILE:HG12	2.43	0.54
1:B:301:TRP:CH2	1:B:472:LYS:HD3	2.43	0.54
1:C:440:VAL:O	1:C:444:LEU:HB2	2.08	0.54
1:D:193:VAL:CG2	1:D:289:ILE:HG22	2.36	0.53
1:D:420:PHE:CG	1:D:430:GLU:CG	2.91	0.53
1:B:360:LEU:CB	3:B:502:3QZ:HAAA	2.39	0.53
1:B:116:LEU:O	1:B:116:LEU:HD23	2.01	0.53
1:B:189:PHE:CD2	1:B:288:PHE:CE2	2.95	0.53
1:B:92:ARG:HE	1:B:425:ARG:NE	2.06	0.53
1:C:479:ARG:HB2	1:C:479:ARG:HH11	1.74	0.53
1:B:313:GLN:HE21	1:B:445:LEU:CD1	2.20	0.53
1:B:83:ILE:CG1	1:B:422:CYS:HB2	2.38	0.53
1:D:293:GLU:OE2	1:D:293:GLU:O	2.27	0.53
1:B:214:LEU:O	1:B:215:ARG:CB	2.55	0.53
1:A:176:LEU:HD21	1:A:287:LEU:HD22	1.90	0.53
1:D:252:TRP:HB2	1:D:257:ASP:HB2	1.90	0.53
1:C:320:LEU:HA	1:C:341:LEU:CD2	2.38	0.53
1:A:113:TYR:O	1:A:114:SER:CB	2.56	0.53
1:C:311:GLU:HG3	1:C:312:ILE:H	1.73	0.53
1:B:62:LEU:HD21	1:B:64:LEU:N	2.21	0.53
1:A:313:GLN:NE2	1:A:450:LEU:HB2	2.24	0.53
1:B:41:LEU:O	1:B:42:GLN:HB2	2.07	0.53
1:A:214:LEU:CD2	1:A:216:PHE:CG	2.90	0.53
1:B:341:LEU:CD1	1:B:344:LEU:HD12	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:PRO:HG2	1:D:336:LYS:HD3	1.90	0.53
1:D:104:ARG:HH21	1:D:278:GLY:CA	2.21	0.53
1:D:143:LEU:HD13	1:D:171:SER:HA	1.90	0.53
1:B:246:SER:HB2	1:B:252:TRP:CZ3	2.44	0.53
1:C:177:THR:HB	1:C:288:PHE:CZ	2.43	0.53
1:C:447:ALA:CB	1:C:448:PHE:CD2	2.90	0.53
1:B:151:MET:CB	1:B:479:ARG:HH22	2.22	0.53
1:D:451:LEU:O	1:D:478:VAL:HG23	2.09	0.53
1:A:62:LEU:HD23	1:A:63:ARG:C	2.27	0.53
1:D:215:ARG:CD	1:D:217:PHE:CE1	2.91	0.53
1:C:106:GLN:O	1:C:107:ASP:CB	2.57	0.53
1:A:205:ILE:O	1:A:205:ILE:HD13	2.09	0.53
1:C:359:PRO:HG2	1:C:360:LEU:H	1.73	0.53
1:D:36:GLY:O	1:D:63:ARG:CD	2.56	0.53
1:B:88:ASP:CB	1:B:89:PHE:CD1	2.91	0.53
1:A:404:ARG:HH22	1:A:414:ASN:CG	2.11	0.53
1:A:170:CYS:SG	1:A:186:VAL:HG11	2.49	0.53
1:D:45:LEU:N	1:D:46:PRO:HD2	2.24	0.53
1:D:54:GLN:NE2	1:D:54:GLN:O	2.42	0.53
1:C:29:HIS:O	1:C:376:ASP:CB	2.56	0.53
1:B:176:LEU:HD12	1:B:287:LEU:CD2	2.36	0.53
1:D:243:HIS:NE2	1:D:254:ASP:OD1	2.42	0.53
1:B:315:ARG:HH11	1:B:343:LEU:HD21	1.73	0.53
1:D:148:CYS:O	1:D:152:ARG:HB2	2.09	0.53
1:D:117:TRP:CZ2	1:D:425:ARG:CZ	2.92	0.53
1:A:109:SER:OG	1:A:110:LEU:N	2.41	0.53
1:A:120:HIS:O	1:A:124:THR:HG22	2.09	0.53
1:B:289:ILE:HG22	1:B:289:ILE:O	2.09	0.53
1:D:41:LEU:O	1:D:42:GLN:HB3	2.09	0.53
1:D:205:ILE:HG23	1:D:206:GLN:N	2.23	0.53
1:D:275:LEU:C	1:D:275:LEU:HD13	2.29	0.53
1:D:404:ARG:HD2	1:D:404:ARG:C	2.26	0.53
1:D:448:PHE:HB3	1:D:479:ARG:C	2.30	0.53
1:D:313:GLN:NE2	1:D:450:LEU:HB2	2.23	0.53
1:A:85:LYS:HB3	1:A:88:ASP:OD2	2.09	0.53
1:B:246:SER:CB	1:B:252:TRP:CH2	2.92	0.53
1:C:243:HIS:ND1	1:C:256:THR:HG21	2.24	0.53
1:C:89:PHE:CZ	1:C:370:SER:OG	2.62	0.53
1:C:232:ARG:HD2	1:C:285:VAL:HG11	1.90	0.53
1:D:316:LEU:HD23	1:D:343:LEU:HB3	1.89	0.53
1:A:403:PHE:CD1	1:A:405:PRO:HD3	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:75:LYS:HG3	1:C:397:TRP:CH2	2.44	0.53
1:D:102:SER:O	1:D:104:ARG:N	2.42	0.52
1:D:162:GLN:HA	1:D:165:PHE:HB2	1.90	0.52
1:C:60:TYR:C	1:C:60:TYR:CD2	2.82	0.52
1:A:180:ASN:C	1:A:182:GLU:H	2.13	0.52
1:A:161:ILE:HG23	1:A:165:PHE:CD2	2.43	0.52
1:A:315:ARG:NH1	1:A:343:LEU:HD21	2.24	0.52
1:B:324:LEU:HG	1:B:340:ARG:CD	2.39	0.52
1:D:315:ARG:NH1	1:D:343:LEU:HD21	2.24	0.52
1:A:136:MET:O	1:A:140:VAL:HG23	2.10	0.52
1:A:45:LEU:HD23	1:A:45:LEU:C	2.29	0.52
1:A:335:TYR:CD2	1:A:336:LYS:HA	2.45	0.52
1:B:89:PHE:HE2	1:B:372:ILE:CG1	2.22	0.52
1:A:298:THR:OG1	1:A:357:VAL:HG23	2.09	0.52
1:B:74:SER:OG	1:B:77:THR:HG23	2.10	0.52
1:C:97:SER:HB2	1:C:209:ASP:CG	2.29	0.52
1:D:177:THR:C	1:D:179:GLY:H	2.12	0.52
1:B:252:TRP:C	1:B:254:ASP:H	2.13	0.52
1:B:100:LEU:HD11	1:B:222:LEU:HD11	1.91	0.52
1:B:214:LEU:C	1:B:215:ARG:CG	2.76	0.52
1:A:335:TYR:HD2	1:A:336:LYS:CA	2.22	0.52
1:D:374:GLY:O	1:D:375:TYR:HB2	2.09	0.52
1:B:473:VAL:HG13	1:B:474:GLN:OE1	2.09	0.52
1:D:432:LEU:CD2	1:D:436:GLU:HG3	2.40	0.52
1:C:320:LEU:HA	1:C:341:LEU:HD21	1.91	0.52
1:A:418:LEU:HD23	1:A:418:LEU:H	1.74	0.52
1:D:172:ILE:HG21	1:D:288:PHE:HA	1.91	0.52
1:B:314:ARG:O	1:B:318:GLU:HG3	2.09	0.52
1:B:178:PHE:HD1	1:B:239:GLN:OE1	1.93	0.52
1:C:177:THR:OG1	1:C:239:GLN:HG2	2.09	0.52
1:D:226:LYS:O	1:D:229:ILE:HG22	2.08	0.52
1:D:254:ASP:OD2	1:D:256:THR:HB	2.09	0.52
1:A:316:LEU:CD2	1:A:343:LEU:HB3	2.40	0.52
1:B:309:HIS:HE1	1:B:403:PHE:HB3	1.74	0.52
1:A:252:TRP:HB2	1:A:257:ASP:OD2	2.08	0.52
1:B:252:TRP:CB	1:B:257:ASP:CG	2.78	0.52
1:A:243:HIS:CD2	1:A:256:THR:CB	2.90	0.52
1:C:97:SER:HB2	1:C:209:ASP:OD2	2.10	0.52
1:D:189:PHE:CE2	1:D:235:MET:HB3	2.45	0.52
1:D:189:PHE:O	1:D:193:VAL:HG23	2.09	0.52
1:A:477:GLN:OE1	1:A:477:GLN:CA	2.56	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:ARG:CZ	1:A:337:ASP:OD1	2.58	0.52
1:C:215:ARG:O	1:C:216:PHE:C	2.48	0.52
1:D:373:PHE:HD1	1:D:374:GLY:CA	2.22	0.52
1:C:31:PRO:CA	1:C:375:TYR:HD1	2.23	0.52
1:C:316:LEU:HD23	1:C:343:LEU:HB3	1.91	0.52
1:C:172:ILE:HG21	1:C:287:LEU:O	2.09	0.52
1:C:37:PHE:O	1:C:65:GLY:O	2.28	0.52
1:C:463:PRO:HG2	1:C:471:LEU:HB2	1.91	0.52
1:B:285:VAL:N	1:B:288:PHE:HB2	2.21	0.52
1:C:173:ILE:HG23	1:C:288:PHE:HZ	1.75	0.52
1:A:332:ARG:O	1:A:333:VAL:CB	2.58	0.52
1:D:350:GLU:OE2	1:D:407:ARG:HD3	2.10	0.52
1:C:31:PRO:CB	1:C:375:TYR:HD1	2.23	0.52
1:B:316:LEU:HD23	1:B:343:LEU:HB3	1.90	0.52
1:C:315:ARG:NH1	1:C:343:LEU:HD21	2.25	0.52
1:B:62:LEU:HD21	1:B:64:LEU:HD23	1.92	0.52
1:B:247:MET:HG3	1:B:248:VAL:H	1.75	0.52
1:D:65:GLY:O	1:D:66:LEU:CD1	2.39	0.52
1:D:262:GLY:O	1:D:263:VAL:CG2	2.57	0.52
1:C:59:VAL:CG2	1:C:72:LEU:HD22	2.40	0.52
1:C:294:THR:HG23	3:C:501:3QZ:CAA	2.39	0.52
1:A:408:PHE:N	1:A:408:PHE:CD1	2.75	0.52
1:C:193:VAL:HG13	1:C:289:ILE:O	2.09	0.52
1:A:87:VAL:HG11	1:A:368:ARG:NH2	2.24	0.52
1:C:279:HIS:CE1	4:C:608:HOH:O	2.63	0.52
1:C:465:PRO:CG	1:C:471:LEU:CD2	2.82	0.51
1:B:205:ILE:HG13	1:B:225:LEU:CD1	2.40	0.51
1:D:413:ALA:HA	4:D:601:HOH:O	2.10	0.51
1:B:136:MET:O	1:B:140:VAL:HG23	2.10	0.51
1:D:357:VAL:CG1	1:D:469:VAL:HG13	2.40	0.51
1:D:177:THR:HB	1:D:288:PHE:CZ	2.46	0.51
1:D:34:VAL:HG11	1:D:52:LEU:HD13	1.92	0.51
1:B:44:ASN:HB3	1:B:47:ILE:HG12	1.91	0.51
1:B:42:GLN:OE1	1:B:48:HIS:CD2	2.63	0.51
1:C:373:PHE:CG	1:C:373:PHE:O	2.61	0.51
1:C:176:LEU:HD11	1:C:287:LEU:HB3	1.91	0.51
1:A:97:SER:HB2	1:A:209:ASP:OD2	2.10	0.51
1:B:231:ASN:O	1:B:235:MET:HB2	2.10	0.51
1:D:172:ILE:CG2	1:D:288:PHE:HA	2.41	0.51
1:A:426:VAL:HG23	1:A:427:CYS:H	1.74	0.51
1:A:299:LEU:HD13	1:A:440:VAL:HG11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:116:LEU:HD23	1:D:117:TRP:HA	1.91	0.51
1:A:284:VAL:O	1:A:288:PHE:N	2.34	0.51
1:A:335:TYR:CG	1:A:336:LYS:N	2.71	0.51
1:B:145:GLN:HE21	1:B:443:ARG:HD3	1.75	0.51
1:D:189:PHE:CD1	1:D:288:PHE:HE2	2.28	0.51
1:D:165:PHE:CZ	1:D:293:GLU:OE2	2.60	0.51
1:C:38:LEU:HB2	1:C:41:LEU:HD11	1.92	0.51
1:C:42:GLN:HG3	1:C:43:PRO:CD	2.41	0.51
1:B:128:LEU:CD2	1:B:432:LEU:HD12	2.40	0.51
1:C:453:PRO:HD3	1:C:476:PHE:O	2.10	0.51
1:D:66:LEU:N	1:D:66:LEU:HD13	2.24	0.51
1:C:178:PHE:N	1:C:254:ASP:OD2	2.41	0.51
1:D:87:VAL:CG1	1:D:88:ASP:N	2.72	0.51
1:D:315:ARG:HH11	1:D:343:LEU:HD21	1.74	0.51
1:C:443:ARG:HA	1:C:446:GLN:HB3	1.92	0.51
1:C:36:GLY:HA3	1:C:39:HIS:CE1	2.46	0.51
1:C:361:ALA:C	1:C:362:LEU:HD22	2.30	0.51
1:A:64:LEU:HD22	3:A:502:3QZ:HABB	1.92	0.51
1:B:460:SER:N	1:B:472:LYS:HE2	2.24	0.51
1:A:106:GLN:HG2	1:A:116:LEU:CD2	2.41	0.51
1:C:70:VAL:HG12	1:C:383:VAL:HG13	1.91	0.51
1:A:309:HIS:HE1	1:A:403:PHE:CB	2.22	0.51
1:A:173:ILE:HD12	1:A:186:VAL:HG13	1.93	0.51
1:C:354:LEU:O	1:C:355:ARG:HD2	2.10	0.51
1:B:223:TRP:HA	1:B:223:TRP:CE3	2.46	0.51
1:B:230:GLU:HG2	1:B:234:HIS:CD2	2.45	0.51
1:D:354:LEU:O	1:D:355:ARG:HD2	2.11	0.51
1:A:161:ILE:CG2	1:A:165:PHE:CE2	2.94	0.51
1:B:315:ARG:NH1	1:B:343:LEU:HD21	2.25	0.51
1:C:109:SER:O	1:C:110:LEU:HD23	2.10	0.51
1:D:308:HIS:CE1	1:D:458:LEU:HB2	2.46	0.51
1:A:214:LEU:HD21	1:A:216:PHE:CB	2.40	0.51
1:B:301:TRP:CE2	1:B:472:LYS:HD3	2.45	0.51
1:D:303:VAL:HG13	1:D:450:LEU:HD21	1.92	0.51
1:B:341:LEU:HD13	1:B:344:LEU:CD1	2.37	0.51
1:C:176:LEU:HD21	1:C:287:LEU:CD2	2.40	0.51
1:A:470:ASN:OD1	1:A:471:LEU:O	2.29	0.51
1:A:301:TRP:CD2	1:A:472:LYS:HG2	2.44	0.51
1:B:252:TRP:H	1:B:257:ASP:HB3	1.76	0.51
1:D:202:HIS:CE1	1:D:203:TRP:NE1	2.79	0.51
1:C:307:LEU:HD22	1:C:458:LEU:CD2	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:447:ALA:CB	1:C:448:PHE:HE2	2.07	0.51
1:B:459:PRO:HB2	1:B:473:VAL:HB	1.93	0.51
1:A:135:SER:O	1:A:138:PRO:HD2	2.11	0.51
1:B:137:GLU:N	1:B:138:PRO:HD2	2.26	0.51
1:A:121:LYS:HD2	1:A:428:LEU:HD13	1.93	0.51
1:B:117:TRP:O	1:B:120:HIS:N	2.43	0.51
1:C:426:VAL:HG23	1:C:427:CYS:H	1.74	0.51
1:D:297:SER:HA	1:D:300:SER:OG	2.11	0.51
1:C:53:THR:HG23	1:C:54:GLN:N	2.26	0.50
1:C:34:VAL:HG22	1:C:62:LEU:HA	1.92	0.50
1:C:358:VAL:HG22	1:C:361:ALA:HA	1.93	0.50
1:B:168:LEU:H	1:B:168:LEU:HD12	1.76	0.50
1:D:407:ARG:CB	1:D:414:ASN:HB2	2.41	0.50
1:C:383:VAL:O	1:C:385:PRO:HD3	2.11	0.50
1:D:176:LEU:HA	1:D:255:MET:H	1.76	0.50
1:D:176:LEU:HD11	1:D:287:LEU:HB3	1.93	0.50
1:C:314:ARG:O	1:C:318:GLU:HG3	2.10	0.50
1:D:220:PRO:O	1:D:224:ARG:HG3	2.11	0.50
1:B:464:ASP:N	1:B:465:PRO:HD2	2.25	0.50
1:A:180:ASN:HD21	1:B:184:THR:HG23	1.76	0.50
1:A:449:THR:O	1:A:450:LEU:CB	2.58	0.50
1:C:105:CYS:HB2	1:C:106:GLN:HE21	1.75	0.50
1:D:72:LEU:HD11	1:D:372:ILE:CD1	2.40	0.50
1:B:58:PRO:HB3	1:B:74:SER:HB3	1.93	0.50
1:D:240:LEU:HD22	1:D:260:LEU:HD13	1.93	0.50
1:B:137:GLU:CD	1:B:334:THR:HG23	2.32	0.50
1:B:225:LEU:CD2	1:B:229:ILE:HD13	2.42	0.50
1:A:372:ILE:O	1:A:373:PHE:CB	2.50	0.50
