Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 12:07 AM GMT

PDB ID	:	1ZRT
Title	:	Rhodobacter capsulatus cytochrome bc1 complex with stigmatellin bound
Authors	:	Berry, E.A.; Huang, L.S.; Saechao, L.K.; Pon, N.G.; Valkova-Valchanov, M.; Daldal, F.
Deposited on	:	2005-05-22
Resolution	:	3.50 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:

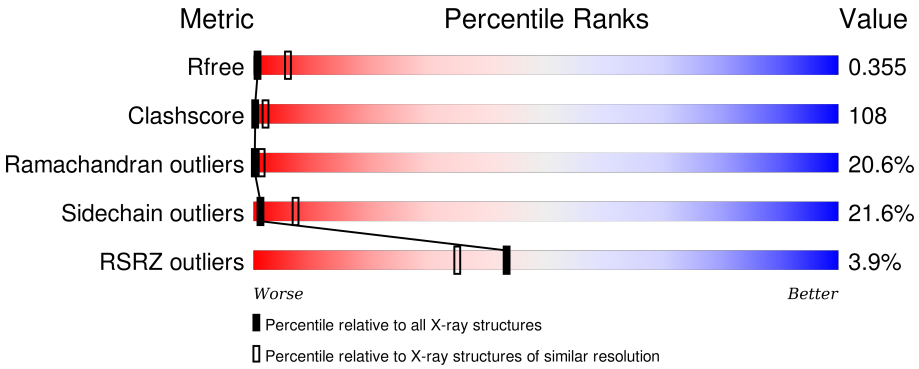
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.50 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	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)

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	C	437	2% 12% 57% 27%
1	P	437	2% 11% 56% 27%
2	D	258	7% 17% 55% 24%
2	Q	258	7% 18% 53% 25%
3	E	191	2% 19% 52% 21% 5%

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Mol	Chain	Length	Quality of chain
3	R	191	4% 17% 53% 21% 5%

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	HEM	C	502	-	-	X	-
4	HEM	P	501	-	-	X	-
4	HEM	P	502	-	-	X	-
5	SMA	C	503	-	-	-	X
6	HEC	D	501	-	-	-	X
6	HEC	Q	501	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 13366 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	427	Total	C	N	O	S	0	0	0
			3272	2202	524	532	14			
1	P	427	Total	C	N	O	S	0	0	0
			3272	2202	524	532	14			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1	MET	-	INITIATING METHIONINE	UNP P08502
P	1	MET	-	INITIATING METHIONINE	UNP P08502

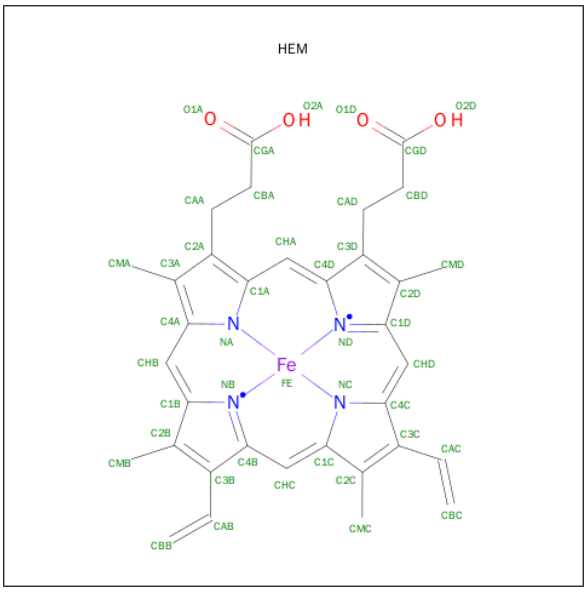
- Molecule 2 is a protein called Cytochrome c1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	252	Total	C	N	O	S	0	0	0
			1876	1191	314	356	15			
2	Q	252	Total	C	N	O	S	0	0	0
			1876	1191	314	356	15			

- Molecule 3 is a protein called Ubiquinol-cytochrome c reductase iron-sulfur subunit.

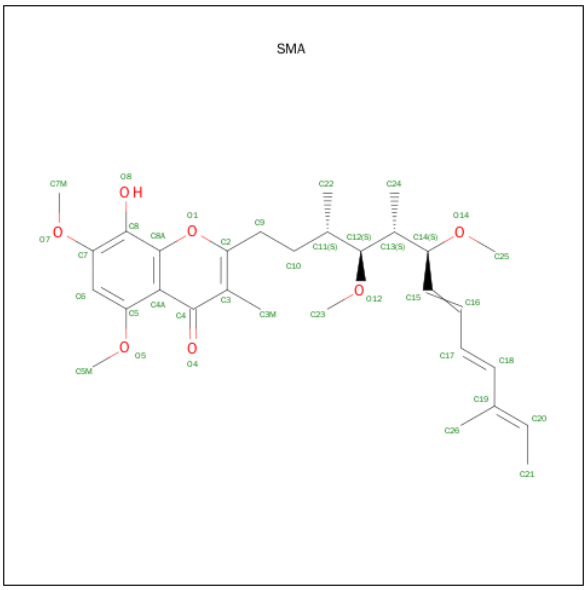
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	181	Total	C	N	O	S	0	0	0
			1365	855	246	256	8			
3	R	181	Total	C	N	O	S	0	0	0
			1365	855	246	256	8			

- Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



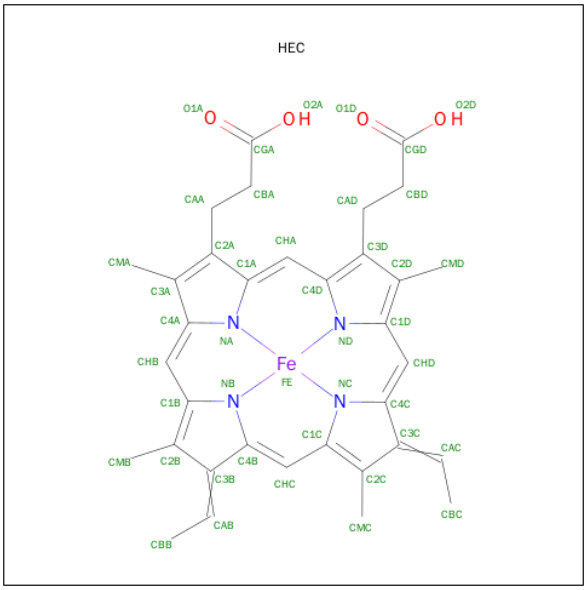
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
4	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
4	P	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
4	P	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 5 is STIGMATELLIN A (three-letter code: SMA) (formula: $C_{30}H_{42}O_7$).



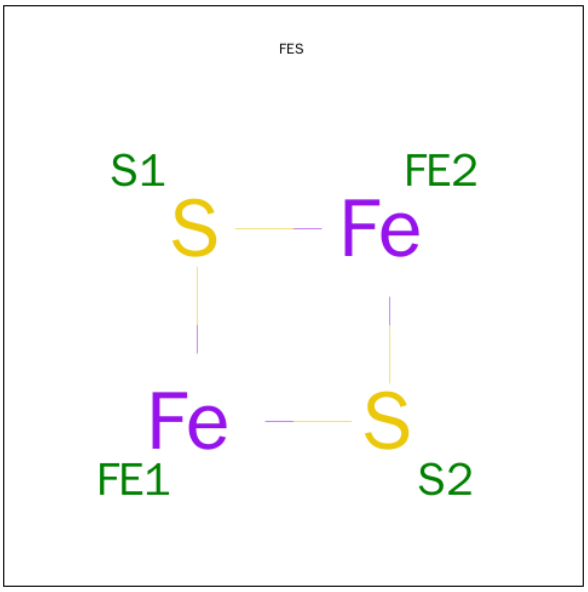
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total C O 37 30 7	0	0
5	P	1	Total C O 37 30 7	0	0

- Molecule 6 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



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

- Molecule 7 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



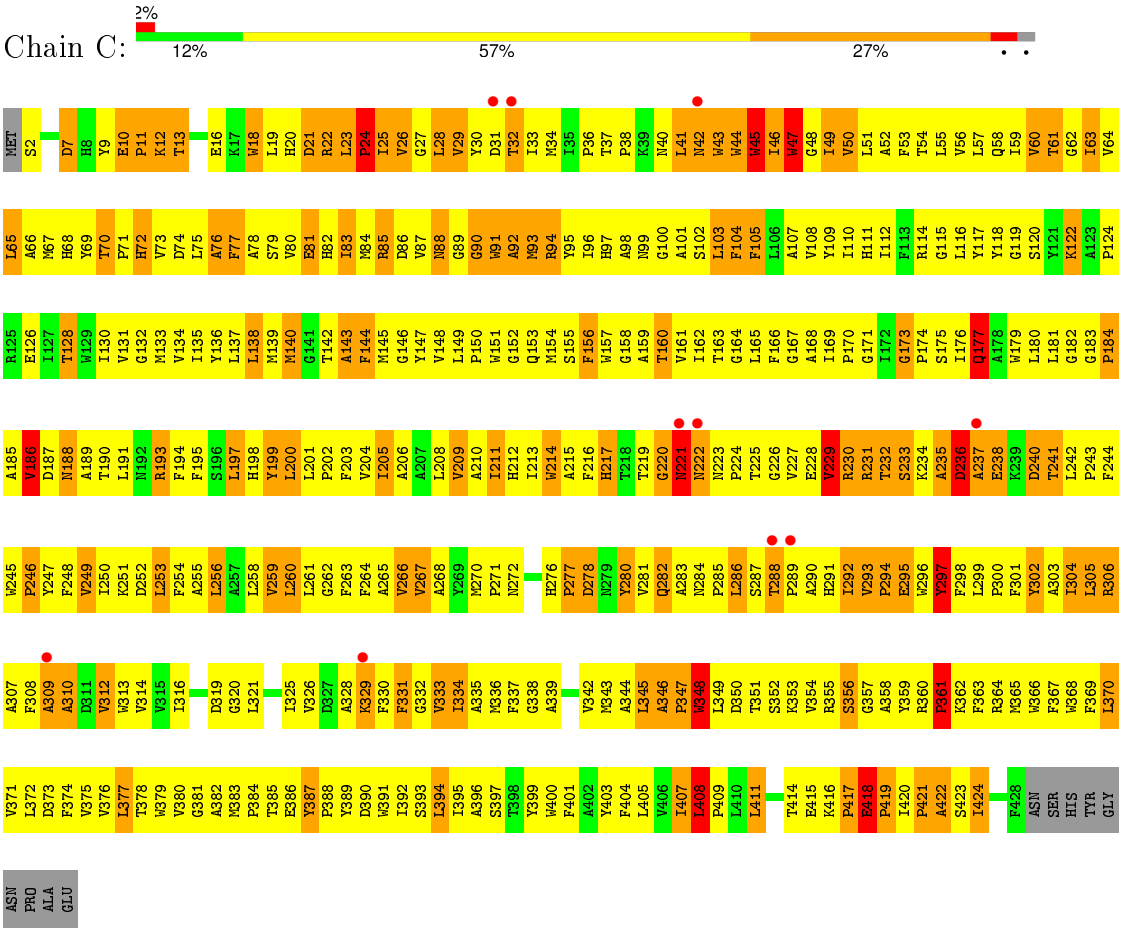
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	E	1	Total Fe S 4 2 2	0	0
7	R	1	Total Fe S 4 2 2	0	0

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.

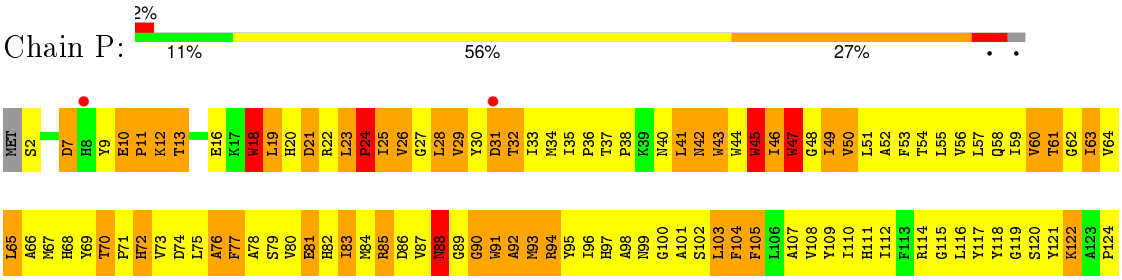
- Molecule 1: Cytochrome b

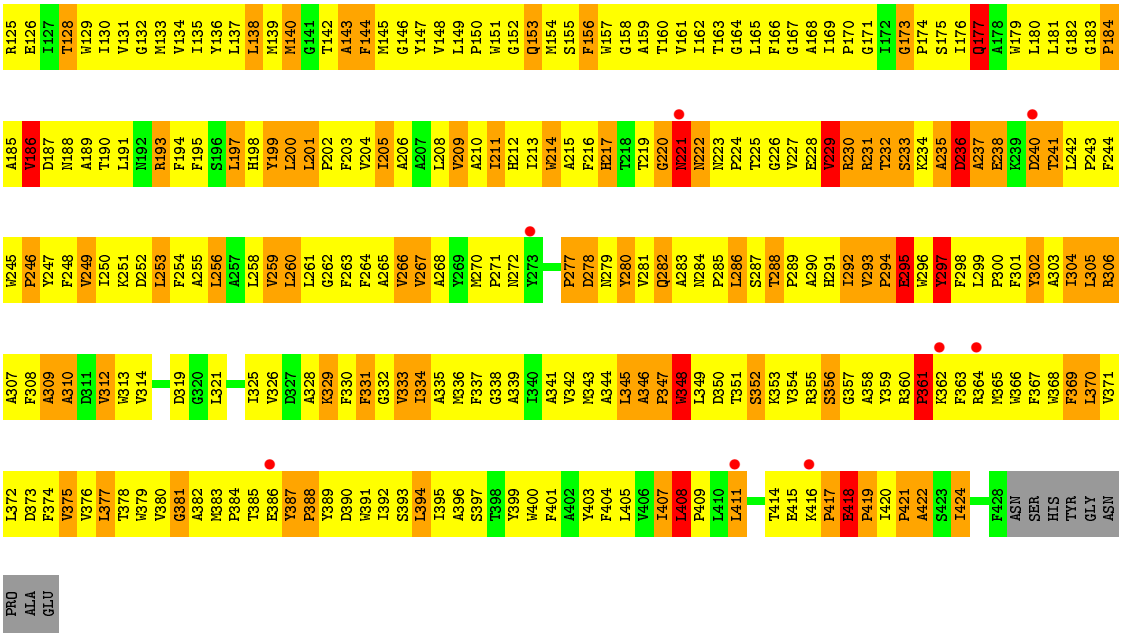
Chain C:



- Molecule 1: Cytochrome b

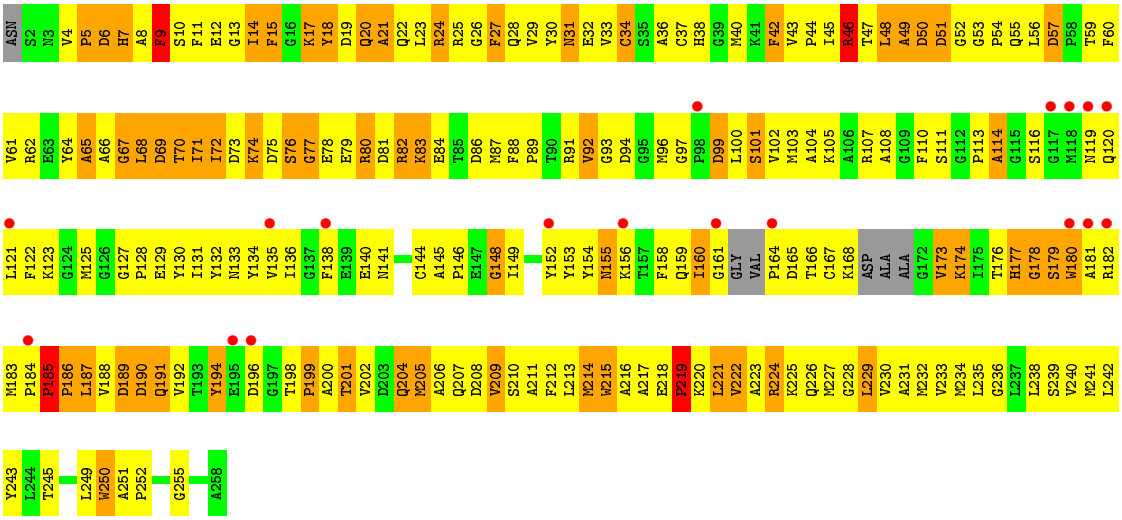
Chain P:





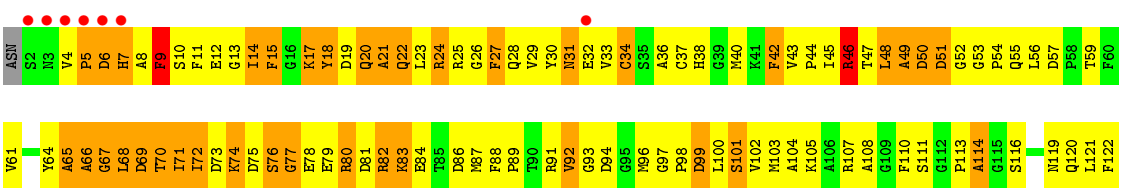
- Molecule 2: Cytochrome c1

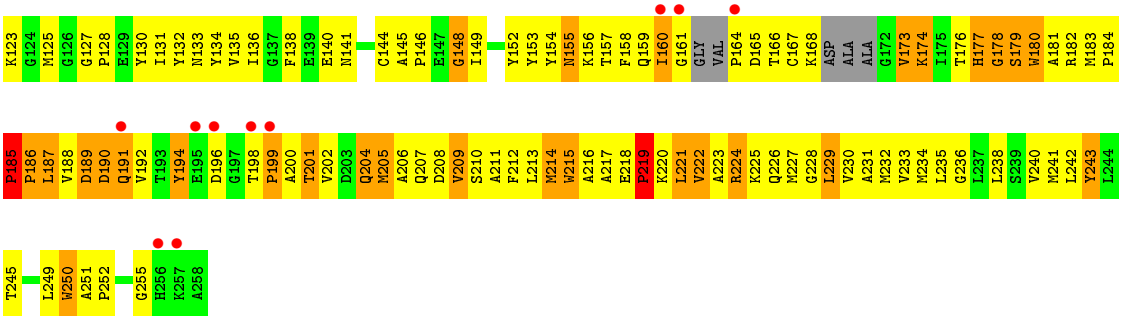
Chain D:



- Molecule 2: Cytochrome c1

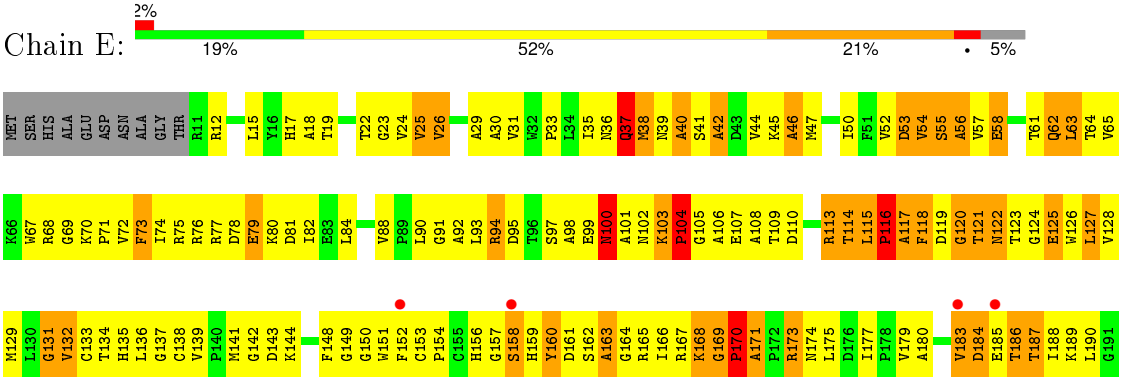
Chain Q:





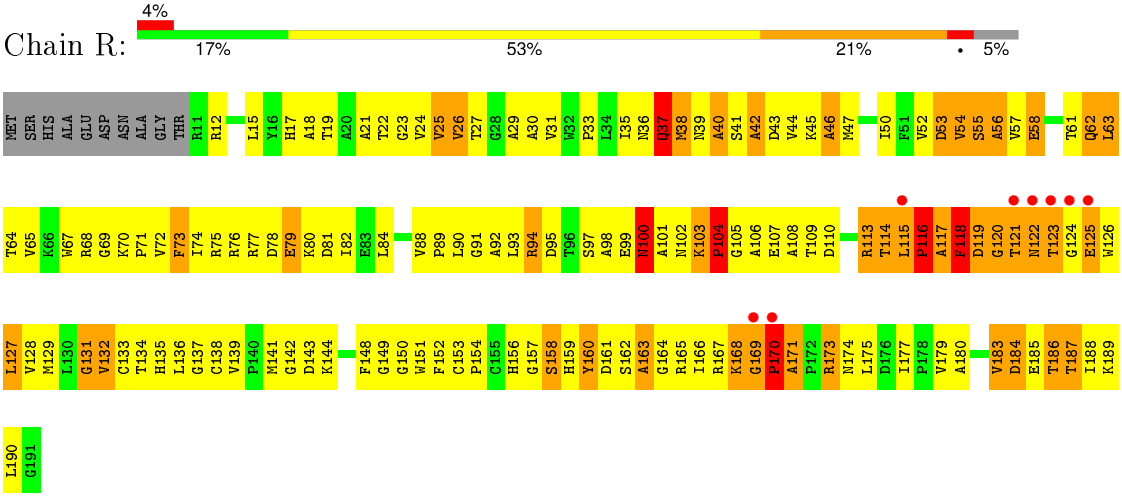
- Molecule 3: Ubiquinol-cytochrome c reductase iron-sulfur subunit

Chain E:



- Molecule 3: Ubiquinol-cytochrome c reductase iron-sulfur subunit

Chain R:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	95.63Å 154.36Å 103.06Å 90.00° 113.57° 90.00°	Depositor
Resolution (Å)	59.39 – 3.50 59.77 – 3.51	Depositor EDS
% Data completeness (in resolution range)	97.6 (59.39-3.50) 96.6 (59.77-3.51)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.91 (at 3.49Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.300 , 0.358 0.300 , 0.355	Depositor DCC
R_{free} test set	1661 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	99.0	Xtriage
Anisotropy	0.858	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.18 , 82.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Outliers	0 of 33265 reflections	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	13366	wwPDB-VP
Average B, all atoms (Å^2)	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.03% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	C	0.67	5/3392 (0.1%)	0.96	11/4657 (0.2%)
1	P	0.65	4/3392 (0.1%)	0.95	11/4657 (0.2%)
2	D	0.46	0/1923	0.78	1/2605 (0.0%)
2	Q	0.40	0/1923	0.76	1/2605 (0.0%)
3	E	0.48	0/1395	0.86	1/1895 (0.1%)
3	R	0.46	0/1395	0.84	1/1895 (0.1%)
All	All	0.57	9/13420 (0.1%)	0.88	26/18314 (0.1%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	47	TRP	CB-CG	8.51	1.65	1.50
1	P	47	TRP	CB-CG	8.37	1.65	1.50
1	C	22	ARG	C-O	7.36	1.37	1.23
1	C	46	ILE	C-O	6.60	1.35	1.23
1	P	46	ILE	C-O	6.46	1.35	1.23
1	P	200	LEU	C-O	6.35	1.35	1.23
1	C	45	TRP	CB-CG	-5.99	1.39	1.50
1	C	200	LEU	C-O	5.69	1.34	1.23
1	P	45	TRP	CB-CG	-5.68	1.40	1.50

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	P	46	ILE	C-N-CA	-12.90	89.44	121.70
1	C	46	ILE	C-N-CA	-12.76	89.80	121.70
1	C	221	ASN	C-N-CA	-11.91	91.92	121.70
1	P	221	ASN	C-N-CA	-11.87	92.02	121.70
1	C	21	ASP	N-CA-C	-6.66	93.01	111.00
1	P	293	VAL	C-N-CD	-6.53	106.24	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	47	TRP	N-CA-C	6.28	127.96	111.00
1	C	293	VAL	C-N-CD	-6.22	106.92	120.60
1	P	21	ASP	N-CA-C	-6.20	94.26	111.00
1	P	47	TRP	N-CA-C	6.11	127.48	111.00
1	C	22	ARG	N-CA-C	5.92	126.97	111.00
1	C	22	ARG	CA-C-O	5.82	132.31	120.10
3	E	169	GLY	N-CA-C	5.31	126.37	113.10
1	C	49	ILE	C-N-CA	-5.28	108.49	121.70
2	Q	48	LEU	N-CA-C	-5.27	96.76	111.00
1	C	222	ASN	N-CA-C	5.26	125.21	111.00
1	P	49	ILE	C-N-CA	-5.26	108.54	121.70
1	P	222	ASN	N-CA-C	5.22	125.11	111.00
1	P	221	ASN	CA-C-N	5.22	128.69	117.20
1	P	201	LEU	CA-CB-CG	-5.21	103.32	115.30
2	D	48	LEU	N-CA-C	-5.17	97.03	111.00
3	R	169	GLY	N-CA-C	5.14	125.95	113.10
1	C	221	ASN	CA-C-N	5.13	128.50	117.20
1	P	295	GLU	N-CA-C	-5.10	97.22	111.00
1	C	220	GLY	N-CA-C	5.10	125.85	113.10
1	P	220	GLY	N-CA-C	5.09	125.83	113.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3272	0	3100	857	0
1	P	3272	0	3100	864	0
2	D	1876	0	1735	326	0
2	Q	1876	0	1735	332	0
3	E	1365	0	1340	253	0
3	R	1365	0	1340	256	0
4	C	86	0	60	46	0
4	P	86	0	60	48	0
5	C	37	0	42	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	P	37	0	42	8	0
6	D	43	0	30	19	0
6	Q	43	0	30	21	0
7	E	4	0	0	1	0
7	R	4	0	0	1	0
All	All	13366	0	12614	2804	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 108.

