



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 08:23 pm BST

PDB ID : 3F3P  
Title : Crystal structure of the nucleoporin pair Nup85-Seh1, space group P21212  
Authors : Debler, E.W.; Hseo, H.; Ma, Y.; Blobel, G.; Hoelz, A.  
Deposited on : 2008-10-31  
Resolution : 3.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

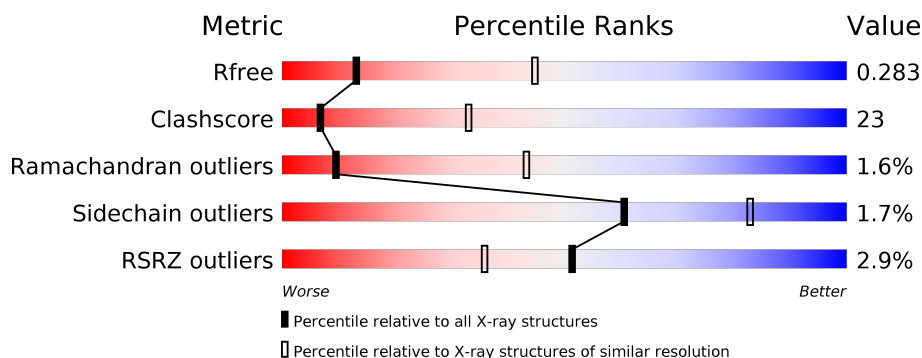
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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))
$R_{free}$	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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

Mol	Chain	Length	Quality of chain
1	A	351	<div> <div>2%</div> <div> <div>49%</div> <div>36%</div> <div>14%</div> </div> </div>
1	B	351	<div> <div>%</div> <div> <div>45%</div> <div>39%</div> <div>14%</div> </div> </div>
1	E	351	<div> <div>%</div> <div> <div>48%</div> <div>37%</div> <div>14%</div> </div> </div>
1	F	351	<div> <div>2%</div> <div> <div>48%</div> <div>38%</div> <div>12%</div> </div> </div>
1	I	351	<div> <div>4%</div> <div> <div>49%</div> <div>36%</div> <div>13%</div> </div> </div>
1	J	351	<div> <div>3%</div> <div> <div>47%</div> <div>38%</div> <div>12%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	C	570	<div><div><div></div><div></div><div></div></div><div>3%52%32%•16%</div></div>
2	D	570	<div><div><div></div><div></div><div></div></div><div>3%50%33%•16%</div></div>
2	G	570	<div><div><div></div><div></div><div></div></div><div>2%52%32%•15%</div></div>
2	H	570	<div><div><div></div><div></div><div></div></div><div>2%50%33%•15%</div></div>
2	K	570	<div><div><div></div><div></div><div></div></div><div>3%53%31%•15%</div></div>
2	L	570	<div><div><div></div><div></div><div></div></div><div>4%49%34%•15%</div></div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 37800 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 Nucleoporin SEH1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	303	Total	C	N	O	S	Se	0	0	0
			2407	1521	416	459	8	3			
1	B	303	Total	C	N	O	S	Se	0	0	0
			2407	1521	416	459	8	3			
1	E	303	Total	C	N	O	S	Se	0	0	0
			2407	1521	416	459	8	3			
1	F	308	Total	C	N	O	S	Se	0	0	0
			2445	1545	424	465	8	3			
1	I	307	Total	C	N	O	S	Se	0	0	0
			2435	1540	422	462	8	3			
1	J	308	Total	C	N	O	S	Se	0	0	0
			2445	1545	424	465	8	3			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	PRO	-	EXPRESSION TAG	UNP P53011
A	0	HIS	-	EXPRESSION TAG	UNP P53011
B	-1	PRO	-	EXPRESSION TAG	UNP P53011
B	0	HIS	-	EXPRESSION TAG	UNP P53011
E	-1	PRO	-	EXPRESSION TAG	UNP P53011
E	0	HIS	-	EXPRESSION TAG	UNP P53011
F	-1	PRO	-	EXPRESSION TAG	UNP P53011
F	0	HIS	-	EXPRESSION TAG	UNP P53011
I	-1	PRO	-	EXPRESSION TAG	UNP P53011
I	0	HIS	-	EXPRESSION TAG	UNP P53011
J	-1	PRO	-	EXPRESSION TAG	UNP P53011
J	0	HIS	-	EXPRESSION TAG	UNP P53011

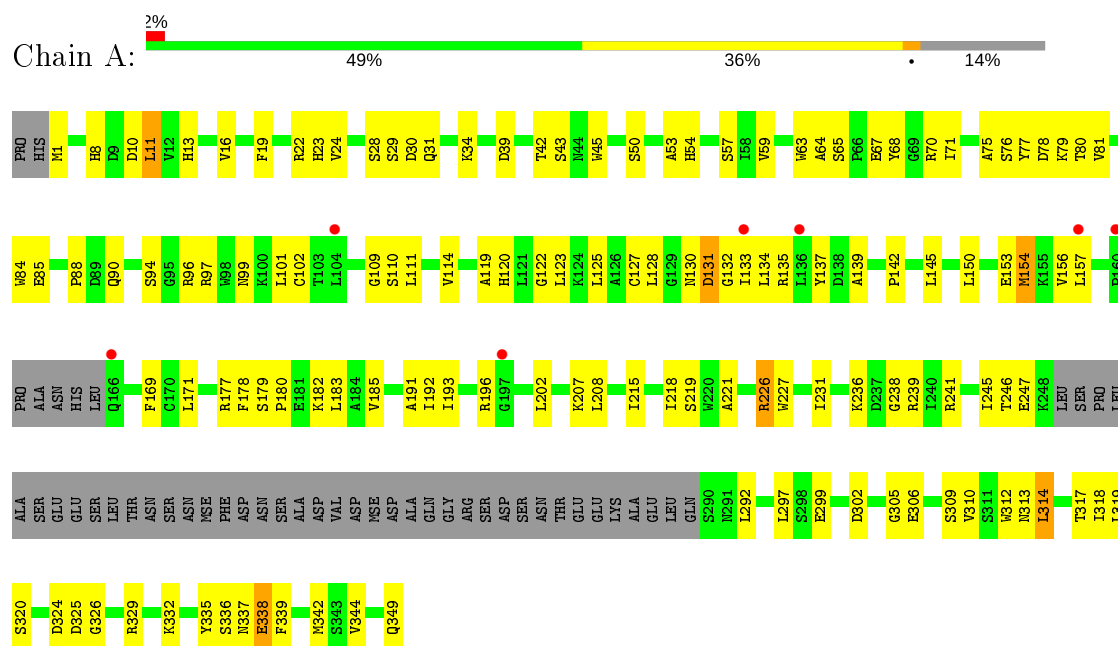
- Molecule 2 is a protein called Nucleoporin NUP85.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	480	Total	C	N	O	S	Se	0	0	0
			3858	2478	617	741	9	13			
2	D	478	Total	C	N	O	S	Se	0	0	0
			3837	2465	612	737	9	14			
2	G	483	Total	C	N	O	S	Se	0	0	0
			3877	2488	620	747	9	13			
2	H	486	Total	C	N	O	S	Se	0	0	0
			3897	2501	624	750	9	13			
2	K	487	Total	C	N	O	S	Se	0	0	0
			3911	2510	628	750	9	14			
2	L	482	Total	C	N	O	S	Se	0	0	0
			3874	2489	620	744	9	12			

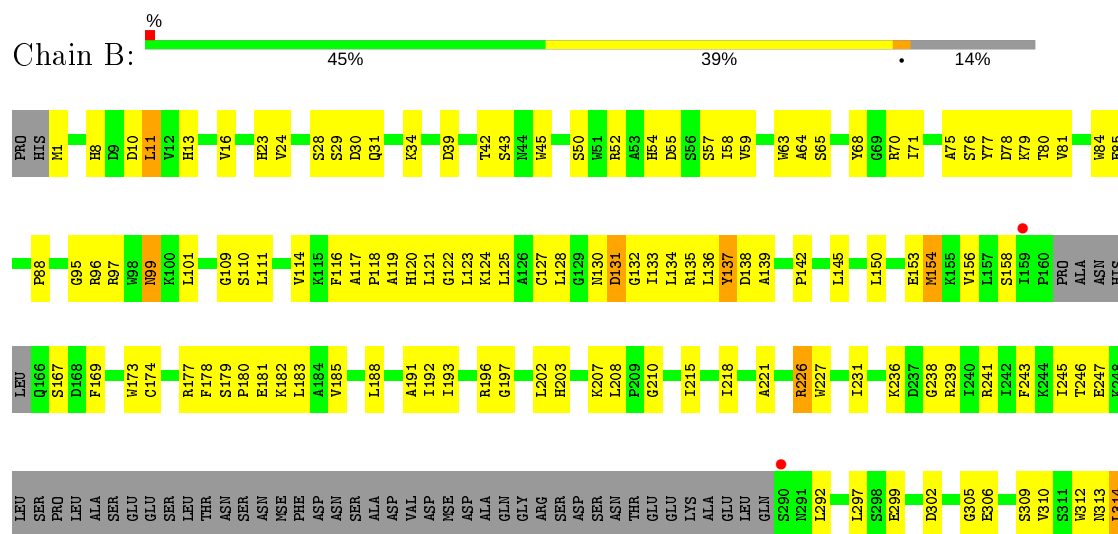
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

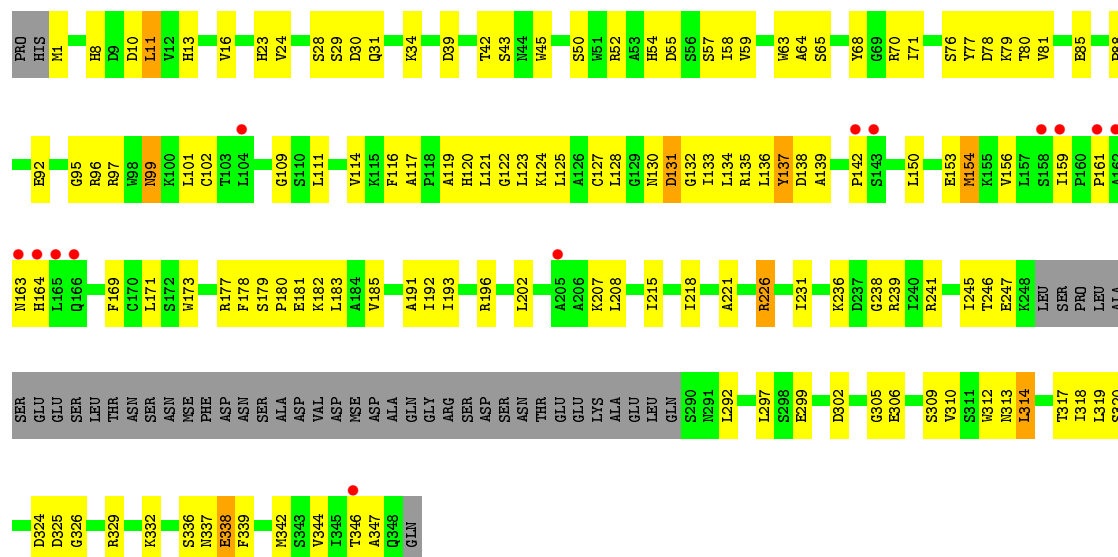
#### • Molecule 1: Nucleoporin SEH1



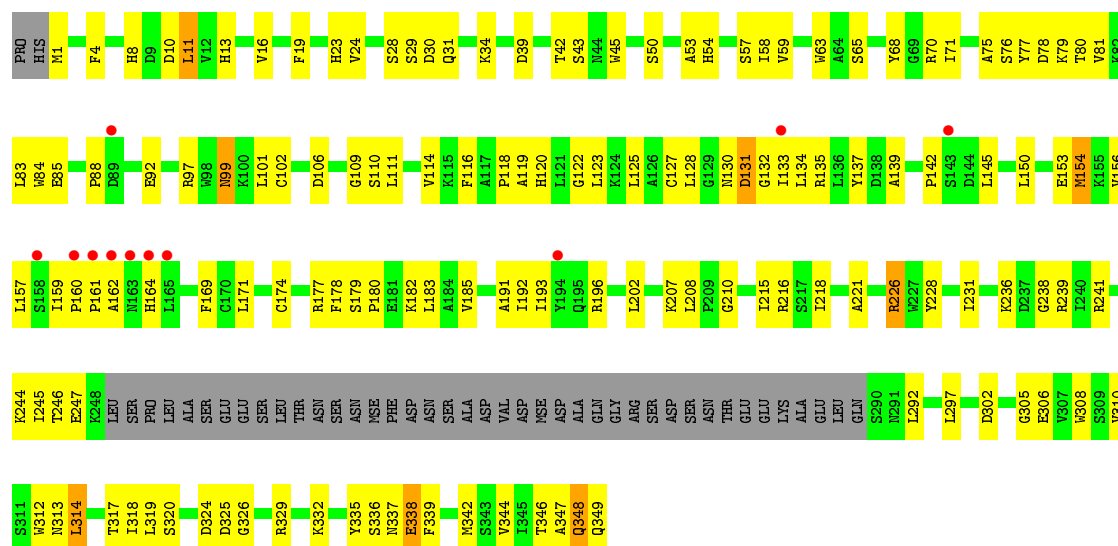
#### • Molecule 1: Nucleoporin SEH1



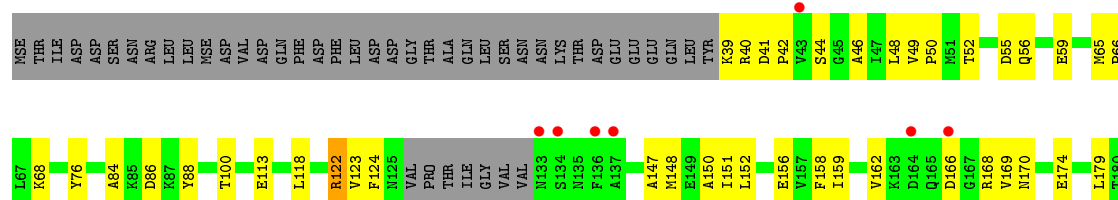




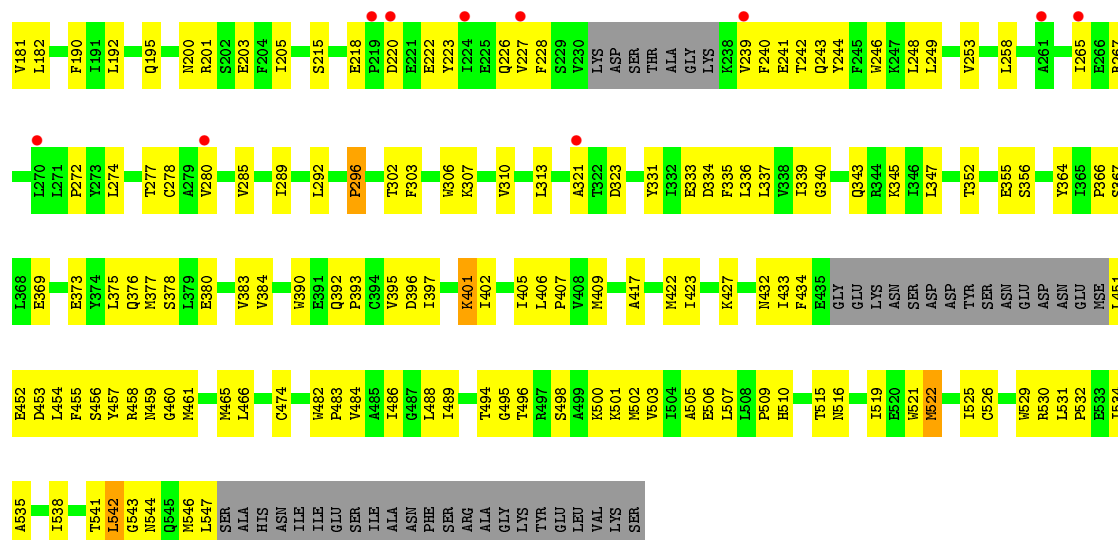
### • Molecule 1: Nucleoporin SEH1

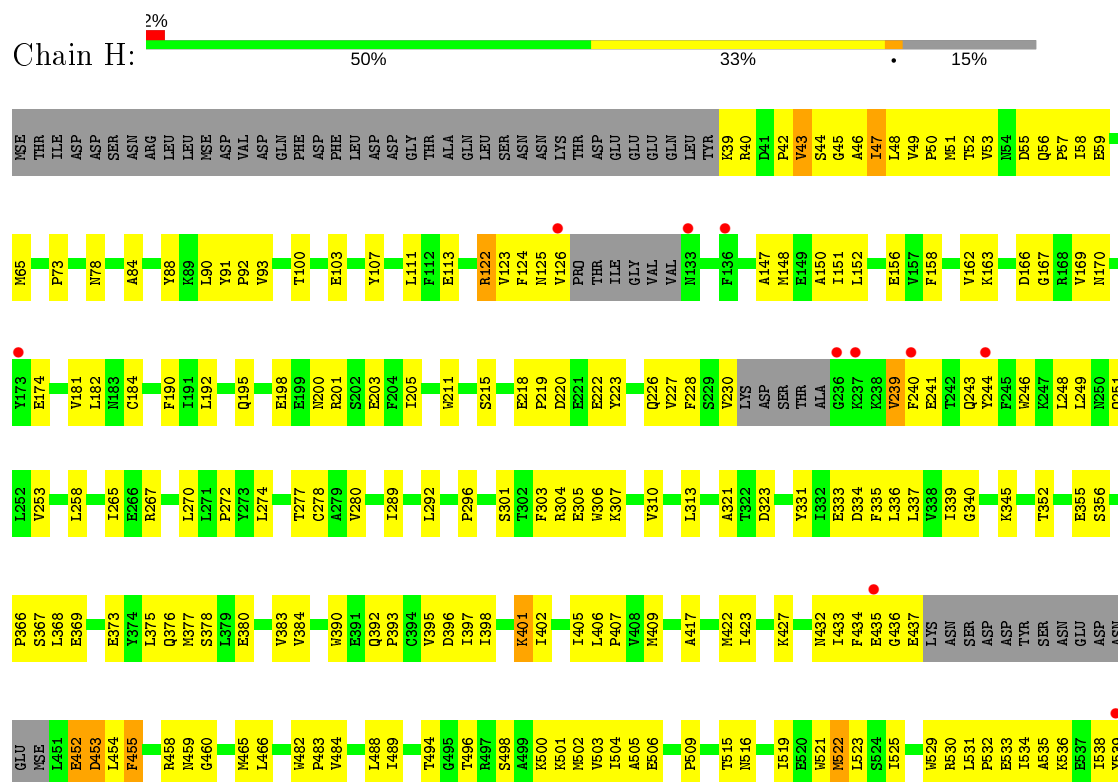
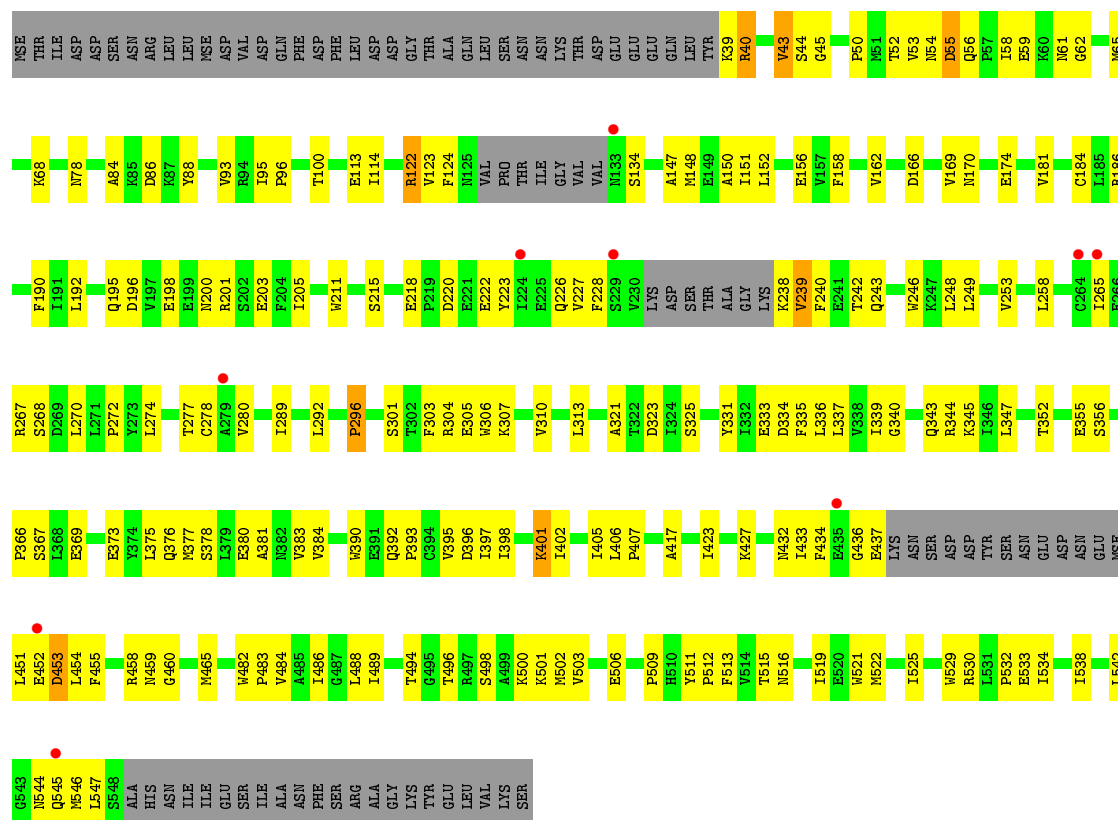