1:B:407:ARG:O	1:B:413:ALA:HB1	2.10	0.50
1:B:223:TRP:HE3	1:B:223:TRP:HA	1.77	0.50
1:D:100:LEU:HD11	1:D:222:LEU:HD11	1.93	0.50
1:D:314:ARG:O	1:D:318:GLU:HG3	2.12	0.50
1:D:109:SER:O	1:D:110:LEU:HD22	2.11	0.50
1:D:174:CYS:SG	1:D:181:LYS:HD3	2.51	0.50
1:B:463:PRO:HG3	1:B:471:LEU:HB2	1.92	0.50
1:A:440:VAL:O	1:A:444:LEU:HB2	2.11	0.50
1:D:72:LEU:HD13	1:D:372:ILE:CD1	2.42	0.50
1:B:313:GLN:HB3	4:B:613:HOH:O	2.11	0.50
1:C:340:ARG:O	1:C:342:PRO:HD3	2.12	0.50
1:C:414:ASN:N	1:C:414:ASN:HD22	2.08	0.50
1:A:286:ASP:O	1:A:290:GLY:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:LEU:HD21	1:A:49:LEU:HG	1.92	0.50
1:D:215:ARG:HG2	1:D:215:ARG:NH2	2.26	0.50
1:C:168:LEU:HD12	1:C:169:THR:H	1.76	0.50
1:A:148:CYS:O	1:A:152:ARG:HB2	2.11	0.50
1:A:407:ARG:CG	1:A:407:ARG:NH1	2.69	0.50
1:A:30:LEU:CG	1:A:31:PRO:HD2	2.40	0.50
1:C:365:ARG:HG2	1:C:380:GLY:HA2	1.93	0.50
1:B:46:PRO:HD3	1:B:466:TYR:CE2	2.46	0.50
1:D:159:VAL:O	1:D:159:VAL:HG23	2.10	0.50
1:D:165:PHE:C	1:D:168:LEU:HD11	2.31	0.50
1:A:463:PRO:CG	1:A:471:LEU:HB2	2.39	0.50
1:B:120:HIS:O	1:B:124:THR:HG22	2.11	0.50
1:A:64:LEU:HD13	3:A:502:3QZ:HABB	1.94	0.50
1:B:226:LYS:O	1:B:229:ILE:HG22	2.11	0.50
1:D:30:LEU:HD21	1:D:61:ARG:NH1	2.26	0.50
1:C:313:GLN:NE2	1:C:450:LEU:CB	2.66	0.50
1:A:312:ILE:HD12	1:A:405:PRO:HG2	1.93	0.50
1:C:225:LEU:C	1:C:225:LEU:HD23	2.32	0.50
1:B:218:PRO:O	1:B:218:PRO:HG2	2.12	0.50
1:A:314:ARG:O	1:A:318:GLU:HG3	2.10	0.50
1:C:178:PHE:CE2	1:C:242:ARG:HB3	2.46	0.50
1:D:81:ALA:CB	1:D:372:ILE:HD11	2.42	0.50
1:D:307:LEU:HD11	1:D:477:GLN:CD	2.32	0.50
1:C:33:LEU:HD22	1:C:34:VAL:N	2.25	0.50
1:B:423:GLY:C	1:B:425:ARG:N	2.61	0.50
1:B:246:SER:CB	1:B:252:TRP:CZ3	2.95	0.50
1:A:102:SER:O	1:A:105:CYS:N	2.45	0.50
1:B:91:GLY:C	1:B:365:ARG:H	2.07	0.50
1:D:168:LEU:CD2	1:D:292:THR:CA	2.90	0.50
1:B:117:TRP:O	1:B:120:HIS:HB3	2.11	0.50
1:D:33:LEU:HD22	1:D:34:VAL:N	2.25	0.50
1:A:71:VAL:HG12	1:A:72:LEU:N	2.27	0.50
1:D:407:ARG:CZ	1:D:407:ARG:HB2	2.38	0.50
1:A:353:ARG:HH22	1:A:404:ARG:HD3	1.76	0.50
1:B:45:LEU:N	1:B:46:PRO:HD2	2.26	0.50
1:C:352:LEU:O	1:C:419:ALA:HB2	2.11	0.49
1:A:81:ALA:CB	1:A:372:ILE:HD13	2.42	0.49
1:C:409:LEU:O	1:C:410:GLU:HB2	2.11	0.49
1:B:410:GLU:N	1:B:411:PRO:CD	2.75	0.49
1:A:404:ARG:NH2	1:A:414:ASN:CG	2.66	0.49
1:C:232:ARG:NH1	3:C:501:3QZ:CAQ	2.74	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:LEU:HD11	1:B:64:LEU:HD23	1.95	0.49
1:A:64:LEU:HD12	1:A:69:VAL:CB	2.42	0.49
1:A:284:VAL:O	1:A:288:PHE:HB2	2.13	0.49
1:A:373:PHE:CD1	1:A:374:GLY:HA3	2.47	0.49
1:D:370:SER:O	4:D:606:HOH:O	2.18	0.49
1:D:377:ILE:N	1:D:377:ILE:HD13	2.26	0.49
1:B:394:GLU:O	1:B:394:GLU:OE1	2.29	0.49
1:D:316:LEU:CD2	1:D:343:LEU:HB3	2.42	0.49
1:D:257:ASP:O	1:D:261:GLN:HB2	2.13	0.49
1:B:410:GLU:CB	1:B:411:PRO:HD3	2.42	0.49
1:B:30:LEU:HD11	1:B:378:PRO:CD	2.40	0.49
1:C:127:ALA:HA	1:C:258:TYR:CD1	2.47	0.49
1:A:205:ILE:HG13	1:A:225:LEU:CD1	2.42	0.49
1:D:463:PRO:O	1:D:463:PRO:CG	2.61	0.49
1:A:210:MET:C	1:A:212:PRO:HD3	2.32	0.49
1:B:406:ASP:C	1:B:408:PHE:N	2.66	0.49
1:A:168:LEU:HD12	1:A:168:LEU:N	2.27	0.49
1:D:283:SER:O	1:D:287:LEU:HD13	2.12	0.49
1:B:218:PRO:O	1:B:218:PRO:CG	2.60	0.49
1:A:231:ASN:O	1:A:235:MET:HB2	2.12	0.49
1:A:141:ASP:HA	1:A:439:VAL:HG11	1.93	0.49
1:C:301:TRP:HZ3	1:C:460:SER:OG	1.96	0.49
1:C:89:PHE:HE2	1:C:372:ILE:HD13	1.76	0.49
1:B:316:LEU:CD2	1:B:343:LEU:HB3	2.42	0.49
1:A:407:ARG:HG3	1:A:407:ARG:NH1	2.18	0.49
1:A:434:ARG:HH11	1:A:434:ARG:HG3	1.77	0.49
1:D:463:PRO:HG2	1:D:463:PRO:O	2.13	0.49
1:C:178:PHE:N	1:C:254:ASP:OD1	2.46	0.49
1:D:196:LEU:CD1	1:D:229:ILE:HA	2.40	0.49
1:A:168:LEU:HD22	1:A:292:THR:HA	1.95	0.49
1:A:418:LEU:HD22	4:A:607:HOH:O	2.12	0.49
1:A:110:LEU:HD11	3:A:501:3QZ:CAH	2.41	0.49
1:B:128:LEU:HG	1:B:287:LEU:CD2	2.35	0.49
1:B:92:ARG:HH12	1:B:362:LEU:C	2.16	0.49
1:B:85:LYS:NZ	1:B:371:SER:O	2.44	0.49
1:B:346:ALA:HB1	1:B:405:PRO:O	2.12	0.49
1:D:29:HIS:HA	1:D:375:TYR:CD1	2.42	0.49
1:C:335:TYR:CG	1:C:336:LYS:N	2.79	0.49
1:D:459:PRO:O	1:D:460:SER:HB3	2.12	0.49
1:A:60:TYR:CE1	1:A:73:ASN:ND2	2.81	0.49
1:B:211:VAL:HG12	1:B:214:LEU:CB	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:VAL:HG21	1:A:280:VAL:HG22	1.95	0.49
1:A:313:GLN:HE22	1:A:450:LEU:CG	2.25	0.49
1:B:473:VAL:O	1:B:475:PRO:HD2	2.12	0.49
1:B:30:LEU:HD12	1:B:376:ASP:O	2.13	0.49
1:A:78:ILE:CD1	1:A:387:LEU:HD23	2.42	0.49
1:B:55:LYS:HG3	1:B:56:LEU:HD22	1.94	0.49
1:D:173:ILE:HG23	1:D:288:PHE:HZ	1.77	0.49
1:B:193:VAL:HG11	1:B:292:THR:OG1	2.12	0.49
1:D:42:GLN:HG3	1:D:43:PRO:HD2	1.94	0.49
1:C:173:ILE:HG23	1:C:288:PHE:CZ	2.48	0.49
1:A:242:ARG:NH2	1:B:187:HIS:ND1	2.60	0.49
1:D:409:LEU:HD13	1:D:410:GLU:HB2	1.94	0.49
1:C:205:ILE:HG13	1:C:225:LEU:CD1	2.42	0.49
1:B:440:VAL:O	1:B:444:LEU:HB2	2.13	0.49
1:D:245:GLU:HG3	1:D:245:GLU:O	2.13	0.49
1:D:459:PRO:CG	1:D:472:LYS:HE3	2.43	0.49
1:A:108:ILE:HD12	1:A:428:LEU:HD22	1.94	0.49
1:A:285:VAL:HG12	1:A:286:ASP:H	1.78	0.49
1:B:40:LEU:C	1:B:40:LEU:HD12	2.32	0.49
1:C:470:ASN:OD1	1:C:471:LEU:O	2.31	0.49
1:C:177:THR:HG22	1:C:177:THR:O	2.12	0.49
1:C:280:VAL:O	1:C:284:VAL:HG23	2.13	0.49
1:A:373:PHE:CD1	1:A:374:GLY:CA	2.96	0.49
1:A:373:PHE:CE1	1:A:374:GLY:HA3	2.48	0.49
1:C:214:LEU:CD2	1:C:216:PHE:CD2	2.96	0.49
1:B:148:CYS:O	1:B:448:PHE:HZ	1.96	0.49
1:D:233:ASP:HB3	1:D:237:GLU:OE2	2.13	0.49
1:D:117:TRP:CH2	1:D:425:ARG:HD3	2.48	0.48
1:A:304:ALA:HB2	4:A:605:HOH:O	2.12	0.48
1:C:208:LEU:HD23	1:C:214:LEU:HD11	1.94	0.48
1:C:211:VAL:O	1:C:214:LEU:HD22	2.12	0.48
1:B:406:ASP:O	1:B:408:PHE:N	2.46	0.48
1:D:376:ASP:C	1:D:377:ILE:HD12	2.32	0.48
1:C:59:VAL:HG22	1:C:72:LEU:CD2	2.43	0.48
1:A:168:LEU:HD12	1:A:168:LEU:H	1.79	0.48
1:D:316:LEU:HG	1:D:343:LEU:HD12	1.95	0.48
1:B:308:HIS:C	1:B:309:HIS:HD2	2.15	0.48
1:C:225:LEU:O	1:C:225:LEU:HD23	2.13	0.48
1:C:75:LYS:HG3	1:C:397:TRP:HH2	1.78	0.48
1:D:462:GLN:OE1	1:D:466:TYR:OH	2.31	0.48
1:C:50:LEU:O	1:C:53:THR:HG22	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:236:VAL:HG22	1:B:288:PHE:CZ	2.48	0.48
1:B:211:VAL:CG1	1:B:214:LEU:HB2	2.42	0.48
1:C:185:LEU:HD11	1:C:239:GLN:NE2	2.28	0.48
1:A:145:GLN:HE21	1:A:443:ARG:HD3	1.78	0.48
1:D:101:VAL:HA	1:D:229:ILE:HD11	1.94	0.48
1:C:414:ASN:HB3	1:C:415:PRO:CD	2.43	0.48
1:D:223:TRP:CE3	1:D:223:TRP:HA	2.48	0.48
1:C:218:PRO:HD3	4:C:622:HOH:O	2.13	0.48
1:D:38:LEU:CD1	1:D:41:LEU:CD1	2.91	0.48
1:C:220:PRO:O	1:C:224:ARG:HG3	2.13	0.48
1:C:407:ARG:CG	1:C:407:ARG:NH1	2.36	0.48
1:C:66:LEU:O	1:C:67:GLN:OE1	2.31	0.48
1:C:299:LEU:O	1:C:303:VAL:HG23	2.14	0.48
1:C:414:ASN:HB3	1:C:415:PRO:HD2	1.96	0.48
1:A:462:GLN:CG	1:A:466:TYR:OH	2.61	0.48
1:A:472:LYS:NZ	1:A:472:LYS:CA	2.74	0.48
1:D:39:HIS:O	1:D:41:LEU:O	2.31	0.48
1:A:284:VAL:CG1	1:A:288:PHE:HB2	2.41	0.48
1:A:332:ARG:HD3	1:A:337:ASP:OD1	2.13	0.48
1:B:85:LYS:CG	1:B:88:ASP:OD2	2.62	0.48
1:A:106:GLN:CB	1:A:279:HIS:CE1	2.96	0.48
1:B:129:LEU:O	1:B:130:LEU:HD23	2.13	0.48
1:D:471:LEU:CD1	1:D:472:LYS:N	2.68	0.48
1:D:173:ILE:CD1	1:D:186:VAL:HA	2.43	0.48
1:D:420:PHE:HB3	1:D:430:GLU:HG3	1.94	0.48
1:D:121:LYS:HD2	1:D:428:LEU:CD2	2.39	0.48
1:A:34:VAL:HG11	1:A:52:LEU:HD12	1.95	0.48
1:D:418:LEU:CD2	1:D:422:CYS:HG	2.23	0.48
1:B:409:LEU:H	1:B:413:ALA:HB2	1.79	0.48
1:C:85:LYS:O	1:C:86:TRP:CB	2.61	0.48
1:A:138:PRO:O	1:A:142:GLN:HG3	2.14	0.48
1:D:470:ASN:OD1	1:D:471:LEU:O	2.31	0.48
1:D:172:ILE:H	1:D:172:ILE:HD13	1.77	0.48
1:A:108:ILE:HG22	2:A:500:HEM:O1D	2.14	0.48
1:A:461:LEU:HD23	1:A:462:GLN:N	2.23	0.48
1:B:42:GLN:OE1	1:B:48:HIS:CE1	2.66	0.48
1:A:104:ARG:HG2	1:A:104:ARG:H	1.43	0.48
1:D:313:GLN:HE22	1:D:450:LEU:CD1	2.26	0.48
1:D:219:ASN:HD21	1:D:222:LEU:HB2	1.78	0.48
1:B:353:ARG:HD3	1:B:391:HIS:O	2.14	0.48
1:D:168:LEU:HD13	1:D:168:LEU:N	2.23	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:429:GLY:O	1:D:433:ALA:N	2.28	0.48
1:B:168:LEU:CD2	1:B:292:THR:O	2.62	0.48
1:B:225:LEU:HD21	1:B:229:ILE:HD13	1.95	0.48
1:D:214:LEU:O	1:D:215:ARG:CB	2.61	0.48
1:A:334:THR:O	1:A:337:ASP:OD2	2.31	0.48
1:A:96:PRO:HG2	1:A:209:ASP:HA	1.96	0.48
1:D:365:ARG:HG2	1:D:366:THR:N	2.29	0.48
1:A:144:THR:HA	1:A:167:LEU:HD21	1.96	0.48
1:B:243:HIS:CD2	1:B:256:THR:HB	2.48	0.48
1:C:162:GLN:C	1:C:162:GLN:NE2	2.67	0.48
1:A:298:THR:OG1	1:A:357:VAL:HG21	2.14	0.48
1:B:29:HIS:O	1:B:375:TYR:HB3	2.14	0.48
1:A:149:GLU:O	1:A:153:VAL:HG13	2.14	0.48
1:A:150:ARG:O	1:A:153:VAL:HG22	2.14	0.48
1:A:151:MET:HE1	1:A:163:LYS:HG3	1.95	0.48
1:C:470:ASN:O	1:C:470:ASN:OD1	2.32	0.48
1:A:284:VAL:O	1:A:288:PHE:CB	2.62	0.48
1:D:207:ILE:O	1:D:208:LEU:C	2.52	0.48
1:D:81:ALA:HB2	1:D:372:ILE:CD1	2.43	0.48
1:B:394:GLU:O	1:B:397:TRP:O	2.32	0.48
1:B:151:MET:HB2	1:B:479:ARG:HH22	1.77	0.48
1:C:316:LEU:CD2	1:C:343:LEU:HB3	2.44	0.48
1:D:279:HIS:O	1:D:280:VAL:C	2.52	0.48
1:D:168:LEU:HD23	1:D:292:THR:CA	2.44	0.48
1:A:423:GLY:O	1:A:426:VAL:HG22	2.14	0.48
1:A:437:LEU:HD11	2:A:500:HEM:HBB1	1.96	0.48
1:A:461:LEU:CD2	1:A:462:GLN:O	2.62	0.48
1:B:62:LEU:CD1	1:B:64:LEU:CD2	2.92	0.48
1:B:286:ASP:O	1:B:290:GLY:CA	2.62	0.48
1:B:178:PHE:HB2	1:B:243:HIS:HE1	1.71	0.48
1:B:298:THR:OG1	1:B:357:VAL:CG2	2.62	0.48
1:D:200:TRP:HD1	1:D:225:LEU:HD11	1.79	0.48
1:B:418:LEU:O	1:B:418:LEU:HD13	2.14	0.48
1:D:449:THR:O	1:D:450:LEU:CB	2.48	0.48
1:B:467:CYS:O	1:B:468:GLY:C	2.52	0.48
1:A:465:PRO:O	1:A:471:LEU:HD11	2.13	0.47
1:B:62:LEU:HD13	1:B:64:LEU:HD21	1.96	0.47
1:C:177:THR:CG2	1:C:177:THR:O	2.61	0.47
1:C:189:PHE:CD1	1:C:288:PHE:HE2	2.31	0.47
1:C:307:LEU:HD13	1:C:458:LEU:CD2	2.35	0.47
