



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:18 AM GMT

PDB ID : 3E1Y  
Title : Crystal structure of human eRF1/eRF3 complex  
Authors : Cheng, Z.; Lim, M.; Kong, C.; Song, H.  
Deposited on : 2008-08-05  
Resolution : 3.80 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

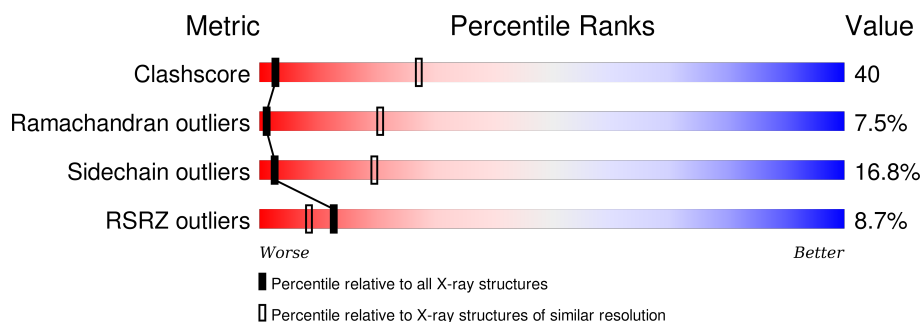
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.80 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))
Clashscore	102246	1458 (4.10-3.50)
Ramachandran outliers	100387	1397 (4.10-3.50)
Sidechain outliers	100360	1392 (4.10-3.50)
RSRZ outliers	91569	1325 (4.10-3.50)

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	451	<div> <div>5%</div> <div>34% 37% 12% 16%</div> </div>
1	B	451	<div> <div>5%</div> <div>35% 37% 12% 16%</div> </div>
1	C	451	<div> <div>5%</div> <div>37% 27% 6% 29%</div> </div>
1	D	451	<div> <div>5%</div> <div>37% 27% 6% 29%</div> </div>
2	E	204	<div> <div>10%</div> <div>26% 50% 17%</div> </div>
2	F	204	<div> <div>12%</div> <div>28% 48% 17%</div> </div>
2	G	204	<div> <div>14%</div> <div>32% 46% 15%</div> </div>

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Mol	Chain	Length	Quality of chain
2	H	204	<div><div></div><div>13%</div><div>31%</div><div>47%</div><div>15%</div><div></div><div></div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17110 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 Eukaryotic peptide chain release factor subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	380	Total	C	N	O	S	0	0	0
			2987	1908	511	558	10			
1	B	380	Total	C	N	O	S	0	0	0
			2987	1908	511	558	10			
1	C	318	Total	C	N	O	S	0	0	0
			2511	1617	414	470	10			
1	D	318	Total	C	N	O	S	0	0	0
			2511	1617	414	470	10			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	EXPRESSION TAG	UNP P62495
A	-12	ARG	-	EXPRESSION TAG	UNP P62495
A	-11	GLY	-	EXPRESSION TAG	UNP P62495
A	-10	SER	-	EXPRESSION TAG	UNP P62495
A	-9	HIS	-	EXPRESSION TAG	UNP P62495
A	-8	HIS	-	EXPRESSION TAG	UNP P62495
A	-7	HIS	-	EXPRESSION TAG	UNP P62495
A	-6	HIS	-	EXPRESSION TAG	UNP P62495
A	-5	HIS	-	EXPRESSION TAG	UNP P62495
A	-4	HIS	-	EXPRESSION TAG	UNP P62495
A	-3	GLY	-	EXPRESSION TAG	UNP P62495
A	-2	MET	-	EXPRESSION TAG	UNP P62495
A	-1	ALA	-	EXPRESSION TAG	UNP P62495
A	0	SER	-	EXPRESSION TAG	UNP P62495
B	-13	MET	-	EXPRESSION TAG	UNP P62495
B	-12	ARG	-	EXPRESSION TAG	UNP P62495
B	-11	GLY	-	EXPRESSION TAG	UNP P62495
B	-10	SER	-	EXPRESSION TAG	UNP P62495
B	-9	HIS	-	EXPRESSION TAG	UNP P62495
B	-8	HIS	-	EXPRESSION TAG	UNP P62495
B	-7	HIS	-	EXPRESSION TAG	UNP P62495

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	HIS	-	EXPRESSION TAG	UNP P62495
B	-5	HIS	-	EXPRESSION TAG	UNP P62495
B	-4	HIS	-	EXPRESSION TAG	UNP P62495
B	-3	GLY	-	EXPRESSION TAG	UNP P62495
B	-2	MET	-	EXPRESSION TAG	UNP P62495
B	-1	ALA	-	EXPRESSION TAG	UNP P62495
B	0	SER	-	EXPRESSION TAG	UNP P62495
C	-13	MET	-	EXPRESSION TAG	UNP P62495
C	-12	ARG	-	EXPRESSION TAG	UNP P62495
C	-11	GLY	-	EXPRESSION TAG	UNP P62495
C	-10	SER	-	EXPRESSION TAG	UNP P62495
C	-9	HIS	-	EXPRESSION TAG	UNP P62495
C	-8	HIS	-	EXPRESSION TAG	UNP P62495
C	-7	HIS	-	EXPRESSION TAG	UNP P62495
C	-6	HIS	-	EXPRESSION TAG	UNP P62495
C	-5	HIS	-	EXPRESSION TAG	UNP P62495
C	-4	HIS	-	EXPRESSION TAG	UNP P62495
C	-3	GLY	-	EXPRESSION TAG	UNP P62495
C	-2	MET	-	EXPRESSION TAG	UNP P62495
C	-1	ALA	-	EXPRESSION TAG	UNP P62495
C	0	SER	-	EXPRESSION TAG	UNP P62495
D	-13	MET	-	EXPRESSION TAG	UNP P62495
D	-12	ARG	-	EXPRESSION TAG	UNP P62495
D	-11	GLY	-	EXPRESSION TAG	UNP P62495
D	-10	SER	-	EXPRESSION TAG	UNP P62495
D	-9	HIS	-	EXPRESSION TAG	UNP P62495
D	-8	HIS	-	EXPRESSION TAG	UNP P62495
D	-7	HIS	-	EXPRESSION TAG	UNP P62495
D	-6	HIS	-	EXPRESSION TAG	UNP P62495
D	-5	HIS	-	EXPRESSION TAG	UNP P62495
D	-4	HIS	-	EXPRESSION TAG	UNP P62495
D	-3	GLY	-	EXPRESSION TAG	UNP P62495
D	-2	MET	-	EXPRESSION TAG	UNP P62495
D	-1	ALA	-	EXPRESSION TAG	UNP P62495
D	0	SER	-	EXPRESSION TAG	UNP P62495

- Molecule 2 is a protein called Eukaryotic peptide chain release factor GTP-binding subunit ERF3A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	195	Total	C	N	O	S	0	0	0
			1513	960	261	280	12			

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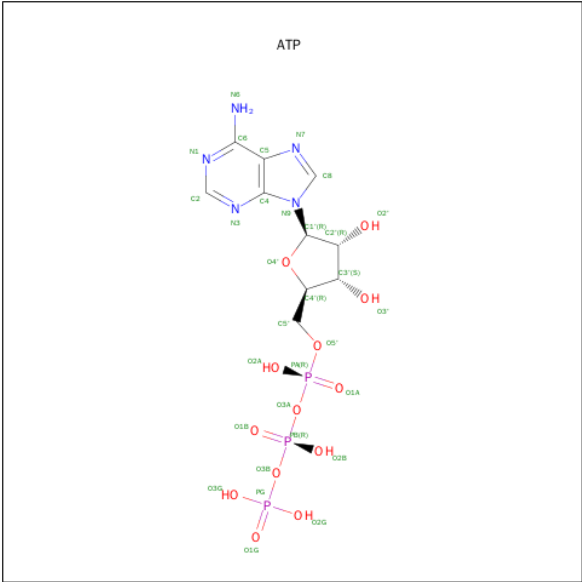
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	195	Total	C	N	O	S	0	0	0
			1513	960	261	280	12			
2	G	195	Total	C	N	O	S	0	0	0
			1513	960	261	280	12			
2	H	195	Total	C	N	O	S	0	0	0
			1513	960	261	280	12			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	434	GLY	-	EXPRESSION TAG	UNP P15170
E	435	PRO	-	EXPRESSION TAG	UNP P15170
E	436	LEU	-	EXPRESSION TAG	UNP P15170
E	437	GLY	-	EXPRESSION TAG	UNP P15170
E	438	SER	-	EXPRESSION TAG	UNP P15170
F	434	GLY	-	EXPRESSION TAG	UNP P15170
F	435	PRO	-	EXPRESSION TAG	UNP P15170
F	436	LEU	-	EXPRESSION TAG	UNP P15170
F	437	GLY	-	EXPRESSION TAG	UNP P15170
F	438	SER	-	EXPRESSION TAG	UNP P15170
G	434	GLY	-	EXPRESSION TAG	UNP P15170
G	435	PRO	-	EXPRESSION TAG	UNP P15170
G	436	LEU	-	EXPRESSION TAG	UNP P15170
G	437	GLY	-	EXPRESSION TAG	UNP P15170
G	438	SER	-	EXPRESSION TAG	UNP P15170
H	434	GLY	-	EXPRESSION TAG	UNP P15170
H	435	PRO	-	EXPRESSION TAG	UNP P15170
H	436	LEU	-	EXPRESSION TAG	UNP P15170
H	437	GLY	-	EXPRESSION TAG	UNP P15170
H	438	SER	-	EXPRESSION TAG	UNP P15170

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).

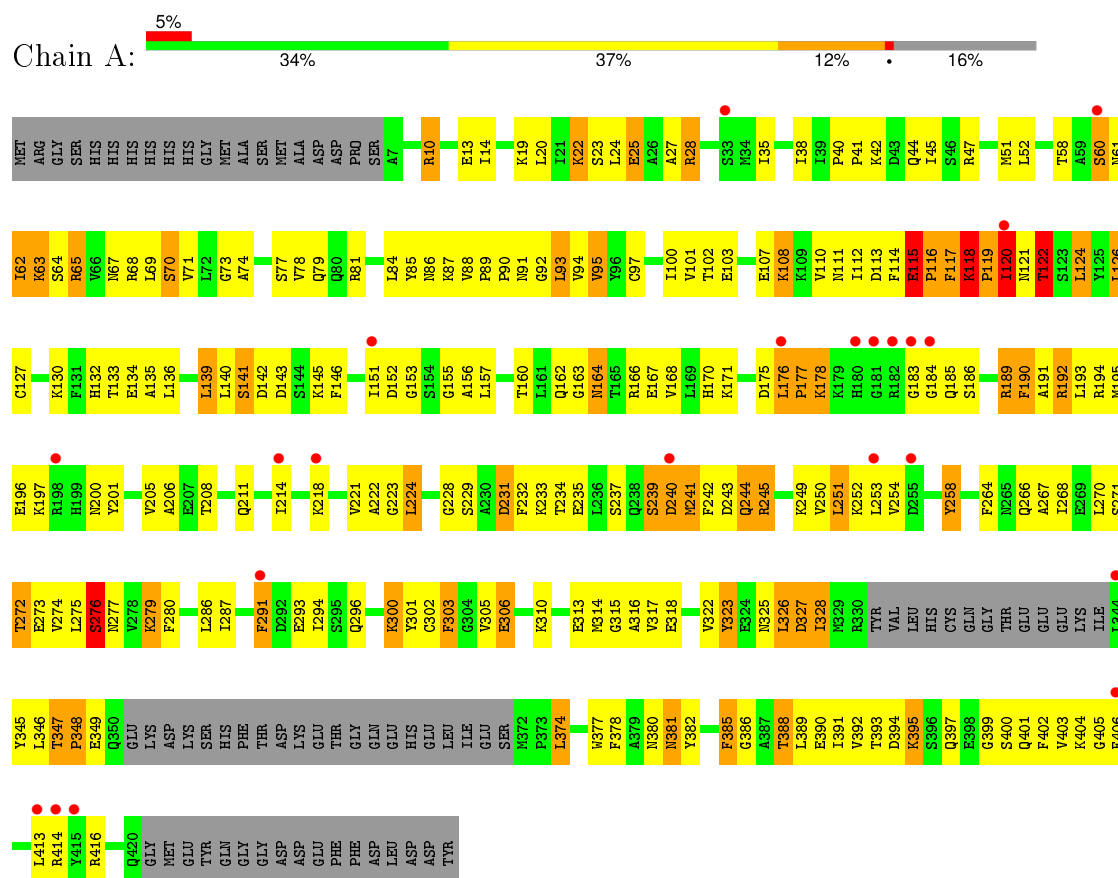


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

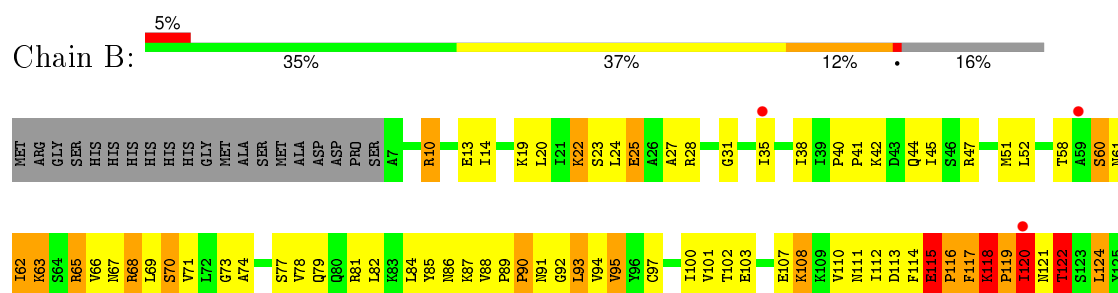
### 3 Residue-property plots

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.

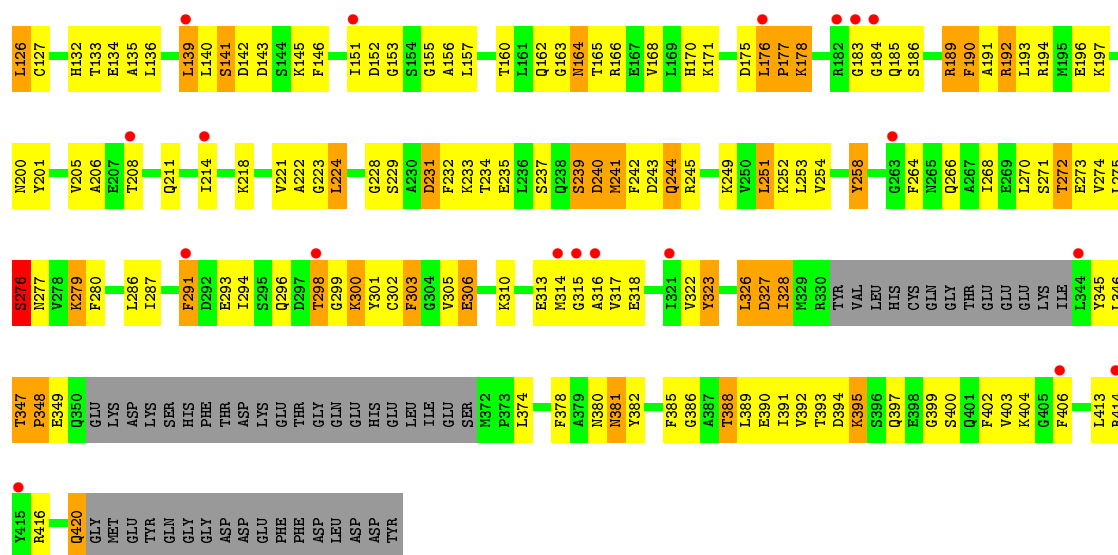
- Molecule 1: Eukaryotic peptide chain release factor subunit 1



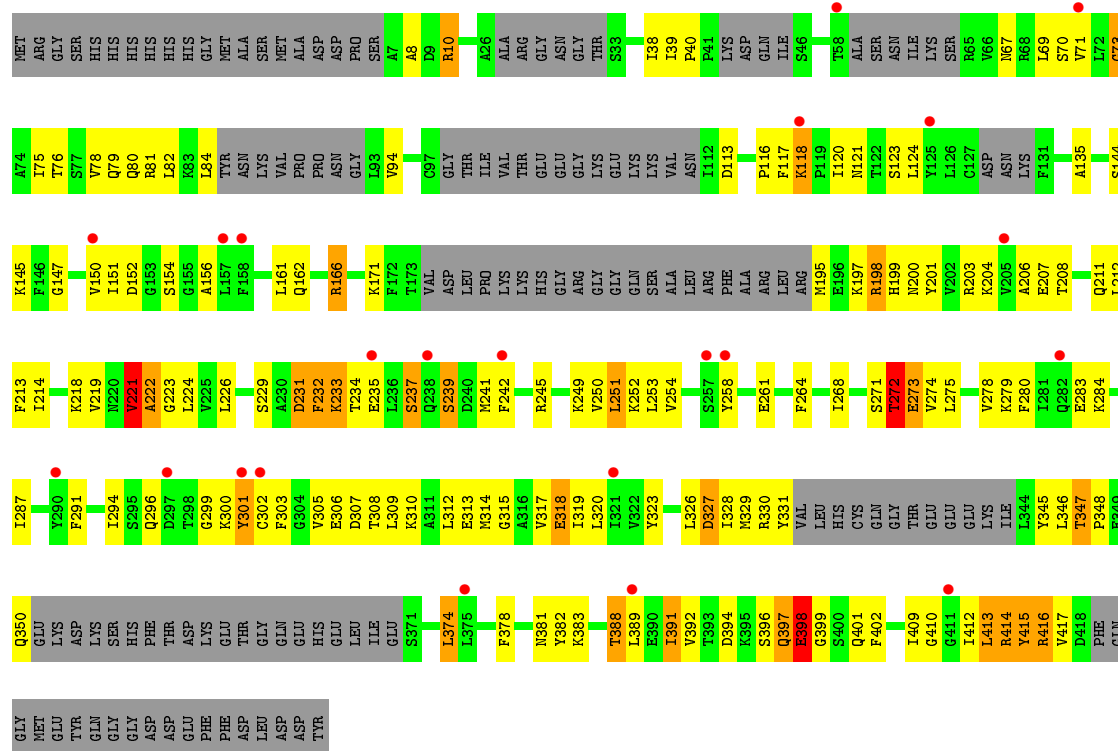
- Molecule 1: Eukaryotic peptide chain release factor subunit 1