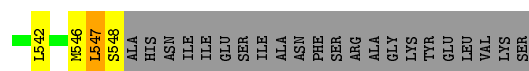
### • Molecule 2: Nucleoporin NUP85



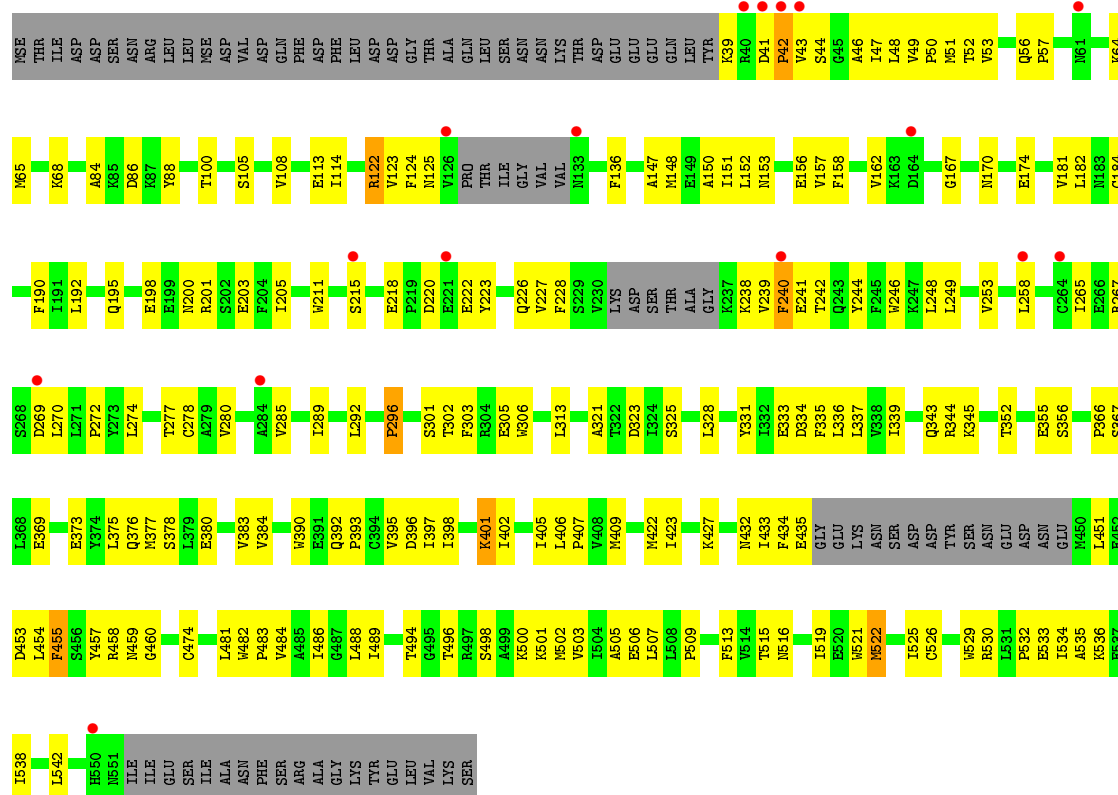




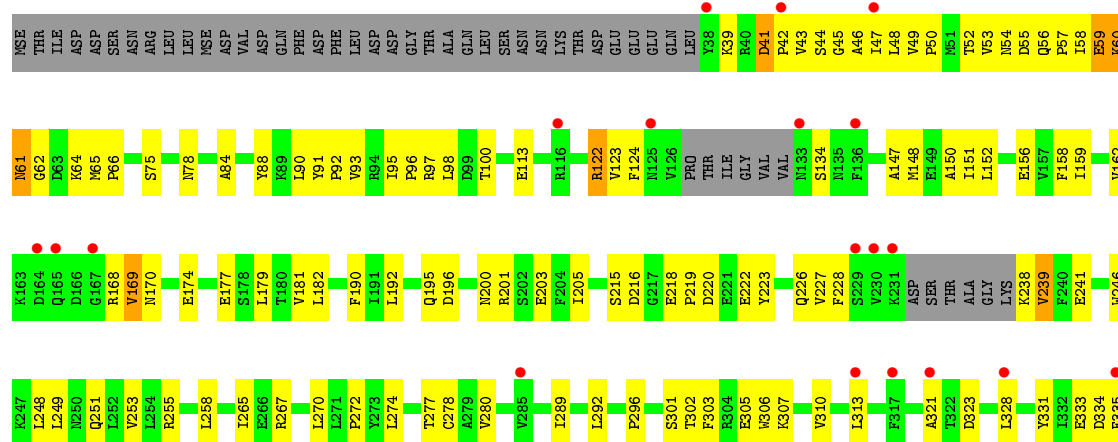


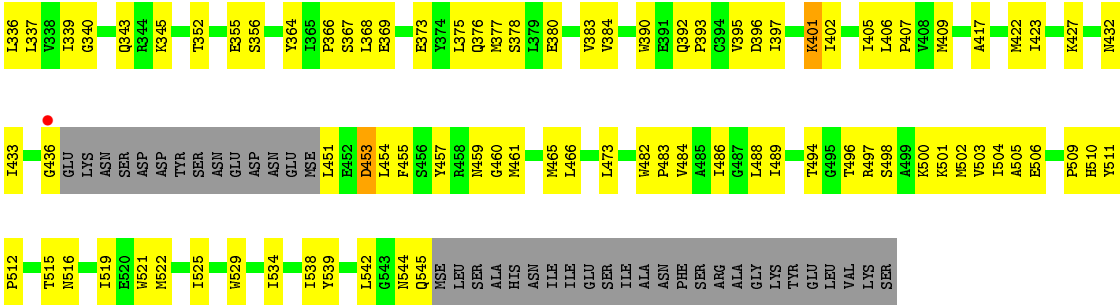


### • Molecule 2: Nucleoporin NUP85



### • Molecule 2: Nucleoporin NUP85





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 <sub>1</sub> 2 <sub>1</sub> 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	210.24 Å   226.48 Å   190.62 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	50.00 – 3.20 49.59 – 3.17	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-3.20) 84.9 (49.59-3.17)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.14	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.55 (at 3.19 Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.261   ,   0.281 0.266   ,   0.283	Depositor DCC
$R_{free}$ test set	7512 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	62.6	Xtriage
Anisotropy	0.754	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 31.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	37800	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 55.01 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.3656e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

<sup>2</sup> Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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	0.44	0/2463	0.69	0/3331
1	B	0.47	2/2463 (0.1%)	0.69	0/3331
1	E	0.44	0/2463	0.70	0/3331
1	F	0.43	0/2504	0.69	0/3390
1	I	0.48	3/2494 (0.1%)	0.70	0/3378
1	J	0.45	0/2504	0.69	0/3390
2	C	0.43	0/3923	0.63	0/5289
2	D	0.45	0/3902	0.63	1/5260 (0.0%)
2	G	0.46	0/3942	0.64	1/5314 (0.0%)
2	H	0.44	0/3962	0.64	1/5340 (0.0%)
2	K	0.45	0/3977	0.63	1/5361 (0.0%)
2	L	0.44	0/3941	0.65	1/5315 (0.0%)
All	All	0.45	5/38538 (0.0%)	0.66	5/52030 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	137	TYR	CE1-CZ	-5.91	1.30	1.38
1	I	137	TYR	CE1-CZ	-5.81	1.31	1.38
1	I	137	TYR	CG-CD2	-5.23	1.32	1.39
1	I	137	TYR	CE2-CZ	-5.13	1.31	1.38
1	B	137	TYR	CG-CD2	-5.07	1.32	1.39

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	455	PHE	N-CA-C	-5.65	95.74	111.00
2	D	455	PHE	N-CA-C	-5.57	95.97	111.00
2	L	62	GLY	N-CA-C	-5.42	99.55	113.10
2	K	455	PHE	N-CA-C	-5.16	97.06	111.00
2	G	134	SER	CB-CA-C	5.13	119.85	110.10

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	2407	0	2343	139	0
1	B	2407	0	2343	140	0
1	E	2407	0	2343	119	0
1	F	2445	0	2380	126	0
1	I	2435	0	2372	124	0
1	J	2445	0	2380	141	0
2	C	3858	0	3806	177	0
2	D	3837	0	3780	180	0
2	G	3877	0	3820	175	0
2	H	3897	0	3845	191	0
2	K	3911	0	3860	172	0
2	L	3874	0	3820	175	0
All	All	37800	0	37092	1742	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 23.

