Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:07 AM GMT

PDB ID	:	3DBL
Title	:	Structural Dissection of a Gating Mechanism Preventing Misactivation of Ubiquitin by NEDD8's E1 (APPBP1-UBA3Arg190wt-NEDD8Ala72Gln)
Authors	:	Souphron, J.; Schulman, B.A.
Deposited on	:	2008-06-01
Resolution	:	2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

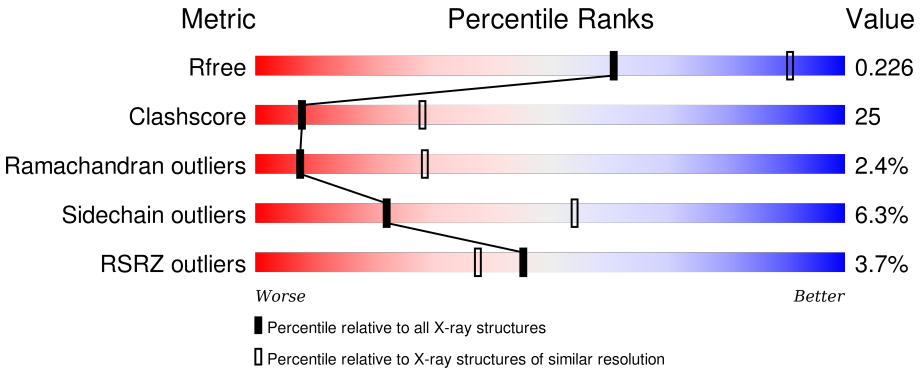
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	531	2% 60% 35%
1	C	531	1% 60% 34%
1	E	531	2% 60% 34%
1	G	531	4% 59% 35%
2	B	434	5% 52% 41% 5%

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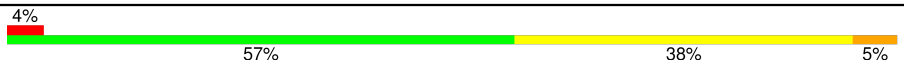
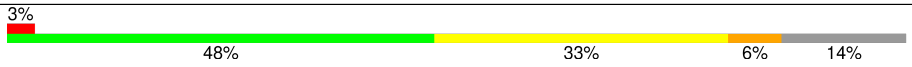
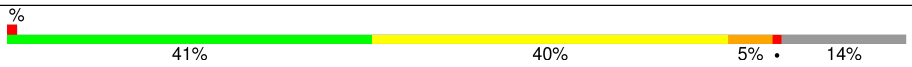
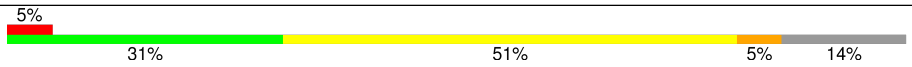
Mol	Chain	Length	Quality of chain
2	D	434	
2	F	434	
2	H	434	
3	I	88	
3	J	88	
3	K	88	
3	L	88	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 32577 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 NEDD8-activating enzyme E1 regulatory subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	522	Total	C	N	O	S	0	0	0
			4138	2621	704	797	16			
1	C	520	Total	C	N	O	S	0	0	0
			4125	2612	702	795	16			
1	E	521	Total	C	N	O	S	0	0	0
			4119	2609	703	792	15			
1	G	518	Total	C	N	O	S	0	0	0
			4113	2605	700	793	15			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	EXPRESSION TAG	UNP Q13564
A	0	SER	-	EXPRESSION TAG	UNP Q13564
A	?	-	ASN	DELETION	UNP Q13564
A	?	-	GLU	DELETION	UNP Q13564
A	?	-	ASN	DELETION	UNP Q13564
A	?	-	GLY	DELETION	UNP Q13564
A	?	-	ALA	DELETION	UNP Q13564
C	-1	GLY	-	EXPRESSION TAG	UNP Q13564
C	0	SER	-	EXPRESSION TAG	UNP Q13564
C	?	-	ASN	DELETION	UNP Q13564
C	?	-	GLU	DELETION	UNP Q13564
C	?	-	ASN	DELETION	UNP Q13564
C	?	-	GLY	DELETION	UNP Q13564
C	?	-	ALA	DELETION	UNP Q13564
E	-1	GLY	-	EXPRESSION TAG	UNP Q13564
E	0	SER	-	EXPRESSION TAG	UNP Q13564
E	?	-	ASN	DELETION	UNP Q13564
E	?	-	GLU	DELETION	UNP Q13564
E	?	-	ASN	DELETION	UNP Q13564
E	?	-	GLY	DELETION	UNP Q13564
E	?	-	ALA	DELETION	UNP Q13564

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-1	GLY	-	EXPRESSION TAG	UNP Q13564
G	0	SER	-	EXPRESSION TAG	UNP Q13564
G	?	-	ASN	DELETION	UNP Q13564
G	?	-	GLU	DELETION	UNP Q13564
G	?	-	ASN	DELETION	UNP Q13564
G	?	-	GLY	DELETION	UNP Q13564
G	?	-	ALA	DELETION	UNP Q13564

- Molecule 2 is a protein called NEDD8-activating enzyme E1 catalytic subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	432	Total	C	N	O	S	0	0	0
			3404	2175	577	635	17			
2	D	432	Total	C	N	O	S	0	0	0
			3408	2178	578	635	17			
2	F	431	Total	C	N	O	S	0	0	0
			3397	2172	576	632	17			
2	H	431	Total	C	N	O	S	0	0	0
			3389	2165	575	632	17			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	9	MET	-	EXPRESSION TAG	UNP Q8TBC4
B	10	LYS	-	EXPRESSION TAG	UNP Q8TBC4
B	11	LEU	-	EXPRESSION TAG	UNP Q8TBC4
B	216	ALA	CYS	ENGINEERED	UNP Q8TBC4
D	9	MET	-	EXPRESSION TAG	UNP Q8TBC4
D	10	LYS	-	EXPRESSION TAG	UNP Q8TBC4
D	11	LEU	-	EXPRESSION TAG	UNP Q8TBC4
D	216	ALA	CYS	ENGINEERED	UNP Q8TBC4
F	9	MET	-	EXPRESSION TAG	UNP Q8TBC4
F	10	LYS	-	EXPRESSION TAG	UNP Q8TBC4
F	11	LEU	-	EXPRESSION TAG	UNP Q8TBC4
F	216	ALA	CYS	ENGINEERED	UNP Q8TBC4
H	9	MET	-	EXPRESSION TAG	UNP Q8TBC4
H	10	LYS	-	EXPRESSION TAG	UNP Q8TBC4
H	11	LEU	-	EXPRESSION TAG	UNP Q8TBC4
H	216	ALA	CYS	ENGINEERED	UNP Q8TBC4

- Molecule 3 is a protein called NEDD8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	86	Total	C	N	O	S	0	0	0
			668	415	121	130	2			
3	J	76	Total	C	N	O	S	0	0	0
			604	380	105	117	2			
3	K	76	Total	C	N	O	S	0	0	0
			604	380	105	117	2			
3	L	76	Total	C	N	O	S	0	0	0
			604	380	105	117	2			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	89	GLY	-	EXPRESSION TAG	UNP Q15843
I	90	SER	-	EXPRESSION TAG	UNP Q15843
I	91	ARG	-	EXPRESSION TAG	UNP Q15843
I	92	ARG	-	EXPRESSION TAG	UNP Q15843
I	93	ALA	-	EXPRESSION TAG	UNP Q15843
I	94	SER	-	EXPRESSION TAG	UNP Q15843
I	95	VAL	-	EXPRESSION TAG	UNP Q15843
I	96	GLY	-	EXPRESSION TAG	UNP Q15843
I	97	SER	-	EXPRESSION TAG	UNP Q15843
I	98	GLY	-	EXPRESSION TAG	UNP Q15843
I	99	GLY	-	EXPRESSION TAG	UNP Q15843
I	100	SER	-	EXPRESSION TAG	UNP Q15843
I	172	GLN	ALA	ENGINEERED	UNP Q15843
J	89	GLY	-	EXPRESSION TAG	UNP Q15843
J	90	SER	-	EXPRESSION TAG	UNP Q15843
J	91	ARG	-	EXPRESSION TAG	UNP Q15843
J	92	ARG	-	EXPRESSION TAG	UNP Q15843
J	93	ALA	-	EXPRESSION TAG	UNP Q15843
J	94	SER	-	EXPRESSION TAG	UNP Q15843
J	95	VAL	-	EXPRESSION TAG	UNP Q15843
J	96	GLY	-	EXPRESSION TAG	UNP Q15843
J	97	SER	-	EXPRESSION TAG	UNP Q15843
J	98	GLY	-	EXPRESSION TAG	UNP Q15843
J	99	GLY	-	EXPRESSION TAG	UNP Q15843
J	100	SER	-	EXPRESSION TAG	UNP Q15843
J	172	GLN	ALA	ENGINEERED	UNP Q15843
K	89	GLY	-	EXPRESSION TAG	UNP Q15843
K	90	SER	-	EXPRESSION TAG	UNP Q15843
K	91	ARG	-	EXPRESSION TAG	UNP Q15843
K	92	ARG	-	EXPRESSION TAG	UNP Q15843
K	93	ALA	-	EXPRESSION TAG	UNP Q15843

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Chain	Residue	Modelled	Actual	Comment	Reference
K	94	SER	-	EXPRESSION TAG	UNP Q15843
K	95	VAL	-	EXPRESSION TAG	UNP Q15843
K	96	GLY	-	EXPRESSION TAG	UNP Q15843
K	97	SER	-	EXPRESSION TAG	UNP Q15843
K	98	GLY	-	EXPRESSION TAG	UNP Q15843
K	99	GLY	-	EXPRESSION TAG	UNP Q15843
K	100	SER	-	EXPRESSION TAG	UNP Q15843
K	172	GLN	ALA	ENGINEERED	UNP Q15843
L	89	GLY	-	EXPRESSION TAG	UNP Q15843
L	90	SER	-	EXPRESSION TAG	UNP Q15843
L	91	ARG	-	EXPRESSION TAG	UNP Q15843
L	92	ARG	-	EXPRESSION TAG	UNP Q15843
L	93	ALA	-	EXPRESSION TAG	UNP Q15843
L	94	SER	-	EXPRESSION TAG	UNP Q15843
L	95	VAL	-	EXPRESSION TAG	UNP Q15843
L	96	GLY	-	EXPRESSION TAG	UNP Q15843
L	97	SER	-	EXPRESSION TAG	UNP Q15843
L	98	GLY	-	EXPRESSION TAG	UNP Q15843
L	99	GLY	-	EXPRESSION TAG	UNP Q15843
L	100	SER	-	EXPRESSION TAG	UNP Q15843
L	172	GLN	ALA	ENGINEERED	UNP Q15843

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

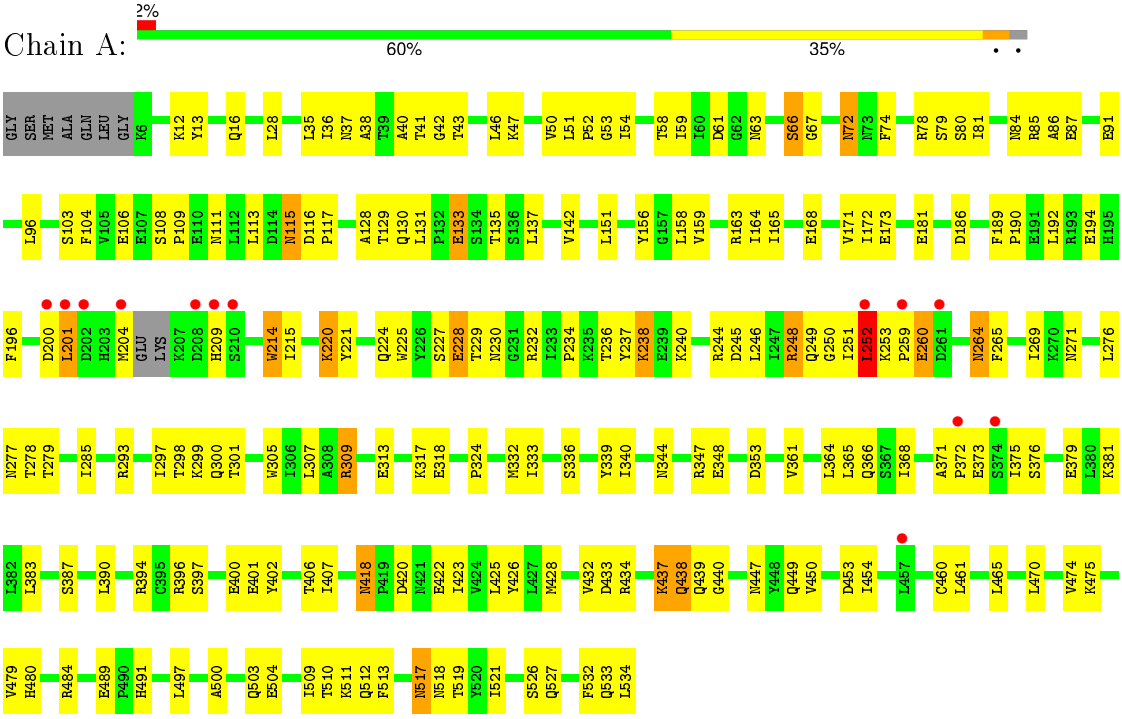
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	H	1	Total Zn 1 1	0	0
4	B	1	Total Zn 1 1	0	0
4	D	1	Total Zn 1 1	0	0
4	F	1	Total Zn 1 1	0	0

3 Residue-property plots (i)

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

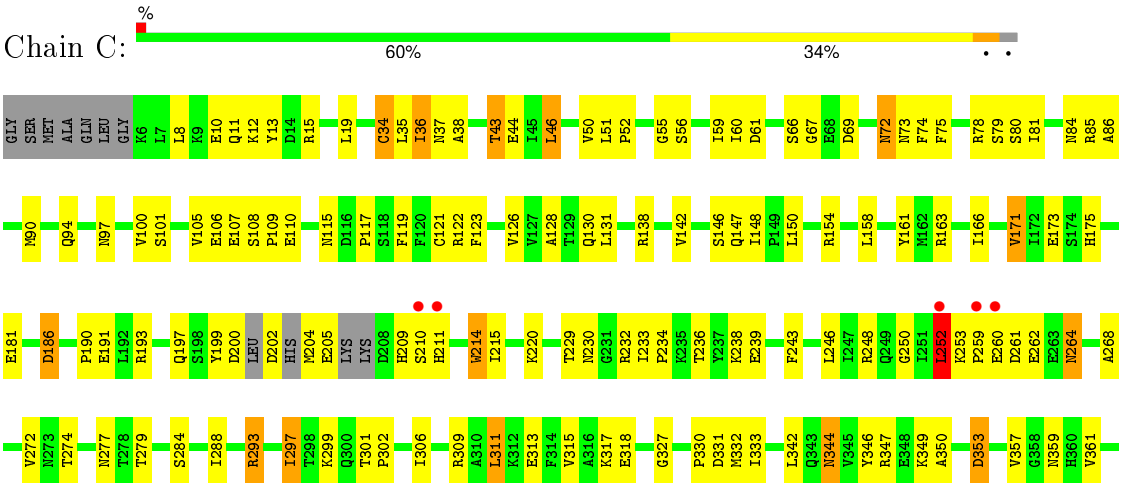
- Molecule 1: NEDD8-activating enzyme E1 regulatory subunit

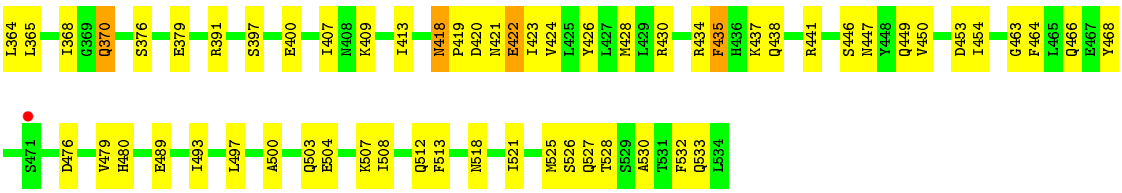
Chain A:



- Molecule 1: NEDD8-activating enzyme E1 regulatory subunit

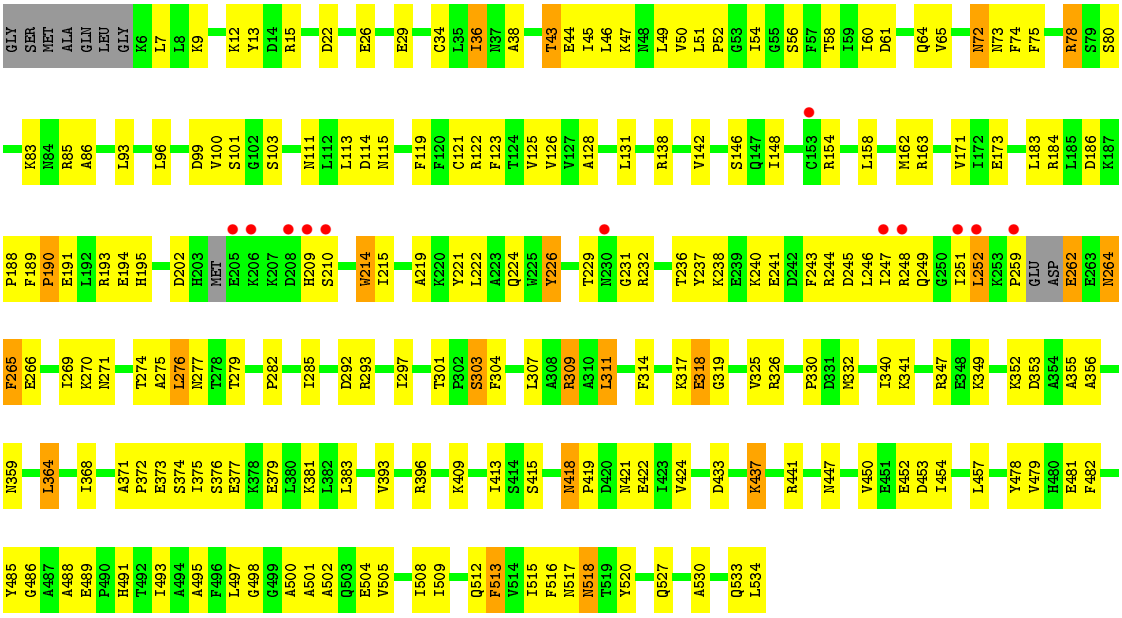
Chain C:





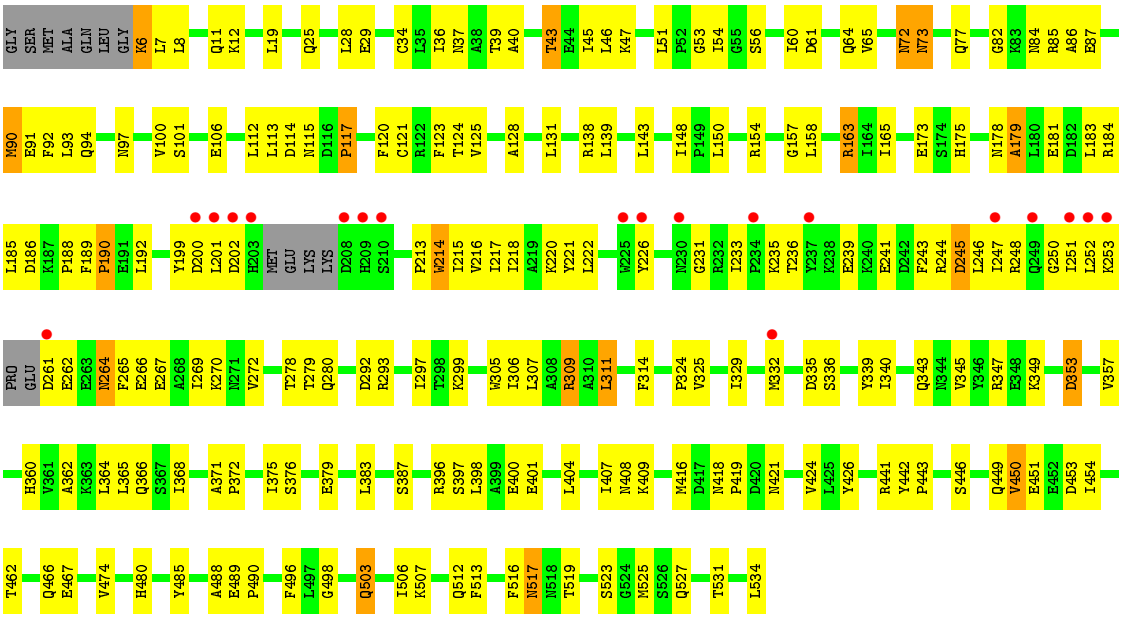
• Molecule 1: NEDD8-activating enzyme E1 regulatory subunit

Chain E:



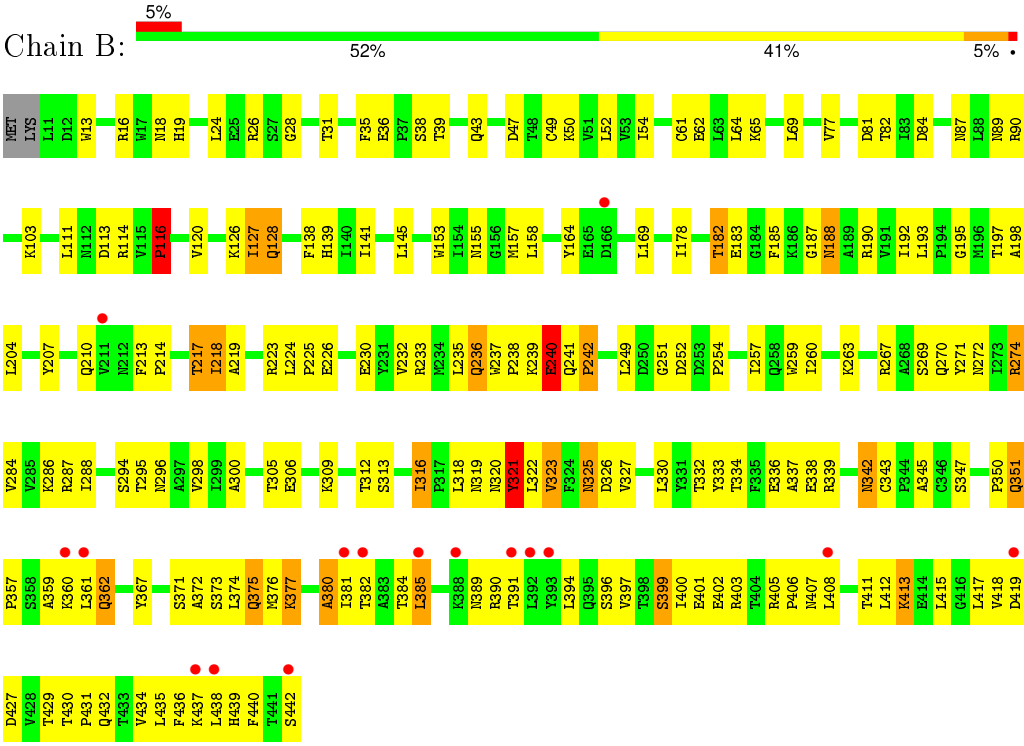
• Molecule 1: NEDD8-activating enzyme E1 regulatory subunit

Chain G:



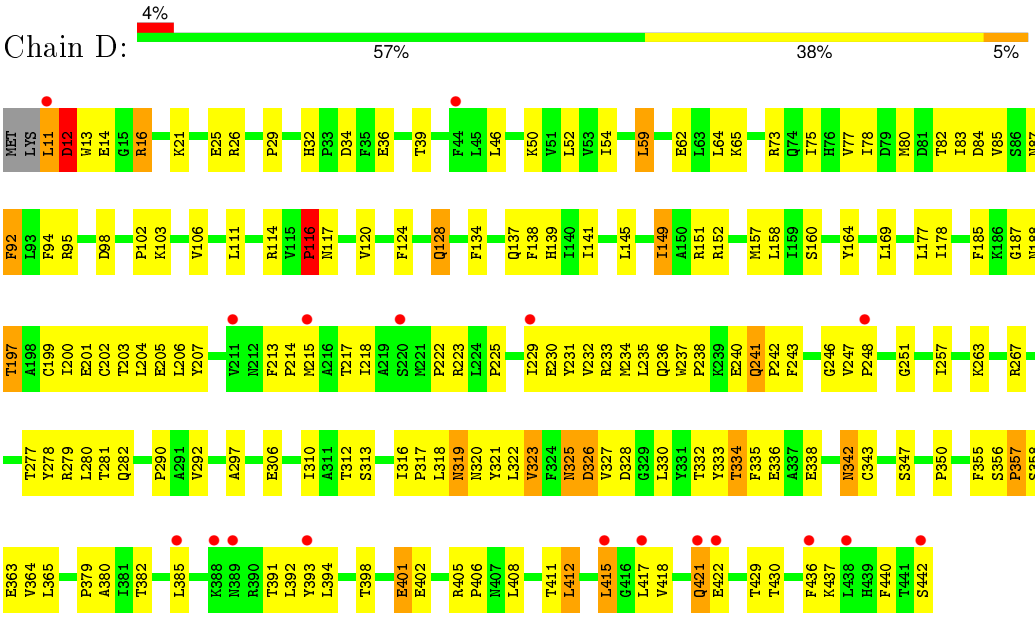
• Molecule 2: NEDD8-activating enzyme E1 catalytic subunit

Chain B:



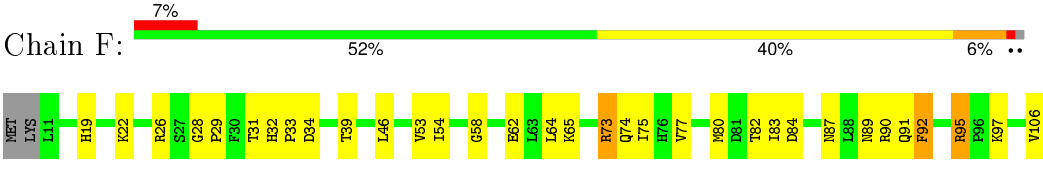
• Molecule 2: NEDD8-activating enzyme E1 catalytic subunit

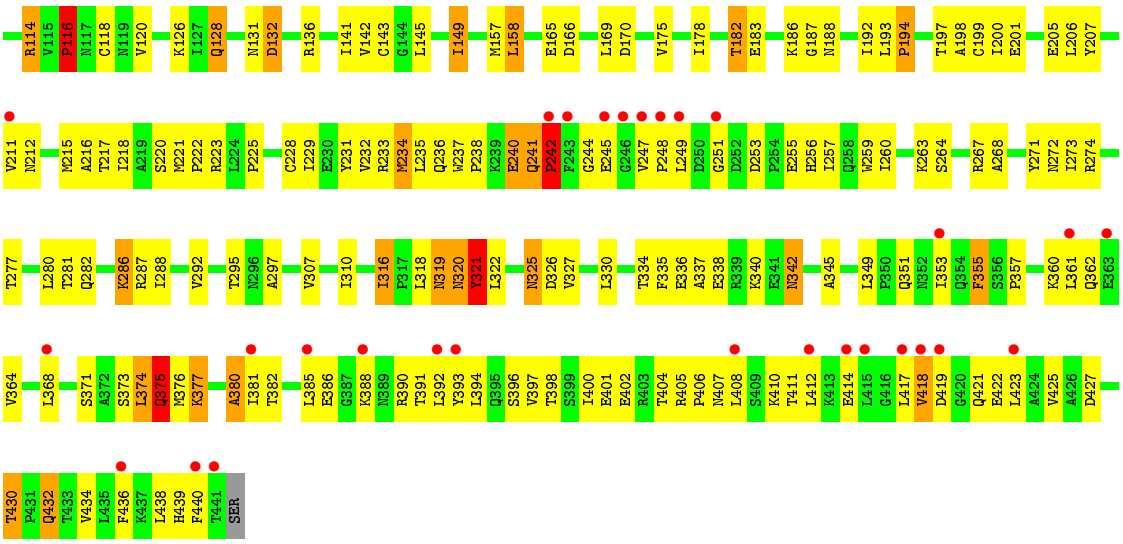
Chain D:



• Molecule 2: NEDD8-activating enzyme E1 catalytic subunit

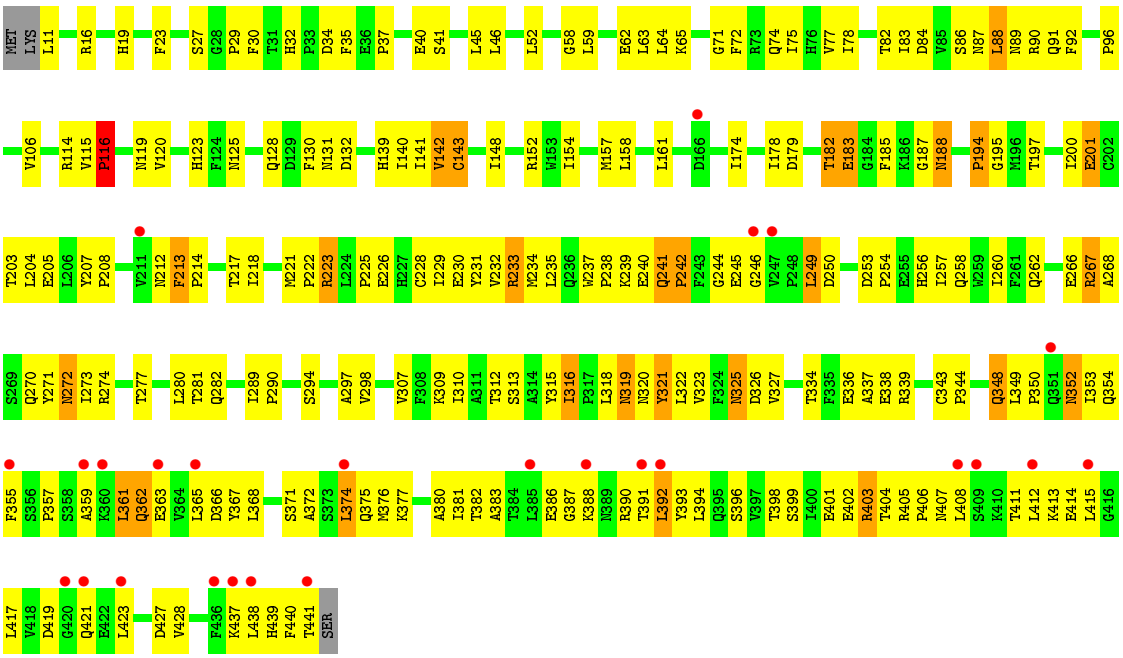
Chain F:





• Molecule 2: NEDD8-activating enzyme E1 catalytic subunit

Chain H:

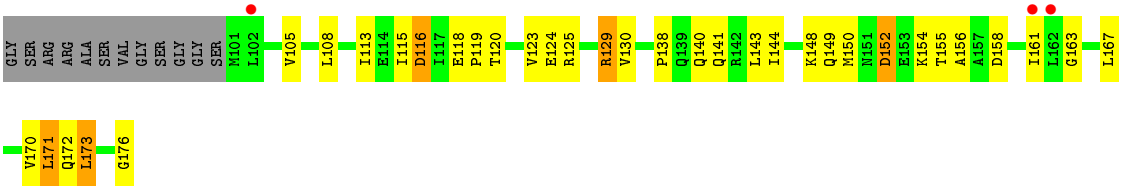


• Molecule 3: NEDD8

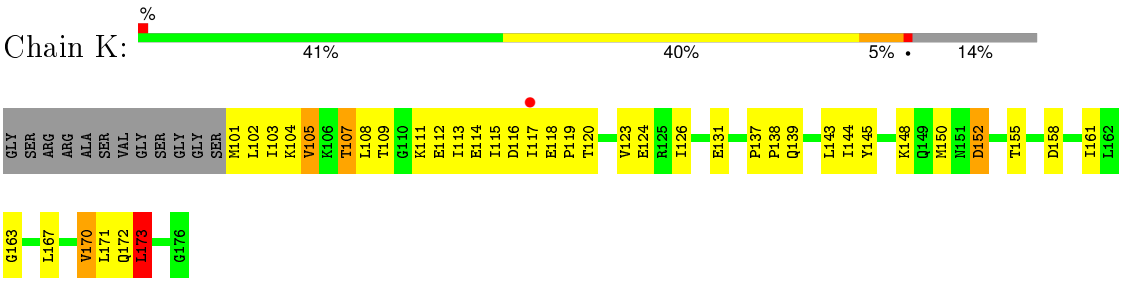
Chain I:

• Molecule 3: NEDD8

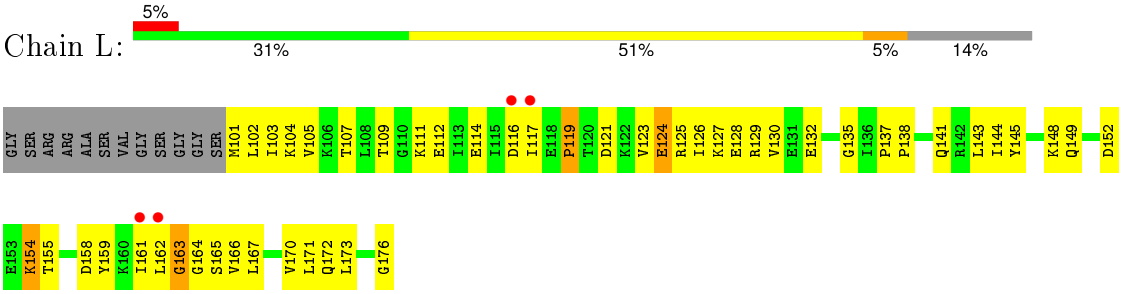
Chain J:



• Molecule 3: NEDD8



• Molecule 3: NEDD8



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	136.12Å 198.95Å 210.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.90 48.99 – 2.91	Depositor EDS
% Data completeness (in resolution range)	92.2 (50.00-2.90) 92.7 (48.99-2.91)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.07 (at 2.91Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.225 , 0.274 0.227 , 0.226	Depositor DCC
R_{free} test set	5854 reflections (5.02%)	DCC
Wilson B-factor (Å^2)	61.0	Xtriage
Anisotropy	0.487	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 46.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Outliers	2 of 116696 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	32577	wwPDB-VP
Average B, all atoms (Å^2)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.15% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0.43	0/4218	0.67	0/5706
1	C	0.41	0/4203	0.62	0/5682
1	E	0.45	0/4198	0.66	0/5678
1	G	0.43	0/4191	0.64	0/5668
2	B	0.47	1/3482 (0.0%)	0.71	2/4738 (0.0%)
2	D	0.44	0/3486	0.67	1/4742 (0.0%)
2	F	0.51	1/3475 (0.0%)	0.75	3/4730 (0.1%)
2	H	0.46	0/3467	0.71	2/4720 (0.0%)
3	I	0.44	0/673	0.68	0/897
3	J	0.42	0/609	0.70	0/813
3	K	0.48	0/609	0.75	1/813 (0.1%)
3	L	0.38	0/609	0.67	0/813
All	All	0.45	2/33220 (0.0%)	0.68	9/45000 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	380	ALA	CA-CB	-9.09	1.33	1.52
2	B	380	ALA	CA-CB	-5.91	1.40	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	165	GLU	N-CA-C	-8.34	88.48	111.00
2	B	240	GLU	N-CA-C	-7.18	91.61	111.00
2	D	12	ASP	N-CA-C	-7.13	91.75	111.00
3	K	173	LEU	CA-CB-CG	-7.12	98.91	115.30
2	H	321	TYR	N-CA-C	5.93	127.03	111.00
2	F	321	TYR	N-CA-C	5.81	126.70	111.00
2	B	321	TYR	N-CA-C	5.71	126.42	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	387	GLY	N-CA-C	-5.14	100.24	113.10
2	F	240	GLU	N-CA-C	-5.03	97.42	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4138	0	4080	177	0
1	C	4125	0	4065	181	0
1	E	4119	0	4054	201	0
1	G	4113	0	4058	171	0
2	B	3404	0	3385	202	0
2	D	3408	0	3396	176	0
2	F	3397	0	3380	234	0
2	H	3389	0	3359	238	0
3	I	668	0	702	36	0
3	J	604	0	638	37	0
3	K	604	0	638	40	0
3	L	604	0	638	53	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
4	F	1	0	0	0	0
4	H	1	0	0	0	0
All	All	32577	0	32393	1615	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 25.