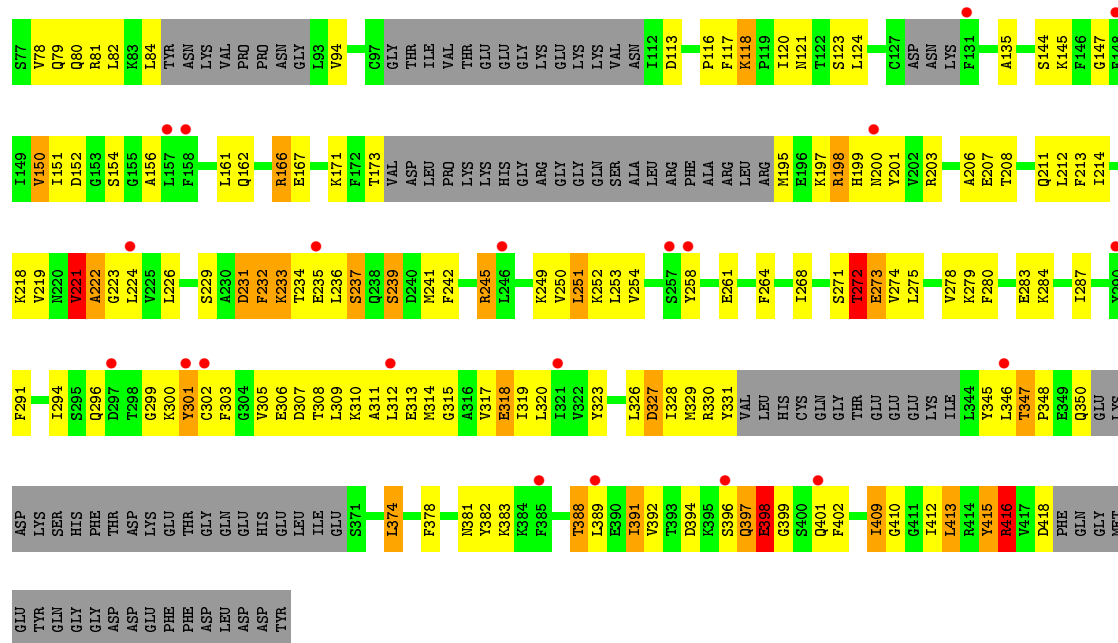


• Molecule 1: Eukaryotic peptide chain release factor subunit 1

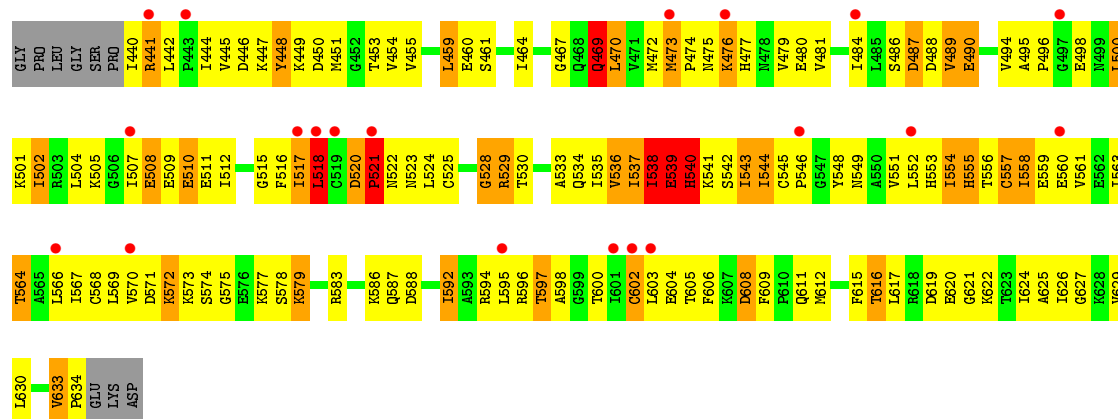


• Molecule 1: Eukaryotic peptide chain release factor subunit 1

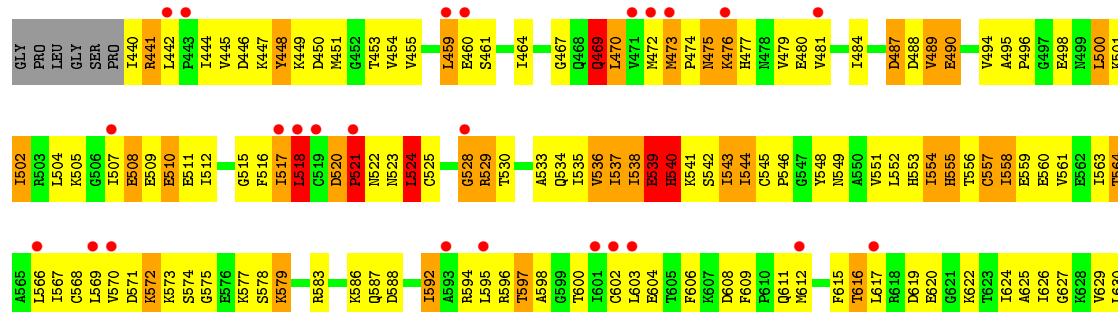




• Molecule 2: Eukaryotic peptide chain release factor GTP-binding subunit ERF3A

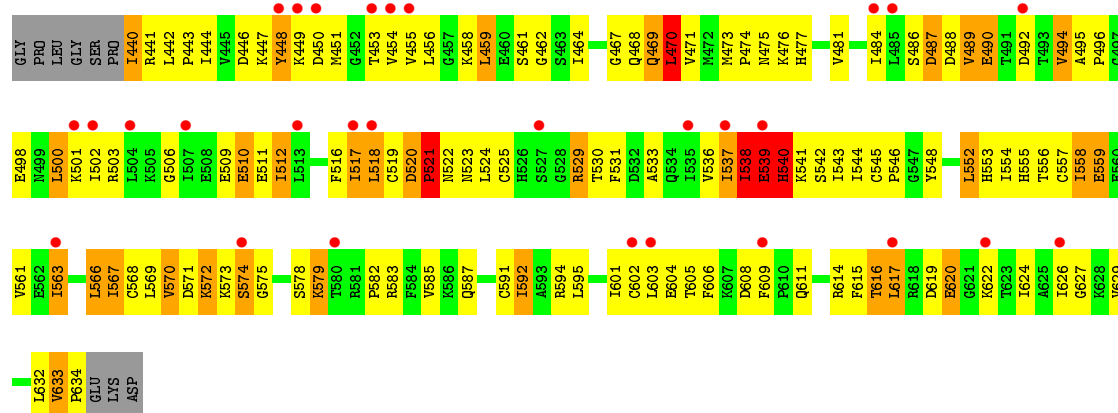


• Molecule 2: Eukaryotic peptide chain release factor GTP-binding subunit ERF3A

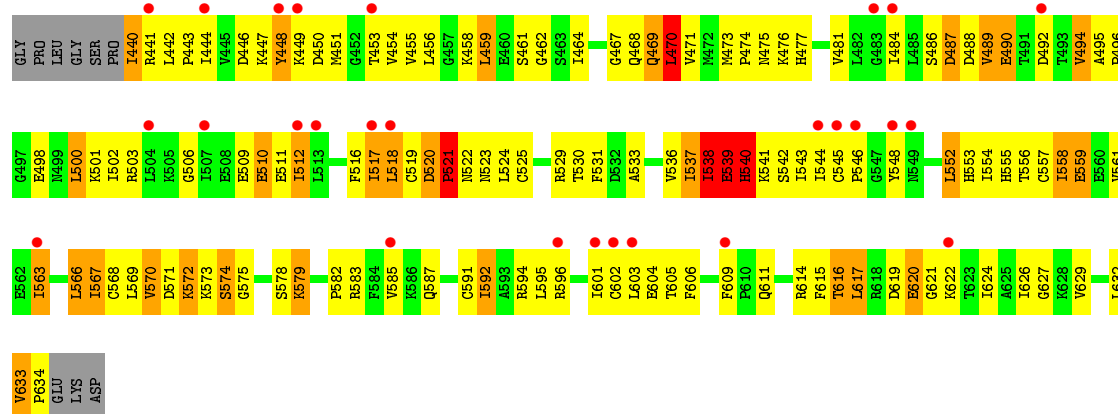




- Molecule 2: Eukaryotic peptide chain release factor GTP-binding subunit ERF3A



- Molecule 2: Eukaryotic peptide chain release factor GTP-binding subunit ERF3A



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	173.97Å 173.97Å 119.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.80 85.83 – 3.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (30.00-3.80) 99.9 (85.83-3.60)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.76 (at 3.58Å)	Xtriage
Refinement program	REFMAC 5.4.0077	Depositor
R, $R_{free}$	0.260 , 0.304 0.277 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	151.8	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 143.6	EDS
Estimated twinning fraction	0.430 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 41590 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	17110	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.21% 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: ATP

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	0.51	2/3033 (0.1%)	0.67	3/4077 (0.1%)
1	B	0.50	0/3033	0.70	4/4077 (0.1%)
1	C	0.37	0/2544	0.55	0/3413
1	D	0.38	0/2544	0.55	0/3413
2	E	0.52	0/1534	0.84	4/2068 (0.2%)
2	F	0.53	0/1534	0.83	3/2068 (0.1%)
2	G	0.45	0/1534	0.79	4/2068 (0.2%)
2	H	0.45	0/1534	0.80	4/2068 (0.2%)
All	All	0.47	2/17290 (0.0%)	0.70	22/23252 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
2	E	0	10
2	F	0	10
2	G	0	5
2	H	0	5
All	All	0	31

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	416	ARG	CD-NE	6.51	1.57	1.46
1	A	416	ARG	CZ-NH2	-5.40	1.26	1.33

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	539	GLU	N-CA-C	-10.60	82.38	111.00
2	H	539	GLU	N-CA-C	-10.26	83.31	111.00
2	E	539	GLU	N-CA-C	-9.96	84.12	111.00
1	B	299	GLY	N-CA-C	-9.82	88.55	113.10
2	E	537	ILE	N-CA-C	-7.47	90.82	111.00
2	F	537	ILE	N-CA-C	-7.36	91.14	111.00
2	F	540	HIS	N-CA-C	7.30	130.71	111.00
2	E	540	HIS	N-CA-C	6.71	129.10	111.00
2	H	518	LEU	N-CA-C	6.49	128.53	111.00
1	A	176	LEU	CA-CB-CG	6.43	130.09	115.30
1	B	176	LEU	CA-CB-CG	6.38	129.98	115.30
2	G	518	LEU	N-CA-C	6.21	127.77	111.00
2	E	518	LEU	N-CA-C	6.02	127.26	111.00
2	G	540	HIS	N-CA-C	6.01	127.23	111.00
2	F	518	LEU	N-CA-C	5.94	127.03	111.00
2	H	540	HIS	N-CA-C	5.81	126.68	111.00
2	H	470	LEU	N-CA-CB	5.79	121.97	110.40
1	A	115	GLU	C-N-CD	-5.39	108.75	120.60
2	G	470	LEU	N-CA-CB	5.35	121.11	110.40
1	B	115	GLU	C-N-CD	-5.18	109.20	120.60
1	A	416	ARG	CD-NE-CZ	5.10	130.75	123.60
1	B	298	THR	N-CA-C	5.02	124.56	111.00

There are no chirality outliers.

All (31) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	298	THR	Peptide
2	E	469	GLN	Peptide
2	E	473	MET	Peptide
2	E	517	ILE	Peptide
2	E	521	PRO	Peptide
2	E	528	GLY	Peptide
2	E	536	VAL	Peptide
2	E	538	ILE	Peptide
2	E	539	GLU	Peptide
2	E	543	ILE	Peptide
2	E	544	ILE	Peptide
2	F	469	GLN	Peptide
2	F	473	MET	Peptide
2	F	517	ILE	Peptide
2	F	521	PRO	Peptide
2	F	524	LEU	Peptide

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Mol	Chain	Res	Type	Group
2	F	528	GLY	Peptide
2	F	536	VAL	Peptide
2	F	539	GLU	Peptide
2	F	543	ILE	Peptide
2	F	544	ILE	Peptide
2	G	469	GLN	Peptide
2	G	517	ILE	Peptide
2	G	521	PRO	Peptide
2	G	538	ILE	Peptide
2	G	539	GLU	Peptide
2	H	469	GLN	Peptide
2	H	517	ILE	Peptide
2	H	521	PRO	Peptide
2	H	538	ILE	Peptide
2	H	539	GLU	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	2987	0	3054	224	0
1	B	2987	0	3054	217	0
1	C	2511	0	2552	119	0
1	D	2511	0	2552	120	0
2	E	1513	0	1582	178	0
2	F	1513	0	1582	180	0
2	G	1513	0	1582	190	0
2	H	1513	0	1582	187	0
3	A	31	0	12	3	0
3	B	31	0	12	0	0
All	All	17110	0	17564	1402	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 40.