All (1742) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:454:LEU:HD13	2:G:459:ASN:HD21	1.02	1.17
2:G:304:ARG:HH12	2:H:437:GLU:HG2	0.94	1.10
2:G:436:GLY:HA2	2:H:198:GLU:OE1	1.50	1.10
2:G:239:VAL:HG12	2:G:240:PHE:H	1.09	1.08
2:C:451:LEU:HD21	2:C:502:MSE:CE	1.86	1.04
2:G:304:ARG:NH1	2:H:437:GLU:HG2	1.72	1.03
2:D:454:LEU:HB2	2:D:459:ASN:HD21	1.21	1.02
1:B:192:ILE:HG22	1:B:207:LYS:HG2	1.43	1.01
1:F:192:ILE:HG22	1:F:207:LYS:HG2	1.44	1.00
2:H:534:ILE:O	2:H:538:ILE:HG12	1.62	1.00
1:J:192:ILE:HG22	1:J:207:LYS:HG2	1.41	1.00
1:F:88:PRO:HA	1:F:97:ARG:HH12	1.24	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:451:LEU:CD2	2:C:502:MSE:HE1	1.91	0.99
1:A:192:ILE:HG22	1:A:207:LYS:HG2	1.44	0.99
1:F:159:ILE:HG13	1:F:161:PRO:HD3	1.43	0.99
1:E:192:ILE:HG22	1:E:207:LYS:HG2	1.44	0.98
2:C:451:LEU:HD21	2:C:502:MSE:HE1	1.01	0.97
2:H:239:VAL:HG23	2:H:240:PHE:H	1.30	0.97
1:I:192:ILE:HG22	1:I:207:LYS:HG2	1.47	0.96
1:I:208:LEU:HD11	1:I:231:ILE:HD11	1.47	0.96
1:A:88:PRO:HA	1:A:97:ARG:HH12	1.29	0.95
1:E:88:PRO:HA	1:E:97:ARG:HH12	1.29	0.95
1:B:88:PRO:HA	1:B:97:ARG:HH12	1.32	0.94
1:A:208:LEU:HD11	1:A:231:ILE:HD11	1.48	0.94
1:J:88:PRO:HA	1:J:97:ARG:HH12	1.32	0.94
2:H:228:PHE:CE2	2:H:267:ARG:HD3	2.03	0.94
2:G:454:LEU:HD13	2:G:459:ASN:ND2	1.84	0.92
2:K:198:GLU:OE1	2:L:436:GLY:HA2	1.68	0.92
1:I:81:VAL:HG23	1:I:111:LEU:HD13	1.51	0.90
2:K:240:PHE:HB2	2:K:269:ASP:OD2	1.72	0.89
1:B:81:VAL:HG23	1:B:111:LEU:HD13	1.55	0.89
2:K:451:LEU:HD11	2:K:502:MSE:HE1	1.53	0.88
2:C:228:PHE:CE2	2:C:267:ARG:HD3	2.08	0.88
1:J:178:PHE:HB3	2:L:502:MSE:HE3	1.55	0.88
2:C:451:LEU:HG	2:C:452:GLU:H	1.37	0.88
2:G:239:VAL:HG12	2:G:240:PHE:N	1.88	0.87
1:J:81:VAL:HG23	1:J:111:LEU:HD13	1.56	0.87
1:B:208:LEU:HD11	1:B:231:ILE:HD11	1.55	0.86
2:D:522:MSE:CE	2:D:538:ILE:HD12	2.06	0.86
1:A:39:ASP:HB3	1:A:42:THR:HG22	1.56	0.86
2:C:454:LEU:HD13	2:C:459:ASN:HD21	1.41	0.85
2:K:242:THR:CG2	2:K:244:TYR:HB2	2.05	0.85
1:A:81:VAL:HG23	1:A:111:LEU:HD13	1.56	0.85
2:H:280:VAL:HG21	2:H:321:ALA:HB3	1.58	0.85
1:I:88:PRO:HA	1:I:97:ARG:HH12	1.41	0.85
1:B:52:ARG:HD2	1:E:95:GLY:O	1.77	0.85
2:D:402:ILE:O	2:D:405:ILE:HG22	1.76	0.85
2:L:241:GLU:OE1	2:L:328:LEU:HD13	1.76	0.85
1:B:247:GLU:HB3	1:B:292:LEU:HD23	1.58	0.85
1:F:78:ASP:OD1	1:F:80:THR:HG22	1.77	0.85
1:A:8:HIS:ND1	1:A:28:SER:HB2	1.91	0.85
2:G:437:GLU:HG3	2:H:304:ARG:HH12	1.40	0.85
1:J:247:GLU:HB3	1:J:292:LEU:HD23	1.57	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:GLU:HB3	1:A:292:LEU:HD23	1.58	0.84
1:I:247:GLU:HB3	1:I:292:LEU:HD23	1.59	0.84
2:K:515:THR:HG22	2:K:516:ASN:H	1.42	0.84
1:A:39:ASP:HB3	1:A:42:THR:CG2	2.08	0.84
1:A:178:PHE:HB3	2:C:502:MSE:HE3	1.58	0.84
2:H:515:THR:HG22	2:H:516:ASN:H	1.44	0.83
1:J:78:ASP:OD1	1:J:80:THR:HG22	1.78	0.83
2:L:280:VAL:HG21	2:L:321:ALA:HB3	1.58	0.83
2:G:451:LEU:HD21	2:G:502:MSE:HE1	1.61	0.83
1:J:39:ASP:HB3	1:J:42:THR:HG22	1.58	0.83
1:I:178:PHE:HB3	2:K:502:MSE:HE3	1.60	0.83
1:B:78:ASP:OD1	1:B:80:THR:HG22	1.79	0.83
2:D:515:THR:HG22	2:D:516:ASN:H	1.43	0.83
1:F:39:ASP:HB3	1:F:42:THR:HG22	1.60	0.83
2:C:280:VAL:HG21	2:C:321:ALA:HB3	1.58	0.83
1:I:39:ASP:HB3	1:I:42:THR:HG22	1.61	0.83
2:D:152:LEU:O	2:D:156:GLU:HG3	1.79	0.82
2:D:454:LEU:CB	2:D:459:ASN:HD21	1.91	0.82
1:E:208:LEU:HD11	1:E:231:ILE:HD11	1.61	0.82
2:H:51:MSE:HE3	2:H:91:TYR:CD2	2.14	0.82
1:I:39:ASP:HB3	1:I:42:THR:CG2	2.09	0.82
2:D:52:THR:HG21	2:D:55:ASP:HB2	1.61	0.82
2:H:454:LEU:HB3	2:H:459:ASN:OD1	1.78	0.82
2:D:453:ASP:O	2:D:454:LEU:HD23	1.78	0.82
2:H:531:LEU:HB3	2:H:534:ILE:HD12	1.59	0.82
1:A:8:HIS:ND1	1:A:28:SER:CB	2.42	0.82
2:C:515:THR:HG22	2:C:516:ASN:H	1.45	0.82
2:G:52:THR:HG22	2:G:53:VAL:H	1.44	0.82
1:J:39:ASP:HB3	1:J:42:THR:CG2	2.09	0.82
2:L:402:ILE:O	2:L:405:ILE:HG22	1.79	0.82
1:E:78:ASP:OD1	1:E:80:THR:HG22	1.80	0.82
2:G:515:THR:HG22	2:G:516:ASN:H	1.44	0.82
2:K:402:ILE:O	2:K:405:ILE:HG22	1.80	0.82
2:G:280:VAL:HG21	2:G:321:ALA:HB3	1.60	0.81
2:K:242:THR:HG22	2:K:244:TYR:HB2	1.62	0.81
1:F:137:TYR:CZ	1:F:150:LEU:HD13	2.15	0.81
1:J:208:LEU:HD11	1:J:231:ILE:HD11	1.62	0.81
2:K:451:LEU:HD21	2:K:502:MSE:HE1	1.59	0.81
1:A:78:ASP:OD1	1:A:80:THR:HG22	1.79	0.81
1:I:78:ASP:OD1	1:I:80:THR:HG22	1.79	0.81
1:J:221:ALA:HB2	1:J:312:TRP:CE2	2.15	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:178:PHE:HB3	2:D:502:MSE:HE3	1.60	0.81
1:E:39:ASP:HB3	1:E:42:THR:CG2	2.11	0.81
2:L:515:THR:HG22	2:L:516:ASN:H	1.45	0.81
2:C:52:THR:HG21	2:C:55:ASP:HB2	1.62	0.81
2:K:280:VAL:HG21	2:K:321:ALA:HB3	1.62	0.81
1:B:28:SER:HB3	1:B:30:ASP:OD1	1.80	0.80
2:G:402:ILE:O	2:G:405:ILE:HG22	1.79	0.80
2:H:454:LEU:HD23	2:H:458:ARG:HB2	1.61	0.80
1:F:39:ASP:HB3	1:F:42:THR:CG2	2.11	0.80
1:A:137:TYR:CZ	1:A:150:LEU:HD13	2.16	0.80
2:D:280:VAL:HG21	2:D:321:ALA:HB3	1.62	0.80
2:C:402:ILE:O	2:C:405:ILE:HG22	1.81	0.80
1:B:39:ASP:HB3	1:B:42:THR:CG2	2.10	0.80
1:B:39:ASP:HB3	1:B:42:THR:HG22	1.62	0.80
2:K:432:ASN:HB2	2:K:460:GLY:HA2	1.62	0.80
1:J:137:TYR:CZ	1:J:150:LEU:HD13	2.17	0.79
2:K:123:VAL:HG12	2:K:124:PHE:H	1.47	0.79
2:K:453:ASP:O	2:K:454:LEU:HD23	1.81	0.79
2:L:522:MSE:HE2	2:L:538:ILE:HD11	1.62	0.79
1:F:95:GLY:O	1:I:52:ARG:HD2	1.82	0.79
2:H:402:ILE:O	2:H:405:ILE:HG22	1.83	0.79
1:E:137:TYR:CZ	1:E:150:LEU:HD13	2.17	0.79
1:E:81:VAL:HG23	1:E:111:LEU:HD13	1.64	0.79
2:G:151:ILE:HD12	2:G:423:ILE:HD12	1.65	0.79
2:D:452:GLU:HG2	2:D:454:LEU:HD21	1.63	0.79
1:F:221:ALA:HB2	1:F:312:TRP:CE2	2.18	0.78
1:F:81:VAL:HG23	1:F:111:LEU:HD13	1.65	0.78
1:A:137:TYR:CE2	1:A:150:LEU:HD13	2.18	0.78
1:J:346:THR:HG22	1:J:347:ALA:H	1.47	0.78
1:E:39:ASP:HB3	1:E:42:THR:HG22	1.63	0.78
2:H:454:LEU:HD13	2:H:459:ASN:HD21	1.47	0.78
1:E:158:SER:O	1:E:159:ILE:HG13	1.83	0.78
2:K:41:ASP:HB3	2:K:46:ALA:O	1.83	0.78
2:D:432:ASN:HB2	2:D:460:GLY:HA2	1.65	0.78
2:G:152:LEU:O	2:G:156:GLU:HG3	1.84	0.78
2:H:152:LEU:O	2:H:156:GLU:HG3	1.84	0.78
2:D:515:THR:HG22	2:D:516:ASN:N	1.99	0.78
2:H:123:VAL:HG12	2:H:124:PHE:H	1.49	0.78
1:E:349:GLN:HB2	2:G:56:GLN:HB2	1.65	0.77
2:D:123:VAL:HG12	2:D:124:PHE:H	1.49	0.77
2:D:228:PHE:CE2	2:D:267:ARG:HD3	2.20	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:123:VAL:HG12	2:C:124:PHE:H	1.49	0.77
2:G:123:VAL:HG12	2:G:124:PHE:H	1.48	0.77
2:K:454:LEU:HB2	2:K:459:ASN:HD21	1.49	0.77
1:F:137:TYR:CE2	1:F:150:LEU:HD13	2.20	0.77
2:K:515:THR:HG22	2:K:516:ASN:N	1.99	0.77
1:E:221:ALA:HB2	1:E:312:TRP:CE2	2.19	0.77
2:L:152:LEU:O	2:L:156:GLU:HG3	1.85	0.77
2:K:152:LEU:O	2:K:156:GLU:HG3	1.83	0.77
2:L:52:THR:HG21	2:L:55:ASP:HB2	1.67	0.77
2:K:434:PHE:CD2	2:K:458:ARG:HA	2.18	0.76
2:C:152:LEU:O	2:C:156:GLU:HG3	1.85	0.76
2:D:454:LEU:HD22	2:D:458:ARG:HD2	1.65	0.76
2:H:454:LEU:CD2	2:H:458:ARG:HB2	2.15	0.76
2:K:258:LEU:HD22	2:K:292:LEU:HD22	1.67	0.76
2:H:531:LEU:HB3	2:H:534:ILE:CD1	2.15	0.76
1:F:88:PRO:HA	1:F:97:ARG:NH1	2.01	0.76
2:C:515:THR:HG22	2:C:516:ASN:N	2.01	0.76
2:L:417:ALA:HB1	2:L:465:MSE:HE1	1.67	0.76
2:L:522:MSE:HE2	2:L:538:ILE:CD1	2.16	0.76
2:K:240:PHE:CD2	2:K:328:LEU:HD11	2.21	0.76
1:B:324:ASP:HB3	2:D:64:LYS:HB3	1.68	0.75
1:J:28:SER:HB3	1:J:30:ASP:OD1	1.86	0.75
1:J:346:THR:HG22	1:J:348:GLN:H	1.51	0.75
2:H:228:PHE:HE2	2:H:267:ARG:HD3	1.51	0.75
2:C:151:ILE:HD12	2:C:423:ILE:HD12	1.67	0.75
2:G:166:ASP:HB3	2:G:169:VAL:HG11	1.66	0.75
2:G:515:THR:HG22	2:G:516:ASN:N	2.01	0.75
2:L:228:PHE:CE2	2:L:267:ARG:HD3	2.21	0.75
1:B:221:ALA:HB2	1:B:312:TRP:CE2	2.21	0.75
2:H:515:THR:HG22	2:H:516:ASN:N	2.01	0.74
2:G:454:LEU:CD1	2:G:459:ASN:HD21	1.91	0.74
2:L:151:ILE:HD12	2:L:423:ILE:HD12	1.69	0.74
1:F:208:LEU:HD11	1:F:231:ILE:HD11	1.69	0.74
1:F:52:ARG:HD2	1:I:95:GLY:O	1.87	0.74
2:H:151:ILE:HD12	2:H:423:ILE:HD12	1.69	0.74
1:J:346:THR:HG22	1:J:347:ALA:N	2.02	0.74
2:L:258:LEU:HD22	2:L:292:LEU:HD22	1.70	0.74
2:L:515:THR:HG22	2:L:516:ASN:N	2.02	0.74
2:D:452:GLU:HG3	2:D:458:ARG:NH1	2.02	0.74
2:C:258:LEU:HD22	2:C:292:LEU:HD22	1.70	0.74
2:D:522:MSE:HE1	2:D:538:ILE:HD12	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:451:LEU:HG	2:G:452:GLU:H	1.52	0.74
2:L:181:VAL:CG1	2:L:405:ILE:HD11	2.18	0.74
2:D:258:LEU:HD22	2:D:292:LEU:HD22	1.69	0.73
2:K:451:LEU:HD11	2:K:502:MSE:CE	2.18	0.73
2:H:258:LEU:HD22	2:H:292:LEU:HD22	1.68	0.73
2:C:334:ASP:OD2	2:C:345:LYS:HE3	1.88	0.73
2:G:52:THR:HG22	2:G:53:VAL:N	2.03	0.73
1:B:344:VAL:O	2:D:48:LEU:HD12	1.88	0.73
1:F:28:SER:HB3	1:F:30:ASP:OD1	1.89	0.73
2:G:228:PHE:CE2	2:G:267:ARG:HD3	2.23	0.73
1:A:8:HIS:CD2	1:A:34:LYS:HD2	2.24	0.73
2:H:383:VAL:HG12	2:H:384:VAL:H	1.53	0.73
2:K:334:ASP:OD2	2:K:345:LYS:HE3	1.89	0.73
2:L:123:VAL:HG12	2:L:124:PHE:H	1.51	0.73
2:D:434:PHE:CD2	2:D:458:ARG:HA	2.23	0.73
1:A:28:SER:HB3	1:A:30:ASP:OD1	1.88	0.73
1:F:30:ASP:HA	1:I:96:ARG:NH1	2.04	0.72
2:L:334:ASP:OD2	2:L:345:LYS:HE3	1.89	0.72
1:I:178:PHE:CB	2:K:502:MSE:HE3	2.19	0.72
2:H:47:ILE:HG22	2:H:48:LEU:N	2.03	0.72
2:D:383:VAL:HG12	2:D:384:VAL:H	1.53	0.72
2:G:258:LEU:HD22	2:G:292:LEU:HD22	1.70	0.72
1:I:221:ALA:HB2	1:I:312:TRP:CE2	2.24	0.72
2:K:228:PHE:CE2	2:K:267:ARG:HD3	2.24	0.72
1:J:1:MSE:HE2	1:J:1:MSE:HA	1.71	0.72
1:A:221:ALA:HB2	1:A:312:TRP:CE2	2.24	0.72
1:B:95:GLY:O	1:E:52:ARG:HD2	1.90	0.72
2:H:239:VAL:HG23	2:H:240:PHE:N	2.04	0.72
2:K:52:THR:HB	2:K:56:GLN:HG2	1.72	0.72
2:C:417:ALA:HB1	2:C:465:MSE:HE1	1.72	0.72
1:E:88:PRO:HA	1:E:97:ARG:NH1	2.04	0.71
2:L:383:VAL:HG12	2:L:384:VAL:H	1.55	0.71
2:L:484:VAL:O	2:L:488:LEU:HD13	1.90	0.71
1:F:247:GLU:HB3	1:F:292:LEU:HD23	1.72	0.71
2:H:538:ILE:O	2:H:542:LEU:HG	1.89	0.71
2:D:534:ILE:O	2:D:538:ILE:HG12	1.90	0.71
2:G:181:VAL:CG1	2:G:405:ILE:HD11	2.20	0.71
1:J:324:ASP:HB3	2:L:64:LYS:HD3	1.72	0.70
2:D:334:ASP:OD2	2:D:345:LYS:HE3	1.90	0.70
2:K:122:ARG:HH11	2:K:122:ARG:HB3	1.56	0.70
2:L:239:VAL:HG12	2:L:239:VAL:O	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:28:SER:HB3	1:E:30:ASP:OD1	1.92	0.70
1:E:314:LEU:O	1:E:314:LEU:HD12	1.91	0.70
2:G:55:ASP:OD1	2:G:55:ASP:N	2.22	0.70
1:B:178:PHE:CB	2:D:502:MSE:HE3	2.21	0.70
1:E:137:TYR:CE2	1:E:150:LEU:HD13	2.26	0.70
2:G:181:VAL:HG12	2:G:405:ILE:HD11	1.73	0.70
2:K:533:GLU:O	2:K:536:LYS:HB3	1.92	0.70
2:K:240:PHE:CB	2:K:269:ASP:OD2	2.40	0.70
2:H:334:ASP:OD2	2:H:345:LYS:HE3	1.91	0.70
2:H:181:VAL:CG1	2:H:405:ILE:HD11	2.22	0.70
2:H:48:LEU:HD12	2:H:49:VAL:N	2.07	0.70
1:E:306:GLU:N	1:E:324:ASP:OD2	2.25	0.70
1:I:28:SER:HB3	1:I:30:ASP:OD1	1.91	0.70
2:G:122:ARG:HB3	2:G:122:ARG:HH11	1.56	0.70
1:A:123:LEU:HB3	1:A:139:ALA:HB3	1.74	0.70
2:C:181:VAL:CG1	2:C:405:ILE:HD11	2.21	0.70
2:H:148:MSE:CE	2:H:152:LEU:HG	2.22	0.70
2:L:181:VAL:HG12	2:L:405:ILE:HD11	1.73	0.70
1:B:226:ARG:HG3	1:B:226:ARG:HH11	1.57	0.69
2:D:148:MSE:CE	2:D:152:LEU:HG	2.22	0.69
2:L:148:MSE:CE	2:L:152:LEU:HG	2.22	0.69
1:A:8:HIS:CD2	1:A:34:LYS:CE	2.74	0.69
2:C:122:ARG:HH11	2:C:122:ARG:HB3	1.57	0.69
2:D:122:ARG:HB3	2:D:122:ARG:HH11	1.58	0.69
2:K:451:LEU:CD1	2:K:502:MSE:HE1	2.22	0.69
2:L:392:GLN:HB3	2:L:393:PRO:HD3	1.74	0.69
2:C:39:LYS:O	2:C:39:LYS:HD3	1.92	0.69
2:C:454:LEU:HD13	2:C:459:ASN:ND2	2.07	0.69
1:F:348:GLN:O	2:H:56:GLN:HG3	1.92	0.69
1:J:88:PRO:HA	1:J:97:ARG:NH1	2.06	0.69
2:C:522:MSE:CE	2:C:538:ILE:HD12	2.23	0.69
2:G:148:MSE:CE	2:G:152:LEU:HG	2.23	0.69
2:H:42:PRO:HA	2:H:46:ALA:O	1.93	0.69
1:J:226:ARG:HH11	1:J:226:ARG:HG3	1.58	0.68
2:K:383:VAL:HG12	2:K:384:VAL:H	1.58	0.68
1:A:226:ARG:HG3	1:A:226:ARG:HH11	1.57	0.68
2:C:484:VAL:O	2:C:488:LEU:HD13	1.92	0.68
1:I:306:GLU:N	1:I:324:ASP:OD2	2.26	0.68
2:D:484:VAL:O	2:D:488:LEU:HD13	1.93	0.68
1:A:8:HIS:HD2	1:A:34:LYS:CE	2.06	0.68
2:D:522:MSE:HE2	2:D:538:ILE:HD12	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:544:ASN:O	2:G:547:LEU:HG	1.92	0.68
1:A:88:PRO:HA	1:A:97:ARG:NH1	2.04	0.68
2:C:181:VAL:HG12	2:C:405:ILE:HD11	1.75	0.68
2:C:454:LEU:HD12	2:C:495:GLY:HA2	1.75	0.68
2:H:392:GLN:HB3	2:H:393:PRO:HD3	1.76	0.68
1:E:123:LEU:HB3	1:E:139:ALA:HB3	1.76	0.68
2:G:334:ASP:OD2	2:G:345:LYS:HE3	1.94	0.68
1:E:247:GLU:HB3	1:E:292:LEU:HD23	1.76	0.68
2:H:454:LEU:CD2	2:H:458:ARG:CB	2.71	0.68
2:K:181:VAL:HG12	2:K:405:ILE:HD11	1.76	0.68
1:J:159:ILE:C	1:J:161:PRO:HD2	2.14	0.68
1:F:226:ARG:HG3	1:F:226:ARG:HH11	1.58	0.67
2:H:484:VAL:O	2:H:488:LEU:HD13	1.93	0.67
1:B:306:GLU:N	1:B:324:ASP:OD2	2.28	0.67
1:F:1:MSE:HE2	1:F:1:MSE:HA	1.76	0.67
1:I:226:ARG:HG3	1:I:226:ARG:HH11	1.59	0.67
2:G:239:VAL:CG1	2:G:240:PHE:H	1.95	0.67
2:L:122:ARG:HB3	2:L:122:ARG:HH11	1.58	0.67
2:L:148:MSE:HE3	2:L:148:MSE:O	1.94	0.67
1:E:226:ARG:HH11	1:E:226:ARG:HG3	1.59	0.67
1:F:314:LEU:HD12	1:F:314:LEU:O	1.94	0.67
2:C:383:VAL:HG12	2:C:384:VAL:H	1.58	0.67
1:B:247:GLU:O	2:D:450:MSE:HE1	1.93	0.67
1:E:178:PHE:HB3	2:G:502:MSE:HE3	1.76	0.67
2:G:39:LYS:HG3	2:G:40:ARG:H	1.58	0.67
2:D:148:MSE:HE3	2:D:148:MSE:O	1.95	0.67
2:D:392:GLN:HB3	2:D:393:PRO:HD3	1.77	0.67
2:H:181:VAL:HG12	2:H:405:ILE:HD11	1.76	0.67
2:K:123:VAL:HG12	2:K:124:PHE:N	2.09	0.67
2:K:148:MSE:CE	2:K:152:LEU:HG	2.24	0.67
1:A:306:GLU:N	1:A:324:ASP:OD2	2.28	0.67
1:I:39:ASP:OD2	1:I:42:THR:HG22	1.95	0.67
2:K:181:VAL:CG1	2:K:405:ILE:HD11	2.25	0.66
2:C:392:GLN:HB3	2:C:393:PRO:HD3	1.77	0.66
1:I:123:LEU:HB3	1:I:139:ALA:HB3	1.76	0.66
2:L:265:ILE:HG21	2:L:289:ILE:HD11	1.77	0.66
2:L:41:ASP:N	2:L:41:ASP:OD1	2.29	0.66
1:A:8:HIS:ND1	1:A:28:SER:HB3	2.09	0.66
2:G:122:ARG:CB	2:G:122:ARG:HH11	2.09	0.66
2:L:454:LEU:HD13	2:L:459:ASN:HD21	1.59	0.66
1:B:39:ASP:OD2	1:B:42:THR:HG22	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:123:VAL:HG12	2:G:124:PHE:N	2.10	0.66
2:D:531:LEU:HB3	2:D:534:ILE:HD12	1.77	0.66
2:H:148:MSE:HE3	2:H:148:MSE:O	1.95	0.66
2:H:166:ASP:HB3	2:H:169:VAL:HG11	1.77	0.66
1:I:139:ALA:O	1:I:142:PRO:HD3	1.96	0.66
1:B:139:ALA:O	1:B:142:PRO:HD3	1.95	0.66
2:C:265:ILE:HG21	2:C:289:ILE:HD11	1.77	0.66
2:D:63:ASP:O	2:D:65:MSE:HG3	1.95	0.66
2:D:51:MSE:HE3	2:D:91:TYR:CD2	2.31	0.66
1:F:77:TYR:CD1	1:F:110:SER:HB3	2.31	0.66
1:J:139:ALA:O	1:J:142:PRO:HD3	1.96	0.66
2:G:265:ILE:HG21	2:G:289:ILE:HD11	1.77	0.66
2:H:265:ILE:HG21	2:H:289:ILE:HD11	1.78	0.66
1:J:306:GLU:N	1:J:324:ASP:OD2	2.28	0.66
1:J:349:GLN:OE1	2:L:59:GLU:HA	1.96	0.66
2:K:151:ILE:HD12	2:K:423:ILE:HD12	1.78	0.66
2:D:239:VAL:HG12	2:D:240:PHE:N	2.11	0.66
2:G:392:GLN:HB3	2:G:393:PRO:HD3	1.78	0.66
2:G:484:VAL:O	2:G:488:LEU:HD13	1.96	0.66
2:C:534:ILE:O	2:C:538:ILE:HG12	1.95	0.65
1:I:324:ASP:HB3	2:K:64:LYS:HG2	1.77	0.65
2:D:243:GLN:HG3	2:D:244:TYR:HD1	1.62	0.65
2:G:122:ARG:HB3	2:G:122:ARG:NH1	2.12	0.65
2:G:383:VAL:HG12	2:G:384:VAL:H	1.61	0.65
1:I:314:LEU:O	1:I:314:LEU:HD12	1.96	0.65
2:H:122:ARG:HB3	2:H:122:ARG:HH11	1.59	0.65
2:C:223:TYR:HA	2:C:226:GLN:OE1	1.96	0.65
2:D:265:ILE:HG21	2:D:289:ILE:HD11	1.77	0.65
2:K:451:LEU:CD2	2:K:502:MSE:HE1	2.26	0.65
1:A:139:ALA:O	1:A:142:PRO:HD3	1.97	0.65
2:D:452:GLU:HG3	2:D:458:ARG:HH11	1.58	0.65
1:F:306:GLU:N	1:F:324:ASP:OD2	2.29	0.65
2:L:544:ASN:O	2:L:545:GLN:HG3	1.97	0.65
2:C:148:MSE:CE	2:C:152:LEU:HG	2.25	0.65
2:K:122:ARG:CB	2:K:122:ARG:HH11	2.10	0.65
2:K:454:LEU:HD22	2:K:458:ARG:HD2	1.79	0.65
1:B:88:PRO:HA	1:B:97:ARG:NH1	2.08	0.65
2:C:535:ALA:HA	2:C:538:ILE:HG12	1.79	0.65
2:G:223:TYR:HA	2:G:226:GLN:OE1	1.97	0.65
2:K:242:THR:HG21	2:K:244:TYR:HB2	1.79	0.65
2:C:123:VAL:HG12	2:C:124:PHE:N	2.12	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:181:VAL:CG1	2:D:405:ILE:HD11	2.27	0.64
2:K:484:VAL:O	2:K:488:LEU:HD13	1.97	0.64
2:H:123:VAL:HG12	2:H:124:PHE:N	2.12	0.64
2:K:223:TYR:HA	2:K:226:GLN:OE1	1.97	0.64
2:D:538:ILE:O	2:D:542:LEU:HG	1.98	0.64
2:H:546:MSE:O	2:H:548:SER:N	2.30	0.64
2:H:454:LEU:CB	2:H:459:ASN:OD1	2.45	0.64
2:L:356:SER:HB2	2:L:378:SER:OG	1.98	0.64
1:A:76:SER:HB3	1:A:78:ASP:OD1	1.98	0.64
2:C:122:ARG:CB	2:C:122:ARG:HH11	2.11	0.64
1:E:39:ASP:OD2	1:E:42:THR:HG22	1.97	0.64
2:K:392:GLN:HB3	2:K:393:PRO:HD3	1.80	0.64
2:D:123:VAL:HG12	2:D:124:PHE:N	2.12	0.64
1:J:160:PRO:N	1:J:161:PRO:CD	2.61	0.64
2:K:538:ILE:HG22	2:K:542:LEU:HD23	1.80	0.64
2:L:223:TYR:HA	2:L:226:GLN:OE1	1.98	0.64
2:D:122:ARG:CB	2:D:122:ARG:HH11	2.11	0.63
2:C:122:ARG:NH1	2:C:122:ARG:HB3	2.13	0.63
1:J:76:SER:HB3	1:J:78:ASP:OD1	1.98	0.63
1:I:128:LEU:HD22	1:I:185:VAL:HG13	1.79	0.63
2:K:122:ARG:NH1	2:K:122:ARG:HB3	2.13	0.63
1:J:178:PHE:CB	2:L:502:MSE:HE3	2.28	0.63
1:A:8:HIS:CD2	1:A:34:LYS:HE2	2.34	0.63
2:K:265:ILE:HG21	2:K:289:ILE:HD11	1.81	0.63
2:L:123:VAL:HG12	2:L:124:PHE:N	2.14	0.63
2:G:240:PHE:HD2	2:G:268:SER:CB	2.12	0.63
2:K:451:LEU:HD21	2:K:502:MSE:CE	2.28	0.63
2:K:496:THR:O	2:K:500:LYS:HG3	1.99	0.63
2:C:496:THR:O	2:C:500:LYS:HG3	1.98	0.63
1:J:221:ALA:HB2	1:J:312:TRP:CD2	2.34	0.63
2:D:181:VAL:HG12	2:D:405:ILE:HD11	1.80	0.63
2:D:535:ALA:HA	2:D:538:ILE:HG12	1.78	0.63
2:G:496:THR:O	2:G:500:LYS:HG3	1.98	0.63
1:A:314:LEU:O	1:A:314:LEU:HD12	1.99	0.63
1:B:346:THR:OG1	2:D:48:LEU:HD11	1.98	0.63
2:D:496:THR:O	2:D:500:LYS:HG3	1.99	0.63
1:E:131:ASP:O	1:E:133:ILE:HG13	1.99	0.63
2:K:242:THR:HG22	2:K:244:TYR:H	1.63	0.62
1:J:81:VAL:CG2	1:J:111:LEU:HD13	2.27	0.62
1:J:24:VAL:HG23	1:J:45:TRP:CZ3	2.34	0.62
2:L:453:ASP:O	2:L:454:LEU:HD23	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:314:LEU:HD12	1:J:314:LEU:O	1.99	0.62
2:G:52:THR:HG22	2:G:54:ASN:H	1.64	0.62
2:L:122:ARG:HB3	2:L:122:ARG:NH1	2.15	0.62
1:F:39:ASP:OD2	1:F:42:THR:HG22	1.98	0.62
1:J:238:GLY:HA2	1:J:305:GLY:O	1.99	0.62
1:A:313:ASN:HD22	1:A:317:THR:HB	1.65	0.62
1:B:128:LEU:HD22	1:B:185:VAL:HG13	1.82	0.62
2:D:223:TYR:HA	2:D:226:GLN:OE1	2.00	0.62
2:D:452:GLU:CG	2:D:454:LEU:HD21	2.30	0.62
1:F:310:VAL:HG13	1:F:319:LEU:HD11	1.82	0.62
2:G:148:MSE:HE2	2:G:152:LEU:HG	1.80	0.62
1:I:131:ASP:O	1:I:133:ILE:HG13	1.99	0.62
1:F:139:ALA:O	1:F:142:PRO:HD3	1.99	0.62
2:K:200:ASN:OD1	2:K:203:GLU:HB2	2.00	0.62
2:L:52:THR:HG22	2:L:53:VAL:N	2.13	0.62
1:B:313:ASN:HD22	1:B:317:THR:HB	1.65	0.62
1:A:178:PHE:CB	2:C:502:MSE:HE3	2.27	0.62
2:G:220:ASP:OD2	2:G:222:GLU:HB3	2.00	0.62
1:E:178:PHE:CB	2:G:502:MSE:HE3	2.29	0.62
1:F:178:PHE:HB3	2:H:502:MSE:HE3	1.80	0.62
1:J:65:SER:HB2	1:J:119:ALA:HB2	1.82	0.62
2:L:496:THR:O	2:L:500:LYS:HG3	1.99	0.62
1:B:238:GLY:HA2	1:B:305:GLY:O	2.00	0.61
2:D:122:ARG:NH1	2:D:122:ARG:HB3	2.14	0.61
1:I:313:ASN:HD22	1:I:317:THR:HB	1.65	0.61
2:C:343:GLN:HE21	2:C:377:MSE:SE	2.33	0.61
1:F:131:ASP:O	1:F:133:ILE:HG13	1.99	0.61
2:G:148:MSE:HE3	2:G:148:MSE:O	1.99	0.61
2:H:122:ARG:HH11	2:H:122:ARG:CB	2.12	0.61
1:J:39:ASP:OD2	1:J:42:THR:HG22	2.00	0.61
2:K:393:PRO:HB3	2:K:405:ILE:HG13	1.82	0.61
2:H:223:TYR:HA	2:H:226:GLN:OE1	2.00	0.61
2:H:535:ALA:O	2:H:539:TYR:HD1	1.84	0.61
1:J:68:TYR:OH	1:J:122:GLY:HA2	2.00	0.61
1:J:348:GLN:HA	2:L:58:ILE:O	2.00	0.61
1:B:24:VAL:HG23	1:B:45:TRP:CZ3	2.35	0.61
2:D:542:LEU:N	2:D:542:LEU:HD23	2.14	0.61
2:H:220:ASP:OD2	2:H:222:GLU:HB3	2.00	0.61
2:H:48:LEU:HD12	2:H:49:VAL:H	1.65	0.61
2:K:343:GLN:HE21	2:K:377:MSE:SE	2.34	0.61
1:A:24:VAL:HG23	1:A:45:TRP:CZ3	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:LEU:HB3	1:B:139:ALA:HB3	1.81	0.61
2:H:122:ARG:HB3	2:H:122:ARG:NH1	2.15	0.61
1:J:160:PRO:N	1:J:161:PRO:HD2	2.16	0.61
2:K:148:MSE:HE3	2:K:148:MSE:O	1.99	0.61
2:K:52:THR:HG22	2:K:53:VAL:N	2.15	0.61
2:L:489:ILE:HD13	2:L:503:VAL:HG11	1.83	0.61
1:A:39:ASP:OD2	1:A:42:THR:HG22	2.01	0.61
2:D:489:ILE:HD13	2:D:503:VAL:HG11	1.83	0.61
1:E:158:SER:C	1:E:159:ILE:HG13	2.21	0.61
1:J:310:VAL:HG13	1:J:319:LEU:HD11	1.81	0.61
2:H:496:THR:O	2:H:500:LYS:HG3	2.00	0.61
2:C:220:ASP:OD2	2:C:222:GLU:HB3	2.01	0.61
2:C:278:CYS:HB2	2:C:323:ASP:HB2	1.83	0.61
2:D:383:VAL:HG12	2:D:384:VAL:N	2.15	0.61
2:G:200:ASN:OD1	2:G:203:GLU:HB2	2.00	0.61
2:K:220:ASP:OD2	2:K:222:GLU:HB3	2.01	0.61
2:L:122:ARG:HH11	2:L:122:ARG:CB	2.12	0.61
2:L:534:ILE:O	2:L:538:ILE:HG13	2.01	0.61
1:B:131:ASP:O	1:B:133:ILE:HG13	2.00	0.60
2:C:333:GLU:O	2:C:337:LEU:HG	2.02	0.60
1:E:139:ALA:O	1:E:142:PRO:HD3	2.01	0.60
1:J:313:ASN:HD22	1:J:317:THR:HB	1.66	0.60
1:A:238:GLY:HA2	1:A:305:GLY:O	2.01	0.60
1:A:335:TYR:CZ	2:C:457:TYR:HA	2.35	0.60
2:C:148:MSE:HE3	2:C:148:MSE:O	2.00	0.60
2:D:151:ILE:HD12	2:D:423:ILE:HD12	1.83	0.60
2:D:505:ALA:HB1	2:D:534:ILE:HD11	1.83	0.60
1:B:96:ARG:HH21	1:E:9:ASP:HB2	1.66	0.60
2:H:393:PRO:HB3	2:H:405:ILE:HG13	1.83	0.60
1:I:81:VAL:CG2	1:I:111:LEU:HD13	2.30	0.60
2:H:505:ALA:HB1	2:H:534:ILE:HD11	1.83	0.60
1:J:134:LEU:HD23	1:J:135:ARG:N	2.16	0.60
1:E:128:LEU:HD22	1:E:185:VAL:HG13	1.83	0.60
2:G:58:ILE:HG22	2:G:59:GLU:N	2.17	0.60
2:K:278:CYS:HB2	2:K:323:ASP:HB2	1.84	0.60
2:D:393:PRO:HB3	2:D:405:ILE:HG13	1.83	0.60
2:L:393:PRO:HB3	2:L:405:ILE:HG13	1.82	0.60
1:A:310:VAL:HG13	1:A:319:LEU:HD11	1.83	0.60
1:I:24:VAL:HG23	1:I:45:TRP:CZ3	2.37	0.60
2:H:52:THR:CG2	2:H:55:ASP:H	2.15	0.60
2:H:148:MSE:HE2	2:H:152:LEU:HG	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:278:CYS:HB2	2:D:323:ASP:HB2	1.84	0.60
2:D:531:LEU:HD22	2:D:534:ILE:HD12	1.83	0.59
1:F:313:ASN:HD22	1:F:317:THR:HB	1.67	0.59
1:F:313:ASN:HB2	1:F:318:ILE:H	1.67	0.59
1:J:71:ILE:HD11	1:J:145:LEU:HD13	1.83	0.59
2:D:105:SER:HB2	2:D:481:LEU:HD21	1.84	0.59
2:H:278:CYS:HB2	2:H:323:ASP:HB2	1.84	0.59
1:I:88:PRO:HA	1:I:97:ARG:NH1	2.16	0.59
1:J:39:ASP:CB	1:J:42:THR:HG22	2.32	0.59
2:L:278:CYS:HB2	2:L:323:ASP:HB2	1.84	0.59
1:A:39:ASP:CB	1:A:42:THR:HG22	2.31	0.59
1:B:81:VAL:CG2	1:B:111:LEU:HD13	2.30	0.59
1:B:137:TYR:CE1	1:B:150:LEU:HD13	2.38	0.59
2:K:489:ILE:HD13	2:K:503:VAL:HG11	1.84	0.59
2:C:522:MSE:HE1	2:C:538:ILE:HD12	1.82	0.59
1:E:313:ASN:HD22	1:E:317:THR:HB	1.66	0.59
2:G:534:ILE:O	2:G:538:ILE:HG12	2.01	0.59
2:H:417:ALA:HB1	2:H:465:MSE:HE1	1.85	0.59
2:H:52:THR:CG2	2:H:53:VAL:N	2.65	0.59
2:K:506:GLU:O	2:K:509:PRO:HD2	2.02	0.59
2:C:451:LEU:HG	2:C:452:GLU:N	2.11	0.59
1:B:55:ASP:HB3	1:E:99:ASN:OD1	2.02	0.59
1:B:314:LEU:O	1:B:314:LEU:HD12	2.03	0.59
2:D:220:ASP:OD2	2:D:222:GLU:HB3	2.02	0.59
2:D:333:GLU:O	2:D:337:LEU:HG	2.03	0.59
2:D:515:THR:CG2	2:D:516:ASN:H	2.15	0.59
2:D:453:ASP:C	2:D:454:LEU:HD23	2.23	0.59
2:H:383:VAL:HG12	2:H:384:VAL:N	2.17	0.59
2:C:313:LEU:C	2:C:313:LEU:HD23	2.23	0.59
1:F:123:LEU:HB3	1:F:139:ALA:HB3	1.84	0.59
2:K:303:PHE:HE2	2:K:366:PRO:HD3	1.68	0.59
2:L:220:ASP:OD2	2:L:222:GLU:HB3	2.02	0.59
2:C:393:PRO:HB3	2:C:405:ILE:HG13	1.84	0.59
1:F:346:THR:HG22	2:H:48:LEU:HD11	1.84	0.59
1:F:134:LEU:HD23	1:F:135:ARG:N	2.18	0.58
1:A:134:LEU:HD23	1:A:135:ARG:N	2.18	0.58
1:B:310:VAL:HG13	1:B:319:LEU:HD11	1.85	0.58
2:D:243:GLN:HG3	2:D:244:TYR:CD1	2.37	0.58
1:E:241:ARG:HG2	1:E:299:GLU:HG3	1.85	0.58
1:E:310:VAL:HG13	1:E:319:LEU:HD11	1.85	0.58
2:H:356:SER:HB2	2:H:378:SER:OG	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:HIS:CD2	1:A:34:LYS:CD	2.85	0.58
1:F:24:VAL:HG23	1:F:45:TRP:CZ3	2.37	0.58
2:G:451:LEU:HD21	2:G:502:MSE:CE	2.32	0.58
2:H:58:ILE:HG22	2:H:59:GLU:N	2.18	0.58
1:J:123:LEU:HB3	1:J:139:ALA:HB3	1.84	0.58
1:J:179:SER:OG	1:J:180:PRO:HD2	2.02	0.58
1:J:81:VAL:HG23	1:J:111:LEU:CD1	2.32	0.58
2:K:432:ASN:HB2	2:K:460:GLY:CA	2.33	0.58
2:L:52:THR:HG22	2:L:54:ASN:H	1.67	0.58
1:B:324:ASP:HB3	2:D:64:LYS:HD3	1.85	0.58
1:E:134:LEU:HD23	1:E:135:ARG:N	2.18	0.58
1:F:128:LEU:HD22	1:F:185:VAL:HG13	1.86	0.58
1:F:238:GLY:HA2	1:F:305:GLY:O	2.04	0.58
2:G:393:PRO:HB3	2:G:405:ILE:HG13	1.85	0.58
1:I:310:VAL:HG13	1:I:319:LEU:HD11	1.85	0.58
1:A:65:SER:HB2	1:A:119:ALA:HB2	1.84	0.58
2:G:455:PHE:CG	2:G:455:PHE:O	2.55	0.58
1:B:134:LEU:HD23	1:B:135:ARG:N	2.19	0.58
1:B:221:ALA:HB2	1:B:312:TRP:CD2	2.38	0.58
1:J:131:ASP:O	1:J:133:ILE:HG13	2.04	0.58
1:J:134:LEU:HD23	1:J:135:ARG:H	1.68	0.58
2:K:148:MSE:HE2	2:K:152:LEU:HG	1.84	0.58
2:D:454:LEU:HD12	2:D:459:ASN:OD1	2.03	0.58
1:F:90:GLN:OE1	1:F:96:ARG:HD2	2.03	0.58
2:C:455:PHE:CG	2:C:455:PHE:O	2.57	0.58
2:D:148:MSE:HE2	2:D:152:LEU:HG	1.86	0.58
2:G:242:THR:HG22	2:G:243:GLN:N	2.18	0.58
2:G:39:LYS:HG3	2:G:40:ARG:N	2.18	0.58
2:L:521:TRP:CZ2	2:L:525:ILE:HD11	2.39	0.58
1:A:134:LEU:HD23	1:A:135:ARG:H	1.69	0.58
2:D:455:PHE:CG	2:D:455:PHE:O	2.57	0.58
1:F:178:PHE:CB	2:H:502:MSE:HE3	2.33	0.58
1:J:313:ASN:HB2	1:J:318:ILE:H	1.67	0.58
2:K:333:GLU:O	2:K:337:LEU:HG	2.03	0.58
2:L:383:VAL:HG12	2:L:384:VAL:N	2.19	0.58
2:H:453:ASP:O	2:H:454:LEU:HG	2.04	0.57
2:D:303:PHE:HE2	2:D:366:PRO:HD3	1.69	0.57
2:D:356:SER:HB2	2:D:378:SER:OG	2.04	0.57
1:E:76:SER:HB3	1:E:78:ASP:OD1	2.04	0.57
1:F:159:ILE:O	1:F:161:PRO:CD	2.52	0.57
1:F:118:PRO:HG2	1:F:174:CYS:O	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:120:HIS:CE1	1:F:177:ARG:HA	2.40	0.57
1:F:76:SER:HB3	1:F:78:ASP:OD1	2.03	0.57
2:H:200:ASN:OD1	2:H:203:GLU:HB2	2.04	0.57
2:G:437:GLU:CG	2:H:304:ARG:HH12	2.13	0.57
2:H:515:THR:CG2	2:H:516:ASN:H	2.16	0.57
1:I:159:ILE:O	1:I:161:PRO:HD2	2.04	0.57
1:I:313:ASN:HB2	1:I:318:ILE:H	1.68	0.57
2:C:489:ILE:HD13	2:C:503:VAL:HG11	1.86	0.57
2:D:200:ASN:OD1	2:D:203:GLU:HB2	2.04	0.57
1:E:131:ASP:OD2	1:E:135:ARG:NH2	2.36	0.57
1:F:221:ALA:HB2	1:F:312:TRP:CD2	2.39	0.57
2:K:313:LEU:C	2:K:313:LEU:HD23	2.25	0.57
2:L:333:GLU:O	2:L:337:LEU:HG	2.03	0.57
1:A:236:LYS:HG3	1:A:306:GLU:OE1	2.05	0.57
2:C:303:PHE:HE2	2:C:366:PRO:HD3	1.70	0.57
2:D:505:ALA:HA	2:D:534:ILE:HD13	1.85	0.57
2:K:43:VAL:HG12	2:K:43:VAL:O	2.05	0.57
2:L:521:TRP:CE2	2:L:525:ILE:HD11	2.40	0.57
1:E:13:HIS:HE2	1:E:29:SER:HG	1.53	0.57
2:G:52:THR:CG2	2:G:53:VAL:H	2.15	0.57
2:K:39:LYS:HD2	2:K:47:ILE:CG2	2.35	0.57
1:E:313:ASN:HB2	1:E:318:ILE:H	1.69	0.57
1:E:24:VAL:HG23	1:E:45:TRP:CZ3	2.40	0.57
2:H:454:LEU:HD23	2:H:458:ARG:CB	2.30	0.57
2:L:303:PHE:HE2	2:L:366:PRO:HD3	1.69	0.57
2:L:343:GLN:HE21	2:L:377:MSE:SE	2.38	0.57
1:F:131:ASP:OD2	1:F:135:ARG:NH2	2.38	0.57
1:J:247:GLU:HB3	1:J:292:LEU:CD2	2.33	0.57
1:B:1:MSE:HE2	1:B:1:MSE:HA	1.87	0.57
2:D:454:LEU:CD2	2:D:458:ARG:HD2	2.35	0.57
2:D:454:LEU:CB	2:D:459:ASN:ND2	2.66	0.57
1:E:134:LEU:HD23	1:E:135:ARG:H	1.69	0.57
2:H:432:ASN:HB2	2:H:460:GLY:HA2	1.87	0.57
2:K:218:GLU:HA	2:K:220:ASP:N	2.20	0.57
2:K:455:PHE:CG	2:K:455:PHE:O	2.56	0.57
