



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:33 PM UTC

PDB ID : 3F3P / pdb_00003f3p
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

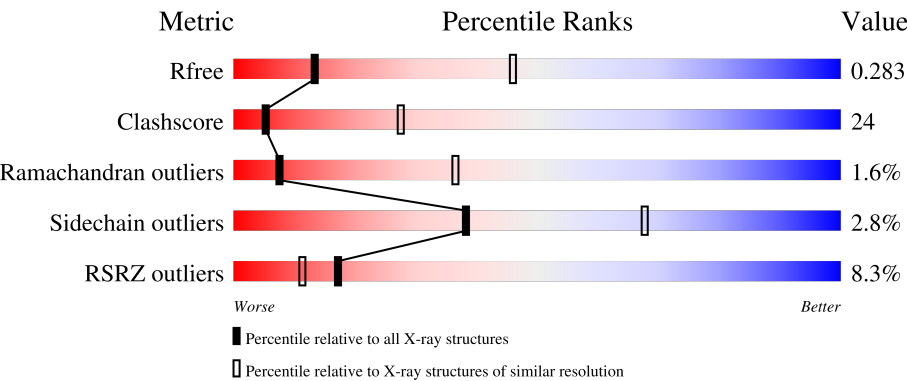
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	4% 47% 36% • • 14%
1	B	351	3% 43% 39% • • 14%
1	E	351	5% 46% 36% • • 14%
1	F	351	7% 45% 38% • • 12%
1	I	351	5% 46% 37% • • 13%

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Mol	Chain	Length	Quality of chain
1	J	351	7% 43% 40% • • 12%
2	C	570	8% 47% 34% • 16%
2	D	570	4% 48% 31% 5% 16%
2	G	570	12% 49% 33% • 15%
2	H	570	10% 47% 34% • 15%
2	K	570	7% 49% 32% • 15%
2	L	570	7% 47% 34% • 15%

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

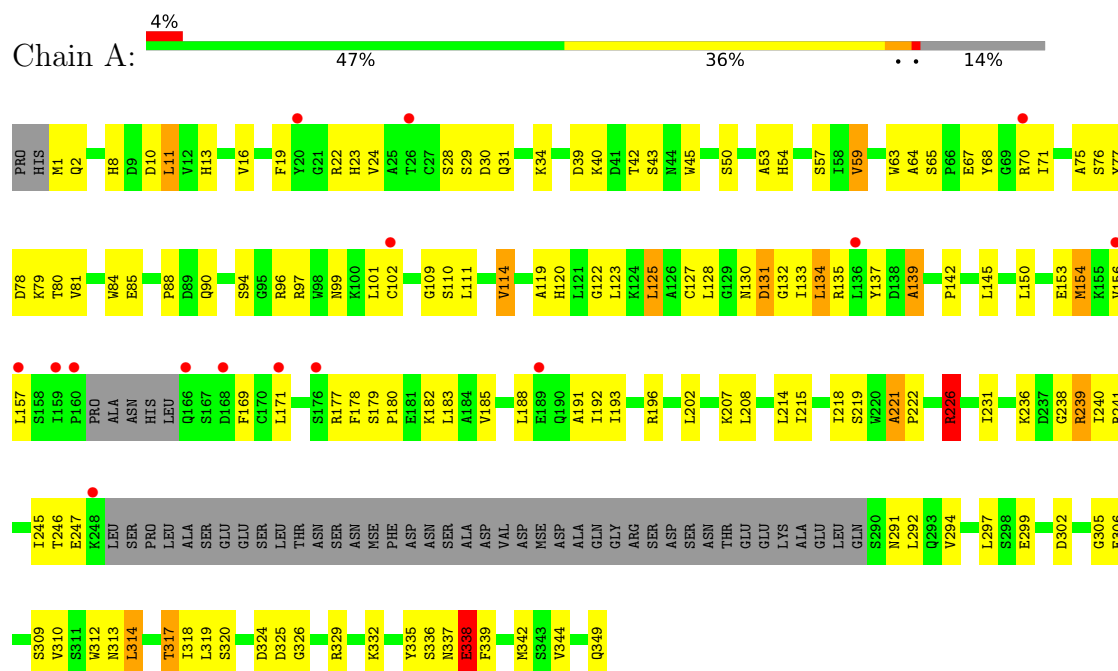
- Molecule 2 is a protein called Nucleoporin NUP85.

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			

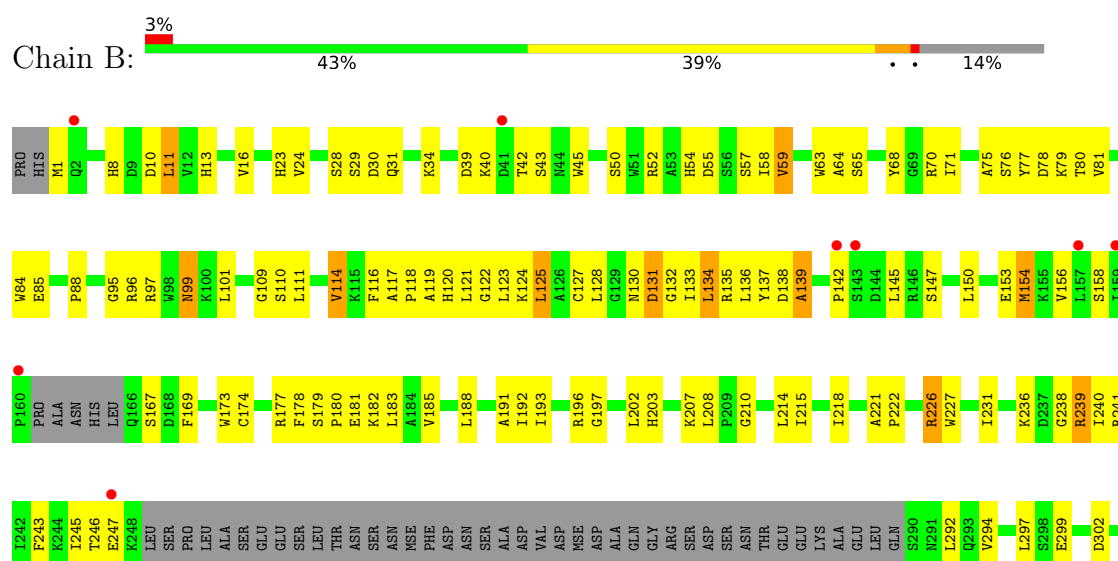
3 Residue-property plots [i](#)

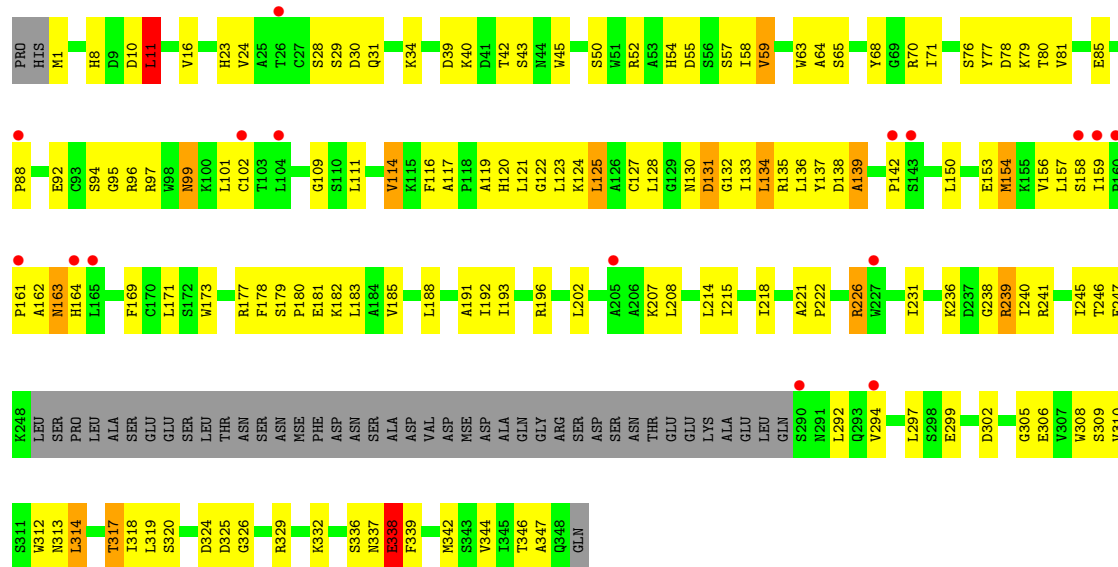
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

