



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:35 AM GMT

PDB ID : 3PDI  
Title : Precursor bound NifEN  
Authors : Kaiser, J.T.; Hu, Y.; Wiig, J.A.; Rees, D.C.; Ribbe, M.W.  
Deposited on : 2010-10-22  
Resolution : 2.40 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

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



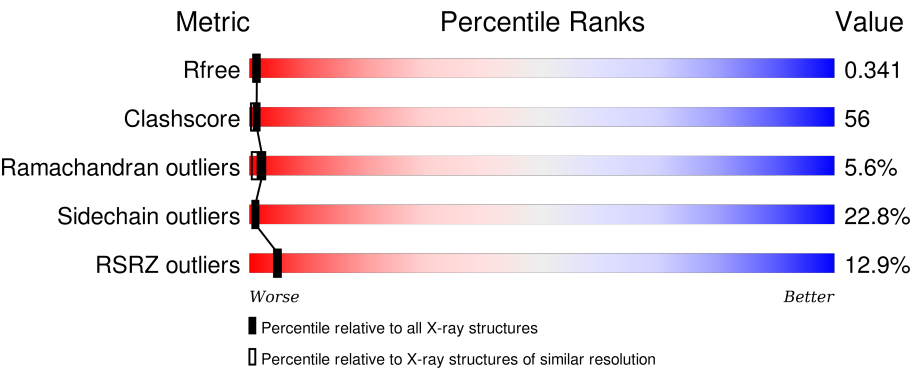
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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 <sub>free</sub>	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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  $\geq 3$ , 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	483	<div><div>13%</div><div>33%40%14%•12%</div></div>
1	C	483	<div><div>17%</div><div>30%42%15%•12%</div></div>
1	E	483	<div><div>14%</div><div>32%42%13%•12%</div></div>
1	G	483	<div><div>17%</div><div>29%44%14%•12%</div></div>
2	B	458	<div><div>6%</div><div>38%41%14%•6%</div></div>

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Mol	Chain	Length	Quality of chain
2	D	458	
2	F	458	
2	H	458	

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
3	SF4	A	501	-	-	X	-
3	SF4	C	501	-	-	X	-
3	SF4	E	501	-	-	X	-
3	SF4	G	501	-	-	X	-



## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 26112 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 Nitrogenase MoFe cofactor biosynthesis protein NifE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	427	Total	C	N	O	S	0	0	0
			3280	2064	577	618	21			
1	C	427	Total	C	N	O	S	0	0	0
			3280	2064	577	618	21			
1	E	427	Total	C	N	O	S	0	0	0
			3280	2064	577	618	21			
1	G	427	Total	C	N	O	S	0	0	0
			3280	2064	577	618	21			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	EXPRESSION TAG	UNP C1DH03
A	-6	HIS	-	EXPRESSION TAG	UNP C1DH03
A	-5	HIS	-	EXPRESSION TAG	UNP C1DH03
A	-4	HIS	-	EXPRESSION TAG	UNP C1DH03
A	-3	HIS	-	EXPRESSION TAG	UNP C1DH03
A	-2	HIS	-	EXPRESSION TAG	UNP C1DH03
A	-1	HIS	-	EXPRESSION TAG	UNP C1DH03
A	0	HIS	-	EXPRESSION TAG	UNP C1DH03
C	-7	MET	-	EXPRESSION TAG	UNP C1DH03
C	-6	HIS	-	EXPRESSION TAG	UNP C1DH03
C	-5	HIS	-	EXPRESSION TAG	UNP C1DH03
C	-4	HIS	-	EXPRESSION TAG	UNP C1DH03
C	-3	HIS	-	EXPRESSION TAG	UNP C1DH03
C	-2	HIS	-	EXPRESSION TAG	UNP C1DH03
C	-1	HIS	-	EXPRESSION TAG	UNP C1DH03
C	0	HIS	-	EXPRESSION TAG	UNP C1DH03
E	-7	MET	-	EXPRESSION TAG	UNP C1DH03
E	-6	HIS	-	EXPRESSION TAG	UNP C1DH03
E	-5	HIS	-	EXPRESSION TAG	UNP C1DH03
E	-4	HIS	-	EXPRESSION TAG	UNP C1DH03
E	-3	HIS	-	EXPRESSION TAG	UNP C1DH03

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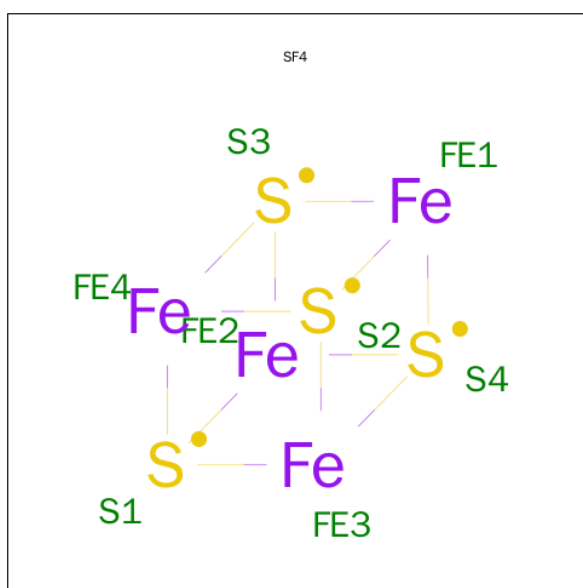
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Chain	Residue	Modelled	Actual	Comment	Reference
E	-2	HIS	-	EXPRESSION TAG	UNP C1DH03
E	-1	HIS	-	EXPRESSION TAG	UNP C1DH03
E	0	HIS	-	EXPRESSION TAG	UNP C1DH03
G	-7	MET	-	EXPRESSION TAG	UNP C1DH03
G	-6	HIS	-	EXPRESSION TAG	UNP C1DH03
G	-5	HIS	-	EXPRESSION TAG	UNP C1DH03
G	-4	HIS	-	EXPRESSION TAG	UNP C1DH03
G	-3	HIS	-	EXPRESSION TAG	UNP C1DH03
G	-2	HIS	-	EXPRESSION TAG	UNP C1DH03
G	-1	HIS	-	EXPRESSION TAG	UNP C1DH03
G	0	HIS	-	EXPRESSION TAG	UNP C1DH03

- Molecule 2 is a protein called Nitrogenase MoFe cofactor biosynthesis protein NifN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	432	Total	C	N	O	S	0	0	0
			3223	2025	573	610	15			
2	D	432	Total	C	N	O	S	0	0	0
			3223	2025	573	610	15			
2	F	432	Total	C	N	O	S	0	0	0
			3223	2025	573	610	15			
2	H	432	Total	C	N	O	S	0	0	0
			3223	2025	573	610	15			

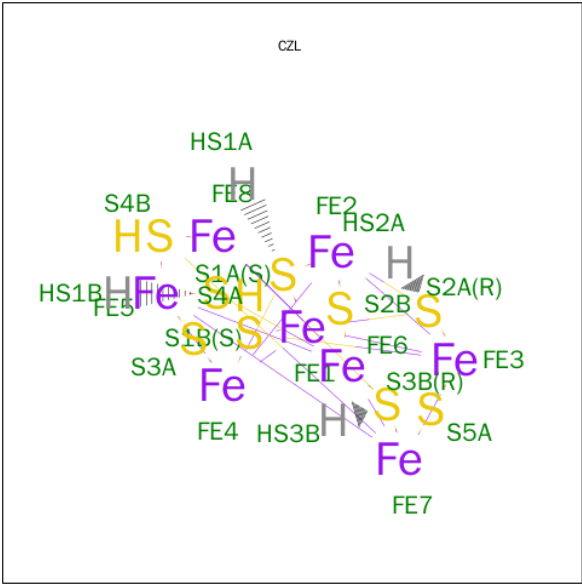
- Molecule 3 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	C	1	Total	Fe	S	0	0
			8	4	4		
3	E	1	Total	Fe	S	0	0
			8	4	4		
3	G	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 4 is L-CLUSTER (FE8S9) (three-letter code: CZL) (formula: Fe<sub>8</sub>H<sub>6</sub>S<sub>9</sub>).



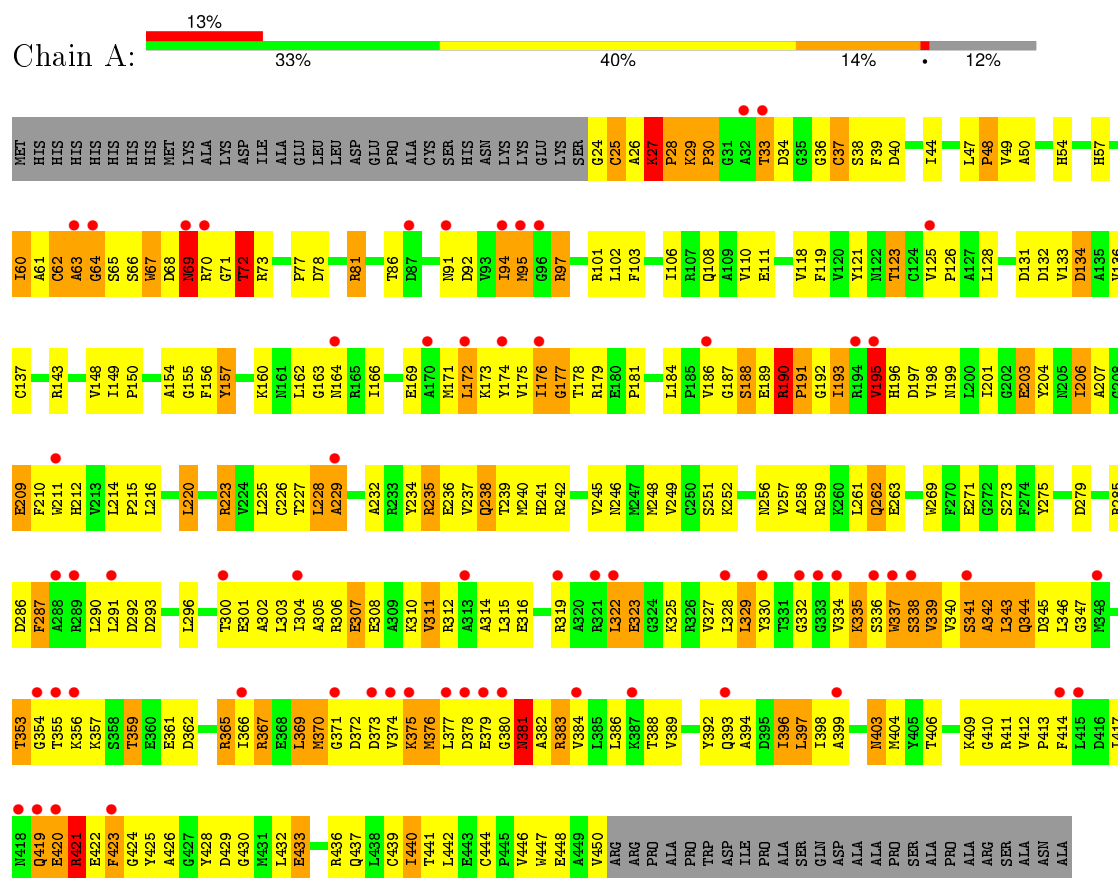
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Fe	S	0	0
			17	8	9		
4	C	1	Total	Fe	S	0	0
			17	8	9		
4	E	1	Total	Fe	S	0	0
			17	8	9		
4	G	1	Total	Fe	S	0	0
			17	8	9		



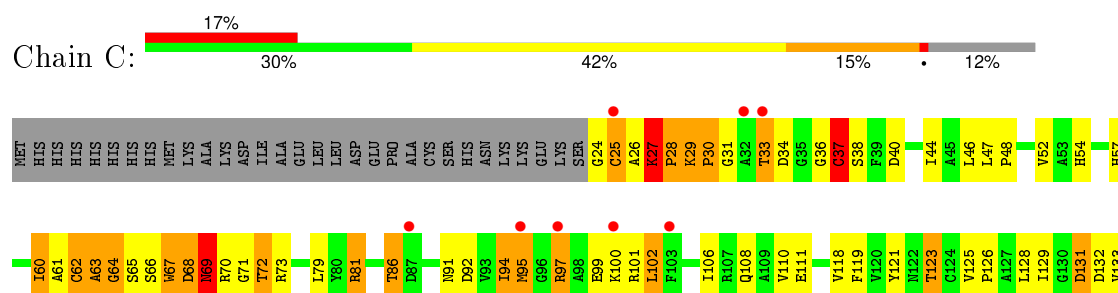
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Nitrogenase MoFe cofactor biosynthesis protein NifE



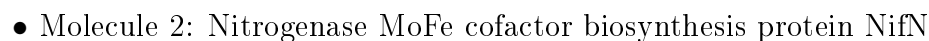
- Molecule 1: Nitrogenase MoFe cofactor biosynthesis protein NifE



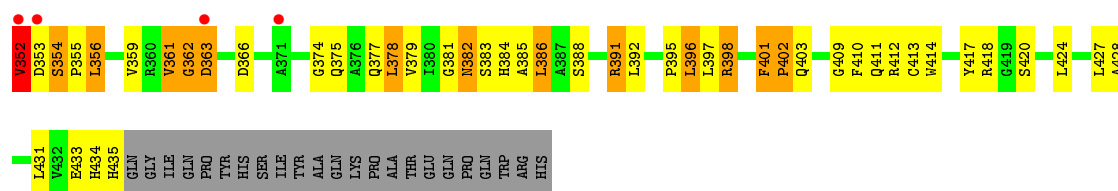




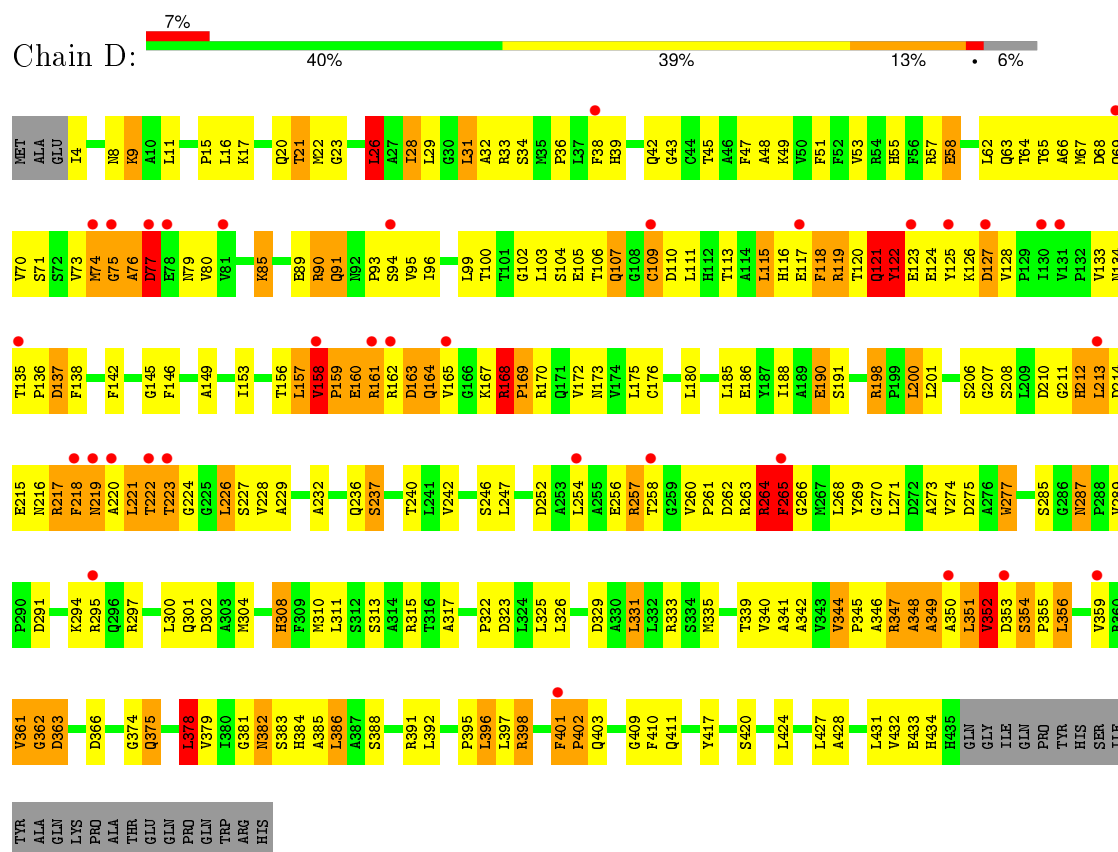




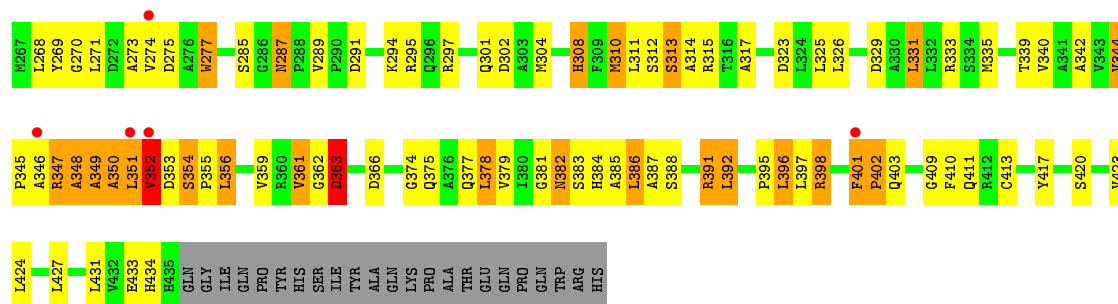




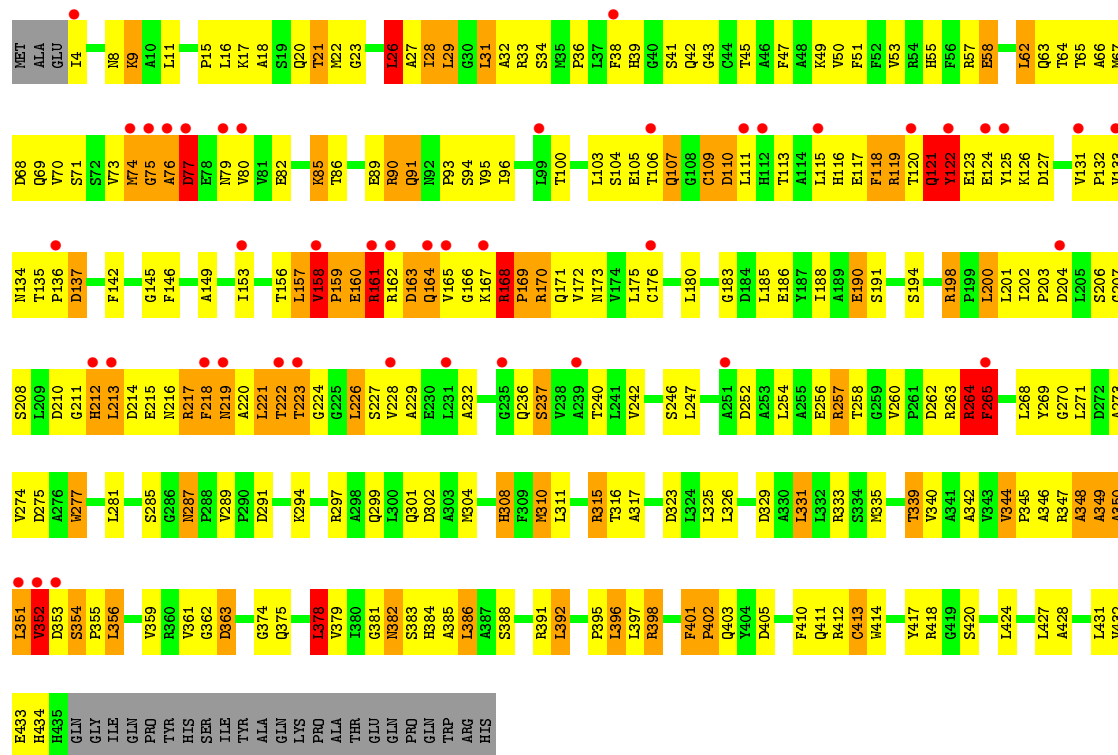
• Molecule 2: Nitrogenase MoFe cofactor biosynthesis protein NifN







- Molecule 2: Nitrogenase MoFe cofactor biosynthesis protein NifN





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	146.07Å 95.22Å 149.98Å 90.00° 95.50° 90.00°	Depositor
Resolution (Å)	39.83 – 2.40 39.83 – 2.40	Depositor EDS
% Data completeness (in resolution range)	87.2 (39.83-2.40) 87.2 (39.83-2.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.91 (at 2.39Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, $R_{free}$	0.294 , 0.341 0.295 , 0.341	Depositor DCC
$R_{free}$ test set	13821 reflections (10.99%)	DCC
Wilson B-factor (Å <sup>2</sup> )	35.9	Xtriage
Anisotropy	0.114	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 22.1	EDS
Estimated twinning fraction	0.075 for l,-k,h	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.39$ , $\langle L^2 \rangle = 0.22$	Xtriage
Outliers	1 of 139612 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.85	EDS
Total number of atoms	26112	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.98% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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: SF4, CZL

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.61	0/3342	0.76	1/4531 (0.0%)
1	C	0.58	2/3342 (0.1%)	0.76	0/4531
1	E	0.61	1/3342 (0.0%)	0.77	0/4531
1	G	0.58	0/3342	0.77	2/4531 (0.0%)
2	B	0.68	2/3283 (0.1%)	0.85	2/4466 (0.0%)
2	D	0.71	4/3283 (0.1%)	0.87	4/4466 (0.1%)
2	F	0.69	4/3283 (0.1%)	0.85	3/4466 (0.1%)
2	H	0.70	4/3283 (0.1%)	0.87	4/4466 (0.1%)
All	All	0.65	17/26500 (0.1%)	0.81	16/35988 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
1	E	0	1
1	G	0	1
2	B	0	4
2	D	0	4
2	F	0	5
2	H	0	4
All	All	0	21

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	122	TYR	CD1-CE1	-7.62	1.27	1.39
2	B	122	TYR	CD1-CE1	-7.59	1.27	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	122	TYR	CD1-CE1	-7.51	1.28	1.39
2	H	122	TYR	CD1-CE1	-7.16	1.28	1.39
2	H	413	CYS	CB-SG	6.81	1.93	1.82
2	D	122	TYR	CD2-CE2	-6.26	1.29	1.39
2	D	122	TYR	CE1-CZ	-6.21	1.30	1.38
2	F	122	TYR	CE1-CZ	-6.15	1.30	1.38
2	F	122	TYR	CD2-CE2	-6.00	1.30	1.39
2	B	122	TYR	CD2-CE2	-5.99	1.30	1.39
1	C	37	CYS	CB-SG	-5.66	1.72	1.81
2	H	122	TYR	CD2-CE2	-5.54	1.31	1.39
2	F	122	TYR	CB-CG	-5.46	1.43	1.51
2	H	122	TYR	CE1-CZ	-5.42	1.31	1.38
1	E	37	CYS	CB-SG	-5.25	1.73	1.81
2	D	122	TYR	CB-CG	-5.10	1.44	1.51
1	C	439	CYS	CB-SG	-5.02	1.73	1.81

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	26	LEU	CA-CB-CG	7.03	131.47	115.30
2	F	26	LEU	CA-CB-CG	6.89	131.14	115.30
2	B	122	TYR	CB-CG-CD1	-6.70	116.98	121.00
2	B	26	LEU	CA-CB-CG	6.53	130.32	115.30
2	H	26	LEU	CA-CB-CG	6.25	129.67	115.30
2	H	122	TYR	CB-CG-CD1	-6.15	117.31	121.00
2	D	122	TYR	CB-CG-CD1	-6.10	117.34	121.00
2	F	122	TYR	CB-CG-CD1	-5.79	117.53	121.00
2	H	392	LEU	CA-CB-CG	5.64	128.28	115.30
1	G	223	ARG	NE-CZ-NH1	-5.33	117.63	120.30
2	F	392	LEU	CA-CB-CG	5.29	127.46	115.30
1	A	223	ARG	NE-CZ-NH1	-5.23	117.68	120.30
2	H	378	LEU	CA-CB-CG	5.22	127.31	115.30
1	G	62	CYS	CA-CB-SG	-5.12	104.78	114.00
2	D	378	LEU	CA-CB-CG	5.10	127.04	115.30
2	D	122	TYR	CG-CD2-CE2	-5.02	117.29	121.30

There are no chirality outliers.

All (21) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	94	ILE	Peptide
2	B	118	PHE	Peptide

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Mol	Chain	Res	Type	Group
2	B	121	GLN	Peptide
2	B	159	PRO	Peptide
2	B	264	ARG	Peptide
1	C	94	ILE	Peptide
2	D	118	PHE	Peptide
2	D	121	GLN	Peptide
2	D	159	PRO	Peptide
2	D	264	ARG	Peptide
1	E	94	ILE	Peptide
2	F	118	PHE	Peptide
2	F	121	GLN	Peptide
2	F	159	PRO	Peptide
2	F	264	ARG	Peptide
2	F	363	ASP	Peptide
1	G	94	ILE	Peptide
2	H	118	PHE	Peptide
2	H	121	GLN	Peptide
2	H	159	PRO	Peptide
2	H	264	ARG	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3280	0	3271	383	0
1	C	3280	0	3271	406	0
1	E	3280	0	3270	396	0
1	G	3280	0	3271	385	0
2	B	3223	0	3197	404	5
2	D	3223	0	3197	399	2
2	F	3223	0	3197	394	0
2	H	3223	0	3197	388	7
3	A	8	0	0	2	0
3	C	8	0	0	2	0
3	E	8	0	0	3	0
3	G	8	0	0	4	0
4	A	17	0	0	3	0
4	C	17	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	17	0	0	2	0
4	G	17	0	0	4	0
All	All	26112	0	25871	2918	7

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 56.