2:L:200:ASN:OD1	2:L:203:GLU:HB2	2.05	0.57
1:A:81:VAL:CG2	1:A:111:LEU:HD13	2.31	0.56
1:F:13:HIS:HE2	1:F:29:SER:HG	1.52	0.56
2:G:151:ILE:CD1	2:G:423:ILE:HD12	2.35	0.56
2:K:515:THR:CG2	2:K:516:ASN:N	2.68	0.56
1:A:131:ASP:OD2	1:A:135:ARG:NH2	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:313:ASN:HB2	1:B:318:ILE:H	1.69	0.56
2:C:406:LEU:HB2	2:C:407:PRO:HD3	1.87	0.56
2:G:417:ALA:HB1	2:G:465:MSE:HE1	1.87	0.56
2:K:42:PRO:HD3	2:K:48:LEU:HB2	1.87	0.56
2:K:451:LEU:CG	2:K:502:MSE:HE1	2.35	0.56
1:J:68:TYR:CG	1:J:123:LEU:HD13	2.41	0.56
1:A:131:ASP:O	1:A:133:ILE:HG13	2.05	0.56
2:G:303:PHE:HE2	2:G:366:PRO:HD3	1.70	0.56
2:G:343:GLN:HE21	2:G:377:MSE:SE	2.38	0.56
2:G:454:LEU:HB3	2:G:459:ASN:OD1	2.05	0.56
2:H:51:MSE:HE3	2:H:91:TYR:CG	2.40	0.56
1:I:137:TYR:CE1	1:I:150:LEU:HD13	2.41	0.56
2:C:521:TRP:CZ2	2:C:525:ILE:HD11	2.41	0.56
1:J:131:ASP:OD2	1:J:135:ARG:NH2	2.38	0.56
1:J:8:HIS:ND1	1:J:28:SER:HB3	2.21	0.56
2:K:383:VAL:HG12	2:K:384:VAL:N	2.20	0.56
1:A:13:HIS:HE2	1:A:29:SER:HG	1.54	0.56
1:A:208:LEU:HD11	1:A:231:ILE:CD1	2.29	0.56
2:G:432:ASN:HB2	2:G:460:GLY:HA2	1.88	0.56
2:G:515:THR:CG2	2:G:516:ASN:H	2.17	0.56
2:H:455:PHE:CG	2:H:455:PHE:O	2.58	0.56
2:K:522:MSE:HE1	2:K:538:ILE:HD12	1.86	0.56
2:L:313:LEU:C	2:L:313:LEU:HD23	2.26	0.56
2:L:422:MSE:HB2	2:L:466:LEU:HD11	1.85	0.56
2:L:496:THR:HG22	2:L:498:SER:H	1.71	0.56
1:I:10:ASP:O	2:K:88:TYR:CE1	2.59	0.56
1:E:8:HIS:ND1	1:E:28:SER:HB3	2.21	0.56
2:L:506:GLU:O	2:L:509:PRO:HD2	2.05	0.56
1:B:10:ASP:O	2:D:88:TYR:CE1	2.59	0.56
2:D:521:TRP:CZ2	2:D:525:ILE:HD11	2.41	0.56
1:E:314:LEU:C	1:E:314:LEU:HD12	2.27	0.56
1:F:179:SER:OG	1:F:180:PRO:HD2	2.06	0.56
1:F:81:VAL:CG2	1:F:111:LEU:HD13	2.36	0.56
2:H:303:PHE:HE2	2:H:366:PRO:HD3	1.70	0.56
1:J:338:GLU:HG3	1:J:339:PHE:N	2.20	0.56
2:K:158:PHE:O	2:K:162:VAL:HG23	2.05	0.56
1:B:96:ARG:NH2	1:E:9:ASP:HB2	2.21	0.56
2:C:200:ASN:OD1	2:C:203:GLU:HB2	2.05	0.56
1:B:76:SER:HB3	1:B:78:ASP:OD1	2.06	0.56
2:H:333:GLU:O	2:H:337:LEU:HG	2.06	0.56
2:H:453:ASP:C	2:H:454:LEU:HG	2.27	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:159:ILE:HD12	2:L:179:LEU:HD22	1.87	0.56
1:E:77:TYR:CD1	1:E:110:SER:HB3	2.40	0.55
2:H:506:GLU:O	2:H:509:PRO:HD2	2.04	0.55
2:K:515:THR:CG2	2:K:516:ASN:H	2.14	0.55
1:B:134:LEU:HD23	1:B:135:ARG:H	1.70	0.55
2:C:40:ARG:HB3	2:C:40:ARG:HH11	1.70	0.55
2:G:218:GLU:HA	2:G:220:ASP:N	2.21	0.55
2:G:406:LEU:HB2	2:G:407:PRO:HD3	1.88	0.55
2:C:546:MSE:HE2	2:C:546:MSE:HA	1.88	0.55
2:G:313:LEU:C	2:G:313:LEU:HD23	2.27	0.55
2:H:533:GLU:O	2:H:536:LYS:HB2	2.07	0.55
1:I:338:GLU:HG3	1:I:339:PHE:N	2.21	0.55
1:A:338:GLU:HG3	1:A:339:PHE:N	2.20	0.55
2:D:506:GLU:O	2:D:509:PRO:HD2	2.06	0.55
1:I:134:LEU:HD23	1:I:135:ARG:H	1.71	0.55
1:B:193:ILE:CD1	1:B:245:ILE:HD13	2.37	0.55
2:C:383:VAL:HG12	2:C:384:VAL:N	2.22	0.55
2:L:148:MSE:HE2	2:L:152:LEU:HG	1.87	0.55
1:B:137:TYR:CZ	1:B:150:LEU:HD13	2.41	0.55
1:B:128:LEU:HD23	1:B:169:PHE:HB3	1.88	0.55
1:E:221:ALA:HB2	1:E:312:TRP:CD2	2.42	0.55
2:H:58:ILE:CG2	2:H:59:GLU:N	2.70	0.55
1:B:329:ARG:HG2	1:B:344:VAL:HG22	1.87	0.55
1:B:336:SER:HB3	2:C:373:GLU:HG2	1.89	0.55
2:G:489:ILE:HD13	2:G:503:VAL:HG11	1.89	0.55
2:H:239:VAL:CG2	2:H:240:PHE:H	2.11	0.55
2:H:535:ALA:O	2:H:539:TYR:CD1	2.59	0.55
1:B:81:VAL:HG23	1:B:111:LEU:CD1	2.34	0.55
2:C:422:MSE:HB2	2:C:466:LEU:HD11	1.89	0.55
1:F:134:LEU:HD23	1:F:135:ARG:H	1.71	0.55
2:G:242:THR:HG22	2:G:243:GLN:H	1.71	0.55
1:I:159:ILE:O	1:I:161:PRO:CD	2.54	0.55
2:K:39:LYS:HD2	2:K:47:ILE:HG21	1.89	0.55
1:J:335:TYR:CZ	2:L:457:TYR:HA	2.42	0.55
1:B:236:LYS:HG3	1:B:306:GLU:OE1	2.07	0.55
1:J:13:HIS:HE2	1:J:29:SER:HG	1.54	0.55
1:B:8:HIS:ND1	1:B:28:SER:HB3	2.21	0.55
1:B:347:ALA:O	2:D:56:GLN:HB3	2.07	0.55
2:G:433:ILE:HG22	2:G:433:ILE:O	2.07	0.55
1:B:131:ASP:OD2	1:B:135:ARG:NH2	2.40	0.54
2:C:159:ILE:HD12	2:C:179:LEU:HD22	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:8:HIS:ND1	1:F:28:SER:HB3	2.22	0.54
2:G:522:MSE:HE1	2:G:538:ILE:HD12	1.88	0.54
2:G:58:ILE:CG2	2:G:59:GLU:N	2.70	0.54
2:H:218:GLU:HA	2:H:220:ASP:N	2.23	0.54
1:A:68:TYR:OH	1:A:122:GLY:HA2	2.07	0.54
2:D:434:PHE:CE2	2:D:458:ARG:HG2	2.42	0.54
1:F:338:GLU:HG3	1:F:339:PHE:N	2.22	0.54
1:F:23:HIS:CE1	1:F:70:ARG:HH22	2.26	0.54
2:G:333:GLU:O	2:G:337:LEU:HG	2.06	0.54
1:I:221:ALA:HB2	1:I:312:TRP:CD2	2.42	0.54
1:A:221:ALA:HB2	1:A:312:TRP:CD2	2.42	0.54
1:A:313:ASN:HB2	1:A:318:ILE:H	1.71	0.54
1:I:134:LEU:HD23	1:I:135:ARG:N	2.21	0.54
1:I:23:HIS:CE1	1:I:70:ARG:HH22	2.25	0.54
2:K:240:PHE:HB2	2:K:269:ASP:CG	2.27	0.54
1:B:346:THR:HG22	1:B:348:GLN:N	2.23	0.54
2:C:158:PHE:O	2:C:162:VAL:HG23	2.07	0.54
2:D:515:THR:CG2	2:D:516:ASN:N	2.69	0.54
1:F:346:THR:CG2	2:H:48:LEU:HD11	2.37	0.54
1:I:156:VAL:HG13	1:I:192:ILE:HD11	1.89	0.54
1:I:208:LEU:HD11	1:I:231:ILE:CD1	2.28	0.54
2:K:496:THR:HG22	2:K:498:SER:H	1.72	0.54
2:L:455:PHE:O	2:L:455:PHE:CG	2.59	0.54
1:A:239:ARG:HG3	1:A:239:ARG:HH11	1.71	0.54
1:B:120:HIS:CE1	1:B:177:ARG:HA	2.43	0.54
2:D:158:PHE:O	2:D:162:VAL:HG23	2.08	0.54
2:D:496:THR:HG22	2:D:498:SER:H	1.72	0.54
1:F:332:LYS:HG3	1:F:342:MSE:SE	2.58	0.54
1:I:121:LEU:CD1	1:I:181:GLU:HG3	2.38	0.54
1:I:329:ARG:HG2	1:I:344:VAL:HG22	1.89	0.54
1:J:236:LYS:HG3	1:J:306:GLU:OE1	2.07	0.54
1:I:336:SER:HB3	2:L:373:GLU:HG2	1.88	0.54
2:L:42:PRO:C	2:L:44:SER:H	2.10	0.54
1:J:1:MSE:HB3	2:L:92:PRO:O	2.08	0.54
1:B:346:THR:HG22	1:B:348:GLN:H	1.70	0.54
2:C:218:GLU:HA	2:C:220:ASP:N	2.22	0.54
2:D:218:GLU:HA	2:D:220:ASP:N	2.22	0.54
1:E:2:GLN:HG3	1:E:2:GLN:O	2.07	0.54
1:E:338:GLU:HG3	1:E:339:PHE:N	2.22	0.54
2:H:124:PHE:CE2	2:H:126:VAL:HB	2.43	0.54
2:K:125:ASN:HB2	2:K:136:PHE:HE2	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:105:SER:HB2	2:K:481:LEU:HD21	1.89	0.54
1:A:16:VAL:HG12	1:A:63:TRP:HD1	1.73	0.54
2:C:170:ASN:O	2:C:174:GLU:HG3	2.08	0.54
2:C:515:THR:CG2	2:C:516:ASN:N	2.71	0.54
1:F:178:PHE:CG	2:H:502:MSE:HE3	2.42	0.54
2:H:523:LEU:HD13	2:H:539:TYR:OH	2.08	0.54
1:I:241:ARG:HG2	1:I:299:GLU:HG3	1.88	0.54
1:I:65:SER:HB2	1:I:119:ALA:HB2	1.90	0.54
1:J:120:HIS:CE1	1:J:177:ARG:HA	2.42	0.54
2:K:242:THR:HG22	2:K:244:TYR:N	2.23	0.54
2:K:434:PHE:CE2	2:K:458:ARG:HG2	2.43	0.54
1:A:90:GLN:HG3	1:A:96:ARG:O	2.08	0.54
1:B:136:LEU:HD11	1:B:202:LEU:HD11	1.89	0.54
2:C:433:ILE:HG22	2:C:433:ILE:O	2.07	0.54
1:E:120:HIS:CE1	1:E:177:ARG:HA	2.43	0.54
1:B:208:LEU:HD11	1:B:231:ILE:CD1	2.33	0.54
2:D:239:VAL:HG12	2:D:240:PHE:H	1.72	0.54
1:E:23:HIS:CE1	1:E:70:ARG:HH22	2.24	0.54
1:F:125:LEU:C	1:F:125:LEU:HD12	2.29	0.54
2:G:228:PHE:CD2	2:G:267:ARG:HD3	2.43	0.54
2:G:278:CYS:HB2	2:G:323:ASP:HB2	1.89	0.54
1:J:77:TYR:CD1	1:J:110:SER:HB3	2.43	0.54
1:J:329:ARG:HG2	1:J:344:VAL:HG22	1.89	0.54
2:L:148:MSE:HE3	2:L:152:LEU:HG	1.89	0.54
1:J:348:GLN:HB3	2:L:60:LYS:HG3	1.90	0.54
2:C:151:ILE:CD1	2:C:423:ILE:HD12	2.37	0.54
2:L:218:GLU:HA	2:L:220:ASP:N	2.23	0.54
2:C:356:SER:HB2	2:C:378:SER:OG	2.07	0.53
2:D:343:GLN:HE21	2:D:377:MSE:SE	2.41	0.53
2:G:240:PHE:CD2	2:G:268:SER:CB	2.91	0.53
2:K:406:LEU:HB2	2:K:407:PRO:HD3	1.90	0.53
1:A:329:ARG:HG2	1:A:344:VAL:HG22	1.90	0.53
2:D:521:TRP:CE2	2:D:525:ILE:HD11	2.42	0.53
1:E:178:PHE:CG	2:G:502:MSE:HE3	2.43	0.53
2:K:521:TRP:CZ2	2:K:525:ILE:HD11	2.42	0.53
1:B:338:GLU:HG3	1:B:339:PHE:N	2.23	0.53
2:C:296:PRO:HG2	2:C:306:TRP:HB2	1.89	0.53
1:E:239:ARG:HH11	1:E:239:ARG:HG3	1.73	0.53
2:G:383:VAL:HG12	2:G:384:VAL:N	2.23	0.53
2:H:521:TRP:CE2	2:H:525:ILE:HD11	2.44	0.53
2:D:433:ILE:HG22	2:D:433:ILE:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:128:LEU:HD23	1:J:169:PHE:HB3	1.90	0.53
1:J:347:ALA:O	2:L:56:GLN:HB3	2.09	0.53
1:B:65:SER:HB2	1:B:119:ALA:HB2	1.89	0.53
1:F:128:LEU:HD23	1:F:169:PHE:HB3	1.89	0.53
1:I:131:ASP:OD2	1:I:135:ARG:NH2	2.42	0.53
1:A:179:SER:OG	1:A:180:PRO:HD2	2.09	0.53
1:B:23:HIS:CE1	1:B:70:ARG:HH22	2.27	0.53
2:H:496:THR:HG22	2:H:498:SER:H	1.72	0.53
1:J:10:ASP:OD1	1:J:11:LEU:HD23	2.09	0.53
2:L:433:ILE:HG22	2:L:433:ILE:O	2.08	0.53
2:L:47:ILE:HD11	2:L:97:ARG:NE	2.24	0.53
1:F:39:ASP:CB	1:F:42:THR:HG22	2.34	0.53
2:H:47:ILE:CG2	2:H:48:LEU:N	2.70	0.53
1:I:137:TYR:CZ	1:I:150:LEU:HD13	2.44	0.53
1:I:193:ILE:CD1	1:I:245:ILE:HD13	2.38	0.53
1:I:39:ASP:CB	1:I:42:THR:HG22	2.34	0.53
1:J:239:ARG:HG3	1:J:239:ARG:HH11	1.74	0.53
2:C:496:THR:HG22	2:C:498:SER:H	1.73	0.53
1:F:239:ARG:HG3	1:F:239:ARG:HH11	1.74	0.53
2:H:521:TRP:CZ2	2:H:525:ILE:HD11	2.44	0.53
2:L:296:PRO:HG2	2:L:306:TRP:HB2	1.90	0.53
2:L:406:LEU:HB2	2:L:407:PRO:HD3	1.90	0.53
2:L:539:TYR:HA	2:L:542:LEU:HD12	1.91	0.53
1:E:81:VAL:CG2	1:E:111:LEU:HD13	2.37	0.53
1:F:121:LEU:CD1	1:F:181:GLU:HG3	2.39	0.53
2:G:496:THR:HG22	2:G:498:SER:H	1.73	0.53
2:H:489:ILE:HD13	2:H:503:VAL:HG11	1.90	0.53
1:B:39:ASP:CB	1:B:42:THR:HG22	2.36	0.53
1:E:39:ASP:CB	1:E:42:THR:HG22	2.37	0.53
2:G:52:THR:CG2	2:G:53:VAL:N	2.72	0.53
1:I:247:GLU:HB3	1:I:292:LEU:CD2	2.36	0.53
2:K:433:ILE:O	2:K:433:ILE:HG22	2.09	0.53
1:A:247:GLU:HB3	1:A:292:LEU:CD2	2.35	0.52
2:G:39:LYS:CG	2:G:40:ARG:N	2.71	0.52
1:I:314:LEU:C	1:I:314:LEU:HD12	2.30	0.52
2:D:432:ASN:HB2	2:D:460:GLY:CA	2.38	0.52
2:D:47:ILE:HG22	2:D:48:LEU:N	2.23	0.52
2:H:39:LYS:HD3	2:H:50:PRO:HD3	1.91	0.52
1:I:13:HIS:HE2	1:I:29:SER:HG	1.57	0.52
2:K:239:VAL:O	2:K:239:VAL:HG12	2.09	0.52
2:C:521:TRP:CE2	2:C:525:ILE:HD11	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:49:VAL:HG13	2:H:50:PRO:HD2	1.91	0.52
1:A:19:PHE:CZ	2:C:510:HIS:CD2	2.97	0.52
1:B:77:TYR:C	1:B:79:LYS:H	2.12	0.52
1:F:16:VAL:HG12	1:F:63:TRP:HD1	1.74	0.52
2:G:521:TRP:CZ2	2:G:525:ILE:HD11	2.45	0.52
2:H:433:ILE:O	2:H:433:ILE:HG22	2.08	0.52
1:J:196:ARG:HH11	1:J:202:LEU:CD2	2.23	0.52
2:K:505:ALA:HA	2:K:534:ILE:CD1	2.40	0.52
2:K:521:TRP:CE2	2:K:525:ILE:HD11	2.44	0.52
2:L:47:ILE:HD11	2:L:97:ARG:HE	1.74	0.52
2:C:451:LEU:CG	2:C:452:GLU:N	2.72	0.52
2:D:148:MSE:HE3	2:D:152:LEU:HG	1.91	0.52
2:D:170:ASN:O	2:D:174:GLU:HG3	2.09	0.52
2:D:49:VAL:CG1	2:D:50:PRO:HD2	2.39	0.52
2:H:313:LEU:C	2:H:313:LEU:HD23	2.30	0.52
2:K:147:ALA:O	2:K:150:ALA:HB3	2.09	0.52
2:C:506:GLU:O	2:C:509:PRO:HD2	2.10	0.52
2:D:296:PRO:HG2	2:D:306:TRP:HB2	1.91	0.52
2:H:227:VAL:HG12	2:H:227:VAL:O	2.09	0.52
2:K:296:PRO:HG2	2:K:306:TRP:HB2	1.91	0.52
1:B:13:HIS:HE2	1:B:29:SER:HG	1.55	0.52
1:E:16:VAL:HG12	1:E:63:TRP:HD1	1.74	0.52
2:H:52:THR:HG22	2:H:53:VAL:N	2.25	0.52
1:I:76:SER:HB3	1:I:78:ASP:OD1	2.08	0.52
1:J:310:VAL:HA	1:J:320:SER:O	2.09	0.52
2:L:249:LEU:O	2:L:253:VAL:HG23	2.10	0.52
2:L:39:LYS:HZ1	2:L:97:ARG:HG2	1.75	0.52
1:A:349:GLN:OE1	2:C:59:GLU:HG3	2.10	0.52
1:I:16:VAL:HG12	1:I:63:TRP:HD1	1.74	0.52
2:K:454:LEU:CB	2:K:459:ASN:HD21	2.19	0.52
1:A:29:SER:C	1:A:31:GLN:H	2.13	0.52
1:B:193:ILE:HD13	1:B:245:ILE:HD13	1.92	0.52
2:C:148:MSE:HE2	2:C:152:LEU:HG	1.89	0.52
1:E:332:LYS:HG3	1:E:342:MSE:SE	2.60	0.52
1:F:10:ASP:OD1	1:F:11:LEU:HD23	2.10	0.52
1:I:120:HIS:CE1	1:I:177:ARG:HA	2.44	0.52
2:K:482:TRP:N	2:K:483:PRO:CD	2.73	0.52
2:L:39:LYS:NZ	2:L:97:ARG:CD	2.73	0.52
1:B:10:ASP:OD1	1:B:11:LEU:HD23	2.09	0.52
1:B:179:SER:OG	1:B:180:PRO:HD2	2.10	0.52
2:C:454:LEU:CB	2:C:459:ASN:OD1	2.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:238:GLY:HA2	1:E:305:GLY:O	2.11	0.52
2:H:170:ASN:O	2:H:174:GLU:HG3	2.10	0.52
2:H:515:THR:CG2	2:H:516:ASN:N	2.70	0.52
2:H:522:MSE:HE1	2:H:538:ILE:HD12	1.91	0.52
1:I:347:ALA:HA	2:K:56:GLN:OE1	2.10	0.52
1:J:125:LEU:C	1:J:125:LEU:HD12	2.30	0.52
2:C:148:MSE:HE3	2:C:152:LEU:HG	1.92	0.51
1:A:177:ARG:NH1	2:C:534:ILE:HD11	2.25	0.51
2:D:313:LEU:C	2:D:313:LEU:HD23	2.31	0.51
2:G:432:ASN:HB2	2:G:460:GLY:CA	2.40	0.51
1:J:16:VAL:HG12	1:J:63:TRP:HD1	1.75	0.51
2:C:515:THR:CG2	2:C:516:ASN:H	2.18	0.51
2:G:506:GLU:O	2:G:509:PRO:HD2	2.11	0.51
1:I:239:ARG:HH11	1:I:239:ARG:HG3	1.75	0.51
1:J:137:TYR:CE1	1:J:150:LEU:HD13	2.44	0.51
1:J:346:THR:CG2	1:J:347:ALA:H	2.21	0.51
2:C:113:GLU:HA	2:C:113:GLU:OE1	2.10	0.51
1:E:125:LEU:C	1:E:125:LEU:HD12	2.30	0.51
1:E:179:SER:OG	1:E:180:PRO:HD2	2.10	0.51
1:E:29:SER:C	1:E:31:GLN:H	2.14	0.51
1:F:136:LEU:HD11	1:F:202:LEU:HD11	1.92	0.51
2:H:52:THR:HG21	2:H:55:ASP:H	1.74	0.51
2:K:356:SER:HB2	2:K:378:SER:OG	2.10	0.51
2:L:158:PHE:O	2:L:162:VAL:HG23	2.11	0.51
2:L:406:LEU:CD1	2:L:461:MSE:HG2	2.40	0.51
1:E:10:ASP:OD1	1:E:11:LEU:HD23	2.11	0.51
1:A:81:VAL:HG23	1:A:111:LEU:CD1	2.36	0.51
2:G:335:PHE:CE2	2:G:339:ILE:HD11	2.45	0.51
1:A:120:HIS:CE1	1:A:177:ARG:HA	2.45	0.51
2:C:227:VAL:O	2:C:227:VAL:HG12	2.11	0.51
2:K:170:ASN:O	2:K:174:GLU:HG3	2.10	0.51
2:L:515:THR:CG2	2:L:516:ASN:H	2.18	0.51
1:A:196:ARG:HH11	1:A:202:LEU:CD2	2.24	0.51
1:B:196:ARG:HH11	1:B:202:LEU:CD2	2.24	0.51
2:C:335:PHE:CE2	2:C:339:ILE:HD11	2.46	0.51
2:G:248:LEU:O	2:G:248:LEU:HD13	2.10	0.51
2:H:436:GLY:O	2:H:437:GLU:C	2.49	0.51
1:I:29:SER:C	1:I:31:GLN:H	2.14	0.51
1:I:81:VAL:HG23	1:I:111:LEU:CD1	2.34	0.51
2:K:242:THR:HG22	2:K:244:TYR:CB	2.36	0.51
1:A:239:ARG:HG3	1:A:239:ARG:NH1	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:VAL:HG21	1:B:77:TYR:CE1	2.46	0.51
1:E:239:ARG:NH1	1:E:239:ARG:HG3	2.26	0.51
2:H:192:LEU:O	2:H:195:GLN:HB2	2.11	0.51
1:F:59:VAL:HG21	1:F:77:TYR:CE1	2.46	0.51
1:I:10:ASP:OD1	1:I:11:LEU:HD23	2.10	0.51
1:J:239:ARG:HG3	1:J:239:ARG:NH1	2.26	0.51
2:K:538:ILE:O	2:K:542:LEU:HD23	2.11	0.51
2:G:521:TRP:CE2	2:G:525:ILE:HD11	2.45	0.51
1:I:218:ILE:O	1:I:218:ILE:HG13	2.10	0.51
2:G:238:LYS:O	2:G:239:VAL:HB	2.11	0.50
2:G:451:LEU:HG	2:G:452:GLU:N	2.25	0.50
1:I:65:SER:CB	1:I:119:ALA:HB2	2.42	0.50
1:B:346:THR:CG2	1:B:348:GLN:H	2.24	0.50
1:F:314:LEU:C	1:F:314:LEU:HD12	2.31	0.50
2:G:296:PRO:HG2	2:G:306:TRP:HB2	1.92	0.50
2:H:296:PRO:HG2	2:H:306:TRP:HB2	1.93	0.50
1:A:314:LEU:C	1:A:314:LEU:HD12	2.31	0.50
1:F:159:ILE:O	1:F:161:PRO:HD2	2.11	0.50
1:F:29:SER:C	1:F:31:GLN:H	2.14	0.50
2:H:546:MSE:C	2:H:548:SER:N	2.64	0.50
1:F:347:ALA:O	2:H:56:GLN:HB3	2.11	0.50
1:I:85:GLU:HB2	1:I:101:LEU:HD11	1.94	0.50
1:B:239:ARG:HH11	1:B:239:ARG:HG3	1.76	0.50
1:B:310:VAL:HA	1:B:320:SER:O	2.12	0.50
1:F:349:GLN:HB2	2:H:56:GLN:HB2	1.94	0.50
2:G:198:GLU:OE1	2:H:436:GLY:HA2	2.12	0.50
1:I:8:HIS:ND1	1:I:28:SER:HB3	2.26	0.50
2:L:335:PHE:CE2	2:L:339:ILE:HD11	2.47	0.50
1:A:68:TYR:CG	1:A:123:LEU:HD13	2.46	0.50
2:G:158:PHE:O	2:G:162:VAL:HG23	2.11	0.50
2:G:522:MSE:HE1	2:G:538:ILE:CD1	2.42	0.50
2:H:230:VAL:O	2:H:230:VAL:HG12	2.11	0.50
2:K:215:SER:HB2	2:K:390:TRP:CZ2	2.46	0.50
2:K:52:THR:CG2	2:K:53:VAL:N	2.74	0.50
1:A:193:ILE:CD1	1:A:245:ILE:HD13	2.42	0.50
1:A:77:TYR:C	1:A:79:LYS:H	2.14	0.50
2:C:248:LEU:HD13	2:C:248:LEU:O	2.10	0.50
2:G:215:SER:HB2	2:G:390:TRP:CZ2	2.46	0.50
2:G:43:VAL:HG12	2:G:44:SER:N	2.27	0.50
1:I:125:LEU:HD12	1:I:125:LEU:C	2.32	0.50
1:J:29:SER:C	1:J:31:GLN:H	2.14	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:170:ASN:O	2:L:174:GLU:HG3	2.11	0.50
2:C:40:ARG:CB	2:C:40:ARG:NH1	2.75	0.50
1:A:178:PHE:HZ	2:C:505:ALA:CB	2.25	0.50
1:E:59:VAL:HG21	1:E:77:TYR:CE1	2.46	0.50
2:H:522:MSE:CE	2:H:538:ILE:HD12	2.42	0.50
1:A:10:ASP:OD1	1:A:11:LEU:HD23	2.12	0.50
1:A:65:SER:CB	1:A:119:ALA:HB2	2.42	0.50
1:A:310:VAL:HA	1:A:320:SER:O	2.12	0.50
1:B:121:LEU:CD1	1:B:181:GLU:HG3	2.42	0.50
2:C:147:ALA:O	2:C:150:ALA:HB3	2.12	0.50
2:D:227:VAL:O	2:D:227:VAL:HG12	2.11	0.50
2:G:356:SER:HB2	2:G:378:SER:OG	2.11	0.50
2:G:532:PRO:HG2	2:G:533:GLU:OE1	2.11	0.50
1:I:68:TYR:CG	1:I:123:LEU:HD13	2.46	0.50
1:J:23:HIS:CE1	1:J:70:ARG:HH22	2.29	0.50
1:J:84:TRP:HA	1:J:99:ASN:O	2.12	0.50
2:K:240:PHE:CG	2:K:269:ASP:OD2	2.65	0.50
1:A:34:LYS:HG2	1:A:50:SER:HB2	1.94	0.50
2:C:343:GLN:NE2	2:C:377:MSE:SE	2.95	0.50
2:C:541:THR:O	2:C:544:ASN:N	2.45	0.50
2:D:239:VAL:CG1	2:D:240:PHE:N	2.75	0.50
2:D:335:PHE:CE2	2:D:339:ILE:HD11	2.47	0.50
2:G:170:ASN:O	2:G:174:GLU:HG3	2.11	0.50
2:G:240:PHE:CD2	2:G:268:SER:HB3	2.47	0.50
1:I:77:TYR:C	1:I:79:LYS:H	2.14	0.50
2:K:227:VAL:HG12	2:K:227:VAL:O	2.12	0.50
2:L:215:SER:HB2	2:L:390:TRP:CZ2	2.47	0.50
1:I:239:ARG:NH1	1:I:239:ARG:HG3	2.27	0.49
1:J:128:LEU:HD22	1:J:185:VAL:HG13	1.94	0.49
1:I:347:ALA:HB2	2:K:51:MSE:CE	2.42	0.49
2:L:39:LYS:CE	2:L:170:ASN:OD1	2.59	0.49
2:L:42:PRO:C	2:L:44:SER:N	2.66	0.49
2:L:544:ASN:C	2:L:545:GLN:HG3	2.33	0.49
1:A:23:HIS:CE1	1:A:70:ARG:HH22	2.30	0.49
1:J:85:GLU:HB2	1:J:101:LEU:HD11	1.94	0.49
2:L:238:LYS:O	2:L:239:VAL:HB	2.12	0.49
2:H:215:SER:HB2	2:H:390:TRP:CZ2	2.46	0.49
2:D:489:ILE:HD13	2:D:503:VAL:CG1	2.42	0.49
1:E:309:SER:HB3	2:G:68:LYS:HA	1.95	0.49
1:J:77:TYR:C	1:J:79:LYS:H	2.15	0.49
2:L:227:VAL:O	2:L:227:VAL:HG12	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:156:VAL:HG13	1:E:192:ILE:HD11	1.94	0.49
1:B:96:ARG:HH21	1:E:9:ASP:CB	2.24	0.49
2:G:166:ASP:HB3	2:G:169:VAL:CG1	2.38	0.49
2:H:39:LYS:HG2	2:H:40:ARG:HG2	1.92	0.49
2:K:335:PHE:CE2	2:K:339:ILE:HD11	2.47	0.49
1:B:34:LYS:HG2	1:B:50:SER:HB2	1.93	0.49
1:F:239:ARG:NH1	1:F:239:ARG:HG3	2.26	0.49
2:K:182:LEU:HG	2:K:409:MSE:HE1	1.95	0.49
2:C:190:PHE:CE2	2:C:427:LYS:HG3	2.47	0.49
2:D:352:THR:OG1	2:D:355:GLU:HG3	2.13	0.49
2:D:452:GLU:CG	2:D:458:ARG:HH11	2.25	0.49
2:G:434:PHE:CD2	2:G:458:ARG:HA	2.47	0.49
1:I:238:GLY:HA2	1:I:305:GLY:O	2.11	0.49
1:J:106:ASP:OD1	1:J:137:TYR:OH	2.30	0.49
1:A:128:LEU:HD22	1:A:185:VAL:HG13	1.94	0.49
1:A:335:TYR:CE1	2:C:457:TYR:HA	2.48	0.49
1:A:297:LEU:HD11	1:A:337:ASN:ND2	2.27	0.49
2:D:147:ALA:O	2:D:150:ALA:HB3	2.12	0.49
2:G:192:LEU:O	2:G:195:GLN:HB2	2.13	0.49
2:H:148:MSE:HE3	2:H:152:LEU:HG	1.91	0.49
2:H:43:VAL:HG12	2:H:44:SER:N	2.28	0.49
1:B:239:ARG:HG3	1:B:239:ARG:NH1	2.28	0.49
2:C:482:TRP:N	2:C:483:PRO:CD	2.76	0.49
2:D:406:LEU:HB2	2:D:407:PRO:HD3	1.94	0.49
2:G:147:ALA:O	2:G:150:ALA:HB3	2.13	0.49
2:G:482:TRP:N	2:G:483:PRO:CD	2.75	0.49
2:K:533:GLU:HG3	2:K:534:ILE:H	1.78	0.49
1:A:125:LEU:HD12	1:A:125:LEU:C	2.32	0.49
1:A:85:GLU:HB2	1:A:101:LEU:HD11	1.94	0.49
1:B:156:VAL:HG13	1:B:192:ILE:HD11	1.95	0.49
1:B:346:THR:HG22	1:B:347:ALA:N	2.28	0.49
1:E:128:LEU:HD23	1:E:169:PHE:HB3	1.95	0.49
1:F:77:TYR:C	1:F:79:LYS:H	2.16	0.49
1:F:84:TRP:HA	1:F:99:ASN:O	2.12	0.49
2:H:151:ILE:CD1	2:H:423:ILE:HD12	2.40	0.49
2:K:248:LEU:O	2:K:248:LEU:HD13	2.13	0.49
2:K:532:PRO:HG2	2:K:533:GLU:H	1.78	0.49
2:L:52:THR:CG2	2:L:53:VAL:N	2.75	0.49
2:C:100:THR:O	2:C:100:THR:HG22	2.13	0.48
2:C:44:SER:C	2:C:46:ALA:H	2.16	0.48
2:D:192:LEU:O	2:D:195:GLN:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:329:ARG:HG2	1:F:344:VAL:HG22	1.94	0.48
2:G:100:THR:O	2:G:100:THR:HG22	2.12	0.48
2:H:223:TYR:O	2:H:227:VAL:HG23	2.13	0.48
1:B:332:LYS:HG3	1:B:342:MSE:SE	2.63	0.48
2:C:313:LEU:HD22	2:C:336:LEU:HD22	1.95	0.48
1:A:67:GLU:HA	2:C:541:THR:OG1	2.12	0.48
2:D:223:TYR:O	2:D:227:VAL:HG23	2.13	0.48
2:D:249:LEU:O	2:D:253:VAL:HG23	2.13	0.48
2:D:375:LEU:HD21	2:D:395:VAL:HG13	1.95	0.48
1:F:34:LYS:HG2	1:F:50:SER:HB2	1.96	0.48
2:G:113:GLU:HA	2:G:113:GLU:OE1	2.13	0.48
2:H:57:PRO:HB3	2:H:91:TYR:OH	2.13	0.48
1:I:179:SER:OG	1:I:180:PRO:HD2	2.13	0.48
1:I:10:ASP:H	1:I:30:ASP:HB3	1.77	0.48
2:K:526:CYS:SG	2:K:535:ALA:HB2	2.53	0.48
2:L:39:LYS:HZ3	2:L:97:ARG:CD	2.26	0.48
1:A:128:LEU:HD23	1:A:169:PHE:HB3	1.95	0.48
1:B:29:SER:C	1:B:31:GLN:H	2.14	0.48
1:B:347:ALA:HB3	2:D:58:ILE:HD12	1.95	0.48
2:L:113:GLU:OE1	2:L:113:GLU:HA	2.14	0.48
2:L:42:PRO:HD3	2:L:48:LEU:HD11	1.95	0.48
2:C:249:LEU:O	2:C:253:VAL:HG23	2.13	0.48
2:D:215:SER:HB2	2:D:390:TRP:CZ2	2.49	0.48
2:K:113:GLU:OE1	2:K:113:GLU:HA	2.13	0.48
1:B:65:SER:CB	1:B:119:ALA:HB2	2.44	0.48
2:D:454:LEU:CD1	2:D:459:ASN:OD1	2.62	0.48
2:D:531:LEU:HD22	2:D:534:ILE:CD1	2.43	0.48
1:E:77:TYR:C	1:E:79:LYS:H	2.17	0.48
1:J:297:LEU:HD11	1:J:337:ASN:ND2	2.29	0.48
1:J:34:LYS:HG2	1:J:50:SER:HB2	1.96	0.48
1:B:125:LEU:C	1:B:125:LEU:HD12	2.34	0.48
2:C:241:GLU:OE1	2:C:241:GLU:HA	2.12	0.48
2:D:373:GLU:O	2:D:377:MSE:HG3	2.13	0.48
2:G:190:PHE:CE2	2:G:427:LYS:HG3	2.49	0.48
2:K:482:TRP:O	2:K:486:ILE:HG12	2.14	0.48
2:L:41:ASP:HA	2:L:46:ALA:O	2.13	0.48
2:C:526:CYS:HA	2:C:531:LEU:HB2	1.96	0.48
1:F:54:HIS:CD2	1:F:58:ILE:HG12	2.49	0.48
1:F:90:GLN:OE1	1:F:96:ARG:CD	2.61	0.48
2:D:531:LEU:HB3	2:D:534:ILE:HB	1.96	0.48
1:E:158:SER:O	1:E:159:ILE:CG1	2.56	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:352:THR:OG1	2:H:355:GLU:HG3	2.13	0.48
1:J:83:LEU:HD12	1:J:102:CYS:SG	2.53	0.48
2:K:100:THR:HG22	2:K:100:THR:O	2.13	0.48
1:B:68:TYR:CG	1:B:123:LEU:HD13	2.48	0.48
2:D:521:TRP:O	2:D:525:ILE:HG13	2.14	0.48
2:D:501:LYS:HE3	2:D:529:TRP:O	2.14	0.48
1:F:218:ILE:O	1:F:218:ILE:HG13	2.14	0.48
1:J:19:PHE:CZ	2:L:510:HIS:CD2	3.02	0.48
2:H:454:LEU:CD2	2:H:458:ARG:HB3	2.44	0.48
2:K:489:ILE:HD13	2:K:503:VAL:CG1	2.44	0.48
2:L:49:VAL:HG12	2:L:50:PRO:N	2.29	0.48
1:A:236:LYS:HG3	1:A:306:GLU:CD	2.35	0.47
1:A:324:ASP:C	1:A:326:GLY:H	2.17	0.47
1:B:54:HIS:CD2	1:B:58:ILE:HG12	2.49	0.47
2:D:434:PHE:CE1	2:D:457:TYR:HE2	2.32	0.47
2:G:239:VAL:CG1	2:G:240:PHE:N	2.62	0.47
2:H:432:ASN:HB2	2:H:460:GLY:CA	2.44	0.47
1:J:193:ILE:HD13	1:J:245:ILE:HD13	1.96	0.47
1:A:59:VAL:HG21	1:A:77:TYR:CE1	2.50	0.47
1:B:191:ALA:HB2	1:B:215:ILE:CD1	2.44	0.47
2:C:313:LEU:O	2:C:313:LEU:HD23	2.14	0.47
2:C:522:MSE:HE2	2:C:538:ILE:CD1	2.44	0.47
1:E:34:LYS:HG2	1:E:50:SER:HB2	1.96	0.47
1:F:336:SER:HB3	2:G:373:GLU:HG2	1.95	0.47
1:I:128:LEU:HD23	1:I:169:PHE:HB3	1.95	0.47
1:J:314:LEU:C	1:J:314:LEU:HD12	2.33	0.47
1:J:75:ALA:HB2	1:J:114:VAL:CG2	2.44	0.47
2:K:375:LEU:HD21	2:K:395:VAL:HG13	1.96	0.47
2:L:52:THR:HG22	2:L:54:ASN:N	2.28	0.47
1:F:226:ARG:HG3	1:F:226:ARG:NH1	2.28	0.47
2:G:39:LYS:HD3	2:G:50:PRO:CG	2.43	0.47
2:G:39:LYS:CE	2:G:50:PRO:HG3	2.44	0.47
2:H:367:SER:C	2:H:369:GLU:H	2.17	0.47
1:I:136:LEU:HD11	1:I:202:LEU:HD11	1.96	0.47
2:L:201:ARG:CZ	2:L:205:ILE:HD11	2.44	0.47
1:F:81:VAL:HG23	1:F:111:LEU:CD1	2.41	0.47
2:G:393:PRO:O	2:G:397:ILE:HG13	2.14	0.47
2:H:434:PHE:CD2	2:H:458:ARG:HA	2.49	0.47
1:I:29:SER:HA	1:I:57:SER:HA	1.97	0.47
1:J:191:ALA:HB2	1:J:215:ILE:CD1	2.44	0.47
1:J:336:SER:HB3	2:K:373:GLU:HG2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:39:LYS:HB3	2:K:47:ILE:HG23	1.96	0.47
2:L:151:ILE:CD1	2:L:423:ILE:HD12	2.42	0.47
1:B:130:ASN:C	1:B:132:GLY:H	2.18	0.47
1:B:97:ARG:HG3	1:B:97:ARG:HH11	1.79	0.47
2:D:169:VAL:HG12	2:D:169:VAL:O	2.14	0.47
1:E:183:LEU:HD12	1:E:183:LEU:O	2.15	0.47
1:F:208:LEU:HD11	1:F:231:ILE:CD1	2.43	0.47
2:H:100:THR:O	2:H:100:THR:HG22	2.15	0.47
2:H:531:LEU:HB3	2:H:534:ILE:HB	1.97	0.47
2:L:454:LEU:HD13	2:L:459:ASN:ND2	2.29	0.47
1:J:178:PHE:HZ	2:L:505:ALA:CB	2.27	0.47
1:F:64:ALA:HB2	1:F:116:PHE:CE2	2.49	0.47
1:F:196:ARG:HH11	1:F:202:LEU:CD2	2.27	0.47
1:F:310:VAL:HA	1:F:320:SER:O	2.15	0.47
2:G:454:LEU:CB	2:G:459:ASN:OD1	2.63	0.47
2:G:453:ASP:O	2:G:454:LEU:HD23	2.15	0.47
1:J:65:SER:CB	1:J:119:ALA:HB2	2.43	0.47
1:J:153:GLU:C	1:J:154:MSE:HG2	2.35	0.47
2:L:367:SER:C	2:L:369:GLU:H	2.18	0.47
1:F:153:GLU:O	1:F:154:MSE:HE3	2.14	0.47
1:F:159:ILE:O	1:F:161:PRO:HD3	2.14	0.47
1:F:191:ALA:HB2	1:F:215:ILE:CD1	2.45	0.47
2:H:249:LEU:O	2:H:253:VAL:HG23	2.15	0.47
2:H:215:SER:HB2	2:H:390:TRP:CH2	2.49	0.47
1:I:191:ALA:HB2	1:I:215:ILE:CD1	2.44	0.47
1:I:59:VAL:HG21	1:I:77:TYR:CE1	2.49	0.47
1:J:324:ASP:C	1:J:326:GLY:H	2.18	0.47
2:L:100:THR:O	2:L:100:THR:HG22	2.15	0.47
2:L:352:THR:OG1	2:L:355:GLU:HG3	2.15	0.47
2:L:55:ASP:O	2:L:56:GLN:C	2.51	0.47
1:A:226:ARG:CG	1:A:226:ARG:HH11	2.26	0.47
1:F:10:ASP:H	1:F:30:ASP:HB3	1.80	0.47
2:G:148:MSE:HE3	2:G:152:LEU:HG	1.96	0.47
1:A:178:PHE:CG	2:C:502:MSE:HG2	2.50	0.47
1:B:16:VAL:HG12	1:B:63:TRP:HD1	1.79	0.47
2:D:100:THR:O	2:D:100:THR:HG22	2.15	0.47
2:H:482:TRP:N	2:H:483:PRO:CD	2.78	0.47
2:H:501:LYS:HE2	2:H:531:LEU:HD23	1.97	0.47
1:I:130:ASN:C	1:I:132:GLY:H	2.19	0.47
2:K:373:GLU:O	2:K:377:MSE:HG3	2.15	0.47
2:L:192:LEU:O	2:L:195:GLN:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:314:LEU:C	1:B:314:LEU:HD12	2.35	0.47
2:C:454:LEU:HB3	2:C:459:ASN:OD1	2.14	0.47
2:C:522:MSE:CE	2:C:538:ILE:CD1	2.91	0.47
2:D:482:TRP:N	2:D:483:PRO:CD	2.78	0.47
2:G:52:THR:HB	2:G:56:GLN:OE1	2.15	0.47
2:H:393:PRO:O	2:H:397:ILE:HG13	2.15	0.47
2:K:434:PHE:CE1	2:K:457:TYR:HE2	2.33	0.47
1:A:180:PRO:HG2	1:A:182:LYS:NZ	2.30	0.47
1:B:10:ASP:H	1:B:30:ASP:HB3	1.79	0.47
2:C:522:MSE:HE2	2:C:538:ILE:HD12	1.98	0.47
2:D:240:PHE:N	2:D:240:PHE:CD1	2.82	0.47
2:G:215:SER:HB2	2:G:390:TRP:CH2	2.50	0.47
2:G:65:MSE:HE2	2:G:84:ALA:HB1	1.97	0.47
2:H:501:LYS:HE3	2:H:529:TRP:O	2.15	0.47
1:I:64:ALA:HB2	1:I:116:PHE:CE2	2.50	0.47
1:I:297:LEU:HD11	1:I:337:ASN:ND2	2.30	0.47
1:I:97:ARG:HH11	1:I:97:ARG:HG3	1.80	0.47
2:K:192:LEU:O	2:K:195:GLN:HB2	2.15	0.47
2:K:474:CYS:SG	2:K:507:LEU:HD22	2.54	0.47
1:A:123:LEU:HD23	1:A:139:ALA:CB	2.45	0.46
1:A:94:SER:C	1:A:96:ARG:H	2.18	0.46
2:C:278:CYS:CB	2:C:323:ASP:HB2	2.45	0.46
1:E:329:ARG:HG2	1:E:344:VAL:HG22	1.96	0.46
1:E:349:GLN:HB2	2:G:56:GLN:CB	2.40	0.46
2:G:396:ASP:OD1	2:G:401:LYS:HE3	2.15	0.46
1:E:10:ASP:O	2:G:88:TYR:CE1	2.69	0.46
1:A:16:VAL:HG12	1:A:63:TRP:CD1	2.49	0.46
1:B:208:LEU:HB3	1:B:243:PHE:CE2	2.50	0.46
2:C:375:LEU:HD21	2:C:395:VAL:HG13	1.96	0.46
2:C:432:ASN:HB2	2:C:460:GLY:HA2	1.97	0.46
1:F:153:GLU:C	1:F:154:MSE:HG2	2.35	0.46
2:H:248:LEU:HD13	2:H:248:LEU:O	2.14	0.46
2:H:52:THR:HB	2:H:56:GLN:OE1	2.15	0.46
1:I:193:ILE:HD13	1:I:245:ILE:HD13	1.97	0.46
1:I:324:ASP:C	1:I:326:GLY:H	2.18	0.46
1:J:208:LEU:HD11	1:J:231:ILE:CD1	2.39	0.46
2:K:343:GLN:NE2	2:K:377:MSE:SE	2.98	0.46
2:L:373:GLU:O	2:L:377:MSE:HG3	2.15	0.46
1:A:75:ALA:HB2	1:A:114:VAL:CG2	2.45	0.46
2:C:489:ILE:HD13	2:C:503:VAL:CG1	2.45	0.46
2:D:239:VAL:CG1	2:D:240:PHE:H	2.27	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:10:ASP:H	1:E:30:ASP:HB3	1.80	0.46
1:E:121:LEU:CD1	1:E:181:GLU:HG3	2.45	0.46
2:K:393:PRO:O	2:K:397:ILE:HG13	2.15	0.46
2:D:113:GLU:OE1	2:D:113:GLU:HA	2.14	0.46
1:E:16:VAL:HG12	1:E:63:TRP:CD1	2.51	0.46
1:F:241:ARG:HG2	1:F:299:GLU:HG3	1.97	0.46
2:G:313:LEU:HD22	2:G:336:LEU:HD22	1.96	0.46
2:K:459:ASN:HB3	2:K:494:THR:OG1	2.16	0.46
2:L:47:ILE:HG22	2:L:49:VAL:HG23	1.98	0.46