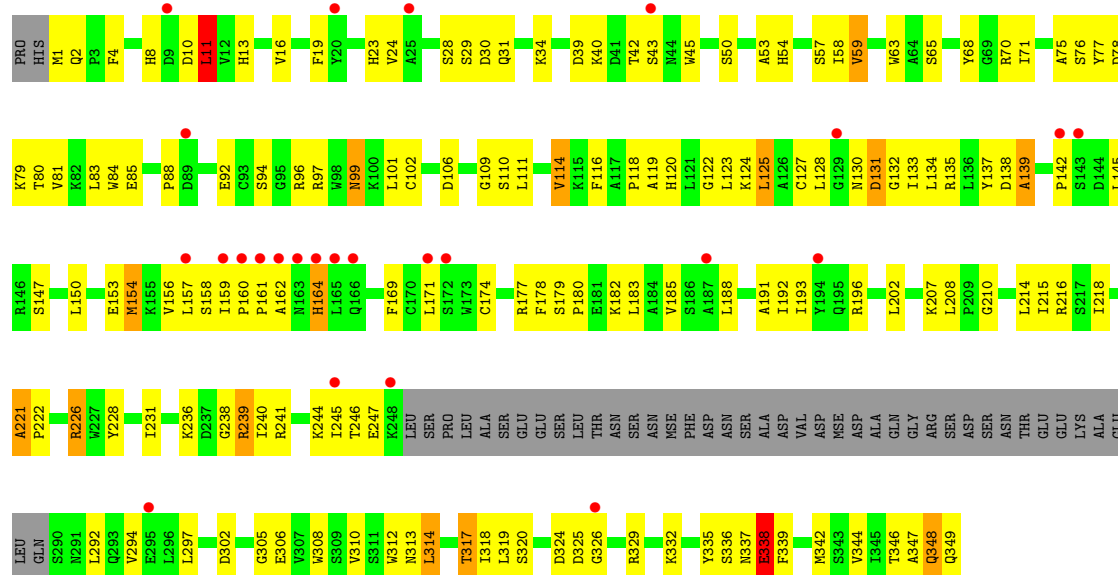


• Molecule 1: Nucleoporin SEH1

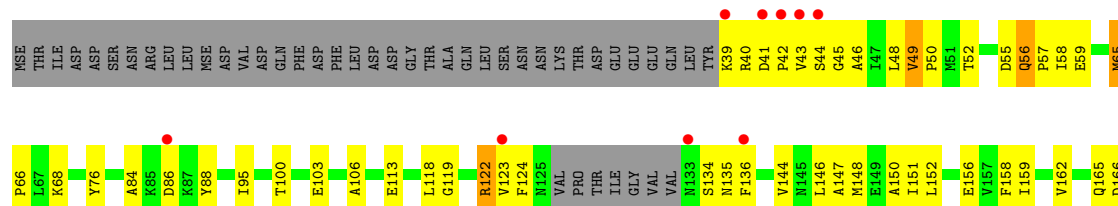


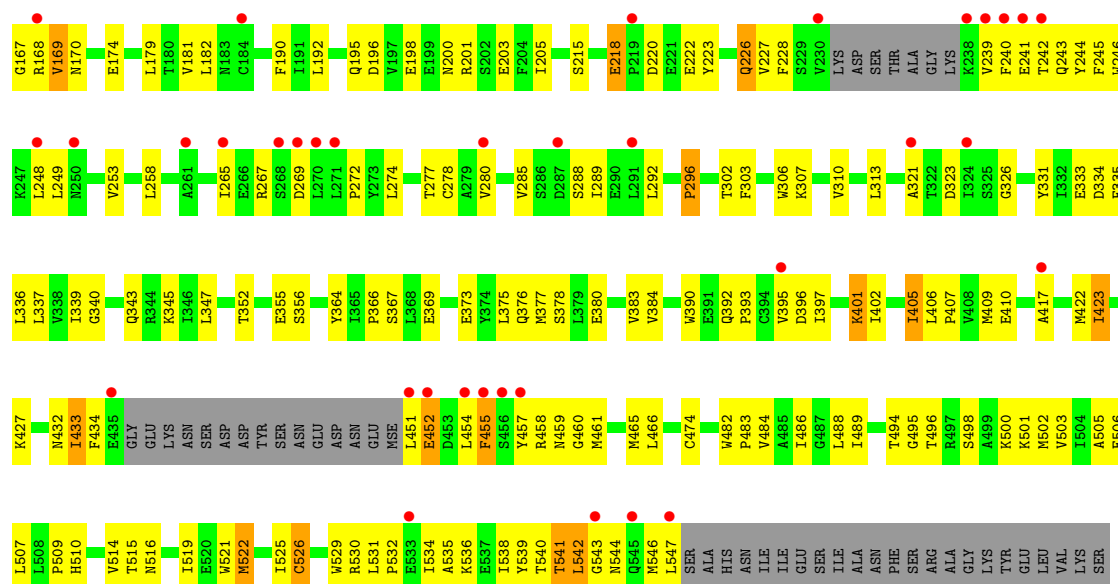


• Molecule 1: Nucleoporin SEH1

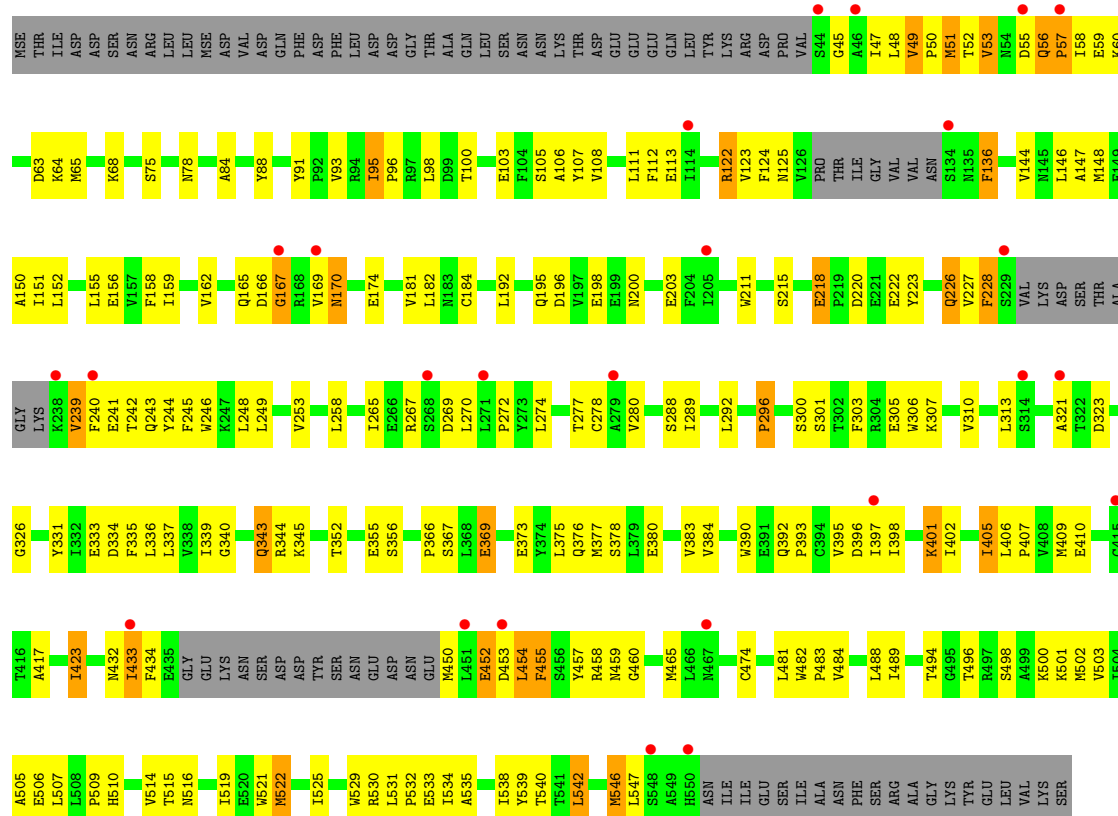


• Molecule 2: Nucleoporin NUP85



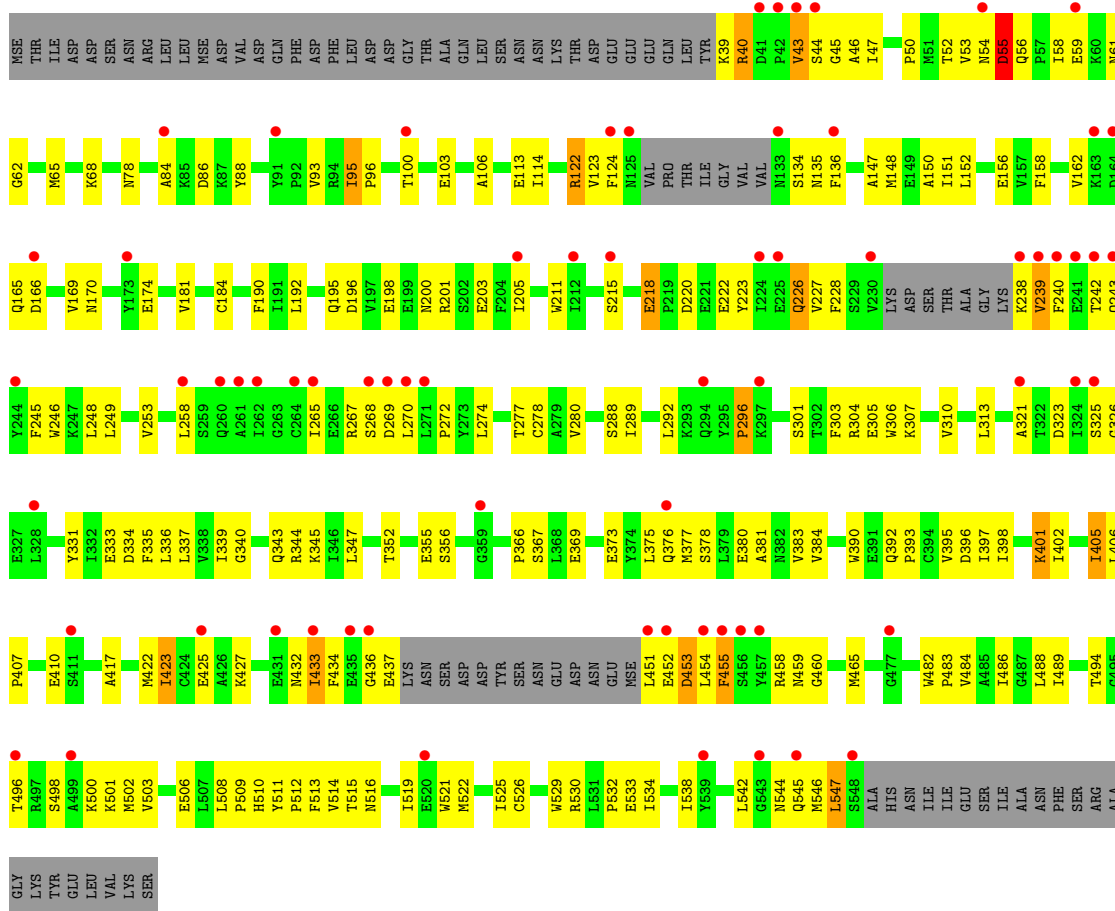


• Molecule 2: Nucleoporin NUP85

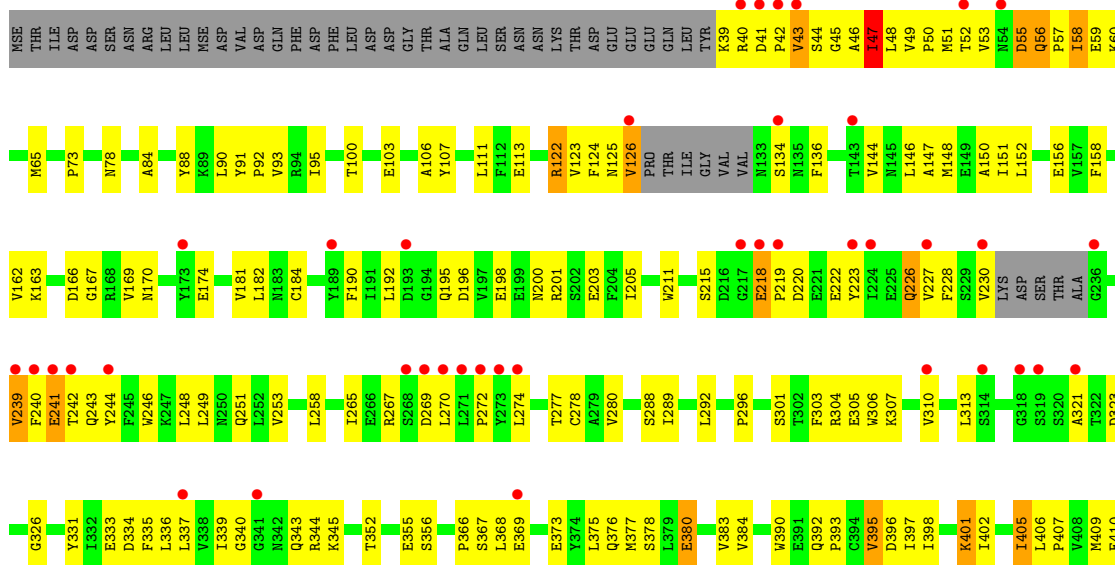


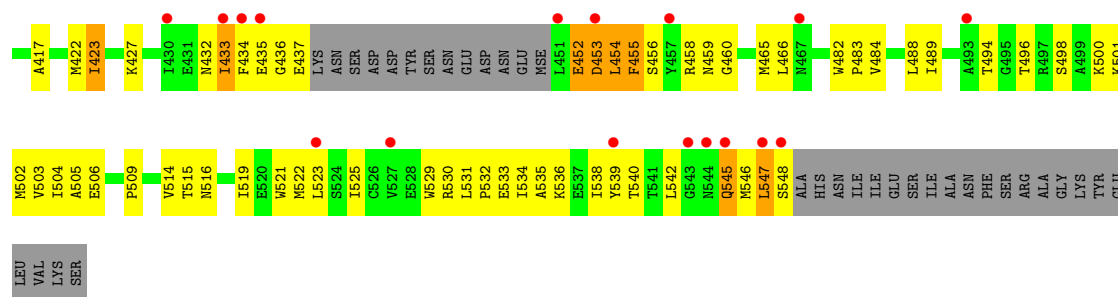
• Molecule 2: Nucleoporin NUP85



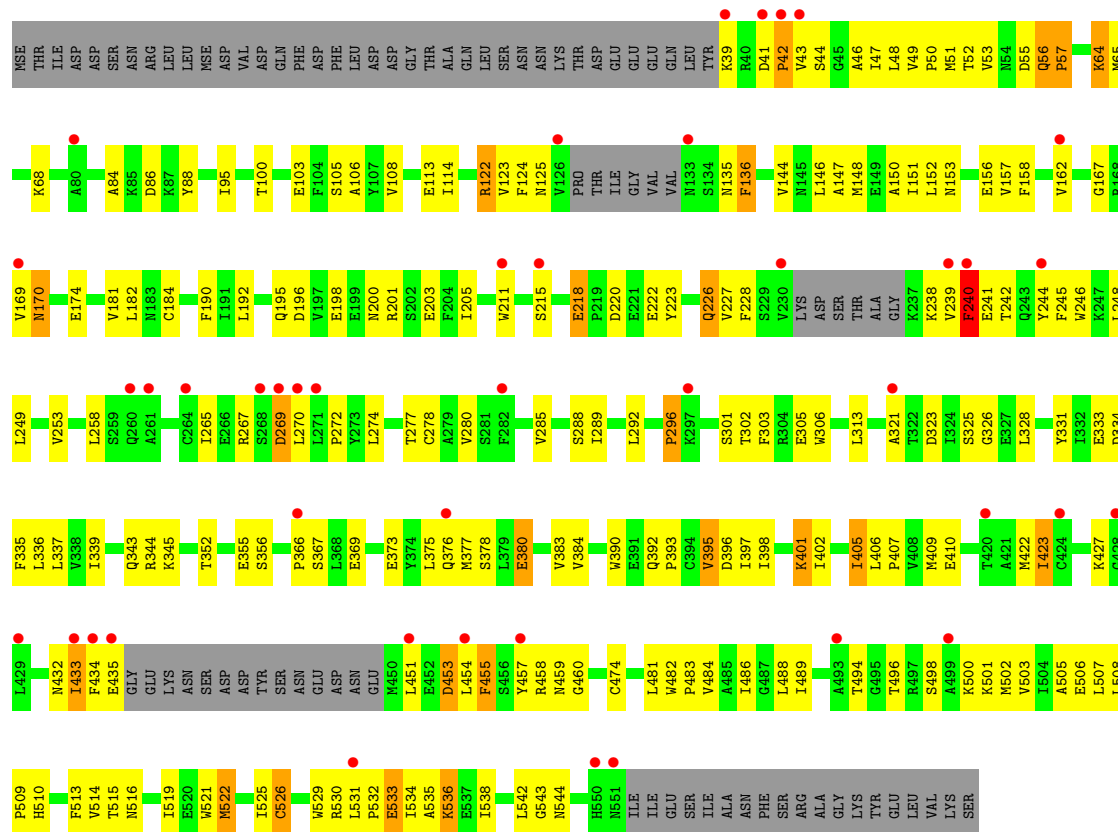


- Molecule 2: Nucleoporin NUP85

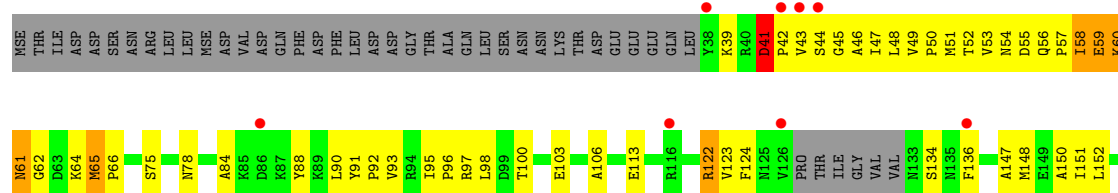




• Molecule 2: Nucleoporin NUP85



• Molecule 2: Nucleoporin NUP85





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	210.24Å 226.48Å 190.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.20 50.00 – 3.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-3.20) 86.5 (50.00-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.55 (at 3.19Å)	Xtrriage
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 ²)	62.6	Xtrriage
Anisotropy	0.754	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 31.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	37800	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtrriage'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.*

¹Intensities estimated from amplitudes.