All (1615) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:143:LEU:HB3	3:J:150:MET:HE3	1.26	1.15
2:D:149:ILE:H	2:D:149:ILE:HD12	1.01	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:359:ALA:HB3	2:H:412:LEU:HD11	1.26	1.13
2:F:149:ILE:H	2:F:149:ILE:HD12	1.15	1.11
1:E:184:ARG:HH12	1:E:325:VAL:HG22	1.11	1.07
3:J:123:VAL:HB	3:J:152:ASP:HA	1.39	1.04
2:B:382:THR:HG22	2:B:391:THR:HA	1.40	1.03
2:D:149:ILE:H	2:D:149:ILE:CD1	1.72	1.02
2:H:316:ILE:HD12	2:H:316:ILE:H	1.21	1.01
2:F:325:ASN:HD21	2:F:327:VAL:HG23	1.22	1.00
1:E:297:ILE:HB	1:E:368:ILE:HD11	1.40	1.00
2:F:342:ASN:HD22	2:F:342:ASN:H	1.10	0.99
2:F:84:ASP:H	2:F:87:ASN:ND2	1.62	0.97
2:F:316:ILE:H	2:F:316:ILE:HD12	1.27	0.96
2:F:277:THR:HG23	2:F:280:LEU:H	1.30	0.95
3:J:150:MET:HE1	3:J:167:LEU:HD13	1.45	0.95
3:K:123:VAL:HB	3:K:152:ASP:HA	1.46	0.95
1:E:184:ARG:NH1	1:E:325:VAL:HG22	1.81	0.94
3:L:107:THR:HG23	3:L:109:THR:H	1.34	0.93
2:B:342:ASN:H	2:B:342:ASN:HD22	0.93	0.93
1:C:297:ILE:H	1:C:297:ILE:HD13	1.33	0.93
2:F:325:ASN:ND2	2:F:327:VAL:HG23	1.84	0.92
1:E:252:LEU:O	1:E:259:PRO:HD3	1.69	0.92
2:H:412:LEU:H	2:H:412:LEU:HD12	1.35	0.92
2:B:376:MET:HB3	2:B:427:ASP:OD2	1.70	0.92
2:F:183:GLU:HG3	3:K:173:LEU:HB3	1.52	0.91
1:A:297:ILE:HG22	1:A:368:ILE:HD11	1.52	0.91
2:B:338:GLU:HG3	3:I:148:LYS:HD3	1.51	0.91
3:I:107:THR:HG22	3:I:109:THR:H	1.37	0.90
2:B:418:VAL:HG23	2:B:421:GLN:HG2	1.53	0.90
2:F:361:LEU:HD23	2:F:408:LEU:HA	1.54	0.90
2:B:342:ASN:HD22	2:B:342:ASN:N	1.70	0.89
2:H:386:GLU:C	2:H:388:LYS:H	1.74	0.89
1:A:365:LEU:HD11	1:A:375:ILE:HD13	1.53	0.89
1:E:447:ASN:HD22	2:F:26:ARG:HH21	1.20	0.89
2:H:320:ASN:HD22	2:H:336:GLU:C	1.75	0.89
1:A:236:THR:HG22	1:A:238:LYS:H	1.37	0.89
2:D:149:ILE:HD12	2:D:149:ILE:N	1.86	0.88
2:D:50:LYS:H	2:D:139:HIS:HD2	1.20	0.88
1:A:253:LYS:O	1:A:260:GLU:N	2.07	0.88
2:H:213:PHE:HB2	2:H:218:ILE:HD11	1.55	0.87
2:B:400:ILE:H	2:B:400:ILE:HD12	1.40	0.87
2:H:277:THR:HG23	2:H:280:LEU:H	1.37	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:447:ASN:ND2	2:D:26:ARG:HE	1.73	0.86
2:H:350:PRO:HB2	2:H:437:LYS:HG3	1.57	0.86
1:C:66:SER:HB2	2:H:262:GLN:HE22	1.37	0.85
2:F:412:LEU:HD13	2:F:440:PHE:HE2	1.38	0.85
2:B:355:PHE:O	2:B:440:PHE:HA	1.75	0.85
3:L:117:ILE:HD13	3:L:126:ILE:HG12	1.59	0.84
2:F:377:LYS:HE2	2:F:377:LYS:HA	1.58	0.84
2:H:380:ALA:HB2	2:H:394:LEU:HD12	1.58	0.83
2:D:342:ASN:H	2:D:342:ASN:HD22	1.26	0.83
1:E:377:GLU:HG2	1:E:381:LYS:HE3	1.61	0.83
2:F:411:THR:H	2:F:414:GLU:CB	1.91	0.83
2:B:359:ALA:O	2:B:412:LEU:HG	1.79	0.83
2:B:413:LYS:HE3	2:B:413:LYS:HA	1.61	0.83
2:F:380:ALA:CB	2:F:394:LEU:HD12	2.08	0.83
2:F:149:ILE:H	2:F:149:ILE:CD1	1.88	0.83
1:G:527:GLN:HB2	2:H:318:LEU:HD13	1.60	0.83
2:B:385:LEU:HD22	2:B:390:ARG:HB3	1.61	0.83
2:H:62:GLU:HG2	2:H:297:ALA:HA	1.61	0.82
2:F:84:ASP:H	2:F:87:ASN:HD22	1.28	0.82
1:E:224:GLN:HE21	1:E:246:LEU:HD11	1.44	0.82
2:H:320:ASN:HD22	2:H:337:ALA:N	1.77	0.82
2:F:362:GLN:HE21	2:F:408:LEU:HD22	1.45	0.81
2:F:401:GLU:HG3	2:F:402:GLU:HG3	1.61	0.81
2:H:338:GLU:HG3	3:L:148:LYS:HD3	1.60	0.81
2:H:217:THR:HG21	2:H:223:ARG:HH21	1.44	0.81
1:C:253:LYS:O	1:C:260:GLU:N	2.13	0.81
2:D:359:ALA:O	2:D:412:LEU:HG	1.81	0.81
2:H:325:ASN:ND2	2:H:327:VAL:HG22	1.95	0.81
2:H:229:ILE:HD13	2:H:281:THR:HA	1.62	0.81
1:E:347:ARG:HH12	2:F:274:ARG:HD2	1.46	0.80
2:H:267:ARG:HA	2:H:270:GLN:HE21	1.43	0.80
2:B:13:TRP:HH2	2:B:116:PRO:HG2	1.45	0.80
2:B:407:ASN:OD1	2:B:415:LEU:HD21	1.82	0.80
1:G:183:LEU:HD22	1:G:215:ILE:HD11	1.64	0.80
3:J:143:LEU:HB3	3:J:150:MET:CE	2.10	0.79
2:B:418:VAL:HG23	2:B:421:GLN:CG	2.12	0.79
1:G:36:ILE:HB	1:G:128:ALA:HA	1.62	0.79
1:G:46:LEU:HD23	1:G:93:LEU:HD13	1.62	0.79
2:B:342:ASN:ND2	2:B:342:ASN:H	1.77	0.79
2:F:342:ASN:HD22	2:F:342:ASN:N	1.80	0.79
1:E:518:ASN:HB2	1:E:533:GLN:HA	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:277:THR:HG23	2:D:280:LEU:H	1.47	0.79
1:G:397:SER:OG	1:G:400:GLU:HG3	1.83	0.79
1:G:37:ASN:HB3	1:G:39:THR:HG23	1.65	0.79
2:D:213:PHE:HB2	2:D:218:ILE:HD11	1.66	0.78
2:F:411:THR:H	2:F:414:GLU:HB3	1.47	0.78
2:F:392:LEU:HD12	2:F:392:LEU:H	1.49	0.78
1:C:299:LYS:HA	1:C:368:ILE:HG23	1.66	0.78
1:G:421:ASN:O	1:G:424:VAL:HG23	1.83	0.78
2:F:418:VAL:HG22	2:F:419:ASP:H	1.49	0.78
2:D:134:PHE:O	2:D:137:GLN:HG2	1.84	0.77
1:C:421:ASN:O	1:C:424:VAL:HG23	1.85	0.77
1:C:43:THR:HG21	1:C:73:ASN:OD1	1.83	0.77
2:H:320:ASN:ND2	2:H:337:ALA:N	2.33	0.77
2:B:188:ASN:OD1	3:I:173:LEU:HD12	1.85	0.76
2:B:240:GLU:O	2:B:241:GLN:HG2	1.85	0.76
1:E:56:SER:HB3	1:E:101:SER:HB2	1.66	0.76
1:C:261:ASP:O	1:C:262:GLU:HG3	1.85	0.76
1:G:340:ILE:HD11	2:H:273:ILE:HG12	1.67	0.76
2:D:325:ASN:HD22	2:D:326:ASP:N	1.84	0.76
1:C:446:SER:HB2	1:C:449:GLN:HG3	1.68	0.76
1:A:347:ARG:HH22	2:B:274:ARG:HH22	1.33	0.76
2:F:382:THR:HG22	2:F:391:THR:HA	1.66	0.75
2:H:132:ASP:HB3	2:H:157:MET:HE1	1.68	0.75
2:F:64:LEU:HD11	2:F:77:VAL:HG21	1.69	0.75
2:B:13:TRP:CH2	2:B:116:PRO:HG2	2.21	0.75
1:C:66:SER:HB2	2:H:262:GLN:NE2	2.02	0.75
2:H:320:ASN:HB2	2:H:336:GLU:HA	1.67	0.74
2:H:178:ILE:HD11	2:H:310:ILE:HD12	1.69	0.74
2:B:325:ASN:HD21	2:B:327:VAL:HG13	1.52	0.74
2:D:193:LEU:H	2:D:197:THR:HG22	1.50	0.74
1:A:437:LYS:HZ3	1:A:437:LYS:HA	1.50	0.74
2:D:50:LYS:H	2:D:139:HIS:CD2	2.05	0.74
1:C:202:ASP:N	1:C:204:MET:HB3	2.03	0.74
2:F:54:ILE:CG2	2:F:145:LEU:HD21	2.17	0.74
1:E:262:GLU:HB3	1:E:265:PHE:HB2	1.70	0.74
3:J:143:LEU:CB	3:J:150:MET:HE3	2.13	0.74
1:C:347:ARG:NH1	2:D:274:ARG:HD2	2.02	0.73
1:G:307:LEU:HB3	1:G:383:LEU:CD2	2.18	0.73
1:A:36:ILE:HB	1:A:128:ALA:HA	1.70	0.73
1:A:299:LYS:HA	1:A:368:ILE:HG23	1.69	0.73
1:E:317:LYS:HB3	1:E:318:GLU:OE1	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:THR:CG2	1:A:232:ARG:HB3	2.18	0.73
1:G:407:ILE:HG23	1:G:409:LYS:HG3	1.70	0.73
1:E:374:SER:C	1:E:375:ILE:HD12	2.09	0.73
3:L:125:ARG:HG3	3:L:128:GLU:OE1	1.88	0.73
2:H:323:VAL:HG21	3:L:170:VAL:HG13	1.69	0.73
2:B:356:SER:HB3	2:B:442:SER:HB3	1.70	0.73
1:G:61:ASP:HB3	1:G:86:ALA:HB2	1.69	0.73
2:F:421:GLN:HG3	2:F:423:LEU:HD21	1.68	0.73
2:D:237:TRP:HB3	2:D:238:PRO:HD3	1.71	0.73
1:A:201:LEU:HD22	1:A:209:HIS:ND1	2.03	0.73
2:F:361:LEU:HD23	2:F:408:LEU:HD23	1.70	0.72
2:H:368:LEU:HB3	2:H:376:MET:HG3	1.70	0.72
2:D:357:PRO:HG3	2:D:440:PHE:CG	2.23	0.72
2:H:325:ASN:HD21	2:H:327:VAL:HG22	1.52	0.72
2:D:193:LEU:H	2:D:197:THR:CG2	2.02	0.72
2:D:380:ALA:HB1	2:D:394:LEU:HD12	1.68	0.72
3:K:104:LYS:HG2	3:K:114:GLU:HG2	1.71	0.72
1:G:360:HIS:O	1:G:364:LEU:HB2	1.90	0.72
1:E:340:ILE:HG21	2:F:272:ASN:ND2	2.03	0.72
2:H:380:ALA:CB	2:H:394:LEU:HD12	2.19	0.72
1:G:450:VAL:O	1:G:454:ILE:HG13	1.90	0.72
2:F:131:ASN:HB3	2:H:131:ASN:HD22	1.55	0.72
2:H:267:ARG:HH11	2:H:267:ARG:HG3	1.54	0.72
2:B:35:PHE:O	2:B:36:GLU:HG3	1.89	0.72
1:G:226:TYR:OH	1:G:233:ILE:HG22	1.90	0.72
2:D:325:ASN:ND2	2:D:327:VAL:HG22	2.06	0.71
1:A:428:MET:HE1	1:A:479:VAL:HA	1.72	0.71
2:B:316:ILE:H	2:B:316:ILE:HD12	1.52	0.71
2:F:242:PRO:HG3	2:F:259:TRP:CZ2	2.25	0.71
1:C:126:VAL:O	1:C:150:LEU:HD12	1.91	0.71
1:A:518:ASN:HD22	1:A:534:LEU:H	1.36	0.71
1:E:78:ARG:HG3	1:E:78:ARG:HH11	1.53	0.71
2:D:320:ASN:HB2	2:D:336:GLU:HA	1.71	0.71
1:E:251:ILE:HG23	1:E:262:GLU:HB2	1.72	0.71
2:B:362:GLN:HB2	2:B:408:LEU:O	1.91	0.71
1:E:491:HIS:NE2	2:F:65:LYS:HE2	2.06	0.70
2:F:32:HIS:CD2	2:F:34:ASP:H	2.08	0.70
1:E:447:ASN:ND2	2:F:26:ARG:HH21	1.88	0.70
1:E:307:LEU:HD13	1:E:383:LEU:HD22	1.73	0.70
1:E:210:SER:HB3	1:E:262:GLU:OE2	1.90	0.70
2:F:237:TRP:HB3	2:F:238:PRO:HD3	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:72:ASN:HD22	1:E:73:ASN:N	1.89	0.70
2:H:381:ILE:H	2:H:381:ILE:HD12	1.56	0.70
2:H:320:ASN:HD22	2:H:336:GLU:CA	2.04	0.70
1:G:376:SER:OG	1:G:379:GLU:HG3	1.92	0.70
1:C:454:ILE:HD13	1:C:480:HIS:ND1	2.06	0.70
1:C:299:LYS:HA	1:C:368:ILE:CG2	2.22	0.70
1:E:236:THR:HG22	1:E:237:TYR:H	1.57	0.69
2:F:142:VAL:HG21	2:F:307:VAL:HG21	1.71	0.69
1:E:226:TYR:CD1	1:E:231:GLY:HA2	2.26	0.69
3:L:155:THR:HG23	3:L:158:ASP:H	1.57	0.69
1:E:186:ASP:OD2	1:E:279:THR:HB	1.92	0.69
1:A:61:ASP:HB3	1:A:86:ALA:HB2	1.75	0.69
2:D:380:ALA:CB	2:D:394:LEU:HD12	2.22	0.69
2:B:380:ALA:CB	2:B:394:LEU:HD12	2.22	0.69
1:G:332:MET:HG2	1:G:339:TYR:HE1	1.56	0.68
1:E:421:ASN:O	1:E:424:VAL:HG23	1.93	0.68
1:E:190:PRO:HG2	1:E:191:GLU:OE2	1.93	0.68
2:F:62:GLU:HG2	2:F:297:ALA:HA	1.76	0.68
2:B:193:LEU:H	2:B:197:THR:HB	1.58	0.68
2:D:151:ARG:HB3	2:D:200:ILE:HD13	1.75	0.68
1:E:236:THR:HG22	1:E:237:TYR:N	2.08	0.68
2:F:201:GLU:HG3	2:F:345:ALA:HB2	1.74	0.68
1:G:246:LEU:O	1:G:246:LEU:HD23	1.93	0.68
3:K:107:THR:CG2	3:K:109:THR:H	2.06	0.68
2:B:338:GLU:HG3	3:I:148:LYS:CD	2.22	0.68
2:H:250:ASP:HB3	2:H:253:ASP:HB2	1.75	0.68
2:F:382:THR:HA	2:F:392:LEU:HD13	1.76	0.68
1:A:437:LYS:HA	1:A:437:LYS:NZ	2.09	0.68
1:C:397:SER:OG	1:C:400:GLU:HG3	1.93	0.68
2:B:351:GLN:HB3	2:B:436:PHE:CD2	2.28	0.68
1:G:309:ARG:CG	1:G:364:LEU:HD21	2.24	0.68
1:E:226:TYR:CE1	1:E:231:GLY:HA2	2.28	0.68
2:D:16:ARG:NH2	2:D:116:PRO:HB2	2.09	0.68
1:C:293:ARG:HG2	1:C:293:ARG:HH11	1.58	0.68
2:B:237:TRP:HB3	2:B:238:PRO:HD3	1.76	0.67
2:F:54:ILE:HB	2:F:143:CYS:HB2	1.75	0.67
1:A:61:ASP:OD2	1:A:85:ARG:HD2	1.94	0.67
2:F:425:VAL:HB	2:F:434:VAL:HG13	1.76	0.67
1:A:264:ASN:N	1:A:264:ASN:HD22	1.91	0.67
2:H:316:ILE:N	2:H:316:ILE:HD12	2.04	0.67
1:E:209:HIS:CD2	1:E:252:LEU:HB2	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:322:LEU:C	2:B:322:LEU:HD23	2.15	0.67
2:B:343:CYS:O	2:B:347:SER:HB3	1.95	0.67
1:C:317:LYS:HB3	1:C:318:GLU:OE1	1.94	0.67
1:G:340:ILE:HD13	2:H:272:ASN:O	1.95	0.67
1:C:347:ARG:NH2	2:D:274:ARG:HE	1.92	0.67
1:E:309:ARG:HD2	1:E:364:LEU:HD21	1.76	0.67
2:B:207:TYR:O	3:I:142:ARG:NH1	2.27	0.67
1:A:461:LEU:O	1:A:465:LEU:HG	1.95	0.67
2:D:325:ASN:HD21	2:D:327:VAL:HG22	1.59	0.67
1:C:61:ASP:OD2	1:C:85:ARG:HD2	1.94	0.67
1:G:201:LEU:HD21	1:G:220:LYS:HB2	1.77	0.67
2:D:73:ARG:HD3	2:D:117:ASN:O	1.94	0.67
2:H:402:GLU:HG3	2:H:405:ARG:HH22	1.60	0.67
3:L:102:LEU:HD13	3:L:116:ASP:OD1	1.94	0.67
3:L:117:ILE:HD11	3:L:126:ILE:HA	1.77	0.66
2:F:54:ILE:HG22	2:F:145:LEU:HD21	1.76	0.66
2:B:217:THR:HB	2:B:223:ARG:NH2	2.11	0.66
2:D:360:LYS:HA	2:D:411:THR:HA	1.78	0.66
3:I:103:ILE:CD1	3:I:117:ILE:HD12	2.26	0.66
2:D:355:PHE:HE1	2:D:364:VAL:HA	1.59	0.66
1:E:340:ILE:HG21	2:F:272:ASN:HD21	1.58	0.66
1:E:311:LEU:HD21	1:E:383:LEU:HD11	1.78	0.66
1:A:173:GLU:O	1:A:512:GLN:O	2.13	0.66
1:C:36:ILE:HG22	1:C:37:ASN:N	2.09	0.66
2:B:257:ILE:HD13	2:B:282:GLN:HG2	1.78	0.66
1:E:43:THR:HG21	1:E:73:ASN:OD1	1.96	0.66
2:H:234:MET:C	2:H:235:LEU:HD22	2.15	0.66
1:G:43:THR:HG21	1:G:73:ASN:OD1	1.94	0.66
2:D:241:GLN:NE2	2:D:246:GLY:H	1.93	0.66
2:F:240:GLU:O	2:F:242:PRO:HD3	1.95	0.66
2:F:438:LEU:HD13	2:F:439:HIS:N	2.10	0.66
1:E:489:GLU:H	2:F:19:HIS:CD2	2.14	0.66
1:C:311:LEU:O	1:C:315:VAL:HG23	1.96	0.66
1:E:34:CYS:HB2	1:E:123:PHE:CD2	2.31	0.66
1:E:193:ARG:HG3	1:E:193:ARG:HH11	1.60	0.65
1:C:236:THR:HG22	1:C:238:LYS:H	1.60	0.65
2:H:257:ILE:HD13	2:H:282:GLN:HG2	1.78	0.65
2:F:242:PRO:HG3	2:F:259:TRP:CE2	2.31	0.65
1:C:297:ILE:CD1	1:C:297:ILE:H	2.07	0.65
2:F:286:LYS:O	2:F:288:ILE:HG13	1.97	0.65
1:E:297:ILE:HG22	1:E:301:THR:HG21	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:355:PHE:O	2:F:440:PHE:HA	1.97	0.65
2:D:327:VAL:HG23	2:D:328:ASP:N	2.12	0.65
2:D:192:ILE:HA	2:D:197:THR:HG21	1.79	0.65
1:E:22:ASP:O	1:E:26:GLU:HG3	1.97	0.65
3:K:107:THR:HG23	3:K:109:THR:H	1.62	0.65
1:G:236:THR:OG1	1:G:239:GLU:HB2	1.97	0.65
2:D:422:GLU:HG2	2:D:437:LYS:HG3	1.77	0.65
2:B:64:LEU:HB3	2:B:111:LEU:HD22	1.79	0.65
2:D:214:PRO:HB2	2:D:217:THR:HG23	1.79	0.65
1:E:396:ARG:HG3	1:E:396:ARG:HH11	1.62	0.65
2:B:380:ALA:HB1	2:B:394:LEU:HD12	1.79	0.64
1:G:143:LEU:HD12	1:G:150:LEU:HD22	1.79	0.64
2:F:381:ILE:H	2:F:381:ILE:HD12	1.62	0.64
1:E:447:ASN:HD22	2:F:26:ARG:NH2	1.94	0.64
1:A:227:SER:C	1:A:229:THR:H	1.99	0.64
1:C:507:LYS:HG2	1:C:513:PHE:HB2	1.78	0.64
1:E:184:ARG:HH11	1:E:184:ARG:HG3	1.62	0.64
1:A:133:GLU:HG3	1:A:433:ASP:HB3	1.79	0.64
1:E:240:LYS:NZ	1:E:276:LEU:HD12	2.11	0.64
2:F:316:ILE:H	2:F:316:ILE:CD1	2.05	0.64
3:I:170:VAL:CG1	3:I:171:LEU:N	2.60	0.64
2:D:342:ASN:HD22	2:D:342:ASN:N	1.93	0.64
1:C:236:THR:HB	1:C:239:GLU:HG3	1.79	0.64
2:B:153:TRP:CE2	2:B:431:PRO:HG3	2.33	0.64
1:E:377:GLU:O	1:E:381:LYS:HG3	1.97	0.64
2:H:267:ARG:HA	2:H:270:GLN:NE2	2.11	0.64
2:D:64:LEU:HD21	2:D:77:VAL:CG2	2.28	0.64
1:A:317:LYS:HB3	1:A:318:GLU:OE1	1.98	0.64
2:B:357:PRO:HG3	2:B:440:PHE:CD2	2.33	0.63
3:K:116:ASP:C	3:K:117:ILE:HD12	2.18	0.63
1:A:137:LEU:HD11	1:A:402:TYR:CD2	2.34	0.63
3:K:155:THR:HG22	3:K:158:ASP:CG	2.18	0.63
1:G:199:TYR:CD2	1:G:216:VAL:HG11	2.32	0.63
1:A:344:ASN:HB3	1:E:111:ASN:ND2	2.14	0.63
1:C:72:ASN:H	1:C:72:ASN:HD22	1.44	0.63
1:A:248:ARG:HG3	1:A:248:ARG:HH11	1.64	0.63
1:G:489:GLU:H	2:H:19:HIS:CD2	2.17	0.63
2:H:362:GLN:HA	2:H:408:LEU:HD22	1.80	0.63
3:I:102:LEU:HD23	3:I:102:LEU:H	1.63	0.63
1:C:441:ARG:NH2	1:C:453:ASP:OD1	2.32	0.63
1:G:307:LEU:HB3	1:G:383:LEU:HD22	1.78	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:293:ARG:HG2	1:C:293:ARG:NH1	2.12	0.63
1:A:87:GLU:O	1:A:91:GLU:HG3	1.97	0.63
1:G:45:ILE:HG12	1:G:498:GLY:HA2	1.81	0.63
2:F:325:ASN:HD21	2:F:327:VAL:CG2	2.04	0.63
2:B:320:ASN:HB2	2:B:336:GLU:HA	1.80	0.63
2:H:201:GLU:HB3	2:H:343:CYS:SG	2.39	0.63
2:H:412:LEU:HD23	2:H:438:LEU:HD21	1.81	0.63
1:E:311:LEU:CD2	1:E:383:LEU:HD11	2.29	0.63
2:B:214:PRO:HG2	2:B:217:THR:HG23	1.80	0.63
1:C:236:THR:HB	1:C:239:GLU:H	1.63	0.63
1:E:12:LYS:O	2:F:89:ASN:HB3	1.98	0.63
3:L:107:THR:HG22	3:L:111:LYS:N	2.13	0.63
2:F:141:ILE:HD12	2:F:158:LEU:HD11	1.80	0.63
1:A:168:GLU:HG3	1:A:394:ARG:HE	1.63	0.63
3:J:170:VAL:HG22	3:J:171:LEU:H	1.63	0.63
1:G:54:ILE:O	1:G:100:VAL:HG13	1.98	0.63
1:A:181:GLU:O	1:A:278:THR:HB	1.98	0.62
2:D:229:ILE:HD13	2:D:281:THR:HA	1.80	0.62
2:H:27:SER:HB3	2:H:37:PRO:CG	2.30	0.62
2:F:398:THR:O	2:F:401:GLU:HG2	1.99	0.62
2:D:322:LEU:C	2:D:322:LEU:HD23	2.19	0.62
2:H:377:LYS:HD3	2:H:428:VAL:HG21	1.81	0.62
2:F:362:GLN:NE2	2:F:408:LEU:HD13	2.13	0.62
2:D:185:PHE:HB3	2:D:326:ASP:HB2	1.81	0.62
2:F:381:ILE:N	2:F:381:ILE:HD12	2.14	0.62
1:A:253:LYS:C	1:A:260:GLU:H	2.02	0.62
2:D:327:VAL:HG23	2:D:328:ASP:H	1.63	0.62
1:E:248:ARG:O	1:E:251:ILE:HG13	1.99	0.62
1:A:371:ALA:O	1:A:373:GLU:N	2.31	0.62
2:D:62:GLU:HG2	2:D:297:ALA:HA	1.82	0.62
3:L:154:LYS:HD2	3:L:159:TYR:OH	1.98	0.62
1:A:209:HIS:CD2	1:A:252:LEU:HD13	2.34	0.62
2:B:384:THR:HG23	2:B:384:THR:O	1.99	0.62
1:E:184:ARG:HH12	1:E:325:VAL:CG2	2.00	0.62
2:F:131:ASN:HD22	2:H:131:ASN:HB3	1.64	0.62
2:B:81:ASP:HB3	2:B:103:LYS:HE3	1.80	0.62
1:G:248:ARG:HH11	1:G:248:ARG:HG3	1.65	0.61
2:F:229:ILE:HD13	2:F:281:THR:HA	1.82	0.61
2:F:169:LEU:HD12	2:F:170:ASP:H	1.64	0.61
3:J:155:THR:HG22	3:J:158:ASP:OD2	2.00	0.61
1:G:307:LEU:HB3	1:G:383:LEU:HD21	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:518:ASN:ND2	1:A:534:LEU:H	1.97	0.61
1:C:115:ASN:O	1:C:117:PRO:HD3	2.00	0.61
2:D:102:PRO:O	2:D:106:VAL:HG23	1.99	0.61
2:H:132:ASP:HB3	2:H:157:MET:CE	2.29	0.61
2:D:141:ILE:HD12	2:D:158:LEU:HD21	1.82	0.61
1:E:46:LEU:O	1:E:50:VAL:HG23	2.01	0.61
3:J:144:ILE:HD13	3:J:149:GLN:HA	1.81	0.61
1:E:516:PHE:HB3	2:F:330:LEU:HD12	1.81	0.61
1:C:43:THR:HG23	1:C:75:PHE:CD1	2.36	0.61
1:C:268:ALA:O	1:C:272:VAL:HG23	2.00	0.61
3:I:107:THR:CG2	3:I:109:THR:HG23	2.30	0.61
2:F:411:THR:H	2:F:414:GLU:HB2	1.66	0.61
2:H:381:ILE:N	2:H:381:ILE:HD12	2.16	0.61
2:H:386:GLU:C	2:H:388:LYS:N	2.46	0.61
2:H:266:GLU:C	2:H:268:ALA:H	2.03	0.61
2:D:330:LEU:H	2:D:330:LEU:HD12	1.64	0.61
1:E:409:LYS:O	1:E:413:ILE:HG13	2.00	0.61
1:C:449:GLN:HB3	1:C:453:ASP:OD2	2.01	0.61
1:C:229:THR:CG2	1:C:232:ARG:HB2	2.31	0.61
2:B:305:THR:HG22	2:B:309:LYS:NZ	2.15	0.61
2:F:393:TYR:HD1	2:F:404:THR:OG1	1.83	0.61
1:C:297:ILE:HD13	1:C:297:ILE:N	2.12	0.60
2:D:342:ASN:ND2	2:D:342:ASN:H	1.95	0.60
1:A:307:LEU:HB3	1:A:383:LEU:HD22	1.81	0.60
3:J:124:GLU:HB2	3:J:152:ASP:O	2.01	0.60
2:B:413:LYS:CA	2:B:413:LYS:HE3	2.30	0.60
1:G:297:ILE:HG21	1:G:368:ILE:HD11	1.84	0.60
1:C:518:ASN:CB	1:C:533:GLN:HA	2.31	0.60
2:D:355:PHE:CE1	2:D:364:VAL:HA	2.36	0.60
2:D:50:LYS:N	2:D:139:HIS:HD2	1.93	0.60
2:B:418:VAL:O	2:B:421:GLN:HG3	2.02	0.60
2:F:380:ALA:HB2	2:F:394:LEU:HD12	1.84	0.60
2:D:323:VAL:HG21	3:J:170:VAL:HG23	1.84	0.60
2:D:325:ASN:HD22	2:D:326:ASP:H	1.50	0.60
2:F:249:LEU:HD11	2:F:260:ILE:HD11	1.83	0.60
2:B:320:ASN:HD22	2:B:337:ALA:N	1.97	0.60
2:B:318:LEU:HD11	2:B:334:THR:CG2	2.32	0.60
3:L:170:VAL:HG12	3:L:171:LEU:N	2.16	0.60
1:G:266:GLU:HA	1:G:269:ILE:HD12	1.84	0.60
3:J:105:VAL:HG11	3:J:130:VAL:HG22	1.83	0.60
3:K:124:GLU:HB2	3:K:152:ASP:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:454:ILE:HD13	1:G:480:HIS:ND1	2.17	0.60
1:G:332:MET:HG2	1:G:339:TYR:CE1	2.36	0.60
2:F:385:LEU:HD12	2:F:390:ARG:HG2	1.84	0.60
2:B:427:ASP:CG	2:B:429:THR:HG22	2.22	0.59
2:F:362:GLN:HE21	2:F:408:LEU:CD2	2.15	0.59
2:F:392:LEU:CD1	2:F:392:LEU:H	2.15	0.59
1:G:12:LYS:HG3	2:H:88:LEU:HB2	1.84	0.59
2:H:143:CYS:HB3	2:H:179:ASP:OD2	2.01	0.59
1:G:25:GLN:O	1:G:29:GLU:HG3	2.02	0.59
1:C:138:ARG:O	1:C:142:VAL:HG23	2.02	0.59
2:H:438:LEU:HD12	2:H:439:HIS:H	1.67	0.59
2:F:54:ILE:HG21	2:F:145:LEU:HD21	1.83	0.59
2:D:393:TYR:CZ	2:D:408:LEU:HD11	2.37	0.59
2:F:361:LEU:CD2	2:F:408:LEU:HA	2.29	0.59
2:H:207:TYR:CE2	3:L:172:GLN:HG2	2.37	0.59
2:D:157:MET:O	2:D:160:SER:HB3	2.02	0.59
2:B:405:ARG:HB3	2:B:406:PRO:HD3	1.84	0.59
2:D:128:GLN:NE2	2:D:128:GLN:H	1.99	0.59
1:C:376:SER:OG	1:C:379:GLU:HG3	2.02	0.59
1:E:229:THR:HG22	1:E:232:ARG:HD2	1.85	0.59
2:F:321:TYR:OH	3:K:172:GLN:HG3	2.01	0.59
1:E:189:PHE:HB2	1:E:190:PRO:HD2	1.85	0.59
2:H:187:GLY:HA2	3:L:173:LEU:HD13	1.85	0.59
2:F:136:ARG:HH11	2:F:136:ARG:HG3	1.68	0.59
2:F:430:THR:OG1	2:F:432:GLN:HB2	2.03	0.59
2:F:95:ARG:HE	2:F:95:ARG:HA	1.67	0.59
2:H:222:PRO:O	2:H:273:ILE:HD11	2.02	0.59
1:E:347:ARG:NH1	2:F:274:ARG:HD2	2.16	0.59
2:F:53:VAL:HB	2:F:77:VAL:HG22	1.84	0.59
2:F:236:GLN:HE22	2:F:263:LYS:HD2	1.68	0.59
1:A:401:GLU:OE2	1:A:534:LEU:HB2	2.02	0.59
2:B:312:THR:O	2:B:313:SER:HB2	2.03	0.59
2:F:368:LEU:HA	2:F:374:LEU:HD11	1.85	0.59
1:A:470:LEU:O	1:A:470:LEU:HD12	2.02	0.59
2:H:349:LEU:HB3	2:H:350:PRO:HD2	1.85	0.59
2:B:418:VAL:CG2	2:B:421:GLN:HG2	2.28	0.58
1:A:371:ALA:C	1:A:373:GLU:H	2.06	0.58
3:L:107:THR:HG21	3:L:111:LYS:HB3	1.85	0.58
3:L:126:ILE:O	3:L:130:VAL:HG23	2.03	0.58
1:G:297:ILE:CG2	1:G:368:ILE:HD11	2.33	0.58
2:H:309:LYS:HD3	2:H:315:TYR:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:121:CYS:HA	1:G:148:ILE:HD11	1.85	0.58
1:C:78:ARG:HH12	2:D:11:LEU:HD22	1.68	0.58
2:F:92:PHE:H	2:F:92:PHE:HD2	1.52	0.58
1:E:447:ASN:ND2	2:F:26:ARG:HE	2.01	0.58
1:C:447:ASN:HD21	2:D:26:ARG:HE	1.51	0.58
2:H:350:PRO:CB	2:H:437:LYS:HG3	2.31	0.58
2:D:59:LEU:HB2	3:J:176:GLY:O	2.04	0.58
1:G:241:GLU:O	1:G:244:ARG:HB2	2.03	0.58
2:B:178:ILE:N	2:B:178:ILE:HD12	2.19	0.58
1:A:434:ARG:O	1:A:437:LYS:HB3	2.04	0.58
2:F:32:HIS:HD2	2:F:34:ASP:H	1.49	0.58
2:D:257:ILE:HG22	2:D:278:TYR:CE1	2.39	0.58
1:A:61:ASP:CB	1:A:86:ALA:HB2	2.33	0.58
2:F:197:THR:CG2	2:F:198:ALA:N	2.66	0.58
1:C:422:GLU:HG3	1:C:530:ALA:HB3	1.86	0.58
1:E:224:GLN:NE2	1:E:246:LEU:HD11	2.15	0.58
2:F:89:ASN:OD1	2:F:90:ARG:HG2	2.03	0.58
2:H:376:MET:HB3	2:H:427:ASP:OD2	2.04	0.58
1:E:78:ARG:NH1	1:E:78:ARG:HG3	2.19	0.58
1:C:236:THR:CB	1:C:239:GLU:HG3	2.34	0.58
2:B:64:LEU:HB3	2:B:111:LEU:CD2	2.34	0.58
2:H:412:LEU:HD22	2:H:440:PHE:CE2	2.38	0.58
2:H:185:PHE:HB3	2:H:326:ASP:HB3	1.86	0.58
1:C:214:TRP:CZ3	1:C:332:MET:HB3	2.39	0.58
3:L:104:LYS:HD3	3:L:112:GLU:OE2	2.03	0.58
2:H:182:THR:O	2:H:183:GLU:HB2	2.04	0.58
1:C:423:ILE:O	1:C:423:ILE:HG13	2.02	0.58
2:H:253:ASP:HB3	2:H:256:HIS:HB2	1.86	0.58
1:A:519:THR:HG22	1:A:521:ILE:CD1	2.34	0.58
3:J:150:MET:CE	3:J:167:LEU:HD13	2.29	0.57
2:B:356:SER:CB	2:B:442:SER:HB3	2.32	0.57
1:G:61:ASP:CB	1:G:86:ALA:HB2	2.35	0.57
2:H:237:TRP:HB3	2:H:238:PRO:HD3	1.86	0.57
2:B:412:LEU:O	2:B:417:LEU:HB2	2.04	0.57
2:B:325:ASN:ND2	2:B:327:VAL:HG13	2.19	0.57
1:G:114:ASP:HA	1:G:138:ARG:HH22	1.68	0.57
2:F:410:LYS:HB3	2:F:414:GLU:HB3	1.86	0.57
1:G:267:GLU:O	1:G:270:LYS:HG2	2.04	0.57
3:I:104:LYS:HD2	3:I:112:GLU:OE2	2.04	0.57
1:A:58:THR:HA	1:A:103:SER:O	2.04	0.57
1:A:434:ARG:HD3	1:A:460:CYS:HB3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:241:GLN:CG	2:F:245:GLU:HA	2.35	0.57
1:C:128:ALA:HB1	1:C:131:LEU:HD11	1.86	0.57
2:D:75:ILE:O	2:D:120:VAL:HA	2.04	0.57
2:F:182:THR:OG1	2:F:295:THR:HG22	2.04	0.57
1:A:236:THR:HG22	1:A:238:LYS:N	2.15	0.57
1:G:244:ARG:HH11	1:G:244:ARG:HG3	1.68	0.57
1:E:371:ALA:O	1:E:373:GLU:N	2.37	0.57
1:C:35:LEU:HD22	1:C:46:LEU:HD22	1.85	0.57
2:F:405:ARG:HB3	2:F:406:PRO:HD3	1.85	0.57
2:B:360:LYS:HA	2:B:411:THR:HA	1.86	0.57
1:E:356:ALA:O	1:E:359:ASN:HB2	2.04	0.57
3:L:105:VAL:O	3:L:105:VAL:HG13	2.04	0.57
1:A:159:VAL:HG22	1:A:425:LEU:HD13	1.86	0.57
1:G:185:LEU:O	1:G:188:PRO:HD3	2.04	0.57
2:B:380:ALA:HB1	2:B:394:LEU:CD1	2.33	0.57
1:C:61:ASP:CB	1:C:86:ALA:HB2	2.34	0.57
3:K:117:ILE:HG12	3:K:126:ILE:HG12	1.86	0.57
2:B:407:ASN:HB3	2:B:415:LEU:HD11	1.86	0.57
2:F:249:LEU:CD1	2:F:260:ILE:HD11	2.34	0.57
1:E:46:LEU:HD23	1:E:93:LEU:HD13	1.87	0.57
2:H:178:ILE:HD12	2:H:307:VAL:HG22	1.87	0.56
3:K:155:THR:HG22	3:K:158:ASP:OD2	2.05	0.56
1:G:264:ASN:N	1:G:264:ASN:HD22	2.02	0.56
1:G:214:TRP:C	1:G:214:TRP:CD1	2.78	0.56
1:C:12:LYS:O	2:D:89:ASN:HB3	2.04	0.56
1:C:19:LEU:HD12	2:D:292:VAL:HG13	1.86	0.56
2:H:249:LEU:HD13	2:H:260:ILE:HD11	1.87	0.56
2:B:182:THR:O	3:I:175:GLY:HA3	2.05	0.56
2:F:228:CYS:SG	2:F:268:ALA:HA	2.45	0.56
3:L:117:ILE:HD12	3:L:126:ILE:HG23	1.88	0.56
1:A:248:ARG:HG3	1:A:248:ARG:NH1	2.20	0.56
1:C:46:LEU:O	1:C:50:VAL:HG23	2.05	0.56
2:H:390:ARG:HH22	2:H:407:ASN:HD21	1.53	0.56
2:H:390:ARG:NH2	2:H:407:ASN:HD21	2.03	0.56
2:H:412:LEU:HA	2:H:417:LEU:HD12	1.87	0.56
1:E:309:ARG:CD	1:E:364:LEU:HD21	2.35	0.56
1:G:264:ASN:HD22	1:G:265:PHE:H	1.53	0.56
1:G:184:ARG:HH12	1:G:325:VAL:HG22	1.70	0.56
2:H:398:THR:O	2:H:401:GLU:HB3	2.06	0.56
1:A:240:LYS:O	1:A:244:ARG:HG3	2.06	0.56
2:B:270:GLN:HG3	2:B:271:TYR:CD1	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:LEU:HD22	1:A:142:VAL:HG21	1.88	0.56
1:G:480:HIS:HB2	2:H:29:PRO:HG2	1.88	0.56
2:H:402:GLU:C	2:H:404:THR:H	2.09	0.56
2:B:201:GLU:HG3	2:B:345:ALA:HB2	1.86	0.56
1:C:264:ASN:HD22	1:C:264:ASN:N	2.04	0.56
2:H:75:ILE:O	2:H:120:VAL:HA	2.06	0.56
2:F:188:ASN:OD1	3:K:173:LEU:HD12	2.06	0.56
3:L:117:ILE:HG23	3:L:121:ASP:HB2	1.87	0.56
2:D:356:SER:HB2	2:D:442:SER:OG	2.05	0.56
2:H:58:GLY:N	2:H:91:GLN:HG2	2.21	0.56
1:A:484:ARG:HH11	1:A:484:ARG:HG2	1.71	0.56
2:B:352:ASN:O	2:B:353:ILE:HD12	2.06	0.56
1:G:307:LEU:HD21	1:G:375:ILE:HG21	1.88	0.56
2:B:213:PHE:HB3	2:B:218:ILE:HD13	1.87	0.56
2:B:54:ILE:HG22	2:B:145:LEU:HD21	1.87	0.56
1:A:186:ASP:OD2	1:A:279:THR:HB	2.06	0.56
2:B:350:PRO:HG2	2:B:437:LYS:HG3	1.88	0.56
1:G:64:GLN:HG2	1:G:82:GLY:O	2.06	0.56
1:E:243:PHE:O	1:E:247:ILE:HG13	2.06	0.56
1:G:87:GLU:O	1:G:91:GLU:HG3	2.05	0.56
2:H:218:ILE:HD13	2:H:230:GLU:HG2	1.88	0.56
1:E:500:ALA:HB1	2:F:330:LEU:CD2	2.36	0.56
2:H:354:GLN:HE22	2:H:439:HIS:HB3	1.70	0.56
2:D:357:PRO:HD2	2:D:442:SER:OG	2.06	0.56
2:H:382:THR:HA	2:H:392:LEU:HG	1.88	0.56
1:C:489:GLU:O	1:C:489:GLU:HG2	2.05	0.56
2:H:212:ASN:O	2:H:214:PRO:HD3	2.06	0.56
2:B:430:THR:HG22	2:B:432:GLN:H	1.70	0.55
3:L:124:GLU:HB2	3:L:152:ASP:O	2.06	0.55
1:A:307:LEU:HD22	1:A:383:LEU:CD2	2.36	0.55
2:B:400:ILE:H	2:B:400:ILE:CD1	2.16	0.55
1:C:36:ILE:HB	1:C:128:ALA:HA	1.87	0.55
1:A:297:ILE:CG2	1:A:368:ILE:HD11	2.30	0.55
2:B:320:ASN:HD22	2:B:336:GLU:C	2.10	0.55
3:L:154:LYS:HD2	3:L:159:TYR:CZ	2.41	0.55
2:D:203:THR:O	2:D:205:GLU:N	2.39	0.55
1:G:77:GLN:HG3	1:G:92:PHE:CZ	2.41	0.55
1:E:340:ILE:HD11	2:F:273:ILE:HG12	1.89	0.55
1:A:307:LEU:HD22	1:A:383:LEU:HD22	1.89	0.55
1:E:56:SER:CB	1:E:101:SER:HB2	2.35	0.55
3:L:170:VAL:CG1	3:L:171:LEU:N	2.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:28:GLY:O	2:F:31:THR:HG22	2.07	0.55
2:D:128:GLN:HE21	2:D:128:GLN:H	1.55	0.55
1:E:9:LYS:HE3	1:E:99:ASP:OD1	2.06	0.55
3:L:117:ILE:CD1	3:L:126:ILE:HG12	2.32	0.55