2:D:165:GLN:O	2:D:167:GLY:N	2.44	0.46
2:D:182:LEU:HG	2:D:409:MSE:HE1	1.98	0.46
1:E:226:ARG:NH1	1:E:226:ARG:HG3	2.29	0.46
2:G:201:ARG:CZ	2:G:205:ILE:HD11	2.46	0.46
2:H:113:GLU:OE1	2:H:113:GLU:HA	2.16	0.46
2:H:335:PHE:CE2	2:H:339:ILE:HD11	2.51	0.46
2:H:452:GLU:O	2:H:452:GLU:HG2	2.16	0.46
1:I:196:ARG:HH11	1:I:202:LEU:CD2	2.28	0.46
1:J:130:ASN:C	1:J:132:GLY:H	2.18	0.46
2:K:249:LEU:O	2:K:253:VAL:HG23	2.15	0.46
2:K:313:LEU:HD22	2:K:336:LEU:HD22	1.97	0.46
1:A:109:GLY:HA3	1:A:130:ASN:HB2	1.97	0.46
1:B:153:GLU:O	1:B:154:MSE:HE3	2.15	0.46
2:D:393:PRO:O	2:D:397:ILE:HG13	2.16	0.46
1:F:130:ASN:C	1:F:132:GLY:H	2.19	0.46
2:H:158:PHE:O	2:H:162:VAL:HG23	2.16	0.46
1:A:218:ILE:HG13	1:A:218:ILE:O	2.15	0.46
2:H:47:ILE:HG22	2:H:48:LEU:H	1.75	0.46
1:I:310:VAL:HA	1:I:320:SER:O	2.16	0.46
1:I:332:LYS:HG3	1:I:342:MSE:SE	2.66	0.46
2:K:435:GLU:HB3	2:L:196:ASP:HB3	1.97	0.46
1:B:226:ARG:HG3	1:B:226:ARG:NH1	2.27	0.46
1:E:1:MSE:HE2	1:E:1:MSE:HA	1.96	0.46
1:F:16:VAL:HG12	1:F:63:TRP:CD1	2.50	0.46
2:G:39:LYS:HD3	2:G:50:PRO:HG3	1.97	0.46
2:H:406:LEU:HB2	2:H:407:PRO:HD3	1.97	0.46
2:K:313:LEU:O	2:K:313:LEU:HD23	2.16	0.46
1:F:180:PRO:HG2	1:F:182:LYS:NZ	2.31	0.46
1:J:16:VAL:HG12	1:J:63:TRP:CD1	2.51	0.46
2:K:278:CYS:CB	2:K:323:ASP:HB2	2.45	0.46
2:L:278:CYS:CB	2:L:323:ASP:HB2	2.45	0.46
2:L:515:THR:CG2	2:L:516:ASN:N	2.72	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:324:ASP:C	1:B:326:GLY:H	2.20	0.46
2:C:222:GLU:O	2:C:226:GLN:HG3	2.16	0.46
1:B:348:GLN:OE1	2:D:60:LYS:HA	2.16	0.46
2:H:163:LYS:O	2:H:167:GLY:HA2	2.16	0.46
2:H:396:ASP:OD1	2:H:401:LYS:HE3	2.15	0.46
1:J:180:PRO:HG2	1:J:182:LYS:NZ	2.31	0.46
1:A:177:ARG:NH1	2:C:534:ILE:CD1	2.79	0.45
1:A:171:LEU:HD23	1:A:185:VAL:HG22	1.98	0.45
2:C:49:VAL:HG13	2:C:50:PRO:CD	2.46	0.45
1:E:196:ARG:HH11	1:E:202:LEU:CD2	2.29	0.45
1:F:227:TRP:CE3	1:F:227:TRP:N	2.82	0.45
2:G:227:VAL:O	2:G:227:VAL:HG12	2.17	0.45
2:K:454:LEU:HB2	2:K:459:ASN:ND2	2.24	0.45
2:L:223:TYR:O	2:L:227:VAL:HG23	2.16	0.45
2:L:489:ILE:HD13	2:L:503:VAL:CG1	2.44	0.45
1:E:183:LEU:HD12	1:E:183:LEU:C	2.36	0.45
1:E:191:ALA:HB2	1:E:215:ILE:CD1	2.46	0.45
1:E:29:SER:HA	1:E:57:SER:HA	1.98	0.45
1:I:183:LEU:O	1:I:183:LEU:HD12	2.15	0.45
2:K:223:TYR:O	2:K:227:VAL:HG23	2.15	0.45
2:K:52:THR:HB	2:K:56:GLN:CG	2.44	0.45
2:L:482:TRP:N	2:L:483:PRO:CD	2.79	0.45
1:A:8:HIS:HD2	1:A:34:LYS:HE3	1.81	0.45
1:B:348:GLN:O	2:D:56:GLN:NE2	2.49	0.45
2:C:396:ASP:OD1	2:C:401:LYS:HE3	2.16	0.45
2:C:482:TRP:O	2:C:486:ILE:HG12	2.16	0.45
2:D:535:ALA:HA	2:D:538:ILE:CG1	2.45	0.45
1:F:10:ASP:O	2:H:88:TYR:CE1	2.69	0.45
1:F:236:LYS:HG3	1:F:306:GLU:OE1	2.16	0.45
1:F:97:ARG:HH11	1:F:97:ARG:HG3	1.81	0.45
2:H:166:ASP:HB3	2:H:169:VAL:CG1	2.46	0.45
2:L:376:GLN:O	2:L:380:GLU:HG3	2.16	0.45
1:A:226:ARG:NH1	1:A:226:ARG:HG3	2.28	0.45
1:B:10:ASP:HB2	1:E:96:ARG:NH2	2.30	0.45
1:E:310:VAL:HA	1:E:320:SER:O	2.16	0.45
2:G:352:THR:OG1	2:G:355:GLU:HG3	2.16	0.45
2:H:375:LEU:HD21	2:H:395:VAL:HG13	1.97	0.45
1:J:193:ILE:CD1	1:J:245:ILE:HD13	2.46	0.45
2:K:376:GLN:O	2:K:380:GLU:HG3	2.16	0.45
1:A:153:GLU:O	1:A:154:MSE:HE3	2.16	0.45
1:A:178:PHE:CD1	2:C:502:MSE:HG2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:192:LEU:O	2:C:195:GLN:HB2	2.16	0.45
2:C:376:GLN:O	2:C:380:GLU:HG3	2.16	0.45
1:J:59:VAL:HG21	1:J:77:TYR:CE1	2.51	0.45
2:K:454:LEU:CD2	2:K:458:ARG:HD2	2.44	0.45
1:A:344:VAL:O	2:C:48:LEU:HD12	2.17	0.45
2:D:313:LEU:HD22	2:D:336:LEU:HD22	1.99	0.45
2:D:278:CYS:CB	2:D:323:ASP:HB2	2.47	0.45
2:D:539:TYR:O	2:D:540:THR:C	2.54	0.45
2:G:511:TYR:HA	2:G:512:PRO:HD3	1.80	0.45
1:F:99:ASN:OD1	1:I:55:ASP:HB3	2.17	0.45
1:J:226:ARG:NH1	1:J:226:ARG:HG3	2.29	0.45
2:K:352:THR:OG1	2:K:355:GLU:HG3	2.16	0.45
2:L:215:SER:HB2	2:L:390:TRP:CH2	2.52	0.45
2:C:223:TYR:O	2:C:227:VAL:HG23	2.16	0.45
2:D:455:PHE:CD2	2:D:455:PHE:O	2.69	0.45
2:G:459:ASN:HB3	2:G:494:THR:OG1	2.16	0.45
2:H:65:MSE:HE2	2:H:84:ALA:HB1	1.98	0.45
1:I:153:GLU:O	1:I:154:MSE:HE3	2.17	0.45
2:K:515:THR:O	2:K:519:ILE:HG13	2.17	0.45
1:A:97:ARG:HG3	1:A:97:ARG:HH11	1.82	0.45
2:H:239:VAL:HB	2:H:240:PHE:CD1	2.52	0.45
2:H:278:CYS:CB	2:H:323:ASP:HB2	2.46	0.45
2:K:148:MSE:HE3	2:K:152:LEU:HG	1.95	0.45
1:B:153:GLU:C	1:B:154:MSE:HG2	2.37	0.45
1:B:180:PRO:HG2	1:B:182:LYS:NZ	2.32	0.45
1:B:218:ILE:O	1:B:218:ILE:HG13	2.16	0.45
1:B:247:GLU:HB3	1:B:292:LEU:CD2	2.38	0.45
2:D:47:ILE:HG22	2:D:48:LEU:H	1.80	0.45
2:G:529:TRP:O	2:G:530:ARG:HB2	2.16	0.45
2:H:306:TRP:O	2:H:310:VAL:HG23	2.16	0.45
2:L:222:GLU:O	2:L:226:GLN:HG3	2.17	0.45
2:L:306:TRP:O	2:L:310:VAL:HG23	2.17	0.45
2:L:343:GLN:NE2	2:L:377:MSE:SE	3.00	0.45
2:L:451:LEU:HB2	2:L:502:MSE:HE1	1.99	0.45
1:A:241:ARG:HG2	1:A:299:GLU:HG3	1.99	0.45
1:B:297:LEU:HD11	1:B:337:ASN:ND2	2.32	0.45
2:G:489:ILE:HD13	2:G:503:VAL:CG1	2.47	0.45
2:G:545:GLN:O	2:G:546:MSE:HE2	2.17	0.45
1:I:236:LYS:HG3	1:I:306:GLU:OE1	2.17	0.45
2:K:65:MSE:HE2	2:K:84:ALA:HB1	1.99	0.45
2:L:147:ALA:O	2:L:150:ALA:HB3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:178:PHE:CG	2:L:502:MSE:HG2	2.52	0.45
2:C:459:ASN:HB3	2:C:494:THR:OG1	2.17	0.44
2:D:515:THR:O	2:D:519:ILE:HG13	2.16	0.44
1:A:191:ALA:HB2	1:A:215:ILE:CD1	2.47	0.44
2:D:376:GLN:O	2:D:380:GLU:HG3	2.17	0.44
1:E:130:ASN:C	1:E:132:GLY:H	2.21	0.44
2:H:546:MSE:O	2:H:547:LEU:C	2.55	0.44
1:J:178:PHE:CD1	2:L:502:MSE:HG2	2.52	0.44
2:K:123:VAL:CG1	2:K:124:PHE:H	2.24	0.44
1:I:309:SER:HB3	2:K:68:LYS:HA	1.99	0.44
1:B:154:MSE:HA	1:B:154:MSE:CE	2.48	0.44
2:C:201:ARG:CZ	2:C:205:ILE:HD11	2.48	0.44
2:C:474:CYS:SG	2:C:507:LEU:HD22	2.58	0.44
2:D:184:CYS:HB2	2:D:211:TRP:NE1	2.32	0.44
2:D:459:ASN:HB3	2:D:494:THR:OG1	2.16	0.44
2:G:249:LEU:O	2:G:253:VAL:HG23	2.17	0.44
2:H:147:ALA:O	2:H:150:ALA:HB3	2.16	0.44
1:I:109:GLY:HA3	1:I:130:ASN:HB2	1.99	0.44
2:C:367:SER:C	2:C:369:GLU:H	2.21	0.44
2:D:52:THR:HG22	2:D:53:VAL:N	2.32	0.44
2:D:65:MSE:HE2	2:D:84:ALA:HB1	1.99	0.44
1:E:64:ALA:HB2	1:E:116:PHE:CE2	2.52	0.44
2:G:39:LYS:HB2	2:G:39:LYS:HE3	1.66	0.44
1:J:162:ALA:C	1:J:164:HIS:H	2.21	0.44
1:J:236:LYS:HG3	1:J:306:GLU:CD	2.37	0.44
2:K:501:LYS:HE3	2:K:529:TRP:O	2.17	0.44
2:L:248:LEU:O	2:L:248:LEU:HD13	2.18	0.44
2:L:396:ASP:OD1	2:L:401:LYS:HE3	2.17	0.44
1:A:130:ASN:C	1:A:132:GLY:H	2.20	0.44
1:A:54:HIS:CE1	1:A:80:THR:HG23	2.52	0.44
2:D:270:LEU:O	2:D:274:LEU:HB2	2.18	0.44
2:D:49:VAL:HG12	2:D:50:PRO:HD2	2.00	0.44
2:D:95:ILE:HA	2:D:96:PRO:HD3	1.85	0.44
1:F:29:SER:HA	1:F:57:SER:HA	1.99	0.44
2:H:107:TYR:CZ	2:H:111:LEU:HD11	2.53	0.44
1:I:16:VAL:HG12	1:I:63:TRP:CD1	2.51	0.44
1:J:154:MSE:HA	1:J:154:MSE:CE	2.48	0.44
2:L:500:LYS:O	2:L:504:ILE:HG13	2.18	0.44
2:L:501:LYS:HE3	2:L:529:TRP:O	2.17	0.44
1:A:10:ASP:H	1:A:30:ASP:HB3	1.82	0.44
1:B:309:SER:HB3	2:D:68:LYS:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:SER:HA	1:B:57:SER:HA	2.00	0.44
2:C:40:ARG:NH2	2:C:174:GLU:OE2	2.51	0.44
2:C:246:TRP:CE2	2:C:331:TYR:HB3	2.53	0.44
2:D:367:SER:C	2:D:369:GLU:H	2.21	0.44
1:F:75:ALA:HB2	1:F:114:VAL:CG2	2.48	0.44
2:G:123:VAL:CG1	2:G:124:PHE:H	2.25	0.44
2:H:125:ASN:O	2:H:126:VAL:HG23	2.18	0.44
1:I:114:VAL:HG22	1:I:127:CYS:HB3	1.98	0.44
2:K:455:PHE:CD2	2:K:455:PHE:O	2.71	0.44
1:A:157:LEU:HA	1:A:157:LEU:HD23	1.86	0.44
1:A:29:SER:HA	1:A:57:SER:HA	2.00	0.44
1:B:75:ALA:HB2	1:B:114:VAL:CG2	2.48	0.44
2:C:215:SER:HB2	2:C:390:TRP:CZ2	2.52	0.44
2:D:474:CYS:SG	2:D:507:LEU:HD22	2.58	0.44
2:G:114:ILE:HD13	2:G:150:ALA:CB	2.47	0.44
2:G:223:TYR:O	2:G:227:VAL:HG23	2.18	0.44
2:G:375:LEU:HD21	2:G:395:VAL:HG13	1.99	0.44
1:I:54:HIS:CD2	1:I:58:ILE:HG12	2.53	0.44
2:K:240:PHE:CD2	2:K:269:ASP:CB	3.01	0.44
2:L:78:ASN:HB2	2:L:93:VAL:O	2.18	0.44
1:B:71:ILE:HD11	1:B:145:LEU:HD13	2.00	0.44
1:B:183:LEU:HD12	1:B:183:LEU:O	2.17	0.44
2:C:373:GLU:O	2:C:377:MSE:HG3	2.18	0.44
1:A:309:SER:HB3	2:C:68:LYS:HA	1.99	0.44
2:D:112:PHE:CE1	2:D:488:LEU:HD12	2.53	0.44
2:D:155:LEU:O	2:D:159:ILE:HG13	2.18	0.44
2:D:396:ASP:OD1	2:D:401:LYS:HE3	2.18	0.44
2:D:57:PRO:HB3	2:D:91:TYR:OH	2.17	0.44
1:E:153:GLU:O	1:E:154:MSE:HE3	2.18	0.44
1:E:81:VAL:HG23	1:E:111:LEU:CD1	2.42	0.44
1:F:114:VAL:HG22	1:F:127:CYS:HB3	1.99	0.44
2:G:61:ASN:O	2:G:62:GLY:C	2.55	0.44
2:H:50:PRO:HB2	2:H:52:THR:O	2.17	0.44
1:J:10:ASP:H	1:J:30:ASP:HB3	1.83	0.44
1:J:114:VAL:HG22	1:J:127:CYS:HB3	2.00	0.44
1:J:29:SER:HA	1:J:57:SER:HA	2.00	0.44
2:K:114:ILE:HD13	2:K:150:ALA:HB1	2.00	0.44
2:L:455:PHE:O	2:L:455:PHE:CD2	2.70	0.44
2:L:521:TRP:O	2:L:525:ILE:HG13	2.18	0.44
1:F:183:LEU:O	1:F:183:LEU:HD12	2.18	0.44
2:H:222:GLU:O	2:H:226:GLN:HG3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:109:GLY:HA3	1:J:130:ASN:HB2	1.99	0.44
1:J:153:GLU:O	1:J:154:MSE:HE3	2.18	0.44
2:L:393:PRO:O	2:L:397:ILE:HG13	2.18	0.44
1:A:178:PHE:CZ	2:C:505:ALA:HB3	2.52	0.43
2:G:482:TRP:O	2:G:486:ILE:HG12	2.18	0.43
2:H:373:GLU:O	2:H:377:MSE:HG3	2.17	0.43
2:H:505:ALA:CB	2:H:534:ILE:HD11	2.49	0.43
1:J:183:LEU:O	1:J:183:LEU:HD12	2.18	0.43
1:J:68:TYR:OH	1:J:122:GLY:CA	2.64	0.43
2:K:246:TRP:CE2	2:K:331:TYR:HB3	2.52	0.43
2:K:49:VAL:HA	2:K:50:PRO:HD3	1.73	0.43
2:L:375:LEU:HD21	2:L:395:VAL:HG13	2.00	0.43
1:A:114:VAL:HG22	1:A:127:CYS:HB3	2.00	0.43
2:C:242:THR:HG22	2:C:244:TYR:HD1	1.82	0.43
2:G:240:PHE:CE2	2:G:268:SER:HB3	2.52	0.43
2:H:459:ASN:HB3	2:H:494:THR:OG1	2.18	0.43
2:H:521:TRP:O	2:H:525:ILE:HG13	2.18	0.43
1:B:114:VAL:HG22	1:B:127:CYS:HB3	2.00	0.43
2:C:541:THR:O	2:C:543:GLY:N	2.52	0.43
2:D:248:LEU:O	2:D:248:LEU:HD13	2.18	0.43
1:E:218:ILE:O	1:E:218:ILE:HG13	2.17	0.43
2:G:313:LEU:O	2:G:313:LEU:HD23	2.17	0.43
1:I:34:LYS:HG2	1:I:50:SER:HB2	2.00	0.43
1:J:332:LYS:HG3	1:J:342:MSE:SE	2.68	0.43
1:J:54:HIS:CD2	1:J:58:ILE:HG12	2.53	0.43
2:K:238:LYS:HB2	2:K:241:GLU:HG3	2.00	0.43
1:A:156:VAL:HG13	1:A:192:ILE:HD11	2.00	0.43
1:A:193:ILE:HD13	1:A:245:ILE:HD13	1.99	0.43
1:B:117:ALA:HB2	1:B:173:TRP:CZ2	2.53	0.43
2:G:515:THR:O	2:G:519:ILE:HG13	2.18	0.43
2:H:455:PHE:CD2	2:H:455:PHE:O	2.72	0.43
1:I:64:ALA:HB3	1:I:71:ILE:HB	2.00	0.43
2:K:367:SER:C	2:K:369:GLU:H	2.22	0.43
2:L:313:LEU:HD22	2:L:336:LEU:HD22	1.99	0.43
2:L:47:ILE:HG22	2:L:48:LEU:N	2.33	0.43
1:A:71:ILE:HD11	1:A:145:LEU:HD13	1.99	0.43
1:B:183:LEU:C	1:B:183:LEU:HD12	2.39	0.43
1:B:64:ALA:HB2	1:B:116:PHE:CE2	2.53	0.43
1:E:178:PHE:CZ	2:G:502:MSE:HG2	2.52	0.43
2:G:455:PHE:CD2	2:G:455:PHE:O	2.71	0.43
2:G:86:ASP:N	2:G:88:TYR:CZ	2.85	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:313:LEU:HD22	2:H:336:LEU:HD22	2.00	0.43
2:H:529:TRP:O	2:H:530:ARG:HB2	2.19	0.43
2:H:532:PRO:O	2:H:535:ALA:HB3	2.19	0.43
2:L:515:THR:O	2:L:519:ILE:HG13	2.18	0.43
1:A:75:ALA:HB2	1:A:114:VAL:HG23	2.00	0.43
1:A:317:THR:HG22	1:A:318:ILE:HG13	2.01	0.43
1:B:77:TYR:CD1	1:B:110:SER:HB3	2.53	0.43
2:C:42:PRO:HA	2:C:46:ALA:O	2.18	0.43
2:C:65:MSE:HE2	2:C:84:ALA:HB1	2.00	0.43
1:E:157:LEU:HG	1:E:187:ALA:HB1	2.00	0.43
1:F:154:MSE:HA	1:F:154:MSE:CE	2.49	0.43
1:F:193:ILE:HD13	1:F:245:ILE:HD13	2.01	0.43
1:J:335:TYR:CE1	2:L:457:TYR:HA	2.52	0.43
2:K:153:ASN:O	2:K:157:VAL:HG23	2.18	0.43
2:K:190:PHE:CE2	2:K:427:LYS:HG3	2.53	0.43
2:K:184:CYS:HB2	2:K:211:TRP:NE1	2.33	0.43
1:A:171:LEU:CD2	1:A:185:VAL:HG22	2.49	0.43
1:B:85:GLU:HB2	1:B:101:LEU:HD11	1.99	0.43
1:A:22:ARG:NH2	2:C:76:TYR:OH	2.52	0.43
1:E:123:LEU:HD23	1:E:139:ALA:CB	2.49	0.43
1:E:208:LEU:HD11	1:E:231:ILE:CD1	2.41	0.43
1:F:193:ILE:CD1	1:F:245:ILE:HD13	2.49	0.43
1:F:318:ILE:HG12	1:F:332:LYS:HE2	2.00	0.43
2:G:373:GLU:O	2:G:377:MSE:HG3	2.19	0.43
2:G:513:PHE:CE2	2:G:542:LEU:HD21	2.53	0.43
2:K:222:GLU:O	2:K:226:GLN:HG3	2.19	0.43
2:L:307:LYS:HE3	2:L:340:GLY:O	2.19	0.43
2:L:313:LEU:O	2:L:313:LEU:HD23	2.18	0.43
2:L:190:PHE:CE2	2:L:427:LYS:HG3	2.53	0.43
1:B:236:LYS:HG3	1:B:306:GLU:CD	2.39	0.43
2:C:538:ILE:O	2:C:542:LEU:HG	2.18	0.43
1:A:336:SER:HB3	2:D:373:GLU:HG2	2.00	0.43
1:E:159:ILE:HG23	1:E:160:PRO:HD2	2.00	0.43
1:F:82:LYS:HG2	1:F:103:THR:HG23	1.99	0.43
2:H:190:PHE:CE2	2:H:427:LYS:HG3	2.54	0.43
2:H:243:GLN:O	2:H:244:TYR:C	2.56	0.43
2:H:535:ALA:O	2:H:538:ILE:HB	2.18	0.43
1:I:178:PHE:CG	2:K:502:MSE:HE3	2.52	0.43
1:J:226:ARG:CG	1:J:226:ARG:HH11	2.28	0.43
1:B:312:TRP:CZ3	1:B:319:LEU:HB2	2.53	0.43
1:B:313:ASN:ND2	1:B:317:THR:HB	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:168:ARG:C	2:C:170:ASN:H	2.22	0.43
2:G:343:GLN:NE2	2:G:377:MSE:SE	3.02	0.43
2:H:39:LYS:HE3	2:H:39:LYS:HB2	1.79	0.43
1:I:123:LEU:HD23	1:I:139:ALA:CB	2.48	0.43
1:I:68:TYR:OH	1:I:122:GLY:HA2	2.19	0.43
1:J:348:GLN:HG3	1:J:348:GLN:H	1.71	0.43
1:J:54:HIS:CE1	1:J:80:THR:HG23	2.54	0.43
1:J:63:TRP:O	1:J:116:PHE:HD2	2.01	0.43
2:L:454:LEU:CB	2:L:459:ASN:OD1	2.66	0.43
2:L:459:ASN:HB3	2:L:494:THR:OG1	2.18	0.43
2:L:95:ILE:HA	2:L:96:PRO:HD3	1.86	0.43
1:A:153:GLU:C	1:A:154:MSE:HG2	2.40	0.43
1:E:136:LEU:HD11	1:E:202:LEU:HD11	2.01	0.43
1:E:153:GLU:C	1:E:154:MSE:HG2	2.39	0.43
1:F:21:GLY:HA3	2:H:73:PRO:HD2	2.00	0.43
1:E:348:GLN:O	2:G:56:GLN:HG3	2.18	0.43
1:I:183:LEU:C	1:I:183:LEU:HD12	2.39	0.43
1:J:75:ALA:HB2	1:J:114:VAL:HG23	2.01	0.43
2:K:513:PHE:HE2	2:K:542:LEU:HD11	1.84	0.43
2:K:529:TRP:O	2:K:530:ARG:HB2	2.19	0.43
2:K:86:ASP:N	2:K:88:TYR:CZ	2.86	0.43
2:L:65:MSE:HA	2:L:66:PRO:HD3	1.85	0.43
2:C:122:ARG:HG3	2:C:123:VAL:HG23	2.01	0.42
1:B:178:PHE:CG	2:D:502:MSE:HE3	2.53	0.42
1:E:109:GLY:HA3	1:E:130:ASN:HB2	2.00	0.42
2:G:95:ILE:HA	2:G:96:PRO:HD3	1.87	0.42
1:I:346:THR:HB	2:K:48:LEU:HD11	2.00	0.42
2:K:521:TRP:O	2:K:525:ILE:HG13	2.18	0.42
2:L:122:ARG:HG3	2:L:123:VAL:HG23	2.01	0.42
1:A:177:ARG:HH12	2:C:534:ILE:HD13	1.84	0.42
1:B:210:GLY:O	1:B:241:ARG:NH1	2.51	0.42
2:C:118:LEU:HD21	2:C:147:ALA:HB2	2.01	0.42
2:C:123:VAL:CG1	2:C:124:PHE:H	2.26	0.42
2:C:307:LYS:HE3	2:C:340:GLY:O	2.18	0.42
2:D:301:SER:O	2:D:305:GLU:HG3	2.19	0.42
1:E:180:PRO:HG2	1:E:182:LYS:NZ	2.34	0.42
2:G:246:TRP:CE2	2:G:331:TYR:HB3	2.54	0.42
2:H:515:THR:O	2:H:519:ILE:HG13	2.18	0.42
2:H:78:ASN:HB2	2:H:93:VAL:O	2.19	0.42
2:K:344:ARG:HG3	2:K:344:ARG:HH11	1.84	0.42
2:K:108:VAL:HG12	2:K:484:VAL:HG11	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:ALA:HB3	1:A:71:ILE:HB	2.01	0.42
2:C:393:PRO:O	2:C:397:ILE:HG13	2.19	0.42
2:C:40:ARG:HB3	2:C:40:ARG:NH1	2.34	0.42
2:C:530:ARG:C	2:C:532:PRO:HD3	2.38	0.42
2:D:307:LYS:HE3	2:D:340:GLY:O	2.19	0.42
1:E:236:LYS:HG3	1:E:306:GLU:OE1	2.20	0.42
2:G:278:CYS:CB	2:G:323:ASP:HB2	2.49	0.42
2:G:376:GLN:O	2:G:380:GLU:HG3	2.19	0.42
2:H:182:LEU:HG	2:H:409:MSE:HE1	2.00	0.42
2:K:396:ASP:OD1	2:K:401:LYS:HE3	2.18	0.42
1:B:109:GLY:HA3	1:B:130:ASN:HB2	2.01	0.42
1:B:167:SER:HB2	1:B:188:LEU:HD21	2.00	0.42
2:D:123:VAL:CG1	2:D:124:PHE:H	2.26	0.42
2:D:417:ALA:HB1	2:D:465:MSE:HE1	2.02	0.42
1:E:114:VAL:HG22	1:E:127:CYS:HB3	1.99	0.42
1:E:64:ALA:HB3	1:E:71:ILE:HB	2.00	0.42
1:F:183:LEU:C	1:F:183:LEU:HD12	2.39	0.42
1:F:55:ASP:HB3	1:I:99:ASN:OD1	2.19	0.42
2:G:114:ILE:HD13	2:G:150:ALA:HB1	2.00	0.42
2:H:500:LYS:O	2:H:504:ILE:HG13	2.19	0.42
1:I:101:LEU:O	1:I:102:CYS:HB3	2.19	0.42
1:I:344:VAL:O	2:K:48:LEU:HD12	2.20	0.42
2:K:422:MSE:C	2:K:422:MSE:SE	3.08	0.42
1:A:70:ARG:O	1:A:85:GLU:HA	2.19	0.42
2:C:352:THR:OG1	2:C:355:GLU:HG3	2.20	0.42
1:B:346:THR:O	2:D:51:MSE:HB2	2.19	0.42
1:E:324:ASP:C	1:E:326:GLY:H	2.22	0.42
1:E:75:ALA:HB2	1:E:114:VAL:CG2	2.49	0.42
1:F:324:ASP:C	1:F:326:GLY:H	2.23	0.42
2:G:307:LYS:HE3	2:G:340:GLY:O	2.20	0.42
2:H:489:ILE:HD13	2:H:503:VAL:CG1	2.49	0.42
1:I:180:PRO:HG2	1:I:182:LYS:NZ	2.34	0.42
1:I:1:MSE:N	1:I:1:MSE:HE2	2.35	0.42
1:I:324:ASP:O	1:I:326:GLY:N	2.52	0.42
1:J:53:ALA:HB1	1:J:84:TRP:CZ2	2.55	0.42
1:J:92:GLU:HA	1:J:97:ARG:CD	2.49	0.42
2:K:274:LEU:HD11	2:K:285:VAL:HG21	2.01	0.42
2:K:301:SER:O	2:K:305:GLU:HG3	2.19	0.42
1:A:135:ARG:HB3	1:A:137:TYR:CE1	2.54	0.42
1:B:331:TRP:CZ3	1:B:341:CYS:HB2	2.54	0.42
1:B:346:THR:CG2	1:B:347:ALA:N	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64:ALA:HB3	1:B:71:ILE:HB	2.02	0.42
2:C:455:PHE:CD2	2:C:455:PHE:O	2.72	0.42
2:C:515:THR:O	2:C:519:ILE:HG13	2.19	0.42
2:D:383:VAL:CG1	2:D:384:VAL:H	2.29	0.42
1:E:70:ARG:O	1:E:85:GLU:HA	2.19	0.42
2:G:196:ASP:HB3	2:H:435:GLU:HB3	2.01	0.42
2:H:52:THR:HG22	2:H:55:ASP:H	1.84	0.42
1:I:171:LEU:HD23	1:I:185:VAL:HG22	2.01	0.42
1:I:226:ARG:CG	1:I:226:ARG:NH1	2.83	0.42
1:J:178:PHE:CZ	2:L:505:ALA:HB3	2.54	0.42
1:A:318:ILE:HG12	1:A:332:LYS:HE2	2.02	0.42
1:A:8:HIS:NE2	1:A:34:LYS:HD2	2.35	0.42
2:C:166:ASP:CG	2:C:166:ASP:O	2.58	0.42
2:H:270:LEU:O	2:H:274:LEU:HB2	2.18	0.42
2:K:201:ARG:CZ	2:K:205:ILE:HD11	2.50	0.42
2:L:511:TYR:HA	2:L:512:PRO:HD3	1.83	0.42
2:C:168:ARG:C	2:C:170:ASN:N	2.73	0.42
2:C:41:ASP:HA	2:C:42:PRO:HD3	1.76	0.42
2:D:198:GLU:HG3	2:D:300:SER:CB	2.50	0.42
1:E:171:LEU:CD2	1:E:185:VAL:HG22	2.50	0.42
2:G:451:LEU:CG	2:G:452:GLU:H	2.20	0.42
2:H:219:PRO:HB3	2:H:251:GLN:OE1	2.20	0.42
2:H:422:MSE:HB2	2:H:466:LEU:HD11	2.02	0.42
1:I:10:ASP:O	2:K:88:TYR:CD1	2.72	0.42
1:I:117:ALA:HB2	1:I:173:TRP:CZ2	2.55	0.42
1:J:77:TYR:HA	1:J:110:SER:HB3	2.01	0.42
2:K:270:LEU:O	2:K:274:LEU:HB2	2.20	0.42
2:L:505:ALA:HB1	2:L:534:ILE:HD11	2.02	0.42
1:A:123:LEU:CD2	1:A:145:LEU:HD22	2.50	0.42
1:A:226:ARG:NH1	1:A:226:ARG:CG	2.81	0.42
2:C:451:LEU:CG	2:C:452:GLU:H	2.09	0.42
1:A:227:TRP:HZ3	2:C:456:SER:HG	1.68	0.42
2:D:222:GLU:O	2:D:226:GLN:HG3	2.19	0.42
1:E:118:PRO:HG2	1:E:174:CYS:O	2.20	0.42
1:E:171:LEU:HD23	1:E:185:VAL:HG22	2.00	0.42
1:F:2:GLN:HA	1:F:3:PRO:HD3	1.91	0.42
1:F:4:PHE:CE1	2:H:90:LEU:HD12	2.55	0.42
2:G:122:ARG:HG3	2:G:123:VAL:HG23	2.02	0.42
2:H:90:LEU:HD23	2:H:90:LEU:HA	1.90	0.42
1:A:53:ALA:HB1	1:A:84:TRP:CZ2	2.55	0.42
2:C:457:TYR:O	2:D:369:GLU:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:406:LEU:CD1	2:C:461:MSE:HG2	2.50	0.42
2:D:242:THR:HG22	2:D:243:GLN:N	2.35	0.42
1:E:65:SER:HB2	1:E:119:ALA:HB2	2.02	0.42
1:E:83:LEU:HD13	1:E:148:TRP:CE2	2.55	0.42
1:E:53:ALA:HB1	1:E:84:TRP:CZ2	2.55	0.42
2:G:344:ARG:HG3	2:G:344:ARG:HH11	1.85	0.42
2:H:122:ARG:HG3	2:H:123:VAL:HG23	2.02	0.42
2:K:454:LEU:CD1	2:K:459:ASN:OD1	2.68	0.42
2:L:301:SER:O	2:L:305:GLU:HG3	2.19	0.42
1:B:346:THR:CG2	1:B:348:GLN:HB2	2.49	0.41
1:B:84:TRP:HA	1:B:99:ASN:O	2.20	0.41
2:C:465:MSE:HB3	2:C:465:MSE:HE2	1.96	0.41
2:C:501:LYS:HE3	2:C:529:TRP:O	2.20	0.41
2:D:108:VAL:HG12	2:D:484:VAL:HG11	2.01	0.41
1:F:71:ILE:HD11	1:F:145:LEU:HD13	2.01	0.41
1:F:197:GLY:HA3	1:F:203:HIS:HD2	1.85	0.41
2:H:301:SER:O	2:H:305:GLU:HG3	2.20	0.41
2:L:216:ASP:OD2	2:L:255:ARG:NH2	2.53	0.41
2:L:42:PRO:O	2:L:44:SER:N	2.53	0.41
2:C:123:VAL:CG1	2:C:124:PHE:N	2.83	0.41
2:C:248:LEU:C	2:C:248:LEU:HD13	2.41	0.41
2:C:531:LEU:O	2:C:534:ILE:HB	2.20	0.41
2:D:103:GLU:H	2:D:103:GLU:CD	2.24	0.41
2:D:122:ARG:HG3	2:D:123:VAL:HG23	2.02	0.41
1:B:227:TRP:CE3	2:D:453:ASP:O	2.73	0.41
2:D:78:ASN:HB2	2:D:93:VAL:O	2.20	0.41
2:G:501:LYS:HE3	2:G:529:TRP:O	2.19	0.41
2:H:103:GLU:H	2:H:103:GLU:CD	2.23	0.41
2:H:201:ARG:CZ	2:H:205:ILE:HD11	2.49	0.41
1:J:346:THR:CG2	1:J:347:ALA:N	2.73	0.41
2:L:296:PRO:HD3	2:L:306:TRP:CD1	2.54	0.41
2:L:182:LEU:HG	2:L:409:MSE:HE1	2.02	0.41
2:K:369:GLU:HG2	2:L:457:TYR:O	2.19	0.41
2:L:91:TYR:O	2:L:93:VAL:HG23	2.19	0.41
1:A:77:TYR:CD1	1:A:110:SER:HB3	2.55	0.41
2:D:75:SER:HB3	2:D:98:LEU:CD1	2.50	0.41
1:F:18:ASP:OD2	1:F:23:HIS:HB2	2.20	0.41
1:F:83:LEU:HD12	1:F:102:CYS:SG	2.61	0.41
1:F:178:PHE:CZ	2:H:502:MSE:HG2	2.55	0.41
1:F:3:PRO:HA	2:H:92:PRO:HD2	2.02	0.41
1:J:118:PRO:HG2	1:J:174:CYS:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:313:ASN:ND2	1:J:317:THR:HB	2.33	0.41
1:A:219:SER:OG	1:A:312:TRP:HD1	2.04	0.41
1:A:313:ASN:ND2	1:A:317:THR:HB	2.33	0.41
2:C:274:LEU:HD11	2:C:285:VAL:HG21	2.01	0.41
2:C:306:TRP:O	2:C:310:VAL:HG23	2.19	0.41
2:C:65:MSE:HA	2:C:66:PRO:HD3	1.81	0.41
2:D:306:TRP:O	2:D:310:VAL:HG23	2.21	0.41
2:D:49:VAL:CG1	2:D:50:PRO:CD	2.98	0.41
2:G:222:GLU:O	2:G:226:GLN:HG3	2.19	0.41
2:G:306:TRP:O	2:G:310:VAL:HG23	2.19	0.41
2:H:313:LEU:HD23	2:H:313:LEU:O	2.20	0.41
1:I:163:ASN:O	1:I:164:HIS:HB2	2.21	0.41
1:J:156:VAL:O	1:J:157:LEU:HD23	2.21	0.41
1:J:134:LEU:HD11	1:J:183:LEU:HD11	2.02	0.41
2:K:248:LEU:HD13	2:K:248:LEU:C	2.40	0.41
2:L:39:LYS:CD	2:L:170:ASN:OD1	2.68	0.41
2:L:60:LYS:O	2:L:61:ASN:HB2	2.20	0.41
1:A:154:MSE:CE	1:A:154:MSE:HA	2.50	0.41
1:A:68:TYR:OH	1:A:122:GLY:CA	2.68	0.41
2:C:86:ASP:N	2:C:88:TYR:CZ	2.86	0.41
2:H:307:LYS:HE3	2:H:340:GLY:O	2.20	0.41
2:H:42:PRO:HA	2:H:46:ALA:C	2.41	0.41
2:H:49:VAL:CG1	2:H:50:PRO:HD2	2.50	0.41
2:L:246:TRP:CE2	2:L:331:TYR:HB3	2.56	0.41
2:C:227:VAL:O	2:C:240:PHE:HE2	2.03	0.41
2:D:49:VAL:HG13	2:D:50:PRO:HD2	2.02	0.41
1:F:226:ARG:CG	1:F:226:ARG:NH1	2.82	0.41
1:F:85:GLU:HB2	1:F:101:LEU:HD11	2.02	0.41
2:G:301:SER:O	2:G:305:GLU:HG3	2.20	0.41
1:E:178:PHE:CE1	2:G:502:MSE:HG2	2.56	0.41
1:J:216:ARG:HD2	1:J:308:TRP:CZ3	2.55	0.41
1:J:318:ILE:HG12	1:J:332:LYS:HE2	2.03	0.41
2:L:65:MSE:HE2	2:L:84:ALA:HB1	2.01	0.41
1:B:134:LEU:HD11	1:B:183:LEU:HD11	2.03	0.41
2:C:49:VAL:CG1	2:C:50:PRO:N	2.83	0.41
2:D:529:TRP:O	2:D:530:ARG:HB2	2.19	0.41
1:E:54:HIS:CD2	1:E:58:ILE:HG12	2.56	0.41
2:G:184:CYS:HB2	2:G:211:TRP:NE1	2.36	0.41
1:I:153:GLU:C	1:I:154:MSE:HG2	2.40	0.41
1:J:171:LEU:HD23	1:J:185:VAL:HG22	2.03	0.41
1:J:226:ARG:NH1	1:J:226:ARG:CG	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:97:ARG:HH11	1:J:97:ARG:HG3	1.85	0.41
2:K:122:ARG:HG3	2:K:123:VAL:HG23	2.03	0.41
1:A:183:LEU:O	1:A:183:LEU:HD12	2.21	0.41
1:B:118:PRO:HG2	1:B:174:CYS:O	2.20	0.41
1:B:197:GLY:HA3	1:B:203:HIS:HD2	1.86	0.41
2:D:532:PRO:HG2	2:D:533:GLU:H	1.85	0.41
1:F:242:ILE:HD11	1:F:319:LEU:HD23	2.03	0.41
1:J:183:LEU:C	1:J:183:LEU:HD12	2.41	0.41
2:L:43:VAL:HG12	2:L:43:VAL:O	2.21	0.41
1:B:124:LYS:HE3	1:B:138:ASP:OD1	2.21	0.41
2:D:546:MSE:CE	2:D:547:LEU:HD23	2.50	0.41
2:G:367:SER:C	2:G:369:GLU:H	2.24	0.41
2:H:376:GLN:O	2:H:380:GLU:HG3	2.21	0.41
1:I:154:MSE:CE	1:I:154:MSE:HA	2.51	0.41
2:L:168:ARG:O	2:L:169:VAL:HG23	2.21	0.41
2:L:177:GLU:O	2:L:181:VAL:HG23	2.21	0.41
1:A:324:ASP:C	1:A:326:GLY:N	2.74	0.41
1:B:68:TYR:OH	1:B:122:GLY:HA2	2.21	0.41
2:D:496:THR:HG22	2:D:497:ARG:N	2.35	0.41
1:F:30:ASP:HA	1:I:96:ARG:CZ	2.49	0.41
2:G:347:LEU:HD22	2:G:381:ALA:HB2	2.02	0.41
1:I:134:LEU:HD11	1:I:183:LEU:HD11	2.01	0.41
1:I:226:ARG:HG3	1:I:226:ARG:NH1	2.29	0.41
1:J:210:GLY:O	1:J:241:ARG:NH1	2.54	0.41
1:J:4:PHE:CE1	2:L:90:LEU:HD12	2.56	0.41
2:L:75:SER:HB3	2:L:98:LEU:CD1	2.51	0.41
2:C:454:LEU:HD13	2:C:459:ASN:OD1	2.20	0.41
2:C:541:THR:O	2:C:542:LEU:C	2.58	0.41
2:D:246:TRP:CE2	2:D:331:TYR:HB3	2.55	0.41
1:E:159:ILE:HG22	1:E:160:PRO:N	2.36	0.41
1:F:135:ARG:HB3	1:F:137:TYR:CE1	2.55	0.41
1:I:92:GLU:HA	1:I:97:ARG:HD2	2.02	0.41
1:J:10:ASP:O	2:L:88:TYR:CE1	2.74	0.41
2:K:532:PRO:HG2	2:K:533:GLU:N	2.35	0.41
2:L:219:PRO:HB3	2:L:251:GLN:OE1	2.20	0.41
2:L:270:LEU:O	2:L:274:LEU:HB2	2.21	0.41
1:A:101:LEU:O	1:A:102:CYS:HB3	2.21	0.40
2:C:169:VAL:O	2:C:169:VAL:HG12	2.21	0.40
2:C:40:ARG:CZ	2:C:40:ARG:HB2	2.51	0.40
2:D:107:TYR:CZ	2:D:111:LEU:HD11	2.56	0.40
2:H:184:CYS:HB2	2:H:211:TRP:NE1	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:218:ILE:HG13	1:J:218:ILE:O	2.20	0.40
2:K:296:PRO:HG3	2:K:302:THR:HG22	2.03	0.40
2:L:123:VAL:CG1	2:L:124:PHE:N	2.84	0.40
2:L:296:PRO:HG3	2:L:302:THR:HG22	2.04	0.40
2:L:432:ASN:HB2	2:L:460:GLY:HA2	2.03	0.40
2:L:496:THR:HG22	2:L:497:ARG:N	2.36	0.40
2:C:215:SER:HB2	2:C:390:TRP:CH2	2.56	0.40
2:C:529:TRP:O	2:C:530:ARG:HB2	2.21	0.40
1:A:88:PRO:HG3	2:C:547:LEU:O	2.21	0.40
2:D:91:TYR:O	2:D:93:VAL:HG23	2.22	0.40
1:F:68:TYR:CG	1:F:123:LEU:HD13	2.57	0.40
2:G:78:ASN:HB2	2:G:93:VAL:O	2.21	0.40
1:F:21:GLY:CA	2:H:73:PRO:HD2	2.51	0.40
1:I:231:ILE:HD13	1:I:231:ILE:HG21	1.84	0.40
1:J:312:TRP:CZ3	1:J:319:LEU:HB2	2.55	0.40
2:L:39:LYS:NZ	2:L:97:ARG:HG2	2.36	0.40
1:A:332:LYS:HG3	1:A:342:MSE:SE	2.71	0.40
1:B:123:LEU:CD2	1:B:145:LEU:HD22	2.51	0.40
2:C:182:LEU:HG	2:C:409:MSE:HE1	2.04	0.40
2:C:242:THR:HG22	2:C:243:GLN:N	2.36	0.40
2:C:296:PRO:HG3	2:C:302:THR:HG22	2.03	0.40
2:C:303:PHE:O	2:C:306:TRP:HB3	2.21	0.40
2:C:434:PHE:CD2	2:C:458:ARG:HA	2.56	0.40
1:E:123:LEU:CD2	1:E:145:LEU:HD22	2.51	0.40
1:E:297:LEU:HA	1:E:297:LEU:HD23	1.95	0.40
2:G:270:LEU:O	2:G:274:LEU:HB2	2.21	0.40
2:G:465:MSE:HB3	2:G:465:MSE:HE2	1.94	0.40
1:J:157:LEU:C	1:J:159:ILE:N	2.73	0.40
1:J:317:THR:HG22	1:J:318:ILE:HG13	2.03	0.40
1:B:226:ARG:NH1	1:B:226:ARG:CG	2.82	0.40
1:B:241:ARG:HG2	1:B:299:GLU:HG3	2.03	0.40
1:B:317:THR:HG22	1:B:318:ILE:HG13	2.02	0.40
1:B:77:TYR:HA	1:B:110:SER:HB3	2.04	0.40
2:C:347:LEU:HD23	2:C:347:LEU:HA	1.91	0.40
2:D:49:VAL:HA	2:D:50:PRO:HD3	1.92	0.40
1:E:141:GLU:O	1:E:143:SER:N	2.55	0.40
1:E:312:TRP:CZ3	1:E:319:LEU:HB2	2.57	0.40
2:H:246:TRP:CE2	2:H:331:TYR:HB3	2.57	0.40
1:I:121:LEU:HD11	1:I:181:GLU:HG3	2.03	0.40
1:J:228:TYR:CG	1:J:244:LYS:HE3	2.56	0.40
2:L:473:LEU:HD23	2:L:473:LEU:HA	1.92	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:125:ASN:HB2	2:D:136:PHE:HE2	1.87	0.40
1:E:224:ILE:HG12	2:G:506:GLU:OE1	2.22	0.40
1:F:101:LEU:O	1:F:102:CYS:HB3	2.21	0.40
2:G:148:MSE:HE2	2:G:152:LEU:CG	2.51	0.40
1:I:124:LYS:HE3	1:I:138:ASP:OD1	2.21	0.40
1:I:54:HIS:CE1	1:I:80:THR:HG23	2.57	0.40
2:L:482:TRP:O	2:L:486:ILE:HG12	2.21	0.40
2:L:57:PRO:HB3	2:L:91:TYR:OH	2.22	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	297/351 (85%)	273 (92%)	21 (7%)	3 (1%)	15	54
1	B	297/351 (85%)	269 (91%)	24 (8%)	4 (1%)	12	47
1	E	297/351 (85%)	271 (91%)	24 (8%)	2 (1%)	22	61
1	F	304/351 (87%)	274 (90%)	27 (9%)	3 (1%)	15	54
1	I	303/351 (86%)	273 (90%)	27 (9%)	3 (1%)	15	54
1	J	304/351 (87%)	277 (91%)	24 (8%)	3 (1%)	15	54
2	C	472/570 (83%)	404 (86%)	61 (13%)	7 (2%)	10	44
2	D	470/570 (82%)	403 (86%)	59 (13%)	8 (2%)	9	42
2	G	475/570 (83%)	404 (85%)	60 (13%)	11 (2%)	6	34
2	H	478/570 (84%)	405 (85%)	61 (13%)	12 (2%)	5	32
2	K	479/570 (84%)	408 (85%)	63 (13%)	8 (2%)	9	42
2	L	474/570 (83%)	402 (85%)	62 (13%)	10 (2%)	7	37
All	All	4650/5526 (84%)	4063 (87%)	513 (11%)	74 (2%)	9	43