1:D:447:ALA:CB	1:D:448:PHE:CE2	2.94	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:309:HIS:ND1	1:C:403:PHE:HD2	2.10	0.47
1:A:398:GLU:O	1:A:399:GLN:C	2.52	0.47
1:B:53:THR:HB	1:B:57:GLY:O	2.14	0.47
1:A:475:PRO:O	1:A:476:PHE:CD2	2.67	0.47
1:B:464:ASP:H	1:B:465:PRO:CD	2.27	0.47
1:A:334:THR:O	1:A:337:ASP:N	2.47	0.47
1:C:85:LYS:HG2	1:C:89:PHE:CE1	2.48	0.47
1:B:313:GLN:NE2	1:B:450:LEU:HB2	2.29	0.47
1:B:445:LEU:HD11	1:B:450:LEU:HD12	1.96	0.47
1:D:151:MET:HA	1:D:154:GLN:HG2	1.96	0.47
1:B:398:GLU:O	1:B:399:GLN:C	2.52	0.47
1:C:31:PRO:CA	1:C:375:TYR:CD1	2.95	0.47
1:D:429:GLY:CA	2:D:500:HEM:HBC2	2.43	0.47
1:A:196:LEU:HD21	3:A:501:3QZ:OAE	2.13	0.47
1:B:39:HIS:ND1	1:B:62:LEU:HG	2.30	0.47
1:B:89:PHE:HE1	1:B:370:SER:HG	1.60	0.47
1:B:313:GLN:HE22	1:B:450:LEU:HD12	1.79	0.47
1:C:128:LEU:HA	1:C:128:LEU:HD22	1.68	0.47
1:A:78:ILE:HD13	1:A:387:LEU:HD23	1.96	0.47
1:C:231:ASN:HB3	1:C:235:MET:HE3	1.96	0.47
1:A:109:SER:HA	1:A:425:ARG:HH21	1.79	0.47
1:C:161:ILE:H	1:C:161:ILE:HG13	1.55	0.47
1:A:113:TYR:CD2	1:A:114:SER:N	2.75	0.47
1:D:176:LEU:HD23	1:D:176:LEU:O	2.13	0.47
1:B:301:TRP:CZ3	1:B:472:LYS:CD	2.96	0.47
1:C:138:PRO:O	1:C:142:GLN:HG3	2.15	0.47
1:D:352:LEU:O	1:D:419:ALA:HB2	2.14	0.47
1:D:121:LYS:CD	1:D:428:LEU:HD21	2.41	0.47
1:C:173:ILE:HD13	1:C:186:VAL:HA	1.96	0.47
1:B:342:PRO:HB2	1:B:408:PHE:CZ	2.50	0.47
1:D:219:ASN:HB2	1:D:220:PRO:HD2	1.96	0.47
1:D:116:LEU:CD2	1:D:116:LEU:C	2.39	0.47
1:D:177:THR:O	1:D:177:THR:HG22	2.14	0.47
1:D:170:CYS:SG	1:D:186:VAL:HG11	2.55	0.47
1:B:62:LEU:CD2	1:B:64:LEU:HD23	2.44	0.47
1:A:62:LEU:CD2	1:A:64:LEU:N	2.77	0.47
1:A:42:GLN:OE1	1:A:48:HIS:CD2	2.67	0.47
1:C:178:PHE:CA	1:C:254:ASP:OD1	2.63	0.47
1:C:474:GLN:O	1:C:474:GLN:OE1	2.32	0.47
1:C:205:ILE:HG13	1:C:225:LEU:HD13	1.97	0.47
1:D:459:PRO:CD	1:D:475:PRO:HB3	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:ILE:HG13	1:B:286:ASP:OD1	2.14	0.47
1:B:169:THR:HG23	1:B:292:THR:HG21	1.97	0.47
1:B:362:LEU:HD12	1:B:362:LEU:HA	1.51	0.47
1:D:387:LEU:CD2	1:D:418:LEU:HB2	2.44	0.47
1:A:263:VAL:HG21	1:A:280:VAL:CG2	2.45	0.47
1:B:71:VAL:HG12	1:B:73:ASN:ND2	2.17	0.47
1:D:252:TRP:CH2	1:D:253:ARG:CZ	2.96	0.47
1:A:342:PRO:HG2	1:A:343:LEU:H	1.80	0.47
1:A:399:GLN:N	1:A:400:PRO:CD	2.78	0.47
1:B:285:VAL:C	1:B:288:PHE:HB3	2.34	0.47
1:A:64:LEU:HD12	1:A:69:VAL:CG2	2.45	0.47
1:A:42:GLN:HA	1:A:43:PRO:HD2	1.72	0.47
1:A:263:VAL:HG13	1:A:275:LEU:O	2.14	0.47
1:A:178:PHE:CB	1:A:243:HIS:CE1	2.88	0.47
1:D:247:MET:HG3	1:D:257:ASP:OD1	2.14	0.47
1:C:350:GLU:HG3	1:C:405:PRO:HA	1.96	0.47
1:B:168:LEU:HD21	1:B:296:ALA:CB	2.35	0.47
1:B:463:PRO:HA	4:B:625:HOH:O	2.15	0.47
1:A:373:PHE:O	1:A:375:TYR:N	2.40	0.47
1:C:72:LEU:HD12	1:C:78:ILE:HA	1.96	0.47
1:C:81:ALA:HB2	1:C:372:ILE:CG1	2.41	0.47
1:A:319:GLU:OE1	1:A:343:LEU:HB2	2.15	0.47
1:C:316:LEU:HG	1:C:343:LEU:HD12	1.97	0.47
1:C:425:ARG:HB3	2:C:500:HEM:O2D	2.14	0.46
1:B:288:PHE:CG	1:B:289:ILE:CD1	2.90	0.46
1:B:168:LEU:HD21	1:B:292:THR:O	2.15	0.46
1:B:92:ARG:HH12	1:B:363:PRO:C	2.18	0.46
1:D:203:TRP:O	1:D:207:ILE:N	2.36	0.46
1:D:232:ARG:HD2	1:D:285:VAL:CG1	2.44	0.46
1:B:473:VAL:CG1	1:B:474:GLN:H	2.27	0.46
1:B:113:TYR:HD2	1:B:114:SER:N	2.02	0.46
1:C:87:VAL:CG1	1:C:368:ARG:HH12	2.18	0.46
1:C:171:SER:O	1:C:175:TYR:CZ	2.68	0.46
1:B:138:PRO:O	1:B:142:GLN:HG3	2.15	0.46
1:D:470:ASN:OD1	1:D:470:ASN:C	2.53	0.46
1:A:62:LEU:O	1:A:69:VAL:N	2.43	0.46
1:A:259:MET:O	1:A:263:VAL:HG23	2.16	0.46
1:D:215:ARG:CG	1:D:215:ARG:HH21	2.26	0.46
1:A:444:LEU:HD21	1:A:479:ARG:NH1	2.30	0.46
1:C:316:LEU:O	1:C:320:LEU:HB2	2.16	0.46
1:D:322:ARG:HA	1:D:322:ARG:HE	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:350:GLU:CG	1:C:405:PRO:HA	2.46	0.46
1:B:177:THR:O	1:B:178:PHE:HB3	2.16	0.46
1:B:174:CYS:HB2	1:B:181:LYS:HB2	1.97	0.46
1:D:52:LEU:O	1:D:55:LYS:HG3	2.16	0.46
1:D:207:ILE:O	1:D:210:MET:N	2.49	0.46
1:D:347:THR:HG23	1:D:403:PHE:HZ	1.81	0.46
1:A:358:VAL:HG12	1:A:361:ALA:CA	2.41	0.46
1:D:58:PRO:HG3	1:D:76:ARG:NH2	2.20	0.46
1:D:148:CYS:O	1:D:152:ARG:N	2.43	0.46
1:C:62:LEU:HD22	1:C:64:LEU:HG	1.98	0.46
1:A:45:LEU:N	1:A:46:PRO:CD	2.77	0.46
1:D:94:GLN:HE22	1:D:99:LYS:NZ	2.13	0.46
1:A:177:THR:OG1	1:A:288:PHE:CD1	2.58	0.46
1:D:101:VAL:HB	1:D:232:ARG:HH12	1.80	0.46
1:D:178:PHE:HA	1:D:243:HIS:CE1	2.51	0.46
1:D:252:TRP:C	1:D:254:ASP:N	2.68	0.46
1:A:174:CYS:SG	1:A:181:LYS:HB2	2.56	0.46
1:B:83:ILE:HD11	1:B:422:CYS:HB2	1.96	0.46
1:B:128:LEU:HD23	1:B:432:LEU:HD12	1.97	0.46
1:A:333:VAL:CG1	1:A:443:ARG:HH12	2.29	0.46
1:D:85:LYS:HB3	1:D:88:ASP:HB2	1.96	0.46
1:C:226:LYS:C	1:C:229:ILE:HG22	2.36	0.46
1:D:313:GLN:HE21	1:D:445:LEU:CD1	2.25	0.46
1:D:397:TRP:O	1:D:400:PRO:HD3	2.15	0.46
1:B:180:ASN:HB3	1:B:185:LEU:HD22	1.97	0.46
1:D:217:PHE:N	1:D:217:PHE:CD1	2.84	0.46
1:B:323:GLU:HG2	1:B:340:ARG:O	2.16	0.46
1:D:276:LEU:HG	1:D:277:GLU:H	1.80	0.46
1:A:141:ASP:HA	1:A:439:VAL:CG1	2.45	0.46
1:C:298:THR:HG21	1:C:437:LEU:HD11	1.97	0.46
1:B:75:LYS:O	1:B:79:GLU:HB2	2.16	0.46
1:D:165:PHE:CA	1:D:168:LEU:HD11	2.46	0.46
1:D:428:LEU:HG	2:D:500:HEM:CMD	2.46	0.46
1:C:43:PRO:O	1:C:44:ASN:HB2	2.15	0.46
1:B:285:VAL:O	1:B:288:PHE:HB3	2.16	0.46
1:B:92:ARG:NH1	1:B:362:LEU:O	2.44	0.46
1:A:50:LEU:CA	1:A:53:THR:HG23	2.46	0.46
1:D:313:GLN:NE2	1:D:449:THR:O	2.49	0.46
1:A:316:LEU:HG	1:A:343:LEU:HD12	1.98	0.46
1:B:82:MET:SD	1:B:364:HIS:CE1	3.09	0.46
1:D:471:LEU:HD13	1:D:472:LYS:H	1.77	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:ARG:HD2	1:A:285:VAL:HG21	1.98	0.46
1:C:55:LYS:HG2	1:C:56:LEU:N	2.31	0.46
1:C:168:LEU:HD22	1:C:292:THR:HA	1.98	0.46
1:A:148:CYS:O	1:A:448:PHE:HZ	1.99	0.46
1:C:324:LEU:HD12	1:C:332:ARG:CB	2.45	0.46
1:A:169:THR:HG21	1:A:190:HIS:CB	2.38	0.46
1:B:69:VAL:HG22	1:B:382:VAL:HG21	1.96	0.46
1:A:248:VAL:HG23	1:A:250:GLY:H	1.81	0.46
1:D:193:VAL:HG13	1:D:289:ILE:O	2.16	0.46
1:D:214:LEU:CG	1:D:216:PHE:H	2.28	0.46
1:D:407:ARG:HB2	1:D:414:ASN:HB2	1.97	0.46
1:D:353:ARG:HD3	1:D:391:HIS:O	2.16	0.46
1:D:333:VAL:N	4:D:602:HOH:O	2.49	0.46
1:A:189:PHE:CD2	1:A:289:ILE:HD13	2.51	0.46
1:D:202:HIS:HE1	1:D:203:TRP:NE1	2.14	0.46
1:A:337:ASP:C	1:A:339:ALA:N	2.68	0.46
1:A:451:LEU:HG	1:A:452:PRO:CD	2.17	0.46
1:C:307:LEU:HD11	1:C:477:GLN:CD	2.35	0.46
1:B:359:PRO:O	1:B:387:LEU:HB2	2.16	0.46
1:B:301:TRP:CH2	1:B:472:LYS:CD	2.98	0.46
1:C:226:LYS:O	1:C:230:GLU:HG3	2.16	0.46
1:D:447:ALA:C	1:D:448:PHE:HD2	2.00	0.46
1:C:246:SER:HB3	1:C:252:TRP:CH2	2.50	0.46
1:A:227:GLN:OE1	1:B:224:ARG:HG2	2.16	0.46
1:A:282:MET:O	1:A:285:VAL:HG12	2.16	0.45
1:B:193:VAL:CG2	1:B:289:ILE:CG2	2.79	0.45
1:C:474:GLN:NE2	1:C:474:GLN:O	2.50	0.45
1:D:309:HIS:HE1	1:D:403:PHE:HB3	1.81	0.45
1:D:219:ASN:ND2	1:D:222:LEU:H	2.13	0.45
1:C:154:GLN:O	1:C:155:ALA:HB3	2.16	0.45
1:A:151:MET:O	1:A:154:GLN:HB2	2.15	0.45
1:A:301:TRP:CZ2	1:A:472:LYS:HG2	2.50	0.45
1:B:176:LEU:CD1	1:B:287:LEU:CD2	2.92	0.45
1:B:286:ASP:O	1:B:290:GLY:HA3	2.16	0.45
1:B:426:VAL:HG23	1:B:427:CYS:H	1.80	0.45
1:D:41:LEU:O	1:D:42:GLN:CB	2.64	0.45
1:B:470:ASN:OD1	1:B:470:ASN:O	2.34	0.45
1:B:214:LEU:CG	1:B:216:PHE:H	2.27	0.45
1:C:177:THR:C	1:C:179:GLY:H	2.19	0.45
1:A:335:TYR:O	1:A:338:ARG:CB	2.64	0.45
1:C:181:LYS:NZ	1:C:181:LYS:HB3	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:LEU:HA	1:A:53:THR:CG2	2.46	0.45
1:C:176:LEU:HD21	1:C:287:LEU:HD22	1.98	0.45
1:B:107:ASP:HB2	1:B:282:MET:HB3	1.98	0.45
1:A:462:GLN:CD	1:A:466:TYR:OH	2.55	0.45
1:D:205:ILE:O	1:D:205:ILE:HD12	2.14	0.45
1:A:128:LEU:CD2	1:A:287:LEU:HD23	2.45	0.45
1:B:42:GLN:HG3	1:B:43:PRO:HD2	1.97	0.45
1:B:313:GLN:NE2	1:B:445:LEU:HD12	2.31	0.45
1:C:128:LEU:HB3	1:C:129:LEU:CD1	2.46	0.45
1:B:309:HIS:ND1	1:B:403:PHE:HD1	2.14	0.45
1:B:154:GLN:C	1:B:156:GLY:H	2.19	0.45
1:A:76:ARG:HB2	1:A:76:ARG:HH11	1.80	0.45
1:B:172:ILE:HG21	1:B:287:LEU:O	2.16	0.45
1:B:109:SER:OG	1:B:110:LEU:HG	2.16	0.45
1:A:243:HIS:CD2	1:A:256:THR:CG2	2.99	0.45
1:D:178:PHE:CA	1:D:243:HIS:CE1	3.00	0.45
1:D:316:LEU:O	1:D:320:LEU:HB2	2.16	0.45
1:C:144:THR:O	1:C:147:PHE:HB3	2.16	0.45
1:C:257:ASP:O	1:C:261:GLN:HB2	2.17	0.45
1:B:83:ILE:HD11	1:B:422:CYS:CB	2.46	0.45
1:D:173:ILE:HD13	1:D:186:VAL:HA	1.98	0.45
1:B:88:ASP:HB2	1:B:89:PHE:CE1	2.50	0.45
1:C:386:ASN:C	1:C:386:ASN:ND2	2.69	0.45
1:C:85:LYS:HG3	1:C:88:ASP:CG	2.37	0.45
1:C:89:PHE:HD1	1:C:89:PHE:N	2.11	0.45
1:B:316:LEU:HG	1:B:343:LEU:HD12	1.99	0.45
1:B:319:GLU:OE1	1:B:343:LEU:HB2	2.16	0.45
1:D:324:LEU:HG	1:D:340:ARG:CG	2.43	0.45
1:C:432:LEU:O	1:C:436:GLU:HG3	2.17	0.45
1:D:116:LEU:O	1:D:120:HIS:N	2.49	0.45
1:A:108:ILE:O	1:A:109:SER:OG	2.17	0.45
1:B:360:LEU:HB3	3:B:502:3QZ:HAAA	1.99	0.45
1:B:459:PRO:C	4:B:604:HOH:O	2.55	0.45
1:C:127:ALA:HB1	1:C:255:MET:HG2	1.99	0.45
1:B:434:ARG:HG3	1:B:434:ARG:HH11	1.81	0.45
1:C:356:PRO:O	1:C:356:PRO:HG2	2.16	0.45
1:D:471:LEU:CD1	1:D:472:LYS:O	2.63	0.45
1:D:426:VAL:O	1:D:427:CYS:HB2	2.17	0.45
1:A:423:GLY:O	1:A:426:VAL:CG1	2.58	0.45
1:A:425:ARG:O	1:A:426:VAL:C	2.54	0.45
1:B:208:LEU:CD2	1:B:214:LEU:HD22	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:173:ILE:HD12	1:C:186:VAL:HG13	1.98	0.45
1:B:78:ILE:HD13	1:B:387:LEU:HD23	1.98	0.45
1:C:246:SER:CB	1:C:252:TRP:CH2	3.00	0.45
1:D:391:HIS:NE2	1:D:417:ALA:HB1	2.32	0.45
1:B:95:ILE:HB	1:B:96:PRO:HD2	1.98	0.45
1:D:152:ARG:HG2	1:D:152:ARG:HH11	1.82	0.45
1:B:154:GLN:OE1	1:B:158:PRO:HB3	2.16	0.45
1:B:115:LEU:HA	1:B:115:LEU:HD23	1.69	0.45
1:D:46:PRO:HD3	1:D:466:TYR:HD2	1.77	0.45
1:A:214:LEU:HD11	1:A:216:PHE:HA	1.99	0.45