All (2804) 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)
3:E:54:VAL:O	3:E:56:ALA:N	1.71	1.24
3:R:54:VAL:O	3:R:56:ALA:N	1.71	1.22
3:R:54:VAL:C	3:R:56:ALA:H	1.40	1.17
3:R:98:ALA:HB2	3:R:108:ALA:HA	1.24	1.12
3:E:54:VAL:C	3:E:56:ALA:H	1.40	1.12
1:C:223:ASN:HD21	1:C:225:THR:HG22	1.06	1.11
1:P:65:LEU:HD11	4:P:501:HEM:O2D	1.49	1.11
1:P:343:MET:HA	1:P:404:PHE:HE2	1.15	1.11
1:C:361:PRO:HD2	1:C:418:GLU:HG3	1.12	1.11
1:P:128:THR:HG22	1:P:215:ALA:HB1	1.34	1.09
1:P:112:ILE:HD12	4:P:502:HEM:HBC2	1.34	1.09
3:E:98:ALA:HB2	3:E:108:ALA:HA	1.24	1.08
1:P:414:THR:HA	1:P:417:PRO:HD2	1.36	1.08
2:D:23:LEU:HB3	2:D:54:PRO:HG3	1.35	1.08
1:P:247:TYR:HB3	2:Q:250:TRP:HE1	1.02	1.08
3:E:159:HIS:HB2	3:E:168:LYS:HB3	1.31	1.07
2:D:74:LYS:HD2	2:D:75:ASP:H	1.19	1.07
1:P:223:ASN:HD21	1:P:225:THR:HG22	1.06	1.07
1:P:145:MET:HE1	1:P:197:LEU:HB3	1.35	1.06
1:C:343:MET:HA	1:C:404:PHE:HE2	1.18	1.06
1:C:128:THR:HG22	1:C:215:ALA:HB1	1.37	1.06
1:C:145:MET:HE1	1:C:197:LEU:HB3	1.37	1.06
1:P:361:PRO:HD2	1:P:418:GLU:HG3	1.11	1.06
2:Q:74:LYS:HD2	2:Q:75:ASP:N	1.71	1.06
1:C:45:TRP:HE1	1:C:222:ASN:N	1.53	1.05
1:C:65:LEU:HD11	4:C:501:HEM:O2D	1.56	1.05
1:C:414:THR:HA	1:C:417:PRO:HD2	1.37	1.05
2:D:74:LYS:HD2	2:D:75:ASP:N	1.71	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:169:ILE:HA	1:C:330:PHE:HE2	1.22	1.04
3:R:159:HIS:HB2	3:R:168:LYS:HB3	1.36	1.04
3:R:53:ASP:O	3:R:55:SER:N	1.91	1.04
1:C:247:TYR:HB3	2:D:250:TRP:NE1	1.71	1.04
3:E:53:ASP:O	3:E:55:SER:N	1.91	1.03
2:Q:23:LEU:HB3	2:Q:54:PRO:HG3	1.35	1.03
1:P:45:TRP:HE1	1:P:222:ASN:N	1.54	1.03
1:C:60:VAL:O	1:C:64:VAL:HG13	1.59	1.03
2:Q:222:VAL:HG23	2:Q:223:ALA:H	1.20	1.02
1:C:112:ILE:HD12	4:C:502:HEM:HBC2	1.37	1.02
2:D:222:VAL:HG23	2:D:223:ALA:H	1.22	1.02
3:E:57:VAL:H	3:E:76:ARG:HH22	1.05	1.02
1:C:33:ILE:HG23	1:C:245:TRP:HB3	1.41	1.01
1:P:169:ILE:HA	1:P:330:PHE:HE2	1.22	1.01
1:C:247:TYR:HB3	2:D:250:TRP:HE1	0.86	1.01
1:C:292:ILE:H	1:C:292:ILE:HD12	1.25	1.01
2:Q:74:LYS:HD2	2:Q:75:ASP:H	1.20	1.01
3:R:57:VAL:H	3:R:76:ARG:HH22	1.07	1.00
2:D:23:LEU:HB3	2:D:54:PRO:CG	1.92	1.00
3:R:100:ASN:HD22	3:R:100:ASN:N	1.58	1.00
1:P:227:VAL:HG23	1:P:229:VAL:HG23	1.42	1.00
1:P:60:VAL:O	1:P:64:VAL:HG13	1.59	1.00
3:E:119:ASP:OD2	3:E:184:ASP:HA	1.62	1.00
1:C:247:TYR:CB	2:D:250:TRP:HE1	1.75	1.00
3:R:53:ASP:O	3:R:54:VAL:C	2.01	0.99
1:C:227:VAL:HG23	1:C:229:VAL:HG23	1.42	0.99
2:Q:23:LEU:HB3	2:Q:54:PRO:CG	1.92	0.99
3:E:100:ASN:HD22	3:E:100:ASN:N	1.58	0.99
1:C:330:PHE:O	1:C:334:ILE:HG22	1.62	0.98
1:P:33:ILE:HG23	1:P:245:TRP:HB3	1.43	0.98
1:P:292:ILE:HD12	1:P:292:ILE:H	1.24	0.98
4:C:501:HEM:HBC2	4:C:501:HEM:HMC1	1.46	0.97
3:R:119:ASP:OD2	3:R:184:ASP:HA	1.62	0.97
1:P:95:TYR:CD2	1:P:271:PRO:HB2	1.99	0.97
1:P:330:PHE:O	1:P:334:ILE:HG22	1.62	0.97
1:C:95:TYR:HE2	1:C:272:ASN:ND2	1.62	0.96
2:D:241:MET:HB3	3:E:19:THR:HG22	1.46	0.96
2:Q:241:MET:HB3	3:R:19:THR:HG22	1.46	0.96
3:E:53:ASP:O	3:E:54:VAL:C	2.02	0.96
2:D:23:LEU:HD13	2:D:54:PRO:HD3	1.47	0.95
1:C:95:TYR:HE2	1:C:272:ASN:HD21	1.01	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:54:THR:HG21	1:P:104:PHE:HB2	1.49	0.95
1:C:229:VAL:HG13	1:C:230:ARG:HG2	1.48	0.94
2:D:224:ARG:HG3	2:D:224:ARG:HH11	1.29	0.94
1:P:89:GLY:O	1:P:92:ALA:HB3	1.66	0.94
2:Q:224:ARG:HG3	2:Q:224:ARG:HH11	1.29	0.94
1:P:167:GLY:HA3	1:P:177:GLN:HE21	1.32	0.94
1:P:114:ARG:HH22	4:P:502:HEM:HBD2	1.33	0.94
2:Q:23:LEU:HD13	2:Q:54:PRO:HD3	1.49	0.93
1:C:167:GLY:HA3	1:C:177:GLN:HE21	1.31	0.93
3:E:53:ASP:C	3:E:55:SER:N	2.17	0.93
1:C:45:TRP:HZ2	1:C:222:ASN:HB3	1.29	0.93
1:P:343:MET:HA	1:P:404:PHE:CE2	2.04	0.93
1:P:223:ASN:ND2	1:P:225:THR:HG22	1.84	0.93
2:D:14:ILE:H	2:D:14:ILE:HD12	1.34	0.93
1:P:45:TRP:HZ2	1:P:222:ASN:HB3	1.29	0.92
1:C:223:ASN:ND2	1:C:225:THR:HG22	1.84	0.92
1:P:51:LEU:HD11	1:P:108:VAL:HA	1.51	0.92
2:Q:14:ILE:HD12	2:Q:14:ILE:H	1.35	0.92
1:C:114:ARG:HH22	4:C:502:HEM:HBD2	1.35	0.92
1:P:47:TRP:HE1	1:P:110:ILE:HG21	1.35	0.92
1:C:89:GLY:O	1:C:92:ALA:HB3	1.69	0.92
1:P:229:VAL:HG13	1:P:230:ARG:HG2	1.49	0.92
2:D:188:VAL:H	2:D:191:GLN:HE22	0.92	0.91
2:Q:188:VAL:H	2:Q:191:GLN:NE2	1.67	0.91
3:R:53:ASP:C	3:R:55:SER:N	2.17	0.91
1:P:145:MET:CE	1:P:197:LEU:HB3	2.01	0.91
1:P:114:ARG:NH2	4:P:502:HEM:HBD2	1.85	0.91
1:C:173:GLY:O	1:C:176:ILE:HG22	1.71	0.91
1:C:51:LEU:HD11	1:C:108:VAL:HA	1.52	0.91
1:P:61:THR:O	1:P:64:VAL:HG22	1.71	0.91
1:C:47:TRP:HE1	1:C:110:ILE:HG21	1.33	0.90
2:Q:188:VAL:H	2:Q:191:GLN:HE22	0.91	0.90
1:C:346:ALA:HB3	1:C:347:PRO:HD3	1.54	0.90
1:C:145:MET:CE	1:C:197:LEU:HB3	2.02	0.90
1:C:416:LYS:HB3	1:C:417:PRO:HD3	1.53	0.90
1:C:131:VAL:HG13	1:C:208:LEU:CD2	2.01	0.90
1:P:45:TRP:CH2	1:P:118:TYR:HD1	1.89	0.90
1:C:114:ARG:NH2	4:C:502:HEM:HBD2	1.86	0.90
1:P:2:SER:CB	1:P:231:ARG:HE	1.85	0.90
2:D:188:VAL:H	2:D:191:GLN:NE2	1.68	0.90
1:P:92:ALA:O	1:P:96:ILE:HG13	1.72	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:189:ALA:O	1:C:193:ARG:HG2	1.70	0.89
1:P:134:VAL:HG12	1:P:208:LEU:HD11	1.55	0.89
3:R:52:VAL:HB	3:R:188:ILE:HG22	1.52	0.89
1:P:54:THR:CG2	1:P:104:PHE:HB2	2.02	0.89
1:P:247:TYR:HB3	2:Q:250:TRP:NE1	1.87	0.89
1:C:343:MET:HA	1:C:404:PHE:CE2	2.06	0.89
1:C:361:PRO:HD2	1:C:418:GLU:CG	2.02	0.89
1:P:189:ALA:O	1:P:193:ARG:HG2	1.73	0.89
1:P:361:PRO:HD2	1:P:418:GLU:CG	2.01	0.89
3:R:52:VAL:HG11	3:R:74:ILE:HD12	1.55	0.89
1:P:187:ASP:O	1:P:190:THR:HG22	1.72	0.89
3:E:52:VAL:HB	3:E:188:ILE:HG22	1.52	0.89
1:C:187:ASP:O	1:C:190:THR:HG22	1.72	0.88
1:P:173:GLY:O	1:P:176:ILE:HG22	1.71	0.88
1:C:45:TRP:CH2	1:C:118:TYR:HD1	1.91	0.88
1:C:92:ALA:O	1:C:96:ILE:HG13	1.72	0.88
1:C:2:SER:CB	1:C:231:ARG:HE	1.86	0.88
1:C:61:THR:O	1:C:64:VAL:HG22	1.72	0.88
1:P:414:THR:CA	1:P:417:PRO:HD2	2.04	0.88
1:C:134:VAL:HG12	1:C:208:LEU:HD11	1.55	0.87
1:P:85:ARG:HH12	2:Q:102:VAL:CG2	1.87	0.87
1:P:416:LYS:HB3	1:P:417:PRO:HD3	1.54	0.87
2:D:44:PRO:HB2	2:D:47:THR:HG23	1.56	0.87
1:C:23:LEU:O	1:C:26:VAL:N	2.07	0.87
2:D:23:LEU:CB	2:D:54:PRO:HG3	2.05	0.86
1:C:54:THR:HG21	1:C:104:PHE:HB2	1.57	0.86
1:P:131:VAL:HG13	1:P:208:LEU:CD2	2.05	0.86
1:C:407:ILE:HD13	1:C:411:LEU:HB2	1.58	0.86
1:P:169:ILE:HA	1:P:330:PHE:CE2	2.10	0.86
3:R:95:ASP:HB2	3:R:173:ARG:HA	1.57	0.86
1:P:226:GLY:HA3	1:P:355:ARG:HB2	1.58	0.86
1:C:414:THR:CA	1:C:417:PRO:HD2	2.05	0.86
1:P:346:ALA:HB3	1:P:347:PRO:HD3	1.58	0.86
3:E:95:ASP:HB2	3:E:173:ARG:HA	1.56	0.85
1:C:169:ILE:HA	1:C:330:PHE:CE2	2.10	0.85
1:P:33:ILE:HG23	1:P:245:TRP:CB	2.07	0.85
1:P:263:PHE:HA	1:P:266:VAL:HG23	1.58	0.85
1:C:226:GLY:HA3	1:C:355:ARG:HB2	1.58	0.85
1:P:247:TYR:CB	2:Q:250:TRP:HE1	1.89	0.85
2:Q:188:VAL:N	2:Q:191:GLN:HE22	1.74	0.85
1:P:262:GLY:O	1:P:265:ALA:HB3	1.76	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:23:LEU:CB	2:Q:54:PRO:HG3	2.06	0.85
1:C:33:ILE:HG23	1:C:245:TRP:CB	2.06	0.85
1:C:108:VAL:O	1:C:112:ILE:HG12	1.77	0.84
1:P:202:PRO:HG3	4:P:501:HEM:HMC1	1.60	0.84
1:P:407:ILE:HD13	1:P:411:LEU:HB2	1.58	0.84
3:E:52:VAL:HG11	3:E:74:ILE:HD12	1.57	0.84
1:C:166:PHE:O	1:C:169:ILE:HG12	1.77	0.84
3:E:159:HIS:HB2	3:E:168:LYS:CB	2.08	0.84
1:C:256:LEU:O	1:C:259:VAL:HG23	1.76	0.84
2:Q:44:PRO:HB2	2:Q:47:THR:HG23	1.58	0.83
1:C:262:GLY:O	1:C:265:ALA:HB3	1.79	0.83
2:D:102:VAL:HG12	2:D:102:VAL:O	1.79	0.83
3:R:142:GLY:HA2	3:R:151:TRP:CD1	2.14	0.83
1:P:148:VAL:C	1:P:150:PRO:HD2	2.00	0.83
1:P:284:ASN:ND2	1:P:287:SER:H	1.77	0.83
2:D:188:VAL:N	2:D:191:GLN:HE22	1.75	0.82
1:C:148:VAL:C	1:C:150:PRO:HD2	2.00	0.82
1:C:45:TRP:HE1	1:C:222:ASN:H	1.27	0.82
1:P:46:ILE:CD1	1:P:252:ASP:HA	2.09	0.82
1:P:256:LEU:O	1:P:259:VAL:HG23	1.79	0.82
1:P:108:VAL:O	1:P:112:ILE:HG12	1.78	0.82
1:C:263:PHE:HA	1:C:266:VAL:HG23	1.61	0.82
3:E:142:GLY:HA2	3:E:151:TRP:CD1	2.15	0.82
1:C:347:PRO:HB2	1:C:348:TRP:HD1	1.43	0.82
3:E:57:VAL:N	3:E:76:ARG:HH22	1.77	0.82
1:C:222:ASN:N	4:C:502:HEM:O1D	2.13	0.82
1:C:286:LEU:HD12	1:C:286:LEU:N	1.95	0.82
1:P:347:PRO:HB2	1:P:348:TRP:HD1	1.44	0.82
1:P:280:TYR:CE1	2:Q:105:LYS:HD2	2.15	0.82
1:C:56:VAL:O	1:C:60:VAL:HG23	1.80	0.82
2:Q:55:GLN:O	2:Q:56:LEU:HG	1.80	0.82
1:P:222:ASN:N	4:P:502:HEM:O1D	2.12	0.82
2:Q:74:LYS:CD	2:Q:75:ASP:H	1.93	0.81
2:D:55:GLN:O	2:D:56:LEU:HG	1.80	0.81
1:C:54:THR:CG2	1:C:104:PHE:HB2	2.10	0.81
1:C:134:VAL:CG1	1:C:208:LEU:HD11	2.10	0.81
1:P:166:PHE:O	1:P:169:ILE:HG12	1.80	0.81
3:E:113:ARG:HG2	3:E:163:ALA:HB1	1.59	0.81
2:Q:71:ILE:HD11	2:Q:89:PRO:HG3	1.61	0.81
3:E:70:LYS:HE3	1:P:185:ALA:HB2	1.59	0.81
1:C:223:ASN:HD21	1:C:227:VAL:HG22	1.46	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:113:ARG:HG2	3:R:163:ALA:HB1	1.60	0.81
1:P:193:ARG:HG3	1:P:193:ARG:HH11	1.44	0.81
3:R:50:ILE:HG22	3:R:190:LEU:HB2	1.62	0.81
1:C:18:TRP:O	1:C:21:ASP:N	2.13	0.81
1:C:46:ILE:CD1	1:C:252:ASP:HA	2.10	0.81
1:P:403:TYR:HA	1:P:407:ILE:HG22	1.63	0.81
1:P:286:LEU:N	1:P:286:LEU:HD12	1.95	0.81
1:P:91:TRP:O	1:P:95:TYR:HB2	1.81	0.81
2:Q:102:VAL:O	2:Q:102:VAL:HG12	1.79	0.81
3:E:50:ILE:HG22	3:E:190:LEU:HB2	1.61	0.81
3:E:54:VAL:O	3:E:56:ALA:CA	2.29	0.80
2:D:74:LYS:CD	2:D:75:ASP:H	1.93	0.80
2:D:71:ILE:HD11	2:D:89:PRO:HG3	1.62	0.80
1:P:227:VAL:CG2	1:P:229:VAL:HG23	2.11	0.80
2:D:241:MET:HB3	3:E:19:THR:CG2	2.11	0.80
1:C:299:LEU:HB2	1:C:378:THR:HG23	1.64	0.80
1:C:26:VAL:HG13	1:C:27:GLY:N	1.96	0.80
2:D:186:PRO:HG2	2:D:187:LEU:H	1.45	0.80
1:P:267:VAL:HG12	1:P:268:ALA:N	1.95	0.80
1:C:414:THR:HA	1:C:417:PRO:CD	2.12	0.80
1:C:22:ARG:O	1:C:23:LEU:O	1.98	0.80
2:Q:186:PRO:HG2	2:Q:187:LEU:H	1.46	0.80
1:P:284:ASN:HD21	1:P:287:SER:N	1.78	0.80
1:C:342:VAL:HG11	1:C:404:PHE:HB3	1.64	0.80
3:E:88:VAL:HB	3:E:165:ARG:NH2	1.97	0.80
1:P:414:THR:HA	1:P:417:PRO:CD	2.11	0.80
3:R:54:VAL:O	3:R:56:ALA:CA	2.30	0.80
3:R:100:ASN:HB3	3:R:177:ILE:HB	1.64	0.80
1:C:227:VAL:CG2	1:C:229:VAL:HG23	2.11	0.80
2:Q:30:TYR:HD1	2:Q:34:CYS:HB2	1.46	0.80
3:R:52:VAL:HB	3:R:188:ILE:CG2	2.10	0.80
1:P:56:VAL:O	1:P:60:VAL:HG23	1.81	0.80
1:C:193:ARG:HH11	1:C:193:ARG:HG3	1.45	0.79
1:C:41:LEU:HD21	1:C:222:ASN:O	1.83	0.79
1:P:134:VAL:CG1	1:P:208:LEU:HD11	2.12	0.79
1:C:193:ARG:HG3	1:C:193:ARG:NH1	1.96	0.79
2:D:158:PHE:O	2:D:179:SER:HA	1.82	0.79
2:Q:241:MET:HB3	3:R:19:THR:CG2	2.11	0.79
3:E:23:GLY:O	3:E:26:VAL:HG23	1.81	0.79
1:C:301:PHE:HA	1:C:304:ILE:HD11	1.65	0.79
1:P:86:ASP:OD1	3:R:42:ALA:HB3	1.82	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:11:PHE:HD1	2:Q:12:GLU:H	1.31	0.79
2:D:30:TYR:HD1	2:D:34:CYS:HB2	1.47	0.79
3:R:88:VAL:HB	3:R:165:ARG:NH2	1.97	0.79
3:R:57:VAL:N	3:R:76:ARG:HH22	1.79	0.79
1:C:403:TYR:HA	1:C:407:ILE:HG22	1.65	0.79
3:E:57:VAL:H	3:E:76:ARG:NH2	1.79	0.79
3:R:23:GLY:O	3:R:26:VAL:HG23	1.81	0.79
1:C:411:LEU:O	1:C:415:GLU:HG2	1.83	0.79
1:P:342:VAL:HG11	1:P:404:PHE:HB3	1.65	0.79
1:P:45:TRP:HE1	1:P:222:ASN:H	1.28	0.79
1:P:45:TRP:CZ2	1:P:222:ASN:HB3	2.16	0.79
3:E:37:GLN:HG3	3:E:38:MET:H	1.46	0.78
3:E:52:VAL:HB	3:E:188:ILE:CG2	2.11	0.78
1:C:91:TRP:O	1:C:95:TYR:HB2	1.83	0.78
1:P:45:TRP:HH2	1:P:118:TYR:HD1	1.31	0.78
3:E:100:ASN:HB3	3:E:177:ILE:HB	1.64	0.78
2:D:188:VAL:O	2:D:189:ASP:HB2	1.83	0.78
1:C:45:TRP:CZ2	1:C:222:ASN:HB3	2.16	0.78
1:C:48:GLY:HA3	4:C:502:HEM:C4A	2.18	0.78
1:P:193:ARG:HG3	1:P:193:ARG:NH1	1.94	0.78
3:E:159:HIS:O	3:E:167:ARG:C	2.21	0.78
1:C:184:PRO:HG2	1:C:185:ALA:H	1.47	0.78
3:R:165:ARG:HA	3:R:174:ASN:HB3	1.66	0.78
1:C:162:ILE:O	1:C:165:LEU:HD12	1.84	0.78
1:C:213:ILE:HA	1:C:216:PHE:CE2	2.17	0.78
1:P:41:LEU:HD21	1:P:222:ASN:O	1.82	0.78
3:E:159:HIS:CB	3:E:168:LYS:HB3	2.13	0.78
2:Q:38:HIS:HB3	2:Q:100:LEU:CD2	2.14	0.78
1:C:193:ARG:HA	1:P:67:MET:HG3	1.66	0.78
1:C:16:GLU:O	1:C:20:HIS:CB	2.31	0.78
1:P:301:PHE:HA	1:P:304:ILE:HD11	1.66	0.78
1:P:334:ILE:HD13	1:P:335:ALA:N	1.99	0.78
1:C:284:ASN:ND2	1:C:287:SER:H	1.81	0.78
3:R:37:GLN:HG3	3:R:38:MET:H	1.48	0.77
2:Q:222:VAL:HG23	2:Q:223:ALA:N	1.99	0.77
1:C:108:VAL:HG13	1:C:112:ILE:HD11	1.65	0.77
1:C:135:ILE:HG12	1:C:208:LEU:HD22	1.67	0.77
2:Q:158:PHE:O	2:Q:179:SER:HA	1.83	0.77
3:E:165:ARG:HA	3:E:174:ASN:HB3	1.65	0.77
1:C:199:TYR:O	1:C:199:TYR:HD2	1.67	0.77
3:R:129:MET:HE1	3:R:164:GLY:HA3	1.65	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:138:PHE:HE1	2:Q:155:ASN:HD22	1.31	0.77
1:C:267:VAL:HG12	1:C:268:ALA:N	2.00	0.77
1:P:157:TRP:O	1:P:161:VAL:HG12	1.84	0.77
1:P:213:ILE:HA	1:P:216:PHE:CE2	2.19	0.77
1:P:411:LEU:O	1:P:415:GLU:HG2	1.85	0.77
2:Q:188:VAL:O	2:Q:189:ASP:HB2	1.84	0.77
1:C:277:PRO:O	1:C:280:TYR:HB2	1.83	0.77
1:P:184:PRO:HG2	1:P:185:ALA:H	1.49	0.77
3:R:57:VAL:H	3:R:76:ARG:NH2	1.81	0.76
1:P:135:ILE:HG12	1:P:208:LEU:HD22	1.66	0.76
2:D:104:ALA:HB3	2:D:217:ALA:CB	2.14	0.76
3:R:100:ASN:CA	3:R:177:ILE:HB	2.15	0.76
1:P:348:TRP:HD1	1:P:348:TRP:H	1.32	0.76
2:Q:104:ALA:HB3	2:Q:217:ALA:HB3	1.68	0.76
3:E:100:ASN:CA	3:E:177:ILE:HB	2.15	0.76
3:E:100:ASN:N	3:E:100:ASN:ND2	2.34	0.76
1:C:284:ASN:HD21	1:C:287:SER:N	1.84	0.76
1:P:223:ASN:HD21	1:P:227:VAL:HG22	1.49	0.76
1:C:85:ARG:HH12	2:D:102:VAL:CG2	1.98	0.76
1:P:277:PRO:O	1:P:280:TYR:HB2	1.84	0.76
1:P:299:LEU:HB2	1:P:378:THR:HG23	1.67	0.76
3:R:159:HIS:HB2	3:R:168:LYS:CB	2.12	0.76
1:C:348:TRP:H	1:C:348:TRP:HD1	1.31	0.76
1:P:383:MET:HB3	1:P:389:TYR:CD1	2.21	0.76
2:Q:104:ALA:HB3	2:Q:217:ALA:CB	2.15	0.76
1:C:185:ALA:HB2	3:R:70:LYS:HE3	1.67	0.76
1:P:312:VAL:O	1:P:314:VAL:N	2.19	0.76
2:D:222:VAL:HG23	2:D:223:ALA:N	2.01	0.76
1:P:48:GLY:HA3	4:P:502:HEM:C4A	2.20	0.76
3:R:36:ASN:O	3:R:39:ASN:N	2.18	0.76
1:C:53:PHE:CE2	1:C:260:LEU:HD21	2.20	0.76
1:P:154:MET:HE1	1:P:292:ILE:HG22	1.68	0.76
2:D:38:HIS:HB3	2:D:100:LEU:CD2	2.15	0.76
1:P:261:LEU:HA	2:Q:235:LEU:HD12	1.68	0.75
1:P:108:VAL:HG13	1:P:112:ILE:HD11	1.67	0.75
2:Q:45:ILE:HB	2:Q:84:GLU:O	1.86	0.75
3:R:54:VAL:HG13	3:R:126:TRP:CH2	2.22	0.75
1:P:162:ILE:O	1:P:165:LEU:HD12	1.87	0.75
1:P:26:VAL:HG13	1:P:27:GLY:N	2.00	0.75
4:P:501:HEM:HMC2	4:P:501:HEM:HBC2	1.68	0.75
2:D:104:ALA:HB3	2:D:217:ALA:HB3	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:45:TRP:HH2	1:C:118:TYR:HD1	1.31	0.75
2:D:221:LEU:O	2:D:224:ARG:HB3	1.87	0.75
1:C:377:LEU:CD2	1:C:396:ALA:HB1	2.17	0.75
1:P:377:LEU:CD2	1:P:396:ALA:HB1	2.17	0.75
2:Q:224:ARG:NH1	2:Q:224:ARG:HG3	2.01	0.75
2:D:138:PHE:HE1	2:D:155:ASN:HD22	1.32	0.75
2:D:145:ALA:HB1	2:D:148:GLY:HA2	1.67	0.75
1:C:193:ARG:HH11	1:C:193:ARG:CG	1.99	0.75
3:E:71:PRO:HG3	1:P:285:PRO:O	1.87	0.75
3:R:100:ASN:HA	3:R:177:ILE:HB	1.68	0.75
3:R:54:VAL:C	3:R:56:ALA:N	2.16	0.74
1:C:334:ILE:HD13	1:C:335:ALA:N	2.00	0.74
1:P:51:LEU:HD21	1:P:108:VAL:HG23	1.68	0.74
1:C:312:VAL:O	1:C:314:VAL:N	2.19	0.74
2:D:45:ILE:HB	2:D:84:GLU:O	1.86	0.74
1:P:146:GLY:HA3	1:P:198:HIS:CE1	2.23	0.74
1:C:154:MET:HE1	1:C:292:ILE:HG22	1.69	0.74
3:E:53:ASP:CG	3:E:55:SER:HB2	2.08	0.74
2:Q:145:ALA:HB1	2:Q:148:GLY:HA2	1.67	0.74
3:R:98:ALA:CB	3:R:108:ALA:HA	2.12	0.74
2:D:25:ARG:HD2	2:D:194:TYR:HD2	1.52	0.74
1:C:51:LEU:HD21	1:C:108:VAL:HG23	1.68	0.74
1:P:193:ARG:CG	1:P:193:ARG:HH11	1.99	0.74
4:P:502:HEM:O2D	4:P:502:HEM:O2A	2.06	0.74
3:E:54:VAL:HG13	3:E:126:TRP:CH2	2.22	0.74
1:C:302:TYR:HA	5:C:503:SMA:H3	1.69	0.74
1:P:280:TYR:CZ	2:Q:105:LYS:HD2	2.23	0.74
3:E:98:ALA:CB	3:E:108:ALA:HA	2.12	0.74
1:C:157:TRP:O	1:C:161:VAL:HG12	1.88	0.74
4:C:502:HEM:O2A	4:C:502:HEM:O2D	2.06	0.74
1:C:51:LEU:CD2	1:C:108:VAL:HG23	2.18	0.74
1:C:223:ASN:ND2	1:C:227:VAL:HG22	2.02	0.74
1:C:278:ASP:O	1:C:281:VAL:HG12	1.88	0.74
1:C:288:THR:HG21	3:R:138:CYS:HB3	1.69	0.74
1:P:114:ARG:HE	1:P:115:GLY:N	1.86	0.74
1:P:16:GLU:O	1:P:20:HIS:CB	2.36	0.74
2:D:97:GLY:CA	6:D:501:HEC:HMD3	2.18	0.74
1:P:51:LEU:CD2	1:P:108:VAL:HG23	2.17	0.73
2:Q:27:PHE:HD1	2:Q:27:PHE:C	1.92	0.73
1:C:383:MET:HB3	1:C:389:TYR:CD1	2.23	0.73
1:C:280:TYR:CE1	2:D:105:LYS:HD2	2.22	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:100:ASN:HA	3:E:177:ILE:HB	1.68	0.73
3:R:129:MET:CE	3:R:164:GLY:HA3	2.17	0.73
2:D:224:ARG:HG3	2:D:224:ARG:NH1	1.99	0.73
1:P:53:PHE:CE2	1:P:260:LEU:HD21	2.24	0.73
3:R:53:ASP:CG	3:R:55:SER:HB2	2.09	0.73
1:C:300:PRO:O	1:C:377:LEU:HD12	1.89	0.73
2:D:27:PHE:HD1	2:D:27:PHE:C	1.92	0.73
1:P:343:MET:O	1:P:346:ALA:HB2	1.89	0.73
1:P:76:ALA:O	1:P:79:SER:HB3	1.88	0.73
2:Q:25:ARG:HD2	2:Q:194:TYR:HD2	1.52	0.73
1:C:41:LEU:CD2	1:C:222:ASN:O	2.37	0.72
1:P:300:PRO:O	1:P:377:LEU:HD12	1.89	0.72
1:P:84:MET:HG3	1:P:91:TRP:HA	1.71	0.72
1:P:41:LEU:CD2	1:P:222:ASN:O	2.37	0.72
3:E:36:ASN:O	3:E:39:ASN:N	2.22	0.72
2:D:11:PHE:HD1	2:D:12:GLU:H	1.37	0.72
1:C:254:PHE:HA	2:D:242:LEU:HD12	1.71	0.72
1:P:55:LEU:HD13	1:P:59:ILE:HD13	1.72	0.72
2:Q:209:VAL:HG23	2:Q:210:SER:H	1.54	0.72
1:P:72:HIS:CE1	1:P:74:ASP:HB2	2.24	0.72
2:D:21:ALA:O	2:D:25:ARG:HG3	1.89	0.72
1:P:263:PHE:O	1:P:266:VAL:HG23	1.89	0.72
3:E:53:ASP:OD2	3:E:55:SER:HB2	1.90	0.72
1:P:54:THR:HG21	1:P:104:PHE:CB	2.19	0.72
1:P:223:ASN:ND2	1:P:227:VAL:HG22	2.05	0.72
1:P:302:TYR:HA	5:P:503:SMA:H3	1.70	0.72
1:P:37:THR:HB	1:P:248:PHE:CE1	2.25	0.72
1:C:76:ALA:O	1:C:79:SER:HB3	1.89	0.72
1:C:84:MET:HG3	1:C:91:TRP:HA	1.71	0.72
1:P:108:VAL:HG21	1:P:139:MET:HE1	1.72	0.72
1:P:57:LEU:O	1:P:61:THR:HG22	1.89	0.72
3:E:102:ASN:O	3:E:103:LYS:HG3	1.89	0.72
1:P:187:ASP:H	1:P:190:THR:HG22	1.54	0.72
3:E:26:VAL:O	3:E:29:ALA:HB3	1.89	0.72
2:D:23:LEU:HB3	2:D:54:PRO:CD	2.20	0.72
1:C:24:PRO:CG	1:C:25:ILE:H	2.02	0.71
1:C:55:LEU:HD13	1:C:59:ILE:HD13	1.72	0.71
1:P:20:HIS:C	1:P:22:ARG:H	1.91	0.71
1:C:114:ARG:HE	1:C:115:GLY:N	1.87	0.71
1:C:67:MET:HG3	1:P:193:ARG:HA	1.71	0.71
1:C:105:PHE:HZ	1:C:140:MET:HG2	1.54	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:294:PRO:HG3	1:C:302:TYR:CD1	2.25	0.71
1:C:57:LEU:O	1:C:61:THR:HG22	1.90	0.71
1:P:153:GLN:NE2	1:P:289:PRO:HD3	2.05	0.71
1:P:395:ILE:HG13	1:P:396:ALA:N	2.04	0.71
2:Q:23:LEU:HB3	2:Q:54:PRO:CD	2.21	0.71
1:P:69:TYR:CE2	1:P:149:LEU:HD23	2.25	0.71
2:Q:51:ASP:O	2:Q:53:GLY:N	2.23	0.71
3:R:102:ASN:O	3:R:103:LYS:HG3	1.89	0.71
1:C:153:GLN:NE2	1:C:289:PRO:HD3	2.05	0.71
3:R:163:ALA:HB3	3:R:165:ARG:HG3	1.72	0.71
1:C:149:LEU:HD21	1:C:195:PHE:HD2	1.56	0.71
1:C:278:ASP:C	1:C:280:TYR:H	1.93	0.71
3:R:159:HIS:CB	3:R:168:LYS:HB3	2.18	0.71
3:R:30:ALA:O	3:R:33:PRO:HG2	1.90	0.71
1:C:226:GLY:HA3	1:C:355:ARG:CB	2.21	0.71
3:E:54:VAL:HG13	3:E:126:TRP:HH2	1.55	0.71
1:P:135:ILE:HG21	4:P:502:HEM:HBB2	1.73	0.71
1:P:149:LEU:HD21	1:P:195:PHE:HD2	1.55	0.71
2:Q:57:ASP:O	2:Q:61:VAL:HG23	1.90	0.71
1:C:343:MET:O	1:C:346:ALA:HB2	1.90	0.71
1:P:95:TYR:CE2	1:P:271:PRO:HB2	2.26	0.71
1:P:226:GLY:HA3	1:P:355:ARG:CB	2.21	0.71
3:E:54:VAL:C	3:E:56:ALA:N	2.16	0.70
1:C:202:PRO:HG3	4:C:501:HEM:HMC3	1.73	0.70
1:C:69:TYR:CE2	1:C:149:LEU:HD23	2.26	0.70
1:P:18:TRP:O	1:P:21:ASP:N	2.22	0.70
2:Q:198:THR:HG23	2:Q:199:PRO:HD2	1.73	0.70
1:P:182:GLY:CA	1:P:193:ARG:NH2	2.55	0.70
1:P:278:ASP:O	1:P:281:VAL:HG12	1.91	0.70
2:Q:221:LEU:O	2:Q:224:ARG:HB3	1.90	0.70
1:C:135:ILE:HG21	4:C:502:HEM:HBB2	1.73	0.70
1:C:187:ASP:H	1:C:190:THR:HG22	1.56	0.70
1:C:348:TRP:N	1:C:348:TRP:CD1	2.58	0.70
1:C:72:HIS:CE1	1:C:74:ASP:HB2	2.25	0.70
1:P:89:GLY:O	1:P:92:ALA:CB	2.39	0.70
1:C:395:ILE:HG13	1:C:396:ALA:N	2.06	0.70
1:P:24:PRO:CG	1:P:25:ILE:H	2.04	0.70
1:P:145:MET:SD	1:P:197:LEU:HB3	2.31	0.70
1:P:390:ASP:OD1	1:P:391:TRP:N	2.23	0.70
3:R:26:VAL:O	3:R:29:ALA:HB3	1.91	0.70
3:E:129:MET:CE	3:E:164:GLY:HA3	2.21	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:54:VAL:HG13	3:R:126:TRP:HH2	1.55	0.70
1:C:23:LEU:HB2	1:P:214:TRP:CZ3	2.26	0.70
1:P:342:VAL:CG1	1:P:404:PHE:HB3	2.22	0.70
1:P:403:TYR:HA	1:P:407:ILE:CG2	2.21	0.70
2:Q:100:LEU:O	2:Q:102:VAL:N	2.24	0.70
3:R:53:ASP:OD2	3:R:55:SER:HB2	1.91	0.70
1:C:225:THR:HG23	1:C:227:VAL:HG13	1.72	0.70
1:C:390:ASP:OD1	1:C:391:TRP:N	2.24	0.70
3:E:37:GLN:HE21	3:E:38:MET:N	1.90	0.70
2:Q:74:LYS:NZ	2:Q:75:ASP:HB3	2.07	0.70
1:P:26:VAL:CG1	1:P:27:GLY:N	2.55	0.70
2:Q:213:LEU:O	2:Q:216:ALA:N	2.25	0.70
1:C:285:PRO:O	3:R:71:PRO:HG3	1.92	0.70
3:E:163:ALA:HB3	3:E:165:ARG:HG3	1.73	0.70
2:D:51:ASP:O	2:D:53:GLY:N	2.23	0.70
1:P:243:PRO:HB2	1:P:245:TRP:O	1.92	0.70
1:C:180:LEU:O	1:C:193:ARG:NH1	2.25	0.70
1:P:152:GLY:O	1:P:155:SER:N	2.25	0.70
1:P:296:TRP:HA	1:P:299:LEU:HG	1.74	0.70
2:Q:128:PRO:HG3	2:Q:214:MET:HG3	1.72	0.70
1:P:254:PHE:HA	2:Q:242:LEU:HD12	1.73	0.70
3:E:100:ASN:CB	3:E:177:ILE:HB	2.21	0.70
2:D:194:TYR:H	2:D:194:TYR:HD1	1.40	0.70
2:D:74:LYS:NZ	2:D:75:ASP:HB3	2.06	0.70
1:C:47:TRP:NE1	1:C:110:ILE:HG21	2.06	0.69
1:C:169:ILE:HG13	1:C:173:GLY:HA2	1.74	0.69
1:C:342:VAL:CG1	1:C:404:PHE:HB3	2.22	0.69
3:R:37:GLN:HE21	3:R:38:MET:N	1.90	0.69
1:C:403:TYR:HA	1:C:407:ILE:CG2	2.22	0.69
1:C:69:TYR:CG	1:C:70:THR:N	2.58	0.69
3:R:52:VAL:HG11	3:R:74:ILE:CD1	2.22	0.69
1:C:205:ILE:HG22	1:C:206:ALA:N	2.07	0.69
1:C:214:TRP:CZ3	1:P:23:LEU:HB2	2.28	0.69
1:C:37:THR:HB	1:C:248:PHE:CE1	2.27	0.69
3:R:45:LYS:O	3:R:47:MET:HG3	1.91	0.69
1:P:278:ASP:C	1:P:280:TYR:H	1.93	0.69
1:P:117:TYR:HB2	1:P:367:PHE:CZ	2.27	0.69
1:P:47:TRP:NE1	1:P:110:ILE:HG21	2.08	0.69
2:Q:27:PHE:CD1	2:Q:27:PHE:C	2.64	0.69
2:Q:97:GLY:CA	6:Q:501:HEC:HMD3	2.22	0.69
3:E:45:LYS:O	3:E:47:MET:HG3	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:90:LEU:O	3:R:93:LEU:HB2	1.93	0.69
1:C:26:VAL:CG1	1:C:27:GLY:N	2.56	0.69
1:P:169:ILE:HD11	1:P:176:ILE:HG21	1.73	0.69
2:Q:21:ALA:O	2:Q:25:ARG:HG3	1.92	0.69
1:C:220:GLY:O	1:C:221:ASN:O	2.09	0.69
3:R:100:ASN:CB	3:R:177:ILE:HB	2.22	0.69
1:C:261:LEU:HA	2:D:235:LEU:HD12	1.73	0.69
1:P:23:LEU:O	1:P:26:VAL:N	2.26	0.69
1:P:281:VAL:HG13	1:P:281:VAL:O	1.93	0.69
3:E:90:LEU:O	3:E:93:LEU:HB2	1.93	0.69
3:E:30:ALA:O	3:E:33:PRO:HG2	1.91	0.69
2:D:190:ASP:HA	2:D:200:ALA:HB1	1.73	0.69
3:R:98:ALA:HB2	3:R:108:ALA:CA	2.13	0.69
1:P:223:ASN:HD21	1:P:225:THR:CG2	1.97	0.69
1:P:180:LEU:O	1:P:193:ARG:NH1	2.25	0.69
2:D:100:LEU:O	2:D:102:VAL:N	2.26	0.69
2:D:27:PHE:CD1	2:D:27:PHE:C	2.65	0.69
1:P:103:LEU:C	1:P:103:LEU:HD12	2.13	0.69
2:D:198:THR:HG23	2:D:199:PRO:HD2	1.73	0.69
1:P:58:GLN:HE21	1:P:101:ALA:HA	1.56	0.69
1:P:105:PHE:HZ	1:P:140:MET:HG2	1.58	0.68
2:D:138:PHE:HE2	2:D:186:PRO:HD3	1.58	0.68
1:P:58:GLN:NE2	1:P:101:ALA:N	2.41	0.68
1:P:169:ILE:HG13	1:P:173:GLY:HA2	1.75	0.68
2:Q:190:ASP:HA	2:Q:200:ALA:HB1	1.74	0.68
1:C:58:GLN:HE21	1:C:101:ALA:HA	1.59	0.68
1:P:32:THR:HG22	1:P:33:ILE:HG13	1.76	0.68
1:C:301:PHE:HA	1:C:304:ILE:CD1	2.23	0.68
1:P:187:ASP:H	1:P:190:THR:CG2	2.06	0.68
1:P:45:TRP:CH2	1:P:118:TYR:CD1	2.80	0.68
2:D:25:ARG:HB3	2:D:194:TYR:CE2	2.28	0.68
1:C:296:TRP:HA	1:C:299:LEU:HG	1.75	0.68
3:R:103:LYS:HB3	3:R:104:PRO:CD	2.24	0.68
1:C:26:VAL:CG1	1:C:27:GLY:H	2.07	0.68
1:P:45:TRP:CZ3	1:P:118:TYR:CD1	2.82	0.68
1:P:297:TYR:C	1:P:298:PHE:HD1	1.96	0.68
1:C:243:PRO:HB2	1:C:245:TRP:O	1.91	0.68
1:C:108:VAL:HG21	1:C:139:MET:HE1	1.75	0.68
1:C:20:HIS:C	1:C:22:ARG:H	1.92	0.68
3:E:139:VAL:HG23	1:P:157:TRP:CH2	2.28	0.68
1:P:26:VAL:CG1	1:P:27:GLY:H	2.07	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:138:PHE:HE2	2:Q:186:PRO:HD3	1.58	0.68
3:E:103:LYS:HB3	3:E:104:PRO:CD	2.23	0.68
3:R:152:PHE:HE2	3:R:154:PRO:HA	1.59	0.68
1:C:263:PHE:O	1:C:266:VAL:HG23	1.94	0.68
1:P:301:PHE:HA	1:P:304:ILE:CD1	2.24	0.68
2:Q:38:HIS:HB3	2:Q:100:LEU:HD21	1.76	0.68
3:R:62:GLN:NE2	3:R:64:THR:HG23	2.08	0.68
1:C:45:TRP:HZ2	1:C:222:ASN:CB	2.07	0.68
1:C:83:ILE:HG22	1:C:84:MET:N	2.09	0.68
2:Q:182:ARG:H	6:Q:501:HEC:HBD2	1.58	0.68
1:C:146:GLY:HA3	1:C:198:HIS:CE1	2.28	0.68
1:P:334:ILE:HG23	1:P:335:ALA:H	1.58	0.68
2:Q:25:ARG:HB3	2:Q:194:TYR:CE2	2.28	0.68
2:Q:158:PHE:HE1	6:Q:501:HEC:O1A	1.77	0.68
1:C:281:VAL:HG13	1:C:281:VAL:O	1.94	0.67
3:R:141:MET:HB2	3:R:152:PHE:O	1.94	0.67
1:P:263:PHE:HA	1:P:266:VAL:CG2	2.24	0.67
1:P:135:ILE:CG1	1:P:208:LEU:HD22	2.24	0.67
1:P:2:SER:N	1:P:231:ARG:HG2	2.09	0.67
1:P:294:PRO:HG3	1:P:302:TYR:CD1	2.29	0.67
2:Q:194:TYR:HD1	2:Q:194:TYR:H	1.40	0.67
2:D:209:VAL:HG23	2:D:210:SER:H	1.58	0.67
1:P:69:TYR:CG	1:P:70:THR:N	2.63	0.67
2:D:182:ARG:H	6:D:501:HEC:HBD2	1.59	0.67
1:P:220:GLY:O	1:P:221:ASN:O	2.11	0.67
3:E:159:HIS:O	3:E:167:ARG:O	2.12	0.67
1:C:416:LYS:HB3	1:C:417:PRO:CD	2.23	0.67
3:R:88:VAL:HB	3:R:165:ARG:HH22	1.58	0.67
1:P:348:TRP:N	1:P:348:TRP:CD1	2.57	0.67
1:P:147:TYR:HA	4:P:501:HEM:CAA	2.23	0.67
2:Q:202:VAL:O	2:Q:205:MET:HB2	1.94	0.67
1:P:205:ILE:HG22	1:P:206:ALA:N	2.09	0.67
1:P:225:THR:HG23	1:P:227:VAL:HG13	1.75	0.67
2:Q:80:ARG:HH22	2:Q:86:ASP:CG	1.97	0.67
3:E:62:GLN:NE2	3:E:64:THR:HG23	2.09	0.67
1:C:334:ILE:HG23	1:C:335:ALA:H	1.60	0.67
1:C:152:GLY:O	1:C:155:SER:N	2.28	0.67
1:C:58:GLN:NE2	1:C:101:ALA:N	2.43	0.67
1:C:64:VAL:HA	1:C:67:MET:CE	2.24	0.67
3:E:152:PHE:HE2	3:E:154:PRO:HA	1.60	0.67
3:E:53:ASP:O	3:E:55:SER:HB3	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2:SER:N	1:C:231:ARG:HG2	2.09	0.67
3:E:117:ALA:O	3:E:118:PHE:HB2	1.94	0.67
2:D:23:LEU:HD22	2:D:212:PHE:HA	1.76	0.67
1:P:293:VAL:HG12	1:P:293:VAL:O	1.94	0.67
3:E:53:ASP:O	3:E:55:SER:CB	2.43	0.67
1:C:169:ILE:HD11	1:C:176:ILE:HG21	1.77	0.67
4:C:501:HEM:O2A	4:C:501:HEM:O1D	2.13	0.67
1:C:73:VAL:HG13	1:C:151:TRP:NE1	2.10	0.67
1:P:58:GLN:NE2	1:P:101:ALA:CA	2.58	0.67
1:P:330:PHE:HA	1:P:333:VAL:CG2	2.25	0.67
1:P:112:ILE:CD1	4:P:502:HEM:HBC2	2.21	0.67
1:C:403:TYR:CA	1:C:407:ILE:HG22	2.25	0.66
1:P:403:TYR:CA	1:P:407:ILE:HG22	2.24	0.66
3:R:37:GLN:HE21	3:R:38:MET:CA	2.08	0.66
3:E:98:ALA:HB2	3:E:108:ALA:CA	2.14	0.66
2:D:80:ARG:HH22	2:D:86:ASP:CG	1.98	0.66
1:P:199:TYR:O	1:P:199:TYR:HD2	1.78	0.66
2:D:57:ASP:O	2:D:61:VAL:HG23	1.94	0.66
1:P:62:GLY:HA2	1:P:97:HIS:CE1	2.31	0.66
2:Q:23:LEU:HD22	2:Q:212:PHE:HA	1.77	0.66
1:C:32:THR:HG22	1:C:33:ILE:HG13	1.77	0.66
3:R:62:GLN:HE22	3:R:64:THR:HG23	1.60	0.66
3:E:116:PRO:O	3:E:117:ALA:HB2	1.96	0.66
3:E:95:ASP:CB	3:E:173:ARG:HA	2.26	0.66
1:P:231:ARG:C	1:P:233:SER:N	2.47	0.66
2:D:202:VAL:O	2:D:205:MET:HB2	1.95	0.66
3:R:116:PRO:O	3:R:117:ALA:HB2	1.96	0.66
1:C:330:PHE:HA	1:C:333:VAL:CG2	2.26	0.66
3:E:37:GLN:HG3	3:E:38:MET:N	2.11	0.66
2:D:97:GLY:HA2	6:D:501:HEC:HMD3	1.78	0.66
3:R:127:LEU:HD12	3:R:128:VAL:N	2.11	0.66
3:R:100:ASN:HA	3:R:177:ILE:O	1.96	0.66
1:C:117:TYR:HB2	1:C:367:PHE:CZ	2.30	0.66
1:C:403:TYR:O	1:C:407:ILE:HG22	1.95	0.66
1:P:319:ASP:C	1:P:321:LEU:H	1.99	0.66
3:R:53:ASP:O	3:R:55:SER:HB3	1.95	0.66
1:C:370:LEU:HD12	1:C:370:LEU:C	2.16	0.66
1:P:138:LEU:HB3	1:P:205:ILE:CD1	2.26	0.66
3:E:114:THR:O	3:E:115:LEU:HB2	1.96	0.66
3:R:95:ASP:CB	3:R:173:ARG:HA	2.26	0.65
1:P:347:PRO:HB2	1:P:348:TRP:CD1	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:61:THR:HG23	1:P:62:GLY:H	1.61	0.65
2:Q:27:PHE:HE2	2:Q:48:LEU:HD13	1.60	0.65
2:D:213:LEU:O	2:D:216:ALA:N	2.28	0.65
2:Q:72:ILE:HG12	2:Q:73:ASP:H	1.58	0.65
1:C:86:ASP:OD1	3:E:42:ALA:HB3	1.95	0.65
3:E:129:MET:HE2	3:E:164:GLY:HA3	1.78	0.65
1:C:166:PHE:CE1	1:C:180:LEU:HD11	2.31	0.65
1:C:301:PHE:HA	1:C:304:ILE:CG1	2.26	0.65
1:C:45:TRP:CZ3	1:C:118:TYR:CD1	2.84	0.65
1:P:370:LEU:HD12	1:P:370:LEU:C	2.15	0.65
3:E:186:THR:O	3:E:186:THR:CG2	2.44	0.65
1:C:182:GLY:CA	1:C:193:ARG:NH2	2.60	0.65
1:C:95:TYR:CE2	1:C:271:PRO:HB2	2.31	0.65
1:C:347:PRO:HB2	1:C:348:TRP:CD1	2.29	0.65
1:C:292:ILE:H	1:C:292:ILE:CD1	1.98	0.65
1:P:284:ASN:ND2	1:P:287:SER:N	2.41	0.65
3:E:88:VAL:HB	3:E:165:ARG:HH22	1.59	0.65
3:R:53:ASP:O	3:R:55:SER:CB	2.45	0.65
1:C:187:ASP:H	1:C:190:THR:CG2	2.09	0.65
1:P:403:TYR:O	1:P:407:ILE:HG22	1.96	0.65
2:D:80:ARG:NH2	2:D:86:ASP:OD1	2.27	0.65
3:R:186:THR:O	3:R:186:THR:HG23	1.97	0.65
1:C:145:MET:SD	1:C:197:LEU:HB3	2.36	0.65
1:P:139:MET:N	1:P:205:ILE:HD11	2.10	0.65
1:P:304:ILE:HG22	1:P:397:SER:OG	1.96	0.65
1:P:416:LYS:HB3	1:P:417:PRO:CD	2.24	0.65
3:E:73:PHE:HE2	3:E:151:TRP:HE1	1.43	0.65
1:C:194:PHE:HE1	5:C:503:SMA:H28	1.61	0.65
1:C:297:TYR:C	1:C:298:PHE:HD1	1.99	0.65
1:C:95:TYR:CD2	1:C:271:PRO:HB2	2.32	0.65
3:E:127:LEU:HD12	3:E:128:VAL:N	2.11	0.65
2:D:27:PHE:HE2	2:D:48:LEU:HD13	1.62	0.65
1:C:225:THR:CG2	1:C:227:VAL:HG22	2.27	0.65
1:P:63:ILE:C	1:P:63:ILE:HD13	2.16	0.65
2:Q:65:ALA:O	2:Q:66:ALA:C	2.35	0.65
2:D:158:PHE:HE1	6:D:501:HEC:O1A	1.80	0.65
2:D:189:ASP:H	2:D:191:GLN:NE2	1.95	0.65
3:R:186:THR:CG2	3:R:186:THR:O	2.44	0.65
1:C:41:LEU:HD13	1:C:45:TRP:CD1	2.32	0.65
1:C:45:TRP:CH2	1:C:118:TYR:CD1	2.81	0.65
1:P:149:LEU:CD2	1:P:195:PHE:HD2	2.10	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:183:VAL:O	3:E:184:ASP:HB2	1.97	0.65
2:D:38:HIS:HB3	2:D:100:LEU:HD21	1.78	0.65
2:D:18:TYR:CZ	2:D:215:TRP:HA	2.32	0.65
3:E:141:MET:HB2	3:E:152:PHE:O	1.97	0.65
1:P:284:ASN:HD21	1:P:287:SER:H	1.38	0.65
3:E:156:HIS:HB2	7:E:501:FES:S1	2.37	0.65
1:C:135:ILE:CG1	1:C:208:LEU:HD22	2.26	0.64
1:C:360:ARG:CZ	1:C:415:GLU:HG3	2.27	0.64
1:C:415:GLU:OE2	1:C:415:GLU:HA	1.97	0.64
2:Q:23:LEU:CD2	2:Q:212:PHE:HA	2.27	0.64
2:D:72:ILE:HG12	2:D:73:ASP:H	1.59	0.64
1:C:305:LEU:HD22	1:C:336:MET:HE3	1.79	0.64
1:P:298:PHE:HD2	5:P:503:SMA:H11	1.63	0.64
3:R:134:THR:OG1	3:R:171:ALA:HB1	1.98	0.64
3:R:100:ASN:N	3:R:100:ASN:ND2	2.34	0.64
1:C:138:LEU:HB3	1:C:205:ILE:CD1	2.28	0.64
1:C:62:GLY:HA2	1:C:97:HIS:CE1	2.32	0.64
3:E:37:GLN:HE21	3:E:38:MET:CA	2.10	0.64
1:P:168:ALA:CB	1:P:333:VAL:HG21	2.27	0.64
1:P:83:ILE:HG22	1:P:84:MET:N	2.11	0.64
3:E:134:THR:OG1	3:E:171:ALA:HB1	1.98	0.64
2:D:11:PHE:HA	2:D:17:LYS:CA	2.26	0.64
2:D:23:LEU:CD1	2:D:54:PRO:HD3	2.24	0.64
1:C:319:ASP:C	1:C:321:LEU:H	2.00	0.64
2:Q:23:LEU:CD1	2:Q:54:PRO:HD3	2.25	0.64
3:R:183:VAL:O	3:R:184:ASP:HB2	1.96	0.64
1:C:148:VAL:HA	1:C:155:SER:OG	1.98	0.64
1:C:46:ILE:O	1:C:49:ILE:HG22	1.98	0.64
3:E:62:GLN:HE22	3:E:64:THR:HG23	1.62	0.64
3:R:78:ASP:HB3	3:R:81:ASP:OD2	1.97	0.64
3:E:186:THR:HG23	3:E:186:THR:O	1.97	0.64
1:C:38:PRO:O	1:C:41:LEU:HG	1.97	0.64
1:C:98:ALA:O	1:C:101:ALA:HB3	1.98	0.64
1:C:395:ILE:HG13	1:C:396:ALA:H	1.63	0.64
1:P:41:LEU:HD13	1:P:45:TRP:CD1	2.32	0.64
4:P:501:HEM:HBC2	4:P:501:HEM:CMC	2.27	0.64
2:D:128:PRO:HG3	2:D:214:MET:HG3	1.77	0.64
3:E:78:ASP:HB3	3:E:81:ASP:OD2	1.98	0.64
1:C:58:GLN:NE2	1:C:101:ALA:CA	2.60	0.64
2:D:221:LEU:C	2:D:221:LEU:HD23	2.18	0.64
1:P:395:ILE:HG13	1:P:396:ALA:H	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:30:TYR:HD1	2:Q:34:CYS:CB	2.11	0.64
1:C:298:PHE:HD2	5:C:503:SMA:H11	1.62	0.64
2:Q:18:TYR:CZ	2:Q:215:TRP:HA	2.33	0.64
3:E:73:PHE:CE2	3:E:151:TRP:NE1	2.65	0.64
1:C:350:ASP:HA	1:C:408:LEU:HD12	1.79	0.64
1:C:54:THR:HG21	1:C:104:PHE:CB	2.26	0.64
1:P:117:TYR:HB2	1:P:367:PHE:CE1	2.33	0.64
1:C:118:TYR:O	1:C:120:SER:N	2.30	0.63
1:P:148:VAL:HA	1:P:155:SER:OG	1.97	0.63
1:P:43:TRP:HA	1:P:43:TRP:CE3	2.33	0.63