All (74) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	272	PRO
2	D	239	VAL
2	D	272	PRO
2	G	239	VAL
2	G	272	PRO
2	H	272	PRO
2	K	272	PRO
2	L	60	LYS
2	L	239	VAL
2	L	272	PRO
2	D	45	GLY
1	F	131	ASP
2	G	453	ASP
2	H	47	ILE
2	H	453	ASP
2	H	547	LEU
2	K	42	PRO
2	L	45	GLY
1	B	131	ASP
1	B	325	ASP
2	C	277	THR
2	C	401	LYS
2	D	166	ASP
2	D	277	THR
2	D	401	LYS
1	E	131	ASP
2	G	40	ARG
2	G	277	THR
2	G	401	LYS
2	H	277	THR
2	H	401	LYS
2	H	452	GLU
1	I	131	ASP
1	I	325	ASP
1	J	131	ASP
2	K	277	THR
2	K	401	LYS
2	L	277	THR
2	L	401	LYS
1	A	131	ASP
1	A	325	ASP
1	B	158	SER

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Mol	Chain	Res	Type
2	C	542	LEU
1	E	325	ASP
1	F	325	ASP
2	H	45	GLY
1	J	325	ASP
2	K	167	GLY
1	A	302	ASP
1	B	302	ASP
2	C	239	VAL
2	C	364	TYR
2	G	45	GLY
2	H	368	LEU
1	I	302	ASP
2	L	61	ASN
2	L	364	TYR
2	G	325	SER
1	J	302	ASP
2	K	325	SER
2	K	398	ILE
2	L	169	VAL
2	L	368	LEU
2	D	398	ILE
2	D	296	PRO
1	F	160	PRO
2	G	398	ILE
2	K	296	PRO
2	C	296	PRO
2	G	43	VAL
2	H	43	VAL
2	H	239	VAL
2	G	296	PRO
2	H	398	ILE