1:D:278:GLY:O	1:D:281:HIS:HB3	2.17	0.45
1:B:216:PHE:O	1:B:217:PHE:C	2.56	0.45
1:C:284:VAL:O	1:C:288:PHE:HB2	2.17	0.45
1:A:89:PHE:CZ	1:A:372:ILE:HD11	2.45	0.45
1:D:29:HIS:O	1:D:30:LEU:HB2	2.17	0.45
1:B:460:SER:H	1:B:472:LYS:NZ	2.15	0.45
1:B:152:ARG:HH11	1:B:152:ARG:HG2	1.81	0.45
1:A:103:GLN:HE21	1:A:104:ARG:H	1.65	0.45
1:B:144:THR:O	1:B:147:PHE:HB3	2.16	0.45
1:D:44:ASN:CB	1:D:47:ILE:HG12	2.44	0.45
1:B:40:LEU:HD23	3:B:502:3QZ:HAJ	1.99	0.45
1:C:464:ASP:O	1:C:466:TYR:N	2.50	0.45
1:C:359:PRO:HG3	1:C:466:TYR:CE2	2.52	0.45
1:D:217:PHE:HB3	1:D:218:PRO:HD2	1.99	0.45
1:A:324:LEU:HG	1:A:340:ARG:CG	2.47	0.45
1:B:372:ILE:HG22	1:B:372:ILE:O	2.17	0.45
1:A:42:GLN:OE1	1:A:48:HIS:CE1	2.70	0.44
1:C:103:GLN:C	1:C:105:CYS:N	2.70	0.44
1:C:145:GLN:HE21	1:C:443:ARG:HD3	1.82	0.44
1:C:154:GLN:C	1:C:156:GLY:H	2.21	0.44
1:A:45:LEU:HD22	1:A:49:LEU:HG	1.98	0.44
1:D:94:GLN:OE1	1:D:99:LYS:NZ	2.50	0.44
1:B:301:TRP:CZ2	1:B:472:LYS:HD3	2.52	0.44
1:A:316:LEU:O	1:A:320:LEU:HB2	2.17	0.44
1:C:323:GLU:HG2	1:C:340:ARG:O	2.17	0.44
1:A:70:VAL:O	1:A:70:VAL:HG13	2.17	0.44
1:D:301:TRP:CE2	1:D:355:ARG:HG2	2.53	0.44
1:C:62:LEU:HD22	1:C:64:LEU:N	2.26	0.44
1:B:168:LEU:HD12	1:B:169:THR:H	1.82	0.44
1:B:432:LEU:O	1:B:436:GLU:HG3	2.16	0.44
1:A:180:ASN:HB3	1:A:185:LEU:HD22	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:72:LEU:HD22	1:B:372:ILE:HG21	1.98	0.44
1:A:214:LEU:HD22	1:A:216:PHE:CD2	2.46	0.44
1:B:152:ARG:HH21	1:C:133:ARG:NH2	2.15	0.44
1:A:447:ALA:HB3	1:A:448:PHE:CE2	2.53	0.44
1:B:107:ASP:HB2	1:B:282:MET:CB	2.47	0.44
1:D:117:TRP:CZ2	1:D:425:ARG:NE	2.85	0.44
1:B:181:LYS:O	1:B:181:LYS:HG2	2.16	0.44
1:A:332:ARG:NH1	1:A:337:ASP:OD2	2.51	0.44
1:C:301:TRP:CE2	1:C:472:LYS:CD	2.99	0.44
1:A:214:LEU:CD2	1:A:216:PHE:HD2	2.22	0.44
1:A:404:ARG:HH21	1:A:414:ASN:ND2	2.10	0.44
1:B:459:PRO:HG3	1:B:475:PRO:HB3	1.99	0.44
1:B:61:ARG:HH12	1:B:68:GLU:CD	2.19	0.44
1:A:225:LEU:C	1:A:225:LEU:HD23	2.38	0.44
1:D:138:PRO:O	1:D:142:GLN:HG3	2.16	0.44
1:D:284:VAL:O	1:D:288:PHE:HB2	2.18	0.44
1:A:40:LEU:CB	1:A:64:LEU:O	2.64	0.44
1:B:200:TRP:CE3	3:B:501:3QZ:CAB	3.00	0.44
1:C:412:GLY:C	4:C:604:HOH:O	2.32	0.44
1:A:254:ASP:OD2	1:A:256:THR:HB	2.18	0.44
1:B:410:GLU:HB3	1:B:411:PRO:HD3	1.98	0.44
1:D:72:LEU:HD13	1:D:372:ILE:HD13	1.99	0.44
1:C:66:LEU:HA	1:C:66:LEU:HD12	1.53	0.44
1:B:316:LEU:O	1:B:320:LEU:HB2	2.16	0.44
1:B:386:ASN:HD21	1:B:389:GLY:N	2.16	0.44
1:C:252:TRP:HB2	1:C:257:ASP:CB	2.47	0.44
1:C:354:LEU:HD12	1:C:354:LEU:HA	1.64	0.44
1:B:62:LEU:HD11	1:B:64:LEU:CD2	2.48	0.44
1:D:55:LYS:HG3	1:D:56:LEU:H	1.83	0.44
1:A:43:PRO:C	1:A:44:ASN:CG	2.77	0.44
1:B:469:VAL:HG12	1:B:470:ASN:H	1.81	0.44
1:C:263:VAL:HG21	1:C:280:VAL:HG23	2.00	0.44
1:A:337:ASP:C	1:A:339:ALA:H	2.19	0.44
1:D:30:LEU:CG	1:D:31:PRO:HD2	2.47	0.44
1:B:148:CYS:O	1:B:152:ARG:HB2	2.18	0.44
1:A:168:LEU:HD12	1:A:169:THR:H	1.82	0.44
1:D:319:GLU:OE1	1:D:343:LEU:HB2	2.17	0.44
1:A:311:GLU:HG3	1:A:312:ILE:N	2.32	0.44
1:D:368:ARG:NH1	1:D:368:ARG:HB3	2.33	0.44
1:D:108:ILE:HG22	1:D:109:SER:N	2.33	0.44
1:A:449:THR:HG22	1:A:450:LEU:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:242:ARG:HD3	1:D:242:ARG:H	1.81	0.44
1:D:136:MET:HG3	1:D:136:MET:H	1.49	0.44
1:D:193:VAL:O	1:D:197:MET:HG2	2.18	0.44
1:A:470:ASN:OD1	1:A:471:LEU:N	2.50	0.44
1:C:160:THR:O	1:C:161:ILE:C	2.54	0.44
1:C:214:LEU:HG	1:C:216:PHE:H	1.83	0.44
1:A:414:ASN:OD1	1:A:415:PRO:HD2	2.18	0.44
1:B:104:ARG:O	1:B:105:CYS:CB	2.66	0.44
1:A:423:GLY:C	1:A:425:ARG:H	2.21	0.44
1:A:60:TYR:HE1	1:A:73:ASN:HD21	1.64	0.44
1:A:449:THR:N	1:A:480:LEU:O	2.46	0.44
1:A:334:THR:HG23	1:A:335:TYR:HB3	1.99	0.44
1:A:89:PHE:CG	1:A:372:ILE:HD11	2.52	0.44
1:C:208:LEU:CD2	1:C:214:LEU:HD11	2.48	0.44
1:A:210:MET:O	1:A:212:PRO:HD3	2.18	0.44
1:D:31:PRO:HA	4:D:605:HOH:O	2.17	0.44
1:A:103:GLN:CA	4:A:610:HOH:O	2.58	0.44
1:B:70:VAL:CG1	1:B:383:VAL:HG22	2.48	0.44
1:C:218:PRO:N	4:C:622:HOH:O	2.51	0.44
1:B:37:PHE:CE1	1:B:63:ARG:HD3	2.53	0.43
1:B:40:LEU:HB2	1:B:64:LEU:O	2.18	0.43
1:C:33:LEU:C	1:C:33:LEU:HD13	2.38	0.43
1:D:37:PHE:O	1:D:65:GLY:O	2.36	0.43
1:A:38:LEU:HD22	1:A:38:LEU:HA	1.69	0.43
1:C:193:VAL:CG2	1:C:289:ILE:HG22	2.48	0.43
1:B:85:LYS:HG2	1:B:88:ASP:OD2	2.18	0.43
1:C:214:LEU:HD23	1:C:216:PHE:CD2	2.53	0.43
1:A:354:LEU:C	1:A:355:ARG:HD3	2.39	0.43
1:A:231:ASN:HD22	1:A:235:MET:CE	2.31	0.43
1:A:386:ASN:ND2	1:A:389:GLY:H	2.16	0.43
1:B:37:PHE:CE1	1:B:63:ARG:CD	3.01	0.43
1:C:425:ARG:HE	1:C:425:ARG:HB3	1.30	0.43
1:B:169:THR:OG1	1:B:292:THR:HB	2.18	0.43
1:B:178:PHE:O	1:B:178:PHE:CG	2.71	0.43
1:C:161:ILE:HD11	1:C:474:GLN:CB	2.47	0.43
1:C:480:LEU:O	1:C:480:LEU:HD12	2.18	0.43
1:C:172:ILE:O	1:C:176:LEU:HB2	2.17	0.43
1:C:176:LEU:HA	1:C:255:MET:H	1.83	0.43
1:D:167:LEU:O	1:D:167:LEU:HD23	2.18	0.43
1:D:462:GLN:CG	1:D:463:PRO:HD2	2.47	0.43
1:D:169:THR:HG21	1:D:190:HIS:CB	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:LEU:C	1:A:60:TYR:HH	2.18	0.43
1:C:162:GLN:O	1:C:165:PHE:HB2	2.18	0.43
1:D:144:THR:O	1:D:147:PHE:HB3	2.17	0.43
1:A:80:GLU:O	1:A:84:ARG:HB2	2.19	0.43
1:A:95:ILE:HB	1:A:96:PRO:HD2	2.00	0.43
1:A:173:ILE:CD1	1:A:186:VAL:HA	2.48	0.43
1:C:325:GLY:N	1:C:326:PRO:HD3	2.32	0.43
1:C:434:ARG:HG3	1:C:434:ARG:HH11	1.82	0.43
1:A:294:THR:HG22	3:A:501:3QZ:CAA	2.25	0.43
1:A:313:GLN:NE2	1:A:450:LEU:HB3	2.25	0.43
1:A:334:THR:O	1:A:335:TYR:C	2.56	0.43
1:A:335:TYR:O	1:A:338:ARG:N	2.52	0.43
1:C:124:THR:HG23	1:C:428:LEU:CD1	2.47	0.43
1:A:216:PHE:O	1:A:217:PHE:C	2.56	0.43
1:D:391:HIS:CE1	1:D:417:ALA:HB1	2.54	0.43
1:B:218:PRO:HB2	1:B:223:TRP:HE1	1.84	0.43
1:C:353:ARG:HH12	1:C:400:PRO:HA	1.83	0.43
1:B:322:ARG:HA	1:B:322:ARG:NE	2.33	0.43
1:D:475:PRO:HA	4:D:610:HOH:O	2.19	0.43
1:A:144:THR:O	1:A:147:PHE:HB3	2.18	0.43
1:D:217:PHE:HD1	1:D:217:PHE:N	2.15	0.43
1:D:123:LEU:HD21	1:D:259:MET:HA	2.01	0.43
1:D:72:LEU:CD2	1:D:372:ILE:CD1	2.97	0.43
1:A:112:ASP:CG	1:A:113:TYR:H	2.21	0.43
1:A:85:LYS:O	1:A:87:VAL:N	2.46	0.43
1:A:354:LEU:O	1:A:355:ARG:CD	2.64	0.43
1:D:75:LYS:HE3	1:D:79:GLU:OE1	2.19	0.43
1:A:267:ARG:O	1:A:268:VAL:HB	2.19	0.43
1:A:203:TRP:O	1:A:207:ILE:HG13	2.18	0.43
1:A:432:LEU:O	1:A:436:GLU:HG3	2.18	0.43
1:D:106:GLN:CG	1:D:116:LEU:CD1	2.96	0.43
1:C:358:VAL:HG12	2:C:500:HEM:HHB	2.00	0.43
1:A:374:GLY:HA3	1:A:375:TYR:CD2	2.53	0.43
1:C:472:LYS:HD2	1:C:472:LYS:HA	1.80	0.43
1:D:407:ARG:O	1:D:413:ALA:HB1	2.19	0.43
1:A:174:CYS:O	1:A:179:GLY:CA	2.64	0.43
1:D:373:PHE:CD1	1:D:374:GLY:N	2.64	0.43
1:C:80:GLU:OE2	1:C:372:ILE:O	2.37	0.43
1:B:136:MET:CB	1:B:175:TYR:CE2	2.93	0.43
1:C:359:PRO:HG3	1:C:466:TYR:HE2	1.83	0.43
1:B:357:VAL:CG1	1:B:469:VAL:HG13	2.29	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:242:ARG:CD	1:D:242:ARG:N	2.82	0.43
1:C:226:LYS:HA	1:C:229:ILE:CG2	2.48	0.43
1:C:226:LYS:CA	1:C:229:ILE:HG22	2.48	0.43
1:A:447:ALA:HB3	1:A:448:PHE:CD2	2.54	0.43
1:C:319:GLU:OE1	1:C:343:LEU:HB2	2.18	0.43
1:D:357:VAL:HG13	1:D:469:VAL:CG1	2.46	0.43
1:A:113:TYR:O	1:A:114:SER:HB2	2.19	0.43
1:B:308:HIS:HE1	1:B:458:LEU:HB2	1.82	0.43
1:C:322:ARG:NE	1:C:322:ARG:HA	2.34	0.43
1:D:180:ASN:C	1:D:182:GLU:H	2.21	0.43
1:A:473:VAL:O	1:A:475:PRO:HD3	2.18	0.43
1:C:44:ASN:HB3	1:C:47:ILE:HG23	2.00	0.43
1:D:39:HIS:HB2	1:D:62:LEU:HD21	2.01	0.43
1:B:152:ARG:HH21	1:C:133:ARG:HH21	1.67	0.43
1:B:62:LEU:CD1	1:B:64:LEU:HD23	2.49	0.43
1:B:116:LEU:HD11	1:B:279:HIS:NE2	2.34	0.43
1:A:478:VAL:O	1:A:479:ARG:HB2	2.19	0.43
1:A:212:PRO:C	1:A:214:LEU:N	2.68	0.43
1:D:178:PHE:HA	1:D:243:HIS:NE2	2.34	0.43
1:C:95:ILE:HB	1:C:96:PRO:HD2	2.01	0.43
1:D:75:LYS:HA	1:D:78:ILE:CG2	2.49	0.43
1:C:468:GLY:HA2	3:C:502:3QZ:OAE	2.19	0.43
1:A:475:PRO:HB2	1:A:477:GLN:CD	2.26	0.43
1:C:361:ALA:HB1	2:C:500:HEM:HAA2	2.00	0.43
1:B:168:LEU:CD1	1:B:169:THR:H	2.31	0.43
1:C:178:PHE:HB2	1:C:243:HIS:NE2	2.34	0.43
1:A:372:ILE:HB	1:A:377:ILE:HG13	1.99	0.43
1:A:208:LEU:HD22	1:A:216:PHE:HD2	1.84	0.43
1:D:81:ALA:HB2	1:D:372:ILE:HD11	2.01	0.43
1:A:50:LEU:O	1:A:53:THR:OG1	2.31	0.43
1:D:473:VAL:HG13	1:D:474:GLN:N	2.10	0.42
1:D:98:TYR:OH	1:D:363:PRO:HG3	2.19	0.42
1:D:427:CYS:SG	2:D:500:HEM:ND	2.92	0.42
1:A:34:VAL:CG1	1:A:52:LEU:HD13	2.49	0.42
1:A:37:PHE:N	4:A:601:HOH:O	2.46	0.42
1:A:44:ASN:HD22	1:A:47:ILE:CD1	2.31	0.42
1:A:72:LEU:HD11	1:A:383:VAL:CG1	2.48	0.42
1:C:162:GLN:NE2	1:C:165:PHE:HB2	2.34	0.42
1:C:168:LEU:N	1:C:168:LEU:HD12	2.34	0.42
1:C:214:LEU:CD2	1:C:216:PHE:HD2	2.33	0.42
1:A:350:GLU:HG3	1:A:404:ARG:C	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:222:LEU:HD11	1:C:226:LYS:HE3	2.01	0.42
1:D:151:MET:HB3	1:D:479:ARG:HH12	1.84	0.42
1:D:448:PHE:HD1	1:D:479:ARG:O	2.00	0.42
1:C:303:VAL:HG13	1:C:450:LEU:CD2	2.48	0.42
1:D:310:PRO:O	1:D:314:ARG:HG2	2.18	0.42
1:A:252:TRP:H	1:A:257:ASP:CB	2.32	0.42
1:B:169:THR:HG21	1:B:190:HIS:HB2	2.01	0.42
1:A:67:GLN:HB2	3:A:502:3QZ:OAD	2.19	0.42
1:B:208:LEU:HD23	1:B:214:LEU:HD22	2.00	0.42
1:C:162:GLN:NE2	1:C:165:PHE:CB	2.80	0.42
1:B:459:PRO:HB3	1:B:473:VAL:HB	2.00	0.42
1:B:113:TYR:O	1:B:114:SER:CB	2.45	0.42
1:B:58:PRO:HG2	1:B:373:PHE:CE1	2.54	0.42
1:C:96:PRO:HG2	1:C:209:ASP:OD1	2.19	0.42
1:D:121:LYS:CD	1:D:428:LEU:CD2	2.98	0.42
1:A:109:SER:CA	1:A:425:ARG:HH21	2.32	0.42
1:B:116:LEU:CD2	1:B:117:TRP:CA	2.90	0.42
1:A:49:LEU:HB3	1:A:60:TYR:OH	2.19	0.42
1:B:85:LYS:HG3	1:B:88:ASP:OD2	2.20	0.42
1:D:151:MET:SD	1:D:163:LYS:HG3	2.59	0.42
1:D:478:VAL:O	1:D:479:ARG:HB2	2.19	0.42
1:C:231:ASN:HB3	1:C:235:MET:CE	2.48	0.42
1:D:117:TRP:HE1	1:D:425:ARG:HH12	1.60	0.42