All (2918) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:ARG:CB	1:A:191:PRO:HD2	1.56	1.33
1:A:190:ARG:HB3	1:A:191:PRO:CD	1.54	1.31
2:H:119:ARG:HA	2:H:122:TYR:CE2	1.66	1.30
2:B:119:ARG:CA	2:B:122:TYR:HE2	1.42	1.29
2:B:119:ARG:HA	2:B:122:TYR:CE2	1.64	1.29
2:H:119:ARG:CA	2:H:122:TYR:HE2	1.44	1.28
1:E:190:ARG:CB	1:E:191:PRO:HD2	1.62	1.27
2:F:119:ARG:CA	2:F:122:TYR:HE2	1.47	1.27
1:E:190:ARG:HB3	1:E:191:PRO:CD	1.63	1.26
1:G:190:ARG:HB3	1:G:191:PRO:CD	1.64	1.26
2:D:119:ARG:HA	2:D:122:TYR:CE2	1.69	1.26
1:C:190:ARG:HB3	1:C:191:PRO:CD	1.63	1.26
2:D:119:ARG:CA	2:D:122:TYR:HE2	1.46	1.25
1:G:190:ARG:CB	1:G:191:PRO:HD2	1.64	1.23
2:F:119:ARG:HA	2:F:122:TYR:CE2	1.72	1.22
1:C:190:ARG:CB	1:C:191:PRO:HD2	1.64	1.21
2:D:122:TYR:HD1	2:D:122:TYR:N	1.37	1.19
2:B:122:TYR:HD1	2:B:122:TYR:N	1.36	1.16
2:B:308:HIS:CE1	1:C:441:THR:HG22	1.82	1.14
1:A:29:LYS:H	1:A:29:LYS:NZ	1.44	1.13
1:A:441:THR:HG22	2:D:308:HIS:CE1	1.84	1.13
1:E:441:THR:HG22	2:H:308:HIS:CE1	1.84	1.13
2:B:173:ASN:HB2	2:B:240:THR:HG22	1.30	1.12
2:F:122:TYR:N	2:F:122:TYR:HD1	1.34	1.11
2:F:308:HIS:HE1	1:G:441:THR:HG22	1.08	1.11
2:H:173:ASN:HB2	2:H:240:THR:HG22	1.32	1.11
1:E:29:LYS:H	1:E:29:LYS:NZ	1.46	1.11
1:A:419:GLN:HE21	1:A:419:GLN:HA	0.96	1.10
1:C:29:LYS:H	1:C:29:LYS:NZ	1.47	1.10
2:H:242:VAL:HB	2:H:264:ARG:HB3	1.33	1.10
2:F:173:ASN:HB2	2:F:240:THR:HG22	1.33	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:441:THR:HG22	2:H:308:HIS:HE1	0.92	1.08
2:D:119:ARG:CA	2:D:122:TYR:CE2	2.32	1.08
2:B:118:PHE:O	2:B:119:ARG:HD2	1.52	1.08
2:F:122:TYR:CD1	2:F:122:TYR:N	2.10	1.08
2:D:173:ASN:HB2	2:D:240:THR:HG22	1.34	1.08
1:G:419:GLN:HE21	1:G:419:GLN:HA	0.97	1.07
2:H:122:TYR:HD1	2:H:122:TYR:N	1.38	1.07
2:B:122:TYR:CD1	2:B:122:TYR:N	2.13	1.07
1:A:419:GLN:NE2	1:A:419:GLN:HA	1.66	1.07
2:H:68:ASP:HB3	2:H:70:VAL:HG22	1.35	1.06
1:E:419:GLN:HA	1:E:419:GLN:NE2	1.69	1.06
1:E:419:GLN:HA	1:E:419:GLN:HE21	0.97	1.06
2:H:122:TYR:N	2:H:122:TYR:CD1	2.15	1.06
2:H:119:ARG:CA	2:H:122:TYR:CE2	2.29	1.05
2:D:242:VAL:HB	2:D:264:ARG:HB3	1.34	1.05
2:D:122:TYR:CD1	2:D:122:TYR:N	2.15	1.05
2:F:118:PHE:O	2:F:119:ARG:HD2	1.56	1.04
1:A:441:THR:HG22	2:D:308:HIS:HE1	0.92	1.04
1:G:29:LYS:H	1:G:29:LYS:NZ	1.53	1.04
2:F:107:GLN:N	2:F:107:GLN:HE21	1.54	1.04
2:F:68:ASP:HB3	2:F:70:VAL:HG22	1.35	1.04
1:C:419:GLN:HE21	1:C:419:GLN:HA	0.90	1.04
2:D:118:PHE:O	2:D:119:ARG:HD2	1.56	1.04
2:F:119:ARG:CA	2:F:122:TYR:CE2	2.33	1.03
1:C:419:GLN:NE2	1:C:419:GLN:HA	1.65	1.03
1:A:57:HIS:HD2	1:A:86:THR:HG21	1.19	1.03
1:A:322:LEU:HD21	1:A:439:CYS:SG	1.99	1.03
2:F:242:VAL:HB	2:F:264:ARG:HB3	1.40	1.03
2:H:208:SER:HA	2:H:223:THR:O	1.59	1.03
2:B:119:ARG:CA	2:B:122:TYR:CE2	2.28	1.02
1:E:206:ILE:HG13	1:E:419:GLN:HB3	1.39	1.02
1:E:57:HIS:CD2	1:E:86:THR:HG21	1.95	1.02
2:H:118:PHE:O	2:H:119:ARG:HD2	1.60	1.02
2:B:308:HIS:HE1	1:C:441:THR:HG22	0.92	1.02
2:B:242:VAL:HB	2:B:264:ARG:HB3	1.38	1.02
2:B:107:GLN:N	2:B:107:GLN:HE21	1.57	1.01
2:D:208:SER:HA	2:D:223:THR:O	1.61	1.00
2:B:68:ASP:HB3	2:B:70:VAL:HG22	1.40	1.00
1:A:57:HIS:CD2	1:A:86:THR:HG21	1.96	1.00
1:G:419:GLN:NE2	1:G:419:GLN:HA	1.69	1.00
2:H:34:SER:H	2:H:221:LEU:HD22	1.24	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:57:HIS:HD2	1:G:86:THR:HG21	1.21	0.99
1:G:57:HIS:CD2	1:G:86:THR:HG21	1.98	0.99
2:F:208:SER:HA	2:F:223:THR:O	1.61	0.99
2:B:301:GLN:HE21	1:C:450:VAL:HG12	1.20	0.99
2:B:34:SER:H	2:B:221:LEU:HD22	1.28	0.99
2:D:107:GLN:N	2:D:107:GLN:HE21	1.59	0.99
1:A:172:LEU:HD12	1:A:173:LYS:N	1.76	0.99
2:D:16:LEU:H	2:D:363:ASP:HB3	1.27	0.98
1:G:172:LEU:HD12	1:G:173:LYS:N	1.76	0.98
1:E:172:LEU:HD12	1:E:173:LYS:N	1.78	0.98
2:D:68:ASP:HB3	2:D:70:VAL:HG22	1.42	0.98
2:F:119:ARG:HA	2:F:122:TYR:HE2	0.83	0.97
1:G:319:ARG:O	1:G:323:GLU:HB2	1.64	0.97
2:H:107:GLN:N	2:H:107:GLN:HE21	1.62	0.97
2:D:34:SER:H	2:D:221:LEU:HD22	1.27	0.97
1:E:450:VAL:HG12	2:H:301:GLN:HE21	1.27	0.97
1:E:176:ILE:O	1:E:178:THR:N	1.98	0.97
2:D:119:ARG:HA	2:D:122:TYR:HE2	0.79	0.96
1:A:174:TYR:CE2	1:A:238:GLN:HG2	2.00	0.96
1:G:206:ILE:HG13	1:G:419:GLN:HB3	1.45	0.96
2:F:308:HIS:CE1	1:G:441:THR:HG22	2.00	0.96
2:F:34:SER:H	2:F:221:LEU:HD22	1.31	0.96
1:E:57:HIS:HD2	1:E:86:THR:HG21	1.23	0.96
1:C:57:HIS:CD2	1:C:86:THR:HG21	2.00	0.96
2:B:16:LEU:H	2:B:363:ASP:HB3	1.31	0.96
1:C:57:HIS:HD2	1:C:86:THR:HG21	1.31	0.96
1:C:174:TYR:CE2	1:C:238:GLN:HG2	2.01	0.95
1:A:450:VAL:HG12	2:D:301:GLN:HE21	1.27	0.95
1:C:206:ILE:HG13	1:C:419:GLN:HB3	1.47	0.95
1:A:206:ILE:HG13	1:A:419:GLN:HB3	1.47	0.95
1:E:201:ILE:HG23	1:E:228:LEU:HD23	1.48	0.95
2:B:20:GLN:HG3	2:B:145:GLY:HA2	1.46	0.95
1:A:367:ARG:HG2	1:A:367:ARG:HH11	1.31	0.95
2:F:100:THR:HG22	2:F:135:THR:H	1.32	0.95
1:E:108:GLN:HE22	2:F:11:LEU:H	1.07	0.95
2:D:39:HIS:CD2	2:D:65:THR:HG21	2.01	0.94
1:E:154:ALA:HB3	1:E:157:TYR:HE1	1.32	0.94
1:A:29:LYS:H	1:A:29:LYS:HZ2	1.12	0.94
1:E:319:ARG:O	1:E:323:GLU:HB2	1.66	0.94
2:H:118:PHE:CA	2:H:122:TYR:OH	2.16	0.94
1:C:367:ARG:HG2	1:C:367:ARG:HH11	1.31	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:20:GLN:HG3	2:F:145:GLY:HA2	1.47	0.94
1:A:319:ARG:O	1:A:323:GLU:HB2	1.66	0.94
2:H:32:ALA:HA	2:H:224:GLY:HA3	1.49	0.94
1:A:176:ILE:O	1:A:178:THR:N	2.00	0.94
1:E:193:ILE:H	1:E:193:ILE:HD12	1.29	0.94
2:F:32:ALA:HA	2:F:224:GLY:HA3	1.50	0.94
1:C:29:LYS:HZ1	1:C:29:LYS:H	1.13	0.93
2:H:119:ARG:HA	2:H:122:TYR:HE2	0.77	0.93
1:G:174:TYR:CE2	1:G:238:GLN:HG2	2.03	0.93
1:C:319:ARG:O	1:C:323:GLU:HB2	1.68	0.93
2:D:158:VAL:HG11	2:D:232:ALA:O	1.69	0.93
1:C:419:GLN:CA	1:C:419:GLN:HE21	1.80	0.93
1:G:176:ILE:O	1:G:178:THR:N	2.02	0.93
2:B:208:SER:HA	2:B:223:THR:O	1.69	0.93
1:C:172:LEU:HD12	1:C:173:LYS:N	1.84	0.93
1:C:322:LEU:HD21	1:C:439:CYS:SG	2.08	0.92
1:G:201:ILE:HG23	1:G:228:LEU:HD23	1.51	0.92
1:E:322:LEU:HD21	1:E:439:CYS:SG	2.09	0.92
1:G:37:CYS:CB	1:G:155:GLY:HA2	1.99	0.92
1:G:367:ARG:HH11	1:G:367:ARG:HG2	1.31	0.92
1:C:37:CYS:SG	2:D:43:GLY:HA3	2.09	0.92
1:G:322:LEU:HD21	1:G:439:CYS:SG	2.09	0.92
1:C:37:CYS:HB3	1:C:155:GLY:CA	2.00	0.92
1:E:29:LYS:H	1:E:29:LYS:HZ1	1.13	0.92
1:G:209:GLU:OE1	1:G:426:ALA:HB2	1.70	0.92
1:E:174:TYR:CE2	1:E:238:GLN:HG2	2.05	0.92
2:H:118:PHE:HA	2:H:122:TYR:CZ	2.05	0.92
1:A:419:GLN:HE21	1:A:419:GLN:CA	1.83	0.92
2:F:39:HIS:CD2	2:F:65:THR:HG21	2.05	0.92
2:F:158:VAL:HG11	2:F:232:ALA:O	1.70	0.92
2:D:351:LEU:C	2:D:353:ASP:H	1.74	0.92
1:A:206:ILE:HB	1:A:419:GLN:C	1.90	0.91
2:H:100:THR:HG22	2:H:135:THR:H	1.35	0.91
2:H:118:PHE:C	2:H:122:TYR:CE2	2.44	0.91
2:D:100:THR:HG22	2:D:135:THR:H	1.34	0.91
2:F:16:LEU:H	2:F:363:ASP:HB3	1.34	0.91
1:G:206:ILE:HB	1:G:419:GLN:C	1.90	0.91
1:G:37:CYS:HB3	1:G:155:GLY:CA	2.01	0.91
2:H:16:LEU:H	2:H:363:ASP:HB3	1.33	0.91
2:D:39:HIS:HD2	2:D:65:THR:HG21	1.35	0.91
1:A:209:GLU:OE1	1:A:426:ALA:HB2	1.70	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:37:CYS:HB3	1:E:155:GLY:CA	2.00	0.90
2:B:32:ALA:HA	2:B:224:GLY:HA3	1.53	0.90
2:H:217:ARG:HD3	2:H:219:ASN:H	1.36	0.90
2:H:158:VAL:HG11	2:H:232:ALA:O	1.71	0.90
1:E:206:ILE:HB	1:E:419:GLN:C	1.91	0.90
1:C:199:ASN:HD21	1:C:225:LEU:HB2	1.36	0.90
1:E:367:ARG:HH11	1:E:367:ARG:HG2	1.35	0.90
2:B:351:LEU:C	2:B:353:ASP:H	1.74	0.90
1:C:176:ILE:O	1:C:178:THR:N	2.04	0.90
2:B:119:ARG:HA	2:B:122:TYR:HE2	0.74	0.90
2:D:120:THR:N	2:D:122:TYR:CZ	2.40	0.90
2:H:20:GLN:HG3	2:H:145:GLY:HA2	1.52	0.90
1:C:193:ILE:H	1:C:193:ILE:HD12	1.35	0.90
2:B:118:PHE:CA	2:B:122:TYR:OH	2.19	0.90
2:F:118:PHE:O	2:F:119:ARG:CD	2.20	0.90
1:C:154:ALA:HB3	1:C:157:TYR:HE1	1.35	0.90
1:A:29:LYS:HB3	1:A:30:PRO:HD2	1.53	0.89
2:B:158:VAL:HG11	2:B:232:ALA:O	1.73	0.89
2:B:120:THR:N	2:B:122:TYR:CZ	2.41	0.89
1:C:206:ILE:HB	1:C:419:GLN:C	1.93	0.89
2:H:39:HIS:CD2	2:H:65:THR:HG21	2.08	0.89
2:F:118:PHE:CA	2:F:122:TYR:OH	2.22	0.88
1:A:37:CYS:HB3	1:A:155:GLY:CA	2.03	0.88
2:F:351:LEU:C	2:F:353:ASP:H	1.75	0.88
1:E:37:CYS:CB	1:E:155:GLY:HA2	2.03	0.88
2:B:39:HIS:CD2	2:B:65:THR:HG21	2.08	0.88
1:E:199:ASN:HD21	1:E:225:LEU:HB2	1.38	0.88
2:D:217:ARG:HD3	2:D:219:ASN:H	1.37	0.88
1:A:191:PRO:HB3	1:E:314:ALA:HB2	1.53	0.88
1:A:174:TYR:OH	1:A:234:TYR:O	1.91	0.88
2:H:351:LEU:C	2:H:353:ASP:H	1.75	0.88
1:E:419:GLN:CA	1:E:419:GLN:HE21	1.86	0.87
2:F:212:HIS:HB3	2:F:223:THR:CG2	2.05	0.87
2:H:17:LYS:HG3	2:H:345:PRO:HB2	1.54	0.87
2:B:118:PHE:C	2:B:122:TYR:CE2	2.47	0.87
2:B:85:LYS:HD2	2:B:118:PHE:CE1	2.10	0.87
1:G:29:LYS:H	1:G:29:LYS:HZ1	1.13	0.87
1:G:108:GLN:HE22	2:H:11:LEU:H	1.19	0.87
2:B:118:PHE:O	2:B:119:ARG:CD	2.22	0.87
2:F:118:PHE:HA	2:F:122:TYR:CZ	2.09	0.87
1:A:199:ASN:HD21	1:A:225:LEU:HB2	1.37	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:20:GLN:HG3	2:D:145:GLY:HA2	1.56	0.87
1:E:37:CYS:HB3	1:E:155:GLY:HA2	1.54	0.87
2:F:122:TYR:HD1	2:F:122:TYR:H	1.21	0.87
2:B:118:PHE:HA	2:B:122:TYR:CZ	2.10	0.87
2:D:118:PHE:C	2:D:122:TYR:CE2	2.48	0.87
2:B:382:ASN:HD21	2:B:384:HIS:HB2	1.37	0.87
2:F:120:THR:N	2:F:122:TYR:CZ	2.43	0.86
1:E:206:ILE:HG13	1:E:419:GLN:CB	2.05	0.86
1:A:307:GLU:O	1:A:311:VAL:HG23	1.75	0.86
2:D:118:PHE:HA	2:D:122:TYR:CZ	2.10	0.86
2:D:118:PHE:CA	2:D:122:TYR:OH	2.22	0.86
1:A:201:ILE:HG23	1:A:228:LEU:HD23	1.57	0.86
1:G:193:ILE:H	1:G:193:ILE:HD12	1.39	0.86
2:D:32:ALA:HA	2:D:224:GLY:HA3	1.56	0.86
2:H:118:PHE:C	2:H:122:TYR:CZ	2.48	0.86
2:H:118:PHE:O	2:H:119:ARG:CD	2.22	0.86
2:B:308:HIS:HE1	1:C:441:THR:CG2	1.86	0.86
1:A:29:LYS:HZ1	1:A:29:LYS:H	1.24	0.86
2:F:17:LYS:HG3	2:F:345:PRO:HB2	1.57	0.86
1:E:307:GLU:O	1:E:311:VAL:HG23	1.76	0.86
2:F:217:ARG:HD3	2:F:219:ASN:H	1.39	0.86
2:H:213:LEU:HD23	2:H:214:ASP:H	1.41	0.85
1:C:177:GLY:HA3	1:C:241:HIS:NE2	1.90	0.85
2:B:118:PHE:C	2:B:122:TYR:CZ	2.50	0.85
2:D:118:PHE:O	2:D:119:ARG:CD	2.22	0.85
1:G:209:GLU:OE1	1:G:419:GLN:OE1	1.94	0.85
1:E:29:LYS:HB3	1:E:30:PRO:HD2	1.58	0.85
2:F:118:PHE:C	2:F:122:TYR:CE2	2.50	0.85
1:E:209:GLU:OE1	1:E:419:GLN:OE1	1.93	0.85
2:B:242:VAL:HB	2:B:264:ARG:CB	2.07	0.85
1:G:29:LYS:HB3	1:G:30:PRO:HD2	1.59	0.85
2:F:39:HIS:HD2	2:F:65:THR:HG21	1.39	0.85
2:D:382:ASN:HD21	2:D:384:HIS:HB2	1.40	0.85
2:H:264:ARG:O	2:H:265:PHE:HB2	1.74	0.85
2:D:17:LYS:HG3	2:D:345:PRO:HB2	1.57	0.85
1:C:209:GLU:OE1	1:C:426:ALA:HB2	1.76	0.85
1:C:30:PRO:HA	2:D:63:GLN:OE1	1.77	0.85
2:H:351:LEU:O	2:H:352:VAL:HG12	1.77	0.85
1:A:154:ALA:HB3	1:A:157:TYR:HE1	1.39	0.85
1:C:307:GLU:HG2	1:C:428:TYR:CD2	2.12	0.84
2:H:382:ASN:HD21	2:H:384:HIS:HB2	1.41	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:242:VAL:HB	2:D:264:ARG:CB	2.07	0.84
2:B:163:ASP:O	2:B:165:VAL:N	2.11	0.84
1:A:307:GLU:HG2	1:A:428:TYR:CD2	2.12	0.84
1:C:201:ILE:HG23	1:C:228:LEU:HD23	1.57	0.84
1:E:307:GLU:HG2	1:E:428:TYR:CD2	2.12	0.84
1:A:193:ILE:H	1:A:193:ILE:HD12	1.43	0.84
1:A:30:PRO:HA	2:B:63:GLN:OE1	1.76	0.84
1:C:411:ARG:HH22	2:D:214:ASP:HA	1.43	0.84
1:G:154:ALA:HB3	1:G:157:TYR:HE1	1.43	0.84
1:E:29:LYS:H	1:E:29:LYS:HZ2	1.26	0.83
1:A:209:GLU:OE1	1:A:426:ALA:CB	2.26	0.83
1:E:37:CYS:SG	2:F:43:GLY:HA3	2.18	0.83
1:G:419:GLN:HE21	1:G:419:GLN:CA	1.88	0.83
2:H:242:VAL:HB	2:H:264:ARG:CB	2.08	0.83
1:A:37:CYS:CB	1:A:155:GLY:HA2	2.08	0.83
1:C:386:LEU:HD21	2:D:216:ASN:HB3	1.59	0.83
2:D:85:LYS:HD2	2:D:118:PHE:CE1	2.13	0.83
2:B:39:HIS:HD2	2:B:65:THR:HG21	1.41	0.83
2:B:100:THR:HG22	2:B:135:THR:H	1.42	0.83
2:F:301:GLN:HE21	1:G:450:VAL:HG12	1.44	0.83
1:E:30:PRO:HA	2:F:63:GLN:OE1	1.78	0.83
2:D:264:ARG:O	2:D:265:PHE:HB2	1.76	0.83
2:B:201:LEU:O	2:B:226:LEU:HD21	1.79	0.83
2:F:351:LEU:O	2:F:352:VAL:HG12	1.78	0.83
2:D:85:LYS:HD2	2:D:118:PHE:HE1	1.44	0.83
1:E:154:ALA:HB3	1:E:157:TYR:CE1	2.14	0.83
2:B:122:TYR:H	2:B:122:TYR:HD1	1.25	0.83
1:G:307:GLU:HG2	1:G:428:TYR:CD2	2.13	0.82
1:C:361:GLU:HG3	4:C:502:CZL:S3B	2.19	0.82
2:B:217:ARG:HD3	2:B:219:ASN:H	1.43	0.82
1:G:199:ASN:HD21	1:G:225:LEU:HB2	1.41	0.82
1:E:209:GLU:OE1	1:E:426:ALA:HB2	1.78	0.82
1:C:307:GLU:O	1:C:311:VAL:HG23	1.78	0.82
2:H:85:LYS:HD2	2:H:118:PHE:CE1	2.13	0.82
2:B:264:ARG:O	2:B:265:PHE:HB2	1.75	0.82
1:G:177:GLY:HA3	1:G:241:HIS:NE2	1.95	0.82
1:C:37:CYS:HB3	1:C:155:GLY:HA2	1.62	0.82
2:D:126:LYS:NZ	2:D:127:ASP:H	1.78	0.82
2:H:122:TYR:HD1	2:H:122:TYR:H	1.28	0.82
1:A:206:ILE:HB	1:A:419:GLN:O	1.80	0.82
1:E:123:THR:HG22	3:E:501:SF4:S4	2.19	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:362:ASP:O	1:G:366:ILE:HG13	1.80	0.82
2:B:85:LYS:HD2	2:B:118:PHE:HE1	1.44	0.82
2:H:39:HIS:HD2	2:H:65:THR:HG21	1.43	0.82
2:H:119:ARG:N	2:H:122:TYR:CE2	2.47	0.81
2:F:85:LYS:HD2	2:F:118:PHE:CE1	2.15	0.81
1:A:206:ILE:HG13	1:A:419:GLN:CB	2.09	0.81
2:D:118:PHE:C	2:D:122:TYR:CZ	2.53	0.81
1:A:209:GLU:OE1	1:A:419:GLN:OE1	1.99	0.81
2:H:120:THR:N	2:H:122:TYR:CZ	2.47	0.81
1:C:206:ILE:HG13	1:C:419:GLN:CB	2.10	0.81
2:F:212:HIS:HB3	2:F:223:THR:HG22	1.59	0.81
2:F:159:PRO:HG3	2:F:257:ARG:HH11	1.46	0.81
2:D:381:GLY:O	2:D:398:ARG:HA	1.78	0.81
1:C:29:LYS:HZ2	1:C:29:LYS:H	1.28	0.81
2:F:118:PHE:C	2:F:122:TYR:CZ	2.54	0.81
1:G:206:ILE:HG13	1:G:419:GLN:CB	2.10	0.81
1:A:66:SER:O	1:A:69:ASN:ND2	2.14	0.81
2:D:159:PRO:HG3	2:D:257:ARG:HH11	1.46	0.81
1:G:72:THR:HG23	1:G:204:TYR:O	1.79	0.81
2:H:163:ASP:O	2:H:165:VAL:N	2.14	0.81
2:F:264:ARG:O	2:F:265:PHE:HB2	1.79	0.81
2:H:397:LEU:HD23	2:H:427:LEU:HD21	1.62	0.81
1:E:174:TYR:CE2	1:E:234:TYR:CZ	2.69	0.80
2:B:126:LYS:NZ	2:B:127:ASP:H	1.79	0.80
1:C:209:GLU:OE1	1:C:419:GLN:OE1	1.98	0.80
1:E:29:LYS:HZ1	1:E:29:LYS:N	1.79	0.80
2:F:242:VAL:HB	2:F:264:ARG:CB	2.10	0.80
2:H:212:HIS:HB3	2:H:223:THR:CG2	2.11	0.80
1:E:91:ASN:O	1:E:94:ILE:HG13	1.81	0.80
1:G:367:ARG:HG2	1:G:367:ARG:NH1	1.93	0.80
1:C:37:CYS:CB	1:C:155:GLY:HA2	2.10	0.80
1:G:209:GLU:OE1	1:G:426:ALA:CB	2.29	0.80
2:B:213:LEU:HD23	2:B:214:ASP:H	1.44	0.80
2:D:133:VAL:HG12	2:D:135:THR:HG23	1.63	0.80
2:H:315:ARG:CG	2:H:340:VAL:HG21	2.11	0.80
1:G:57:HIS:HA	1:G:86:THR:CG2	2.12	0.80
1:G:26:ALA:O	1:G:27:LYS:HB3	1.80	0.80
2:D:163:ASP:O	2:D:165:VAL:N	2.14	0.80
1:C:29:LYS:HB3	1:C:30:PRO:HD2	1.61	0.80
1:E:29:LYS:NZ	1:E:29:LYS:N	2.30	0.79
1:E:206:ILE:HB	1:E:419:GLN:O	1.80	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:213:LEU:HD23	2:D:214:ASP:H	1.46	0.79
1:C:154:ALA:HB3	1:C:157:TYR:CE1	2.16	0.79
2:D:201:LEU:O	2:D:226:LEU:HD21	1.81	0.79
1:E:177:GLY:HA3	1:E:241:HIS:NE2	1.97	0.79
2:D:120:THR:N	2:D:122:TYR:CE2	2.50	0.79
1:C:91:ASN:O	1:C:94:ILE:HG13	1.82	0.79
2:H:168:ARG:HE	2:H:169:PRO:HD3	1.45	0.79
1:C:383:ARG:CA	2:D:217:ARG:HH12	1.96	0.79
2:B:212:HIS:HB3	2:B:223:THR:CG2	2.13	0.79
2:H:159:PRO:CG	2:H:257:ARG:HH11	1.94	0.79
2:F:85:LYS:HD2	2:F:118:PHE:HE1	1.46	0.79
1:G:206:ILE:HB	1:G:419:GLN:O	1.83	0.79
1:G:37:CYS:HB3	1:G:155:GLY:HA2	1.61	0.79
2:F:159:PRO:CG	2:F:257:ARG:HH11	1.94	0.79
2:B:258:THR:OG1	2:B:260:VAL:HG23	1.82	0.79
2:B:120:THR:N	2:B:122:TYR:CE2	2.51	0.79
2:F:163:ASP:O	2:F:165:VAL:N	2.15	0.79
2:H:85:LYS:HD2	2:H:118:PHE:HE1	1.48	0.79
2:D:42:GLN:HA	2:D:64:THR:HG21	1.62	0.79
1:C:27:LYS:HD3	2:D:66:ALA:HB1	1.65	0.79
1:C:409:LYS:HB3	2:D:218:PHE:CZ	2.18	0.79
2:H:118:PHE:CA	2:H:122:TYR:CZ	2.65	0.79
2:F:42:GLN:HA	2:F:64:THR:HG21	1.65	0.79
1:C:29:LYS:HZ1	1:C:29:LYS:N	1.81	0.79
2:B:221:LEU:O	2:B:223:THR:N	2.16	0.79
1:C:206:ILE:HB	1:C:419:GLN:O	1.83	0.79
2:F:213:LEU:HD23	2:F:214:ASP:H	1.48	0.79
2:H:126:LYS:NZ	2:H:127:ASP:H	1.80	0.78
2:F:118:PHE:HA	2:F:122:TYR:OH	1.83	0.78
1:E:193:ILE:HD12	1:E:193:ILE:N	1.97	0.78
1:G:29:LYS:N	1:G:29:LYS:HZ1	1.81	0.78
2:B:351:LEU:O	2:B:352:VAL:HG12	1.82	0.78
2:B:159:PRO:HG3	2:B:257:ARG:HH11	1.47	0.78
2:B:17:LYS:HG3	2:B:345:PRO:HB2	1.64	0.78
2:F:119:ARG:N	2:F:122:TYR:CE2	2.51	0.78
1:A:29:LYS:N	1:A:29:LYS:NZ	2.27	0.78
1:A:174:TYR:CE2	1:A:234:TYR:CZ	2.71	0.78
1:A:252:LYS:HB2	1:A:361:GLU:OE2	1.82	0.78
2:B:119:ARG:N	2:B:122:TYR:CE2	2.50	0.78
1:G:177:GLY:CA	1:G:241:HIS:CE1	2.66	0.78
2:F:315:ARG:CG	2:F:340:VAL:HG21	2.13	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:118:PHE:HA	2:H:122:TYR:OH	1.80	0.78
1:G:37:CYS:HB2	1:G:155:GLY:HA2	1.63	0.78
2:F:201:LEU:O	2:F:226:LEU:HD21	1.84	0.78
2:F:133:VAL:HG12	2:F:135:THR:HG23	1.66	0.78
1:E:66:SER:O	1:E:69:ASN:ND2	2.16	0.78
2:F:382:ASN:HD21	2:F:384:HIS:HB2	1.49	0.78
1:A:27:LYS:HD3	2:B:66:ALA:HB1	1.64	0.78
1:A:386:LEU:HD21	2:B:216:ASN:HB3	1.63	0.78
2:F:126:LYS:NZ	2:F:127:ASP:H	1.82	0.78
1:C:57:HIS:HA	1:C:86:THR:HG22	1.66	0.78
1:G:413:PRO:HA	1:G:447:TRP:CZ2	2.19	0.78
2:F:240:THR:HG21	2:F:254:LEU:HD11	1.66	0.78
1:E:386:LEU:HD21	2:F:216:ASN:HB3	1.65	0.78
1:E:72:THR:HG23	1:E:204:TYR:O	1.85	0.77
1:A:362:ASP:O	1:A:366:ILE:HG13	1.83	0.77
2:D:168:ARG:HE	2:D:169:PRO:HD3	1.48	0.77
2:H:159:PRO:HG3	2:H:257:ARG:HH11	1.49	0.77
2:H:270:GLY:O	2:H:274:VAL:HG23	1.84	0.77
1:A:91:ASN:O	1:A:94:ILE:HG13	1.84	0.77
2:B:64:THR:HG22	2:B:66:ALA:H	1.50	0.77
2:D:351:LEU:O	2:D:352:VAL:HG12	1.84	0.77
2:H:133:VAL:HG12	2:H:135:THR:HG23	1.66	0.77
2:B:326:LEU:HD11	2:B:350:ALA:HB1	1.66	0.77
1:C:177:GLY:CA	1:C:241:HIS:CE1	2.67	0.77
2:D:122:TYR:H	2:D:122:TYR:HD1	1.28	0.77
1:A:26:ALA:O	1:A:27:LYS:HB3	1.85	0.77
1:E:361:GLU:HG3	4:E:502:CZL:S3B	2.25	0.77
1:C:174:TYR:OH	1:C:234:TYR:O	2.02	0.77
2:B:168:ARG:HE	2:B:169:PRO:HD3	1.49	0.77
2:B:119:ARG:N	2:B:122:TYR:OH	2.16	0.77
2:D:119:ARG:N	2:D:122:TYR:CE2	2.52	0.77
2:H:64:THR:HG22	2:H:66:ALA:H	1.48	0.77
2:F:39:HIS:HA	2:F:65:THR:OG1	1.84	0.77
1:E:362:ASP:O	1:E:366:ILE:HG13	1.85	0.77
1:E:94:ILE:O	1:E:94:ILE:HD12	1.85	0.77
1:A:27:LYS:HD3	2:B:66:ALA:CB	2.15	0.77
1:E:26:ALA:O	1:E:27:LYS:HB3	1.82	0.77
1:C:26:ALA:O	1:C:27:LYS:HB3	1.85	0.77
2:F:120:THR:N	2:F:122:TYR:CE2	2.52	0.76
1:A:206:ILE:C	1:A:419:GLN:O	2.24	0.76
2:D:240:THR:HG21	2:D:254:LEU:HD11	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:212:HIS:HB3	2:D:223:THR:CG2	2.14	0.76
2:D:118:PHE:HA	2:D:122:TYR:OH	1.85	0.76
1:A:57:HIS:HA	1:A:86:THR:CG2	2.16	0.76
2:F:26:LEU:HA	2:F:29:LEU:HB2	1.67	0.76
2:F:64:THR:HG22	2:F:66:ALA:H	1.49	0.76
1:A:72:THR:HG23	1:A:204:TYR:O	1.85	0.76
2:H:173:ASN:CB	2:H:240:THR:HG22	2.14	0.76
2:H:212:HIS:HB3	2:H:223:THR:HG22	1.66	0.76
2:H:381:GLY:O	2:H:398:ARG:HA	1.84	0.76
2:H:119:ARG:N	2:H:122:TYR:OH	2.19	0.76
1:E:206:ILE:CG1	1:E:419:GLN:HB3	2.13	0.76
2:B:118:PHE:CA	2:B:122:TYR:CZ	2.69	0.76
1:C:57:HIS:HA	1:C:86:THR:CG2	2.16	0.76
2:B:315:ARG:CG	2:B:340:VAL:HG21	2.15	0.76
2:B:42:GLN:HA	2:B:64:THR:HG21	1.67	0.75
1:A:177:GLY:HA2	1:A:241:HIS:CE1	2.21	0.75
1:G:177:GLY:HA2	1:G:241:HIS:CE1	2.20	0.75
2:B:159:PRO:CG	2:B:257:ARG:HH11	1.99	0.75
1:A:191:PRO:HG2	1:E:310:LYS:NZ	2.01	0.75
2:F:125:TYR:O	2:F:126:LYS:HB3	1.86	0.75
1:A:37:CYS:HB3	1:A:155:GLY:HA2	1.65	0.75
1:C:174:TYR:CE2	1:C:234:TYR:CZ	2.75	0.75
1:A:154:ALA:HB3	1:A:157:TYR:CE1	2.21	0.75
1:G:252:LYS:HB2	1:G:361:GLU:OE2	1.85	0.75
1:G:91:ASN:O	1:G:94:ILE:HG13	1.86	0.75
2:F:173:ASN:CB	2:F:240:THR:HG22	2.15	0.75
2:B:118:PHE:HA	2:B:122:TYR:OH	1.86	0.75
2:D:159:PRO:CG	2:D:257:ARG:HH11	1.98	0.75
2:D:168:ARG:HG3	2:D:236:GLN:HB2	1.67	0.75
2:H:201:LEU:O	2:H:226:LEU:HD21	1.85	0.75
1:C:209:GLU:OE1	1:C:426:ALA:CB	2.34	0.75
1:E:381:ASN:H	1:E:381:ASN:HD22	1.34	0.75
2:B:212:HIS:HB3	2:B:223:THR:HG22	1.68	0.75
1:E:66:SER:HB3	2:F:47:PHE:CE1	2.22	0.75
2:H:168:ARG:HG3	2:H:236:GLN:HB2	1.67	0.75
2:B:168:ARG:HG3	2:B:236:GLN:HB2	1.67	0.75
1:G:190:ARG:O	1:G:192:GLY:N	2.20	0.75
2:D:39:HIS:HA	2:D:65:THR:OG1	1.87	0.75
2:D:159:PRO:CB	2:D:257:ARG:HD3	2.17	0.75
1:A:191:PRO:CB	1:E:314:ALA:HB2	2.17	0.74
2:D:212:HIS:HB3	2:D:223:THR:HG22	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:108:GLN:NE2	2:F:11:LEU:H	1.81	0.74
2:F:168:ARG:HG3	2:F:236:GLN:HB2	1.68	0.74
1:E:57:HIS:HA	1:E:86:THR:CG2	2.17	0.74
2:H:117:GLU:C	2:H:122:TYR:OH	2.25	0.74
2:F:20:GLN:HG3	2:F:145:GLY:CA	2.17	0.74
1:C:220:LEU:HG	1:C:300:THR:HG22	1.69	0.74
2:B:107:GLN:N	2:B:107:GLN:NE2	2.34	0.74
2:D:118:PHE:CA	2:D:122:TYR:CZ	2.70	0.74
2:B:173:ASN:CB	2:B:240:THR:HG22	2.12	0.74
2:D:16:LEU:H	2:D:363:ASP:CB	1.98	0.74
2:B:20:GLN:HG3	2:B:145:GLY:CA	2.17	0.74
2:B:351:LEU:C	2:B:353:ASP:N	2.40	0.74
2:F:168:ARG:HE	2:F:169:PRO:HD3	1.51	0.74
1:A:190:ARG:O	1:A:192:GLY:N	2.19	0.74
2:H:125:TYR:O	2:H:126:LYS:HB3	1.86	0.74
2:F:121:GLN:N	2:F:122:TYR:CE1	2.56	0.74
2:F:159:PRO:HB2	2:F:257:ARG:HB2	1.67	0.74
1:A:361:GLU:HG3	4:A:502:CZL:S3B	2.27	0.74
1:E:67:TRP:CZ3	2:F:15:PRO:O	2.40	0.74
2:D:16:LEU:N	2:D:363:ASP:HB3	2.00	0.74
2:D:382:ASN:ND2	2:D:384:HIS:HB2	2.03	0.74
1:C:206:ILE:CG1	1:C:419:GLN:HB3	2.17	0.74
1:A:383:ARG:CA	2:B:217:ARG:HH12	2.00	0.74
1:E:174:TYR:OH	1:E:234:TYR:O	2.04	0.74
1:G:38:SER:OG	1:G:162:LEU:HD12	1.87	0.74
1:G:30:PRO:HA	2:H:63:GLN:OE1	1.87	0.74
2:B:363:ASP:N	2:B:363:ASP:OD2	2.20	0.74
1:C:367:ARG:HG2	1:C:367:ARG:NH1	1.94	0.74
2:B:159:PRO:HB2	2:B:257:ARG:HB2	1.69	0.74
2:B:302:ASP:CB	2:D:211:GLY:HA3	2.17	0.74
2:F:107:GLN:N	2:F:107:GLN:NE2	2.36	0.73
1:G:175:VAL:O	1:G:176:ILE:C	2.26	0.73
1:E:106:ILE:O	1:E:110:VAL:HG22	1.87	0.73
1:E:417:ILE:HG22	1:E:417:ILE:O	1.87	0.73
2:H:351:LEU:C	2:H:353:ASP:N	2.42	0.73
1:G:67:TRP:CZ3	2:H:15:PRO:O	2.41	0.73
2:D:168:ARG:HB2	2:D:169:PRO:HD3	1.69	0.73
2:B:198:ARG:O	2:B:198:ARG:HG3	1.88	0.73
2:B:119:ARG:C	2:B:122:TYR:CE2	2.61	0.73
2:B:125:TYR:O	2:B:126:LYS:HB3	1.87	0.73
1:A:57:HIS:HA	1:A:86:THR:HG22	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:SER:HB3	2:B:47:PHE:CE1	2.23	0.73
2:H:297:ARG:HD2	2:H:417:TYR:OH	1.88	0.73
2:D:121:GLN:N	2:D:122:TYR:CE1	2.57	0.73
2:D:125:TYR:O	2:D:126:LYS:HB3	1.87	0.73
1:E:209:GLU:OE1	1:E:426:ALA:CB	2.36	0.73
1:G:62:CYS:SG	1:G:123:THR:HG21	2.28	0.73
2:B:382:ASN:ND2	2:B:384:HIS:HB2	2.03	0.73
1:G:154:ALA:HB3	1:G:157:TYR:CE1	2.24	0.73
1:E:206:ILE:C	1:E:419:GLN:O	2.27	0.73
1:A:367:ARG:NH1	1:A:367:ARG:HG2	1.93	0.73
1:C:175:VAL:O	1:C:176:ILE:C	2.26	0.73
1:C:67:TRP:CZ3	2:D:15:PRO:O	2.42	0.73
2:H:242:VAL:CB	2:H:264:ARG:HB3	2.16	0.73
1:E:175:VAL:O	1:E:176:ILE:C	2.23	0.73
1:G:174:TYR:CE2	1:G:234:TYR:CZ	2.76	0.73
1:E:38:SER:OG	1:E:162:LEU:HD12	1.87	0.73
1:C:193:ILE:N	1:C:193:ILE:HD12	2.03	0.73
1:C:413:PRO:HA	1:C:447:TRP:CZ2	2.23	0.73
1:A:206:ILE:HG13	1:A:419:GLN:CG	2.19	0.73
1:E:177:GLY:CA	1:E:241:HIS:CE1	2.72	0.73
1:A:314:ALA:HB2	1:E:191:PRO:HB3	1.70	0.73
2:F:119:ARG:N	2:F:122:TYR:OH	2.21	0.73
1:C:29:LYS:NZ	1:C:29:LYS:N	2.31	0.73
2:H:149:ALA:O	2:H:153:ILE:HG13	1.88	0.73
2:B:240:THR:HG21	2:B:254:LEU:HD11	1.71	0.72
2:D:107:GLN:N	2:D:107:GLN:NE2	2.36	0.72
1:G:174:TYR:OH	1:G:234:TYR:O	2.06	0.72
1:G:367:ARG:HH11	1:G:367:ARG:CG	2.02	0.72
1:G:307:GLU:O	1:G:311:VAL:HG23	1.87	0.72
2:B:121:GLN:N	2:B:122:TYR:CE1	2.57	0.72
2:F:118:PHE:CA	2:F:122:TYR:CZ	2.71	0.72
1:C:191:PRO:HB3	1:G:314:ALA:HB2	1.69	0.72
1:G:206:ILE:CG1	1:G:419:GLN:HB3	2.18	0.72
1:E:57:HIS:HA	1:E:86:THR:HG22	1.70	0.72
2:F:270:GLY:O	2:F:274:VAL:HG23	1.90	0.72
2:D:315:ARG:CG	2:D:340:VAL:HG21	2.18	0.72
2:H:120:THR:N	2:H:122:TYR:CE2	2.57	0.72
1:A:367:ARG:CG	1:A:367:ARG:HH11	2.01	0.72
1:A:177:GLY:CA	1:A:241:HIS:CE1	2.72	0.72
1:C:177:GLY:HA2	1:C:241:HIS:CE1	2.24	0.72
1:E:252:LYS:HB2	1:E:361:GLU:OE2	1.88	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:108:GLN:HE22	2:D:11:LEU:H	1.37	0.72
1:A:436:ARG:O	1:A:440:ILE:HG23	1.88	0.72
1:C:383:ARG:HG2	1:C:384:VAL:H	1.55	0.72
1:C:66:SER:O	1:C:69:ASN:ND2	2.21	0.72
2:D:351:LEU:C	2:D:353:ASP:N	2.40	0.72
1:C:190:ARG:O	1:C:192:GLY:N	2.22	0.72
2:H:240:THR:HG21	2:H:254:LEU:HD11	1.72	0.72
2:B:302:ASP:HB2	2:D:211:GLY:HA3	1.70	0.72
1:G:301:GLU:O	1:G:304:ILE:HG13	1.90	0.72
1:E:441:THR:CG2	2:H:308:HIS:HE1	1.87	0.72
1:E:382:ALA:HB3	2:F:217:ARG:HG3	1.71	0.72
1:G:193:ILE:N	1:G:193:ILE:HD12	2.04	0.72
1:C:382:ALA:HB3	2:D:217:ARG:HG3	1.70	0.72
1:G:29:LYS:H	1:G:29:LYS:HZ2	1.37	0.72
1:A:174:TYR:HE2	1:A:238:GLN:HG2	1.53	0.72
2:F:159:PRO:CB	2:F:257:ARG:HD3	2.19	0.72
2:F:351:LEU:C	2:F:353:ASP:N	2.42	0.72
1:C:66:SER:HB3	2:D:47:PHE:CE1	2.25	0.72
2:D:119:ARG:N	2:D:122:TYR:OH	2.23	0.72
1:A:383:ARG:HA	2:B:217:ARG:HH12	1.55	0.72
2:B:218:PHE:CD2	2:B:218:PHE:N	2.58	0.72
2:H:168:ARG:HB2	2:H:169:PRO:HD3	1.71	0.72
1:C:362:ASP:O	1:C:366:ILE:HG13	1.90	0.72
1:G:27:LYS:HD3	2:H:66:ALA:HB1	1.71	0.71
1:A:177:GLY:HA3	1:A:241:HIS:NE2	2.05	0.71
1:E:367:ARG:NH1	1:E:367:ARG:HG2	1.97	0.71
1:C:94:ILE:HD12	1:C:94:ILE:O	1.90	0.71
2:H:119:ARG:N	2:H:122:TYR:CZ	2.59	0.71
2:D:39:HIS:HD2	2:D:65:THR:CG2	2.01	0.71
2:B:26:LEU:HA	2:B:29:LEU:HB2	1.72	0.71
2:B:344:VAL:HG22	2:B:345:PRO:HD2	1.71	0.71
1:C:27:LYS:HD3	2:D:66:ALA:CB	2.19	0.71
2:H:159:PRO:CB	2:H:257:ARG:HD3	2.20	0.71
1:E:397:LEU:HD22	1:E:398:ILE:N	2.06	0.71
2:D:397:LEU:HD23	2:D:427:LEU:HD21	1.71	0.71
1:A:108:GLN:HE22	2:B:11:LEU:H	1.37	0.71
1:G:381:ASN:HD22	1:G:381:ASN:H	1.38	0.71
2:D:117:GLU:C	2:D:122:TYR:OH	2.29	0.71
2:D:64:THR:HG22	2:D:66:ALA:H	1.55	0.71
1:A:409:LYS:HB3	2:B:218:PHE:CZ	2.25	0.71
2:D:363:ASP:OD2	2:D:363:ASP:N	2.22	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:67:MET:CE	2:B:71:SER:HB2	2.20	0.71
2:F:397:LEU:HD23	2:F:427:LEU:HD21	1.70	0.71
2:B:133:VAL:HG12	2:B:135:THR:HG23	1.72	0.71
1:A:175:VAL:O	1:A:176:ILE:C	2.29	0.71
2:B:117:GLU:C	2:B:122:TYR:OH	2.29	0.71
2:H:221:LEU:O	2:H:223:THR:N	2.23	0.71
2:D:218:PHE:N	2:D:218:PHE:CD2	2.58	0.71
2:F:159:PRO:HB3	2:F:257:ARG:HD3	1.72	0.71
2:B:159:PRO:CB	2:B:257:ARG:HD3	2.21	0.71
2:H:344:VAL:HG22	2:H:345:PRO:HD2	1.70	0.71
2:B:381:GLY:O	2:B:398:ARG:HA	1.90	0.71
1:A:383:ARG:HG2	1:A:384:VAL:H	1.56	0.71
1:A:62:CYS:SG	1:A:123:THR:HG21	2.30	0.70
2:D:217:ARG:C	2:D:218:PHE:HD2	1.94	0.70
2:H:16:LEU:H	2:H:363:ASP:CB	2.03	0.70
2:H:121:GLN:N	2:H:122:TYR:CE1	2.59	0.70
1:E:193:ILE:H	1:E:193:ILE:CD1	2.02	0.70
2:D:159:PRO:HB2	2:D:257:ARG:HB2	1.73	0.70
1:E:262:GLN:HG3	1:E:263:GLU:N	2.05	0.70
2:D:221:LEU:O	2:D:223:THR:N	2.24	0.70
2:F:221:LEU:O	2:F:223:THR:N	2.24	0.70
1:E:108:GLN:CD	2:F:11:LEU:HB3	2.11	0.70
2:D:20:GLN:HG2	2:D:135:THR:HB	1.73	0.70
2:H:382:ASN:ND2	2:H:384:HIS:HB2	2.05	0.70
1:A:301:GLU:O	1:A:304:ILE:HG13	1.91	0.70
1:E:220:LEU:HG	1:E:300:THR:HG22	1.72	0.70
1:C:174:TYR:HE2	1:C:238:GLN:HG2	1.51	0.70
1:E:108:GLN:NE2	2:F:11:LEU:HB3	2.06	0.70
2:D:220:ALA:O	2:D:221:LEU:HB3	1.89	0.70
1:A:383:ARG:H	2:B:217:ARG:HH22	1.39	0.70
2:F:16:LEU:H	2:F:363:ASP:CB	2.04	0.70
1:E:67:TRP:CH2	2:F:15:PRO:O	2.44	0.70
1:G:332:GLY:H	1:G:334:VAL:HG22	1.56	0.70
2:H:198:ARG:HG3	2:H:198:ARG:O	1.91	0.70
2:F:363:ASP:OD2	2:F:363:ASP:N	2.24	0.70
1:E:367:ARG:HH11	1:E:367:ARG:CG	2.04	0.70
1:C:397:LEU:HD22	1:C:398:ILE:N	2.06	0.70
2:F:381:GLY:O	2:F:398:ARG:HA	1.91	0.70
2:D:173:ASN:CB	2:D:240:THR:HG22	2.16	0.70
2:H:20:GLN:HG3	2:H:145:GLY:CA	2.21	0.70
1:C:314:ALA:HB2	1:G:191:PRO:HB3	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:191:PRO:CB	1:G:314:ALA:HB2	2.20	0.69
1:G:410:GLY:O	1:G:412:VAL:HG23	1.91	0.69
2:B:119:ARG:N	2:B:122:TYR:CZ	2.61	0.69
2:D:119:ARG:C	2:D:122:TYR:CE2	2.65	0.69
1:C:206:ILE:HG13	1:C:419:GLN:CG	2.21	0.69
2:H:218:PHE:N	2:H:218:PHE:CD2	2.56	0.69
2:H:379:VAL:O	2:H:396:LEU:HD23	1.92	0.69
1:E:329:LEU:HD13	1:E:340:VAL:HG22	1.74	0.69
2:D:242:VAL:CB	2:D:264:ARG:HB3	2.17	0.69
1:G:383:ARG:HG2	1:G:384:VAL:H	1.56	0.69
1:C:383:ARG:HA	2:D:217:ARG:HH12	1.58	0.69
2:F:168:ARG:HH21	2:F:169:PRO:HG3	1.56	0.69
1:G:197:ASP:OD2	1:G:223:ARG:HD3	1.92	0.69
1:E:413:PRO:HA	1:E:447:TRP:CZ2	2.27	0.69
2:F:39:HIS:HD2	2:F:65:THR:CG2	2.04	0.69
1:A:106:ILE:O	1:A:110:VAL:HG22	1.92	0.69
2:F:119:ARG:C	2:F:122:TYR:CE2	2.65	0.69
1:G:57:HIS:HA	1:G:86:THR:HG22	1.73	0.69
2:B:16:LEU:H	2:B:363:ASP:CB	2.03	0.69
1:C:367:ARG:CG	1:C:367:ARG:HH11	2.03	0.69
2:H:363:ASP:OD2	2:H:363:ASP:N	2.25	0.69
2:H:159:PRO:HB2	2:H:257:ARG:HB2	1.72	0.69
1:A:314:ALA:HB2	1:E:191:PRO:CB	2.22	0.69
2:H:42:GLN:HA	2:H:64:THR:HG21	1.73	0.69
1:G:48:PRO:HG2	1:G:229:ALA:HB1	1.75	0.69
1:A:206:ILE:CG1	1:A:419:GLN:HB3	2.21	0.69
1:E:421:ARG:CZ	1:E:422:GLU:H	2.06	0.69
1:A:37:CYS:HB2	1:A:155:GLY:HA2	1.74	0.69
1:E:177:GLY:HA2	1:E:241:HIS:CE1	2.28	0.69
2:B:159:PRO:HB3	2:B:257:ARG:HD3	1.75	0.69
2:F:326:LEU:HD11	2:F:350:ALA:HB1	1.74	0.69
1:C:359:THR:HG22	4:C:502:CZL:S2A	2.33	0.69
2:H:67:MET:CE	2:H:71:SER:HB2	2.22	0.69
1:G:66:SER:HB3	2:H:47:PHE:CE1	2.28	0.69
2:H:289:VAL:HG23	2:H:294:LYS:HD3	1.74	0.69
1:E:403:ASN:N	1:E:403:ASN:OD1	2.26	0.69
1:C:206:ILE:C	1:C:419:GLN:O	2.32	0.69
2:F:344:VAL:HG22	2:F:345:PRO:HD2	1.74	0.69
2:D:168:ARG:CB	2:D:169:PRO:HD3	2.22	0.69
2:H:107:GLN:N	2:H:107:GLN:NE2	2.39	0.69
1:G:417:ILE:O	1:G:417:ILE:HG22	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:197:ASP:OD2	1:C:223:ARG:HD3	1.93	0.69
1:A:220:LEU:HG	1:A:300:THR:HG22	1.75	0.69
1:G:71:GLY:HA2	1:G:420:GLU:O	1.92	0.68
2:B:220:ALA:O	2:B:221:LEU:HB3	1.91	0.68
2:H:168:ARG:CB	2:H:169:PRO:HD3	2.24	0.68
2:D:93:PRO:HG3	2:D:96:ILE:HD11	1.75	0.68
1:A:209:GLU:HG2	1:A:210:PHE:N	2.07	0.68
1:E:332:GLY:H	1:E:334:VAL:HG22	1.57	0.68
2:D:20:GLN:HG3	2:D:145:GLY:CA	2.22	0.68
2:B:159:PRO:HB2	2:B:257:ARG:CB	2.24	0.68
1:E:190:ARG:O	1:E:192:GLY:N	2.21	0.68
1:E:206:ILE:HG13	1:E:419:GLN:CG	2.24	0.68
2:H:34:SER:H	2:H:221:LEU:CD2	2.03	0.68
1:E:381:ASN:N	1:E:381:ASN:HD22	1.91	0.68
2:F:100:THR:CG2	2:F:135:THR:H	2.05	0.68
2:D:344:VAL:HG22	2:D:345:PRO:HD2	1.74	0.68
2:F:333:ARG:HB2	2:F:333:ARG:HH11	1.58	0.68
2:F:117:GLU:C	2:F:122:TYR:OH	2.32	0.68
1:G:206:ILE:C	1:G:419:GLN:O	2.32	0.68
2:F:218:PHE:N	2:F:218:PHE:CD2	2.61	0.68
1:C:339:VAL:O	1:C:343:LEU:HD23	1.94	0.68
2:F:191:SER:HB3	2:F:277:TRP:HZ3	1.58	0.68
2:D:159:PRO:HB3	2:D:257:ARG:HD3	1.75	0.68
2:D:159:PRO:HB2	2:D:257:ARG:CB	2.24	0.68
1:E:404:MET:HB2	1:E:414:PHE:CE1	2.29	0.68
1:G:220:LEU:HG	1:G:300:THR:HG22	1.74	0.68
1:A:207:ALA:HB2	1:A:421:ARG:O	1.94	0.68
1:C:27:LYS:O	1:C:27:LYS:HD2	1.93	0.68
1:C:381:ASN:H	1:C:381:ASN:HD22	1.40	0.68
1:C:252:LYS:HB2	1:C:361:GLU:OE2	1.94	0.68
1:G:359:THR:HG22	4:G:502:CZL:S2A	2.34	0.68
1:E:383:ARG:HG2	1:E:384:VAL:H	1.58	0.68
1:E:409:LYS:HB3	2:F:218:PHE:CZ	2.28	0.68
1:A:381:ASN:H	1:A:381:ASN:HD22	1.40	0.68
1:G:381:ASN:HD22	1:G:381:ASN:N	1.92	0.68
2:D:67:MET:CE	2:D:71:SER:HB2	2.24	0.68
1:C:383:ARG:H	2:D:217:ARG:HH22	1.42	0.68
1:G:37:CYS:CB	1:G:155:GLY:CA	2.67	0.68
2:H:188:ILE:HD11	2:H:268:LEU:HD12	1.74	0.68
2:F:383:SER:OG	2:F:403:GLN:HA	1.94	0.68
2:B:106:THR:C	2:B:107:GLN:HE21	1.97	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:36:GLY:HA2	2:D:43:GLY:HA2	1.76	0.67
2:D:382:ASN:HB2	2:D:402:PRO:O	1.93	0.67
2:D:258:THR:OG1	2:D:260:VAL:HG23	1.94	0.67
1:G:206:ILE:HG13	1:G:419:GLN:CG	2.23	0.67
1:A:36:GLY:HA2	2:B:43:GLY:HA2	1.76	0.67
1:A:332:GLY:H	1:A:334:VAL:HG22	1.58	0.67
1:E:410:GLY:O	1:E:412:VAL:HG23	1.94	0.67
2:H:126:LYS:O	2:H:127:ASP:HB2	1.94	0.67
1:E:450:VAL:HG12	2:H:301:GLN:NE2	2.05	0.67
2:F:333:ARG:NH1	2:F:333:ARG:HB2	2.10	0.67
1:A:29:LYS:N	1:A:29:LYS:HZ1	1.87	0.67
2:B:207:GLY:O	2:B:223:THR:O	2.12	0.67
1:A:382:ALA:HB3	2:B:217:ARG:HG3	1.75	0.67
1:C:123:THR:O	1:C:126:PRO:HD2	1.93	0.67
2:H:159:PRO:HB3	2:H:257:ARG:HD3	1.75	0.67
2:H:315:ARG:HG2	2:H:340:VAL:HG21	1.76	0.67
2:F:315:ARG:HG2	2:F:340:VAL:HG21	1.75	0.67
2:F:289:VAL:HG23	2:F:294:LYS:HD3	1.76	0.67
2:H:119:ARG:C	2:H:122:TYR:CE2	2.67	0.67
2:H:213:LEU:HD13	2:H:218:PHE:HB3	1.77	0.67
2:B:16:LEU:N	2:B:363:ASP:HB3	2.05	0.67
1:G:174:TYR:CE1	1:G:237:VAL:HB	2.30	0.67
2:F:159:PRO:HB2	2:F:257:ARG:CB	2.24	0.67
2:B:191:SER:HB3	2:B:277:TRP:HZ3	1.59	0.67
1:E:37:CYS:HB2	1:E:155:GLY:HA2	1.76	0.67
1:G:339:VAL:O	1:G:343:LEU:HD23	1.95	0.67
1:A:411:ARG:HH22	2:B:214:ASP:HA	1.59	0.67
1:A:174:TYR:CE1	1:A:237:VAL:HB	2.30	0.67
2:D:158:VAL:O	2:D:158:VAL:HG13	1.92	0.67
2:H:382:ASN:HB2	2:H:402:PRO:O	1.94	0.67
2:H:220:ALA:O	2:H:221:LEU:HB3	1.95	0.67
1:C:62:CYS:SG	1:C:123:THR:HG21	2.34	0.67
2:H:16:LEU:N	2:H:363:ASP:HB3	2.06	0.67
2:F:258:THR:OG1	2:F:260:VAL:HG23	1.94	0.67
2:B:270:GLY:O	2:B:274:VAL:HG23	1.95	0.67
2:F:93:PRO:HG3	2:F:96:ILE:HD11	1.77	0.67
2:D:104:SER:O	2:D:109:CYS:HB3	1.94	0.67
2:F:119:ARG:N	2:F:122:TYR:CZ	2.63	0.67
1:C:48:PRO:HB3	1:C:72:THR:HG21	1.77	0.67