All (1402) 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)
2:G:541:LYS:HG2	2:G:587:GLN:NE2	1.21	1.53
2:H:541:LYS:HG2	2:H:587:GLN:NE2	1.20	1.45
2:E:541:LYS:HG2	2:E:587:GLN:NE2	1.27	1.41
2:F:541:LYS:HG2	2:F:587:GLN:NE2	1.30	1.38
2:H:540:HIS:HB3	2:H:541:LYS:CA	1.52	1.37
2:F:540:HIS:HB3	2:F:541:LYS:CA	1.50	1.37
2:G:540:HIS:HB3	2:G:541:LYS:CA	1.52	1.37
1:C:252:LYS:HE2	1:C:274:VAL:CG2	1.56	1.35
2:E:540:HIS:HB3	2:E:541:LYS:CA	1.50	1.34
1:D:252:LYS:HE2	1:D:274:VAL:CG2	1.56	1.34
2:E:540:HIS:CB	2:E:541:LYS:HA	1.51	1.33
1:B:118:LYS:CD	1:B:119:PRO:HD3	1.57	1.33
2:G:540:HIS:CB	2:G:541:LYS:HA	1.56	1.32
1:A:118:LYS:CD	1:A:119:PRO:HD3	1.58	1.31
1:A:118:LYS:CE	1:A:119:PRO:HD3	1.61	1.30
1:A:91:ASN:O	1:A:120:ILE:HG22	1.16	1.28
1:B:118:LYS:CE	1:B:119:PRO:HD3	1.64	1.26
2:E:541:LYS:HB3	2:E:587:GLN:OE1	1.35	1.26
2:F:540:HIS:CB	2:F:541:LYS:HA	1.51	1.25
1:A:118:LYS:HE3	1:A:119:PRO:CD	1.65	1.25
2:H:633:VAL:HG12	2:H:634:PRO:CD	1.66	1.25
2:G:633:VAL:HG12	2:G:634:PRO:CD	1.66	1.25
1:B:91:ASN:O	1:B:120:ILE:HG22	1.18	1.25
2:H:540:HIS:CB	2:H:541:LYS:HA	1.55	1.24
2:G:541:LYS:HB3	2:G:587:GLN:OE1	1.33	1.23
2:G:541:LYS:HG2	2:G:587:GLN:CD	1.59	1.23
2:F:541:LYS:HB3	2:F:587:GLN:OE1	1.36	1.23
2:E:541:LYS:HG2	2:E:587:GLN:CD	1.59	1.22
1:B:118:LYS:HE3	1:B:119:PRO:CD	1.69	1.21
2:H:541:LYS:HB3	2:H:587:GLN:OE1	1.38	1.20
2:H:541:LYS:HG2	2:H:587:GLN:CD	1.62	1.20
2:G:633:VAL:CG1	2:G:634:PRO:HD3	1.71	1.20
2:E:541:LYS:CG	2:E:587:GLN:NE2	2.05	1.19
2:H:633:VAL:CG1	2:H:634:PRO:HD3	1.71	1.19
2:F:541:LYS:HG2	2:F:587:GLN:CD	1.62	1.18
1:D:252:LYS:HE2	1:D:274:VAL:HG21	1.19	1.18
2:H:545:CYS:HB2	2:H:546:PRO:HD2	1.20	1.16
1:C:347:THR:HB	1:C:348:PRO:HD2	1.28	1.15
2:H:541:LYS:CG	2:H:587:GLN:NE2	2.08	1.15
2:F:541:LYS:CG	2:F:587:GLN:NE2	2.09	1.15
2:G:541:LYS:CG	2:G:587:GLN:NE2	2.09	1.14
1:C:252:LYS:HE2	1:C:274:VAL:HG21	1.20	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:GLU:CG	1:A:116:PRO:HD2	1.78	1.12
2:G:545:CYS:HB2	2:G:546:PRO:HD2	1.19	1.12
2:H:541:LYS:CG	2:H:587:GLN:HE22	1.62	1.12
2:E:545:CYS:HB2	2:E:546:PRO:HD2	1.12	1.11
2:F:473:MET:HE1	2:F:525:CYS:O	1.48	1.11
1:D:347:THR:HB	1:D:348:PRO:HD2	1.29	1.11
2:G:541:LYS:CB	2:G:587:GLN:OE1	1.97	1.11
1:B:115:GLU:CG	1:B:116:PRO:HD2	1.78	1.11
2:G:541:LYS:CG	2:G:587:GLN:HE22	1.64	1.10
2:F:545:CYS:HB2	2:F:546:PRO:HD2	1.14	1.09
2:G:444:ILE:HG23	2:G:455:VAL:HG13	1.35	1.08
2:E:541:LYS:CD	2:E:587:GLN:HE22	1.64	1.08
2:E:541:LYS:CE	2:E:587:GLN:HE22	1.66	1.08
2:H:440:ILE:HB	2:H:462:GLY:HA3	1.09	1.08
2:G:440:ILE:HB	2:G:462:GLY:HA3	1.08	1.08
1:A:347:THR:HB	1:A:348:PRO:HD2	1.13	1.08
1:B:347:THR:HB	1:B:348:PRO:HD2	1.14	1.07
1:B:115:GLU:HG3	1:B:116:PRO:CD	1.83	1.07
1:B:115:GLU:HG3	1:B:116:PRO:HD2	1.35	1.07
2:F:473:MET:CE	2:F:525:CYS:O	2.03	1.06
1:D:287:ILE:HG21	1:D:398:GLU:O	1.53	1.06
2:H:444:ILE:HG23	2:H:455:VAL:HG13	1.37	1.06
2:H:541:LYS:CB	2:H:587:GLN:OE1	2.03	1.06
2:F:541:LYS:CE	2:F:587:GLN:HE22	1.69	1.06
1:A:115:GLU:HG3	1:A:116:PRO:CD	1.85	1.05
1:C:287:ILE:HG21	1:C:398:GLU:O	1.55	1.05
2:F:541:LYS:CD	2:F:587:GLN:HE22	1.68	1.05
1:D:252:LYS:HE2	1:D:274:VAL:HG23	1.37	1.05
1:D:312:LEU:HD12	1:D:317:VAL:HG21	1.36	1.04
2:E:541:LYS:CB	2:E:587:GLN:OE1	2.05	1.04
1:D:391:ILE:HD12	1:D:391:ILE:H	1.23	1.04
1:A:115:GLU:HG3	1:A:116:PRO:HD2	1.36	1.03
1:C:312:LEU:HD12	1:C:317:VAL:HG21	1.36	1.02
2:F:541:LYS:CB	2:F:587:GLN:OE1	2.06	1.02
2:H:440:ILE:CB	2:H:462:GLY:HA3	1.90	1.02
1:A:118:LYS:HE3	1:A:119:PRO:CG	1.88	1.02
1:C:391:ILE:HD12	1:C:391:ILE:H	1.24	1.01
1:B:118:LYS:HE3	1:B:119:PRO:CG	1.89	1.01
1:A:115:GLU:CG	1:A:116:PRO:CD	2.39	1.01
2:G:440:ILE:CB	2:G:462:GLY:HA3	1.90	1.01
2:F:541:LYS:HE2	2:F:587:GLN:HE22	1.26	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:456:LEU:HD21	2:G:501:LYS:HE2	1.43	1.01
1:C:252:LYS:HE2	1:C:274:VAL:HG23	1.38	1.00
2:H:456:LEU:HD21	2:H:501:LYS:HE2	1.44	0.99
2:E:541:LYS:HE2	2:E:587:GLN:HE22	1.26	0.98
2:F:479:VAL:HG21	2:F:504:LEU:HD23	1.44	0.98
1:A:91:ASN:O	1:A:120:ILE:CG2	2.12	0.97
2:E:541:LYS:CG	2:E:587:GLN:CD	2.31	0.97
2:F:541:LYS:CG	2:F:587:GLN:CD	2.33	0.96
1:D:252:LYS:CE	1:D:274:VAL:CG2	2.43	0.96
2:E:479:VAL:HG21	2:E:504:LEU:HD23	1.47	0.96
2:E:473:MET:HE1	2:E:525:CYS:O	1.64	0.96
1:B:115:GLU:CG	1:B:116:PRO:CD	2.39	0.96
1:D:291:PHE:HE1	1:D:401:GLN:NE2	1.63	0.96
1:B:91:ASN:O	1:B:120:ILE:CG2	2.13	0.96
2:G:530:THR:O	2:G:633:VAL:HG23	1.66	0.95
1:C:291:PHE:HE1	1:C:401:GLN:NE2	1.62	0.95
1:C:252:LYS:CE	1:C:274:VAL:CG2	2.44	0.95
2:H:633:VAL:CG1	2:H:634:PRO:CD	2.37	0.95
1:C:252:LYS:CE	1:C:274:VAL:HG23	1.96	0.95
2:E:489:VAL:HG12	2:E:490:GLU:N	1.81	0.95
1:D:252:LYS:CE	1:D:274:VAL:HG23	1.96	0.95
1:B:118:LYS:CE	1:B:119:PRO:CD	2.37	0.95
1:B:118:LYS:CD	1:B:119:PRO:CD	2.45	0.94
2:G:541:LYS:CG	2:G:587:GLN:CD	2.36	0.94
1:B:118:LYS:HD2	1:B:119:PRO:HD3	1.47	0.94
2:E:541:LYS:CG	2:E:587:GLN:HE22	1.72	0.94
2:F:489:VAL:HG12	2:F:490:GLU:N	1.83	0.94
2:G:633:VAL:CG1	2:G:634:PRO:CD	2.37	0.94
1:A:347:THR:CB	1:A:348:PRO:HD2	1.97	0.93
1:A:118:LYS:HE3	1:A:119:PRO:HD3	1.28	0.93
2:H:530:THR:O	2:H:633:VAL:HG23	1.67	0.93
2:F:545:CYS:CB	2:F:546:PRO:HD2	1.97	0.93
1:B:347:THR:CB	1:B:348:PRO:HD2	1.99	0.93
1:A:118:LYS:CD	1:A:119:PRO:CD	2.46	0.92
2:H:440:ILE:HB	2:H:462:GLY:CA	1.99	0.92
1:A:118:LYS:HD2	1:A:119:PRO:HD3	1.51	0.91
1:B:347:THR:HB	1:B:348:PRO:CD	2.00	0.91
2:G:440:ILE:HB	2:G:462:GLY:CA	1.99	0.91
1:A:114:PHE:CD1	1:A:115:GLU:O	2.24	0.91
1:B:114:PHE:CD1	1:B:115:GLU:O	2.24	0.91
1:A:41:PRO:O	1:A:42:LYS:HG2	1.71	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:GLU:HG2	1:B:116:PRO:HD2	1.53	0.90
2:H:489:VAL:HG12	2:H:490:GLU:N	1.85	0.90
1:A:347:THR:HB	1:A:348:PRO:CD	1.98	0.90
2:G:541:LYS:HG2	2:G:587:GLN:HE22	1.10	0.90
1:A:115:GLU:HG2	1:A:116:PRO:HD2	1.53	0.90
2:E:489:VAL:HG12	2:E:490:GLU:H	1.36	0.90
1:B:223:GLY:O	1:B:249:LYS:O	1.90	0.90
2:G:489:VAL:HG12	2:G:490:GLU:H	1.35	0.90
1:B:118:LYS:CG	1:B:119:PRO:CD	2.50	0.90
1:A:118:LYS:CG	1:A:119:PRO:CD	2.50	0.89
2:H:489:VAL:HG12	2:H:490:GLU:H	1.34	0.89
2:G:489:VAL:HG12	2:G:490:GLU:N	1.85	0.89
2:H:541:LYS:CG	2:H:587:GLN:CD	2.38	0.89
2:F:541:LYS:CG	2:F:587:GLN:HE22	1.75	0.88
2:H:541:LYS:HG2	2:H:587:GLN:HE22	1.08	0.88
2:H:541:LYS:CD	2:H:587:GLN:HE22	1.86	0.88
2:E:541:LYS:HE2	2:E:587:GLN:NE2	1.89	0.88
2:E:473:MET:CE	2:E:525:CYS:O	2.22	0.88
2:F:489:VAL:HG12	2:F:490:GLU:H	1.38	0.88
2:G:541:LYS:CG	2:G:587:GLN:OE1	2.22	0.87
1:A:223:GLY:O	1:A:249:LYS:O	1.91	0.87
2:G:521:PRO:HB2	2:G:522:ASN:HB2	1.56	0.87
2:F:521:PRO:HB2	2:F:522:ASN:HB2	1.56	0.86
2:G:541:LYS:CD	2:G:587:GLN:HE22	1.87	0.86
1:C:317:VAL:HG12	1:C:413:LEU:HD23	1.57	0.86
1:B:231:ASP:O	1:B:235:GLU:HB2	1.76	0.86
2:E:521:PRO:HB2	2:E:522:ASN:HB2	1.56	0.86
1:C:245:ARG:HD2	1:C:245:ARG:H	1.40	0.86
1:B:41:PRO:O	1:B:42:LYS:HG2	1.76	0.86
2:H:521:PRO:HB2	2:H:522:ASN:HB2	1.56	0.85
1:A:231:ASP:O	1:A:235:GLU:HB2	1.76	0.85
2:F:541:LYS:HE2	2:F:587:GLN:NE2	1.91	0.85
1:D:315:GLY:HA3	1:D:415:TYR:OH	1.75	0.85
2:E:529:ARG:HA	2:E:597:THR:CG2	2.07	0.85
1:A:107:GLU:O	1:A:108:LYS:HB2	1.77	0.85
2:F:447:LYS:HG3	2:F:512:ILE:HG23	1.56	0.85
1:D:245:ARG:HD2	1:D:245:ARG:H	1.40	0.85
1:B:245:ARG:HD2	1:B:245:ARG:H	1.42	0.84
1:C:347:THR:HB	1:C:348:PRO:CD	2.08	0.84
1:B:107:GLU:O	1:B:108:LYS:HB2	1.77	0.84
2:H:603:LEU:O	2:H:604:GLU:HG2	1.78	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:633:VAL:CB	2:G:634:PRO:CD	2.56	0.84
2:E:447:LYS:HG3	2:E:512:ILE:HG23	1.57	0.84
1:D:347:THR:HB	1:D:348:PRO:CD	2.08	0.84
2:G:558:ILE:O	2:G:559:GLU:HB2	1.78	0.84
2:G:603:LEU:O	2:G:604:GLU:HG2	1.78	0.83
1:B:300:LYS:O	1:B:413:LEU:N	2.11	0.83
1:B:118:LYS:CG	1:B:119:PRO:HD2	2.08	0.83
1:C:291:PHE:HE1	1:C:401:GLN:HE21	1.21	0.83
1:B:316:ALA:HB1	1:B:386:GLY:HA3	1.61	0.83
2:E:473:MET:HB3	2:E:474:PRO:HD3	1.58	0.83
2:G:495:ALA:HB1	2:G:496:PRO:HD2	1.61	0.83
1:A:118:LYS:HG3	1:A:119:PRO:HD2	1.61	0.82
2:H:633:VAL:CB	2:H:634:PRO:CD	2.56	0.82
2:G:633:VAL:HB	2:G:634:PRO:HD2	1.61	0.82
2:H:444:ILE:CG2	2:H:455:VAL:HG13	2.09	0.82
2:H:633:VAL:HB	2:H:634:PRO:HD2	1.62	0.82
1:B:118:LYS:HG3	1:B:119:PRO:HD2	1.60	0.82
2:H:558:ILE:O	2:H:559:GLU:HB2	1.78	0.82
1:D:291:PHE:HE1	1:D:401:GLN:HE21	1.22	0.82
2:H:541:LYS:CG	2:H:587:GLN:OE1	2.27	0.82
2:H:545:CYS:CB	2:H:546:PRO:HD2	1.99	0.82
1:B:92:GLY:HA3	1:B:120:ILE:CG2	2.10	0.82
1:C:223:GLY:O	1:C:249:LYS:O	1.99	0.81
1:A:316:ALA:HB1	1:A:386:GLY:HA3	1.62	0.81
2:G:444:ILE:CG2	2:G:455:VAL:HG13	2.08	0.81
1:A:118:LYS:CE	1:A:119:PRO:CD	2.35	0.81
1:A:118:LYS:CG	1:A:119:PRO:HD2	2.11	0.81
2:F:473:MET:HB3	2:F:474:PRO:HD3	1.63	0.81
1:A:92:GLY:HA3	1:A:120:ILE:CG2	2.11	0.81
2:F:447:LYS:O	2:F:448:TYR:HB3	1.81	0.81
2:H:495:ALA:HB1	2:H:496:PRO:HD2	1.61	0.81
1:A:118:LYS:CG	1:A:119:PRO:HD3	2.10	0.81
1:D:223:GLY:O	1:D:249:LYS:O	1.99	0.81
2:F:545:CYS:HB2	2:F:546:PRO:CD	2.06	0.80
2:E:541:LYS:CG	2:E:587:GLN:OE1	2.28	0.80
2:E:540:HIS:NE2	2:E:543:ILE:O	2.14	0.80
1:B:291:PHE:HE2	1:B:406:PHE:HE1	1.28	0.80
1:A:245:ARG:H	1:A:245:ARG:HD2	1.43	0.80
2:H:441:ARG:CG	2:H:525:CYS:SG	2.70	0.80
1:C:315:GLY:HA3	1:C:415:TYR:OH	1.80	0.80
1:B:176:LEU:O	1:B:178:LYS:N	2.15	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:540:HIS:NE2	2:F:543:ILE:O	2.15	0.79
1:A:176:LEU:O	1:A:178:LYS:N	2.15	0.79
2:H:441:ARG:HD3	2:H:525:CYS:SG	2.23	0.79
1:A:291:PHE:HE2	1:A:406:PHE:HE1	1.27	0.79
1:A:118:LYS:HE3	1:A:119:PRO:HG3	1.62	0.79
2:E:545:CYS:HB2	2:E:546:PRO:CD	2.05	0.79
1:C:195:MET:HA	1:C:198:ARG:HB3	1.65	0.78
2:E:545:CYS:CB	2:E:546:PRO:HD2	1.96	0.78
2:G:441:ARG:HD3	2:G:525:CYS:SG	2.24	0.78
1:B:118:LYS:HE3	1:B:119:PRO:HG3	1.63	0.78
1:C:317:VAL:HG12	1:C:413:LEU:CD2	2.14	0.78
2:F:524:LEU:HD12	2:F:525:CYS:H	1.46	0.78
2:G:441:ARG:CG	2:G:525:CYS:SG	2.72	0.78
1:A:300:LYS:O	1:A:413:LEU:N	2.16	0.78
2:E:447:LYS:O	2:E:448:TYR:HB3	1.83	0.77
2:H:540:HIS:NE2	2:H:543:ILE:O	2.17	0.77
1:B:118:LYS:CG	1:B:119:PRO:HD3	2.12	0.77
2:E:453:THR:OG1	2:E:509:GLU:HB3	1.84	0.77
2:E:473:MET:HG2	2:E:602:CYS:CB	2.12	0.77
2:G:489:VAL:CG1	2:G:490:GLU:H	1.97	0.77
2:F:606:PHE:H	2:F:629:VAL:HG13	1.50	0.77
2:G:545:CYS:CB	2:G:546:PRO:HD2	1.98	0.77
2:G:546:PRO:HD2	2:G:583:ARG:O	1.84	0.77
2:G:456:LEU:CD2	2:G:501:LYS:HG2	2.15	0.77
2:E:473:MET:HG2	2:E:602:CYS:HB3	1.64	0.77
1:D:195:MET:HA	1:D:198:ARG:HB3	1.65	0.77
1:A:81:ARG:HD2	1:A:111:ASN:HB3	1.65	0.77
1:B:81:ARG:HD2	1:B:111:ASN:HB3	1.66	0.77
1:B:120:ILE:HD12	1:B:121:ASN:H	1.50	0.77
2:H:489:VAL:CG1	2:H:490:GLU:H	1.96	0.77
2:F:541:LYS:CG	2:F:587:GLN:OE1	2.30	0.77
2:H:546:PRO:HD2	2:H:583:ARG:O	1.84	0.77
1:A:279:LYS:HD3	1:A:279:LYS:H	1.49	0.77
2:G:540:HIS:NE2	2:G:543:ILE:O	2.18	0.76
2:H:530:THR:HG22	2:H:633:VAL:HG21	1.67	0.76
2:F:453:THR:OG1	2:F:509:GLU:HB3	1.84	0.76
2:H:633:VAL:HG12	2:H:634:PRO:HD3	0.81	0.76
2:E:541:LYS:CD	2:E:587:GLN:NE2	2.40	0.76
2:H:510:GLU:HG3	2:H:511:GLU:H	1.51	0.76
2:E:606:PHE:H	2:E:629:VAL:HG13	1.50	0.76
2:H:456:LEU:CD2	2:H:501:LYS:HG2	2.16	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:ILE:HD12	1:A:121:ASN:H	1.51	0.76
1:A:114:PHE:HD1	1:A:115:GLU:O	1.69	0.75
2:H:441:ARG:HG2	2:H:525:CYS:SG	2.25	0.75
1:B:279:LYS:H	1:B:279:LYS:HD3	1.49	0.75
2:F:494:VAL:HG21	2:F:500:LEU:HD11	1.68	0.75
1:A:118:LYS:CB	1:A:119:PRO:CD	2.64	0.75
1:B:118:LYS:CB	1:B:119:PRO:CD	2.64	0.75
2:G:541:LYS:CE	2:G:587:GLN:HE22	2.00	0.75
2:G:456:LEU:HD21	2:G:501:LYS:CE	2.17	0.75
2:G:530:THR:HG22	2:G:633:VAL:HG21	1.69	0.75
2:F:473:MET:HG2	2:F:602:CYS:HB3	1.67	0.75
1:A:275:LEU:O	1:A:277:ASN:N	2.18	0.74
2:G:510:GLU:HG3	2:G:511:GLU:H	1.52	0.74
2:F:543:ILE:HG22	2:F:544:ILE:N	2.02	0.74
2:F:473:MET:HG2	2:F:602:CYS:CB	2.17	0.74
2:G:441:ARG:HG2	2:G:525:CYS:SG	2.28	0.74
1:B:316:ALA:CB	1:B:386:GLY:HA3	2.17	0.74
2:F:469:GLN:OE1	2:F:480:GLU:HB2	1.88	0.74
2:E:543:ILE:HG22	2:E:544:ILE:N	2.03	0.74
1:D:75:ILE:O	1:D:78:VAL:HG12	1.87	0.74
1:B:115:GLU:HG3	1:B:116:PRO:HD3	1.69	0.73
2:H:541:LYS:CE	2:H:587:GLN:HE22	2.01	0.73
1:C:252:LYS:CE	1:C:274:VAL:HG21	2.12	0.73
1:B:114:PHE:HD1	1:B:115:GLU:O	1.70	0.73
1:A:316:ALA:CB	1:A:386:GLY:HA3	2.18	0.73
2:F:553:HIS:HB2	2:F:616:THR:HG23	1.69	0.73
2:H:530:THR:C	2:H:633:VAL:HG23	2.09	0.73
2:E:494:VAL:HG21	2:E:500:LEU:HD11	1.71	0.73
2:H:456:LEU:HD21	2:H:501:LYS:CE	2.18	0.73
1:D:195:MET:HG2	1:D:198:ARG:HH11	1.52	0.73
2:H:555:HIS:C	2:H:557:CYS:H	1.90	0.73
2:G:530:THR:C	2:G:633:VAL:HG23	2.08	0.73
2:E:469:GLN:OE1	2:E:480:GLU:HB2	1.88	0.73
2:G:555:HIS:C	2:G:557:CYS:H	1.91	0.72
1:C:195:MET:HG2	1:C:198:ARG:HH11	1.54	0.72
2:G:545:CYS:HB2	2:G:583:ARG:O	1.90	0.72
1:A:275:LEU:C	1:A:277:ASN:H	1.90	0.72
1:B:275:LEU:O	1:B:277:ASN:N	2.22	0.72
1:C:75:ILE:O	1:C:78:VAL:HG12	1.88	0.72
2:F:541:LYS:CD	2:F:587:GLN:NE2	2.44	0.72
2:G:573:LYS:O	2:G:573:LYS:HG3	1.90	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:537:ILE:HG21	2:H:587:GLN:HA	1.71	0.72
1:B:275:LEU:C	1:B:277:ASN:H	1.92	0.72
2:G:456:LEU:CD2	2:G:501:LYS:HE2	2.20	0.72
1:A:115:GLU:HG3	1:A:116:PRO:HD3	1.70	0.71
2:H:633:VAL:CB	2:H:634:PRO:HD2	2.19	0.71
2:H:489:VAL:CG1	2:H:490:GLU:N	2.53	0.71
2:F:530:THR:HB	2:F:633:VAL:O	1.91	0.71
2:E:553:HIS:HB2	2:E:616:THR:HG23	1.71	0.71
1:C:291:PHE:CE1	1:C:401:GLN:NE2	2.54	0.71
2:H:456:LEU:CD2	2:H:501:LYS:HE2	2.20	0.71
2:H:545:CYS:HB2	2:H:583:ARG:O	1.89	0.71
2:H:444:ILE:HG23	2:H:455:VAL:CG1	2.19	0.71
1:D:252:LYS:CE	1:D:274:VAL:HG21	2.11	0.71
2:E:489:VAL:CG1	2:E:490:GLU:N	2.54	0.71
1:A:38:ILE:HD12	1:A:124:LEU:HD13	1.73	0.71
2:G:633:VAL:CB	2:G:634:PRO:HD2	2.20	0.70
1:A:276:SER:HA	1:A:279:LYS:HE3	1.72	0.70
2:G:545:CYS:HB2	2:G:546:PRO:CD	2.12	0.70
2:E:489:VAL:CG1	2:E:490:GLU:H	2.04	0.70
2:F:489:VAL:CG1	2:F:490:GLU:N	2.55	0.70
1:C:152:ASP:OD1	1:C:258:TYR:O	2.10	0.70
2:G:633:VAL:HG12	2:G:634:PRO:HD3	0.81	0.70
1:D:291:PHE:CE1	1:D:401:GLN:NE2	2.55	0.70
2:G:444:ILE:HG23	2:G:455:VAL:CG1	2.17	0.70
1:B:276:SER:HA	1:B:279:LYS:HE3	1.71	0.70
2:H:573:LYS:O	2:H:573:LYS:HG3	1.92	0.70
2:G:543:ILE:HG22	2:G:544:ILE:N	2.07	0.70
2:G:447:LYS:HG3	2:G:512:ILE:HG23	1.74	0.70
1:A:118:LYS:HE2	3:A:1526:ATP:PG	2.31	0.69
2:G:447:LYS:O	2:G:448:TYR:HB3	1.92	0.69
2:F:444:ILE:HG23	2:F:455:VAL:HG13	1.74	0.69
2:E:444:ILE:HG23	2:E:455:VAL:HG13	1.74	0.69
2:H:486:SER:HA	2:H:500:LEU:HD12	1.73	0.69
2:H:537:ILE:CG2	2:H:587:GLN:HA	2.23	0.69
2:G:554:ILE:HD12	2:G:601:ILE:HG21	1.74	0.69
2:G:533:ALA:O	2:G:592:ILE:HA	1.92	0.69
2:H:533:ALA:O	2:H:592:ILE:HA	1.93	0.69
2:G:486:SER:HA	2:G:500:LEU:HD12	1.74	0.69
1:D:283:GLU:HG3	1:D:392:VAL:HG12	1.75	0.69
2:H:447:LYS:O	2:H:448:TYR:HB3	1.92	0.69
2:H:554:ILE:HD12	2:H:601:ILE:HG21	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:537:ILE:HG21	2:G:587:GLN:HA	1.75	0.69
1:D:152:ASP:OD1	1:D:258:TYR:O	2.11	0.69
2:H:543:ILE:HG22	2:H:544:ILE:N	2.09	0.68
2:F:529:ARG:H	2:F:529:ARG:HD3	1.56	0.68
2:E:540:HIS:CG	2:E:542:SER:H	2.12	0.68
2:F:473:MET:HE2	2:F:525:CYS:O	1.93	0.68
2:G:489:VAL:CG1	2:G:490:GLU:N	2.53	0.68
1:B:13:GLU:HA	1:B:13:GLU:OE1	1.91	0.68
2:E:530:THR:HB	2:E:633:VAL:O	1.93	0.68
1:A:277:ASN:O	1:A:280:PHE:HB2	1.94	0.68
1:B:38:ILE:HD12	1:B:124:LEU:HD13	1.75	0.68
2:G:536:VAL:HG22	2:G:536:VAL:O	1.92	0.68
1:B:305:VAL:HG23	1:B:306:GLU:N	2.09	0.68
1:B:91:ASN:HB2	1:B:116:PRO:HD2	1.76	0.68
1:D:156:ALA:HB2	1:D:201:TYR:OH	1.94	0.68
1:B:91:ASN:HB3	1:B:119:PRO:HA	1.75	0.68
1:A:91:ASN:HB3	1:A:119:PRO:HA	1.75	0.68
1:B:327:ASP:HB3	1:B:347:THR:CG2	2.23	0.68
2:E:529:ARG:HA	2:E:597:THR:HG22	1.76	0.68
1:C:233:LYS:O	1:C:237:SER:HB2	1.93	0.67
2:E:554:ILE:HG23	2:E:615:PHE:HB3	1.77	0.67