1:A:449:THR:H	1:A:480:LEU:C	2.21	0.42
1:D:178:PHE:CB	1:D:243:HIS:HE1	2.33	0.42
1:B:244:LYS:CG	1:B:260:LEU:HD21	2.48	0.42
1:D:335:TYR:CG	1:D:336:LYS:N	2.87	0.42
1:B:420:PHE:CE1	2:B:500:HEM:HBB2	2.54	0.42
1:D:137:GLU:CD	1:D:334:THR:HG23	2.40	0.42
1:A:308:HIS:CE1	1:A:458:LEU:HB2	2.54	0.42
1:A:409:LEU:HG	4:A:609:HOH:O	2.18	0.42
1:B:325:GLY:N	1:B:326:PRO:HD3	2.34	0.42
1:D:459:PRO:CB	1:D:473:VAL:HB	2.47	0.42
1:D:106:GLN:CB	1:D:279:HIS:ND1	2.70	0.42
1:A:477:GLN:CD	1:A:477:GLN:H	2.22	0.42
1:B:37:PHE:CE1	1:B:63:ARG:CZ	3.03	0.42
1:A:45:LEU:CD2	1:A:49:LEU:CG	2.87	0.42
1:A:180:ASN:O	1:A:182:GLU:N	2.53	0.42
1:D:396:VAL:O	1:D:415:PRO:HG2	2.19	0.42
1:A:96:PRO:CG	1:A:209:ASP:HA	2.49	0.42
1:B:159:VAL:HG23	1:B:162:GLN:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:178:PHE:CD2	1:B:252:TRP:HZ3	2.16	0.42
1:C:216:PHE:CD2	1:C:216:PHE:N	2.87	0.42
1:D:97:SER:N	1:D:209:ASP:OD1	2.52	0.42
1:A:172:ILE:CG2	1:A:176:LEU:HD13	2.49	0.42
1:C:88:ASP:CB	1:C:89:PHE:CD1	2.93	0.42
1:B:91:GLY:HA3	1:B:365:ARG:HB3	2.02	0.42
1:B:164:GLU:C	1:B:166:SER:H	2.21	0.42
1:D:189:PHE:CG	1:D:288:PHE:HE2	2.38	0.42
1:A:461:LEU:HD23	1:A:462:GLN:HG2	1.97	0.42
1:C:297:SER:HB3	1:C:357:VAL:CG2	2.48	0.42
1:C:38:LEU:HD23	1:C:38:LEU:HA	1.70	0.42
1:D:38:LEU:HD23	1:D:38:LEU:HA	1.75	0.42
1:A:125:ARG:HA	1:A:128:LEU:HD12	2.02	0.42
1:D:413:ALA:CA	4:D:601:HOH:O	2.67	0.42
1:B:148:CYS:O	1:B:152:ARG:N	2.53	0.42
1:B:350:GLU:CD	1:B:404:ARG:O	2.58	0.42
1:A:80:GLU:CG	1:A:84:ARG:HD3	2.42	0.42
1:A:93:PRO:CD	1:A:365:ARG:HB2	2.41	0.42
1:C:171:SER:O	1:C:175:TYR:CE1	2.73	0.42
1:C:311:GLU:HG3	1:C:312:ILE:N	2.34	0.42
1:D:177:THR:O	1:D:179:GLY:N	2.53	0.42
1:D:292:THR:OG1	1:D:293:GLU:N	2.50	0.42
1:C:463:PRO:HB2	1:C:465:PRO:CD	2.46	0.42
1:A:34:VAL:CG2	1:A:62:LEU:HA	2.49	0.42
1:C:458:LEU:HG	1:C:458:LEU:H	1.67	0.42
1:C:80:GLU:CD	1:C:372:ILE:O	2.59	0.42
1:D:353:ARG:HH12	1:D:400:PRO:CA	2.29	0.42
1:B:333:VAL:HB	1:B:443:ARG:HH12	1.84	0.42
1:B:443:ARG:HG3	1:B:443:ARG:HH11	1.84	0.42
1:D:311:GLU:HG3	1:D:312:ILE:N	2.34	0.42
1:D:108:ILE:C	1:D:110:LEU:H	2.22	0.42
1:D:180:ASN:ND2	1:D:185:LEU:HD13	2.35	0.42
1:A:196:LEU:HD21	1:A:232:ARG:HD3	2.02	0.42
1:A:154:GLN:C	1:A:156:GLY:H	2.23	0.42
1:A:475:PRO:HG2	1:A:477:GLN:HE21	1.81	0.42
1:A:39:HIS:O	1:A:41:LEU:O	2.37	0.42
1:B:470:ASN:HA	1:B:471:LEU:HD12	2.01	0.42
1:C:260:LEU:HA	1:C:280:VAL:HG21	2.02	0.42
1:A:89:PHE:CD2	1:A:383:VAL:HG21	2.55	0.42
1:C:375:TYR:CD2	1:C:375:TYR:N	2.88	0.42
1:A:83:ILE:HD11	1:A:422:CYS:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:396:VAL:HG12	1:D:415:PRO:HG2	2.01	0.42
1:B:309:HIS:CE1	1:B:403:PHE:HB3	2.53	0.42
1:B:391:HIS:NE2	1:B:417:ALA:HB1	2.35	0.42
1:D:189:PHE:CZ	1:D:235:MET:HB3	2.55	0.41
1:B:246:SER:HB3	1:B:252:TRP:CZ2	2.55	0.41
1:C:173:ILE:HG12	1:C:288:PHE:CZ	2.55	0.41
1:C:31:PRO:HG2	1:C:61:ARG:CG	2.40	0.41
1:C:336:LYS:O	1:C:336:LYS:HG3	2.20	0.41
1:D:298:THR:OG1	1:D:357:VAL:CG2	2.68	0.41
1:C:69:VAL:HG12	1:C:70:VAL:N	2.35	0.41
1:B:308:HIS:C	1:B:309:HIS:CD2	2.94	0.41
1:D:141:ASP:OD1	1:D:443:ARG:CZ	2.68	0.41
1:C:199:THR:O	1:C:225:LEU:HD12	2.20	0.41
1:D:168:LEU:CD2	1:D:292:THR:CB	2.97	0.41
1:B:62:LEU:CD1	1:B:64:LEU:HD21	2.50	0.41
1:B:116:LEU:HD23	1:B:117:TRP:HA	1.95	0.41
1:B:464:ASP:H	1:B:465:PRO:HD3	1.85	0.41
1:A:178:PHE:CZ	1:A:242:ARG:HB3	2.56	0.41
1:C:373:PHE:CD1	1:C:373:PHE:O	2.73	0.41
1:B:459:PRO:HB2	1:B:472:LYS:HZ3	1.81	0.41
1:D:313:GLN:HE22	1:D:450:LEU:CB	2.32	0.41
1:D:298:THR:OG1	1:D:357:VAL:HG23	2.20	0.41
1:C:98:TYR:CD1	1:C:110:LEU:HD22	2.55	0.41
1:C:141:ASP:HA	1:C:439:VAL:HG11	2.02	0.41
1:B:180:ASN:O	1:B:181:LYS:HB3	2.20	0.41
1:C:280:VAL:HG12	1:C:281:HIS:N	2.32	0.41
1:A:263:VAL:CG1	1:A:275:LEU:HD12	2.40	0.41
1:D:212:PRO:CD	1:D:213:PHE:H	2.33	0.41
1:A:335:TYR:O	1:A:338:ARG:HB3	2.21	0.41
1:D:414:ASN:HA	1:D:414:ASN:HD22	1.66	0.41
1:D:75:LYS:CA	1:D:78:ILE:HG22	2.50	0.41
1:B:298:THR:OG1	1:B:357:VAL:HG23	2.20	0.41
1:B:215:ARG:HB3	1:B:215:ARG:HE	1.68	0.41
1:D:387:LEU:HD21	1:D:418:LEU:HB2	2.02	0.41
1:C:182:GLU:O	1:C:186:VAL:HG23	2.20	0.41
1:A:443:ARG:HG3	1:A:443:ARG:HH11	1.85	0.41
1:C:219:ASN:CB	1:C:220:PRO:HD2	2.51	0.41
1:C:167:LEU:HD22	1:C:168:LEU:N	2.35	0.41
1:D:71:VAL:C	1:D:72:LEU:HD23	2.40	0.41
1:B:473:VAL:HG13	1:B:474:GLN:H	1.85	0.41
1:D:396:VAL:HB	1:D:397:TRP:CE3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:100:LEU:HD11	1:D:222:LEU:CD1	2.50	0.41
1:D:112:ASP:OD2	1:D:365:ARG:NH1	2.53	0.41
1:D:181:LYS:HG2	1:D:181:LYS:O	2.20	0.41
1:B:185:LEU:HD11	1:B:239:GLN:HE22	1.84	0.41
1:D:199:THR:O	1:D:225:LEU:HD12	2.19	0.41
1:A:172:ILE:HG21	1:A:287:LEU:O	2.20	0.41
1:C:214:LEU:HD21	1:C:216:PHE:CD2	2.54	0.41
1:C:85:LYS:HB3	1:C:88:ASP:OD2	2.20	0.41
1:C:79:GLU:HG2	1:C:83:ILE:HD12	2.02	0.41
1:D:364:HIS:CD2	1:D:385:PRO:HG3	2.56	0.41
1:B:37:PHE:O	1:B:65:GLY:O	2.39	0.41
1:B:208:LEU:CD1	1:B:222:LEU:HD13	2.50	0.41
1:D:215:ARG:CG	1:D:215:ARG:NH2	2.83	0.41
1:C:473:VAL:O	1:C:475:PRO:HD3	2.21	0.41
1:D:61:ARG:HA	1:D:70:VAL:HA	2.03	0.41
1:D:76:ARG:HG3	1:D:77:THR:N	2.36	0.41
1:B:74:SER:HG	1:B:77:THR:CB	2.33	0.41
1:B:354:LEU:O	1:B:355:ARG:CD	2.66	0.41
1:D:111:GLY:C	1:D:425:ARG:HH22	2.19	0.41
1:C:45:LEU:N	1:C:46:PRO:CD	2.82	0.41
1:C:278:GLY:O	1:C:281:HIS:HB3	2.21	0.41
1:A:89:PHE:CE1	1:A:372:ILE:CG1	2.86	0.41
1:B:408:PHE:CD2	1:B:410:GLU:N	2.69	0.41
1:B:324:LEU:CB	1:B:340:ARG:HB3	2.48	0.41
1:D:240:LEU:CD2	1:D:260:LEU:HD13	2.50	0.41
1:B:369:PRO:HD3	1:B:379:GLU:OE2	2.20	0.41
1:D:177:THR:C	1:D:179:GLY:N	2.74	0.41
1:C:307:LEU:HD11	1:C:477:GLN:NE2	2.35	0.41
1:D:374:GLY:O	1:D:375:TYR:HD2	1.99	0.41
1:D:299:LEU:O	1:D:303:VAL:HG23	2.21	0.41
1:A:341:LEU:HD13	1:A:344:LEU:CD1	2.40	0.41
1:B:30:LEU:HD12	1:B:30:LEU:HA	1.93	0.41
1:A:30:LEU:HD12	1:A:376:ASP:O	2.21	0.41
1:C:108:ILE:HD11	1:C:121:LYS:CD	2.50	0.41
1:B:311:GLU:HG3	1:B:312:ILE:N	2.34	0.41
1:B:336:LYS:HD3	1:C:326:PRO:HG2	2.02	0.41
1:D:420:PHE:CG	1:D:430:GLU:HG2	2.56	0.41
1:A:473:VAL:HG12	1:A:474:GLN:OE1	2.21	0.41
1:A:463:PRO:O	1:A:466:TYR:HD1	1.90	0.41
1:B:100:LEU:HD23	1:B:100:LEU:O	2.20	0.41
1:C:173:ILE:HA	1:C:288:PHE:CZ	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:202:HIS:CE1	1:D:203:TRP:CD1	3.09	0.41
1:D:211:VAL:CG1	1:D:214:LEU:HB2	2.38	0.41
1:A:337:ASP:HA	1:A:340:ARG:HG2	2.02	0.41
1:A:374:GLY:HA3	1:A:375:TYR:CE2	2.56	0.41
1:C:410:GLU:C	1:C:412:GLY:N	2.73	0.41
1:D:232:ARG:HD2	1:D:285:VAL:HG11	2.01	0.41
1:B:78:ILE:CD1	1:B:385:PRO:HB2	2.51	0.41
1:B:307:LEU:HD11	1:B:477:GLN:CD	2.40	0.41
1:B:112:ASP:CG	1:B:365:ARG:CZ	2.88	0.41
1:C:252:TRP:HB2	1:C:257:ASP:CG	2.41	0.41
1:C:69:VAL:HG13	1:C:382:VAL:CB	2.48	0.41
1:B:354:LEU:C	1:B:355:ARG:HD3	2.41	0.41
1:D:137:GLU:OE1	1:D:334:THR:HG23	2.21	0.41
1:B:76:ARG:HG2	1:B:76:ARG:H	1.62	0.41
1:A:467:CYS:HB3	1:A:468:GLY:H	1.72	0.41
1:D:472:LYS:HG3	1:D:472:LYS:HZ3	1.63	0.41
1:C:62:LEU:HD21	1:C:64:LEU:CA	2.51	0.41
1:B:243:HIS:NE2	1:B:256:THR:HB	2.36	0.41
1:C:159:VAL:HG12	1:C:476:PHE:CD2	2.41	0.41
1:A:41:LEU:H	1:A:41:LEU:HG	1.21	0.41
1:A:189:PHE:CD2	1:A:289:ILE:CD1	3.04	0.41
1:B:460:SER:N	1:B:472:LYS:HZ1	2.19	0.41
1:A:344:LEU:C	1:A:346:ALA:N	2.74	0.41
1:B:443:ARG:HG3	1:B:443:ARG:NH1	2.36	0.41
1:A:202:HIS:O	1:A:203:TRP:C	2.59	0.41
1:A:44:ASN:C	1:A:46:PRO:HD2	2.42	0.40
1:C:177:THR:C	1:C:179:GLY:N	2.74	0.40
1:C:160:THR:OG1	1:C:161:ILE:N	2.53	0.40
1:A:143:LEU:HD13	1:A:171:SER:CA	2.51	0.40
1:A:143:LEU:HD21	1:A:181:LYS:HD2	2.03	0.40
1:B:437:LEU:HD11	2:B:500:HEM:HBB1	2.02	0.40
1:A:70:VAL:HG12	1:A:381:MET:HG3	2.04	0.40
1:D:304:ALA:HB2	1:D:472:LYS:HE3	2.02	0.40
1:C:352:LEU:HD13	1:C:420:PHE:HE2	1.86	0.40
1:B:423:GLY:O	1:B:424:ALA:C	2.59	0.40
1:C:178:PHE:C	1:C:180:ASN:H	2.25	0.40
1:A:214:LEU:HD21	1:A:216:PHE:HD2	1.78	0.40
1:B:291:GLY:O	1:B:295:THR:OG1	2.40	0.40
1:D:322:ARG:NH2	1:D:326:PRO:HB3	2.36	0.40
1:A:233:ASP:O	1:A:237:GLU:HG3	2.21	0.40
1:B:125:ARG:HH12	1:B:426:VAL:CG2	2.34	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:432:LEU:O	1:B:432:LEU:HD23	2.21	0.40
1:C:177:THR:HG23	1:C:239:GLN:CG	2.51	0.40
1:A:329:SER:O	1:A:331:SER:OG	2.37	0.40
1:A:443:ARG:NH1	1:A:443:ARG:HG3	2.37	0.40
1:D:178:PHE:N	1:D:243:HIS:NE2	2.69	0.40
1:C:59:VAL:HG22	1:C:72:LEU:HD22	2.02	0.40
1:D:432:LEU:C	1:D:432:LEU:HD22	2.41	0.40
1:A:50:LEU:O	1:A:53:THR:CB	2.68	0.40
1:A:78:ILE:CG2	1:A:418:LEU:HD11	2.51	0.40
1:C:338:ARG:HA	1:C:438:PHE:CZ	2.56	0.40
1:B:471:LEU:N	1:B:471:LEU:CD1	2.33	0.40
1:D:376:ASP:HA	4:D:606:HOH:O	2.20	0.40
1:B:460:SER:H	1:B:472:LYS:HZ1	1.68	0.40
1:C:31:PRO:HA	1:C:375:TYR:HD1	1.77	0.40
1:C:69:VAL:HG22	1:C:382:VAL:HB	2.04	0.40
1:D:443:ARG:HG3	1:D:443:ARG:HH11	1.87	0.40
1:B:299:LEU:O	1:B:303:VAL:HG23	2.21	0.40
1:B:299:LEU:HD13	1:B:440:VAL:HG11	2.03	0.40
1:B:379:GLU:C	1:B:381:MET:H	2.24	0.40
1:A:187:HIS:CE1	1:B:238:LYS:HE2	2.57	0.40
1:A:133:ARG:HG2	1:A:133:ARG:HH11	1.86	0.40
1:B:400:PRO:HD2	1:B:401:HIS:H	1.86	0.40
1:B:40:LEU:C	1:B:40:LEU:HD13	2.37	0.40
1:A:64:LEU:HD12	1:A:69:VAL:HG21	2.02	0.40
1:B:291:GLY:HA2	2:B:500:HEM:HMC3	2.03	0.40
1:B:74:SER:OG	1:B:77:THR:CB	2.70	0.40
1:A:76:ARG:HB2	1:A:76:ARG:NH1	2.36	0.40
1:A:267:ARG:O	1:A:268:VAL:CB	2.70	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:404:ARG:NH2	4:A:618:HOH:O[2_556]	1.67	0.53
1:A:39:HIS:NE2	1:D:35:PRO:O[1_556]	2.07	0.13
1:D:38:LEU:N	4:A:601:HOH:O[1_554]	2.13	0.07
1:B:35:PRO:O	1:C:35:PRO:O[1_556]	2.14	0.06
1:B:38:LEU:N	4:C:601:HOH:O[1_556]	2.14	0.06