1:C:34:CYS:HB2	1:C:123:PHE:CE2	2.42	0.55
2:H:320:ASN:ND2	2:H:336:GLU:CG	2.70	0.55
1:E:347:ARG:HH22	2:F:274:ARG:NH1	2.04	0.55
2:H:362:GLN:O	2:H:362:GLN:NE2	2.39	0.55
2:B:164:TYR:CE2	2:B:169:LEU:HB2	2.42	0.55
1:C:15:ARG:HG3	2:D:90:ARG:NH1	2.22	0.55
1:G:6:LYS:C	1:G:8:LEU:H	2.09	0.55
1:A:201:LEU:HD13	1:A:209:HIS:CE1	2.42	0.55
2:H:402:GLU:HG3	2:H:405:ARG:NH2	2.21	0.55
3:I:170:VAL:HG13	3:I:171:LEU:H	1.72	0.55
2:B:419:ASP:HB2	2:B:440:PHE:CD1	2.42	0.55
1:E:282:PRO:HB2	1:E:285:ILE:HD13	1.88	0.55
2:F:64:LEU:HD21	2:F:77:VAL:CG2	2.37	0.54
1:C:518:ASN:HB3	1:C:532:PHE:O	2.07	0.54
1:E:61:ASP:HB3	1:E:86:ALA:HB2	1.89	0.54
2:D:187:GLY:HA2	3:J:173:LEU:HD13	1.89	0.54
2:B:353:ILE:HG23	2:B:355:PHE:HD1	1.73	0.54
1:E:513:PHE:N	1:E:513:PHE:CD1	2.74	0.54
2:D:241:GLN:HE21	2:D:246:GLY:H	1.53	0.54
1:E:307:LEU:HD22	1:E:383:LEU:CD2	2.38	0.54
1:C:409:LYS:O	1:C:413:ILE:HG13	2.07	0.54
2:H:348:GLN:HB3	2:H:349:LEU:HD12	1.89	0.54
2:B:187:GLY:HA2	3:I:173:LEU:HD13	1.88	0.54
2:H:235:LEU:HD22	2:H:235:LEU:N	2.22	0.54
2:D:158:LEU:HD12	2:D:177:LEU:HD22	1.89	0.54
2:F:319:ASN:O	2:F:320:ASN:HB2	2.07	0.54
1:G:246:LEU:HD23	1:G:246:LEU:C	2.28	0.54
3:K:101:MET:HB3	3:K:117:ILE:O	2.07	0.54
2:F:404:THR:HA	2:F:407:ASN:HD22	1.71	0.54
1:C:264:ASN:HD22	1:C:264:ASN:H	1.55	0.54
1:C:146:SER:O	1:C:147:GLN:HB2	2.08	0.54
2:F:234:MET:HG2	2:F:234:MET:O	2.06	0.54
1:E:505:VAL:O	1:E:509:ILE:HG13	2.07	0.54
1:A:201:LEU:HD23	1:A:204:MET:SD	2.47	0.54
2:B:380:ALA:HB2	2:B:394:LEU:HD12	1.88	0.54
1:C:500:ALA:HB1	2:D:330:LEU:HD21	1.90	0.54
1:A:214:TRP:CD1	1:A:214:TRP:C	2.81	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:357:PRO:HG3	2:H:440:PHE:CD2	2.42	0.54
2:F:64:LEU:HD21	2:F:77:VAL:HG23	1.89	0.54
2:H:368:LEU:HD13	2:H:376:MET:HE3	1.90	0.54
1:G:309:ARG:HG3	1:G:364:LEU:HD21	1.89	0.54
2:H:27:SER:HB3	2:H:37:PRO:HG3	1.88	0.54
1:G:175:HIS:HD2	1:G:512:GLN:O	1.90	0.54
2:H:417:LEU:HD23	2:H:421:GLN:NE2	2.23	0.54
2:F:251:GLY:O	2:F:286:LYS:HD3	2.07	0.54
1:A:46:LEU:O	1:A:50:VAL:HG23	2.07	0.54
1:G:84:ASN:CG	1:G:106:GLU:HG2	2.28	0.54
1:C:56:SER:HB3	1:C:101:SER:HB3	1.90	0.54
1:E:264:ASN:HD22	1:E:265:PHE:H	1.55	0.54
1:E:264:ASN:ND2	1:E:265:PHE:N	2.56	0.54
2:F:425:VAL:HB	2:F:434:VAL:CG1	2.37	0.54
2:H:392:LEU:HD23	2:H:392:LEU:H	1.73	0.54
2:H:46:LEU:HD23	2:H:71:GLY:O	2.08	0.54
2:B:397:VAL:HG12	2:B:399:SER:H	1.72	0.53
2:F:417:LEU:HB3	2:F:421:GLN:OE1	2.08	0.53
1:G:184:ARG:NH1	1:G:325:VAL:HG22	2.23	0.53
1:E:437:LYS:HE3	1:E:437:LYS:O	2.08	0.53
2:F:183:GLU:HB2	3:K:173:LEU:HD22	1.89	0.53
2:D:225:PRO:HB2	2:D:280:LEU:HD21	1.89	0.53
1:A:518:ASN:HB3	1:A:532:PHE:O	2.08	0.53
1:C:72:ASN:ND2	1:C:73:ASN:N	2.56	0.53
1:E:188:PRO:HG2	1:E:193:ARG:NH2	2.23	0.53
3:J:125:ARG:HD3	3:J:129:ARG:NH2	2.23	0.53
1:A:74:PHE:CD1	2:B:65:LYS:HG3	2.43	0.53
2:B:49:CYS:HA	2:B:139:HIS:HD2	1.71	0.53
2:D:16:ARG:HH22	2:D:116:PRO:HB2	1.72	0.53
2:B:214:PRO:HG2	2:B:217:THR:CG2	2.38	0.53
1:E:450:VAL:O	1:E:454:ILE:HG13	2.08	0.53
2:B:235:LEU:O	2:B:238:PRO:HD2	2.09	0.53
2:B:323:VAL:HG23	2:B:333:TYR:HB3	1.89	0.53
1:A:423:ILE:O	1:A:426:TYR:HB3	2.09	0.53
2:F:197:THR:HG22	2:F:198:ALA:N	2.23	0.53
3:I:122:LYS:HA	3:I:155:THR:HA	1.91	0.53
2:H:412:LEU:C	2:H:417:LEU:HB2	2.29	0.53
2:H:267:ARG:CG	2:H:267:ARG:HH11	2.21	0.53
1:C:368:ILE:O	1:C:368:ILE:HG22	2.07	0.53
2:H:88:LEU:HD13	2:H:96:PRO:HG3	1.91	0.53
2:F:178:ILE:HD11	2:F:310:ILE:CD1	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:74:GLN:NE2	2:F:74:GLN:HA	2.23	0.53
1:E:325:VAL:HG21	1:E:349:LYS:HG3	1.90	0.53
3:K:123:VAL:HG22	3:K:150:MET:HE2	1.91	0.53
1:C:447:ASN:ND2	2:D:26:ARG:NE	2.53	0.53
1:C:66:SER:H	1:C:69:ASP:HB2	1.74	0.53
1:A:227:SER:O	1:A:229:THR:N	2.37	0.53
2:B:320:ASN:ND2	2:B:337:ALA:O	2.41	0.53
2:H:405:ARG:HB3	2:H:405:ARG:HH11	1.74	0.53
1:C:214:TRP:CE3	1:C:332:MET:HB3	2.44	0.53
2:H:320:ASN:ND2	2:H:336:GLU:C	2.56	0.53
1:G:201:LEU:HD22	1:G:221:TYR:HE1	1.73	0.53
1:C:209:HIS:NE2	1:C:252:LEU:HD23	2.24	0.53
2:H:32:HIS:HD2	2:H:34:ASP:H	1.57	0.53
1:E:347:ARG:HH22	2:F:274:ARG:HH11	1.57	0.53
1:G:213:PRO:HB3	1:G:332:MET:SD	2.49	0.53
2:H:32:HIS:CD2	2:H:34:ASP:H	2.25	0.53
1:A:366:GLN:C	1:A:368:ILE:H	2.12	0.52
2:D:412:LEU:O	2:D:415:LEU:HD12	2.10	0.52
1:G:503:GLN:NE2	2:H:185:PHE:CE2	2.77	0.52
2:H:325:ASN:HD22	2:H:326:ASP:H	1.56	0.52
1:E:240:LYS:HZ3	1:E:276:LEU:HD12	1.73	0.52
2:F:95:ARG:HG3	2:F:97:LYS:NZ	2.24	0.52
2:B:381:ILE:CG2	2:B:423:LEU:HD22	2.39	0.52
2:F:380:ALA:HB1	2:F:394:LEU:HD12	1.90	0.52
2:H:231:TYR:CD2	2:H:267:ARG:HG2	2.44	0.52
1:C:518:ASN:HB2	1:C:533:GLN:HA	1.90	0.52
2:D:405:ARG:HB3	2:D:405:ARG:NH1	2.23	0.52
1:A:189:PHE:CE1	1:A:192:LEU:HB2	2.44	0.52
1:E:377:GLU:CG	1:E:381:LYS:HE3	2.37	0.52
2:D:240:GLU:O	2:D:241:GLN:C	2.48	0.52
1:G:124:THR:HG22	1:G:125:VAL:HG23	1.90	0.52
1:E:49:LEU:O	1:E:52:PRO:HG2	2.10	0.52
3:K:118:GLU:O	3:K:120:THR:N	2.43	0.52
1:C:438:GLN:O	1:C:438:GLN:HG2	2.08	0.52
2:H:228:CYS:SG	2:H:268:ALA:HA	2.48	0.52
2:B:183:GLU:HG3	3:I:173:LEU:HB3	1.91	0.52
1:E:222:LEU:O	1:E:226:TYR:HB3	2.09	0.52
1:C:434:ARG:HH11	1:C:464:PHE:HA	1.74	0.52
1:A:450:VAL:O	1:A:454:ILE:HG13	2.09	0.52
2:F:316:ILE:N	2:F:316:ILE:HD12	2.10	0.52
2:D:411:THR:O	2:D:415:LEU:HG	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:178:ILE:HD12	2:H:307:VAL:CG2	2.39	0.52
2:B:326:ASP:HB3	2:B:330:LEU:HD23	1.91	0.52
1:C:61:ASP:HB3	1:C:86:ALA:HB2	1.91	0.52
2:D:64:LEU:HD21	2:D:77:VAL:HG22	1.91	0.52
2:D:330:LEU:N	2:D:330:LEU:HD12	2.25	0.52
1:E:45:ILE:HG12	1:E:498:GLY:HA2	1.92	0.52
1:E:65:VAL:HG22	1:E:85:ARG:HG3	1.91	0.52
1:A:66:SER:OG	1:A:67:GLY:N	2.43	0.52
2:H:440:PHE:O	2:H:441:THR:HG23	2.09	0.52
2:B:182:THR:HG21	2:B:296:ASN:OD1	2.10	0.52
1:C:121:CYS:HA	1:C:148:ILE:HD11	1.92	0.52
1:E:504:GLU:O	1:E:508:ILE:HG13	2.09	0.52
1:G:115:ASN:O	1:G:117:PRO:HD3	2.10	0.52
2:B:361:LEU:HB3	2:B:407:ASN:O	2.10	0.52
2:H:267:ARG:O	2:H:267:ARG:HG3	2.10	0.52
2:D:251:GLY:O	2:D:257:ILE:HD11	2.10	0.52
2:H:240:GLU:O	2:H:242:PRO:HD3	2.09	0.52
2:F:282:GLN:O	2:F:286:LYS:HG3	2.10	0.52
1:G:262:GLU:HB2	1:G:265:PHE:HB2	1.91	0.52
2:H:87:ASN:HB3	2:H:91:GLN:CD	2.30	0.52
1:A:196:PHE:O	1:A:220:LYS:HE2	2.10	0.52
2:H:123:HIS:HB3	2:H:125:ASN:HD22	1.75	0.52
1:G:158:LEU:HD22	1:G:158:LEU:N	2.24	0.52
2:D:178:ILE:HD11	2:D:310:ILE:HD12	1.92	0.52
1:C:72:ASN:HD22	1:C:73:ASN:N	2.08	0.52
1:A:428:MET:CE	1:A:479:VAL:HA	2.39	0.52
2:H:249:LEU:HA	2:H:256:HIS:ND1	2.24	0.52
3:I:117:ILE:HD11	3:I:126:ILE:HG23	1.91	0.52
1:A:418:ASN:ND2	1:A:420:ASP:H	2.08	0.52
2:B:61:CYS:HB3	2:B:93:LEU:HG	1.91	0.52
1:E:47:LYS:HG2	1:E:96:LEU:HD11	1.92	0.51
3:L:161:ILE:HG23	3:L:165:SER:OG	2.10	0.51
2:H:52:LEU:HD11	2:H:78:ILE:HG13	1.91	0.51
2:H:354:GLN:NE2	2:H:354:GLN:HA	2.25	0.51
2:B:197:THR:HG22	2:B:198:ALA:O	2.10	0.51
1:C:357:VAL:O	1:C:361:VAL:HG23	2.09	0.51
2:B:427:ASP:OD1	2:B:429:THR:HG22	2.10	0.51
3:K:104:LYS:HD2	3:K:112:GLU:OE2	2.10	0.51
1:C:115:ASN:C	1:C:117:PRO:HD3	2.29	0.51
1:A:224:GLN:NE2	1:A:246:LEU:HD11	2.25	0.51
1:E:36:ILE:HG21	1:E:131:LEU:HD21	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:162:MET:HE1	1:E:501:ALA:HA	1.92	0.51
2:H:16:ARG:NH2	2:H:116:PRO:HB2	2.25	0.51
2:F:199:CYS:SG	2:F:201:GLU:HB2	2.51	0.51
2:H:233:ARG:HG2	2:H:233:ARG:HH11	1.75	0.51
2:B:81:ASP:CB	2:B:103:LYS:HE3	2.40	0.51
1:E:158:LEU:HA	1:E:493:ILE:HG12	1.93	0.51
2:F:259:TRP:CH2	2:F:263:LYS:HG3	2.45	0.51
1:C:51:LEU:N	1:C:52:PRO:HD2	2.25	0.51
1:E:376:SER:OG	1:E:379:GLU:HG2	2.10	0.51
2:B:353:ILE:HG22	2:B:438:LEU:HD12	1.91	0.51
1:A:78:ARG:C	1:A:80:SER:H	2.13	0.51
2:D:319:ASN:ND2	2:D:336:GLU:HG3	2.25	0.51
1:E:162:MET:CE	1:E:501:ALA:HA	2.41	0.51
2:D:87:ASN:HD21	2:D:103:LYS:HE2	1.76	0.51
2:B:232:VAL:HA	2:B:236:GLN:HB2	1.93	0.51
2:F:75:ILE:O	2:F:120:VAL:HA	2.11	0.51
2:B:353:ILE:HD11	2:B:367:TYR:HE2	1.74	0.51
2:F:232:VAL:HG11	2:F:263:LYS:HB2	1.93	0.51
1:E:307:LEU:HB3	1:E:383:LEU:CD2	2.41	0.51
1:A:527:GLN:HG3	2:B:306:GLU:OE1	2.09	0.51
2:B:267:ARG:HA	2:B:270:GLN:HE21	1.76	0.51
1:C:430:ARG:HH11	1:C:430:ARG:HB3	1.75	0.51
1:C:130:GLN:HA	1:C:154:ARG:HD2	1.92	0.51
2:F:411:THR:N	2:F:414:GLU:HB3	2.22	0.51
2:D:361:LEU:HD21	2:D:392:LEU:HB3	1.93	0.51
1:E:264:ASN:N	1:E:264:ASN:HD22	2.07	0.51
3:J:115:ILE:HG23	3:J:129:ARG:HB3	1.92	0.51
2:D:393:TYR:CE2	2:D:408:LEU:HD11	2.45	0.51
2:F:374:LEU:O	2:F:375:GLN:C	2.49	0.51
1:A:163:ARG:HG2	1:A:163:ARG:HH11	1.76	0.51
2:H:354:GLN:HE21	2:H:354:GLN:HA	1.76	0.51
2:F:241:GLN:O	2:F:242:PRO:C	2.49	0.51
2:D:84:ASP:O	2:D:87:ASN:HB2	2.10	0.51
1:C:430:ARG:NH1	1:C:430:ARG:HB3	2.25	0.51
1:A:225:TRP:CE2	1:A:234:PRO:HG3	2.46	0.51
2:H:197:THR:CG2	2:H:320:ASN:OD1	2.59	0.51
1:C:293:ARG:HH11	1:C:293:ARG:CG	2.24	0.51
1:C:229:THR:HG21	1:C:232:ARG:HB2	1.92	0.51
2:H:84:ASP:H	2:H:87:ASN:ND2	2.08	0.51
1:A:454:ILE:HD13	1:A:480:HIS:CD2	2.45	0.51
1:G:336:SER:HB2	2:H:221:MET:HA	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:231:TYR:CE2	2:F:267:ARG:HD3	2.46	0.51
1:E:352:LYS:O	1:E:355:ALA:HB3	2.10	0.51
1:E:264:ASN:HD22	1:E:265:PHE:N	2.09	0.50
3:L:104:LYS:O	3:L:166:VAL:HA	2.11	0.50
2:F:349:LEU:CD1	2:F:349:LEU:H	2.24	0.50
1:G:407:ILE:HG13	1:G:408:ASN:N	2.26	0.50
1:E:74:PHE:CD1	2:F:65:LYS:HG3	2.45	0.50
1:C:84:ASN:OD1	1:C:106:GLU:HG2	2.11	0.50
2:D:141:ILE:CD1	2:D:158:LEU:HD21	2.41	0.50
1:G:441:ARG:NH2	1:G:453:ASP:OD2	2.43	0.50
3:J:138:PRO:O	3:J:141:GLN:HB2	2.11	0.50
1:C:528:THR:HG22	2:D:334:THR:OG1	2.11	0.50
3:L:107:THR:CG2	3:L:111:LYS:HB3	2.41	0.50
1:C:67:GLY:H	2:H:262:GLN:HE22	1.59	0.50
1:C:67:GLY:H	2:H:262:GLN:NE2	2.09	0.50
2:H:223:ARG:HH11	2:H:223:ARG:HG3	1.76	0.50
1:A:251:ILE:O	1:A:252:LEU:C	2.49	0.50
3:I:139:GLN:O	3:I:142:ARG:NH2	2.43	0.50
2:B:64:LEU:HD21	2:B:77:VAL:HG22	1.92	0.50
1:A:13:TYR:O	1:A:16:GLN:HG2	2.12	0.50
1:A:376:SER:OG	1:A:379:GLU:HG3	2.11	0.50
1:A:108:SER:HB3	1:A:111:ASN:HB2	1.92	0.50
1:A:116:ASP:N	1:A:117:PRO:HD3	2.26	0.50
2:D:357:PRO:HG3	2:D:440:PHE:CD1	2.46	0.50
2:F:241:GLN:HG3	2:F:245:GLU:HA	1.94	0.50
1:C:407:ILE:HG23	1:C:409:LYS:HG3	1.93	0.50
1:C:214:TRP:CD1	1:C:215:ILE:N	2.79	0.50
3:L:105:VAL:HG23	3:L:167:LEU:HB2	1.92	0.50
1:A:38:ALA:HB2	1:A:59:ILE:HG21	1.93	0.50
1:E:241:GLU:OE1	1:E:244:ARG:HD2	2.12	0.50
1:A:204:MET:O	1:A:209:HIS:HB2	2.11	0.50
2:B:251:GLY:O	2:B:257:ILE:HD11	2.11	0.50
2:F:257:ILE:HG21	2:F:282:GLN:HG2	1.94	0.50
2:B:267:ARG:HA	2:B:270:GLN:HG2	1.93	0.50
1:C:34:CYS:HB2	1:C:123:PHE:CZ	2.46	0.50
1:E:58:THR:HA	1:E:103:SER:O	2.11	0.50
2:F:205:GLU:O	2:F:207:TYR:N	2.45	0.50
1:E:72:ASN:ND2	1:E:72:ASN:C	2.65	0.50
2:F:158:LEU:HD12	2:F:175:VAL:HB	1.92	0.50
1:E:502:ALA:O	1:E:505:VAL:HB	2.11	0.50
2:H:372:ALA:HA	2:H:375:GLN:NE2	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:412:LEU:HD23	2:F:417:LEU:HD13	1.93	0.50
2:B:434:VAL:HG13	2:B:436:PHE:HE1	1.77	0.50
1:A:229:THR:O	1:A:230:ASN:HB2	2.12	0.50
2:F:374:LEU:O	2:F:376:MET:HG3	2.12	0.50
2:B:54:ILE:CG2	2:B:145:LEU:HD21	2.42	0.50
1:A:163:ARG:NH1	1:A:165:ILE:HG12	2.27	0.50
2:H:383:ALA:HB2	2:H:423:LEU:CD2	2.42	0.50
1:A:264:ASN:HD22	1:A:265:PHE:H	1.60	0.50
1:G:201:LEU:HD22	1:G:221:TYR:CE1	2.47	0.50
3:I:103:ILE:HD11	3:I:117:ILE:HD12	1.91	0.50
1:A:168:GLU:HG3	1:A:394:ARG:CG	2.41	0.50
3:J:115:ILE:HG22	3:J:116:ASP:N	2.26	0.50
2:H:63:LEU:HD22	2:H:142:VAL:HG11	1.93	0.50
2:D:398:THR:O	2:D:402:GLU:HG3	2.12	0.50
1:G:72:ASN:C	1:G:72:ASN:ND2	2.63	0.50
1:G:233:ILE:O	1:G:235:LYS:HG3	2.12	0.49
1:A:221:TYR:OH	1:A:250:GLY:HA3	2.11	0.49
1:G:264:ASN:ND2	1:G:265:PHE:H	2.08	0.49
2:H:438:LEU:HD12	2:H:439:HIS:N	2.27	0.49
2:F:434:VAL:HG13	2:F:436:PHE:HE1	1.76	0.49
2:D:206:LEU:HB2	3:J:172:GLN:NE2	2.27	0.49
1:A:489:GLU:H	2:B:19:HIS:HD2	1.60	0.49
1:A:491:HIS:CD2	2:B:69:LEU:HD12	2.47	0.49
2:F:392:LEU:HD12	2:F:392:LEU:N	2.22	0.49
2:H:240:GLU:O	2:H:242:PRO:CD	2.60	0.49
2:F:216:ALA:O	2:F:220:SER:HB2	2.12	0.49
1:G:19:LEU:HG	2:H:290:PRO:HB3	1.94	0.49
1:A:190:PRO:O	1:A:194:GLU:HG3	2.13	0.49
1:E:422:GLU:H	1:E:422:GLU:CD	2.15	0.49
2:H:349:LEU:HB3	2:H:350:PRO:CD	2.42	0.49
1:G:84:ASN:OD1	1:G:86:ALA:HB3	2.11	0.49
1:G:299:LYS:HE2	1:G:368:ILE:O	2.13	0.49
2:B:197:THR:CG2	2:B:198:ALA:N	2.75	0.49
3:I:117:ILE:HG22	3:I:118:GLU:N	2.27	0.49
2:F:229:ILE:HA	2:F:264:SER:OG	2.12	0.49
1:C:66:SER:CB	2:H:262:GLN:HE22	2.19	0.49
2:H:232:VAL:HG11	2:H:260:ILE:HA	1.93	0.49
1:A:248:ARG:HG2	1:A:269:ILE:HD11	1.94	0.49
2:D:323:VAL:HG23	2:D:333:TYR:HB3	1.95	0.49
3:J:170:VAL:HG22	3:J:171:LEU:N	2.28	0.49
3:J:171:LEU:HD12	3:J:172:GLN:H	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:123:VAL:HB	3:L:152:ASP:HA	1.92	0.49
1:A:214:TRP:CZ3	1:A:332:MET:HG2	2.46	0.49
2:D:429:THR:HG23	2:D:430:THR:HG22	1.93	0.49
1:C:8:LEU:O	1:C:11:GLN:HB2	2.13	0.49
2:H:319:ASN:HD22	2:H:320:ASN:N	2.10	0.49
2:D:415:LEU:CD1	2:D:417:LEU:HG	2.43	0.49
2:F:54:ILE:HG22	2:F:145:LEU:CD2	2.42	0.49
1:E:340:ILE:HD13	2:F:272:ASN:O	2.13	0.49
1:C:426:TYR:HB2	1:C:521:ILE:CD1	2.43	0.49
1:C:309:ARG:HD2	1:C:313:GLU:OE2	2.12	0.49
1:C:158:LEU:HD12	1:C:525:MET:HG2	1.94	0.49
2:H:380:ALA:CB	2:H:394:LEU:CD1	2.89	0.49
2:H:318:LEU:HD11	2:H:334:THR:CG2	2.43	0.49
2:H:270:GLN:HB2	2:H:271:TYR:CE1	2.48	0.49
1:E:72:ASN:HD22	1:E:72:ASN:C	2.13	0.49
1:G:349:LYS:O	1:G:353:ASP:HB2	2.13	0.49
1:A:53:GLY:O	1:A:54:ILE:C	2.49	0.49
2:B:62:GLU:HG2	2:B:300:ALA:HB3	1.95	0.49
2:H:35:PHE:HB2	2:H:313:SER:O	2.13	0.49
2:H:158:LEU:HA	2:H:161:LEU:HD12	1.94	0.49
1:G:186:ASP:OD2	1:G:279:THR:HB	2.13	0.49
2:F:338:GLU:HG3	3:K:148:LYS:HA	1.95	0.49
2:H:357:PRO:HA	2:H:440:PHE:CE2	2.47	0.49
3:K:107:THR:HG22	3:K:109:THR:H	1.78	0.49
2:B:62:GLU:OE2	2:B:65:LYS:NZ	2.36	0.49
2:H:394:LEU:HG	2:H:396:SER:H	1.78	0.49
1:E:309:ARG:HD3	1:E:309:ARG:O	2.13	0.49
2:B:207:TYR:CE2	3:I:172:GLN:HG2	2.48	0.49
1:A:104:PHE:CE1	1:A:106:GLU:HG3	2.48	0.49
2:B:190:ARG:HH22	2:B:203:THR:CG2	2.24	0.49
1:A:253:LYS:CB	1:A:260:GLU:HG3	2.43	0.48
2:B:399:SER:HB3	2:B:400:ILE:HD12	1.95	0.48
1:A:78:ARG:HD2	2:B:13:TRP:CE3	2.48	0.48
1:A:36:ILE:HG22	1:A:36:ILE:O	2.13	0.48
1:A:201:LEU:HD22	1:A:209:HIS:CE1	2.47	0.48
3:K:104:LYS:CG	3:K:114:GLU:HG2	2.42	0.48
2:D:187:GLY:CA	3:J:173:LEU:HD13	2.42	0.48
2:D:271:TYR:O	2:D:272:ASN:HB2	2.12	0.48
1:G:488:ALA:C	1:G:490:PRO:HD3	2.33	0.48
3:I:102:LEU:CD2	3:I:102:LEU:H	2.27	0.48
2:F:419:ASP:N	2:F:419:ASP:OD1	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:526:SER:O	1:A:527:GLN:HB2	2.13	0.48
3:K:131:GLU:OE2	3:K:138:PRO:HD3	2.13	0.48
1:A:51:LEU:N	1:A:52:PRO:HD2	2.28	0.48
1:A:366:GLN:C	1:A:368:ILE:N	2.67	0.48
2:D:237:TRP:CE3	2:D:242:PRO:HG3	2.48	0.48
3:I:170:VAL:HG12	3:I:171:LEU:N	2.28	0.48
1:G:264:ASN:ND2	1:G:265:PHE:N	2.61	0.48
1:A:41:THR:CG2	1:A:497:LEU:HD23	2.43	0.48
2:H:322:LEU:HD23	2:H:322:LEU:C	2.34	0.48
2:H:320:ASN:HD22	2:H:336:GLU:HA	1.77	0.48
2:H:325:ASN:HD22	2:H:326:ASP:N	2.12	0.48
1:A:227:SER:C	1:A:229:THR:N	2.65	0.48
1:G:265:PHE:O	1:G:269:ILE:HG13	2.14	0.48
1:A:519:THR:HG22	1:A:521:ILE:HD12	1.96	0.48
1:E:38:ALA:O	1:E:85:ARG:HD3	2.13	0.48
2:H:125:ASN:ND2	2:H:130:PHE:HZ	2.10	0.48
1:C:90:MET:O	1:C:94:GLN:HB2	2.13	0.48
2:F:192:ILE:HG22	2:F:194:PRO:HD3	1.95	0.48
1:G:181:GLU:O	1:G:278:THR:HB	2.13	0.48
2:H:354:GLN:NE2	2:H:439:HIS:HB3	2.28	0.48
2:H:213:PHE:H	2:H:213:PHE:HD1	1.61	0.48
2:H:223:ARG:O	2:H:273:ILE:HD13	2.12	0.48
2:B:16:ARG:NH2	2:B:116:PRO:HB2	2.29	0.48
1:C:344:ASN:HD21	1:C:347:ARG:NH2	2.12	0.48
1:G:40:ALA:O	1:G:43:THR:HG22	2.14	0.48
1:E:500:ALA:HB1	2:F:330:LEU:HD21	1.95	0.48
2:B:411:THR:C	2:B:413:LYS:H	2.17	0.48
1:E:307:LEU:HB3	1:E:383:LEU:HD22	1.95	0.48
2:B:197:THR:HG23	2:B:320:ASN:OD1	2.14	0.48
2:B:321:TYR:OH	3:I:172:GLN:HG3	2.13	0.48
1:A:484:ARG:NH1	1:A:484:ARG:HG2	2.27	0.48
1:C:74:PHE:CE2	2:D:92:PHE:HE1	2.30	0.48
2:D:279:ARG:O	2:D:282:GLN:HB2	2.14	0.48
1:C:428:MET:CE	1:C:479:VAL:HA	2.44	0.48
3:I:107:THR:CG2	3:I:109:THR:H	2.19	0.48
3:I:117:ILE:HD13	3:I:126:ILE:HG12	1.96	0.48
1:A:248:ARG:C	1:A:250:GLY:H	2.17	0.48
2:B:413:LYS:HA	2:B:413:LYS:CE	2.34	0.48
1:E:34:CYS:HB2	1:E:123:PHE:CE2	2.49	0.48
2:B:126:LYS:O	2:B:128:GLN:N	2.47	0.48
3:J:105:VAL:HG13	3:J:113:ILE:CG1	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:50:VAL:HG13	1:C:100:VAL:HG21	1.96	0.48
2:F:178:ILE:HD11	2:F:310:ILE:HD12	1.95	0.48
1:C:158:LEU:HA	1:C:493:ILE:HG13	1.96	0.48
1:G:65:VAL:CG2	1:G:85:ARG:HA	2.43	0.48
1:E:527:GLN:OE1	1:E:527:GLN:HA	2.14	0.48
2:F:132:ASP:HA	2:F:157:MET:HE2	1.95	0.48
1:A:361:VAL:HG12	1:A:365:LEU:HD12	1.95	0.48
1:G:226:TYR:CZ	1:G:233:ILE:HG22	2.48	0.48
2:H:405:ARG:HB3	2:H:405:ARG:NH1	2.29	0.48
3:K:103:ILE:HG12	3:K:117:ILE:HD13	1.96	0.48
2:H:413:LYS:C	2:H:415:LEU:H	2.16	0.48
1:C:342:LEU:HD11	1:C:346:TYR:HE1	1.79	0.48
2:B:434:VAL:HG13	2:B:436:PHE:CE1	2.49	0.47
2:B:415:LEU:O	2:B:417:LEU:HD22	2.14	0.47
1:A:418:ASN:C	1:A:418:ASN:HD22	2.17	0.47
1:C:38:ALA:HB2	1:C:59:ILE:CG2	2.44	0.47
3:L:149:GLN:HG3	3:L:149:GLN:O	2.15	0.47
2:H:316:ILE:CD1	2:H:316:ILE:H	1.99	0.47
2:H:270:GLN:HB2	2:H:271:TYR:CD1	2.49	0.47
1:E:236:THR:CG2	1:E:237:TYR:N	2.77	0.47
1:C:36:ILE:HG21	1:C:131:LEU:HD21	1.96	0.47
1:C:500:ALA:O	1:C:504:GLU:HG2	2.13	0.47
1:C:229:THR:HG22	1:C:232:ARG:HB2	1.94	0.47
2:F:92:PHE:CD2	2:F:92:PHE:N	2.79	0.47
1:C:105:VAL:HG12	1:C:107:GLU:H	1.79	0.47
2:F:58:GLY:H	2:F:91:GLN:HG2	1.79	0.47
3:K:143:LEU:O	3:K:144:ILE:HD12	2.14	0.47
2:F:217:THR:HG21	2:F:223:ARG:HH22	1.79	0.47
1:A:375:ILE:HD12	1:A:375:ILE:N	2.29	0.47
2:F:225:PRO:HG3	2:F:274:ARG:O	2.15	0.47
2:D:306:GLU:OE2	2:D:317:PRO:HA	2.14	0.47
2:B:190:ARG:NH2	2:B:203:THR:CG2	2.77	0.47
1:G:192:LEU:HD12	1:G:345:VAL:HG11	1.94	0.47
2:D:231:TYR:CD1	2:D:235:LEU:HD12	2.48	0.47
1:G:347:ARG:HH22	2:H:274:ARG:HD2	1.78	0.47
1:E:121:CYS:HA	1:E:148:ILE:HD11	1.95	0.47
2:D:355:PHE:O	2:D:440:PHE:HA	2.14	0.47
1:E:191:GLU:O	1:E:194:GLU:HB2	2.13	0.47
1:A:264:ASN:N	1:A:264:ASN:ND2	2.59	0.47
3:I:103:ILE:HD13	3:I:117:ILE:HD12	1.95	0.47
1:C:500:ALA:HB1	2:D:330:LEU:CD2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:320:ASN:OD1	2:F:337:ALA:N	2.47	0.47
2:D:87:ASN:ND2	2:D:103:LYS:HE2	2.29	0.47
1:C:158:LEU:HD22	1:C:493:ILE:HD11	1.95	0.47
2:B:371:SER:O	2:B:373:SER:N	2.48	0.47
2:H:59:LEU:HB2	3:L:176:GLY:O	2.15	0.47
2:B:353:ILE:O	2:B:439:HIS:HB2	2.13	0.47
1:G:226:TYR:O	1:G:231:GLY:N	2.41	0.47
1:A:518:ASN:CB	1:A:533:GLN:HA	2.44	0.47
2:B:384:THR:HA	2:B:389:ASN:ND2	2.28	0.47
2:D:306:GLU:CD	2:D:318:LEU:H	2.17	0.47
1:A:156:TYR:CZ	1:A:432:VAL:HG11	2.49	0.47
2:D:21:LYS:HD3	2:D:25:GLU:OE2	2.15	0.47
2:D:325:ASN:ND2	2:D:327:VAL:H	2.11	0.47
2:B:321:TYR:HH	3:I:172:GLN:CD	2.17	0.47
3:L:145:TYR:HB2	3:L:167:LEU:HD22	1.97	0.47
2:F:215:MET:SD	2:F:218:ILE:HD12	2.54	0.47
2:H:213:PHE:CD1	2:H:213:PHE:N	2.82	0.47
2:H:266:GLU:C	2:H:268:ALA:N	2.68	0.47
2:H:266:GLU:O	2:H:270:GLN:HG3	2.15	0.47
1:G:424:VAL:CG1	1:G:474:VAL:HG13	2.44	0.47
1:E:307:LEU:HD22	1:E:383:LEU:HD22	1.96	0.47
2:F:235:LEU:O	2:F:238:PRO:HD2	2.15	0.47
2:F:142:VAL:HG21	2:F:307:VAL:CG2	2.42	0.47
1:C:252:LEU:HA	1:C:252:LEU:HD13	1.67	0.47
1:G:7:LEU:O	1:G:7:LEU:HD23	2.14	0.47
1:G:462:THR:O	1:G:466:GLN:HG3	2.15	0.47
1:G:113:LEU:HD11	1:G:139:LEU:HB2	1.97	0.47
1:A:298:THR:C	1:A:300:GLN:H	2.18	0.47
2:D:343:CYS:O	2:D:347:SER:HB3	2.14	0.47
2:F:241:GLN:OE1	2:F:245:GLU:HA	2.15	0.47
2:F:193:LEU:H	2:F:197:THR:HB	1.80	0.47
1:A:336:SER:O	1:A:340:ILE:HG12	2.14	0.47
2:H:245:GLU:HG2	2:H:246:GLY:N	2.30	0.47
2:F:232:VAL:HG12	2:F:260:ILE:HG23	1.97	0.47
3:K:102:LEU:HD12	3:K:116:ASP:OD1	2.15	0.47
2:D:188:ASN:HA	2:D:322:LEU:O	2.14	0.47
1:C:12:LYS:HE3	1:C:13:TYR:CZ	2.50	0.47
2:H:218:ILE:HD13	2:H:230:GLU:CG	2.45	0.47
2:B:64:LEU:HD21	2:B:77:VAL:CG2	2.45	0.47
2:B:350:PRO:HB3	2:B:435:LEU:CB	2.45	0.47
1:C:426:TYR:O	1:C:430:ARG:HG2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:349:LEU:CD1	2:F:349:LEU:N	2.78	0.46
2:H:312:THR:O	2:H:313:SER:HB2	2.14	0.46
2:H:419:ASP:HB2	2:H:440:PHE:HD1	1.80	0.46
2:B:419:ASP:HB2	2:B:440:PHE:HD1	1.80	0.46
2:B:188:ASN:C	2:B:188:ASN:HD22	2.18	0.46
2:H:249:LEU:HA	2:H:256:HIS:CE1	2.50	0.46
1:C:36:ILE:HD13	1:C:60:ILE:HD12	1.98	0.46
1:G:97:ASN:HB3	1:G:100:VAL:HG23	1.97	0.46
2:B:233:ARG:NH1	2:B:287:ARG:HH12	2.13	0.46
2:B:284:VAL:O	2:B:287:ARG:NH1	2.48	0.46
3:L:152:ASP:OD1	3:L:152:ASP:N	2.46	0.46
1:E:162:MET:HB2	1:E:520:TYR:HB3	1.97	0.46
2:H:16:ARG:HH22	2:H:116:PRO:HB2	1.80	0.46
1:A:96:LEU:HD23	2:B:95:ARG:NH2	2.30	0.46
3:K:105:VAL:HG22	3:K:113:ILE:HG12	1.97	0.46
1:A:348:GLU:HG3	1:E:115:ASN:ND2	2.30	0.46
2:F:386:GLU:C	2:F:388:LYS:H	2.17	0.46
2:H:203:THR:O	2:H:205:GLU:N	2.48	0.46
2:B:155:ASN:HB2	2:B:200:ILE:HD13	1.96	0.46
2:H:223:ARG:NH1	2:H:223:ARG:HG3	2.30	0.46
1:G:128:ALA:HB1	1:G:131:LEU:CD1	2.45	0.46
2:B:232:VAL:HG11	2:B:263:LYS:HB2	1.98	0.46
2:D:52:LEU:HB2	2:D:138:PHE:CE2	2.50	0.46
2:D:418:VAL:HG22	2:D:421:GLN:CD	2.35	0.46
2:D:335:PHE:HE2	3:J:170:VAL:HG21	1.80	0.46
2:B:271:TYR:O	2:B:272:ASN:HB2	2.14	0.46
1:E:61:ASP:CB	1:E:86:ALA:HB2	2.45	0.46
2:F:74:GLN:HE21	2:F:74:GLN:HA	1.79	0.46
1:A:489:GLU:H	2:B:19:HIS:CD2	2.34	0.46
2:D:222:PRO:HD2	2:D:271:TYR:CE2	2.50	0.46
1:C:108:SER:OG	1:C:109:PRO:HD2	2.14	0.46
1:A:151:LEU:HD13	1:A:164:ILE:HD13	1.97	0.46
2:F:362:GLN:HG2	2:F:408:LEU:HD22	1.98	0.46
1:E:47:LYS:HG3	1:E:75:PHE:CZ	2.50	0.46
1:E:188:PRO:HG2	1:E:193:ARG:CZ	2.45	0.46
2:B:192:ILE:CD1	2:B:200:ILE:HD12	2.46	0.46
1:C:173:GLU:O	1:C:512:GLN:O	2.33	0.46
2:H:174:ILE:HG23	2:H:194:PRO:HG2	1.97	0.46
2:F:340:LYS:HB3	2:F:342:ASN:ND2	2.30	0.46
2:F:398:THR:C	2:F:401:GLU:HG2	2.36	0.46
1:C:421:ASN:O	1:C:423:ILE:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:356:SER:O	2:D:358:SER:N	2.49	0.46
1:E:138:ARG:HG2	1:E:138:ARG:HH11	1.80	0.46
1:E:314:PHE:CE2	1:E:319:GLY:HA3	2.50	0.46
2:F:83:ILE:CD1	2:F:106:VAL:HG21	2.45	0.46
2:H:239:LYS:O	2:H:239:LYS:HG3	2.15	0.46
1:A:299:LYS:HG2	1:A:368:ILE:O	2.16	0.46
2:F:418:VAL:HG22	2:F:419:ASP:N	2.25	0.46
1:C:72:ASN:N	1:C:72:ASN:HD22	2.08	0.46
1:A:36:ILE:CG2	1:A:36:ILE:O	2.64	0.46
1:G:53:GLY:O	1:G:54:ILE:C	2.54	0.46
1:G:245:ASP:HA	1:G:248:ARG:HG3	1.98	0.46
2:F:95:ARG:HE	2:F:95:ARG:CA	2.29	0.46
1:A:214:TRP:CD1	1:A:215:ILE:N	2.84	0.46
1:G:441:ARG:HH22	1:G:453:ASP:CG	2.18	0.46
1:C:119:PHE:O	1:C:122:ARG:HG2	2.16	0.46
2:D:385:LEU:HD23	2:D:385:LEU:HA	1.74	0.46
1:A:253:LYS:C	1:A:260:GLU:N	2.60	0.46
1:G:28:LEU:HD11	1:G:506:ILE:HD13	1.98	0.46
2:F:259:TRP:CZ2	2:F:263:LYS:HG3	2.51	0.46
1:E:44:GLU:OE2	2:F:65:LYS:HE3	2.15	0.46
1:E:219:ALA:O	1:E:222:LEU:HB3	2.16	0.46
2:D:46:LEU:O	2:D:73:ARG:HB2	2.15	0.46
1:G:244:ARG:NH1	1:G:272:VAL:HB	2.30	0.46
1:E:113:LEU:HD13	1:E:138:ARG:HG2	1.97	0.46
2:F:253:ASP:OD1	2:F:255:GLU:HB2	2.16	0.46
1:E:125:VAL:HG12	1:E:126:VAL:N	2.31	0.46
1:A:474:VAL:O	1:A:475:LYS:C	2.54	0.46
2:D:392:LEU:HD21	2:D:417:LEU:HD21	1.98	0.46
2:B:185:PHE:HB3	2:B:326:ASP:OD2	2.16	0.46
2:B:326:ASP:CB	2:B:330:LEU:HD23	2.46	0.46
2:D:192:ILE:HA	2:D:197:THR:CG2	2.45	0.46
2:D:355:PHE:CE1	2:D:364:VAL:HG22	2.51	0.46
1:A:264:ASN:ND2	1:A:265:PHE:H	2.13	0.46
2:B:321:TYR:OH	3:I:172:GLN:CG	2.64	0.46
1:E:489:GLU:O	1:E:489:GLU:HG2	2.15	0.46
2:H:64:LEU:HD21	2:H:77:VAL:HG22	1.98	0.46
1:C:243:PHE:O	1:C:246:LEU:HB3	2.16	0.46
1:G:47:LYS:HZ1	2:H:65:LYS:HE2	1.79	0.46
1:A:407:ILE:HG23	1:A:407:ILE:O	2.16	0.46
2:B:199:CYS:O	2:B:202:CYS:HB2	2.15	0.46
1:C:435:PHE:C	1:C:435:PHE:CD2	2.88	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:149:ILE:N	2:F:149:ILE:HD12	2.01	0.46
3:L:102:LEU:O	3:L:163:GLY:O	2.34	0.46
3:I:103:ILE:HD11	3:I:117:ILE:CD1	2.45	0.46
2:D:90:ARG:HG2	2:D:90:ARG:HH11	1.81	0.46
1:C:171:VAL:HG13	1:C:391:ARG:HB2	1.97	0.46
1:G:398:LEU:HD12	1:G:401:GLU:OE2	2.16	0.46
2:F:410:LYS:HB3	2:F:414:GLU:CG	2.46	0.45
1:C:214:TRP:CD1	1:C:214:TRP:C	2.89	0.45
1:C:527:GLN:HG3	2:D:306:GLU:OE1	2.15	0.45
2:H:254:PRO:O	2:H:258:GLN:HB2	2.16	0.45
2:D:230:GLU:O	2:D:234:MET:HB3	2.16	0.45
2:B:28:GLY:O	2:B:31:THR:HG23	2.15	0.45
2:H:45:LEU:HD11	2:H:72:PHE:CE2	2.52	0.45
3:K:145:TYR:HB2	3:K:167:LEU:HD22	1.98	0.45
1:A:396:ARG:NH2	1:A:406:THR:O	2.41	0.45
1:E:318:GLU:HG3	1:E:356:ALA:HB1	1.99	0.45
1:G:299:LYS:HG2	1:G:368:ILE:HG23	1.98	0.45
