



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:09 PM UTC

PDB ID : 8QWB / pdb_00008qwb
Title : Crystal structure of citrate synthase from Methylophaga sulfidovorans
Authors : Mais, C.-N.; Bange, G.; Sendker, F.L.; Hochberg, G.
Deposited on : 2023-10-19
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
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

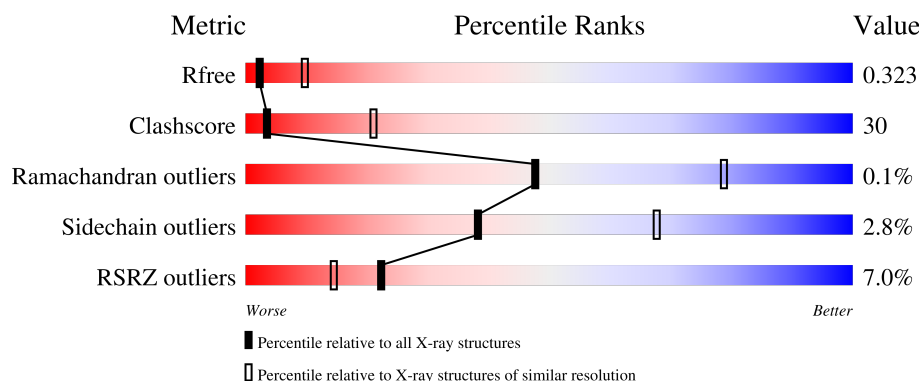
1 Overall quality at a glance i

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	397	6% 43% 38% • 18%
1	B	397	7% 42% 38% • 18%
1	C	397	5% 43% 34% • 22%
1	D	397	4% 48% 33% • 18%
1	E	397	7% 42% 37% • 19%

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Mol	Chain	Length	Quality of chain
1	F	397	
1	G	397	
1	H	397	
1	I	397	
1	J	397	
1	K	397	
1	L	397	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 30057 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 Citrate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	324	Total	C	N	O	S	0	0	0
			2555	1628	434	475	18			
1	B	327	Total	C	N	O	S	0	0	0
			2580	1642	437	482	19			
1	C	311	Total	C	N	O	S	0	0	0
			2441	1552	409	463	17			
1	D	324	Total	C	N	O	S	0	0	0
			2552	1623	434	477	18			
1	E	321	Total	C	N	O	S	0	0	0
			2533	1611	431	473	18			
1	F	318	Total	C	N	O	S	0	0	0
			2509	1597	427	468	17			
1	G	313	Total	C	N	O	S	0	0	0
			2457	1564	414	462	17			
1	H	315	Total	C	N	O	S	0	0	0
			2484	1581	421	465	17			
1	I	311	Total	C	N	O	S	0	0	0
			2446	1555	416	458	17			
1	J	326	Total	C	N	O	S	0	0	0
			2563	1632	433	480	18			
1	K	309	Total	C	N	O	S	0	0	0
			2433	1552	409	456	16			
1	L	317	Total	C	N	O	S	0	0	0
			2504	1594	423	469	18			

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	386	LEU	-	expression tag	UNP A0A1I4B681
A	387	VAL	-	expression tag	UNP A0A1I4B681
A	388	PRO	-	expression tag	UNP A0A1I4B681
A	389	ARG	-	expression tag	UNP A0A1I4B681
A	390	LEU	-	expression tag	UNP A0A1I4B681

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Chain	Residue	Modelled	Actual	Comment	Reference
A	391	GLU	-	expression tag	UNP A0A1I4B681
A	392	HIS	-	expression tag	UNP A0A1I4B681
A	393	HIS	-	expression tag	UNP A0A1I4B681
A	394	HIS	-	expression tag	UNP A0A1I4B681
A	395	HIS	-	expression tag	UNP A0A1I4B681
A	396	HIS	-	expression tag	UNP A0A1I4B681
A	397	HIS	-	expression tag	UNP A0A1I4B681
B	386	LEU	-	expression tag	UNP A0A1I4B681
B	387	VAL	-	expression tag	UNP A0A1I4B681
B	388	PRO	-	expression tag	UNP A0A1I4B681
B	389	ARG	-	expression tag	UNP A0A1I4B681
B	390	LEU	-	expression tag	UNP A0A1I4B681
B	391	GLU	-	expression tag	UNP A0A1I4B681
B	392	HIS	-	expression tag	UNP A0A1I4B681
B	393	HIS	-	expression tag	UNP A0A1I4B681
B	394	HIS	-	expression tag	UNP A0A1I4B681
B	395	HIS	-	expression tag	UNP A0A1I4B681
B	396	HIS	-	expression tag	UNP A0A1I4B681
B	397	HIS	-	expression tag	UNP A0A1I4B681
C	386	LEU	-	expression tag	UNP A0A1I4B681
C	387	VAL	-	expression tag	UNP A0A1I4B681
C	388	PRO	-	expression tag	UNP A0A1I4B681
C	389	ARG	-	expression tag	UNP A0A1I4B681
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C	391	GLU	-	expression tag	UNP A0A1I4B681
C	392	HIS	-	expression tag	UNP A0A1I4B681
C	393	HIS	-	expression tag	UNP A0A1I4B681
C	394	HIS	-	expression tag	UNP A0A1I4B681
C	395	HIS	-	expression tag	UNP A0A1I4B681
C	396	HIS	-	expression tag	UNP A0A1I4B681
C	397	HIS	-	expression tag	UNP A0A1I4B681
D	386	LEU	-	expression tag	UNP A0A1I4B681
D	387	VAL	-	expression tag	UNP A0A1I4B681
D	388	PRO	-	expression tag	UNP A0A1I4B681
D	389	ARG	-	expression tag	UNP A0A1I4B681
D	390	LEU	-	expression tag	UNP A0A1I4B681
D	391	GLU	-	expression tag	UNP A0A1I4B681
D	392	HIS	-	expression tag	UNP A0A1I4B681
D	393	HIS	-	expression tag	UNP A0A1I4B681
D	394	HIS	-	expression tag	UNP A0A1I4B681
D	395	HIS	-	expression tag	UNP A0A1I4B681
D	396	HIS	-	expression tag	UNP A0A1I4B681

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Chain	Residue	Modelled	Actual	Comment	Reference
D	397	HIS	-	expression tag	UNP A0A1I4B681
E	386	LEU	-	expression tag	UNP A0A1I4B681
E	387	VAL	-	expression tag	UNP A0A1I4B681
E	388	PRO	-	expression tag	UNP A0A1I4B681
E	389	ARG	-	expression tag	UNP A0A1I4B681
E	390	LEU	-	expression tag	UNP A0A1I4B681
E	391	GLU	-	expression tag	UNP A0A1I4B681
E	392	HIS	-	expression tag	UNP A0A1I4B681
E	393	HIS	-	expression tag	UNP A0A1I4B681
E	394	HIS	-	expression tag	UNP A0A1I4B681
E	395	HIS	-	expression tag	UNP A0A1I4B681
E	396	HIS	-	expression tag	UNP A0A1I4B681
E	397	HIS	-	expression tag	UNP A0A1I4B681
F	386	LEU	-	expression tag	UNP A0A1I4B681
F	387	VAL	-	expression tag	UNP A0A1I4B681
F	388	PRO	-	expression tag	UNP A0A1I4B681
F	389	ARG	-	expression tag	UNP A0A1I4B681
F	390	LEU	-	expression tag	UNP A0A1I4B681
F	391	GLU	-	expression tag	UNP A0A1I4B681
F	392	HIS	-	expression tag	UNP A0A1I4B681
F	393	HIS	-	expression tag	UNP A0A1I4B681
F	394	HIS	-	expression tag	UNP A0A1I4B681
F	395	HIS	-	expression tag	UNP A0A1I4B681
F	396	HIS	-	expression tag	UNP A0A1I4B681
F	397	HIS	-	expression tag	UNP A0A1I4B681
G	386	LEU	-	expression tag	UNP A0A1I4B681
G	387	VAL	-	expression tag	UNP A0A1I4B681
G	388	PRO	-	expression tag	UNP A0A1I4B681
G	389	ARG	-	expression tag	UNP A0A1I4B681
G	390	LEU	-	expression tag	UNP A0A1I4B681
G	391	GLU	-	expression tag	UNP A0A1I4B681
G	392	HIS	-	expression tag	UNP A0A1I4B681
G	393	HIS	-	expression tag	UNP A0A1I4B681
G	394	HIS	-	expression tag	UNP A0A1I4B681
G	395	HIS	-	expression tag	UNP A0A1I4B681
G	396	HIS	-	expression tag	UNP A0A1I4B681
G	397	HIS	-	expression tag	UNP A0A1I4B681
H	386	LEU	-	expression tag	UNP A0A1I4B681
H	387	VAL	-	expression tag	UNP A0A1I4B681
H	388	PRO	-	expression tag	UNP A0A1I4B681
H	389	ARG	-	expression tag	UNP A0A1I4B681
H	390	LEU	-	expression tag	UNP A0A1I4B681

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Chain	Residue	Modelled	Actual	Comment	Reference
H	391	GLU	-	expression tag	UNP A0A1I4B681
H	392	HIS	-	expression tag	UNP A0A1I4B681
H	393	HIS	-	expression tag	UNP A0A1I4B681
H	394	HIS	-	expression tag	UNP A0A1I4B681
H	395	HIS	-	expression tag	UNP A0A1I4B681
H	396	HIS	-	expression tag	UNP A0A1I4B681
H	397	HIS	-	expression tag	UNP A0A1I4B681
I	386	LEU	-	expression tag	UNP A0A1I4B681
I	387	VAL	-	expression tag	UNP A0A1I4B681
I	388	PRO	-	expression tag	UNP A0A1I4B681
I	389	ARG	-	expression tag	UNP A0A1I4B681
I	390	LEU	-	expression tag	UNP A0A1I4B681
I	391	GLU	-	expression tag	UNP A0A1I4B681
I	392	HIS	-	expression tag	UNP A0A1I4B681
I	393	HIS	-	expression tag	UNP A0A1I4B681
I	394	HIS	-	expression tag	UNP A0A1I4B681
I	395	HIS	-	expression tag	UNP A0A1I4B681
I	396	HIS	-	expression tag	UNP A0A1I4B681
I	397	HIS	-	expression tag	UNP A0A1I4B681
J	386	LEU	-	expression tag	UNP A0A1I4B681
J	387	VAL	-	expression tag	UNP A0A1I4B681
J	388	PRO	-	expression tag	UNP A0A1I4B681
J	389	ARG	-	expression tag	UNP A0A1I4B681
J	390	LEU	-	expression tag	UNP A0A1I4B681
J	391	GLU	-	expression tag	UNP A0A1I4B681
J	392	HIS	-	expression tag	UNP A0A1I4B681
J	393	HIS	-	expression tag	UNP A0A1I4B681
J	394	HIS	-	expression tag	UNP A0A1I4B681
J	395	HIS	-	expression tag	UNP A0A1I4B681
J	396	HIS	-	expression tag	UNP A0A1I4B681
J	397	HIS	-	expression tag	UNP A0A1I4B681
K	386	LEU	-	expression tag	UNP A0A1I4B681
K	387	VAL	-	expression tag	UNP A0A1I4B681
K	388	PRO	-	expression tag	UNP A0A1I4B681
K	389	ARG	-	expression tag	UNP A0A1I4B681
K	390	LEU	-	expression tag	UNP A0A1I4B681
K	391	GLU	-	expression tag	UNP A0A1I4B681
K	392	HIS	-	expression tag	UNP A0A1I4B681
K	393	HIS	-	expression tag	UNP A0A1I4B681
K	394	HIS	-	expression tag	UNP A0A1I4B681
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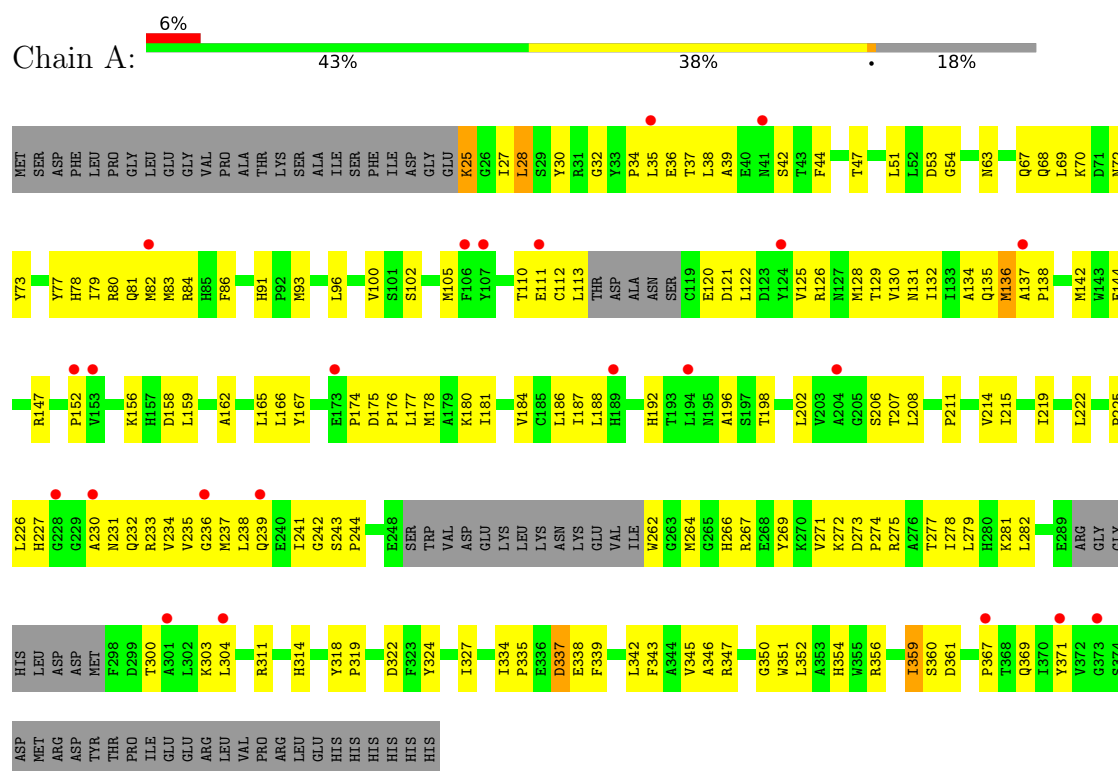
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Chain	Residue	Modelled	Actual	Comment	Reference
K	397	HIS	-	expression tag	UNP A0A1I4B681
L	386	LEU	-	expression tag	UNP A0A1I4B681
L	387	VAL	-	expression tag	UNP A0A1I4B681
L	388	PRO	-	expression tag	UNP A0A1I4B681
L	389	ARG	-	expression tag	UNP A0A1I4B681
L	390	LEU	-	expression tag	UNP A0A1I4B681
L	391	GLU	-	expression tag	UNP A0A1I4B681
L	392	HIS	-	expression tag	UNP A0A1I4B681
L	393	HIS	-	expression tag	UNP A0A1I4B681
L	394	HIS	-	expression tag	UNP A0A1I4B681
L	395	HIS	-	expression tag	UNP A0A1I4B681
L	396	HIS	-	expression tag	UNP A0A1I4B681
L	397	HIS	-	expression tag	UNP A0A1I4B681

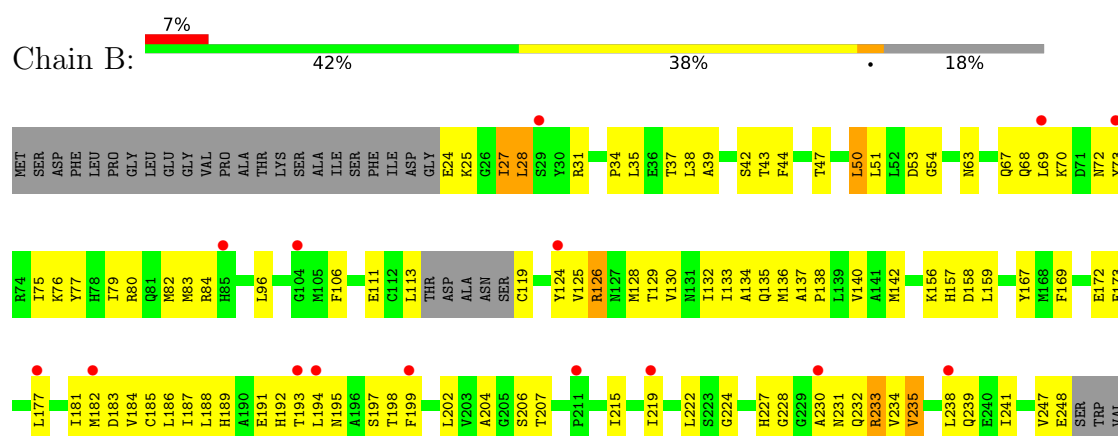
3 Residue-property plots [i](#)

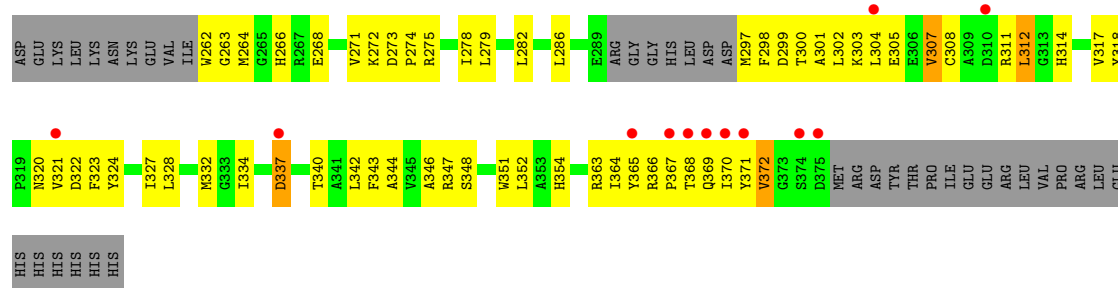
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

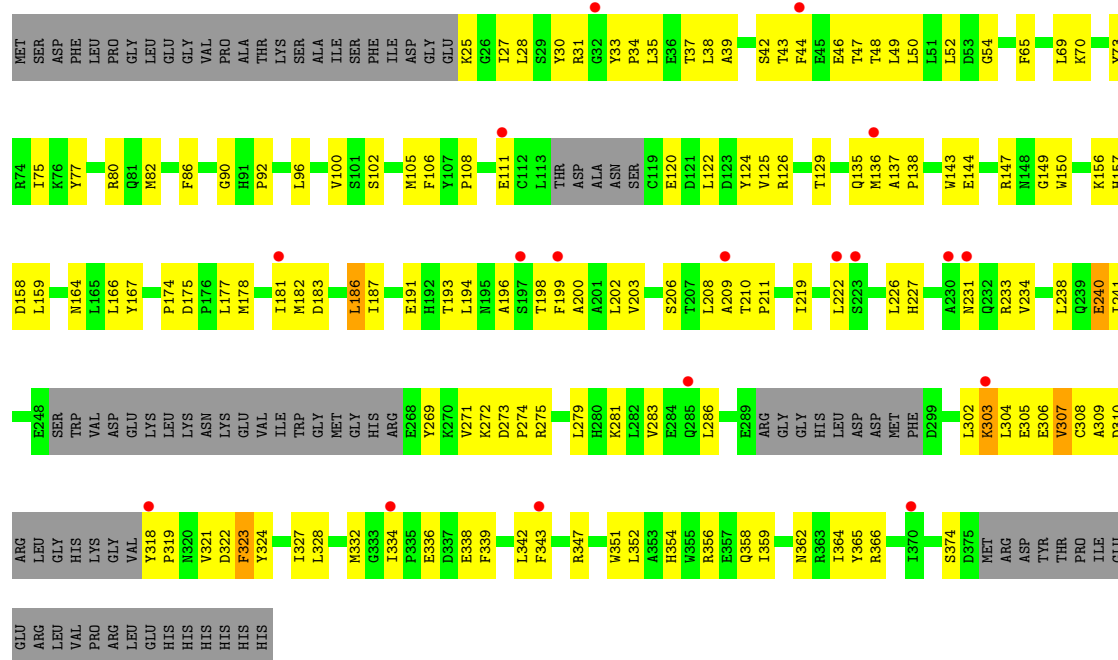
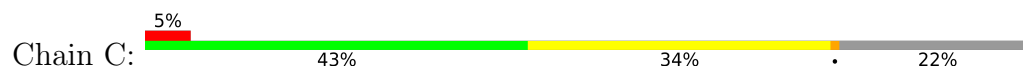


• Molecule 1: Citrate synthase

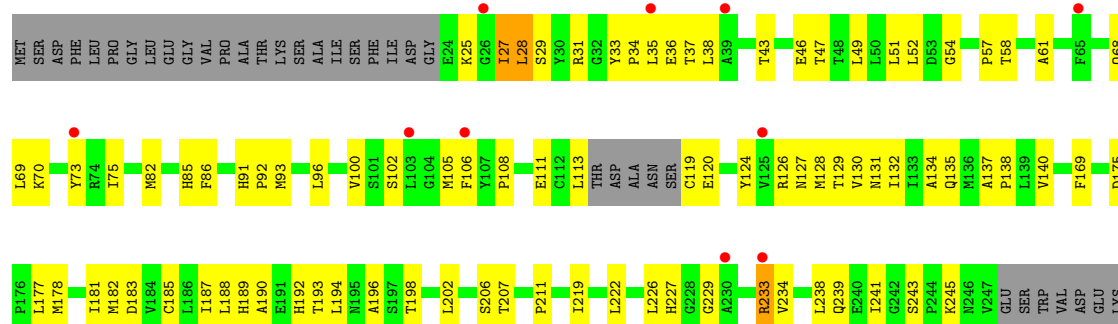


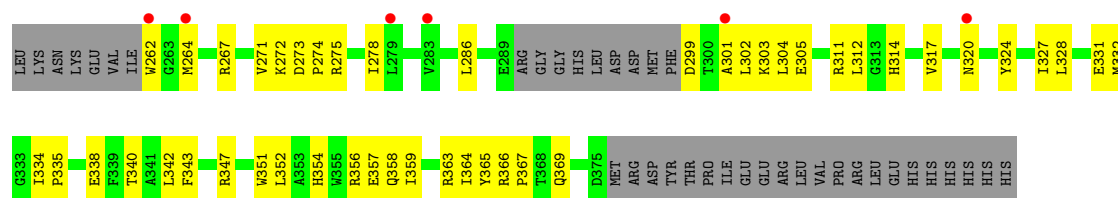


• Molecule 1: Citrate synthase

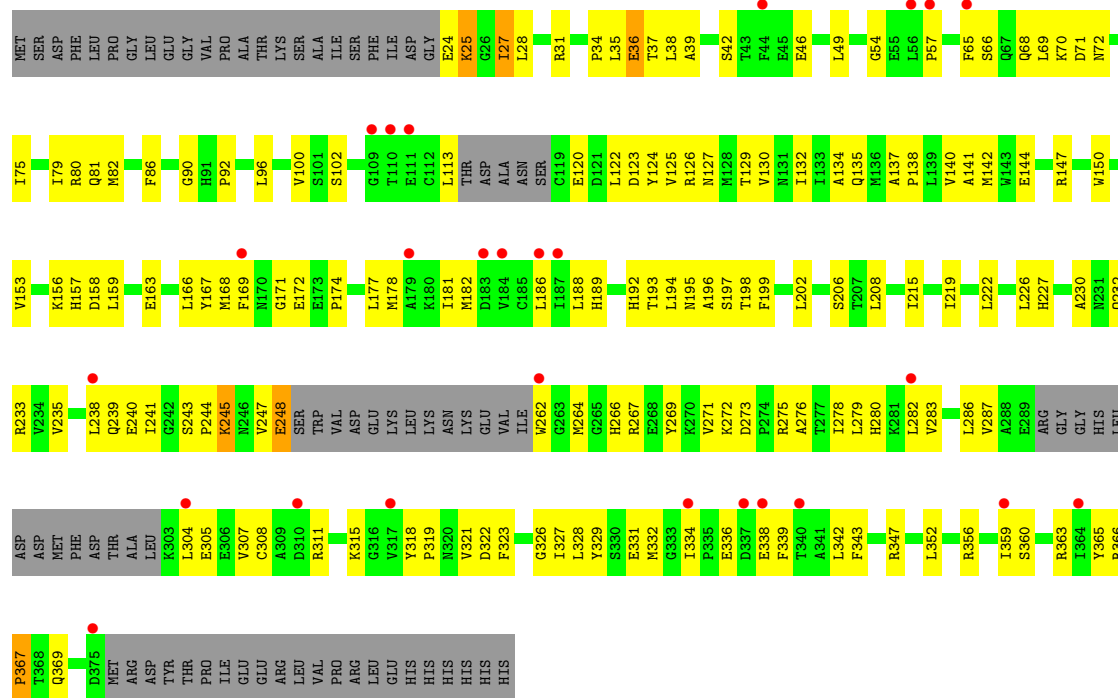
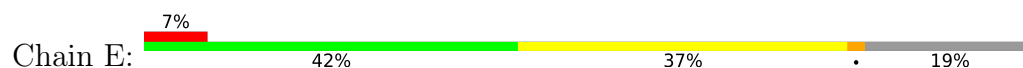