2:H:326:LEU:HD11	2:H:350:ALA:HB1	1.75	0.67
2:B:93:PRO:HG3	2:B:96:ILE:CG1	2.25	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:149:ALA:O	2:B:153:ILE:HG13	1.95	0.67
2:F:302:ASP:CB	2:H:211:GLY:HA3	2.25	0.67
1:C:71:GLY:HA2	1:C:420:GLU:O	1.95	0.66
1:A:450:VAL:HG12	2:D:301:GLN:NE2	2.06	0.66
2:H:93:PRO:HG3	2:H:96:ILE:HD11	1.77	0.66
2:B:176:CYS:O	2:B:247:LEU:HD11	1.95	0.66
1:C:403:ASN:OD1	1:C:403:ASN:N	2.28	0.66
2:F:93:PRO:HG3	2:F:96:ILE:CG1	2.26	0.66
2:F:67:MET:CE	2:F:71:SER:HB2	2.25	0.66
2:D:252:ASP:O	2:D:256:GLU:HG2	1.95	0.66
2:H:39:HIS:HD2	2:H:65:THR:CG2	2.08	0.66
1:C:177:GLY:HA3	1:C:241:HIS:CE1	2.30	0.66
1:G:68:ASP:HA	1:G:81:ARG:HH22	1.59	0.66
1:G:398:ILE:HG23	1:G:417:ILE:HG12	1.78	0.66
1:E:197:ASP:OD2	1:E:223:ARG:HD3	1.95	0.66
1:A:30:PRO:HD3	2:B:64:THR:O	1.95	0.66
1:C:37:CYS:HB3	1:C:155:GLY:HA3	1.77	0.66
1:A:94:ILE:HD12	1:A:94:ILE:O	1.96	0.66
2:F:297:ARG:HD2	2:F:417:TYR:OH	1.95	0.66
1:A:397:LEU:HD22	1:A:398:ILE:N	2.11	0.66
2:B:301:GLN:NE2	1:C:450:VAL:HG12	2.03	0.66
1:A:67:TRP:CZ3	2:B:15:PRO:O	2.48	0.66
1:C:68:ASP:HA	1:C:81:ARG:HH22	1.60	0.66
1:C:106:ILE:O	1:C:110:VAL:HG22	1.94	0.66
2:H:124:GLU:CD	2:H:126:LYS:H	2.00	0.66
1:C:310:LYS:NZ	1:G:191:PRO:HG2	2.11	0.66
2:H:258:THR:OG1	2:H:260:VAL:HG23	1.96	0.66
1:E:27:LYS:HD2	1:E:27:LYS:O	1.96	0.66
1:G:174:TYR:HE2	1:G:238:GLN:HG2	1.57	0.66
1:E:346:LEU:O	1:E:346:LEU:HD23	1.96	0.66
2:F:212:HIS:HB3	2:F:223:THR:HG21	1.78	0.66
1:A:380:GLY:HA3	1:A:384:VAL:HG23	1.78	0.66
2:B:168:ARG:HB2	2:B:169:PRO:HD3	1.78	0.66
1:C:301:GLU:O	1:C:304:ILE:HG13	1.96	0.66
2:F:104:SER:O	2:F:109:CYS:HB3	1.96	0.65
1:A:322:LEU:CD2	1:A:439:CYS:SG	2.82	0.65
1:A:71:GLY:HA2	1:A:420:GLU:O	1.96	0.65
1:E:199:ASN:HB2	1:E:246:ASN:ND2	2.12	0.65
1:A:38:SER:OG	1:A:162:LEU:HD12	1.95	0.65
1:C:332:GLY:H	1:C:334:VAL:HG22	1.60	0.65
2:D:119:ARG:N	2:D:122:TYR:CZ	2.64	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:39:HIS:HD2	2:B:65:THR:CG2	2.09	0.65
1:A:381:ASN:N	1:A:381:ASN:HD22	1.92	0.65
2:F:16:LEU:N	2:F:363:ASP:HB3	2.08	0.65
2:F:198:ARG:O	2:F:198:ARG:HG3	1.95	0.65
2:D:379:VAL:O	2:D:396:LEU:HD23	1.96	0.65
1:C:417:ILE:O	1:C:417:ILE:HG22	1.97	0.65
2:D:289:VAL:HG23	2:D:294:LYS:HD3	1.77	0.65
2:H:126:LYS:HZ3	2:H:127:ASP:H	1.45	0.65
1:G:380:GLY:HA3	1:G:384:VAL:HG23	1.76	0.65
2:B:315:ARG:HG2	2:B:340:VAL:HG21	1.76	0.65
2:B:93:PRO:HG3	2:B:96:ILE:HD11	1.77	0.65
1:G:245:VAL:CG1	1:G:290:LEU:HD23	2.26	0.65
2:F:149:ALA:O	2:F:153:ILE:HG13	1.97	0.65
2:H:118:PHE:N	2:H:122:TYR:OH	2.28	0.65
2:B:118:PHE:C	2:B:122:TYR:OH	2.35	0.65
2:H:217:ARG:C	2:H:218:PHE:HD2	2.00	0.65
1:E:108:GLN:HE22	2:F:11:LEU:N	1.89	0.65
1:E:436:ARG:O	1:E:440:ILE:HG23	1.96	0.65
1:G:421:ARG:CZ	1:G:422:GLU:H	2.09	0.65
2:H:39:HIS:HA	2:H:65:THR:OG1	1.96	0.65
1:C:380:GLY:HA3	1:C:384:VAL:HG23	1.78	0.65
1:A:108:GLN:NE2	2:B:11:LEU:HB3	2.11	0.65
1:C:262:GLN:HG3	1:C:263:GLU:N	2.12	0.65
2:B:289:VAL:HG23	2:B:294:LYS:HD3	1.77	0.65
1:G:346:LEU:HD23	1:G:346:LEU:O	1.97	0.65
2:B:126:LYS:O	2:B:127:ASP:HB2	1.97	0.65
1:A:206:ILE:HB	1:A:420:GLU:N	2.11	0.65
2:H:20:GLN:HG2	2:H:135:THR:HB	1.78	0.65
2:F:126:LYS:O	2:F:127:ASP:HB2	1.96	0.65
2:D:126:LYS:O	2:D:127:ASP:HB2	1.96	0.65
1:C:206:ILE:CG2	1:C:420:GLU:HA	2.27	0.65
2:F:382:ASN:HB2	2:F:402:PRO:O	1.96	0.65
1:A:330:TYR:HB3	1:A:399:ALA:HB2	1.78	0.65
2:H:118:PHE:C	2:H:122:TYR:OH	2.35	0.65
2:F:121:GLN:C	2:F:122:TYR:CD1	2.69	0.65
1:A:413:PRO:HA	1:A:447:TRP:CZ2	2.32	0.65
2:H:160:GLU:CG	2:H:161:ARG:H	2.10	0.65
1:E:27:LYS:HD3	2:F:66:ALA:HB1	1.79	0.65
1:E:206:ILE:HB	1:E:420:GLU:N	2.11	0.65
1:G:37:CYS:HB3	1:G:155:GLY:HA3	1.79	0.65
2:D:159:PRO:HB2	2:D:257:ARG:CG	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:168:ARG:NE	2:D:169:PRO:HD3	2.11	0.65
1:G:397:LEU:HD22	1:G:398:ILE:N	2.12	0.65
2:H:82:GLU:O	2:H:86:THR:OG1	2.10	0.65
1:C:209:GLU:HG2	1:C:210:PHE:N	2.07	0.64
1:G:436:ARG:O	1:G:440:ILE:HG23	1.97	0.64
2:D:326:LEU:HD11	2:D:350:ALA:HB1	1.79	0.64
2:H:159:PRO:HB2	2:H:257:ARG:CB	2.28	0.64
2:D:26:LEU:HA	2:D:29:LEU:HB2	1.80	0.64
2:F:28:ILE:HD12	2:F:34:SER:OG	1.97	0.64
1:A:174:TYR:CZ	1:A:234:TYR:CE2	2.86	0.64
1:G:245:VAL:HG13	1:G:290:LEU:HD23	1.76	0.64
2:B:382:ASN:HB2	2:B:402:PRO:O	1.96	0.64
2:H:168:ARG:NE	2:H:169:PRO:HD3	2.12	0.64
1:C:329:LEU:HD13	1:C:340:VAL:HG22	1.79	0.64
1:G:403:ASN:N	1:G:403:ASN:OD1	2.30	0.64
2:F:340:VAL:O	2:F:340:VAL:HG12	1.97	0.64
2:F:302:ASP:HB2	2:H:211:GLY:HA3	1.79	0.64
2:F:160:GLU:CG	2:F:161:ARG:H	2.09	0.64
1:E:206:ILE:HB	1:E:420:GLU:HA	1.80	0.64
1:E:71:GLY:HA2	1:E:420:GLU:O	1.98	0.64
1:G:174:TYR:CZ	1:G:238:GLN:HG2	2.32	0.64
2:H:67:MET:HE2	2:H:71:SER:HB2	1.78	0.64
2:D:198:ARG:O	2:D:198:ARG:HG3	1.98	0.64
1:A:37:CYS:HB3	1:A:155:GLY:HA3	1.76	0.64
1:E:123:THR:O	1:E:126:PRO:HD2	1.96	0.64
2:D:315:ARG:HG2	2:D:340:VAL:HG21	1.79	0.64
1:E:369:LEU:HD23	1:E:370:MET:HB3	1.79	0.64
1:G:329:LEU:HD13	1:G:340:VAL:HG22	1.80	0.64
2:F:420:SER:O	2:F:424:LEU:HD12	1.97	0.64
1:C:191:PRO:CG	1:G:314:ALA:HB2	2.27	0.64
1:E:125:VAL:HB	1:E:126:PRO:HD3	1.80	0.64
1:C:381:ASN:HD22	1:C:381:ASN:N	1.95	0.64
2:B:217:ARG:C	2:B:218:PHE:HD2	2.01	0.64
1:G:177:GLY:HA3	1:G:241:HIS:CE1	2.32	0.64
2:D:100:THR:CG2	2:D:135:THR:H	2.10	0.64
2:F:378:LEU:HD13	2:F:379:VAL:N	2.11	0.64
1:A:417:ILE:HG22	1:A:417:ILE:O	1.96	0.64
2:D:149:ALA:O	2:D:153:ILE:HG13	1.97	0.64
2:D:160:GLU:CG	2:D:161:ARG:H	2.11	0.64
2:D:270:GLY:O	2:D:274:VAL:HG23	1.97	0.64
1:G:421:ARG:NH2	1:G:422:GLU:HB3	2.12	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:LEU:HD23	2:B:106:THR:HG21	1.80	0.64
1:C:369:LEU:HD23	1:C:370:MET:HB3	1.79	0.64
1:C:287:PHE:O	1:C:291:LEU:HD23	1.97	0.64
2:B:160:GLU:CG	2:B:161:ARG:H	2.10	0.64
1:A:369:LEU:HD23	1:A:370:MET:HB3	1.78	0.64
1:E:68:ASP:HA	1:E:81:ARG:HH22	1.62	0.64
1:C:346:LEU:O	1:C:346:LEU:HD23	1.98	0.64
2:B:378:LEU:HD13	2:B:379:VAL:N	2.13	0.64
1:A:432:LEU:O	1:A:436:ARG:HD2	1.98	0.63
1:E:123:THR:CG2	3:E:501:SF4:S4	2.85	0.63
2:D:106:THR:C	2:D:107:GLN:HE21	2.01	0.63
1:E:174:TYR:CZ	1:E:234:TYR:CE2	2.86	0.63
2:D:121:GLN:C	2:D:122:TYR:CD1	2.72	0.63
1:C:420:GLU:HG2	1:C:421:ARG:N	2.13	0.63
1:A:193:ILE:N	1:A:193:ILE:HD12	2.14	0.63
1:C:398:ILE:HG23	1:C:417:ILE:HG12	1.80	0.63
1:A:398:ILE:HG23	1:A:417:ILE:HG12	1.80	0.63
1:C:38:SER:OG	1:C:162:LEU:HD12	1.98	0.63
2:F:207:GLY:O	2:F:223:THR:O	2.16	0.63
2:F:220:ALA:O	2:F:221:LEU:HB3	1.97	0.63
1:C:37:CYS:HB2	1:C:155:GLY:HA2	1.80	0.63
1:A:68:ASP:HA	1:A:81:ARG:HH22	1.62	0.63
1:A:403:ASN:OD1	1:A:403:ASN:N	2.31	0.63
1:C:206:ILE:HB	1:C:420:GLU:N	2.13	0.63
1:G:206:ILE:CG2	1:G:420:GLU:HA	2.27	0.63
1:A:206:ILE:CG2	1:A:420:GLU:HA	2.29	0.63
1:E:411:ARG:HH22	2:F:214:ASP:HA	1.63	0.63
2:B:168:ARG:CB	2:B:169:PRO:HD3	2.29	0.63
2:D:176:CYS:O	2:D:247:LEU:HD11	1.98	0.63
1:A:206:ILE:HG13	1:A:419:GLN:HG3	1.80	0.63
1:C:30:PRO:HD3	2:D:64:THR:O	1.97	0.63
1:E:174:TYR:CZ	1:E:238:GLN:HG2	2.32	0.63
2:B:246:SER:HB3	2:B:323:ASP:OD2	1.98	0.63
2:B:57:ARG:O	2:B:58:GLU:CD	2.37	0.63
1:A:191:PRO:HG2	1:E:310:LYS:HZ3	1.60	0.63
1:A:420:GLU:HG2	1:A:421:ARG:N	2.14	0.63
1:C:123:THR:HG22	3:C:501:SF4:S4	2.38	0.63
2:H:168:ARG:HH21	2:H:169:PRO:HG3	1.63	0.63
2:F:168:ARG:HB2	2:F:169:PRO:HD3	1.81	0.63
2:H:26:LEU:HA	2:H:29:LEU:HB2	1.80	0.63
2:D:31:LEU:O	2:D:221:LEU:HD21	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:379:VAL:O	2:F:396:LEU:HD23	1.97	0.63
2:H:93:PRO:HG3	2:H:96:ILE:CG1	2.29	0.63
1:E:206:ILE:CG2	1:E:420:GLU:HA	2.28	0.63
2:H:31:LEU:O	2:H:221:LEU:HD21	1.99	0.63
2:B:242:VAL:CB	2:B:264:ARG:HB3	2.21	0.63
2:H:106:THR:C	2:H:107:GLN:HE21	2.02	0.63
2:F:38:PHE:HB2	2:F:45:THR:CG2	2.29	0.63
1:A:389:VAL:HG13	1:A:394:ALA:HB3	1.80	0.63
2:F:126:LYS:HZ3	2:F:127:ASP:H	1.45	0.62
1:A:37:CYS:SG	2:B:43:GLY:HA3	2.39	0.62
2:H:382:ASN:HD22	2:H:382:ASN:C	2.02	0.62
1:C:102:LEU:CD2	1:C:106:ILE:HD11	2.29	0.62
2:B:124:GLU:CD	2:B:126:LYS:H	2.02	0.62
1:C:72:THR:HG23	1:C:204:TYR:O	1.99	0.62
1:G:355:THR:HB	1:G:377:LEU:HD11	1.79	0.62
2:D:168:ARG:HH21	2:D:169:PRO:HG3	1.64	0.62
1:G:66:SER:O	1:G:69:ASN:ND2	2.32	0.62
1:A:262:GLN:HG3	1:A:263:GLU:N	2.13	0.62
1:G:404:MET:HB2	1:G:414:PHE:CE1	2.33	0.62
1:E:355:THR:HB	1:E:377:LEU:HD11	1.80	0.62
2:H:121:GLN:C	2:H:122:TYR:CD1	2.72	0.62
1:G:206:ILE:HB	1:G:420:GLU:N	2.13	0.62
1:E:48:PRO:HG2	1:E:229:ALA:HB1	1.81	0.62
1:E:380:GLY:HA3	1:E:384:VAL:HG23	1.80	0.62
1:C:125:VAL:HB	1:C:126:PRO:HD3	1.80	0.62
1:G:193:ILE:H	1:G:193:ILE:CD1	2.11	0.62
1:A:346:LEU:O	1:A:346:LEU:HD23	2.00	0.62
1:A:421:ARG:CZ	1:A:422:GLU:H	2.12	0.62
1:E:48:PRO:HB3	1:E:72:THR:HG21	1.81	0.62
1:C:404:MET:HB2	1:C:414:PHE:CE1	2.34	0.62
2:B:379:VAL:O	2:B:396:LEU:HD23	1.98	0.62
2:H:191:SER:HB3	2:H:277:TRP:HZ3	1.64	0.62
1:E:382:ALA:HB2	1:E:406:THR:HB	1.82	0.62
2:F:100:THR:HG22	2:F:135:THR:N	2.11	0.62
2:H:164:GLN:O	2:H:167:LYS:HG2	2.00	0.62
2:B:121:GLN:C	2:B:122:TYR:CD1	2.72	0.62
2:F:126:LYS:HG3	2:F:127:ASP:N	2.15	0.62
1:A:421:ARG:NH2	1:A:422:GLU:HB3	2.14	0.62
2:F:242:VAL:CB	2:F:264:ARG:HB3	2.26	0.62
1:C:174:TYR:CZ	1:C:238:GLN:HG2	2.34	0.62
1:G:94:ILE:O	1:G:95:MET:O	2.18	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:104:SER:O	2:B:109:CYS:HB3	1.98	0.62
1:C:421:ARG:CZ	1:C:422:GLU:H	2.12	0.62
2:D:213:LEU:HG	2:D:223:THR:HG23	1.81	0.62
1:G:36:GLY:HA2	2:H:43:GLY:HA2	1.82	0.62
2:F:388:SER:O	2:F:392:LEU:HD22	1.99	0.62
2:D:246:SER:HB3	2:D:323:ASP:OD2	1.99	0.62
2:D:164:GLN:O	2:D:167:LYS:HG2	2.00	0.62
1:G:92:ASP:HA	1:G:97:ARG:HB3	1.81	0.62
2:F:158:VAL:HG13	2:F:158:VAL:O	2.00	0.62
2:H:4:ILE:N	2:H:353:ASP:OD2	2.33	0.62
2:F:168:ARG:CB	2:F:169:PRO:HD3	2.29	0.62
2:B:8:ASN:O	2:B:9:LYS:CB	2.46	0.62
1:C:330:TYR:HB3	1:C:399:ALA:HB2	1.81	0.62
2:D:124:GLU:CD	2:D:126:LYS:H	2.03	0.62
2:H:213:LEU:CD2	2:H:214:ASP:H	2.13	0.62
1:A:383:ARG:H	2:B:217:ARG:NH2	1.97	0.62
2:B:348:ALA:O	2:B:349:ALA:O	2.18	0.62
1:C:206:ILE:HG13	1:C:419:GLN:HG3	1.81	0.62
2:B:31:LEU:O	2:B:221:LEU:HD21	2.00	0.62
1:A:410:GLY:O	1:A:412:VAL:HG23	2.00	0.62
2:B:38:PHE:HB2	2:B:45:THR:CG2	2.30	0.62
2:B:118:PHE:N	2:B:122:TYR:OH	2.33	0.61
1:E:383:ARG:CA	2:F:217:ARG:HH12	2.13	0.61
1:G:92:ASP:OD2	1:G:97:ARG:HG2	1.98	0.61
2:F:164:GLN:O	2:F:167:LYS:HG2	2.00	0.61
2:H:388:SER:O	2:H:392:LEU:HD22	2.00	0.61
1:G:125:VAL:HB	1:G:126:PRO:HD3	1.80	0.61
2:H:158:VAL:O	2:H:158:VAL:HG13	2.00	0.61
1:C:193:ILE:H	1:C:193:ILE:CD1	2.10	0.61
1:E:94:ILE:O	1:E:95:MET:O	2.19	0.61
1:C:245:VAL:CG1	1:C:290:LEU:HD23	2.31	0.61
2:H:126:LYS:HG3	2:H:127:ASP:N	2.15	0.61
1:C:421:ARG:NH2	1:C:422:GLU:HB3	2.16	0.61
1:A:27:LYS:CD	2:B:66:ALA:HB1	2.30	0.61
1:G:94:ILE:O	1:G:94:ILE:HD12	2.00	0.61
2:D:34:SER:H	2:D:221:LEU:CD2	2.09	0.61
1:A:172:LEU:HD12	1:A:173:LYS:CA	2.30	0.61
2:F:382:ASN:ND2	2:F:384:HIS:HB2	2.14	0.61
1:G:389:VAL:HG13	1:G:394:ALA:HB3	1.83	0.61
1:G:155:GLY:N	3:G:501:SF4:S4	2.72	0.61
1:E:172:LEU:HD12	1:E:172:LEU:C	2.20	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:349:ALA:O	2:H:350:ALA:C	2.39	0.61
1:G:67:TRP:CH2	2:H:15:PRO:O	2.53	0.61
2:F:168:ARG:NE	2:F:169:PRO:HD3	2.15	0.61
2:B:388:SER:O	2:B:392:LEU:HD22	2.01	0.61
2:D:191:SER:HB3	2:D:277:TRP:HZ3	1.65	0.61
1:E:432:LEU:O	1:E:436:ARG:HD2	2.01	0.61
2:D:42:GLN:CA	2:D:64:THR:HG21	2.30	0.61
1:G:37:CYS:SG	2:H:43:GLY:HA3	2.41	0.61
1:E:172:LEU:HD12	1:E:173:LYS:CA	2.30	0.61
1:C:174:TYR:CZ	1:C:234:TYR:CE2	2.88	0.61
1:E:174:TYR:CE1	1:E:237:VAL:HB	2.35	0.61
2:D:93:PRO:HG3	2:D:96:ILE:CG1	2.30	0.61
1:G:262:GLN:HG3	1:G:263:GLU:N	2.14	0.61
1:E:154:ALA:O	1:E:157:TYR:CD1	2.53	0.61
1:A:176:ILE:O	1:A:177:GLY:C	2.39	0.61
1:A:329:LEU:HD13	1:A:340:VAL:HG22	1.82	0.61
2:H:75:GLY:O	2:H:76:ALA:HB2	2.01	0.61
1:A:310:LYS:NZ	1:E:191:PRO:HG2	2.16	0.61
1:G:48:PRO:HB3	1:G:72:THR:HG21	1.81	0.61
1:A:174:TYR:CZ	1:A:238:GLN:HG2	2.36	0.61
2:H:17:LYS:HG3	2:H:345:PRO:CB	2.28	0.61
2:H:333:ARG:HB2	2:H:333:ARG:NH1	2.15	0.61
1:E:339:VAL:O	1:E:343:LEU:HD23	2.00	0.61
2:F:382:ASN:C	2:F:382:ASN:HD22	2.04	0.61
1:A:404:MET:HB2	1:A:414:PHE:CE1	2.36	0.61
2:F:217:ARG:C	2:F:218:PHE:HD2	2.04	0.61
2:D:317:ALA:HB3	2:D:379:VAL:HG22	1.81	0.61
1:C:314:ALA:HB2	1:G:191:PRO:CB	2.31	0.60
1:E:421:ARG:NH2	1:E:422:GLU:HB3	2.16	0.60
2:H:33:ARG:N	2:H:221:LEU:HD23	2.15	0.60
1:C:67:TRP:CH2	2:D:15:PRO:O	2.54	0.60
2:H:100:THR:CG2	2:H:135:THR:H	2.12	0.60
1:G:306:ARG:NH2	1:G:307:GLU:OE1	2.35	0.60
2:B:340:VAL:HG12	2:B:340:VAL:O	2.01	0.60
1:E:398:ILE:HG23	1:E:417:ILE:HG12	1.83	0.60
2:D:8:ASN:O	2:D:9:LYS:CB	2.48	0.60
1:A:355:THR:HB	1:A:377:LEU:HD11	1.82	0.60
1:C:410:GLY:O	1:C:412:VAL:HG23	2.01	0.60
1:G:369:LEU:HD23	1:G:370:MET:HB3	1.83	0.60
1:C:432:LEU:O	1:C:436:ARG:HD2	2.01	0.60
2:F:93:PRO:HG3	2:F:96:ILE:CD1	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:VAL:HB	1:A:126:PRO:HD3	1.82	0.60
1:G:382:ALA:HB2	1:G:406:THR:HB	1.84	0.60
2:H:28:ILE:HG13	2:H:29:LEU:N	2.15	0.60
2:F:331:LEU:HD22	2:F:331:LEU:O	2.01	0.60
2:F:118:PHE:C	2:F:122:TYR:OH	2.40	0.60
1:A:48:PRO:HB3	1:A:72:THR:HG21	1.84	0.60
2:B:27:ALA:HB2	2:B:146:PHE:CD1	2.36	0.60
1:C:172:LEU:HD12	1:C:173:LYS:CA	2.32	0.60
1:E:68:ASP:HB3	2:F:384:HIS:HE1	1.67	0.60
1:A:339:VAL:O	1:A:343:LEU:HD23	2.02	0.60
2:D:118:PHE:N	2:D:122:TYR:OH	2.35	0.60
1:G:432:LEU:O	1:G:436:ARG:HD2	2.02	0.60
2:F:159:PRO:HG3	2:F:257:ARG:NH1	2.16	0.60
2:B:158:VAL:HG13	2:B:158:VAL:O	2.00	0.60
1:C:108:GLN:NE2	2:D:11:LEU:HB3	2.16	0.60
1:E:176:ILE:O	1:E:177:GLY:C	2.40	0.60
1:E:177:GLY:HA3	1:E:241:HIS:CE1	2.35	0.60
1:G:108:GLN:NE2	2:H:11:LEU:H	1.95	0.60
2:B:168:ARG:HH21	2:B:169:PRO:HG3	1.66	0.60
2:D:388:SER:O	2:D:392:LEU:HD22	2.01	0.60
1:A:356:LYS:HG2	1:A:376:MET:SD	2.42	0.60
2:B:186:GLU:O	2:B:190:GLU:HG2	2.02	0.60
2:B:213:LEU:CD2	2:B:214:ASP:H	2.15	0.60
1:G:54:HIS:HD2	1:G:121:TYR:OH	1.85	0.60
2:H:38:PHE:HB2	2:H:45:THR:CG2	2.32	0.60
2:H:104:SER:O	2:H:109:CYS:HB3	2.02	0.60
1:G:420:GLU:HG2	1:G:421:ARG:N	2.15	0.60
2:F:176:CYS:O	2:F:247:LEU:HD11	2.01	0.60
1:C:310:LYS:HZ3	1:G:191:PRO:HG2	1.67	0.60
1:C:207:ALA:HB2	1:C:421:ARG:O	2.02	0.60
1:E:209:GLU:HG2	1:E:210:PHE:N	2.13	0.60
1:C:128:LEU:HD23	2:D:106:THR:HG21	1.84	0.60
1:E:397:LEU:HD22	1:E:398:ILE:H	1.67	0.60
1:G:106:ILE:O	1:G:110:VAL:HG22	2.02	0.60
1:C:436:ARG:O	1:C:440:ILE:HG23	2.01	0.59
1:E:420:GLU:HG2	1:E:421:ARG:N	2.16	0.59
1:G:359:THR:CG2	4:G:502:CZL:S2A	2.90	0.59
1:C:245:VAL:HG13	1:C:290:LEU:HD23	1.83	0.59
1:A:92:ASP:HA	1:A:97:ARG:HB3	1.84	0.59
2:F:186:GLU:O	2:F:190:GLU:HG2	2.02	0.59
2:B:126:LYS:HZ2	2:B:127:ASP:H	1.48	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:126:LYS:HZ3	2:D:127:ASP:H	1.49	0.59
2:D:217:ARG:C	2:D:218:PHE:CD2	2.76	0.59
2:B:213:LEU:HD13	2:B:218:PHE:HB3	1.83	0.59
1:A:94:ILE:O	1:A:95:MET:O	2.21	0.59
2:B:168:ARG:NE	2:B:169:PRO:HD3	2.16	0.59
1:A:419:GLN:HE22	1:A:424:GLY:H	1.50	0.59
1:C:355:THR:HB	1:C:377:LEU:HD11	1.84	0.59
2:B:38:PHE:HB2	2:B:45:THR:HG22	1.85	0.59
2:F:75:GLY:O	2:F:76:ALA:HB2	2.02	0.59
2:D:331:LEU:HD22	2:D:331:LEU:O	2.02	0.59
1:C:383:ARG:H	2:D:217:ARG:NH2	2.00	0.59
2:B:212:HIS:HB3	2:B:223:THR:HG21	1.84	0.59
1:G:176:ILE:O	1:G:177:GLY:C	2.41	0.59
1:A:67:TRP:O	1:A:81:ARG:NH2	2.36	0.59
2:B:382:ASN:ND2	2:B:384:HIS:H	2.01	0.59
1:G:232:ALA:HA	1:G:236:GLU:OE1	2.03	0.59
1:E:245:VAL:HG13	1:E:290:LEU:HD23	1.83	0.59
1:E:174:TYR:HE2	1:E:238:GLN:HG2	1.60	0.59
1:E:389:VAL:HG13	1:E:394:ALA:HB3	1.84	0.59
1:C:149:ILE:N	1:C:149:ILE:HD12	2.17	0.59
2:D:156:THR:HG22	2:D:157:LEU:HD13	1.83	0.59
1:G:172:LEU:HD12	1:G:172:LEU:C	2.22	0.59
1:G:172:LEU:HD12	1:G:173:LYS:CA	2.32	0.59
2:B:20:GLN:HG2	2:B:135:THR:HB	1.85	0.59
2:B:349:ALA:O	2:B:350:ALA:C	2.41	0.59
1:A:193:ILE:C	1:A:195:VAL:H	2.06	0.59
1:A:92:ASP:OD2	1:A:97:ARG:HG2	2.02	0.59
2:H:212:HIS:HB3	2:H:223:THR:HG21	1.83	0.59
2:F:433:GLU:HG3	2:F:434:HIS:CD2	2.37	0.59
2:D:300:LEU:O	2:D:300:LEU:HD12	2.02	0.59
1:C:389:VAL:HG13	1:C:394:ALA:HB3	1.85	0.59
1:C:382:ALA:HB2	1:C:406:THR:HB	1.85	0.59
2:D:213:LEU:HD13	2:D:218:PHE:HB3	1.84	0.59
1:C:199:ASN:ND2	1:C:225:LEU:HB2	2.14	0.59
1:E:245:VAL:CG1	1:E:290:LEU:HD23	2.33	0.59
2:D:297:ARG:HD2	2:D:417:TYR:OH	2.03	0.59
1:E:421:ARG:NH2	1:E:422:GLU:H	2.00	0.59
1:A:172:LEU:C	1:A:172:LEU:HD12	2.23	0.59
2:H:100:THR:HG22	2:H:135:THR:N	2.13	0.59
1:G:108:GLN:NE2	2:H:11:LEU:HB3	2.17	0.59
2:D:410:PHE:CE2	2:D:411:GLN:HB2	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:36:GLY:HA2	2:F:43:GLY:HA2	1.84	0.58
2:H:93:PRO:HG3	2:H:96:ILE:CD1	2.33	0.58
1:C:337:TRP:CE3	1:C:337:TRP:O	2.56	0.58
1:A:196:HIS:HB3	1:A:291:LEU:HD11	1.85	0.58
1:A:27:LYS:O	1:A:27:LYS:HD2	2.02	0.58
2:B:173:ASN:HB2	2:B:240:THR:CG2	2.20	0.58
1:E:27:LYS:HD3	2:F:66:ALA:CB	2.33	0.58
1:E:206:ILE:HB	1:E:420:GLU:CA	2.33	0.58
1:A:382:ALA:HB2	1:A:406:THR:HB	1.85	0.58
2:F:159:PRO:CG	2:F:257:ARG:NH1	2.65	0.58
1:C:154:ALA:O	1:C:157:TYR:CD1	2.56	0.58
1:C:92:ASP:OD2	1:C:97:ARG:HG2	2.04	0.58
2:H:252:ASP:O	2:H:256:GLU:HG2	2.04	0.58
1:E:330:TYR:HB3	1:E:399:ALA:HB2	1.86	0.58
2:B:76:ALA:O	2:B:77:ASP:C	2.42	0.58
1:E:29:LYS:CB	1:E:30:PRO:HD2	2.30	0.58
2:F:106:THR:C	2:F:107:GLN:HE21	2.05	0.58
2:H:213:LEU:HG	2:H:223:THR:HG23	1.86	0.58
2:B:100:THR:CG2	2:B:135:THR:H	2.16	0.58
2:D:348:ALA:O	2:D:349:ALA:O	2.21	0.58
1:C:94:ILE:O	1:C:95:MET:O	2.22	0.58
1:A:359:THR:HG22	4:A:502:CZL:S2A	2.43	0.58
1:C:108:GLN:CD	2:D:11:LEU:HB3	2.23	0.58
1:E:327:VAL:HG21	1:E:343:LEU:CD1	2.34	0.58
2:F:246:SER:HB3	2:F:323:ASP:OD2	2.03	0.58
2:F:118:PHE:N	2:F:122:TYR:OH	2.36	0.58
2:F:124:GLU:CD	2:F:126:LYS:H	2.06	0.58
2:D:382:ASN:HD22	2:D:382:ASN:C	2.06	0.58
2:B:67:MET:HE3	2:B:71:SER:HB2	1.85	0.58
1:G:29:LYS:HG3	2:H:66:ALA:HB3	1.85	0.58
2:F:213:LEU:HD13	2:F:218:PHE:HB3	1.85	0.58
2:F:38:PHE:CD2	2:F:45:THR:HG22	2.38	0.58
1:C:232:ALA:HA	1:C:236:GLU:OE1	2.04	0.58
2:B:297:ARG:HD2	2:B:417:TYR:OH	2.03	0.58
1:E:92:ASP:OD2	1:E:97:ARG:HG2	2.03	0.58
2:B:117:GLU:C	2:B:122:TYR:HH	2.07	0.58
1:C:174:TYR:CE1	1:C:237:VAL:HB	2.39	0.58
1:E:193:ILE:C	1:E:195:VAL:H	2.06	0.58
2:B:211:GLY:HA3	2:D:302:ASP:CB	2.34	0.58
2:F:38:PHE:HB2	2:F:45:THR:HG22	1.86	0.58
1:C:190:ARG:HB3	1:C:191:PRO:HD2	0.73	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:27:LYS:CD	2:D:66:ALA:HB1	2.32	0.58
1:C:409:LYS:HB3	2:D:218:PHE:HZ	1.65	0.58
1:E:92:ASP:HA	1:E:97:ARG:HB3	1.85	0.58
2:F:188:ILE:HD11	2:F:268:LEU:HD12	1.86	0.58
1:G:30:PRO:HD3	2:H:64:THR:O	2.03	0.58
1:A:204:TYR:CE1	1:A:229:ALA:HB3	2.39	0.57
1:C:176:ILE:O	1:C:177:GLY:C	2.43	0.57
2:D:17:LYS:HG3	2:D:345:PRO:CB	2.32	0.57
1:G:199:ASN:ND2	1:G:225:LEU:HB2	2.17	0.57
2:H:397:LEU:CD2	2:H:427:LEU:HD21	2.33	0.57
2:H:156:THR:HG22	2:H:157:LEU:HD13	1.86	0.57
2:H:8:ASN:O	2:H:9:LYS:CB	2.51	0.57
2:H:410:PHE:CE2	2:H:411:GLN:HB2	2.39	0.57
1:G:373:ASP:CG	1:G:374:VAL:H	2.08	0.57
2:H:126:LYS:HG3	2:H:127:ASP:H	1.68	0.57
1:E:86:THR:HG23	1:E:86:THR:O	2.04	0.57
1:E:54:HIS:HD2	1:E:121:TYR:OH	1.87	0.57
2:D:38:PHE:HB2	2:D:45:THR:CG2	2.33	0.57
1:C:27:LYS:C	1:C:27:LYS:HD2	2.25	0.57
1:A:37:CYS:CB	1:A:155:GLY:CA	2.72	0.57
2:D:20:GLN:HG2	2:D:135:THR:CB	2.35	0.57
1:A:370:MET:O	1:A:370:MET:HG2	2.02	0.57
2:B:42:GLN:CA	2:B:64:THR:HG21	2.35	0.57
2:D:382:ASN:ND2	2:D:384:HIS:H	2.02	0.57
2:D:168:ARG:HB2	2:D:169:PRO:CD	2.34	0.57
2:B:191:SER:CB	2:B:277:TRP:HZ3	2.16	0.57
1:G:287:PHE:O	1:G:291:LEU:HD23	2.04	0.57
2:D:118:PHE:C	2:D:122:TYR:OH	2.40	0.57
1:C:206:ILE:HB	1:C:420:GLU:HA	1.87	0.57
1:A:206:ILE:HB	1:A:420:GLU:HA	1.87	0.57
1:C:193:ILE:C	1:C:195:VAL:H	2.08	0.57
1:C:68:ASP:O	1:C:81:ARG:NH2	2.38	0.57
2:F:49:LYS:O	2:F:53:VAL:HG13	2.03	0.57
2:B:39:HIS:HA	2:B:65:THR:OG1	2.05	0.57
1:E:206:ILE:CB	1:E:420:GLU:HA	2.35	0.57
1:G:27:LYS:HD3	2:H:66:ALA:CB	2.33	0.57
2:H:317:ALA:HB3	2:H:379:VAL:HG22	1.85	0.57
1:C:204:TYR:HA	1:C:229:ALA:O	2.05	0.57
1:C:37:CYS:CB	1:C:155:GLY:CA	2.72	0.57
2:F:349:ALA:O	2:F:350:ALA:C	2.43	0.57
1:G:108:GLN:CD	2:H:11:LEU:HB3	2.24	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:340:VAL:CG1	2:F:340:VAL:O	2.51	0.57
2:F:382:ASN:ND2	2:F:384:HIS:H	2.03	0.57
2:F:8:ASN:O	2:F:9:LYS:CB	2.52	0.57
1:C:181:PRO:HD3	1:C:242:ARG:HG3	1.86	0.57
2:H:176:CYS:O	2:H:247:LEU:HD11	2.04	0.57
1:C:204:TYR:CE1	1:C:229:ALA:HB3	2.40	0.57
1:A:29:LYS:N	1:A:29:LYS:HZ2	1.93	0.57
2:D:212:HIS:HB3	2:D:223:THR:HG21	1.85	0.57
2:B:213:LEU:HG	2:B:223:THR:HG23	1.86	0.57
1:C:172:LEU:HD12	1:C:172:LEU:C	2.24	0.57
1:G:193:ILE:C	1:G:195:VAL:H	2.07	0.57
2:B:340:VAL:CG1	2:B:340:VAL:O	2.53	0.57
2:D:340:VAL:O	2:D:340:VAL:HG12	2.04	0.57
1:E:118:VAL:C	1:E:119:PHE:HD1	2.08	0.57
2:D:95:VAL:HG22	2:D:228:VAL:CG1	2.34	0.57
1:E:301:GLU:O	1:E:304:ILE:HG13	2.05	0.57
2:D:85:LYS:O	2:D:89:GLU:HG2	2.05	0.57
2:H:173:ASN:HB2	2:H:240:THR:CG2	2.23	0.57
2:D:213:LEU:HD12	2:D:223:THR:OG1	2.05	0.57
2:B:27:ALA:HB2	2:B:146:PHE:CE1	2.40	0.57
1:E:199:ASN:ND2	1:E:225:LEU:HB2	2.14	0.57
2:B:93:PRO:HG3	2:B:96:ILE:CD1	2.34	0.57
2:D:75:GLY:O	2:D:76:ALA:HB2	2.05	0.57
1:C:397:LEU:HD22	1:C:398:ILE:H	1.70	0.56
1:A:102:LEU:CD2	1:A:106:ILE:HD11	2.35	0.56
1:A:337:TRP:O	1:A:337:TRP:CE3	2.58	0.56
2:D:433:GLU:HG3	2:D:434:HIS:HD2	1.69	0.56
2:H:331:LEU:HD22	2:H:331:LEU:O	2.05	0.56
1:G:353:THR:HG22	1:G:377:LEU:HD23	1.85	0.56
2:D:33:ARG:N	2:D:221:LEU:HD23	2.20	0.56
2:H:397:LEU:CD2	2:H:427:LEU:CD2	2.83	0.56
1:E:370:MET:O	1:E:370:MET:HG2	2.04	0.56
1:G:102:LEU:CD2	1:G:106:ILE:HD11	2.36	0.56
1:A:245:VAL:HG13	1:A:290:LEU:HD23	1.87	0.56
2:H:117:GLU:C	2:H:122:TYR:HH	2.04	0.56
1:G:421:ARG:HH22	1:G:422:GLU:HB3	1.71	0.56
1:G:425:TYR:HD1	1:G:433:GLU:OE1	1.89	0.56
1:A:48:PRO:HG2	1:A:229:ALA:HB1	1.87	0.56
1:E:207:ALA:HB2	1:E:421:ARG:O	2.05	0.56
2:F:31:LEU:O	2:F:221:LEU:HD21	2.05	0.56
2:F:34:SER:H	2:F:221:LEU:CD2	2.13	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:34:SER:H	2:B:221:LEU:CD2	2.09	0.56
2:H:159:PRO:CG	2:H:257:ARG:NH1	2.67	0.56
1:A:68:ASP:HB3	2:B:384:HIS:HE1	1.71	0.56
1:G:67:TRP:HZ3	2:H:15:PRO:O	1.87	0.56
2:D:93:PRO:HG3	2:D:96:ILE:CD1	2.34	0.56
2:H:160:GLU:CD	2:H:161:ARG:H	2.08	0.56
2:D:191:SER:CB	2:D:277:TRP:HZ3	2.16	0.56
2:D:433:GLU:HG3	2:D:434:HIS:CD2	2.39	0.56
2:H:383:SER:OG	2:H:403:GLN:HA	2.04	0.56
2:F:82:GLU:O	2:F:86:THR:OG1	2.16	0.56
2:F:118:PHE:O	2:F:119:ARG:HD3	2.04	0.56
1:E:181:PRO:CD	1:E:242:ARG:HG3	2.36	0.56
2:D:126:LYS:HG3	2:D:127:ASP:N	2.20	0.56
1:A:29:LYS:CB	1:A:30:PRO:HD2	2.28	0.56
1:G:356:LYS:HG2	1:G:376:MET:SD	2.45	0.56
2:H:213:LEU:HD12	2:H:223:THR:OG1	2.05	0.56
2:B:433:GLU:HG3	2:B:434:HIS:CD2	2.41	0.56
2:D:173:ASN:HD22	2:D:240:THR:HG22	1.70	0.56
1:G:27:LYS:HD2	1:G:27:LYS:O	2.04	0.56
2:B:28:ILE:HG13	2:B:29:LEU:N	2.21	0.56
2:B:100:THR:HG22	2:B:134:ASN:HA	1.88	0.56
1:E:226:CYS:HB3	1:E:240:MET:HE2	1.88	0.56
2:F:17:LYS:HG3	2:F:345:PRO:CB	2.33	0.56
1:G:67:TRP:O	1:G:81:ARG:NH2	2.39	0.56
2:D:38:PHE:CD2	2:D:45:THR:HG22	2.41	0.56
2:D:213:LEU:CD2	2:D:214:ASP:H	2.16	0.56
2:F:100:THR:HG22	2:F:134:ASN:HA	1.88	0.56
2:D:158:VAL:N	2:D:159:PRO:CD	2.69	0.56
2:B:158:VAL:N	2:B:159:PRO:CD	2.69	0.56
1:G:337:TRP:O	1:G:337:TRP:CE3	2.58	0.56
1:E:287:PHE:O	1:E:291:LEU:HD23	2.05	0.56
1:A:204:TYR:HB2	1:A:206:ILE:HD13	1.88	0.56
1:A:409:LYS:HB3	2:B:218:PHE:HZ	1.71	0.56
1:E:173:LYS:HG3	1:E:173:LYS:O	2.04	0.56
1:E:176:ILE:HG13	1:E:178:THR:HG23	1.88	0.56
1:A:306:ARG:NH2	1:A:307:GLU:OE1	2.39	0.56
1:A:193:ILE:HD13	1:A:293:ASP:OD1	2.06	0.56
1:A:373:ASP:CG	1:A:374:VAL:H	2.09	0.56
2:H:185:LEU:HB2	2:H:206:SER:OG	2.06	0.56
2:B:397:LEU:HD23	2:B:427:LEU:HD21	1.86	0.56
1:E:337:TRP:CE3	1:E:337:TRP:O	2.59	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:173:ASN:HB2	2:D:240:THR:CG2	2.23	0.56
2:F:68:ASP:CB	2:F:70:VAL:HG22	2.24	0.56
2:F:126:LYS:HG3	2:F:127:ASP:H	1.69	0.55
2:D:28:ILE:HD12	2:D:34:SER:OG	2.06	0.55
2:H:158:VAL:N	2:H:159:PRO:CD	2.69	0.55
1:A:67:TRP:C	1:A:67:TRP:CD1	2.79	0.55
2:B:269:TYR:O	2:B:273:ALA:HB3	2.06	0.55
1:G:330:TYR:HB3	1:G:399:ALA:HB2	1.88	0.55
2:H:124:GLU:OE1	2:H:126:LYS:N	2.38	0.55
1:G:421:ARG:NH2	1:G:422:GLU:H	2.03	0.55
1:E:421:ARG:NE	1:E:422:GLU:H	2.03	0.55
2:D:207:GLY:O	2:D:223:THR:O	2.25	0.55
1:E:174:TYR:CZ	1:E:234:TYR:CZ	2.94	0.55
1:A:67:TRP:CH2	2:B:15:PRO:O	2.60	0.55
1:G:67:TRP:C	1:G:67:TRP:CD1	2.79	0.55
1:G:370:MET:HG2	1:G:370:MET:O	2.04	0.55
1:C:275:TYR:CD2	1:C:338:SER:HB2	2.41	0.55
1:A:197:ASP:OD2	1:A:223:ARG:HD3	2.06	0.55
1:A:123:THR:O	1:A:126:PRO:HD2	2.06	0.55
2:D:185:LEU:HB2	2:D:206:SER:OG	2.06	0.55
2:F:213:LEU:CD2	2:F:214:ASP:H	2.16	0.55
2:F:95:VAL:HG22	2:F:228:VAL:CG1	2.37	0.55
2:F:26:LEU:HD21	2:F:401:PHE:CZ	2.42	0.55
1:A:108:GLN:CD	2:B:11:LEU:HB3	2.26	0.55
2:B:67:MET:HE2	2:B:71:SER:HB2	1.88	0.55
2:D:67:MET:HE2	2:D:71:SER:HB2	1.88	0.55
2:H:160:GLU:O	2:H:161:ARG:C	2.45	0.55
1:C:370:MET:O	1:C:370:MET:HG2	2.05	0.55
2:H:191:SER:CB	2:H:277:TRP:HZ3	2.19	0.55
1:A:287:PHE:O	1:A:291:LEU:HD23	2.06	0.55
2:B:75:GLY:O	2:B:76:ALA:HB2	2.06	0.55
1:E:232:ALA:HA	1:E:236:GLU:OE1	2.05	0.55
2:B:110:ASP:HB2	2:B:113:THR:HB	1.89	0.55
1:E:204:TYR:CE1	1:E:229:ALA:HB3	2.41	0.55
1:C:356:LYS:HG2	1:C:376:MET:SD	2.46	0.55
1:C:383:ARG:HE	2:D:90:ARG:HH12	1.54	0.55
1:G:169:GLU:O	1:G:172:LEU:HG	2.05	0.55
2:F:20:GLN:HG2	2:F:135:THR:HB	1.87	0.55
2:F:158:VAL:N	2:F:159:PRO:CD	2.70	0.55
2:B:159:PRO:HB2	2:B:257:ARG:CG	2.37	0.55
2:F:93:PRO:HG3	2:F:96:ILE:HG13	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:93:PRO:HG3	2:H:96:ILE:HG13	1.88	0.55
1:C:92:ASP:HA	1:C:97:ARG:HB3	1.87	0.55
2:B:433:GLU:HG3	2:B:434:HIS:HD2	1.71	0.55
2:D:188:ILE:HD11	2:D:268:LEU:HD12	1.87	0.55
2:H:118:PHE:O	2:H:119:ARG:HD3	2.06	0.55
1:G:190:ARG:HB3	1:G:191:PRO:HD2	0.74	0.55
1:C:383:ARG:N	2:D:217:ARG:HH12	2.05	0.55
1:E:383:ARG:HD2	2:F:217:ARG:HH22	1.72	0.55
2:B:185:LEU:HB2	2:B:206:SER:OG	2.06	0.55
2:B:212:HIS:NE2	2:D:295:ARG:NE	2.54	0.55
2:B:401:PHE:HD2	2:B:401:PHE:O	1.89	0.55
1:G:362:ASP:C	1:G:366:ILE:HG13	2.27	0.55
1:G:174:TYR:CZ	1:G:234:TYR:CE2	2.94	0.55
2:D:349:ALA:O	2:D:350:ALA:C	2.45	0.55
2:H:340:VAL:O	2:H:340:VAL:HG12	2.06	0.55
2:B:164:GLN:O	2:B:167:LYS:HG2	2.06	0.55
1:G:137:CYS:SG	1:G:150:PRO:HB3	2.47	0.55
2:D:396:LEU:HD22	2:D:397:LEU:N	2.21	0.55
1:A:275:TYR:CD2	1:A:338:SER:HB2	2.41	0.55
2:H:246:SER:HB3	2:H:323:ASP:OD2	2.07	0.55
1:E:137:CYS:SG	1:E:150:PRO:HB3	2.47	0.55
1:E:206:ILE:HG13	1:E:419:GLN:HG3	1.88	0.55
1:C:169:GLU:O	1:C:172:LEU:HG	2.07	0.55
1:A:199:ASN:ND2	1:A:225:LEU:HB2	2.13	0.55
2:B:395:PRO:HG3	2:B:434:HIS:CG	2.42	0.55
2:B:285:SER:HB3	2:B:287:ASN:HD21	1.72	0.55
1:E:275:TYR:CD2	1:E:338:SER:HB2	2.41	0.55
1:E:356:LYS:HG2	1:E:376:MET:SD	2.47	0.55
1:A:314:ALA:HB2	1:E:191:PRO:CG	2.37	0.55
1:C:383:ARG:HD2	2:D:217:ARG:HH22	1.72	0.55
1:G:123:THR:O	1:G:126:PRO:HD2	2.06	0.55
1:A:383:ARG:HE	2:B:90:ARG:HH12	1.55	0.55
1:G:173:LYS:HG3	1:G:173:LYS:O	2.05	0.55
1:A:199:ASN:HB2	1:A:246:ASN:ND2	2.21	0.55
1:C:306:ARG:NH2	1:C:307:GLU:OE1	2.40	0.55
1:G:302:ALA:O	1:G:305:ALA:HB3	2.07	0.55
2:F:185:LEU:HB2	2:F:206:SER:OG	2.06	0.55
1:G:409:LYS:HB3	2:H:218:PHE:CZ	2.41	0.55
2:F:213:LEU:HD12	2:F:223:THR:OG1	2.06	0.55
1:C:199:ASN:HB2	1:C:246:ASN:ND2	2.22	0.55
1:C:40:ASP:O	1:C:44:ILE:HG12	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:419:GLN:HE22	1:G:424:GLY:H	1.55	0.54
1:E:27:LYS:C	1:E:27:LYS:HD2	2.27	0.54
1:E:424:GLY:O	1:E:433:GLU:OE2	2.23	0.54
1:G:386:LEU:HD21	2:H:216:ASN:HB3	1.87	0.54
2:H:401:PHE:O	2:H:401:PHE:HD2	1.90	0.54
1:C:67:TRP:O	1:C:81:ARG:NH2	2.39	0.54
2:F:191:SER:CB	2:F:277:TRP:HZ3	2.20	0.54
1:A:355:THR:O	1:A:357:LYS:N	2.37	0.54
1:C:133:VAL:HG23	1:C:134:ASP:OD1	2.07	0.54
1:C:48:PRO:HG2	1:C:229:ALA:HB1	1.89	0.54
1:G:204:TYR:HA	1:G:229:ALA:O	2.06	0.54
2:F:4:ILE:N	2:F:353:ASP:OD2	2.41	0.54
1:E:68:ASP:HB3	2:F:384:HIS:CE1	2.43	0.54
1:G:165:ARG:NH1	4:G:502:CZL:S4B	2.77	0.54
2:D:228:VAL:HG23	2:D:229:ALA:N	2.21	0.54
1:A:54:HIS:HD2	1:A:121:TYR:OH	1.90	0.54
1:E:190:ARG:CB	1:E:191:PRO:CD	2.48	0.54
1:G:440:ILE:HG13	1:G:441:THR:N	2.22	0.54
2:F:42:GLN:CA	2:F:64:THR:HG21	2.35	0.54
1:A:424:GLY:O	1:A:433:GLU:OE2	2.25	0.54
2:H:20:GLN:HG2	2:H:135:THR:CB	2.37	0.54
2:B:160:GLU:CD	2:B:161:ARG:H	2.10	0.54
2:D:55:HIS:CE1	2:D:403:GLN:HG2	2.43	0.54
1:E:132:ASP:O	1:E:136:VAL:HG23	2.07	0.54
1:E:190:ARG:HB3	1:E:191:PRO:HD2	0.72	0.54
1:G:433:GLU:O	1:G:437:GLN:HG2	2.07	0.54
2:F:29:LEU:O	2:F:221:LEU:HD11	2.06	0.54
1:A:421:ARG:NH2	1:A:422:GLU:H	2.06	0.54
2:D:354:SER:HB2	2:D:355:PRO:HD2	1.89	0.54
1:G:68:ASP:HB3	2:H:384:HIS:HE1	1.72	0.54
2:H:76:ALA:O	2:H:77:ASP:C	2.44	0.54
1:G:181:PRO:HD3	1:G:242:ARG:HG3	1.87	0.54
2:D:126:LYS:HG3	2:D:127:ASP:H	1.72	0.54
1:E:71:GLY:HA2	1:E:420:GLU:CA	2.37	0.54
1:C:86:THR:O	1:C:86:THR:HG23	2.07	0.54
2:D:159:PRO:HG3	2:D:257:ARG:NH1	2.18	0.54
2:H:397:LEU:HD22	2:H:427:LEU:HD23	1.89	0.54
1:G:209:GLU:HG2	1:G:210:PHE:N	2.15	0.54
1:G:206:ILE:HB	1:G:420:GLU:HA	1.88	0.54
2:H:64:THR:HG22	2:H:66:ALA:N	2.22	0.54
1:E:57:HIS:O	1:E:126:PRO:HG2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:68:ASP:CA	1:C:81:ARG:HH22	2.21	0.54
1:G:68:ASP:O	1:G:81:ARG:NH2	2.40	0.54
2:H:175:LEU:HB3	2:H:247:LEU:HD13	1.89	0.54
2:B:420:SER:O	2:B:424:LEU:HD12	2.07	0.54
2:H:374:GLY:O	2:H:375:GLN:HB2	2.07	0.54
2:B:173:ASN:HD22	2:B:240:THR:HG22	1.73	0.54
2:B:382:ASN:C	2:B:382:ASN:HD22	2.10	0.54
1:A:193:ILE:H	1:A:193:ILE:CD1	2.16	0.54
1:G:397:LEU:HD22	1:G:398:ILE:H	1.72	0.54
2:F:67:MET:HE2	2:F:71:SER:HB2	1.89	0.54
2:F:160:GLU:CD	2:F:161:ARG:H	2.11	0.54
1:G:196:HIS:HB3	1:G:291:LEU:HD11	1.88	0.54
1:E:373:ASP:CG	1:E:374:VAL:H	2.11	0.54
1:G:444:CYS:SG	1:G:446:VAL:HG23	2.47	0.54
1:G:228:LEU:O	1:G:229:ALA:HB3	2.08	0.54
1:A:206:ILE:HB	1:A:420:GLU:CA	2.37	0.54
1:G:37:CYS:HB2	1:G:39:PHE:H	1.72	0.54
1:C:359:THR:CG2	4:C:502:CZL:S2A	2.96	0.54
1:E:94:ILE:O	1:E:94:ILE:CD1	2.56	0.54
2:B:89:GLU:OE2	2:B:124:GLU:HB2	2.07	0.54
1:C:29:LYS:CB	1:C:30:PRO:HD2	2.33	0.54
1:C:355:THR:O	1:C:357:LYS:N	2.37	0.54
1:E:193:ILE:C	1:E:195:VAL:N	2.62	0.54
1:A:154:ALA:O	1:A:157:TYR:CD1	2.61	0.54
1:G:199:ASN:HB2	1:G:246:ASN:ND2	2.22	0.54
2:B:17:LYS:HG3	2:B:345:PRO:CB	2.35	0.54
2:F:24:ALA:HB1	2:F:149:ALA:HB2	1.90	0.54
2:D:331:LEU:C	2:D:331:LEU:HD22	2.28	0.54
2:D:26:LEU:HD21	2:D:401:PHE:CZ	2.43	0.53
2:D:160:GLU:CD	2:D:161:ARG:H	2.12	0.53
1:A:353:THR:HG22	1:A:377:LEU:HD23	1.90	0.53
2:F:76:ALA:O	2:F:77:ASP:C	2.45	0.53
2:F:125:TYR:O	2:F:126:LYS:CB	2.56	0.53
1:G:206:ILE:HG13	1:G:419:GLN:HG3	1.89	0.53
1:G:421:ARG:NE	1:G:422:GLU:H	2.05	0.53
2:H:95:VAL:HG22	2:H:228:VAL:CG1	2.38	0.53
1:E:362:ASP:C	1:E:366:ILE:HG13	2.28	0.53
1:A:196:HIS:ND1	1:A:291:LEU:HD12	2.23	0.53
2:D:76:ALA:O	2:D:77:ASP:C	2.47	0.53
1:E:421:ARG:HH22	1:E:422:GLU:HB3	1.73	0.53
1:E:62:CYS:HA	3:E:501:SF4:S3	2.49	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:354:SER:CB	2:B:355:PRO:HD2	2.38	0.53
2:D:256:GLU:OE2	2:D:256:GLU:HA	2.08	0.53
2:H:420:SER:O	2:H:424:LEU:HD12	2.07	0.53
2:H:186:GLU:O	2:H:190:GLU:HG2	2.08	0.53
2:H:49:LYS:O	2:H:53:VAL:HG13	2.08	0.53
2:H:110:ASP:HB2	2:H:113:THR:HB	1.89	0.53
2:B:126:LYS:HG3	2:B:127:ASP:N	2.23	0.53
1:C:206:ILE:HB	1:C:420:GLU:CA	2.38	0.53
1:A:433:GLU:O	1:A:437:GLN:HG2	2.07	0.53
2:F:173:ASN:HD22	2:F:240:THR:HG22	1.73	0.53
1:G:29:LYS:HG2	2:H:65:THR:O	2.09	0.53
1:G:380:GLY:HA2	1:G:383:ARG:HD3	1.90	0.53
1:G:383:ARG:H	2:H:217:ARG:HH22	1.56	0.53
2:D:344:VAL:O	2:D:361:VAL:HA	2.08	0.53
2:H:315:ARG:HG3	2:H:340:VAL:HG21	1.89	0.53
2:F:269:TYR:O	2:F:273:ALA:HB3	2.08	0.53
2:H:85:LYS:O	2:H:89:GLU:HG2	2.08	0.53
1:C:353:THR:HG22	1:C:377:LEU:HD23	1.89	0.53
2:B:33:ARG:N	2:B:221:LEU:HD23	2.22	0.53
1:C:123:THR:CG2	3:C:501:SF4:S4	2.97	0.53
1:A:241:HIS:N	1:A:241:HIS:ND1	2.52	0.53
2:H:275:ASP:OD1	2:H:297:ARG:NE	2.29	0.53
2:H:333:ARG:HB2	2:H:333:ARG:HH11	1.72	0.53
2:D:333:ARG:HB2	2:D:333:ARG:NH1	2.23	0.53
1:C:54:HIS:HD2	1:C:121:TYR:OH	1.92	0.53
2:B:4:ILE:N	2:B:353:ASP:OD2	2.42	0.53
1:A:68:ASP:HB3	2:B:384:HIS:CE1	2.43	0.53
2:B:95:VAL:HG22	2:B:228:VAL:CG1	2.38	0.53