1:G:264:ASN:HD22	1:G:265:PHE:N	2.14	0.45
1:A:35:LEU:HD21	1:A:42:GLY:C	2.37	0.45
1:G:158:LEU:HD21	2:H:23:PHE:CE2	2.51	0.45
2:D:429:THR:CG2	2:D:430:THR:HG22	2.46	0.45
2:H:353:ILE:O	2:H:439:HIS:HB2	2.16	0.45
2:F:232:VAL:HA	2:F:236:GLN:HB3	1.96	0.45
2:H:237:TRP:CE2	2:H:249:LEU:HB3	2.51	0.45
1:C:128:ALA:HB1	1:C:131:LEU:CD1	2.45	0.45
1:E:396:ARG:NH1	1:E:534:LEU:O	2.49	0.45
1:C:166:ILE:HD11	1:C:508:ILE:HD13	1.98	0.45
2:D:405:ARG:HH11	2:D:405:ARG:HB3	1.81	0.45
2:D:405:ARG:O	2:D:408:LEU:HB2	2.17	0.45
1:C:434:ARG:NH1	1:C:463:GLY:C	2.69	0.45
2:H:125:ASN:ND2	2:H:130:PHE:CZ	2.84	0.45
2:H:399:SER:HB2	2:H:403:ARG:HH22	1.81	0.45
2:B:249:LEU:HD13	2:B:260:ILE:HD11	1.98	0.45
3:I:156:ALA:HA	3:I:161:ILE:HD12	1.97	0.45
3:L:138:PRO:HA	3:L:141:GLN:NE2	2.32	0.45
2:F:280:LEU:HD12	2:F:280:LEU:O	2.16	0.45
2:F:361:LEU:HB3	2:F:408:LEU:HA	1.97	0.45
2:F:405:ARG:O	2:F:408:LEU:HB2	2.16	0.45
1:A:518:ASN:HB3	1:A:533:GLN:HA	1.99	0.45
2:B:239:LYS:HA	2:B:239:LYS:HD2	1.76	0.45
2:B:427:ASP:HB3	2:B:429:THR:HG22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:233:ARG:HG2	2:H:233:ARG:NH1	2.31	0.45
2:F:319:ASN:C	2:F:319:ASN:HD22	2.20	0.45
2:H:392:LEU:HD23	2:H:392:LEU:N	2.30	0.45
1:E:113:LEU:HD13	1:E:138:ARG:CG	2.47	0.45
2:H:139:HIS:C	2:H:140:ILE:HG13	2.36	0.45
2:B:226:GLU:CD	2:B:226:GLU:H	2.19	0.45
1:C:327:GLY:CA	1:C:350:ALA:HB2	2.46	0.45
1:A:285:ILE:HG12	1:A:387:SER:O	2.16	0.45
2:F:412:LEU:HA	2:F:417:LEU:HD12	1.98	0.45
3:K:107:THR:HG22	3:K:111:LYS:H	1.81	0.45
2:F:321:TYR:O	2:F:334:THR:HG23	2.17	0.45
2:B:50:LYS:H	2:B:139:HIS:CD2	2.34	0.45
2:H:59:LEU:HD12	3:L:176:GLY:CA	2.46	0.45
2:D:164:TYR:CE2	2:D:169:LEU:HB2	2.51	0.45
3:L:103:ILE:C	3:L:103:ILE:HD12	2.36	0.45
1:E:209:HIS:CG	1:E:252:LEU:HB2	2.52	0.45
1:E:209:HIS:CD2	1:E:252:LEU:H	2.35	0.45
2:B:318:LEU:HD11	2:B:334:THR:HG21	1.96	0.45
1:C:434:ARG:NH1	1:C:464:PHE:HA	2.31	0.45
2:D:94:PHE:N	2:D:94:PHE:CD2	2.82	0.45
2:B:187:GLY:CA	3:I:173:LEU:HD13	2.47	0.45
1:A:298:THR:C	1:A:300:GLN:N	2.70	0.45
2:D:54:ILE:HG22	2:D:145:LEU:HD21	1.98	0.45
2:D:149:ILE:CD1	2:D:149:ILE:N	2.54	0.45
2:H:320:ASN:ND2	2:H:336:GLU:HG2	2.32	0.45
2:H:218:ILE:CD1	2:H:230:GLU:HG2	2.47	0.45
2:F:357:PRO:HD3	2:F:440:PHE:CD2	2.52	0.45
2:B:351:GLN:O	2:B:436:PHE:HA	2.16	0.45
1:A:78:ARG:O	1:A:80:SER:N	2.46	0.45
1:E:317:LYS:HD3	1:E:318:GLU:OE1	2.16	0.45
1:E:236:THR:CG2	1:E:237:TYR:H	2.26	0.45
1:C:78:ARG:C	1:C:80:SER:H	2.20	0.45
3:K:155:THR:HG22	3:K:158:ASP:OD1	2.17	0.45
2:F:349:LEU:HD12	2:F:349:LEU:N	2.32	0.45
1:G:7:LEU:O	1:G:11:GLN:HG3	2.17	0.45
1:E:138:ARG:HG2	1:E:138:ARG:NH1	2.32	0.45
1:G:485:TYR:OH	1:G:525:MET:SD	2.75	0.45
2:H:344:PRO:HG3	2:H:374:LEU:HD22	1.98	0.45
1:E:447:ASN:HD22	1:E:447:ASN:N	2.13	0.45
2:H:320:ASN:CB	2:H:336:GLU:HA	2.44	0.45
1:G:503:GLN:O	1:G:507:LYS:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:120:PHE:O	1:G:148:ILE:HD13	2.16	0.45
1:C:38:ALA:HB2	1:C:59:ILE:HG21	1.99	0.45
2:D:232:VAL:HG11	2:D:263:LYS:HB2	1.99	0.45
2:H:74:GLN:HE22	2:H:119:ASN:HD22	1.64	0.45
1:A:236:THR:HG22	1:A:237:TYR:N	2.32	0.44
1:G:340:ILE:HD11	2:H:273:ILE:CG1	2.42	0.44
2:H:266:GLU:O	2:H:268:ALA:N	2.48	0.44
1:C:503:GLN:CD	2:D:185:PHE:HE2	2.21	0.44
1:E:340:ILE:HD12	2:F:271:TYR:O	2.17	0.44
1:E:47:LYS:HG2	1:E:96:LEU:CD1	2.46	0.44
3:L:105:VAL:HA	3:L:167:LEU:O	2.17	0.44
2:H:241:GLN:O	2:H:242:PRO:C	2.55	0.44
1:C:109:PRO:HG2	1:C:110:GLU:H	1.82	0.44
1:C:512:GLN:HE21	1:C:512:GLN:HB2	1.55	0.44
2:B:84:ASP:H	2:B:87:ASN:ND2	2.16	0.44
2:D:338:GLU:HG3	3:J:148:LYS:HD3	1.99	0.44
3:L:129:ARG:O	3:L:132:GLU:HB3	2.17	0.44
2:H:40:GLU:HG2	2:H:40:GLU:O	2.16	0.44
1:A:397:SER:OG	1:A:400:GLU:HG3	2.17	0.44
2:F:221:MET:N	2:F:222:PRO:HD3	2.33	0.44
1:G:325:VAL:HG21	1:G:349:LYS:CG	2.47	0.44
2:F:106:VAL:O	2:F:109:GLU:HB3	2.16	0.44
1:G:157:GLY:HA3	1:G:485:TYR:CG	2.52	0.44
2:H:225:PRO:HD2	2:H:226:GLU:OE1	2.17	0.44
1:G:503:GLN:OE1	1:G:506:ILE:HB	2.17	0.44
1:G:396:ARG:HD3	1:G:534:LEU:O	2.18	0.44
1:G:426:TYR:CE2	1:G:534:LEU:HD13	2.52	0.44
1:E:359:ASN:HA	1:E:359:ASN:HD22	1.63	0.44
1:A:332:MET:O	1:A:333:ILE:C	2.55	0.44
1:E:422:GLU:HG3	1:E:530:ALA:HB3	1.99	0.44
1:G:311:LEU:O	1:G:314:PHE:HB3	2.18	0.44
2:B:342:ASN:ND2	2:B:342:ASN:N	2.44	0.44
2:F:398:THR:HA	2:F:401:GLU:HG2	1.99	0.44
2:B:357:PRO:HD3	2:B:440:PHE:HB3	1.99	0.44
1:C:480:HIS:HB2	2:D:29:PRO:HG2	1.97	0.44
2:B:217:THR:HB	2:B:223:ARG:HH21	1.81	0.44
1:C:518:ASN:HB3	1:C:533:GLN:HA	1.99	0.44
2:D:85:VAL:C	2:D:87:ASN:H	2.21	0.44
3:K:113:ILE:HG13	3:K:113:ILE:O	2.17	0.44
1:G:311:LEU:HD21	1:G:387:SER:HB2	1.98	0.44
1:E:457:LEU:HD23	1:E:479:VAL:HG13	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:173:GLU:O	1:E:512:GLN:O	2.34	0.44
2:B:374:LEU:O	2:B:376:MET:HG3	2.18	0.44
2:F:362:GLN:HG2	2:F:408:LEU:HB3	1.99	0.44
1:C:80:SER:O	1:C:81:ILE:C	2.55	0.44
1:E:12:LYS:HG3	1:E:13:TYR:CD2	2.52	0.44
1:E:15:ARG:HG3	2:F:90:ARG:NH1	2.33	0.44
2:F:320:ASN:HB3	2:F:321:TYR:H	1.26	0.44
1:G:120:PHE:HA	1:G:123:PHE:CD1	2.53	0.44
1:A:12:LYS:HE3	1:A:13:TYR:CE2	2.52	0.44
2:B:225:PRO:HB2	2:B:280:LEU:HD21	1.99	0.44
2:H:361:LEU:C	2:H:363:GLU:H	2.21	0.44
3:L:117:ILE:CD1	3:L:126:ILE:HA	2.45	0.44
1:G:424:VAL:HG13	1:G:474:VAL:HG13	2.00	0.44
1:C:72:ASN:HD22	1:C:73:ASN:H	1.65	0.44
1:E:265:PHE:O	1:E:269:ILE:HG13	2.18	0.44
2:H:233:ARG:NH1	2:H:234:MET:HB2	2.32	0.44
2:B:323:VAL:O	2:B:332:THR:HA	2.17	0.44
2:D:230:GLU:OE2	2:D:233:ARG:NH1	2.51	0.44
1:A:500:ALA:O	1:A:504:GLU:HG2	2.17	0.44
1:G:371:ALA:HA	1:G:372:PRO:HD3	1.89	0.44
2:D:243:PHE:O	2:D:247:VAL:HG21	2.17	0.44
2:H:294:SER:O	2:H:298:VAL:HG23	2.17	0.44
1:E:221:TYR:HD1	1:E:221:TYR:H	1.65	0.44
2:D:325:ASN:ND2	2:D:326:ASP:N	2.59	0.44
1:A:229:THR:HG22	1:A:232:ARG:H	1.83	0.44
3:I:108:LEU:CD2	3:I:171:LEU:HD23	2.47	0.44
1:G:114:ASP:HA	1:G:138:ARG:NH2	2.32	0.44
2:B:350:PRO:CG	2:B:437:LYS:HG3	2.47	0.44
1:G:6:LYS:N	1:G:6:LYS:HD2	2.33	0.44
1:E:36:ILE:HB	1:E:128:ALA:HA	1.99	0.44
3:I:113:ILE:HD13	3:I:134:GLU:HG2	2.00	0.44
1:C:349:LYS:HE3	1:C:353:ASP:OD1	2.17	0.44
1:A:434:ARG:HD3	1:A:460:CYS:CB	2.47	0.44
2:D:13:TRP:HZ3	2:D:116:PRO:HG2	1.83	0.44
1:A:248:ARG:HG2	1:A:269:ILE:CD1	2.48	0.44
2:F:376:MET:HB3	2:F:427:ASP:OD1	2.18	0.44
1:C:74:PHE:CD2	2:D:65:LYS:HD3	2.53	0.44
2:H:83:ILE:CD1	2:H:106:VAL:HG21	2.48	0.44
1:G:442:TYR:HB3	1:G:443:PRO:HD2	1.99	0.44
1:E:393:VAL:HG11	1:E:515:ILE:HD11	2.00	0.44
2:F:353:ILE:O	2:F:353:ILE:HG22	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:352:ASN:HD22	2:H:437:LYS:HB2	1.83	0.44
2:H:27:SER:HB3	2:H:37:PRO:HG2	2.00	0.44
1:C:19:LEU:HG	2:D:290:PRO:HB3	2.00	0.44
1:G:325:VAL:HG23	1:G:353:ASP:OD2	2.17	0.44
2:H:123:HIS:O	2:H:125:ASN:N	2.51	0.44
2:D:231:TYR:HD1	2:D:235:LEU:HD12	1.83	0.44
1:E:183:LEU:HD22	1:E:215:ILE:HD11	2.00	0.44
1:G:34:CYS:SG	1:G:60:ILE:HD13	2.57	0.44
2:H:365:LEU:O	2:H:365:LEU:HG	2.18	0.44
2:F:187:GLY:HA2	3:K:173:LEU:HD13	2.00	0.43
2:F:318:LEU:HD12	2:F:319:ASN:N	2.33	0.43
2:H:267:ARG:CG	2:H:267:ARG:NH1	2.81	0.43
2:B:241:GLN:HA	2:B:242:PRO:HD2	1.68	0.43
3:L:170:VAL:CG1	3:L:171:LEU:H	2.31	0.43
1:E:72:ASN:ND2	1:E:73:ASN:N	2.62	0.43
1:E:415:SER:HB3	1:E:421:ASN:OD1	2.18	0.43
1:E:50:VAL:HG13	1:E:100:VAL:HG21	2.00	0.43
2:B:182:THR:OG1	2:B:295:THR:HG22	2.17	0.43
2:F:157:MET:O	2:F:157:MET:HE3	2.18	0.43
1:A:285:ILE:HD11	1:A:390:LEU:H	1.82	0.43
1:E:184:ARG:HD3	1:E:279:THR:OG1	2.17	0.43
3:L:101:MET:HB3	3:L:117:ILE:O	2.17	0.43
2:H:338:GLU:HG3	3:L:148:LYS:CD	2.41	0.43
3:L:144:ILE:HD13	3:L:170:VAL:HB	2.00	0.43
1:C:84:ASN:OD1	1:C:86:ALA:HB3	2.19	0.43
1:G:253:LYS:CB	1:G:261:ASP:N	2.81	0.43
1:A:50:VAL:HA	1:A:54:ILE:HG22	1.99	0.43
1:A:192:LEU:HD11	1:A:196:PHE:CZ	2.53	0.43
2:D:401:GLU:HG3	2:D:402:GLU:N	2.33	0.43
3:L:103:ILE:HD12	3:L:103:ILE:O	2.18	0.43
1:E:54:ILE:HD12	1:E:54:ILE:HA	1.73	0.43
1:G:507:LYS:HG2	1:G:513:PHE:HB2	2.01	0.43
3:L:125:ARG:C	3:L:127:LYS:N	2.70	0.43
1:G:297:ILE:HD11	1:G:309:ARG:HG2	1.99	0.43
2:H:232:VAL:HG12	2:H:260:ILE:HG23	1.99	0.43
1:A:339:TYR:CD2	2:B:223:ARG:HB3	2.53	0.43
3:J:105:VAL:HG11	3:J:115:ILE:HD11	2.00	0.43
2:F:267:ARG:HG2	2:F:267:ARG:HH11	1.83	0.43
3:K:137:PRO:HA	3:K:138:PRO:HD3	1.87	0.43
2:D:199:CYS:O	2:D:202:CYS:HB2	2.18	0.43
1:E:418:ASN:HD22	1:E:419:PRO:HD2	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:ILE:HG23	1:A:109:PRO:HG3	2.00	0.43
1:E:340:ILE:HD11	2:F:273:ILE:CG1	2.48	0.43
1:A:84:ASN:OD1	1:A:86:ALA:HB3	2.19	0.43
2:D:393:TYR:CD2	2:D:408:LEU:HD21	2.53	0.43
3:I:104:LYS:O	3:I:166:VAL:HA	2.18	0.43
1:G:184:ARG:HH11	1:G:184:ARG:HG3	1.84	0.43
1:G:362:ALA:O	1:G:366:GLN:HG3	2.18	0.43
2:H:412:LEU:O	2:H:417:LEU:HB2	2.19	0.43
2:F:422:GLU:O	2:F:423:LEU:HD23	2.18	0.43
1:C:202:ASP:O	1:C:204:MET:HE3	2.18	0.43
1:A:527:GLN:HB2	2:B:318:LEU:HD13	2.00	0.43
3:J:105:VAL:CG1	3:J:115:ILE:HD11	2.49	0.43
1:E:51:LEU:HD11	2:F:92:PHE:HB3	1.99	0.43
2:H:390:ARG:HG3	2:H:390:ARG:HH11	1.83	0.43
1:E:138:ARG:O	1:E:142:VAL:HG23	2.19	0.43
1:G:329:ILE:HD11	1:G:343:GLN:HA	2.01	0.43
1:E:325:VAL:O	1:E:326:ARG:C	2.55	0.43
1:A:513:PHE:CZ	2:B:185:PHE:HE1	2.36	0.43
1:C:344:ASN:HD22	1:C:344:ASN:HA	1.53	0.43
1:A:517:ASN:OD1	1:A:533:GLN:NE2	2.52	0.43
1:C:78:ARG:CZ	2:D:13:TRP:HB3	2.48	0.43
1:G:324:PRO:HA	1:G:353:ASP:OD2	2.18	0.43
1:C:527:GLN:OE1	1:C:527:GLN:HA	2.18	0.43
2:B:224:LEU:HB3	2:B:226:GLU:OE1	2.19	0.43
2:H:30:PHE:N	2:H:30:PHE:CD1	2.85	0.43
1:G:496:PHE:CD2	1:G:496:PHE:C	2.92	0.43
2:F:54:ILE:HB	2:F:143:CYS:CB	2.48	0.43
2:B:111:LEU:HD23	2:B:120:VAL:HG21	2.01	0.43
1:E:128:ALA:HB1	1:E:131:LEU:CD1	2.48	0.43
2:H:115:VAL:HA	2:H:116:PRO:HD2	1.90	0.43
2:F:205:GLU:C	2:F:207:TYR:H	2.21	0.43
1:A:324:PRO:HB3	1:A:353:ASP:HB3	1.99	0.43
1:E:214:TRP:CE2	1:E:271:ASN:ND2	2.86	0.43
1:C:199:TYR:HB3	1:C:200:ASP:H	1.61	0.43
1:C:301:THR:HA	1:C:302:PRO:HD3	1.82	0.43
2:B:141:ILE:HD12	2:B:158:LEU:HD21	2.00	0.43
1:E:303:SER:O	1:E:304:PHE:C	2.57	0.43
2:D:319:ASN:C	2:D:319:ASN:HD22	2.21	0.43
1:E:15:ARG:HG3	2:F:90:ARG:HH12	1.83	0.43
2:D:59:LEU:HD12	3:J:176:GLY:HA3	2.01	0.43
2:H:383:ALA:HB2	2:H:423:LEU:HD22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:95:ARG:HA	2:B:95:ARG:HD3	1.73	0.43
1:G:51:LEU:HD11	2:H:92:PHE:HB3	2.01	0.43
2:D:312:THR:O	2:D:313:SER:HB2	2.18	0.43
2:H:367:TYR:O	2:H:371:SER:CB	2.67	0.43
1:C:43:THR:HG22	1:C:44:GLU:N	2.34	0.43
1:E:190:PRO:O	1:E:191:GLU:C	2.57	0.43
3:K:155:THR:N	3:K:158:ASP:OD2	2.43	0.43
2:H:187:GLY:CA	3:L:173:LEU:HD13	2.48	0.43
1:A:215:ILE:HD11	1:A:332:MET:HE2	2.01	0.43
1:A:42:GLY:HA2	1:A:129:THR:HG21	2.00	0.43
2:D:152:ARG:NE	2:D:201:GLU:OE1	2.52	0.43
1:A:309:ARG:HD2	1:A:313:GLU:HG2	2.01	0.43
1:A:447:ASN:ND2	2:B:26:ARG:HE	2.17	0.43
2:F:400:ILE:O	2:F:400:ILE:HG22	2.18	0.43
2:F:182:THR:O	2:F:183:GLU:HG2	2.19	0.42
2:B:353:ILE:HD13	2:B:436:PHE:HD2	1.84	0.42
1:C:441:ARG:HG2	1:C:441:ARG:HH11	1.84	0.42
2:B:384:THR:HA	2:B:389:ASN:HD22	1.83	0.42
2:H:382:THR:HG22	2:H:391:THR:HA	2.00	0.42
1:G:173:GLU:O	1:G:512:GLN:O	2.37	0.42
2:B:89:ASN:OD1	2:B:90:ARG:NH1	2.47	0.42
2:D:382:THR:HG22	2:D:391:THR:HA	2.00	0.42
1:A:438:GLN:O	1:A:440:GLY:N	2.52	0.42
2:H:320:ASN:ND2	2:H:336:GLU:HG3	2.34	0.42
2:H:393:TYR:CG	2:H:394:LEU:N	2.87	0.42
1:G:307:LEU:HD13	1:G:383:LEU:HD22	2.01	0.42
1:A:128:ALA:HB1	1:A:131:LEU:HD11	2.02	0.42
1:A:246:LEU:O	1:A:249:GLN:HB3	2.19	0.42
1:E:114:ASP:OD1	1:E:138:ARG:NH2	2.48	0.42
2:F:371:SER:C	2:F:373:SER:N	2.71	0.42
1:C:186:ASP:OD2	1:C:279:THR:HB	2.19	0.42
2:F:397:VAL:HG23	2:F:397:VAL:O	2.19	0.42
1:E:184:ARG:NH1	1:E:184:ARG:HG3	2.29	0.42
2:F:335:PHE:CE2	3:K:170:VAL:HG21	2.54	0.42
2:H:188:ASN:OD1	3:L:173:LEU:HD12	2.18	0.42
1:C:46:LEU:HA	1:C:46:LEU:HD12	1.86	0.42
2:B:145:LEU:O	3:I:176:GLY:HA2	2.19	0.42
1:C:146:SER:O	1:C:147:GLN:CB	2.67	0.42
2:F:233:ARG:HG2	2:F:234:MET:N	2.35	0.42
2:F:74:GLN:NE2	2:F:74:GLN:CA	2.83	0.42
2:F:58:GLY:N	2:F:91:GLN:HG2	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:418:ASN:HD22	1:E:418:ASN:C	2.23	0.42
1:C:248:ARG:C	1:C:250:GLY:H	2.23	0.42
2:F:212:ASN:HA	2:F:212:ASN:HD22	1.62	0.42
2:F:342:ASN:ND2	2:F:342:ASN:N	2.52	0.42
2:F:256:HIS:O	2:F:260:ILE:HG13	2.19	0.42
2:F:236:GLN:NE2	2:F:263:LYS:HD2	2.32	0.42
1:G:221:TYR:CD2	1:G:247:ILE:HA	2.55	0.42
1:C:332:MET:O	1:C:333:ILE:C	2.58	0.42
1:A:35:LEU:CD2	1:A:46:LEU:HD22	2.49	0.42
1:C:428:MET:HE2	1:C:479:VAL:HA	2.01	0.42
1:E:221:TYR:N	1:E:221:TYR:CD1	2.85	0.42
1:G:165:ILE:HG22	1:G:165:ILE:O	2.20	0.42
1:C:181:GLU:OE1	1:C:330:PRO:HD3	2.19	0.42
2:B:43:GLN:HG3	2:B:47:ASP:OD2	2.19	0.42
2:B:380:ALA:CB	2:B:394:LEU:CD1	2.92	0.42
1:E:193:ARG:HG3	1:E:193:ARG:NH1	2.30	0.42
2:F:257:ILE:HD13	2:F:282:GLN:HG2	2.00	0.42
1:E:274:THR:O	1:E:276:LEU:N	2.53	0.42
1:C:504:GLU:O	1:C:508:ILE:HG13	2.19	0.42
2:B:233:ARG:HH11	2:B:287:ARG:HH12	1.65	0.42
2:H:411:THR:OG1	2:H:414:GLU:HB2	2.19	0.42
1:C:233:ILE:O	1:C:234:PRO:C	2.57	0.42
1:C:418:ASN:C	1:C:420:ASP:N	2.73	0.42
1:E:297:ILE:HB	1:E:368:ILE:CD1	2.30	0.42
2:H:132:ASP:OD1	2:H:132:ASP:N	2.52	0.42
2:B:185:PHE:HB2	2:B:327:VAL:HG12	2.02	0.42
1:E:374:SER:O	1:E:375:ILE:HD12	2.20	0.42
2:B:322:LEU:HD23	2:B:323:VAL:N	2.35	0.42
2:B:126:LYS:O	2:B:127:ILE:C	2.58	0.42
2:B:128:GLN:HG3	2:B:153:TRP:CE2	2.54	0.42
2:F:320:ASN:HA	2:F:320:ASN:HD22	1.56	0.42
2:F:364:VAL:O	2:F:368:LEU:HG	2.19	0.42
1:A:28:LEU:HA	1:A:509:ILE:HG21	2.02	0.42
3:I:124:GLU:HB2	3:I:152:ASP:O	2.19	0.42
1:E:119:PHE:O	1:E:122:ARG:HG2	2.19	0.42
3:J:156:ALA:O	3:J:161:ILE:HB	2.20	0.42
2:B:294:SER:O	2:B:298:VAL:HG23	2.19	0.42
2:F:128:GLN:H	2:F:128:GLN:HE21	1.66	0.42
2:D:359:ALA:HB1	2:D:363:GLU:CD	2.40	0.42
2:D:325:ASN:CG	2:D:327:VAL:HG22	2.39	0.42
1:G:407:ILE:CG2	1:G:409:LYS:HE3	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:236:THR:HG22	1:E:238:LYS:H	1.83	0.42
1:E:240:LYS:HZ2	1:E:276:LEU:HD12	1.82	0.42
2:H:183:GLU:HG3	2:H:289:ILE:CG2	2.49	0.42
1:G:523:SER:OG	1:G:525:MET:HG2	2.20	0.42
2:F:128:GLN:H	2:F:128:GLN:NE2	2.18	0.42
1:A:510:THR:O	1:A:511:LYS:HB2	2.19	0.42
1:C:331:ASP:OD2	2:D:223:ARG:NH1	2.53	0.42
2:B:385:LEU:HA	2:B:385:LEU:HD12	1.77	0.42
2:H:235:LEU:O	2:H:238:PRO:HD2	2.19	0.42
3:K:115:ILE:HG13	3:K:117:ILE:CD1	2.49	0.42
1:G:163:ARG:NH1	1:G:165:ILE:HG12	2.34	0.42
2:D:95:ARG:HH11	2:D:95:ARG:HG3	1.85	0.42
2:D:350:PRO:HB2	2:D:437:LYS:HD3	2.01	0.42
1:G:251:ILE:HG12	1:G:265:PHE:HB3	2.02	0.42
2:H:77:VAL:HG23	2:H:120:VAL:CG1	2.50	0.42
3:K:105:VAL:HG22	3:K:113:ILE:CG1	2.50	0.42
1:G:47:LYS:NZ	2:H:65:LYS:HE2	2.34	0.42
2:B:157:MET:HE2	2:B:157:MET:O	2.20	0.42
1:A:236:THR:CG2	1:A:238:LYS:HB3	2.49	0.42
1:C:67:GLY:HA3	2:D:14:GLU:O	2.20	0.42
1:A:229:THR:HG21	1:A:232:ARG:HB3	2.01	0.42
1:G:226:TYR:CE2	1:G:233:ILE:HG22	2.55	0.42
3:K:107:THR:HG23	3:K:108:LEU:N	2.34	0.42
1:E:34:CYS:HB2	1:E:123:PHE:CG	2.55	0.42
2:D:335:PHE:CE2	3:J:170:VAL:HG21	2.55	0.42
1:G:324:PRO:CG	1:G:357:VAL:HG21	2.50	0.42
2:F:114:ARG:O	2:F:116:PRO:HD3	2.20	0.42
3:L:135:GLY:O	3:L:137:PRO:HD3	2.20	0.42
1:A:276:LEU:HD23	1:A:276:LEU:HA	1.83	0.42
1:G:306:ILE:HD13	1:G:365:LEU:HD23	2.02	0.42
2:D:241:GLN:HA	2:D:242:PRO:HD2	1.89	0.41
2:F:34:ASP:OD1	2:F:34:ASP:N	2.53	0.41
1:A:168:GLU:HG3	1:A:394:ARG:NE	2.34	0.41
1:G:244:ARG:HH11	1:G:244:ARG:CG	2.32	0.41
1:C:51:LEU:HD11	2:D:92:PHE:HB3	2.02	0.41
1:E:330:PRO:O	1:E:332:MET:HG3	2.20	0.41
2:B:195:GLY:C	2:B:339:ARG:HH12	2.24	0.41
2:D:80:MET:O	2:D:124:PHE:HE1	2.03	0.41
2:D:32:HIS:CD2	2:D:34:ASP:H	2.38	0.41
2:F:32:HIS:CG	2:F:33:PRO:HD2	2.55	0.41
3:L:155:THR:HG22	3:L:158:ASP:CG	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:207:TYR:HA	2:H:208:PRO:HD3	1.89	0.41
2:B:213:PHE:HD1	2:B:230:GLU:HG2	1.85	0.41
2:D:318:LEU:HD11	2:D:334:THR:CG2	2.50	0.41
2:H:245:GLU:CG	2:H:246:GLY:N	2.83	0.41
2:H:140:ILE:C	2:H:141:ILE:HD12	2.41	0.41
1:C:418:ASN:HD22	1:C:419:PRO:HD2	1.84	0.41
3:L:162:LEU:O	3:L:164:GLY:N	2.53	0.41
1:A:301:THR:CG2	1:A:305:TRP:HB2	2.50	0.41
2:F:80:MET:HE2	2:F:126:LYS:HB2	2.02	0.41
1:C:437:LYS:HD2	1:C:437:LYS:HA	1.73	0.41
1:G:90:MET:O	1:G:94:GLN:HB2	2.19	0.41
1:A:366:GLN:O	1:A:368:ILE:N	2.54	0.41
1:A:236:THR:HG21	1:A:238:LYS:HB3	2.02	0.41
2:B:413:LYS:HE3	2:B:413:LYS:O	2.20	0.41
2:F:351:GLN:HB2	2:F:436:PHE:CD2	2.56	0.41
2:H:402:GLU:O	2:H:404:THR:N	2.54	0.41
2:H:405:ARG:HB3	2:H:406:PRO:HD3	2.01	0.41
2:F:319:ASN:HD22	2:F:320:ASN:N	2.18	0.41
2:H:392:LEU:CD2	2:H:392:LEU:H	2.30	0.41
1:C:74:PHE:HE2	2:D:92:PHE:HE1	1.69	0.41
1:A:172:ILE:HA	1:A:390:LEU:HD23	2.01	0.41
1:G:90:MET:CE	1:G:94:GLN:OE1	2.68	0.41
2:B:401:GLU:HG3	2:B:402:GLU:N	2.35	0.41
1:G:519:THR:O	1:G:531:THR:HA	2.20	0.41
1:C:284:SER:O	1:C:288:ILE:HG13	2.21	0.41
1:E:486:GLY:HA3	2:F:22:LYS:HD3	2.02	0.41
2:B:286:LYS:HB2	2:B:288:ILE:HG13	2.00	0.41
1:G:404:LEU:HD21	1:G:467:GLU:HG2	2.02	0.41
2:B:403:ARG:HH11	2:B:403:ARG:HG3	1.85	0.41
1:G:218:ILE:O	1:G:222:LEU:HB2	2.20	0.41
1:E:44:GLU:HG3	1:E:495:ALA:HA	2.03	0.41
2:D:207:TYR:CE2	3:J:172:GLN:HG2	2.55	0.41
1:E:229:THR:CG2	1:E:232:ARG:HD2	2.49	0.41
2:H:84:ASP:OD1	2:H:86:SER:N	2.47	0.41
2:B:218:ILE:HD12	2:B:218:ILE:HA	1.91	0.41
1:E:332:MET:O	2:F:223:ARG:NE	2.54	0.41
2:B:87:ASN:HB3	2:B:91:GLN:CD	2.40	0.41
2:H:361:LEU:C	2:H:363:GLU:N	2.74	0.41
1:E:488:ALA:HB2	2:F:22:LYS:HD2	2.03	0.41
2:H:89:ASN:OD1	2:H:90:ARG:NH1	2.50	0.41
1:G:189:PHE:HB2	1:G:190:PRO:HD2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:402:GLU:HG2	2:F:405:ARG:NH2	2.34	0.41
2:F:361:LEU:CD2	2:F:408:LEU:HD23	2.45	0.41
2:F:410:LYS:HB3	2:F:414:GLU:HG2	2.03	0.41
2:B:385:LEU:CD2	2:B:390:ARG:HB3	2.40	0.41
1:A:78:ARG:O	1:A:81:ILE:HG13	2.20	0.41
1:G:299:LYS:HG2	1:G:368:ILE:CG2	2.50	0.41
2:F:222:PRO:O	2:F:273:ILE:HD11	2.20	0.41
2:H:249:LEU:CD1	2:H:260:ILE:HD11	2.49	0.41
1:G:251:ILE:O	1:G:253:LYS:N	2.54	0.41
2:D:405:ARG:N	2:D:406:PRO:CD	2.84	0.41
2:B:24:LEU:HD21	2:B:312:THR:HG21	2.01	0.41
2:H:195:GLY:O	2:H:339:ARG:NH1	2.53	0.41
1:E:341:LYS:HE2	1:E:341:LYS:HB3	1.93	0.41
2:H:355:PHE:O	2:H:440:PHE:HA	2.20	0.41
2:F:377:LYS:HE2	2:F:377:LYS:CA	2.39	0.41
2:D:319:ASN:HD22	2:D:320:ASN:N	2.19	0.41
2:B:217:THR:CB	2:B:223:ARG:NH2	2.81	0.41
1:G:45:ILE:CG1	1:G:498:GLY:HA2	2.48	0.41
2:D:323:VAL:O	2:D:332:THR:HA	2.21	0.41
1:C:97:ASN:HB3	1:C:100:VAL:HG23	2.01	0.41
1:C:175:HIS:HD2	1:C:512:GLN:O	2.03	0.41
3:J:118:GLU:O	3:J:120:THR:N	2.54	0.41
1:G:178:ASN:O	1:G:179:ALA:HB2	2.20	0.41
2:D:365:LEU:HD12	2:D:379:PRO:HG2	2.01	0.41
3:K:150:MET:CE	3:K:161:ILE:HD11	2.50	0.41
2:H:352:ASN:ND2	2:H:437:LYS:HB2	2.35	0.41
1:G:396:ARG:HH21	1:G:400:GLU:HB3	1.86	0.41
1:A:517:ASN:HD22	1:A:517:ASN:C	2.20	0.41
2:F:142:VAL:CG2	2:F:307:VAL:CG2	2.99	0.41
1:E:424:VAL:HG11	1:E:478:TYR:CD1	2.55	0.41
1:G:248:ARG:HG3	1:G:248:ARG:NH1	2.31	0.41
1:G:72:ASN:C	1:G:72:ASN:HD22	2.23	0.41
1:G:488:ALA:O	1:G:490:PRO:HD3	2.20	0.41
1:A:51:LEU:HD11	2:B:92:PHE:HB3	2.03	0.41
1:C:365:LEU:O	1:C:370:GLN:HB2	2.19	0.41
1:E:482:PHE:HA	1:E:485:TYR:CD1	2.55	0.41
1:A:40:ALA:O	1:A:43:THR:HG22	2.20	0.41
2:F:46:LEU:HD22	2:F:73:ARG:CZ	2.50	0.41
2:F:247:VAL:HA	2:F:248:PRO:HD3	1.87	0.41
2:D:246:GLY:O	2:D:248:PRO:HD3	2.21	0.41
1:E:489:GLU:C	2:F:19:HIS:HD2	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:222:LEU:HD13	1:G:243:PHE:CZ	2.55	0.41
1:E:64:GLN:HA	1:E:83:LYS:O	2.20	0.41
2:B:38:SER:OG	2:B:39:THR:N	2.53	0.41
2:D:36:GLU:OE1	2:D:36:GLU:HA	2.21	0.41
3:J:140:GLN:HG3	3:J:140:GLN:O	2.20	0.41
1:A:115:ASN:N	1:A:115:ASN:OD1	2.54	0.41
1:E:266:GLU:HG3	1:E:270:LYS:NZ	2.36	0.41
2:H:412:LEU:H	2:H:412:LEU:CD1	2.13	0.41
2:H:354:GLN:HE21	2:H:354:GLN:CA	2.31	0.41
2:B:427:ASP:CB	2:B:429:THR:HG22	2.50	0.41
1:A:368:ILE:HA	1:A:368:ILE:HD13	1.86	0.41
1:A:307:LEU:HB3	1:A:383:LEU:CD2	2.49	0.41
2:B:240:GLU:OE1	2:B:259:TRP:HZ2	2.03	0.41
1:C:204:MET:HG3	1:C:205:GLU:N	2.36	0.41
1:G:235:LYS:HB3	1:G:235:LYS:NZ	2.35	0.41
2:B:394:LEU:HG	2:B:396:SER:H	1.86	0.41
2:B:218:ILE:HG22	2:B:219:ALA:N	2.36	0.41
1:C:409:LYS:HE2	1:C:468:TYR:O	2.19	0.41
2:F:192:ILE:CD1	2:F:200:ILE:HG12	2.51	0.41
2:D:231:TYR:CD2	2:D:267:ARG:HD2	2.56	0.41
2:D:52:LEU:HD11	2:D:78:ILE:HG13	2.02	0.41
2:H:139:HIS:O	2:H:140:ILE:HG13	2.21	0.41
1:G:446:SER:HB2	1:G:449:GLN:HG3	2.02	0.41
2:D:83:ILE:HD12	2:D:98:ASP:HB3	2.03	0.41
2:H:200:ILE:HD13	2:H:200:ILE:HA	1.96	0.41
1:C:193:ARG:O	1:C:197:GLN:HG3	2.21	0.41
1:A:449:GLN:HB3	1:A:453:ASP:OD2	2.20	0.41
1:E:7:LEU:HD23	1:E:7:LEU:O	2.21	0.41
1:E:297:ILE:O	1:E:297:ILE:HD12	2.21	0.41
1:E:43:THR:HG23	1:E:75:PHE:CD1	2.56	0.41
3:J:105:VAL:O	3:J:113:ILE:HG12	2.21	0.41
1:G:214:TRP:O	1:G:217:ILE:HB	2.21	0.41
1:E:36:ILE:O	1:E:60:ILE:O	2.38	0.41
1:A:72:ASN:C	1:A:72:ASN:ND2	2.73	0.41
1:A:130:GLN:OE1	1:A:130:GLN:HA	2.21	0.41
1:E:441:ARG:NH2	1:E:453:ASP:OD1	2.54	0.41
1:E:377:GLU:HG2	1:E:381:LYS:CE	2.41	0.40
1:C:347:ARG:HH12	2:D:274:ARG:HD2	1.84	0.40
1:G:407:ILE:CG2	1:G:409:LYS:HG3	2.48	0.40
3:K:108:LEU:HD21	3:K:171:LEU:HB2	2.03	0.40
3:K:170:VAL:HG13	3:K:171:LEU:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:102:LEU:HG	3:L:114:GLU:HG2	2.02	0.40
3:J:115:ILE:CG2	3:J:129:ARG:HB3	2.51	0.40
2:D:408:LEU:HD23	2:D:408:LEU:HA	1.94	0.40
1:G:112:LEU:C	1:G:114:ASP:N	2.73	0.40
1:A:35:LEU:HD23	1:A:46:LEU:HD22	2.03	0.40
1:E:65:VAL:HB	1:E:80:SER:O	2.20	0.40
2:F:231:TYR:CG	2:F:267:ARG:NH1	2.89	0.40
1:C:119:PHE:CE1	1:C:122:ARG:NH1	2.89	0.40
2:H:374:LEU:O	2:H:374:LEU:HD12	2.21	0.40
2:F:371:SER:C	2:F:373:SER:H	2.24	0.40
1:E:195:HIS:HE1	1:E:341:LYS:HE2	1.86	0.40
1:G:293:ARG:HG2	1:G:305:TRP:NE1	2.36	0.40
2:H:267:ARG:CG	2:H:267:ARG:O	2.69	0.40
1:A:229:THR:HG22	1:A:232:ARG:HB3	1.99	0.40
2:H:250:ASP:N	2:H:256:HIS:ND1	2.59	0.40
1:C:36:ILE:CG2	1:C:37:ASN:N	2.79	0.40
3:J:154:LYS:HB3	3:J:158:ASP:OD2	2.21	0.40
1:G:269:ILE:O	1:G:269:ILE:HG22	2.20	0.40
3:J:113:ILE:O	3:J:113:ILE:HG13	2.21	0.40
2:B:350:PRO:HB3	2:B:435:LEU:HB3	2.02	0.40
2:B:190:ARG:HH22	2:B:203:THR:HG23	1.87	0.40
1:C:301:THR:HG22	1:C:306:ILE:HG13	2.04	0.40
1:C:418:ASN:C	1:C:420:ASP:H	2.22	0.40
1:G:416:MET:C	1:G:418:ASN:N	2.75	0.40
2:B:252:ASP:O	2:B:254:PRO:HD3	2.21	0.40
1:C:220:LYS:HD2	1:C:220:LYS:HA	1.90	0.40
3:L:143:LEU:C	3:L:144:ILE:HD12	2.42	0.40
1:E:340:ILE:O	1:E:340:ILE:HG22	2.22	0.40
1:C:311:LEU:HA	1:C:311:LEU:HD12	1.85	0.40
2:F:336:GLU:O	2:F:337:ALA:C	2.60	0.40
1:E:371:ALA:C	1:E:373:GLU:H	2.24	0.40
2:H:125:ASN:HD22	2:H:130:PHE:HZ	1.69	0.40
2:D:54:ILE:CG2	2:D:145:LEU:HD21	2.51	0.40
2:H:148:ILE:O	2:H:152:ARG:HG3	2.21	0.40
1:E:481:GLU:OE1	2:F:29:PRO:HD2	2.21	0.40
1:G:56:SER:HB3	1:G:101:SER:OG	2.21	0.40
3:L:107:THR:HG22	3:L:111:LYS:H	1.82	0.40
2:B:374:LEU:O	2:B:375:GLN:C	2.59	0.40
2:H:386:GLU:O	2:H:388:LYS:N	2.49	0.40
1:A:307:LEU:HD21	1:A:375:ILE:HG21	2.03	0.40
2:H:157:MET:O	2:H:157:MET:HE3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:13:TRP:CZ3	2:D:116:PRO:HG2	2.56	0.40
2:D:422:GLU:HA	2:D:436:PHE:O	2.22	0.40
1:G:216:VAL:O	1:G:216:VAL:HG12	2.22	0.40
1:C:154:ARG:HB3	1:C:161:TYR:HB3	2.03	0.40
2:D:52:LEU:HB2	2:D:138:PHE:CD2	2.56	0.40
1:E:183:LEU:HD22	1:E:215:ILE:CD1	2.51	0.40
3:K:139:GLN:H	3:K:139:GLN:HG2	1.61	0.40
1:A:344:ASN:HB3	1:E:111:ASN:HD21	1.83	0.40
2:B:230:GLU:OE2	2:B:233:ARG:NH1	2.54	0.40
1:C:526:SER:O	1:C:527:GLN:HB2	2.19	0.40
1:C:210:SER:O	1:C:211:HIS:HD2	2.05	0.40
2:B:52:LEU:HB2	2:B:138:PHE:CE2	2.57	0.40
1:E:154:ARG:HH12	1:E:433:ASP:CG	2.25	0.40
2:F:322:LEU:C	2:F:322:LEU:HD23	2.41	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	518/531 (98%)	451 (87%)	54 (10%)	13 (2%)	7 27
1	C	513/531 (97%)	452 (88%)	52 (10%)	9 (2%)	11 37
1	E	515/531 (97%)	464 (90%)	42 (8%)	9 (2%)	11 38
1	G	512/531 (96%)	447 (87%)	56 (11%)	9 (2%)	11 37
2	B	430/434 (99%)	376 (87%)	46 (11%)	8 (2%)	10 35
2	D	430/434 (99%)	370 (86%)	50 (12%)	10 (2%)	8 30
2	F	429/434 (99%)	360 (84%)	55 (13%)	14 (3%)	5 20
2	H	429/434 (99%)	355 (83%)	60 (14%)	14 (3%)	5 20
3	I	84/88 (96%)	78 (93%)	4 (5%)	2 (2%)	7 29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	J	74/88 (84%)	70 (95%)	1 (1%)	3 (4%)	3 14
3	K	74/88 (84%)	65 (88%)	6 (8%)	3 (4%)	3 14
3	L	74/88 (84%)	65 (88%)	5 (7%)	4 (5%)	2 7
All	All	4082/4212 (97%)	3553 (87%)	431 (11%)	98 (2%)	7 29