²Theoretical 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	0.49	0/2463	1.02	15/3331 (0.5%)
1	B	0.51	0/2463	1.01	11/3331 (0.3%)
1	E	0.53	0/2463	1.02	13/3331 (0.4%)
1	F	0.51	0/2504	1.03	16/3390 (0.5%)
1	I	0.52	0/2494	1.03	15/3378 (0.4%)
1	J	0.53	1/2504 (0.0%)	1.03	15/3390 (0.4%)
2	C	0.50	0/3923	1.04	24/5289 (0.5%)
2	D	0.52	3/3902 (0.1%)	1.03	25/5260 (0.5%)
2	G	0.57	0/3942	1.04	22/5314 (0.4%)
2	H	0.56	0/3962	1.04	25/5340 (0.5%)
2	K	0.52	1/3977 (0.0%)	1.05	28/5361 (0.5%)
2	L	0.51	0/3941	1.04	22/5315 (0.4%)
All	All	0.52	5/38538 (0.0%)	1.03	231/52030 (0.4%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	343	GLN	CD-NE2	-5.67	1.21	1.33
2	K	510	HIS	CG-ND1	-5.61	1.32	1.38
2	D	510	HIS	CG-ND1	-5.50	1.32	1.38
2	D	343	GLN	CD-OE1	-5.50	1.13	1.23
1	J	164	HIS	CG-ND1	-5.12	1.32	1.38

All (231) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	226	GLN	N-CA-C	-9.54	101.77	113.50
2	G	55	ASP	N-CA-C	9.36	122.40	109.11
2	K	226	GLN	N-CA-C	-9.15	102.24	113.50
2	C	226	GLN	N-CA-C	-9.06	102.35	113.50
1	E	59	VAL	N-CA-C	9.05	119.04	110.53
1	B	59	VAL	N-CA-C	9.05	119.04	110.53
1	F	59	VAL	N-CA-C	9.04	119.03	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	226	GLN	N-CA-C	-9.03	102.39	113.50
2	L	226	GLN	N-CA-C	-8.94	102.50	113.50
2	H	269	ASP	N-CA-C	8.82	123.46	112.87
2	K	56	GLN	CA-C-N	8.79	130.83	119.84
2	K	56	GLN	C-N-CA	8.79	130.83	119.84
2	G	547	LEU	N-CA-C	-8.78	102.57	113.28
2	C	269	ASP	N-CA-C	8.75	123.36	112.87
1	I	59	VAL	N-CA-C	8.74	118.74	110.53
2	G	226	GLN	N-CA-C	-8.73	102.76	113.50
1	J	59	VAL	N-CA-C	8.72	118.73	110.53
2	L	269	ASP	N-CA-C	8.67	123.27	112.87
2	K	269	ASP	N-CA-C	8.63	123.37	113.01
2	G	269	ASP	N-CA-C	8.60	123.19	112.87
2	D	269	ASP	N-CA-C	8.43	123.13	113.01
2	G	288	SER	N-CA-C	-8.33	100.87	112.45
2	G	134	SER	N-CA-C	-8.28	102.74	113.17
2	K	288	SER	N-CA-C	-8.25	100.98	112.45
2	C	288	SER	N-CA-C	-8.23	101.01	112.45
2	C	56	GLN	CA-C-N	8.23	127.95	119.56
2	C	56	GLN	C-N-CA	8.23	127.95	119.56
2	H	288	SER	N-CA-C	-8.20	101.06	112.45
2	H	41	ASP	N-CA-C	8.14	115.31	108.07
2	K	55	ASP	N-CA-C	8.12	121.97	110.68
2	D	288	SER	N-CA-C	-8.11	101.18	112.45
2	L	288	SER	N-CA-C	-8.11	101.18	112.45
2	L	170	ASN	N-CA-C	-7.75	102.83	111.82
2	D	241	GLU	N-CA-C	-7.70	100.30	111.30
1	A	59	VAL	N-CA-C	7.69	118.49	110.72
2	L	241	GLU	N-CA-C	-7.48	102.39	112.94
2	D	56	GLN	CA-C-N	7.30	126.93	119.19
2	D	56	GLN	C-N-CA	7.30	126.93	119.19
1	I	163	ASN	N-CA-C	-7.29	104.01	113.12
2	D	167	GLY	N-CA-C	-7.22	102.46	112.13
2	H	241	GLU	N-CA-C	-7.19	102.53	113.89
2	K	170	ASN	N-CA-C	-7.15	103.48	111.71
2	K	531	LEU	CA-C-N	7.09	126.57	118.85
2	K	531	LEU	C-N-CA	7.09	126.57	118.85
2	H	455	PHE	N-CA-C	-7.07	95.74	110.80
1	I	162	ALA	N-CA-C	7.06	119.11	108.46
2	G	165	GLN	N-CA-C	7.03	119.97	111.40
2	D	228	PHE	N-CA-C	6.99	118.40	108.54
2	D	455	PHE	N-CA-C	-6.96	95.97	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	64	LYS	N-CA-C	-6.95	97.92	109.46
1	I	338	GLU	N-CA-C	-6.90	99.34	110.32
1	F	338	GLU	N-CA-C	-6.87	99.41	110.32
1	B	338	GLU	N-CA-C	-6.86	99.41	110.32
1	F	139	ALA	N-CA-C	-6.79	99.44	109.62
1	E	338	GLU	N-CA-C	-6.78	99.54	110.32
1	J	338	GLU	N-CA-C	-6.73	99.62	110.32
1	A	338	GLU	N-CA-C	-6.72	99.64	110.32
2	C	165	GLN	N-CA-C	-6.67	101.54	110.55
2	C	58	ILE	N-CA-C	6.65	117.87	108.36
2	C	169	VAL	N-CA-C	-6.63	104.38	113.00
1	E	139	ALA	N-CA-C	-6.62	99.70	109.62
2	L	166	ASP	N-CA-C	6.59	120.63	112.59
2	C	536	LYS	N-CA-C	-6.58	104.03	111.07
2	H	60	LYS	N-CA-C	6.55	119.01	111.02
2	D	218	GLU	N-CA-C	6.52	119.07	110.08
2	L	218	GLU	N-CA-C	6.51	119.06	110.08
2	H	56	GLN	N-CA-C	-6.50	101.87	109.93
2	K	455	PHE	N-CA-C	-6.45	97.06	110.80
2	H	47	ILE	N-CA-C	6.38	122.61	109.34
1	F	239	ARG	N-CA-C	6.36	119.83	109.59
2	H	218	GLU	N-CA-C	6.35	118.84	110.08
2	L	51	MSE	N-CA-C	-6.34	104.28	111.07
1	F	164	HIS	N-CA-C	-6.33	103.19	113.19
1	A	139	ALA	N-CA-C	-6.31	100.16	109.62
1	J	239	ARG	N-CA-C	6.31	119.75	109.59
2	C	218	GLU	N-CA-C	6.30	118.77	110.08
2	K	453	ASP	N-CA-C	-6.26	100.09	110.17
1	I	139	ALA	N-CA-C	-6.25	100.24	109.62
2	H	134	SER	N-CA-C	-6.24	105.63	113.18
2	H	540	THR	N-CA-C	-6.23	104.78	112.38
2	K	169	VAL	N-CA-C	-6.22	105.21	112.98
2	L	65	MSE	N-CA-C	6.21	120.25	109.82
1	B	139	ALA	N-CA-C	-6.20	100.32	109.62
2	L	433	ILE	N-CA-C	-6.16	107.29	113.20
1	B	348	GLN	N-CA-C	6.15	118.48	110.43
1	I	239	ARG	N-CA-C	6.13	119.45	109.59
2	C	167	GLY	N-CA-C	-6.11	103.94	112.13
2	C	135	ASN	N-CA-C	-6.11	105.79	113.18
2	G	218	GLU	N-CA-C	6.10	118.50	110.08
1	J	214	LEU	N-CA-C	6.09	119.44	110.30
2	K	218	GLU	N-CA-C	6.09	118.48	110.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	239	ARG	N-CA-C	6.05	119.33	109.59
1	J	139	ALA	N-CA-C	-6.03	100.57	109.62
2	D	49	VAL	N-CA-C	6.03	114.13	109.19
1	E	221	ALA	N-CA-C	5.99	117.36	109.93
2	L	136	PHE	N-CA-C	-5.99	104.75	111.28
2	D	170	ASN	N-CA-C	-5.98	104.89	111.82
1	J	221	ALA	N-CA-C	5.97	117.33	109.93
1	E	239	ARG	N-CA-C	5.97	119.20	109.59
2	K	326	GLY	N-CA-C	-5.97	105.37	113.37
2	H	454	LEU	N-CA-C	5.96	118.38	108.13
2	G	136	PHE	N-CA-C	-5.95	104.79	111.28
1	F	221	ALA	N-CA-C	5.94	117.29	109.93
2	D	136	PHE	N-CA-C	-5.92	104.83	111.28
2	K	136	PHE	N-CA-C	-5.90	104.85	111.28
2	C	455	PHE	N-CA-C	-5.89	98.26	110.80
2	D	106	ALA	N-CA-C	-5.89	104.22	111.40
1	A	40	LYS	N-CA-C	5.88	117.36	111.07
1	E	40	LYS	N-CA-C	5.88	117.36	111.07
2	G	455	PHE	N-CA-C	-5.88	98.28	110.80
1	A	2	GLN	CA-C-N	5.87	125.78	119.85
1	A	2	GLN	C-N-CA	5.87	125.78	119.85
2	L	455	PHE	N-CA-C	-5.86	98.31	110.80
2	H	136	PHE	N-CA-C	-5.85	104.90	111.28
2	G	134	SER	CB-CA-C	5.84	119.85	110.09
2	H	545	GLN	N-CA-C	5.84	117.51	111.03
2	C	136	PHE	N-CA-C	-5.83	104.92	111.28
2	G	135	ASN	N-CA-C	-5.83	106.17	113.28
2	L	106	ALA	N-CA-C	-5.82	104.30	111.40
2	K	135	ASN	N-CA-C	-5.81	106.19	113.28
1	E	2	GLN	N-CA-C	-5.80	100.58	109.64
1	J	40	LYS	N-CA-C	5.80	117.28	111.07
1	A	214	LEU	N-CA-C	5.80	119.00	110.30
2	L	326	GLY	N-CA-C	-5.79	105.36	112.77
1	E	240	ILE	N-CA-C	-5.79	100.09	108.36
2	L	267	ARG	N-CA-C	-5.78	107.47	114.75
2	D	326	GLY	N-CA-C	-5.78	105.38	112.77
1	A	239	ARG	N-CA-C	5.77	118.88	109.59
1	A	221	ALA	N-CA-C	5.76	117.07	109.93
1	E	11	LEU	N-CA-C	5.76	118.63	109.24
2	H	433	ILE	N-CA-C	-5.75	107.68	113.20
2	L	62	GLY	N-CA-C	-5.75	99.55	113.18
2	C	433	ILE	N-CA-C	-5.74	107.69	113.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	58	ILE	N-CA-C	5.73	117.37	109.46
2	H	106	ALA	N-CA-C	-5.73	104.41	111.40
2	G	47	ILE	N-CA-C	5.72	121.23	109.34
2	K	433	ILE	N-CA-C	-5.70	107.73	113.20
1	F	40	LYS	N-CA-C	5.70	117.16	111.07
2	C	106	ALA	N-CA-C	-5.69	104.46	111.40
2	G	106	ALA	N-CA-C	-5.68	104.47	111.40
1	I	214	LEU	N-CA-C	5.67	118.81	110.30
1	F	214	LEU	N-CA-C	5.67	118.80	110.30
1	J	2	GLN	CA-C-N	5.66	125.57	119.85
1	J	2	GLN	C-N-CA	5.66	125.57	119.85
1	A	240	ILE	N-CA-C	-5.65	100.28	108.36
2	C	326	GLY	N-CA-C	-5.59	105.61	112.77
2	H	326	GLY	N-CA-C	-5.59	105.88	113.37
2	K	106	ALA	N-CA-C	-5.59	104.58	111.40
2	C	95	ILE	CA-C-N	5.56	125.88	119.93
2	C	95	ILE	C-N-CA	5.56	125.88	119.93
1	E	214	LEU	N-CA-C	5.55	118.62	110.30
1	B	294	VAL	N-CA-C	5.53	115.86	108.11
2	K	410	GLU	N-CA-C	-5.53	105.79	112.54
2	C	410	GLU	N-CA-C	-5.53	105.80	112.54
1	F	240	ILE	N-CA-C	-5.53	100.45	108.36
1	B	40	LYS	N-CA-C	5.51	116.97	111.07
2	D	95	ILE	CA-C-N	5.51	125.82	119.93
2	D	95	ILE	C-N-CA	5.51	125.82	119.93
2	D	433	ILE	N-CA-C	-5.50	107.92	113.20
2	G	326	GLY	N-CA-C	-5.50	106.00	113.37
2	K	240	PHE	N-CA-C	-5.50	106.62	113.38
1	J	222	PRO	N-CA-C	-5.49	102.57	111.14
2	G	46	ALA	N-CA-C	5.48	115.26	108.19
2	C	134	SER	N-CA-C	-5.48	106.59	113.72
1	I	40	LYS	N-CA-C	5.48	116.93	111.07
2	L	167	GLY	N-CA-C	-5.46	106.08	113.24
2	K	57	PRO	N-CA-C	5.44	123.69	112.47
1	B	134	LEU	N-CA-C	-5.42	102.46	110.48
2	H	410	GLU	N-CA-C	-5.39	105.96	112.54
2	C	526	CYS	N-CA-C	-5.39	105.57	111.82
2	K	395	VAL	N-CA-C	-5.39	105.12	110.62
2	L	58	ILE	N-CA-C	5.39	116.14	107.73
2	L	537	GLU	N-CA-C	-5.38	105.52	111.71
1	J	240	ILE	N-CA-C	-5.38	100.67	108.36
1	J	158	SER	N-CA-C	-5.37	106.42	112.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	11	LEU	N-CA-C	5.37	117.99	109.24
2	D	57	PRO	N-CA-C	5.35	120.58	113.57
2	D	51	MSE	N-CA-C	-5.35	105.62	111.82
1	B	222	PRO	N-CA-C	-5.33	102.82	111.14
2	C	65	MSE	N-CA-C	5.33	118.78	109.82
2	H	55	ASP	N-CA-C	5.31	118.36	107.37
2	H	395	VAL	N-CA-C	-5.30	105.37	110.72
1	B	214	LEU	N-CA-C	5.29	118.23	110.30
2	G	526	CYS	N-CA-C	-5.28	105.70	111.82
2	C	57	PRO	N-CA-C	5.27	120.69	113.84
2	D	410	GLU	N-CA-C	-5.26	106.13	112.54
1	A	188	LEU	CB-CA-C	-5.25	110.09	117.23
1	I	294	VAL	N-CA-C	5.24	115.44	108.11
1	J	188	LEU	CB-CA-C	-5.24	110.11	117.23
1	A	222	PRO	N-CA-C	-5.23	102.98	111.14
1	A	294	VAL	N-CA-C	5.22	115.42	108.11
2	L	410	GLU	N-CA-C	-5.21	106.18	112.54
2	G	433	ILE	N-CA-C	-5.21	108.20	113.20
2	G	410	GLU	N-CA-C	-5.21	106.19	112.54
1	F	222	PRO	N-CA-C	-5.21	103.02	111.14
1	F	308	TRP	N-CA-C	5.20	118.78	112.23
2	D	454	LEU	N-CA-C	5.17	117.50	108.76
2	D	53	VAL	N-CA-C	5.16	115.82	110.82
2	K	95	ILE	CA-C-N	5.15	125.44	119.93
2	K	95	ILE	C-N-CA	5.15	125.44	119.93
1	F	134	LEU	N-CA-C	-5.15	102.86	110.48
1	A	226	ARG	N-CA-C	5.15	117.69	109.81
2	D	452	GLU	N-CA-C	5.13	118.01	107.69
1	I	240	ILE	N-CA-C	-5.13	101.02	108.36
1	J	294	VAL	N-CA-C	5.13	115.29	108.11
1	I	222	PRO	N-CA-C	-5.12	103.14	111.14
2	L	41	ASP	N-CA-C	-5.12	103.08	110.40
1	E	188	LEU	CB-CA-C	-5.12	110.27	117.23
1	F	11	LEU	N-CA-C	5.11	118.13	109.76
2	G	95	ILE	CA-C-N	5.09	125.38	119.93
2	G	95	ILE	C-N-CA	5.09	125.38	119.93
1	I	11	LEU	N-CA-C	5.09	118.11	109.76
1	F	188	LEU	CB-CA-C	-5.08	110.33	117.23
1	F	294	VAL	N-CA-C	5.07	115.20	108.11
2	H	380	GLU	N-CA-C	-5.07	105.84	111.36
2	G	425	GLU	N-CA-C	-5.06	105.84	111.36
2	L	395	VAL	N-CA-C	-5.06	105.61	110.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	95	ILE	CA-C-N	5.06	125.34	119.93
2	H	95	ILE	C-N-CA	5.06	125.34	119.93
1	E	222	PRO	N-CA-C	-5.04	103.28	111.14
1	A	134	LEU	N-CA-C	-5.04	103.02	110.48
1	B	240	ILE	N-CA-C	-5.04	101.16	108.36
2	K	536	LYS	N-CA-C	-5.04	105.48	110.97
1	E	15	VAL	N-CA-C	-5.03	100.82	108.17
1	I	188	LEU	CB-CA-C	-5.03	110.39	117.23
2	K	526	CYS	N-CA-C	-5.03	105.99	111.82
1	I	134	LEU	N-CA-C	-5.03	103.04	110.48
2	K	380	GLU	N-CA-C	-5.02	105.88	111.36
1	F	15	VAL	N-CA-C	-5.02	100.84	108.17
1	I	308	TRP	N-CA-C	5.00	118.53	112.23
2	D	369	GLU	N-CA-C	-5.00	106.69	112.89