### 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	265/302 (88%)	256 (97%)	9 (3%)	37	70
1	B	265/302 (88%)	257 (97%)	8 (3%)	41	73
1	E	265/302 (88%)	257 (97%)	8 (3%)	41	73
1	F	269/302 (89%)	262 (97%)	7 (3%)	46	76
1	I	268/302 (89%)	260 (97%)	8 (3%)	41	73
1	J	269/302 (89%)	260 (97%)	9 (3%)	38	71
2	C	430/494 (87%)	426 (99%)	4 (1%)	78	91
2	D	427/494 (86%)	423 (99%)	4 (1%)	78	91
2	G	432/494 (87%)	429 (99%)	3 (1%)	84	94
2	H	434/494 (88%)	431 (99%)	3 (1%)	84	94
2	K	436/494 (88%)	431 (99%)	5 (1%)	73	88
2	L	431/494 (87%)	426 (99%)	5 (1%)	71	88
All	All	4191/4776 (88%)	4118 (98%)	73 (2%)	60	83

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MSE
1	A	11	LEU
1	A	43	SER
1	A	99	ASN
1	A	154	MSE
1	A	226	ARG
1	A	246	THR
1	A	314	LEU
1	A	338	GLU
1	B	11	LEU
1	B	43	SER
1	B	99	ASN
1	B	154	MSE
1	B	226	ARG
1	B	246	THR
1	B	314	LEU
1	B	338	GLU
2	C	56	GLN
2	C	122	ARG
2	C	453	ASP
2	C	522	MSE
2	D	59	GLU