• Molecule 1: Citrate synthase

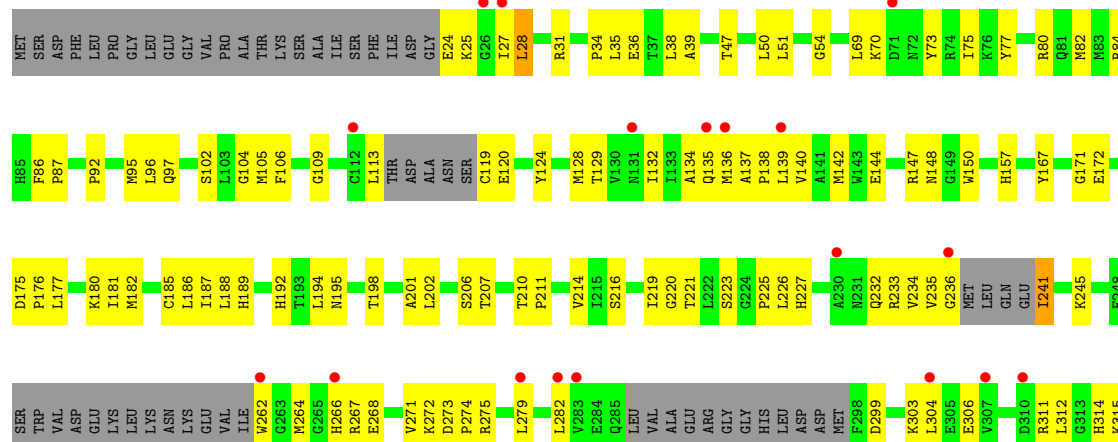


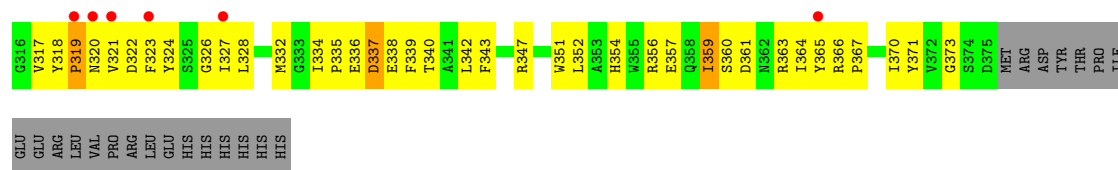


- Molecule 1: Citrate synthase

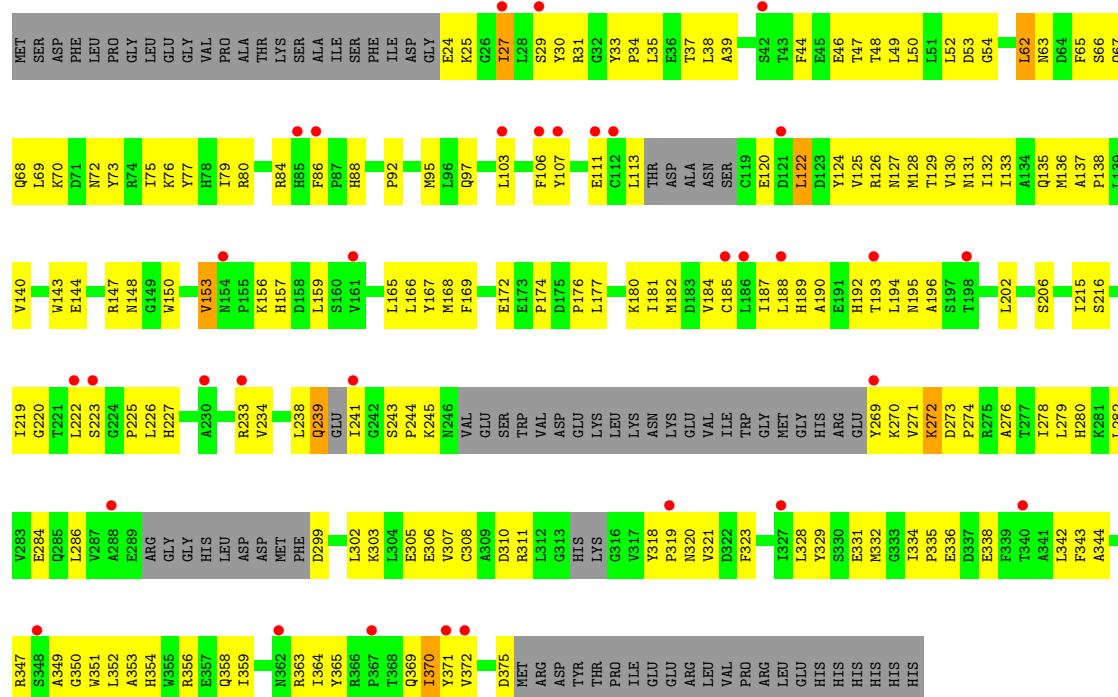


- Molecule 1: Citrate synthase

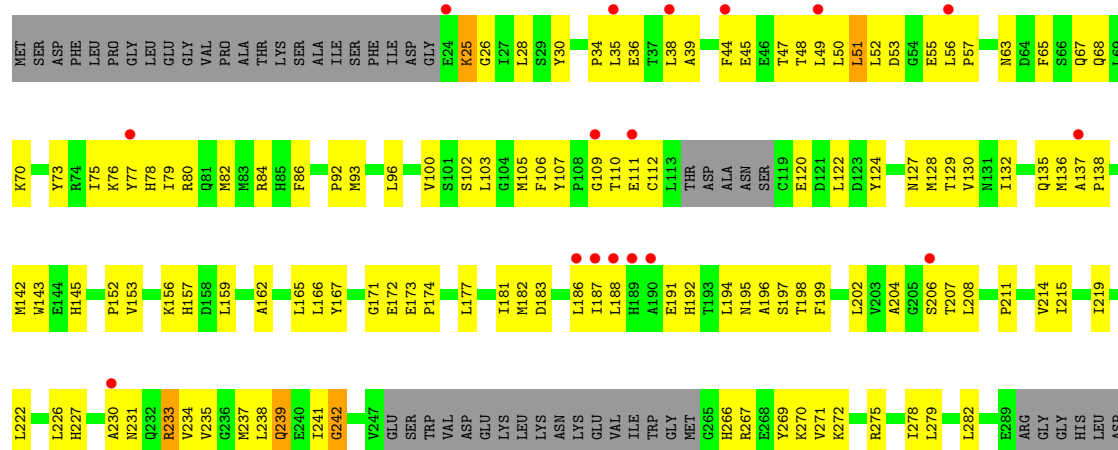


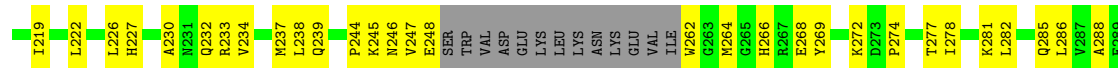
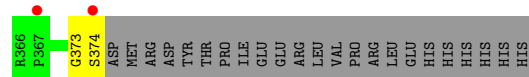


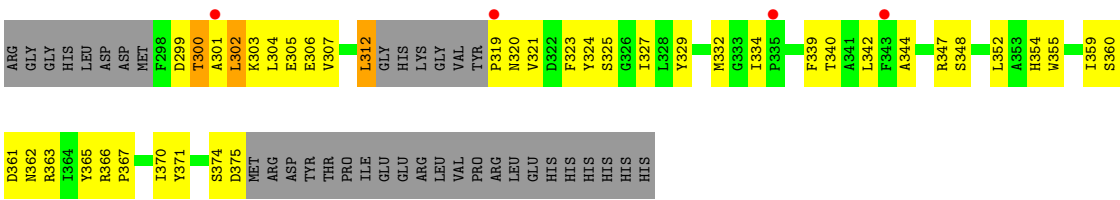
● Molecule 1: Citrate synthase



● Molecule 1: Citrate synthase







4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	155.69Å 96.61Å 203.10Å 90.00° 110.41° 90.00°	Depositor
Resolution (Å)	48.31 – 3.20 48.31 – 3.20	Depositor EDS
% Data completeness (in resolution range)	98.8 (48.31-3.20) 99.0 (48.31-3.20)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.18.2-3874	Depositor
R, R_{free}	0.282 , 0.325 0.324 , 0.323	Depositor DCC
R_{free} test set	4638 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	114.5	Xtriage
Anisotropy	0.406	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 136.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.019 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	30057	wwPDB-VP
Average B, all atoms (Å ²)	134.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.13% of the height of the origin peak. No significant pseudotranslation is detected.*

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	0.90	0/2615	1.15	0/3547
1	B	0.89	0/2640	1.17	0/3580
1	C	0.87	0/2494	1.18	0/3385
1	D	0.89	0/2611	1.18	0/3542
1	E	0.90	0/2592	1.16	0/3515
1	F	0.87	0/2568	1.18	2/3482 (0.1%)
1	G	0.92	0/2510	1.16	1/3404 (0.0%)
1	H	0.90	0/2539	1.16	1/3444 (0.0%)
1	I	0.87	0/2498	1.17	0/3384
1	J	0.90	0/2622	1.16	0/3557
1	K	0.89	0/2487	1.17	1/3372 (0.0%)
1	L	0.89	0/2561	1.15	0/3474
All	All	0.89	0/30737	1.17	5/41686 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	109	GLY	CA-C-O	-5.75	118.17	122.37
1	F	319	PRO	CB-CA-C	-5.24	102.92	111.56
1	G	364	ILE	N-CA-C	-5.20	108.43	113.53
1	K	137	ALA	N-CA-C	-5.10	106.62	113.25
1	F	211	PRO	N-CA-C	-5.03	106.25	113.75

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	2555	0	2508	138	0
1	B	2580	0	2527	155	0
1	C	2441	0	2391	133	0
1	D	2552	0	2503	136	0
1	E	2533	0	2482	155	0
1	F	2509	0	2452	169	0
1	G	2457	0	2415	160	0
1	H	2484	0	2443	160	0
1	I	2446	0	2402	165	0
1	J	2563	0	2507	149	0
1	K	2433	0	2377	157	0
1	L	2504	0	2452	178	0
All	All	30057	0	29459	1761	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 30.