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	140	0
1	B	2407	0	2343	143	0
1	E	2407	0	2343	119	0
1	F	2445	0	2380	129	0
1	I	2435	0	2372	127	0
1	J	2445	0	2380	152	0
2	C	3858	0	3806	187	0
2	D	3837	0	3780	187	0
2	G	3877	0	3820	185	0
2	H	3897	0	3845	201	0
2	K	3911	0	3860	182	0
2	L	3874	0	3820	184	0
All	All	37800	0	37092	1820	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 24.

All (1820) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:I:178:PHE:HB3	2:K:502:MSE:HE3	1.60	0.83
1:J:39:ASP:HB3	1:J:42:THR:HG22	1.58	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:78:ASP:OD1	1:A:80:THR:HG22	1.79	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: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
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:81:VAL:HG23	1:F:111:LEU:HD13	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:221:ALA:HB2	1:F:312:TRP:CE2	2.18	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:L:515:THR:HG22	2:L:516:ASN:N	2.02	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
1:J:159:ILE:C	1:J:161:PRO:HD2	2.14	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HB3	2:K:122:ARG:HH11	1.56	0.70
2:L:239:VAL:HG12	2:L:239:VAL:O	1.92	0.70
1:E:28:SER:HB3	1:E:30:ASP:OD1	1.92	0.70
1:E:314:LEU:HD12	1:E:314:LEU:O	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:48:LEU:HD12	2:H:49:VAL:N	2.07	0.70
2:H:181:VAL:CG1	2:H:405:ILE:HD11	2.22	0.70
2:H:334:ASP:OD2	2:H:345:LYS:HE3	1.91	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:HB3	2:C:122:ARG:HH11	1.57	0.69
2:D:122:ARG:HB3	2:D:122:ARG:HH11	1.58	0.69
2:C:39:LYS:O	2:C:39:LYS:HD3	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:HG3	1:J:226:ARG:HH11	1.58	0.68
2:K:383:VAL:HG12	2:K:384:VAL:H	1.58	0.68
1:A:226:ARG:HH11	1:A:226:ARG:HG3	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
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:F:226:ARG:HH11	1:F:226:ARG:HG3	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:HH11	1:I:226:ARG:HG3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:OD1	2:L:41:ASP:N	2.29	0.66
1:A:8:HIS:ND1	1:A:28:SER:HB3	2.09	0.66
2:G:122:ARG:HH11	2:G:122:ARG:CB	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
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:O	2:H:148:MSE:HE3	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:51:MSE:HE3	2:D:91:TYR:CD2	2.31	0.66
2:D:63:ASP:O	2:D:65:MSE:HG3	1.95	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
1:E:158:SER:C	1:E:159:ILE:HG13	2.21	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:HD12	1:I:314:LEU:O	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HH11	2:K:122:ARG:CB	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
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:HH11	2:C:122:ARG:CB	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
2:D:453:ASP:C	2:D:454:LEU:HD23	2.23	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:HH11	2:D:122:ARG:CB	2.11	0.63
2:C:122:ARG:HB3	2:C:122:ARG:NH1	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
1:J:178:PHE:CB	2:L:502:MSE:HE3	2.28	0.63
2:K:122:ARG:HB3	2:K:122:ARG:NH1	2.13	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:313:LEU:C	2:C:313:LEU:HD23	2.23	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:HD12	1:A:314:LEU:O	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:24:VAL:HG23	1:J:45:TRP:CZ3	2.34	0.62
1:J:81:VAL:CG2	1:J:111:LEU:HD13	2.27	0.62
2:L:453:ASP:O	2:L:454:LEU:HD23	2.00	0.62
1:J:314:LEU:O	1:J:314:LEU:HD12	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:K:313:LEU:C	2:K:313:LEU:HD23	2.25	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:A:178:PHE:CB	2:C:502:MSE:HE3	2.27	0.62
1:B:313:ASN:HD22	1:B:317:THR:HB	1.65	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
2:G:220:ASP:OD2	2:G:222:GLU:HB3	2.00	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:238:GLY:HA2	1:B:305:GLY:O	2.00	0.61
2:D:122:ARG:HB3	2:D:122:ARG:NH1	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:48:LEU:HD12	2:H:49:VAL:H	1.65	0.61
2:H:220:ASP:OD2	2:H:222:GLU:HB3	2.00	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
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:52:THR:HG22	2:K:53:VAL:N	2.15	0.61
2:K:148:MSE:O	2:K:148:MSE:HE3	1.99	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: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:L:313:LEU:HD23	2:L:313:LEU:C	2.26	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:96:ARG:HH21	1:E:9:ASP:HB2	1.66	0.60
2:C:148:MSE:O	2:C:148:MSE:HE3	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:E:314:LEU:HD12	1:E:314:LEU:C	2.27	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:453:ASP:C	2:H:454:LEU:HG	2.27	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:G:313:LEU:HD23	2:G:313:LEU:C	2.27	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
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:39:LYS:HZ1	2:L:97:ARG:HG2	1.66	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:52:THR:CG2	2:H:53:VAL:N	2.65	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:417:ALA:HB1	2:H:465:MSE:HE1	1.85	0.59
2:K:506:GLU:O	2:K:509:PRO:HD2	2.02	0.59
1:B:55:ASP:HB3	1:E:99:ASN:OD1	2.02	0.59
2:C:451:LEU:HG	2:C:452:GLU:N	2.11	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:K:240:PHE:HB2	2:K:269:ASP:CG	2.27	0.59
2:H:383:VAL:HG12	2:H:384:VAL:N	2.17	0.59
2:L:42:PRO:C	2:L:44:SER:H	2.10	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:13:HIS:HE2	1:E:29:SER:HG	1.51	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
1:F:125:LEU:C	1:F:125:LEU:HD12	2.29	0.58
2:H:356:SER:HB2	2:H:378:SER:OG	2.04	0.58
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:81:VAL:HG23	1:J:111:LEU:CD1	2.32	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O	2:C:455:PHE:CG	2.57	0.58
2:D:148:MSE:HE2	2:D:152:LEU:HG	1.86	0.58
2:G:39:LYS:HG3	2:G:40:ARG:N	2.18	0.58
2:G:242:THR:HG22	2:G:243:GLN: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:13:HIS:HE2	1:F:29:SER:HG	1.51	0.57
1:F:76:SER:HB3	1:F:78:ASP:OD1	2.03	0.57
1:F:118:PRO:HG2	1:F:174:CYS:O	2.03	0.57
1:F:120:HIS:CE1	1:F:177:ARG:HA	2.40	0.57
1:F:159:ILE:O	1:F:161:PRO:CD	2.52	0.57
2:G:437:GLU:CG	2:H:304:ARG:HH12	2.13	0.57
2:H:200:ASN:OD1	2:H:203:GLU:HB2	2.04	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
1:I:314:LEU:HD12	1:I:314:LEU:C	2.30	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:505:ALA:HA	2:D:534:ILE:HD13	1.85	0.57
2:L:521:TRP:CE2	2:L:525:ILE:HD11	2.40	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
2:K:43:VAL:O	2:K:43:VAL:HG12	2.05	0.57
1:E:24:VAL:HG23	1:E:45:TRP:CZ3	2.40	0.57
1:E:313:ASN:HB2	1:E:318:ILE:H	1.69	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:B:77:TYR:C	1:B:79:LYS:H	2.12	0.57
1:F:131:ASP:OD2	1:F:135:ARG:NH2	2.38	0.57
2:H:313:LEU:C	2:H:313:LEU:HD23	2.30	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:CB	2:D:459:ASN:ND2	2.66	0.57
2:D:454:LEU:CD2	2:D:458:ARG:HD2	2.35	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
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
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: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
1:J:68:TYR:CG	1:J:123:LEU:HD13	2.41	0.56
1:J:125:LEU:HD12	1:J:125:LEU:C	2.30	0.56
2:C:521:TRP:CZ2	2:C:525:ILE:HD11	2.41	0.56
1:J:8:HIS:ND1	1:J:28:SER:HB3	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:131:ASP:OD2	1:J:135:ARG:NH2	2.38	0.56
2:K:383:VAL:HG12	2:K:384:VAL:N	2.20	0.56
1:A:29:SER:C	1:A:31:GLN:H	2.13	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: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:E:125:LEU:C	1:E:125:LEU:HD12	2.30	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:29:SER:C	1:E:31:GLN:H	2.14	0.56
1:F:81:VAL:CG2	1:F:111:LEU:HD13	2.36	0.56
1:F:179:SER:OG	1:F:180:PRO:HD2	2.06	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
2:D:313:LEU:HD23	2:D:313:LEU:C	2.31	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:436:GLY:O	2:H:437:GLU:C	2.49	0.56
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
1:A:13:HIS:HE2	1:A:29:SER:HG	1.55	0.55
2:C:546:MSE:HA	2:C:546:MSE:HE2	1.88	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:F:314:LEU:HD12	1:F:314:LEU:C	2.31	0.55
2:L:148:MSE:HE2	2:L:152:LEU:HG	1.87	0.55
1:A:314:LEU:HD12	1:A:314:LEU:C	2.31	0.55
1:B:128:LEU:HD23	1:B:169:PHE:HB3	1.88	0.55
1:B:137:TYR:CZ	1:B:150:LEU:HD13	2.41	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:I:29:SER:C	1:I:31:GLN:H	2.14	0.55
1:A:77:TYR:C	1:A:79:LYS:H	2.14	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:29:SER:C	1:F:31:GLN:H	2.14	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
1:J:335:TYR:CZ	2:L:457:TYR:HA	2.42	0.55
2:K:39:LYS:HD2	2:K:47:ILE:HG21	1.89	0.55
1:B:236:LYS:HG3	1:B:306:GLU:OE1	2.07	0.55
2:H:546:MSE:C	2:H:548:SER:N	2.64	0.55
1:I:125:LEU:C	1:I:125:LEU:HD12	2.32	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:J:29:SER:C	1:J:31:GLN:H	2.14	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
1:F:8:HIS:ND1	1:F:28:SER:HB3	2.22	0.54
2:G:58:ILE:CG2	2:G:59:GLU:N	2.70	0.54
2:G:522:MSE:HE1	2:G:538:ILE:HD12	1.88	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:23:HIS:CE1	1:F:70:ARG:HH22	2.26	0.54
1:F:338:GLU:HG3	1:F:339:PHE:N	2.22	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:23:HIS:CE1	1:I:70:ARG:HH22	2.25	0.54
1:I:134:LEU:HD23	1:I:135:ARG:N	2.21	0.54
2:L:544:ASN:C	2:L:545:GLN:HG3	2.33	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:77:TYR:C	1:I:79:LYS:H	2.14	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:CG	2:L:455:PHE:O	2.59	0.54
1:A:239:ARG:HH11	1:A:239:ARG:HG3	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:I:336:SER:HB3	2:L:373:GLU:HG2	1.88	0.54
1:J:1:MSE:HB3	2:L:92:PRO:O	2.08	0.54
1:J:236:LYS:HG3	1:J:306:GLU:OE1	2.07	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: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
1:J:13:HIS:HE2	1:J:29:SER:HG	1.55	0.54
1:J:77:TYR:C	1:J:79:LYS:H	2.15	0.54
2:K:105:SER:HB2	2:K:481:LEU:HD21	1.89	0.54
2:K:125:ASN:HB2	2:K:136:PHE:HE2	1.71	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:523:LEU:HD13	2:H:539:TYR:OH	2.08	0.54
1:I:65:SER:HB2	1:I:119:ALA:HB2	1.90	0.54
1:I:241:ARG:HG2	1:I:299:GLU:HG3	1.88	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:29:SER:C	1:B:31:GLN:H	2.14	0.54
1:B:136:LEU:HD11	1:B:202:LEU:HD11	1.89	0.54
2:C:433:ILE:O	2:C:433:ILE:HG22	2.07	0.54
1:E:2:GLN:HG3	1:E:2:GLN: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
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
1:J:348:GLN:HB3	2:L:60:LYS:HG3	1.90	0.54
2:L:148:MSE:HE3	2:L:152:LEU:HG	1.89	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:125:LEU:C	1:A:125:LEU:HD12	2.32	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
1:F:77:TYR:C	1:F:79:LYS:H	2.16	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:HG3	1:E:239:ARG:HH11	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:C:44:SER:C	2:C:46:ALA:H	2.16	0.53
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:SER:HB2	1:B:119:ALA:HB2	1.89	0.53
1:E:77:TYR:C	1:E:79:LYS:H	2.17	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:J:314:LEU:HD12	1:J:314:LEU:C	2.33	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:47:ILE:HD11	2:L:97:ARG:NE	2.24	0.53
2:L:433:ILE:HG22	2:L:433:ILE:O	2.08	0.53
2:D:433:ILE:HG22	2:D:433:ILE:O	2.08	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:39:ASP:CB	1:I:42:THR:HG22	2.34	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:J:239:ARG:HG3	1:J:239:ARG:HH11	1.74	0.53
1:B:125:LEU:HD12	1:B:125:LEU:C	2.34	0.53
2:C:496:THR:HG22	2:C:498:SER:H	1.73	0.53
1:F:239:ARG:HH11	1:F:239:ARG:HG3	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
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
2:D:47:ILE:HG22	2:D:48:LEU:N	2.23	0.52
2:D:432:ASN:HB2	2:D:460:GLY:CA	2.38	0.52
2:H:39:LYS:HD3	2:H:50:PRO:HD3	1.91	0.52
2:K:239:VAL:O	2:K:239:VAL:HG12	2.09	0.52
1:A:236:LYS:HG3	1:A:306:GLU:CD	2.35	0.52
1:A:324:ASP:C	1:A:326:GLY:H	2.17	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:521:TRP:CE2	2:C:525:ILE:HD11	2.44	0.52
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: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:49:VAL:CG1	2:D:50:PRO:HD2	2.39	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:H:367:SER:C	2:H:369:GLU:H	2.17	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:O	2:H:227:VAL:HG12	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:B:130:ASN:C	1:B:132:GLY:H	2.18	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:K:433:ILE:O	2:K:433:ILE:HG22	2.09	0.52