1:A:397:LEU:HD22	1:A:398:ILE:H	1.74	0.53
2:H:38:PHE:CD2	2:H:45:THR:HG22	2.44	0.53
2:D:385:ALA:O	2:D:386:LEU:C	2.46	0.53
2:B:85:LYS:O	2:B:89:GLU:HG2	2.09	0.53
2:D:28:ILE:HD11	2:D:36:PRO:N	2.23	0.53
2:D:351:LEU:O	2:D:353:ASP:N	2.42	0.53
1:A:307:GLU:O	1:A:311:VAL:CG2	2.54	0.53
1:G:193:ILE:C	1:G:195:VAL:N	2.62	0.53
1:E:102:LEU:HD23	1:E:102:LEU:O	2.09	0.53
1:G:327:VAL:O	1:G:327:VAL:HG23	2.09	0.53
1:C:337:TRP:CD1	1:C:365:ARG:HG2	2.44	0.53
1:E:228:LEU:O	1:E:229:ALA:HB3	2.09	0.53
1:A:380:GLY:HA2	1:A:383:ARG:HD3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:128:LEU:HD23	2:H:106:THR:HG21	1.90	0.53
2:D:353:ASP:O	2:D:354:SER:OG	2.21	0.53
1:C:193:ILE:C	1:C:195:VAL:N	2.62	0.53
2:F:333:ARG:CB	2:F:333:ARG:HH11	2.20	0.53
2:H:75:GLY:O	2:H:76:ALA:CB	2.57	0.53
2:D:38:PHE:HB2	2:D:45:THR:HG22	1.91	0.53
1:A:335:LYS:O	1:A:338:SER:OG	2.27	0.53
2:F:252:ASP:O	2:F:256:GLU:HG2	2.09	0.53
1:E:133:VAL:HG23	1:E:134:ASP:OD1	2.09	0.53
2:H:118:PHE:O	2:H:122:TYR:CE2	2.61	0.53
1:C:380:GLY:HA2	1:C:383:ARG:HD3	1.91	0.53
2:D:401:PHE:HD2	2:D:401:PHE:O	1.92	0.53
2:D:57:ARG:O	2:D:58:GLU:CD	2.47	0.53
1:G:300:THR:O	1:G:304:ILE:HG23	2.09	0.53
1:A:327:VAL:HG21	1:A:343:LEU:CD1	2.39	0.53
2:H:256:GLU:HA	2:H:256:GLU:OE2	2.09	0.53
1:G:181:PRO:CD	1:G:242:ARG:HG3	2.39	0.53
2:B:333:ARG:NH1	2:B:333:ARG:HB2	2.24	0.53
1:A:191:PRO:HG2	1:E:310:LYS:HZ2	1.74	0.53
1:G:440:ILE:HG13	1:G:441:THR:H	1.74	0.53
1:A:57:HIS:HE1	1:A:131:ASP:OD1	1.92	0.53
1:G:68:ASP:CA	1:G:81:ARG:HH22	2.22	0.53
2:D:110:ASP:HB2	2:D:113:THR:HB	1.91	0.52
2:H:28:ILE:HD11	2:H:36:PRO:N	2.24	0.52
1:G:367:ARG:HH21	1:G:375:LYS:HD2	1.74	0.52
2:B:354:SER:HB2	2:B:355:PRO:HD2	1.92	0.52
1:C:241:HIS:N	1:C:241:HIS:ND1	2.49	0.52
2:B:159:PRO:HG3	2:B:257:ARG:NH1	2.19	0.52
1:G:67:TRP:CZ3	2:H:15:PRO:HG2	2.44	0.52
1:A:362:ASP:C	1:A:366:ILE:HG13	2.28	0.52
2:F:433:GLU:HG3	2:F:434:HIS:HD2	1.74	0.52
1:C:337:TRP:CD1	1:C:365:ARG:HB3	2.43	0.52
1:E:40:ASP:O	1:E:44:ILE:HG12	2.10	0.52
2:F:105:GLU:HG2	2:F:136:PRO:HG3	1.91	0.52
1:G:132:ASP:O	1:G:136:VAL:HG23	2.08	0.52
2:D:117:GLU:C	2:D:122:TYR:HH	2.09	0.52
1:G:206:ILE:HG22	1:G:420:GLU:HA	1.90	0.52
1:A:206:ILE:CB	1:A:420:GLU:HA	2.40	0.52
1:A:430:GLY:O	1:A:433:GLU:OE1	2.27	0.52
2:H:31:LEU:HD12	2:H:226:LEU:HB2	1.91	0.52
1:E:380:GLY:HA2	1:E:383:ARG:HD3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:28:ILE:HG13	2:F:29:LEU:N	2.23	0.52
2:B:36:PRO:HB2	2:B:62:LEU:HD13	1.90	0.52
1:A:174:TYR:O	1:A:174:TYR:CD2	2.63	0.52
1:E:154:ALA:O	1:E:157:TYR:HD1	1.92	0.52
2:F:39:HIS:CD2	2:F:80:VAL:HG22	2.44	0.52
2:H:354:SER:CB	2:H:355:PRO:HD2	2.39	0.52
2:H:396:LEU:HD22	2:H:397:LEU:N	2.24	0.52
1:E:67:TRP:O	1:E:81:ARG:NH2	2.42	0.52
2:B:211:GLY:HA3	2:D:302:ASP:HB2	1.90	0.52
2:B:118:PHE:O	2:B:122:TYR:CE2	2.62	0.52
1:C:419:GLN:HE22	1:C:424:GLY:H	1.57	0.52
1:C:421:ARG:NH2	1:C:422:GLU:H	2.07	0.52
1:G:176:ILE:HG13	1:G:178:THR:HG23	1.91	0.52
2:H:348:ALA:O	2:H:349:ALA:O	2.27	0.52
1:A:199:ASN:OD1	1:A:240:MET:HG2	2.09	0.52
1:G:68:ASP:HB3	2:H:384:HIS:CE1	2.44	0.52
1:E:102:LEU:CD2	1:E:106:ILE:HD11	2.40	0.52
1:C:287:PHE:O	1:C:291:LEU:CD2	2.57	0.52
2:H:27:ALA:HB2	2:H:146:PHE:CD1	2.44	0.52
1:A:172:LEU:CD1	1:A:173:LYS:N	2.64	0.52
1:E:241:HIS:N	1:E:241:HIS:ND1	2.45	0.52
2:D:159:PRO:CG	2:D:257:ARG:NH1	2.70	0.52
1:E:67:TRP:CD1	1:E:67:TRP:C	2.82	0.52
1:C:108:GLN:NE2	2:D:11:LEU:H	2.07	0.52
1:C:327:VAL:HG21	1:C:343:LEU:CD1	2.39	0.52
1:G:253:ALA:HA	4:G:502:CZL:S5A	2.49	0.52
2:F:75:GLY:O	2:F:76:ALA:CB	2.57	0.52
1:E:337:TRP:CD1	1:E:365:ARG:HB3	2.44	0.52
1:C:228:LEU:O	1:C:229:ALA:HB3	2.09	0.52
1:C:323:GLU:OE2	1:C:323:GLU:HA	2.09	0.52
2:H:397:LEU:HD23	2:H:427:LEU:CD2	2.35	0.52
1:A:337:TRP:CD1	1:A:365:ARG:HB3	2.45	0.52
2:B:82:GLU:O	2:B:86:THR:OG1	2.20	0.52
1:C:206:ILE:CB	1:C:420:GLU:HA	2.40	0.52
1:C:71:GLY:HA2	1:C:420:GLU:CA	2.40	0.52
2:H:264:ARG:O	2:H:265:PHE:CB	2.54	0.52
1:E:307:GLU:O	1:E:311:VAL:CG2	2.55	0.52
1:C:373:ASP:CG	1:C:374:VAL:H	2.13	0.52
1:C:206:ILE:HG22	1:C:420:GLU:HA	1.90	0.52
1:G:322:LEU:HD22	1:G:322:LEU:N	2.25	0.52
1:E:30:PRO:HD3	2:F:64:THR:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:20:GLN:HG2	2:B:135:THR:CB	2.39	0.52
1:G:336:SER:O	1:G:339:VAL:HG23	2.09	0.52
2:H:118:PHE:HA	2:H:122:TYR:CE1	2.44	0.52
1:G:383:ARG:CA	2:H:217:ARG:HH12	2.22	0.52
2:F:228:VAL:HG23	2:F:229:ALA:N	2.25	0.52
1:C:174:TYR:CZ	1:C:234:TYR:CZ	2.98	0.52
2:F:159:PRO:HB2	2:F:257:ARG:CG	2.39	0.52
2:F:67:MET:HE3	2:F:71:SER:HB2	1.90	0.52
1:A:327:VAL:HG23	1:A:327:VAL:O	2.10	0.52
2:B:331:LEU:HD22	2:B:331:LEU:O	2.10	0.52
1:C:206:ILE:CD1	1:C:419:GLN:HB3	2.40	0.52
1:G:174:TYR:O	1:G:174:TYR:CD2	2.63	0.52
1:C:65:SER:O	1:C:68:ASP:OD1	2.28	0.52
2:B:93:PRO:HG3	2:B:96:ILE:HG13	1.90	0.52
1:C:421:ARG:NE	1:C:422:GLU:H	2.07	0.52
2:B:51:PHE:CE1	2:B:402:PRO:HB3	2.46	0.52
2:F:317:ALA:HB3	2:F:379:VAL:HG22	1.91	0.52
1:G:143:ARG:HB3	1:G:143:ARG:NH1	2.25	0.52
1:A:444:CYS:SG	1:A:446:VAL:HG23	2.50	0.52
2:F:156:THR:HG22	2:F:157:LEU:HD13	1.92	0.52
2:D:126:LYS:HZ2	2:D:127:ASP:H	1.52	0.51
1:A:48:PRO:HG2	1:A:204:TYR:HD1	1.75	0.51
1:A:421:ARG:NE	1:A:422:GLU:H	2.07	0.51
2:F:348:ALA:O	2:F:349:ALA:O	2.27	0.51
1:A:337:TRP:CD1	1:A:365:ARG:HG2	2.45	0.51
1:G:337:TRP:CD1	1:G:365:ARG:HB3	2.44	0.51
1:G:206:ILE:HB	1:G:420:GLU:CA	2.40	0.51
1:A:86:THR:O	1:A:86:THR:HG23	2.09	0.51
2:B:26:LEU:HD21	2:B:401:PHE:CZ	2.45	0.51
1:E:169:GLU:O	1:E:172:LEU:HG	2.10	0.51
1:G:179:ARG:NH2	1:G:239:THR:CG2	2.73	0.51
1:A:252:LYS:CB	1:A:361:GLU:OE2	2.56	0.51
1:G:38:SER:O	1:G:163:GLY:HA3	2.10	0.51
1:C:362:ASP:C	1:C:366:ILE:HG13	2.31	0.51
1:G:328:LEU:HD22	1:G:389:VAL:HG22	1.92	0.51
1:E:353:THR:HG22	1:E:377:LEU:HD23	1.91	0.51
1:E:181:PRO:HD3	1:E:242:ARG:HG3	1.91	0.51
1:A:373:ASP:CG	1:A:374:VAL:N	2.64	0.51
2:F:110:ASP:HB2	2:F:113:THR:HB	1.92	0.51
2:F:85:LYS:O	2:F:89:GLU:HG2	2.10	0.51
2:D:118:PHE:O	2:D:119:ARG:HD3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:ILE:HG22	1:A:420:GLU:HA	1.91	0.51
1:C:30:PRO:HB3	2:D:63:GLN:HG3	1.92	0.51
1:E:306:ARG:NH2	1:E:307:GLU:OE1	2.43	0.51
2:H:57:ARG:O	2:H:58:GLU:CD	2.49	0.51
2:D:228:VAL:CG2	2:D:229:ALA:N	2.73	0.51
1:A:245:VAL:CG1	1:A:290:LEU:HD23	2.39	0.51
1:G:40:ASP:O	1:G:44:ILE:HG12	2.10	0.51
2:D:325:LEU:HD11	2:D:342:ALA:HB1	1.92	0.51
1:E:227:THR:O	1:E:229:ALA:N	2.43	0.51
1:G:355:THR:C	1:G:357:LYS:H	2.14	0.51
2:H:354:SER:HB2	2:H:355:PRO:HD2	1.92	0.51
2:H:382:ASN:ND2	2:H:384:HIS:H	2.07	0.51
1:C:196:HIS:ND1	1:C:291:LEU:HD12	2.26	0.51
2:F:256:GLU:HA	2:F:256:GLU:OE2	2.10	0.51
2:F:89:GLU:OE2	2:F:124:GLU:HB2	2.11	0.51
2:D:124:GLU:OE1	2:D:126:LYS:N	2.42	0.51
1:A:204:TYR:CE1	1:A:229:ALA:CB	2.93	0.51
2:F:213:LEU:HG	2:F:223:THR:HG23	1.93	0.51
1:C:67:TRP:HZ3	2:D:15:PRO:O	1.91	0.51
1:C:94:ILE:O	1:C:94:ILE:CD1	2.56	0.51
1:E:68:ASP:O	1:E:81:ARG:NH2	2.43	0.51
2:D:340:VAL:O	2:D:340:VAL:CG1	2.59	0.51
2:B:228:VAL:HG23	2:B:229:ALA:N	2.24	0.51
2:B:74:MET:O	2:B:76:ALA:N	2.44	0.51
1:A:179:ARG:NH2	1:A:239:THR:CG2	2.73	0.51
1:A:421:ARG:HH22	1:A:422:GLU:HB3	1.74	0.51
1:E:57:HIS:HE1	1:E:131:ASP:OD1	1.94	0.51
1:G:323:GLU:HA	1:G:323:GLU:OE2	2.09	0.51
2:F:396:LEU:HD22	2:F:397:LEU:N	2.25	0.51
2:B:191:SER:HB3	2:B:277:TRP:CZ3	2.43	0.51
2:H:160:GLU:CG	2:H:161:ARG:N	2.72	0.51
1:E:357:LYS:HD2	1:E:357:LYS:N	2.25	0.51
2:B:125:TYR:O	2:B:126:LYS:CB	2.57	0.51
1:C:421:ARG:HH22	1:C:422:GLU:HB3	1.76	0.51
2:H:173:ASN:HD22	2:H:240:THR:HG22	1.76	0.51
1:A:193:ILE:C	1:A:195:VAL:N	2.61	0.51
1:G:252:LYS:CB	1:G:361:GLU:OE2	2.57	0.51
1:A:38:SER:O	1:A:163:GLY:HA3	2.10	0.51
1:E:327:VAL:HG21	1:E:343:LEU:HD11	1.92	0.51
1:A:339:VAL:O	1:A:342:ALA:HB3	2.11	0.51
2:F:175:LEU:HB3	2:F:247:LEU:HD13	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:204:TYR:HB2	1:E:206:ILE:HD13	1.92	0.51
1:E:47:LEU:N	1:E:48:PRO:HD3	2.26	0.51
1:E:367:ARG:HH21	1:E:375:LYS:HD2	1.76	0.51
1:C:336:SER:O	1:C:339:VAL:HG23	2.11	0.51
1:G:198:VAL:HG22	1:G:223:ARG:O	2.11	0.51
1:G:327:VAL:HG21	1:G:343:LEU:CD1	2.40	0.51
2:B:160:GLU:CG	2:B:161:ARG:N	2.74	0.51
1:E:355:THR:C	1:E:357:LYS:H	2.15	0.51
1:A:336:SER:O	1:A:339:VAL:HG23	2.10	0.51
2:H:204:ASP:OD1	2:H:206:SER:HB2	2.11	0.51
2:H:269:TYR:O	2:H:273:ALA:HB3	2.10	0.51
1:C:433:GLU:O	1:C:437:GLN:HG2	2.11	0.51
1:E:204:TYR:CE1	1:E:229:ALA:CB	2.93	0.51
1:G:355:THR:O	1:G:357:LYS:N	2.39	0.51
1:A:169:GLU:O	1:A:172:LEU:HG	2.10	0.51
1:C:174:TYR:OH	1:C:238:GLN:CG	2.59	0.51
1:C:173:LYS:O	1:C:173:LYS:HG3	2.10	0.51
2:D:100:THR:HG22	2:D:135:THR:N	2.15	0.51
2:B:354:SER:CB	2:B:355:PRO:CD	2.89	0.51
2:D:160:GLU:CG	2:D:161:ARG:N	2.73	0.51
2:B:156:THR:HG22	2:B:157:LEU:HD13	1.92	0.51
1:G:133:VAL:HG23	1:G:134:ASP:OD1	2.10	0.51
1:C:204:TYR:CE1	1:C:229:ALA:CB	2.94	0.51
1:C:439:CYS:O	1:C:440:ILE:C	2.49	0.51
1:G:206:ILE:CB	1:G:420:GLU:HA	2.40	0.51
1:G:71:GLY:HA2	1:G:420:GLU:CA	2.41	0.51
1:E:204:TYR:HA	1:E:229:ALA:O	2.11	0.51
1:E:383:ARG:H	2:F:217:ARG:HH22	1.59	0.51
2:B:36:PRO:HB2	2:B:62:LEU:CD1	2.41	0.51
1:C:339:VAL:O	1:C:342:ALA:HB3	2.11	0.51
1:A:296:LEU:O	1:A:300:THR:HG23	2.11	0.51
2:F:55:HIS:CE1	2:F:403:GLN:HG2	2.46	0.51
1:A:330:TYR:HB3	1:A:399:ALA:CB	2.41	0.51
2:F:160:GLU:CG	2:F:161:ARG:N	2.73	0.51
1:C:38:SER:O	1:C:163:GLY:HA3	2.11	0.51
2:B:38:PHE:CD2	2:B:45:THR:HG22	2.46	0.51
2:D:75:GLY:O	2:D:76:ALA:CB	2.59	0.51
1:E:388:THR:O	1:E:392:TYR:HD2	1.94	0.51
2:D:118:PHE:CD2	2:D:118:PHE:O	2.64	0.50
1:A:174:TYR:CZ	1:A:234:TYR:CZ	2.99	0.50
1:G:171:MET:O	1:G:175:VAL:HB	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:138:LYS:NZ	1:C:142:GLU:OE1	2.36	0.50
1:A:143:ARG:HB3	1:A:143:ARG:NH1	2.25	0.50
1:A:132:ASP:O	1:A:136:VAL:HG23	2.10	0.50
2:H:85:LYS:CD	2:H:118:PHE:HE1	2.22	0.50
2:B:124:GLU:OE1	2:B:126:LYS:N	2.43	0.50
2:B:126:LYS:HZ3	2:B:127:ASP:H	1.56	0.50
2:F:117:GLU:C	2:F:122:TYR:HH	2.14	0.50
2:D:126:LYS:NZ	2:D:127:ASP:N	2.55	0.50
2:B:39:HIS:CD2	2:B:80:VAL:HG22	2.46	0.50
1:C:29:LYS:CG	2:D:65:THR:O	2.60	0.50
2:H:28:ILE:HD12	2:H:34:SER:OG	2.11	0.50
1:E:381:ASN:ND2	1:E:381:ASN:N	2.59	0.50
1:A:323:GLU:OE2	1:A:347:GLY:O	2.30	0.50
1:C:327:VAL:HG23	1:C:327:VAL:O	2.11	0.50
2:B:118:PHE:O	2:B:118:PHE:CD2	2.64	0.50
2:B:126:LYS:HG3	2:B:127:ASP:H	1.75	0.50
2:B:264:ARG:O	2:B:265:PHE:CB	2.55	0.50
1:C:355:THR:C	1:C:357:LYS:H	2.14	0.50
1:A:367:ARG:HH21	1:A:375:LYS:HD2	1.76	0.50
1:A:68:ASP:CA	1:A:81:ARG:HH22	2.24	0.50
1:G:154:ALA:O	1:G:157:TYR:CD1	2.64	0.50
2:F:385:ALA:O	2:F:386:LEU:C	2.50	0.50
2:F:118:PHE:CD2	2:F:118:PHE:O	2.64	0.50
1:G:190:ARG:CB	1:G:191:PRO:CD	2.49	0.50
2:D:264:ARG:O	2:D:265:PHE:CB	2.55	0.50
1:C:357:LYS:HD2	1:C:357:LYS:N	2.25	0.50
2:F:36:PRO:HB2	2:F:62:LEU:CD1	2.42	0.50
2:F:401:PHE:HD2	2:F:401:PHE:O	1.94	0.50
2:B:213:LEU:HD22	2:B:215:GLU:H	1.76	0.50
2:B:351:LEU:O	2:B:353:ASP:N	2.44	0.50
1:A:67:TRP:HZ3	2:B:15:PRO:O	1.93	0.50
2:F:275:ASP:OD1	2:F:297:ARG:NE	2.33	0.50
1:E:355:THR:O	1:E:357:LYS:N	2.40	0.50
1:E:377:LEU:HD12	1:E:378:ASP:O	2.12	0.50
1:C:149:ILE:CD1	1:C:149:ILE:N	2.75	0.50
1:E:143:ARG:NH1	1:E:143:ARG:HB3	2.27	0.50
1:A:322:LEU:N	1:A:322:LEU:HD22	2.26	0.50
1:A:57:HIS:O	1:A:126:PRO:HG2	2.11	0.50
1:A:37:CYS:HB2	1:A:39:PHE:H	1.76	0.50
1:G:57:HIS:O	1:G:126:PRO:HG2	2.12	0.50
2:F:31:LEU:HD23	2:F:95:VAL:HG11	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:383:ARG:HE	2:F:90:ARG:HH12	1.58	0.50
1:E:37:CYS:CB	1:E:155:GLY:CA	2.73	0.50
1:E:65:SER:O	1:E:68:ASP:OD1	2.29	0.50
1:G:66:SER:HB3	2:H:47:PHE:CZ	2.47	0.50
2:H:311:LEU:HD23	2:H:431:LEU:HD12	1.93	0.50
1:G:275:TYR:CD2	1:G:338:SER:HB2	2.45	0.50
1:E:153:SER:HB3	1:E:166:ILE:HG21	1.93	0.50
1:A:27:LYS:HD2	1:A:27:LYS:C	2.32	0.50
1:E:322:LEU:HD22	1:E:322:LEU:N	2.27	0.50
1:G:204:TYR:CE1	1:G:229:ALA:HB3	2.47	0.50
1:E:433:GLU:O	1:E:437:GLN:HG2	2.10	0.50
2:H:207:GLY:O	2:H:223:THR:O	2.29	0.50
2:H:213:LEU:HD22	2:H:215:GLU:H	1.76	0.50
1:G:382:ALA:HB3	2:H:217:ARG:HG3	1.93	0.50
1:C:367:ARG:HH21	1:C:375:LYS:HD2	1.75	0.50
1:E:37:CYS:HB3	1:E:155:GLY:HA3	1.86	0.50
1:E:199:ASN:OD1	1:E:240:MET:HG2	2.12	0.50
1:C:94:ILE:O	1:C:94:ILE:CG1	2.60	0.50
1:A:357:LYS:HD2	1:A:357:LYS:N	2.26	0.50
2:F:410:PHE:CE2	2:F:411:GLN:HB2	2.47	0.50
2:F:285:SER:HB3	2:F:287:ASN:HD21	1.75	0.50
2:B:252:ASP:O	2:B:256:GLU:HG2	2.11	0.50
1:E:52:VAL:O	1:E:79:LEU:HD23	2.12	0.50
2:D:374:GLY:O	2:D:375:GLN:HB2	2.11	0.50
1:C:206:ILE:O	1:C:207:ALA:HB3	2.12	0.50
2:F:304:MET:O	2:F:308:HIS:HB3	2.12	0.50
1:C:29:LYS:HG2	2:D:65:THR:O	2.11	0.50
2:H:228:VAL:HG23	2:H:229:ALA:N	2.27	0.50
2:D:353:ASP:O	2:D:354:SER:CB	2.59	0.50
2:H:340:VAL:O	2:H:340:VAL:CG1	2.58	0.50
1:G:339:VAL:O	1:G:342:ALA:HB3	2.11	0.50
2:F:160:GLU:HG2	2:F:161:ARG:H	1.75	0.50
1:E:28:PRO:HD3	1:E:357:LYS:NZ	2.27	0.50
1:E:52:VAL:C	1:E:79:LEU:HD23	2.32	0.50
1:A:227:THR:O	1:A:229:ALA:N	2.44	0.50
2:H:39:HIS:CD2	2:H:80:VAL:HG22	2.47	0.50
2:B:100:THR:HG22	2:B:135:THR:N	2.20	0.50
2:D:354:SER:CB	2:D:355:PRO:HD2	2.42	0.50
1:E:404:MET:CB	1:E:414:PHE:CE1	2.95	0.50
1:E:38:SER:O	1:E:163:GLY:HA3	2.11	0.50
1:E:296:LEU:O	1:E:300:THR:HG23	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:335:LYS:O	1:G:338:SER:OG	2.29	0.50
2:F:124:GLU:O	2:F:125:TYR:C	2.50	0.50
1:G:411:ARG:HH22	2:H:214:ASP:HA	1.77	0.50
2:D:26:LEU:CD1	2:D:146:PHE:CD1	2.94	0.50
1:E:409:LYS:HB3	2:F:218:PHE:HZ	1.73	0.50
1:A:174:TYR:OH	1:A:238:GLN:HG3	2.11	0.50
1:C:179:ARG:NH2	1:C:239:THR:CG2	2.75	0.50
1:C:67:TRP:C	1:C:67:TRP:CD1	2.84	0.50
2:D:93:PRO:HG3	2:D:96:ILE:HG13	1.94	0.50
1:G:373:ASP:CG	1:G:374:VAL:N	2.64	0.50
1:C:312:ARG:HB2	1:C:312:ARG:HH11	1.77	0.50
2:B:118:PHE:HA	2:B:122:TYR:CE1	2.46	0.49
2:F:121:GLN:CA	2:F:122:TYR:CD1	2.95	0.49
1:A:440:ILE:HG13	1:A:441:THR:N	2.27	0.49
1:G:424:GLY:O	1:G:433:GLU:OE2	2.29	0.49
1:C:383:ARG:N	2:D:217:ARG:NH1	2.59	0.49
1:C:181:PRO:CD	1:C:242:ARG:HG3	2.42	0.49
2:H:213:LEU:HD13	2:H:218:PHE:CG	2.47	0.49
1:E:383:ARG:HA	2:F:217:ARG:HH12	1.78	0.49
1:A:177:GLY:HA3	1:A:241:HIS:CE1	2.41	0.49
2:F:354:SER:CB	2:F:355:PRO:HD2	2.41	0.49
1:A:65:SER:O	1:A:68:ASP:OD1	2.30	0.49
1:G:196:HIS:ND1	1:G:291:LEU:HD12	2.27	0.49
1:A:149:ILE:HD12	1:A:149:ILE:N	2.27	0.49
1:A:133:VAL:HG23	1:A:134:ASP:OD1	2.12	0.49
1:C:190:ARG:CB	1:C:191:PRO:CD	2.48	0.49
2:F:27:ALA:HB2	2:F:146:PHE:CD1	2.46	0.49
1:C:57:HIS:HE1	1:C:131:ASP:OD1	1.96	0.49
1:G:367:ARG:HD2	1:G:372:ASP:HA	1.94	0.49
2:B:126:LYS:NZ	2:B:127:ASP:N	2.55	0.49
2:F:118:PHE:HA	2:F:122:TYR:CE1	2.48	0.49
1:G:204:TYR:HB2	1:G:206:ILE:HD13	1.94	0.49
1:C:29:LYS:HG3	2:D:66:ALA:HB3	1.94	0.49
1:G:380:GLY:HA3	1:G:384:VAL:CG2	2.42	0.49
2:D:28:ILE:HG13	2:D:29:LEU:N	2.27	0.49
2:B:159:PRO:CG	2:B:257:ARG:NH1	2.71	0.49
1:A:226:CYS:HB3	1:A:240:MET:HE2	1.94	0.49
1:A:355:THR:C	1:A:357:LYS:H	2.14	0.49
1:G:337:TRP:CD1	1:G:365:ARG:HG2	2.48	0.49
2:F:183:GLY:O	2:F:413:CYS:HB2	2.12	0.49
2:D:118:PHE:O	2:D:122:TYR:CE2	2.66	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:125:TYR:O	2:D:126:LYS:CB	2.58	0.49
1:C:237:VAL:O	1:C:238:GLN:C	2.50	0.49
2:D:4:ILE:N	2:D:353:ASP:OD2	2.46	0.49
1:E:68:ASP:CA	1:E:81:ARG:HH22	2.25	0.49
1:C:220:LEU:CD2	1:C:303:LEU:HD13	2.42	0.49
1:G:381:ASN:N	1:G:381:ASN:ND2	2.60	0.49
2:H:333:ARG:CB	2:H:333:ARG:HH11	2.25	0.49
2:H:126:LYS:HZ3	2:H:127:ASP:N	2.09	0.49
1:A:204:TYR:HA	1:A:229:ALA:O	2.12	0.49
2:D:31:LEU:HD12	2:D:226:LEU:HB2	1.95	0.49
1:C:307:GLU:O	1:C:311:VAL:CG2	2.55	0.49
2:F:297:ARG:HG3	2:F:417:TYR:CE2	2.47	0.49
2:D:49:LYS:O	2:D:53:VAL:HG13	2.11	0.49
2:B:105:GLU:HG2	2:B:136:PRO:HG3	1.93	0.49
2:B:85:LYS:CD	2:B:118:PHE:HE1	2.20	0.49
1:G:209:GLU:HG3	1:G:426:ALA:HB3	1.94	0.49
1:G:207:ALA:HB2	1:G:421:ARG:O	2.12	0.49
1:A:209:GLU:CD	1:A:419:GLN:OE1	2.50	0.49
1:E:206:ILE:CD1	1:E:419:GLN:HB3	2.42	0.49
1:E:206:ILE:HG22	1:E:420:GLU:HA	1.95	0.49
1:E:425:TYR:HD1	1:E:433:GLU:OE1	1.96	0.49
2:F:107:GLN:HE21	2:F:107:GLN:H	1.55	0.49
1:C:381:ASN:HB2	2:D:217:ARG:HH21	1.77	0.49
2:F:351:LEU:O	2:F:353:ASP:N	2.46	0.49
2:H:297:ARG:HG3	2:H:417:TYR:CE2	2.47	0.49
2:H:74:MET:O	2:H:75:GLY:C	2.51	0.49
2:H:38:PHE:HB2	2:H:45:THR:HG22	1.93	0.49
2:F:74:MET:O	2:F:76:ALA:N	2.45	0.49
2:F:387:ALA:O	2:F:391:ARG:HB2	2.13	0.49
1:G:423:PHE:O	1:G:423:PHE:HD2	1.95	0.49
1:C:383:ARG:CD	2:D:217:ARG:HH22	2.26	0.49
1:A:302:ALA:O	1:A:305:ALA:HB3	2.12	0.49
2:D:109:CYS:O	2:D:109:CYS:SG	2.70	0.49
2:B:188:ILE:HD11	2:B:268:LEU:HD12	1.94	0.49
1:C:204:TYR:HB2	1:C:206:ILE:HD13	1.95	0.49
1:C:48:PRO:HB3	1:C:72:THR:CG2	2.43	0.49
1:A:126:PRO:O	1:A:131:ASP:HB2	2.12	0.49
2:B:401:PHE:CD2	2:B:401:PHE:O	2.65	0.49
1:E:179:ARG:NH2	1:E:239:THR:CG2	2.76	0.49
1:G:108:GLN:HE22	2:H:11:LEU:N	2.00	0.49
2:F:344:VAL:HG13	2:F:346:ALA:H	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:LYS:HD2	1:A:361:GLU:HG2	1.94	0.49
2:D:168:ARG:CB	2:D:169:PRO:CD	2.90	0.49
2:D:160:GLU:HG2	2:D:161:ARG:H	1.77	0.49
1:E:336:SER:O	1:E:339:VAL:HG23	2.12	0.49
1:G:61:ALA:HB2	2:H:137:ASP:CG	2.32	0.49
2:F:122:TYR:O	2:F:123:GLU:C	2.50	0.49
2:D:118:PHE:HA	2:D:122:TYR:CE1	2.48	0.49
1:G:48:PRO:HG2	1:G:204:TYR:HD1	1.77	0.49
1:G:28:PRO:HD3	1:G:357:LYS:NZ	2.28	0.49
1:A:409:LYS:C	1:A:411:ARG:H	2.16	0.49
2:D:333:ARG:CB	2:D:333:ARG:HH11	2.26	0.49
2:B:311:LEU:HD23	2:B:431:LEU:HD12	1.94	0.49
1:A:214:LEU:N	1:A:215:PRO:CD	2.76	0.49
2:B:49:LYS:O	2:B:53:VAL:HG13	2.13	0.49
2:B:385:ALA:O	2:B:386:LEU:C	2.50	0.49
1:E:444:CYS:SG	1:E:446:VAL:HG23	2.52	0.49
2:H:125:TYR:O	2:H:126:LYS:CB	2.57	0.48
2:F:126:LYS:HZ3	2:F:127:ASP:N	2.11	0.48
1:C:171:MET:O	1:C:175:VAL:HB	2.13	0.48
1:G:252:LYS:HD2	1:G:361:GLU:HG2	1.95	0.48
2:B:160:GLU:O	2:B:161:ARG:C	2.52	0.48
2:B:160:GLU:HG2	2:B:161:ARG:H	1.78	0.48
1:A:327:VAL:HG21	1:A:343:LEU:HD11	1.95	0.48
2:B:74:MET:O	2:B:75:GLY:C	2.50	0.48
2:D:420:SER:O	2:D:424:LEU:HD12	2.12	0.48
1:E:149:ILE:HD12	1:E:149:ILE:N	2.28	0.48
2:H:126:LYS:CG	2:H:127:ASP:H	2.26	0.48
1:C:425:TYR:HD1	1:C:433:GLU:OE1	1.96	0.48
2:D:378:LEU:HD13	2:D:379:VAL:N	2.28	0.48
1:E:337:TRP:CD1	1:E:365:ARG:HG2	2.48	0.48
1:E:373:ASP:CG	1:E:374:VAL:N	2.66	0.48
2:D:105:GLU:HG2	2:D:136:PRO:HG3	1.95	0.48
2:F:126:LYS:CG	2:F:127:ASP:H	2.26	0.48
2:D:115:LEU:O	2:D:119:ARG:N	2.47	0.48
1:A:27:LYS:CG	2:B:66:ALA:HB1	2.44	0.48
1:G:209:GLU:CD	1:G:419:GLN:OE1	2.51	0.48
1:A:228:LEU:O	1:A:229:ALA:HB3	2.14	0.48
1:C:174:TYR:OH	1:C:238:GLN:HG3	2.12	0.48
2:H:159:PRO:HB2	2:H:257:ARG:CG	2.43	0.48
1:A:67:TRP:CZ3	2:B:15:PRO:HG2	2.47	0.48
1:C:68:ASP:HB3	2:D:384:HIS:CE1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:359:THR:HG22	4:E:502:CZL:S2A	2.53	0.48
2:F:374:GLY:O	2:F:375:GLN:HB2	2.12	0.48
1:A:40:ASP:O	1:A:44:ILE:HG12	2.12	0.48
2:H:385:ALA:O	2:H:386:LEU:C	2.51	0.48
2:F:162:ARG:NE	2:F:162:ARG:HA	2.28	0.48
2:B:315:ARG:HG3	2:B:340:VAL:HG21	1.94	0.48
1:G:343:LEU:HD23	1:G:343:LEU:H	1.77	0.48
2:H:74:MET:O	2:H:76:ALA:N	2.45	0.48
1:C:148:VAL:C	1:C:149:ILE:HD12	2.34	0.48
2:B:256:GLU:HA	2:B:256:GLU:OE2	2.13	0.48
2:D:121:GLN:CA	2:D:122:TYR:CD1	2.97	0.48
1:G:383:ARG:HA	2:H:217:ARG:HH12	1.79	0.48
1:E:323:GLU:OE2	1:E:323:GLU:HA	2.13	0.48
1:G:362:ASP:O	1:G:366:ILE:CG1	2.58	0.48
1:C:64:GLY:O	1:C:67:TRP:HE3	1.95	0.48
1:G:65:SER:O	1:G:68:ASP:OD1	2.30	0.48
1:E:67:TRP:HZ3	2:F:15:PRO:O	1.92	0.48
2:D:397:LEU:CD2	2:D:427:LEU:HD21	2.43	0.48
1:C:330:TYR:HB3	1:C:399:ALA:CB	2.43	0.48
1:G:423:PHE:O	1:G:423:PHE:CD2	2.67	0.48
2:H:124:GLU:O	2:H:125:TYR:C	2.51	0.48
2:D:39:HIS:CD2	2:D:80:VAL:HG22	2.49	0.48
1:E:209:GLU:HG3	1:E:426:ALA:HB3	1.96	0.48
2:B:206:SER:O	2:D:295:ARG:NH2	2.47	0.48
2:H:354:SER:CB	2:H:355:PRO:CD	2.91	0.48
1:C:354:GLY:N	1:C:366:ILE:CD1	2.75	0.48
2:B:228:VAL:CG2	2:B:229:ALA:N	2.76	0.48
1:G:166:ILE:O	1:G:166:ILE:HG22	2.14	0.48
1:A:310:LYS:HZ2	1:E:191:PRO:HG2	1.78	0.48
2:D:304:MET:O	2:D:308:HIS:HB3	2.13	0.48
2:H:401:PHE:O	2:H:401:PHE:CD2	2.67	0.48
2:B:31:LEU:HD12	2:B:226:LEU:HB2	1.96	0.48
1:C:57:HIS:O	1:C:126:PRO:HG2	2.14	0.48
1:E:367:ARG:HD2	1:E:372:ASP:HA	1.96	0.48
1:C:296:LEU:O	1:C:300:THR:HG23	2.13	0.48
2:B:160:GLU:O	2:B:162:ARG:O	2.32	0.48
1:E:304:ILE:HD12	1:E:305:ALA:N	2.28	0.48
1:A:187:GLY:O	1:A:188:SER:HB3	2.12	0.48
1:C:409:LYS:C	1:C:411:ARG:H	2.17	0.48
1:C:300:THR:O	1:C:304:ILE:HG23	2.13	0.48
1:C:328:LEU:HD22	1:C:389:VAL:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:333:ARG:HB2	2:B:333:ARG:HH11	1.78	0.48
2:F:126:LYS:CG	2:F:127:ASP:N	2.76	0.48
1:C:191:PRO:HG2	1:G:310:LYS:NZ	2.29	0.48
1:A:429:ASP:O	1:A:432:LEU:HB2	2.13	0.48
2:B:217:ARG:C	2:B:218:PHE:CD2	2.84	0.48
2:B:28:ILE:HD12	2:B:34:SER:OG	2.14	0.48
1:A:323:GLU:HA	1:A:323:GLU:OE2	2.14	0.48
1:A:171:MET:O	1:A:175:VAL:HB	2.14	0.48
2:F:191:SER:HB3	2:F:277:TRP:CZ3	2.43	0.48
2:D:237:SER:O	2:D:260:VAL:HG13	2.13	0.48
2:D:410:PHE:CD2	2:D:411:GLN:HB2	2.49	0.48
2:B:75:GLY:O	2:B:76:ALA:CB	2.61	0.48
2:D:335:MET:SD	2:D:424:LEU:CD2	3.01	0.48
1:C:388:THR:O	1:C:392:TYR:HD2	1.96	0.48
1:G:214:LEU:N	1:G:215:PRO:CD	2.77	0.48
1:G:353:THR:CG2	1:G:377:LEU:HD23	2.44	0.48
2:B:213:LEU:HD12	2:B:223:THR:OG1	2.13	0.48
2:F:16:LEU:O	2:F:16:LEU:HD12	2.13	0.48
2:F:354:SER:CB	2:F:355:PRO:CD	2.91	0.48
1:G:220:LEU:CD2	1:G:303:LEU:HD13	2.44	0.48
2:D:67:MET:HE3	2:D:71:SER:HB2	1.92	0.48
2:D:175:LEU:HB3	2:D:247:LEU:HD13	1.95	0.48
1:E:196:HIS:HB3	1:E:291:LEU:HD11	1.95	0.48
1:C:52:VAL:C	1:C:79:LEU:HD23	2.35	0.48
1:A:166:ILE:O	1:A:166:ILE:HG22	2.14	0.48
2:F:124:GLU:OE1	2:F:126:LYS:N	2.44	0.47
2:D:85:LYS:CD	2:D:118:PHE:HE1	2.23	0.47
2:F:20:GLN:HG2	2:F:135:THR:CB	2.44	0.47
1:E:174:TYR:OH	1:E:238:GLN:CG	2.62	0.47
1:A:63:ALA:O	1:A:65:SER:N	2.47	0.47
1:A:66:SER:HB3	2:B:47:PHE:CZ	2.49	0.47
2:D:397:LEU:CD2	2:D:427:LEU:CD2	2.92	0.47
2:F:93:PRO:CG	2:F:96:ILE:HG13	2.44	0.47
2:D:95:VAL:CG2	2:D:228:VAL:CG1	2.92	0.47
1:C:335:LYS:O	1:C:338:SER:OG	2.32	0.47
2:H:105:GLU:HG2	2:H:136:PRO:HG3	1.96	0.47
2:B:409:GLY:C	2:B:411:GLN:H	2.17	0.47
1:E:248:MET:SD	1:E:258:ALA:HB2	2.53	0.47
2:B:121:GLN:CA	2:B:122:TYR:CD1	2.97	0.47
2:B:42:GLN:HA	2:B:64:THR:CG2	2.39	0.47
2:B:173:ASN:HD22	2:B:240:THR:CG2	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:42:GLN:HA	2:D:64:THR:CG2	2.38	0.47
1:G:383:ARG:HE	2:H:90:ARG:HH12	1.61	0.47
1:G:172:LEU:CD1	1:G:173:LYS:N	2.65	0.47
2:H:349:ALA:O	2:H:351:LEU:N	2.47	0.47
2:H:351:LEU:O	2:H:353:ASP:N	2.47	0.47
1:A:68:ASP:O	1:A:81:ARG:NH2	2.47	0.47
2:B:382:ASN:HD22	2:B:384:HIS:N	2.12	0.47
2:F:397:LEU:CD2	2:F:427:LEU:CD2	2.92	0.47
2:D:160:GLU:O	2:D:161:ARG:C	2.52	0.47
2:D:74:MET:O	2:D:76:ALA:N	2.47	0.47
2:H:412:ARG:HB3	2:H:414:TRP:CZ3	2.49	0.47
2:F:211:GLY:HA3	2:H:302:ASP:CB	2.44	0.47
2:B:116:HIS:C	2:B:119:ARG:H	2.17	0.47
2:B:124:GLU:O	2:B:125:TYR:C	2.52	0.47
1:C:48:PRO:HG2	1:C:204:TYR:HD1	1.79	0.47
1:C:322:LEU:N	1:C:322:LEU:HD22	2.29	0.47
1:C:430:GLY:O	1:C:433:GLU:OE1	2.32	0.47
1:G:204:TYR:CE1	1:G:229:ALA:CB	2.97	0.47
1:A:206:ILE:O	1:A:419:GLN:O	2.31	0.47
2:H:36:PRO:HB2	2:H:62:LEU:CD1	2.45	0.47
1:A:383:ARG:N	2:B:217:ARG:HH22	2.10	0.47
1:A:193:ILE:CD1	1:A:293:ASP:OD1	2.63	0.47
2:D:397:LEU:HD23	2:D:427:LEU:CD2	2.43	0.47
2:F:38:PHE:CG	2:F:45:THR:HG22	2.48	0.47
2:D:74:MET:O	2:D:75:GLY:C	2.52	0.47
2:H:331:LEU:HD22	2:H:331:LEU:C	2.33	0.47
2:D:383:SER:OG	2:D:403:GLN:HA	2.15	0.47
2:B:410:PHE:CE2	2:B:411:GLN:HB2	2.49	0.47
1:G:138:LYS:NZ	1:G:142:GLU:OE1	2.37	0.47
1:A:137:CYS:SG	1:A:150:PRO:HB3	2.54	0.47
2:D:89:GLU:OE2	2:D:124:GLU:HB2	2.14	0.47
2:D:173:ASN:HD22	2:D:240:THR:CG2	2.26	0.47
1:G:357:LYS:HD2	1:G:357:LYS:N	2.29	0.47
1:C:383:ARG:HD2	2:D:217:ARG:NH2	2.29	0.47
2:F:213:LEU:HD22	2:F:215:GLU:H	1.79	0.47
1:A:380:GLY:HA3	1:A:384:VAL:CG2	2.44	0.47
1:G:174:TYR:CZ	1:G:234:TYR:CZ	3.02	0.47
2:F:397:LEU:HD23	2:F:427:LEU:CD2	2.40	0.47
1:E:343:LEU:HD23	1:E:343:LEU:H	1.79	0.47
2:D:186:GLU:O	2:D:190:GLU:HG2	2.14	0.47
2:D:21:THR:HG21	2:D:137:ASP:OD1	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:285:SER:CB	2:H:287:ASN:HD21	2.27	0.47
1:G:118:VAL:C	1:G:119:PHE:HD1	2.17	0.47
2:H:310:MET:HE3	2:H:310:MET:N	2.30	0.47
2:H:126:LYS:CG	2:H:127:ASP:N	2.77	0.47
1:E:47:LEU:N	1:E:48:PRO:CD	2.78	0.47
1:G:27:LYS:HD2	1:G:27:LYS:C	2.34	0.47
1:A:383:ARG:HD2	2:B:217:ARG:HH22	1.79	0.47
2:B:213:LEU:HD13	2:B:218:PHE:CG	2.50	0.47
1:E:66:SER:HB3	2:F:47:PHE:CZ	2.50	0.47
2:F:325:LEU:HD11	2:F:342:ALA:HB1	1.97	0.47
1:E:61:ALA:HB2	2:F:137:ASP:CG	2.35	0.47
2:H:121:GLN:HB2	2:H:122:TYR:CE1	2.50	0.47
2:D:116:HIS:C	2:D:119:ARG:H	2.18	0.47
1:C:322:LEU:CD2	1:C:439:CYS:SG	2.95	0.47
1:G:377:LEU:HD12	1:G:378:ASP:O	2.15	0.47
2:D:34:SER:N	2:D:221:LEU:HD22	2.11	0.47
2:B:16:LEU:O	2:B:16:LEU:HD12	2.15	0.47
2:D:168:ARG:HE	2:D:168:ARG:HB2	1.54	0.47
1:G:328:LEU:HD23	1:G:397:LEU:HD23	1.95	0.47
2:H:160:GLU:HG2	2:H:161:ARG:H	1.78	0.47
2:D:191:SER:HG	2:D:277:TRP:HZ3	1.62	0.47
1:A:28:PRO:HD3	1:A:357:LYS:NZ	2.29	0.47
2:H:121:GLN:CA	2:H:122:TYR:CD1	2.97	0.47
1:G:206:ILE:O	1:G:207:ALA:HB3	2.13	0.47
1:G:322:LEU:CD2	1:G:439:CYS:SG	2.95	0.47
1:A:207:ALA:CB	1:A:421:ARG:O	2.63	0.47
1:C:28:PRO:HD3	1:C:357:LYS:NZ	2.30	0.47
2:H:100:THR:HG22	2:H:134:ASN:HA	1.97	0.47
2:H:159:PRO:HG3	2:H:257:ARG:NH1	2.21	0.47
2:F:349:ALA:O	2:F:351:LEU:N	2.48	0.47
1:G:64:GLY:O	1:G:67:TRP:HE3	1.97	0.47
2:H:236:GLN:HG2	2:H:236:GLN:O	2.14	0.47
2:F:168:ARG:HB2	2:F:169:PRO:CD	2.45	0.47
2:F:74:MET:O	2:F:75:GLY:C	2.53	0.47
1:E:358:SER:HB2	1:E:363:LYS:HE3	1.97	0.47
1:A:181:PRO:HD3	1:A:242:ARG:HG3	1.94	0.47
2:H:428:ALA:O	2:H:432:VAL:HG23	2.15	0.47
1:A:29:LYS:CG	2:B:65:THR:O	2.62	0.47
1:A:27:LYS:HG3	2:B:66:ALA:HB1	1.97	0.47
1:G:421:ARG:NH2	1:G:422:GLU:CB	2.77	0.47
1:A:209:GLU:OE1	1:A:426:ALA:HB3	2.10	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:GLY:HA2	1:A:420:GLU:CA	2.44	0.47
1:E:206:ILE:CB	1:E:419:GLN:O	2.58	0.47
1:C:367:ARG:HD3	1:C:367:ARG:HA	1.40	0.47
2:D:159:PRO:HB2	2:D:257:ARG:CD	2.44	0.47
1:A:94:ILE:O	1:A:94:ILE:CG1	2.63	0.47
1:A:304:ILE:HD12	1:A:305:ALA:N	2.30	0.47
1:C:327:VAL:HG21	1:C:343:LEU:HD11	1.95	0.47
1:C:396:ILE:HD11	1:C:442:LEU:HD23	1.95	0.47
1:A:232:ALA:HA	1:A:236:GLU:OE1	2.14	0.47
2:B:412:ARG:HB3	2:B:414:TRP:CZ3	2.50	0.47
1:A:62:CYS:HA	3:A:501:SF4:S3	2.55	0.47
2:D:401:PHE:CD2	2:D:401:PHE:O	2.68	0.47
2:F:217:ARG:C	2:F:218:PHE:CD2	2.85	0.47
1:G:323:GLU:OE2	1:G:347:GLY:O	2.33	0.47
1:E:323:GLU:OE2	1:E:347:GLY:O	2.33	0.47
1:E:37:CYS:HB2	1:E:39:PHE:H	1.80	0.47
1:G:404:MET:CB	1:G:414:PHE:CE1	2.97	0.47
1:E:335:LYS:O	1:E:338:SER:OG	2.32	0.47
1:C:373:ASP:CG	1:C:374:VAL:N	2.68	0.47
2:B:310:MET:HG3	2:B:428:ALA:HB1	1.97	0.47
1:A:191:PRO:CG	1:E:314:ALA:HB2	2.44	0.47
2:B:29:LEU:O	2:B:221:LEU:HD11	2.14	0.47
2:B:55:HIS:CE1	2:B:403:GLN:HG2	2.50	0.47
2:D:269:TYR:O	2:D:273:ALA:HB3	2.15	0.47
2:F:113:THR:O	2:F:116:HIS:N	2.47	0.46
1:A:48:PRO:HG2	1:A:204:TYR:CD1	2.50	0.46
1:G:29:LYS:N	1:G:29:LYS:NZ	2.37	0.46
2:H:42:GLN:CA	2:H:64:THR:HG21	2.41	0.46
1:G:354:GLY:N	1:G:366:ILE:CD1	2.78	0.46
1:E:328:LEU:HD22	1:E:389:VAL:HG22	1.97	0.46
1:G:304:ILE:HD12	1:G:305:ALA:N	2.30	0.46
2:H:410:PHE:CD2	2:H:411:GLN:HB2	2.50	0.46
1:E:118:VAL:O	1:E:119:PHE:HD1	1.98	0.46
1:C:31:GLY:N	1:C:33:THR:OG1	2.48	0.46
2:F:121:GLN:HB2	2:F:122:TYR:CE1	2.49	0.46
1:A:206:ILE:CB	1:A:419:GLN:O	2.59	0.46
1:G:27:LYS:CD	2:H:66:ALA:HB1	2.43	0.46
1:E:123:THR:C	1:E:126:PRO:HD2	2.36	0.46
2:D:29:LEU:O	2:D:221:LEU:HD11	2.15	0.46
1:G:58:GLY:O	1:G:86:THR:O	2.33	0.46
1:E:171:MET:O	1:E:175:VAL:HB	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:367:ARG:HD2	1:C:372:ASP:HA	1.97	0.46
1:G:307:GLU:O	1:G:311:VAL:CG2	2.60	0.46
2:H:285:SER:HB3	2:H:287:ASN:HD21	1.79	0.46
2:H:171:GLN:O	2:H:237:SER:HB2	2.16	0.46
2:H:89:GLU:OE2	2:H:124:GLU:HB2	2.14	0.46
1:A:439:CYS:O	1:A:440:ILE:C	2.53	0.46
1:G:424:GLY:C	1:G:433:GLU:OE2	2.54	0.46
1:A:209:GLU:HG3	1:A:426:ALA:HB3	1.96	0.46
2:B:295:ARG:NE	2:D:212:HIS:NE2	2.63	0.46
1:E:409:LYS:C	1:E:411:ARG:H	2.18	0.46
1:A:367:ARG:HD2	1:A:372:ASP:HA	1.98	0.46
2:D:159:PRO:CB	2:D:257:ARG:CD	2.90	0.46
2:H:168:ARG:CB	2:H:169:PRO:CD	2.92	0.46
2:H:93:PRO:CG	2:H:96:ILE:HG13	2.46	0.46
1:A:343:LEU:H	1:A:343:LEU:HD23	1.80	0.46
2:F:311:LEU:HD23	2:F:431:LEU:HD12	1.97	0.46
1:C:214:LEU:N	1:C:215:PRO:CD	2.78	0.46
1:G:388:THR:O	1:G:392:TYR:HD2	1.97	0.46
1:E:48:PRO:HG2	1:E:204:TYR:HD1	1.81	0.46
1:G:409:LYS:HD2	2:H:218:PHE:CZ	2.50	0.46
2:H:228:VAL:CG2	2:H:229:ALA:N	2.78	0.46
2:H:27:ALA:HB2	2:H:146:PHE:CE1	2.50	0.46
2:D:213:LEU:HD22	2:D:215:GLU:H	1.80	0.46
2:F:33:ARG:N	2:F:221:LEU:HD23	2.30	0.46
1:A:381:ASN:HB2	2:B:217:ARG:HH21	1.80	0.46
2:B:212:HIS:CE1	2:D:295:ARG:NE	2.83	0.46
2:B:168:ARG:HB2	2:B:169:PRO:CD	2.44	0.46
2:D:311:LEU:HD23	2:D:431:LEU:HD12	1.97	0.46
1:A:206:ILE:HG12	1:A:206:ILE:H	1.33	0.46
2:B:218:PHE:O	2:B:220:ALA:N	2.49	0.46
2:B:36:PRO:HD2	2:B:61:PRO:O	2.16	0.46
2:H:378:LEU:HD13	2:H:379:VAL:N	2.30	0.46
1:A:404:MET:CB	1:A:414:PHE:CE1	2.99	0.46
1:A:24:GLY:O	1:A:25:CYS:HB3	2.16	0.46
1:G:52:VAL:O	1:G:79:LEU:HD23	2.16	0.46
1:E:440:ILE:HG13	1:E:441:THR:N	2.31	0.46
1:G:206:ILE:CD1	1:G:419:GLN:HB3	2.45	0.46
1:E:174:TYR:CD2	1:E:174:TYR:O	2.68	0.46
2:F:354:SER:HB2	2:F:355:PRO:HD2	1.97	0.46
1:A:78:ASP:O	1:A:81:ARG:HB2	2.16	0.46
1:E:328:LEU:HD23	1:E:397:LEU:HD23	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:95:VAL:HG22	2:B:228:VAL:HG11	1.97	0.46
1:A:214:LEU:HB3	1:A:215:PRO:HD3	1.97	0.46
2:F:116:HIS:HA	2:F:119:ARG:HB2	1.98	0.46
1:C:440:ILE:HG13	1:C:441:THR:N	2.30	0.46
1:E:421:ARG:CZ	1:E:422:GLU:N	2.75	0.46
2:H:226:LEU:HD22	2:H:226:LEU:HA	1.67	0.46
2:H:36:PRO:HB2	2:H:62:LEU:HD13	1.98	0.46
1:E:383:ARG:CD	2:F:217:ARG:HH22	2.29	0.46
2:B:221:LEU:C	2:B:223:THR:N	2.68	0.46
1:G:179:ARG:HB3	1:G:238:GLN:CB	2.46	0.46
1:E:354:GLY:N	1:E:366:ILE:CD1	2.78	0.46
1:C:68:ASP:HB3	2:D:384:HIS:HE1	1.81	0.46
1:C:252:LYS:HD2	1:C:361:GLU:HG2	1.97	0.46
2:H:156:THR:C	2:H:157:LEU:HD13	2.36	0.46
2:B:269:TYR:O	2:B:273:ALA:CB	2.64	0.46
2:B:383:SER:OG	2:B:403:GLN:HA	2.16	0.46
2:D:285:SER:HB3	2:D:287:ASN:HD21	1.81	0.46
1:A:61:ALA:HB2	2:B:137:ASP:CG	2.36	0.46
1:G:155:GLY:HA3	3:G:501:SF4:S4	2.56	0.46
2:F:36:PRO:HB2	2:F:62:LEU:HD13	1.98	0.46
2:F:401:PHE:CD2	2:F:401:PHE:O	2.69	0.46
1:A:382:ALA:O	1:A:386:LEU:N	2.48	0.46
2:B:212:HIS:CE1	2:D:295:ARG:HG3	2.51	0.46
1:G:286:ASP:O	1:G:290:LEU:HB2	2.15	0.46
1:C:196:HIS:HB3	1:C:291:LEU:HD11	1.97	0.46
2:D:38:PHE:CG	2:D:45:THR:HG22	2.51	0.46
2:H:55:HIS:CE1	2:H:403:GLN:HG2	2.51	0.46
2:B:179:ASN:HB3	2:B:324:LEU:HD11	1.98	0.46
2:F:42:GLN:HA	2:F:64:THR:CG2	2.41	0.46
2:D:159:PRO:CB	2:D:257:ARG:CG	2.93	0.46
2:D:100:THR:HG22	2:D:134:ASN:HA	1.98	0.46
2:H:257:ARG:HB3	2:H:257:ARG:CZ	2.45	0.46
1:C:339:VAL:HG11	1:C:417:ILE:HD11	1.98	0.46
1:C:343:LEU:HD23	1:C:343:LEU:H	1.81	0.46
2:B:175:LEU:HB3	2:B:247:LEU:HD13	1.98	0.46
2:H:162:ARG:NE	2:H:162:ARG:HA	2.31	0.46
1:E:339:VAL:O	1:E:342:ALA:HB3	2.16	0.46
2:B:167:LYS:O	2:B:167:LYS:HG3	2.15	0.46
2:B:121:GLN:HB2	2:B:122:TYR:CE1	2.51	0.46
2:H:33:ARG:N	2:H:221:LEU:CD2	2.79	0.46
1:G:174:TYR:OH	1:G:238:GLN:CG	2.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:LEU:HD22	1:A:389:VAL:HG22	1.96	0.46
2:H:160:GLU:O	2:H:162:ARG:O	2.34	0.46
1:A:377:LEU:HD12	1:A:378:ASP:O	2.15	0.46
2:D:91:GLN:HE21	2:D:91:GLN:HB2	1.63	0.46
1:A:310:LYS:HZ3	1:E:191:PRO:HG2	1.81	0.45
1:E:29:LYS:HG3	2:F:66:ALA:HB3	1.98	0.45
2:H:29:LEU:O	2:H:221:LEU:HD11	2.16	0.45
1:A:383:ARG:N	2:B:217:ARG:NH2	2.63	0.45
1:G:316:GLU:HA	1:G:319:ARG:HG3	1.98	0.45
1:C:174:TYR:CD2	1:C:174:TYR:O	2.68	0.45
1:C:323:GLU:OE2	1:C:347:GLY:O	2.34	0.45
1:A:362:ASP:O	1:A:366:ILE:CG1	2.61	0.45
1:C:404:MET:CB	1:C:414:PHE:CE1	2.99	0.45
1:E:341:SER:HA	1:E:344:GLN:HE21	1.80	0.45
2:B:300:LEU:HD12	2:B:300:LEU:O	2.16	0.45
1:E:24:GLY:O	1:E:25:CYS:HB3	2.16	0.45
1:E:189:GLU:O	1:E:190:ARG:O	2.34	0.45
2:D:126:LYS:C	2:D:128:VAL:H	2.20	0.45
2:H:213:LEU:HD13	2:H:218:PHE:CB	2.45	0.45
1:C:179:ARG:HB3	1:C:238:GLN:CB	2.46	0.45
2:B:302:ASP:OD2	2:D:58:GLU:CD	2.55	0.45
2:F:57:ARG:O	2:F:58:GLU:CD	2.55	0.45
1:E:196:HIS:ND1	1:E:291:LEU:HD12	2.31	0.45