4:P:501:HEM:HBB2	4:P:501:HEM:CMB	2.28	0.63
1:P:85:ARG:HH12	2:Q:102:VAL:HG22	1.63	0.63
2:Q:221:LEU:C	2:Q:221:LEU:HD23	2.18	0.63
2:D:23:LEU:CD2	2:D:212:PHE:HA	2.28	0.63
2:D:14:ILE:H	2:D:14:ILE:CD1	2.10	0.63
3:R:114:THR:O	3:R:115:LEU:HB2	1.96	0.63
1:C:43:TRP:CE3	1:C:43:TRP:HA	2.34	0.63
1:P:305:LEU:HD22	1:P:336:MET:HE3	1.80	0.63
3:E:100:ASN:HA	3:E:177:ILE:O	1.98	0.63
2:D:138:PHE:HD2	2:D:185:PRO:HA	1.63	0.63
1:C:354:VAL:HG12	1:C:355:ARG:H	1.63	0.63
1:P:350:ASP:HA	1:P:408:LEU:HD12	1.80	0.63
3:E:159:HIS:O	3:E:167:ARG:HB2	1.98	0.63
1:C:243:PRO:O	1:C:244:PHE:C	2.37	0.63
2:D:55:GLN:O	2:D:56:LEU:CG	2.46	0.63
1:C:168:ALA:CB	1:C:333:VAL:HG21	2.28	0.63
1:C:69:TYR:N	1:C:83:ILE:HD11	2.13	0.63
1:P:47:TRP:HE1	1:P:110:ILE:CG2	2.10	0.63
1:P:240:ASP:O	1:P:241:THR:HG23	1.98	0.63
1:C:134:VAL:HG12	1:C:208:LEU:CD1	2.28	0.63
1:P:330:PHE:HA	1:P:333:VAL:HG23	1.79	0.63
1:P:304:ILE:HG23	1:P:377:LEU:HD11	1.81	0.63
2:Q:127:GLY:O	2:Q:130:TYR:N	2.31	0.63
2:D:249:LEU:HD23	2:D:249:LEU:O	1.98	0.63
1:C:263:PHE:HA	1:C:266:VAL:CG2	2.29	0.63
1:C:103:LEU:C	1:C:103:LEU:HD12	2.19	0.63
1:C:147:TYR:HA	4:C:501:HEM:CAA	2.29	0.63
3:E:138:CYS:HB3	1:P:288:THR:HG21	1.79	0.63
1:P:159:ALA:O	1:P:163:THR:HG23	1.98	0.63
2:Q:25:ARG:HE	2:Q:194:TYR:HE2	1.46	0.63
1:C:199:TYR:O	1:C:199:TYR:CD2	2.50	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:160:TYR:CE1	3:E:175:LEU:HG	2.34	0.63
1:C:390:ASP:O	1:C:393:SER:HB2	1.99	0.63
3:R:103:LYS:HB3	3:R:104:PRO:HD2	1.80	0.63
1:C:159:ALA:O	1:C:163:THR:HG23	1.98	0.63
1:C:43:TRP:CZ3	1:C:251:LYS:HE2	2.34	0.63
1:C:112:ILE:CD1	4:C:502:HEM:HBC2	2.24	0.63
1:P:103:LEU:HG	1:P:104:PHE:N	2.13	0.63
2:Q:181:ALA:HB1	6:Q:501:HEC:CBD	2.29	0.63
1:C:240:ASP:O	1:C:241:THR:HG23	1.99	0.63
2:Q:15:PHE:N	2:Q:15:PHE:CD2	2.66	0.63
3:R:100:ASN:C	3:R:102:ASN:H	2.02	0.63
1:C:231:ARG:C	1:C:233:SER:H	2.00	0.63
1:P:98:ALA:O	1:P:101:ALA:HB3	1.99	0.63
2:D:23:LEU:HB3	2:D:54:PRO:HD3	1.81	0.63
3:E:61:THR:O	3:E:62:GLN:HB2	1.99	0.63
3:R:73:PHE:CE2	3:R:151:TRP:NE1	2.66	0.63
2:Q:82:ARG:O	2:Q:83:LYS:O	2.16	0.63
1:C:117:TYR:HB2	1:C:367:PHE:CE1	2.34	0.62
1:P:231:ARG:C	1:P:233:SER:H	2.01	0.62
1:P:305:LEU:HD12	1:P:305:LEU:O	1.98	0.62
1:P:38:PRO:O	1:P:41:LEU:HG	1.98	0.62
1:P:86:ASP:OD1	3:R:42:ALA:CB	2.46	0.62
2:Q:97:GLY:HA2	6:Q:501:HEC:HMD3	1.80	0.62
3:R:37:GLN:HG3	3:R:38:MET:N	2.12	0.62
2:Q:15:PHE:HD2	2:Q:15:PHE:N	1.97	0.62
1:C:304:ILE:HG23	1:C:377:LEU:HD11	1.80	0.62
1:C:61:THR:HG23	1:C:62:GLY:H	1.64	0.62
1:P:343:MET:O	1:P:346:ALA:CB	2.47	0.62
1:P:69:TYR:N	1:P:83:ILE:HD11	2.14	0.62
2:D:25:ARG:HE	2:D:194:TYR:HE2	1.46	0.62
2:Q:14:ILE:H	2:Q:14:ILE:CD1	2.10	0.62
1:C:108:VAL:CG1	1:C:112:ILE:HD11	2.29	0.62
1:C:229:VAL:O	1:C:231:ARG:N	2.28	0.62
1:C:304:ILE:HG22	1:C:397:SER:OG	1.99	0.62
1:C:46:ILE:O	1:C:49:ILE:CG2	2.47	0.62
1:P:118:TYR:O	1:P:120:SER:N	2.32	0.62
1:P:267:VAL:O	1:P:271:PRO:HD3	1.99	0.62
1:P:415:GLU:HA	1:P:415:GLU:OE2	1.99	0.62
4:P:501:HEM:O1D	4:P:501:HEM:O2A	2.17	0.62
3:E:52:VAL:HG11	3:E:74:ILE:CD1	2.27	0.62
1:C:411:LEU:O	1:C:411:LEU:HD22	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:182:GLY:HA2	1:P:193:ARG:NH2	2.14	0.62
1:P:360:ARG:CZ	1:P:415:GLU:HG3	2.29	0.62
1:P:407:ILE:O	1:P:411:LEU:HB2	1.99	0.62
3:R:73:PHE:HE2	3:R:151:TRP:HE1	1.45	0.62
1:P:45:TRP:CZ3	1:P:118:TYR:HD1	2.17	0.62
1:P:73:VAL:HG13	1:P:151:TRP:NE1	2.14	0.62
2:Q:11:PHE:HA	2:Q:17:LYS:CA	2.30	0.62
2:Q:138:PHE:HD2	2:Q:185:PRO:HA	1.64	0.62
1:C:20:HIS:C	1:C:22:ARG:N	2.47	0.62
1:P:45:TRP:HE1	1:P:222:ASN:CA	2.13	0.62
3:E:77:ARG:HD3	3:E:82:ILE:CG1	2.30	0.62
1:P:151:TRP:CE3	1:P:191:LEU:HD12	2.35	0.62
1:P:43:TRP:CZ3	1:P:251:LYS:HE2	2.34	0.62
2:D:134:TYR:CE1	2:D:158:PHE:HB2	2.34	0.62
2:D:29:VAL:CG1	2:D:209:VAL:HG13	2.29	0.62
1:P:354:VAL:HG12	1:P:355:ARG:H	1.64	0.62
2:Q:55:GLN:O	2:Q:56:LEU:CG	2.46	0.62
2:D:15:PHE:N	2:D:15:PHE:CD2	2.66	0.62
1:C:231:ARG:C	1:C:233:SER:N	2.47	0.62
1:P:390:ASP:O	1:P:393:SER:HB2	2.00	0.62
1:P:64:VAL:HA	1:P:67:MET:CE	2.30	0.62
3:R:156:HIS:HB2	7:R:501:FES:S1	2.39	0.62
1:C:54:THR:O	1:C:57:LEU:HB3	2.00	0.62
1:P:45:TRP:HZ2	1:P:222:ASN:CB	2.07	0.62
2:Q:25:ARG:HD2	2:Q:194:TYR:CD2	2.35	0.62
3:E:114:THR:O	3:E:116:PRO:HD2	2.00	0.62
3:R:114:THR:O	3:R:116:PRO:HD2	2.00	0.62
2:D:102:VAL:O	2:D:102:VAL:CG1	2.48	0.62
2:D:181:ALA:HB1	6:D:501:HEC:CBD	2.30	0.62
3:R:158:SER:HA	3:R:168:LYS:O	2.00	0.62
2:Q:241:MET:CB	3:R:19:THR:HG22	2.28	0.62
1:C:69:TYR:OH	1:C:149:LEU:O	2.17	0.61
1:C:47:TRP:HE1	1:C:110:ILE:CG2	2.08	0.61
1:P:134:VAL:HG12	1:P:208:LEU:CD1	2.29	0.61
1:P:69:TYR:OH	1:P:149:LEU:HB3	1.99	0.61
2:Q:29:VAL:CG1	2:Q:209:VAL:HG13	2.29	0.61
2:D:127:GLY:O	2:D:130:TYR:N	2.33	0.61
3:E:62:GLN:HB2	3:E:75:ARG:HG3	1.82	0.61
2:Q:189:ASP:H	2:Q:191:GLN:NE2	1.97	0.61
1:C:284:ASN:ND2	1:C:287:SER:N	2.45	0.61
1:C:11:PRO:O	1:C:13:THR:N	2.32	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:163:THR:OG1	1:C:181:LEU:HD21	2.00	0.61
1:C:230:ARG:C	1:C:232:THR:H	2.02	0.61
1:C:330:PHE:HA	1:C:333:VAL:HG23	1.81	0.61
1:C:63:ILE:C	1:C:63:ILE:HD13	2.20	0.61
2:D:222:VAL:CG2	2:D:223:ALA:H	2.06	0.61
1:P:114:ARG:HE	1:P:115:GLY:CA	2.13	0.61
1:P:194:PHE:HE1	5:P:503:SMA:H28	1.66	0.61
1:C:293:VAL:O	1:C:293:VAL:HG12	1.98	0.61
1:C:114:ARG:HE	1:C:115:GLY:CA	2.14	0.61
2:Q:23:LEU:HB3	2:Q:54:PRO:HD3	1.82	0.61
2:D:65:ALA:O	2:D:66:ALA:C	2.37	0.61
2:Q:71:ILE:O	2:Q:72:ILE:O	2.18	0.61
1:P:225:THR:CG2	1:P:227:VAL:HG22	2.30	0.61
1:P:229:VAL:O	1:P:231:ARG:N	2.26	0.61
1:P:301:PHE:HA	1:P:304:ILE:CG1	2.31	0.61
1:P:61:THR:HG23	1:P:62:GLY:N	2.15	0.61
3:E:100:ASN:C	3:E:102:ASN:H	2.01	0.61
2:Q:249:LEU:HD23	2:Q:249:LEU:O	2.00	0.61
1:C:103:LEU:HG	1:C:104:PHE:N	2.15	0.61
1:C:305:LEU:HD12	1:C:305:LEU:O	1.99	0.61
1:P:58:GLN:NE2	1:P:101:ALA:HA	2.15	0.61
3:E:103:LYS:HB3	3:E:104:PRO:HD2	1.80	0.61
3:E:158:SER:HA	3:E:168:LYS:O	1.99	0.61
2:D:15:PHE:HD2	2:D:15:PHE:N	1.97	0.61
1:C:43:TRP:HZ3	1:C:251:LYS:CG	2.13	0.61
1:C:45:TRP:HE1	1:C:222:ASN:CA	2.13	0.61
1:P:74:ASP:O	1:P:75:LEU:HD23	2.01	0.61
2:Q:222:VAL:CG2	2:Q:223:ALA:H	2.04	0.61
1:P:243:PRO:O	1:P:244:PHE:C	2.37	0.61
1:C:286:LEU:HD12	1:C:286:LEU:H	1.63	0.61
3:E:179:VAL:HG13	3:E:179:VAL:O	2.00	0.61
2:Q:173:VAL:O	2:Q:174:LYS:HD2	2.00	0.61
3:R:61:THR:O	3:R:62:GLN:HB2	2.00	0.61
3:R:62:GLN:HB2	3:R:75:ARG:HG3	1.81	0.61
1:C:305:LEU:C	1:C:305:LEU:HD12	2.21	0.61
1:P:166:PHE:CE1	1:P:180:LEU:HD11	2.34	0.61
1:P:249:VAL:HG12	1:P:250:ILE:N	2.15	0.61
2:Q:80:ARG:NH2	2:Q:86:ASP:OD1	2.27	0.61
1:C:245:TRP:C	1:C:245:TRP:CD1	2.74	0.61
1:C:418:GLU:CD	1:C:419:PRO:N	2.54	0.61
1:C:42:ASN:O	1:C:45:TRP:HB2	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:143:ALA:HA	4:C:501:HEM:HMB1	1.83	0.61
1:P:169:ILE:HG13	1:P:173:GLY:CA	2.31	0.61
1:P:418:GLU:CD	1:P:419:PRO:N	2.54	0.61
1:P:74:ASP:C	1:P:75:LEU:HD23	2.21	0.61
2:D:30:TYR:HD1	2:D:34:CYS:CB	2.12	0.61
1:P:286:LEU:H	1:P:286:LEU:HD12	1.66	0.61
1:C:188:ASN:O	1:C:191:LEU:HB3	2.01	0.61
1:C:131:VAL:HG13	1:C:208:LEU:HD21	1.79	0.61
1:C:300:PRO:HG2	1:C:301:PHE:H	1.66	0.61
1:C:343:MET:O	1:C:346:ALA:CB	2.49	0.61
1:C:360:ARG:NE	1:C:415:GLU:HG3	2.16	0.61
1:P:348:TRP:HD1	1:P:348:TRP:N	1.97	0.61
1:P:143:ALA:HA	4:P:501:HEM:HMB1	1.83	0.61
1:P:77:PHE:O	1:P:80:VAL:HB	2.01	0.61
3:E:18:ALA:O	3:E:22:THR:HG23	2.01	0.61
1:P:263:PHE:CA	1:P:266:VAL:HG23	2.30	0.61
3:E:55:SER:O	3:E:56:ALA:HB3	2.01	0.61
2:Q:205:MET:CE	2:Q:205:MET:HA	2.30	0.61
2:D:72:ILE:HG12	2:D:73:ASP:N	2.16	0.61
1:P:230:ARG:C	1:P:232:THR:H	2.03	0.60
3:R:160:TYR:CE1	3:R:175:LEU:HG	2.35	0.60
1:P:11:PRO:O	1:P:13:THR:N	2.34	0.60
1:C:23:LEU:C	1:C:26:VAL:HG12	2.21	0.60
1:C:298:PHE:C	1:C:300:PRO:HD2	2.21	0.60
1:C:348:TRP:N	1:C:348:TRP:HD1	1.97	0.60
1:C:36:PRO:HB3	1:C:241:THR:HB	1.83	0.60
3:R:77:ARG:HD3	3:R:82:ILE:CG1	2.30	0.60
1:C:18:TRP:C	1:C:20:HIS:H	2.04	0.60
1:P:20:HIS:C	1:P:22:ARG:N	2.52	0.60
1:P:41:LEU:HB2	1:P:248:PHE:HE2	1.66	0.60
2:D:27:PHE:CE1	2:D:31:ASN:HB2	2.36	0.60
2:D:38:HIS:CG	2:D:100:LEU:HD21	2.37	0.60
1:C:169:ILE:HG13	1:C:173:GLY:CA	2.31	0.60
1:P:102:SER:OG	1:P:296:TRP:NE1	2.34	0.60
1:P:300:PRO:HG2	1:P:301:PHE:H	1.67	0.60
1:P:52:ALA:N	4:P:502:HEM:HMB3	2.16	0.60
3:E:121:THR:HG23	3:E:122:ASN:N	2.15	0.60
1:C:71:PRO:O	1:C:72:HIS:HB2	1.99	0.60
1:P:43:TRP:HE3	1:P:43:TRP:HA	1.66	0.60
2:Q:27:PHE:HE1	2:Q:31:ASN:HB2	1.67	0.60
3:R:36:ASN:O	3:R:37:GLN:C	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:71:ILE:O	2:D:72:ILE:O	2.18	0.60
3:R:25:VAL:HG12	3:R:26:VAL:N	2.16	0.60
1:C:43:TRP:HZ3	1:C:251:LYS:HG2	1.66	0.60
1:C:377:LEU:HD23	1:C:396:ALA:HB1	1.84	0.60
1:P:108:VAL:CG1	1:P:112:ILE:HD11	2.31	0.60
2:Q:198:THR:CG2	2:Q:199:PRO:HD2	2.30	0.60
2:D:135:VAL:CG2	6:D:501:HEC:HMB2	2.30	0.60
2:D:72:ILE:HG23	2:D:73:ASP:H	1.66	0.60
1:P:46:ILE:O	1:P:49:ILE:HG22	2.01	0.60
2:Q:102:VAL:O	2:Q:102:VAL:CG1	2.49	0.60
2:Q:72:ILE:HG12	2:Q:73:ASP:N	2.16	0.60
2:D:251:ALA:HB3	2:D:252:PRO:HD3	1.84	0.60
2:D:82:ARG:O	2:D:83:LYS:O	2.19	0.60
1:P:375:VAL:HG12	1:P:376:VAL:N	2.16	0.60
3:E:118:PHE:C	3:E:120:GLY:H	2.05	0.60
1:C:292:ILE:HD12	1:C:292:ILE:N	2.07	0.60
3:R:121:THR:O	3:R:122:ASN:HB3	2.01	0.60
3:R:121:THR:HG23	3:R:122:ASN:N	2.16	0.60
1:C:346:ALA:HB3	1:C:347:PRO:CD	2.30	0.60
1:C:61:THR:HG23	1:C:62:GLY:N	2.16	0.60
3:E:36:ASN:O	3:E:37:GLN:C	2.38	0.60
2:Q:134:TYR:CE1	2:Q:158:PHE:HB2	2.35	0.60
1:C:32:THR:CG2	1:C:33:ILE:HG13	2.32	0.60
3:E:25:VAL:HG12	3:E:26:VAL:N	2.16	0.60
3:R:18:ALA:O	3:R:22:THR:HG23	2.02	0.60
1:P:95:TYR:HE2	1:P:272:ASN:OD1	1.84	0.60
2:D:96:MET:O	6:D:501:HEC:HMD3	2.02	0.60
2:Q:13:GLY:O	2:Q:15:PHE:N	2.35	0.60
2:Q:231:ALA:O	2:Q:234:MET:HB2	2.02	0.60
1:C:45:TRP:CZ3	1:C:118:TYR:HD1	2.18	0.59
1:C:249:VAL:HG12	1:C:250:ILE:N	2.16	0.59
1:P:188:ASN:O	1:P:191:LEU:HB3	2.02	0.59
1:P:77:PHE:CD1	1:P:282:GLN:HG3	2.37	0.59
2:Q:29:VAL:O	2:Q:33:VAL:HG12	2.02	0.59
2:Q:49:ALA:O	2:Q:51:ASP:N	2.35	0.59
3:R:37:GLN:NE2	3:R:38:MET:HG2	2.16	0.59
1:P:414:THR:C	1:P:417:PRO:HD2	2.22	0.59
3:R:159:HIS:O	3:R:167:ARG:HB2	2.02	0.59
3:E:121:THR:O	3:E:122:ASN:HB3	2.02	0.59
1:C:227:VAL:O	1:C:229:VAL:N	2.35	0.59
1:C:41:LEU:HB2	1:C:248:PHE:HE2	1.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:367:PHE:HD2	1:C:368:TRP:CD1	2.21	0.59
1:C:77:PHE:O	1:C:80:VAL:HB	2.02	0.59
1:P:54:THR:HG21	1:P:104:PHE:CA	2.32	0.59
1:P:411:LEU:O	1:P:411:LEU:HD22	2.02	0.59
6:Q:501:HEC:HMB1	6:Q:501:HEC:HBB3	1.84	0.59
2:D:27:PHE:HE1	2:D:31:ASN:HB2	1.66	0.59
2:D:49:ALA:O	2:D:51:ASP:N	2.35	0.59
2:Q:233:VAL:HG22	2:Q:234:MET:N	2.17	0.59
3:R:179:VAL:O	3:R:179:VAL:HG13	2.02	0.59
1:C:403:TYR:HD2	1:C:404:PHE:CD1	2.20	0.59
1:C:52:ALA:N	4:C:502:HEM:HMB3	2.17	0.59
1:P:87:VAL:O	1:P:89:GLY:N	2.34	0.59
1:C:179:TRP:HE1	3:R:38:MET:HB2	1.66	0.59
1:P:245:TRP:C	1:P:245:TRP:CD1	2.75	0.59
2:D:242:LEU:O	2:D:243:TYR:C	2.40	0.59
1:P:377:LEU:HD23	1:P:396:ALA:HB1	1.84	0.59
1:P:51:LEU:HD11	1:P:108:VAL:CA	2.29	0.59
3:R:53:ASP:C	3:R:55:SER:H	2.03	0.59
1:C:140:MET:HE2	5:C:503:SMA:H37	1.83	0.59
1:P:304:ILE:HG22	1:P:397:SER:CB	2.32	0.59
2:Q:38:HIS:CG	2:Q:100:LEU:HD21	2.36	0.59
2:Q:27:PHE:CE1	2:Q:31:ASN:HB2	2.37	0.59
2:D:198:THR:CG2	2:D:199:PRO:HD2	2.31	0.59
3:R:152:PHE:CE2	3:R:154:PRO:HA	2.38	0.59
1:P:32:THR:CG2	1:P:33:ILE:HG13	2.32	0.59
1:P:36:PRO:HB3	1:P:241:THR:HB	1.84	0.59
2:D:13:GLY:O	2:D:15:PHE:N	2.35	0.59
1:C:49:ILE:HG23	1:C:50:VAL:N	2.17	0.59
1:C:69:TYR:OH	1:C:149:LEU:HB3	2.01	0.59
1:P:305:LEU:HD12	1:P:305:LEU:C	2.23	0.59
1:P:91:TRP:CE3	2:Q:224:ARG:HG2	2.37	0.59
2:D:72:ILE:HG23	2:D:73:ASP:N	2.17	0.59
3:R:180:ALA:CB	3:R:190:LEU:HD23	2.31	0.59
3:E:53:ASP:C	3:E:55:SER:H	2.02	0.59
3:R:55:SER:O	3:R:56:ALA:HB3	2.01	0.59
1:P:140:MET:HE2	5:P:503:SMA:H37	1.83	0.59
1:P:367:PHE:HD2	1:P:368:TRP:CD1	2.21	0.59
2:Q:131:ILE:O	2:Q:134:TYR:HB3	2.03	0.59
2:D:138:PHE:CE2	2:D:186:PRO:HD3	2.38	0.59
2:D:205:MET:CE	2:D:205:MET:HA	2.33	0.59
6:D:501:HEC:HBB3	6:D:501:HEC:HMB1	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:80:LYS:O	3:R:84:LEU:HG	2.03	0.59
1:C:47:TRP:NE1	1:C:110:ILE:CG2	2.66	0.59
2:Q:132:TYR:CZ	2:Q:136:ILE:HD12	2.38	0.59
2:Q:72:ILE:HG23	2:Q:73:ASP:N	2.17	0.59
2:Q:72:ILE:HG23	2:Q:73:ASP:H	1.66	0.59
1:C:133:MET:HE2	1:C:344:ALA:N	2.18	0.59
1:C:294:PRO:HD3	1:C:302:TYR:CE1	2.38	0.59
1:P:163:THR:OG1	1:P:181:LEU:HD21	2.01	0.59
1:C:407:ILE:O	1:C:411:LEU:HB2	2.02	0.58
1:P:43:TRP:HZ3	1:P:251:LYS:CG	2.15	0.58
2:D:132:TYR:CZ	2:D:136:ILE:HD12	2.38	0.58
1:C:375:VAL:HG12	1:C:376:VAL:N	2.17	0.58
2:Q:138:PHE:CE2	2:Q:186:PRO:HD3	2.38	0.58
1:P:68:HIS:HE1	3:R:37:GLN:NE2	2.00	0.58
3:R:67:TRP:CE2	3:R:68:ARG:HD2	2.38	0.58
1:C:297:TYR:CD1	1:C:297:TYR:N	2.71	0.58
1:C:299:LEU:N	1:C:300:PRO:HD2	2.18	0.58
1:P:331:PHE:O	1:P:334:ILE:HG23	2.04	0.58
1:P:42:ASN:O	1:P:45:TRP:HB2	2.03	0.58
2:Q:135:VAL:CG2	6:Q:501:HEC:HMB2	2.33	0.58
2:Q:242:LEU:O	2:Q:243:TYR:C	2.40	0.58
2:D:186:PRO:CG	2:D:187:LEU:H	2.16	0.58
2:Q:251:ALA:HB3	2:Q:252:PRO:HD3	1.85	0.58
3:R:100:ASN:HB3	3:R:177:ILE:CB	2.33	0.58
1:C:157:TRP:CH2	3:R:139:VAL:HG23	2.38	0.58
1:C:139:MET:N	1:C:205:ILE:HD11	2.18	0.58
1:P:227:VAL:O	1:P:229:VAL:N	2.36	0.58
1:C:43:TRP:HE3	1:C:43:TRP:HA	1.67	0.58
1:P:80:VAL:O	1:P:83:ILE:HB	2.04	0.58
2:D:173:VAL:O	2:D:174:LYS:HD2	2.03	0.58
1:C:294:PRO:HG3	1:C:302:TYR:HD1	1.67	0.58
3:E:91:GLY:O	3:E:92:ALA:HB3	2.04	0.58
3:E:152:PHE:CE2	3:E:154:PRO:HA	2.38	0.58
3:R:162:SER:C	3:R:164:GLY:H	2.07	0.58
1:C:149:LEU:CD2	1:C:195:PHE:HD2	2.16	0.58
1:P:109:TYR:CE2	1:P:374:PHE:HZ	2.22	0.58
1:P:145:MET:SD	1:P:197:LEU:CB	2.92	0.58
1:P:43:TRP:HZ3	1:P:251:LYS:HG2	1.69	0.58
1:P:292:ILE:HD12	1:P:292:ILE:N	2.07	0.58
1:P:54:THR:O	1:P:57:LEU:HB3	2.03	0.58
1:P:68:HIS:C	1:P:83:ILE:HD11	2.23	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:186:PRO:HG2	2:D:187:LEU:N	2.17	0.58
3:E:80:LYS:O	3:E:84:LEU:HG	2.04	0.58
1:C:182:GLY:HA2	1:C:193:ARG:NH2	2.18	0.58
1:C:230:ARG:C	1:C:232:THR:N	2.57	0.58
1:P:135:ILE:HG21	4:P:502:HEM:CBB	2.33	0.58
3:R:100:ASN:HB2	3:R:115:LEU:HD11	1.85	0.58
1:C:58:GLN:NE2	1:C:101:ALA:HA	2.18	0.58
1:C:280:TYR:CZ	2:D:105:LYS:HD2	2.38	0.58
1:C:46:ILE:HD11	1:C:252:ASP:HA	1.86	0.58
4:C:501:HEM:HBB2	4:C:501:HEM:CMB	2.33	0.58
3:E:37:GLN:NE2	3:E:38:MET:HG2	2.19	0.58
1:P:360:ARG:NE	1:P:415:GLU:HG3	2.18	0.58
1:P:69:TYR:CZ	1:P:149:LEU:HB3	2.38	0.58
2:Q:44:PRO:HB3	2:Q:46:ARG:HE	1.68	0.58
3:E:180:ALA:CB	3:E:190:LEU:HD23	2.33	0.58
1:C:153:GLN:HE21	1:C:289:PRO:HD3	1.69	0.58
1:P:46:ILE:O	1:P:49:ILE:CG2	2.52	0.58
1:P:89:GLY:O	1:P:90:GLY:C	2.42	0.58
1:C:414:THR:C	1:C:417:PRO:HD2	2.24	0.58
2:D:190:ASP:C	2:D:192:VAL:H	2.07	0.58
1:P:286:LEU:N	1:P:286:LEU:CD1	2.67	0.58
3:R:186:THR:O	3:R:187:THR:HG23	2.04	0.57
3:R:74:ILE:HA	3:R:128:VAL:HG22	1.84	0.57
1:C:223:ASN:HD21	1:C:225:THR:CG2	1.97	0.57
1:C:304:ILE:HG22	1:C:397:SER:CB	2.34	0.57
1:C:69:TYR:CZ	1:C:149:LEU:HB3	2.39	0.57
1:P:363:PHE:HB2	1:P:415:GLU:OE1	2.04	0.57
2:Q:204:GLN:NE2	2:Q:208:ASP:OD2	2.37	0.57
3:E:170:PRO:O	3:E:171:ALA:C	2.42	0.57
2:D:233:VAL:HG22	2:D:234:MET:N	2.18	0.57
1:C:24:PRO:O	1:C:25:ILE:C	2.42	0.57
1:C:23:LEU:HA	1:C:26:VAL:CG1	2.34	0.57
1:P:403:TYR:HD2	1:P:404:PHE:CD1	2.22	0.57
1:P:45:TRP:HZ3	1:P:118:TYR:CE1	2.22	0.57
2:Q:190:ASP:C	2:Q:192:VAL:H	2.07	0.57
2:D:45:ILE:O	2:D:47:THR:N	2.37	0.57
1:C:225:THR:HG22	1:C:227:VAL:HG22	1.86	0.57
2:D:29:VAL:O	2:D:33:VAL:HG12	2.03	0.57
4:C:501:HEM:HBC2	4:C:501:HEM:CMC	2.28	0.57
1:C:68:HIS:C	1:C:83:ILE:HD11	2.23	0.57
1:P:133:MET:HE2	1:P:344:ALA:N	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:298:PHE:C	1:P:300:PRO:HD2	2.24	0.57
2:Q:74:LYS:HZ3	2:Q:75:ASP:HB3	1.70	0.57
3:E:162:SER:C	3:E:164:GLY:H	2.07	0.57
1:C:363:PHE:HB2	1:C:415:GLU:OE1	2.05	0.57
1:P:23:LEU:C	1:P:26:VAL:HG12	2.24	0.57
2:D:25:ARG:HD2	2:D:194:TYR:CD2	2.36	0.57
3:E:67:TRP:CE2	3:E:68:ARG:HD2	2.39	0.57
1:C:54:THR:HG21	1:C:104:PHE:CA	2.35	0.57
2:Q:45:ILE:O	2:Q:47:THR:N	2.36	0.57
2:Q:96:MET:O	6:Q:501:HEC:HMD3	2.03	0.57
3:R:170:PRO:O	3:R:171:ALA:C	2.43	0.57
2:Q:40:MET:HB3	2:Q:43:VAL:CG2	2.34	0.57
1:C:149:LEU:N	1:C:150:PRO:HD2	2.20	0.57
1:C:222:ASN:CG	1:C:223:ASN:H	2.08	0.57
1:P:41:LEU:O	1:P:251:LYS:NZ	2.38	0.57
2:D:138:PHE:CD2	2:D:185:PRO:HA	2.40	0.57
2:D:241:MET:CB	3:E:19:THR:HG22	2.27	0.57
3:E:55:SER:O	3:E:56:ALA:CB	2.52	0.57
2:D:204:GLN:NE2	2:D:208:ASP:OD2	2.37	0.57
2:D:73:ASP:OD2	2:D:74:LYS:HE3	2.05	0.57
2:D:40:MET:HB3	2:D:43:VAL:CG2	2.35	0.57
1:P:131:VAL:HG13	1:P:208:LEU:HD21	1.83	0.57
1:P:294:PRO:HD3	1:P:302:TYR:CE1	2.39	0.57
1:P:40:ASN:ND2	1:P:224:PRO:HG2	2.20	0.57
3:E:74:ILE:HA	3:E:128:VAL:HG22	1.86	0.57
3:E:99:GLU:O	3:E:100:ASN:C	2.43	0.57
1:C:86:ASP:CG	2:D:46:ARG:HH22	2.07	0.57
1:C:142:THR:OG1	1:C:201:LEU:HB3	2.05	0.57
2:D:131:ILE:O	2:D:134:TYR:HB3	2.05	0.57
3:E:67:TRP:HE3	3:E:72:VAL:HG21	1.69	0.57
3:R:93:LEU:HD21	3:R:165:ARG:HB3	1.87	0.56
1:C:403:TYR:CD2	1:C:404:PHE:CD1	2.93	0.56
1:C:89:GLY:O	1:C:92:ALA:CB	2.47	0.56
1:P:329:LYS:O	1:P:333:VAL:HG22	2.05	0.56
1:P:49:ILE:HG23	1:P:50:VAL:N	2.20	0.56
2:Q:19:ASP:O	2:Q:21:ALA:N	2.38	0.56
1:C:403:TYR:HD2	1:C:404:PHE:HD1	1.53	0.56
1:P:256:LEU:HA	1:P:259:VAL:CG2	2.36	0.56
1:P:388:PRO:O	1:P:392:ILE:HG13	2.06	0.56
3:E:113:ARG:HD2	3:E:177:ILE:HD11	1.87	0.56
3:E:115:LEU:HD12	3:E:177:ILE:HG21	1.85	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:360:ARG:O	1:C:363:PHE:HB3	2.05	0.56
1:P:45:TRP:NE1	1:P:222:ASN:N	2.39	0.56
2:Q:221:LEU:HD23	2:Q:222:VAL:N	2.21	0.56
1:C:144:PHE:CG	1:C:145:MET:N	2.74	0.56
1:C:41:LEU:O	1:C:251:LYS:NZ	2.37	0.56
1:C:256:LEU:HA	1:C:259:VAL:CG2	2.35	0.56
1:C:330:PHE:O	1:C:333:VAL:HG23	2.05	0.56
1:C:135:ILE:HG21	4:C:502:HEM:CBB	2.35	0.56
1:C:51:LEU:HD11	1:C:108:VAL:CA	2.30	0.56
1:P:114:ARG:NE	1:P:115:GLY:N	2.52	0.56
1:P:66:ALA:HB2	4:P:501:HEM:HHD	1.87	0.56
1:P:71:PRO:O	1:P:72:HIS:HB2	2.06	0.56
3:E:100:ASN:HB2	3:E:115:LEU:HD11	1.86	0.56
2:D:19:ASP:O	2:D:21:ALA:N	2.38	0.56
2:Q:113:PRO:O	2:Q:114:ALA:CB	2.54	0.56
1:P:290:ALA:O	1:P:291:HIS:HB2	2.06	0.56
1:P:93:MET:O	1:P:94:ARG:C	2.42	0.56
3:R:55:SER:O	3:R:56:ALA:CB	2.52	0.56
1:P:377:LEU:HD22	1:P:396:ALA:HB1	1.86	0.56
1:P:111:HIS:CE1	4:P:502:HEM:O1A	2.58	0.56
1:P:309:ALA:O	1:P:310:ALA:HB3	2.06	0.56
3:R:115:LEU:O	3:R:116:PRO:O	2.23	0.56
1:C:377:LEU:HD22	1:C:396:ALA:HB1	1.86	0.56
1:C:87:VAL:O	1:C:89:GLY:N	2.38	0.56
1:P:230:ARG:C	1:P:232:THR:N	2.57	0.56
1:P:23:LEU:HA	1:P:26:VAL:CG1	2.35	0.56
2:Q:181:ALA:HB1	6:Q:501:HEC:HBD1	1.88	0.56
1:C:309:ALA:O	1:C:310:ALA:HB3	2.06	0.56
1:C:169:ILE:O	1:C:173:GLY:HA3	2.05	0.56
1:C:305:LEU:CD2	1:C:336:MET:CE	2.83	0.56
1:C:45:TRP:HZ3	1:C:118:TYR:CE1	2.24	0.56
1:P:147:TYR:HD1	4:P:501:HEM:HAA2	1.70	0.56
2:Q:33:VAL:O	2:Q:34:CYS:HB2	2.05	0.56
3:E:100:ASN:HB3	3:E:177:ILE:CB	2.33	0.56
1:P:9:TYR:O	1:P:10:GLU:CB	2.54	0.56
1:C:151:TRP:CE3	1:C:191:LEU:HD12	2.41	0.56
1:C:361:PRO:HG3	1:C:364:ARG:CZ	2.35	0.56
1:P:22:ARG:O	1:P:23:LEU:O	2.24	0.56
3:R:124:GLY:O	3:R:125:GLU:HB2	2.05	0.56
1:C:23:LEU:CA	1:C:26:VAL:HG12	2.35	0.56
3:E:38:MET:HB2	1:P:179:TRP:HE1	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:222:ASN:CG	1:P:223:ASN:H	2.08	0.56
1:P:46:ILE:HD11	1:P:252:ASP:HA	1.84	0.56
1:P:72:HIS:C	1:P:72:HIS:ND1	2.59	0.56
2:Q:242:LEU:O	2:Q:245:THR:N	2.39	0.56
2:D:33:VAL:O	2:D:34:CYS:HB2	2.05	0.56
2:D:241:MET:HB3	3:E:19:THR:CB	2.35	0.56
3:R:67:TRP:HE3	3:R:72:VAL:HG21	1.70	0.56
1:C:144:PHE:CD1	1:C:162:ILE:HD13	2.41	0.56
1:C:302:TYR:C	1:C:302:TYR:CD2	2.80	0.56
1:C:331:PHE:O	1:C:334:ILE:HG23	2.05	0.56
1:C:202:PRO:HG3	4:C:501:HEM:CMC	2.35	0.56
1:P:144:PHE:O	1:P:148:VAL:HG23	2.05	0.56
1:P:297:TYR:CD1	1:P:297:TYR:N	2.73	0.56
1:P:330:PHE:O	1:P:333:VAL:HG23	2.05	0.56
1:P:294:PRO:HA	5:P:503:SMA:H10	1.87	0.56
3:E:118:PHE:O	3:E:119:ASP:HB2	2.06	0.56
3:E:124:GLY:O	3:E:125:GLU:HB2	2.06	0.56
1:P:7:ASP:C	1:P:9:TYR:H	2.09	0.56
1:P:384:PRO:O	1:P:386:GLU:N	2.35	0.56
2:D:92:VAL:HG12	2:D:93:GLY:N	2.21	0.56
3:E:186:THR:O	3:E:187:THR:HG23	2.06	0.56
1:C:305:LEU:C	1:C:307:ALA:H	2.08	0.56
1:P:227:VAL:C	1:P:229:VAL:N	2.60	0.56
3:R:91:GLY:O	3:R:92:ALA:HB3	2.06	0.55
1:P:169:ILE:O	1:P:173:GLY:HA3	2.07	0.55
1:P:19:LEU:O	1:P:22:ARG:O	2.25	0.55
1:P:24:PRO:O	1:P:25:ILE:C	2.43	0.55
2:D:113:PRO:O	2:D:114:ALA:CB	2.54	0.55
3:R:99:GLU:O	3:R:100:ASN:C	2.43	0.55
1:C:114:ARG:NE	1:C:115:GLY:N	2.53	0.55
1:C:131:VAL:HG13	1:C:208:LEU:HD23	1.86	0.55
1:C:380:VAL:O	1:C:382:ALA:N	2.39	0.55
1:C:77:PHE:CD1	1:C:282:GLN:HG3	2.41	0.55
1:P:346:ALA:HB3	1:P:347:PRO:CD	2.35	0.55
3:E:93:LEU:HD21	3:E:165:ARG:HB3	1.88	0.55
1:P:242:LEU:N	1:P:242:LEU:HD12	2.21	0.55
3:E:58:GLU:N	3:E:76:ARG:HH12	2.04	0.55
3:R:58:GLU:N	3:R:76:ARG:NH1	2.54	0.55
1:C:158:GLY:O	1:C:159:ALA:C	2.44	0.55
1:C:45:TRP:NE1	1:C:222:ASN:N	2.38	0.55
1:P:158:GLY:O	1:P:159:ALA:C	2.44	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:18:TRP:C	1:P:20:HIS:H	2.08	0.55
1:P:281:VAL:O	1:P:282:GLN:O	2.25	0.55
2:Q:70:THR:HG22	2:Q:80:ARG:O	2.06	0.55
1:C:7:ASP:C	1:C:9:TYR:H	2.09	0.55
1:C:368:TRP:O	1:C:371:VAL:HG12	2.07	0.55
1:P:77:PHE:HD1	1:P:282:GLN:HG3	1.70	0.55
1:P:299:LEU:N	1:P:300:PRO:HD2	2.21	0.55
1:P:360:ARG:O	1:P:363:PHE:HB3	2.07	0.55
1:P:114:ARG:CZ	4:P:502:HEM:HBD2	2.37	0.55
1:P:72:HIS:CE1	1:P:74:ASP:H	2.21	0.55
2:D:104:ALA:HB1	2:D:214:MET:HA	1.88	0.55
2:Q:75:ASP:O	2:Q:77:GLY:N	2.38	0.55
1:C:242:LEU:HD12	1:C:242:LEU:N	2.22	0.55
2:D:107:ARG:HG2	2:D:107:ARG:HH11	1.70	0.55
1:C:102:SER:OG	1:C:296:TRP:NE1	2.40	0.55
1:C:126:GLU:O	1:C:130:ILE:HG12	2.07	0.55
1:C:24:PRO:CG	1:C:25:ILE:N	2.68	0.55
1:C:74:ASP:O	1:C:75:LEU:HD23	2.07	0.55
1:P:62:GLY:CA	1:P:97:HIS:CE1	2.89	0.55
2:D:33:VAL:O	2:D:34:CYS:CB	2.54	0.55
2:Q:238:LEU:CD1	3:R:23:GLY:HA2	2.35	0.55
3:R:99:GLU:C	3:R:100:ASN:HD22	2.09	0.55
1:C:209:VAL:HG12	1:C:210:ALA:N	2.22	0.55
1:C:227:VAL:C	1:C:229:VAL:N	2.59	0.55
1:C:237:ALA:O	1:C:238:GLU:CG	2.55	0.55
1:P:64:VAL:CG2	1:P:65:LEU:N	2.70	0.55
2:Q:33:VAL:O	2:Q:34:CYS:CB	2.54	0.55
1:P:199:TYR:O	1:P:199:TYR:CD2	2.59	0.55
3:R:117:ALA:O	3:R:118:PHE:HB2	2.06	0.55
3:R:127:LEU:C	3:R:127:LEU:HD12	2.26	0.55
1:C:136:TYR:OH	1:C:301:PHE:HE1	1.89	0.55
1:C:105:PHE:CZ	1:C:140:MET:HG2	2.38	0.55
1:C:187:ASP:O	1:C:188:ASN:C	2.45	0.55
1:C:281:VAL:O	1:C:282:GLN:O	2.24	0.55
1:C:387:TYR:HD2	1:C:388:PRO:N	2.05	0.55
4:C:502:HEM:O1A	4:C:502:HEM:HBD1	2.07	0.55
1:C:84:MET:HG3	1:C:91:TRP:CA	2.36	0.55
2:D:221:LEU:HD23	2:D:222:VAL:N	2.21	0.55
1:P:144:PHE:CG	1:P:145:MET:N	2.73	0.55
1:P:69:TYR:OH	1:P:149:LEU:O	2.23	0.55
1:P:305:LEU:C	1:P:307:ALA:H	2.09	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:387:TYR:HD2	1:P:388:PRO:N	2.05	0.55
2:Q:127:GLY:O	2:Q:130:TYR:HB3	2.06	0.55
2:Q:9:PHE:N	2:Q:9:PHE:CD1	2.75	0.55
2:D:127:GLY:O	2:D:130:TYR:HB3	2.07	0.55
3:E:54:VAL:HG22	3:E:126:TRP:CZ3	2.42	0.55
1:C:162:ILE:HA	1:C:165:LEU:HD12	1.88	0.55
1:C:251:LYS:O	1:C:254:PHE:HB3	2.06	0.55
1:C:95:TYR:CE2	1:C:272:ASN:ND2	2.54	0.55
1:C:301:PHE:HD2	1:C:304:ILE:HD11	1.72	0.55
1:C:46:ILE:HG13	1:C:49:ILE:CG2	2.36	0.55
1:P:47:TRP:NE1	1:P:110:ILE:CG2	2.67	0.55
1:P:144:PHE:CD1	1:P:162:ILE:HD13	2.42	0.55
1:P:222:ASN:CG	1:P:223:ASN:N	2.60	0.55
2:Q:104:ALA:HB1	2:Q:214:MET:HA	1.89	0.55
1:P:319:ASP:C	1:P:321:LEU:N	2.57	0.55
1:C:319:ASP:C	1:C:321:LEU:N	2.58	0.55
2:D:231:ALA:O	2:D:234:MET:HB2	2.07	0.55
2:D:40:MET:HB3	2:D:43:VAL:HG23	1.89	0.55
1:P:105:PHE:CG	1:P:297:TYR:HD2	2.24	0.55
3:E:115:LEU:O	3:E:116:PRO:O	2.24	0.55
3:E:127:LEU:HD12	3:E:127:LEU:C	2.27	0.55
2:D:68:LEU:O	2:D:69:ASP:O	2.25	0.55
2:Q:73:ASP:OD2	2:Q:74:LYS:HE3	2.06	0.55
2:D:44:PRO:HB3	2:D:46:ARG:HE	1.70	0.55
1:P:142:THR:OG1	1:P:201:LEU:HB3	2.07	0.55
1:P:84:MET:HG3	1:P:91:TRP:CA	2.35	0.55
3:E:58:GLU:N	3:E:76:ARG:NH1	2.54	0.55
1:P:356:SER:C	1:P:358:ALA:N	2.61	0.55
2:Q:107:ARG:HH11	2:Q:107:ARG:HG2	1.71	0.55
3:E:54:VAL:CG1	3:E:126:TRP:CH2	2.91	0.54
3:R:54:VAL:CG1	3:R:126:TRP:CH2	2.90	0.54
3:R:98:ALA:O	3:R:100:ASN:ND2	2.40	0.54
3:R:58:GLU:N	3:R:76:ARG:HH12	2.05	0.54
1:C:294:PRO:HA	5:C:503:SMA:H10	1.88	0.54
1:C:362:LYS:HB2	1:C:411:LEU:HD21	1.89	0.54
1:P:233:SER:O	1:P:235:ALA:N	2.40	0.54
1:P:24:PRO:CG	1:P:25:ILE:N	2.70	0.54
2:Q:68:LEU:O	2:Q:69:ASP:O	2.25	0.54
2:D:26:GLY:O	2:D:29:VAL:CG1	2.55	0.54
2:D:218:GLU:O	2:D:220:LYS:N	2.41	0.54
1:C:133:MET:O	1:C:136:TYR:HB3	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:195:PHE:HE1	1:P:195:PHE:CE1	2.25	0.54
1:C:66:ALA:HB2	4:C:501:HEM:HHD	1.90	0.54
1:P:403:TYR:CD2	1:P:404:PHE:CD1	2.95	0.54
1:C:290:ALA:O	1:C:291:HIS:HB2	2.06	0.54
1:C:23:LEU:HA	1:C:26:VAL:HG12	1.89	0.54
1:C:26:VAL:HG13	1:C:27:GLY:H	1.64	0.54
1:P:105:PHE:CB	1:P:297:TYR:HD2	2.21	0.54
1:P:126:GLU:O	1:P:130:ILE:HG12	2.07	0.54
1:P:362:LYS:O	1:P:366:TRP:HD1	1.91	0.54
1:C:263:PHE:CA	1:C:266:VAL:HG23	2.34	0.54
3:R:54:VAL:HG22	3:R:126:TRP:CZ3	2.42	0.54
1:C:268:ALA:HA	2:D:224:ARG:HD3	1.90	0.54
3:E:159:HIS:O	3:E:167:ARG:CA	2.55	0.54
1:P:309:ALA:O	1:P:310:ALA:CB	2.55	0.54
1:C:309:ALA:O	1:C:310:ALA:CB	2.55	0.54
2:Q:92:VAL:HG12	2:Q:93:GLY:N	2.21	0.54
3:R:113:ARG:HD2	3:R:177:ILE:HD11	1.88	0.54
1:C:109:TYR:CE2	1:C:374:PHE:HZ	2.25	0.54
1:C:222:ASN:CG	1:C:223:ASN:N	2.61	0.54
1:C:233:SER:O	1:C:235:ALA:N	2.41	0.54
1:C:80:VAL:O	1:C:83:ILE:HB	2.08	0.54
1:P:128:THR:HG22	1:P:215:ALA:CB	2.23	0.54
1:P:131:VAL:HG13	1:P:208:LEU:HD23	1.89	0.54
2:D:134:TYR:CE2	2:D:183:MET:HE1	2.42	0.54
2:D:26:GLY:HA2	2:D:29:VAL:HG12	1.89	0.54
2:D:181:ALA:HB1	6:D:501:HEC:HBD1	1.89	0.54
3:R:128:VAL:O	3:R:177:ILE:HG23	2.08	0.54
1:C:89:GLY:O	1:C:90:GLY:C	2.46	0.54
1:P:111:HIS:HE1	4:P:502:HEM:O1A	1.91	0.54
1:P:156:PHE:CD2	1:P:157:TRP:N	2.75	0.54
1:P:237:ALA:O	1:P:238:GLU:CG	2.55	0.54
1:P:249:VAL:HG13	1:P:253:LEU:CD1	2.37	0.54
1:P:251:LYS:O	1:P:254:PHE:HB3	2.08	0.54
1:P:334:ILE:HG23	1:P:335:ALA:N	2.23	0.54
1:P:380:VAL:O	1:P:382:ALA:N	2.41	0.54
4:P:502:HEM:O1A	4:P:502:HEM:HBD1	2.07	0.54
2:D:184:PRO:CG	6:D:501:HEC:HBC2	2.38	0.54
2:D:9:PHE:CD1	2:D:9:PHE:N	2.74	0.54
2:Q:241:MET:HB3	3:R:19:THR:CB	2.37	0.54
2:Q:40:MET:HB3	2:Q:43:VAL:HG23	1.87	0.54
3:R:115:LEU:HD12	3:R:177:ILE:HG21	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:236:ASP:C	1:C:238:GLU:H	2.11	0.54
1:P:305:LEU:CD2	1:P:336:MET:CE	2.85	0.54
1:P:370:LEU:O	1:P:373:ASP:HB3	2.08	0.54
1:P:67:MET:SD	3:R:38:MET:SD	3.05	0.54
3:E:152:PHE:CD1	3:E:159:HIS:NE2	2.76	0.54
3:R:53:ASP:O	3:R:55:SER:CA	2.56	0.54
1:C:118:TYR:C	1:C:120:SER:H	2.12	0.54
1:C:145:MET:SD	1:C:197:LEU:CB	2.96	0.54
1:C:249:VAL:HG13	1:C:253:LEU:CD1	2.38	0.54
1:C:268:ALA:HB2	2:D:227:MET:HE1	1.90	0.54
1:P:110:ILE:O	1:P:111:HIS:C	2.46	0.54
1:P:227:VAL:C	1:P:229:VAL:H	2.11	0.54
1:P:232:THR:O	1:P:233:SER:HB2	2.08	0.54
1:P:301:PHE:HA	1:P:304:ILE:HG12	1.90	0.54
1:P:302:TYR:CD2	1:P:302:TYR:C	2.81	0.54
2:Q:186:PRO:CG	2:Q:187:LEU:H	2.16	0.54
3:R:37:GLN:NE2	3:R:38:MET:CG	2.71	0.54
2:Q:46:ARG:NH1	3:R:43:ASP:HA	2.22	0.54
1:C:162:ILE:HA	1:C:165:LEU:CD1	2.37	0.54
1:C:18:TRP:O	1:C:20:HIS:N	2.41	0.54
1:C:227:VAL:C	1:C:229:VAL:H	2.12	0.54
1:C:232:THR:O	1:C:233:SER:HB2	2.07	0.54
1:C:302:TYR:HE2	1:C:306:ARG:CZ	2.20	0.54
1:C:72:HIS:C	1:C:72:HIS:ND1	2.60	0.54
1:P:162:ILE:HA	1:P:165:LEU:HD12	1.88	0.54
1:P:45:TRP:NE1	1:P:222:ASN:O	2.41	0.54
2:Q:138:PHE:CD2	2:Q:185:PRO:HA	2.41	0.54
3:E:98:ALA:O	3:E:100:ASN:ND2	2.40	0.54
3:R:115:LEU:O	3:R:116:PRO:C	2.46	0.54
1:C:408:LEU:HB3	1:C:409:PRO:CD	2.38	0.54
1:C:64:VAL:HA	1:C:67:MET:HE2	1.89	0.54
1:P:153:GLN:HE21	1:P:289:PRO:HD3	1.69	0.54
1:P:296:TRP:HA	1:P:299:LEU:CG	2.38	0.54
2:Q:11:PHE:HD2	2:Q:18:TYR:CD1	2.25	0.54
2:Q:37:CYS:HA	2:Q:96:MET:SD	2.48	0.54
1:C:9:TYR:O	1:C:10:GLU:CB	2.55	0.54
1:C:18:TRP:CE3	1:C:18:TRP:HA	2.42	0.53
1:C:301:PHE:HA	1:C:304:ILE:HG12	1.88	0.53
1:C:67:MET:SD	3:E:38:MET:SD	3.06	0.53
1:P:162:ILE:HA	1:P:165:LEU:CD1	2.38	0.53
2:Q:153:TYR:O	2:Q:180:TRP:CE3	2.61	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:218:GLU:O	2:Q:220:LYS:N	2.41	0.53
1:C:286:LEU:CD1	1:C:286:LEU:N	2.67	0.53
2:Q:76:SER:O	2:Q:78:GLU:N	2.41	0.53
1:C:227:VAL:O	1:C:227:VAL:HG23	2.08	0.53
1:C:294:PRO:HB3	5:C:503:SMA:C8A	2.38	0.53
1:P:243:PRO:HD2	1:P:247:TYR:HE1	1.73	0.53
1:C:243:PRO:HD2	1:C:247:TYR:HE1	1.73	0.53
3:R:95:ASP:OD2	3:R:174:ASN:ND2	2.41	0.53
1:C:294:PRO:HD3	1:C:302:TYR:HE1	1.74	0.53
1:C:302:TYR:HE2	1:C:306:ARG:NH1	2.06	0.53
1:C:388:PRO:O	1:C:392:ILE:HG13	2.08	0.53
1:C:71:PRO:O	1:C:72:HIS:CB	2.57	0.53
1:P:403:TYR:HD2	1:P:404:PHE:HD1	1.55	0.53
2:Q:149:ILE:CG2	2:Q:152:TYR:HB2	2.38	0.53
2:Q:153:TYR:CZ	2:Q:184:PRO:HB3	2.43	0.53
2:Q:184:PRO:CG	6:Q:501:HEC:HBC2	2.39	0.53
2:D:11:PHE:HD2	2:D:18:TYR:CD1	2.26	0.53
2:D:209:VAL:HG23	2:D:210:SER:N	2.23	0.53
2:D:76:SER:O	2:D:78:GLU:N	2.41	0.53
1:C:231:ARG:HD3	1:C:231:ARG:O	2.08	0.53
1:C:345:LEU:O	1:C:346:ALA:C	2.46	0.53
1:C:45:TRP:CE2	1:C:222:ASN:O	2.62	0.53
1:P:112:ILE:CD1	4:P:502:HEM:HMC1	2.39	0.53
1:P:138:LEU:HB3	1:P:205:ILE:HD11	1.90	0.53
1:P:209:VAL:HG12	1:P:210:ALA:N	2.23	0.53
2:Q:186:PRO:HG2	2:Q:187:LEU:N	2.17	0.53
2:D:70:THR:HG22	2:D:80:ARG:O	2.08	0.53
1:P:356:SER:C	1:P:358:ALA:H	2.12	0.53
2:D:196:ASP:C	2:D:196:ASP:OD2	2.47	0.53
1:C:195:PHE:CE1	1:P:195:PHE:HE1	2.27	0.53
1:P:45:TRP:HZ3	1:P:118:TYR:CD1	2.26	0.53
1:P:112:ILE:HG23	4:P:502:HEM:HBC2	1.89	0.53
1:P:89:GLY:O	1:P:92:ALA:N	2.42	0.53
2:D:149:ILE:CG2	2:D:152:TYR:HB2	2.38	0.53
3:R:79:GLU:O	3:R:82:ILE:N	2.42	0.53
1:C:356:SER:C	1:C:358:ALA:N	2.62	0.53
1:C:140:MET:O	1:C:143:ALA:HB3	2.08	0.53
1:C:156:PHE:CD2	1:C:157:TRP:N	2.77	0.53
1:C:201:LEU:N	1:C:202:PRO:HD2	2.24	0.53
1:P:236:ASP:C	1:P:238:GLU:H	2.12	0.53
2:Q:179:SER:O	2:Q:180:TRP:HB2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:45:ILE:HD13	2:Q:88:PHE:CD1	2.44	0.53
2:Q:8:ALA:O	2:Q:9:PHE:O	2.27	0.53
3:R:166:ILE:HD11	3:R:171:ALA:HB3	1.91	0.53
1:C:33:ILE:CG2	1:C:245:TRP:HB3	2.27	0.53
2:D:238:LEU:CD1	3:E:23:GLY:HA2	2.39	0.53
1:C:73:VAL:HG23	1:C:188:ASN:HA	1.91	0.53
1:C:49:ILE:O	1:C:50:VAL:C	2.44	0.53
1:P:149:LEU:N	1:P:150:PRO:HD2	2.23	0.53
1:P:45:TRP:CE2	1:P:222:ASN:O	2.61	0.53
1:P:302:TYR:HE2	1:P:306:ARG:CZ	2.22	0.53
1:P:85:ARG:NH1	2:Q:102:VAL:CG2	2.64	0.53
3:E:99:GLU:C	3:E:100:ASN:HD22	2.10	0.53
1:C:138:LEU:HB3	1:C:205:ILE:HD11	1.90	0.53
1:P:133:MET:O	1:P:136:TYR:HB3	2.08	0.53
1:P:109:TYR:CE2	1:P:374:PHE:CZ	2.97	0.53
1:P:58:GLN:HA	1:P:58:GLN:OE1	2.09	0.53
2:D:179:SER:O	2:D:180:TRP:HB2	2.09	0.53
1:C:414:THR:O	1:C:417:PRO:HB2	2.09	0.53