All (1761) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:264:MET:HA	1:F:319:PRO:HB3	1.34	1.05
1:A:28:LEU:HD12	1:A:35:LEU:HB2	1.42	1.02
1:A:334:ILE:HG21	1:A:342:LEU:HD11	1.42	0.99
1:K:266:HIS:HB3	1:K:269:TYR:HB2	1.45	0.98
1:I:233:ARG:HB2	1:I:323:PHE:HA	1.47	0.96
1:D:28:LEU:HA	1:D:35:LEU:HD13	1.47	0.96
1:J:28:LEU:HG	1:J:35:LEU:H	1.31	0.95
1:I:28:LEU:HB3	1:I:34:PRO:HA	1.50	0.94
1:D:239:GLN:HA	1:D:303:LYS:HD2	1.51	0.93
1:K:52:LEU:HD22	1:K:126:ARG:HH22	1.34	0.92
1:K:28:LEU:HB3	1:K:34:PRO:HA	1.51	0.91
1:A:28:LEU:HB3	1:A:34:PRO:HA	1.53	0.91
1:A:233:ARG:HG2	1:A:262:TRP:HB3	1.53	0.91
1:C:28:LEU:HA	1:C:35:LEU:HD13	1.52	0.90
1:G:369:GLN:HA	1:G:375:ASP:HB3	1.51	0.90
1:K:334:ILE:HG21	1:K:342:LEU:HD11	1.54	0.90
1:L:266:HIS:HB3	1:L:269:TYR:HB2	1.52	0.90
1:J:363:ARG:HG2	1:J:365:TYR:H	1.37	0.89
1:B:27:ILE:HG13	1:B:274:PRO:HG3	1.53	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:LEU:HD21	1:B:354:HIS:HB3	1.54	0.88
1:A:266:HIS:HB3	1:A:269:TYR:HB2	1.55	0.87
1:B:28:LEU:HB3	1:B:34:PRO:HA	1.53	0.87
1:H:166:LEU:HB2	1:H:174:PRO:HG3	1.57	0.87
1:B:233:ARG:HG2	1:B:263:GLY:HA3	1.54	0.86
1:F:189:HIS:CE1	1:F:321:VAL:HG21	2.10	0.86
1:I:129:THR:HG23	1:I:352:LEU:HD13	1.58	0.86
1:B:27:ILE:HG12	1:B:28:LEU:HD13	1.58	0.85
1:G:68:GLN:HG2	1:G:130:VAL:HG11	1.59	0.85
1:D:181:ILE:HD13	1:D:286:LEU:HD11	1.58	0.85
1:I:28:LEU:HA	1:I:35:LEU:HD13	1.59	0.85
1:F:233:ARG:HH21	1:F:327:ILE:HD11	1.41	0.84
1:F:96:LEU:HG	1:F:219:ILE:HD13	1.58	0.84
1:G:233:ARG:HE	1:G:323:PHE:HA	1.43	0.83
1:F:202:LEU:HD21	1:F:354:HIS:HB3	1.59	0.82
1:G:286:LEU:HD21	1:G:331:GLU:HG2	1.61	0.82
1:J:202:LEU:HD21	1:J:354:HIS:HB3	1.61	0.82
1:G:238:LEU:HD23	1:G:238:LEU:H	1.43	0.81
1:D:202:LEU:HD21	1:D:354:HIS:HB3	1.61	0.81
1:D:178:MET:HA	1:D:181:ILE:HD12	1.63	0.81
1:D:182:MET:HB2	1:D:332:MET:HE1	1.62	0.81
1:H:129:THR:HG23	1:H:352:LEU:HD13	1.61	0.80
1:A:241:ILE:HG22	1:A:244:PRO:HG2	1.64	0.80
1:J:272:LYS:HE3	1:J:319:PRO:HB2	1.64	0.79
1:F:27:ILE:HG13	1:F:274:PRO:HG3	1.63	0.79
1:F:80:ARG:HD3	1:F:84:ARG:HE	1.46	0.79
1:J:113:LEU:HD22	1:J:119:CYS:HB3	1.64	0.79
1:A:27:ILE:HG12	1:A:28:LEU:HD13	1.64	0.79
1:H:369:GLN:HE21	1:H:375:ASP:HB3	1.45	0.79
1:K:129:THR:HG23	1:K:352:LEU:HD13	1.65	0.79
1:B:304:LEU:HG	1:B:327:ILE:HD11	1.63	0.78
1:I:307:VAL:HA	1:I:311:ARG:HB2	1.64	0.78
1:L:83:MET:HG2	1:L:95:MET:HE2	1.63	0.78
1:B:312:LEU:H	1:B:312:LEU:HD22	1.49	0.78
1:A:102:SER:HB2	1:C:86:PHE:CE2	2.19	0.78
1:E:24:GLU:HB2	1:E:27:ILE:HG23	1.65	0.78
1:D:28:LEU:HG	1:D:35:LEU:H	1.49	0.78
1:A:222:LEU:HD11	1:A:343:PHE:HD1	1.46	0.77
1:F:27:ILE:HG12	1:F:28:LEU:HD13	1.66	0.77
1:F:267:ARG:HH21	1:H:363:ARG:HE	1.30	0.77
1:D:189:HIS:HB3	1:D:343:PHE:HD1	1.49	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:197:SER:H	1:E:227:HIS:HE1	1.33	0.76
1:F:233:ARG:HG3	1:F:323:PHE:HA	1.67	0.76
1:K:25:LYS:HE2	1:K:271:VAL:H	1.51	0.76
1:H:192:HIS:CE1	1:H:266:HIS:HE2	2.03	0.76
1:F:335:PRO:HG2	1:F:338:GLU:HG3	1.68	0.76
1:I:367:PRO:HG2	1:L:194:LEU:HB3	1.65	0.76
1:B:75:ILE:HG21	1:B:142:MET:HE1	1.68	0.75
1:E:79:ILE:O	1:E:82:MET:HG3	1.85	0.75
1:G:129:THR:HG23	1:G:352:LEU:HD13	1.69	0.75
1:E:264:MET:HG2	1:E:319:PRO:HA	1.68	0.75
1:G:177:LEU:HD22	1:G:177:LEU:H	1.51	0.74
1:J:312:LEU:H	1:J:312:LEU:HD12	1.52	0.74
1:K:68:GLN:HG2	1:K:130:VAL:HG11	1.68	0.74
1:F:327:ILE:HD12	1:F:327:ILE:H	1.53	0.74
1:J:311:ARG:HA	1:J:314:HIS:HB2	1.67	0.74
1:J:137:ALA:HB3	1:J:138:PRO:HD3	1.69	0.74
1:A:129:THR:HB	1:A:352:LEU:HD13	1.70	0.74
1:E:286:LEU:HB3	1:E:331:GLU:HG2	1.70	0.74
1:G:47:THR:HG21	1:G:187:ILE:HG23	1.70	0.74
1:C:196:ALA:HB3	1:C:227:HIS:HD2	1.52	0.73
1:L:327:ILE:H	1:L:327:ILE:HD12	1.52	0.73
1:E:138:PRO:HA	1:E:168:MET:HE1	1.71	0.73
1:I:304:LEU:HD13	1:I:324:TYR:CE2	2.24	0.73
1:B:75:ILE:HD11	1:B:138:PRO:HB2	1.71	0.72
1:D:189:HIS:HB3	1:D:343:PHE:CD1	2.24	0.72
1:E:126:ARG:HH21	1:E:356:ARG:HH12	1.34	0.72
1:H:303:LYS:HD3	1:H:327:ILE:HG21	1.68	0.72
1:L:239:GLN:HA	1:L:303:LYS:HB3	1.71	0.72
1:B:193:THR:HG22	1:B:194:LEU:H	1.53	0.72
1:D:96:LEU:HG	1:D:219:ILE:HD13	1.71	0.72
1:E:334:ILE:HG21	1:E:342:LEU:HD11	1.69	0.72
1:A:202:LEU:HD21	1:A:354:HIS:HB3	1.70	0.72
1:L:334:ILE:HG21	1:L:342:LEU:HD11	1.72	0.72
1:D:102:SER:HB2	1:E:86:PHE:CE1	2.24	0.72
1:H:49:LEU:HD23	1:H:57:PRO:HG3	1.70	0.72
1:I:334:ILE:HG21	1:I:342:LEU:HD11	1.72	0.72
1:F:181:ILE:HG22	1:F:328:LEU:HD21	1.72	0.72
1:B:368:THR:HA	1:B:372:VAL:HA	1.71	0.71
1:D:34:PRO:HB2	1:D:36:GLU:OE1	1.90	0.71
1:A:311:ARG:HA	1:A:314:HIS:NE2	2.05	0.71
1:E:245:LYS:HE3	1:E:245:LYS:HA	1.70	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:314:HIS:HB3	1:B:317:VAL:HG23	1.71	0.71
1:F:241:ILE:HD11	1:F:306:GLU:HB2	1.72	0.71
1:G:350:GLY:O	1:G:354:HIS:HD2	1.74	0.71
1:B:68:GLN:HG2	1:B:130:VAL:HG11	1.72	0.71
1:B:300:THR:HA	1:B:327:ILE:HD13	1.72	0.71
1:B:368:THR:HA	1:B:372:VAL:CA	2.21	0.71
1:G:140:VAL:HG12	1:G:169:PHE:HZ	1.56	0.71
1:G:181:ILE:HG21	1:G:328:LEU:HD11	1.72	0.71
1:B:239:GLN:HG2	1:B:298:PHE:CE1	2.26	0.70
1:J:364:ILE:HG23	1:J:366:ARG:HG2	1.71	0.70
1:G:272:LYS:HG2	1:G:273:ASP:H	1.55	0.70
1:H:233:ARG:HE	1:H:323:PHE:HA	1.56	0.70
1:I:126:ARG:HH22	1:I:356:ARG:HH11	1.39	0.70
1:J:58:THR:HG23	1:J:61:ALA:H	1.57	0.70
1:F:28:LEU:HB3	1:F:35:LEU:H	1.54	0.70
1:A:96:LEU:HG	1:A:219:ILE:HD13	1.72	0.70
1:L:232:GLN:HB2	1:L:262:TRP:CE2	2.27	0.70
1:H:48:THR:HG22	1:H:349:ALA:HB2	1.73	0.70
1:D:312:LEU:H	1:D:312:LEU:HD22	1.57	0.70
1:K:137:ALA:HB3	1:K:138:PRO:HD3	1.72	0.70
1:J:245:LYS:HA	1:J:245:LYS:HE3	1.73	0.70
1:L:97:GLN:HA	1:L:219:ILE:HD11	1.73	0.69
1:D:105:MET:HE3	1:E:90:GLY:HA3	1.73	0.69
1:J:28:LEU:HB3	1:J:34:PRO:HA	1.74	0.69
1:L:96:LEU:HG	1:L:219:ILE:HD12	1.74	0.69
1:K:202:LEU:HD21	1:K:354:HIS:HB3	1.72	0.69
1:J:314:HIS:HB3	1:J:317:VAL:O	1.93	0.69
1:A:34:PRO:HG2	1:A:37:THR:HB	1.74	0.69
1:D:354:HIS:O	1:D:357:GLU:HG2	1.92	0.69
1:F:194:LEU:HB3	1:H:367:PRO:HD2	1.74	0.69
1:G:182:MET:HE1	1:G:329:TYR:HE1	1.58	0.69
1:K:44:PHE:CD1	1:K:186:LEU:HB3	2.27	0.69
1:I:103:LEU:HG	1:I:107:TYR:HE1	1.58	0.69
1:D:192:HIS:HB2	1:D:347:ARG:NH2	2.08	0.69
1:I:233:ARG:HH11	1:I:234:VAL:HA	1.57	0.69
1:D:366:ARG:NE	1:E:195:ASN:HA	2.09	0.68
1:J:177:LEU:HD22	1:J:177:LEU:H	1.58	0.68
1:A:304:LEU:HG	1:A:327:ILE:HD11	1.74	0.68
1:F:334:ILE:HG12	1:F:342:LEU:HD21	1.75	0.68
1:J:233:ARG:HH21	1:J:322:ASP:HB2	1.58	0.68
1:E:129:THR:HG23	1:E:352:LEU:HD13	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:197:SER:H	1:E:227:HIS:CE1	2.12	0.68
1:J:129:THR:HG23	1:J:352:LEU:HD13	1.75	0.68
1:L:264:MET:HA	1:L:320:ASN:H	1.58	0.68
1:H:70:LYS:HE3	1:H:157:HIS:CE1	2.29	0.68
1:C:96:LEU:HG	1:C:219:ILE:HD13	1.73	0.68
1:F:96:LEU:HD13	1:F:139:LEU:HD11	1.76	0.68
1:H:197:SER:H	1:H:227:HIS:CE1	2.12	0.68
1:K:28:LEU:HA	1:K:35:LEU:HD13	1.74	0.68
1:L:181:ILE:HG13	1:L:286:LEU:HD11	1.74	0.68
1:L:264:MET:HA	1:L:319:PRO:HA	1.75	0.68
1:D:68:GLN:HG2	1:D:130:VAL:HG11	1.76	0.68
1:E:195:ASN:ND2	1:E:198:THR:H	1.93	0.67
1:L:233:ARG:HH12	1:L:325:SER:HB2	1.58	0.67
1:B:307:VAL:HG13	1:B:323:PHE:HZ	1.58	0.67
1:D:229:GLY:HA3	1:D:262:TRP:HE1	1.60	0.67
1:F:113:LEU:HD21	1:F:120:GLU:HB2	1.75	0.67
1:I:233:ARG:NH1	1:I:234:VAL:HA	2.10	0.67
1:J:286:LEU:HD22	1:J:331:GLU:HB3	1.76	0.67
1:K:229:GLY:HA3	1:K:262:TRP:HE1	1.60	0.67
1:B:311:ARG:HD2	1:B:318:TYR:HD1	1.58	0.67
1:A:238:LEU:HD11	1:A:241:ILE:HB	1.77	0.67
1:E:137:ALA:HB3	1:E:138:PRO:HD3	1.77	0.67
1:E:271:VAL:HG22	1:E:272:LYS:H	1.60	0.67
1:G:308:CYS:HA	1:G:319:PRO:HG3	1.77	0.67
1:I:202:LEU:HD22	1:I:358:GLN:HE21	1.58	0.67
1:L:334:ILE:HG12	1:L:342:LEU:HD11	1.77	0.67
1:B:70:LYS:HD3	1:B:157:HIS:O	1.95	0.67
1:C:233:ARG:HD2	1:C:323:PHE:HA	1.77	0.67
1:F:304:LEU:HD12	1:F:323:PHE:CZ	2.29	0.67
1:J:335:PRO:HG2	1:J:338:GLU:HG2	1.76	0.67
1:B:192:HIS:HD2	1:B:195:ASN:HD21	1.42	0.66
1:D:137:ALA:HB3	1:D:138:PRO:HD3	1.77	0.66
1:B:300:THR:HB	1:B:327:ILE:HG21	1.77	0.66
1:G:128:MET:HE2	1:G:128:MET:HA	1.77	0.66
1:D:28:LEU:HB3	1:D:34:PRO:HA	1.75	0.66
1:I:230:ALA:HA	1:I:322:ASP:HB3	1.77	0.66
1:L:244:PRO:HD2	1:L:245:LYS:HZ2	1.60	0.66
1:D:334:ILE:HG12	1:D:342:LEU:HD21	1.76	0.66
1:A:77:TYR:O	1:A:80:ARG:HG2	1.94	0.66
1:H:35:LEU:HD21	1:H:188:LEU:HG	1.77	0.66
1:I:25:LYS:NZ	1:I:274:PRO:HD3	2.09	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:70:LYS:HA	1:I:73:TYR:CE2	2.31	0.66
1:I:233:ARG:HD3	1:I:234:VAL:N	2.11	0.66
1:L:264:MET:HA	1:L:320:ASN:N	2.10	0.66
1:F:177:LEU:H	1:F:177:LEU:HD22	1.61	0.66
1:I:34:PRO:O	1:I:37:THR:HG22	1.96	0.66
1:B:368:THR:HA	1:B:372:VAL:HB	1.77	0.66
1:D:52:LEU:HD22	1:D:126:ARG:HH22	1.60	0.66
1:E:75:ILE:HG21	1:E:142:MET:HE1	1.77	0.66
1:E:177:LEU:HD22	1:E:177:LEU:H	1.61	0.66
1:J:132:ILE:HG21	1:J:215:ILE:HG13	1.78	0.66
1:E:188:LEU:HD21	1:E:278:ILE:HB	1.77	0.65
1:H:70:LYS:HA	1:H:73:TYR:CE2	2.32	0.65
1:K:75:ILE:HD11	1:K:138:PRO:HB2	1.78	0.65
1:L:370:ILE:HG22	1:L:371:TYR:H	1.60	0.65
1:A:206:SER:HA	1:A:361:ASP:OD1	1.97	0.65
1:I:280:HIS:O	1:I:283:VAL:HG22	1.96	0.65
1:C:196:ALA:HB3	1:C:227:HIS:CD2	2.32	0.65
1:G:79:ILE:HD11	1:G:106:PHE:HE2	1.62	0.65
1:J:28:LEU:HG	1:J:35:LEU:N	2.09	0.65
1:C:129:THR:HG23	1:C:352:LEU:HD13	1.79	0.65
1:I:216:SER:HA	1:I:219:ILE:HD11	1.78	0.65
1:L:129:THR:HG23	1:L:352:LEU:HD13	1.78	0.65
1:B:206:SER:HB2	1:B:364:ILE:HA	1.79	0.65
1:C:334:ILE:HG12	1:C:342:LEU:HD21	1.78	0.65
1:G:182:MET:HB2	1:G:332:MET:HE1	1.77	0.65
1:G:202:LEU:HD21	1:G:354:HIS:HB3	1.79	0.65
1:F:363:ARG:HG2	1:F:365:TYR:H	1.63	0.64
1:L:182:MET:HE1	1:L:329:TYR:HE1	1.62	0.64
1:G:97:GLN:HA	1:G:219:ILE:HD11	1.78	0.64
1:G:196:ALA:HB3	1:G:227:HIS:HD2	1.62	0.64
1:I:31:ARG:HD3	1:I:54:GLY:HA2	1.78	0.64
1:J:156:LYS:HE3	1:J:167:TYR:CZ	2.32	0.64
1:L:31:ARG:HD2	1:L:35:LEU:HB2	1.77	0.64
1:L:70:LYS:HA	1:L:73:TYR:CE2	2.32	0.64
1:H:222:LEU:HD13	1:H:227:HIS:HD2	1.61	0.64
1:K:28:LEU:HD12	1:K:35:LEU:HD13	1.79	0.64
1:I:301:ALA:O	1:I:304:LEU:HG	1.96	0.64
1:B:129:THR:HG23	1:B:352:LEU:HD13	1.78	0.64
1:L:137:ALA:HB3	1:L:138:PRO:HD3	1.80	0.64
1:L:206:SER:HB2	1:L:363:ARG:O	1.96	0.64
1:B:247:VAL:HG22	1:B:248:GLU:HG2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:301:ALA:O	1:J:305:GLU:HG2	1.98	0.64
1:G:176:PRO:O	1:G:180:LYS:HG2	1.97	0.64
1:D:70:LYS:HA	1:D:73:TYR:CE2	2.32	0.63
1:K:222:LEU:HD12	1:K:351:TRP:HZ2	1.63	0.63
1:J:243:SER:HB3	1:J:244:PRO:HD3	1.79	0.63
1:C:200:ALA:O	1:C:203:VAL:HG22	1.99	0.63
1:J:182:MET:HA	1:J:182:MET:HE3	1.80	0.63
1:G:189:HIS:HB3	1:G:343:PHE:HD1	1.62	0.63
1:H:271:VAL:HG22	1:H:272:LYS:H	1.62	0.63
1:A:38:LEU:O	1:A:42:SER:HB3	1.98	0.63
1:A:102:SER:HB2	1:C:86:PHE:HE2	1.61	0.63
1:B:34:PRO:O	1:B:37:THR:HG22	1.99	0.63
1:J:111:GLU:OE2	1:J:120:GLU:HG2	1.98	0.63
1:C:38:LEU:HD21	1:C:50:LEU:HD23	1.81	0.63
1:D:58:THR:HG23	1:D:61:ALA:H	1.64	0.63
1:D:328:LEU:O	1:D:332:MET:HG3	1.99	0.63
1:H:96:LEU:HG	1:H:219:ILE:HD13	1.81	0.63
1:H:238:LEU:HA	1:H:304:LEU:HD11	1.81	0.63
1:J:49:LEU:HD13	1:J:57:PRO:HG3	1.80	0.63
1:L:244:PRO:HD2	1:L:245:LYS:NZ	2.14	0.63
1:G:189:HIS:HB3	1:G:343:PHE:CD1	2.34	0.63
1:K:75:ILE:HD13	1:K:139:LEU:HD23	1.80	0.63
1:L:177:LEU:O	1:L:181:ILE:HG12	1.99	0.63
1:C:304:LEU:O	1:C:307:VAL:HG22	1.99	0.62
1:C:177:LEU:O	1:C:181:ILE:HG12	1.99	0.62
1:G:206:SER:HB3	1:G:365:TYR:CD2	2.34	0.62
1:J:132:ILE:O	1:J:136:MET:HG2	1.99	0.62
1:J:197:SER:H	1:J:227:HIS:CE1	2.18	0.62
1:A:156:LYS:HE3	1:A:167:TYR:CZ	2.34	0.62
1:G:166:LEU:HB3	1:G:174:PRO:HB3	1.81	0.62
1:L:266:HIS:CE1	1:L:268:GLU:HB2	2.34	0.62
1:H:25:LYS:HE3	1:H:270:LYS:H	1.65	0.62
1:L:222:LEU:HA	1:L:227:HIS:HD1	1.64	0.62
1:L:304:LEU:HB3	1:L:324:TYR:CE1	2.35	0.62
1:A:264:MET:HG3	1:A:319:PRO:HA	1.81	0.62
1:J:127:ASN:O	1:J:130:VAL:HG12	1.99	0.62
1:A:86:PHE:CE1	1:C:102:SER:HB2	2.34	0.62
1:E:34:PRO:O	1:E:37:THR:HG22	1.99	0.62
1:I:137:ALA:HB3	1:I:138:PRO:HD3	1.81	0.62
1:B:132:ILE:HG21	1:B:215:ILE:HG13	1.82	0.62
1:D:27:ILE:HG13	1:D:274:PRO:HG3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:238:LEU:HB3	1:E:241:ILE:HG23	1.80	0.62
1:F:47:THR:HG21	1:F:187:ILE:HG23	1.80	0.62
1:H:192:HIS:HE1	1:H:266:HIS:HE2	1.48	0.62
1:L:44:PHE:O	1:L:48:THR:HG23	2.00	0.62
1:A:27:ILE:HG23	1:A:28:LEU:HD22	1.82	0.62
1:A:267:ARG:HD2	1:C:366:ARG:HB3	1.81	0.62
1:B:79:ILE:O	1:B:82:MET:HG2	1.99	0.62
1:J:240:GLU:H	1:J:303:LYS:HD3	1.64	0.62
1:F:137:ALA:HB3	1:F:138:PRO:HD3	1.82	0.61
1:I:25:LYS:HD3	1:I:27:ILE:HD13	1.82	0.61
1:H:28:LEU:HD23	1:H:35:LEU:HD22	1.82	0.61
1:A:226:LEU:HD12	1:C:206:SER:O	2.00	0.61
1:D:106:PHE:O	1:D:108:PRO:HD3	2.00	0.61
1:G:137:ALA:HB3	1:G:138:PRO:HD3	1.81	0.61
1:F:27:ILE:HG12	1:F:28:LEU:HD22	1.81	0.61
1:G:24:GLU:HB2	1:G:270:LYS:HB3	1.82	0.61
1:H:47:THR:HG21	1:H:187:ILE:HG23	1.83	0.61
1:J:275:ARG:HB2	1:J:321:VAL:HG22	1.82	0.61
1:K:206:SER:HA	1:K:362:ASN:OD1	2.01	0.61
1:K:230:ALA:HA	1:K:233:ARG:HH22	1.65	0.61
1:K:328:LEU:O	1:K:332:MET:HG3	2.01	0.61
1:F:267:ARG:HH12	1:H:366:ARG:HB3	1.64	0.61
1:G:311:ARG:HD2	1:G:318:TYR:CE2	2.36	0.61
1:E:75:ILE:HD11	1:E:138:PRO:HB2	1.83	0.61
1:F:198:THR:HG1	1:F:351:TRP:CD1	2.18	0.61
1:F:364:ILE:HG12	1:H:226:LEU:HD23	1.81	0.61
1:G:233:ARG:NE	1:G:323:PHE:HA	2.12	0.61
1:C:206:SER:HA	1:C:362:ASN:OD1	2.01	0.61
1:E:182:MET:HA	1:E:182:MET:HE3	1.83	0.61
1:E:286:LEU:HD12	1:E:328:LEU:HD12	1.81	0.61
1:K:222:LEU:HD12	1:K:351:TRP:CZ2	2.36	0.61
1:C:47:THR:HG21	1:C:187:ILE:HG23	1.82	0.61
1:F:264:MET:HA	1:F:319:PRO:CB	2.21	0.61
1:G:193:THR:HG22	1:G:194:LEU:H	1.66	0.61
1:G:46:GLU:HB2	1:G:62:LEU:HD11	1.82	0.61
1:F:279:LEU:HD23	1:F:282:LEU:HD12	1.83	0.60
1:F:336:GLU:HA	1:F:339:PHE:CE2	2.36	0.60
1:I:243:SER:N	1:I:311:ARG:HE	1.99	0.60
1:B:25:LYS:NZ	1:B:27:ILE:HD12	2.16	0.60
1:A:105:MET:HE3	1:C:90:GLY:HA3	1.83	0.60
1:J:97:GLN:HA	1:J:219:ILE:HD11	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:233:ARG:HH21	1:K:326:GLY:H	1.49	0.60
1:L:131:ASN:O	1:L:135:GLN:HG2	2.02	0.60
1:L:239:GLN:CG	1:L:299:ASP:HA	2.32	0.60
1:B:125:VAL:HG23	1:B:126:ARG:H	1.66	0.60
1:B:140:VAL:HG12	1:B:169:PHE:HZ	1.65	0.60
1:F:189:HIS:HB3	1:F:343:PHE:CD1	2.37	0.60
1:F:233:ARG:NH1	1:F:234:VAL:HA	2.16	0.60
1:I:28:LEU:HG	1:I:35:LEU:H	1.66	0.60
1:J:241:ILE:O	1:J:244:PRO:HD2	2.01	0.60
1:B:369:GLN:HG3	1:B:370:ILE:HG12	1.83	0.60
1:C:70:LYS:HA	1:C:73:TYR:CE2	2.37	0.60
1:D:131:ASN:O	1:D:135:GLN:HG2	2.01	0.60
1:F:28:LEU:HD12	1:F:35:LEU:HB3	1.83	0.60
1:F:233:ARG:HD3	1:F:234:VAL:N	2.16	0.60
1:J:197:SER:H	1:J:227:HIS:HE1	1.48	0.60
1:L:167:TYR:HA	1:L:172:GLU:O	2.00	0.60
1:L:177:LEU:H	1:L:177:LEU:HD22	1.67	0.60
1:A:102:SER:HB2	1:C:86:PHE:CZ	2.37	0.60
1:H:156:LYS:HE3	1:H:167:TYR:CZ	2.36	0.60
1:J:189:HIS:HB3	1:J:343:PHE:CD1	2.37	0.60
1:J:189:HIS:HB3	1:J:343:PHE:HD1	1.67	0.60
1:L:34:PRO:O	1:L:37:THR:HG22	2.01	0.60
1:D:28:LEU:HG	1:D:35:LEU:N	2.16	0.60
1:D:271:VAL:HG22	1:D:272:LYS:H	1.66	0.60
1:G:76:LYS:HB2	1:G:79:ILE:HG12	1.83	0.60
1:G:369:GLN:HA	1:G:375:ASP:CB	2.30	0.60
1:H:328:LEU:O	1:H:332:MET:HG3	2.01	0.60
1:I:182:MET:HB2	1:I:332:MET:HE1	1.84	0.60
1:B:77:TYR:O	1:B:80:ARG:HG2	2.02	0.60
1:C:356:ARG:O	1:C:359:ILE:HG12	2.02	0.60
1:E:238:LEU:HG	1:E:240:GLU:H	1.67	0.60
1:F:195:ASN:HB2	1:F:227:HIS:HE2	1.67	0.60
1:H:369:GLN:HE22	1:H:372:VAL:HG22	1.67	0.60
1:A:243:SER:HB3	1:A:244:PRO:HD3	1.84	0.59
1:H:181:ILE:HG22	1:H:328:LEU:HD21	1.84	0.59
1:K:355:TRP:O	1:K:359:ILE:HG12	2.02	0.59
1:G:24:GLU:HG3	1:G:25:LYS:N	2.15	0.59
1:I:38:LEU:O	1:I:42:SER:HB3	2.02	0.59
1:L:300:THR:HG23	1:L:301:ALA:H	1.67	0.59
1:C:323:PHE:CD1	1:C:324:TYR:N	2.70	0.59
1:D:113:LEU:HD22	1:D:119:CYS:HB3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:70:LYS:HA	1:F:73:TYR:CE2	2.37	0.59
1:F:363:ARG:HG3	1:H:267:ARG:HH22	1.66	0.59
1:B:132:ILE:O	1:B:136:MET:HG2	2.01	0.59
1:G:25:LYS:NZ	1:G:272:LYS:HB2	2.16	0.59
1:I:25:LYS:HE2	1:I:271:VAL:CG2	2.32	0.59
1:C:303:LYS:O	1:C:307:VAL:HG13	2.03	0.59
1:F:189:HIS:HE1	1:F:321:VAL:HG21	1.66	0.59
1:F:266:HIS:CE1	1:F:268:GLU:HB3	2.38	0.59
1:D:369:GLN:OE1	1:E:193:THR:HG23	2.03	0.59
1:H:319:PRO:HB3	1:H:323:PHE:CG	2.37	0.59
1:D:25:LYS:HE2	1:D:271:VAL:HG11	1.84	0.59
1:L:176:PRO:O	1:L:180:LYS:HG3	2.02	0.59
1:L:247:VAL:O	1:L:248:GLU:C	2.46	0.59
1:A:222:LEU:HD11	1:A:343:PHE:CD1	2.34	0.59
1:F:28:LEU:HD13	1:F:28:LEU:H	1.68	0.59
1:G:24:GLU:HG3	1:G:25:LYS:H	1.67	0.59
1:B:195:ASN:ND2	1:B:347:ARG:HH21	2.01	0.59
1:F:181:ILE:HG21	1:F:328:LEU:HD11	1.84	0.59
1:F:206:SER:O	1:H:226:LEU:HD22	2.03	0.59
1:K:75:ILE:HA	1:K:135:GLN:NE2	2.18	0.59
1:A:70:LYS:HA	1:A:73:TYR:CE2	2.37	0.58
1:F:182:MET:HE2	1:F:332:MET:SD	2.42	0.58
1:G:33:TYR:HB3	1:G:38:LEU:HD21	1.85	0.58
1:J:275:ARG:HH12	1:J:347:ARG:HH22	1.51	0.58
1:D:363:ARG:HE	1:D:365:TYR:HA	1.67	0.58
1:H:239:GLN:HG3	1:H:304:LEU:HD22	1.85	0.58
1:L:69:LEU:HD12	1:L:134:ALA:HB2	1.84	0.58
1:G:70:LYS:HA	1:G:73:TYR:CE2	2.39	0.58
1:H:102:SER:HA	1:H:105:MET:HE2	1.86	0.58
1:L:38:LEU:O	1:L:42:SER:HB3	2.03	0.58
1:L:122:LEU:HD13	1:L:123:ASP:N	2.19	0.58
1:L:359:ILE:HG13	1:L:360:SER:N	2.18	0.58
1:H:159:LEU:HD21	1:H:173:GLU:HG2	1.86	0.58
1:J:77:TYR:O	1:J:80:ARG:HG2	2.03	0.58
1:K:373:GLY:O	1:K:374:SER:C	2.46	0.58
1:E:192:HIS:CE1	1:E:266:HIS:HE2	2.22	0.58
1:A:137:ALA:HB3	1:A:138:PRO:HD3	1.86	0.58
1:B:273:ASP:CG	1:B:275:ARG:HE	2.12	0.58
1:B:297:MET:HA	1:B:297:MET:HE3	1.85	0.58
1:C:166:LEU:HB2	1:C:174:PRO:HG3	1.84	0.58
1:E:276:ALA:HB2	1:E:321:VAL:HA	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:34:PRO:O	1:G:37:THR:HG22	2.04	0.58
1:G:225:PRO:HG2	1:G:226:LEU:HD12	1.86	0.58
1:H:329:TYR:HB3	1:H:334:ILE:HB	1.86	0.58
1:I:328:LEU:O	1:I:332:MET:HG3	2.03	0.58
1:J:47:THR:HG21	1:J:187:ILE:HG23	1.86	0.58
1:K:276:ALA:HA	1:K:279:LEU:HD12	1.86	0.58
1:I:233:ARG:CB	1:I:323:PHE:HA	2.28	0.58
1:A:356:ARG:O	1:A:359:ILE:HG23	2.04	0.58
1:B:334:ILE:HG12	1:B:342:LEU:HD11	1.85	0.58
1:G:75:ILE:HD11	1:G:138:PRO:HB2	1.86	0.58
1:K:156:LYS:HB2	1:K:159:LEU:HB2	1.85	0.58
1:D:196:ALA:HB3	1:D:227:HIS:CD2	2.38	0.57
1:E:140:VAL:HG12	1:E:169:PHE:HZ	1.69	0.57
1:B:126:ARG:HH21	1:B:129:THR:HG21	1.68	0.57
1:B:311:ARG:HA	1:B:314:HIS:ND1	2.19	0.57
1:B:328:LEU:O	1:B:332:MET:HG3	2.04	0.57
1:C:34:PRO:HB2	1:C:37:THR:HG23	1.86	0.57
1:H:231:ASN:OD1	1:H:336:GLU:HB3	2.05	0.57
1:K:299:ASP:HA	1:K:303:LYS:HD2	1.86	0.57
1:L:230:ALA:HA	1:L:233:ARG:HG2	1.87	0.57
1:D:369:GLN:HB2	1:E:194:LEU:HD23	1.85	0.57
1:G:195:ASN:HB2	1:G:227:HIS:NE2	2.19	0.57
1:K:241:ILE:O	1:K:244:PRO:HD2	2.04	0.57
1:A:211:PRO:O	1:A:214:VAL:HG22	2.05	0.57
1:C:92:PRO:HA	1:C:143:TRP:CD1	2.39	0.57
1:C:182:MET:HE2	1:C:332:MET:SD	2.44	0.57
1:K:27:ILE:HG12	1:K:28:LEU:HD22	1.85	0.57
1:L:38:LEU:HA	1:L:42:SER:HB3	1.87	0.57
1:D:196:ALA:HB3	1:D:227:HIS:HD2	1.70	0.57
1:E:230:ALA:HA	1:E:233:ARG:HD3	1.87	0.57
1:K:28:LEU:HG	1:K:35:LEU:H	1.70	0.57
1:K:70:LYS:HA	1:K:73:TYR:CE2	2.39	0.57
1:C:44:PHE:CD1	1:C:186:LEU:HB3	2.40	0.57
1:C:233:ARG:NH2	1:C:234:VAL:HB	2.19	0.57
1:D:33:TYR:HB3	1:D:38:LEU:HD11	1.87	0.57
1:F:370:ILE:HD12	1:F:370:ILE:H	1.70	0.57
1:G:156:LYS:HE2	1:G:167:TYR:CE1	2.40	0.57
1:J:47:THR:O	1:J:51:LEU:HG	2.05	0.57
1:L:136:MET:SD	1:L:348:SER:HB3	2.44	0.57
1:H:195:ASN:HB2	1:H:227:HIS:HE1	1.70	0.57
1:J:133:ILE:HG13	1:J:352:LEU:HD12	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:367:PRO:O	1:E:369:GLN:HG2	2.03	0.57
1:G:226:LEU:HD12	1:G:226:LEU:H	1.68	0.57
1:J:75:ILE:HD11	1:J:138:PRO:HB2	1.87	0.57
1:G:182:MET:HA	1:G:182:MET:HE3	1.87	0.57
1:H:233:ARG:NE	1:H:323:PHE:HA	2.18	0.57
1:I:58:THR:HG23	1:I:61:ALA:H	1.69	0.57
1:K:192:HIS:HE1	1:K:266:HIS:CE1	2.22	0.57
1:A:28:LEU:CD1	1:A:35:LEU:HB2	2.28	0.56
1:A:136:MET:HG2	1:A:345:VAL:HA	1.87	0.56
1:B:79:ILE:HD11	1:B:106:PHE:CE2	2.40	0.56
1:B:368:THR:HA	1:B:372:VAL:CB	2.35	0.56
1:G:103:LEU:HD21	1:G:135:GLN:HG3	1.86	0.56
1:H:52:LEU:HD13	1:H:353:ALA:HA	1.87	0.56
1:B:159:LEU:HD21	1:B:173:GLU:HG2	1.85	0.56
1:D:92:PRO:HG2	1:D:338:GLU:HG2	1.86	0.56
1:G:328:LEU:O	1:G:332:MET:HG3	2.06	0.56
1:G:335:PRO:HG2	1:G:338:GLU:HG2	1.86	0.56
1:H:44:PHE:O	1:H:48:THR:HG23	2.05	0.56
1:K:211:PRO:O	1:K:214:VAL:HG22	2.05	0.56
1:B:167:TYR:HA	1:B:172:GLU:O	2.06	0.56
1:B:298:PHE:HA	1:B:302:LEU:HD12	1.87	0.56
1:E:182:MET:HB2	1:E:332:MET:HE1	1.88	0.56
1:F:28:LEU:HD13	1:F:28:LEU:N	2.20	0.56
1:F:232:GLN:HB3	1:F:262:TRP:NE1	2.21	0.56
1:B:28:LEU:HD12	1:B:35:LEU:HB3	1.87	0.56
1:E:195:ASN:HD21	1:E:198:THR:H	1.53	0.56
1:F:267:ARG:HD3	1:H:364:ILE:HD11	1.86	0.56
1:L:132:ILE:HD12	1:L:352:LEU:HD21	1.86	0.56
1:B:366:ARG:HH11	1:B:367:PRO:HD2	1.70	0.56
1:D:190:ALA:O	1:D:347:ARG:HA	2.05	0.56
1:C:231:ASN:O	1:C:234:VAL:HG12	2.05	0.56
1:F:272:LYS:HA	1:F:318:TYR:HB3	1.87	0.56
1:H:145:HIS:CD2	1:H:153:VAL:H	2.22	0.56
1:I:304:LEU:HD13	1:I:324:TYR:HE2	1.69	0.56
1:B:156:LYS:HE3	1:B:167:TYR:CZ	2.40	0.56
1:D:286:LEU:HB3	1:D:331:GLU:HG2	1.88	0.56
1:K:231:ASN:ND2	1:K:339:PHE:HB2	2.21	0.56
1:A:311:ARG:HA	1:A:314:HIS:CE1	2.41	0.56
1:C:202:LEU:HD21	1:C:354:HIS:HB3	1.87	0.56
1:H:177:LEU:O	1:H:181:ILE:HG13	2.06	0.56
1:J:113:LEU:HD11	1:J:120:GLU:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:312:LEU:HD22	1:L:312:LEU:C	2.31	0.56
1:D:311:ARG:HD3	1:D:311:ARG:H	1.70	0.56
1:E:194:LEU:O	1:E:198:THR:HB	2.06	0.56
1:G:234:VAL:HG11	1:G:336:GLU:HG2	1.87	0.56
1:J:314:HIS:CD2	1:J:317:VAL:HG23	2.41	0.56
1:K:156:LYS:HB3	1:K:158:ASP:OD1	2.06	0.56
1:I:194:LEU:HB3	1:L:367:PRO:HD2	1.88	0.56
1:L:264:MET:CA	1:L:319:PRO:HA	2.36	0.56
1:E:92:PRO:HG3	1:E:147:ARG:NH1	2.21	0.55
1:E:150:TRP:CH2	1:I:74:ARG:HG3	2.42	0.55
1:L:49:LEU:HD12	1:L:57:PRO:HG3	1.88	0.55
1:L:304:LEU:HD12	1:L:323:PHE:CE1	2.42	0.55
1:A:27:ILE:HG13	1:A:274:PRO:HG3	1.88	0.55
1:A:28:LEU:HD13	1:A:28:LEU:N	2.21	0.55
1:I:102:SER:HB2	1:L:86:PHE:CZ	2.41	0.55
1:J:44:PHE:CZ	1:J:346:ALA:HA	2.42	0.55
1:J:327:ILE:H	1:J:327:ILE:HD12	1.71	0.55
1:K:31:ARG:CD	1:K:54:GLY:HA2	2.37	0.55
1:D:28:LEU:HB3	1:D:34:PRO:CA	2.35	0.55
1:D:129:THR:HG23	1:D:352:LEU:HD13	1.88	0.55
1:I:25:LYS:HE2	1:I:271:VAL:HG23	1.88	0.55
1:J:303:LYS:O	1:J:306:GLU:HG2	2.05	0.55
1:L:266:HIS:CB	1:L:269:TYR:HB2	2.30	0.55
1:A:272:LYS:HG3	1:A:319:PRO:HB2	1.88	0.55
1:C:203:VAL:HA	1:C:365:TYR:CD2	2.41	0.55
1:D:198:THR:HG1	1:D:351:TRP:CD1	2.25	0.55
1:E:126:ARG:HH21	1:E:356:ARG:NH1	2.01	0.55
1:E:141:ALA:HB3	1:E:168:MET:HE2	1.88	0.55
1:K:96:LEU:HG	1:K:219:ILE:HD13	1.87	0.55
1:K:103:LEU:HD22	1:K:135:GLN:HG2	1.88	0.55
1:L:216:SER:O	1:L:219:ILE:HG12	2.06	0.55
1:D:86:PHE:CE1	1:E:102:SER:HB2	2.41	0.55
1:F:206:SER:HA	1:F:361:ASP:CG	2.31	0.55
1:F:335:PRO:HG2	1:F:338:GLU:CG	2.35	0.55
1:G:206:SER:HB3	1:G:365:TYR:HD2	1.71	0.55
1:H:67:GLN:HA	1:H:70:LYS:HD3	1.88	0.55
1:I:231:ASN:OD1	1:I:336:GLU:HB3	2.07	0.55
1:K:31:ARG:NE	1:K:54:GLY:HA2	2.21	0.55
1:K:279:LEU:HA	1:K:282:LEU:HD12	1.88	0.55
1:L:91:HIS:CE1	1:L:93:MET:HB2	2.42	0.55
1:A:359:ILE:HD13	1:A:359:ILE:H	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:LYS:HE3	1:B:167:TYR:CE1	2.42	0.55
1:E:365:TYR:O	1:E:367:PRO:HD3	2.06	0.55
1:H:326:GLY:HA2	1:H:329:TYR:CD2	2.42	0.55
1:L:303:LYS:O	1:L:307:VAL:HG23	2.06	0.55
1:C:309:ALA:O	1:C:310:ASP:C	2.50	0.55
1:E:68:GLN:HG2	1:E:130:VAL:HG21	1.88	0.55
1:F:167:TYR:HA	1:F:172:GLU:O	2.07	0.55
1:I:371:TYR:HB2	1:L:268:GLU:OE2	2.07	0.55
1:K:47:THR:HG21	1:K:187:ILE:HG23	1.89	0.55
1:L:33:TYR:CE1	1:L:50:LEU:HD11	2.41	0.55
1:C:106:PHE:O	1:C:108:PRO:HD3	2.07	0.55
1:D:28:LEU:CG	1:D:35:LEU:H	2.19	0.55
1:D:364:ILE:HB	1:E:267:ARG:HH12	1.71	0.55
1:G:272:LYS:HG2	1:G:273:ASP:N	2.20	0.55
1:B:233:ARG:CG	1:B:263:GLY:HA3	2.32	0.55
1:C:77:TYR:O	1:C:80:ARG:HG2	2.06	0.55
1:F:102:SER:HB2	1:H:86:PHE:CE1	2.42	0.55
1:F:167:TYR:O	1:F:171:GLY:N	2.40	0.55
1:F:334:ILE:H	1:F:334:ILE:HD12	1.72	0.55
1:G:44:PHE:O	1:G:48:THR:HG23	2.07	0.55
1:G:69:LEU:HA	1:G:130:VAL:HG22	1.88	0.55
1:I:311:ARG:O	1:I:312:LEU:C	2.49	0.55
1:K:273:ASP:OD2	1:K:275:ARG:HB2	2.07	0.55
1:A:232:GLN:O	1:A:235:VAL:HG12	2.07	0.54
1:B:230:ALA:HA	1:B:322:ASP:HB3	1.89	0.54
1:C:206:SER:HB2	1:C:364:ILE:HA	1.89	0.54
1:F:272:LYS:HZ2	1:F:319:PRO:CD	2.20	0.54
1:G:131:ASN:O	1:G:135:GLN:HG2	2.07	0.54
1:H:100:VAL:HG21	1:H:219:ILE:HD11	1.89	0.54
1:H:241:ILE:O	1:H:242:GLY:C	2.50	0.54
1:I:82:MET:HG2	1:I:86:PHE:HE2	1.72	0.54
1:J:166:LEU:HD21	1:J:178:MET:HG2	1.88	0.54
1:K:222:LEU:HD11	1:K:343:PHE:CD2	2.43	0.54
1:D:82:MET:HG3	1:E:82:MET:HE2	1.87	0.54
1:G:113:LEU:CD2	1:G:120:GLU:HB3	2.37	0.54
1:J:27:ILE:HG22	1:J:269:TYR:HE1	1.71	0.54
1:J:31:ARG:NE	1:J:54:GLY:HA2	2.22	0.54
1:K:334:ILE:H	1:K:334:ILE:HD12	1.72	0.54
1:D:238:LEU:HD11	1:D:241:ILE:HB	1.89	0.54
1:E:235:VAL:HG23	1:E:304:LEU:HD22	1.90	0.54
1:G:113:LEU:HD21	1:G:120:GLU:HB3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:75:ILE:HA	1:K:135:GLN:HE22	1.71	0.54
1:L:140:VAL:HG12	1:L:169:PHE:HZ	1.72	0.54
1:B:272:LYS:HD2	1:B:311:ARG:HH22	1.73	0.54
1:D:234:VAL:HG21	1:D:303:LYS:HE2	1.88	0.54
1:G:77:TYR:O	1:G:80:ARG:HG2	2.07	0.54
1:G:127:ASN:O	1:G:130:VAL:HG12	2.08	0.54
1:L:166:LEU:HB3	1:L:174:PRO:HG3	1.89	0.54
1:B:38:LEU:O	1:B:42:SER:HB3	2.08	0.54
1:G:33:TYR:CD1	1:G:50:LEU:HD11	2.42	0.54
1:G:350:GLY:O	1:G:354:HIS:CD2	2.58	0.54
1:J:112:CYS:O	1:J:113:LEU:C	2.50	0.54
1:J:216:SER:O	1:J:219:ILE:HG12	2.07	0.54
1:A:53:ASP:OD1	1:A:54:GLY:N	2.40	0.54
1:B:301:ALA:HA	1:B:305:GLU:CD	2.33	0.54
1:C:305:GLU:O	1:C:308:CYS:HB3	2.07	0.54
1:D:49:LEU:HD23	1:D:57:PRO:HB3	1.88	0.54
1:D:301:ALA:O	1:D:305:GLU:HG2	2.07	0.54
1:F:371:TYR:CE1	1:F:373:GLY:HA3	2.43	0.54
1:J:63:ASN:O	1:J:67:GLN:HG2	2.08	0.54
1:B:135:GLN:C	1:B:138:PRO:HD2	2.32	0.54
1:C:33:TYR:CE1	1:C:50:LEU:HD11	2.43	0.54
1:C:100:VAL:HG21	1:C:219:ILE:CD1	2.38	0.54
1:E:70:LYS:C	1:E:72:ASN:H	2.15	0.54
1:F:75:ILE:HD12	1:F:142:MET:HE3	1.89	0.54
1:F:102:SER:HA	1:F:105:MET:HE2	1.90	0.54
1:F:235:VAL:O	1:F:236:GLY:C	2.50	0.54
1:I:86:PHE:CZ	1:L:102:SER:HB2	2.42	0.54
1:L:195:ASN:ND2	1:L:347:ARG:HE	2.06	0.54
1:C:318:TYR:N	1:C:319:PRO:HD2	2.23	0.54
1:F:132:ILE:O	1:F:136:MET:HG2	2.08	0.54
1:H:103:LEU:HG	1:H:107:TYR:HE2	1.71	0.54
1:H:369:GLN:NE2	1:H:372:VAL:HG22	2.23	0.54
1:I:243:SER:H	1:I:311:ARG:HE	1.55	0.54
1:I:266:HIS:CE1	1:I:268:GLU:HB2	2.43	0.54
1:J:327:ILE:O	1:J:331:GLU:HG2	2.07	0.54