2:E:464:ILE:HG23	2:E:494:VAL:CG1	2.25	0.67
2:F:568:CYS:HB2	2:F:592:ILE:HD11	1.75	0.67
1:A:92:GLY:HA3	1:A:120:ILE:HG21	1.77	0.67
2:G:537:ILE:CG2	2:G:587:GLN:HA	2.25	0.67
2:G:540:HIS:CE1	2:G:542:SER:HG	2.13	0.67
2:F:489:VAL:CG1	2:F:490:GLU:H	2.05	0.67
1:A:13:GLU:HA	1:A:13:GLU:OE1	1.94	0.67
1:B:277:ASN:O	1:B:280:PHE:HB2	1.94	0.67
1:A:305:VAL:HG23	1:A:306:GLU:N	2.09	0.67
1:D:118:LYS:HE2	1:D:120:ILE:HG12	1.77	0.67
2:F:464:ILE:HG23	2:F:494:VAL:CG1	2.24	0.67
2:F:540:HIS:CG	2:F:542:SER:H	2.12	0.67
2:H:447:LYS:HG3	2:H:512:ILE:HG23	1.76	0.67
2:G:553:HIS:HB2	2:G:616:THR:HG23	1.77	0.67
2:F:573:LYS:O	2:F:573:LYS:HG3	1.95	0.67
1:D:233:LYS:O	1:D:237:SER:HB2	1.94	0.67
2:E:473:MET:CB	2:E:474:PRO:HD3	2.24	0.67
1:C:378:PHE:O	1:C:382:TYR:HB3	1.95	0.66
2:G:540:HIS:CE1	2:G:542:SER:OG	2.48	0.66
1:B:92:GLY:HA3	1:B:120:ILE:HG21	1.75	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:312:LEU:HD12	1:C:317:VAL:CG2	2.21	0.66
2:G:467:GLY:HA2	2:G:481:VAL:O	1.96	0.66
1:A:327:ASP:HB3	1:A:347:THR:CG2	2.24	0.66
1:A:157:LEU:HD12	1:A:171:LYS:HD3	1.78	0.66
2:F:554:ILE:HG23	2:F:615:PHE:HB3	1.78	0.66
2:H:536:VAL:O	2:H:536:VAL:HG22	1.95	0.66
1:C:283:GLU:HG3	1:C:392:VAL:HG12	1.76	0.66
2:H:467:GLY:HA2	2:H:481:VAL:O	1.96	0.66
2:F:546:PRO:HD2	2:F:583:ARG:O	1.96	0.66
2:G:440:ILE:HG13	2:G:440:ILE:O	1.95	0.66
1:D:378:PHE:O	1:D:382:TYR:HB3	1.95	0.66
1:A:91:ASN:HB2	1:A:116:PRO:HD2	1.76	0.66
1:C:156:ALA:HB2	1:C:201:TYR:OH	1.95	0.66
1:B:120:ILE:HD12	1:B:121:ASN:N	2.10	0.65
2:H:553:HIS:HB2	2:H:616:THR:HG23	1.79	0.65
2:H:540:HIS:CE1	2:H:542:SER:OG	2.49	0.65
2:F:539:GLU:O	2:F:624:ILE:HA	1.96	0.65
1:A:146:PHE:CE2	1:A:275:LEU:HG	2.30	0.65
2:E:573:LYS:HG3	2:E:573:LYS:O	1.95	0.65
2:H:633:VAL:CG1	2:H:634:PRO:HD2	2.26	0.65
1:A:120:ILE:HD12	1:A:121:ASN:N	2.11	0.65
1:B:146:PHE:CE2	1:B:275:LEU:HG	2.32	0.64
2:E:473:MET:CG	2:E:602:CYS:HB3	2.26	0.64
2:E:568:CYS:HB2	2:E:592:ILE:HD11	1.78	0.64
1:D:151:ILE:CG2	1:D:232:PHE:HB3	2.27	0.64
1:A:177:PRO:HG2	1:A:193:LEU:HD22	1.79	0.64
2:G:517:ILE:HG12	2:G:602:CYS:SG	2.36	0.64
1:C:118:LYS:HE2	1:C:120:ILE:HG12	1.79	0.64
1:A:382:TYR:HE1	1:A:388:THR:HA	1.63	0.64
2:E:521:PRO:HB2	2:E:522:ASN:CB	2.26	0.64
2:H:441:ARG:CD	2:H:525:CYS:SG	2.84	0.64
1:D:397:GLN:C	1:D:399:GLY:H	2.00	0.64
2:G:626:ILE:CG2	2:G:627:GLY:N	2.61	0.64
1:B:141:SER:O	1:B:143:ASP:N	2.30	0.64
2:F:551:VAL:HG12	2:F:558:ILE:HD11	1.80	0.64
1:C:76:THR:O	1:C:80:GLN:HG2	1.98	0.64
2:F:464:ILE:HG23	2:F:494:VAL:HG13	1.77	0.63
2:F:561:VAL:HG23	2:F:596:ARG:O	1.97	0.63
2:H:545:CYS:HB2	2:H:546:PRO:CD	2.12	0.63
2:H:440:ILE:O	2:H:440:ILE:HG13	1.97	0.63
2:E:464:ILE:HG23	2:E:494:VAL:HG13	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:521:PRO:HB2	2:F:522:ASN:CB	2.26	0.63
2:H:510:GLU:HG3	2:H:511:GLU:N	2.13	0.63
1:B:157:LEU:HD12	1:B:171:LYS:HD3	1.80	0.63
2:H:517:ILE:HG12	2:H:602:CYS:SG	2.38	0.63
1:B:10:ARG:O	1:B:13:GLU:HB2	1.98	0.63
2:E:546:PRO:HD2	2:E:583:ARG:O	1.98	0.63
2:G:633:VAL:CG1	2:G:634:PRO:HD2	2.28	0.63
2:F:473:MET:CB	2:F:474:PRO:HD3	2.28	0.63
1:A:10:ARG:O	1:A:13:GLU:HB2	1.98	0.63
1:D:317:VAL:HG12	1:D:413:LEU:HD23	1.80	0.63
1:B:177:PRO:HG2	1:B:193:LEU:HD22	1.81	0.63
1:B:382:TYR:HE1	1:B:388:THR:HA	1.63	0.63
1:B:95:VAL:HG13	1:B:113:ASP:HB3	1.80	0.63
2:G:456:LEU:HG	2:G:501:LYS:HG2	1.80	0.62
1:D:76:THR:O	1:D:80:GLN:HG2	1.98	0.62
1:C:151:ILE:CG2	1:C:232:PHE:HB3	2.29	0.62
2:F:473:MET:CG	2:F:602:CYS:HB3	2.29	0.62
2:G:441:ARG:CD	2:G:525:CYS:SG	2.86	0.62
2:G:510:GLU:HG3	2:G:511:GLU:N	2.14	0.62
2:F:554:ILE:HB	2:F:557:CYS:SG	2.40	0.62
2:H:464:ILE:HG23	2:H:494:VAL:HG13	1.81	0.62
2:F:559:GLU:HG3	2:F:560:GLU:N	2.13	0.62
2:F:564:THR:OG1	2:F:594:ARG:HB3	2.00	0.62
2:H:456:LEU:HG	2:H:501:LYS:HG2	1.80	0.62
1:B:326:LEU:HD21	1:B:328:ILE:HD12	1.80	0.62
1:C:397:GLN:C	1:C:399:GLY:H	2.00	0.62
2:F:508:GLU:HB3	2:F:511:GLU:HB2	1.80	0.62
1:C:166:ARG:HE	1:C:166:ARG:H	1.47	0.62
2:E:554:ILE:HB	2:E:557:CYS:SG	2.40	0.62
2:G:540:HIS:CB	2:G:541:LYS:CA	2.37	0.62
2:E:540:HIS:CE1	2:E:542:SER:OG	2.53	0.62
1:D:391:ILE:CD1	1:D:391:ILE:H	1.92	0.62
1:A:214:ILE:HD12	1:A:245:ARG:HD3	1.82	0.62
2:E:559:GLU:HG3	2:E:560:GLU:N	2.14	0.62
1:A:141:SER:O	1:A:143:ASP:N	2.32	0.62
2:F:473:MET:SD	2:F:525:CYS:HB2	2.39	0.62
1:A:291:PHE:CE2	1:A:406:PHE:HE1	2.14	0.62
2:G:533:ALA:CB	2:G:629:VAL:HA	2.30	0.62
2:E:508:GLU:HB3	2:E:511:GLU:HB2	1.81	0.62
1:B:233:LYS:HD2	1:B:253:LEU:HD22	1.81	0.61
1:A:190:PHE:O	1:A:194:ARG:HB2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:190:PHE:O	1:B:194:ARG:HB2	2.00	0.61
1:A:233:LYS:HE3	1:A:254:VAL:O	2.00	0.61
1:A:22:LYS:O	1:A:25:GLU:HG2	2.01	0.61
2:H:540:HIS:CG	2:H:542:SER:H	2.17	0.61
2:F:540:HIS:CB	2:F:541:LYS:CA	2.37	0.61
1:D:166:ARG:HE	1:D:166:ARG:H	1.49	0.61
2:E:606:PHE:N	2:E:629:VAL:HG13	2.15	0.61
2:H:626:ILE:CG2	2:H:627:GLY:N	2.61	0.61
2:F:441:ARG:CZ	2:F:525:CYS:SG	2.88	0.61
1:D:312:LEU:HD12	1:D:317:VAL:CG2	2.22	0.61
2:G:521:PRO:HB2	2:G:522:ASN:CB	2.30	0.61
2:G:464:ILE:HG23	2:G:494:VAL:HG13	1.81	0.61
1:C:284:LYS:HG2	1:C:396:SER:HB2	1.83	0.61
2:H:521:PRO:HB2	2:H:522:ASN:CB	2.31	0.61
1:B:291:PHE:CE2	1:B:406:PHE:HE1	2.15	0.61
1:B:22:LYS:O	1:B:25:GLU:HG2	2.01	0.61
1:A:326:LEU:HD21	1:A:328:ILE:HD12	1.81	0.61
2:G:540:HIS:CG	2:G:542:SER:H	2.18	0.61
1:D:252:LYS:HE3	1:D:274:VAL:HG23	1.83	0.61
1:D:284:LYS:HG2	1:D:396:SER:HB2	1.83	0.61
2:E:540:HIS:HB3	2:E:541:LYS:HA	0.68	0.60
1:A:95:VAL:HG13	1:A:113:ASP:HB3	1.82	0.60
2:E:495:ALA:HB1	2:E:496:PRO:HD2	1.83	0.60
1:A:327:ASP:O	1:A:347:THR:HA	2.02	0.60
2:E:484:ILE:HG12	2:E:502:ILE:HG23	1.84	0.60
1:B:233:LYS:HE3	1:B:254:VAL:O	2.01	0.60
2:E:544:ILE:HG12	2:E:548:TYR:CD1	2.35	0.60
1:A:118:LYS:HE2	3:A:1526:ATP:O2G	2.02	0.60
1:D:391:ILE:N	1:D:391:ILE:HD12	2.05	0.60
2:F:447:LYS:HZ3	2:F:510:GLU:HB2	1.64	0.60
2:E:615:PHE:CE1	2:E:627:GLY:HA3	2.37	0.60
2:F:528:GLY:O	2:F:600:THR:HG23	2.02	0.60
1:A:323:TYR:HA	1:A:392:VAL:O	2.02	0.60
2:H:533:ALA:CB	2:H:629:VAL:HA	2.31	0.60
2:H:540:HIS:HB3	2:H:541:LYS:HA	0.69	0.60
2:E:494:VAL:HG23	2:E:498:GLU:OE1	2.02	0.60
1:D:245:ARG:O	1:D:249:LYS:HG2	2.01	0.60
1:B:190:PHE:O	1:B:194:ARG:CB	2.50	0.60
2:E:564:THR:OG1	2:E:594:ARG:HB3	2.02	0.60
1:C:252:LYS:HE3	1:C:274:VAL:HG23	1.82	0.60
1:B:214:ILE:HD12	1:B:245:ARG:HD3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:609:PHE:HB3	2:E:611:GLN:HE22	1.67	0.60
1:B:196:GLU:O	1:B:200:ASN:HB2	2.02	0.60
1:A:196:GLU:O	1:A:200:ASN:HB2	2.01	0.60
1:A:27:ALA:HB1	1:A:100:ILE:HG21	1.83	0.60
1:A:152:ASP:OD1	1:A:153:GLY:N	2.35	0.59
2:F:540:HIS:CE1	2:F:542:SER:OG	2.55	0.59
1:A:190:PHE:O	1:A:194:ARG:CB	2.49	0.59
1:A:91:ASN:HB3	1:A:118:LYS:O	2.01	0.59
2:F:615:PHE:CE1	2:F:627:GLY:HA3	2.37	0.59
1:B:152:ASP:OD1	1:B:153:GLY:N	2.35	0.59
2:E:473:MET:SD	2:E:525:CYS:HB2	2.42	0.59
2:H:555:HIS:C	2:H:557:CYS:N	2.56	0.59
1:A:245:ARG:O	1:A:249:LYS:HG2	2.03	0.59
2:E:442:LEU:O	2:E:517:ILE:HA	2.03	0.59
2:F:442:LEU:HB3	2:F:518:LEU:HB2	1.85	0.59
1:C:245:ARG:O	1:C:249:LYS:HG2	2.01	0.59
1:B:91:ASN:HB3	1:B:118:LYS:O	2.02	0.59
2:H:555:HIS:O	2:H:557:CYS:N	2.36	0.59
2:F:495:ALA:HB1	2:F:496:PRO:HD2	1.84	0.59
2:F:484:ILE:HG12	2:F:502:ILE:HG23	1.84	0.59
2:F:529:ARG:HA	2:F:597:THR:CG2	2.33	0.59
1:A:233:LYS:HD2	1:A:253:LEU:HD22	1.84	0.59
1:B:133:THR:HG22	1:B:136:LEU:HD12	1.84	0.59
2:G:540:HIS:HB3	2:G:541:LYS:HA	0.70	0.58
2:E:563:ILE:HG22	2:E:595:LEU:HG	1.86	0.58
1:B:118:LYS:CB	1:B:119:PRO:HD2	2.32	0.58
2:G:555:HIS:C	2:G:557:CYS:N	2.57	0.58
1:B:116:PRO:O	1:B:118:LYS:N	2.36	0.58
1:B:400:SER:O	1:B:404:LYS:HB2	2.03	0.58
2:F:540:HIS:CE1	2:F:542:SER:HG	2.21	0.58
1:A:118:LYS:CB	1:A:119:PRO:HD2	2.33	0.58
2:H:545:CYS:CB	2:H:546:PRO:CD	2.78	0.58
2:F:477:HIS:CE1	2:F:507:ILE:HB	2.38	0.58
2:F:445:VAL:HG22	2:F:556:THR:CG2	2.34	0.58
2:G:555:HIS:O	2:G:557:CYS:N	2.37	0.58
2:E:477:HIS:CE1	2:E:507:ILE:HB	2.38	0.58
1:B:186:SER:HB3	1:B:189:ARG:H	1.68	0.58
2:E:445:VAL:HG22	2:E:556:THR:CG2	2.33	0.58
2:F:540:HIS:CE1	2:F:624:ILE:HD11	2.39	0.58
1:A:121:ASN:C	1:A:122:THR:HG22	2.24	0.58
2:F:442:LEU:O	2:F:517:ILE:HA	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:442:LEU:HB3	2:E:518:LEU:HB2	1.86	0.58
1:A:252:LYS:HG2	1:A:253:LEU:O	2.03	0.58
1:A:286:LEU:HD13	1:A:390:GLU:HG3	1.84	0.58
1:B:327:ASP:O	1:B:347:THR:HA	2.04	0.58
2:F:606:PHE:N	2:F:629:VAL:HG13	2.16	0.58
2:E:551:VAL:HG12	2:E:558:ILE:HD11	1.83	0.58
2:H:540:HIS:CB	2:H:541:LYS:CA	2.37	0.58
2:E:447:LYS:HZ3	2:E:510:GLU:HB2	1.67	0.58
1:D:233:LYS:HE3	1:D:254:VAL:O	2.03	0.58
2:E:540:HIS:CE1	2:E:543:ILE:O	2.57	0.58
2:F:563:ILE:HG22	2:F:595:LEU:HG	1.86	0.58
1:B:252:LYS:HG2	1:B:253:LEU:O	2.04	0.58
2:G:543:ILE:CG2	2:G:544:ILE:N	2.67	0.57
1:B:121:ASN:C	1:B:122:THR:HG22	2.24	0.57
2:E:543:ILE:CG2	2:E:544:ILE:N	2.67	0.57
1:A:116:PRO:O	1:A:118:LYS:N	2.37	0.57
2:E:459:LEU:HD11	2:E:464:ILE:HG22	1.85	0.57
1:D:151:ILE:HG22	1:D:232:PHE:CG	2.39	0.57
1:B:286:LEU:HD13	1:B:390:GLU:HG3	1.85	0.57
1:A:400:SER:O	1:A:404:LYS:HB2	2.03	0.57
2:E:489:VAL:HG11	2:H:575:GLY:HA2	1.87	0.57
1:A:118:LYS:HG3	1:A:119:PRO:CD	2.27	0.57
1:A:126:LEU:HD13	1:A:132:HIS:CD2	2.40	0.57
2:E:559:GLU:HG2	2:E:597:THR:OG1	2.04	0.57
1:A:382:TYR:CE1	1:A:388:THR:HA	2.39	0.57
2:F:540:HIS:CE1	2:F:543:ILE:O	2.58	0.57
2:F:544:ILE:HG12	2:F:548:TYR:CD1	2.40	0.57
2:F:538:ILE:HG12	2:F:625:ALA:HA	1.87	0.57
1:C:391:ILE:N	1:C:391:ILE:HD12	2.06	0.57
2:E:464:ILE:CD1	2:E:470:LEU:HD11	2.35	0.57
2:F:494:VAL:HG23	2:F:498:GLU:OE1	2.04	0.57
1:C:233:LYS:HE3	1:C:254:VAL:O	2.04	0.57
1:C:224:LEU:O	1:C:250:VAL:HA	2.05	0.57
2:F:609:PHE:HB3	2:F:611:GLN:HE22	1.69	0.57
1:B:27:ALA:HB1	1:B:100:ILE:HG21	1.85	0.57
2:F:540:HIS:HB3	2:F:541:LYS:HA	0.67	0.57
1:B:116:PRO:C	1:B:118:LYS:N	2.58	0.57
1:A:116:PRO:C	1:A:118:LYS:N	2.58	0.57
2:F:464:ILE:HD11	2:F:470:LEU:HD11	1.87	0.57
1:B:382:TYR:CE1	1:B:388:THR:HA	2.39	0.57
1:C:151:ILE:HG22	1:C:232:PHE:CG	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:323:TYR:CE2	1:D:394:ASP:HB3	2.40	0.57
1:A:186:SER:HB3	1:A:189:ARG:H	1.69	0.57
2:F:464:ILE:CD1	2:F:470:LEU:HD11	2.35	0.56
2:E:539:GLU:O	2:E:624:ILE:HA	2.05	0.56
2:E:540:HIS:CE1	2:E:542:SER:HG	2.23	0.56
2:F:543:ILE:CG2	2:F:544:ILE:N	2.67	0.56
2:E:441:ARG:CZ	2:E:525:CYS:SG	2.93	0.56
1:A:347:THR:O	1:A:349:GLU:N	2.34	0.56
2:F:489:VAL:HG11	2:G:575:GLY:HA2	1.87	0.56
2:G:533:ALA:HB2	2:G:629:VAL:HA	1.87	0.56
1:B:126:LEU:HD13	1:B:132:HIS:CD2	2.40	0.56
2:G:456:LEU:CG	2:G:501:LYS:HG2	2.35	0.56
2:F:467:GLY:H	2:F:481:VAL:HB	1.69	0.56
1:D:271:SER:O	1:D:273:GLU:N	2.38	0.56
2:H:594:ARG:C	2:H:595:LEU:HD12	2.26	0.56
1:D:294:ILE:C	1:D:296:GLN:H	2.09	0.56
1:B:117:PHE:CE1	1:B:139:LEU:HD22	2.40	0.56
1:B:323:TYR:HA	1:B:392:VAL:O	2.06	0.56
1:D:224:LEU:O	1:D:250:VAL:HA	2.05	0.56
2:E:543:ILE:HG22	2:E:544:ILE:C	2.26	0.56
2:F:543:ILE:HG22	2:F:544:ILE:C	2.26	0.56
2:E:467:GLY:H	2:E:481:VAL:HB	1.70	0.56
2:H:533:ALA:HB2	2:H:629:VAL:HA	1.88	0.56
2:H:543:ILE:CG2	2:H:544:ILE:N	2.69	0.56
1:B:245:ARG:O	1:B:249:LYS:HG2	2.05	0.56
1:B:275:LEU:C	1:B:277:ASN:N	2.59	0.56
2:F:529:ARG:HB2	2:F:597:THR:HG23	1.86	0.56
1:A:305:VAL:HG23	1:A:306:GLU:H	1.70	0.56
1:B:327:ASP:HB3	1:B:347:THR:HG22	1.87	0.56
2:E:561:VAL:HG23	2:E:596:ARG:O	2.05	0.56
1:C:318:GLU:O	1:C:388:THR:HB	2.06	0.56
2:G:456:LEU:HD21	2:G:501:LYS:HG2	1.88	0.56
2:F:454:VAL:HG12	2:F:455:VAL:N	2.21	0.56
2:H:633:VAL:HB	2:H:634:PRO:CD	2.26	0.56
2:E:464:ILE:HD11	2:E:470:LEU:HD11	1.88	0.56
1:C:271:SER:O	1:C:273:GLU:N	2.39	0.56
2:F:538:ILE:O	2:F:540:HIS:N	2.39	0.55
2:H:500:LEU:HD23	2:H:502:ILE:HD11	1.87	0.55
1:A:116:PRO:C	1:A:118:LYS:H	2.09	0.55
2:H:531:PHE:HA	2:H:633:VAL:CG2	2.35	0.55
2:F:545:CYS:CB	2:F:546:PRO:CD	2.77	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:456:LEU:CG	2:H:501:LYS:HG2	2.35	0.55
1:B:176:LEU:O	1:B:178:LYS:HG3	2.06	0.55
1:B:10:ARG:HA	1:B:13:GLU:HG2	1.89	0.55
1:C:264:PHE:O	1:C:268:ILE:HG13	2.07	0.55
1:A:38:ILE:O	1:A:38:ILE:HG22	2.06	0.55
1:C:233:LYS:O	1:C:237:SER:CB	2.54	0.55
1:C:294:ILE:C	1:C:296:GLN:H	2.10	0.55
2:G:500:LEU:HD23	2:G:502:ILE:HD11	1.87	0.55
1:B:378:PHE:O	1:B:382:TYR:HB3	2.07	0.55
1:A:117:PHE:CE1	1:A:139:LEU:HD22	2.42	0.55
1:B:116:PRO:C	1:B:118:LYS:H	2.09	0.55
2:G:531:PHE:HA	2:G:633:VAL:CG2	2.36	0.55
1:A:378:PHE:O	1:A:382:TYR:HB3	2.07	0.55
1:D:326:LEU:HD13	1:D:328:ILE:HD12	1.87	0.55
1:A:133:THR:HG22	1:A:136:LEU:HD12	1.88	0.55
2:H:531:PHE:HA	2:H:633:VAL:HG23	1.89	0.55
1:B:347:THR:O	1:B:349:GLU:N	2.31	0.55
2:H:455:VAL:HG22	2:H:512:ILE:CD1	2.37	0.55
2:G:571:ASP:OD2	2:G:573:LYS:HG2	2.07	0.55
1:B:305:VAL:HG23	1:B:306:GLU:H	1.68	0.55
1:D:318:GLU:O	1:D:388:THR:HB	2.06	0.55
2:E:538:ILE:O	2:E:540:HIS:N	2.40	0.55
1:A:327:ASP:HB3	1:A:347:THR:HG22	1.88	0.55
2:G:594:ARG:C	2:G:595:LEU:HD12	2.27	0.55
1:A:10:ARG:HA	1:A:13:GLU:HG2	1.89	0.55
2:F:459:LEU:HD11	2:F:464:ILE:HG22	1.88	0.55
2:F:475:ASN:O	2:F:476:LYS:C	2.45	0.55
1:D:264:PHE:O	1:D:268:ILE:HG13	2.06	0.55
1:B:91:ASN:HB3	1:B:116:PRO:HG2	1.89	0.55
2:G:531:PHE:HA	2:G:633:VAL:HG23	1.89	0.55
2:F:571:ASP:OD2	2:F:573:LYS:HG2	2.07	0.55
1:B:191:ALA:O	1:B:192:ARG:C	2.46	0.55
2:H:548:TYR:HB3	2:H:563:ILE:HD11	1.89	0.54
1:C:264:PHE:CE1	1:C:268:ILE:HD11	2.42	0.54
1:B:162:GLN:O	1:B:164:ASN:N	2.40	0.54
1:D:320:LEU:HD21	1:D:378:PHE:CD2	2.42	0.54
1:B:394:ASP:HB3	1:B:403:VAL:HG21	1.88	0.54
2:G:544:ILE:HG12	2:G:548:TYR:CD1	2.42	0.54
2:H:520:ASP:CG	2:H:521:PRO:HD2	2.27	0.54
2:E:571:ASP:OD2	2:E:573:LYS:HG2	2.07	0.54
2:G:615:PHE:HE1	2:G:617:LEU:HD22	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:ARG:H	1:A:245:ARG:CD	2.18	0.54
1:C:326:LEU:HD13	1:C:328:ILE:HD12	1.89	0.54
2:G:585:VAL:O	2:G:585:VAL:HG13	2.06	0.54
2:H:442:LEU:HB2	2:H:459:LEU:HD23	1.88	0.54
2:E:540:HIS:HB3	2:E:541:LYS:C	2.25	0.54
2:E:529:ARG:HA	2:E:597:THR:HG21	1.90	0.54
2:H:585:VAL:HG13	2:H:585:VAL:O	2.06	0.54
2:E:473:MET:HE2	2:E:525:CYS:O	2.06	0.54
1:D:145:LYS:HE2	1:D:162:GLN:HE21	1.72	0.54
1:C:391:ILE:CD1	1:C:391:ILE:H	1.94	0.54
1:D:233:LYS:O	1:D:237:SER:CB	2.55	0.54
2:E:571:ASP:OD1	2:E:572:LYS:N	2.41	0.54
1:A:394:ASP:HB3	1:A:403:VAL:HG21	1.89	0.54
2:G:548:TYR:HB3	2:G:563:ILE:HD11	1.89	0.54
2:H:486:SER:OG	2:H:498:GLU:HB3	2.08	0.54
2:G:443:PRO:HA	2:G:517:ILE:HA	1.89	0.54
1:A:191:ALA:O	1:A:192:ARG:C	2.47	0.54
2:F:545:CYS:HB2	2:F:583:ARG:O	2.08	0.53
2:H:486:SER:OG	2:H:498:GLU:OE1	2.26	0.53
2:G:486:SER:OG	2:G:498:GLU:HB3	2.08	0.53
2:G:633:VAL:HB	2:G:634:PRO:CD	2.25	0.53
2:H:456:LEU:HD21	2:H:501:LYS:HG2	1.89	0.53
1:A:176:LEU:O	1:A:178:LYS:HG3	2.08	0.53
1:A:274:VAL:O	1:A:277:ASN:HB2	2.08	0.53
1:B:274:VAL:O	1:B:277:ASN:HB2	2.09	0.53
2:F:559:GLU:HG2	2:F:597:THR:OG1	2.07	0.53
2:F:548:TYR:HB3	2:F:563:ILE:HD11	1.90	0.53
2:F:520:ASP:CG	2:F:521:PRO:HD2	2.29	0.53
1:A:91:ASN:HB3	1:A:116:PRO:HG2	1.90	0.53
2:E:520:ASP:CG	2:E:521:PRO:HD2	2.28	0.53
2:F:571:ASP:OD1	2:F:572:LYS:N	2.41	0.53
1:C:145:LYS:HE2	1:C:162:GLN:HE21	1.72	0.53
2:E:541:LYS:CB	2:E:587:GLN:CD	2.72	0.53
2:H:615:PHE:HE1	2:H:617:LEU:HD22	1.73	0.53
1:C:346:LEU:HD11	1:C:350:GLN:HB3	1.90	0.53
1:B:67:ASN:O	1:B:71:VAL:HG23	2.08	0.53
2:H:454:VAL:HG12	2:H:455:VAL:N	2.23	0.53
2:H:455:VAL:HG22	2:H:512:ILE:HD11	1.90	0.53
2:E:536:VAL:HG12	2:E:626:ILE:O	2.08	0.53
1:C:323:TYR:CE2	1:C:394:ASP:HB3	2.43	0.53
2:E:548:TYR:HB3	2:E:563:ILE:HD11	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:447:LYS:O	2:F:448:TYR:CB	2.53	0.53
2:H:486:SER:CB	2:H:498:GLU:OE1	2.57	0.53
2:G:626:ILE:HG22	2:G:627:GLY:N	2.24	0.53
1:B:151:ILE:HG21	1:B:232:PHE:HB3	1.91	0.53