2:L:249:LEU:O	2:L:253:VAL:HG23	2.10	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
1:J:153:GLU:C	1:J:154:MSE:HG2	2.35	0.52
2:K:454:LEU:CB	2:K:459:ASN:HD21	2.19	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
1:J:324:ASP:C	1:J:326:GLY:H	2.18	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
2:L:42:PRO:C	2:L:44:SER:N	2.66	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:177:ARG:NH1	2:C:534:ILE:HD11	2.25	0.51
2:C:148:MSE:HE3	2:C:152:LEU:HG	1.92	0.51
2:G:432:ASN:HB2	2:G:460:GLY:CA	2.40	0.51
1:I:130:ASN:C	1:I:132:GLY:H	2.19	0.51
1:J:16:VAL:HG12	1:J:63:TRP:HD1	1.75	0.51
1:B:314:LEU:HD12	1:B:314:LEU:C	2.35	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:L:367:SER:C	2:L:369:GLU:H	2.18	0.51
1:E:179:SER:OG	1:E:180:PRO:HD2	2.10	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
1:A:94:SER:C	1:A:96:ARG:H	2.18	0.51
1:F:153:GLU:C	1:F:154:MSE:HG2	2.35	0.51
2:G:335:PHE:CE2	2:G:339:ILE:HD11	2.45	0.51
2:L:55:ASP:O	2:L:56:GLN:C	2.51	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
1:I:81:VAL:HG23	1:I:111:LEU:CD1	2.34	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:59:VAL:HG21	1:B:77:TYR:CE1	2.46	0.51
1:E:239:ARG:HG3	1:E:239:ARG:NH1	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:F:130:ASN:C	1:F:132:GLY:H	2.19	0.51
1:I:10:ASP:OD1	1:I:11:LEU:HD23	2.10	0.51
1:J:130:ASN:C	1:J:132:GLY:H	2.18	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
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:B:324:ASP:C	1:B:326:GLY:H	2.20	0.50
1:F:159:ILE:O	1:F:161:PRO:HD2	2.11	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:I:324:ASP:C	1:I:326:GLY:H	2.18	0.50
1:B:239:ARG:HG3	1:B:239:ARG:HH11	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
1:E:183:LEU:C	1:E:183:LEU:HD12	2.36	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:52:THR:CG2	2:K:53:VAL:N	2.74	0.50
2:K:215:SER:HB2	2:K:390:TRP:CZ2	2.46	0.50
1:A:193:ILE:CD1	1:A:245:ILE:HD13	2.42	0.50
2:C:248:LEU:O	2:C:248:LEU:HD13	2.10	0.50
2:G:43:VAL:HG12	2:G:44:SER:N	2.27	0.50
2:G:215:SER:HB2	2:G:390:TRP:CZ2	2.46	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
1:A:178:PHE:HZ	2:C:505:ALA:CB	2.25	0.50
2:C:40:ARG:CB	2:C:40:ARG:NH1	2.75	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:113:GLU:OE1	2:C:113:GLU:HA	2.10	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
1:B:153:GLU:C	1:B:154:MSE:HG2	2.37	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:D:539:TYR:O	2:D:540:THR:C	2.54	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
2:L:215:SER:HB2	2:L:390:TRP:CZ2	2.47	0.50
1:I:239:ARG:HG3	1:I:239:ARG:NH1	2.27	0.49
1:I:347:ALA:HB2	2:K:51:MSE:CE	2.42	0.49
1:J:128:LEU:HD22	1:J:185:VAL:HG13	1.94	0.49
2:L:39:LYS:CE	2:L:170:ASN:OD1	2.59	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
2:L:227:VAL:O	2:L:227:VAL:HG12	2.13	0.49
1:B:96:ARG:HH21	1:E:9:ASP:CB	2.24	0.49
1:E:156:VAL:HG13	1:E:192:ILE:HD11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HG3	1:F:239:ARG:NH1	2.26	0.49
2:H:546:MSE:O	2:H:547:LEU:C	2.55	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:236:LYS:HG3	1:J:306:GLU:CD	2.37	0.49
1:A:128:LEU:HD22	1:A:185:VAL:HG13	1.94	0.49
1:A:297:LEU:HD11	1:A:337:ASN:ND2	2.27	0.49
1:A:335:TYR:CE1	2:C:457:TYR:HA	2.48	0.49
2:C:367:SER:C	2:C:369:GLU:H	2.21	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:43:VAL:HG12	2:H:44:SER:N	2.28	0.49
2:H:148:MSE:HE3	2:H:152:LEU:HG	1.91	0.49
1:J:162:ALA:C	1:J:164:HIS:H	2.21	0.49
2:K:227:VAL:O	2:K:227:VAL:HG12	2.12	0.49
1:A:130:ASN:C	1:A:132:GLY:H	2.20	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: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
2:D:367:SER:C	2:D:369:GLU:H	2.21	0.49
1:E:128:LEU:HD23	1:E:169:PHE:HB3	1.95	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:HG22	2:C:100:THR:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:192:LEU:O	2:D:195:GLN:HB2	2.13	0.48
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:A:67:GLU:HA	2:C:541:THR:OG1	2.12	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
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:61:ASN:O	2:G:62:GLY:C	2.55	0.48
2:G:113:GLU:OE1	2:G:113:GLU:HA	2.13	0.48
2:H:57:PRO:HB3	2:H:91:TYR:OH	2.13	0.48
1:I:10:ASP:H	1:I:30:ASP:HB3	1.77	0.48
1:I:179:SER:OG	1:I:180:PRO:HD2	2.13	0.48
2:K:526:CYS:SG	2:K:535:ALA:HB2	2.53	0.48
1:A:128:LEU:HD23	1:A:169:PHE:HB3	1.95	0.48
1:B:347:ALA:HB3	2:D:58:ILE:HD12	1.95	0.48
2:L:42:PRO:HD3	2:L:48:LEU:HD11	1.95	0.48
2:L:113:GLU:HA	2:L:113:GLU:OE1	2.14	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
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:J:34:LYS:HG2	1:J:50:SER:HB2	1.96	0.48
1:J:297:LEU:HD11	1:J:337:ASN:ND2	2.29	0.48
1:B:183:LEU:C	1:B:183:LEU:HD12	2.39	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:501:LYS:HE3	2:D:529:TRP:O	2.14	0.48
2:D:521:TRP:O	2:D:525:ILE:HG13	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
1:E:153:GLU:C	1:E:154:MSE:HG2	2.39	0.48
2:H:243:GLN:O	2:H:244:TYR:C	2.56	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:B:54:HIS:CD2	1:B:58:ILE:HG12	2.49	0.47
1:B:236:LYS:HG3	1:B:306:GLU:CD	2.39	0.47
2:D:434:PHE:CE1	2:D:457:TYR:HE2	2.32	0.47
1:E:130:ASN:C	1:E:132:GLY:H	2.21	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:HD23	2:C:313:LEU:O	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: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
2:C:168:ARG:C	2:C:170:ASN:H	2.22	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
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:I:183:LEU:C	1:I:183:LEU:HD12	2.39	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:97:ARG:HG3	1:B:97:ARG:HH11	1.79	0.47
2:D:169:VAL:O	2:D:169:VAL:HG12	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
1:J:178:PHE:HZ	2:L:505:ALA:CB	2.27	0.47
2:L:454:LEU:HD13	2:L:459:ASN:ND2	2.29	0.47
2:C:530:ARG:C	2:C:532:PRO:HD3	2.38	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:453:ASP:O	2:G:454:LEU:HD23	2.15	0.47
2:G:454:LEU:CB	2:G:459:ASN:OD1	2.63	0.47
1:J:65:SER:CB	1:J:119:ALA:HB2	2.43	0.47
1:A:226:ARG:HH11	1:A:226:ARG:CG	2.26	0.47
1:F:10:ASP:H	1:F:30:ASP:HB3	1.80	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:183:LEU:C	1:F:183:LEU:HD12	2.39	0.47
1:F:191:ALA:HB2	1:F:215:ILE:CD1	2.45	0.47
1:F:324:ASP:C	1:F:326:GLY:H	2.23	0.47
2:G:148:MSE:HE3	2:G:152:LEU:HG	1.96	0.47
2:H:215:SER:HB2	2:H:390:TRP:CH2	2.49	0.47
2:H:249:LEU:O	2:H:253:VAL:HG23	2.15	0.47
1:I:59:VAL:HG21	1:I:77:TYR:CE1	2.49	0.47
1:I:191:ALA:HB2	1:I:215:ILE:CD1	2.44	0.47
2:K:367:SER:C	2:K:369:GLU:H	2.22	0.47
2:K:422:MSE:C	2:K:422:MSE:SE	3.08	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
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
1:E:324:ASP:C	1:E:326:GLY:H	2.22	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
2:K:113:GLU:OE1	2:K:113:GLU:HA	2.13	0.47
2:K:373:GLU:O	2:K:377:MSE:HG3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:192:LEU:O	2:L:195:GLN:HB2	2.14	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:65:MSE:HE2	2:G:84:ALA:HB1	1.97	0.47
2:G:215:SER:HB2	2:G:390:TRP:CH2	2.50	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:97:ARG:HH11	1:I:97:ARG:HG3	1.80	0.47
1:I:297:LEU:HD11	1:I:337:ASN:ND2	2.30	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
2:C:278:CYS:CB	2:C:323:ASP:HB2	2.45	0.46
1:E:10:ASP:O	2:G:88:TYR:CE1	2.69	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: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
2:H:52:THR:HB	2:H:56:GLN:OE1	2.15	0.46
2:H:248:LEU:HD13	2:H:248:LEU:O	2.14	0.46
1:I:193:ILE:HD13	1:I:245:ILE:HD13	1.97	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:248:LEU:HD13	2:C:248:LEU:C	2.41	0.46
2:D:103:GLU:CD	2:D:103:GLU:H	2.24	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
1:A:153:GLU:C	1:A:154:MSE:HG2	2.40	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:HG3	1:E:226:ARG:NH1	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:HG2	2:H:452:GLU:O	2.16	0.46
1:I:196:ARG:HH11	1:I:202:LEU:CD2	2.28	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:A:324:ASP:C	1:A:326:GLY:N	2.74	0.46
1:B:153:GLU:O	1:B:154:MSE:HE3	2.15	0.46
2:C:166:ASP:CG	2:C:166:ASP:O	2.58	0.46
2:D:393:PRO:O	2:D:397:ILE:HG13	2.16	0.46
2:H:158:PHE:O	2:H:162:VAL:HG23	2.16	0.46
1:I:153:GLU:C	1:I:154:MSE:HG2	2.40	0.46
1:A:218:ILE:O	1:A:218:ILE:HG13	2.15	0.46
2:H:42:PRO:HA	2:H:46:ALA:C	2.41	0.46
2:H:47:ILE:HG22	2:H:48:LEU:H	1.75	0.46
2:H:103:GLU:H	2:H:103:GLU:CD	2.23	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:248:LEU:HD13	2:K:248:LEU:C	2.40	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:HD23	2:K:313:LEU:O	2.16	0.46
1:F:180:PRO:HG2	1:F:182:LYS:NZ	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:348:GLN:OE1	2:D:60:LYS:HA	2.16	0.46
2:C:222:GLU:O	2:C:226:GLN:HG3	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:171:LEU:HD23	1:A:185:VAL:HG22	1.98	0.45
1:A:177:ARG:NH1	2:C:534:ILE:CD1	2.79	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:N	1:F:227:TRP:CE3	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:29:SER:HA	1:E:57:SER:HA	1.98	0.45
1:E:191:ALA:HB2	1:E:215:ILE:CD1	2.46	0.45
1:I:183:LEU:HD12	1:I:183:LEU:O	2.15	0.45
2:K:52:THR:HB	2:K:56:GLN:CG	2.44	0.45
2:K:223:TYR:O	2:K:227:VAL:HG23	2.15	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:C:541:THR:O	2:C:542:LEU:C	2.58	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:97:ARG:HH11	1:F:97:ARG:HG3	1.81	0.45
1:F:236:LYS:HG3	1:F:306:GLU:OE1	2.16	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:HG3	1:A:226:ARG:NH1	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:278:CYS:CB	2:D:323:ASP:HB2	2.47	0.45
2:D:313:LEU:HD22	2:D:336:LEU:HD22	1.99	0.45
1:F:99:ASN:OD1	1:I:55:ASP:HB3	2.17	0.45
2:G:511:TYR:HA	2:G:512:PRO:HD3	1.80	0.45
1:J:226:ARG:HG3	1:J:226:ARG:NH1	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:O	2:D:455:PHE:CD2	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:HH11	1:A:97:ARG:HG3	1.82	0.45
2:G:367:SER:C	2:G:369:GLU:H	2.24	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
1:J:157:LEU:C	1:J:159:ILE:N	2.73	0.45
2:K:148:MSE:HE3	2:K:152:LEU:HG	1.95	0.45
2:L:541:THR:O	2:L:542:LEU:C	2.59	0.45
1:B:180:PRO:HG2	1:B:182:LYS:NZ	2.32	0.45
1:B:247:GLU:HB3	1:B:292:LEU:CD2	2.38	0.45
2:C:168:ARG:C	2:C:170:ASN:N	2.73	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:K:103:GLU:H	2:K:103:GLU:CD	2.25	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:J:178:PHE:CG	2:L:502:MSE:HG2	2.52	0.45
1:J:183:LEU:C	1:J:183:LEU:HD12	2.41	0.45
1:J:324:ASP:C	1:J:326:GLY:N	2.75	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
1:B:218:ILE:O	1:B:218:ILE:HG13	2.16	0.44
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
2:G:248:LEU:HD13	2:G:248:LEU:C	2.42	0.44
1:J:210:GLY:C	1:J:241:ARG:NH1	2.75	0.44
1:A:183:LEU:C	1:A:183:LEU:HD12	2.41	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
2:H:545:GLN:C	2:H:547:LEU:N	2.75	0.44
1:I:309:SER:HB3	2:K:68:LYS:HA	1.99	0.44
1:I:324:ASP:C	1:I:326:GLY:N	2.75	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: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
1:I:236:LYS:HG3	1:I:306:GLU:CD	2.43	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:HE3	2:G:39:LYS:HB2	1.66	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:54:HIS:CE1	1:A:80:THR:HG23	2.52	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
2:D:270:LEU:O	2:D:274:LEU:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:29:SER:HA	1:B:57:SER:HA	2.00	0.44
1:B:309:SER:HB3	2:D:68:LYS: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
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:G:196:ASP:C	2:G:198:GLU:N	2.75	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
1:J:63:TRP:C	1:J:116:PHE:CD2	2.96	0.44
2:K:200:ASN:CG	2:K:203:GLU:HB2	2.42	0.44
2:K:455:PHE:O	2:K:455:PHE:CD2	2.71	0.44
2:L:103:GLU:CD	2:L:103:GLU:H	2.26	0.44
1:A:29:SER:HA	1:A:57:SER:HA	2.00	0.44
1:A:157:LEU:HD23	1:A:157:LEU:HA	1.86	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:A:309:SER:HB3	2:C:68:LYS:HA	1.99	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:196:ASP:C	2:C:198:GLU:N	2.75	0.44
2:C:373:GLU:O	2:C:377:MSE:HG3	2.18	0.44
2:D:57:PRO:HB3	2:D:91:TYR:OH	2.17	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
1:E:81:VAL:HG23	1:E:111:LEU:CD1	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:153:GLU:O	1:E:154:MSE:HE3	2.18	0.44
1:F:114:VAL:HG22	1:F:127:CYS:HB3	1.99	0.44
2:G:103:GLU:CD	2:G:103:GLU:H	2.25	0.44