1:B:137:ALA:HB3	1:B:138:PRO:HD3	1.90	0.54
1:E:264:MET:HE1	1:E:311:ARG:HB2	1.90	0.54
1:I:98:THR:HG21	1:L:102:SER:HB3	1.90	0.54
1:J:264:MET:SD	1:J:319:PRO:HA	2.48	0.54
1:L:182:MET:HA	1:L:182:MET:HE3	1.90	0.54
1:B:27:ILE:CG1	1:B:28:LEU:HD13	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:102:SER:HA	1:C:105:MET:HE2	1.90	0.54
1:D:27:ILE:HG13	1:D:28:LEU:HD13	1.90	0.54
1:F:86:PHE:CZ	1:H:102:SER:HB2	2.42	0.54
1:I:28:LEU:HD23	1:I:34:PRO:HB3	1.89	0.54
1:A:135:GLN:C	1:A:138:PRO:HD2	2.33	0.53
1:C:27:ILE:HG23	1:C:274:PRO:HG3	1.89	0.53
1:C:100:VAL:HG21	1:C:219:ILE:HD11	1.90	0.53
1:K:196:ALA:HB3	1:K:227:HIS:HD2	1.72	0.53
1:L:334:ILE:HG21	1:L:342:LEU:CD1	2.37	0.53
1:A:369:GLN:HB2	1:C:193:THR:CG2	2.38	0.53
1:F:96:LEU:CD1	1:F:139:LEU:HD11	2.37	0.53
1:I:160:SER:H	1:I:163:GLU:HB2	1.73	0.53
1:A:120:GLU:H	1:A:120:GLU:CD	2.15	0.53
1:I:28:LEU:HG	1:I:35:LEU:N	2.23	0.53
1:I:123:ASP:HB2	1:I:127:ASN:CG	2.34	0.53
1:K:144:GLU:HG2	1:K:147:ARG:NH2	2.24	0.53
1:L:159:LEU:HD21	1:L:173:GLU:HG2	1.90	0.53
1:D:34:PRO:HG2	1:D:37:THR:HG22	1.91	0.53
1:E:100:VAL:HG21	1:E:219:ILE:HD11	1.89	0.53
1:F:77:TYR:HB3	1:J:151:ASP:OD1	2.07	0.53
1:L:300:THR:HA	1:L:303:LYS:NZ	2.24	0.53
1:A:225:PRO:HD2	1:C:208:LEU:O	2.08	0.53
1:D:140:VAL:HG12	1:D:169:PHE:HZ	1.73	0.53
1:D:175:ASP:OD1	1:D:178:MET:HB2	2.09	0.53
1:F:264:MET:SD	1:F:319:PRO:HD3	2.47	0.53
1:K:182:MET:HB2	1:K:332:MET:HE1	1.90	0.53
1:K:335:PRO:HG2	1:K:338:GLU:HG2	1.91	0.53
1:L:365:TYR:O	1:L:367:PRO:HD3	2.08	0.53
1:A:162:ALA:HA	1:A:165:LEU:HD12	1.91	0.53
1:C:120:GLU:CD	1:C:120:GLU:H	2.16	0.53
1:K:34:PRO:HG2	1:K:37:THR:HB	1.89	0.53
1:E:196:ALA:HB3	1:E:227:HIS:ND1	2.24	0.53
1:G:222:LEU:HD11	1:G:343:PHE:HD2	1.73	0.53
1:E:233:ARG:HH12	1:E:326:GLY:HA3	1.72	0.53
1:F:27:ILE:CG1	1:F:28:LEU:HD13	2.37	0.53
1:F:275:ARG:HB3	1:F:321:VAL:CG1	2.39	0.53
1:G:276:ALA:HB2	1:G:321:VAL:HA	1.91	0.53
1:K:320:ASN:CG	1:K:321:VAL:H	2.17	0.53
1:F:102:SER:HB2	1:H:86:PHE:CZ	2.44	0.53
1:F:225:PRO:HG2	1:F:226:LEU:HD13	1.91	0.53
1:G:92:PRO:HA	1:G:143:TRP:CD1	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:311:ARG:HD2	1:G:318:TYR:HE2	1.74	0.53
1:H:239:GLN:H	1:H:239:GLN:CD	2.17	0.53
1:I:206:SER:O	1:L:226:LEU:HD12	2.09	0.53
1:K:69:LEU:HA	1:K:130:VAL:HG22	1.91	0.53
1:K:195:ASN:HB3	1:K:227:HIS:NE2	2.23	0.53
1:K:327:ILE:O	1:K:331:GLU:HG2	2.09	0.53
1:L:28:LEU:HD11	1:L:192:HIS:CE1	2.44	0.53
1:B:182:MET:O	1:B:186:LEU:HG	2.09	0.53
1:I:44:PHE:HA	1:I:187:ILE:HG12	1.90	0.53
1:I:370:ILE:HG13	1:I:370:ILE:O	2.09	0.53
1:L:132:ILE:HG21	1:L:215:ILE:HG13	1.90	0.53
1:L:142:MET:HG3	1:L:152:PRO:HB3	1.90	0.53
1:F:113:LEU:HD22	1:F:119:CYS:HB3	1.91	0.52
1:F:226:LEU:HD22	1:H:208:LEU:HG	1.90	0.52
1:F:264:MET:O	1:F:318:TYR:C	2.52	0.52
1:J:68:GLN:HG2	1:J:130:VAL:HG11	1.91	0.52
1:J:76:LYS:HB2	1:J:79:ILE:HG12	1.90	0.52
1:L:300:THR:HA	1:L:303:LYS:HZ3	1.73	0.52
1:D:128:MET:HE2	1:D:128:MET:HA	1.91	0.52
1:D:206:SER:O	1:E:226:LEU:HD12	2.09	0.52
1:E:127:ASN:O	1:E:130:VAL:HG12	2.08	0.52
1:E:156:LYS:HE3	1:E:167:TYR:CZ	2.44	0.52
1:F:31:ARG:HG3	1:F:50:LEU:O	2.09	0.52
1:F:177:LEU:O	1:F:181:ILE:HG13	2.08	0.52
1:K:127:ASN:O	1:K:130:VAL:HG12	2.09	0.52
1:K:241:ILE:HB	1:K:244:PRO:HG2	1.92	0.52
1:B:63:ASN:HD21	1:B:67:GLN:HE21	1.57	0.52
1:C:30:TYR:HD2	1:C:38:LEU:HD22	1.74	0.52
1:I:28:LEU:HB3	1:I:34:PRO:CA	2.32	0.52
1:I:135:GLN:O	1:I:136:MET:C	2.53	0.52
1:K:28:LEU:HD13	1:K:28:LEU:N	2.24	0.52
1:C:198:THR:HA	1:C:351:TRP:CD1	2.44	0.52
1:C:279:LEU:O	1:C:283:VAL:HG23	2.09	0.52
1:C:281:LYS:C	1:C:281:LYS:HD3	2.34	0.52
1:J:211:PRO:O	1:J:214:VAL:HG22	2.10	0.52
1:J:222:LEU:HD13	1:J:343:PHE:CD2	2.44	0.52
1:J:335:PRO:HG2	1:J:338:GLU:CG	2.39	0.52
1:L:126:ARG:HA	1:L:129:THR:HB	1.89	0.52
1:B:27:ILE:O	1:B:28:LEU:HB2	2.09	0.52
1:D:366:ARG:HB3	1:E:267:ARG:HD2	1.92	0.52
1:E:135:GLN:C	1:E:138:PRO:HD2	2.34	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:137:ALA:HB3	1:H:138:PRO:HD3	1.91	0.52
1:I:125:VAL:HG13	1:I:355:TRP:CZ3	2.44	0.52
1:I:279:LEU:HD23	1:I:282:LEU:HD12	1.92	0.52
1:L:239:GLN:HG2	1:L:299:ASP:HA	1.90	0.52
1:I:304:LEU:HD12	1:I:305:GLU:N	2.24	0.52
1:K:25:LYS:HE2	1:K:271:VAL:HG12	1.92	0.52
1:B:76:LYS:NZ	1:B:106:PHE:HB3	2.25	0.52
1:H:198:THR:O	1:H:202:LEU:HG	2.09	0.52
1:I:126:ARG:HA	1:I:129:THR:HB	1.91	0.52
1:J:243:SER:HB2	1:J:306:GLU:OE1	2.09	0.52
1:J:363:ARG:HG2	1:J:365:TYR:N	2.17	0.52
1:A:166:LEU:HB2	1:A:174:PRO:HG3	1.92	0.52
1:A:177:LEU:O	1:A:181:ILE:HG13	2.10	0.52
1:G:272:LYS:NZ	1:G:272:LYS:HB3	2.24	0.52
1:K:30:TYR:CD1	1:K:35:LEU:HD11	2.45	0.52
1:K:222:LEU:HD11	1:K:343:PHE:HD2	1.75	0.52
1:B:195:ASN:HB3	1:B:227:HIS:HE1	1.74	0.52
1:E:222:LEU:HD13	1:E:343:PHE:HD2	1.75	0.52
1:E:275:ARG:HH12	1:E:347:ARG:HH22	1.58	0.52
1:K:203:VAL:HA	1:K:365:TYR:CD2	2.45	0.52
1:K:211:PRO:HG3	1:K:355:TRP:CH2	2.45	0.52
1:A:63:ASN:O	1:A:67:GLN:HG2	2.10	0.52
1:D:183:ASP:O	1:D:187:ILE:HG13	2.10	0.52
1:G:66:SER:O	1:G:70:LYS:HG3	2.10	0.52
1:G:144:GLU:HG2	1:G:147:ARG:NH2	2.25	0.52
1:H:192:HIS:HE1	1:H:266:HIS:NE2	2.08	0.52
1:H:278:ILE:O	1:H:282:LEU:HG	2.10	0.52
1:A:72:ASN:HB3	1:A:131:ASN:HA	1.93	0.51
1:D:311:ARG:HA	1:D:314:HIS:HB2	1.91	0.51
1:E:49:LEU:HD11	1:E:65:PHE:HB3	1.91	0.51
1:H:355:TRP:NE1	1:H:359:ILE:HD11	2.25	0.51
1:I:368:THR:HA	1:I:371:TYR:HB3	1.92	0.51
1:J:24:GLU:OE1	1:J:25:LYS:HG3	2.10	0.51
1:G:48:THR:HG22	1:G:349:ALA:HB2	1.92	0.51
1:G:238:LEU:HD22	1:G:245:LYS:HZ2	1.75	0.51
1:G:278:ILE:O	1:G:282:LEU:HG	2.10	0.51
1:K:233:ARG:HH21	1:K:326:GLY:N	2.08	0.51
1:L:198:THR:O	1:L:202:LEU:HG	2.10	0.51
1:B:195:ASN:HB3	1:B:227:HIS:CE1	2.45	0.51
1:B:215:ILE:HD11	1:B:352:LEU:HG	1.92	0.51
1:C:70:LYS:HE3	1:C:157:HIS:CD2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:231:ASN:OD1	1:C:336:GLU:HB3	2.11	0.51
1:E:264:MET:HA	1:E:319:PRO:HA	1.91	0.51
1:F:129:THR:HG23	1:F:352:LEU:HD13	1.91	0.51
1:G:97:GLN:HA	1:G:219:ILE:CD1	2.39	0.51
1:H:266:HIS:CG	1:H:269:TYR:HB2	2.44	0.51
1:B:70:LYS:HA	1:B:73:TYR:CE2	2.44	0.51
1:B:206:SER:HB3	1:B:365:TYR:CD2	2.46	0.51
1:B:304:LEU:HB3	1:B:324:TYR:CE1	2.46	0.51
1:F:272:LYS:HZ1	1:F:319:PRO:CG	2.24	0.51
1:G:356:ARG:O	1:G:359:ILE:HG12	2.11	0.51
1:J:70:LYS:HA	1:J:73:TYR:CZ	2.45	0.51
1:J:334:ILE:HG12	1:J:342:LEU:HD21	1.91	0.51
1:K:24:GLU:C	1:K:25:LYS:HG3	2.35	0.51
1:L:59:LYS:HG3	1:L:60:LYS:HD2	1.92	0.51
1:L:233:ARG:NH1	1:L:325:SER:HB2	2.25	0.51
1:B:303:LYS:O	1:B:307:VAL:HG12	2.11	0.51
1:F:314:HIS:HB3	1:F:317:VAL:HB	1.93	0.51
1:I:70:LYS:HA	1:I:73:TYR:CZ	2.45	0.51
1:J:96:LEU:HG	1:J:219:ILE:HD12	1.92	0.51
1:A:32:GLY:HA2	1:C:374:SER:O	2.10	0.51
1:B:82:MET:HG3	1:B:83:MET:N	2.26	0.51
1:D:28:LEU:O	1:D:34:PRO:HA	2.11	0.51
1:D:124:TYR:HE2	1:D:211:PRO:HD2	1.76	0.51
1:I:111:GLU:CD	1:I:111:GLU:H	2.19	0.51
1:I:194:LEU:HD12	1:L:367:PRO:HG2	1.92	0.51
1:K:43:THR:H	1:K:46:GLU:HB3	1.75	0.51
1:L:272:LYS:HD3	1:L:277:THR:HG22	1.93	0.51
1:D:43:THR:HG23	1:D:46:GLU:H	1.75	0.51
1:F:38:LEU:O	1:F:39:ALA:C	2.54	0.51
1:I:241:ILE:HA	1:I:311:ARG:NH2	2.26	0.51
1:A:215:ILE:O	1:A:219:ILE:HG13	2.11	0.51
1:D:28:LEU:HG	1:D:35:LEU:HB2	1.93	0.51
1:D:367:PRO:HG2	1:E:194:LEU:HD12	1.92	0.51
1:E:132:ILE:HG21	1:E:215:ILE:HG13	1.93	0.51
1:I:127:ASN:O	1:I:130:VAL:HG22	2.11	0.51
1:K:263:GLY:O	1:K:323:PHE:HB2	2.11	0.51
1:B:197:SER:H	1:B:227:HIS:CE1	2.28	0.51
1:B:199:PHE:HA	1:B:202:LEU:HD12	1.93	0.51
1:C:149:GLY:HA2	1:L:77:TYR:CE2	2.45	0.51
1:G:49:LEU:CD1	1:G:62:LEU:HA	2.41	0.51
1:G:238:LEU:H	1:G:238:LEU:CD2	2.19	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:334:ILE:HG21	1:G:342:LEU:HD11	1.93	0.51
1:K:121:ASP:C	1:K:122:LEU:HD12	2.35	0.51
1:L:47:THR:O	1:L:51:LEU:HG	2.10	0.51
1:F:272:LYS:HZ2	1:F:319:PRO:HD2	1.75	0.51
1:I:73:TYR:HD1	1:I:134:ALA:HB1	1.76	0.51
1:K:275:ARG:O	1:K:279:LEU:HG	2.11	0.51
1:G:167:TYR:HA	1:G:172:GLU:O	2.11	0.50
1:G:279:LEU:HD23	1:G:282:LEU:HD12	1.92	0.50
1:K:28:LEU:HG	1:K:35:LEU:N	2.26	0.50
1:K:215:ILE:O	1:K:219:ILE:HG13	2.11	0.50
1:L:303:LYS:HG3	1:L:304:LEU:HD22	1.94	0.50
1:A:222:LEU:HD12	1:A:351:TRP:CZ2	2.46	0.50
1:B:366:ARG:O	1:B:369:GLN:HG2	2.12	0.50
1:E:308:CYS:HB3	1:E:323:PHE:CE2	2.46	0.50
1:F:323:PHE:HD2	1:F:324:TYR:CE1	2.29	0.50
1:F:366:ARG:HB3	1:H:267:ARG:HD2	1.92	0.50
1:G:369:GLN:CA	1:G:375:ASP:HB3	2.34	0.50
1:I:83:MET:SD	1:I:142:MET:HE3	2.51	0.50
1:I:97:GLN:HA	1:I:219:ILE:CD1	2.41	0.50
1:I:302:LEU:O	1:I:305:GLU:HG3	2.11	0.50
1:J:238:LEU:HB3	1:J:303:LYS:HE3	1.92	0.50
1:A:269:TYR:CE1	1:A:274:PRO:HD2	2.46	0.50
1:E:24:GLU:CB	1:E:27:ILE:HG23	2.36	0.50
1:G:25:LYS:HZ2	1:G:272:LYS:HB2	1.75	0.50
1:H:182:MET:HB2	1:H:332:MET:HE1	1.93	0.50
1:H:237:MET:SD	1:H:237:MET:N	2.80	0.50
1:D:47:THR:HG21	1:D:187:ILE:HG23	1.93	0.50
1:I:156:LYS:HD3	1:I:159:LEU:HD11	1.94	0.50
1:K:52:LEU:HB3	1:K:126:ARG:HH12	1.76	0.50
1:K:203:VAL:HA	1:K:365:TYR:HD2	1.76	0.50
1:A:30:TYR:CE1	1:A:35:LEU:HD21	2.46	0.50
1:A:125:VAL:O	1:A:126:ARG:HB2	2.11	0.50
1:A:231:ASN:HA	1:A:234:VAL:HG23	1.91	0.50
1:A:238:LEU:HD21	1:A:242:GLY:HA2	1.93	0.50
1:A:271:VAL:HG22	1:A:272:LYS:H	1.77	0.50
1:B:31:ARG:NE	1:B:54:GLY:HA2	2.26	0.50
1:E:38:LEU:O	1:E:42:SER:HB3	2.11	0.50
1:F:181:ILE:HB	1:F:332:MET:CE	2.41	0.50
1:F:311:ARG:HE	1:F:318:TYR:HE1	1.60	0.50
1:H:206:SER:HB2	1:H:364:ILE:HA	1.93	0.50
1:J:36:GLU:H	1:J:36:GLU:CD	2.19	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:110:THR:HG22	1:K:112:CYS:H	1.77	0.50
1:K:243:SER:HB2	1:K:244:PRO:HD3	1.93	0.50
1:L:156:LYS:HE2	1:L:167:TYR:CZ	2.46	0.50
1:A:156:LYS:HB2	1:A:159:LEU:HB2	1.92	0.50
1:H:327:ILE:O	1:H:331:GLU:HG2	2.11	0.50
1:I:279:LEU:O	1:I:283:VAL:HG13	2.12	0.50
1:E:167:TYR:HB2	1:E:174:PRO:HD3	1.93	0.50
1:F:28:LEU:HD12	1:F:35:LEU:CB	2.42	0.50
1:H:47:THR:O	1:H:50:LEU:HG	2.11	0.50
1:H:358:GLN:HE22	1:H:365:TYR:HE1	1.60	0.50
1:I:28:LEU:HG	1:I:35:LEU:HB2	1.94	0.50
1:K:199:PHE:HA	1:K:202:LEU:HD12	1.92	0.50
1:L:195:ASN:HD21	1:L:347:ARG:HE	1.59	0.50
1:L:264:MET:CB	1:L:319:PRO:HA	2.41	0.50
1:B:311:ARG:HD2	1:B:318:TYR:CD1	2.44	0.50
1:G:153:VAL:HG21	1:G:168:MET:O	2.12	0.50
1:I:104:GLY:O	1:I:108:PRO:HB3	2.11	0.50
1:J:372:VAL:HB	1:J:375:ASP:CA	2.41	0.50
1:K:222:LEU:HG	1:K:227:HIS:CE1	2.46	0.50
1:A:111:GLU:O	1:A:113:LEU:HG	2.12	0.50
1:C:199:PHE:O	1:C:203:VAL:HG13	2.12	0.50
1:D:91:HIS:HD2	1:D:93:MET:HB2	1.77	0.50
1:L:33:TYR:CZ	1:L:50:LEU:HD11	2.46	0.50
1:C:198:THR:O	1:C:202:LEU:HD23	2.13	0.49
1:H:70:LYS:HB3	1:H:157:HIS:CD2	2.47	0.49
1:I:86:PHE:CE1	1:L:102:SER:HB2	2.47	0.49
1:J:247:VAL:O	1:J:248:GLU:C	2.54	0.49
1:K:49:LEU:HD11	1:K:65:PHE:HB3	1.94	0.49
1:L:246:ASN:O	1:L:248:GLU:HG3	2.12	0.49
1:C:206:SER:HB3	1:C:365:TYR:CD2	2.47	0.49
1:D:28:LEU:CD1	1:D:35:LEU:HB2	2.41	0.49
1:D:335:PRO:HG2	1:D:338:GLU:HG3	1.93	0.49
1:E:182:MET:O	1:E:186:LEU:HG	2.13	0.49
1:G:233:ARG:HE	1:G:323:PHE:CA	2.19	0.49
1:H:36:GLU:CD	1:H:36:GLU:H	2.20	0.49
1:K:123:ASP:CG	1:K:124:TYR:H	2.18	0.49
1:B:271:VAL:HA	1:B:318:TYR:CD2	2.47	0.49
1:D:85:HIS:HD2	1:E:81:GLN:NE2	2.09	0.49
1:E:198:THR:O	1:E:202:LEU:HG	2.13	0.49
1:F:27:ILE:CG1	1:F:274:PRO:HG3	2.40	0.49
1:F:109:GLY:HA3	1:F:210:THR:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:233:ARG:HB3	1:H:233:ARG:CZ	2.42	0.49
1:J:31:ARG:CZ	1:J:54:GLY:HA2	2.42	0.49
1:K:156:LYS:HD2	1:K:159:LEU:CD1	2.42	0.49
1:A:34:PRO:HG2	1:A:37:THR:CB	2.39	0.49
1:C:156:LYS:HE3	1:C:167:TYR:CZ	2.47	0.49
1:C:273:ASP:OD1	1:C:274:PRO:HD2	2.12	0.49
1:D:47:THR:O	1:D:51:LEU:HG	2.12	0.49
1:D:314:HIS:HB3	1:D:317:VAL:HG23	1.94	0.49
1:D:367:PRO:HG3	1:E:199:PHE:CD1	2.47	0.49
1:I:68:GLN:HG2	1:I:130:VAL:HG21	1.94	0.49
1:L:285:GLN:O	1:L:288:ALA:HB3	2.12	0.49
1:A:269:TYR:C	1:A:271:VAL:N	2.71	0.49
1:B:368:THR:HG23	1:B:372:VAL:HB	1.93	0.49
1:C:75:ILE:HD11	1:C:138:PRO:HB2	1.93	0.49
1:H:195:ASN:HB2	1:H:227:HIS:CE1	2.47	0.49
1:L:156:LYS:HB3	1:L:158:ASP:OD1	2.12	0.49
1:C:38:LEU:O	1:C:39:ALA:C	2.55	0.49
1:C:302:LEU:O	1:C:306:GLU:HG2	2.13	0.49
1:E:71:ASP:CG	1:E:157:HIS:HE1	2.21	0.49
1:J:175:ASP:OD1	1:J:175:ASP:N	2.46	0.49
1:A:79:ILE:O	1:A:82:MET:HG2	2.13	0.49
1:D:364:ILE:HG13	1:E:267:ARG:HH22	1.78	0.49
1:H:80:ARG:O	1:H:84:ARG:HG3	2.12	0.49
1:D:334:ILE:H	1:D:334:ILE:HD12	1.78	0.49
1:J:68:GLN:CD	1:J:130:VAL:HG11	2.38	0.49
1:J:304:LEU:HD12	1:J:323:PHE:CE1	2.47	0.49
1:J:374:SER:O	1:J:375:ASP:C	2.56	0.49
1:K:177:LEU:O	1:K:181:ILE:HG13	2.12	0.49
1:A:100:VAL:HG21	1:A:219:ILE:HD11	1.93	0.49
1:E:363:ARG:NH2	1:E:365:TYR:HA	2.28	0.49
1:G:222:LEU:HD23	1:G:344:ALA:HB2	1.94	0.49
1:G:271:VAL:HB	1:G:318:TYR:CE1	2.48	0.49
1:H:334:ILE:HD13	1:H:342:LEU:CD1	2.42	0.49
1:K:299:ASP:H	1:K:303:LYS:HE2	1.78	0.49
1:L:28:LEU:HD12	1:L:31:ARG:HH21	1.78	0.49
1:D:354:HIS:O	1:D:358:GLN:HG2	2.13	0.49
1:J:176:PRO:O	1:J:180:LYS:HG2	2.13	0.49
1:J:241:ILE:HD12	1:J:242:GLY:N	2.27	0.49
1:B:215:ILE:O	1:B:219:ILE:HG13	2.14	0.48
1:B:222:LEU:HD23	1:B:344:ALA:HB2	1.94	0.48
1:F:69:LEU:HD12	1:F:134:ALA:HB2	1.93	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:124:TYR:O	1:F:128:MET:HG2	2.13	0.48
1:F:267:ARG:NH1	1:H:366:ARG:HB3	2.27	0.48
1:J:27:ILE:O	1:J:28:LEU:HB2	2.13	0.48
1:L:59:LYS:HG3	1:L:60:LYS:N	2.28	0.48
1:L:125:VAL:HG13	1:L:355:TRP:CZ3	2.48	0.48
1:A:238:LEU:HB3	1:A:303:LYS:HD2	1.94	0.48
1:C:27:ILE:HD12	1:C:274:PRO:HD3	1.94	0.48
1:D:127:ASN:O	1:D:130:VAL:HG12	2.13	0.48
1:F:24:GLU:OE1	1:F:25:LYS:HG3	2.13	0.48
1:G:272:LYS:HE2	1:G:274:PRO:HD3	1.95	0.48
1:I:338:GLU:O	1:I:342:LEU:HG	2.13	0.48
1:H:63:ASN:O	1:H:67:GLN:HG2	2.13	0.48
1:I:75:ILE:HD11	1:I:138:PRO:HB2	1.95	0.48
1:L:188:LEU:HD21	1:L:278:ILE:HB	1.95	0.48
1:D:233:ARG:CZ	1:D:233:ARG:HA	2.43	0.48
1:E:35:LEU:O	1:E:39:ALA:N	2.46	0.48
1:H:93:MET:SD	1:H:341:ALA:HA	2.54	0.48
1:H:222:LEU:CD1	1:H:227:HIS:HD2	2.25	0.48
1:I:198:THR:O	1:I:202:LEU:HG	2.13	0.48
1:J:192:HIS:HB3	1:J:195:ASN:HD22	1.78	0.48
1:L:183:ASP:O	1:L:187:ILE:HG13	2.12	0.48
1:A:343:PHE:CE1	1:A:347:ARG:HG3	2.48	0.48
1:C:31:ARG:NE	1:C:54:GLY:HA2	2.28	0.48
1:D:25:LYS:C	1:D:27:ILE:H	2.21	0.48
1:D:91:HIS:CD2	1:D:93:MET:H	2.32	0.48
1:F:194:LEU:O	1:H:367:PRO:HD2	2.14	0.48
1:F:233:ARG:HH21	1:F:327:ILE:CD1	2.21	0.48
1:F:356:ARG:O	1:F:359:ILE:HG23	2.13	0.48
1:J:347:ARG:HB3	1:J:351:TRP:CE2	2.49	0.48
1:K:335:PRO:HG2	1:K:338:GLU:CG	2.43	0.48
1:L:34:PRO:HB2	1:L:37:THR:HB	1.96	0.48
1:L:303:LYS:O	1:L:306:GLU:HG2	2.13	0.48
1:A:318:TYR:HB3	1:A:319:PRO:HD2	1.95	0.48
1:B:181:ILE:HD13	1:B:286:LEU:HG	1.96	0.48
1:E:144:GLU:O	1:E:147:ARG:HG2	2.13	0.48
1:F:104:GLY:C	1:F:106:PHE:H	2.21	0.48
1:F:139:LEU:HD12	1:F:140:VAL:N	2.28	0.48
1:H:77:TYR:O	1:H:80:ARG:HG2	2.13	0.48
1:I:245:LYS:H	1:I:245:LYS:HD3	1.78	0.48
1:J:363:ARG:NE	1:J:365:TYR:HA	2.28	0.48
1:K:25:LYS:HD3	1:K:269:TYR:HA	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:49:LEU:HD11	1:L:65:PHE:HB3	1.94	0.48
1:L:239:GLN:CA	1:L:303:LYS:HB3	2.42	0.48
1:A:86:PHE:CZ	1:C:102:SER:HB2	2.49	0.48
1:A:192:HIS:HE1	1:A:266:HIS:CE1	2.32	0.48
1:B:235:VAL:C	1:B:303:LYS:HZ2	2.21	0.48
1:C:31:ARG:CD	1:C:54:GLY:HA2	2.44	0.48
1:C:150:TRP:CE2	1:L:74:ARG:HD3	2.49	0.48
1:E:28:LEU:HD23	1:E:35:LEU:HD22	1.95	0.48
1:E:192:HIS:CD2	1:E:193:THR:H	2.31	0.48
1:E:206:SER:HB2	1:E:363:ARG:O	2.13	0.48
1:F:273:ASP:OD2	1:F:320:ASN:HA	2.14	0.48
1:G:216:SER:O	1:G:219:ILE:HG12	2.13	0.48
1:I:82:MET:HG2	1:I:86:PHE:CE2	2.48	0.48
1:I:245:LYS:HD3	1:I:245:LYS:N	2.29	0.48
1:K:323:PHE:O	1:K:324:TYR:HB2	2.14	0.48
1:A:241:ILE:O	1:A:244:PRO:HD2	2.14	0.48
1:B:156:LYS:HD2	1:B:159:LEU:HD22	1.95	0.48
1:C:304:LEU:HB3	1:C:324:TYR:CE1	2.48	0.48
1:E:318:TYR:HB3	1:E:319:PRO:HD2	1.95	0.48
1:G:49:LEU:HD11	1:G:65:PHE:HB3	1.96	0.48
1:G:215:ILE:HD11	1:G:352:LEU:HD23	1.95	0.48
1:I:202:LEU:HB3	1:I:365:TYR:CZ	2.49	0.48
1:A:91:HIS:HD2	1:A:93:MET:HB2	1.78	0.48
1:B:96:LEU:HG	1:B:219:ILE:HD13	1.95	0.48
1:E:243:SER:N	1:E:244:PRO:HD2	2.29	0.48
1:H:323:PHE:O	1:H:324:TYR:HB2	2.13	0.48
1:I:31:ARG:H	1:L:374:SER:HA	1.77	0.48
1:K:40:GLU:HG2	1:K:41:ASN:CG	2.39	0.48
1:L:93:MET:HE1	1:L:344:ALA:HB2	1.95	0.48
1:A:277:THR:O	1:A:281:LYS:HD3	2.14	0.48
1:B:366:ARG:NH1	1:B:367:PRO:HD2	2.28	0.48
1:E:166:LEU:HB3	1:E:174:PRO:HB3	1.96	0.48
1:E:356:ARG:O	1:E:359:ILE:HG12	2.14	0.48
1:F:194:LEU:HD12	1:H:367:PRO:HG2	1.95	0.48
1:F:272:LYS:HZ1	1:F:319:PRO:HG3	1.78	0.48
1:F:367:PRO:HG2	1:H:194:LEU:HB3	1.95	0.48
1:H:92:PRO:HA	1:H:143:TRP:CD1	2.49	0.48
1:H:311:ARG:O	1:H:312:LEU:C	2.56	0.48
1:K:156:LYS:HE3	1:K:167:TYR:CZ	2.48	0.48
1:L:129:THR:HG23	1:L:352:LEU:HB3	1.96	0.48
1:B:324:TYR:HD1	1:B:327:ILE:HD12	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:266:HIS:HB3	1:E:269:TYR:HB2	1.95	0.47
1:G:72:ASN:HD22	1:G:130:VAL:HG13	1.79	0.47
1:G:202:LEU:HD22	1:G:358:GLN:HB2	1.96	0.47
1:H:233:ARG:O	1:H:235:VAL:HG23	2.14	0.47
1:A:144:GLU:O	1:A:147:ARG:HG2	2.15	0.47
1:E:125:VAL:O	1:E:126:ARG:HB3	2.12	0.47
1:L:324:TYR:HA	1:L:327:ILE:HD13	1.95	0.47
1:A:91:HIS:CD2	1:A:93:MET:H	2.32	0.47
1:D:273:ASP:CG	1:D:275:ARG:HE	2.22	0.47
1:D:363:ARG:HG3	1:D:365:TYR:H	1.78	0.47
1:G:53:ASP:OD1	1:G:54:GLY:N	2.47	0.47
1:G:320:ASN:H	1:G:323:PHE:HE2	1.61	0.47
1:H:55:GLU:O	1:H:56:LEU:C	2.57	0.47
1:J:356:ARG:O	1:J:359:ILE:HG12	2.14	0.47
1:K:24:GLU:CG	1:K:25:LYS:H	2.27	0.47
1:A:359:ILE:HG12	1:A:360:SER:N	2.30	0.47
1:B:304:LEU:CG	1:B:327:ILE:HD11	2.39	0.47
1:C:124:TYR:HE2	1:C:211:PRO:HD2	1.80	0.47
1:F:207:THR:HA	1:H:226:LEU:HB2	1.96	0.47
1:F:366:ARG:HH22	1:H:192:HIS:HD1	1.61	0.47
1:G:33:TYR:CB	1:G:38:LEU:HD21	2.45	0.47
1:L:135:GLN:C	1:L:138:PRO:HD2	2.39	0.47
1:A:68:GLN:NE2	1:A:130:VAL:HG11	2.29	0.47
1:A:175:ASP:OD1	1:A:178:MET:HB2	2.14	0.47
1:C:202:LEU:HD21	1:C:354:HIS:CB	2.45	0.47
1:D:86:PHE:CZ	1:E:102:SER:HB2	2.49	0.47
1:D:222:LEU:HD11	1:D:343:PHE:CD2	2.49	0.47
1:E:279:LEU:HD12	1:E:321:VAL:O	2.15	0.47
1:F:27:ILE:HG12	1:F:28:LEU:CD1	2.40	0.47
1:G:79:ILE:HD11	1:G:106:PHE:CE2	2.46	0.47
1:G:137:ALA:HB1	1:G:165:LEU:HG	1.96	0.47
1:I:28:LEU:O	1:I:34:PRO:HA	2.15	0.47
1:K:175:ASP:OD2	1:K:177:LEU:HB3	2.13	0.47
1:L:202:LEU:HD21	1:L:354:HIS:HB3	1.95	0.47
1:L:274:PRO:O	1:L:278:ILE:HG13	2.15	0.47
1:B:38:LEU:O	1:B:39:ALA:C	2.55	0.47
1:D:177:LEU:O	1:D:181:ILE:HG13	2.15	0.47
1:E:122:LEU:HG	1:E:123:ASP:N	2.29	0.47
1:E:280:HIS:O	1:E:283:VAL:HG22	2.14	0.47
1:E:328:LEU:O	1:E:332:MET:HG3	2.14	0.47
1:F:28:LEU:O	1:F:34:PRO:HA	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:30:TYR:CE1	1:I:191:GLU:HB3	2.49	0.47
1:J:314:HIS:HD2	1:J:317:VAL:HG23	1.77	0.47
1:L:155:PRO:HG3	1:L:168:MET:SD	2.55	0.47
1:A:121:ASP:C	1:A:122:LEU:HD12	2.40	0.47
1:A:142:MET:HA	1:A:152:PRO:HB3	1.96	0.47
1:A:269:TYR:C	1:A:271:VAL:H	2.21	0.47
1:B:247:VAL:O	1:B:248:GLU:C	2.58	0.47
1:C:283:VAL:HG21	1:C:327:ILE:HD11	1.97	0.47
1:C:327:ILE:HG13	1:C:328:LEU:N	2.29	0.47
1:D:267:ARG:NH1	1:E:366:ARG:HB3	2.29	0.47
1:E:232:GLN:HG2	1:E:262:TRP:CZ2	2.49	0.47
1:F:135:GLN:C	1:F:138:PRO:HD2	2.40	0.47
1:F:273:ASP:CG	1:F:275:ARG:HE	2.23	0.47
1:G:233:ARG:HD3	1:G:233:ARG:C	2.40	0.47
1:H:135:GLN:C	1:H:138:PRO:HD2	2.40	0.47
1:I:31:ARG:CD	1:I:54:GLY:HA2	2.45	0.47
1:K:100:VAL:HG21	1:K:219:ILE:HD11	1.97	0.47
1:K:111:GLU:H	1:K:111:GLU:CD	2.23	0.47
1:K:196:ALA:HB3	1:K:227:HIS:CD2	2.49	0.47
1:B:222:LEU:HD12	1:B:227:HIS:HD2	1.80	0.47
1:D:49:LEU:HD23	1:D:57:PRO:CB	2.44	0.47
1:D:111:GLU:CD	1:D:111:GLU:H	2.21	0.47
1:F:28:LEU:CB	1:F:35:LEU:H	2.24	0.47
1:H:53:ASP:HB2	1:H:356:ARG:NH1	2.30	0.47
1:H:128:MET:O	1:H:132:ILE:HG13	2.14	0.47
1:I:70:LYS:HE3	1:I:157:HIS:CE1	2.50	0.47
1:I:233:ARG:NE	1:I:326:GLY:HA3	2.30	0.47
1:J:206:SER:HB2	1:J:363:ARG:O	2.15	0.47
1:L:184:VAL:O	1:L:188:LEU:HD13	2.15	0.47
1:B:53:ASP:OD1	1:B:54:GLY:N	2.47	0.47
1:B:125:VAL:HG23	1:B:126:ARG:N	2.30	0.47
1:B:232:GLN:HG2	1:B:262:TRP:CZ2	2.50	0.47
1:C:159:LEU:HB2	1:C:164:ASN:OD1	2.15	0.47
1:D:206:SER:HB2	1:D:363:ARG:O	2.15	0.47
1:F:27:ILE:O	1:F:28:LEU:C	2.56	0.47
1:F:272:LYS:NZ	1:F:319:PRO:CD	2.78	0.47
1:G:48:THR:HG22	1:G:349:ALA:CB	2.45	0.47
1:H:182:MET:O	1:H:186:LEU:HG	2.15	0.47
1:I:226:LEU:HD12	1:L:206:SER:O	2.14	0.47
1:K:35:LEU:O	1:K:39:ALA:N	2.45	0.47
1:L:132:ILE:HB	1:L:352:LEU:HD11	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:LYS:HZ2	1:B:27:ILE:HD12	1.78	0.47
1:B:177:LEU:O	1:B:181:ILE:HG13	2.15	0.47
1:B:204:ALA:O	1:B:207:THR:HG22	2.14	0.47
1:F:31:ARG:CD	1:F:54:GLY:HA2	2.45	0.47
1:F:266:HIS:HE1	1:F:268:GLU:HB3	1.79	0.47
1:G:358:GLN:OE1	1:G:363:ARG:HB3	2.15	0.47
1:I:75:ILE:HG21	1:I:142:MET:HE1	1.96	0.47
1:I:82:MET:HE2	1:L:86:PHE:HZ	1.80	0.47
1:J:272:LYS:HD3	1:J:319:PRO:HD2	1.96	0.47
1:K:169:PHE:HE2	1:K:338:GLU:HG3	1.80	0.47
1:A:27:ILE:HG12	1:A:28:LEU:CD1	2.41	0.46
1:A:47:THR:HG21	1:A:187:ILE:HG23	1.98	0.46
1:A:369:GLN:NE2	1:A:371:TYR:HB3	2.30	0.46
1:B:192:HIS:HB2	1:B:275:ARG:NH1	2.30	0.46
1:C:137:ALA:HB3	1:C:138:PRO:HD3	1.97	0.46
1:C:231:ASN:CG	1:C:336:GLU:HB3	2.40	0.46
1:F:97:GLN:HG3	1:F:216:SER:O	2.14	0.46
1:H:167:TYR:HA	1:H:172:GLU:O	2.15	0.46
1:J:31:ARG:HG3	1:J:50:LEU:HG	1.97	0.46
1:K:60:LYS:HZ3	1:K:64:ASP:CG	2.22	0.46
1:L:27:ILE:CD1	1:L:269:TYR:HA	2.45	0.46
1:A:184:VAL:O	1:A:188:LEU:HG	2.14	0.46
1:F:47:THR:O	1:F:51:LEU:HG	2.14	0.46
1:G:156:LYS:HB2	1:G:159:LEU:HB2	1.97	0.46
1:H:222:LEU:HD13	1:H:227:HIS:CD2	2.47	0.46
1:I:30:TYR:HA	1:L:374:SER:OG	2.15	0.46
1:J:238:LEU:CB	1:J:303:LYS:HE3	2.45	0.46
1:K:31:ARG:HD2	1:K:54:GLY:HA2	1.98	0.46
1:K:241:ILE:C	1:K:244:PRO:HD2	2.41	0.46
1:K:278:ILE:O	1:K:282:LEU:HG	2.15	0.46
1:L:239:GLN:CG	1:L:302:LEU:HD13	2.45	0.46
1:B:43:THR:HA	1:B:183:ASP:OD2	2.14	0.46
1:D:102:SER:HB2	1:E:86:PHE:CZ	2.50	0.46
1:D:135:GLN:C	1:D:138:PRO:HD2	2.40	0.46
1:D:238:LEU:CD1	1:D:241:ILE:HB	2.45	0.46
1:F:221:THR:HG22	1:H:207:THR:HG21	1.97	0.46
1:F:299:ASP:HA	1:F:303:LYS:HG2	1.98	0.46
1:G:29:SER:HA	1:G:31:ARG:HH22	1.80	0.46
1:I:38:LEU:O	1:I:39:ALA:C	2.58	0.46
1:J:364:ILE:CG2	1:J:366:ARG:HG2	2.44	0.46
1:K:72:ASN:HD22	1:K:130:VAL:HG13	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:80:ARG:O	1:L:84:ARG:HG3	2.15	0.46
1:L:182:MET:O	1:L:186:LEU:HG	2.16	0.46
1:D:31:ARG:NE	1:D:54:GLY:HA2	2.31	0.46
1:D:264:MET:O	1:D:320:ASN:HB2	2.15	0.46
1:F:334:ILE:HD12	1:F:334:ILE:N	2.30	0.46
1:G:308:CYS:HA	1:G:319:PRO:CG	2.45	0.46
1:H:204:ALA:HB3	1:H:214:VAL:HG13	1.96	0.46
1:H:230:ALA:HA	1:H:233:ARG:HH11	1.81	0.46
1:I:216:SER:HA	1:I:219:ILE:CD1	2.45	0.46
1:J:56:LEU:HD23	1:J:57:PRO:O	2.16	0.46
1:B:308:CYS:O	1:B:311:ARG:HG2	2.16	0.46
1:D:222:LEU:HD11	1:D:343:PHE:CE2	2.51	0.46
1:E:96:LEU:HG	1:E:219:ILE:HD13	1.97	0.46
1:F:264:MET:SD	1:F:319:PRO:HB3	2.55	0.46
1:G:35:LEU:HD11	1:G:188:LEU:HD23	1.97	0.46
1:G:86:PHE:CG	1:G:95:MET:HE1	2.51	0.46
1:G:125:VAL:O	1:G:126:ARG:HB3	2.15	0.46
1:I:191:GLU:OE1	1:I:354:HIS:HE1	1.97	0.46
1:J:166:LEU:HB2	1:J:174:PRO:HG3	1.97	0.46
1:A:25:LYS:HB2	1:A:25:LYS:NZ	2.30	0.46
1:E:156:LYS:HE3	1:E:167:TYR:CE1	2.51	0.46
1:F:347:ARG:HB3	1:F:351:TRP:CE2	2.50	0.46
1:G:347:ARG:HB3	1:G:351:TRP:CE2	2.51	0.46
1:H:35:LEU:HD11	1:H:188:LEU:HD12	1.97	0.46
1:H:336:GLU:HA	1:H:339:PHE:CZ	2.51	0.46
1:I:25:LYS:HZ1	1:I:274:PRO:HD3	1.77	0.46
1:I:25:LYS:HZ2	1:I:274:PRO:HD3	1.79	0.46
1:I:367:PRO:HB3	1:I:370:ILE:HG23	1.96	0.46
1:A:36:GLU:O	1:A:39:ALA:HB3	2.16	0.46
1:B:334:ILE:H	1:B:334:ILE:HD12	1.80	0.46
1:H:233:ARG:HB3	1:H:233:ARG:NH1	2.30	0.46
1:I:135:GLN:C	1:I:138:PRO:HD2	2.41	0.46
1:J:177:LEU:O	1:J:181:ILE:HG13	2.16	0.46
1:L:124:TYR:CE1	1:L:128:MET:HE2	2.51	0.46
1:A:128:MET:O	1:A:132:ILE:HG13	2.15	0.46
1:A:238:LEU:HB3	1:A:303:LYS:CD	2.46	0.46
1:B:367:PRO:O	1:B:371:TYR:N	2.49	0.46
1:C:38:LEU:O	1:C:42:SER:HB3	2.16	0.46
1:D:229:GLY:CA	1:D:262:TRP:HE1	2.27	0.46
1:G:27:ILE:HG21	1:G:30:TYR:CZ	2.50	0.46
1:G:302:LEU:O	1:G:305:GLU:HG3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:67:GLN:HA	1:I:70:LYS:HD3	1.97	0.46
1:I:123:ASP:HB2	1:I:127:ASN:ND2	2.30	0.46
1:J:184:VAL:O	1:J:188:LEU:HG	2.16	0.46
1:K:273:ASP:CG	1:K:275:ARG:HE	2.24	0.46
1:K:338:GLU:O	1:K:342:LEU:HG	2.15	0.46
1:L:78:HIS:HB2	1:L:106:PHE:HZ	1.81	0.46
1:A:278:ILE:O	1:A:282:LEU:HG	2.16	0.46
1:A:335:PRO:HG2	1:A:338:GLU:CG	2.46	0.46
1:B:70:LYS:C	1:B:72:ASN:H	2.24	0.46
1:B:80:ARG:O	1:B:84:ARG:HG3	2.15	0.46
1:B:126:ARG:NE	1:B:126:ARG:HA	2.31	0.46
1:B:307:VAL:HG13	1:B:323:PHE:CZ	2.44	0.46
1:D:267:ARG:HD2	1:E:366:ARG:HB3	1.98	0.46
1:G:33:TYR:CE1	1:G:50:LEU:HD11	2.51	0.46
1:H:67:GLN:HE22	1:H:157:HIS:CE1	2.34	0.46
1:H:124:TYR:O	1:H:128:MET:HG2	2.16	0.46
1:I:356:ARG:O	1:I:359:ILE:HG23	2.16	0.46
1:K:280:HIS:HB2	1:K:324:TYR:CZ	2.51	0.46
1:A:273:ASP:CG	1:A:275:ARG:HE	2.24	0.46
1:E:215:ILE:O	1:E:219:ILE:HG13	2.15	0.46
1:F:86:PHE:CE1	1:H:102:SER:HB2	2.51	0.46
1:G:133:ILE:HG13	1:G:352:LEU:CD1	2.46	0.46
1:H:35:LEU:O	1:H:39:ALA:N	2.47	0.46
1:H:215:ILE:O	1:H:219:ILE:HG13	2.16	0.46
1:H:363:ARG:O	1:H:364:ILE:C	2.59	0.46
1:I:27:ILE:HB	1:I:274:PRO:HG3	1.97	0.46
1:K:24:GLU:HB2	1:K:25:LYS:NZ	2.31	0.46
1:L:113:LEU:HG	1:L:119:CYS:HB3	1.97	0.46
1:A:196:ALA:HB3	1:A:227:HIS:HD2	1.81	0.45
1:A:206:SER:O	1:C:226:LEU:HD12	2.16	0.45
1:A:211:PRO:O	1:A:215:ILE:HG12	2.15	0.45
1:A:232:GLN:HB3	1:A:262:TRP:CD2	2.51	0.45
1:D:366:ARG:HH22	1:E:192:HIS:CE1	2.34	0.45
1:F:75:ILE:HD11	1:F:138:PRO:CB	2.46	0.45
1:J:53:ASP:OD1	1:J:54:GLY:N	2.49	0.45
1:J:312:LEU:H	1:J:312:LEU:CD1	2.27	0.45
1:K:52:LEU:HD13	1:K:126:ARG:HH12	1.80	0.45
1:K:65:PHE:CZ	1:K:69:LEU:HD12	2.51	0.45
1:K:178:MET:HA	1:K:181:ILE:HD12	1.97	0.45
1:L:107:TYR:HB3	1:L:128:MET:HE3	1.98	0.45
1:A:111:GLU:CD	1:A:111:GLU:H	2.24	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:VAL:HG21	1:A:339:PHE:CE2	2.52	0.45
1:B:185:CYS:O	1:B:189:HIS:HD2	1.99	0.45
1:E:273:ASP:CG	1:E:275:ARG:HE	2.24	0.45
1:G:370:ILE:HG23	1:G:375:ASP:HB2	1.96	0.45
1:I:137:ALA:O	1:I:138:PRO:C	2.60	0.45
1:I:181:ILE:HG21	1:I:328:LEU:HD11	1.97	0.45
1:J:59:LYS:HD2	1:J:59:LYS:C	2.41	0.45
1:B:192:HIS:CD2	1:B:195:ASN:HD21	2.29	0.45
1:B:238:LEU:HD23	1:B:238:LEU:H	1.81	0.45
1:C:25:LYS:HD2	1:C:25:LYS:N	2.32	0.45
1:C:28:LEU:CA	1:C:35:LEU:HD13	2.35	0.45
1:F:181:ILE:HG23	1:F:282:LEU:HD22	1.98	0.45
1:G:70:LYS:HB3	1:G:157:HIS:CD2	2.52	0.45
1:I:301:ALA:HA	1:I:304:LEU:CD2	2.46	0.45