2:H:506:GLY:HA3	2:H:509:GLU:CD	2.29	0.53
2:H:578:SER:OG	2:H:579:LYS:N	2.41	0.53
2:G:506:GLY:HA3	2:G:509:GLU:CD	2.29	0.53
2:G:455:VAL:HG22	2:G:512:ILE:HD11	1.91	0.53
2:H:440:ILE:CG2	2:H:462:GLY:HA3	2.38	0.53
2:G:520:ASP:CG	2:G:521:PRO:HD2	2.28	0.53
1:D:310:LYS:O	1:D:314:MET:HG2	2.09	0.53
2:H:538:ILE:O	2:H:540:HIS:N	2.42	0.53
2:F:540:HIS:HB3	2:F:541:LYS:C	2.25	0.53
2:G:454:VAL:HG12	2:G:455:VAL:N	2.23	0.53
2:G:440:ILE:CG2	2:G:462:GLY:HA3	2.38	0.53
1:D:264:PHE:CE1	1:D:268:ILE:HD11	2.44	0.53
2:H:571:ASP:OD2	2:H:573:LYS:HG2	2.09	0.52
1:B:393:THR:HB	1:B:395:LYS:HG3	1.90	0.52
2:F:441:ARG:NH2	2:F:525:CYS:SG	2.82	0.52
1:C:320:LEU:HD21	1:C:378:PHE:CD2	2.43	0.52
2:G:538:ILE:O	2:G:540:HIS:N	2.42	0.52
2:H:544:ILE:HG12	2:H:548:TYR:CD1	2.43	0.52
2:E:520:ASP:OD1	2:E:522:ASN:ND2	2.39	0.52
2:E:454:VAL:HG12	2:E:455:VAL:N	2.24	0.52
2:H:484:ILE:CG2	2:H:500:LEU:HG	2.40	0.52
1:C:271:SER:O	1:C:272:THR:C	2.48	0.52
1:A:19:LYS:O	1:A:20:LEU:C	2.48	0.52
2:E:540:HIS:CE1	2:E:624:ILE:HD11	2.45	0.52
2:G:459:LEU:HD11	2:G:464:ILE:HG22	1.90	0.52
2:G:484:ILE:CG2	2:G:500:LEU:HG	2.39	0.52
2:G:543:ILE:HG22	2:G:544:ILE:C	2.29	0.52
2:H:563:ILE:HG22	2:H:595:LEU:HG	1.91	0.52
2:E:545:CYS:HB2	2:E:583:ARG:O	2.09	0.52
2:E:472:MET:HG2	2:E:473:MET:H	1.73	0.52
2:H:459:LEU:HD11	2:H:464:ILE:HG22	1.90	0.52
2:H:484:ILE:HG12	2:H:502:ILE:HD13	1.92	0.52
2:G:486:SER:OG	2:G:498:GLU:OE1	2.28	0.52
1:D:416:ARG:HH11	1:D:418:ASP:HA	1.75	0.52
2:G:578:SER:OG	2:G:579:LYS:N	2.41	0.52
1:C:79:GLN:HA	1:C:82:LEU:HB3	1.92	0.52
2:G:442:LEU:HB2	2:G:459:LEU:HD23	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:558:ILE:O	2:F:558:ILE:HG13	2.10	0.52
1:D:346:LEU:HD11	1:D:350:GLN:HB3	1.90	0.52
1:D:208:THR:HG22	1:D:212:LEU:HD23	1.91	0.52
1:A:151:ILE:HG21	1:A:232:PHE:HB3	1.92	0.52
2:F:540:HIS:ND1	2:F:624:ILE:HD11	2.25	0.52
2:H:443:PRO:HA	2:H:517:ILE:HA	1.91	0.52
1:B:118:LYS:CE	1:B:119:PRO:HG3	2.39	0.52
1:C:264:PHE:CZ	1:C:268:ILE:HD11	2.45	0.52
1:A:67:ASN:O	1:A:71:VAL:HG23	2.10	0.52
1:A:110:VAL:CG2	1:A:112:ILE:HD11	2.40	0.52
2:H:543:ILE:HG22	2:H:544:ILE:C	2.30	0.52
1:B:176:LEU:O	1:B:178:LYS:CG	2.58	0.52
2:F:540:HIS:HE2	2:F:544:ILE:HG13	1.74	0.52
2:F:472:MET:HG2	2:F:473:MET:H	1.75	0.52
1:B:244:GLN:HB3	1:B:245:ARG:HD2	1.92	0.52
1:B:117:PHE:CE1	1:B:139:LEU:O	2.63	0.52
1:A:14:ILE:HG23	1:A:140:LEU:HD22	1.91	0.52
1:C:252:LYS:HG2	1:C:253:LEU:O	2.10	0.51
2:E:477:HIS:HE1	2:E:508:GLU:H	1.57	0.51
2:E:529:ARG:CA	2:E:597:THR:HG22	2.38	0.51
2:G:558:ILE:O	2:G:559:GLU:CB	2.54	0.51
1:C:326:LEU:C	1:C:328:ILE:H	2.14	0.51
2:E:540:HIS:HE2	2:E:544:ILE:HG13	1.76	0.51
2:G:455:VAL:HG22	2:G:512:ILE:CD1	2.39	0.51
2:E:459:LEU:O	2:E:496:PRO:HA	2.10	0.51
2:G:486:SER:CB	2:G:498:GLU:OE1	2.58	0.51
1:A:170:HIS:CD2	1:A:208:THR:HG21	2.45	0.51
1:A:302:CYS:HB3	1:A:413:LEU:HD11	1.93	0.51
2:F:477:HIS:HE1	2:F:508:GLU:H	1.58	0.51
1:A:117:PHE:CE1	1:A:139:LEU:O	2.63	0.51
1:C:208:THR:HG22	1:C:212:LEU:HD23	1.92	0.51
1:B:19:LYS:O	1:B:20:LEU:C	2.48	0.51
1:B:58:THR:C	1:B:60:SER:H	2.14	0.51
1:B:115:GLU:HG2	1:B:116:PRO:CD	2.27	0.51
2:G:495:ALA:HB1	2:G:496:PRO:CD	2.39	0.51
1:A:176:LEU:O	1:A:178:LYS:CG	2.59	0.51
2:G:554:ILE:CD1	2:G:601:ILE:HG21	2.40	0.51
1:A:94:VAL:O	1:A:113:ASP:HA	2.10	0.51
1:A:394:ASP:C	1:A:395:LYS:HG2	2.30	0.51
1:B:394:ASP:C	1:B:395:LYS:HG2	2.31	0.51
2:H:536:VAL:O	2:H:537:ILE:C	2.48	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:546:PRO:CD	2:H:583:ARG:O	2.57	0.51
2:H:484:ILE:HG23	2:H:500:LEU:HG	1.92	0.51
1:B:170:HIS:CD2	1:B:208:THR:HG21	2.46	0.51
2:F:441:ARG:NE	2:F:525:CYS:SG	2.83	0.51
2:G:484:ILE:HG12	2:G:502:ILE:HD13	1.92	0.51
2:F:460:GLU:HB3	2:F:611:GLN:HG3	1.93	0.51
1:D:81:ARG:HH21	1:D:84:LEU:HD11	1.76	0.51
2:E:473:MET:HB3	2:E:474:PRO:CD	2.36	0.51
2:F:536:VAL:HG12	2:F:626:ILE:O	2.10	0.51
1:A:322:VAL:O	1:A:391:ILE:HA	2.11	0.51
1:A:393:THR:HB	1:A:395:LYS:HG3	1.91	0.51
1:D:271:SER:O	1:D:272:THR:C	2.47	0.51
1:D:252:LYS:HG2	1:D:253:LEU:O	2.09	0.51
2:E:474:PRO:HG3	2:E:602:CYS:HB3	1.92	0.51
1:C:397:GLN:C	1:C:399:GLY:N	2.64	0.51
1:B:322:VAL:HG12	1:B:323:TYR:N	2.25	0.51
1:A:303:PHE:HD2	1:A:303:PHE:N	2.08	0.51
1:B:110:VAL:CG2	1:B:112:ILE:HD11	2.41	0.51
1:B:118:LYS:HB3	1:B:119:PRO:HD2	1.93	0.51
1:A:117:PHE:CZ	1:A:139:LEU:O	2.64	0.51
2:H:468:GLN:HB3	2:H:470:LEU:HD13	1.93	0.51
1:B:303:PHE:N	1:B:303:PHE:HD2	2.09	0.51
2:G:536:VAL:O	2:G:537:ILE:C	2.49	0.50
2:G:571:ASP:OD1	2:G:572:LYS:N	2.43	0.50
2:E:543:ILE:O	2:E:544:ILE:HG13	2.11	0.50
1:D:326:LEU:C	1:D:328:ILE:H	2.14	0.50
1:A:303:PHE:N	1:A:303:PHE:CD2	2.79	0.50
1:A:162:GLN:O	1:A:164:ASN:N	2.44	0.50
2:E:529:ARG:CA	2:E:597:THR:CG2	2.86	0.50
2:H:494:VAL:HG21	2:H:500:LEU:HD11	1.93	0.50
2:G:484:ILE:HG23	2:G:500:LEU:HG	1.93	0.50
1:B:94:VAL:O	1:B:113:ASP:HA	2.10	0.50
1:B:52:LEU:HB2	1:B:79:GLN:OE1	2.11	0.50
1:D:79:GLN:HA	1:D:82:LEU:HB3	1.93	0.50
2:F:551:VAL:HG12	2:F:558:ILE:CD1	2.42	0.50
2:F:578:SER:OG	2:F:579:LYS:N	2.44	0.50
2:G:563:ILE:HG22	2:G:595:LEU:HG	1.91	0.50
1:C:206:ALA:HB2	1:C:242:PHE:HB2	1.94	0.50
1:A:118:LYS:HB3	1:A:119:PRO:CD	2.40	0.50
2:G:494:VAL:HG21	2:G:500:LEU:HD11	1.93	0.50
1:C:81:ARG:HH21	1:C:84:LEU:HD11	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:171:LYS:NZ	1:D:261:GLU:OE1	2.44	0.50
1:A:58:THR:C	1:A:60:SER:H	2.14	0.50
2:F:459:LEU:O	2:F:496:PRO:HA	2.11	0.50
2:H:571:ASP:OD1	2:H:572:LYS:N	2.44	0.50
1:B:322:VAL:O	1:B:391:ILE:HA	2.12	0.50
1:A:61:ASN:O	1:A:63:LYS:N	2.41	0.50
2:G:542:SER:O	2:G:543:ILE:HG12	2.12	0.50
1:A:118:LYS:HB3	1:A:119:PRO:HD2	1.93	0.50
1:A:97:CYS:SG	1:A:111:ASN:ND2	2.85	0.50
1:B:277:ASN:O	1:B:280:PHE:N	2.44	0.50
1:D:397:GLN:C	1:D:399:GLY:N	2.64	0.50
1:B:252:LYS:HG2	1:B:253:LEU:N	2.27	0.50
2:H:626:ILE:HG22	2:H:627:GLY:N	2.25	0.50
2:E:445:VAL:HG22	2:E:556:THR:HG21	1.93	0.50
1:D:264:PHE:CZ	1:D:268:ILE:HD11	2.46	0.50
1:B:303:PHE:N	1:B:303:PHE:CD2	2.79	0.50
1:B:310:LYS:HA	1:B:313:GLU:HB2	1.93	0.50
1:D:402:PHE:HZ	1:D:410:GLY:H	1.58	0.50
2:H:563:ILE:HA	2:H:594:ARG:O	2.12	0.49
2:H:554:ILE:CD1	2:H:601:ILE:HG21	2.41	0.49
2:F:529:ARG:HA	2:F:597:THR:HG22	1.94	0.49
2:H:467:GLY:H	2:H:481:VAL:HG12	1.76	0.49
2:E:475:ASN:HB3	2:E:477:HIS:HB2	1.93	0.49
1:C:310:LYS:O	1:C:314:MET:HG2	2.11	0.49
1:B:44:GLN:O	1:B:47:ARG:HB3	2.12	0.49
2:G:541:LYS:CB	2:G:587:GLN:CD	2.75	0.49
1:B:38:ILE:O	1:B:38:ILE:HG22	2.11	0.49
1:C:252:LYS:HG2	1:C:253:LEU:N	2.27	0.49
1:B:97:CYS:SG	1:B:111:ASN:ND2	2.85	0.49
1:B:117:PHE:CZ	1:B:139:LEU:O	2.65	0.49
1:B:61:ASN:O	1:B:63:LYS:N	2.40	0.49
2:F:441:ARG:HB2	2:F:461:SER:HB3	1.94	0.49
1:A:275:LEU:N	1:A:275:LEU:HD12	2.28	0.49
2:H:486:SER:HB2	2:H:500:LEU:HD11	1.94	0.49
1:C:151:ILE:CG2	1:C:232:PHE:CG	2.96	0.49
1:A:51:MET:O	1:A:51:MET:HG2	2.13	0.49
1:C:226:LEU:HB2	1:C:253:LEU:HD23	1.95	0.49
1:D:226:LEU:HB2	1:D:253:LEU:HD23	1.95	0.49
1:A:40:PRO:HB3	1:A:122:THR:H	1.78	0.49
2:E:520:ASP:O	2:E:524:LEU:HB3	2.13	0.49
1:B:276:SER:HA	1:B:279:LYS:CE	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:LEU:CD1	1:A:390:GLU:HG3	2.43	0.49
1:A:310:LYS:HA	1:A:313:GLU:HB2	1.94	0.49
2:H:441:ARG:N	2:H:461:SER:O	2.45	0.49
2:G:456:LEU:CD2	2:G:501:LYS:CG	2.90	0.49
1:A:244:GLN:HB3	1:A:245:ARG:HD2	1.93	0.49
2:G:467:GLY:H	2:G:481:VAL:HG12	1.77	0.49
1:D:252:LYS:HG2	1:D:253:LEU:N	2.27	0.49
1:B:40:PRO:HB3	1:B:122:THR:H	1.78	0.49
2:H:456:LEU:CD2	2:H:501:LYS:CE	2.86	0.49
2:H:540:HIS:HE2	2:H:544:ILE:HG13	1.78	0.49
2:E:441:ARG:HB2	2:E:461:SER:HB3	1.94	0.49
2:F:520:ASP:OD1	2:F:522:ASN:ND2	2.42	0.49
1:C:78:VAL:O	1:C:82:LEU:HB2	2.12	0.49
1:D:206:ALA:HB2	1:D:242:PHE:HB2	1.94	0.49
1:A:44:GLN:O	1:A:47:ARG:HB3	2.12	0.49
1:B:118:LYS:HB3	1:B:119:PRO:CD	2.41	0.49
2:F:467:GLY:N	2:F:481:VAL:HB	2.28	0.49
2:F:467:GLY:O	2:F:480:GLU:HG3	2.13	0.49
2:F:633:VAL:HA	2:F:634:PRO:HA	1.65	0.49
2:H:554:ILE:HD12	2:H:601:ILE:CG2	2.42	0.49
2:F:551:VAL:CG1	2:F:558:ILE:HD11	2.42	0.49
2:E:609:PHE:HB3	2:E:611:GLN:NE2	2.27	0.49
2:E:578:SER:OG	2:E:579:LYS:N	2.44	0.49
1:C:171:LYS:NZ	1:C:261:GLU:OE1	2.45	0.49
2:H:456:LEU:CD2	2:H:501:LYS:CG	2.90	0.49
1:B:41:PRO:O	1:B:42:LYS:CG	2.55	0.49
1:D:78:VAL:O	1:D:82:LEU:HB2	2.13	0.49
2:G:540:HIS:HE2	2:G:544:ILE:HG13	1.78	0.48
2:E:441:ARG:NE	2:E:525:CYS:SG	2.86	0.48
1:A:52:LEU:HB2	1:A:79:GLN:OE1	2.12	0.48
2:G:563:ILE:HA	2:G:594:ARG:O	2.14	0.48
2:E:544:ILE:CG2	2:E:563:ILE:HD11	2.43	0.48
2:G:441:ARG:N	2:G:461:SER:O	2.44	0.48
2:E:529:ARG:O	2:E:597:THR:HG22	2.13	0.48
1:D:233:LYS:O	1:D:237:SER:N	2.44	0.48
1:D:317:VAL:HG12	1:D:413:LEU:CD2	2.42	0.48
1:A:277:ASN:O	1:A:280:PHE:N	2.46	0.48
1:C:320:LEU:HD23	1:C:389:LEU:HD13	1.96	0.48
1:D:40:PRO:HD3	1:D:123:SER:HB2	1.95	0.48
2:G:554:ILE:HD12	2:G:601:ILE:CG2	2.42	0.48
1:A:305:VAL:CG2	1:A:306:GLU:N	2.76	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:LYS:HG2	1:A:253:LEU:N	2.29	0.48
2:F:445:VAL:HG22	2:F:556:THR:HG21	1.94	0.48
2:G:447:LYS:CD	2:G:512:ILE:O	2.62	0.48
2:E:473:MET:HG2	2:E:602:CYS:HB2	1.94	0.48
2:E:460:GLU:HB3	2:E:611:GLN:HG3	1.95	0.48
1:A:399:GLY:O	1:A:403:VAL:HG23	2.14	0.48
1:A:133:THR:C	1:A:135:ALA:N	2.64	0.48
2:H:542:SER:O	2:H:543:ILE:HG12	2.13	0.48
1:A:89:PRO:O	1:A:91:ASN:N	2.47	0.48
2:E:473:MET:HG3	2:E:474:PRO:HA	1.96	0.48
2:E:502:ILE:HB	2:E:504:LEU:CD1	2.44	0.48
1:B:52:LEU:HD12	1:B:79:GLN:HG3	1.95	0.48
1:B:318:GLU:HB2	1:B:414:ARG:HG2	1.94	0.48
1:D:203:ARG:O	1:D:207:GLU:HB2	2.14	0.48
1:D:330:ARG:HB2	1:D:374:LEU:HD23	1.96	0.48
1:A:121:ASN:O	1:A:121:ASN:OD1	2.32	0.48
2:H:469:GLN:O	2:H:521:PRO:HG3	2.14	0.48
1:A:275:LEU:C	1:A:277:ASN:N	2.57	0.48
2:G:486:SER:HB2	2:G:500:LEU:HD11	1.94	0.48
1:D:151:ILE:CG2	1:D:232:PHE:CG	2.96	0.48
1:B:399:GLY:O	1:B:403:VAL:HG23	2.14	0.48
1:B:81:ARG:CD	1:B:111:ASN:HB3	2.40	0.48
2:G:468:GLN:HB3	2:G:470:LEU:HD13	1.95	0.48
1:B:234:THR:O	1:B:234:THR:HG22	2.13	0.48
1:A:119:PRO:O	1:A:120:ILE:C	2.52	0.48
2:F:546:PRO:CD	2:F:583:ARG:O	2.62	0.48
1:D:317:VAL:HA	1:D:413:LEU:HA	1.95	0.48
1:A:41:PRO:O	1:A:42:LYS:CG	2.52	0.48
1:A:151:ILE:O	1:A:228:GLY:HA2	2.14	0.48
2:F:473:MET:HG3	2:F:474:PRO:HA	1.96	0.48
1:B:275:LEU:HD12	1:B:275:LEU:N	2.29	0.48
2:F:529:ARG:CA	2:F:597:THR:CG2	2.92	0.48
2:F:502:ILE:HB	2:F:504:LEU:CD1	2.44	0.47
2:H:520:ASP:OD1	2:H:522:ASN:ND2	2.37	0.47
2:E:467:GLY:O	2:E:480:GLU:HG3	2.14	0.47
1:C:233:LYS:O	1:C:237:SER:N	2.44	0.47
2:E:551:VAL:HG12	2:E:558:ILE:CD1	2.44	0.47
2:F:609:PHE:HB3	2:F:611:GLN:NE2	2.29	0.47
2:E:569:LEU:H	2:E:578:SER:CB	2.27	0.47
2:E:540:HIS:HA	2:E:624:ILE:HG13	1.95	0.47
1:B:119:PRO:O	1:B:120:ILE:C	2.53	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:467:GLY:N	2:E:481:VAL:HB	2.29	0.47
1:D:320:LEU:HD23	1:D:389:LEU:HD13	1.97	0.47
2:G:611:GLN:H	2:G:611:GLN:CD	2.18	0.47
1:A:239:SER:C	1:A:241:MET:H	2.18	0.47
1:B:286:LEU:CD1	1:B:390:GLU:HG3	2.43	0.47
1:C:319:ILE:HD12	1:C:412:ILE:HD12	1.97	0.47
1:C:330:ARG:HB2	1:C:374:LEU:HD23	1.96	0.47
1:B:51:MET:O	1:B:51:MET:HG2	2.13	0.47
1:B:121:ASN:OD1	1:B:121:ASN:O	2.33	0.47
2:H:447:LYS:CD	2:H:512:ILE:O	2.61	0.47
1:B:146:PHE:O	1:B:160:THR:HA	2.14	0.47
1:B:303:PHE:H	1:B:303:PHE:HD2	1.63	0.47
1:A:234:THR:O	1:A:234:THR:HG22	2.13	0.47
2:G:456:LEU:CD2	2:G:501:LYS:CE	2.85	0.47
2:F:450:ASP:CG	2:F:451:MET:N	2.68	0.47
2:F:543:ILE:O	2:F:544:ILE:HG13	2.13	0.47
2:F:540:HIS:HA	2:F:624:ILE:HG13	1.96	0.47
2:G:546:PRO:CD	2:G:583:ARG:O	2.57	0.47
1:C:317:VAL:HA	1:C:413:LEU:HA	1.96	0.47
2:H:495:ALA:HB1	2:H:496:PRO:CD	2.39	0.47
1:C:151:ILE:HG22	1:C:232:PHE:CD2	2.50	0.47
1:D:323:TYR:HE2	1:D:394:ASP:HB3	1.80	0.47
1:C:318:GLU:HB2	1:C:414:ARG:HH21	1.79	0.47
2:E:569:LEU:H	2:E:578:SER:HB3	1.79	0.47
1:B:239:SER:C	1:B:241:MET:H	2.18	0.47
1:B:14:ILE:HG23	1:B:140:LEU:HD22	1.95	0.47
2:G:530:THR:C	2:G:633:VAL:CG2	2.82	0.47
2:F:473:MET:HB3	2:F:474:PRO:CD	2.39	0.47
2:G:469:GLN:O	2:G:521:PRO:HG3	2.15	0.47
1:A:176:LEU:HA	1:A:197:LYS:HD2	1.96	0.47
1:B:275:LEU:H	1:B:275:LEU:CD1	2.28	0.47
1:A:322:VAL:HG12	1:A:323:TYR:N	2.29	0.47
1:C:203:ARG:O	1:C:207:GLU:HB2	2.14	0.47
2:E:537:ILE:O	2:E:588:ASP:N	2.44	0.47
2:H:540:HIS:CE1	2:H:624:ILE:HD11	2.49	0.47
2:H:473:MET:HE2	2:H:525:CYS:O	2.15	0.47
2:E:473:MET:CB	2:E:474:PRO:CD	2.93	0.47
1:B:305:VAL:CG2	1:B:306:GLU:N	2.77	0.47
2:G:569:LEU:H	2:G:578:SER:CB	2.28	0.47
1:A:62:ILE:HG21	1:A:68:ARG:HB2	1.95	0.47
2:F:544:ILE:CG2	2:F:563:ILE:HD11	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:LYS:CE	1:B:119:PRO:CG	2.79	0.47
1:A:303:PHE:HD2	1:A:303:PHE:H	1.62	0.47
2:H:611:GLN:CD	2:H:611:GLN:H	2.18	0.47
1:C:402:PHE:HZ	1:C:410:GLY:H	1.62	0.47
2:E:528:GLY:O	2:E:600:THR:HG23	2.14	0.47
2:G:540:HIS:CE1	2:G:624:ILE:HD11	2.50	0.46
2:G:520:ASP:OD1	2:G:522:ASN:ND2	2.38	0.46
2:G:605:THR:O	2:G:606:PHE:C	2.53	0.46
2:F:529:ARG:CA	2:F:597:THR:HG22	2.45	0.46
1:D:151:ILE:HG22	1:D:232:PHE:CD2	2.51	0.46
2:G:609:PHE:HB3	2:G:611:GLN:HE22	1.80	0.46
2:H:609:PHE:HB3	2:H:611:GLN:HE22	1.81	0.46
1:C:40:PRO:HD3	1:C:123:SER:HB2	1.97	0.46
2:G:538:ILE:O	2:G:539:GLU:C	2.52	0.46
2:H:538:ILE:O	2:H:539:GLU:C	2.54	0.46
2:E:544:ILE:HG12	2:E:548:TYR:CG	2.50	0.46
1:A:271:SER:O	1:A:273:GLU:N	2.48	0.46
1:B:68:ARG:O	1:B:70:SER:N	2.48	0.46
2:G:473:MET:HB3	2:G:474:PRO:HA	1.96	0.46
1:C:214:ILE:HD12	1:C:245:ARG:HD3	1.98	0.46
2:E:529:ARG:HB2	2:E:597:THR:HG23	1.97	0.46
1:A:146:PHE:O	1:A:160:THR:HA	2.15	0.46
1:B:151:ILE:CG2	1:B:232:PHE:HB3	2.45	0.46
2:F:569:LEU:H	2:F:578:SER:CB	2.29	0.46
1:B:89:PRO:O	1:B:91:ASN:N	2.49	0.46
2:G:446:ASP:HB3	2:G:456:LEU:HD13	1.98	0.46
2:E:551:VAL:CG1	2:E:558:ILE:HD11	2.46	0.46
1:B:117:PHE:CD1	1:B:139:LEU:HD13	2.51	0.46
2:H:569:LEU:H	2:H:578:SER:CB	2.29	0.46
2:F:474:PRO:HG3	2:F:602:CYS:HB3	1.98	0.46
1:C:413:LEU:HD13	1:C:417:VAL:HG23	1.97	0.46
1:D:214:ILE:HD12	1:D:245:ARG:HD3	1.98	0.46
1:B:302:CYS:HB3	1:B:413:LEU:HD11	1.98	0.46
1:A:276:SER:HA	1:A:279:LYS:CE	2.43	0.46
2:F:529:ARG:HB2	2:F:597:THR:CG2	2.46	0.46
1:D:319:ILE:HD12	1:D:412:ILE:HD12	1.98	0.46
2:E:540:HIS:CB	2:E:541:LYS:CA	2.36	0.46
1:B:176:LEU:HA	1:B:197:LYS:HD2	1.97	0.46
2:G:453:THR:OG1	2:G:509:GLU:HB3	2.16	0.46
2:F:604:GLU:HB2	2:F:612:MET:HB2	1.98	0.46
1:B:347:THR:CB	1:B:348:PRO:CD	2.70	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:LEU:CD1	1:A:275:LEU:H	2.29	0.46
1:B:151:ILE:O	1:B:228:GLY:HA2	2.16	0.46
2:H:453:THR:OG1	2:H:509:GLU:HB3	2.16	0.46
2:E:620:GLU:HB3	2:E:621:GLY:H	1.48	0.46
2:H:541:LYS:CB	2:H:587:GLN:CD	2.77	0.45
2:G:520:ASP:O	2:G:524:LEU:HB3	2.16	0.45
2:G:603:LEU:O	2:G:604:GLU:CG	2.59	0.45
1:D:79:GLN:HG2	1:D:82:LEU:HD23	1.98	0.45
2:G:442:LEU:HD12	2:G:458:LYS:O	2.16	0.45
2:G:609:PHE:HB3	2:G:611:GLN:NE2	2.31	0.45
1:B:62:ILE:HG21	1:B:68:ARG:HB2	1.97	0.45
1:B:93:LEU:HA	1:B:93:LEU:HD23	1.48	0.45
2:F:619:ASP:C	2:F:619:ASP:OD1	2.55	0.45
1:C:303:PHE:HE1	2:G:583:ARG:HE	1.62	0.45
1:A:300:LYS:H	1:A:300:LYS:HD2	1.80	0.45
2:E:633:VAL:HA	2:E:634:PRO:HA	1.67	0.45
2:E:515:GLY:HA2	2:E:557:CYS:N	2.30	0.45
2:H:450:ASP:CG	2:H:451:MET:N	2.70	0.45
2:G:486:SER:HB2	2:G:500:LEU:CD1	2.46	0.45
2:E:552:LEU:HD21	2:E:554:ILE:HD11	1.97	0.45
1:B:133:THR:C	1:B:135:ALA:N	2.64	0.45
1:D:268:ILE:O	1:D:268:ILE:HG22	2.17	0.45
1:B:397:GLN:NE2	2:E:549:ASN:H	2.14	0.45
1:A:347:THR:CB	1:A:348:PRO:CD	2.68	0.45
2:H:605:THR:HA	2:H:629:VAL:HG13	1.97	0.45
1:A:318:GLU:HB2	1:A:414:ARG:HG2	1.99	0.45
1:C:197:LYS:HA	1:C:200:ASN:HB2	1.97	0.45
2:H:474:PRO:HD2	2:H:516:PHE:CD1	2.52	0.45
2:E:444:ILE:HD12	2:E:516:PHE:HB2	1.98	0.45
2:E:538:ILE:HG12	2:E:625:ALA:HA	1.99	0.45
1:B:91:ASN:CB	1:B:118:LYS:O	2.64	0.45
2:F:479:VAL:CG2	2:F:504:LEU:HD23	2.32	0.45