2:Q:196:ASP:C	2:Q:196:ASP:OD2	2.46	0.53
1:C:384:PRO:O	1:C:386:GLU:N	2.37	0.53
1:C:362:LYS:O	1:C:366:TRP:HD1	1.91	0.53
1:C:268:ALA:HB2	2:D:227:MET:CE	2.39	0.53
1:P:105:PHE:CZ	1:P:140:MET:HG2	2.41	0.53
1:P:361:PRO:HG3	1:P:364:ARG:CZ	2.39	0.53
3:E:115:LEU:O	3:E:116:PRO:C	2.47	0.53
2:D:153:TYR:O	2:D:180:TRP:CE3	2.61	0.53
1:C:153:GLN:HE21	1:C:289:PRO:CG	2.21	0.53
1:C:45:TRP:NE1	1:C:222:ASN:O	2.42	0.53
1:C:91:TRP:CE3	2:D:224:ARG:HG2	2.44	0.53
1:P:40:ASN:HD22	1:P:224:PRO:HG2	1.74	0.53
1:P:65:LEU:CD1	4:P:501:HEM:O2D	2.40	0.53
3:E:166:ILE:HD11	3:E:171:ALA:HB3	1.90	0.53
2:D:37:CYS:HA	2:D:96:MET:SD	2.49	0.53
2:D:75:ASP:O	2:D:77:GLY:N	2.39	0.53
3:E:53:ASP:O	3:E:55:SER:CA	2.55	0.52
1:P:136:TYR:OH	1:P:301:PHE:HE1	1.92	0.52
1:P:144:PHE:CD2	1:P:145:MET:N	2.78	0.52
1:P:213:ILE:HA	1:P:216:PHE:CD2	2.44	0.52
1:P:95:TYR:CE2	1:P:272:ASN:OD1	2.63	0.52
1:P:294:PRO:HG3	1:P:302:TYR:HD1	1.73	0.52
1:P:133:MET:HG3	1:P:344:ALA:HA	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:362:LYS:HB2	1:P:411:LEU:HD21	1.90	0.52
1:P:47:TRP:N	4:P:502:HEM:O2A	2.42	0.52
2:Q:26:GLY:O	2:Q:29:VAL:CG1	2.56	0.52
2:Q:38:HIS:CE1	6:Q:501:HEC:ND	2.77	0.52
1:P:414:THR:O	1:P:417:PRO:HB2	2.08	0.52
1:C:144:PHE:O	1:C:148:VAL:HG23	2.08	0.52
1:C:213:ILE:HA	1:C:216:PHE:CD2	2.44	0.52
1:C:133:MET:HG3	1:C:344:ALA:HA	1.91	0.52
1:C:114:ARG:CZ	4:C:502:HEM:HBD2	2.38	0.52
1:P:147:TYR:HA	4:P:501:HEM:HAA1	1.91	0.52
1:P:187:ASP:O	1:P:188:ASN:C	2.47	0.52
3:R:183:VAL:O	3:R:183:VAL:HG12	2.09	0.52
1:C:40:ASN:ND2	1:C:224:PRO:HG2	2.24	0.52
1:P:225:THR:HG22	1:P:227:VAL:HG22	1.90	0.52
1:P:49:ILE:O	1:P:50:VAL:C	2.46	0.52
3:E:55:SER:HA	3:E:186:THR:HG23	1.91	0.52
1:C:229:VAL:O	1:C:229:VAL:HG12	2.09	0.52
1:P:301:PHE:HD2	1:P:304:ILE:HD11	1.74	0.52
1:P:345:LEU:O	1:P:346:ALA:C	2.48	0.52
3:E:104:PRO:C	3:E:106:ALA:H	2.11	0.52
2:D:8:ALA:O	2:D:9:PHE:O	2.28	0.52
3:E:79:GLU:O	3:E:82:ILE:N	2.42	0.52
1:P:268:ALA:HB2	2:Q:227:MET:HE1	1.92	0.52
1:P:408:LEU:HB3	1:P:409:PRO:CD	2.39	0.52
2:Q:30:TYR:CD1	2:Q:34:CYS:HB2	2.36	0.52
2:D:27:PHE:HZ	2:D:64:TYR:CE2	2.27	0.52
3:R:152:PHE:CD1	3:R:159:HIS:NE2	2.78	0.52
3:R:159:HIS:O	3:R:167:ARG:C	2.48	0.52
1:C:86:ASP:OD1	3:E:42:ALA:CB	2.58	0.52
3:E:150:GLY:O	3:E:151:TRP:CD2	2.62	0.52
3:R:77:ARG:HH12	3:R:110:ASP:CG	2.13	0.52
1:C:145:MET:HE1	1:C:197:LEU:C	2.30	0.52
1:C:329:LYS:O	1:C:333:VAL:HG22	2.09	0.52
1:C:338:GLY:O	1:C:342:VAL:HG23	2.09	0.52
1:C:403:TYR:CD2	1:C:404:PHE:HD1	2.28	0.52
1:P:136:TYR:HH	1:P:301:PHE:HE1	1.50	0.52
1:P:72:HIS:HE1	1:P:74:ASP:HB2	1.74	0.52
1:P:268:ALA:HB2	2:Q:227:MET:CE	2.40	0.52
2:Q:181:ALA:HB1	6:Q:501:HEC:HBD2	1.92	0.52
2:D:18:TYR:CE2	2:D:215:TRP:HB2	2.44	0.52
1:C:416:LYS:CB	1:C:417:PRO:CD	2.87	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:104:PRO:C	3:R:106:ALA:H	2.12	0.52
1:C:105:PHE:CG	1:C:297:TYR:HD2	2.28	0.52
1:C:111:HIS:CE1	4:C:502:HEM:O1A	2.62	0.52
1:C:147:TYR:HD1	4:C:501:HEM:HAA2	1.74	0.52
1:C:153:GLN:HE22	1:C:157:TRP:HE1	1.58	0.52
1:C:205:ILE:CG2	1:C:206:ALA:N	2.73	0.52
1:C:249:VAL:CG1	1:C:250:ILE:N	2.73	0.52
1:C:112:ILE:CD1	4:C:502:HEM:HMC1	2.40	0.52
1:P:254:PHE:HA	2:Q:242:LEU:CD1	2.39	0.52
1:P:154:MET:CE	1:P:292:ILE:HG22	2.39	0.52
1:P:305:LEU:HD13	1:P:332:GLY:HA3	1.91	0.52
1:P:168:ALA:HB1	1:P:333:VAL:HG21	1.92	0.52
1:P:294:PRO:HB3	5:P:503:SMA:C8A	2.40	0.52
2:D:74:LYS:HZ2	2:D:75:ASP:HB3	1.73	0.52
1:C:242:LEU:HB3	1:C:243:PRO:HD2	1.91	0.52
2:D:45:ILE:HD13	2:D:88:PHE:CD1	2.44	0.52
1:C:18:TRP:C	1:C:20:HIS:N	2.62	0.52
1:C:195:PHE:CE1	1:P:195:PHE:CE1	2.97	0.52
1:P:249:VAL:CG1	1:P:250:ILE:N	2.72	0.52
1:P:278:ASP:C	1:P:280:TYR:N	2.60	0.52
1:P:153:GLN:HE21	1:P:289:PRO:CG	2.22	0.52
4:P:501:HEM:CBC	4:P:501:HEM:HMC2	2.39	0.52
1:P:71:PRO:HD2	1:P:71:PRO:O	2.09	0.52
1:P:85:ARG:HG2	1:P:85:ARG:O	2.10	0.52
1:P:352:SER:OG	1:P:354:VAL:HG23	2.10	0.52
1:C:48:GLY:HA3	4:C:502:HEM:C3A	2.45	0.52
1:P:18:TRP:CE3	1:P:18:TRP:HA	2.44	0.52
1:P:46:ILE:HG23	1:P:47:TRP:CE3	2.45	0.52
2:Q:64:TYR:CE1	2:Q:68:LEU:HD11	2.45	0.52
3:E:153:CYS:HB3	3:E:158:SER:OG	2.10	0.52
1:C:370:LEU:O	1:C:373:ASP:HB3	2.10	0.52
1:C:377:LEU:HD22	1:C:396:ALA:CB	2.40	0.52
1:C:58:GLN:OE1	1:C:58:GLN:HA	2.10	0.52
1:P:100:GLY:O	1:P:101:ALA:C	2.48	0.52
1:P:136:TYR:OH	1:P:301:PHE:CE1	2.63	0.52
1:P:48:GLY:HA3	4:P:502:HEM:C3A	2.45	0.52
1:P:51:LEU:HD22	1:P:108:VAL:HG23	1.92	0.52
3:E:133:CYS:HA	3:E:160:TYR:OH	2.10	0.52
2:Q:159:GLN:O	2:Q:160:ILE:CB	2.58	0.52
3:R:55:SER:HA	3:R:186:THR:HG23	1.93	0.51
1:C:45:TRP:HZ3	1:C:118:TYR:CD1	2.27	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:49:ILE:HG23	1:C:50:VAL:H	1.75	0.51
1:P:114:ARG:C	1:P:114:ARG:HD2	2.31	0.51
2:D:238:LEU:HD13	3:E:26:VAL:HG21	1.91	0.51
1:C:93:MET:O	1:C:94:ARG:C	2.46	0.51
1:C:110:ILE:O	1:C:111:HIS:C	2.48	0.51
1:C:223:ASN:HD22	1:C:227:VAL:H	1.58	0.51
1:C:332:GLY:O	1:C:333:VAL:C	2.47	0.51
1:C:361:PRO:HA	1:C:364:ARG:HD2	1.91	0.51
1:P:294:PRO:HD3	1:P:302:TYR:HE1	1.75	0.51
3:E:95:ASP:OD2	3:E:174:ASN:ND2	2.43	0.51
2:D:38:HIS:CB	2:D:100:LEU:HD21	2.40	0.51
2:D:153:TYR:CZ	2:D:184:PRO:HB3	2.45	0.51
3:R:150:GLY:O	3:R:151:TRP:CD2	2.63	0.51
1:C:136:TYR:OH	1:C:301:PHE:CE1	2.61	0.51
2:D:242:LEU:O	2:D:245:THR:N	2.43	0.51
1:P:231:ARG:O	1:P:231:ARG:HD3	2.11	0.51
1:P:43:TRP:CE3	1:P:251:LYS:HE2	2.45	0.51
2:Q:194:TYR:N	2:Q:194:TYR:CD1	2.78	0.51
2:Q:27:PHE:CE2	2:Q:48:LEU:HD13	2.44	0.51
3:E:122:ASN:CG	3:E:124:GLY:H	2.14	0.51
3:E:132:VAL:HG22	3:E:137:GLY:HA2	1.92	0.51
3:R:97:SER:O	3:R:98:ALA:HB3	2.10	0.51
1:C:302:TYR:CE2	1:C:306:ARG:HG2	2.46	0.51
1:C:47:TRP:N	4:C:502:HEM:O2A	2.42	0.51
1:P:302:TYR:HE2	1:P:306:ARG:NH1	2.08	0.51
1:P:403:TYR:CD2	1:P:404:PHE:HD1	2.29	0.51
2:Q:132:TYR:CD2	2:Q:133:ASN:N	2.78	0.51
2:Q:209:VAL:HG23	2:Q:210:SER:N	2.23	0.51
2:Q:182:ARG:N	6:Q:501:HEC:HBD2	2.26	0.51
2:D:21:ALA:C	2:D:25:ARG:HG3	2.30	0.51
3:R:148:PHE:O	3:R:149:GLY:C	2.49	0.51
1:C:252:ASP:O	1:C:253:LEU:C	2.48	0.51
1:P:104:PHE:C	1:P:104:PHE:CD1	2.84	0.51
1:P:54:THR:HG22	1:P:104:PHE:HB2	1.91	0.51
1:P:149:LEU:HD21	1:P:195:PHE:CD2	2.42	0.51
1:P:86:ASP:CG	2:Q:46:ARG:HH22	2.13	0.51
2:Q:149:ILE:HG21	2:Q:152:TYR:HB2	1.92	0.51
2:Q:47:THR:HA	2:Q:50:ASP:OD2	2.11	0.51
2:D:128:PRO:O	2:D:131:ILE:HB	2.11	0.51
2:D:149:ILE:HG21	2:D:152:TYR:HB2	1.92	0.51
1:C:240:ASP:O	1:C:241:THR:OG1	2.23	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:114:ARG:HD2	1:C:114:ARG:C	2.31	0.51
3:E:37:GLN:NE2	3:E:38:MET:CG	2.74	0.51
1:P:252:ASP:O	1:P:253:LEU:C	2.48	0.51
2:Q:38:HIS:CB	2:Q:100:LEU:HD21	2.38	0.51
3:E:97:SER:O	3:E:98:ALA:HB3	2.09	0.51
2:D:194:TYR:CD1	2:D:194:TYR:N	2.77	0.51
1:P:242:LEU:HB3	1:P:243:PRO:HD2	1.93	0.51
2:D:74:LYS:HZ3	2:D:75:ASP:HB3	1.74	0.51
2:D:57:ASP:OD1	2:D:59:THR:HB	2.09	0.51
3:E:148:PHE:O	3:E:149:GLY:C	2.49	0.51
1:C:166:PHE:CD1	1:C:180:LEU:HD11	2.45	0.51
1:C:22:ARG:O	1:C:23:LEU:C	2.48	0.51
1:C:77:PHE:HD1	1:C:282:GLN:HG3	1.76	0.51
1:C:305:LEU:HD13	1:C:332:GLY:HA3	1.92	0.51
4:C:501:HEM:CBC	4:C:501:HEM:HMC1	2.30	0.51
1:P:105:PHE:CG	1:P:297:TYR:CD2	2.99	0.51
1:P:140:MET:O	1:P:143:ALA:HB3	2.10	0.51
1:P:153:GLN:HE22	1:P:157:TRP:HE1	1.58	0.51
1:P:194:PHE:O	1:P:195:PHE:C	2.49	0.51
1:P:23:LEU:CA	1:P:26:VAL:HG12	2.41	0.51
1:P:46:ILE:HG13	1:P:49:ILE:CG2	2.40	0.51
2:Q:19:ASP:O	2:Q:20:GLN:C	2.48	0.51
2:Q:26:GLY:HA2	2:Q:29:VAL:HG12	1.92	0.51
3:E:183:VAL:HG12	3:E:183:VAL:O	2.11	0.51
2:D:184:PRO:O	2:D:185:PRO:C	2.49	0.51
1:C:168:ALA:HB1	1:C:333:VAL:HG21	1.93	0.51
1:C:361:PRO:HA	1:C:364:ARG:CD	2.41	0.51
1:C:74:ASP:C	1:C:75:LEU:HD23	2.31	0.51
1:C:72:HIS:CE1	1:C:74:ASP:H	2.25	0.51
2:D:235:LEU:O	2:D:236:GLY:C	2.46	0.51
1:P:103:LEU:CG	1:P:104:PHE:N	2.74	0.51
1:P:118:TYR:C	1:P:120:SER:H	2.13	0.51
1:P:296:TRP:HA	1:P:299:LEU:CD1	2.41	0.51
2:Q:128:PRO:O	2:Q:131:ILE:HB	2.10	0.51
3:E:77:ARG:HH12	3:E:110:ASP:CG	2.14	0.51
1:P:227:VAL:O	1:P:227:VAL:HG23	2.10	0.51
2:Q:224:ARG:O	2:Q:227:MET:HB3	2.11	0.51
1:C:330:PHE:O	1:C:331:PHE:C	2.50	0.51
1:C:112:ILE:HG23	4:C:502:HEM:HBC2	1.93	0.51
1:C:62:GLY:CA	1:C:97:HIS:CE1	2.93	0.51
2:Q:206:ALA:O	2:Q:207:GLN:C	2.50	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:48:LEU:O	2:D:49:ALA:HB2	2.11	0.51
1:C:191:LEU:HD23	1:C:191:LEU:C	2.32	0.50
1:C:258:LEU:O	1:C:261:LEU:HB3	2.10	0.50
1:P:157:TRP:CD2	1:P:288:THR:HG22	2.46	0.50
1:P:380:VAL:HG21	1:P:392:ILE:CG2	2.42	0.50
1:P:387:TYR:CD2	1:P:388:PRO:HB3	2.46	0.50
3:E:117:ALA:O	3:E:118:PHE:CB	2.58	0.50
2:D:104:ALA:HB3	2:D:217:ALA:HB2	1.90	0.50
1:C:154:MET:HE2	1:C:292:ILE:O	2.11	0.50
1:C:99:ASN:O	1:C:100:GLY:C	2.50	0.50
1:C:371:VAL:HG13	1:C:372:LEU:N	2.26	0.50
1:C:60:VAL:O	1:C:61:THR:C	2.48	0.50
3:E:157:GLY:O	3:E:159:HIS:CD2	2.64	0.50
2:D:159:GLN:O	2:D:160:ILE:CB	2.58	0.50
1:C:43:TRP:CE3	1:C:251:LYS:HE2	2.45	0.50
1:P:166:PHE:CD2	1:P:166:PHE:N	2.78	0.50
1:P:89:GLY:O	1:P:90:GLY:O	2.30	0.50
2:Q:21:ALA:C	2:Q:25:ARG:HG3	2.31	0.50
1:P:416:LYS:CB	1:P:417:PRO:CD	2.88	0.50
3:R:115:LEU:CB	3:R:116:PRO:CD	2.90	0.50
1:C:72:HIS:HE1	1:C:74:ASP:HB2	1.76	0.50
1:P:138:LEU:HB3	1:P:205:ILE:HD12	1.92	0.50
1:P:377:LEU:HD22	1:P:396:ALA:CB	2.41	0.50
2:Q:227:MET:O	2:Q:228:GLY:C	2.50	0.50
2:Q:48:LEU:O	2:Q:49:ALA:HB2	2.12	0.50
2:D:155:ASN:O	2:D:179:SER:OG	2.29	0.50
2:Q:57:ASP:OD1	2:Q:59:THR:HB	2.11	0.50
2:Q:251:ALA:N	2:Q:252:PRO:CD	2.74	0.50
1:C:144:PHE:CD2	1:C:145:MET:N	2.80	0.50
1:C:216:PHE:CE1	1:C:217:HIS:ND1	2.74	0.50
1:C:370:LEU:HD23	1:C:403:TYR:CZ	2.47	0.50
1:C:387:TYR:CD2	1:C:388:PRO:HB3	2.47	0.50
1:P:202:PRO:O	1:P:205:ILE:N	2.45	0.50
1:P:216:PHE:CE1	1:P:217:HIS:ND1	2.73	0.50
3:E:115:LEU:CB	3:E:116:PRO:CD	2.89	0.50
1:P:242:LEU:HB3	1:P:247:TYR:CD1	2.46	0.50
3:R:30:ALA:O	3:R:33:PRO:CG	2.58	0.50
1:C:194:PHE:O	1:C:195:PHE:C	2.49	0.50
1:C:334:ILE:HG23	1:C:335:ALA:N	2.25	0.50
1:C:370:LEU:O	1:C:371:VAL:C	2.49	0.50
1:C:64:VAL:CG2	1:C:65:LEU:N	2.73	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:37:GLN:CG	3:E:38:MET:N	2.74	0.50
1:P:170:PRO:HD2	1:P:330:PHE:CE2	2.47	0.50
2:D:100:LEU:HD12	2:D:103:MET:HG2	1.94	0.50
2:Q:238:LEU:HD13	3:R:26:VAL:HG21	1.94	0.50
1:C:356:SER:C	1:C:358:ALA:H	2.13	0.50
1:C:421:PRO:O	1:C:422:ALA:HB2	2.12	0.50
1:C:109:TYR:CE2	1:C:374:PHE:CZ	3.00	0.50
1:P:99:ASN:O	1:P:100:GLY:C	2.50	0.50
1:P:73:VAL:HG23	1:P:188:ASN:HA	1.94	0.50
1:P:70:THR:HG21	1:P:75:LEU:HB2	1.94	0.50
2:Q:11:PHE:O	2:Q:12:GLU:C	2.49	0.50
3:E:180:ALA:HB2	3:E:190:LEU:HA	1.94	0.50
3:R:62:GLN:CB	3:R:75:ARG:HG3	2.42	0.50
1:C:157:TRP:CD2	1:C:288:THR:HG22	2.47	0.50
1:C:301:PHE:O	1:C:302:TYR:C	2.50	0.50
1:P:332:GLY:O	1:P:333:VAL:C	2.47	0.50
1:C:72:HIS:CD2	1:P:75:LEU:CD1	2.95	0.50
2:Q:100:LEU:O	2:Q:101:SER:C	2.51	0.50
2:Q:235:LEU:O	2:Q:236:GLY:C	2.47	0.50
2:Q:27:PHE:HZ	2:Q:64:TYR:CE2	2.29	0.50
2:D:132:TYR:CD2	2:D:133:ASN:N	2.80	0.50
2:D:181:ALA:HB1	6:D:501:HEC:HBD2	1.93	0.50
2:D:19:ASP:O	2:D:20:GLN:C	2.49	0.50
1:C:28:LEU:O	1:C:29:VAL:C	2.51	0.50
2:D:241:MET:HE3	3:E:19:THR:HA	1.94	0.50
1:C:352:SER:OG	1:C:354:VAL:HG23	2.11	0.50
1:C:367:PHE:O	1:C:370:LEU:HB3	2.12	0.49
1:C:380:VAL:HG21	1:C:392:ILE:CG2	2.42	0.49
1:C:91:TRP:CZ3	2:D:224:ARG:HG2	2.47	0.49
1:P:305:LEU:HD22	1:P:336:MET:CE	2.42	0.49
1:P:81:GLU:O	1:P:82:HIS:C	2.51	0.49
2:Q:18:TYR:CE2	2:Q:215:TRP:HB2	2.46	0.49
2:D:11:PHE:O	2:D:12:GLU:C	2.49	0.49
2:D:47:THR:HA	2:D:50:ASP:OD2	2.11	0.49
1:C:47:TRP:HB3	1:C:111:HIS:HD1	1.76	0.49
2:Q:184:PRO:O	2:Q:185:PRO:C	2.49	0.49
3:E:30:ALA:O	3:E:33:PRO:CG	2.59	0.49
3:E:79:GLU:O	3:E:80:LYS:C	2.50	0.49
3:R:132:VAL:O	3:R:132:VAL:HG13	2.12	0.49
1:C:255:ALA:O	1:C:258:LEU:HB2	2.12	0.49
2:D:224:ARG:O	2:D:227:MET:HB3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:330:PHE:O	1:P:331:PHE:C	2.50	0.49
2:Q:191:GLN:O	2:Q:192:VAL:HG13	2.12	0.49
1:P:263:PHE:HD1	1:P:264:PHE:HD1	1.61	0.49
1:C:187:ASP:N	1:C:190:THR:HG22	2.26	0.49
1:C:37:THR:HG22	1:C:41:LEU:CD1	2.42	0.49
1:C:55:LEU:HD13	1:C:55:LEU:C	2.33	0.49
1:P:258:LEU:O	1:P:261:LEU:HB3	2.13	0.49
2:Q:100:LEU:HD12	2:Q:103:MET:HG2	1.93	0.49
1:C:85:ARG:HG2	1:C:85:ARG:O	2.13	0.49
1:C:111:HIS:HE1	4:C:502:HEM:O1A	1.95	0.49
1:C:254:PHE:HA	2:D:242:LEU:CD1	2.42	0.49
1:C:377:LEU:CD2	1:C:396:ALA:CB	2.88	0.49
2:D:227:MET:O	2:D:228:GLY:C	2.50	0.49
1:P:37:THR:HG22	1:P:41:LEU:CD1	2.42	0.49
1:P:298:PHE:CD2	5:P:503:SMA:H11	2.45	0.49
2:Q:201:THR:O	2:Q:202:VAL:C	2.51	0.49
3:R:79:GLU:O	3:R:80:LYS:C	2.50	0.49
3:R:62:GLN:HE22	3:R:64:THR:CG2	2.24	0.49
1:C:105:PHE:CB	1:C:297:TYR:HD2	2.25	0.49
1:C:201:LEU:O	1:C:202:PRO:C	2.50	0.49
1:C:232:THR:O	1:C:233:SER:CB	2.60	0.49
1:C:81:GLU:O	1:C:82:HIS:C	2.51	0.49
1:P:301:PHE:O	1:P:302:TYR:C	2.50	0.49
1:P:50:VAL:CG1	1:P:51:LEU:N	2.75	0.49
1:P:60:VAL:O	1:P:61:THR:C	2.51	0.49
2:D:209:VAL:O	2:D:210:SER:C	2.50	0.49
3:R:180:ALA:HB2	3:R:190:LEU:HD23	1.95	0.49
1:C:100:GLY:O	1:C:101:ALA:C	2.49	0.49
1:C:43:TRP:CZ3	1:C:251:LYS:HG2	2.48	0.49
1:C:45:TRP:NE1	4:C:502:HEM:O1D	2.45	0.49
1:P:46:ILE:HD12	1:P:252:ASP:HA	1.90	0.49
2:Q:209:VAL:O	2:Q:210:SER:C	2.51	0.49
3:E:128:VAL:O	3:E:177:ILE:HG23	2.13	0.49
3:E:73:PHE:HE2	3:E:151:TRP:NE1	2.07	0.49
2:D:251:ALA:N	2:D:252:PRO:CD	2.76	0.49
2:D:226:GLN:O	2:D:230:VAL:HG23	2.12	0.49
1:C:179:TRP:HE1	3:R:38:MET:CB	2.26	0.49
1:P:147:TYR:HA	4:P:501:HEM:HAA2	1.93	0.49
1:P:18:TRP:C	1:P:20:HIS:N	2.64	0.49
2:D:135:VAL:HG21	6:D:501:HEC:HMB2	1.93	0.49
1:P:242:LEU:H	1:P:242:LEU:HD12	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:74:LYS:HZ2	2:Q:75:ASP:HB3	1.78	0.49
3:E:160:TYR:HD1	3:E:164:GLY:O	1.96	0.49
1:C:296:TRP:HA	1:C:299:LEU:CG	2.41	0.49
1:C:301:PHE:O	1:C:304:ILE:CG1	2.61	0.49
1:C:370:LEU:O	1:C:373:ASP:N	2.46	0.49
1:C:46:ILE:HG23	1:C:47:TRP:CE3	2.48	0.49
1:P:187:ASP:N	1:P:190:THR:HG22	2.24	0.49
1:P:201:LEU:O	1:P:202:PRO:C	2.47	0.49
2:D:155:ASN:OD1	2:D:158:PHE:N	2.39	0.49
2:D:19:ASP:C	2:D:21:ALA:N	2.66	0.49
2:D:97:GLY:HA3	6:D:501:HEC:HMD3	1.95	0.49
1:C:354:VAL:HG12	1:C:355:ARG:N	2.28	0.49
1:C:210:ALA:O	1:C:213:ILE:HB	2.13	0.49
1:C:147:TYR:HA	4:C:501:HEM:HAA1	1.95	0.49
1:P:210:ALA:O	1:P:213:ILE:HB	2.12	0.49
1:P:41:LEU:HD12	1:P:248:PHE:CE2	2.47	0.49
1:P:377:LEU:CD2	1:P:396:ALA:CB	2.89	0.49
1:P:91:TRP:CZ3	2:Q:224:ARG:HG2	2.47	0.49
3:R:37:GLN:CG	3:R:38:MET:N	2.75	0.49
3:E:116:PRO:O	3:E:117:ALA:CB	2.61	0.49
2:D:187:LEU:HB3	2:D:202:VAL:HG13	1.94	0.49
2:D:131:ILE:HD13	2:D:213:LEU:CD1	2.43	0.49
3:R:157:GLY:O	3:R:159:HIS:CD2	2.65	0.49
2:D:177:HIS:O	2:D:178:GLY:O	2.31	0.49
1:C:128:THR:HG22	1:C:215:ALA:CB	2.26	0.48
1:P:230:ARG:HD2	1:P:238:GLU:HB2	1.95	0.48
1:P:370:LEU:HD23	1:P:403:TYR:CZ	2.48	0.48
2:D:186:PRO:CG	2:D:187:LEU:N	2.76	0.48
1:C:263:PHE:HD1	1:C:264:PHE:HD1	1.61	0.48
1:C:383:MET:CB	1:C:389:TYR:CD1	2.94	0.48
1:C:240:ASP:O	1:C:241:THR:CB	2.61	0.48
2:D:113:PRO:O	2:D:114:ALA:HB3	2.13	0.48
1:C:114:ARG:CD	1:C:114:ARG:C	2.82	0.48
1:C:298:PHE:CD2	5:C:503:SMA:H11	2.46	0.48
1:P:47:TRP:HB3	1:P:111:HIS:HD1	1.76	0.48
1:P:166:PHE:C	1:P:168:ALA:N	2.66	0.48
1:P:217:HIS:C	1:P:219:THR:N	2.66	0.48
1:P:363:PHE:O	1:P:364:ARG:C	2.52	0.48
1:P:387:TYR:CE2	1:P:388:PRO:HB3	2.47	0.48
2:Q:42:PHE:O	2:Q:44:PRO:HD3	2.12	0.48
3:E:113:ARG:NH1	3:E:177:ILE:HD11	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:241:MET:HE2	3:R:19:THR:HA	1.96	0.48
1:P:319:ASP:O	1:P:321:LEU:N	2.46	0.48
1:P:240:ASP:O	1:P:241:THR:OG1	2.21	0.48
3:E:77:ARG:HD3	3:E:82:ILE:HG12	1.95	0.48
1:P:356:SER:O	1:P:358:ALA:N	2.46	0.48
3:E:132:VAL:O	3:E:132:VAL:HG13	2.13	0.48
1:C:200:LEU:CD2	1:P:203:PHE:HZ	2.26	0.48
1:C:223:ASN:ND2	1:C:227:VAL:H	2.11	0.48
1:C:23:LEU:O	1:C:24:PRO:C	2.50	0.48
1:C:50:VAL:CG1	1:C:51:LEU:N	2.75	0.48
1:P:153:GLN:HA	1:P:153:GLN:OE1	2.13	0.48
1:P:158:GLY:O	1:P:161:VAL:HG12	2.13	0.48
2:D:100:LEU:O	2:D:101:SER:C	2.51	0.48
3:R:159:HIS:O	3:R:167:ARG:O	2.32	0.48
1:C:242:LEU:HD12	1:C:242:LEU:H	1.78	0.48
1:C:242:LEU:HB3	1:C:247:TYR:CD1	2.49	0.48
1:C:214:TRP:CH2	1:P:23:LEU:HB2	2.48	0.48
1:C:46:ILE:HG13	1:C:49:ILE:HG23	1.94	0.48
1:P:182:GLY:HA2	1:P:193:ARG:HH21	1.75	0.48
1:P:357:GLY:HA3	1:P:363:PHE:HD2	1.78	0.48
1:P:368:TRP:O	1:P:371:VAL:HG12	2.13	0.48
1:P:371:VAL:HG13	1:P:372:LEU:N	2.28	0.48
1:P:52:ALA:H	4:P:502:HEM:HMB3	1.76	0.48
1:P:64:VAL:HA	1:P:67:MET:HE2	1.94	0.48
1:P:75:LEU:O	1:P:76:ALA:C	2.52	0.48
2:D:206:ALA:O	2:D:209:VAL:HG23	2.13	0.48
1:C:28:LEU:HA	1:C:32:THR:HB	1.95	0.48
1:P:354:VAL:HG12	1:P:355:ARG:N	2.29	0.48
3:R:180:ALA:HB2	3:R:190:LEU:HA	1.94	0.48
3:R:132:VAL:HG22	3:R:137:GLY:HA2	1.95	0.48
1:C:46:ILE:HD12	1:C:252:ASP:HA	1.91	0.48
1:P:166:PHE:CD1	1:P:180:LEU:HD11	2.49	0.48
1:P:18:TRP:O	1:P:20:HIS:N	2.46	0.48
1:P:67:MET:SD	3:R:38:MET:CE	3.02	0.48
1:P:414:THR:HA	1:P:417:PRO:CG	2.43	0.48
2:D:182:ARG:N	6:D:501:HEC:HBD2	2.27	0.48
2:D:210:SER:O	2:D:211:ALA:C	2.51	0.48
3:R:163:ALA:CB	3:R:165:ARG:HG3	2.41	0.48
1:C:104:PHE:C	1:C:104:PHE:CD1	2.87	0.48
1:C:278:ASP:N	1:C:278:ASP:OD2	2.46	0.48
1:C:288:THR:HG21	3:R:138:CYS:CB	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:300:PRO:HA	1:C:377:LEU:HD12	1.95	0.48
1:C:91:TRP:CD2	1:C:92:ALA:N	2.81	0.48
1:P:217:HIS:O	1:P:219:THR:N	2.47	0.48
1:P:23:LEU:O	1:P:24:PRO:C	2.52	0.48
2:D:29:VAL:HG11	2:D:209:VAL:HG13	1.95	0.48
3:E:62:GLN:C	3:E:62:GLN:CD	2.72	0.48
3:E:62:GLN:HE22	3:E:64:THR:CG2	2.27	0.48
3:E:15:LEU:O	3:E:18:ALA:HB3	2.14	0.48
1:C:166:PHE:N	1:C:166:PHE:CD2	2.80	0.48
1:C:295:GLU:HB3	1:C:297:TYR:CE1	2.49	0.48
1:C:387:TYR:CE2	1:C:388:PRO:HB3	2.48	0.48
3:E:139:VAL:O	1:P:288:THR:OG1	2.32	0.48
1:P:114:ARG:C	1:P:114:ARG:CD	2.82	0.48
1:P:302:TYR:CE2	1:P:306:ARG:HG2	2.48	0.48
1:P:361:PRO:HA	1:P:364:ARG:HD2	1.95	0.48
2:Q:218:GLU:N	2:Q:219:PRO:HD3	2.28	0.48
3:E:100:ASN:C	3:E:102:ASN:N	2.67	0.48
2:D:22:GLN:HA	2:D:25:ARG:NH1	2.29	0.48
1:C:230:ARG:HD2	1:C:238:GLU:HB2	1.96	0.48
1:C:153:GLN:HE21	1:C:289:PRO:CD	2.26	0.48
1:C:52:ALA:H	4:C:502:HEM:HMB3	1.79	0.48
1:C:67:MET:SD	3:E:38:MET:CE	3.02	0.48
1:P:153:GLN:HE21	1:P:289:PRO:CD	2.26	0.48
1:P:232:THR:O	1:P:233:SER:CB	2.61	0.48
1:P:372:LEU:O	1:P:376:VAL:HG23	2.14	0.48
1:P:68:HIS:HB2	1:P:83:ILE:HG13	1.96	0.48
2:Q:104:ALA:HB3	2:Q:217:ALA:HB2	1.93	0.48
2:D:64:TYR:CE1	2:D:68:LEU:HD11	2.49	0.48
3:R:122:ASN:CG	3:R:124:GLY:H	2.16	0.48
2:Q:113:PRO:O	2:Q:114:ALA:HB3	2.12	0.48
1:C:202:PRO:O	1:C:205:ILE:N	2.47	0.48
1:C:305:LEU:HD23	1:C:336:MET:CE	2.43	0.48
1:C:48:GLY:HA3	4:C:502:HEM:CHB	2.42	0.48
1:P:108:VAL:HG21	1:P:139:MET:CE	2.43	0.48
1:P:166:PHE:O	1:P:168:ALA:N	2.46	0.48
1:P:334:ILE:O	1:P:335:ALA:C	2.52	0.48
1:P:338:GLY:O	1:P:342:VAL:HG23	2.13	0.48
1:P:370:LEU:O	1:P:373:ASP:N	2.46	0.48
1:P:45:TRP:NE1	4:P:502:HEM:O1D	2.46	0.48
2:Q:132:TYR:C	2:Q:134:TYR:N	2.66	0.48
3:R:133:CYS:HA	3:R:160:TYR:OH	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:205:MET:HE3	2:Q:205:MET:HA	1.96	0.48
2:Q:222:VAL:O	2:Q:225:LYS:N	2.47	0.48
2:D:194:TYR:OH	2:D:205:MET:HE3	2.13	0.48
3:E:129:MET:HE1	3:E:164:GLY:HA3	1.96	0.48
2:D:229:LEU:O	2:D:233:VAL:HG13	2.13	0.48
1:C:363:PHE:O	1:C:364:ARG:C	2.51	0.47
1:C:75:LEU:O	1:C:76:ALA:C	2.53	0.47
1:P:117:TYR:CD2	1:P:118:TYR:CE2	3.02	0.47
1:P:223:ASN:HD22	1:P:227:VAL:H	1.60	0.47
1:P:231:ARG:O	1:P:233:SER:N	2.47	0.47
1:P:255:ALA:O	1:P:258:LEU:HB2	2.13	0.47
4:P:501:HEM:HMB2	4:P:501:HEM:HBB2	1.96	0.47
1:P:88:ASN:HB2	3:R:36:ASN:HD22	1.79	0.47
2:D:134:TYR:HE1	2:D:158:PHE:HB2	1.78	0.47
2:D:26:GLY:O	2:D:29:VAL:HG13	2.14	0.47
3:R:153:CYS:HB3	3:R:158:SER:OG	2.14	0.47
3:E:180:ALA:HB2	3:E:190:LEU:HD23	1.96	0.47
1:P:240:ASP:O	1:P:241:THR:CB	2.61	0.47
3:R:116:PRO:O	3:R:117:ALA:CB	2.61	0.47
1:C:78:ALA:O	1:C:79:SER:C	2.52	0.47
1:P:77:PHE:HD1	1:P:282:GLN:CG	2.26	0.47
2:Q:155:ASN:O	2:Q:179:SER:OG	2.31	0.47
3:E:173:ARG:HG3	3:E:173:ARG:HH11	1.79	0.47
2:D:24:ARG:O	2:D:27:PHE:HB3	2.14	0.47
2:D:26:GLY:O	2:D:29:VAL:HG12	2.14	0.47
3:R:77:ARG:HD3	3:R:82:ILE:HG12	1.95	0.47
1:C:331:PHE:CD2	1:C:331:PHE:C	2.88	0.47
1:C:48:GLY:H	4:C:502:HEM:CGA	2.28	0.47
1:C:73:VAL:O	1:C:73:VAL:HG12	2.14	0.47
1:P:177:GLN:O	1:P:180:LEU:N	2.47	0.47
1:P:151:TRP:CZ3	1:P:191:LEU:HB2	2.49	0.47
1:C:75:LEU:CD1	1:P:72:HIS:CD2	2.97	0.47
2:Q:135:VAL:HG21	6:Q:501:HEC:HMB2	1.96	0.47
2:Q:186:PRO:CG	2:Q:187:LEU:N	2.77	0.47
2:D:132:TYR:C	2:D:134:TYR:N	2.67	0.47
2:D:27:PHE:HD1	2:D:27:PHE:O	1.96	0.47
2:Q:251:ALA:H	2:Q:252:PRO:CD	2.27	0.47
1:C:209:VAL:CG1	1:C:210:ALA:N	2.77	0.47
1:C:65:LEU:CD1	4:C:501:HEM:O2D	2.45	0.47
1:C:89:GLY:O	1:C:90:GLY:O	2.33	0.47
1:C:268:ALA:O	2:D:224:ARG:CD	2.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:71:PRO:O	1:P:72:HIS:CB	2.62	0.47
3:E:62:GLN:NE2	3:E:63:LEU:C	2.67	0.47
3:E:62:GLN:CB	3:E:75:ARG:HG3	2.44	0.47
2:Q:40:MET:HE3	2:Q:43:VAL:HG21	1.95	0.47
1:C:166:PHE:CD1	1:C:180:LEU:CD1	2.97	0.47
1:C:166:PHE:C	1:C:168:ALA:N	2.68	0.47
1:C:177:GLN:O	1:C:180:LEU:N	2.47	0.47
1:C:302:TYR:CE2	1:C:306:ARG:CZ	2.97	0.47
1:C:334:ILE:O	1:C:335:ALA:C	2.51	0.47
1:C:362:LYS:CB	1:C:411:LEU:HD21	2.44	0.47
1:C:58:GLN:O	1:C:59:ILE:C	2.53	0.47
1:P:215:ALA:O	1:P:216:PHE:C	2.51	0.47
1:P:361:PRO:HA	1:P:364:ARG:CD	2.44	0.47
1:P:81:GLU:O	1:P:84:MET:N	2.48	0.47
2:Q:210:SER:O	2:Q:211:ALA:C	2.51	0.47
2:Q:22:GLN:HA	2:Q:25:ARG:NH1	2.30	0.47
1:P:33:ILE:HG22	1:P:34:MET:N	2.28	0.47
1:C:73:VAL:HG22	1:C:151:TRP:CE2	2.50	0.47
1:C:231:ARG:O	1:C:233:SER:N	2.48	0.47
1:C:249:VAL:O	1:C:253:LEU:HD12	2.14	0.47
1:C:46:ILE:HD13	1:C:255:ALA:HB3	1.95	0.47
1:C:294:PRO:CD	1:C:302:TYR:CE1	2.97	0.47
1:C:63:ILE:HD13	1:C:67:MET:HE2	1.97	0.47
1:P:201:LEU:N	1:P:202:PRO:HD2	2.30	0.47
1:P:331:PHE:CD2	1:P:331:PHE:C	2.88	0.47
2:Q:187:LEU:HB3	2:Q:202:VAL:HG13	1.95	0.47
3:E:135:HIS:O	3:E:136:LEU:HG	2.15	0.47
2:D:201:THR:HB	2:D:204:GLN:H	1.79	0.47
1:C:138:LEU:HB3	1:C:205:ILE:HD12	1.94	0.47
1:P:107:ALA:O	1:P:108:VAL:C	2.52	0.47
1:P:23:LEU:HA	1:P:26:VAL:HG12	1.95	0.47
1:P:278:ASP:OD2	1:P:278:ASP:N	2.44	0.47
1:P:362:LYS:CB	1:P:411:LEU:HD21	2.44	0.47
1:P:370:LEU:O	1:P:371:VAL:C	2.52	0.47
2:Q:10:SER:HB2	2:Q:17:LYS:C	2.35	0.47
2:Q:26:GLY:O	2:Q:29:VAL:HG12	2.13	0.47
1:C:108:VAL:HG21	1:C:139:MET:CE	2.44	0.47
1:P:303:ALA:HB3	1:P:377:LEU:HD13	1.97	0.47
1:P:305:LEU:C	1:P:307:ALA:N	2.68	0.47
2:D:27:PHE:CE2	2:D:48:LEU:HD13	2.45	0.47
2:D:67:GLY:O	2:D:68:LEU:O	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:33:ILE:CG2	1:P:245:TRP:HB3	2.30	0.47
3:R:160:TYR:HD1	3:R:164:GLY:O	1.97	0.47
1:P:421:PRO:O	1:P:422:ALA:HB2	2.13	0.47
2:D:165:ASP:O	2:D:167:CYS:N	2.48	0.47
1:C:25:ILE:HD13	1:C:25:ILE:C	2.35	0.47
1:P:248:PHE:O	1:P:252:ASP:OD2	2.33	0.47
1:P:254:PHE:O	1:P:255:ALA:C	2.53	0.47
1:P:295:GLU:HB3	1:P:297:TYR:CE1	2.50	0.47
1:P:347:PRO:O	1:P:349:LEU:N	2.48	0.47
1:P:49:ILE:HG23	1:P:50:VAL:H	1.79	0.47
1:P:90:GLY:O	1:P:91:TRP:C	2.53	0.47
3:E:113:ARG:O	3:E:114:THR:C	2.53	0.47
2:D:53:GLY:HA3	2:D:215:TRP:CE3	2.50	0.47
2:D:38:HIS:CE1	6:D:501:HEC:ND	2.83	0.47
2:Q:173:VAL:O	2:Q:174:LYS:CD	2.63	0.47
2:D:218:GLU:HG3	2:D:218:GLU:O	2.14	0.47
1:C:200:LEU:C	1:C:202:PRO:HD2	2.35	0.47
1:C:170:PRO:HD2	1:C:330:PHE:CE2	2.50	0.47
1:P:104:PHE:CE1	1:P:139:MET:SD	3.08	0.47
1:P:394:LEU:O	1:P:395:ILE:C	2.53	0.47
2:D:25:ARG:NE	2:D:194:TYR:HE2	2.11	0.47
3:E:152:PHE:HD1	3:E:159:HIS:NE2	2.13	0.47
3:E:63:LEU:HD11	3:E:65:VAL:CG2	2.44	0.47
2:Q:177:HIS:O	2:Q:178:GLY:O	2.33	0.47
1:C:103:LEU:CG	1:C:104:PHE:N	2.77	0.47
1:C:152:GLY:O	1:C:155:SER:CB	2.63	0.47
1:C:236:ASP:CG	1:C:238:GLU:H	2.18	0.47
1:C:392:ILE:O	1:C:395:ILE:HG13	2.14	0.47
3:E:39:ASN:O	3:E:40:ALA:C	2.52	0.47
1:P:205:ILE:CG2	1:P:206:ALA:N	2.75	0.47
1:P:297:TYR:N	1:P:297:TYR:HD1	2.13	0.47
1:P:78:ALA:O	1:P:79:SER:C	2.53	0.47
1:C:33:ILE:HG22	1:C:34:MET:N	2.30	0.47
3:R:30:ALA:O	3:R:33:PRO:CD	2.63	0.47
2:D:191:GLN:O	2:D:192:VAL:HG13	2.15	0.47
1:C:40:ASN:HD22	1:C:224:PRO:HG2	1.79	0.46
1:C:299:LEU:O	1:C:302:TYR:HB3	2.15	0.46
1:C:357:GLY:HA3	1:C:363:PHE:HD2	1.80	0.46
1:C:370:LEU:CD1	1:C:370:LEU:C	2.84	0.46
1:P:105:PHE:CD2	1:P:297:TYR:HB2	2.50	0.46
1:P:108:VAL:O	1:P:109:TYR:C	2.53	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:187:ASP:CG	1:P:188:ASN:H	2.18	0.46
1:P:334:ILE:C	1:P:334:ILE:HD13	2.36	0.46
1:P:367:PHE:O	1:P:370:LEU:HB3	2.15	0.46
1:P:91:TRP:O	1:P:92:ALA:O	2.33	0.46
2:Q:194:TYR:OH	2:Q:205:MET:HE3	2.14	0.46
2:Q:29:VAL:HG13	2:Q:209:VAL:CG1	2.45	0.46
3:R:71:PRO:HG2	3:R:139:VAL:HG22	1.95	0.46
2:D:29:VAL:HG13	2:D:209:VAL:CG1	2.45	0.46
3:E:180:ALA:HA	3:E:189:LYS:O	2.15	0.46
1:C:296:TRP:HA	1:C:299:LEU:CD1	2.45	0.46
1:C:305:LEU:HD22	1:C:336:MET:CE	2.41	0.46
1:C:91:TRP:O	1:C:95:TYR:HD1	1.98	0.46
1:P:111:HIS:HE1	4:P:502:HEM:NA	2.06	0.46
1:P:140:MET:HE2	1:P:140:MET:HB3	1.85	0.46
1:P:163:THR:O	1:P:164:GLY:C	2.53	0.46
1:P:151:TRP:CD1	1:P:283:ALA:HB3	2.50	0.46
1:P:294:PRO:CD	1:P:302:TYR:CE1	2.98	0.46
2:Q:132:TYR:C	2:Q:134:TYR:H	2.18	0.46
2:Q:201:THR:HB	2:Q:204:GLN:H	1.79	0.46
2:Q:131:ILE:HD13	2:Q:213:LEU:CD1	2.46	0.46
3:E:29:ALA:O	3:E:33:PRO:HD2	2.15	0.46
3:E:30:ALA:O	3:E:31:VAL:C	2.53	0.46
3:R:57:VAL:N	3:R:76:ARG:HH12	2.13	0.46
1:C:145:MET:HE1	1:C:197:LEU:CB	2.27	0.46
1:C:68:HIS:HB2	1:C:83:ILE:HG13	1.96	0.46
1:P:229:VAL:HG12	1:P:229:VAL:O	2.14	0.46
1:P:347:PRO:C	1:P:349:LEU:H	2.18	0.46
1:P:392:ILE:O	1:P:395:ILE:HG13	2.16	0.46
1:P:40:ASN:OD1	1:P:40:ASN:N	2.49	0.46
1:P:48:GLY:H	4:P:502:HEM:CGA	2.27	0.46
1:P:58:GLN:HA	1:P:61:THR:CG2	2.45	0.46
1:P:91:TRP:O	1:P:95:TYR:HD1	1.98	0.46
2:Q:99:ASP:OD1	2:Q:101:SER:N	2.47	0.46
2:Q:154:TYR:O	2:Q:155:ASN:HB2	2.15	0.46
2:Q:27:PHE:O	2:Q:27:PHE:HD1	1.98	0.46
3:R:37:GLN:HE21	3:R:38:MET:CG	2.28	0.46
3:E:135:HIS:CD2	3:E:170:PRO:HB3	2.50	0.46
2:D:45:ILE:CD1	2:D:88:PHE:CD1	2.98	0.46
2:Q:229:LEU:HD12	2:Q:229:LEU:HA	1.72	0.46
3:R:62:GLN:CD	3:R:62:GLN:C	2.74	0.46
3:R:62:GLN:NE2	3:R:63:LEU:C	2.69	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:63:LEU:HD11	3:R:65:VAL:CG2	2.45	0.46
1:C:248:PHE:O	1:C:249:VAL:C	2.54	0.46
1:C:105:PHE:CG	1:C:297:TYR:CD2	3.03	0.46
1:C:331:PHE:O	1:C:335:ALA:HB2	2.15	0.46
1:C:195:PHE:HE1	1:P:195:PHE:CZ	2.33	0.46
2:Q:23:LEU:O	2:Q:24:ARG:C	2.54	0.46
2:D:30:TYR:CD1	2:D:34:CYS:HB2	2.38	0.46
1:C:414:THR:HA	1:C:417:PRO:CG	2.44	0.46
3:E:61:THR:O	3:E:62:GLN:CB	2.63	0.46
1:P:240:ASP:O	1:P:241:THR:CG2	2.61	0.46
1:C:117:TYR:HD1	1:C:363:PHE:HE2	1.63	0.46
1:C:200:LEU:HD23	1:P:203:PHE:HZ	1.80	0.46
1:C:209:VAL:O	1:C:212:HIS:HB3	2.16	0.46
1:C:23:LEU:HB2	1:P:214:TRP:CH2	2.50	0.46
1:C:303:ALA:HB3	1:C:377:LEU:CD1	2.45	0.46
1:C:394:LEU:O	1:C:395:ILE:C	2.54	0.46
1:P:40:ASN:ND2	1:P:223:ASN:OD1	2.44	0.46
1:P:90:GLY:C	1:P:92:ALA:N	2.68	0.46
2:Q:206:ALA:O	2:Q:209:VAL:HG23	2.16	0.46
3:E:57:VAL:N	3:E:76:ARG:HH12	2.13	0.46
1:C:399:TYR:O	1:C:400:TRP:C	2.53	0.46
1:C:51:LEU:HD22	1:C:108:VAL:HG23	1.93	0.46
1:C:302:TYR:O	1:C:305:LEU:HB3	2.15	0.46
1:C:69:TYR:HA	1:C:79:SER:OG	2.15	0.46
1:C:92:ALA:C	1:C:96:ILE:HG13	2.36	0.46
2:Q:158:PHE:CE1	6:Q:501:HEC:O1A	2.65	0.46
1:C:245:TRP:CD1	1:C:246:PRO:N	2.84	0.46
1:P:184:PRO:CG	1:P:185:ALA:H	2.25	0.46
2:Q:233:VAL:CG2	2:Q:234:MET:N	2.79	0.46
3:R:102:ASN:HB3	3:R:115:LEU:CD1	2.46	0.46
1:C:43:TRP:HZ3	1:C:251:LYS:HE2	1.80	0.46
1:C:195:PHE:CZ	1:P:195:PHE:HE1	2.34	0.46
1:P:46:ILE:HG13	1:P:49:ILE:HG23	1.96	0.46
4:P:501:HEM:CBC	4:P:501:HEM:CMC	2.94	0.46
1:P:51:LEU:O	1:P:52:ALA:C	2.54	0.46
1:P:53:PHE:O	1:P:54:THR:C	2.54	0.46
1:P:62:GLY:HA2	1:P:97:HIS:ND1	2.31	0.46
2:Q:127:GLY:O	2:Q:128:PRO:C	2.54	0.46
2:Q:215:TRP:O	2:Q:219:PRO:HD3	2.15	0.46
2:Q:218:GLU:O	2:Q:218:GLU:HG3	2.15	0.46
2:Q:67:GLY:O	2:Q:68:LEU:O	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:65:ALA:O	2:D:68:LEU:HD12	2.15	0.46
3:R:61:THR:O	3:R:62:GLN:CB	2.64	0.46
1:C:204:VAL:HG12	1:C:205:ILE:N	2.31	0.46
1:C:237:ALA:O	1:C:238:GLU:O	2.34	0.46
1:C:70:THR:HG21	1:C:75:LEU:HB2	1.97	0.46
1:P:166:PHE:HD2	1:P:166:PHE:N	2.14	0.46
1:P:334:ILE:HD13	1:P:335:ALA:CA	2.46	0.46
1:P:300:PRO:HA	1:P:377:LEU:HD12	1.96	0.46
1:P:366:TRP:CD2	1:P:407:ILE:HG13	2.51	0.46
2:Q:9:PHE:HB2	2:Q:11:PHE:CE1	2.51	0.46
2:Q:206:ALA:O	2:Q:209:VAL:CG2	2.64	0.46
2:Q:29:VAL:HG11	2:Q:209:VAL:HG13	1.97	0.46
1:P:28:LEU:HA	1:P:32:THR:HB	1.98	0.46
3:E:159:HIS:O	3:E:167:ARG:CB	2.63	0.46
3:E:30:ALA:O	3:E:33:PRO:CD	2.63	0.46
2:Q:240:VAL:O	2:Q:241:MET:C	2.54	0.46
2:Q:165:ASP:O	2:Q:167:CYS:N	2.48	0.46
1:C:305:LEU:C	1:C:307:ALA:N	2.68	0.46
1:P:138:LEU:HD12	1:P:204:VAL:HG12	1.97	0.46
1:P:157:TRP:CZ2	1:P:288:THR:HG23	2.51	0.46
1:P:223:ASN:ND2	1:P:227:VAL:H	2.14	0.46
1:P:25:ILE:HD13	1:P:26:VAL:N	2.31	0.46
1:P:88:ASN:HB2	3:R:36:ASN:ND2	2.30	0.46
3:E:62:GLN:HE22	3:E:63:LEU:C	2.19	0.46
2:D:233:VAL:CG2	2:D:234:MET:N	2.78	0.46
3:R:173:ARG:HH11	3:R:173:ARG:HG3	1.80	0.46
1:C:134:VAL:HG11	1:C:208:LEU:HD11	1.94	0.46
1:C:215:ALA:O	1:C:216:PHE:C	2.54	0.46
1:C:117:TYR:HD1	1:C:363:PHE:CE2	2.34	0.46
2:D:222:VAL:O	2:D:225:LYS:N	2.49	0.46
1:P:160:THR:OG1	1:P:186:VAL:HG21	2.16	0.46
1:P:43:TRP:CZ3	1:P:251:LYS:HG2	2.50	0.46
1:P:305:LEU:HD23	1:P:336:MET:CE	2.46	0.46
1:P:71:PRO:CD	1:P:71:PRO:O	2.64	0.46
2:Q:29:VAL:HG13	2:Q:209:VAL:HG13	1.98	0.46
3:R:15:LEU:O	3:R:18:ALA:HB3	2.16	0.46
2:D:40:MET:HE3	2:D:43:VAL:HG21	1.98	0.46
1:C:117:TYR:CD2	1:C:118:TYR:CE2	3.03	0.45
1:C:147:TYR:HA	4:C:501:HEM:HAA2	1.98	0.45
1:C:153:GLN:HA	1:C:153:GLN:OE1	2.15	0.45
1:C:151:TRP:CZ3	1:C:191:LEU:HB2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:254:PHE:O	1:C:255:ALA:C	2.55	0.45
1:C:372:LEU:O	1:C:376:VAL:HG23	2.15	0.45
1:P:46:ILE:HD13	1:P:255:ALA:HB3	1.97	0.45
1:P:23:LEU:O	1:P:25:ILE:N	2.48	0.45
1:P:48:GLY:HA3	4:P:502:HEM:CHB	2.45	0.45
1:P:50:VAL:HG12	1:P:51:LEU:N	2.30	0.45
3:E:102:ASN:HB3	3:E:115:LEU:CD1	2.46	0.45
3:E:118:PHE:C	3:E:120:GLY:N	2.69	0.45
2:D:23:LEU:O	2:D:24:ARG:C	2.54	0.45
1:C:240:ASP:O	1:C:241:THR:CG2	2.63	0.45
1:P:7:ASP:C	1:P:9:TYR:N	2.70	0.45
3:R:100:ASN:C	3:R:102:ASN:N	2.68	0.45
3:R:113:ARG:O	3:R:114:THR:C	2.54	0.45
1:C:107:ALA:O	1:C:108:VAL:C	2.54	0.45
1:C:149:LEU:N	1:C:150:PRO:CD	2.78	0.45
1:C:217:HIS:C	1:C:219:THR:N	2.68	0.45
1:P:407:ILE:O	1:P:411:LEU:CB	2.63	0.45
2:D:153:TYR:N	2:D:153:TYR:CD1	2.85	0.45
2:D:206:ALA:O	2:D:209:VAL:CG2	2.64	0.45
1:P:383:MET:CB	1:P:389:TYR:CD1	2.93	0.45
1:C:356:SER:O	1:C:358:ALA:N	2.49	0.45
1:C:138:LEU:HD12	1:C:204:VAL:HG12	1.98	0.45
1:C:191:LEU:O	1:C:194:PHE:HB2	2.16	0.45
1:C:347:PRO:O	1:C:349:LEU:N	2.49	0.45
1:C:403:TYR:C	1:C:407:ILE:HG22	2.36	0.45
1:C:41:LEU:HD12	1:C:248:PHE:CE2	2.51	0.45