1:K:48:THR:O	1:K:52:LEU:HG	2.17	0.45
1:L:363:ARG:HG2	1:L:365:TYR:H	1.81	0.45
1:A:230:ALA:HA	1:A:322:ASP:HB3	1.98	0.45
1:H:75:ILE:HD11	1:H:138:PRO:HB2	1.98	0.45
1:H:132:ILE:O	1:H:136:MET:HG2	2.16	0.45
1:I:245:LYS:HG2	1:I:247:VAL:H	1.81	0.45
1:K:81:GLN:O	1:K:85:HIS:HD2	1.99	0.45
1:K:83:MET:SD	1:K:142:MET:HE3	2.56	0.45
1:K:301:ALA:O	1:K:305:GLU:HG2	2.16	0.45
1:A:69:LEU:HD12	1:A:134:ALA:HB2	1.99	0.45
1:D:69:LEU:HD12	1:D:134:ALA:HB2	1.98	0.45
1:D:185:CYS:O	1:D:189:HIS:HD2	1.99	0.45
1:E:70:LYS:O	1:E:71:ASP:HB2	2.17	0.45
1:F:267:ARG:HH21	1:H:363:ARG:NE	2.05	0.45
1:G:269:TYR:CD2	1:G:274:PRO:HD2	2.51	0.45
1:H:110:THR:HG22	1:H:112:CYS:H	1.82	0.45
1:H:198:THR:HG1	1:H:351:TRP:CD1	2.34	0.45
1:I:305:GLU:HA	1:I:308:CYS:SG	2.56	0.45
1:K:159:LEU:HD11	1:K:173:GLU:HG2	1.98	0.45
1:C:177:LEU:HD23	1:C:177:LEU:C	2.41	0.45
1:D:43:THR:HA	1:D:187:ILE:HD11	1.99	0.45
1:D:113:LEU:HD21	1:D:120:GLU:HG3	1.97	0.45
1:F:321:VAL:HG23	1:F:322:ASP:N	2.31	0.45
1:G:29:SER:HA	1:G:31:ARG:NH2	2.31	0.45
1:H:111:GLU:H	1:H:111:GLU:CD	2.25	0.45
1:I:183:ASP:O	1:I:187:ILE:HG13	2.17	0.45
1:I:195:ASN:O	1:I:196:ALA:C	2.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:233:ARG:HE	1:I:339:PHE:HE2	1.64	0.45
1:L:181:ILE:HD12	1:L:282:LEU:HD22	1.99	0.45
1:D:36:GLU:OE1	1:D:36:GLU:N	2.49	0.45
1:J:133:ILE:CG1	1:J:352:LEU:HD12	2.47	0.45
1:K:44:PHE:CZ	1:K:346:ALA:HA	2.51	0.45
1:K:75:ILE:HD11	1:K:138:PRO:CB	2.46	0.45
1:C:125:VAL:O	1:C:126:ARG:HB3	2.17	0.45
1:F:271:VAL:O	1:F:272:LYS:HB2	2.17	0.45
1:F:370:ILE:HD12	1:F:370:ILE:N	2.32	0.45
1:G:75:ILE:HD13	1:G:135:GLN:OE1	2.16	0.45
1:G:122:LEU:HD13	1:G:124:TYR:H	1.82	0.45
1:G:144:GLU:HG2	1:G:147:ARG:HH21	1.81	0.45
1:H:122:LEU:C	1:H:122:LEU:HD12	2.42	0.45
1:J:44:PHE:CD1	1:J:186:LEU:HB3	2.52	0.45
1:J:60:LYS:HB3	1:J:60:LYS:HE3	1.76	0.45
1:J:233:ARG:NE	1:J:263:GLY:HA3	2.32	0.45
1:J:323:PHE:HD2	1:J:324:TYR:CZ	2.35	0.45
1:J:372:VAL:O	1:J:375:ASP:HB2	2.17	0.45
1:A:78:HIS:HA	1:A:81:GLN:NE2	2.32	0.45
1:B:266:HIS:HE1	1:B:268:GLU:HB2	1.82	0.45
1:E:206:SER:HB3	1:E:365:TYR:HD1	1.82	0.45
1:I:27:ILE:HD12	1:I:274:PRO:HG3	1.98	0.45
1:I:125:VAL:HG22	1:I:355:TRP:CH2	2.52	0.45
1:J:79:ILE:HG22	1:J:83:MET:HE3	1.97	0.45
1:J:103:LEU:HG	1:J:107:TYR:HE1	1.82	0.45
1:J:133:ILE:HG13	1:J:352:LEU:CD1	2.47	0.45
1:A:156:LYS:HB3	1:A:158:ASP:OD1	2.17	0.45
1:B:63:ASN:O	1:B:67:GLN:HG2	2.17	0.45
1:B:239:GLN:C	1:B:241:ILE:H	2.24	0.45
1:B:347:ARG:O	1:B:348:SER:C	2.59	0.45
1:F:185:CYS:O	1:F:189:HIS:HD2	1.99	0.45
1:H:142:MET:HA	1:H:152:PRO:HB3	1.98	0.45
1:I:27:ILE:HG13	1:I:28:LEU:HD13	1.98	0.45
1:I:241:ILE:HG22	1:I:244:PRO:HD3	1.98	0.45
1:J:69:LEU:HD12	1:J:134:ALA:HB2	1.99	0.45
1:J:218:ALA:HB1	1:J:351:TRP:CE2	2.52	0.45
1:J:233:ARG:O	1:J:235:VAL:HG12	2.17	0.45
1:J:279:LEU:HA	1:J:282:LEU:HD12	1.99	0.45
1:L:93:MET:HE3	1:L:340:THR:HG22	1.98	0.45
1:L:156:LYS:HE3	1:L:159:LEU:HD22	1.98	0.45
1:L:300:THR:O	1:L:304:LEU:HD23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:HIS:CE1	1:C:366:ARG:HH22	2.35	0.44
1:C:28:LEU:O	1:C:34:PRO:HA	2.17	0.44
1:C:269:TYR:CE1	1:C:273:ASP:HB2	2.53	0.44
1:F:192:HIS:HE1	1:F:266:HIS:CE1	2.35	0.44
1:J:57:PRO:HB2	1:J:61:ALA:HB3	1.98	0.44
1:L:239:GLN:HG2	1:L:302:LEU:HD13	2.00	0.44
1:B:113:LEU:HA	1:B:119:CYS:HB3	1.99	0.44
1:D:27:ILE:CG1	1:D:28:LEU:HD13	2.47	0.44
1:E:113:LEU:HD21	1:E:120:GLU:HB3	1.99	0.44
1:G:192:HIS:HB3	1:G:347:ARG:HH22	1.82	0.44
1:H:35:LEU:HA	1:H:38:LEU:HB2	1.99	0.44
1:I:49:LEU:HD13	1:I:57:PRO:HB3	1.98	0.44
1:J:135:GLN:C	1:J:138:PRO:HD2	2.42	0.44
1:J:310:ASP:HB2	1:J:314:HIS:CE1	2.52	0.44
1:L:50:LEU:HB2	1:L:56:LEU:HD23	1.99	0.44
1:B:133:ILE:HG13	1:B:352:LEU:HD12	2.00	0.44
1:B:158:ASP:HB2	1:F:315:LYS:HG2	1.99	0.44
1:C:238:LEU:HD12	1:C:238:LEU:N	2.33	0.44
1:E:36:GLU:N	1:E:36:GLU:OE1	2.51	0.44
1:E:192:HIS:HB2	1:E:347:ARG:NH2	2.32	0.44
1:E:287:VAL:HG11	1:E:305:GLU:OE1	2.17	0.44
1:I:159:LEU:HB2	1:I:164:ASN:OD1	2.17	0.44
1:I:160:SER:N	1:I:163:GLU:HB2	2.32	0.44
1:J:239:GLN:O	1:J:241:ILE:HG13	2.17	0.44
1:K:103:LEU:HG	1:K:107:TYR:HE1	1.82	0.44
1:B:31:ARG:HB2	1:B:50:LEU:HD21	1.98	0.44
1:E:192:HIS:HD2	1:E:193:THR:H	1.65	0.44
1:G:334:ILE:HG21	1:G:342:LEU:CD1	2.47	0.44
1:H:127:ASN:O	1:H:130:VAL:HG22	2.17	0.44
1:I:356:ARG:O	1:I:359:ILE:HG12	2.17	0.44
1:K:281:LYS:HA	1:K:284:GLU:CD	2.42	0.44
1:C:273:ASP:OD2	1:C:275:ARG:HB2	2.17	0.44
1:E:264:MET:HG2	1:E:319:PRO:CA	2.44	0.44
1:G:63:ASN:O	1:G:67:GLN:HG2	2.17	0.44
1:G:192:HIS:HB3	1:G:347:ARG:NH2	2.32	0.44
1:G:274:PRO:O	1:G:278:ILE:HG13	2.17	0.44
1:H:329:TYR:HB2	1:H:339:PHE:CE1	2.53	0.44
1:I:216:SER:O	1:I:219:ILE:HG12	2.18	0.44
1:L:239:GLN:HB3	1:L:302:LEU:HB3	1.99	0.44
1:B:192:HIS:HB3	1:B:347:ARG:NH2	2.32	0.44
1:C:30:TYR:CE1	1:C:191:GLU:HB3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:135:GLN:C	1:C:138:PRO:HD2	2.43	0.44
1:E:338:GLU:O	1:E:342:LEU:HG	2.18	0.44
1:F:128:MET:O	1:F:132:ILE:HG13	2.18	0.44
1:F:233:ARG:HH11	1:F:234:VAL:HA	1.81	0.44
1:G:184:VAL:O	1:G:188:LEU:HG	2.18	0.44
1:G:272:LYS:HB3	1:G:272:LYS:HZ3	1.82	0.44
1:J:327:ILE:HD12	1:J:327:ILE:N	2.31	0.44
1:A:78:HIS:HE1	1:I:149:GLY:HA2	1.83	0.44
1:A:236:GLY:O	1:A:237:MET:C	2.60	0.44
1:B:156:LYS:HB3	1:B:158:ASP:OD1	2.18	0.44
1:C:272:LYS:HG3	1:C:318:TYR:O	2.17	0.44
1:E:322:ASP:O	1:E:323:PHE:C	2.61	0.44
1:E:329:TYR:HB3	1:E:339:PHE:CE1	2.52	0.44
1:F:220:GLY:HA2	1:F:223:SER:HB3	1.99	0.44
1:F:326:GLY:O	1:F:327:ILE:C	2.61	0.44
1:H:202:LEU:HB3	1:H:358:GLN:OE1	2.17	0.44
1:J:124:TYR:CD2	1:J:128:MET:HG3	2.53	0.44
1:K:92:PRO:HA	1:K:143:TRP:CD1	2.53	0.44
1:K:300:THR:O	1:K:304:LEU:HD23	2.18	0.44
1:A:82:MET:HG3	1:A:83:MET:N	2.32	0.44
1:C:28:LEU:HB3	1:C:34:PRO:HA	2.00	0.44
1:E:238:LEU:N	1:E:241:ILE:HG12	2.32	0.44
1:F:175:ASP:O	1:F:176:PRO:C	2.61	0.44
1:F:321:VAL:O	1:F:322:ASP:C	2.60	0.44
1:G:34:PRO:HG2	1:G:37:THR:CG2	2.48	0.44
1:G:220:GLY:O	1:G:223:SER:HB3	2.17	0.44
1:H:76:LYS:HB2	1:H:79:ILE:HG12	1.99	0.44
1:J:72:ASN:HD22	1:J:130:VAL:HG13	1.82	0.44
1:K:301:ALA:HA	1:K:304:LEU:HB2	1.99	0.44
1:B:264:MET:HA	1:B:320:ASN:H	1.83	0.44
1:D:124:TYR:HE2	1:D:211:PRO:CD	2.31	0.44
1:F:271:VAL:O	1:F:318:TYR:CG	2.71	0.44
1:G:70:LYS:C	1:G:72:ASN:N	2.75	0.44
1:G:182:MET:HE3	1:G:185:CYS:HB3	1.99	0.44
1:H:30:TYR:CD1	1:H:51:LEU:HD21	2.52	0.44
1:I:25:LYS:HE2	1:I:271:VAL:HG21	2.00	0.44
1:I:50:LEU:O	1:I:54:GLY:N	2.50	0.44
1:I:221:THR:O	1:L:207:THR:HG21	2.18	0.44
1:J:193:THR:O	1:J:194:LEU:C	2.60	0.44
1:L:178:MET:SD	1:L:332:MET:HG2	2.58	0.44
1:C:304:LEU:HD12	1:C:327:ILE:HG21	1.98	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:28:LEU:HG	1:F:36:GLU:OE2	2.18	0.43
1:H:120:GLU:N	1:H:120:GLU:OE1	2.50	0.43
1:H:222:LEU:HD11	1:H:343:PHE:CD2	2.53	0.43
1:K:34:PRO:O	1:K:38:LEU:HG	2.17	0.43
1:K:184:VAL:O	1:K:188:LEU:HD13	2.17	0.43
1:L:144:GLU:HG2	1:L:147:ARG:NH2	2.32	0.43
1:L:195:ASN:O	1:L:196:ALA:C	2.61	0.43
1:A:166:LEU:N	1:A:166:LEU:HD12	2.33	0.43
1:D:28:LEU:CB	1:D:35:LEU:H	2.30	0.43
1:D:243:SER:HA	1:D:245:LYS:NZ	2.33	0.43
1:E:72:ASN:ND2	1:E:130:VAL:HG13	2.33	0.43
1:F:86:PHE:HB3	1:F:87:PRO:HD2	2.00	0.43
1:F:144:GLU:HA	1:F:147:ARG:HE	1.82	0.43
1:F:148:ASN:HB2	1:F:150:TRP:CD1	2.53	0.43
1:F:304:LEU:HD22	1:F:304:LEU:N	2.33	0.43
1:G:70:LYS:C	1:G:72:ASN:H	2.26	0.43
1:H:206:SER:HB3	1:H:365:TYR:HD1	1.82	0.43
1:H:355:TRP:O	1:H:359:ILE:HG12	2.17	0.43
1:I:283:VAL:HA	1:I:286:LEU:HD12	1.99	0.43
1:K:274:PRO:O	1:K:278:ILE:HG13	2.18	0.43
1:L:35:LEU:O	1:L:39:ALA:N	2.40	0.43
1:L:319:PRO:HB3	1:L:323:PHE:CD2	2.53	0.43
1:A:44:PHE:CE1	1:A:346:ALA:HA	2.53	0.43
1:C:322:ASP:O	1:C:323:PHE:C	2.61	0.43
1:D:233:ARG:O	1:D:234:VAL:C	2.60	0.43
1:D:239:GLN:C	1:D:241:ILE:H	2.25	0.43
1:E:177:LEU:HD22	1:E:177:LEU:N	2.30	0.43
1:F:206:SER:HA	1:F:361:ASP:OD1	2.18	0.43
1:G:80:ARG:O	1:G:84:ARG:HG3	2.17	0.43
1:G:111:GLU:H	1:G:111:GLU:CD	2.27	0.43
1:H:239:GLN:H	1:H:239:GLN:NE2	2.16	0.43
1:I:28:LEU:HD21	1:I:36:GLU:CD	2.42	0.43
1:I:233:ARG:NE	1:I:339:PHE:HE2	2.16	0.43
1:I:243:SER:HB2	1:I:244:PRO:HD3	2.00	0.43
1:J:300:THR:O	1:J:304:LEU:HD22	2.18	0.43
1:K:182:MET:O	1:K:186:LEU:HD13	2.18	0.43
1:A:207:THR:CG2	1:C:227:HIS:HB2	2.49	0.43
1:B:25:LYS:HZ2	1:B:27:ILE:HB	1.82	0.43
1:B:44:PHE:CD1	1:B:186:LEU:HB3	2.53	0.43
1:B:44:PHE:CZ	1:B:346:ALA:HA	2.53	0.43
1:B:224:GLY:O	1:B:228:GLY:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:231:ASN:O	1:B:234:VAL:HG12	2.17	0.43
1:C:240:GLU:O	1:C:241:ILE:C	2.62	0.43
1:E:34:PRO:O	1:E:38:LEU:HG	2.19	0.43
1:F:357:GLU:OE2	1:H:372:VAL:HG23	2.19	0.43
1:G:216:SER:HA	1:G:219:ILE:HD11	1.99	0.43
1:G:270:LYS:HG3	1:G:271:VAL:HG13	2.00	0.43
1:I:202:LEU:HD21	1:I:354:HIS:HB3	2.00	0.43
1:J:135:GLN:O	1:J:136:MET:C	2.61	0.43
1:J:238:LEU:HB3	1:J:242:GLY:HA3	2.00	0.43
1:K:135:GLN:O	1:K:139:LEU:HG	2.18	0.43
1:B:184:VAL:O	1:B:188:LEU:HD13	2.18	0.43
1:B:347:ARG:HB3	1:B:351:TRP:CE2	2.53	0.43
1:C:182:MET:O	1:C:186:LEU:HD13	2.19	0.43
1:E:193:THR:O	1:E:195:ASN:N	2.45	0.43
1:E:241:ILE:C	1:E:244:PRO:HD2	2.44	0.43
1:F:182:MET:O	1:F:186:LEU:HG	2.19	0.43
1:H:124:TYR:HE2	1:H:211:PRO:HD2	1.83	0.43
1:H:358:GLN:HE21	1:H:358:GLN:HB3	1.51	0.43
1:J:122:LEU:HD12	1:J:127:ASN:HD22	1.83	0.43
1:J:233:ARG:HD2	1:J:323:PHE:HA	2.00	0.43
1:K:230:ALA:CA	1:K:233:ARG:HH22	2.31	0.43
1:C:209:ALA:O	1:C:210:THR:C	2.61	0.43
1:C:332:MET:HB2	1:C:334:ILE:HD13	1.99	0.43
1:D:128:MET:O	1:D:132:ILE:HG13	2.19	0.43
1:E:336:GLU:HA	1:E:339:PHE:CE1	2.53	0.43
1:F:135:GLN:O	1:F:136:MET:C	2.61	0.43
1:F:340:THR:O	1:F:343:PHE:HB3	2.19	0.43
1:I:178:MET:HE3	1:I:332:MET:HA	1.99	0.43
1:J:43:THR:O	1:J:44:PHE:C	2.62	0.43
1:J:111:GLU:CD	1:J:120:GLU:HG2	2.43	0.43
1:L:177:LEU:HD22	1:L:177:LEU:N	2.32	0.43
1:A:232:GLN:HB3	1:A:262:TRP:CE2	2.54	0.43
1:A:338:GLU:O	1:A:339:PHE:C	2.62	0.43
1:B:69:LEU:HD12	1:B:134:ALA:HB2	2.01	0.43
1:B:70:LYS:C	1:B:72:ASN:N	2.76	0.43
1:B:222:LEU:CD1	1:B:227:HIS:HD2	2.32	0.43
1:C:222:LEU:CD2	1:C:343:PHE:HD2	2.32	0.43
1:D:68:GLN:CG	1:D:130:VAL:HG11	2.47	0.43
1:E:238:LEU:HB3	1:E:241:ILE:CG2	2.48	0.43
1:E:271:VAL:HG22	1:E:272:LYS:N	2.30	0.43
1:F:361:ASP:C	1:F:363:ARG:H	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:366:ARG:H	1:H:267:ARG:NH1	2.16	0.43
1:G:135:GLN:C	1:G:138:PRO:HD2	2.43	0.43
1:G:241:ILE:O	1:G:244:PRO:HD2	2.19	0.43
1:G:299:ASP:O	1:G:303:LYS:HB3	2.18	0.43
1:H:25:LYS:HE3	1:H:270:LYS:HG2	2.00	0.43
1:J:165:LEU:O	1:J:169:PHE:HB2	2.19	0.43
1:L:111:GLU:OE2	1:L:208:LEU:HB3	2.19	0.43
1:B:192:HIS:O	1:B:192:HIS:CG	2.70	0.43
1:C:43:THR:HG23	1:C:46:GLU:H	1.84	0.43
1:C:175:ASP:OD1	1:C:178:MET:HG2	2.18	0.43
1:D:25:LYS:C	1:D:27:ILE:N	2.76	0.43
1:E:28:LEU:HD22	1:E:275:ARG:HD2	2.00	0.43
1:E:367:PRO:HB2	1:E:369:GLN:HE21	1.83	0.43
1:H:34:PRO:O	1:H:38:LEU:HG	2.17	0.43
1:H:279:LEU:HD23	1:H:282:LEU:HD12	2.01	0.43
1:H:340:THR:O	1:H:343:PHE:HB3	2.17	0.43
1:I:112:CYS:SG	1:I:113:LEU:N	2.91	0.43
1:B:264:MET:HE1	1:B:314:HIS:CE1	2.53	0.43
1:C:203:VAL:HA	1:C:365:TYR:HD2	1.83	0.43
1:D:324:TYR:HD1	1:D:327:ILE:HD11	1.83	0.43
1:E:192:HIS:HB2	1:E:347:ARG:CZ	2.49	0.43
1:I:207:THR:HA	1:L:226:LEU:HB2	2.01	0.43
1:K:211:PRO:HG3	1:K:355:TRP:CZ2	2.54	0.43
1:L:327:ILE:H	1:L:327:ILE:CD1	2.28	0.43
1:B:334:ILE:HD12	1:B:334:ILE:N	2.33	0.43
1:E:31:ARG:CD	1:E:54:GLY:HA2	2.48	0.43
1:E:308:CYS:SG	1:E:327:ILE:HD11	2.59	0.43
1:F:92:PRO:HG2	1:F:337:ASP:O	2.17	0.43
1:K:49:LEU:HD11	1:K:65:PHE:CB	2.49	0.43
1:L:361:ASP:OD1	1:L:362:ASN:N	2.52	0.43
1:A:186:LEU:O	1:A:346:ALA:HB1	2.19	0.42
1:A:300:THR:O	1:A:304:LEU:HD23	2.19	0.42
1:B:183:ASP:O	1:B:187:ILE:HG13	2.18	0.42
1:G:30:TYR:HB3	1:G:33:TYR:O	2.19	0.42
1:H:142:MET:HG3	1:H:152:PRO:CG	2.49	0.42
1:J:144:GLU:OE1	1:J:147:ARG:NH2	2.52	0.42
1:A:235:VAL:HG13	1:A:235:VAL:O	2.19	0.42
1:C:65:PHE:CE2	1:C:69:LEU:HD11	2.54	0.42
1:E:153:VAL:O	1:E:168:MET:HE3	2.19	0.42
1:F:201:ALA:HA	1:F:214:VAL:HG13	2.00	0.42
1:G:39:ALA:HB1	1:G:184:VAL:HG13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:370:ILE:HG23	1:G:375:ASP:H	1.84	0.42
1:H:183:ASP:O	1:H:187:ILE:HG13	2.20	0.42
1:H:347:ARG:O	1:H:348:SER:C	2.61	0.42
1:I:166:LEU:HD23	1:I:178:MET:HE2	2.00	0.42
1:K:44:PHE:CG	1:K:186:LEU:HB3	2.53	0.42
1:K:231:ASN:HD21	1:K:340:THR:H	1.67	0.42
1:L:185:CYS:O	1:L:189:HIS:HD2	2.02	0.42
1:L:232:GLN:OE1	1:L:232:GLN:N	2.49	0.42
1:A:350:GLY:O	1:A:354:HIS:HD2	2.02	0.42
1:C:28:LEU:HG	1:C:35:LEU:HB2	2.01	0.42
1:C:82:MET:HE3	1:C:82:MET:HB3	1.92	0.42
1:C:82:MET:O	1:C:86:PHE:HD1	2.02	0.42
1:D:111:GLU:O	1:D:113:LEU:HG	2.19	0.42
1:F:181:ILE:HB	1:F:332:MET:HE2	2.01	0.42
1:F:323:PHE:HD2	1:F:324:TYR:HE1	1.63	0.42
1:G:132:ILE:O	1:G:136:MET:HG2	2.19	0.42
1:G:238:LEU:HD22	1:G:245:LYS:NZ	2.33	0.42
1:I:29:SER:HB2	1:L:375:ASP:OD1	2.19	0.42
1:J:233:ARG:NH1	1:J:262:TRP:CD1	2.87	0.42
1:K:25:LYS:HE3	1:K:270:LYS:H	1.84	0.42
1:L:128:MET:O	1:L:132:ILE:HG13	2.19	0.42
1:B:286:LEU:HD23	1:B:286:LEU:HA	1.91	0.42
1:D:75:ILE:HD11	1:D:138:PRO:HB2	2.01	0.42
1:E:239:GLN:NE2	1:E:307:VAL:HA	2.35	0.42
1:H:271:VAL:HG22	1:H:272:LYS:N	2.32	0.42
1:I:268:GLU:HG3	1:L:366:ARG:NH1	2.35	0.42
1:A:208:LEU:HD12	1:C:226:LEU:HD21	2.02	0.42
1:B:24:GLU:CD	1:B:25:LYS:HB2	2.45	0.42
1:B:239:GLN:HG2	1:B:298:PHE:HE1	1.79	0.42
1:E:25:LYS:HA	1:E:25:LYS:CE	2.49	0.42
1:F:176:PRO:O	1:F:180:LYS:HG3	2.20	0.42
1:G:52:LEU:HD23	1:G:353:ALA:HA	2.00	0.42
1:G:370:ILE:O	1:G:371:TYR:C	2.62	0.42
1:I:230:ALA:O	1:I:233:ARG:HD2	2.19	0.42
1:J:341:ALA:O	1:J:345:VAL:HG23	2.20	0.42
1:J:372:VAL:HG12	1:J:374:SER:H	1.84	0.42
1:K:42:SER:HA	1:K:46:GLU:OE2	2.19	0.42
1:K:70:LYS:C	1:K:72:ASN:N	2.77	0.42
1:K:222:LEU:O	1:K:222:LEU:HD23	2.19	0.42
1:L:352:LEU:O	1:L:355:TRP:HB3	2.20	0.42
1:B:83:MET:SD	1:B:142:MET:HE3	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:300:THR:O	1:B:305:GLU:HG3	2.19	0.42
1:C:30:TYR:CD1	1:C:35:LEU:HD11	2.55	0.42
1:C:70:LYS:HE3	1:C:157:HIS:NE2	2.35	0.42
1:D:356:ARG:O	1:D:359:ILE:HG23	2.19	0.42
1:E:238:LEU:H	1:E:241:ILE:CD1	2.33	0.42
1:E:271:VAL:HA	1:E:318:TYR:CD2	2.54	0.42
1:G:335:PRO:HG2	1:G:338:GLU:CG	2.50	0.42
1:H:30:TYR:CE2	1:H:35:LEU:HD13	2.54	0.42
1:I:36:GLU:OE1	1:I:36:GLU:N	2.53	0.42
1:I:77:TYR:HE2	1:I:81:GLN:HE21	1.65	0.42
1:L:59:LYS:HZ2	1:L:60:LYS:HD2	1.85	0.42
1:L:281:LYS:NZ	1:L:282:LEU:HG	2.35	0.42
1:A:239:GLN:HG3	1:A:241:ILE:HD11	2.02	0.42
1:B:278:ILE:O	1:B:282:LEU:HG	2.19	0.42
1:D:271:VAL:HG22	1:D:272:LYS:N	2.33	0.42
1:E:66:SER:O	1:E:70:LYS:HG3	2.19	0.42
1:E:156:LYS:HB3	1:E:158:ASP:OD1	2.19	0.42
1:E:167:TYR:O	1:E:171:GLY:N	2.52	0.42
1:F:31:ARG:HD3	1:H:374:SER:HB2	2.02	0.42
1:H:275:ARG:HB3	1:H:321:VAL:HG23	2.02	0.42
1:J:166:LEU:HB3	1:J:174:PRO:HB3	2.02	0.42
1:J:312:LEU:HD12	1:J:312:LEU:N	2.29	0.42
1:K:334:ILE:HD12	1:K:334:ILE:N	2.34	0.42
1:B:192:HIS:HB2	1:B:275:ARG:HH12	1.85	0.42
1:C:31:ARG:HG3	1:C:50:LEU:O	2.19	0.42
1:C:347:ARG:HD3	1:C:347:ARG:HA	1.86	0.42
1:D:207:THR:HA	1:E:226:LEU:HB2	2.01	0.42
1:E:28:LEU:CD2	1:E:275:ARG:HD2	2.49	0.42
1:E:70:LYS:HD3	1:E:157:HIS:CD2	2.55	0.42
1:J:177:LEU:HD22	1:J:177:LEU:N	2.30	0.42
1:K:156:LYS:HE3	1:K:167:TYR:CE2	2.54	0.42
1:K:198:THR:O	1:K:202:LEU:HG	2.19	0.42
1:K:214:VAL:CG2	1:K:215:ILE:N	2.83	0.42
1:L:239:GLN:HG3	1:L:299:ASP:HA	1.99	0.42
1:B:275:ARG:O	1:B:279:LEU:HG	2.19	0.42
1:C:42:SER:HA	1:C:46:GLU:OE1	2.20	0.42
1:D:301:ALA:H	1:D:304:LEU:HD23	1.85	0.42
1:F:35:LEU:HD11	1:F:188:LEU:HD12	2.02	0.42
1:H:76:LYS:HE2	1:H:107:TYR:OH	2.20	0.42
1:I:135:GLN:O	1:I:139:LEU:HG	2.20	0.42
1:I:368:THR:O	1:I:371:TYR:HD1	2.03	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:68:GLN:HG2	1:L:72:ASN:ND2	2.35	0.42
1:L:181:ILE:CG1	1:L:286:LEU:HD11	2.46	0.42
1:L:303:LYS:HA	1:L:306:GLU:HG2	2.02	0.42
1:A:96:LEU:HD11	1:A:136:MET:HE2	2.02	0.42
1:A:271:VAL:HG22	1:A:272:LYS:N	2.33	0.42
1:B:124:TYR:CE1	1:B:128:MET:HE3	2.55	0.42
1:C:144:GLU:OE1	1:C:147:ARG:NH2	2.53	0.42
1:C:183:ASP:O	1:C:186:LEU:HB2	2.19	0.42
1:F:27:ILE:HG12	1:F:28:LEU:N	2.35	0.42
1:G:128:MET:O	1:G:132:ILE:HG13	2.19	0.42
1:J:72:ASN:ND2	1:J:130:VAL:HG13	2.35	0.42
1:K:45:GLU:H	1:K:45:GLU:CD	2.27	0.42
1:L:159:LEU:HA	1:L:163:GLU:OE1	2.20	0.42
1:L:181:ILE:HG13	1:L:286:LEU:HD21	2.02	0.42
1:A:337:ASP:OD1	1:A:337:ASP:N	2.53	0.41
1:C:233:ARG:CZ	1:C:322:ASP:O	2.68	0.41
1:H:68:GLN:CD	1:H:130:VAL:HG21	2.45	0.41
1:J:76:LYS:HE3	1:J:106:PHE:HB3	2.02	0.41
1:J:347:ARG:HB3	1:J:351:TRP:CZ2	2.55	0.41
1:L:122:LEU:O	1:L:123:ASP:C	2.63	0.41
1:L:122:LEU:HD22	1:L:123:ASP:H	1.85	0.41
1:B:47:THR:O	1:B:51:LEU:HG	2.20	0.41
1:C:48:THR:O	1:C:52:LEU:HG	2.20	0.41
1:D:226:LEU:HD22	1:E:208:LEU:HG	2.02	0.41
1:E:279:LEU:HD23	1:E:282:LEU:HD12	2.02	0.41
1:E:315:LYS:O	1:E:315:LYS:HD3	2.20	0.41
1:F:182:MET:N	1:F:332:MET:HE1	2.35	0.41
1:F:189:HIS:HB3	1:F:343:PHE:CE1	2.54	0.41
1:G:196:ALA:HB3	1:G:227:HIS:CD2	2.50	0.41
1:G:239:GLN:HE21	1:G:239:GLN:HB2	1.66	0.41
1:J:112:CYS:SG	1:J:113:LEU:N	2.93	0.41
1:K:102:SER:HA	1:K:105:MET:HE2	2.01	0.41
1:L:110:THR:HG22	1:L:113:LEU:H	1.85	0.41
1:L:122:LEU:HD13	1:L:123:ASP:H	1.84	0.41
1:L:327:ILE:HD12	1:L:327:ILE:N	2.28	0.41
1:A:47:THR:O	1:A:51:LEU:HG	2.19	0.41
1:A:166:LEU:CB	1:A:174:PRO:HG3	2.50	0.41
1:E:123:ASP:O	1:E:124:TYR:C	2.63	0.41
1:E:336:GLU:HA	1:E:339:PHE:CD1	2.56	0.41
1:F:95:MET:HE2	1:H:105:MET:SD	2.60	0.41
1:F:367:PRO:HD2	1:H:194:LEU:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:45:GLU:H	1:H:45:GLU:CD	2.27	0.41
1:H:49:LEU:HD13	1:H:65:PHE:CD1	2.56	0.41
1:I:66:SER:O	1:I:70:LYS:HG3	2.20	0.41
1:I:336:GLU:HA	1:I:339:PHE:CD1	2.55	0.41
1:I:336:GLU:HA	1:I:339:PHE:CE1	2.55	0.41
1:J:60:LYS:HD2	1:J:60:LYS:C	2.45	0.41
1:J:363:ARG:CG	1:J:365:TYR:H	2.22	0.41
1:K:136:MET:O	1:K:137:ALA:C	2.63	0.41
1:L:199:PHE:HD1	1:L:202:LEU:HD12	1.85	0.41
1:A:110:THR:HG22	1:A:112:CYS:H	1.85	0.41
1:C:70:LYS:HA	1:C:73:TYR:CD2	2.55	0.41
1:C:111:GLU:CD	1:C:111:GLU:H	2.28	0.41
1:C:269:TYR:CZ	1:C:273:ASP:HB2	2.56	0.41
1:D:82:MET:HE3	1:D:82:MET:HB3	1.93	0.41
1:D:299:ASP:O	1:D:303:LYS:HD3	2.21	0.41
1:E:206:SER:HB3	1:E:365:TYR:CD1	2.56	0.41
1:E:206:SER:CB	1:E:365:TYR:HD1	2.34	0.41
1:E:247:VAL:O	1:E:248:GLU:HG2	2.21	0.41
1:F:195:ASN:HB2	1:F:227:HIS:NE2	2.33	0.41
1:F:366:ARG:HH22	1:H:192:HIS:CE1	2.39	0.41
1:F:367:PRO:HG3	1:H:199:PHE:CG	2.55	0.41
1:G:190:ALA:O	1:G:347:ARG:HA	2.20	0.41
1:I:211:PRO:O	1:I:215:ILE:HG12	2.21	0.41
1:I:222:LEU:HD11	1:I:351:TRP:CZ2	2.55	0.41
1:I:300:THR:N	1:I:303:LYS:HD3	2.36	0.41
1:K:24:GLU:HB2	1:K:25:LYS:HZ3	1.86	0.41
1:L:68:GLN:HG2	1:L:72:ASN:HD21	1.85	0.41
1:L:334:ILE:CG2	1:L:342:LEU:HD11	2.46	0.41
1:G:34:PRO:O	1:G:38:LEU:HG	2.21	0.41
1:G:226:LEU:HD12	1:G:226:LEU:N	2.33	0.41
1:I:264:MET:HE2	1:I:264:MET:HB2	1.94	0.41
1:I:306:GLU:HG2	1:I:311:ARG:HD3	2.01	0.41
1:K:323:PHE:HD1	1:K:324:TYR:CD2	2.38	0.41
1:L:68:GLN:CD	1:L:130:VAL:HG11	2.45	0.41
1:B:27:ILE:HG12	1:B:28:LEU:CD1	2.40	0.41
1:B:239:GLN:HG2	1:B:298:PHE:CZ	2.55	0.41
1:B:264:MET:HE2	1:B:264:MET:HB3	1.93	0.41
1:D:363:ARG:HG3	1:D:365:TYR:CD1	2.56	0.41
1:E:120:GLU:H	1:E:120:GLU:CD	2.27	0.41
1:G:67:GLN:HA	1:G:70:LYS:HD2	2.02	0.41
1:G:148:ASN:HB2	1:G:150:TRP:CD1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:280:HIS:O	1:G:284:GLU:HG3	2.20	0.41
1:H:103:LEU:HA	1:H:106:PHE:HD2	1.85	0.41
1:H:167:TYR:O	1:H:171:GLY:N	2.53	0.41
1:I:225:PRO:HG3	1:L:112:CYS:SG	2.61	0.41
1:I:362:ASN:N	1:I:362:ASN:HD22	2.18	0.41
1:K:27:ILE:HG12	1:K:28:LEU:HD13	2.02	0.41
1:K:28:LEU:CB	1:K:34:PRO:HA	2.35	0.41
1:K:280:HIS:O	1:K:284:GLU:HG3	2.20	0.41
1:L:59:LYS:NZ	1:L:60:LYS:HD2	2.36	0.41
1:L:102:SER:HA	1:L:105:MET:HE2	2.01	0.41
1:B:312:LEU:H	1:B:312:LEU:CD2	2.25	0.41
1:C:234:VAL:HG11	1:C:339:PHE:HE2	1.85	0.41
1:D:100:VAL:HG21	1:D:219:ILE:HD11	2.02	0.41
1:D:193:THR:O	1:D:194:LEU:C	2.64	0.41
1:E:177:LEU:O	1:E:181:ILE:HG13	2.21	0.41
1:H:326:GLY:HA2	1:H:329:TYR:HD2	1.85	0.41
1:J:31:ARG:NH2	1:J:51:LEU:O	2.53	0.41
1:J:38:LEU:O	1:J:42:SER:HB3	2.20	0.41
1:K:40:GLU:HG2	1:K:41:ASN:ND2	2.35	0.41
1:L:77:TYR:O	1:L:80:ARG:HG2	2.21	0.41
1:L:91:HIS:ND1	1:L:93:MET:HB2	2.36	0.41
1:A:324:TYR:HD1	1:A:327:ILE:HD12	1.85	0.41
1:C:49:LEU:HD21	1:C:65:PHE:CG	2.56	0.41
1:C:206:SER:HA	1:C:362:ASN:CG	2.46	0.41
1:C:286:LEU:HD23	1:C:286:LEU:C	2.46	0.41
1:C:338:GLU:O	1:C:342:LEU:HD13	2.21	0.41
1:D:126:ARG:HH21	1:D:129:THR:HG21	1.84	0.41
1:D:286:LEU:HD22	1:D:328:LEU:HD12	2.03	0.41
1:E:167:TYR:HA	1:E:172:GLU:O	2.20	0.41
1:E:178:MET:SD	1:E:332:MET:HG2	2.61	0.41
1:F:264:MET:SD	1:F:319:PRO:CG	3.09	0.41
1:H:196:ALA:HB3	1:H:227:HIS:ND1	2.35	0.41
1:I:27:ILE:O	1:I:28:LEU:C	2.62	0.41
1:J:59:LYS:HB3	1:J:59:LYS:HE3	1.89	0.41
1:J:211:PRO:O	1:J:215:ILE:HG12	2.20	0.41
1:J:285:GLN:O	1:J:289:GLU:HG2	2.21	0.41
1:K:233:ARG:NH2	1:K:322:ASP:O	2.53	0.41
1:L:320:ASN:CG	1:L:321:VAL:H	2.29	0.41
1:A:156:LYS:HE3	1:A:167:TYR:CE1	2.56	0.41
1:A:367:PRO:HG2	1:C:194:LEU:HB3	2.03	0.41
1:B:24:GLU:OE1	1:B:25:LYS:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:340:THR:O	1:B:343:PHE:HB3	2.21	0.41
1:C:304:LEU:HA	1:C:307:VAL:HG22	2.02	0.41
1:D:85:HIS:CD2	1:E:81:GLN:HE21	2.38	0.41
1:D:304:LEU:HD22	1:D:304:LEU:N	2.35	0.41
1:E:156:LYS:HB2	1:E:159:LEU:HB2	2.03	0.41
1:E:359:ILE:HG13	1:E:360:SER:N	2.36	0.41
1:F:28:LEU:N	1:F:28:LEU:CD1	2.84	0.41
1:F:82:MET:HE2	1:F:82:MET:HB3	1.90	0.41
1:F:233:ARG:HD3	1:F:233:ARG:C	2.46	0.41
1:G:88:HIS:O	1:G:147:ARG:HG3	2.20	0.41
1:G:306:GLU:O	1:G:307:VAL:HB	2.21	0.41
1:H:329:TYR:HA	1:H:334:ILE:HD12	2.02	0.41
1:H:371:TYR:CG	1:H:371:TYR:O	2.72	0.41
1:I:42:SER:HA	1:I:46:GLU:OE1	2.20	0.41
1:I:68:GLN:CD	1:I:130:VAL:HG21	2.46	0.41
1:I:76:LYS:HE3	1:I:106:PHE:HB3	2.03	0.41
1:I:102:SER:HB2	1:L:86:PHE:CE1	2.55	0.41
1:I:283:VAL:O	1:I:287:VAL:HG23	2.21	0.41
1:J:68:GLN:HA	1:J:71:ASP:OD2	2.21	0.41
1:J:283:VAL:O	1:J:287:VAL:HG23	2.21	0.41
1:J:338:GLU:O	1:J:342:LEU:HD13	2.21	0.41
1:K:80:ARG:O	1:K:84:ARG:HG3	2.21	0.41
1:K:135:GLN:C	1:K:138:PRO:HD2	2.46	0.41
1:L:199:PHE:HA	1:L:202:LEU:HD12	2.01	0.41
1:L:202:LEU:CD2	1:L:354:HIS:HB3	2.51	0.41
1:L:237:MET:O	1:L:238:LEU:HB2	2.21	0.41
1:A:44:PHE:CD1	1:A:186:LEU:HB3	2.56	0.41
1:A:231:ASN:HA	1:A:234:VAL:CG2	2.50	0.41
1:A:241:ILE:CG2	1:A:244:PRO:HG2	2.45	0.41
1:A:267:ARG:NH1	1:C:366:ARG:HB3	2.36	0.41
1:A:275:ARG:O	1:A:279:LEU:HG	2.21	0.41
1:B:198:THR:HA	1:B:351:TRP:CD1	2.56	0.41
1:B:297:MET:HE2	1:B:302:LEU:HD21	2.03	0.41
1:B:321:VAL:HG13	1:B:322:ASP:OD1	2.21	0.41
1:C:323:PHE:C	1:C:324:TYR:HD1	2.29	0.41
1:I:69:LEU:HD12	1:I:130:VAL:O	2.20	0.41
1:I:278:ILE:O	1:I:282:LEU:HG	2.21	0.41
1:J:110:THR:HG22	1:J:112:CYS:H	1.86	0.41
1:J:233:ARG:HA	1:J:233:ARG:HH11	1.86	0.41
1:K:222:LEU:HG	1:K:227:HIS:ND1	2.36	0.41
1:K:305:GLU:OE2	1:K:324:TYR:HE1	2.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:337:ASP:OD1	1:B:337:ASP:N	2.53	0.40
1:C:358:GLN:O	1:C:362:ASN:HB2	2.21	0.40
1:E:46:GLU:HG3	1:E:57:PRO:HD2	2.02	0.40
1:E:69:LEU:HD12	1:E:134:ALA:HB2	2.03	0.40
1:E:189:HIS:HB3	1:E:343:PHE:CD1	2.56	0.40
1:F:36:GLU:H	1:F:36:GLU:CD	2.29	0.40
1:F:359:ILE:HG13	1:F:360:SER:H	1.85	0.40
1:G:177:LEU:O	1:G:181:ILE:HG13	2.20	0.40
1:H:192:HIS:CE1	1:H:266:HIS:NE2	2.79	0.40
1:I:27:ILE:HD12	1:I:274:PRO:HB3	2.02	0.40
1:I:159:LEU:HA	1:I:163:GLU:OE1	2.22	0.40
1:J:372:VAL:HB	1:J:375:ASP:HA	2.03	0.40
1:K:24:GLU:HG3	1:K:25:LYS:H	1.86	0.40
1:B:126:ARG:NH2	1:B:129:THR:HG21	2.36	0.40
1:C:324:TYR:O	1:C:327:ILE:HG12	2.21	0.40
1:D:188:LEU:HD21	1:D:278:ILE:HB	2.04	0.40
1:E:159:LEU:HA	1:E:163:GLU:OE1	2.22	0.40
1:H:26:GLY:H	1:H:269:TYR:HE1	1.68	0.40
1:H:231:ASN:O	1:H:234:VAL:HG12	2.21	0.40
1:H:323:PHE:C	1:H:325:SER:H	2.30	0.40
1:I:121:ASP:OD1	1:I:122:LEU:N	2.55	0.40
1:I:194:LEU:O	1:L:367:PRO:HD2	2.22	0.40
1:I:222:LEU:HD13	1:I:343:PHE:CD2	2.57	0.40
1:K:266:HIS:CB	1:K:269:TYR:HB2	2.34	0.40
1:K:273:ASP:OD2	1:K:321:VAL:HB	2.21	0.40
1:L:140:VAL:HG12	1:L:169:PHE:CZ	2.54	0.40
1:L:312:LEU:H	1:L:312:LEU:CD1	2.34	0.40
1:A:27:ILE:HD11	1:A:274:PRO:HB3	2.03	0.40
1:A:126:ARG:HH22	1:A:356:ARG:HD2	1.86	0.40
1:A:198:THR:O	1:A:202:LEU:HG	2.21	0.40
1:B:363:ARG:HH21	1:B:369:GLN:NE2	2.19	0.40
1:C:122:LEU:HD12	1:C:122:LEU:C	2.46	0.40
1:E:356:ARG:O	1:E:359:ILE:HG23	2.21	0.40
1:F:70:LYS:HD3	1:F:157:HIS:O	2.21	0.40
1:F:136:MET:O	1:F:140:VAL:HG23	2.21	0.40
1:G:156:LYS:HD2	1:G:159:LEU:HD22	2.04	0.40
1:G:238:LEU:O	1:G:239:GLN:C	2.64	0.40
1:G:243:SER:HB2	1:G:244:PRO:HD3	2.03	0.40
1:I:207:THR:O	1:I:208:LEU:HB2	2.21	0.40
1:K:206:SER:HA	1:K:362:ASN:CG	2.46	0.40
1:K:283:VAL:O	1:K:287:VAL:HG23	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:301:ALA:O	1:B:302:LEU:HD23	2.22	0.40
1:C:304:LEU:HD12	1:C:327:ILE:HD13	2.03	0.40
1:G:27:ILE:HG13	1:G:193:THR:OG1	2.21	0.40
1:H:162:ALA:HA	1:H:165:LEU:HD12	2.03	0.40
1:I:366:ARG:NH1	1:L:195:ASN:HA	2.36	0.40
1:K:350:GLY:O	1:K:354:HIS:HD2	2.04	0.40
1:A:80:ARG:O	1:A:84:ARG:HG3	2.21	0.40
1:A:176:PRO:HB2	1:A:180:LYS:NZ	2.37	0.40
1:C:273:ASP:OD2	1:C:321:VAL:HB	2.21	0.40
1:D:177:LEU:HG	1:D:181:ILE:HD11	2.03	0.40
1:D:194:LEU:N	1:D:194:LEU:HD22	2.37	0.40
1:D:340:THR:O	1:D:343:PHE:HB3	2.22	0.40
1:E:80:ARG:HG3	1:E:81:GLN:N	2.37	0.40
1:G:49:LEU:HD11	1:G:62:LEU:HA	2.04	0.40
1:G:169:PHE:HE2	1:G:338:GLU:HG3	1.87	0.40
1:H:82:MET:HE3	1:H:82:MET:HB3	1.95	0.40
1:I:182:MET:HE2	1:I:332:MET:SD	2.61	0.40
1:K:125:VAL:HA	1:K:128:MET:SD	2.61	0.40
1:K:129:THR:O	1:K:133:ILE:HG13	2.22	0.40
1:L:234:VAL:HG21	1:L:339:PHE:CE2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	316/397 (80%)	297 (94%)	19 (6%)	0	100	100
1	B	319/397 (80%)	292 (92%)	27 (8%)	0	100	100
1	C	301/397 (76%)	283 (94%)	18 (6%)	0	100	100
1	D	316/397 (80%)	300 (95%)	16 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	313/397 (79%)	297 (95%)	15 (5%)	1 (0%)	36	68
1	F	308/397 (78%)	284 (92%)	24 (8%)	0	100	100
1	G	301/397 (76%)	282 (94%)	19 (6%)	0	100	100
1	H	305/397 (77%)	283 (93%)	21 (7%)	1 (0%)	36	68
1	I	297/397 (75%)	280 (94%)	16 (5%)	1 (0%)	36	68
1	J	318/397 (80%)	299 (94%)	19 (6%)	0	100	100
1	K	295/397 (74%)	280 (95%)	15 (5%)	0	100	100
1	L	307/397 (77%)	286 (93%)	21 (7%)	0	100	100
All	All	3696/4764 (78%)	3463 (94%)	230 (6%)	3 (0%)	48	79