1:C:79:GLN:HG2	1:C:82:LEU:HD23	1.97	0.45
2:H:486:SER:HB2	2:H:500:LEU:CD1	2.46	0.45
1:C:166:ARG:HE	1:C:166:ARG:N	2.12	0.45
2:F:445:VAL:HG22	2:F:556:THR:HG22	1.99	0.45
2:E:558:ILE:O	2:E:558:ILE:HG13	2.17	0.45
2:E:619:ASP:OD1	2:E:620:GLU:N	2.50	0.45
2:F:619:ASP:OD1	2:F:620:GLU:N	2.50	0.45
2:E:450:ASP:CG	2:E:451:MET:N	2.69	0.45
1:A:87:LYS:HD3	1:A:88:VAL:H	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:327:ASP:HB3	1:C:348:PRO:HD3	1.99	0.45
2:H:473:MET:HB3	2:H:474:PRO:HA	1.97	0.45
2:E:536:VAL:HG21	2:H:488:ASP:HB2	1.98	0.45
1:C:268:ILE:O	1:C:268:ILE:HG22	2.17	0.45
1:A:52:LEU:HD12	1:A:79:GLN:HG3	1.99	0.45
2:H:620:GLU:HB3	2:H:621:GLY:H	1.47	0.45
1:A:93:LEU:HA	1:A:93:LEU:HD23	1.48	0.45
1:A:118:LYS:CE	1:A:119:PRO:HG3	2.39	0.45
1:A:81:ARG:CD	1:A:111:ASN:HB3	2.41	0.45
2:H:442:LEU:HD12	2:H:458:LYS:O	2.17	0.45
2:G:629:VAL:HG13	2:G:629:VAL:O	2.17	0.45
2:E:475:ASN:O	2:E:476:LYS:C	2.54	0.45
2:F:594:ARG:C	2:F:595:LEU:HD12	2.37	0.45
1:B:91:ASN:CB	1:B:119:PRO:HA	2.46	0.45
1:B:45:ILE:HG13	1:B:88:VAL:HG22	1.99	0.45
1:A:45:ILE:HG13	1:A:88:VAL:HG22	1.97	0.45
2:H:520:ASP:O	2:H:524:LEU:HB3	2.16	0.45
2:F:569:LEU:H	2:F:578:SER:HB3	1.81	0.45
1:A:271:SER:O	1:A:272:THR:C	2.55	0.45
1:A:397:GLN:NE2	2:F:549:ASN:H	2.15	0.45
1:C:301:TYR:HD2	1:C:301:TYR:H	1.65	0.45
2:F:517:ILE:HD11	2:F:602:CYS:HB2	1.99	0.45
1:B:223:GLY:HA2	1:B:251:LEU:HD22	1.98	0.45
2:E:447:LYS:HD2	2:E:512:ILE:O	2.17	0.45
2:F:515:GLY:HA2	2:F:557:CYS:N	2.32	0.45
1:C:147:GLY:HA3	1:C:224:LEU:HD22	1.99	0.45
1:C:69:LEU:O	1:C:70:SER:C	2.55	0.45
1:C:226:LEU:HD12	1:C:253:LEU:HD21	2.00	0.44
1:D:327:ASP:HB3	1:D:348:PRO:HD3	1.99	0.44
2:H:446:ASP:HB3	2:H:456:LEU:HD13	1.99	0.44
1:B:275:LEU:H	1:B:275:LEU:HD12	1.82	0.44
2:E:535:ILE:HG22	2:E:536:VAL:N	2.31	0.44
1:A:151:ILE:CG2	1:A:232:PHE:HB3	2.46	0.44
2:H:609:PHE:HB3	2:H:611:GLN:NE2	2.32	0.44
1:D:329:MET:HB3	1:D:331:TYR:HE1	1.82	0.44
2:G:605:THR:HA	2:G:629:VAL:HG13	1.99	0.44
1:D:166:ARG:HE	1:D:166:ARG:N	2.13	0.44
1:A:326:LEU:CD2	1:A:328:ILE:HD12	2.47	0.44
2:G:450:ASP:CG	2:G:451:MET:N	2.69	0.44
2:F:535:ILE:HG22	2:F:536:VAL:N	2.33	0.44
1:D:214:ILE:HA	1:D:219:VAL:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:552:LEU:HD21	2:F:554:ILE:HD11	1.99	0.44
2:F:555:HIS:N	2:F:557:CYS:SG	2.90	0.44
1:B:22:LYS:C	1:B:24:LEU:H	2.20	0.44
1:B:287:ILE:HD13	1:B:402:PHE:HB2	1.98	0.44
2:G:540:HIS:HB2	2:G:587:GLN:HG3	2.00	0.44
1:A:223:GLY:HA2	1:A:251:LEU:HD22	2.00	0.44
2:F:529:ARG:O	2:F:597:THR:HG22	2.17	0.44
1:A:328:ILE:HG22	1:A:345:TYR:HB3	2.00	0.44
1:A:270:LEU:HA	1:A:270:LEU:HD13	1.87	0.44
2:H:530:THR:C	2:H:633:VAL:CG2	2.83	0.44
1:D:234:THR:O	1:D:234:THR:HG22	2.18	0.44
2:E:594:ARG:C	2:E:595:LEU:HD12	2.37	0.44
1:B:87:LYS:HD3	1:B:88:VAL:H	1.82	0.44
2:G:473:MET:HE2	2:G:525:CYS:O	2.18	0.44
2:E:619:ASP:OD1	2:E:619:ASP:C	2.55	0.44
2:G:619:ASP:OD1	2:G:620:GLU:N	2.51	0.44
1:D:197:LYS:HA	1:D:200:ASN:HB2	1.99	0.44
1:D:69:LEU:O	1:D:70:SER:C	2.55	0.44
1:A:314:MET:O	1:A:315:GLY:C	2.55	0.44
2:G:474:PRO:HD2	2:G:516:PHE:CD1	2.52	0.44
2:F:502:ILE:H	2:F:502:ILE:HG12	1.65	0.44
2:E:447:LYS:O	2:E:448:TYR:CB	2.55	0.44
2:E:555:HIS:N	2:E:557:CYS:SG	2.91	0.44
1:B:233:LYS:O	1:B:237:SER:CB	2.66	0.44
1:B:133:THR:O	1:B:134:GLU:C	2.55	0.44
2:E:604:GLU:HB2	2:E:612:MET:HB2	2.00	0.44
2:G:566:LEU:CD1	2:G:582:PRO:O	2.65	0.44
1:B:271:SER:O	1:B:273:GLU:N	2.51	0.44
1:A:380:ASN:O	1:A:381:ASN:HB3	2.17	0.44
1:B:293:GLU:O	1:B:296:GLN:N	2.49	0.44
1:A:287:ILE:HD13	1:A:402:PHE:HB2	1.98	0.44
1:A:121:ASN:O	1:A:122:THR:CB	2.65	0.44
2:E:575:GLY:HA2	2:H:489:VAL:HG11	1.99	0.44
1:B:22:LYS:O	1:B:24:LEU:N	2.51	0.44
1:D:147:GLY:HA3	1:D:224:LEU:HD22	2.00	0.44
1:B:151:ILE:CD1	1:B:205:VAL:HG11	2.48	0.44
2:F:447:LYS:HD2	2:F:512:ILE:O	2.18	0.43
1:B:326:LEU:CD2	1:B:328:ILE:HD12	2.46	0.43
1:C:319:ILE:HB	1:C:412:ILE:HB	2.00	0.43
2:F:487:ASP:HB3	2:F:488:ASP:H	1.73	0.43
1:A:275:LEU:H	1:A:275:LEU:HD12	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:552:LEU:HD11	2:H:554:ILE:HG12	2.00	0.43
2:E:533:ALA:O	2:E:592:ILE:HA	2.18	0.43
1:A:233:LYS:O	1:A:237:SER:CB	2.66	0.43
1:A:68:ARG:O	1:A:70:SER:N	2.51	0.43
2:H:619:ASP:C	2:H:619:ASP:OD1	2.56	0.43
1:D:94:VAL:O	1:D:113:ASP:HA	2.18	0.43
1:D:301:TYR:HD2	1:D:301:TYR:H	1.65	0.43
2:H:443:PRO:HD2	2:H:458:LYS:O	2.19	0.43
2:F:561:VAL:CG2	2:F:596:ARG:O	2.65	0.43
1:A:110:VAL:CG2	1:A:112:ILE:CD1	2.96	0.43
1:C:329:MET:HB3	1:C:331:TYR:HE1	1.82	0.43
1:C:234:THR:HG22	1:C:234:THR:O	2.18	0.43
2:G:541:LYS:CD	2:G:587:GLN:NE2	2.64	0.43
1:A:91:ASN:CB	1:A:119:PRO:HA	2.46	0.43
1:D:151:ILE:HG21	1:D:232:PHE:HB3	1.98	0.43
1:B:206:ALA:HB2	1:B:242:PHE:HB2	2.00	0.43
1:A:293:GLU:O	1:A:296:GLN:N	2.51	0.43
1:D:8:ALA:C	1:D:10:ARG:H	2.22	0.43
1:D:124:LEU:HD23	1:D:124:LEU:C	2.39	0.43
1:B:121:ASN:O	1:B:122:THR:CB	2.65	0.43
3:A:1526:ATP:H5'1	3:A:1526:ATP:O2G	2.18	0.43
1:A:91:ASN:CB	1:A:118:LYS:O	2.64	0.43
2:H:605:THR:O	2:H:606:PHE:C	2.56	0.43
2:G:486:SER:CA	2:G:500:LEU:HD12	2.47	0.43
1:B:110:VAL:CG2	1:B:112:ILE:CD1	2.97	0.43
1:D:329:MET:HB3	1:D:331:TYR:CE1	2.53	0.43
2:G:619:ASP:OD1	2:G:619:ASP:C	2.57	0.43
1:A:156:ALA:HB2	1:A:201:TYR:OH	2.19	0.43
1:B:156:ALA:HB2	1:B:201:TYR:OH	2.19	0.43
2:F:577:LYS:HE2	2:F:577:LYS:HB3	1.87	0.43
1:B:118:LYS:HG3	1:B:119:PRO:CD	2.28	0.43
2:F:517:ILE:HG12	2:F:602:CYS:SG	2.58	0.43
2:E:524:LEU:CD1	2:E:525:CYS:H	2.32	0.43
2:E:517:ILE:HD11	2:E:602:CYS:HB2	2.00	0.43
2:F:575:GLY:HA2	2:G:489:VAL:HG11	2.01	0.43
2:G:603:LEU:C	2:G:604:GLU:HG2	2.39	0.43
2:F:536:VAL:HG21	2:G:488:ASP:HB2	1.99	0.43
1:B:271:SER:O	1:B:272:THR:C	2.56	0.43
1:B:380:ASN:O	1:B:381:ASN:HB3	2.19	0.43
2:G:552:LEU:HD11	2:G:554:ILE:HG12	2.01	0.43
1:A:22:LYS:C	1:A:24:LEU:H	2.22	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:24:LEU:HA	1:B:24:LEU:HD23	1.77	0.43
1:A:151:ILE:CD1	1:A:205:VAL:HG11	2.49	0.43
1:C:221:VAL:HB	1:C:222:ALA:H	1.61	0.43
1:B:270:LEU:HA	1:B:270:LEU:HD13	1.86	0.43
2:H:566:LEU:CD1	2:H:582:PRO:O	2.67	0.43
1:B:89:PRO:HB2	1:B:115:GLU:CD	2.39	0.43
2:G:567:ILE:HB	2:G:568:CYS:H	1.71	0.43
2:H:629:VAL:HG13	2:H:629:VAL:O	2.18	0.43
1:C:294:ILE:C	1:C:296:GLN:N	2.72	0.43
1:B:85:TYR:CZ	1:B:93:LEU:HD21	2.53	0.43
2:H:619:ASP:OD1	2:H:620:GLU:N	2.51	0.43
1:D:221:VAL:HB	1:D:222:ALA:H	1.60	0.43
1:D:231:ASP:O	1:D:235:GLU:HB2	2.18	0.43
1:C:124:LEU:HD23	1:C:124:LEU:C	2.38	0.43
1:B:118:LYS:HA	1:B:118:LYS:HD2	1.51	0.43
2:H:633:VAL:O	2:H:634:PRO:C	2.57	0.43
1:C:308:THR:O	1:C:312:LEU:N	2.43	0.43
1:C:326:LEU:HD23	1:C:326:LEU:HA	1.79	0.43
1:C:329:MET:HB3	1:C:331:TYR:CE1	2.53	0.43
1:B:314:MET:O	1:B:315:GLY:C	2.56	0.43
1:D:302:CYS:HB2	1:D:307:ASP:HB3	2.01	0.43
1:D:309:LEU:O	1:D:313:GLU:HG2	2.19	0.43
1:A:206:ALA:HB2	1:A:242:PHE:HB2	1.99	0.43
1:A:74:ALA:O	1:A:78:VAL:HG12	2.19	0.43
2:F:444:ILE:HG12	2:F:455:VAL:HG11	2.00	0.43
1:C:239:SER:C	1:C:241:MET:H	2.22	0.43
1:B:420:GLN:H	1:B:420:GLN:NE2	2.17	0.43
2:H:540:HIS:CE1	2:H:543:ILE:O	2.71	0.42
2:F:524:LEU:CD1	2:F:525:CYS:H	2.26	0.42
1:B:244:GLN:HE21	1:B:244:GLN:HB2	1.51	0.42
2:E:444:ILE:HG12	2:E:455:VAL:HG11	2.01	0.42
2:F:533:ALA:O	2:F:592:ILE:HA	2.19	0.42
2:E:445:VAL:HG22	2:E:556:THR:HG22	1.99	0.42
2:E:487:ASP:HB3	2:E:488:ASP:H	1.74	0.42
2:G:486:SER:O	2:G:488:ASP:N	2.52	0.42
1:A:139:LEU:HA	1:A:139:LEU:HD23	1.74	0.42
1:A:258:TYR:CD1	1:A:266:GLN:NE2	2.87	0.42
2:G:633:VAL:O	2:G:634:PRO:C	2.57	0.42
2:E:545:CYS:CB	2:E:546:PRO:CD	2.75	0.42
2:E:546:PRO:CD	2:E:583:ARG:O	2.64	0.42
1:B:124:LEU:C	1:B:124:LEU:CD2	2.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:PHE:CD1	1:A:139:LEU:HD13	2.54	0.42
2:E:486:SER:O	2:E:488:ASP:N	2.53	0.42
1:C:302:CYS:HB2	1:C:307:ASP:HB3	2.02	0.42
2:H:561:VAL:HG23	2:H:596:ARG:O	2.20	0.42
2:H:563:ILE:CG2	2:H:595:LEU:HG	2.50	0.42
2:F:543:ILE:HG22	2:F:544:ILE:CA	2.50	0.42
1:A:88:VAL:HA	1:A:89:PRO:HD2	1.74	0.42
1:A:405:GLY:O	2:F:583:ARG:HB3	2.20	0.42
2:E:464:ILE:CG2	2:E:494:VAL:HG13	2.48	0.42
2:F:464:ILE:CG2	2:F:494:VAL:HG13	2.47	0.42
1:C:382:TYR:CD1	1:C:389:LEU:HB2	2.54	0.42
2:F:534:GLN:HB2	2:F:630:LEU:HD11	2.02	0.42
2:G:540:HIS:CE1	2:G:543:ILE:O	2.72	0.42
1:D:226:LEU:HD12	1:D:253:LEU:HD21	2.01	0.42
2:H:474:PRO:HD2	2:H:516:PHE:CE1	2.55	0.42
1:B:328:ILE:HG22	1:B:345:TYR:HB3	2.02	0.42
1:A:133:THR:O	1:A:134:GLU:C	2.57	0.42
1:B:258:TYR:CD1	1:B:266:GLN:NE2	2.88	0.42
2:E:605:THR:OG1	2:E:608:ASP:HB2	2.20	0.42
2:G:529:ARG:HG2	2:G:530:THR:OG1	2.20	0.42
2:G:447:LYS:CG	2:G:512:ILE:HG23	2.48	0.42
2:H:447:LYS:HD3	2:H:512:ILE:O	2.19	0.42
1:A:243:ASP:O	1:A:244:GLN:HB2	2.19	0.42
1:A:85:TYR:CZ	1:A:93:LEU:HD21	2.54	0.42
1:B:420:GLN:HG2	1:B:420:GLN:O	2.18	0.42
1:A:28:ARG:HG3	1:A:130:LYS:HB3	2.01	0.42
1:B:74:ALA:O	1:B:78:VAL:HG12	2.19	0.42
1:D:413:LEU:HG	1:D:413:LEU:H	1.74	0.42
2:H:603:LEU:O	2:H:604:GLU:CG	2.59	0.42
1:C:279:LYS:O	1:C:283:GLU:HB2	2.20	0.42
1:D:294:ILE:C	1:D:296:GLN:N	2.71	0.42
2:G:470:LEU:HG	2:G:519:CYS:O	2.20	0.42
2:F:537:ILE:O	2:F:588:ASP:N	2.47	0.42
1:D:251:LEU:HD21	1:D:278:VAL:HG22	2.02	0.42
2:G:548:TYR:OH	2:G:624:ILE:HG21	2.20	0.42
2:E:543:ILE:HG22	2:E:544:ILE:CA	2.50	0.42
2:F:473:MET:CB	2:F:474:PRO:CD	2.96	0.42
2:H:486:SER:O	2:H:488:ASP:N	2.52	0.42
1:C:251:LEU:HD21	1:C:278:VAL:HG22	2.01	0.42
2:E:540:HIS:ND1	2:E:624:ILE:HD11	2.34	0.42
1:A:267:ALA:O	1:A:271:SER:HB3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:231:ASP:O	1:C:235:GLU:HB2	2.20	0.42
1:C:8:ALA:C	1:C:10:ARG:H	2.22	0.42
2:E:500:LEU:C	2:E:501:LYS:HG3	2.41	0.42
2:E:520:ASP:OD1	2:E:521:PRO:HD2	2.20	0.42
2:F:454:VAL:CG1	2:F:455:VAL:N	2.83	0.42
1:A:323:TYR:CD1	1:A:325:ASN:O	2.73	0.42
1:A:206:ALA:CB	1:A:242:PHE:HB2	2.50	0.42
2:G:595:LEU:HD12	2:G:595:LEU:N	2.34	0.41
2:G:568:CYS:O	2:G:592:ILE:HG12	2.20	0.41
1:A:152:ASP:HB3	1:A:155:GLY:O	2.20	0.41
1:A:64:SER:O	1:A:67:ASN:N	2.48	0.41
1:C:213:PHE:CD2	1:C:221:VAL:HG11	2.55	0.41
2:F:537:ILE:HD13	2:F:537:ILE:HA	1.83	0.41
1:D:239:SER:C	1:D:241:MET:H	2.23	0.41
2:H:455:VAL:CG2	2:H:512:ILE:CD1	2.99	0.41
1:C:413:LEU:HD13	1:C:417:VAL:CG2	2.50	0.41
1:A:124:LEU:CD2	1:A:124:LEU:C	2.88	0.41
1:B:322:VAL:CG1	1:B:323:TYR:N	2.83	0.41
2:H:617:LEU:HA	2:H:617:LEU:HD12	1.84	0.41
1:C:8:ALA:C	1:C:10:ARG:N	2.73	0.41
1:A:264:PHE:O	1:A:268:ILE:HG13	2.21	0.41
1:B:294:ILE:HG23	1:B:301:TYR:CZ	2.55	0.41
2:E:534:GLN:HB2	2:E:630:LEU:HD11	2.03	0.41
1:A:121:ASN:O	1:A:122:THR:HG22	2.21	0.41
1:A:223:GLY:O	1:A:224:LEU:HB2	2.20	0.41
2:F:555:HIS:CD2	2:F:555:HIS:H	2.37	0.41
1:D:319:ILE:HB	1:D:412:ILE:HB	2.02	0.41
1:A:73:GLY:O	1:A:77:SER:HB2	2.19	0.41
1:B:121:ASN:O	1:B:122:THR:HG22	2.20	0.41
1:B:223:GLY:O	1:B:224:LEU:HB2	2.19	0.41
1:D:78:VAL:O	1:D:82:LEU:CB	2.69	0.41
2:G:517:ILE:CG1	2:G:602:CYS:SG	3.08	0.41
1:A:399:GLY:O	1:A:400:SER:C	2.59	0.41
1:B:139:LEU:HA	1:B:139:LEU:HD23	1.76	0.41
1:D:8:ALA:C	1:D:10:ARG:N	2.73	0.41
1:B:102:THR:HG23	1:B:103:GLU:N	2.36	0.41
2:F:544:ILE:HG12	2:F:548:TYR:CG	2.55	0.41
2:G:447:LYS:HD3	2:G:512:ILE:O	2.21	0.41
1:A:176:LEU:O	1:A:177:PRO:C	2.58	0.41
1:A:24:LEU:HD23	1:A:24:LEU:HA	1.75	0.41
1:A:191:ALA:O	1:A:195:MET:N	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:264:PHE:O	1:B:268:ILE:HG13	2.21	0.41
1:D:38:ILE:CD1	1:D:135:ALA:CB	2.99	0.41
1:B:115:GLU:CG	1:B:116:PRO:N	2.83	0.41
1:C:214:ILE:HA	1:C:219:VAL:HA	2.01	0.41
2:E:555:HIS:CD2	2:E:555:HIS:H	2.36	0.41
1:D:382:TYR:CD1	1:D:389:LEU:HB2	2.55	0.41
1:B:294:ILE:HG12	1:B:301:TYR:CD1	2.55	0.41
1:C:94:VAL:O	1:C:113:ASP:HA	2.19	0.41
1:C:309:LEU:O	1:C:313:GLU:HG2	2.21	0.41
1:A:167:GLU:HG3	1:B:66:VAL:HG21	2.02	0.41
2:G:471:VAL:HG13	2:G:477:HIS:H	1.84	0.41
1:B:73:GLY:O	1:B:77:SER:HB2	2.20	0.41
1:D:308:THR:O	1:D:312:LEU:N	2.44	0.41
1:B:178:LYS:H	1:B:178:LYS:HG3	1.65	0.41
2:F:467:GLY:HA2	2:F:481:VAL:O	2.21	0.41
2:H:486:SER:CA	2:H:500:LEU:HD12	2.46	0.41
2:H:568:CYS:O	2:H:592:ILE:HG12	2.21	0.41
2:H:470:LEU:HG	2:H:519:CYS:O	2.21	0.41
1:D:236:LEU:O	1:D:242:PHE:HD2	2.04	0.41
1:B:266:GLN:O	1:B:270:LEU:HD23	2.20	0.41
1:D:213:PHE:CD2	1:D:221:VAL:HG11	2.56	0.41
1:B:82:LEU:HD12	1:B:82:LEU:HA	1.95	0.41
1:A:374:LEU:HA	1:A:374:LEU:HD23	1.87	0.41
2:G:474:PRO:HD2	2:G:516:PHE:CE1	2.56	0.41
1:B:245:ARG:CD	1:B:245:ARG:H	2.18	0.41
2:H:567:ILE:HB	2:H:568:CYS:H	1.71	0.41
1:A:102:THR:HG23	1:A:103:GLU:N	2.36	0.41
1:D:409:ILE:HG23	1:D:409:ILE:O	2.21	0.41
2:H:595:LEU:HD12	2:H:595:LEU:N	2.35	0.41
1:D:303:PHE:HE1	2:H:583:ARG:HE	1.63	0.41
1:A:401:GLN:HB3	2:F:545:CYS:SG	2.61	0.41
2:G:444:ILE:HD12	2:G:516:PHE:HB2	2.03	0.41
2:H:447:LYS:CG	2:H:512:ILE:HG23	2.49	0.41
2:E:473:MET:CG	2:E:474:PRO:HD3	2.50	0.41
2:E:517:ILE:HG12	2:E:602:CYS:SG	2.61	0.41
1:B:243:ASP:O	1:B:244:GLN:HB2	2.20	0.41
1:A:224:LEU:O	1:A:250:VAL:HA	2.20	0.41
1:B:176:LEU:O	1:B:177:PRO:C	2.59	0.41
2:F:464:ILE:HD12	2:F:470:LEU:HD21	2.03	0.41
1:B:233:LYS:O	1:B:237:SER:HB2	2.21	0.41
1:A:233:LYS:O	1:A:237:SER:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:561:VAL:HG11	2:G:617:LEU:HD11	2.03	0.41
1:D:329:MET:O	1:D:345:TYR:HA	2.20	0.41
1:A:266:GLN:O	1:A:270:LEU:HD23	2.20	0.41
1:C:329:MET:O	1:C:345:TYR:HA	2.21	0.41
1:C:38:ILE:CD1	1:C:135:ALA:CB	2.98	0.41
1:A:377:TRP:CZ3	1:A:385:PHE:HE2	2.39	0.41
2:G:570:VAL:HG12	2:G:591:CYS:HA	2.03	0.41
2:G:543:ILE:HG22	2:G:544:ILE:CA	2.51	0.41
1:C:416:ARG:HE	1:C:417:VAL:C	2.24	0.41
2:F:444:ILE:HD12	2:F:516:PHE:HB2	2.03	0.41
2:G:606:PHE:O	2:G:608:ASP:N	2.54	0.41
1:A:61:ASN:C	1:A:63:LYS:H	2.24	0.41
1:C:204:LYS:HA	1:C:207:GLU:HB3	2.03	0.41
1:B:206:ALA:CB	1:B:242:PHE:HB2	2.50	0.41
2:G:563:ILE:H	2:G:563:ILE:HG13	1.59	0.40
2:H:540:HIS:HB2	2:H:587:GLN:HG3	2.03	0.40
2:E:544:ILE:HG21	2:E:563:ILE:HD11	2.04	0.40
1:B:88:VAL:HA	1:B:89:PRO:HD2	1.75	0.40
2:E:470:LEU:HD13	2:E:518:LEU:HD13	2.03	0.40
1:C:78:VAL:O	1:C:82:LEU:CB	2.68	0.40
1:D:150:VAL:O	1:D:156:ALA:HA	2.21	0.40
1:C:396:SER:O	1:C:399:GLY:N	2.54	0.40
1:C:71:VAL:C	1:C:73:GLY:H	2.24	0.40
2:H:570:VAL:HG12	2:H:591:CYS:HA	2.03	0.40
1:C:401:GLN:OE1	2:G:548:TYR:HB2	2.21	0.40
2:H:548:TYR:OH	2:H:624:ILE:HG21	2.21	0.40
1:A:110:VAL:HG23	1:A:112:ILE:HD11	2.03	0.40
1:A:294:ILE:HG12	1:A:301:TYR:CD1	2.56	0.40
2:H:471:VAL:HG13	2:H:477:HIS:H	1.85	0.40
2:H:543:ILE:O	2:H:544:ILE:HG13	2.22	0.40
1:D:396:SER:O	1:D:399:GLY:N	2.53	0.40
1:B:152:ASP:HB3	1:B:155:GLY:O	2.22	0.40
1:A:377:TRP:CH2	1:A:385:PHE:HE2	2.40	0.40
1:B:89:PRO:HA	1:B:90:PRO:HD2	1.87	0.40
2:F:520:ASP:OD1	2:F:521:PRO:HD2	2.21	0.40
2:F:500:LEU:C	2:F:501:LYS:HG3	2.42	0.40
1:D:279:LYS:O	1:D:283:GLU:HB2	2.22	0.40
1:A:22:LYS:O	1:A:24:LEU:N	2.54	0.40
1:D:166:ARG:O	1:D:167:GLU:HG3	2.21	0.40
2:E:577:LYS:HB3	2:E:577:LYS:HE2	1.87	0.40
2:H:563:ILE:H	2:H:563:ILE:HG13	1.59	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:473:MET:CE	2:F:525:CYS:HB2	2.51	0.40
2:H:444:ILE:HD12	2:H:516:PHE:HB2	2.04	0.40
2:E:470:LEU:N	2:E:479:VAL:O	2.54	0.40
1:A:279:LYS:H	1:A:279:LYS:CD	2.18	0.40
2:G:533:ALA:HB1	2:G:629:VAL:HA	2.03	0.40
1:A:305:VAL:O	1:A:306:GLU:C	2.59	0.40
1:D:307:ASP:O	1:D:311:ALA:N	2.52	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	374/451 (83%)	289 (77%)	55 (15%)	30 (8%)	1	19
1	B	374/451 (83%)	290 (78%)	51 (14%)	33 (9%)	1	16
1	C	298/451 (66%)	230 (77%)	51 (17%)	17 (6%)	2	28
1	D	298/451 (66%)	229 (77%)	52 (17%)	17 (6%)	2	28
2	E	193/204 (95%)	143 (74%)	34 (18%)	16 (8%)	1	18
2	F	193/204 (95%)	146 (76%)	30 (16%)	17 (9%)	1	16
2	G	193/204 (95%)	148 (77%)	31 (16%)	14 (7%)	1	22
2	H	193/204 (95%)	148 (77%)	31 (16%)	14 (7%)	1	22
All	All	2116/2620 (81%)	1623 (77%)	335 (16%)	158 (8%)	1	20