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Mol	Chain	Res	Type
2	D	122	ARG
2	D	522	MSE
2	D	546	MSE
1	E	11	LEU
1	E	43	SER
1	E	96	ARG
1	E	99	ASN
1	E	154	MSE
1	E	226	ARG
1	E	246	THR
1	E	314	LEU
1	F	11	LEU
1	F	43	SER
1	F	99	ASN
1	F	154	MSE
1	F	226	ARG
1	F	246	THR
1	F	314	LEU
2	G	55	ASP
2	G	122	ARG
2	G	186	ARG
2	H	122	ARG
2	H	241	GLU
2	H	522	MSE
1	I	11	LEU
1	I	43	SER
1	I	99	ASN
1	I	154	MSE
1	I	226	ARG
1	I	246	THR
1	I	314	LEU
1	I	338	GLU
1	J	11	LEU
1	J	43	SER
1	J	99	ASN
1	J	154	MSE
1	J	226	ARG
1	J	246	THR
1	J	314	LEU
1	J	338	GLU
1	J	348	GLN
2	K	44	SER

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Mol	Chain	Res	Type
2	K	57	PRO
2	K	122	ARG
2	K	240	PHE
2	K	522	MSE
2	L	41	ASP
2	L	59	GLU
2	L	122	ARG
2	L	134	SER
2	L	453	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	343	GLN
2	D	343	GLN
2	G	343	GLN
2	K	343	GLN
2	K	545	GLN
2	L	343	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 ⓘ

There are no ligands in this entry.

## 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<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
1	A	300/351 (85%)	0.14	7 (2%)	60 47	54, 74, 98, 129	0
1	B	300/351 (85%)	0.10	3 (1%)	82 72	56, 74, 99, 120	0
1	E	300/351 (85%)	0.17	4 (1%)	77 65	53, 72, 97, 114	0
1	F	305/351 (86%)	0.20	8 (2%)	56 40	53, 72, 101, 143	0
1	I	304/351 (86%)	0.16	13 (4%)	35 22	55, 74, 102, 139	0
1	J	305/351 (86%)	0.22	11 (3%)	42 27	54, 75, 101, 144	0
2	C	467/570 (81%)	0.19	17 (3%)	42 27	58, 81, 123, 138	0
2	D	464/570 (81%)	0.19	17 (3%)	41 26	57, 80, 120, 133	0
2	G	470/570 (82%)	0.18	9 (1%)	66 53	55, 80, 117, 134	0
2	H	473/570 (82%)	0.20	10 (2%)	63 49	56, 80, 121, 150	0
2	K	473/570 (82%)	0.21	16 (3%)	45 29	58, 81, 122, 137	0
2	L	470/570 (82%)	0.21	20 (4%)	35 22	57, 80, 123, 142	0
All	All	4631/5526 (83%)	0.18	135 (2%)	51 36	53, 76, 117, 150	0

All (135) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	163	ASN	7.9
1	I	164	HIS	6.6
1	J	164	HIS	6.2
2	G	133	ASN	5.9
1	F	164	HIS	5.8
1	B	349	GLN	5.7
2	K	41	ASP	5.4
2	K	240	PHE	5.3
2	H	133	ASN	5.1
1	J	162	ALA	5.1
2	C	261	ALA	4.9

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Mol	Chain	Res	Type	RSRZ
2	K	133	ASN	4.9
1	J	163	ASN	4.8
2	L	136	PHE	4.7
1	I	158	SER	4.6
2	C	133	ASN	4.5
1	A	160	PRO	4.4
1	F	162	ALA	4.3
2	G	265	ILE	4.3
1	F	158	SER	4.3
2	L	133	ASN	4.3
1	J	161	PRO	4.3
2	D	271	LEU	4.2
1	J	165	LEU	4.2
1	I	165	LEU	4.1
2	K	40	ARG	4.0
1	I	142	PRO	3.9
2	D	324	ILE	3.9
2	K	61	ASN	3.9
2	C	265	ILE	3.8
2	L	313	LEU	3.8
1	E	290	SER	3.8
1	F	290	SER	3.7
2	L	38	TYR	3.6
2	C	136	PHE	3.6
2	K	264	CYS	3.5
2	K	43	VAL	3.5
2	K	269	ASP	3.4
2	G	545	GLN	3.4
2	H	539	TYR	3.4
2	H	236	GLY	3.4
2	H	435	GLU	3.3
1	A	136	LEU	3.2
2	D	164	ASP	3.2
2	D	61	ASN	3.2
2	H	136	PHE	3.2
2	K	126	VAL	3.1
1	I	166	GLN	3.1
2	C	220	ASP	3.1
2	K	164	ASP	3.0
1	I	159	ILE	3.0
2	C	239	VAL	3.0
1	B	159	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	I	162	ALA	2.9
2	L	165	GLN	2.9
2	L	116	ARG	2.9
2	L	230	VAL	2.9
2	L	335	PHE	2.8
1	J	160	PRO	2.8
2	H	237	LYS	2.8
2	C	219	PRO	2.8
1	A	133	ILE	2.8
2	D	245	PHE	2.8
1	I	163	ASN	2.7
2	D	240	PHE	2.7
2	C	227	VAL	2.7
1	E	198	LYS	2.7
1	I	143	SER	2.7
2	C	224	ILE	2.7
1	J	89	ASP	2.6
1	I	104	LEU	2.6
2	C	137	ALA	2.6
2	K	42	PRO	2.6
2	D	550	HIS	2.6
2	D	136	PHE	2.6
1	A	166	GLN	2.5
2	L	231	LYS	2.5
2	K	284	ALA	2.5
2	C	280	VAL	2.5
1	I	205	ALA	2.5
2	D	248	LEU	2.5
1	F	159	ILE	2.5
2	G	264	CYS	2.5
2	D	335	PHE	2.5
1	A	104	LEU	2.4
1	B	290	SER	2.4
2	C	134	SER	2.4
2	D	166	ASP	2.4
2	H	126	VAL	2.4
2	D	44	SER	2.4
1	J	194	TYR	2.4
2	L	285	VAL	2.4
1	F	161	PRO	2.3
2	H	244	TYR	2.3
2	L	229	SER	2.3

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Mol	Chain	Res	Type	RSRZ
2	L	125	ASN	2.3
2	K	215	SER	2.3
2	C	164	ASP	2.3
2	G	229	SER	2.3
1	A	157	LEU	2.3
2	L	317	PHE	2.3
2	L	436	GLY	2.3
2	G	435	GLU	2.3
2	L	164	ASP	2.3
2	C	321	ALA	2.3
2	H	240	PHE	2.2
2	D	260	GLN	2.2
2	D	317	PHE	2.2
1	F	248	LYS	2.2
2	G	279	ALA	2.2
2	D	58	ILE	2.2
2	L	167	GLY	2.2
1	E	136	LEU	2.2
1	J	158	SER	2.2
2	C	270	LEU	2.1
2	D	57	PRO	2.1
2	D	272	PRO	2.1
1	A	197	GLY	2.1
2	H	173	TYR	2.1
2	C	43	VAL	2.1
2	L	42	PRO	2.1
2	C	166	ASP	2.1
2	L	47	ILE	2.1
1	J	143	SER	2.1
1	I	346	THR	2.1
1	I	161	PRO	2.1
2	L	321	ALA	2.1
2	K	258	LEU	2.0
2	K	550	HIS	2.0
2	K	221	GLU	2.0
1	J	133	ILE	2.0
1	E	248	LYS	2.0
2	G	224	ILE	2.0
2	L	328	LEU	2.0
2	G	452	GLU	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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.