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	242	GLY
1	I	108	PRO
1	E	367	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	275/340 (81%)	270 (98%)	5 (2%)	51	74
1	B	278/340 (82%)	265 (95%)	13 (5%)	23	57
1	C	265/340 (78%)	257 (97%)	8 (3%)	36	66
1	D	275/340 (81%)	270 (98%)	5 (2%)	51	74
1	E	273/340 (80%)	268 (98%)	5 (2%)	51	74
1	F	270/340 (79%)	264 (98%)	6 (2%)	45	71
1	G	266/340 (78%)	256 (96%)	10 (4%)	29	62
1	H	269/340 (79%)	261 (97%)	8 (3%)	36	66
1	I	264/340 (78%)	255 (97%)	9 (3%)	32	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	275/340 (81%)	266 (97%)	9 (3%)	33	65
1	K	262/340 (77%)	258 (98%)	4 (2%)	57	76
1	L	271/340 (80%)	261 (96%)	10 (4%)	30	63
All	All	3243/4080 (80%)	3151 (97%)	92 (3%)	38	68

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	LYS
1	A	28	LEU
1	A	136	MET
1	A	337	ASP
1	A	359	ILE
1	B	27	ILE
1	B	28	LEU
1	B	50	LEU
1	B	111	GLU
1	B	126	ARG
1	B	191	GLU
1	B	233	ARG
1	B	235	VAL
1	B	299	ASP
1	B	307	VAL
1	B	312	LEU
1	B	337	ASP
1	B	372	VAL
1	C	136	MET
1	C	158	ASP
1	C	186	LEU
1	C	240	GLU
1	C	271	VAL
1	C	303	LYS
1	C	307	VAL
1	C	323	PHE
1	D	27	ILE
1	D	28	LEU
1	D	29	SER
1	D	233	ARG
1	D	302	LEU
1	E	25	LYS
1	E	27	ILE