All (98) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	252	LEU
1	C	252	LEU
2	D	116	PRO
2	D	204	LEU
1	E	202	ASP
1	E	252	LEU
1	E	275	ALA
2	F	396	SER
3	K	119	PRO
2	H	116	PRO
2	H	204	LEU
2	H	241	GLN
2	H	244	GLY
2	H	361	LEU
3	L	119	PRO
3	L	163	GLY
1	A	63	ASN
1	A	79	SER
1	A	228	GLU
1	A	439	GLN
2	B	116	PRO
2	B	127	ILE
3	I	147	GLY
3	I	163	GLY
1	C	230	ASN
1	C	422	GLU
2	D	12	ASP
2	D	92	PHE
2	D	412	LEU
3	J	119	PRO
3	J	163	GLY
1	E	249	GLN
1	E	318	GLU

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Mol	Chain	Res	Type
1	E	372	PRO
2	F	92	PHE
2	F	116	PRO
2	F	206	LEU
2	F	244	GLY
2	F	287	ARG
2	F	360	LYS
2	F	418	VAL
1	G	252	LEU
1	G	451	GLU
2	H	183	GLU
2	H	392	LEU
2	H	403	ARG
1	A	201	LEU
1	A	260	GLU
1	A	372	PRO
1	A	438	GLN
2	B	372	ALA
2	B	399	SER
1	C	36	ILE
1	C	259	PRO
2	D	357	PRO
2	F	132	ASP
2	F	166	ASP
3	K	152	ASP
1	G	190	PRO
1	G	517	ASN
2	H	88	LEU
2	H	267	ARG
3	L	124	GLU
1	A	271	ASN
2	B	204	LEU
2	B	375	GLN
1	C	79	SER
1	C	450	VAL
1	E	36	ILE
1	E	190	PRO
1	E	276	LEU
2	F	375	GLN
1	G	250	GLY
2	H	272	ASN
1	A	133	GLU