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	437/496 (88%)	369 (84%)	49 (11%)	19 (4%)	3	19
1	B	428/496 (86%)	357 (83%)	53 (12%)	18 (4%)	3	20
1	C	429/496 (86%)	361 (84%)	50 (12%)	18 (4%)	3	20
1	D	426/496 (86%)	361 (85%)	42 (10%)	23 (5%)	2	14
All	All	1720/1984 (87%)	1448 (84%)	194 (11%)	78 (4%)	3	18

All (78) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	107	ASP
1	A	114	SER
1	A	335	TYR
1	A	338	ARG
1	A	426	VAL
1	A	460	SER
1	A	482	PRO
1	B	114	SER
1	B	324	LEU
1	B	335	TYR
1	B	410	GLU
1	B	411	PRO
1	B	474	GLN
1	B	482	PRO
1	C	107	ASP
1	C	114	SER
1	C	178	PHE
1	C	335	TYR
1	C	409	LEU
1	C	410	GLU
1	C	459	PRO
1	C	475	PRO

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Mol	Chain	Res	Type
1	D	103	GLN
1	D	114	SER
1	D	335	TYR
1	D	375	TYR
1	D	426	VAL
1	A	105	CYS
1	A	373	PHE
1	B	42	GLN
1	B	253	ARG
1	B	361	ALA
1	B	427	CYS
1	B	459	PRO
1	C	86	TRP
1	C	333	VAL
1	D	253	ARG
1	D	324	LEU
1	D	427	CYS
1	D	462	GLN
1	A	42	GLN
1	A	109	SER
1	A	359	PRO
1	A	407	ARG
1	A	461	LEU
1	B	359	PRO
1	C	105	CYS
1	C	203	TRP
1	C	427	CYS
1	C	462	GLN
1	D	105	CYS
1	D	178	PHE
1	D	342	PRO
1	D	450	LEU
1	D	459	PRO
1	A	462	GLN
1	B	429	GLY
1	B	450	LEU
1	B	462	GLN
1	C	42	GLN
1	C	342	PRO
1	A	106	GLN
1	A	333	VAL
1	C	359	PRO