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Mol	Chain	Res	Type
1	E	36	GLU
1	E	245	LYS
1	E	248	GLU
1	F	28	LEU
1	F	241	ILE
1	F	245	LYS
1	F	312	LEU
1	F	337	ASP
1	F	359	ILE
1	G	27	ILE
1	G	62	LEU
1	G	107	TYR
1	G	122	LEU
1	G	153	VAL
1	G	239	GLN
1	G	272	LYS
1	G	310	ASP
1	G	370	ILE
1	G	372	VAL
1	H	25	LYS
1	H	51	LEU
1	H	78	HIS
1	H	191	GLU
1	H	233	ARG
1	H	239	GLN
1	H	303	LYS
1	H	358	GLN
1	I	29	SER
1	I	36	GLU
1	I	82	MET
1	I	107	TYR
1	I	219	ILE
1	I	271	VAL
1	I	283	VAL
1	I	310	ASP
1	I	362	ASN
1	J	40	GLU
1	J	49	LEU
1	J	107	TYR
1	J	124	TYR
1	J	165	LEU
1	J	169	PHE

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Mol	Chain	Res	Type
1	J	245	LYS
1	J	304	LEU
1	J	368	THR
1	K	24	GLU
1	K	28	LEU
1	K	107	TYR
1	K	214	VAL
1	L	28	LEU
1	L	37	THR
1	L	122	LEU
1	L	126	ARG
1	L	128	MET
1	L	139	LEU
1	L	300	THR
1	L	302	LEU
1	L	305	GLU
1	L	312	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (91) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	A	67	GLN
1	A	68	GLN
1	A	81	GLN
1	A	91	HIS
1	A	145	HIS
1	A	157	HIS
1	A	232	GLN
1	B	41	ASN
1	B	63	ASN
1	B	68	GLN
1	B	127	ASN
1	B	157	HIS
1	B	195	ASN
1	B	227	HIS
1	B	232	GLN
1	B	358	GLN
1	B	369	GLN
1	C	41	ASN
1	C	72	ASN
1	C	81	GLN