2:H:50:PRO:HB2	2:H:52:THR:O	2.17	0.44
2:H:196:ASP:C	2:H:198:GLU:N	2.76	0.44
1:J:10:ASP:H	1:J:30:ASP:HB3	1.83	0.44
1:J:29:SER:HA	1:J:57:SER:HA	2.00	0.44
1:J:114:VAL:HG22	1:J:127:CYS:HB3	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:HD12	1:F:183:LEU:O	2.18	0.44
2:H:222:GLU:O	2:H:226:GLN:HG3	2.17	0.44
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:68:TYR:OH	1:J:122:GLY:CA	2.64	0.43
1:J:183:LEU:HD12	1:J:183:LEU:O	2.18	0.43
2:K:49:VAL:HA	2:K:50:PRO:HD3	1.73	0.43
2:K:246:TRP:CE2	2:K:331:TYR:HB3	2.52	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
1:B:324:ASP:C	1:B:326:GLY:N	2.77	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:227:VAL:C	2:G:228:PHE:HD1	2.25	0.43
2:G:245:PHE:CD1	2:G:245:PHE:C	2.96	0.43
2:G:313:LEU:HD23	2:G:313:LEU:O	2.17	0.43
1:I:34:LYS:HG2	1:I:50:SER:HB2	2.00	0.43
1:I:94:SER:C	1:I:96:ARG:H	2.26	0.43
1:J:54:HIS:CD2	1:J:58:ILE:HG12	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:332:LYS:HG3	1:J:342:MSE:SE	2.68	0.43
2:K:238:LYS:HB2	2:K:241:GLU:HG3	2.00	0.43
2:L:541:THR:C	2:L:543:GLY:N	2.77	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:D:406:LEU:O	2:D:407:PRO:C	2.60	0.43
2:G:515:THR:O	2:G:519:ILE:HG13	2.18	0.43
2:H:455:PHE:O	2:H:455:PHE:CD2	2.72	0.43
1:I:64:ALA:HB3	1:I:71:ILE:HB	2.00	0.43
2:L:47:ILE:HG22	2:L:48:LEU:N	2.33	0.43
2:L:313:LEU:HD22	2:L:336:LEU:HD22	1.99	0.43
1:A:71:ILE:HD11	1:A:145:LEU:HD13	1.99	0.43
1:B:64:ALA:HB2	1:B:116:PHE:CE2	2.53	0.43
2:D:63:ASP:O	2:D:64:LYS:C	2.59	0.43
1:E:178:PHE:CZ	2:G:502:MSE:HG2	2.52	0.43
2:G:86:ASP:N	2:G:88:TYR:CZ	2.85	0.43
2:G:455:PHE:O	2:G:455:PHE:CD2	2.71	0.43
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
1:J:94:SER:C	1:J:96:ARG:H	2.25	0.43
1:J:157:LEU:C	1:J:159:ILE:H	2.26	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:CE	1:F:154:MSE:HA	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:184:CYS:HB2	2:K:211:TRP:NE1	2.33	0.43
2:K:190:PHE:CE2	2:K:427:LYS:HG3	2.53	0.43
1:A:22:ARG:NH2	2:C:76:TYR:OH	2.52	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
2:C:43:VAL:C	2:C:45:GLY:H	2.26	0.43
1:E:123:LEU:HD23	1:E:139:ALA:CB	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:406:LEU:O	2:H:407:PRO:C	2.60	0.43
2:K:222:GLU:O	2:K:226:GLN:HG3	2.19	0.43
2:L:190:PHE:CE2	2:L:427:LYS:HG3	2.53	0.43
2:L:307:LYS:HE3	2:L:340:GLY:O	2.19	0.43
2:L:313:LEU:HD23	2:L:313:LEU:O	2.18	0.43
1:A:336:SER:HB3	2:D:373:GLU:HG2	2.00	0.43
2:C:538:ILE:O	2:C:542:LEU:HG	2.18	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: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:HH11	1:J:226:ARG:CG	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
2:G:343:GLN:NE2	2:G:377:MSE:SE	3.02	0.43
2:G:422:MSE:SE	2:G:422:MSE:C	3.11	0.43
2:H:39:LYS:HB2	2:H:39:LYS:HE3	1.79	0.43
1:I:68:TYR:OH	1:I:122:GLY:HA2	2.19	0.43
1:I:123:LEU:HD23	1:I:139:ALA:CB	2.48	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
1:J:348:GLN:H	1:J:348:GLN:HG3	1.71	0.43
2:K:245:PHE:CD1	2:K:245:PHE:C	2.97	0.43
2:L:95:ILE:HA	2:L:96:PRO:HD3	1.86	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
1:E:136:LEU:HD11	1:E:202:LEU:HD11	2.01	0.43
1:E:348:GLN:O	2:G:56:GLN:HG3	2.18	0.43
1:F:21:GLY:HA3	2:H:73:PRO:HD2	2.00	0.43
2:G:508:LEU:O	2:G:509:PRO:C	2.61	0.43
1:J:75:ALA:HB2	1:J:114:VAL:HG23	2.01	0.43
2:K:86:ASP:N	2:K:88:TYR:CZ	2.86	0.43
2:K:196:ASP:C	2:K:198:GLU:N	2.76	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:65:MSE:HA	2:L:66:PRO:HD3	1.85	0.43
1:B:178:PHE:CG	2:D:502:MSE:HE3	2.53	0.42
2:C:122:ARG:HG3	2:C:123:VAL:HG23	2.01	0.42
2:C:454:LEU:HD13	2:C:459:ASN:CG	2.43	0.42
2:D:144:VAL:C	2:D:146:LEU:N	2.77	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
2:H:367:SER:C	2:H:369:GLU:N	2.77	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
2:L:196:ASP:C	2:L:198:GLU:N	2.77	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:78:ASN:HB2	2:H:93:VAL:O	2.19	0.42
2:H:515:THR:O	2:H:519:ILE:HG13	2.18	0.42
2:K:108:VAL:HG12	2:K:484:VAL:HG11	2.00	0.42
2:K:344:ARG:HH11	2:K:344:ARG:HG3	1.84	0.42
1:A:64:ALA:HB3	1:A:71:ILE:HB	2.01	0.42
2:C:40:ARG:HB3	2:C:40:ARG:NH1	2.34	0.42
2:C:393:PRO:O	2:C:397:ILE:HG13	2.19	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:64:ALA:HB3	1:E:71:ILE:HB	2.00	0.42
1:E:114:VAL:HG22	1:E:127:CYS:HB3	1.99	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:227:VAL:C	2:G:228:PHE:CD1	2.98	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:508:LEU:O	2:K:509:PRO:C	2.61	0.42
2:L:343:GLN:O	2:L:344:ARG:C	2.63	0.42
1:A:70:ARG:O	1:A:85:GLU:HA	2.19	0.42
1:B:346:THR:O	2:D:51:MSE:HB2	2.19	0.42
2:C:352:THR:OG1	2:C:355:GLU:HG3	2.20	0.42
1:E:75:ALA:HB2	1:E:114:VAL:CG2	2.49	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:1:MSE:HE2	1:I:1:MSE:N	2.35	0.42
1:I:180:PRO:HG2	1:I:182:LYS:NZ	2.34	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
1:J:106:ASP:CG	1:J:137:TYR:OH	2.61	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
2:L:48:LEU:C	2:L:49:VAL:HG23	2.44	0.42
1:A:29:SER:C	1:A:31:GLN:N	2.78	0.42
1:A:135:ARG:HB3	1:A:137:TYR:CE1	2.54	0.42
1:B:64:ALA:HB3	1:B:71:ILE:HB	2.02	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
2:C:245:PHE:CD1	2:C:245:PHE:C	2.97	0.42
2:C:455:PHE:O	2:C:455:PHE:CD2	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:NH1	1:I:226:ARG:CG	2.83	0.42
1:J:106:ASP:CG	1:J:137:TYR:HH	2.23	0.42
1:J:178:PHE:CZ	2:L:505:ALA:HB3	2.54	0.42
2:L:200:ASN:CG	2:L:203:GLU:HB2	2.44	0.42
1:A:8:HIS:NE2	1:A:34:LYS:HD2	2.35	0.42
1:A:318:ILE:HG12	1:A:332:LYS:HE2	2.02	0.42
1:E:324:ASP:C	1:E:326:GLY:N	2.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:200:ASN:CG	2:G:203:GLU:HB2	2.43	0.42
2:H:270:LEU:O	2:H:274:LEU:HB2	2.18	0.42
2:H:546:MSE:C	2:H:548:SER:H	2.28	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
1:B:210:GLY:C	1:B:241:ARG:NH1	2.78	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
2:D:200:ASN:CG	2:D:203:GLU:HB2	2.44	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:K:313:LEU:C	2:K:313:LEU:CD2	2.92	0.42
2:K:543:GLY:O	2:K:544:ASN:C	2.62	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:CG	1:A:226:ARG:NH1	2.81	0.42
2:C:451:LEU:CG	2:C:452:GLU:H	2.09	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
2:K:144:VAL:C	2:K:146:LEU:N	2.76	0.42
1:A:53:ALA:HB1	1:A:84:TRP:CZ2	2.55	0.42
1:B:29:SER:C	1:B:31:GLN:N	2.78	0.42
2:C:406:LEU:CD1	2:C:461:MSE:HG2	2.50	0.42
2:C:457:TYR:O	2:D:369:GLU:HG2	2.19	0.42
2:D:242:THR:HG22	2:D:243:GLN:N	2.35	0.42
1:E:53:ALA:HB1	1:E:84:TRP:CZ2	2.55	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
2:G:344:ARG:HH11	2:G:344:ARG:HG3	1.85	0.42
2:H:122:ARG:HG3	2:H:123:VAL:HG23	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:84:TRP:HA	1:B:99:ASN:O	2.20	0.41
1:B:346:THR:CG2	1:B:348:GLN:HB2	2.49	0.41
2:C:200:ASN:CG	2:C:203:GLU:HB2	2.45	0.41
2:C:465:MSE:HE2	2:C:465:MSE:HB3	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
2:D:343:GLN:O	2:D:344:ARG:C	2.63	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:42:PRO:O	2:L:44:SER:N	2.53	0.41
2:L:216:ASP:OD2	2:L:255:ARG:NH2	2.53	0.41
1:B:227:TRP:CE3	2:D:453:ASP:O	2.73	0.41
2:C:123:VAL:CG1	2:C:124:PHE:N	2.83	0.41
2:C:531:LEU:O	2:C:534:ILE:HB	2.20	0.41
2:D:78:ASN:HB2	2:D:93:VAL:O	2.20	0.41
2:D:122:ARG:HG3	2:D:123:VAL:HG23	2.02	0.41
2:G:501:LYS:HE3	2:G:529:TRP:O	2.19	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: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
2:L:182:LEU:HG	2:L:409:MSE:HE1	2.02	0.41
2:L:296:PRO:HD3	2:L:306:TRP:CD1	2.54	0.41
2:L:367:SER:C	2:L:369:GLU:N	2.78	0.41
1:A:77:TYR:CD1	1:A:110:SER:HB3	2.55	0.41
2:C:118:LEU:O	2:C:119:GLY:C	2.63	0.41
2:C:539:TYR:O	2:C:540:THR:C	2.61	0.41
2:D:75:SER:HB3	2:D:98:LEU:CD1	2.50	0.41
1:F:3:PRO:HA	2:H:92:PRO:HD2	2.02	0.41
1:F:18:ASP:OD2	1:F:23:HIS:HB2	2.20	0.41
1:F:29:SER:C	1:F:31:GLN:N	2.78	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
2:H:343:GLN:O	2:H:344:ARG:C	2.63	0.41
1:J:118:PRO:HG2	1:J:174:CYS:O	2.20	0.41
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:65:MSE:HA	2:C:66:PRO:HD3	1.81	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:D:49:VAL:CG1	2:D:50:PRO:CD	2.98	0.41
2:D:306:TRP:O	2:D:310:VAL:HG23	2.21	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:200:ASN:CG	2:H:203:GLU:HB2	2.45	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:106:ASP:OD1	1:J:137:TYR:OH	2.30	0.41
1:J:134:LEU:HD11	1:J:183:LEU:HD11	2.02	0.41
1:J:156:VAL:O	1:J:157:LEU:HD23	2.21	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
2:L:406:LEU:O	2:L:407:PRO:C	2.63	0.41
1:A:68:TYR:OH	1:A:122:GLY:CA	2.68	0.41
1:A:154:MSE:HA	1:A:154:MSE:CE	2.50	0.41
2:C:86:ASP:N	2:C:88:TYR:CZ	2.86	0.41
2:H:49:VAL:CG1	2:H:50:PRO:HD2	2.50	0.41
2:H:307:LYS:HE3	2:H:340:GLY:O	2.20	0.41
2:H:456:SER:C	2:H:458:ARG:H	2.29	0.41
2:L:246:TRP:CE2	2:L:331:TYR:HB3	2.56	0.41
2:C:103:GLU:H	2:C:103:GLU:CD	2.28	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
2:D:248:LEU:HD13	2:D:248:LEU:C	2.45	0.41
1:E:178:PHE:CE1	2:G:502:MSE:HG2	2.56	0.41
1:F:85:GLU:HB2	1:F:101:LEU:HD11	2.02	0.41
1:F:226:ARG:NH1	1:F:226:ARG:CG	2.82	0.41
2:G:301:SER:O	2:G:305:GLU:HG3	2.20	0.41
2:H:248:LEU:HD13	2:H:248:LEU:C	2.45	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
2:G:508:LEU:C	2:G:510:HIS:N	2.77	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:97:ARG:HG3	1:J:97:ARG:HH11	1.85	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
2:K:122:ARG:HG3	2:K:123:VAL:HG23	2.03	0.41
2:L:313:LEU:C	2:L:313:LEU:CD2	2.93	0.41
1:A:183:LEU:HD12	1:A:183:LEU:O	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:63:TRP:C	1:J:116:PHE:HD2	2.29	0.41
2:L:248:LEU:HD13	2:L:248:LEU:C	2.45	0.41
1:B:68:TYR:OH	1:B:122:GLY:HA2	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
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
2:H:376:GLN:O	2:H:380:GLU:HG3	2.21	0.41
1:I:134:LEU:HD11	1:I:183:LEU:HD11	2.01	0.41
1:I:154:MSE:CE	1:I:154:MSE:HA	2.51	0.41
1:I:226:ARG:HG3	1:I:226:ARG:NH1	2.29	0.41
1:J:4:PHE:CE1	2:L:90:LEU:HD12	2.56	0.41
1:J:210:GLY:O	1:J:241:ARG:NH1	2.54	0.41
2:L:75:SER:HB3	2:L:98:LEU:CD1	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
2:C:313:LEU:C	2:C:313:LEU:CD2	2.91	0.41
2:C:454:LEU:HD13	2:C:459:ASN:OD1	2.20	0.41
2:D:246:TRP:CE2	2:D:331:TYR:HB3	2.55	0.41
1:F:135:ARG:HB3	1:F:137:TYR:CE1	2.55	0.41
1:F:159:ILE:C	1:F:161:PRO:HD3	2.45	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:406:LEU:O	2:K:407:PRO:C	2.64	0.41
2:K:532:PRO:HG2	2:K:533:GLU:N	2.35	0.41
2:L:43:VAL:O	2:L:43:VAL:HG12	2.21	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:40:ARG:CZ	2:C:40:ARG:HB2	2.51	0.40
2:C:169:VAL:O	2:C:169:VAL:HG12	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:J:218:ILE:O	1:J:218:ILE:HG13	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
1:A:88:PRO:HG3	2:C:547:LEU:O	2.21	0.40
2:C:144:VAL:C	2:C:146:LEU:N	2.79	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
2:D:91:TYR:O	2:D:93:VAL:HG23	2.22	0.40
2:D:196:ASP:C	2:D:198:GLU:N	2.79	0.40
1:F:21:GLY:CA	2:H:73:PRO:HD2	2.51	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:I:231:ILE:HD13	1:I:231:ILE:HG21	1.84	0.40
1:J:124:LYS:HG3	1:J:138:ASP:CG	2.45	0.40
1:J:312:TRP:CZ3	1:J:319:LEU:HB2	2.55	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:HD23	1:E:297:LEU:HA	1.95	0.40
2:G:270:LEU:O	2:G:274:LEU:HB2	2.21	0.40
2:G:465:MSE:HE2	2:G:465:MSE:HB3	1.94	0.40
1:J:317:THR:HG22	1:J:318:ILE:HG13	2.03	0.40
2:K:536:LYS:HD2	2:K:536:LYS:C	2.47	0.40
1:B:77:TYR:HA	1:B:110:SER:HB3	2.04	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
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
2:D:245:PHE:CD1	2:D:245:PHE:C	2.98	0.40
1:E:141:GLU:O	1:E:143:SER:N	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:312:TRP:CZ3	1:E:319:LEU:HB2	2.57	0.40
1:F:324:ASP:C	1:F:326:GLY:N	2.78	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:I:157:LEU:O	1:I:158:SER:C	2.64	0.40
1:J:78:ASP:CG	1:J:80:THR:HG22	2.46	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
2:C:422:MSE:C	2:C:422:MSE:SE	3.14	0.40
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
2:H:144:VAL:C	2:H:146:LEU:N	2.78	0.40
1:I:54:HIS:CE1	1:I:80:THR:HG23	2.57	0.40
1:I:124:LYS:HE3	1:I:138:ASP:OD1	2.21	0.40
1:J:29:SER:C	1:J:31:GLN:N	2.79	0.40
2:L:57:PRO:HB3	2:L:91:TYR:OH	2.22	0.40
2:L:482:TRP:O	2:L:486:ILE:HG12	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	297/351 (85%)	273 (92%)	21 (7%)	3 (1%)	12	45
1	B	297/351 (85%)	269 (91%)	24 (8%)	4 (1%)	9	40
1	E	297/351 (85%)	271 (91%)	24 (8%)	2 (1%)	18	52
1	F	304/351 (87%)	274 (90%)	27 (9%)	3 (1%)	12	45
1	I	303/351 (86%)	273 (90%)	27 (9%)	3 (1%)	12	45