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Mol	Chain	Res	Type
1	D	86	TRP
1	D	373	PHE
1	A	324	LEU
1	B	203	TRP
1	B	455	VAL
1	D	42	GLN
1	D	359	PRO
1	D	465	PRO
1	A	374	GLY
1	C	429	GLY
1	D	463	PRO
1	D	473	VAL
1	D	357	VAL
1	D	410	GLU

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	393/430 (91%)	304 (77%)	89 (23%)	1 5
1	B	387/430 (90%)	314 (81%)	73 (19%)	2 10
1	C	386/430 (90%)	299 (78%)	87 (22%)	1 5
1	D	385/430 (90%)	301 (78%)	84 (22%)	1 6
All	All	1551/1720 (90%)	1218 (78%)	333 (22%)	1 6

All (333) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	PHE
1	A	38	LEU
1	A	40	LEU
1	A	41	LEU
1	A	42	GLN
1	A	44	ASN
1	A	45	LEU

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Mol	Chain	Res	Type
1	A	54	GLN
1	A	56	LEU
1	A	62	LEU
1	A	67	GLN
1	A	85	LYS
1	A	92	ARG
1	A	100	LEU
1	A	102	SER
1	A	103	GLN
1	A	104	ARG
1	A	106	GLN
1	A	108	ILE
1	A	113	TYR
1	A	134	SER
1	A	165	PHE
1	A	167	LEU
1	A	168	LEU
1	A	176	LEU
1	A	178	PHE
1	A	191	ASP
1	A	194	GLN
1	A	196	LEU
1	A	205	ILE
1	A	213	PHE
1	A	214	LEU
1	A	215	ARG
1	A	217	PHE
1	A	244	LYS
1	A	245	GLU
1	A	246	SER
1	A	247	MET
1	A	252	TRP
1	A	253	ARG
1	A	257	ASP
1	A	267	ARG
1	A	275	LEU
1	A	276	LEU
1	A	285	VAL
1	A	286	ASP
1	A	287	LEU
1	A	289	ILE
1	A	292	THR

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Mol	Chain	Res	Type
1	A	293	GLU
1	A	295	THR
1	A	323	GLU
1	A	324	LEU
1	A	330	CYS
1	A	331	SER
1	A	332	ARG
1	A	333	VAL
1	A	334	THR
1	A	335	TYR
1	A	336	LYS
1	A	337	ASP
1	A	343	LEU
1	A	366	THR
1	A	371	SER
1	A	372	ILE
1	A	373	PHE
1	A	375	TYR
1	A	386	ASN
1	A	392	LEU
1	A	404	ARG
1	A	405	PRO
1	A	406	ASP
1	A	407	ARG
1	A	408	PHE
1	A	418	LEU
1	A	422	CYS
1	A	426	VAL
1	A	428	LEU
1	A	445	LEU
1	A	446	GLN
1	A	448	PHE
1	A	449	THR
1	A	451	LEU
1	A	461	LEU
1	A	471	LEU
1	A	472	LYS
1	A	474	GLN
1	A	477	GLN
1	A	482	PRO
1	B	37	PHE
1	B	40	LEU

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Mol	Chain	Res	Type
1	B	41	LEU
1	B	45	LEU
1	B	62	LEU
1	B	66	LEU
1	B	73	ASN
1	B	84	ARG
1	B	87	VAL
1	B	89	PHE
1	B	102	SER
1	B	103	GLN
1	B	104	ARG
1	B	105	CYS
1	B	107	ASP
1	B	110	LEU
1	B	113	TYR
1	B	116	LEU
1	B	167	LEU
1	B	168	LEU
1	B	170	CYS
1	B	172	ILE
1	B	173	ILE
1	B	184	THR
1	B	191	ASP
1	B	194	GLN
1	B	196	LEU
1	B	205	ILE
1	B	213	PHE
1	B	214	LEU
1	B	216	PHE
1	B	218	PRO
1	B	219	ASN
1	B	223	TRP
1	B	231	ASN
1	B	257	ASP
1	B	275	LEU
1	B	286	ASP
1	B	287	LEU
1	B	289	ILE
1	B	293	GLU
1	B	295	THR
1	B	323	GLU
1	B	324	LEU

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Mol	Chain	Res	Type
1	B	343	LEU
1	B	358	VAL
1	B	362	LEU
1	B	373	PHE
1	B	375	TYR
1	B	382	VAL
1	B	386	ASN
1	B	392	LEU
1	B	394	GLU
1	B	395	THR
1	B	402	GLU
1	B	404	ARG
1	B	407	ARG
1	B	408	PHE
1	B	410	GLU
1	B	416	SER
1	B	418	LEU
1	B	422	CYS
1	B	426	VAL
1	B	428	LEU
1	B	461	LEU
1	B	464	ASP
1	B	466	TYR
1	B	470	ASN
1	B	471	LEU
1	B	474	GLN
1	B	476	PHE
1	B	480	LEU
1	B	482	PRO
1	C	40	LEU
1	C	41	LEU
1	C	45	LEU
1	C	53	THR
1	C	54	GLN
1	C	55	LYS
1	C	56	LEU
1	C	59	VAL
1	C	62	LEU
1	C	66	LEU
1	C	67	GLN
1	C	70	VAL
1	C	89	PHE

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Mol	Chain	Res	Type
1	C	101	VAL
1	C	102	SER
1	C	104	ARG
1	C	105	CYS
1	C	106	GLN
1	C	108	ILE
1	C	113	TYR
1	C	116	LEU
1	C	125	ARG
1	C	126	SER
1	C	128	LEU
1	C	129	LEU
1	C	137	GLU
1	C	160	THR
1	C	162	GLN
1	C	163	LYS
1	C	165	PHE
1	C	167	LEU
1	C	168	LEU
1	C	169	THR
1	C	175	TYR
1	C	176	LEU
1	C	177	THR
1	C	180	ASN
1	C	191	ASP
1	C	194	GLN
1	C	196	LEU
1	C	205	ILE
1	C	217	PHE
1	C	219	ASN
1	C	247	MET
1	C	252	TRP
1	C	253	ARG
1	C	257	ASP
1	C	275	LEU
1	C	276	LEU
1	C	279	HIS
1	C	280	VAL
1	C	288	PHE
1	C	289	ILE
1	C	293	GLU
1	C	295	THR

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Mol	Chain	Res	Type
1	C	323	GLU
1	C	324	LEU
1	C	334	THR
1	C	343	LEU
1	C	354	LEU
1	C	357	VAL
1	C	366	THR
1	C	371	SER
1	C	372	ILE
1	C	373	PHE
1	C	386	ASN
1	C	388	GLN
1	C	404	ARG
1	C	406	ASP
1	C	407	ARG
1	C	408	PHE
1	C	409	LEU
1	C	418	LEU
1	C	425	ARG
1	C	426	VAL
1	C	428	LEU
1	C	448	PHE
1	C	449	THR
1	C	450	LEU
1	C	451	LEU
1	C	458	LEU
1	C	466	TYR
1	C	470	ASN
1	C	472	LYS
1	C	474	GLN
1	C	476	PHE
1	C	479	ARG
1	D	40	LEU
1	D	41	LEU
1	D	45	LEU
1	D	53	THR
1	D	54	GLN
1	D	55	LYS
1	D	56	LEU
1	D	62	LEU
1	D	87	VAL
1	D	103	GLN

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Mol	Chain	Res	Type
1	D	106	GLN
1	D	110	LEU
1	D	113	TYR
1	D	114	SER
1	D	115	LEU
1	D	116	LEU
1	D	136	MET
1	D	160	THR
1	D	162	GLN
1	D	163	LYS
1	D	168	LEU
1	D	169	THR
1	D	172	ILE
1	D	176	LEU
1	D	178	PHE
1	D	180	ASN
1	D	191	ASP
1	D	194	GLN
1	D	196	LEU
1	D	202	HIS
1	D	205	ILE
1	D	208	LEU
1	D	213	PHE
1	D	214	LEU
1	D	215	ARG
1	D	216	PHE
1	D	223	TRP
1	D	242	ARG
1	D	244	LYS
1	D	245	GLU
1	D	247	MET
1	D	248	VAL
1	D	252	TRP
1	D	253	ARG
1	D	257	ASP
1	D	275	LEU
1	D	276	LEU
1	D	288	PHE
1	D	289	ILE
1	D	292	THR
1	D	293	GLU
1	D	294	THR

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Mol	Chain	Res	Type
1	D	297	SER
1	D	323	GLU
1	D	324	LEU
1	D	334	THR
1	D	337	ASP
1	D	343	LEU
1	D	371	SER
1	D	372	ILE
1	D	373	PHE
1	D	376	ASP
1	D	377	ILE
1	D	386	ASN
1	D	402	GLU
1	D	404	ARG
1	D	406	ASP
1	D	407	ARG
1	D	408	PHE
1	D	410	GLU
1	D	414	ASN
1	D	418	LEU
1	D	422	CYS
1	D	426	VAL
1	D	430	GLU
1	D	432	LEU
1	D	434	ARG
1	D	448	PHE
1	D	449	THR
1	D	450	LEU
1	D	461	LEU
1	D	472	LYS
1	D	474	GLN
1	D	480	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (70) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	GLN
1	A	142	GLN
1	A	145	GLN
1	A	187	HIS
1	A	202	HIS
1	A	231	ASN

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Mol	Chain	Res	Type
1	A	239	GLN
1	A	243	HIS
1	A	261	GLN
1	A	266	GLN
1	A	309	HIS
1	A	313	GLN
1	A	317	GLN
1	A	345	ASN
1	A	386	ASN
1	A	401	HIS
1	A	414	ASN
1	A	477	GLN
1	B	73	ASN
1	B	103	GLN
1	B	142	GLN
1	B	145	GLN
1	B	202	HIS
1	B	206	GLN
1	B	231	ASN
1	B	234	HIS
1	B	239	GLN
1	B	274	GLN
1	B	309	HIS
1	B	313	GLN
1	B	317	GLN
1	B	345	ASN
1	B	386	ASN
1	B	414	ASN
1	B	481	GLN
1	C	39	HIS
1	C	48	HIS
1	C	54	GLN
1	C	106	GLN
1	C	142	GLN
1	C	145	GLN
1	C	162	GLN
1	C	180	ASN
1	C	202	HIS
1	C	239	GLN
1	C	313	GLN
1	C	317	GLN
1	C	345	ASN

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Mol	Chain	Res	Type
1	C	386	ASN
1	C	414	ASN
1	C	446	GLN
1	C	481	GLN
1	D	54	GLN
1	D	67	GLN
1	D	103	GLN
1	D	106	GLN
1	D	120	HIS
1	D	142	GLN
1	D	145	GLN
1	D	154	GLN
1	D	180	ASN
1	D	231	ASN
1	D	239	GLN
1	D	308	HIS
1	D	309	HIS
1	D	313	GLN
1	D	345	ASN
1	D	386	ASN
1	D	401	HIS
1	D	481	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

12 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	2.67	9 (30%)	24,82,82	3.05	11 (45%)
3	3QZ	A	501	-	27,27,27	1.21	3 (11%)	42,45,45	1.53	11 (26%)
3	3QZ	A	502	-	27,27,27	1.11	3 (11%)	42,45,45	1.39	9 (21%)
2	HEM	B	500	-	30,50,50	2.68	9 (30%)	24,82,82	3.02	11 (45%)
3	3QZ	B	501	-	27,27,27	1.18	3 (11%)	42,45,45	1.58	11 (26%)
3	3QZ	B	502	-	27,27,27	1.11	3 (11%)	42,45,45	1.41	8 (19%)
2	HEM	C	500	-	30,50,50	2.64	9 (30%)	24,82,82	2.95	10 (41%)
3	3QZ	C	501	-	27,27,27	1.06	4 (14%)	42,45,45	1.46	10 (23%)
3	3QZ	C	502	-	27,27,27	1.14	2 (7%)	42,45,45	1.41	9 (21%)
2	HEM	D	500	-	30,50,50	2.53	9 (30%)	24,82,82	2.89	11 (45%)
3	3QZ	D	501	-	27,27,27	1.31	3 (11%)	42,45,45	1.61	10 (23%)
3	3QZ	D	502	-	27,27,27	1.34	2 (7%)	42,45,45	1.41	7 (16%)

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
3	3QZ	A	501	-	-	0/6/68/68	0/4/4/4
3	3QZ	A	502	-	-	0/6/68/68	0/4/4/4
2	HEM	B	500	-	-	0/10/54/54	0/0/8/8
3	3QZ	B	501	-	-	0/6/68/68	0/4/4/4
3	3QZ	B	502	-	-	0/6/68/68	0/4/4/4
2	HEM	C	500	-	-	0/10/54/54	0/0/8/8
3	3QZ	C	501	-	-	0/6/68/68	0/4/4/4
3	3QZ	C	502	-	-	0/6/68/68	0/4/4/4
2	HEM	D	500	-	-	0/10/54/54	0/0/8/8
3	3QZ	D	501	-	-	0/6/68/68	0/4/4/4
3	3QZ	D	502	-	-	0/6/68/68	0/4/4/4

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	HEM	C3B-C4B	-8.59	1.44	1.51
2	B	500	HEM	C3B-C4B	-8.24	1.44	1.51
2	C	500	HEM	C3B-C4B	-7.81	1.44	1.51
2	D	500	HEM	C3B-C4B	-6.77	1.45	1.51
2	D	500	HEM	C2D-C3D	-6.48	1.35	1.54
2	B	500	HEM	C2D-C3D	-6.44	1.35	1.54
2	A	500	HEM	C2D-C3D	-6.29	1.35	1.54
2	C	500	HEM	C2D-C3D	-6.27	1.35	1.54
2	C	500	HEM	C3D-C4D	-4.92	1.45	1.51
2	B	500	HEM	C3D-C4D	-4.61	1.45	1.51
2	D	500	HEM	C3D-C4D	-4.60	1.45	1.51
2	A	500	HEM	C3D-C4D	-4.16	1.46	1.51
3	D	501	3QZ	CAG-CAQ	-3.06	1.38	1.45
3	D	502	3QZ	CAG-CAQ	-2.99	1.39	1.45
3	B	501	3QZ	CAG-CAQ	-2.63	1.39	1.45
3	A	501	3QZ	CAG-CAQ	-2.60	1.39	1.45
3	C	502	3QZ	CAG-CAQ	-2.56	1.39	1.45
2	B	500	HEM	C2C-C1C	-2.55	1.47	1.52
2	C	500	HEM	C2C-C1C	-2.47	1.47	1.52
3	B	502	3QZ	CAG-CAQ	-2.43	1.40	1.45
3	A	502	3QZ	CAG-CAQ	-2.35	1.40	1.45
2	D	500	HEM	C2C-C1C	-2.35	1.48	1.52
3	A	501	3QZ	CAX-CAW	-2.32	1.53	1.57
3	D	501	3QZ	CAX-CAW	-2.31	1.53	1.57
3	B	501	3QZ	CAX-CAW	-2.25	1.53	1.57
3	C	501	3QZ	CAX-CAW	-2.21	1.53	1.57
3	C	501	3QZ	CAG-CAQ	-2.13	1.40	1.45
2	A	500	HEM	C2C-C1C	-2.08	1.48	1.52
2	C	500	HEM	C2D-C1D	-2.06	1.45	1.51
3	C	501	3QZ	CAH-CAR	2.03	1.53	1.50
2	D	500	HEM	C3C-CAC	2.03	1.55	1.51
2	B	500	HEM	FE-NC	2.09	2.04	1.95
3	B	502	3QZ	CAH-CAR	2.09	1.53	1.50
2	A	500	HEM	FE-NC	2.10	2.04	1.95
3	A	502	3QZ	CAH-CAR	2.11	1.53	1.50
2	B	500	HEM	C4C-NC	2.18	1.38	1.36
2	D	500	HEM	C1C-NC	2.25	1.38	1.36
2	D	500	HEM	CAA-C2A	2.29	1.55	1.52
2	C	500	HEM	C4C-NC	2.47	1.39	1.36
2	A	500	HEM	C4C-NC	2.61	1.39	1.36
2	C	500	HEM	CAA-C2A	2.71	1.56	1.52
3	C	501	3QZ	CAG-CAR	2.78	1.38	1.34
2	B	500	HEM	C1C-NC	2.87	1.39	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	HEM	C1C-NC	3.10	1.39	1.36
3	B	502	3QZ	CAG-CAR	3.28	1.38	1.34
3	A	502	3QZ	CAG-CAR	3.33	1.38	1.34
3	B	501	3QZ	CAG-CAR	3.51	1.39	1.34
3	C	502	3QZ	CAG-CAR	3.69	1.39	1.34
3	A	501	3QZ	CAG-CAR	3.72	1.39	1.34
2	D	500	HEM	CBB-CAB	4.11	1.53	1.29
2	C	500	HEM	CBB-CAB	4.17	1.53	1.29
2	A	500	HEM	CBB-CAB	4.18	1.53	1.29
2	A	500	HEM	CBC-CAC	4.31	1.54	1.29
2	B	500	HEM	CBB-CAB	4.38	1.54	1.29
2	C	500	HEM	CBC-CAC	4.39	1.54	1.29
3	D	501	3QZ	CAG-CAR	4.41	1.40	1.34
2	B	500	HEM	CBC-CAC	4.42	1.54	1.29
2	D	500	HEM	CBC-CAC	4.55	1.55	1.29
3	D	502	3QZ	CAG-CAR	4.80	1.40	1.34