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Mol	Chain	Res	Type
1	A	200	ASP
2	B	242	PRO
2	B	377	LYS
2	D	88	LEU
2	D	90	ARG
3	J	152	ASP
2	F	211	VAL
2	F	242	PRO
2	F	320	ASN
3	K	163	GLY
1	G	179	ALA
2	H	352	ASN
1	A	259	PRO
2	D	16	ARG
2	D	241	GLN
1	G	280	GLN
2	H	194	PRO
3	L	154	LYS
1	G	419	PRO
2	H	242	PRO
1	C	55	GLY
1	C	190	PRO
1	G	450	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	452/462 (98%)	426 (94%)	26 (6%)	25 58
1	C	451/462 (98%)	424 (94%)	27 (6%)	24 57
1	E	448/462 (97%)	420 (94%)	28 (6%)	22 54
1	G	450/462 (97%)	429 (95%)	21 (5%)	32 68
2	B	378/382 (99%)	350 (93%)	28 (7%)	17 44
2	D	379/382 (99%)	354 (93%)	25 (7%)	21 51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	F	377/382 (99%)	346 (92%)	31 (8%)	14 39
2	H	375/382 (98%)	351 (94%)	24 (6%)	22 53
3	I	73/74 (99%)	67 (92%)	6 (8%)	14 39
3	J	67/74 (90%)	62 (92%)	5 (8%)	17 44
3	K	67/74 (90%)	63 (94%)	4 (6%)	24 57
3	L	67/74 (90%)	66 (98%)	1 (2%)	72 92
All	All	3584/3672 (98%)	3358 (94%)	226 (6%)	22 54