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	J	304/351 (87%)	277 (91%)	24 (8%)	3 (1%)	12	45
2	C	472/570 (83%)	404 (86%)	61 (13%)	7 (2%)	8	37
2	D	470/570 (82%)	403 (86%)	59 (13%)	8 (2%)	7	35
2	G	475/570 (83%)	404 (85%)	60 (13%)	11 (2%)	5	29
2	H	478/570 (84%)	405 (85%)	61 (13%)	12 (2%)	4	27
2	K	479/570 (84%)	408 (85%)	63 (13%)	8 (2%)	7	35
2	L	474/570 (83%)	402 (85%)	62 (13%)	10 (2%)	5	31
All	All	4650/5526 (84%)	4063 (87%)	513 (11%)	74 (2%)	7	36

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
2	H	43	VAL
2	H	239	VAL
2	G	296	PRO
2	H	398	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	265/302 (88%)	252 (95%)	13 (5%)	22	55
1	B	265/302 (88%)	252 (95%)	13 (5%)	22	55
1	E	265/302 (88%)	253 (96%)	12 (4%)	24	58
1	F	269/302 (89%)	258 (96%)	11 (4%)	27	60
1	I	268/302 (89%)	257 (96%)	11 (4%)	27	60
1	J	269/302 (89%)	256 (95%)	13 (5%)	23	56
2	C	430/494 (87%)	421 (98%)	9 (2%)	47	71
2	D	427/494 (86%)	419 (98%)	8 (2%)	50	73
2	G	432/494 (87%)	427 (99%)	5 (1%)	63	79
2	H	434/494 (88%)	427 (98%)	7 (2%)	55	75
2	K	436/494 (88%)	427 (98%)	9 (2%)	47	71
2	L	431/494 (87%)	424 (98%)	7 (2%)	55	75
All	All	4191/4776 (88%)	4073 (97%)	118 (3%)	38	68

All (118) 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	114	VAL
1	A	125	LEU

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Mol	Chain	Res	Type
1	A	154	MSE
1	A	226	ARG
1	A	246	THR
1	A	291	ASN
1	A	314	LEU
1	A	317	THR
1	A	338	GLU
1	B	11	LEU
1	B	43	SER
1	B	99	ASN
1	B	114	VAL
1	B	125	LEU
1	B	147	SER
1	B	154	MSE
1	B	226	ARG
1	B	246	THR
1	B	314	LEU
1	B	317	THR
1	B	338	GLU
1	B	348	GLN
2	C	49	VAL
2	C	56	GLN
2	C	122	ARG
2	C	405	ILE
2	C	423	ILE
2	C	452	GLU
2	C	514	VAL
2	C	522	MSE
2	C	541	THR
2	D	59	GLU
2	D	122	ARG
2	D	405	ILE
2	D	423	ILE
2	D	514	VAL
2	D	522	MSE
2	D	542	LEU
2	D	546	MSE
1	E	11	LEU
1	E	43	SER
1	E	96	ARG
1	E	99	ASN
1	E	114	VAL

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Mol	Chain	Res	Type
1	E	125	LEU
1	E	154	MSE
1	E	226	ARG
1	E	246	THR
1	E	314	LEU
1	E	317	THR
1	E	338	GLU
1	F	11	LEU
1	F	43	SER
1	F	99	ASN
1	F	114	VAL
1	F	125	LEU
1	F	154	MSE
1	F	226	ARG
1	F	246	THR
1	F	314	LEU
1	F	317	THR
1	F	338	GLU
2	G	55	ASP
2	G	122	ARG
2	G	405	ILE
2	G	423	ILE
2	G	514	VAL
2	H	122	ARG
2	H	126	VAL
2	H	241	GLU
2	H	242	THR
2	H	405	ILE
2	H	423	ILE
2	H	514	VAL
1	I	11	LEU
1	I	43	SER
1	I	99	ASN
1	I	114	VAL
1	I	125	LEU
1	I	154	MSE
1	I	226	ARG
1	I	246	THR
1	I	314	LEU
1	I	317	THR
1	I	338	GLU
1	J	11	LEU

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Mol	Chain	Res	Type
1	J	43	SER
1	J	99	ASN
1	J	114	VAL
1	J	125	LEU
1	J	147	SER
1	J	154	MSE
1	J	226	ARG
1	J	246	THR
1	J	314	LEU
1	J	317	THR
1	J	338	GLU
1	J	348	GLN
2	K	44	SER
2	K	57	PRO
2	K	122	ARG
2	K	240	PHE
2	K	405	ILE
2	K	423	ILE
2	K	514	VAL
2	K	522	MSE
2	K	533	GLU
2	L	41	ASP
2	L	59	GLU
2	L	122	ARG
2	L	134	SER
2	L	405	ILE
2	L	423	ILE
2	L	514	VAL

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

Mol	Chain	Res	Type
1	A	99	ASN
1	A	166	GLN
2	C	343	GLN
2	C	382	ASN
2	C	388	ASN
2	C	467	ASN
2	C	545	GLN
2	D	56	GLN
2	D	342	ASN
2	D	343	GLN