1:P:331:PHE:O	1:P:335:ALA:HB2	2.16	0.45
1:P:367:PHE:CD2	1:P:368:TRP:CD1	3.03	0.45
2:Q:134:TYR:CE2	2:Q:183:MET:HE2	2.51	0.45
2:Q:34:CYS:C	2:Q:36:ALA:H	2.19	0.45
2:D:99:ASP:OD1	2:D:101:SER:N	2.49	0.45
2:D:190:ASP:O	2:D:192:VAL:HG22	2.17	0.45
3:R:78:ASP:O	3:R:81:ASP:HB2	2.16	0.45
1:C:328:ALA:O	1:C:329:LYS:C	2.55	0.45
1:C:43:TRP:C	1:C:45:TRP:H	2.20	0.45
1:P:73:VAL:HG22	1:P:151:TRP:CE2	2.51	0.45
1:P:90:GLY:O	1:P:92:ALA:N	2.50	0.45
2:Q:104:ALA:CB	2:Q:214:MET:HA	2.46	0.45
2:Q:11:PHE:HD1	2:Q:12:GLU:N	2.08	0.45
2:Q:155:ASN:OD1	2:Q:158:PHE:N	2.41	0.45
3:R:37:GLN:C	3:R:39:ASN:H	2.18	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:93:LEU:O	3:E:94:ARG:C	2.55	0.45
2:D:27:PHE:CZ	2:D:64:TYR:CE2	3.04	0.45
1:C:7:ASP:C	1:C:9:TYR:N	2.69	0.45
3:E:143:ASP:HB3	3:E:144:LYS:H	1.63	0.45
2:Q:5:PRO:O	2:Q:6:ASP:C	2.54	0.45
2:Q:6:ASP:O	2:Q:7:HIS:C	2.54	0.45
1:C:182:GLY:HA2	1:C:193:ARG:HH21	1.80	0.45
1:C:217:HIS:O	1:C:219:THR:N	2.50	0.45
1:C:50:VAL:HG12	1:C:51:LEU:N	2.32	0.45
1:C:65:LEU:HD22	4:C:501:HEM:HMD1	1.97	0.45
3:E:37:GLN:C	3:E:39:ASN:H	2.19	0.45
1:P:130:ILE:O	1:P:131:VAL:C	2.54	0.45
1:P:143:ALA:O	1:P:144:PHE:C	2.55	0.45
1:P:357:GLY:HA3	1:P:363:PHE:CD2	2.51	0.45
1:P:370:LEU:CD1	1:P:370:LEU:C	2.83	0.45
1:P:379:TRP:O	1:P:380:VAL:C	2.54	0.45
1:P:81:GLU:OE2	2:Q:102:VAL:HG21	2.17	0.45
2:Q:19:ASP:C	2:Q:21:ALA:N	2.68	0.45
2:Q:45:ILE:CD1	2:Q:88:PHE:CD1	2.99	0.45
2:D:96:MET:O	6:D:501:HEC:CMD	2.65	0.45
1:C:319:ASP:O	1:C:321:LEU:N	2.49	0.45
2:D:218:GLU:N	2:D:219:PRO:HD3	2.32	0.45
3:E:54:VAL:O	3:E:56:ALA:HA	2.14	0.45
1:C:347:PRO:C	1:C:349:LEU:H	2.18	0.45
1:P:102:SER:OG	1:P:296:TRP:CZ2	2.70	0.45
1:P:152:GLY:O	1:P:155:SER:CB	2.64	0.45
1:P:361:PRO:O	1:P:362:LYS:C	2.53	0.45
1:P:403:TYR:C	1:P:407:ILE:HG22	2.37	0.45
2:D:215:TRP:CD1	2:D:216:ALA:N	2.85	0.45
1:P:245:TRP:CD1	1:P:246:PRO:N	2.85	0.45
3:R:73:PHE:HE2	3:R:151:TRP:NE1	2.09	0.45
3:R:102:ASN:HB3	3:R:115:LEU:HD13	1.99	0.45
1:C:203:PHE:HZ	1:P:200:LEU:HD23	1.82	0.45
1:C:213:ILE:O	1:C:214:TRP:C	2.53	0.45
1:C:40:ASN:ND2	1:C:223:ASN:OD1	2.44	0.45
1:C:297:TYR:N	1:C:297:TYR:HD1	2.12	0.45
1:P:202:PRO:O	1:P:203:PHE:C	2.55	0.45
1:P:301:PHE:O	1:P:304:ILE:HG12	2.17	0.45
1:P:350:ASP:HB2	1:P:408:LEU:HD11	1.99	0.45
2:Q:11:PHE:CD1	2:Q:12:GLU:N	2.80	0.45
2:Q:153:TYR:N	2:Q:153:TYR:CD1	2.84	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:163:ALA:CB	3:E:165:ARG:HG3	2.43	0.45
2:D:154:TYR:O	2:D:155:ASN:HB2	2.17	0.45
2:D:184:PRO:HG2	6:D:501:HEC:HBC2	1.99	0.45
2:D:201:THR:O	2:D:202:VAL:C	2.55	0.45
2:D:6:ASP:O	2:D:7:HIS:C	2.54	0.45
2:Q:110:PHE:HB3	2:Q:125:MET:O	2.17	0.45
1:C:156:PHE:CE1	1:C:186:VAL:HB	2.52	0.45
1:C:302:TYR:CE2	1:C:306:ARG:NH1	2.85	0.45
1:C:407:ILE:O	1:C:411:LEU:CB	2.65	0.45
1:C:43:TRP:O	1:C:45:TRP:N	2.50	0.45
3:E:71:PRO:HG2	3:E:139:VAL:HG22	1.99	0.45
1:P:236:ASP:CG	1:P:238:GLU:H	2.19	0.45
2:D:205:MET:HE2	2:D:205:MET:HA	1.99	0.45
2:D:206:ALA:O	2:D:207:GLN:C	2.55	0.45
2:Q:190:ASP:O	2:Q:192:VAL:HG22	2.16	0.45
3:R:160:TYR:CD1	3:R:175:LEU:HD12	2.52	0.45
2:D:229:LEU:HA	2:D:229:LEU:HD12	1.74	0.45
3:R:90:LEU:O	3:R:91:GLY:C	2.55	0.45
1:C:156:PHE:O	1:C:157:TRP:C	2.55	0.45
1:C:360:ARG:O	1:C:364:ARG:HG3	2.17	0.45
1:P:157:TRP:CE2	1:P:288:THR:HG23	2.52	0.45
1:P:267:VAL:O	1:P:271:PRO:CD	2.65	0.45
1:P:64:VAL:HG23	1:P:65:LEU:N	2.31	0.45
2:Q:199:PRO:C	2:Q:201:THR:H	2.21	0.45
2:D:104:ALA:CB	2:D:214:MET:HA	2.46	0.45
3:R:152:PHE:HD1	3:R:159:HIS:NE2	2.15	0.45
1:C:53:PHE:CD2	1:C:260:LEU:HD21	2.51	0.45
1:C:151:TRP:CD1	1:C:283:ALA:HB3	2.52	0.45
1:C:330:PHE:C	1:C:334:ILE:HG22	2.33	0.45
1:P:152:GLY:O	1:P:153:GLN:C	2.55	0.45
1:P:302:TYR:CE2	1:P:306:ARG:CZ	3.00	0.45
1:P:330:PHE:C	1:P:334:ILE:HG22	2.35	0.45
1:P:303:ALA:HB3	1:P:377:LEU:CD1	2.46	0.45
3:E:113:ARG:HD2	3:E:177:ILE:CD1	2.47	0.45
2:Q:189:ASP:O	2:Q:190:ASP:HB2	2.17	0.45
3:E:150:GLY:O	3:E:151:TRP:CG	2.70	0.45
1:C:144:PHE:O	1:C:145:MET:C	2.56	0.44
1:C:145:MET:HG2	1:C:194:PHE:CD1	2.52	0.44
1:C:256:LEU:HA	1:C:259:VAL:HG23	1.99	0.44
1:C:379:TRP:O	1:C:380:VAL:C	2.54	0.44
1:P:138:LEU:HD12	1:P:204:VAL:CG1	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:104:PRO:O	3:E:106:ALA:N	2.50	0.44
3:E:75:ARG:HG2	3:E:76:ARG:O	2.16	0.44
3:R:163:ALA:C	3:R:165:ARG:H	2.20	0.44
1:C:173:GLY:O	1:C:176:ILE:N	2.50	0.44
1:P:305:LEU:HD13	1:P:332:GLY:CA	2.46	0.44
1:P:230:ARG:CZ	1:P:424:ILE:CB	2.96	0.44
3:R:135:HIS:CD2	3:R:170:PRO:HB3	2.52	0.44
3:E:135:HIS:CE1	3:E:136:LEU:HD12	2.52	0.44
2:D:132:TYR:C	2:D:134:TYR:H	2.19	0.44
3:R:152:PHE:C	3:R:152:PHE:CD2	2.89	0.44
3:R:46:ALA:O	3:R:47:MET:HB2	2.17	0.44
3:R:100:ASN:CB	3:R:115:LEU:HD11	2.47	0.44
1:C:130:ILE:O	1:C:131:VAL:C	2.55	0.44
1:C:135:ILE:CD1	1:C:208:LEU:HB3	2.48	0.44
1:C:158:GLY:O	1:C:161:VAL:HG12	2.17	0.44
1:C:211:ILE:O	1:C:212:HIS:C	2.56	0.44
1:C:68:HIS:HE1	3:E:37:GLN:NE2	2.15	0.44
1:P:45:TRP:CZ2	1:P:222:ASN:C	2.91	0.44
1:P:256:LEU:HA	1:P:259:VAL:HG23	2.00	0.44
1:P:392:ILE:O	1:P:393:SER:C	2.55	0.44
4:P:501:HEM:CMB	4:P:501:HEM:CBB	2.94	0.44
2:Q:132:TYR:O	2:Q:134:TYR:N	2.50	0.44
1:P:242:LEU:HB3	1:P:247:TYR:CE1	2.53	0.44
2:D:190:ASP:C	2:D:192:VAL:N	2.71	0.44
2:Q:190:ASP:O	2:Q:192:VAL:N	2.51	0.44
2:D:110:PHE:HB3	2:D:125:MET:O	2.17	0.44
1:C:138:LEU:HD12	1:C:204:VAL:CG1	2.47	0.44
1:C:330:PHE:C	1:C:332:GLY:N	2.70	0.44
1:C:37:THR:HG22	1:C:41:LEU:HD11	2.00	0.44
1:P:134:VAL:O	1:P:135:ILE:C	2.55	0.44
1:P:156:PHE:CE1	1:P:186:VAL:HB	2.53	0.44
1:P:145:MET:HG2	1:P:194:PHE:CD1	2.52	0.44
1:P:249:VAL:O	1:P:253:LEU:HD12	2.16	0.44
1:P:25:ILE:HD13	1:P:25:ILE:C	2.37	0.44
1:P:80:VAL:O	1:P:81:GLU:C	2.55	0.44
2:Q:26:GLY:O	2:Q:29:VAL:HG13	2.18	0.44
2:Q:9:PHE:CG	2:Q:11:PHE:CZ	3.06	0.44
1:C:288:THR:OG1	3:R:139:VAL:O	2.36	0.44
1:P:28:LEU:O	1:P:32:THR:HB	2.17	0.44
1:C:242:LEU:HB3	1:C:247:TYR:CE1	2.53	0.44
2:D:238:LEU:HD11	3:E:23:GLY:HA2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:312:VAL:C	1:C:314:VAL:H	2.20	0.44
2:Q:226:GLN:O	2:Q:230:VAL:HG23	2.18	0.44
1:C:23:LEU:O	1:C:25:ILE:N	2.51	0.44
1:C:371:VAL:CG1	1:C:372:LEU:N	2.80	0.44
3:E:37:GLN:HE21	3:E:38:MET:CG	2.30	0.44
1:P:182:GLY:HA3	1:P:193:ARG:NH2	2.31	0.44
1:P:213:ILE:O	1:P:214:TRP:C	2.53	0.44
2:Q:97:GLY:HA3	6:Q:501:HEC:HMD3	1.99	0.44
2:Q:53:GLY:HA3	2:Q:215:TRP:CE3	2.52	0.44
2:Q:27:PHE:CZ	2:Q:64:TYR:CE2	3.06	0.44
3:R:180:ALA:HA	3:R:189:LYS:O	2.18	0.44
2:D:173:VAL:O	2:D:174:LYS:CD	2.65	0.44
3:E:131:GLY:O	3:E:132:VAL:HB	2.16	0.44
1:C:108:VAL:O	1:C:109:TYR:C	2.56	0.44
1:C:140:MET:HE2	1:C:140:MET:HB3	1.75	0.44
1:C:361:PRO:O	1:C:362:LYS:C	2.54	0.44
1:P:132:GLY:O	1:P:133:MET:C	2.56	0.44
1:P:144:PHE:O	1:P:145:MET:C	2.56	0.44
1:P:248:PHE:O	1:P:249:VAL:C	2.55	0.44
1:P:297:TYR:O	1:P:298:PHE:HD1	2.00	0.44
4:P:502:HEM:CGA	4:P:502:HEM:O2D	2.65	0.44
1:P:92:ALA:C	1:P:96:ILE:HG13	2.35	0.44
3:E:163:ALA:C	3:E:165:ARG:H	2.21	0.44
2:D:29:VAL:HG13	2:D:209:VAL:HG13	1.99	0.44
2:D:34:CYS:C	2:D:36:ALA:H	2.21	0.44
1:C:243:PRO:HD2	1:C:247:TYR:CE1	2.53	0.44
2:D:238:LEU:CD1	3:E:26:VAL:HG21	2.48	0.44
2:D:42:PHE:O	2:D:44:PRO:HD3	2.18	0.44
1:P:263:PHE:C	1:P:266:VAL:HG23	2.36	0.44
2:D:5:PRO:O	2:D:6:ASP:C	2.55	0.44
3:R:93:LEU:O	3:R:94:ARG:C	2.55	0.44
3:R:94:ARG:NH1	3:R:169:GLY:O	2.51	0.44
1:C:163:THR:O	1:C:164:GLY:C	2.54	0.44
1:C:160:THR:OG1	1:C:186:VAL:HG21	2.18	0.44
1:C:190:THR:HA	1:C:193:ARG:HG3	2.00	0.44
1:C:295:GLU:CB	1:C:297:TYR:HE1	2.31	0.44
4:C:502:HEM:CGA	4:C:502:HEM:O2D	2.64	0.44
1:P:328:ALA:O	1:P:329:LYS:C	2.56	0.44
2:Q:149:ILE:HG22	2:Q:180:TRP:CZ3	2.53	0.44
2:Q:65:ALA:O	2:Q:68:LEU:HD12	2.17	0.44
3:E:100:ASN:CB	3:E:115:LEU:HD11	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:94:ARG:NH1	3:E:169:GLY:O	2.50	0.44
3:R:150:GLY:O	3:R:151:TRP:CG	2.71	0.44
1:C:183:GLY:HA3	1:C:184:PRO:HD2	1.82	0.44
3:R:104:PRO:O	3:R:106:ALA:N	2.51	0.44
1:C:357:GLY:HA2	1:C:360:ARG:HB2	2.00	0.44
1:C:373:ASP:O	1:C:374:PHE:C	2.55	0.44
1:C:45:TRP:CZ2	1:C:222:ASN:C	2.91	0.44
1:P:104:PHE:HE1	1:P:139:MET:SD	2.40	0.44
1:P:209:VAL:CG1	1:P:210:ALA:N	2.79	0.44
1:P:270:MET:N	1:P:271:PRO:CD	2.80	0.44
1:P:407:ILE:HD13	1:P:407:ILE:O	2.17	0.44
1:P:37:THR:HG22	1:P:41:LEU:HD11	2.00	0.44
2:D:11:PHE:HD1	2:D:12:GLU:N	2.12	0.44
2:Q:32:GLU:OE2	2:Q:192:VAL:HG12	2.18	0.44
3:R:68:ARG:O	3:R:70:LYS:N	2.49	0.44
2:Q:230:VAL:O	2:Q:234:MET:CG	2.65	0.44
1:C:166:PHE:O	1:C:168:ALA:N	2.51	0.44
1:C:236:ASP:C	1:C:238:GLU:N	2.71	0.44
1:C:357:GLY:HA3	1:C:363:PHE:CD2	2.53	0.44
1:C:43:TRP:C	1:C:45:TRP:N	2.71	0.44
1:P:156:PHE:O	1:P:157:TRP:C	2.56	0.44
1:P:387:TYR:HD2	1:P:388:PRO:CA	2.31	0.44
1:P:58:GLN:O	1:P:59:ILE:C	2.52	0.44
2:Q:25:ARG:NE	2:Q:194:TYR:CE2	2.81	0.44
3:E:152:PHE:C	3:E:152:PHE:CD2	2.91	0.44
2:Q:43:VAL:O	2:Q:87:MET:HA	2.18	0.44
1:P:369:PHE:HA	1:P:369:PHE:HD2	1.66	0.44
3:R:143:ASP:HB3	3:R:144:LYS:H	1.65	0.44
1:P:399:TYR:O	1:P:400:TRP:C	2.56	0.44
3:R:57:VAL:HG12	3:R:57:VAL:O	2.18	0.43
3:R:61:THR:HB	3:R:62:GLN:H	1.55	0.43
1:C:152:GLY:O	1:C:153:GLN:C	2.56	0.43
1:C:225:THR:CG2	1:C:227:VAL:HG13	2.46	0.43
1:C:350:ASP:HB2	1:C:408:LEU:HD11	1.99	0.43
4:C:502:HEM:HBD1	4:C:502:HEM:CGA	2.48	0.43
1:C:51:LEU:O	1:C:52:ALA:C	2.57	0.43
1:P:190:THR:HA	1:P:193:ARG:HG3	2.00	0.43
1:P:211:ILE:O	1:P:212:HIS:C	2.56	0.43
1:P:301:PHE:O	1:P:304:ILE:CG1	2.66	0.43
2:Q:204:GLN:HE22	2:Q:208:ASP:CG	2.20	0.43
2:Q:30:TYR:HA	2:Q:33:VAL:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:39:ASN:O	3:R:40:ALA:C	2.56	0.43
2:D:138:PHE:HB2	2:D:185:PRO:HG3	2.00	0.43
2:D:131:ILE:HG21	2:D:213:LEU:HD12	2.00	0.43
3:E:57:VAL:O	3:E:57:VAL:HG12	2.18	0.43
1:P:312:VAL:C	1:P:314:VAL:H	2.21	0.43
3:E:78:ASP:O	3:E:81:ASP:HB2	2.18	0.43
1:P:11:PRO:O	1:P:12:LYS:C	2.56	0.43
3:R:63:LEU:HD13	3:R:63:LEU:C	2.39	0.43
1:C:118:TYR:C	1:C:120:SER:N	2.71	0.43
1:C:153:GLN:HE21	1:C:289:PRO:HG3	1.83	0.43
1:C:102:SER:OG	1:C:296:TRP:CZ2	2.71	0.43
1:C:371:VAL:O	1:C:374:PHE:HB3	2.18	0.43
1:P:112:ILE:HG23	4:P:502:HEM:CBC	2.48	0.43
1:P:299:LEU:O	1:P:302:TYR:HB3	2.18	0.43
1:P:304:ILE:HD12	1:P:339:ALA:CB	2.48	0.43
1:P:380:VAL:HG21	1:P:392:ILE:HG22	1.99	0.43
2:Q:99:ASP:OD1	2:Q:100:LEU:N	2.51	0.43
3:E:159:HIS:CG	3:E:168:LYS:HB3	2.53	0.43
2:D:241:MET:HE3	3:E:22:THR:HG21	2.00	0.43
2:Q:238:LEU:C	2:Q:238:LEU:HD23	2.39	0.43
3:R:63:LEU:HD22	3:R:64:THR:N	2.33	0.43
1:C:138:LEU:HA	1:C:138:LEU:HD22	1.71	0.43
1:C:203:PHE:HZ	1:P:200:LEU:CD2	2.31	0.43
1:C:77:PHE:HD1	1:C:282:GLN:CG	2.30	0.43
1:C:40:ASN:N	1:C:40:ASN:OD1	2.49	0.43
1:C:58:GLN:HA	1:C:61:THR:CG2	2.48	0.43
1:C:81:GLU:O	1:C:84:MET:N	2.51	0.43
1:P:135:ILE:CD1	1:P:208:LEU:HB3	2.49	0.43
1:P:45:TRP:HH2	1:P:118:TYR:CD1	2.21	0.43
3:E:63:LEU:HD22	3:E:64:THR:N	2.33	0.43
3:R:29:ALA:O	3:R:33:PRO:HD2	2.19	0.43
3:R:113:ARG:NH1	3:R:177:ILE:HD11	2.34	0.43
1:C:105:PHE:CD2	1:C:297:TYR:HB2	2.54	0.43
1:C:122:LYS:HD3	1:C:350:ASP:OD2	2.18	0.43
1:C:62:GLY:HA2	1:C:97:HIS:ND1	2.33	0.43
1:C:80:VAL:O	1:C:81:GLU:C	2.54	0.43
1:P:209:VAL:O	1:P:212:HIS:HB3	2.18	0.43
1:P:237:ALA:O	1:P:238:GLU:O	2.35	0.43
1:P:292:ILE:CD1	1:P:292:ILE:H	1.98	0.43
1:P:50:VAL:CG2	1:P:259:VAL:HG21	2.48	0.43
2:Q:25:ARG:NE	2:Q:194:TYR:HE2	2.11	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:127:GLY:O	2:D:128:PRO:C	2.55	0.43
2:D:26:GLY:HA2	2:D:29:VAL:CG1	2.48	0.43
2:D:26:GLY:O	2:D:27:PHE:C	2.57	0.43
2:D:28:GLN:O	2:D:29:VAL:C	2.56	0.43
3:E:57:VAL:CA	3:E:76:ARG:HH22	2.32	0.43
2:D:43:VAL:O	2:D:87:MET:HA	2.18	0.43
1:C:276:HIS:HA	1:C:277:PRO:HD2	1.52	0.43
1:C:281:VAL:O	1:C:281:VAL:CG1	2.65	0.43
1:C:301:PHE:O	1:C:304:ILE:HG13	2.17	0.43
1:C:334:ILE:C	1:C:334:ILE:HD13	2.39	0.43
1:C:305:LEU:HD23	1:C:336:MET:HE1	2.00	0.43
1:C:230:ARG:CZ	1:C:424:ILE:CB	2.97	0.43
1:P:153:GLN:HE21	1:P:289:PRO:HG3	1.83	0.43
1:P:346:ALA:O	1:P:347:PRO:C	2.56	0.43
1:C:85:ARG:HH12	2:D:102:VAL:HG22	1.81	0.43
2:D:183:MET:HB2	6:D:501:HEC:C3D	2.49	0.43
2:D:70:THR:O	2:D:71:ILE:C	2.56	0.43
2:Q:70:THR:O	2:Q:71:ILE:C	2.57	0.43
1:C:154:MET:CE	1:C:292:ILE:HG22	2.42	0.43
2:Q:190:ASP:C	2:Q:192:VAL:N	2.70	0.43
1:P:308:PHE:N	1:P:308:PHE:CD1	2.86	0.43
3:R:62:GLN:HE22	3:R:63:LEU:C	2.22	0.43
1:C:346:ALA:O	1:C:347:PRO:C	2.56	0.43
1:C:45:TRP:HH2	1:C:118:TYR:CD1	2.21	0.43
1:P:281:VAL:CG1	1:P:281:VAL:O	2.64	0.43
1:P:330:PHE:C	1:P:332:GLY:N	2.71	0.43
4:P:502:HEM:CGA	4:P:502:HEM:HBD1	2.48	0.43
1:P:73:VAL:O	1:P:73:VAL:HG12	2.17	0.43
2:Q:134:TYR:HE1	2:Q:158:PHE:HB2	1.80	0.43
2:Q:138:PHE:HB2	2:Q:185:PRO:HG3	2.01	0.43
2:D:21:ALA:O	2:D:22:GLN:C	2.56	0.43
2:D:30:TYR:HA	2:D:33:VAL:O	2.19	0.43
2:D:70:THR:O	2:D:71:ILE:O	2.37	0.43
2:D:240:VAL:O	2:D:241:MET:C	2.55	0.43
2:D:56:LEU:HD13	2:D:60:PHE:CE2	2.54	0.43
3:R:160:TYR:HE1	3:R:175:LEU:HG	1.84	0.43
1:C:176:ILE:HG23	1:C:177:GLN:N	2.33	0.43
1:C:177:GLN:O	1:C:180:LEU:HB2	2.18	0.43
1:C:366:TRP:CD2	1:C:407:ILE:HG13	2.53	0.43
1:P:204:VAL:HG12	1:P:205:ILE:N	2.32	0.43
1:P:357:GLY:C	1:P:359:TYR:N	2.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:40:ASN:ND2	1:P:224:PRO:HD2	2.33	0.43
2:Q:209:VAL:O	2:Q:212:PHE:N	2.51	0.43
2:Q:26:GLY:O	2:Q:27:PHE:C	2.56	0.43
2:Q:34:CYS:C	2:Q:36:ALA:N	2.72	0.43
2:D:33:VAL:HG13	6:D:501:HEC:HBB1	1.99	0.43
1:P:243:PRO:HD2	1:P:247:TYR:CE1	2.53	0.43
2:Q:229:LEU:O	2:Q:233:VAL:HG13	2.18	0.43
3:R:54:VAL:O	3:R:56:ALA:HA	2.15	0.43
1:C:162:ILE:CA	1:C:165:LEU:HD12	2.48	0.43
1:C:278:ASP:C	1:C:280:TYR:N	2.61	0.43
1:C:303:ALA:HB3	1:C:377:LEU:HD13	2.00	0.43
1:C:303:ALA:HA	1:C:306:ARG:CG	2.49	0.43
1:C:334:ILE:HD13	1:C:335:ALA:CA	2.47	0.43
1:C:336:MET:O	1:C:337:PHE:C	2.57	0.43
1:C:380:VAL:HG21	1:C:392:ILE:HG22	2.00	0.43
1:C:342:VAL:HG12	1:C:404:PHE:HD2	1.83	0.43
1:P:380:VAL:C	1:P:382:ALA:H	2.22	0.43
1:P:135:ILE:CG2	4:P:502:HEM:CBB	2.97	0.43
1:P:65:LEU:HD22	4:P:501:HEM:HMD1	2.01	0.43
2:Q:25:ARG:HH21	2:Q:204:GLN:NE2	2.17	0.43
2:Q:26:GLY:HA3	2:Q:212:PHE:HB2	2.00	0.43
3:E:102:ASN:HB3	3:E:115:LEU:HD13	2.00	0.43
2:D:134:TYR:CD1	2:D:158:PHE:HB2	2.54	0.43
3:R:30:ALA:O	3:R:31:VAL:C	2.55	0.43
3:R:117:ALA:O	3:R:118:PHE:CB	2.66	0.43
1:C:367:PHE:CD2	1:C:368:TRP:CD1	3.04	0.43
1:P:149:LEU:N	1:P:150:PRO:CD	2.82	0.43
1:P:300:PRO:O	1:P:377:LEU:CD1	2.63	0.43
1:P:379:TRP:C	1:P:381:GLY:N	2.72	0.43
1:C:32:THR:HG23	1:C:32:THR:O	2.19	0.43
1:C:143:ALA:O	1:C:144:PHE:C	2.56	0.43
1:C:18:TRP:O	1:C:21:ASP:CB	2.66	0.43
1:C:380:VAL:C	1:C:382:ALA:N	2.72	0.43
1:P:71:PRO:HA	1:P:191:LEU:HD21	2.00	0.43
1:P:191:LEU:C	1:P:191:LEU:HD23	2.39	0.43
1:P:203:PHE:O	1:P:204:VAL:C	2.55	0.43
1:P:366:TRP:CE3	1:P:407:ILE:HG13	2.54	0.43
2:Q:184:PRO:HG2	6:Q:501:HEC:HBC2	2.00	0.43
3:E:90:LEU:O	3:E:91:GLY:C	2.56	0.43
2:D:149:ILE:HG22	2:D:180:TRP:CZ3	2.54	0.43
2:D:199:PRO:C	2:D:201:THR:H	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:131:ILE:HD13	2:D:213:LEU:HD12	2.01	0.43
1:C:11:PRO:O	1:C:12:LYS:C	2.56	0.43
1:C:308:PHE:N	1:C:308:PHE:CD1	2.86	0.43
2:Q:111:SER:HB2	2:Q:122:PHE:C	2.39	0.43
3:R:62:GLN:CA	3:R:75:ARG:HG3	2.49	0.42
1:C:157:TRP:CE2	1:C:288:THR:HG23	2.54	0.42
1:C:248:PHE:O	1:C:252:ASP:OD2	2.37	0.42
1:C:305:LEU:HD13	1:C:332:GLY:CA	2.48	0.42
1:P:118:TYR:C	1:P:120:SER:N	2.72	0.42
1:P:144:PHE:CD1	1:P:162:ILE:CD1	3.02	0.42
1:P:294:PRO:HB2	1:P:295:GLU:H	1.59	0.42
1:P:117:TYR:HD1	1:P:363:PHE:CE2	2.37	0.42
1:P:84:MET:HA	1:P:90:GLY:CA	2.49	0.42
2:Q:213:LEU:C	2:Q:215:TRP:N	2.70	0.42
2:Q:215:TRP:CD1	2:Q:216:ALA:N	2.87	0.42
2:Q:23:LEU:HA	2:Q:23:LEU:HD23	1.87	0.42
2:Q:28:GLN:O	2:Q:29:VAL:C	2.56	0.42
3:R:135:HIS:O	3:R:136:LEU:HG	2.19	0.42
2:D:138:PHE:CB	2:D:185:PRO:HG3	2.49	0.42
3:E:68:ARG:O	3:E:70:LYS:N	2.51	0.42
3:R:35:ILE:HG22	3:R:35:ILE:O	2.19	0.42
3:R:113:ARG:HD2	3:R:177:ILE:CD1	2.48	0.42
1:C:157:TRP:CZ2	1:C:288:THR:HG23	2.54	0.42
1:C:392:ILE:O	1:C:393:SER:C	2.57	0.42
1:C:56:VAL:O	1:C:57:LEU:C	2.58	0.42
1:C:71:PRO:O	1:C:71:PRO:HD2	2.18	0.42
1:P:137:LEU:HA	1:P:137:LEU:HD23	1.73	0.42
1:P:173:GLY:O	1:P:176:ILE:N	2.53	0.42
1:P:300:PRO:C	1:P:377:LEU:HD12	2.40	0.42
2:Q:96:MET:O	6:Q:501:HEC:CMD	2.68	0.42
2:D:99:ASP:OD1	2:D:100:LEU:N	2.52	0.42
1:C:247:TYR:CE2	2:D:249:LEU:CD2	3.03	0.42
2:Q:238:LEU:HD11	3:R:23:GLY:HA2	2.00	0.42
1:C:352:SER:C	1:C:354:VAL:H	2.23	0.42
1:C:112:ILE:HG23	4:C:502:HEM:CBC	2.50	0.42
1:C:66:ALA:CA	4:C:501:HEM:HMD2	2.48	0.42
1:P:162:ILE:CA	1:P:165:LEU:HD12	2.48	0.42
1:P:304:ILE:HD12	1:P:339:ALA:HB3	2.01	0.42
1:P:373:ASP:O	1:P:374:PHE:C	2.57	0.42
1:P:65:LEU:HD22	4:P:501:HEM:CMD	2.49	0.42
2:Q:100:LEU:N	2:Q:100:LEU:HD22	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:38:HIS:HE1	2:Q:98:PRO:HD2	1.84	0.42
1:C:161:VAL:HG23	3:R:136:LEU:HD13	2.01	0.42
2:D:9:PHE:CG	2:D:11:PHE:CZ	3.07	0.42
3:R:142:GLY:HA2	3:R:151:TRP:NE1	2.33	0.42
1:C:105:PHE:HD2	1:C:109:TYR:HE1	1.67	0.42
1:C:47:TRP:CZ2	1:C:110:ILE:HD12	2.55	0.42
4:C:501:HEM:HMB2	4:C:501:HEM:HBB2	2.02	0.42
1:C:53:PHE:O	1:C:54:THR:C	2.55	0.42
1:C:91:TRP:CG	1:C:92:ALA:N	2.87	0.42
1:P:117:TYR:HD1	1:P:363:PHE:HE2	1.67	0.42
1:P:155:SER:N	1:P:279:ASN:OD1	2.44	0.42
1:P:66:ALA:CA	4:P:501:HEM:HMD2	2.49	0.42
2:Q:31:ASN:O	2:Q:31:ASN:ND2	2.48	0.42
2:Q:42:PHE:HD1	2:Q:101:SER:HG	1.64	0.42
1:C:85:ARG:NH1	2:D:102:VAL:CG2	2.75	0.42
2:D:9:PHE:HB2	2:D:11:PHE:CE1	2.54	0.42
2:D:204:GLN:HE22	2:D:208:ASP:CG	2.21	0.42
1:C:184:PRO:CG	1:C:185:ALA:H	2.22	0.42
1:C:132:GLY:O	1:C:133:MET:C	2.56	0.42
1:C:166:PHE:HD2	1:C:166:PHE:N	2.17	0.42
1:C:50:VAL:CG2	1:C:259:VAL:HG21	2.49	0.42
1:C:304:ILE:HD12	1:C:339:ALA:HB3	2.01	0.42
1:C:387:TYR:HD2	1:C:388:PRO:CA	2.33	0.42
1:C:408:LEU:O	1:C:411:LEU:HB3	2.19	0.42
1:C:90:GLY:O	1:C:91:TRP:C	2.57	0.42
1:P:104:PHE:HE1	1:P:139:MET:CE	2.32	0.42
1:P:166:PHE:CD1	1:P:180:LEU:CD1	3.02	0.42
1:P:236:ASP:C	1:P:238:GLU:N	2.72	0.42
1:P:295:GLU:CB	1:P:297:TYR:HE1	2.32	0.42
1:P:371:VAL:CG1	1:P:372:LEU:N	2.81	0.42
3:E:119:ASP:O	3:E:120:GLY:O	2.36	0.42
3:E:63:LEU:HD13	3:E:63:LEU:C	2.39	0.42
3:E:122:ASN:HD21	3:E:124:GLY:C	2.21	0.42
2:Q:91:ARG:O	2:Q:92:VAL:C	2.58	0.42
3:E:35:ILE:HG22	3:E:35:ILE:O	2.18	0.42
1:C:316:ILE:O	1:C:320:GLY:N	2.42	0.42
1:P:103:LEU:O	1:P:103:LEU:HD12	2.19	0.42
1:P:250:ILE:O	1:P:251:LYS:C	2.58	0.42
1:P:43:TRP:HZ3	1:P:251:LYS:HE2	1.81	0.42
1:P:302:TYR:O	1:P:305:LEU:HB3	2.20	0.42
1:P:350:ASP:CA	1:P:408:LEU:HD12	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:121:THR:O	3:E:122:ASN:CB	2.67	0.42
1:C:236:ASP:O	1:C:238:GLU:N	2.52	0.42
1:C:300:PRO:O	1:C:377:LEU:CD1	2.64	0.42
1:C:331:PHE:HA	1:C:334:ILE:CG2	2.50	0.42
2:D:224:ARG:CG	2:D:224:ARG:NH1	2.74	0.42
1:P:136:TYR:O	1:P:137:LEU:C	2.58	0.42
1:P:357:GLY:HA2	1:P:360:ARG:HB2	2.01	0.42
1:P:379:TRP:O	1:P:381:GLY:N	2.52	0.42
1:P:91:TRP:CD2	1:P:92:ALA:N	2.88	0.42
2:Q:205:MET:HE2	2:Q:205:MET:HA	1.99	0.42
2:Q:27:PHE:CD2	2:Q:48:LEU:HD22	2.55	0.42
1:C:161:VAL:CG2	3:R:136:LEU:HD13	2.49	0.42
1:C:243:PRO:C	1:C:245:TRP:N	2.71	0.42
3:E:63:LEU:HD11	3:E:65:VAL:HG23	2.02	0.42
2:D:190:ASP:O	2:D:192:VAL:N	2.52	0.42
2:D:56:LEU:HD13	2:D:60:PHE:HE2	1.85	0.42
1:P:35:ILE:HA	1:P:36:PRO:HD3	1.75	0.42
2:D:91:ARG:O	2:D:92:VAL:C	2.58	0.42
1:C:103:LEU:O	1:C:103:LEU:HD12	2.20	0.42
1:C:212:HIS:CE1	4:C:502:HEM:ND	2.88	0.42
1:P:236:ASP:O	1:P:238:GLU:N	2.53	0.42
1:P:338:GLY:O	1:P:339:ALA:C	2.57	0.42
1:P:342:VAL:HG12	1:P:404:PHE:HD2	1.84	0.42
1:P:41:LEU:HD12	1:P:248:PHE:CD2	2.55	0.42
2:Q:183:MET:HB2	6:Q:501:HEC:C3D	2.50	0.42
3:R:136:LEU:HA	3:R:136:LEU:HD23	1.88	0.42
3:E:157:GLY:O	3:E:158:SER:C	2.58	0.42
1:C:221:ASN:ND2	1:C:244:PHE:HE1	2.18	0.42
3:R:22:THR:O	3:R:26:VAL:HG22	2.19	0.42
2:D:32:GLU:OE2	2:D:192:VAL:HG12	2.19	0.42
3:R:114:THR:OG1	3:R:123:THR:HB	2.20	0.42
3:R:75:ARG:HG2	3:R:76:ARG:O	2.20	0.42
1:C:139:MET:O	1:C:140:MET:C	2.58	0.42
1:C:202:PRO:O	1:C:203:PHE:C	2.58	0.42
1:C:135:ILE:HD11	1:C:208:LEU:HB3	2.01	0.42
1:C:380:VAL:C	1:C:382:ALA:H	2.23	0.42
3:E:38:MET:CB	1:P:179:TRP:HE1	2.31	0.42
1:P:268:ALA:HA	2:Q:224:ARG:HD3	2.02	0.42
1:P:278:ASP:O	1:P:280:TYR:N	2.53	0.42
1:P:331:PHE:HA	1:P:334:ILE:CG2	2.50	0.42
2:Q:134:TYR:CD1	2:Q:158:PHE:HB2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:154:TYR:CD2	2:Q:155:ASN:N	2.87	0.42
2:Q:209:VAL:O	2:Q:212:PHE:HB3	2.20	0.42
3:R:135:HIS:CE1	3:R:136:LEU:HD12	2.55	0.42
3:E:104:PRO:C	3:E:106:ALA:N	2.73	0.42
2:D:132:TYR:O	2:D:134:TYR:N	2.53	0.42
1:C:28:LEU:O	1:C:32:THR:HB	2.19	0.42
3:R:122:ASN:HD21	3:R:124:GLY:C	2.23	0.42
1:C:51:LEU:CD1	1:C:108:VAL:HA	2.37	0.42
1:C:134:VAL:O	1:C:135:ILE:C	2.58	0.42
1:C:250:ILE:O	1:C:251:LYS:C	2.57	0.42
1:C:301:PHE:O	1:C:304:ILE:HG12	2.19	0.42
1:C:73:VAL:HG13	1:C:151:TRP:CD1	2.54	0.42
1:C:91:TRP:O	1:C:95:TYR:CD1	2.73	0.42
1:P:350:ASP:HB2	1:P:408:LEU:CD1	2.50	0.42
1:P:63:ILE:HA	4:P:501:HEM:CBC	2.50	0.42
1:P:70:THR:HG22	1:P:70:THR:O	2.20	0.42
1:P:284:ASN:OD1	1:P:286:LEU:HD13	2.19	0.42
3:E:46:ALA:O	3:E:47:MET:HB2	2.20	0.42
3:R:119:ASP:O	3:R:120:GLY:O	2.38	0.41
1:C:176:ILE:O	1:C:179:TRP:HB3	2.20	0.41
1:C:357:GLY:C	1:C:359:TYR:N	2.71	0.41
1:C:135:ILE:CG2	4:C:502:HEM:CBB	2.98	0.41
1:C:80:VAL:HG12	1:C:81:GLU:N	2.35	0.41
1:P:177:GLN:O	1:P:180:LEU:HB2	2.20	0.41
1:P:135:ILE:CD1	1:P:208:LEU:HD22	2.50	0.41
1:P:296:TRP:CA	1:P:299:LEU:HG	2.47	0.41
1:P:302:TYR:CE2	1:P:306:ARG:NH1	2.87	0.41
1:P:85:ARG:CG	1:P:85:ARG:O	2.68	0.41
1:P:91:TRP:O	1:P:95:TYR:CD1	2.73	0.41
2:Q:10:SER:HB2	2:Q:18:TYR:N	2.34	0.41
2:Q:33:VAL:HG13	6:Q:501:HEC:HBB1	2.02	0.41
2:D:23:LEU:CD1	2:D:53:GLY:HA2	2.50	0.41
2:D:62:ARG:O	2:D:65:ALA:HB3	2.20	0.41
1:P:28:LEU:O	1:P:29:VAL:C	2.56	0.41
3:E:63:LEU:CD1	3:E:65:VAL:HG23	2.50	0.41
3:E:22:THR:O	3:E:26:VAL:HG22	2.20	0.41
3:E:162:SER:O	3:E:164:GLY:N	2.53	0.41
2:Q:107:ARG:HG2	2:Q:107:ARG:NH1	2.35	0.41
3:R:131:GLY:O	3:R:132:VAL:HB	2.20	0.41
1:C:162:ILE:O	1:C:163:THR:C	2.58	0.41
1:C:173:GLY:O	1:C:174:PRO:C	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:18:TRP:HE3	1:C:18:TRP:HA	1.83	0.41
1:C:48:GLY:N	1:C:111:HIS:CE1	2.88	0.41
4:C:501:HEM:CBB	4:C:501:HEM:CMB	2.97	0.41
1:P:45:TRP:CZ3	1:P:118:TYR:CE1	3.06	0.41
1:P:131:VAL:HG21	1:P:211:ILE:CG2	2.50	0.41
1:P:31:ASP:O	1:P:217:HIS:NE2	2.53	0.41
2:Q:11:PHE:CD2	2:Q:18:TYR:CE1	3.08	0.41
2:Q:24:ARG:O	2:Q:27:PHE:HB3	2.20	0.41
1:P:221:ASN:ND2	1:P:244:PHE:HE1	2.18	0.41
3:R:30:ALA:O	3:R:33:PRO:HD2	2.20	0.41
3:R:113:ARG:HB3	3:R:114:THR:H	1.67	0.41
1:C:104:PHE:CE1	1:C:139:MET:SD	3.13	0.41
1:C:131:VAL:HG21	1:C:211:ILE:CG2	2.49	0.41
1:C:187:ASP:CG	1:C:188:ASN:H	2.24	0.41
1:C:91:TRP:O	1:C:92:ALA:O	2.38	0.41
1:P:138:LEU:HD23	1:P:138:LEU:N	2.35	0.41
1:P:336:MET:O	1:P:337:PHE:C	2.58	0.41
1:P:408:LEU:O	1:P:411:LEU:HB3	2.20	0.41
1:P:63:ILE:C	1:P:63:ILE:CD1	2.85	0.41
1:P:80:VAL:HG12	1:P:81:GLU:N	2.34	0.41
2:D:25:ARG:NE	2:D:194:TYR:CE2	2.81	0.41
3:E:30:ALA:O	3:E:33:PRO:HD2	2.20	0.41
3:E:162:SER:C	3:E:164:GLY:N	2.73	0.41
3:R:163:ALA:C	3:R:165:ARG:N	2.73	0.41
1:C:136:TYR:O	1:C:137:LEU:C	2.59	0.41
1:C:139:MET:HB2	1:C:139:MET:HE2	1.87	0.41
1:C:163:THR:HG21	1:C:181:LEU:HD23	2.02	0.41
1:C:304:ILE:HD12	1:C:339:ALA:CB	2.51	0.41
1:C:58:GLN:HE21	1:C:101:ALA:CA	2.25	0.41
1:P:145:MET:HE3	1:P:198:HIS:HA	2.02	0.41
1:P:154:MET:HE3	5:P:503:SMA:H10	2.03	0.41
1:P:58:GLN:O	1:P:61:THR:HG23	2.20	0.41
3:R:36:ASN:O	3:R:38:MET:N	2.53	0.41
3:R:37:GLN:HE21	3:R:38:MET:HA	1.84	0.41
3:E:100:ASN:HB3	3:E:177:ILE:CG2	2.50	0.41
2:Q:70:THR:O	2:Q:71:ILE:O	2.38	0.41
3:E:62:GLN:CA	3:E:75:ARG:HG3	2.50	0.41
3:E:68:ARG:C	3:E:70:LYS:H	2.23	0.41
3:R:162:SER:C	3:R:164:GLY:N	2.73	0.41
1:C:278:ASP:HA	1:C:281:VAL:HG12	2.01	0.41
1:C:350:ASP:HB2	1:C:408:LEU:CD1	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:37:GLN:O	3:E:39:ASN:N	2.53	0.41
1:P:117:TYR:CE2	1:P:118:TYR:HE2	2.38	0.41
1:P:146:GLY:HA2	1:P:198:HIS:CG	2.55	0.41
1:P:46:ILE:CD1	1:P:255:ALA:HB3	2.50	0.41
2:D:134:TYR:OH	2:D:183:MET:HE1	2.19	0.41
1:C:245:TRP:HA	1:C:246:PRO:HA	1.61	0.41
1:P:183:GLY:HA3	1:P:184:PRO:HD2	1.81	0.41
3:R:68:ARG:C	3:R:70:LYS:H	2.24	0.41
1:C:301:PHE:CA	1:C:304:ILE:HG12	2.50	0.41
1:P:144:PHE:HE1	1:P:159:ALA:HA	1.85	0.41
1:P:176:ILE:O	1:P:179:TRP:HB3	2.20	0.41
1:P:267:VAL:O	1:P:271:PRO:HB3	2.19	0.41
1:P:303:ALA:O	1:P:307:ALA:HB2	2.19	0.41
1:P:367:PHE:C	1:P:367:PHE:CD2	2.93	0.41
2:Q:133:ASN:HB3	2:Q:157:THR:HG21	2.02	0.41
2:Q:218:GLU:N	2:Q:219:PRO:CD	2.82	0.41
2:Q:46:ARG:NH1	3:R:43:ASP:CA	2.83	0.41
2:D:19:ASP:O	2:D:22:GLN:N	2.53	0.41
1:P:242:LEU:CD1	1:P:242:LEU:H	2.33	0.41
1:P:32:THR:HG23	1:P:32:THR:O	2.19	0.41
3:R:162:SER:O	3:R:164:GLY:N	2.53	0.41
2:Q:229:LEU:O	2:Q:230:VAL:C	2.59	0.41
1:C:135:ILE:HG12	1:C:208:LEU:CD2	2.45	0.41
1:C:25:ILE:HD13	1:C:26:VAL:N	2.36	0.41
1:C:64:VAL:HG23	1:C:65:LEU:N	2.36	0.41
1:P:135:ILE:HG12	1:P:208:LEU:CD2	2.43	0.41
1:P:122:LYS:HD3	1:P:350:ASP:OD2	2.21	0.41
1:P:91:TRP:O	1:P:95:TYR:CB	2.61	0.41
2:Q:134:TYR:CE2	6:Q:501:HEC:HAA1	2.55	0.41
2:D:25:ARG:HH21	2:D:204:GLN:NE2	2.18	0.41
1:C:242:LEU:CD1	1:C:242:LEU:H	2.33	0.41
1:C:263:PHE:C	1:C:266:VAL:HG23	2.41	0.41
1:C:240:ASP:OD1	1:C:241:THR:N	2.54	0.41
2:D:111:SER:HB2	2:D:122:PHE:C	2.40	0.41
1:C:187:ASP:O	1:C:190:THR:N	2.53	0.41
1:P:186:VAL:O	1:P:187:ASP:HB2	2.21	0.41
1:P:138:LEU:C	1:P:205:ILE:HD11	2.40	0.41
1:P:157:TRP:CE2	1:P:288:THR:CG2	3.04	0.41
1:P:305:LEU:CD1	1:P:332:GLY:HA3	2.50	0.41
2:Q:138:PHE:CB	2:Q:185:PRO:HG3	2.51	0.41
2:Q:18:TYR:CG	2:Q:23:LEU:HD11	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:27:PHE:CE2	2:Q:48:LEU:HD22	2.56	0.41
2:D:134:TYR:CZ	2:D:183:MET:HE1	2.56	0.41
2:D:205:MET:HE3	2:D:205:MET:HA	2.01	0.41
2:D:26:GLY:HA3	2:D:212:PHE:HB2	2.02	0.41
2:D:229:LEU:O	2:D:230:VAL:C	2.58	0.41
3:R:161:ASP:OD1	3:R:165:ARG:N	2.54	0.41
3:R:101:ALA:C	3:R:103:LYS:H	2.24	0.41
1:C:144:PHE:HE1	1:C:159:ALA:HA	1.85	0.41
1:C:200:LEU:O	1:C:201:LEU:C	2.59	0.41
1:C:361:PRO:O	1:C:364:ARG:N	2.53	0.41
1:C:387:TYR:CD2	1:C:387:TYR:C	2.94	0.41
1:P:121:TYR:CG	1:P:122:LYS:N	2.88	0.41
1:P:303:ALA:HA	1:P:306:ARG:CG	2.50	0.41
1:P:48:GLY:N	1:P:111:HIS:CE1	2.89	0.41
2:Q:21:ALA:O	2:Q:22:GLN:C	2.59	0.41
1:C:193:ARG:HH11	1:C:193:ARG:CB	2.33	0.41
1:C:302:TYR:HD2	1:C:303:ALA:N	2.18	0.41
1:C:366:TRP:CE3	1:C:407:ILE:HG13	2.56	0.41
1:C:407:ILE:O	1:C:407:ILE:HD13	2.21	0.41
1:C:70:THR:HA	1:C:71:PRO:HD3	1.86	0.41
1:P:371:VAL:O	1:P:374:PHE:HB3	2.20	0.41
1:P:380:VAL:C	1:P:382:ALA:N	2.73	0.41
3:E:163:ALA:C	3:E:165:ARG:N	2.74	0.41
2:D:27:PHE:CD2	2:D:48:LEU:HD22	2.56	0.41
2:D:127:GLY:C	2:D:129:GLU:N	2.74	0.41
2:D:31:ASN:O	2:D:31:ASN:ND2	2.49	0.41
2:D:241:MET:HB3	3:E:19:THR:HB	2.03	0.41
2:D:230:VAL:O	2:D:234:MET:CG	2.69	0.41
2:D:107:ARG:HG2	2:D:107:ARG:NH1	2.34	0.41
1:P:125:ARG:HH21	1:P:125:ARG:HG2	1.86	0.41
3:R:89:PRO:O	3:R:90:LEU:C	2.59	0.41
1:C:117:TYR:CE2	1:C:118:TYR:HE2	2.39	0.41
1:C:143:ALA:O	1:C:146:GLY:N	2.54	0.41
1:C:331:PHE:CD2	1:C:331:PHE:O	2.74	0.41
1:C:91:TRP:O	1:C:95:TYR:CB	2.63	0.41
1:P:166:PHE:C	1:P:168:ALA:H	2.25	0.41
1:P:43:TRP:C	1:P:45:TRP:H	2.24	0.41
3:R:37:GLN:NE2	3:R:38:MET:N	2.64	0.41
2:D:154:TYR:CD2	2:D:155:ASN:N	2.89	0.41
3:R:63:LEU:HD12	3:R:74:ILE:HD12	2.01	0.40
1:C:190:THR:HG23	1:C:191:LEU:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:338:GLY:O	1:C:339:ALA:C	2.60	0.40
1:C:367:PHE:C	1:C:367:PHE:CD2	2.93	0.40
2:D:105:LYS:HB2	2:D:105:LYS:HE3	1.81	0.40
1:P:105:PHE:HD2	1:P:109:TYR:HE1	1.69	0.40
1:P:296:TRP:CD2	1:P:297:TYR:N	2.89	0.40
1:P:55:LEU:HB2	1:P:104:PHE:HE2	1.85	0.40
2:Q:30:TYR:CD1	2:Q:34:CYS:CB	2.99	0.40
3:E:161:ASP:OD1	3:E:165:ARG:N	2.53	0.40
1:C:144:PHE:CD1	1:C:162:ILE:CD1	3.03	0.40
1:C:216:PHE:C	1:C:216:PHE:CD1	2.94	0.40
1:C:23:LEU:HB2	1:P:214:TRP:CE3	2.55	0.40
1:C:302:TYR:CD2	1:C:306:ARG:HG2	2.55	0.40
1:C:300:PRO:C	1:C:377:LEU:HD12	2.42	0.40
1:C:363:PHE:HB2	1:C:411:LEU:HD11	2.02	0.40
1:P:162:ILE:O	1:P:163:THR:C	2.58	0.40
1:P:182:GLY:CA	1:P:193:ARG:HH21	2.28	0.40
1:P:235:ALA:O	1:P:236:ASP:OD1	2.40	0.40
1:P:297:TYR:C	1:P:298:PHE:CD1	2.86	0.40
1:P:296:TRP:C	1:P:298:PHE:H	2.25	0.40
1:P:341:ALA:O	1:P:342:VAL:C	2.59	0.40
1:P:41:LEU:HA	1:P:41:LEU:HD23	1.77	0.40
2:Q:10:SER:C	2:Q:17:LYS:CA	2.90	0.40
2:Q:64:TYR:CD1	2:Q:64:TYR:C	2.93	0.40
3:E:101:ALA:C	3:E:103:LYS:H	2.25	0.40
3:E:113:ARG:HB3	3:E:114:THR:H	1.68	0.40
2:D:34:CYS:C	2:D:36:ALA:N	2.74	0.40
2:Q:72:ILE:CG1	2:Q:73:ASP:N	2.79	0.40
3:R:157:GLY:O	3:R:158:SER:C	2.58	0.40
2:Q:241:MET:HB3	3:R:19:THR:HB	2.04	0.40
3:R:118:PHE:O	3:R:119:ASP:CB	2.69	0.40
1:C:46:ILE:CD1	1:C:255:ALA:HB3	2.52	0.40
1:C:47:TRP:CE3	1:C:50:VAL:HB	2.57	0.40
1:C:58:GLN:O	1:C:61:THR:HG23	2.22	0.40
1:C:268:ALA:O	2:D:224:ARG:HD3	2.21	0.40
1:P:51:LEU:CD1	1:P:108:VAL:HA	2.37	0.40
1:P:128:THR:OG1	1:P:129:TRP:N	2.54	0.40
1:P:205:ILE:O	1:P:206:ALA:C	2.60	0.40
3:E:166:ILE:HB	3:E:174:ASN:HA	2.03	0.40
2:D:10:SER:HB2	2:D:17:LYS:C	2.42	0.40
2:D:23:LEU:C	2:D:54:PRO:HG3	2.42	0.40
2:Q:241:MET:HE2	3:R:22:THR:HG21	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:104:PHE:HE1	1:C:139:MET:SD	2.44	0.40
1:C:203:PHE:O	1:C:204:VAL:C	2.58	0.40
1:C:45:TRP:NE1	1:C:222:ASN:CA	2.82	0.40
1:C:270:MET:N	1:C:271:PRO:CD	2.84	0.40
1:P:73:VAL:HG13	1:P:151:TRP:CD1	2.57	0.40
1:P:191:LEU:O	1:P:194:PHE:HB2	2.20	0.40
1:P:135:ILE:HD11	1:P:209:VAL:N	2.37	0.40
1:P:40:ASN:O	1:P:41:LEU:C	2.59	0.40
2:Q:213:LEU:O	2:Q:216:ALA:HB3	2.21	0.40
3:E:91:GLY:O	3:E:92:ALA:CB	2.69	0.40
2:D:11:PHE:CD2	2:D:18:TYR:CE1	3.09	0.40
2:D:238:LEU:O	2:D:239:SER:C	2.60	0.40
3:R:100:ASN:HB3	3:R:177:ILE:CG2	2.52	0.40
1:C:176:ILE:CG2	1:C:177:GLN:N	2.84	0.40
1:P:173:GLY:O	1:P:174:PRO:C	2.58	0.40
1:P:193:ARG:CB	1:P:193:ARG:HH11	2.35	0.40
1:P:234:LYS:HB2	1:P:235:ALA:H	1.64	0.40
1:P:261:LEU:C	1:P:261:LEU:HD23	2.42	0.40
1:P:331:PHE:CD2	1:P:331:PHE:O	2.75	0.40
1:C:72:HIS:CD2	1:P:75:LEU:HD12	2.57	0.40
2:Q:131:ILE:HG21	2:Q:213:LEU:HD12	2.03	0.40
3:R:37:GLN:O	3:R:39:ASN:N	2.54	0.40
3:E:166:ILE:CD1	3:E:171:ALA:HB3	2.52	0.40
2:D:100:LEU:N	2:D:100:LEU:HD22	2.35	0.40
2:D:64:TYR:CD1	2:D:64:TYR:C	2.93	0.40
3:E:23:GLY:O	3:E:24:VAL:C	2.60	0.40
1:C:284:ASN:OD1	1:C:286:LEU:HD13	2.21	0.40
2:D:40:MET:HB3	2:D:43:VAL:HG21	2.03	0.40
3:R:21:ALA:O	3:R:24:VAL:HB	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	425/437 (97%)	214 (50%)	138 (32%)	73 (17%)	0 2
1	P	425/437 (97%)	209 (49%)	145 (34%)	71 (17%)	0 3
2	D	250/258 (97%)	123 (49%)	63 (25%)	64 (26%)	0 1
2	Q	250/258 (97%)	122 (49%)	61 (24%)	67 (27%)	0 0
3	E	179/191 (94%)	104 (58%)	37 (21%)	38 (21%)	0 1
3	R	179/191 (94%)	106 (59%)	34 (19%)	39 (22%)	0 1
All	All	1708/1772 (96%)	878 (51%)	478 (28%)	352 (21%)	0 1