All (226) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	ASN
1	A	47	LYS
1	A	66	SER
1	A	72	ASN
1	A	115	ASN
1	A	135	THR
1	A	158	LEU
1	A	171	VAL
1	A	214	TRP
1	A	220	LYS
1	A	228	GLU
1	A	238	LYS
1	A	245	ASP
1	A	248	ARG
1	A	252	LEU
1	A	264	ASN
1	A	277	ASN
1	A	293	ARG
1	A	309	ARG
1	A	364	LEU
1	A	381	LYS
1	A	418	ASN
1	A	422	GLU
1	A	437	LYS
1	A	503	GLN
1	A	517	ASN
2	B	18	ASN
2	B	82	THR
2	B	113	ASP

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Mol	Chain	Res	Type
2	B	114	ARG
2	B	116	PRO
2	B	128	GLN
2	B	182	THR
2	B	188	ASN
2	B	210	GLN
2	B	217	THR
2	B	218	ILE
2	B	236	GLN
2	B	240	GLU
2	B	269	SER
2	B	274	ARG
2	B	316	ILE
2	B	319	ASN
2	B	321	TYR
2	B	323	VAL
2	B	325	ASN
2	B	342	ASN
2	B	351	GLN
2	B	353	ILE
2	B	362	GLN
2	B	377	LYS
2	B	385	LEU
2	B	413	LYS
2	B	421	GLN
3	I	101	MET
3	I	105	VAL
3	I	107	THR
3	I	109	THR
3	I	165	SER
3	I	171	LEU
1	C	10	GLU
1	C	34	CYS
1	C	43	THR
1	C	46	LEU
1	C	72	ASN
1	C	163	ARG
1	C	171	VAL
1	C	186	ASP
1	C	191	GLU
1	C	214	TRP
1	C	252	LEU

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Mol	Chain	Res	Type
1	C	264	ASN
1	C	274	THR
1	C	277	ASN
1	C	293	ARG
1	C	297	ILE
1	C	311	LEU
1	C	344	ASN
1	C	353	ASP
1	C	359	ASN
1	C	364	LEU
1	C	370	GLN
1	C	418	ASN
1	C	435	PHE
1	C	466	GLN
1	C	476	ASP
1	C	497	LEU
2	D	11	LEU
2	D	12	ASP
2	D	39	THR
2	D	59	LEU
2	D	82	THR
2	D	111	LEU
2	D	114	ARG
2	D	116	PRO
2	D	128	GLN
2	D	149	ILE
2	D	197	THR
2	D	215	MET
2	D	236	GLN
2	D	316	ILE
2	D	319	ASN
2	D	321	TYR
2	D	323	VAL
2	D	325	ASN
2	D	326	ASP
2	D	334	THR
2	D	342	ASN
2	D	362	GLN
2	D	401	GLU
2	D	415	LEU
2	D	421	GLN
3	J	108	LEU

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Mol	Chain	Res	Type
3	J	116	ASP
3	J	129	ARG
3	J	171	LEU
3	J	173	LEU
1	E	29	GLU
1	E	43	THR
1	E	72	ASN
1	E	78	ARG
1	E	146	SER
1	E	163	ARG
1	E	171	VAL
1	E	214	TRP
1	E	226	TYR
1	E	245	ASP
1	E	262	GLU
1	E	264	ASN
1	E	265	PHE
1	E	277	ASN
1	E	292	ASP
1	E	293	ARG
1	E	303	SER
1	E	309	ARG
1	E	311	LEU
1	E	353	ASP
1	E	364	LEU
1	E	418	ASN
1	E	437	LYS
1	E	452	GLU
1	E	497	LEU
1	E	513	PHE
1	E	517	ASN
1	E	518	ASN
2	F	39	THR
2	F	73	ARG
2	F	82	THR
2	F	95	ARG
2	F	111	LEU
2	F	114	ARG
2	F	116	PRO
2	F	118	CYS
2	F	128	GLN
2	F	149	ILE

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Mol	Chain	Res	Type
2	F	158	LEU
2	F	182	THR
2	F	186	LYS
2	F	194	PRO
2	F	234	MET
2	F	241	GLN
2	F	242	PRO
2	F	286	LYS
2	F	292	VAL
2	F	316	ILE
2	F	319	ASN
2	F	321	TYR
2	F	325	ASN
2	F	326	ASP
2	F	342	ASN
2	F	355	PHE
2	F	374	LEU
2	F	375	GLN
2	F	377	LYS
2	F	430	THR
2	F	432	GLN
3	K	105	VAL
3	K	107	THR
3	K	170	VAL
3	K	173	LEU
1	G	6	LYS
1	G	43	THR
1	G	72	ASN
1	G	73	ASN
1	G	90	MET
1	G	117	PRO
1	G	154	ARG
1	G	163	ARG
1	G	200	ASP
1	G	202	ASP
1	G	214	TRP
1	G	245	ASP
1	G	264	ASN
1	G	292	ASP
1	G	309	ARG
1	G	311	LEU
1	G	335	ASP

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Mol	Chain	Res	Type
1	G	353	ASP
1	G	503	GLN
1	G	516	PHE
1	G	517	ASN
2	H	11	LEU
2	H	41	SER
2	H	82	THR
2	H	114	ARG
2	H	116	PRO
2	H	128	GLN
2	H	142	VAL
2	H	143	CYS
2	H	154	ILE
2	H	182	THR
2	H	188	ASN
2	H	201	GLU
2	H	213	PHE
2	H	223	ARG
2	H	233	ARG
2	H	249	LEU
2	H	316	ILE
2	H	319	ASN
2	H	321	TYR
2	H	325	ASN
2	H	348	GLN
2	H	362	GLN
2	H	366	ASP
2	H	374	LEU
3	L	119	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (145) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	ASN
1	A	63	ASN
1	A	72	ASN
1	A	77	GLN
1	A	175	HIS
1	A	197	GLN
1	A	209	HIS
1	A	224	GLN
1	A	264	ASN

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Mol	Chain	Res	Type
1	A	277	ASN
1	A	320	GLN
1	A	359	ASN
1	A	370	GLN
1	A	418	ASN
1	A	438	GLN
1	A	439	GLN
1	A	447	ASN
1	A	480	HIS
1	A	518	ASN
1	A	533	GLN
2	B	19	HIS
2	B	74	GLN
2	B	87	ASN
2	B	128	GLN
2	B	139	HIS
2	B	210	GLN
2	B	270	GLN
2	B	272	ASN
2	B	319	ASN
2	B	320	ASN
2	B	325	ASN
2	B	342	ASN
2	B	351	GLN
2	B	389	ASN
2	B	395	GLN
2	B	439	HIS
1	C	11	GLN
1	C	72	ASN
1	C	211	HIS
1	C	224	GLN
1	C	264	ASN
1	C	280	GLN
1	C	320	GLN
1	C	344	ASN
1	C	359	ASN
1	C	370	GLN
1	C	418	ASN
1	C	439	GLN
1	C	447	ASN
1	C	512	GLN
1	C	517	ASN

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Mol	Chain	Res	Type
2	D	18	ASN
2	D	32	HIS
2	D	74	GLN
2	D	128	GLN
2	D	139	HIS
2	D	210	GLN
2	D	241	GLN
2	D	270	GLN
2	D	282	GLN
2	D	319	ASN
2	D	325	ASN
2	D	342	ASN
2	D	362	GLN
2	D	375	GLN
2	D	421	GLN
2	D	432	GLN
3	J	149	GLN
3	J	172	GLN
1	E	37	ASN
1	E	64	GLN
1	E	72	ASN
1	E	111	ASN
1	E	115	ASN
1	E	195	HIS
1	E	197	GLN
1	E	211	HIS
1	E	224	GLN
1	E	264	ASN
1	E	271	ASN
1	E	277	ASN
1	E	359	ASN
1	E	386	ASN
1	E	418	ASN
1	E	436	HIS
1	E	438	GLN
1	E	439	GLN
1	E	447	ASN
1	E	517	ASN
1	E	518	ASN
2	F	19	HIS
2	F	32	HIS
2	F	74	GLN

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Mol	Chain	Res	Type
2	F	87	ASN
2	F	125	ASN
2	F	128	GLN
2	F	131	ASN
2	F	212	ASN
2	F	236	GLN
2	F	272	ASN
2	F	319	ASN
2	F	325	ASN
2	F	342	ASN
2	F	362	GLN
2	F	375	GLN
2	F	395	GLN
2	F	407	ASN
2	F	439	HIS
3	K	172	GLN
1	G	37	ASN
1	G	72	ASN
1	G	197	GLN
1	G	264	ASN
1	G	271	ASN
1	G	277	ASN
1	G	343	GLN
1	G	344	ASN
1	G	359	ASN
1	G	360	HIS
1	G	436	HIS
1	G	438	GLN
1	G	517	ASN
1	G	533	GLN
2	H	19	HIS
2	H	32	HIS
2	H	74	GLN
2	H	87	ASN
2	H	125	ASN
2	H	128	GLN
2	H	131	ASN
2	H	262	GLN
2	H	270	GLN
2	H	272	ASN
2	H	319	ASN
2	H	320	ASN

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Mol	Chain	Res	Type
2	H	325	ASN
2	H	351	GLN
2	H	352	ASN
2	H	354	GLN
2	H	362	GLN
2	H	375	GLN
2	H	407	ASN
2	H	421	GLN
2	H	439	HIS
3	L	141	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	522/531 (98%)	0.07	13 (2%) 61 55	33, 67, 99, 122	0
1	C	520/531 (97%)	0.08	6 (1%) 81 78	41, 68, 102, 130	0
1	E	521/531 (98%)	0.13	12 (2%) 64 59	32, 56, 116, 134	0
1	G	518/531 (97%)	0.15	19 (3%) 45 38	34, 64, 124, 137	0
2	B	432/434 (99%)	0.17	20 (4%) 36 30	36, 59, 109, 117	0
2	D	432/434 (99%)	0.29	18 (4%) 40 33	40, 70, 109, 117	0
2	F	431/434 (99%)	0.40	29 (6%) 21 15	37, 61, 116, 124	0
2	H	431/434 (99%)	0.31	26 (6%) 25 18	37, 69, 116, 122	0
3	I	86/88 (97%)	-0.04	0 100 100	47, 68, 93, 97	0
3	J	76/88 (86%)	0.36	3 (3%) 43 36	58, 77, 96, 98	0
3	K	76/88 (86%)	0.14	1 (1%) 79 78	56, 73, 90, 91	0
3	L	76/88 (86%)	0.55	4 (5%) 30 23	67, 93, 115, 121	0
All	All	4121/4212 (97%)	0.19	151 (3%) 45 38	32, 66, 113, 137	0

All (151) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	408	LEU	5.7
2	F	441	THR	5.6
2	H	360	LYS	5.4
1	C	259	PRO	5.2
1	G	201	LEU	5.0
2	D	417	LEU	5.0
2	H	408	LEU	4.9
2	B	408	LEU	4.8
1	E	209	HIS	4.7
1	E	210	SER	4.5
1	E	259	PRO	4.5

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Mol	Chain	Res	Type	RSRZ
1	G	210	SER	4.5
2	B	385	LEU	4.4
1	A	209	HIS	4.3
1	G	252	LEU	4.3
2	F	353	ILE	4.2
2	B	166	ASP	4.2
2	F	417	LEU	4.1
2	H	385	LEU	4.1
2	D	442	SER	4.1
1	E	252	LEU	4.1
1	G	209	HIS	4.1
2	D	385	LEU	4.1
1	G	247	ILE	4.0
3	L	162	LEU	4.0
2	F	412	LEU	4.0
2	F	385	LEU	4.0
1	C	260	GLU	3.9
3	J	162	LEU	3.8
1	A	252	LEU	3.8
1	A	259	PRO	3.8
2	D	415	LEU	3.8
2	B	392	LEU	3.8
2	H	438	LEU	3.7
2	H	436	PHE	3.6
2	B	381	ILE	3.6
3	L	161	ILE	3.6
1	A	208	ASP	3.5
3	L	117	ILE	3.4
2	D	389	ASN	3.3
2	B	442	SER	3.3
2	H	412	LEU	3.3
2	H	415	LEU	3.3
2	H	409	SER	3.3
2	H	211	VAL	3.2
2	D	438	LEU	3.2
3	L	116	ASP	3.2
1	A	201	LEU	3.2
2	B	438	LEU	3.1
2	H	391	THR	3.1
2	F	248	PRO	3.1
1	G	261	ASP	3.1
2	H	437	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	210	SER	3.0
1	A	261	ASP	3.0
2	H	365	LEU	3.0
1	E	247	ILE	3.0
2	F	440	PHE	3.0
2	H	246	GLY	2.9
2	H	392	LEU	2.9
2	H	363	GLU	2.9
1	A	204	MET	2.9
2	H	420	GLY	2.9
1	G	208	ASP	2.8
2	F	245	GLU	2.8
2	F	247	VAL	2.8
2	B	423	LEU	2.8
2	B	420	GLY	2.8
2	H	247	VAL	2.8
2	F	381	ILE	2.8
1	G	237	TYR	2.8
1	G	230	ASN	2.8
2	B	353	ILE	2.8
3	J	161	ILE	2.8
2	F	418	VAL	2.8
1	E	205	GLU	2.8
2	F	361	LEU	2.8
2	H	351	GLN	2.7
2	H	423	LEU	2.7
2	H	388	LYS	2.7
2	D	388	LYS	2.7
2	F	246	GLY	2.7
2	B	421	GLN	2.7
1	E	208	ASP	2.7
1	G	332	MET	2.6
1	G	234	PRO	2.6
1	A	200	ASP	2.6
2	B	391	THR	2.6
1	A	210	SER	2.6
2	D	422	GLU	2.6
2	B	361	LEU	2.6
2	F	243	PHE	2.6
2	F	368	LEU	2.6
1	G	203	HIS	2.6
2	F	242	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	G	226	TYR	2.5
2	B	382	THR	2.5
2	H	441	THR	2.5
2	F	251	GLY	2.5
1	G	249	GLN	2.5
2	B	393	TYR	2.5
2	D	11	LEU	2.5
1	E	230	ASN	2.5
2	B	360	LYS	2.4
1	A	202	ASP	2.4
2	H	374	LEU	2.4
1	G	253	LYS	2.4
1	A	372	PRO	2.4
1	E	251	ILE	2.4
2	F	415	LEU	2.4
1	C	211	HIS	2.4
2	F	392	LEU	2.3
2	D	215	MET	2.3
2	D	436	PHE	2.3
2	D	220	SER	2.3
3	K	117	ILE	2.3
2	H	359	ALA	2.3
2	D	393	TYR	2.3
2	H	355	PHE	2.3
1	G	202	ASP	2.2
2	F	393	TYR	2.2
1	G	200	ASP	2.2
2	F	423	LEU	2.2
2	D	248	PRO	2.2
2	B	388	LYS	2.2
2	F	388	LYS	2.2
1	A	457	LEU	2.2
2	F	419	ASP	2.2
2	F	436	PHE	2.2
3	J	102	LEU	2.2
2	D	421	GLN	2.2
2	F	249	LEU	2.2
2	B	419	ASP	2.2
2	H	166	ASP	2.2
2	F	363	GLU	2.2
2	D	211	VAL	2.2
1	E	248	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	229	ILE	2.1
1	E	206	LYS	2.1
2	H	421	GLN	2.1
1	C	252	LEU	2.1
1	E	153	CYS	2.1
1	G	251	ILE	2.1
2	F	414	GLU	2.0
1	A	374	SER	2.0
2	B	211	VAL	2.0
2	B	437	LYS	2.0
1	G	225	TRP	2.0
2	F	211	VAL	2.0
2	D	44	PHE	2.0
1	C	471	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	ZN	D	3	1/1	0.99	0.19	0.56	74,74,74,74	0
4	ZN	F	4	1/1	0.97	0.18	0.34	62,62,62,62	0
4	ZN	H	2	1/1	0.99	0.17	0.07	80,80,80,80	0
4	ZN	B	1	1/1	0.99	0.16	-0.01	65,65,65,65	0

6.5 Other polymers (i)

There are no such residues in this entry.