1:C:46:LEU:HB2	1:C:121:TYR:OH	2.16	0.45
2:H:33:ARG:H	2:H:221:LEU:HD23	1.80	0.45
1:A:94:ILE:O	1:A:94:ILE:CD1	2.62	0.45
2:H:188:ILE:HD11	2:H:268:LEU:CD1	2.44	0.45
2:D:160:GLU:O	2:D:162:ARG:O	2.34	0.45
1:A:181:PRO:CD	1:A:242:ARG:HG3	2.47	0.45
1:C:118:VAL:C	1:C:119:PHE:HD1	2.20	0.45
2:H:116:HIS:C	2:H:119:ARG:H	2.20	0.45
2:F:113:THR:O	2:F:117:GLU:N	2.47	0.45
1:C:190:ARG:CG	1:C:191:PRO:HD2	2.42	0.45
1:C:383:ARG:HG2	1:C:384:VAL:N	2.28	0.45
1:G:126:PRO:O	1:G:131:ASP:HB2	2.16	0.45
1:G:62:CYS:HA	3:G:501:SF4:S3	2.56	0.45
2:F:26:LEU:CD1	2:F:146:PHE:CD1	2.99	0.45
2:D:16:LEU:HB2	2:D:363:ASP:HA	1.98	0.45
1:G:328:LEU:HD22	1:G:389:VAL:CG2	2.46	0.45
1:A:341:SER:HA	1:A:344:GLN:HE21	1.81	0.45
2:H:299:GLN:OE1	2:H:418:ARG:NH2	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:91:GLN:HB2	2:B:91:GLN:HE21	1.56	0.45
2:D:122:TYR:O	2:D:123:GLU:C	2.55	0.45
1:G:421:ARG:HE	1:G:421:ARG:HB3	1.15	0.45
1:E:382:ALA:CB	2:F:217:ARG:HG3	2.45	0.45
2:D:159:PRO:HB2	2:D:257:ARG:HD3	1.97	0.45
2:F:315:ARG:HG3	2:F:340:VAL:HG21	1.94	0.45
1:C:337:TRP:HE3	1:C:337:TRP:O	1.98	0.45
2:F:102:GLY:HA2	2:F:138:PHE:CE1	2.52	0.45
1:C:295:ASP:O	1:C:299:ARG:HG3	2.17	0.45
2:D:126:LYS:HZ3	2:D:127:ASP:N	2.14	0.45
1:A:174:TYR:OH	1:A:238:GLN:CG	2.64	0.45
1:E:396:ILE:HG23	1:E:413:PRO:HB2	1.98	0.45
1:A:328:LEU:HD22	1:A:389:VAL:CG2	2.47	0.45
2:F:160:GLU:O	2:F:161:ARG:C	2.54	0.45
1:G:52:VAL:C	1:G:79:LEU:HD23	2.37	0.45
2:B:197:LEU:HD12	2:B:281:LEU:HD22	1.98	0.45
1:A:191:PRO:HB2	1:E:310:LYS:HG2	1.98	0.45
1:C:203:GLU:HB3	1:C:227:THR:HG23	1.99	0.45
1:A:425:TYR:HD1	1:A:433:GLU:OE1	1.99	0.45
1:E:419:GLN:HE22	1:E:424:GLY:H	1.65	0.45
1:A:381:ASN:ND2	1:A:381:ASN:N	2.60	0.45
1:C:316:GLU:HA	1:C:319:ARG:HG3	1.99	0.45
2:D:382:ASN:HD22	2:D:384:HIS:N	2.14	0.45
1:E:94:ILE:CG1	1:E:94:ILE:O	2.65	0.45
1:E:78:ASP:O	1:E:81:ARG:HB2	2.17	0.45
1:E:417:ILE:HD13	1:E:417:ILE:HA	1.63	0.45
1:A:220:LEU:CD2	1:A:303:LEU:HD13	2.46	0.45
1:G:340:VAL:O	1:G:344:GLN:HB3	2.17	0.45
2:B:317:ALA:HB3	2:B:379:VAL:HG22	1.97	0.45
1:C:444:CYS:SG	1:C:446:VAL:HG23	2.57	0.45
1:A:190:ARG:CB	1:A:191:PRO:CD	2.41	0.45
2:H:113:THR:O	2:H:117:GLU:N	2.48	0.45
1:C:314:ALA:HB2	1:G:191:PRO:CG	2.46	0.45
1:A:27:LYS:HD3	2:B:66:ALA:HB3	1.95	0.45
1:A:30:PRO:HA	1:A:33:THR:HG1	1.82	0.45
2:B:64:THR:HG22	2:B:66:ALA:N	2.26	0.45
1:G:419:GLN:NE2	1:G:424:GLY:H	2.15	0.45
1:E:172:LEU:CD1	1:E:172:LEU:C	2.84	0.45
1:C:123:THR:C	1:C:126:PRO:HD2	2.37	0.45
2:H:16:LEU:O	2:H:16:LEU:HD12	2.17	0.45
2:D:382:ASN:ND2	2:D:384:HIS:N	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:316:THR:OG1	2:H:339:THR:HA	2.17	0.45
2:H:433:GLU:HG3	2:H:434:HIS:CD2	2.51	0.45
1:A:312:ARG:HH11	1:A:312:ARG:HB2	1.81	0.45
1:G:203:GLU:HB3	1:G:227:THR:HG23	1.99	0.45
2:B:435:HIS:CD2	1:C:422:GLU:HG2	2.51	0.45
1:C:209:GLU:HG3	1:C:426:ALA:HB3	1.98	0.45
1:E:126:PRO:O	1:E:131:ASP:HB2	2.17	0.45
2:B:295:ARG:HG3	2:D:212:HIS:CE1	2.52	0.45
1:E:381:ASN:HB2	2:F:217:ARG:HH21	1.81	0.45
2:D:382:ASN:HD22	2:D:384:HIS:H	1.65	0.45
1:E:252:LYS:HD2	1:E:361:GLU:HG2	1.99	0.45
1:E:341:SER:HA	1:E:344:GLN:NE2	2.32	0.45
2:B:38:PHE:CG	2:B:45:THR:HG22	2.51	0.45
2:B:76:ALA:HA	2:B:79:ASN:OD1	2.17	0.45
2:F:204:ASP:OD1	2:F:206:SER:HB2	2.17	0.45
2:B:156:THR:C	2:B:157:LEU:HD13	2.36	0.45
1:C:132:ASP:O	1:C:136:VAL:HG23	2.15	0.45
1:A:60:ILE:H	1:A:60:ILE:HG12	1.44	0.45
2:F:121:GLN:HB2	2:F:122:TYR:HE1	1.82	0.45
1:A:209:GLU:O	1:A:209:GLU:HG3	2.16	0.45
1:G:354:GLY:O	1:G:375:LYS:O	2.35	0.45
1:E:164:ASN:O	1:E:254:MET:HE2	2.17	0.45
1:A:423:PHE:O	1:A:423:PHE:HD2	1.99	0.45
2:H:304:MET:O	2:H:308:HIS:HB3	2.17	0.44
1:G:209:GLU:OE1	1:G:426:ALA:HB3	2.13	0.44
2:F:363:ASP:O	2:F:366:ASP:HB2	2.17	0.44
2:D:315:ARG:HG3	2:D:340:VAL:HG21	1.96	0.44
1:G:245:VAL:HG11	1:G:290:LEU:HD23	1.99	0.44
2:B:160:GLU:CD	2:B:160:GLU:H	2.21	0.44
1:A:423:PHE:O	1:A:423:PHE:CD2	2.70	0.44
1:A:249:VAL:O	1:A:251:SER:N	2.50	0.44
2:B:113:THR:O	2:B:116:HIS:N	2.47	0.44
2:B:126:LYS:CG	2:B:127:ASP:H	2.31	0.44
2:D:265:PHE:HB3	2:D:266:GLY:H	1.56	0.44
2:H:26:LEU:HD21	2:H:401:PHE:CZ	2.53	0.44
2:F:228:VAL:CG2	2:F:229:ALA:N	2.80	0.44
1:E:108:GLN:NE2	2:F:11:LEU:N	2.55	0.44
2:D:168:ARG:CG	2:D:169:PRO:HD3	2.47	0.44
1:G:94:ILE:O	1:G:94:ILE:CG1	2.66	0.44
2:B:175:LEU:HA	2:B:175:LEU:HD23	1.81	0.44
1:E:187:GLY:O	1:E:188:SER:HB3	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:117:GLU:O	2:F:122:TYR:OH	2.35	0.44
1:G:190:ARG:CG	1:G:191:PRO:HD2	2.41	0.44
1:A:421:ARG:CZ	1:A:422:GLU:N	2.80	0.44
1:E:421:ARG:NH2	1:E:422:GLU:CB	2.80	0.44
1:G:383:ARG:H	2:H:217:ARG:NH2	2.14	0.44
1:C:377:LEU:HD12	1:C:378:ASP:O	2.16	0.44
1:A:316:GLU:HA	1:A:319:ARG:HG3	2.00	0.44
1:A:176:ILE:HG13	1:A:178:THR:HG23	2.00	0.44
2:F:257:ARG:HB3	2:F:257:ARG:CZ	2.47	0.44
2:B:382:ASN:HD22	2:B:384:HIS:H	1.63	0.44
2:D:344:VAL:HG13	2:D:346:ALA:H	1.83	0.44
2:B:344:VAL:HG13	2:B:346:ALA:H	1.83	0.44
2:B:168:ARG:HE	2:B:168:ARG:HB2	1.64	0.44
1:E:404:MET:HB2	1:E:414:PHE:HE1	1.77	0.44
2:H:67:MET:HE3	2:H:71:SER:HB2	1.96	0.44
2:D:162:ARG:NE	2:D:162:ARG:HA	2.31	0.44
1:C:286:ASP:O	1:C:290:LEU:HB2	2.17	0.44
2:D:95:VAL:HG22	2:D:228:VAL:HG11	1.98	0.44
2:B:316:THR:OG1	2:B:339:THR:HA	2.17	0.44
2:H:18:ALA:HB1	2:H:22:MET:CE	2.47	0.44
1:C:187:GLY:O	1:C:188:SER:HB3	2.16	0.44
1:C:60:ILE:HG12	1:C:60:ILE:H	1.50	0.44
1:E:190:ARG:CG	1:E:191:PRO:HD2	2.41	0.44
2:D:124:GLU:O	2:D:125:TYR:C	2.55	0.44
2:F:218:PHE:O	2:F:220:ALA:N	2.50	0.44
2:B:349:ALA:O	2:B:351:LEU:N	2.51	0.44
2:H:353:ASP:O	2:H:354:SER:CB	2.64	0.44
2:H:168:ARG:HB2	2:H:169:PRO:CD	2.37	0.44
1:E:64:GLY:O	1:E:67:TRP:HE3	1.99	0.44
1:A:179:ARG:NH2	1:A:235:ARG:O	2.50	0.44
1:A:388:THR:O	1:A:392:TYR:HD2	2.00	0.44
1:G:379:GLU:H	1:G:379:GLU:HG2	1.53	0.44
1:E:175:VAL:O	1:E:177:GLY:N	2.50	0.44
2:B:20:GLN:HG2	2:B:135:THR:CG2	2.47	0.44
1:C:316:GLU:N	1:C:317:PRO:CD	2.80	0.44
1:G:417:ILE:CG2	1:G:417:ILE:O	2.65	0.44
2:B:362:GLY:HA3	2:B:366:ASP:OD1	2.16	0.44
2:D:271:LEU:HA	2:D:271:LEU:HD23	1.83	0.44
2:F:94:SER:O	2:F:129:PRO:HD2	2.17	0.44
2:D:121:GLN:HB2	2:D:122:TYR:CE1	2.52	0.44
1:E:439:CYS:O	1:E:440:ILE:C	2.54	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:322:LEU:O	1:G:325:LYS:HG2	2.17	0.44
2:D:354:SER:CB	2:D:355:PRO:CD	2.96	0.44
2:B:176:CYS:C	2:B:247:LEU:HD11	2.38	0.44
1:A:198:VAL:HG22	1:A:223:ARG:O	2.18	0.44
1:A:103:PHE:HZ	1:A:143:ARG:HD3	1.83	0.44
1:A:118:VAL:C	1:A:119:PHE:HD1	2.21	0.44
1:E:184:LEU:HG	1:E:184:LEU:H	1.67	0.44
2:F:271:LEU:HD23	2:F:271:LEU:HA	1.83	0.44
2:F:28:ILE:HD11	2:F:36:PRO:N	2.33	0.44
1:E:383:ARG:NE	2:F:90:ARG:HH12	2.16	0.44
1:A:174:TYR:CE2	1:A:234:TYR:CE2	3.05	0.44
1:G:179:ARG:NH2	1:G:235:ARG:O	2.50	0.44
2:B:382:ASN:ND2	2:B:384:HIS:N	2.64	0.44
1:C:302:ALA:O	1:C:305:ALA:HB3	2.17	0.44
1:E:220:LEU:CD2	1:E:303:LEU:HD13	2.47	0.44
2:H:191:SER:HG	2:H:277:TRP:HZ3	1.66	0.44
2:D:191:SER:HB3	2:D:277:TRP:CZ3	2.48	0.44
1:A:340:VAL:O	1:A:344:GLN:HB3	2.17	0.44
2:F:395:PRO:HG3	2:F:434:HIS:CG	2.53	0.44
2:H:185:LEU:CB	2:H:206:SER:OG	2.66	0.44
1:E:166:ILE:O	1:E:166:ILE:HG22	2.18	0.44
1:G:231:ASP:OD1	1:G:233:ARG:NH2	2.50	0.44
2:F:23:GLY:HA3	2:F:142:PHE:O	2.18	0.44
2:H:118:PHE:CD2	2:H:118:PHE:O	2.71	0.44
2:B:89:GLU:OE2	2:B:124:GLU:CB	2.66	0.44
2:D:126:LYS:CG	2:D:127:ASP:H	2.31	0.44
1:A:29:LYS:HG2	2:B:65:THR:O	2.18	0.44
2:F:295:ARG:NE	2:H:212:HIS:NE2	2.66	0.44
1:C:380:GLY:HA3	1:C:384:VAL:CG2	2.46	0.44
2:F:226:LEU:HD22	2:F:226:LEU:HA	1.67	0.44
1:G:68:ASP:N	1:G:68:ASP:OD1	2.51	0.44
2:F:255:ALA:O	2:F:258:THR:O	2.36	0.44
2:H:191:SER:HB3	2:H:277:TRP:CZ3	2.47	0.44
2:B:102:GLY:HA2	2:B:138:PHE:CE1	2.53	0.44
1:E:249:VAL:O	1:E:251:SER:N	2.49	0.44
1:C:24:GLY:O	1:C:25:CYS:HB3	2.17	0.44
2:B:113:THR:O	2:B:117:GLU:N	2.50	0.44
2:B:122:TYR:O	2:B:123:GLU:C	2.55	0.44
1:G:429:ASP:O	1:G:432:LEU:HB2	2.17	0.44
1:A:155:GLY:N	3:A:501:SF4:S4	2.90	0.44
1:A:64:GLY:O	1:A:67:TRP:HE3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:307:GLU:HG2	1:G:428:TYR:CG	2.52	0.44
2:H:38:PHE:CG	2:H:45:THR:HG22	2.52	0.44
1:G:287:PHE:O	1:G:291:LEU:CD2	2.65	0.44
1:E:152:ASP:O	1:E:166:ILE:HG21	2.18	0.44
1:E:149:ILE:N	1:E:149:ILE:CD1	2.81	0.44
2:H:23:GLY:HA3	2:H:142:PHE:O	2.18	0.44
1:G:285:ARG:O	1:G:288:ALA:HB3	2.18	0.44
1:A:310:LYS:HG2	1:E:191:PRO:HB2	2.00	0.43
2:F:116:HIS:C	2:F:119:ARG:H	2.21	0.43
1:E:27:LYS:CD	2:F:66:ALA:HB1	2.48	0.43
1:E:424:GLY:C	1:E:433:GLU:OE2	2.56	0.43
1:E:125:VAL:CB	1:E:126:PRO:HD3	2.47	0.43
2:D:351:LEU:H	2:D:351:LEU:HG	1.54	0.43
2:D:99:LEU:HD23	2:D:133:VAL:HB	2.00	0.43
1:C:193:ILE:HD13	1:C:293:ASP:OD1	2.18	0.43
2:H:315:ARG:HG3	2:H:340:VAL:CG2	2.48	0.43
1:A:108:GLN:NE2	2:B:11:LEU:H	2.12	0.43
1:G:327:VAL:HG21	1:G:343:LEU:HD11	1.98	0.43
2:B:95:VAL:CG2	2:B:228:VAL:CG1	2.96	0.43
2:B:93:PRO:CG	2:B:96:ILE:HG13	2.47	0.43
1:G:404:MET:HB2	1:G:414:PHE:HE1	1.81	0.43
1:A:353:THR:CG2	1:A:377:LEU:HD23	2.48	0.43
2:H:175:LEU:HA	2:H:175:LEU:HD23	1.88	0.43
1:E:275:TYR:HD2	1:E:338:SER:HB2	1.81	0.43
2:D:105:GLU:O	2:D:105:GLU:HG3	2.18	0.43
1:C:231:ASP:OD1	1:C:233:ARG:NH2	2.51	0.43
2:B:271:LEU:HA	2:B:271:LEU:HD23	1.73	0.43
2:F:125:TYR:CD1	2:F:125:TYR:N	2.84	0.43
2:F:173:ASN:HD22	2:F:240:THR:CG2	2.30	0.43
1:G:355:THR:N	1:G:358:SER:OG	2.45	0.43
2:D:218:PHE:O	2:D:220:ALA:N	2.51	0.43
2:B:226:LEU:HA	2:B:226:LEU:HD22	1.69	0.43
1:E:397:LEU:O	1:E:414:PHE:HD2	2.01	0.43
1:A:396:ILE:HG23	1:A:413:PRO:HB2	2.00	0.43
2:H:329:ASP:OD2	2:H:333:ARG:NH1	2.41	0.43
1:G:54:HIS:CD2	1:G:121:TYR:OH	2.69	0.43
1:G:102:LEU:HD23	1:G:102:LEU:O	2.17	0.43
1:A:189:GLU:O	1:A:190:ARG:O	2.35	0.43
2:H:126:LYS:NZ	2:H:127:ASP:N	2.56	0.43
1:C:189:GLU:O	1:C:190:ARG:O	2.36	0.43
1:G:377:LEU:O	1:G:384:VAL:HG11	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:358:SER:HB2	1:C:363:LYS:HE3	1.99	0.43
2:B:301:GLN:HB3	1:C:450:VAL:HG11	1.99	0.43
1:A:383:ARG:N	2:B:217:ARG:HH12	2.17	0.43
1:C:307:GLU:HG2	1:C:428:TYR:CG	2.53	0.43
2:F:315:ARG:HG3	2:F:340:VAL:CG2	2.49	0.43
1:A:102:LEU:HD23	1:A:102:LEU:O	2.17	0.43
2:B:95:VAL:HG12	2:B:96:ILE:N	2.32	0.43
2:F:76:ALA:HA	2:F:79:ASN:OD1	2.19	0.43
1:E:330:TYR:HB3	1:E:399:ALA:CB	2.47	0.43
2:D:76:ALA:HA	2:D:79:ASN:OD1	2.18	0.43
2:F:200:LEU:C	2:F:200:LEU:HD22	2.38	0.43
2:F:118:PHE:O	2:F:122:TYR:CE2	2.70	0.43
1:G:48:PRO:HG2	1:G:204:TYR:CD1	2.52	0.43
2:F:70:VAL:C	2:F:72:SER:H	2.22	0.43
2:H:26:LEU:CD1	2:H:146:PHE:CD1	3.01	0.43
1:C:409:LYS:HD2	2:D:218:PHE:CZ	2.52	0.43
2:B:26:LEU:CD1	2:B:146:PHE:CD1	3.01	0.43
2:B:20:GLN:HG2	2:B:135:THR:HG22	2.01	0.43
2:B:168:ARG:CB	2:B:169:PRO:CD	2.97	0.43
2:B:24:ALA:HB1	2:B:149:ALA:HB2	1.99	0.43
1:A:287:PHE:O	1:A:291:LEU:CD2	2.66	0.43
1:A:286:ASP:O	1:A:290:LEU:HB2	2.18	0.43
2:B:314:ALA:HA	2:B:377:GLN:OE1	2.17	0.43
1:G:312:ARG:HH11	1:G:312:ARG:HB2	1.84	0.43
1:C:204:TYR:CD1	1:C:229:ALA:O	2.71	0.43
2:H:213:LEU:CD1	2:H:218:PHE:HB3	2.46	0.43
1:C:382:ALA:O	1:C:386:LEU:N	2.50	0.43
1:A:382:ALA:CB	2:B:217:ARG:HG3	2.46	0.43
1:C:126:PRO:O	1:C:131:ASP:HB2	2.19	0.43
1:E:157:TYR:HD1	1:E:157:TYR:H	1.67	0.43
2:H:16:LEU:HB2	2:H:363:ASP:HA	2.01	0.43
1:E:362:ASP:O	1:E:366:ILE:CG1	2.63	0.43
2:F:347:ARG:O	2:F:348:ALA:O	2.36	0.43
1:G:94:ILE:O	1:G:94:ILE:CD1	2.66	0.43
2:F:168:ARG:H	2:F:236:GLN:HB2	1.84	0.43
1:C:340:VAL:O	1:C:344:GLN:HB3	2.18	0.43
2:B:94:SER:O	2:B:129:PRO:HD2	2.19	0.43
1:C:137:CYS:SG	1:C:150:PRO:HB3	2.58	0.43
2:F:312:SER:O	2:F:313:SER:CB	2.67	0.43
2:D:116:HIS:HA	2:D:119:ARG:HB2	2.00	0.43
1:C:440:ILE:HG13	1:C:441:THR:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:LEU:O	1:A:325:LYS:HG2	2.18	0.43
1:G:155:GLY:CA	3:G:501:SF4:S4	3.05	0.43
1:C:179:ARG:NH2	1:C:235:ARG:O	2.51	0.43
2:B:236:GLN:HG2	2:B:236:GLN:O	2.18	0.43
1:A:341:SER:HA	1:A:344:GLN:NE2	2.32	0.43
2:F:331:LEU:C	2:F:331:LEU:HD22	2.38	0.43
1:C:328:LEU:HD22	1:C:389:VAL:CG2	2.49	0.43
2:B:395:PRO:HG3	2:B:434:HIS:ND1	2.33	0.43
2:H:105:GLU:HG3	2:H:105:GLU:O	2.19	0.43
1:G:187:GLY:O	1:G:188:SER:HB3	2.19	0.43
2:B:183:GLY:O	2:B:413:CYS:HB2	2.19	0.43
1:C:47:LEU:N	1:C:48:PRO:HD3	2.34	0.43
1:A:204:TYR:CD1	1:A:229:ALA:O	2.72	0.43
1:A:71:GLY:O	1:A:72:THR:O	2.36	0.43
2:H:39:HIS:HD2	2:H:65:THR:OG1	2.01	0.43
2:D:26:LEU:HD13	2:D:146:PHE:CE1	2.54	0.43
1:C:304:ILE:O	1:C:308:GLU:HG3	2.18	0.43
1:C:304:ILE:HD12	1:C:305:ALA:N	2.34	0.43
2:D:260:VAL:HA	2:D:261:PRO:HD3	1.88	0.43
1:E:286:ASP:O	1:E:290:LEU:HB2	2.18	0.43
2:H:21:THR:HG21	2:H:137:ASP:OD1	2.18	0.43
2:H:299:GLN:OE1	2:H:418:ARG:NE	2.48	0.43
2:F:91:GLN:HB2	2:F:91:GLN:HE21	1.61	0.43
2:F:122:TYR:C	2:F:124:GLU:N	2.72	0.43
2:H:173:ASN:HD22	2:H:240:THR:CG2	2.31	0.43
1:C:382:ALA:CB	2:D:217:ARG:HG3	2.42	0.43
1:E:409:LYS:HD2	2:F:218:PHE:CZ	2.53	0.43
1:A:383:ARG:CG	1:A:384:VAL:H	2.30	0.43
1:A:383:ARG:CD	2:B:217:ARG:HH22	2.32	0.43
2:B:221:LEU:HG	2:B:221:LEU:O	2.19	0.43
1:G:172:LEU:CD1	1:G:172:LEU:C	2.86	0.43
1:E:179:ARG:HB3	1:E:238:GLN:CB	2.49	0.43
1:A:345:ASP:OD1	1:A:346:LEU:N	2.52	0.43
2:F:185:LEU:CB	2:F:206:SER:OG	2.67	0.43
2:B:329:ASP:OD2	2:B:333:ARG:NH1	2.47	0.43
1:G:103:PHE:HZ	1:G:143:ARG:HD3	1.84	0.43
1:G:152:ASP:O	1:G:166:ILE:HG21	2.18	0.43
1:E:99:GLU:O	1:E:100:LYS:C	2.57	0.43
2:B:299:GLN:OE1	2:B:418:ARG:NH2	2.49	0.43
2:H:109:CYS:O	2:H:110:ASP:C	2.57	0.43
2:B:39:HIS:HD2	2:B:65:THR:CB	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:47:LEU:N	1:G:48:PRO:HD3	2.34	0.43
1:C:27:LYS:C	1:C:27:LYS:CD	2.87	0.43
1:E:58:GLY:O	1:E:86:THR:O	2.36	0.43
1:C:353:THR:CG2	1:C:377:LEU:HD23	2.48	0.43
1:E:383:ARG:H	2:F:217:ARG:NH2	2.16	0.43
2:B:100:THR:CG2	2:B:134:ASN:HA	2.49	0.43
2:D:158:VAL:N	2:D:159:PRO:HD2	2.34	0.43
2:H:352:VAL:CG1	2:H:354:SER:H	2.32	0.43
1:G:293:ASP:OD2	1:G:294:PRO:HD2	2.19	0.43
1:C:252:LYS:CB	1:C:361:GLU:OE2	2.64	0.43
1:C:304:ILE:HD12	1:C:304:ILE:C	2.40	0.43
2:H:329:ASP:OD1	2:H:356:LEU:HD22	2.19	0.43
1:G:149:ILE:HD12	1:G:149:ILE:N	2.34	0.43
2:H:126:LYS:HZ2	2:H:127:ASP:H	1.61	0.43
2:F:126:LYS:O	2:F:127:ASP:CB	2.65	0.43
1:A:206:ILE:CD1	1:A:419:GLN:HB3	2.48	0.43
1:G:384:VAL:O	1:G:387:LYS:HG2	2.19	0.43
2:F:344:VAL:O	2:F:361:VAL:HA	2.18	0.43
1:E:68:ASP:N	1:E:68:ASP:OD1	2.51	0.43
1:E:340:VAL:O	1:E:344:GLN:HB3	2.19	0.43
2:H:160:GLU:H	2:H:160:GLU:CD	2.22	0.43
2:H:325:LEU:HD11	2:H:342:ALA:HB1	2.00	0.43
2:H:91:GLN:HB2	2:H:91:GLN:HE21	1.58	0.43
1:C:166:ILE:HG22	1:C:166:ILE:O	2.19	0.43
2:H:125:TYR:HB2	2:H:126:LYS:O	2.18	0.42
2:D:126:LYS:CG	2:D:127:ASP:N	2.82	0.42
1:C:322:LEU:O	1:C:325:LYS:HG2	2.19	0.42
1:C:47:LEU:N	1:C:48:PRO:CD	2.82	0.42
2:F:173:ASN:HB2	2:F:240:THR:CG2	2.24	0.42
2:D:173:ASN:ND2	2:D:240:THR:HG22	2.34	0.42
1:E:128:LEU:HD23	2:F:106:THR:HG21	2.00	0.42
2:H:217:ARG:C	2:H:218:PHE:CD2	2.82	0.42
2:F:221:LEU:O	2:F:221:LEU:HG	2.19	0.42
1:C:154:ALA:O	1:C:157:TYR:HD1	2.01	0.42
1:G:78:ASP:O	1:G:81:ARG:HB2	2.18	0.42
1:A:304:ILE:O	1:A:308:GLU:HG3	2.19	0.42
1:C:198:VAL:HG22	1:C:223:ARG:O	2.19	0.42
1:E:46:LEU:HB2	1:E:121:TYR:OH	2.19	0.42
1:C:289:ARG:HB3	1:C:289:ARG:HE	1.70	0.42
2:H:113:THR:O	2:H:116:HIS:N	2.49	0.42
1:A:421:ARG:NH2	1:A:422:GLU:CB	2.80	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:383:ARG:N	2:F:217:ARG:HH12	2.17	0.42
2:F:213:LEU:HD13	2:F:218:PHE:CG	2.54	0.42
1:G:179:ARG:HB3	1:G:238:GLN:HB2	2.00	0.42
2:H:347:ARG:O	2:H:348:ALA:O	2.37	0.42
1:C:65:SER:C	1:C:67:TRP:H	2.22	0.42
2:F:168:ARG:CB	2:F:169:PRO:CD	2.97	0.42
1:A:337:TRP:O	1:A:337:TRP:HE3	2.01	0.42
2:F:285:SER:CB	2:F:287:ASN:HD21	2.31	0.42
2:B:391:ARG:HE	2:B:391:ARG:HB2	1.61	0.42
1:E:379:GLU:H	1:E:379:GLU:HG2	1.56	0.42
2:D:117:GLU:O	2:D:122:TYR:OH	2.32	0.42
2:D:126:LYS:O	2:D:127:ASP:CB	2.63	0.42
2:B:304:MET:O	2:B:308:HIS:HB3	2.19	0.42
1:E:48:PRO:HG2	1:E:204:TYR:CD1	2.55	0.42
1:A:383:ARG:HD2	2:B:217:ARG:NH2	2.34	0.42
2:F:159:PRO:CB	2:F:257:ARG:CD	2.93	0.42
2:H:149:ALA:O	2:H:153:ILE:CG1	2.62	0.42
2:D:291:ASP:HA	2:D:294:LYS:HG3	2.01	0.42
2:H:386:LEU:HA	2:H:386:LEU:HD23	1.91	0.42
1:G:248:MET:SD	1:G:258:ALA:HB2	2.59	0.42
2:B:126:LYS:CG	2:B:127:ASP:N	2.82	0.42
1:C:207:ALA:CB	1:C:421:ARG:O	2.67	0.42
1:E:440:ILE:HG13	1:E:441:THR:H	1.85	0.42
2:F:265:PHE:HB3	2:F:266:GLY:H	1.56	0.42
2:F:221:LEU:C	2:F:223:THR:N	2.73	0.42
1:A:172:LEU:C	1:A:172:LEU:CD1	2.87	0.42
2:D:16:LEU:HD12	2:D:16:LEU:O	2.18	0.42
1:G:316:GLU:C	1:G:316:GLU:CD	2.77	0.42
1:C:179:ARG:HB3	1:C:238:GLN:HB3	2.01	0.42
1:E:174:TYR:CE2	1:E:234:TYR:CE2	3.07	0.42
1:E:308:GLU:O	1:E:312:ARG:HD3	2.18	0.42
1:E:287:PHE:O	1:E:291:LEU:CD2	2.66	0.42
1:G:184:LEU:HA	1:G:185:PRO:HD3	1.82	0.42
1:G:31:GLY:N	1:G:33:THR:OG1	2.52	0.42
2:F:89:GLU:OE2	2:F:124:GLU:CB	2.67	0.42
1:G:433:GLU:HA	1:G:436:ARG:HD2	2.01	0.42
1:E:27:LYS:CD	1:E:27:LYS:C	2.87	0.42
2:B:295:ARG:NE	2:D:212:HIS:CE1	2.87	0.42
2:D:26:LEU:HD12	2:D:146:PHE:CD1	2.55	0.42
2:F:100:THR:CG2	2:F:134:ASN:HA	2.49	0.42
2:D:322:PRO:HG2	2:D:348:ALA:CB	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:220:LEU:HD21	1:E:303:LEU:HD13	2.01	0.42
1:C:341:SER:HA	1:C:344:GLN:HE21	1.84	0.42
2:D:175:LEU:HD23	2:D:175:LEU:HA	1.86	0.42
2:B:167:LYS:HA	2:B:237:SER:H	1.84	0.42
2:F:105:GLU:HG2	2:F:136:PRO:CG	2.50	0.42
2:D:335:MET:SD	2:D:424:LEU:HD21	2.59	0.42
2:H:200:LEU:C	2:H:200:LEU:HD22	2.39	0.42
1:C:71:GLY:HA2	1:C:420:GLU:C	2.40	0.42
1:A:26:ALA:O	1:A:27:LYS:CB	2.63	0.42
2:D:213:LEU:HD13	2:D:218:PHE:CG	2.55	0.42
1:C:383:ARG:NE	2:D:90:ARG:HH12	2.16	0.42
1:A:174:TYR:CZ	1:A:234:TYR:CD2	3.08	0.42
2:D:352:VAL:CG1	2:D:354:SER:H	2.33	0.42
1:C:397:LEU:O	1:C:414:PHE:HD2	2.02	0.42
1:E:327:VAL:HG23	1:E:327:VAL:O	2.20	0.42
1:E:103:PHE:HZ	1:E:143:ARG:HD3	1.84	0.42
1:C:312:ARG:HB2	1:C:312:ARG:NH1	2.35	0.42
2:H:50:VAL:O	2:H:51:PHE:C	2.57	0.42
1:C:30:PRO:HA	2:D:63:GLN:CD	2.38	0.42
2:H:39:HIS:HD2	2:H:65:THR:CB	2.32	0.42
1:C:172:LEU:CD1	1:C:172:LEU:C	2.87	0.42
1:E:174:TYR:OH	1:E:238:GLN:HG2	2.20	0.42
1:E:174:TYR:OH	1:E:238:GLN:HG3	2.20	0.42
2:F:158:VAL:N	2:F:159:PRO:HD2	2.34	0.42
1:G:193:ILE:O	1:G:195:VAL:N	2.53	0.42
1:A:193:ILE:O	1:A:195:VAL:N	2.52	0.42
2:B:168:ARG:HG3	2:B:236:GLN:CB	2.44	0.42
2:H:398:ARG:NH1	2:H:405:ASP:OD1	2.52	0.42
1:C:220:LEU:HD21	1:C:303:LEU:HD13	2.00	0.42
1:A:346:LEU:HD23	1:A:346:LEU:C	2.40	0.42
1:E:312:ARG:HB2	1:E:312:ARG:HH11	1.85	0.42
2:D:55:HIS:HE1	2:D:403:GLN:HG2	1.83	0.42
2:B:335:MET:SD	2:B:424:LEU:CD2	3.08	0.42
2:D:22:MET:SD	2:D:48:ALA:HA	2.60	0.42
1:C:184:LEU:HA	1:C:185:PRO:HD3	1.80	0.42
2:B:117:GLU:O	2:B:122:TYR:OH	2.32	0.42
2:B:116:HIS:HA	2:B:119:ARG:HB2	2.02	0.42
1:C:191:PRO:HG3	1:G:314:ALA:HB2	2.00	0.42
1:E:62:CYS:SG	1:E:123:THR:HG21	2.60	0.42
1:E:367:ARG:HD3	1:E:367:ARG:HA	1.43	0.42
1:E:246:ASN:HD22	1:E:246:ASN:HA	1.69	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:68:ASP:N	1:C:68:ASP:OD1	2.53	0.42
1:G:304:ILE:C	1:G:304:ILE:HD12	2.40	0.42
1:C:417:ILE:HD13	1:C:417:ILE:HA	1.64	0.42
1:G:417:ILE:HA	1:G:417:ILE:HD13	1.62	0.42
1:E:346:LEU:C	1:E:346:LEU:HD23	2.39	0.42
2:B:162:ARG:HA	2:B:162:ARG:NE	2.34	0.42
2:F:310:MET:N	2:F:310:MET:HE3	2.35	0.42
2:B:121:GLN:HB2	2:B:122:TYR:HE1	1.85	0.42
2:F:109:CYS:O	2:F:110:ASP:C	2.59	0.42
1:E:322:LEU:CD2	1:E:439:CYS:SG	2.95	0.42
1:E:201:ILE:HA	1:E:228:LEU:HB3	2.01	0.42
1:E:209:GLU:OE1	1:E:426:ALA:HB3	2.19	0.42
1:G:29:LYS:CG	2:H:65:THR:O	2.68	0.42
1:C:355:THR:N	1:C:358:SER:OG	2.46	0.42
2:D:185:LEU:CB	2:D:206:SER:OG	2.67	0.42
2:B:213:LEU:CD1	2:B:218:PHE:HB3	2.48	0.42
2:F:99:LEU:HD23	2:F:133:VAL:HB	2.02	0.42
1:C:293:ASP:OD2	1:C:294:PRO:HD2	2.19	0.42
2:H:168:ARG:HE	2:H:168:ARG:HB2	1.58	0.42
1:C:66:SER:HB3	2:D:47:PHE:CZ	2.54	0.42
1:A:417:ILE:HD13	1:A:417:ILE:HA	1.66	0.42
1:E:270:PHE:CD2	1:E:286:ASP:OD2	2.73	0.42
2:D:395:PRO:HG3	2:D:434:HIS:CG	2.55	0.42
2:B:329:ASP:OD1	2:B:356:LEU:HD22	2.19	0.42
2:F:409:GLY:C	2:F:411:GLN:H	2.23	0.42
2:H:131:VAL:HA	2:H:132:PRO:HD3	1.90	0.42
1:C:206:ILE:O	1:C:419:GLN:O	2.38	0.42
2:F:64:THR:HG22	2:F:66:ALA:N	2.25	0.42
1:A:201:ILE:HA	1:A:228:LEU:HB3	2.02	0.42
1:C:29:LYS:HZ2	1:C:29:LYS:HB2	1.84	0.42
2:H:68:ASP:CB	2:H:70:VAL:HG22	2.25	0.42
2:B:265:PHE:HB3	2:B:266:GLY:H	1.61	0.42
1:C:377:LEU:O	1:C:384:VAL:HG11	2.19	0.42
2:B:33:ARG:N	2:B:221:LEU:CD2	2.83	0.42
2:D:362:GLY:HA3	2:D:366:ASP:OD1	2.20	0.42
1:C:323:GLU:OE2	1:C:324:GLY:N	2.53	0.42
2:H:168:ARG:CG	2:H:169:PRO:HD3	2.50	0.42
2:D:236:GLN:O	2:D:236:GLN:HG2	2.19	0.42
2:B:374:GLY:O	2:B:375:GLN:HB2	2.19	0.42
2:F:397:LEU:HD22	2:F:427:LEU:HD23	2.01	0.42
1:G:339:VAL:HG11	1:G:417:ILE:HD11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:353:THR:CG2	1:E:377:LEU:HD23	2.50	0.42
2:D:333:ARG:HH11	2:D:333:ARG:HB2	1.83	0.42
2:D:200:LEU:HD22	2:D:200:LEU:C	2.40	0.42
2:H:122:TYR:O	2:H:123:GLU:C	2.57	0.41
2:D:113:THR:O	2:D:117:GLU:N	2.52	0.41
1:C:48:PRO:CB	1:C:72:THR:HG21	2.48	0.41
1:A:440:ILE:HG13	1:A:441:THR:H	1.85	0.41
1:G:421:ARG:CZ	1:G:422:GLU:N	2.78	0.41
1:A:203:GLU:HB3	1:A:227:THR:HG23	2.02	0.41
2:F:215:GLU:O	2:F:218:PHE:CE2	2.73	0.41
1:G:174:TYR:OH	1:G:238:GLN:HG2	2.19	0.41
2:F:159:PRO:CB	2:F:257:ARG:HH11	2.32	0.41
2:D:349:ALA:O	2:D:351:LEU:N	2.53	0.41
1:A:359:THR:CG2	4:A:502:CZL:S2A	3.07	0.41
1:C:102:LEU:HD23	1:C:102:LEU:O	2.20	0.41
2:H:160:GLU:HG2	2:H:161:ARG:N	2.35	0.41
1:G:341:SER:HA	1:G:344:GLN:HE21	1.85	0.41
1:C:270:PHE:CD2	1:C:286:ASP:OD2	2.73	0.41
1:A:47:LEU:C	1:A:49:VAL:H	2.23	0.41
1:C:206:ILE:H	1:C:206:ILE:HG12	1.35	0.41
1:G:47:LEU:N	1:G:48:PRO:CD	2.83	0.41
1:A:419:GLN:NE2	1:A:424:GLY:H	2.15	0.41
2:B:295:ARG:HH22	2:D:206:SER:HB3	1.85	0.41
2:D:33:ARG:H	2:D:221:LEU:HD23	1.86	0.41
1:A:383:ARG:N	2:B:217:ARG:NH1	2.68	0.41
2:B:33:ARG:H	2:B:221:LEU:HD23	1.85	0.41
1:G:175:VAL:O	1:G:177:GLY:N	2.52	0.41
1:C:63:ALA:O	1:C:65:SER:N	2.53	0.41
2:H:382:ASN:CB	2:H:402:PRO:HD2	2.50	0.41
1:C:341:SER:HA	1:C:344:GLN:NE2	2.34	0.41
2:B:105:GLU:HG2	2:B:136:PRO:CG	2.51	0.41
2:H:183:GLY:O	2:H:413:CYS:HB2	2.20	0.41
1:A:248:MET:SD	1:A:258:ALA:HB2	2.59	0.41
2:H:121:GLN:N	2:H:122:TYR:CD1	2.89	0.41
2:B:126:LYS:HZ2	2:B:127:ASP:N	2.16	0.41
1:C:201:ILE:HA	1:C:228:LEU:HB3	2.01	0.41
1:E:71:GLY:HA2	1:E:420:GLU:C	2.40	0.41
1:G:356:LYS:HD3	1:G:378:ASP:HA	2.00	0.41
2:H:31:LEU:HD23	2:H:95:VAL:HG11	2.01	0.41
1:C:246:ASN:O	1:C:269:TRP:HA	2.20	0.41
1:E:354:GLY:O	1:E:375:LYS:O	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:344:VAL:O	2:B:361:VAL:HA	2.21	0.41
2:B:340:VAL:CG1	2:B:374:GLY:HA3	2.50	0.41
1:G:346:LEU:HD23	1:G:346:LEU:C	2.40	0.41
1:C:345:ASP:OD1	1:C:346:LEU:N	2.54	0.41
2:F:171:GLN:O	2:F:237:SER:HB2	2.20	0.41
1:E:304:ILE:C	1:E:304:ILE:HD12	2.40	0.41
2:H:136:PRO:O	2:H:137:ASP:C	2.56	0.41
2:F:314:ALA:HA	2:F:377:GLN:OE1	2.19	0.41
2:F:131:VAL:HA	2:F:132:PRO:HD3	1.86	0.41
2:B:126:LYS:C	2:B:128:VAL:H	2.24	0.41
2:F:125:TYR:HB2	2:F:126:LYS:O	2.20	0.41
1:C:433:GLU:HA	1:C:436:ARG:HD2	2.02	0.41
1:C:48:PRO:HG2	1:C:204:TYR:CD1	2.55	0.41
1:G:71:GLY:HA2	1:G:420:GLU:C	2.40	0.41
2:F:107:GLN:NE2	2:F:107:GLN:H	2.16	0.41
2:H:221:LEU:C	2:H:223:THR:N	2.74	0.41
1:C:316:GLU:C	1:C:316:GLU:CD	2.78	0.41
2:D:159:PRO:CB	2:D:257:ARG:HG3	2.51	0.41
1:C:293:ASP:OD2	1:C:294:PRO:CD	2.69	0.41
1:A:154:ALA:O	1:A:157:TYR:HD1	2.03	0.41
2:D:397:LEU:HD22	2:D:427:LEU:HD23	2.02	0.41
2:H:291:ASP:HA	2:H:294:LYS:HG3	2.03	0.41
2:F:291:ASP:HA	2:F:294:LYS:HG3	2.03	0.41
2:B:149:ALA:O	2:B:153:ILE:CG1	2.66	0.41
1:C:346:LEU:C	1:C:346:LEU:HD23	2.41	0.41
2:F:38:PHE:CB	2:F:45:THR:HG22	2.50	0.41
2:H:335:MET:SD	2:H:424:LEU:CD2	3.09	0.41
2:B:333:ARG:CB	2:B:333:ARG:HH11	2.32	0.41
2:B:332:LEU:HB3	2:B:337:ALA:HB3	2.01	0.41
1:E:421:ARG:HB3	1:E:421:ARG:HE	1.15	0.41
2:H:95:VAL:HG22	2:H:228:VAL:HG11	2.02	0.41
1:E:380:GLY:HA3	1:E:384:VAL:CG2	2.47	0.41
1:E:381:ASN:HB2	2:F:217:ARG:NH2	2.36	0.41
2:F:20:GLN:HA	2:F:141:CYS:O	2.20	0.41
1:C:199:ASN:OD1	1:C:240:MET:HG2	2.21	0.41
1:A:246:ASN:HD22	1:A:246:ASN:HA	1.70	0.41
1:E:67:TRP:CZ3	2:F:15:PRO:HG2	2.56	0.41
2:F:51:PHE:CE1	2:F:402:PRO:HB3	2.54	0.41
1:A:220:LEU:HD21	1:A:303:LEU:HD13	2.03	0.41
2:F:329:ASP:OD1	2:F:356:LEU:HD22	2.21	0.41
2:F:55:HIS:HE1	2:F:403:GLN:HG2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:160:GLU:HG2	2:D:161:ARG:N	2.35	0.41
1:C:31:GLY:C	1:C:33:THR:N	2.73	0.41
1:C:249:VAL:O	1:C:251:SER:N	2.53	0.41
1:C:143:ARG:HB3	1:C:143:ARG:NH1	2.35	0.41
2:B:125:TYR:CD1	2:B:125:TYR:N	2.83	0.41
1:G:322:LEU:N	1:G:322:LEU:CD2	2.83	0.41
1:G:439:CYS:O	1:G:440:ILE:C	2.57	0.41
1:E:209:GLU:CD	1:E:419:GLN:OE1	2.56	0.41
1:G:29:LYS:CB	1:G:30:PRO:HD2	2.32	0.41
1:G:316:GLU:N	1:G:317:PRO:CD	2.84	0.41
2:D:347:ARG:O	2:D:348:ALA:O	2.38	0.41
2:F:351:LEU:H	2:F:351:LEU:HG	1.54	0.41
2:H:344:VAL:HG13	2:H:346:ALA:H	1.86	0.41
2:F:168:ARG:CG	2:F:169:PRO:HD3	2.50	0.41
2:D:93:PRO:CG	2:D:96:ILE:HG13	2.50	0.41
2:B:396:LEU:HD22	2:B:397:LEU:N	2.36	0.41
1:E:304:ILE:O	1:E:308:GLU:HG3	2.20	0.41
2:F:156:THR:C	2:F:157:LEU:HD13	2.41	0.41
2:H:395:PRO:HG3	2:H:434:HIS:CG	2.55	0.41
1:G:24:GLY:O	1:G:25:CYS:HB3	2.21	0.41
1:G:182:ASP:HA	1:G:183:PRO:HD3	1.91	0.41
1:A:50:ALA:HB3	1:A:77:PRO:HG2	2.01	0.41
2:B:125:TYR:HB2	2:B:126:LYS:O	2.20	0.41
1:A:322:LEU:N	1:A:322:LEU:CD2	2.84	0.41
1:G:47:LEU:C	1:G:49:VAL:H	2.24	0.41
1:G:358:SER:HB2	1:G:363:LYS:HE3	2.03	0.41
1:E:383:ARG:HD2	2:F:217:ARG:NH2	2.34	0.41
1:G:128:LEU:C	1:G:130:GLY:H	2.23	0.41
2:H:159:PRO:HB2	2:H:257:ARG:HD3	2.01	0.41
2:H:166:GLY:O	2:H:236:GLN:HA	2.21	0.41
2:B:168:ARG:H	2:B:236:GLN:HB2	1.85	0.41
1:G:304:ILE:O	1:G:308:GLU:HG3	2.20	0.41
1:A:328:LEU:HD23	1:A:397:LEU:HD23	2.03	0.41
1:C:247:MET:HB2	1:C:270:PHE:CE1	2.55	0.41
2:H:256:GLU:OE2	2:H:256:GLU:CA	2.68	0.41
2:F:53:VAL:O	2:F:57:ARG:HA	2.21	0.41
2:F:263:ARG:HE	2:F:263:ARG:HB2	1.60	0.41
1:C:227:THR:O	1:C:229:ALA:N	2.54	0.41
1:C:429:ASP:O	1:C:432:LEU:HB2	2.20	0.41
1:A:209:GLU:O	1:A:212:HIS:HB2	2.21	0.41
2:B:100:THR:HG21	2:B:134:ASN:OD1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:193:ILE:O	1:E:195:VAL:N	2.53	0.41
1:E:174:TYR:CZ	1:E:234:TYR:CD2	3.08	0.41
2:B:354:SER:HB2	2:B:355:PRO:CD	2.50	0.41
1:E:328:LEU:HD22	1:E:389:VAL:CG2	2.50	0.41
2:F:302:ASP:OD2	2:H:58:GLU:CD	2.59	0.41
2:B:58:GLU:CD	2:D:302:ASP:OD2	2.59	0.41
1:G:404:MET:HE2	1:G:405:TYR:CE2	2.56	0.41
1:C:247:MET:HB2	1:C:270:PHE:CZ	2.56	0.41
1:C:245:VAL:HG11	1:C:290:LEU:HD23	2.00	0.41
2:D:102:GLY:HA2	2:D:138:PHE:CE1	2.55	0.41
2:F:85:LYS:CD	2:F:118:PHE:HE1	2.23	0.41
1:C:424:GLY:O	1:C:433:GLU:OE2	2.39	0.41
1:C:421:ARG:NH2	1:C:422:GLU:CB	2.81	0.41
1:A:29:LYS:HG3	2:B:66:ALA:HB3	2.02	0.41
1:E:322:LEU:N	1:E:322:LEU:CD2	2.84	0.41
1:G:48:PRO:HB3	1:G:72:THR:CG2	2.51	0.41
1:C:27:LYS:CG	2:D:66:ALA:HB1	2.50	0.41
2:H:42:GLN:HA	2:H:64:THR:CG2	2.47	0.41
1:G:355:THR:CB	1:G:377:LEU:HD11	2.50	0.41
2:H:95:VAL:CG2	2:H:228:VAL:CG1	2.99	0.41
1:G:57:HIS:HE1	1:G:131:ASP:OD1	2.04	0.41
2:F:27:ALA:HB2	2:F:146:PHE:CE1	2.56	0.41
2:F:31:LEU:HD12	2:F:226:LEU:HB2	2.03	0.41
2:B:28:ILE:HD11	2:B:36:PRO:N	2.36	0.41
1:C:174:TYR:CZ	1:C:234:TYR:CD2	3.09	0.41
2:F:16:LEU:HB2	2:F:363:ASP:HA	2.02	0.41
2:H:159:PRO:CB	2:H:257:ARG:HH11	2.31	0.41
2:B:353:ASP:O	2:B:354:SER:CB	2.69	0.41
2:B:352:VAL:CG1	2:B:354:SER:H	2.34	0.41
2:B:257:ARG:CZ	2:B:257:ARG:HB3	2.51	0.41
1:G:193:ILE:HD13	1:G:293:ASP:OD1	2.20	0.41
2:D:51:PHE:CE1	2:D:402:PRO:HB3	2.56	0.41
1:G:65:SER:C	1:G:67:TRP:H	2.22	0.41
2:H:382:ASN:ND2	2:H:384:HIS:N	2.69	0.41
1:E:63:ALA:O	1:E:65:SER:N	2.54	0.41
1:E:417:ILE:CG2	1:E:417:ILE:O	2.59	0.41
2:B:191:SER:HG	2:B:277:TRP:HZ3	1.67	0.41
2:B:291:ASP:HA	2:B:294:LYS:HG3	2.03	0.41
2:F:335:MET:SD	2:F:424:LEU:CD2	3.09	0.41
2:D:176:CYS:C	2:D:247:LEU:HD11	2.41	0.41
2:F:175:LEU:HD23	2:F:175:LEU:HA	1.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:409:GLY:C	2:D:411:GLN:H	2.23	0.41
1:G:337:TRP:HE3	1:G:337:TRP:O	2.02	0.41
2:F:269:TYR:O	2:F:273:ALA:CB	2.69	0.41
1:A:148:VAL:C	1:A:149:ILE:HD12	2.40	0.41
1:A:149:ILE:CD1	1:A:149:ILE:N	2.84	0.41
2:F:211:GLY:HA3	2:H:302:ASP:HB2	2.03	0.41
1:C:61:ALA:HB2	2:D:137:ASP:CG	2.42	0.41
2:D:329:ASP:OD1	2:D:356:LEU:HD22	2.20	0.41
1:G:60:ILE:HG12	1:G:60:ILE:H	1.45	0.41
1:G:249:VAL:O	1:G:251:SER:N	2.53	0.41
1:E:146:THR:O	1:E:148:VAL:HG23	2.21	0.41
2:F:119:ARG:HH11	2:F:119:ARG:HG2	1.86	0.41
1:C:419:GLN:NE2	1:C:424:GLY:H	2.19	0.41
1:E:430:GLY:O	1:E:433:GLU:OE1	2.39	0.41
1:C:356:LYS:HD3	1:C:378:ASP:HA	2.02	0.41
1:C:381:ASN:HB2	2:D:217:ARG:NH2	2.36	0.41
2:D:33:ARG:N	2:D:221:LEU:CD2	2.84	0.41
1:E:381:ASN:H	1:E:381:ASN:ND2	2.10	0.41
1:E:384:VAL:O	1:E:387:LYS:HG2	2.21	0.41
2:B:326:LEU:N	2:B:326:LEU:HD23	2.35	0.41
1:C:405:TYR:CE1	2:D:57:ARG:O	2.74	0.41
2:H:76:ALA:HA	2:H:79:ASN:OD1	2.21	0.41
2:D:297:ARG:HG3	2:D:417:TYR:CE2	2.56	0.41
1:E:335:LYS:HG3	1:E:335:LYS:H	1.64	0.41
1:E:52:VAL:CG1	1:E:53:ALA:N	2.84	0.41
1:C:99:GLU:O	1:C:100:LYS:C	2.58	0.41
1:E:316:GLU:N	1:E:317:PRO:CD	2.84	0.41
1:E:316:GLU:OE1	1:E:317:PRO:HD3	2.21	0.41
1:E:60:ILE:HG12	1:E:60:ILE:H	1.40	0.41
2:B:118:PHE:O	2:B:119:ARG:HD3	2.15	0.40
2:F:126:LYS:NZ	2:F:127:ASP:N	2.59	0.40
1:A:30:PRO:HB3	2:B:63:GLN:HG3	2.02	0.40
2:H:240:THR:HG23	2:H:260:VAL:HG11	2.03	0.40
1:C:125:VAL:CB	1:C:126:PRO:HD3	2.50	0.40
2:F:329:ASP:OD2	2:F:333:ARG:NH1	2.44	0.40
2:B:109:CYS:SG	2:B:109:CYS:O	2.80	0.40
1:G:52:VAL:CG1	1:G:53:ALA:N	2.83	0.40
2:H:121:GLN:HB2	2:H:122:TYR:HE1	1.85	0.40
2:H:126:LYS:O	2:H:127:ASP:CB	2.63	0.40
2:D:125:TYR:HB2	2:D:126:LYS:O	2.22	0.40
1:E:382:ALA:O	1:E:386:LEU:N	2.48	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:159:PRO:CB	2:B:257:ARG:CD	2.94	0.40
2:F:352:VAL:CG1	2:F:354:SER:H	2.35	0.40
1:G:373:ASP:OD2	1:G:374:VAL:N	2.55	0.40
1:E:134:ASP:OD1	1:E:134:ASP:N	2.54	0.40
1:E:316:GLU:C	1:E:316:GLU:CD	2.80	0.40
2:F:423:VAL:HG12	2:F:423:VAL:O	2.21	0.40
1:G:51:ASP:N	1:G:51:ASP:OD1	2.54	0.40
1:C:310:LYS:HZ2	1:G:191:PRO:HG2	1.84	0.40
1:G:322:LEU:HD11	1:G:439:CYS:SG	2.61	0.40
1:A:424:GLY:C	1:A:433:GLU:OE2	2.60	0.40
1:E:206:ILE:O	1:E:207:ALA:HB3	2.21	0.40
2:D:221:LEU:O	2:D:221:LEU:HG	2.22	0.40
2:D:226:LEU:HD22	2:D:226:LEU:HA	1.65	0.40
2:F:159:PRO:CB	2:F:257:ARG:CG	2.99	0.40
2:F:353:ASP:O	2:F:354:SER:CB	2.69	0.40
2:H:17:LYS:HE3	2:H:17:LYS:HB3	1.90	0.40
1:C:311:VAL:CG2	1:C:428:TYR:HB3	2.51	0.40
1:G:199:ASN:OD1	1:G:240:MET:HG2	2.21	0.40
1:A:354:GLY:N	1:A:366:ILE:CD1	2.83	0.40
2:F:105:GLU:HG3	2:F:105:GLU:O	2.22	0.40
2:B:271:LEU:O	2:B:272:ASP:C	2.57	0.40
2:D:23:GLY:HA3	2:D:142:PHE:O	2.21	0.40
1:E:140:ALA:O	1:E:141:ALA:C	2.60	0.40
2:H:281:LEU:HD23	2:H:281:LEU:HA	1.92	0.40
2:F:117:GLU:O	2:F:121:GLN:OE1	2.39	0.40
2:D:121:GLN:N	2:D:122:TYR:CD1	2.88	0.40
2:D:122:TYR:C	2:D:124:GLU:N	2.72	0.40
2:D:39:HIS:HD2	2:D:65:THR:CB	2.34	0.40
2:F:295:ARG:NE	2:H:212:HIS:CE1	2.90	0.40
1:A:383:ARG:HG2	1:A:384:VAL:N	2.31	0.40
1:C:174:TYR:OH	1:C:238:GLN:HG2	2.21	0.40
1:C:174:TYR:OH	1:C:234:TYR:CD1	2.74	0.40
1:C:375:LYS:HG2	1:C:375:LYS:O	2.21	0.40
2:B:159:PRO:HB2	2:B:257:ARG:CD	2.52	0.40
2:D:256:GLU:OE2	2:D:256:GLU:CA	2.68	0.40
2:F:167:LYS:HA	2:F:237:SER:H	1.85	0.40
2:B:287:ASN:N	2:B:287:ASN:ND2	2.69	0.40
2:D:386:LEU:HA	2:D:386:LEU:HD23	1.86	0.40
1:G:153:SER:HB3	1:G:166:ILE:HG21	2.04	0.40
1:C:214:LEU:HA	1:C:214:LEU:HD12	1.83	0.40
2:F:200:LEU:HA	2:F:200:LEU:HD23	1.78	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:428:ALA:O	2:D:432:VAL:HG23	2.21	0.40
2:H:202:ILE:HA	2:H:203:PRO:HA	1.70	0.40
2:H:271:LEU:HA	2:H:271:LEU:HD23	1.70	0.40
2:D:121:GLN:HB2	2:D:122:TYR:HE1	1.86	0.40
1:G:206:ILE:H	1:G:206:ILE:HG12	1.33	0.40
1:E:206:ILE:O	1:E:419:GLN:O	2.39	0.40
1:G:382:ALA:O	1:G:386:LEU:N	2.51	0.40
2:H:221:LEU:HG	2:H:221:LEU:O	2.22	0.40
2:H:32:ALA:N	2:H:226:LEU:O	2.44	0.40
2:D:213:LEU:CG	2:D:223:THR:HG23	2.51	0.40
2:D:363:ASP:O	2:D:366:ASP:HB2	2.21	0.40
2:H:159:PRO:CB	2:H:257:ARG:CD	2.96	0.40
2:H:351:LEU:O	2:H:352:VAL:CG1	2.60	0.40
2:F:168:ARG:HB2	2:F:168:ARG:HE	1.61	0.40
2:D:275:ASP:OD1	2:D:297:ARG:NE	2.37	0.40
1:E:119:PHE:N	1:E:119:PHE:CD1	2.89	0.40
2:F:285:SER:HB3	2:F:287:ASN:ND2	2.37	0.40