All (352) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	7	ASP
1	C	10	GLU
1	C	12	LYS
1	C	23	LEU
1	C	24	PRO
1	C	30	TYR
1	C	72	HIS
1	C	76	ALA
1	C	85	ARG
1	C	90	GLY
1	C	92	ALA
1	C	186	VAL
1	C	221	ASN
1	C	229	VAL
1	C	233	SER
1	C	238	GLU
1	C	241	THR
1	C	277	PRO
1	C	282	GLN
1	C	294	PRO
1	C	310	ALA
1	C	312	VAL
1	C	313	TRP
1	C	325	ILE
1	C	346	ALA
1	C	385	THR
1	C	418	GLU
1	C	419	PRO
1	C	421	PRO
1	C	424	ILE

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Mol	Chain	Res	Type
2	D	4	VAL
2	D	5	PRO
2	D	6	ASP
2	D	9	PHE
2	D	14	ILE
2	D	17	LYS
2	D	18	TYR
2	D	49	ALA
2	D	51	ASP
2	D	52	GLY
2	D	68	LEU
2	D	69	ASP
2	D	71	ILE
2	D	72	ILE
2	D	81	ASP
2	D	83	LYS
2	D	92	VAL
2	D	101	SER
2	D	108	ALA
2	D	114	ALA
2	D	120	GLN
2	D	121	LEU
2	D	140	GLU
2	D	160	ILE
2	D	164	PRO
2	D	166	THR
2	D	168	LYS
2	D	178	GLY
2	D	189	ASP
2	D	219	PRO
3	E	40	ALA
3	E	42	ALA
3	E	46	ALA
3	E	54	VAL
3	E	55	SER
3	E	56	ALA
3	E	62	GLN
3	E	103	LYS
3	E	113	ARG
3	E	114	THR
3	E	115	LEU
3	E	116	PRO