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Mol	Chain	Res	Type
2	D	382	ASN
2	D	388	ASN
1	F	163	ASN
2	G	343	GLN
2	G	382	ASN
2	G	388	ASN
2	G	467	ASN
2	H	260	GLN
2	H	382	ASN
2	H	388	ASN
2	H	467	ASN
1	I	90	GLN
1	J	99	ASN
1	J	293	GLN
2	K	183	ASN
2	K	343	GLN
2	K	382	ASN
2	K	388	ASN
2	K	467	ASN
2	L	165	GLN
2	L	343	GLN
2	L	382	ASN
2	L	388	ASN
2	L	467	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides 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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	300/351 (85%)	0.68	15 (5%)	34	22	54, 74, 98, 129	0
1	B	300/351 (85%)	0.68	12 (4%)	42	26	56, 74, 99, 120	0
1	E	300/351 (85%)	0.80	16 (5%)	32	20	53, 72, 97, 114	0
1	F	305/351 (86%)	0.86	24 (7%)	18	12	53, 72, 101, 143	0
1	I	304/351 (86%)	0.74	16 (5%)	32	20	55, 74, 102, 139	0
1	J	305/351 (86%)	0.85	25 (8%)	17	11	54, 75, 101, 144	0
2	C	467/570 (81%)	0.85	44 (9%)	14	9	58, 81, 123, 138	0
2	D	464/570 (81%)	0.81	25 (5%)	31	20	57, 80, 120, 133	0
2	G	470/570 (82%)	1.03	68 (14%)	6	5	55, 80, 117, 134	0
2	H	473/570 (82%)	1.03	57 (12%)	8	6	56, 80, 121, 150	0
2	K	473/570 (82%)	0.87	42 (8%)	15	10	58, 81, 122, 137	0
2	L	470/570 (82%)	0.85	42 (8%)	15	10	57, 80, 123, 142	0
All	All	4631/5526 (83%)	0.85	386 (8%)	17	11	53, 76, 117, 150	0

All (386) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	K	240	PHE	6.4
2	H	539	TYR	5.3
1	I	142	PRO	5.2
2	L	42	PRO	5.2
2	L	451	LEU	5.0
1	I	161	PRO	5.0
2	C	547	LEU	4.9
1	I	165	LEU	4.9
1	B	160	PRO	4.8
1	B	143	SER	4.7
2	K	230	VAL	4.7

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Mol	Chain	Res	Type	RSRZ
2	C	230	VAL	4.6
1	I	143	SER	4.5
1	F	163	ASN	4.5
2	D	451	LEU	4.5
2	G	548	SER	4.4
1	F	165	LEU	4.4
2	D	240	PHE	4.3
2	C	240	PHE	4.3
2	G	269	ASP	4.3
2	K	451	LEU	4.2
2	H	173	TYR	4.1
2	H	230	VAL	4.1
2	C	39	LYS	4.1
1	F	161	PRO	4.1
2	G	539	TYR	4.0
2	G	265	ILE	4.0
2	C	451	LEU	4.0
1	J	165	LEU	3.9
2	H	241	GLU	3.9
2	C	43	VAL	3.9
2	H	126	VAL	3.9
2	H	240	PHE	3.9
2	C	271	LEU	3.9
1	J	142	PRO	3.9
2	H	270	LEU	3.8
2	C	261	ALA	3.8
2	H	548	SER	3.8
2	D	229	SER	3.8
2	H	271	LEU	3.7
2	H	547	LEU	3.7
2	G	239	VAL	3.7
2	C	452	GLU	3.6
2	G	230	VAL	3.6
2	H	453	ASP	3.6
1	B	142	PRO	3.6
2	C	265	ILE	3.6
1	I	159	ILE	3.6
2	L	126	VAL	3.6
1	E	248	LYS	3.6
2	D	271	LEU	3.6
2	G	270	LEU	3.6
2	G	242	THR	3.6

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Mol	Chain	Res	Type	RSRZ
2	K	43	VAL	3.6
2	G	240	PHE	3.5
2	C	241	GLU	3.5
2	L	545	GLN	3.5
2	D	453	ASP	3.5
1	J	159	ILE	3.5
2	G	173	TYR	3.4
2	K	239	VAL	3.4
1	J	248	LYS	3.4
2	C	270	LEU	3.4
2	K	41	ASP	3.4
2	G	451	LEU	3.4
2	L	230	VAL	3.4
2	G	41	ASP	3.4
2	H	451	LEU	3.4
2	G	42	PRO	3.4
2	G	452	GLU	3.3
2	L	271	LEU	3.3
2	G	244	TYR	3.3
2	G	241	GLU	3.3
2	G	271	LEU	3.2
2	C	238	LYS	3.2
2	C	457	TYR	3.2
2	C	454	LEU	3.2
2	K	215	SER	3.2
2	L	240	PHE	3.2
1	J	164	HIS	3.2
1	J	326	GLY	3.2
2	H	242	THR	3.2
2	D	314	SER	3.1
2	K	268	SER	3.1
2	K	270	LEU	3.1
2	C	545	GLN	3.1
2	C	543	GLY	3.1
2	D	44	SER	3.1
1	I	227	TRP	3.1
1	A	20	TYR	3.1
2	H	341	GLY	3.1
2	D	169	VAL	3.1
2	K	169	VAL	3.1
1	I	164	HIS	3.0
2	L	505	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
2	C	239	VAL	3.0
2	C	533	GLU	3.0
1	A	159	ILE	3.0
2	H	314	SER	3.0
2	K	271	LEU	3.0
1	E	20	TYR	3.0
2	G	457	TYR	3.0
2	H	273	TYR	3.0
2	K	493	ALA	3.0
2	K	264	CYS	3.0
2	G	238	LYS	3.0
2	G	324	ILE	3.0
2	L	452	GLU	3.0
2	L	239	VAL	3.0
2	K	39	LYS	3.0
2	L	86	ASP	3.0
2	D	550	HIS	3.0
1	B	349	GLN	3.0
2	L	433	ILE	3.0
2	C	242	THR	2.9
2	G	454	LEU	2.9
1	F	142	PRO	2.9
2	D	134	SER	2.9
1	E	160	PRO	2.9
2	H	272	PRO	2.9
2	C	268	SER	2.9
2	K	551	ASN	2.9
1	E	227	TRP	2.9
2	G	268	SER	2.9
2	L	44	SER	2.9
2	L	454	LEU	2.9
2	C	42	PRO	2.9
1	B	159	ILE	2.9
1	F	290	SER	2.8
2	G	545	GLN	2.8
1	E	218	ILE	2.8
2	G	215	SER	2.8
2	K	42	PRO	2.8
2	C	435	GLU	2.8
2	L	494	THR	2.8
2	L	313	LEU	2.8
2	H	42	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
2	H	337	LEU	2.8
2	G	359	GLY	2.8
2	H	544	ASN	2.8
1	F	164	HIS	2.8
2	L	490	ALA	2.8
1	I	88	PRO	2.8
1	A	160	PRO	2.8
2	H	227	VAL	2.8
2	L	270	LEU	2.8
2	G	455	PHE	2.7
1	F	248	LYS	2.7
2	K	162	VAL	2.7
1	F	343	SER	2.7
2	H	435	GLU	2.7
1	E	198	LYS	2.7
2	L	457	TYR	2.7
2	C	321	ALA	2.7
1	F	159	ILE	2.7
2	H	244	TYR	2.7
2	K	260	GLN	2.7
2	L	136	PHE	2.7
2	C	41	ASP	2.7
2	D	46	ALA	2.7
2	L	321	ALA	2.7
2	G	136	PHE	2.7
1	E	310	VAL	2.7
1	J	20	TYR	2.7
1	B	41	ASP	2.7
1	J	161	PRO	2.6
2	K	433	ILE	2.6
2	C	44	SER	2.6
1	F	89	ASP	2.6
2	G	225	GLU	2.6
2	H	321	ALA	2.6
1	J	194	TYR	2.6
2	G	433	ILE	2.6
1	J	89	ASP	2.6
2	K	321	ALA	2.6
1	E	102	CYS	2.6
1	F	158	SER	2.6
1	E	130	ASN	2.6
2	G	133	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
2	G	436	GLY	2.6
2	K	428	GLY	2.6
1	I	104	LEU	2.6
2	G	477	GLY	2.6
2	C	168	ARG	2.6
2	D	433	ILE	2.5
1	I	158	SER	2.5
2	H	217	GLY	2.5
2	H	236	GLY	2.5
1	J	157	LEU	2.5
2	H	43	VAL	2.5
2	G	100	THR	2.5
2	D	415	CYS	2.5
1	E	167	SER	2.5
2	H	239	VAL	2.5
2	G	262	ILE	2.5
2	L	436	GLY	2.5
1	J	166	GLN	2.5
1	A	168	ASP	2.5
1	F	308	TRP	2.5
2	G	543	GLY	2.5
2	H	310	VAL	2.5
2	D	548	SER	2.5
2	G	261	ALA	2.5
2	G	520	GLU	2.5
2	L	486	ILE	2.5
1	F	41	ASP	2.5
2	C	455	PHE	2.5
2	G	125	ASN	2.5
2	D	57	PRO	2.5
2	G	43	VAL	2.5
2	G	321	ALA	2.4
1	J	143	SER	2.4
1	J	295	GLU	2.4
2	K	211	TRP	2.4
1	A	136	LEU	2.4
1	E	142	PRO	2.4
2	H	543	GLY	2.4
2	L	477	GLY	2.4
2	H	218	GLU	2.4
2	C	250	ASN	2.4
2	H	223	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
2	K	244	TYR	2.4
2	C	417	ALA	2.4
2	D	321	ALA	2.4
1	A	176	SER	2.4
2	G	264	CYS	2.4
2	L	523	LEU	2.4
2	G	166	ASP	2.4
2	G	499	ALA	2.4
2	D	238	LYS	2.4
2	K	297	LYS	2.4
2	C	291	LEU	2.4
2	G	258	LEU	2.4
2	G	325	SER	2.4
2	G	456	SER	2.4
1	F	160	PRO	2.4
2	H	143	THR	2.4
2	H	527	VAL	2.4
2	G	91	TYR	2.4
2	H	269	ASP	2.4
2	G	260	GLN	2.4
2	L	245	PHE	2.4
2	L	410	GLU	2.4
2	C	456	SER	2.4
1	A	248	LYS	2.3
1	J	187	ALA	2.3
2	K	80	ALA	2.3
2	H	41	ASP	2.3
1	A	171	LEU	2.3
1	B	2	GLN	2.3
2	H	219	PRO	2.3
2	L	371	SER	2.3
2	L	375	LEU	2.3
2	G	431	GLU	2.3
1	E	290	SER	2.3
1	J	25	ALA	2.3
1	J	163	ASN	2.3
1	I	160	PRO	2.3
2	D	167	GLY	2.3
2	D	205	ILE	2.3
2	G	224	ILE	2.3
2	K	269	ASP	2.3
2	L	238	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	46	GLU	2.3
1	F	294	VAL	2.3
2	D	397	ILE	2.3
2	K	366	PRO	2.3
2	K	429	LEU	2.3
2	D	268	SER	2.3
2	G	163	LYS	2.3
1	I	294	VAL	2.3
2	C	86	ASP	2.3
2	C	269	ASP	2.3
1	J	245	ILE	2.2
1	F	69	GLY	2.2
2	C	136	PHE	2.2
2	H	54	ASN	2.2
2	H	467	ASN	2.2
2	K	126	VAL	2.2
2	K	133	ASN	2.2
2	G	425	GLU	2.2
2	H	224	ILE	2.2
2	H	274	LEU	2.2
2	K	454	LEU	2.2
1	I	26	THR	2.2
2	G	496	THR	2.2
2	H	457	TYR	2.2
2	L	38	TYR	2.2
2	C	395	VAL	2.2
2	L	285	VAL	2.2
2	G	54	ASN	2.2
1	F	189	GLU	2.2
1	E	145	LEU	2.2
1	F	214	LEU	2.2
2	D	55	ASP	2.2
2	C	219	PRO	2.2
2	H	523	LEU	2.2
2	L	116	ARG	2.2
1	E	65	SER	2.2
1	A	189	GLU	2.2
2	D	467	ASN	2.2
2	G	59	GLU	2.2
1	F	324	ASP	2.2
2	G	297	LYS	2.2
2	G	205	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
2	H	268	SER	2.2
1	J	171	LEU	2.2
2	L	418	ALA	2.2
2	H	318	GLY	2.2
2	C	184	CYS	2.2
2	L	43	VAL	2.1
2	L	169	VAL	2.1
2	D	114	ILE	2.1
1	B	157	LEU	2.1
1	E	166	GLN	2.1
2	G	328	LEU	2.1
2	H	545	GLN	2.1
1	I	205	ALA	2.1
1	J	172	SER	2.1
2	H	319	SER	2.1
1	A	70	ARG	2.1
1	J	160	PRO	2.1
2	L	455	PHE	2.1
1	J	9	ASP	2.1
2	C	280	VAL	2.1
2	H	52	THR	2.1
2	C	324	ILE	2.1
2	G	212	ILE	2.1
2	K	531	LEU	2.1
1	F	326	GLY	2.1
2	L	404	SER	2.1
2	C	123	VAL	2.1
2	H	430	ILE	2.1
2	K	457	TYR	2.1
1	A	166	GLN	2.1
2	G	243	GLN	2.1
2	G	376	GLN	2.1
2	K	261	ALA	2.1
1	B	326	GLY	2.1
1	F	295	GLU	2.1
2	G	411	SER	2.1
2	C	248	LEU	2.1
2	H	193	ASP	2.1
2	H	433	ILE	2.1
2	K	550	HIS	2.1
1	A	26	THR	2.1
2	H	189	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
2	K	420	THR	2.1
1	J	129	GLY	2.1
2	G	124	PHE	2.1
2	H	369	GLU	2.1
2	K	434	PHE	2.1
2	G	44	SER	2.1
1	A	156	VAL	2.1
1	B	332	LYS	2.1
2	C	133	ASN	2.1
2	H	493	ALA	2.1
1	F	323	GLY	2.1
1	F	243	PHE	2.1
2	G	435	GLU	2.1
2	H	434	PHE	2.1
2	L	325	SER	2.0
2	G	84	ALA	2.0
2	L	166	ASP	2.0
2	L	242	THR	2.0
2	K	376	GLN	2.0
2	K	435	GLU	2.0
2	L	168	ARG	2.0
1	B	345	ILE	2.0
1	I	290	SER	2.0
1	J	43	SER	2.0
2	H	134	SER	2.0
1	J	162	ALA	2.0
2	D	279	ALA	2.0
2	K	499	ALA	2.0
1	F	87	ASP	2.0
2	C	287	ASP	2.0
2	G	164	ASP	2.0
1	A	102	CYS	2.0
1	I	102	CYS	2.0
2	K	282	PHE	2.0
2	K	424	CYS	2.0
2	G	294	GLN	2.0
1	B	247	GLU	2.0
2	H	40	ARG	2.0
1	A	157	LEU	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 oligosaccharides 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.