All (7) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:170:ARG:NH1	2:H:161:ARG:NH1[1_455]	1.89	0.31
2:B:170:ARG:NH1	2:H:161:ARG:O[1_455]	2.03	0.17
2:B:170:ARG:CZ	2:H:161:ARG:CZ[1_455]	2.04	0.16
2:D:169:PRO:CA	2:H:170:ARG:NH1[1_455]	2.09	0.11
2:B:170:ARG:NE	2:H:161:ARG:NE[1_455]	2.10	0.10
2:D:169:PRO:C	2:H:170:ARG:NH1[1_455]	2.11	0.09
2:B:170:ARG:NH1	2:H:161:ARG:CZ[1_455]	2.18	0.02

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	425/483 (88%)	348 (82%)	54 (13%)	23 (5%)	2	1
1	C	425/483 (88%)	350 (82%)	50 (12%)	25 (6%)	2	0
1	E	425/483 (88%)	355 (84%)	47 (11%)	23 (5%)	2	1
1	G	425/483 (88%)	347 (82%)	53 (12%)	25 (6%)	2	0
2	B	430/458 (94%)	361 (84%)	46 (11%)	23 (5%)	2	1
2	D	430/458 (94%)	359 (84%)	48 (11%)	23 (5%)	2	1
2	F	430/458 (94%)	359 (84%)	47 (11%)	24 (6%)	2	1
2	H	430/458 (94%)	356 (83%)	49 (11%)	25 (6%)	2	1
All	All	3420/3764 (91%)	2835 (83%)	394 (12%)	191 (6%)	2	1