All (158) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	65	ARG
1	A	108	LYS
1	A	115	GLU

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Mol	Chain	Res	Type
1	A	116	PRO
1	A	118	LYS
1	A	120	ILE
1	A	122	THR
1	A	142	ASP
1	A	177	PRO
1	A	222	ALA
1	A	276	SER
1	A	347	THR
1	A	381	ASN
1	B	65	ARG
1	B	108	LYS
1	B	115	GLU
1	B	116	PRO
1	B	118	LYS
1	B	120	ILE
1	B	122	THR
1	B	142	ASP
1	B	177	PRO
1	B	222	ALA
1	B	276	SER
1	B	347	THR
1	B	381	ASN
1	B	416	ARG
1	C	116	PRO
1	C	409	ILE
1	D	116	PRO
1	D	409	ILE
2	E	489	VAL
2	E	510	GLU
2	E	538	ILE
2	E	540	HIS
2	E	567	ILE
2	F	489	VAL
2	F	510	GLU
2	F	538	ILE
2	F	540	HIS
2	F	567	ILE
2	G	489	VAL
2	G	540	HIS
2	H	489	VAL
2	H	540	HIS

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Mol	Chain	Res	Type
1	A	90	PRO
1	A	117	PHE
1	A	119	PRO
1	A	163	GLY
1	B	117	PHE
1	B	119	PRO
1	B	163	GLY
1	C	222	ALA
1	C	273	GLU
1	C	306	GLU
1	C	318	GLU
1	D	222	ALA
1	D	273	GLU
1	D	306	GLU
1	D	318	GLU
2	E	523	ASN
2	E	564	THR
2	F	523	ASN
2	F	539	GLU
2	F	564	THR
2	G	487	ASP
2	G	518	LEU
2	G	523	ASN
2	G	556	THR
2	G	559	GLU
2	H	487	ASP
2	H	518	LEU
2	H	523	ASN
2	H	556	THR
2	H	559	GLU
1	A	184	GLY
1	A	258	TYR
1	A	272	THR
1	A	388	THR
1	B	90	PRO
1	B	184	GLY
1	B	258	TYR
1	B	272	THR
1	B	388	THR
1	C	154	SER
1	C	229	SER
1	C	272	THR