All (118) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	500	HEM	C3C-CAC-CBC	-6.92	113.84	124.46
2	B	500	HEM	C3B-CAB-CBB	-6.80	114.03	124.46
2	A	500	HEM	C3B-CAB-CBB	-6.74	114.11	124.46
2	C	500	HEM	C3B-CAB-CBB	-6.58	114.37	124.46
2	B	500	HEM	C3C-CAC-CBC	-6.52	114.46	124.46
2	C	500	HEM	C3C-CAC-CBC	-6.39	114.66	124.46
2	D	500	HEM	C3C-CAC-CBC	-6.28	114.83	124.46
2	D	500	HEM	C3B-CAB-CBB	-6.08	115.13	124.46
3	B	501	3QZ	CAO-CAX-CAP	-3.79	109.40	113.70
3	C	502	3QZ	CAO-CAX-CAP	-3.69	109.52	113.70
3	D	502	3QZ	CAO-CAX-CAP	-3.68	109.53	113.70
3	A	501	3QZ	CAO-CAX-CAP	-3.54	109.69	113.70
3	D	501	3QZ	CAO-CAX-CAP	-3.27	109.99	113.70
3	A	501	3QZ	CAX-CAW-CAU	-3.11	96.30	99.81
3	A	502	3QZ	CAO-CAX-CAP	-3.08	110.21	113.70
3	D	501	3QZ	CAJ-CAS-CAU	-3.06	106.94	112.02
3	B	501	3QZ	CAX-CAW-CAU	-3.06	96.36	99.81
3	D	501	3QZ	CAH-CAR-CAG	-3.05	117.02	120.89
3	C	501	3QZ	CAO-CAX-CAP	-2.97	110.34	113.70
3	D	501	3QZ	CAL-CAU-CAS	-2.92	114.42	119.03
3	B	502	3QZ	CAO-CAX-CAP	-2.89	110.42	113.70
2	B	500	HEM	CAA-C2A-C1A	-2.86	123.90	127.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	500	HEM	CMA-C3A-C4A	-2.86	123.64	128.36
3	C	501	3QZ	CAL-CAU-CAS	-2.84	114.55	119.03
3	A	502	3QZ	CAL-CAU-CAW	-2.80	100.13	103.75
3	D	501	3QZ	CAX-CAW-CAU	-2.79	96.66	99.81
3	B	501	3QZ	CAL-CAU-CAS	-2.74	114.69	119.03
3	B	502	3QZ	CAH-CAR-CAG	-2.73	117.43	120.89
3	C	501	3QZ	CAJ-CAS-CAU	-2.72	107.52	112.02
3	A	501	3QZ	CAH-CAR-CAG	-2.67	117.50	120.89
3	C	502	3QZ	CAL-CAU-CAS	-2.65	114.83	119.03
3	B	501	3QZ	CAH-CAR-CAG	-2.63	117.55	120.89
3	B	502	3QZ	CAL-CAU-CAS	-2.62	114.88	119.03
2	B	500	HEM	CMA-C3A-C4A	-2.61	124.05	128.36
3	B	502	3QZ	CAJ-CAS-CAU	-2.59	107.73	112.02
3	C	501	3QZ	CAH-CAR-CAG	-2.58	117.62	120.89
3	A	501	3QZ	CAL-CAU-CAS	-2.57	114.96	119.03
3	C	501	3QZ	CAX-CAW-CAU	-2.56	96.92	99.81
3	A	502	3QZ	CAH-CAR-CAG	-2.55	117.65	120.89
3	D	501	3QZ	CAO-CAL-CAU	-2.54	99.53	104.44
2	A	500	HEM	CAA-C2A-C1A	-2.47	124.32	127.01
3	B	501	3QZ	CAJ-CAS-CAU	-2.46	107.94	112.02
3	A	501	3QZ	CAJ-CAS-CAU	-2.46	107.95	112.02
3	C	501	3QZ	CAL-CAU-CAW	-2.44	100.59	103.75
3	A	502	3QZ	CAJ-CAS-CAU	-2.43	107.99	112.02
3	C	502	3QZ	CAL-CAU-CAW	-2.38	100.67	103.75
3	D	502	3QZ	CAL-CAU-CAW	-2.37	100.68	103.75
2	D	500	HEM	CMA-C3A-C4A	-2.31	124.54	128.36
3	D	502	3QZ	CAL-CAU-CAS	-2.28	115.42	119.03
3	D	501	3QZ	CAL-CAU-CAW	-2.25	100.84	103.75
3	C	501	3QZ	CAO-CAL-CAU	-2.24	100.11	104.44
3	B	501	3QZ	CAO-CAL-CAU	-2.20	100.17	104.44
3	B	501	3QZ	CAL-CAU-CAW	-2.17	100.94	103.75
2	D	500	HEM	CAA-C2A-C1A	-2.16	124.66	127.01
3	A	501	3QZ	CAO-CAL-CAU	-2.16	100.26	104.44
2	C	500	HEM	CAA-C2A-C1A	-2.16	124.67	127.01
3	B	502	3QZ	CAX-CAW-CAU	-2.15	97.39	99.81
3	A	501	3QZ	CAL-CAU-CAW	-2.12	101.01	103.75
3	A	502	3QZ	CAL-CAU-CAS	-2.11	115.69	119.03
3	B	502	3QZ	CAL-CAU-CAW	-2.09	101.05	103.75
3	C	502	3QZ	CAK-CAN-CAW	-2.08	109.25	112.80
3	A	502	3QZ	CAO-CAL-CAU	-2.07	100.42	104.44
3	C	502	3QZ	CAJ-CAS-CAU	-2.04	108.64	112.02
3	C	501	3QZ	CAK-CAN-CAW	-2.04	109.33	112.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	502	3QZ	CAH-CAR-CAG	-2.03	118.31	120.89
3	D	502	3QZ	CAH-CAR-CAG	-2.02	118.33	120.89
3	A	501	3QZ	CAK-CAN-CAW	-2.01	109.39	112.80
3	B	501	3QZ	OAF-CAX-CAP	2.02	110.90	107.65
3	A	502	3QZ	CAI-CAQ-CAG	2.02	119.81	116.70
3	A	501	3QZ	CAO-CAX-CAW	2.05	105.17	103.20
3	B	501	3QZ	CAI-CAQ-CAG	2.17	120.05	116.70
3	C	502	3QZ	OAF-CAX-CAP	2.25	111.29	107.65
3	D	501	3QZ	OAF-CAX-CAP	2.26	111.30	107.65
3	D	502	3QZ	CAC-CAW-CAX	2.29	111.79	109.13
2	B	500	HEM	C3B-C4B-CHC	2.30	126.40	123.16
3	A	502	3QZ	CAC-CAW-CAX	2.32	111.83	109.13
2	A	500	HEM	C3B-C4B-CHC	2.33	126.45	123.16
3	A	501	3QZ	CAC-CAW-CAX	2.34	111.85	109.13
2	D	500	HEM	C3B-C4B-CHC	2.38	126.52	123.16
3	C	501	3QZ	CAC-CAW-CAX	2.40	111.92	109.13
3	C	502	3QZ	CAH-CAR-CAV	2.51	119.57	116.71
3	D	502	3QZ	OAF-CAX-CAP	2.61	111.86	107.65
3	D	501	3QZ	CAC-CAW-CAX	2.68	112.25	109.13
2	C	500	HEM	C3B-C4B-CHC	2.73	127.00	123.16
3	A	502	3QZ	CAH-CAR-CAV	2.76	119.84	116.71
3	D	502	3QZ	CAH-CAR-CAV	2.78	119.86	116.71
3	C	502	3QZ	CAC-CAW-CAX	2.79	112.38	109.13
3	B	501	3QZ	CAC-CAW-CAX	2.81	112.40	109.13
3	B	502	3QZ	CAC-CAW-CAX	2.82	112.41	109.13
2	C	500	HEM	C2D-C3D-C4D	2.84	106.32	101.50
2	B	500	HEM	CMD-C2D-C3D	2.96	127.44	114.35
2	A	500	HEM	C2D-C3D-C4D	2.96	106.53	101.50
2	D	500	HEM	CMD-C2D-C3D	2.97	127.47	114.35
2	D	500	HEM	C2D-C3D-C4D	3.00	106.58	101.50
3	C	501	3QZ	CAH-CAR-CAV	3.00	120.12	116.71
2	B	500	HEM	C2D-C3D-C4D	3.06	106.68	101.50
2	A	500	HEM	CMD-C2D-C3D	3.06	127.88	114.35
3	B	502	3QZ	CAH-CAR-CAV	3.06	120.19	116.71
2	C	500	HEM	CMD-C2D-C3D	3.11	128.10	114.35
3	A	501	3QZ	CAH-CAR-CAV	3.17	120.31	116.71
3	B	501	3QZ	CAH-CAR-CAV	3.28	120.43	116.71
3	D	501	3QZ	CAH-CAR-CAV	3.35	120.52	116.71
2	C	500	HEM	CAD-C3D-C4D	4.02	126.64	112.47
2	B	500	HEM	CAD-C3D-C4D	4.07	126.84	112.47
2	A	500	HEM	CAD-C3D-C4D	4.08	126.84	112.47
2	D	500	HEM	CAD-C3D-C4D	4.13	127.05	112.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	500	HEM	CMB-C2B-C3B	4.53	127.83	116.53
2	D	500	HEM	CAD-C3D-C2D	4.57	126.37	113.22
2	B	500	HEM	CAD-C3D-C2D	4.61	126.48	113.22
2	A	500	HEM	CAD-C3D-C2D	4.66	126.63	113.22
2	B	500	HEM	CMB-C2B-C3B	4.69	128.25	116.53
2	C	500	HEM	CMB-C2B-C3B	4.72	128.31	116.53
2	A	500	HEM	CMB-C2B-C3B	4.76	128.40	116.53
2	C	500	HEM	CAD-C3D-C2D	4.81	127.05	113.22
2	A	500	HEM	CMC-C2C-C3C	5.00	129.00	116.53
2	C	500	HEM	CMC-C2C-C3C	5.07	129.19	116.53
2	B	500	HEM	CMC-C2C-C3C	5.08	129.21	116.53
2	D	500	HEM	CMC-C2C-C3C	5.12	129.31	116.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 97 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	HEM	6	0
3	A	501	3QZ	14	0
3	A	502	3QZ	5	0
2	B	500	HEM	5	0
3	B	501	3QZ	12	0
3	B	502	3QZ	8	0
2	C	500	HEM	13	0
3	C	501	3QZ	12	0
3	C	502	3QZ	1	0
2	D	500	HEM	11	0
3	D	501	3QZ	10	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	445/496 (89%)	-0.02	6 (1%) 79 53	61, 112, 161, 252	0
1	B	436/496 (87%)	0.03	18 (4%) 41 16	61, 113, 169, 252	0
1	C	437/496 (88%)	0.07	14 (3%) 51 23	61, 117, 177, 252	0
1	D	434/496 (87%)	0.06	18 (4%) 41 16	61, 116, 175, 252	0
All	All	1752/1984 (88%)	0.03	56 (3%) 51 23	61, 115, 171, 252	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	317	GLN	4.8
1	D	466	TYR	4.6
1	B	479	ARG	4.5
1	A	479	ARG	4.5
1	B	337	ASP	4.4
1	B	412	GLY	4.4
1	D	288	PHE	4.2
1	D	106	GLN	4.1
1	D	326	PRO	3.9
1	D	104	ARG	3.8
1	D	410	GLU	3.8
1	C	319	GLU	3.7
1	D	412	GLY	3.7
1	A	288	PHE	3.6
1	C	466	TYR	3.6
1	C	456	GLY	3.6
1	B	326	PRO	3.4
1	B	477	GLN	3.3
1	A	178	PHE	3.2
1	C	477	GLN	3.2
1	B	336	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	106	GLN	3.0
1	D	91	GLY	2.9
1	D	195	ASP	2.8
1	D	320	LEU	2.7
1	C	257	ASP	2.7
1	D	455	VAL	2.7
1	C	439	VAL	2.7
1	D	175	TYR	2.6
1	D	400	PRO	2.6
1	A	467	CYS	2.6
1	C	215	ARG	2.6
1	C	326	PRO	2.5
1	B	257	ASP	2.5
1	D	411	PRO	2.4
1	B	288	PHE	2.4
1	B	411	PRO	2.4
1	B	65	GLY	2.4
1	C	289	ILE	2.4
1	C	133	ARG	2.4
1	D	319	GLU	2.4
1	C	288	PHE	2.3
1	C	295	THR	2.3
1	B	476	PHE	2.3
1	B	323	GLU	2.2
1	B	170	CYS	2.2
1	C	467	CYS	2.2
1	B	227	GLN	2.1
1	B	438	PHE	2.1
1	B	128	LEU	2.1
1	D	188	ALA	2.1
1	B	175	TYR	2.1
1	B	215	ARG	2.1
1	C	336	LYS	2.1
1	A	337	ASP	2.1
1	D	215	ARG	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, 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
3	3QZ	B	501	24/24	0.88	0.45	4.41	54,87,104,137	0
3	3QZ	B	502	24/24	0.80	0.48	2.96	75,84,91,91	24
3	3QZ	A	501	24/24	0.93	0.34	2.74	54,79,87,91	0
3	3QZ	C	502	24/24	0.90	0.41	2.63	82,86,91,92	0
3	3QZ	A	502	24/24	0.78	0.42	2.50	76,86,93,93	0
3	3QZ	D	501	24/24	0.90	0.29	1.15	59,96,103,111	0
3	3QZ	C	501	24/24	0.90	0.28	1.03	54,82,101,101	0
3	3QZ	D	502	24/24	0.87	0.29	1.01	83,88,91,110	0
2	HEM	D	500	43/43	0.97	0.28	0.64	51,96,125,140	0
2	HEM	B	500	43/43	0.97	0.27	0.47	51,105,127,139	0
2	HEM	C	500	43/43	0.96	0.28	0.46	51,95,132,162	0
2	HEM	A	500	43/43	0.96	0.25	0.06	51,77,92,113	0

6.5 Other polymers (i)

There are no such residues in this entry.