All (191) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	30	PRO
1	A	64	GLY
1	A	95	MET
1	A	177	GLY
1	A	190	ARG
1	A	191	PRO
1	A	381	ASN
2	B	9	LYS
2	B	76	ALA
2	B	121	GLN
2	B	158	VAL
2	B	164	GLN
2	B	169	PRO
2	B	219	ASN
2	B	222	THR
2	B	265	PHE
2	B	348	ALA
2	B	349	ALA
2	B	352	VAL
2	B	354	SER
1	C	30	PRO
1	C	64	GLY
1	C	95	MET
1	C	190	ARG
1	C	191	PRO
1	C	381	ASN
1	C	421	ARG

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Mol	Chain	Res	Type
2	D	9	LYS
2	D	73	VAL
2	D	76	ALA
2	D	121	GLN
2	D	158	VAL
2	D	164	GLN
2	D	169	PRO
2	D	219	ASN
2	D	222	THR
2	D	265	PHE
2	D	348	ALA
2	D	349	ALA
2	D	352	VAL
2	D	354	SER
1	E	30	PRO
1	E	64	GLY
1	E	95	MET
1	E	177	GLY
1	E	190	ARG
1	E	191	PRO
1	E	381	ASN
1	E	421	ARG
2	F	76	ALA
2	F	121	GLN
2	F	158	VAL
2	F	164	GLN
2	F	169	PRO
2	F	219	ASN
2	F	222	THR
2	F	265	PHE
2	F	348	ALA
2	F	349	ALA
2	F	352	VAL
2	F	354	SER
1	G	30	PRO
1	G	64	GLY
1	G	95	MET
1	G	177	GLY
1	G	190	ARG
1	G	191	PRO
1	G	381	ASN
2	H	73	VAL