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Mol	Chain	Res	Type
1	C	381	ASN
1	D	154	SER
1	D	229	SER
1	D	272	THR
1	D	327	ASP
1	D	381	ASN
1	D	416	ARG
2	E	469	GLN
2	E	487	ASP
2	E	555	HIS
2	E	557	CYS
2	F	469	GLN
2	F	487	ASP
2	F	555	HIS
2	G	475	ASN
1	A	69	LEU
1	A	183	GLY
1	A	229	SER
1	A	240	ASP
1	B	23	SER
1	B	69	LEU
1	B	183	GLY
1	B	240	ASP
1	C	327	ASP
1	C	388	THR
1	D	388	THR
2	E	518	LEU
2	E	598	ALA
2	F	557	CYS
2	G	521	PRO
2	G	538	ILE
2	G	574	SER
2	H	475	ASN
2	H	521	PRO
2	H	538	ILE
2	H	574	SER
1	A	23	SER
1	A	190	PHE
1	A	224	LEU
1	B	190	PHE
1	B	224	LEU
1	B	229	SER

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Mol	Chain	Res	Type
1	C	221	VAL
1	D	221	VAL
1	D	398	GLU
2	E	521	PRO
2	F	518	LEU
2	F	521	PRO
2	F	598	ALA
2	G	470	LEU
2	G	537	ILE
2	G	567	ILE
2	H	470	LEU
2	H	567	ILE
1	A	221	VAL
1	B	68	ARG
1	B	221	VAL
1	C	299	GLY
1	C	398	GLU
1	D	299	GLY
2	H	537	ILE
2	E	554	ILE
2	F	554	ILE
1	C	347	THR
1	D	347	THR
2	E	558	ILE
2	F	558	ILE
1	B	31	GLY
1	B	348	PRO
1	A	348	PRO
1	C	73	GLY

### 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	325/387 (84%)	268 (82%)	57 (18%)	2	17
1	B	325/387 (84%)	267 (82%)	58 (18%)	2	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	275/387 (71%)	239 (87%)	36 (13%)	5	31
1	D	275/387 (71%)	238 (86%)	37 (14%)	5	30
2	E	173/180 (96%)	142 (82%)	31 (18%)	2	16
2	F	173/180 (96%)	141 (82%)	32 (18%)	2	15
2	G	173/180 (96%)	140 (81%)	33 (19%)	2	13
2	H	173/180 (96%)	140 (81%)	33 (19%)	2	13
All	All	1892/2268 (83%)	1575 (83%)	317 (17%)	2	19

All (317) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ARG
1	A	22	LYS
1	A	25	GLU
1	A	28	ARG
1	A	35	ILE
1	A	60	SER
1	A	62	ILE
1	A	63	LYS
1	A	65	ARG
1	A	70	SER
1	A	84	LEU
1	A	86	ASN
1	A	93	LEU
1	A	95	VAL
1	A	101	VAL
1	A	118	LYS
1	A	120	ILE
1	A	122	THR
1	A	124	LEU
1	A	126	LEU
1	A	127	CYS
1	A	139	LEU
1	A	141	SER
1	A	145	LYS
1	A	164	ASN
1	A	166	ARG
1	A	168	VAL
1	A	175	ASP
1	A	178	LYS

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Mol	Chain	Res	Type
1	A	185	GLN
1	A	189	ARG
1	A	192	ARG
1	A	211	GLN
1	A	218	LYS
1	A	231	ASP
1	A	239	SER
1	A	240	ASP
1	A	241	MET
1	A	244	GLN
1	A	245	ARG
1	A	251	LEU
1	A	276	SER
1	A	279	LYS
1	A	291	PHE
1	A	300	LYS
1	A	303	PHE
1	A	306	GLU
1	A	317	VAL
1	A	323	TYR
1	A	326	LEU
1	A	327	ASP
1	A	328	ILE
1	A	346	LEU
1	A	374	LEU
1	A	385	PHE
1	A	389	LEU
1	A	395	LYS
1	B	10	ARG
1	B	22	LYS
1	B	25	GLU
1	B	28	ARG
1	B	35	ILE
1	B	60	SER
1	B	62	ILE
1	B	63	LYS
1	B	65	ARG
1	B	70	SER
1	B	84	LEU
1	B	86	ASN
1	B	93	LEU
1	B	95	VAL

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Mol	Chain	Res	Type
1	B	101	VAL
1	B	118	LYS
1	B	120	ILE
1	B	122	THR
1	B	124	LEU
1	B	126	LEU
1	B	127	CYS
1	B	139	LEU
1	B	141	SER
1	B	145	LYS
1	B	164	ASN
1	B	165	THR
1	B	166	ARG
1	B	168	VAL
1	B	175	ASP
1	B	178	LYS
1	B	185	GLN
1	B	189	ARG
1	B	192	ARG
1	B	211	GLN
1	B	218	LYS
1	B	231	ASP
1	B	239	SER
1	B	240	ASP
1	B	241	MET
1	B	244	GLN
1	B	251	LEU
1	B	276	SER
1	B	279	LYS
1	B	291	PHE
1	B	300	LYS
1	B	303	PHE
1	B	306	GLU
1	B	317	VAL
1	B	323	TYR
1	B	326	LEU
1	B	327	ASP
1	B	328	ILE
1	B	346	LEU
1	B	374	LEU
1	B	385	PHE
1	B	389	LEU

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Mol	Chain	Res	Type
1	B	395	LYS
1	B	420	GLN
1	C	10	ARG
1	C	39	ILE
1	C	67	ASN
1	C	117	PHE
1	C	118	LYS
1	C	121	ASN
1	C	144	SER
1	C	150	VAL
1	C	161	LEU
1	C	166	ARG
1	C	198	ARG
1	C	199	HIS
1	C	211	GLN
1	C	218	LYS
1	C	221	VAL
1	C	231	ASP
1	C	232	PHE
1	C	233	LYS
1	C	237	SER
1	C	239	SER
1	C	251	LEU
1	C	272	THR
1	C	275	LEU
1	C	280	PHE
1	C	300	LYS
1	C	301	TYR
1	C	305	VAL
1	C	374	LEU
1	C	383	LYS
1	C	391	ILE
1	C	397	GLN
1	C	398	GLU
1	C	413	LEU
1	C	414	ARG
1	C	415	TYR
1	C	416	ARG
1	D	10	ARG
1	D	39	ILE
1	D	67	ASN
1	D	117	PHE

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Mol	Chain	Res	Type
1	D	118	LYS
1	D	121	ASN
1	D	144	SER
1	D	150	VAL
1	D	161	LEU
1	D	166	ARG
1	D	173	THR
1	D	198	ARG
1	D	199	HIS
1	D	211	GLN
1	D	218	LYS
1	D	221	VAL
1	D	231	ASP
1	D	232	PHE
1	D	233	LYS
1	D	237	SER
1	D	239	SER
1	D	245	ARG
1	D	251	LEU
1	D	272	THR
1	D	275	LEU
1	D	280	PHE
1	D	300	LYS
1	D	301	TYR
1	D	305	VAL
1	D	374	LEU
1	D	383	LYS
1	D	391	ILE
1	D	397	GLN
1	D	398	GLU
1	D	413	LEU
1	D	415	TYR
1	D	416	ARG
2	E	440	ILE
2	E	441	ARG
2	E	446	ASP
2	E	448	TYR
2	E	449	LYS
2	E	459	LEU
2	E	470	LEU
2	E	476	LYS
2	E	490	GLU

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Mol	Chain	Res	Type
2	E	500	LEU
2	E	502	ILE
2	E	505	LYS
2	E	508	GLU
2	E	520	ASP
2	E	529	ARG
2	E	540	HIS
2	E	566	LEU
2	E	570	VAL
2	E	572	LYS
2	E	574	SER
2	E	579	LYS
2	E	586	LYS
2	E	592	ILE
2	E	597	THR
2	E	602	CYS
2	E	603	LEU
2	E	608	ASP
2	E	616	THR
2	E	617	LEU
2	E	622	LYS
2	E	633	VAL
2	F	440	ILE
2	F	441	ARG
2	F	446	ASP
2	F	448	TYR
2	F	449	LYS
2	F	459	LEU
2	F	470	LEU
2	F	475	ASN
2	F	476	LYS
2	F	490	GLU
2	F	500	LEU
2	F	502	ILE
2	F	505	LYS
2	F	508	GLU
2	F	520	ASP
2	F	524	LEU
2	F	529	ARG
2	F	540	HIS
2	F	566	LEU
2	F	570	VAL

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Mol	Chain	Res	Type
2	F	572	LYS
2	F	574	SER
2	F	579	LYS
2	F	586	LYS
2	F	592	ILE
2	F	597	THR
2	F	603	LEU
2	F	608	ASP
2	F	616	THR
2	F	617	LEU
2	F	622	LYS
2	F	633	VAL
2	G	440	ILE
2	G	448	TYR
2	G	449	LYS
2	G	459	LEU
2	G	470	LEU
2	G	476	LYS
2	G	487	ASP
2	G	490	GLU
2	G	492	ASP
2	G	494	VAL
2	G	500	LEU
2	G	503	ARG
2	G	510	GLU
2	G	512	ILE
2	G	520	ASP
2	G	529	ARG
2	G	540	HIS
2	G	552	LEU
2	G	558	ILE
2	G	563	ILE
2	G	566	LEU
2	G	570	VAL
2	G	572	LYS
2	G	574	SER
2	G	579	LYS
2	G	592	ILE
2	G	614	ARG
2	G	616	THR
2	G	617	LEU
2	G	620	GLU

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Mol	Chain	Res	Type
2	G	622	LYS
2	G	632	LEU
2	G	633	VAL
2	H	440	ILE
2	H	448	TYR
2	H	449	LYS
2	H	459	LEU
2	H	470	LEU
2	H	476	LYS
2	H	487	ASP
2	H	490	GLU
2	H	492	ASP
2	H	494	VAL
2	H	500	LEU
2	H	503	ARG
2	H	510	GLU
2	H	512	ILE
2	H	520	ASP
2	H	529	ARG
2	H	540	HIS
2	H	552	LEU
2	H	558	ILE
2	H	563	ILE
2	H	566	LEU
2	H	570	VAL
2	H	572	LYS
2	H	574	SER
2	H	579	LYS
2	H	592	ILE
2	H	614	ARG
2	H	616	THR
2	H	617	LEU
2	H	620	GLU
2	H	622	LYS
2	H	632	LEU
2	H	633	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	111	ASN
1	A	164	ASN

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Mol	Chain	Res	Type
1	A	244	GLN
1	A	266	GLN
1	A	397	GLN
1	B	111	ASN
1	B	164	ASN
1	B	244	GLN
1	B	266	GLN
1	B	397	GLN
1	B	420	GLN
1	C	67	ASN
1	C	121	ASN
1	C	162	GLN
1	C	244	GLN
1	C	266	GLN
1	C	350	GLN
1	D	67	ASN
1	D	121	ASN
1	D	162	GLN
1	D	244	GLN
1	D	266	GLN
1	D	350	GLN
2	E	477	HIS
2	E	587	GLN
2	F	477	HIS
2	F	587	GLN
2	G	477	HIS
2	G	499	ASN
2	G	549	ASN
2	H	499	ASN
2	H	534	GLN
2	H	549	ASN
2	H	553	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	ATP	A	1526	-	24,33,33	1.04	1 (4%)	31,52,52	1.90	5 (16%)
3	ATP	B	1526	-	24,33,33	1.06	2 (8%)	31,52,52	1.75	4 (12%)

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	ATP	A	1526	-	-	0/18/38/38	0/3/3/3
3	ATP	B	1526	-	-	0/18/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1526	ATP	O4'-C1'	2.40	1.44	1.41
3	B	1526	ATP	C5-C4	3.36	1.48	1.40
3	A	1526	ATP	C5-C4	3.42	1.48	1.40

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1526	ATP	N3-C2-N1	-6.41	123.99	128.89
3	A	1526	ATP	N3-C2-N1	-6.34	124.04	128.89
3	A	1526	ATP	PA-O3A-PB	-4.32	120.61	132.73
3	B	1526	ATP	PA-O3A-PB	-3.36	123.30	132.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1526	ATP	PB-O3B-PG	-3.20	121.94	132.67
3	B	1526	ATP	PB-O3B-PG	-2.96	122.74	132.67
3	A	1526	ATP	C4-C5-N7	-2.93	106.79	109.48
3	B	1526	ATP	C4-C5-N7	-2.48	107.20	109.48
3	A	1526	ATP	O4'-C1'-N9	2.25	112.81	108.10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1526	ATP	3	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	380/451 (84%)	0.60	22 (5%) 26 16	71, 89, 96, 100	0
1	B	380/451 (84%)	0.64	22 (5%) 26 16	71, 89, 96, 100	0
1	C	318/451 (70%)	0.50	22 (6%) 20 12	73, 90, 93, 100	0
1	D	318/451 (70%)	0.49	22 (6%) 20 12	73, 90, 93, 100	0
2	E	195/204 (95%)	0.82	20 (10%) 9 6	56, 87, 93, 97	0
2	F	195/204 (95%)	0.83	25 (12%) 5 4	56, 87, 93, 97	0
2	G	195/204 (95%)	0.85	29 (14%) 3 2	55, 87, 92, 96	0
2	H	195/204 (95%)	0.80	27 (13%) 4 3	55, 87, 92, 96	0
All	All	2176/2620 (83%)	0.66	189 (8%) 13 8	55, 89, 95, 100	0

All (189) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	183	GLY	6.3
1	A	181	GLY	5.9
2	F	570	VAL	5.6
2	G	502	ILE	5.4
1	B	184	GLY	5.4
1	A	183	GLY	5.3
1	B	414	ARG	4.8
2	E	519	CYS	4.7
1	B	176	LEU	4.6
1	B	415	TYR	4.6
2	F	518	LEU	4.5
2	F	507	ILE	4.4
2	G	501	LYS	4.3
2	F	519	CYS	4.2
1	D	297	ASP	4.1
2	G	448	TYR	4.1

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Mol	Chain	Res	Type	RSRZ
2	H	545	CYS	3.9
1	C	297	ASP	3.8
2	G	484	ILE	3.8
2	G	603	LEU	3.7
2	H	484	ILE	3.6
2	F	473	MET	3.6
2	E	518	LEU	3.6
2	F	602	CYS	3.5
2	E	566	LEU	3.5
1	C	157	LEU	3.5
1	B	315	GLY	3.4
2	G	492	ASP	3.4
1	D	58	THR	3.4
2	G	449	LYS	3.3
1	D	224	LEU	3.3
2	H	441	ARG	3.3
2	H	517	ILE	3.3
1	A	182	ARG	3.3
1	D	258	TYR	3.2
2	F	595	LEU	3.2
1	D	346	LEU	3.1
1	D	321	ILE	3.1
1	C	125	TYR	3.1
1	C	258	TYR	3.1
2	F	472	MET	3.1
1	A	414	ARG	3.1
2	H	602	CYS	3.0
1	A	184	GLY	3.0
2	E	443	PRO	3.0
1	D	200	ASN	3.0
2	F	566	LEU	3.0
2	H	548	TYR	3.0
2	G	622	LYS	2.9
2	H	596	ARG	2.9
2	F	601	ILE	2.9
1	D	396	SER	2.9
2	E	507	ILE	2.9
2	H	603	LEU	2.9
2	H	544	ILE	2.8
1	C	389	LEU	2.8
1	C	118	LYS	2.8
2	H	453	THR	2.8

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Mol	Chain	Res	Type	RSRZ
2	E	473	MET	2.8
2	H	518	LEU	2.8
2	E	595	LEU	2.8
2	G	504	LEU	2.8
2	E	517	ILE	2.8
2	H	622	LYS	2.8
1	A	151	ILE	2.7
2	E	601	ILE	2.7
2	F	521	PRO	2.7
2	H	492	ASP	2.7
2	G	518	LEU	2.7
2	F	517	ILE	2.7
1	C	302	CYS	2.7
1	B	314	MET	2.7
1	D	302	CYS	2.7
1	B	151	ILE	2.6
1	A	198	ARG	2.6
2	E	521	PRO	2.6
1	A	120	ILE	2.6
1	A	180	HIS	2.6
1	D	157	LEU	2.6
2	E	603	LEU	2.6
1	A	291	PHE	2.6
1	D	385	PHE	2.6
2	E	602	CYS	2.6
2	G	539	GLU	2.6
1	D	389	LEU	2.6
1	D	131	PHE	2.6
1	A	415	TYR	2.5
1	C	321	ILE	2.5
2	G	527	SER	2.5
1	C	150	VAL	2.5
1	B	406	PHE	2.5
2	G	580	THR	2.5
1	C	238	GLN	2.5
2	F	593	ALA	2.5
2	H	585	VAL	2.5
2	H	546	PRO	2.5
1	B	291	PHE	2.5
2	E	570	VAL	2.5
1	C	290	TYR	2.4
1	C	235	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
2	F	612	MET	2.4
1	C	257	SER	2.4
1	C	375	LEU	2.4
2	F	603	LEU	2.4
2	H	483	GLY	2.4
1	A	176	LEU	2.4
2	G	454	VAL	2.4
2	G	617	LEU	2.4
1	A	406	PHE	2.4
1	B	316	ALA	2.4
1	C	411	GLY	2.4
2	H	513	LEU	2.3
2	H	449	LYS	2.3
1	D	158	PHE	2.3
1	B	263	GLY	2.3
2	G	485	LEU	2.3
1	D	401	GLN	2.3
2	H	549	ASN	2.3
1	B	35	ILE	2.3
1	C	205	VAL	2.3
2	H	444	ILE	2.3
1	B	214	ILE	2.3
1	A	60	SER	2.3
2	E	441	ARG	2.3
1	B	120	ILE	2.3
2	G	602	CYS	2.3
2	E	560	GLU	2.3
2	G	450	ASP	2.3
1	C	158	PHE	2.3
1	D	148	PHE	2.3
1	D	257	SER	2.3
2	F	442	LEU	2.3
2	G	513	LEU	2.3
2	G	507	ILE	2.2
2	F	528	GLY	2.2
2	G	453	THR	2.2
1	C	301	TYR	2.2
2	G	455	VAL	2.2
1	A	255	ASP	2.2
1	B	182	ARG	2.2
1	B	344	LEU	2.2
1	B	298	THR	2.2

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Mol	Chain	Res	Type	RSRZ
2	F	471	VAL	2.2
1	A	344	LEU	2.2
1	B	59	ALA	2.2
2	H	504	LEU	2.2
2	H	609	PHE	2.2
2	H	563	ILE	2.2
1	C	71	VAL	2.1
2	F	460	GLU	2.1
2	H	448	TYR	2.1
1	A	218	LYS	2.1
2	G	609	PHE	2.1
1	B	208	THR	2.1
1	D	235	GLU	2.1
2	H	512	ILE	2.1
2	G	537	ILE	2.1
1	C	242	PHE	2.1
2	F	443	PRO	2.1
2	E	497	GLY	2.1
2	E	476	LYS	2.1
1	A	413	LEU	2.1
2	E	552	LEU	2.1
2	F	569	LEU	2.1
2	H	507	ILE	2.1
2	H	601	ILE	2.1
1	B	321	ILE	2.1
2	G	517	ILE	2.1
2	F	459	LEU	2.1
2	F	481	VAL	2.1
2	E	546	PRO	2.1
1	A	214	ILE	2.1
1	C	282	GLN	2.1
1	D	290	TYR	2.1
1	C	58	THR	2.1
1	D	246	LEU	2.1
2	F	617	LEU	2.1
2	F	476	LYS	2.1
2	E	484	ILE	2.1
2	G	574	SER	2.1
1	D	312	LEU	2.0
1	D	301	TYR	2.0
1	A	33	SER	2.0
1	B	139	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	253	LEU	2.0
2	G	563	ILE	2.0
2	G	626	ILE	2.0
2	G	535	ILE	2.0
1	A	240	ASP	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(Å <sup>2</sup> )	Q<0.9
3	ATP	A	1526	31/31	0.78	0.36	0.01	171,173,180,180	0
3	ATP	B	1526	31/31	0.75	0.34	0.00	169,171,179,179	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.