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Mol	Chain	Res	Type
3	E	117	ALA
3	E	118	PHE
3	E	125	GLU
3	E	168	LYS
1	P	7	ASP
1	P	10	GLU
1	P	12	LYS
1	P	23	LEU
1	P	24	PRO
1	P	30	TYR
1	P	72	HIS
1	P	76	ALA
1	P	85	ARG
1	P	90	GLY
1	P	92	ALA
1	P	221	ASN
1	P	229	VAL
1	P	230	ARG
1	P	233	SER
1	P	238	GLU
1	P	241	THR
1	P	277	PRO
1	P	282	GLN
1	P	294	PRO
1	P	310	ALA
1	P	312	VAL
1	P	313	TRP
1	P	325	ILE
1	P	346	ALA
1	P	385	THR
1	P	418	GLU
1	P	419	PRO
1	P	421	PRO
1	P	424	ILE
2	Q	4	VAL
2	Q	5	PRO
2	Q	6	ASP
2	Q	9	PHE
2	Q	14	ILE
2	Q	17	LYS
2	Q	18	TYR
2	Q	46	ARG

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Mol	Chain	Res	Type
2	Q	49	ALA
2	Q	51	ASP
2	Q	52	GLY
2	Q	68	LEU
2	Q	69	ASP
2	Q	71	ILE
2	Q	72	ILE
2	Q	81	ASP
2	Q	83	LYS
2	Q	92	VAL
2	Q	101	SER
2	Q	108	ALA
2	Q	114	ALA
2	Q	120	GLN
2	Q	121	LEU
2	Q	140	GLU
2	Q	160	ILE
2	Q	164	PRO
2	Q	166	THR
2	Q	168	LYS
2	Q	189	ASP
2	Q	219	PRO
3	R	40	ALA
3	R	42	ALA
3	R	46	ALA
3	R	55	SER
3	R	56	ALA
3	R	62	GLN
3	R	103	LYS
3	R	113	ARG
3	R	114	THR
3	R	115	LEU
3	R	116	PRO
3	R	117	ALA
3	R	125	GLU
3	R	168	LYS
1	C	11	PRO
1	C	41	LEU
1	C	88	ASN
1	C	119	GLY
1	C	122	LYS
1	C	156	PHE