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Mol	Chain	Res	Type
2	H	76	ALA
2	H	121	GLN
2	H	158	VAL
2	H	164	GLN
2	H	169	PRO
2	H	219	ASN
2	H	222	THR
2	H	265	PHE
2	H	348	ALA
2	H	349	ALA
2	H	352	VAL
2	H	354	SER
1	A	25	CYS
1	A	27	LYS
1	A	229	ALA
1	A	421	ARG
2	B	73	VAL
2	B	75	GLY
2	B	77	ASP
1	C	27	LYS
1	C	63	ALA
1	C	177	GLY
1	C	229	ALA
2	D	75	GLY
2	D	77	ASP
2	D	237	SER
1	E	25	CYS
1	E	27	LYS
1	E	63	ALA
1	E	211	TRP
1	E	229	ALA
2	F	9	LYS
2	F	73	VAL
2	F	75	GLY
2	F	77	ASP
1	G	25	CYS
1	G	27	LYS
1	G	63	ALA
1	G	176	ILE
1	G	211	TRP
1	G	342	ALA
1	G	421	ARG

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Mol	Chain	Res	Type
2	H	9	LYS
2	H	75	GLY
2	H	77	ASP
1	A	28	PRO
1	A	63	ALA
1	A	188	SER
1	A	211	TRP
1	A	342	ALA
2	B	111	LEU
2	B	237	SER
1	C	25	CYS
1	C	28	PRO
1	C	69	ASN
1	C	176	ILE
1	C	211	TRP
1	C	228	LEU
1	C	342	ALA
1	E	28	PRO
1	E	69	ASN
1	E	176	ILE
1	E	188	SER
1	E	342	ALA
1	E	371	GLY
2	F	111	LEU
1	G	28	PRO
1	G	69	ASN
1	G	229	ALA
2	H	111	LEU
2	H	237	SER
1	A	69	ASN
1	A	176	ILE
1	A	238	GLN
2	B	350	ALA
2	B	362	GLY
2	B	402	PRO
2	D	111	LEU
2	D	362	GLY
2	D	402	PRO
1	E	228	LEU
1	E	250	CYS
2	F	237	SER
2	F	350	ALA

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Mol	Chain	Res	Type
2	F	362	GLY
1	G	72	THR
1	G	188	SER
2	H	29	LEU
2	H	161	ARG
2	H	362	GLY
2	H	402	PRO
1	A	72	THR
1	A	228	LEU
1	A	371	GLY
2	B	168	ARG
1	C	188	SER
1	C	238	GLN
1	C	250	CYS
1	C	371	GLY
1	C	399	ALA
2	D	168	ARG
2	D	341	ALA
2	D	375	GLN
1	E	399	ALA
2	F	168	ARG
2	F	402	PRO
1	G	371	GLY
2	H	168	ARG
2	B	271	LEU
2	F	161	ARG
1	G	141	ALA
1	G	228	LEU
1	G	250	CYS
2	H	110	ASP
2	H	350	ALA
1	G	129	ILE
1	A	195	VAL
1	C	129	ILE
1	C	195	VAL
1	E	195	VAL
1	G	195	VAL
2	F	132	PRO



### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	343/388 (88%)	260 (76%)	83 (24%)	1	1
1	C	343/388 (88%)	257 (75%)	86 (25%)	1	1
1	E	343/388 (88%)	257 (75%)	86 (25%)	1	1
1	G	343/388 (88%)	260 (76%)	83 (24%)	1	1
2	B	335/363 (92%)	266 (79%)	69 (21%)	1	1
2	D	335/363 (92%)	265 (79%)	70 (21%)	1	1
2	F	335/363 (92%)	265 (79%)	70 (21%)	1	1
2	H	335/363 (92%)	265 (79%)	70 (21%)	1	1
All	All	2712/3004 (90%)	2095 (77%)	617 (23%)	1	1

All (617) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	LYS
1	A	29	LYS
1	A	33	THR
1	A	34	ASP
1	A	37	CYS
1	A	48	PRO
1	A	60	ILE
1	A	62	CYS
1	A	67	TRP
1	A	69	ASN
1	A	70	ARG
1	A	72	THR
1	A	73	ARG
1	A	81	ARG
1	A	97	ARG
1	A	101	ARG
1	A	111	GLU
1	A	123	THR
1	A	134	ASP

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Mol	Chain	Res	Type
1	A	156	PHE
1	A	157	TYR
1	A	160	LYS
1	A	164	ASN
1	A	172	LEU
1	A	184	LEU
1	A	186	VAL
1	A	190	ARG
1	A	193	ILE
1	A	195	VAL
1	A	203	GLU
1	A	206	ILE
1	A	209	GLU
1	A	216	LEU
1	A	220	LEU
1	A	235	ARG
1	A	256	ASN
1	A	257	VAL
1	A	259	ARG
1	A	261	LEU
1	A	262	GLN
1	A	269	TRP
1	A	271	GLU
1	A	273	SER
1	A	279	ASP
1	A	285	ARG
1	A	287	PHE
1	A	292	ASP
1	A	307	GLU
1	A	311	VAL
1	A	315	LEU
1	A	322	LEU
1	A	323	GLU
1	A	329	LEU
1	A	335	LYS
1	A	337	TRP
1	A	338	SER
1	A	339	VAL
1	A	341	SER
1	A	343	LEU
1	A	344	GLN
1	A	353	THR

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Mol	Chain	Res	Type
1	A	359	THR
1	A	365	ARG
1	A	367	ARG
1	A	369	LEU
1	A	370	MET
1	A	375	LYS
1	A	376	MET
1	A	379	GLU
1	A	381	ASN
1	A	383	ARG
1	A	393	GLN
1	A	396	ILE
1	A	397	LEU
1	A	403	ASN
1	A	419	GLN
1	A	420	GLU
1	A	421	ARG
1	A	423	PHE
1	A	433	GLU
1	A	440	ILE
1	A	442	LEU
1	A	448	GLU
2	B	17	LYS
2	B	21	THR
2	B	26	LEU
2	B	28	ILE
2	B	31	LEU
2	B	41	SER
2	B	58	GLU
2	B	62	LEU
2	B	69	GLN
2	B	74	MET
2	B	77	ASP
2	B	85	LYS
2	B	90	ARG
2	B	91	GLN
2	B	94	SER
2	B	103	LEU
2	B	107	GLN
2	B	109	CYS
2	B	115	LEU
2	B	119	ARG

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Mol	Chain	Res	Type
2	B	122	TYR
2	B	123	GLU
2	B	137	ASP
2	B	157	LEU
2	B	158	VAL
2	B	160	GLU
2	B	161	ARG
2	B	168	ARG
2	B	170	ARG
2	B	172	VAL
2	B	180	LEU
2	B	190	GLU
2	B	194	SER
2	B	198	ARG
2	B	200	LEU
2	B	210	ASP
2	B	212	HIS
2	B	213	LEU
2	B	217	ARG
2	B	218	PHE
2	B	221	LEU
2	B	222	THR
2	B	223	THR
2	B	226	LEU
2	B	227	SER
2	B	257	ARG
2	B	262	ASP
2	B	263	ARG
2	B	264	ARG
2	B	265	PHE
2	B	277	TRP
2	B	287	ASN
2	B	308	HIS
2	B	310	MET
2	B	339	THR
2	B	344	VAL
2	B	351	LEU
2	B	352	VAL
2	B	356	LEU
2	B	359	VAL
2	B	361	VAL
2	B	363	ASP

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Mol	Chain	Res	Type
2	B	378	LEU
2	B	382	ASN
2	B	386	LEU
2	B	391	ARG
2	B	396	LEU
2	B	398	ARG
2	B	401	PHE
1	C	27	LYS
1	C	29	LYS
1	C	33	THR
1	C	34	ASP
1	C	37	CYS
1	C	60	ILE
1	C	62	CYS
1	C	67	TRP
1	C	68	ASP
1	C	69	ASN
1	C	70	ARG
1	C	72	THR
1	C	73	ARG
1	C	81	ARG
1	C	86	THR
1	C	97	ARG
1	C	101	ARG
1	C	102	LEU
1	C	111	GLU
1	C	123	THR
1	C	131	ASP
1	C	134	ASP
1	C	156	PHE
1	C	157	TYR
1	C	159	THR
1	C	160	LYS
1	C	164	ASN
1	C	172	LEU
1	C	184	LEU
1	C	186	VAL
1	C	190	ARG
1	C	193	ILE
1	C	195	VAL
1	C	203	GLU
1	C	206	ILE

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Mol	Chain	Res	Type
1	C	209	GLU
1	C	216	LEU
1	C	220	LEU
1	C	235	ARG
1	C	256	ASN
1	C	257	VAL
1	C	259	ARG
1	C	261	LEU
1	C	262	GLN
1	C	269	TRP
1	C	271	GLU
1	C	273	SER
1	C	279	ASP
1	C	285	ARG
1	C	287	PHE
1	C	292	ASP
1	C	307	GLU
1	C	311	VAL
1	C	315	LEU
1	C	322	LEU
1	C	323	GLU
1	C	329	LEU
1	C	335	LYS
1	C	337	TRP
1	C	338	SER
1	C	339	VAL
1	C	341	SER
1	C	343	LEU
1	C	344	GLN
1	C	353	THR
1	C	359	THR
1	C	365	ARG
1	C	367	ARG
1	C	369	LEU
1	C	370	MET
1	C	375	LYS
1	C	376	MET
1	C	379	GLU
1	C	381	ASN
1	C	383	ARG
1	C	393	GLN
1	C	396	ILE

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Mol	Chain	Res	Type
1	C	397	LEU
1	C	403	ASN
1	C	419	GLN
1	C	420	GLU
1	C	421	ARG
1	C	423	PHE
1	C	433	GLU
1	C	442	LEU
1	C	448	GLU
2	D	21	THR
2	D	26	LEU
2	D	28	ILE
2	D	31	LEU
2	D	58	GLU
2	D	62	LEU
2	D	69	GLN
2	D	74	MET
2	D	77	ASP
2	D	85	LYS
2	D	90	ARG
2	D	91	GLN
2	D	94	SER
2	D	103	LEU
2	D	107	GLN
2	D	109	CYS
2	D	115	LEU
2	D	119	ARG
2	D	122	TYR
2	D	127	ASP
2	D	137	ASP
2	D	157	LEU
2	D	158	VAL
2	D	160	GLU
2	D	161	ARG
2	D	163	ASP
2	D	168	ARG
2	D	170	ARG
2	D	172	VAL
2	D	180	LEU
2	D	190	GLU
2	D	198	ARG
2	D	200	LEU

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Mol	Chain	Res	Type
2	D	210	ASP
2	D	212	HIS
2	D	213	LEU
2	D	217	ARG
2	D	218	PHE
2	D	221	LEU
2	D	222	THR
2	D	223	THR
2	D	226	LEU
2	D	227	SER
2	D	257	ARG
2	D	262	ASP
2	D	263	ARG
2	D	264	ARG
2	D	265	PHE
2	D	277	TRP
2	D	287	ASN
2	D	308	HIS
2	D	310	MET
2	D	313	SER
2	D	331	LEU
2	D	339	THR
2	D	344	VAL
2	D	347	ARG
2	D	351	LEU
2	D	352	VAL
2	D	356	LEU
2	D	359	VAL
2	D	361	VAL
2	D	363	ASP
2	D	378	LEU
2	D	382	ASN
2	D	386	LEU
2	D	391	ARG
2	D	396	LEU
2	D	398	ARG
2	D	401	PHE
1	E	27	LYS
1	E	29	LYS
1	E	33	THR
1	E	34	ASP
1	E	37	CYS

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Mol	Chain	Res	Type
1	E	60	ILE
1	E	62	CYS
1	E	67	TRP
1	E	69	ASN
1	E	70	ARG
1	E	72	THR
1	E	73	ARG
1	E	78	ASP
1	E	81	ARG
1	E	86	THR
1	E	95	MET
1	E	97	ARG
1	E	101	ARG
1	E	111	GLU
1	E	123	THR
1	E	131	ASP
1	E	134	ASP
1	E	156	PHE
1	E	157	TYR
1	E	159	THR
1	E	160	LYS
1	E	164	ASN
1	E	172	LEU
1	E	184	LEU
1	E	190	ARG
1	E	193	ILE
1	E	195	VAL
1	E	203	GLU
1	E	206	ILE
1	E	209	GLU
1	E	216	LEU
1	E	220	LEU
1	E	235	ARG
1	E	256	ASN
1	E	257	VAL
1	E	259	ARG
1	E	261	LEU
1	E	262	GLN
1	E	269	TRP
1	E	271	GLU
1	E	273	SER
1	E	279	ASP

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Mol	Chain	Res	Type
1	E	285	ARG
1	E	287	PHE
1	E	292	ASP
1	E	307	GLU
1	E	311	VAL
1	E	315	LEU
1	E	322	LEU
1	E	323	GLU
1	E	329	LEU
1	E	337	TRP
1	E	338	SER
1	E	339	VAL
1	E	341	SER
1	E	343	LEU
1	E	344	GLN
1	E	353	THR
1	E	359	THR
1	E	365	ARG
1	E	367	ARG
1	E	369	LEU
1	E	370	MET
1	E	375	LYS
1	E	376	MET
1	E	379	GLU
1	E	381	ASN
1	E	383	ARG
1	E	393	GLN
1	E	396	ILE
1	E	397	LEU
1	E	402	ARG
1	E	403	ASN
1	E	419	GLN
1	E	420	GLU
1	E	421	ARG
1	E	423	PHE
1	E	433	GLU
1	E	440	ILE
1	E	442	LEU
1	E	448	GLU
2	F	14	SER
2	F	21	THR
2	F	26	LEU

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Mol	Chain	Res	Type
2	F	28	ILE
2	F	31	LEU
2	F	41	SER
2	F	58	GLU
2	F	62	LEU
2	F	69	GLN
2	F	74	MET
2	F	77	ASP
2	F	85	LYS
2	F	90	ARG
2	F	91	GLN
2	F	94	SER
2	F	103	LEU
2	F	107	GLN
2	F	109	CYS
2	F	115	LEU
2	F	119	ARG
2	F	122	TYR
2	F	157	LEU
2	F	158	VAL
2	F	160	GLU
2	F	161	ARG
2	F	168	ARG
2	F	170	ARG
2	F	172	VAL
2	F	180	LEU
2	F	190	GLU
2	F	194	SER
2	F	198	ARG
2	F	200	LEU
2	F	210	ASP
2	F	212	HIS
2	F	213	LEU
2	F	217	ARG
2	F	218	PHE
2	F	221	LEU
2	F	222	THR
2	F	223	THR
2	F	226	LEU
2	F	227	SER
2	F	257	ARG
2	F	262	ASP

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Mol	Chain	Res	Type
2	F	263	ARG
2	F	264	ARG
2	F	265	PHE
2	F	277	TRP
2	F	287	ASN
2	F	308	HIS
2	F	310	MET
2	F	313	SER
2	F	331	LEU
2	F	339	THR
2	F	344	VAL
2	F	347	ARG
2	F	351	LEU
2	F	352	VAL
2	F	356	LEU
2	F	359	VAL
2	F	361	VAL
2	F	363	ASP
2	F	378	LEU
2	F	382	ASN
2	F	386	LEU
2	F	391	ARG
2	F	396	LEU
2	F	398	ARG
2	F	401	PHE
1	G	27	LYS
1	G	29	LYS
1	G	33	THR
1	G	34	ASP
1	G	37	CYS
1	G	60	ILE
1	G	67	TRP
1	G	69	ASN
1	G	70	ARG
1	G	72	THR
1	G	73	ARG
1	G	81	ARG
1	G	86	THR
1	G	101	ARG
1	G	111	GLU
1	G	123	THR
1	G	131	ASP

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Mol	Chain	Res	Type
1	G	134	ASP
1	G	156	PHE
1	G	157	TYR
1	G	160	LYS
1	G	164	ASN
1	G	172	LEU
1	G	184	LEU
1	G	190	ARG
1	G	193	ILE
1	G	195	VAL
1	G	203	GLU
1	G	206	ILE
1	G	209	GLU
1	G	216	LEU
1	G	220	LEU
1	G	235	ARG
1	G	240	MET
1	G	256	ASN
1	G	257	VAL
1	G	259	ARG
1	G	261	LEU
1	G	262	GLN
1	G	269	TRP
1	G	271	GLU
1	G	273	SER
1	G	279	ASP
1	G	285	ARG
1	G	287	PHE
1	G	292	ASP
1	G	307	GLU
1	G	311	VAL
1	G	315	LEU
1	G	322	LEU
1	G	323	GLU
1	G	329	LEU
1	G	335	LYS
1	G	337	TRP
1	G	338	SER
1	G	339	VAL
1	G	341	SER
1	G	343	LEU
1	G	344	GLN

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Mol	Chain	Res	Type
1	G	353	THR
1	G	359	THR
1	G	365	ARG
1	G	367	ARG
1	G	369	LEU
1	G	370	MET
1	G	375	LYS
1	G	376	MET
1	G	379	GLU
1	G	381	ASN
1	G	383	ARG
1	G	393	GLN
1	G	396	ILE
1	G	397	LEU
1	G	402	ARG
1	G	403	ASN
1	G	419	GLN
1	G	420	GLU
1	G	421	ARG
1	G	423	PHE
1	G	433	GLU
1	G	440	ILE
1	G	442	LEU
1	G	448	GLU
2	H	21	THR
2	H	26	LEU
2	H	28	ILE
2	H	31	LEU
2	H	41	SER
2	H	58	GLU
2	H	62	LEU
2	H	69	GLN
2	H	74	MET
2	H	77	ASP
2	H	85	LYS
2	H	90	ARG
2	H	91	GLN
2	H	94	SER
2	H	103	LEU
2	H	107	GLN
2	H	109	CYS
2	H	115	LEU

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Mol	Chain	Res	Type
2	H	119	ARG
2	H	122	TYR
2	H	137	ASP
2	H	157	LEU
2	H	158	VAL
2	H	160	GLU
2	H	161	ARG
2	H	163	ASP
2	H	168	ARG
2	H	170	ARG
2	H	172	VAL
2	H	180	LEU
2	H	190	GLU
2	H	194	SER
2	H	198	ARG
2	H	200	LEU
2	H	210	ASP
2	H	212	HIS
2	H	213	LEU
2	H	217	ARG
2	H	218	PHE
2	H	221	LEU
2	H	222	THR
2	H	223	THR
2	H	226	LEU
2	H	227	SER
2	H	257	ARG
2	H	262	ASP
2	H	263	ARG
2	H	264	ARG
2	H	265	PHE
2	H	277	TRP
2	H	287	ASN
2	H	308	HIS
2	H	310	MET
2	H	315	ARG
2	H	331	LEU
2	H	339	THR
2	H	344	VAL
2	H	351	LEU
2	H	352	VAL
2	H	356	LEU

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Mol	Chain	Res	Type
2	H	359	VAL
2	H	361	VAL
2	H	363	ASP
2	H	378	LEU
2	H	382	ASN
2	H	386	LEU
2	H	391	ARG
2	H	396	LEU
2	H	398	ARG
2	H	401	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (88) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	HIS
1	A	57	HIS
1	A	69	ASN
1	A	108	GLN
1	A	199	ASN
1	A	246	ASN
1	A	344	GLN
1	A	381	ASN
1	A	419	GLN
2	B	39	HIS
2	B	91	GLN
2	B	107	GLN
2	B	112	HIS
2	B	173	ASN
2	B	287	ASN
2	B	301	GLN
2	B	308	HIS
2	B	382	ASN
2	B	384	HIS
2	B	434	HIS
2	B	435	HIS
1	C	54	HIS
1	C	57	HIS
1	C	69	ASN
1	C	108	GLN
1	C	199	ASN
1	C	246	ASN
1	C	256	ASN

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Mol	Chain	Res	Type
1	C	344	GLN
1	C	381	ASN
1	C	419	GLN
2	D	39	HIS
2	D	91	GLN
2	D	107	GLN
2	D	112	HIS
2	D	121	GLN
2	D	173	ASN
2	D	287	ASN
2	D	301	GLN
2	D	308	HIS
2	D	382	ASN
2	D	384	HIS
2	D	434	HIS
2	D	435	HIS
1	E	54	HIS
1	E	57	HIS
1	E	69	ASN
1	E	108	GLN
1	E	164	ASN
1	E	199	ASN
1	E	246	ASN
1	E	256	ASN
1	E	344	GLN
1	E	381	ASN
1	E	419	GLN
2	F	20	GLN
2	F	39	HIS
2	F	91	GLN
2	F	107	GLN
2	F	112	HIS
2	F	121	GLN
2	F	287	ASN
2	F	301	GLN
2	F	308	HIS
2	F	382	ASN
2	F	384	HIS
2	F	434	HIS
1	G	54	HIS
1	G	57	HIS
1	G	69	ASN

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Mol	Chain	Res	Type
1	G	108	GLN
1	G	199	ASN
1	G	246	ASN
1	G	256	ASN
1	G	344	GLN
1	G	381	ASN
1	G	393	GLN
1	G	419	GLN
2	H	39	HIS
2	H	91	GLN
2	H	107	GLN
2	H	121	GLN
2	H	287	ASN
2	H	301	GLN
2	H	308	HIS
2	H	382	ASN
2	H	384	HIS
2	H	434	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

8 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	$\# Z  > 2$
3	SF4	A	501	1,2	0,12,12	0.00	-	0,24,24	0.00	-
4	CZL	A	502	-	1,34,34	0.38	0	0,122,122	0.00	-
3	SF4	C	501	1,2	0,12,12	0.00	-	0,24,24	0.00	-
4	CZL	C	502	-	1,34,34	0.31	0	0,122,122	0.00	-
3	SF4	E	501	1,2	0,12,12	0.00	-	0,24,24	0.00	-
4	CZL	E	502	-	1,34,34	0.31	0	0,122,122	0.00	-
3	SF4	G	501	1,2	0,12,12	0.00	-	0,24,24	0.00	-
4	CZL	G	502	-	1,34,34	0.32	0	0,122,122	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
3	SF4	A	501	1,2	-	0/0/48/48	0/6/5/5
4	CZL	A	502	-	-	0/0/365/365	0/0/18/18
3	SF4	C	501	1,2	-	0/0/48/48	0/6/5/5
4	CZL	C	502	-	-	0/0/365/365	0/0/18/18
3	SF4	E	501	1,2	-	0/0/48/48	0/6/5/5
4	CZL	E	502	-	-	0/0/365/365	0/0/18/18
3	SF4	G	501	1,2	-	0/0/48/48	0/6/5/5
4	CZL	G	502	-	-	0/0/365/365	0/0/18/18

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	SF4	2	0
4	A	502	CZL	3	0
3	C	501	SF4	2	0
4	C	502	CZL	3	0
3	E	501	SF4	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	502	CZL	2	0
3	G	501	SF4	4	0
4	G	502	CZL	4	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	427/483 (88%)	0.88	63 (14%) 3 3	14, 42, 91, 112	0
1	C	427/483 (88%)	1.07	80 (18%) 2 1	17, 44, 91, 117	0
1	E	427/483 (88%)	1.05	69 (16%) 3 2	15, 43, 91, 117	0
1	G	427/483 (88%)	1.09	80 (18%) 2 1	17, 44, 93, 114	0
2	B	432/458 (94%)	0.58	28 (6%) 22 22	14, 35, 72, 89	0
2	D	432/458 (94%)	0.63	34 (7%) 15 15	12, 36, 75, 91	0
2	F	432/458 (94%)	0.78	44 (10%) 9 8	14, 37, 73, 90	0
2	H	432/458 (94%)	0.66	44 (10%) 9 8	13, 37, 74, 89	0
All	All	3436/3764 (91%)	0.84	442 (12%) 5 5	12, 40, 82, 117	0

All (442) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	376	MET	23.0
1	E	371	GLY	11.3
1	G	337	TRP	11.2
1	C	334	VAL	10.6
1	G	376	MET	10.0
1	G	32	ALA	9.5
2	D	165	VAL	9.1
1	G	366	ILE	8.5
1	E	376	MET	8.3
2	D	161	ARG	8.1
1	C	377	LEU	8.1
1	G	334	VAL	7.8
1	E	31	GLY	7.7
1	E	379	GLU	7.6
2	D	222	THR	7.6
2	H	218	PHE	7.6

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Mol	Chain	Res	Type	RSRZ
2	B	158	VAL	7.4
1	E	95	MET	7.0
1	E	419	GLN	6.9
2	H	74	MET	6.8
1	E	420	GLU	6.8
1	G	419	GLN	6.7
2	F	222	THR	6.6
2	F	104	SER	6.5
1	C	350	VAL	6.5
1	C	32	ALA	6.4
1	C	25	CYS	6.2
1	C	393	GLN	6.0
1	G	382	ALA	6.0
2	F	165	VAL	6.0
1	G	378	ASP	5.9
1	C	420	GLU	5.8
2	F	127	ASP	5.7
2	D	109	CYS	5.7
1	G	381	ASN	5.6
1	A	375	LYS	5.5
1	E	361	GLU	5.2
1	C	371	GLY	5.1
1	A	337	TRP	5.1
2	H	265	PHE	5.1
1	E	375	LYS	5.1
1	G	352	ALA	5.0
1	C	95	MET	5.0
2	H	125	TYR	5.0
2	H	165	VAL	5.0
1	G	71	GLY	5.0
2	D	75	GLY	5.0
1	G	420	GLU	5.0
1	G	354	GLY	5.0
1	G	338	SER	4.9
1	E	195	VAL	4.9
1	C	340	VAL	4.9
1	C	375	LYS	4.8
1	C	378	ASP	4.8
1	C	194	ARG	4.8
1	A	423	PHE	4.8
2	H	77	ASP	4.8
1	E	32	ALA	4.8

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Mol	Chain	Res	Type	RSRZ
2	B	154	VAL	4.8
1	G	339	VAL	4.7
2	B	109	CYS	4.6
1	G	369	LEU	4.6
2	F	118	PHE	4.6
1	C	354	GLY	4.5
1	G	377	LEU	4.5
2	H	164	GLN	4.5
1	G	365	ARG	4.5
1	E	291	LEU	4.5
1	G	359	THR	4.5
2	B	77	ASP	4.4
1	C	336	SER	4.4
1	A	32	ALA	4.4
1	G	353	THR	4.4
1	C	355	THR	4.3
2	D	223	THR	4.3
2	D	69	GLN	4.3
2	H	231	LEU	4.3
1	C	402	ARG	4.3
1	E	338	SER	4.2
2	F	274	VAL	4.2
1	A	387	LYS	4.2
2	F	77	ASP	4.2
1	G	195	VAL	4.2
1	G	360	GLU	4.2
2	D	353	ASP	4.2
1	G	379	GLU	4.2
2	F	251	ALA	4.2
2	D	125	TYR	4.1
1	E	357	LYS	4.1
1	G	386	LEU	4.1
1	G	324	GLY	4.1
2	H	158	VAL	4.1
1	C	382	ALA	4.1
1	G	414	PHE	4.1
1	C	322	LEU	4.1
2	H	213	LEU	4.1
1	E	312	ARG	4.0
1	E	374	VAL	4.0
1	C	368	GLU	4.0
1	E	336	SER	3.9

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Mol	Chain	Res	Type	RSRZ
1	G	333	GLY	3.9
1	G	340	VAL	3.9
1	A	348	MET	3.9
1	G	336	SER	3.9
1	E	394	ALA	3.9
2	D	127	ASP	3.9
2	H	212	HIS	3.9
1	G	348	MET	3.9
2	H	352	VAL	3.8
2	F	98	LEU	3.8
1	G	345	ASP	3.8
2	H	219	ASN	3.8
1	G	349	LYS	3.8
2	F	90	ARG	3.8
2	D	74	MET	3.8
1	E	391	GLU	3.7
1	E	65	SER	3.7
1	G	361	GLU	3.7
1	A	374	VAL	3.7
1	C	370	MET	3.7
1	A	420	GLU	3.7
1	G	387	LYS	3.7
2	F	112	HIS	3.6
1	A	170	ALA	3.6
2	F	346	ALA	3.6
1	C	365	ARG	3.6
2	H	176	CYS	3.6
1	A	377	LEU	3.6
1	C	369	LEU	3.6
1	A	63	ALA	3.5
1	A	336	SER	3.5
1	C	290	LEU	3.5
2	B	165	VAL	3.5
2	F	241	LEU	3.5
1	A	373	ASP	3.5
1	C	229	ALA	3.5
1	E	337	TRP	3.4
1	A	393	GLN	3.4
2	F	111	LEU	3.4
1	G	380	GLY	3.4
1	C	360	GLU	3.4
1	C	296	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
2	F	202	ILE	3.4
2	B	64	THR	3.4
1	G	346	LEU	3.3
1	G	350	VAL	3.3
1	C	353	THR	3.3
1	E	393	GLN	3.3
1	A	322	LEU	3.3
1	C	361	GLU	3.3
1	E	423	PHE	3.3
2	F	64	THR	3.3
1	E	328	LEU	3.3
1	C	338	SER	3.3
1	A	334	VAL	3.3
1	E	33	THR	3.3
1	G	362	ASP	3.2
1	C	379	GLU	3.2
1	G	292	ASP	3.2
1	A	291	LEU	3.2
2	H	112	HIS	3.2
1	E	343	LEU	3.2
1	G	393	GLN	3.2
1	A	87	ASP	3.2
2	B	213	LEU	3.2
1	A	356	LYS	3.2
1	E	288	ALA	3.2
1	C	337	TRP	3.2
1	G	172	LEU	3.2
1	E	421	ARG	3.2
1	G	91	ASN	3.2
2	B	74	MET	3.2
1	A	33	THR	3.1
1	C	325	LYS	3.1
2	D	123	GLU	3.1
1	A	176	ILE	3.1
2	B	222	THR	3.1
2	F	188	ILE	3.1
2	F	265	PHE	3.1
1	C	151	VAL	3.1
1	A	341	SER	3.1
1	C	330	TYR	3.1
1	E	174	TYR	3.1
1	G	255	LEU	3.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	H	235	GLY	3.1
2	H	106	THR	3.1
1	C	384	VAL	3.1
1	A	419	GLN	3.1
1	E	355	THR	3.1
1	G	355	THR	3.1
1	C	352	ALA	3.1
1	G	314	ALA	3.1
1	E	381	ASN	3.0
1	E	290	LEU	3.0
1	C	419	GLN	3.0
1	G	315	LEU	3.0
2	D	213	LEU	3.0
1	E	25	CYS	3.0
1	A	378	ASP	3.0
1	G	290	LEU	3.0
2	B	212	HIS	3.0
1	C	97	ARG	2.9
2	F	66	ALA	2.9
2	B	112	HIS	2.9
2	F	154	VAL	2.9
1	C	255	LEU	2.9
1	A	371	GLY	2.9
1	A	174	TYR	2.9
1	E	70	ARG	2.9
2	F	158	VAL	2.9
2	H	228	VAL	2.9
1	E	364	ALA	2.9
1	C	367	ARG	2.9
1	C	326	ARG	2.9
1	E	96	GLY	2.9
2	B	111	LEU	2.8
1	A	399	ALA	2.8
1	A	338	SER	2.8
2	F	125	TYR	2.8
1	A	415	LEU	2.8
2	B	161	ARG	2.8
1	C	389	VAL	2.8
2	H	222	THR	2.8
2	B	169	PRO	2.8
1	C	390	ASP	2.8
1	G	384	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	379	GLU	2.8
1	C	421	ARG	2.8
2	B	118	PHE	2.8
2	F	352	VAL	2.8
1	C	358	SER	2.8
1	A	384	VAL	2.7
1	C	174	TYR	2.7
1	C	335	LYS	2.7
2	F	101	THR	2.7
1	C	435	VAL	2.7
2	H	353	ASP	2.7
2	D	220	ALA	2.7
1	E	176	ILE	2.7
1	A	172	LEU	2.7
1	E	372	ASP	2.7
1	C	160	LYS	2.7
1	G	95	MET	2.7
2	F	100	THR	2.7
2	D	131	VAL	2.7
1	A	96	GLY	2.7
2	B	347	ARG	2.6
1	A	288	ALA	2.6
1	E	319	ARG	2.6
1	E	365	ARG	2.6
1	G	358	SER	2.6
1	E	34	ASP	2.6
2	B	265	PHE	2.6
1	A	321	ARG	2.6
2	F	170	ARG	2.6
1	A	300	THR	2.6
1	C	87	ASP	2.6
1	A	289	ARG	2.6
1	E	326	ARG	2.6
2	H	351	LEU	2.6
1	C	155	GLY	2.6
1	G	168	GLY	2.6
1	C	187	GLY	2.6
1	E	194	ARG	2.6
1	E	44	ILE	2.6
1	G	343	LEU	2.6
2	H	115	LEU	2.6
2	D	401	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	348	MET	2.6
1	E	339	VAL	2.5
1	G	266	GLY	2.5
2	F	254	LEU	2.5
1	A	95	MET	2.5
2	H	161	ARG	2.5
2	D	135	THR	2.5
1	E	358	SER	2.5
2	H	133	VAL	2.5
1	C	303	LEU	2.5
2	D	130	ILE	2.5
1	G	372	ASP	2.5
1	A	195	VAL	2.5
1	G	385	LEU	2.5
1	C	33	THR	2.5
2	H	4	ILE	2.5
2	D	295	ARG	2.5
2	B	117	GLU	2.5
2	D	81	VAL	2.5
1	E	415	LEU	2.5
1	E	353	THR	2.5
1	E	35	GLY	2.5
1	G	70	ARG	2.5
1	G	330	TYR	2.5
2	F	166	GLY	2.5
1	C	167	ALA	2.5
1	A	194	ARG	2.4
2	H	75	GLY	2.4
1	E	348	MET	2.4
1	E	370	MET	2.4
1	A	313	ALA	2.4
1	C	394	ALA	2.4
1	G	374	VAL	2.4
2	F	161	ARG	2.4
1	C	211	TRP	2.4
1	G	64	GLY	2.4
2	H	120	THR	2.4
2	D	162	ARG	2.4
1	A	328	LEU	2.4
1	E	329	LEU	2.4
2	F	75	GLY	2.4
2	B	363	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
2	D	78	GLU	2.4
1	A	229	ALA	2.4
1	C	383	ARG	2.4
2	H	38	PHE	2.4
1	A	330	TYR	2.4
1	G	368	GLU	2.4
1	E	397	LEU	2.4
2	H	131	VAL	2.4
1	G	436	ARG	2.4
1	C	363	LYS	2.4
2	D	258	THR	2.4
2	H	76	ALA	2.4
1	E	38	SER	2.3
1	C	387	LYS	2.3
1	G	253	ALA	2.3
1	G	357	LYS	2.3
1	G	332	GLY	2.3
1	C	103	PHE	2.3
1	E	289	ARG	2.3
1	A	418	ASN	2.3
1	C	372	ASP	2.3
2	F	169	PRO	2.3
2	H	124	GLU	2.3
2	D	254	LEU	2.3
2	F	213	LEU	2.3
2	F	172	VAL	2.3
1	E	24	GLY	2.3
1	G	335	LYS	2.3
2	B	159	PRO	2.3
1	A	414	PHE	2.3
2	D	218	PHE	2.3
1	C	397	LEU	2.3
1	G	211	TRP	2.3
2	F	223	THR	2.3
1	A	333	GLY	2.3
1	A	366	ILE	2.3
1	C	328	LEU	2.3
1	E	131	ASP	2.3
1	C	195	VAL	2.3
1	A	211	TRP	2.3
2	H	162	ARG	2.3
2	B	291	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	339	VAL	2.2
1	C	392	TYR	2.2
2	H	251	ALA	2.2
1	A	94	ILE	2.2
1	A	69	ASN	2.2
1	E	346	LEU	2.2
1	E	369	LEU	2.2
1	G	284	LEU	2.2
1	G	331	THR	2.2
1	C	357	LYS	2.2
1	E	340	VAL	2.2
1	A	125	VAL	2.2
1	C	422	GLU	2.2
1	G	87	ASP	2.2
2	D	117	GLU	2.2
1	C	100	LYS	2.2
2	F	401	PHE	2.2
2	B	351	LEU	2.2
1	A	70	ARG	2.2
1	E	97	ARG	2.2
1	G	279	ASP	2.2
1	E	386	LEU	2.2
1	C	345	ASP	2.2
2	F	119	ARG	2.2
1	G	351	VAL	2.2
2	B	352	VAL	2.2
1	A	64	GLY	2.2
2	F	74	MET	2.2
2	F	115	LEU	2.2
2	H	99	LEU	2.2
1	G	185	PRO	2.2
2	H	79	ASN	2.2
1	E	66	SER	2.1
1	E	407	ALA	2.1
2	D	94	SER	2.1
1	C	366	ILE	2.1
2	H	153	ILE	2.1
1	C	289	ARG	2.1
1	G	162	LEU	2.1
2	H	204	ASP	2.1
1	A	164	ASN	2.1
1	E	412	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
2	F	235	GLY	2.1
2	D	350	ALA	2.1
2	F	103	LEU	2.1
1	C	316	GLU	2.1
1	E	436	ARG	2.1
2	B	371	ALA	2.1
2	D	158	VAL	2.1
1	A	91	ASN	2.1
2	D	265	PHE	2.1
2	F	157	LEU	2.1
2	F	258	THR	2.1
2	H	136	PRO	2.1
1	A	380	GLY	2.1
1	G	418	ASN	2.1
1	G	291	LEU	2.1
1	A	354	GLY	2.1
1	G	177	GLY	2.1
2	B	75	GLY	2.1
2	H	80	VAL	2.1
1	A	355	THR	2.1
1	E	373	ASP	2.1
2	D	219	ASN	2.1
2	D	359	VAL	2.1
1	C	250	CYS	2.1
2	F	351	LEU	2.1
2	H	111	LEU	2.1
1	A	319	ARG	2.0
1	C	257	VAL	2.0
1	A	304	ILE	2.0
1	E	356	LYS	2.0
2	H	167	LYS	2.0
1	G	174	TYR	2.0
2	B	223	THR	2.0
2	D	38	PHE	2.0
1	G	65	SER	2.0
2	D	77	ASP	2.0
2	B	283	GLU	2.0
1	G	277	ILE	2.0
1	C	386	LEU	2.0
2	B	353	ASP	2.0
2	H	122	TYR	2.0
2	F	162	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
2	H	239	ALA	2.0
1	A	186	VAL	2.0
1	A	332	GLY	2.0
1	E	377	LEU	2.0
1	G	341	SER	2.0
2	H	223	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<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
3	SF4	G	501	8/8	0.95	0.16	-0.24	25,29,31,44	0
3	SF4	C	501	8/8	0.96	0.16	-0.39	16,26,34,53	0
3	SF4	A	501	8/8	0.96	0.15	-0.76	17,21,23,28	0
4	CZL	A	502	17/17	0.96	0.14	-1.42	26,47,58,62	0
4	CZL	E	502	17/17	0.96	0.12	-1.53	74,89,128,134	0
4	CZL	G	502	17/17	0.95	0.11	-1.68	55,87,123,129	0
4	CZL	C	502	17/17	0.96	0.09	-1.88	59,81,108,114	0
3	SF4	E	501	8/8	0.96	0.13	-2.19	14,32,40,43	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.