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Mol	Chain	Res	Type
1	C	173	GLY
1	C	228	GLU
1	C	230	ARG
1	C	235	ALA
1	C	326	VAL
1	C	348	TRP
1	C	381	GLY
1	C	420	ILE
1	C	422	ALA
2	D	34	CYS
2	D	46	ARG
2	D	77	GLY
2	D	116	SER
2	D	146	PRO
2	D	173	VAL
2	D	222	VAL
3	E	38	MET
3	E	58	GLU
3	E	94	ARG
3	E	100	ASN
3	E	104	PRO
3	E	120	GLY
3	E	132	VAL
3	E	163	ALA
3	E	184	ASP
3	E	185	GLU
1	P	11	PRO
1	P	41	LEU
1	P	88	ASN
1	P	119	GLY
1	P	122	LYS
1	P	156	PHE
1	P	173	GLY
1	P	186	VAL
1	P	228	GLU
1	P	235	ALA
1	P	326	VAL
1	P	348	TRP
1	P	381	GLY
1	P	420	ILE
1	P	422	ALA
2	Q	34	CYS

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Mol	Chain	Res	Type
2	Q	77	GLY
2	Q	79	GLU
2	Q	116	SER
2	Q	146	PRO
2	Q	173	VAL
2	Q	178	GLY
2	Q	222	VAL
3	R	38	MET
3	R	41	SER
3	R	54	VAL
3	R	58	GLU
3	R	94	ARG
3	R	100	ASN
3	R	104	PRO
3	R	118	PHE
3	R	119	ASP
3	R	120	GLY
3	R	132	VAL
3	R	163	ALA
3	R	184	ASP
3	R	185	GLU
1	C	13	THR
1	C	19	LEU
1	C	177	GLN
1	C	236	ASP
1	C	237	ALA
1	C	309	ALA
1	C	394	LEU
2	D	7	HIS
2	D	20	GLN
2	D	50	ASP
2	D	65	ALA
2	D	79	GLU
2	D	155	ASN
2	D	156	LYS
2	D	176	THR
2	D	180	TRP
3	E	41	SER
3	E	105	GLY
3	E	107	GLU
3	E	170	PRO
1	P	19	LEU

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Mol	Chain	Res	Type
1	P	91	TRP
1	P	177	GLN
1	P	236	ASP
1	P	237	ALA
1	P	309	ALA
1	P	356	SER
1	P	394	LEU
2	Q	7	HIS
2	Q	20	GLN
2	Q	50	ASP
2	Q	65	ALA
2	Q	155	ASN
2	Q	156	LYS
2	Q	176	THR
2	Q	180	TRP
3	R	69	GLY
3	R	107	GLU
3	R	170	PRO
1	C	44	TRP
1	C	143	ALA
1	C	297	TYR
1	C	329	LYS
1	C	353	LYS
1	C	356	SER
2	D	82	ARG
2	D	94	ASP
2	D	123	LYS
2	D	174	LYS
2	D	179	SER
2	D	185	PRO
3	E	37	GLN
3	E	69	GLY
3	E	122	ASN
3	E	158	SER
1	P	13	THR
1	P	28	LEU
1	P	29	VAL
1	P	93	MET
1	P	143	ALA
1	P	297	TYR
1	P	329	LYS
1	P	353	LYS

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Mol	Chain	Res	Type
2	Q	82	ARG
2	Q	94	ASP
2	Q	123	LYS
2	Q	148	GLY
2	Q	174	LYS
2	Q	179	SER
2	Q	185	PRO
3	R	37	GLN
3	R	105	GLY
3	R	122	ASN
1	C	28	LEU
1	C	93	MET
1	C	160	THR
1	C	361	PRO
1	C	365	MET
1	C	423	SER
2	D	76	SER
2	D	119	ASN
2	D	148	GLY
2	D	161	GLY
2	D	186	PRO
2	D	221	LEU
3	E	44	VAL
1	P	153	GLN
1	P	171	GLY
1	P	361	PRO
1	P	365	MET
2	Q	21	ALA
2	Q	66	ALA
2	Q	76	SER
2	Q	119	ASN
2	Q	161	GLY
2	Q	190	ASP
2	Q	191	GLN
2	Q	221	LEU
3	R	44	VAL
3	R	131	GLY
3	R	158	SER
1	C	91	TRP
1	C	188	ASN
1	C	234	LYS
1	C	408	LEU

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Mol	Chain	Res	Type
2	D	21	ALA
2	D	190	ASP
2	D	191	GLN
3	E	131	GLY
3	E	171	ALA
1	P	18	TRP
1	P	352	SER
1	P	408	LEU
2	Q	22	GLN
2	Q	67	GLY
2	Q	186	PRO
2	Q	243	TYR
3	R	171	ALA
1	C	347	PRO
1	P	347	PRO
1	C	29	VAL
1	C	171	GLY
2	D	67	GLY
2	D	255	GLY
1	P	26	VAL
2	Q	255	GLY
1	C	26	VAL
2	Q	199	PRO
1	C	184	PRO
2	D	199	PRO
1	P	184	PRO
3	R	183	VAL
3	E	183	VAL

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	C	304/360 (84%)	220 (72%)	84 (28%)	0 3
1	P	304/360 (84%)	218 (72%)	86 (28%)	0 3
2	D	182/206 (88%)	153 (84%)	29 (16%)	3 18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	Q	182/206 (88%)	154 (85%)	28 (15%)	3 20
3	E	142/149 (95%)	121 (85%)	21 (15%)	4 22
3	R	142/149 (95%)	119 (84%)	23 (16%)	3 17
All	All	1256/1430 (88%)	985 (78%)	271 (22%)	1 7

All (271) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	18	TRP
1	C	24	PRO
1	C	25	ILE
1	C	31	ASP
1	C	32	THR
1	C	42	ASN
1	C	43	TRP
1	C	44	TRP
1	C	45	TRP
1	C	47	TRP
1	C	50	VAL
1	C	60	VAL
1	C	61	THR
1	C	63	ILE
1	C	65	LEU
1	C	70	THR
1	C	77	PHE
1	C	81	GLU
1	C	83	ILE
1	C	88	ASN
1	C	94	ARG
1	C	103	LEU
1	C	104	PHE
1	C	105	PHE
1	C	116	LEU
1	C	124	PRO
1	C	128	THR
1	C	138	LEU
1	C	140	MET
1	C	144	PHE
1	C	175	SER
1	C	177	GLN
1	C	186	VAL

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Mol	Chain	Res	Type
1	C	193	ARG
1	C	197	LEU
1	C	199	TYR
1	C	205	ILE
1	C	209	VAL
1	C	211	ILE
1	C	214	TRP
1	C	217	HIS
1	C	221	ASN
1	C	229	VAL
1	C	231	ARG
1	C	232	THR
1	C	236	ASP
1	C	240	ASP
1	C	246	PRO
1	C	249	VAL
1	C	253	LEU
1	C	256	LEU
1	C	259	VAL
1	C	260	LEU
1	C	266	VAL
1	C	267	VAL
1	C	278	ASP
1	C	280	TYR
1	C	286	LEU
1	C	288	THR
1	C	292	ILE
1	C	295	GLU
1	C	297	TYR
1	C	302	TYR
1	C	304	ILE
1	C	305	LEU
1	C	306	ARG
1	C	331	PHE
1	C	333	VAL
1	C	334	ILE
1	C	345	LEU
1	C	348	TRP
1	C	351	THR
1	C	361	PRO
1	C	369	PHE
1	C	370	LEU

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Mol	Chain	Res	Type
1	C	377	LEU
1	C	387	TYR
1	C	401	PHE
1	C	405	LEU
1	C	407	ILE
1	C	408	LEU
1	C	411	LEU
1	C	417	PRO
1	C	418	GLU
2	D	9	PHE
2	D	15	PHE
2	D	24	ARG
2	D	27	PHE
2	D	31	ASN
2	D	42	PHE
2	D	46	ARG
2	D	57	ASP
2	D	70	THR
2	D	74	LYS
2	D	80	ARG
2	D	99	ASP
2	D	141	ASN
2	D	144	CYS
2	D	177	HIS
2	D	185	PRO
2	D	187	LEU
2	D	194	TYR
2	D	201	THR
2	D	204	GLN
2	D	205	MET
2	D	209	VAL
2	D	214	MET
2	D	215	TRP
2	D	219	PRO
2	D	224	ARG
2	D	229	LEU
2	D	232	MET
2	D	250	TRP
3	E	12	ARG
3	E	17	HIS
3	E	25	VAL
3	E	26	VAL

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Mol	Chain	Res	Type
3	E	37	GLN
3	E	53	ASP
3	E	63	LEU
3	E	73	PHE
3	E	79	GLU
3	E	100	ASN
3	E	104	PRO
3	E	109	THR
3	E	116	PRO
3	E	121	THR
3	E	123	THR
3	E	127	LEU
3	E	160	TYR
3	E	170	PRO
3	E	173	ARG
3	E	186	THR
3	E	187	THR
1	P	18	TRP
1	P	24	PRO
1	P	25	ILE
1	P	31	ASP
1	P	32	THR
1	P	42	ASN
1	P	43	TRP
1	P	44	TRP
1	P	45	TRP
1	P	47	TRP
1	P	50	VAL
1	P	60	VAL
1	P	61	THR
1	P	63	ILE
1	P	65	LEU
1	P	70	THR
1	P	77	PHE
1	P	81	GLU
1	P	83	ILE
1	P	88	ASN
1	P	94	ARG
1	P	103	LEU
1	P	104	PHE
1	P	105	PHE
1	P	116	LEU

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Mol	Chain	Res	Type
1	P	124	PRO
1	P	128	THR
1	P	138	LEU
1	P	140	MET
1	P	144	PHE
1	P	175	SER
1	P	177	GLN
1	P	186	VAL
1	P	193	ARG
1	P	197	LEU
1	P	199	TYR
1	P	205	ILE
1	P	209	VAL
1	P	211	ILE
1	P	214	TRP
1	P	217	HIS
1	P	221	ASN
1	P	229	VAL
1	P	231	ARG
1	P	232	THR
1	P	236	ASP
1	P	240	ASP
1	P	246	PRO
1	P	249	VAL
1	P	253	LEU
1	P	256	LEU
1	P	259	VAL
1	P	260	LEU
1	P	266	VAL
1	P	267	VAL
1	P	278	ASP
1	P	280	TYR
1	P	286	LEU
1	P	288	THR
1	P	292	ILE
1	P	295	GLU
1	P	297	TYR
1	P	302	TYR
1	P	304	ILE
1	P	305	LEU
1	P	306	ARG
1	P	331	PHE

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Mol	Chain	Res	Type
1	P	333	VAL
1	P	334	ILE
1	P	345	LEU
1	P	348	TRP
1	P	351	THR
1	P	361	PRO
1	P	369	PHE
1	P	370	LEU
1	P	375	VAL
1	P	377	LEU
1	P	387	TYR
1	P	388	PRO
1	P	401	PHE
1	P	405	LEU
1	P	407	ILE
1	P	408	LEU
1	P	411	LEU
1	P	417	PRO
1	P	418	GLU
2	Q	9	PHE
2	Q	15	PHE
2	Q	24	ARG
2	Q	27	PHE
2	Q	31	ASN
2	Q	42	PHE
2	Q	46	ARG
2	Q	70	THR
2	Q	74	LYS
2	Q	80	ARG
2	Q	99	ASP
2	Q	141	ASN
2	Q	144	CYS
2	Q	177	HIS
2	Q	185	PRO
2	Q	187	LEU
2	Q	194	TYR
2	Q	201	THR
2	Q	204	GLN
2	Q	205	MET
2	Q	209	VAL
2	Q	214	MET
2	Q	215	TRP

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Mol	Chain	Res	Type
2	Q	219	PRO
2	Q	224	ARG
2	Q	229	LEU
2	Q	232	MET
2	Q	250	TRP
3	R	12	ARG
3	R	17	HIS
3	R	25	VAL
3	R	26	VAL
3	R	27	THR
3	R	37	GLN
3	R	53	ASP
3	R	63	LEU
3	R	73	PHE
3	R	79	GLU
3	R	100	ASN
3	R	104	PRO
3	R	109	THR
3	R	116	PRO
3	R	118	PHE
3	R	121	THR
3	R	123	THR
3	R	127	LEU
3	R	160	TYR
3	R	170	PRO
3	R	173	ARG
3	R	186	THR
3	R	187	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	58	GLN
1	C	68	HIS
1	C	99	ASN
1	C	177	GLN
1	C	276	HIS
1	C	284	ASN
2	D	28	GLN
2	D	191	GLN
2	D	204	GLN
3	E	36	ASN

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Mol	Chain	Res	Type
3	E	37	GLN
3	E	62	GLN
3	E	100	ASN
1	P	58	GLN
1	P	68	HIS
1	P	99	ASN
1	P	177	GLN
1	P	276	HIS
1	P	284	ASN
2	Q	28	GLN
2	Q	159	GLN
2	Q	191	GLN
2	Q	204	GLN
3	R	36	ASN
3	R	37	GLN
3	R	62	GLN
3	R	100	ASN

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

10 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	$\#\|Z\|>2$
4	HEM	C	501	1	30,50,50	3.06	12 (40%)	24,82,82	3.64	12 (50%)
4	HEM	C	502	1	30,50,50	3.10	13 (43%)	24,82,82	2.96	7 (29%)
5	SMA	C	503	-	35,38,38	1.83	7 (20%)	40,52,52	1.83	4 (10%)
6	HEC	D	501	2	24,50,50	1.58	2 (8%)	19,82,82	4.43	8 (42%)
7	FES	E	501	3	0,4,4	0.00	-	0,4,4	0.00	-
4	HEM	P	501	1	30,50,50	3.04	12 (40%)	24,82,82	3.47	13 (54%)
4	HEM	P	502	1	30,50,50	3.26	14 (46%)	24,82,82	3.03	8 (33%)
5	SMA	P	503	-	35,38,38	1.70	5 (14%)	40,52,52	1.83	5 (12%)
6	HEC	Q	501	2	24,50,50	1.65	2 (8%)	19,82,82	4.55	9 (47%)
7	FES	R	501	3	0,4,4	0.00	-	0,4,4	0.00	-

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
4	HEM	C	501	1	-	0/10/54/54	0/0/8/8
4	HEM	C	502	1	-	0/10/54/54	0/0/8/8
5	SMA	C	503	-	-	0/33/34/34	0/2/2/2
6	HEC	D	501	2	-	1/6/54/54	0/0/8/8
7	FES	E	501	3	-	0/0/4/4	0/1/1/1
4	HEM	P	501	1	-	0/10/54/54	0/0/8/8
4	HEM	P	502	1	-	0/10/54/54	0/0/8/8
5	SMA	P	503	-	-	0/33/34/34	0/2/2/2
6	HEC	Q	501	2	-	1/6/54/54	0/0/8/8
7	FES	R	501	3	-	0/0/4/4	0/1/1/1

All (67) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	P	502	HEM	C3B-CAB	-8.31	1.35	1.51
4	C	501	HEM	C3C-CAC	-7.75	1.36	1.51
4	C	502	HEM	C3B-CAB	-7.52	1.37	1.51
4	P	501	HEM	C3B-CAB	-7.21	1.37	1.51
4	C	501	HEM	C2D-C3D	-7.15	1.33	1.54
4	P	502	HEM	C3B-C4B	-7.01	1.45	1.51
4	C	501	HEM	C3B-CAB	-6.79	1.38	1.51
4	P	501	HEM	C3C-CAC	-6.76	1.38	1.51
4	P	501	HEM	C2D-C3D	-6.62	1.34	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	P	502	HEM	C3C-CAC	-6.57	1.39	1.51
4	C	502	HEM	C3C-CAC	-6.22	1.39	1.51
6	Q	501	HEC	C3B-C2B	-5.55	1.35	1.40
4	C	502	HEM	C3B-C4B	-5.47	1.47	1.51
4	P	502	HEM	C3D-C4D	-5.25	1.44	1.51
6	D	501	HEC	C3B-C2B	-5.24	1.35	1.40
4	P	501	HEM	C3D-C4D	-5.11	1.45	1.51
4	P	502	HEM	C2C-C1C	-4.83	1.43	1.52
4	C	502	HEM	C3D-C4D	-4.77	1.45	1.51
4	C	502	HEM	C2C-C1C	-4.61	1.43	1.52
4	C	502	HEM	C2D-C3D	-4.07	1.42	1.54
4	P	502	HEM	C2D-C3D	-4.02	1.42	1.54
4	C	501	HEM	FE-NC	-3.83	1.80	1.95
4	P	501	HEM	C2C-C1C	-3.65	1.45	1.52
4	C	501	HEM	C3D-C4D	-3.63	1.46	1.51
6	Q	501	HEC	C3C-C2C	-3.38	1.37	1.40
6	D	501	HEC	C3C-C2C	-3.12	1.37	1.40
4	C	501	HEM	FE-NB	-2.97	1.81	1.97
4	P	501	HEM	FE-NB	-2.79	1.82	1.97
4	C	501	HEM	C2C-C1C	-2.44	1.48	1.52
4	P	501	HEM	C4A-CHB	-2.42	1.33	1.39
4	P	502	HEM	C2B-C1B	-2.39	1.44	1.51
4	C	502	HEM	C2B-C1B	-2.14	1.44	1.51
4	C	502	HEM	C4A-CHB	-2.06	1.34	1.39
4	P	502	HEM	C4A-CHB	-2.02	1.34	1.39
4	P	502	HEM	C1C-NC	2.01	1.38	1.36
4	P	502	HEM	CHD-C4C	2.15	1.41	1.36
5	C	503	SMA	C4A-C8A	2.29	1.44	1.41
4	C	501	HEM	C1C-NC	2.33	1.38	1.36
5	P	503	SMA	C7-C8	2.36	1.43	1.40
5	C	503	SMA	O7-C7	2.36	1.40	1.37
4	C	501	HEM	CAA-C2A	2.37	1.56	1.52
4	P	501	HEM	CHD-C4C	2.51	1.42	1.36
4	P	501	HEM	C4C-NC	2.54	1.39	1.36
4	P	502	HEM	C4C-NC	2.60	1.39	1.36
4	C	502	HEM	CHD-C4C	2.65	1.42	1.36
4	P	501	HEM	CAA-C2A	2.91	1.57	1.52
4	C	501	HEM	C4C-NC	2.97	1.39	1.36
5	P	503	SMA	C4-C3	3.01	1.50	1.41
5	C	503	SMA	C7-C8	3.39	1.44	1.40
5	C	503	SMA	C4-C3	3.40	1.51	1.41
4	C	502	HEM	CBB-CAB	3.43	1.49	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	P	503	SMA	C6-C7	3.45	1.45	1.38
4	P	502	HEM	CBB-CAB	3.58	1.50	1.29
5	C	503	SMA	C6-C7	3.86	1.46	1.38
4	C	501	HEM	CBC-CAC	3.89	1.51	1.29
4	C	502	HEM	C4C-NC	4.09	1.41	1.36
4	P	501	HEM	CBC-CAC	4.19	1.53	1.29
4	C	502	HEM	CBC-CAC	4.33	1.54	1.29
4	P	502	HEM	CAD-C3D	4.36	1.62	1.54
4	C	502	HEM	CAD-C3D	4.44	1.63	1.54
4	P	502	HEM	CBC-CAC	4.46	1.55	1.29
5	P	503	SMA	O1-C2	4.57	1.40	1.35
5	C	503	SMA	O1-C2	4.67	1.40	1.35
4	P	501	HEM	CBB-CAB	4.89	1.57	1.29
4	C	501	HEM	CBB-CAB	5.25	1.59	1.29
5	P	503	SMA	C4-C4A	5.44	1.48	1.41
5	C	503	SMA	C4-C4A	5.61	1.49	1.41

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	Q	501	HEC	CBC-CAC-C3C	-8.44	108.61	127.35
6	D	501	HEC	CBC-CAC-C3C	-7.97	109.64	127.35
6	Q	501	HEC	CBB-CAB-C3B	-7.00	111.81	127.35
6	D	501	HEC	CBB-CAB-C3B	-6.94	111.93	127.35
6	Q	501	HEC	CAA-C2A-C1A	-6.93	119.49	127.01
6	D	501	HEC	CAA-C2A-C1A	-6.87	119.54	127.01
5	P	503	SMA	C9-C10-C11	-6.68	106.88	114.75
5	C	503	SMA	C9-C10-C11	-6.49	107.10	114.75
4	P	502	HEM	C3B-CAB-CBB	-5.11	116.62	124.46
5	C	503	SMA	C3-C4-C4A	-4.94	114.50	121.35
5	P	503	SMA	C3-C4-C4A	-4.67	114.88	121.35
4	C	502	HEM	C3B-CAB-CBB	-4.52	117.52	124.46
4	C	501	HEM	CAA-C2A-C3A	-3.34	119.46	129.00
6	Q	501	HEC	CAD-C3D-C2D	-3.27	119.67	129.00
6	D	501	HEC	CAD-C3D-C2D	-3.26	119.69	129.00
4	P	501	HEM	CAA-C2A-C3A	-3.11	120.13	129.00
4	P	502	HEM	C2D-C3D-C4D	-2.69	96.93	101.50
4	P	501	HEM	C3B-CAB-CBB	-2.61	120.45	124.46
4	C	501	HEM	CHD-C1D-ND	-2.52	118.46	124.52
4	C	502	HEM	C2D-C3D-C4D	-2.42	97.40	101.50
5	C	503	SMA	C4-C4A-C5	-2.30	121.40	125.02
4	P	501	HEM	CHD-C1D-ND	-2.22	119.19	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	P	503	SMA	C4-C4A-C5	-2.08	121.74	125.02
4	C	501	HEM	C4B-CHC-C1C	-2.08	122.34	125.82
4	P	501	HEM	CMD-C2D-C3D	2.02	123.30	114.35
6	Q	501	HEC	CMB-C2B-C1B	2.05	131.76	128.36
4	C	501	HEM	CMD-C2D-C3D	2.05	123.43	114.35
6	Q	501	HEC	CMD-C2D-C1D	2.18	131.98	128.36
4	P	501	HEM	C3B-C4B-CHC	2.23	126.31	123.16
6	D	501	HEC	CMD-C2D-C1D	2.27	132.13	128.36
4	P	501	HEM	C2C-C1C-NC	2.30	114.08	110.21
5	P	503	SMA	O8-C8-C8A	2.37	124.01	119.78
4	P	502	HEM	C3C-CAC-CBC	2.38	128.11	124.46
4	C	502	HEM	CAD-C3D-C4D	2.60	121.66	112.47
4	P	502	HEM	CAD-C3D-C4D	2.70	121.99	112.47
4	P	501	HEM	CAD-C3D-C4D	3.08	123.34	112.47
4	C	501	HEM	C2C-C1C-NC	3.15	115.52	110.21
4	C	501	HEM	CAD-C3D-C4D	3.48	124.76	112.47
4	P	501	HEM	C2D-C3D-C4D	3.50	107.44	101.50
4	P	501	HEM	CMC-C2C-C3C	3.69	125.75	116.53
4	C	501	HEM	C2D-C3D-C4D	3.90	108.12	101.50
4	P	502	HEM	CMD-C2D-C3D	3.96	131.88	114.35
4	C	502	HEM	CMD-C2D-C3D	4.01	132.09	114.35
4	P	502	HEM	CMC-C2C-C3C	4.38	127.48	116.53
4	C	502	HEM	CMC-C2C-C3C	4.41	127.55	116.53
4	C	501	HEM	CMC-C2C-C3C	4.57	127.94	116.53
4	C	501	HEM	CAD-C3D-C2D	4.81	127.03	113.22
4	P	501	HEM	CMB-C2B-C3B	5.01	129.04	116.53
4	C	501	HEM	CMB-C2B-C3B	5.34	129.87	116.53
4	C	502	HEM	CMB-C2B-C3B	5.40	130.00	116.53
4	P	502	HEM	CMB-C2B-C3B	5.42	130.05	116.53
4	P	501	HEM	CAD-C3D-C2D	5.50	129.02	113.22
5	C	503	SMA	C9-C2-C3	5.62	127.97	120.56
5	P	503	SMA	C9-C2-C3	5.67	128.04	120.56
6	Q	501	HEC	CBA-CAA-C2A	5.71	122.76	112.53
6	D	501	HEC	CBA-CAA-C2A	5.93	123.15	112.53
6	D	501	HEC	CBD-CAD-C3D	7.56	126.08	112.53
6	Q	501	HEC	CBD-CAD-C3D	7.57	126.11	112.53
4	P	501	HEM	CAA-C2A-C1A	8.62	136.37	127.01
4	P	501	HEM	CBA-CAA-C2A	8.73	128.18	112.53
4	C	501	HEM	CAA-C2A-C1A	8.74	136.50	127.01
4	C	501	HEM	CBA-CAA-C2A	9.27	129.14	112.53
4	C	502	HEM	CAD-C3D-C2D	9.49	140.51	113.22
4	P	502	HEM	CAD-C3D-C2D	9.52	140.59	113.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	D	501	HEC	CAD-C3D-C4D	9.68	137.52	127.01
6	Q	501	HEC	CAD-C3D-C4D	10.33	138.22	127.01

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	Q	501	HEC	C2D-C3D-CAD-CBD
6	D	501	HEC	C2D-C3D-CAD-CBD

There are no ring outliers.

10 monomers are involved in 151 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	501	HEM	19	0
4	C	502	HEM	27	0
5	C	503	SMA	7	0
6	D	501	HEC	19	0
7	E	501	FES	1	0
4	P	501	HEM	21	0
4	P	502	HEM	27	0
5	P	503	SMA	8	0
6	Q	501	HEC	21	0
7	R	501	FES	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

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	C	427/437 (97%)	-0.32	10 (2%)	64	54	18, 89, 138, 180	0
1	P	427/437 (97%)	-0.32	10 (2%)	64	54	13, 78, 137, 168	0
2	D	252/258 (97%)	0.15	18 (7%)	19	15	65, 122, 173, 183	0
2	Q	252/258 (97%)	0.14	17 (6%)	21	16	33, 110, 166, 188	0
3	E	181/191 (94%)	-0.21	4 (2%)	65	55	50, 110, 154, 179	0
3	R	181/191 (94%)	-0.15	8 (4%)	38	29	50, 121, 158, 170	0
All	All	1720/1772 (97%)	-0.15	67 (3%)	43	35	13, 101, 159, 188	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	119	ASN	11.5
2	D	120	GLN	7.8
1	C	221	ASN	5.8
2	D	121	LEU	5.6
2	Q	256	HIS	5.4
2	Q	164	PRO	5.1
2	Q	5	PRO	5.0
2	D	118	MET	4.8
2	Q	7	HIS	4.7
3	E	185	GLU	4.6
3	R	123	THR	4.5
2	Q	161	GLY	4.5
2	Q	4	VAL	4.0
3	R	122	ASN	3.6
1	C	42	ASN	3.5
3	R	170	PRO	3.5
1	C	222	ASN	3.5
2	D	164	PRO	3.4
1	P	221	ASN	3.3

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Mol	Chain	Res	Type	RSRZ
1	P	273	TYR	3.2
2	D	181	ALA	3.2
1	P	362	LYS	3.1
2	Q	6	ASP	3.1
2	D	152	TYR	3.0
2	D	156	LYS	3.0
2	D	182	ARG	2.9
2	Q	198	THR	2.9
1	P	240	ASP	2.8
1	C	309	ALA	2.8
2	Q	191	GLN	2.7
3	R	115	LEU	2.6
3	R	169	GLY	2.6
2	Q	2	SER	2.5
1	C	288	THR	2.5
2	Q	199	PRO	2.5
3	E	152	PHE	2.5
1	C	31	ASP	2.5
1	C	329	LYS	2.5
2	Q	3	ASN	2.4
2	Q	196	ASP	2.4
1	P	416	LYS	2.4
3	R	121	THR	2.4
2	Q	257	LYS	2.3
1	C	289	PRO	2.3
2	D	196	ASP	2.3
1	P	8	HIS	2.3
2	D	161	GLY	2.3
2	D	180	TRP	2.2
3	E	183	VAL	2.2
2	D	195	GLU	2.2
3	E	158	SER	2.2
1	P	411	LEU	2.2
2	D	117	GLY	2.2
1	P	31	ASP	2.2
2	Q	160	ILE	2.2
1	P	386	GLU	2.1
1	P	364	ARG	2.1
2	D	184	PRO	2.1
2	Q	32	GLU	2.1
1	C	237	ALA	2.1
2	Q	195	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	138	PHE	2.0
2	D	98	PRO	2.0
3	R	125	GLU	2.0
3	R	124	GLY	2.0
2	D	135	VAL	2.0
1	C	32	THR	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
5	SMA	C	503	37/37	0.87	0.39	2.75	4,62,108,137	0
4	HEM	C	501	43/43	0.95	0.27	0.83	3,3,71,116	0
6	HEC	Q	501	43/43	0.96	0.36	0.31	39,102,139,149	0
6	HEC	D	501	43/43	0.93	0.46	0.28	74,101,126,139	0
4	HEM	P	502	43/43	0.94	0.29	0.24	11,74,128,155	0
4	HEM	P	501	43/43	0.96	0.23	0.18	3,16,68,87	0
5	SMA	P	503	37/37	0.94	0.23	-0.06	15,60,113,120	0
4	HEM	C	502	43/43	0.95	0.27	-0.14	14,67,129,139	0
7	FES	R	501	4/4	0.96	0.19	-0.50	105,113,145,197	0
7	FES	E	501	4/4	0.97	0.16	-1.07	50,70,85,98	0

6.5 Other polymers (i)

There are no such residues in this entry.