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Mol	Chain	Res	Type
1	C	127	ASN
1	C	154	ASN
1	C	170	ASN
1	D	85	HIS
1	D	91	HIS
1	D	157	HIS
1	D	227	HIS
1	D	246	ASN
1	D	358	GLN
1	E	41	ASN
1	E	81	GLN
1	E	192	HIS
1	E	195	ASN
1	E	227	HIS
1	E	239	GLN
1	E	246	ASN
1	F	91	HIS
1	F	148	ASN
1	F	157	HIS
1	F	189	HIS
1	F	358	GLN
1	G	68	GLN
1	G	72	ASN
1	G	148	ASN
1	G	154	ASN
1	G	157	HIS
1	G	170	ASN
1	G	189	HIS
1	G	232	GLN
1	G	239	GLN
1	G	354	HIS
1	G	358	GLN
1	H	67	GLN
1	H	72	ASN
1	H	145	HIS
1	H	148	ASN
1	H	192	HIS
1	H	227	HIS
1	H	239	GLN
1	H	369	GLN
1	I	41	ASN
1	I	67	GLN

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Mol	Chain	Res	Type
1	I	72	ASN
1	I	97	GLN
1	I	131	ASN
1	I	135	GLN
1	I	148	ASN
1	I	157	HIS
1	I	227	HIS
1	I	354	HIS
1	I	362	ASN
1	J	135	GLN
1	J	148	ASN
1	J	192	HIS
1	J	227	HIS
1	J	280	HIS
1	K	41	ASN
1	K	63	ASN
1	K	67	GLN
1	K	72	ASN
1	K	85	HIS
1	K	154	ASN
1	K	231	ASN
1	L	72	ASN
1	L	131	ASN
1	L	145	HIS
1	L	148	ASN
1	L	157	HIS
1	L	170	ASN
1	L	280	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no 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	324/397 (81%)	0.65	23 (7%)	22	14	86, 118, 157, 237	0
1	B	327/397 (82%)	0.65	27 (8%)	17	11	84, 114, 187, 280	0
1	C	311/397 (78%)	0.62	18 (5%)	29	18	89, 135, 208, 286	0
1	D	324/397 (81%)	0.58	16 (4%)	35	22	85, 117, 172, 218	0
1	E	321/397 (80%)	0.62	26 (8%)	18	11	85, 116, 171, 259	0
1	F	318/397 (80%)	0.58	24 (7%)	20	13	30, 122, 183, 255	0
1	G	313/397 (78%)	0.84	33 (10%)	11	8	96, 127, 207, 286	0
1	H	315/397 (79%)	0.74	24 (7%)	20	13	89, 140, 207, 271	0
1	I	311/397 (78%)	0.52	12 (3%)	43	27	94, 135, 209, 262	0
1	J	326/397 (82%)	0.67	25 (7%)	19	13	96, 131, 187, 285	0
1	K	309/397 (77%)	0.70	27 (8%)	16	11	92, 132, 205, 241	0
1	L	317/397 (79%)	0.64	11 (3%)	47	29	30, 147, 209, 288	0
All	All	3816/4764 (80%)	0.65	266 (6%)	22	14	30, 128, 199, 288	0

All (266) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	374	SER	8.3
1	B	370	ILE	6.4
1	J	304	LEU	5.8
1	F	319	PRO	5.4
1	E	44	PHE	5.2
1	H	35	LEU	5.1
1	G	29	SER	4.7
1	A	194	LEU	4.6
1	E	186	LEU	4.5
1	B	375	ASP	4.4
1	F	304	LEU	4.3

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Mol	Chain	Res	Type	RSRZ
1	F	321	VAL	4.2
1	J	39	ALA	4.2
1	D	279	LEU	4.1
1	J	233	ARG	4.1
1	G	230	ALA	4.0
1	B	69	LEU	3.9
1	F	279	LEU	3.9
1	J	38	LEU	3.9
1	F	230	ALA	3.9
1	C	44	PHE	3.8
1	J	348	SER	3.8
1	A	111	GLU	3.7
1	H	44	PHE	3.7
1	H	189	HIS	3.7
1	H	230	ALA	3.7
1	G	27	ILE	3.6
1	J	230	ALA	3.5
1	B	310	ASP	3.5
1	L	301	ALA	3.5
1	G	106	PHE	3.5
1	D	301	ALA	3.5
1	E	364	ILE	3.5
1	J	323	PHE	3.4
1	J	193	THR	3.4
1	J	351	TRP	3.4
1	B	124	TYR	3.4
1	H	188	LEU	3.4
1	K	302	LEU	3.4
1	A	304	LEU	3.3
1	D	39	ALA	3.3
1	F	236	GLY	3.3
1	F	320	ASN	3.3
1	E	111	GLU	3.3
1	C	136	MET	3.2
1	B	211	PRO	3.2
1	C	343	PHE	3.2
1	F	26	GLY	3.2
1	L	343	PHE	3.2
1	K	39	ALA	3.2
1	F	131	ASN	3.1
1	H	375	ASP	3.1
1	E	183	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	194	LEU	3.0
1	H	109	GLY	3.0
1	H	302	LEU	3.0
1	B	104	GLY	3.0
1	H	187	ILE	3.0
1	L	108	PRO	3.0
1	F	282	LEU	3.0
1	H	56	LEU	3.0
1	C	318	TYR	3.0
1	A	173	GLU	3.0
1	E	57	PRO	2.9
1	K	191	GLU	2.9
1	A	107	TYR	2.9
1	C	111	GLU	2.9
1	A	204	ALA	2.9
1	C	197	SER	2.9
1	G	103	LEU	2.9
1	K	367	PRO	2.9
1	H	301	ALA	2.9
1	L	93	MET	2.9
1	G	340	THR	2.9
1	G	372	VAL	2.9
1	F	27	ILE	2.9
1	A	301	ALA	2.8
1	D	283	VAL	2.8
1	H	310	ASP	2.8
1	L	202	LEU	2.8
1	F	135	GLN	2.8
1	G	223	SER	2.8
1	J	375	ASP	2.8
1	K	121	ASP	2.8
1	J	307	VAL	2.8
1	L	319	PRO	2.8
1	E	334	ILE	2.8
1	I	121	ASP	2.8
1	I	200	ALA	2.8
1	G	193	THR	2.8
1	B	371	TYR	2.7
1	H	190	ALA	2.7
1	I	201	ALA	2.7
1	F	112	CYS	2.7
1	K	150	TRP	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	371	TYR	2.7
1	G	85	HIS	2.7
1	H	38	LEU	2.7
1	J	165	LEU	2.7
1	C	334	ILE	2.7
1	C	370	ILE	2.7
1	D	106	PHE	2.7
1	G	107	TYR	2.7
1	G	319	PRO	2.7
1	A	230	ALA	2.7
1	I	369	GLN	2.7
1	C	222	LEU	2.7
1	I	202	LEU	2.7
1	E	110	THR	2.6
1	K	230	ALA	2.6
1	F	266	HIS	2.6
1	J	361	ASP	2.6
1	G	154	ASN	2.6
1	B	193	THR	2.6
1	B	177	LEU	2.6
1	I	230	ALA	2.6
1	G	241	ILE	2.6
1	A	367	PRO	2.6
1	B	367	PRO	2.6
1	K	236	GLY	2.6
1	B	238	LEU	2.6
1	K	283	VAL	2.6
1	C	223	SER	2.6
1	G	371	TYR	2.6
1	J	29	SER	2.6
1	D	35	LEU	2.6
1	A	373	GLY	2.6
1	E	338	GLU	2.6
1	E	317	VAL	2.6
1	E	340	THR	2.6
1	I	266	HIS	2.5
1	G	42	SER	2.5
1	A	153	VAL	2.5
1	J	301	ALA	2.5
1	F	327	ILE	2.5
1	J	368	THR	2.5
1	B	73	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	307	VAL	2.5
1	C	231	ASN	2.5
1	E	310	ASP	2.5
1	E	262	TRP	2.5
1	G	233	ARG	2.5
1	G	348	SER	2.5
1	F	310	ASP	2.5
1	G	121	ASP	2.5
1	B	85	HIS	2.5
1	G	161	VAL	2.5
1	H	372	VAL	2.5
1	A	239	GLN	2.5
1	E	179	ALA	2.4
1	F	323	PHE	2.4
1	G	362	ASN	2.4
1	A	124	TYR	2.4
1	K	125	VAL	2.4
1	I	27	ILE	2.4
1	D	65	PHE	2.4
1	K	193	THR	2.4
1	G	367	PRO	2.4
1	C	209	ALA	2.4
1	K	101	SER	2.4
1	K	374	SER	2.4
1	J	109	GLY	2.4
1	A	82	MET	2.4
1	D	320	ASN	2.4
1	F	71	ASP	2.4
1	H	137	ALA	2.4
1	L	35	LEU	2.4
1	H	111	GLU	2.4
1	H	374	SER	2.4
1	A	41	ASN	2.3
1	C	303	LYS	2.3
1	I	362	ASN	2.3
1	A	106	PHE	2.3
1	C	285	GLN	2.3
1	K	188	LEU	2.3
1	L	335	PRO	2.3
1	E	187	ILE	2.3
1	K	241	ILE	2.3
1	J	322	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	29	SER	2.3
1	B	219	ILE	2.3
1	A	35	LEU	2.3
1	K	211	PRO	2.3
1	C	32	GLY	2.3
1	B	199	PHE	2.3
1	D	125	VAL	2.3
1	I	184	VAL	2.3
1	E	359	ILE	2.3
1	J	27	ILE	2.3
1	D	262	TRP	2.3
1	G	269	TYR	2.3
1	F	283	VAL	2.3
1	G	111	GLU	2.2
1	B	182	MET	2.2
1	K	263	GLY	2.2
1	E	282	LEU	2.2
1	K	355	TRP	2.2
1	G	327	ILE	2.2
1	H	49	LEU	2.2
1	A	228	GLY	2.2
1	D	103	LEU	2.2
1	I	285	GLN	2.2
1	C	181	ILE	2.2
1	B	304	LEU	2.2
1	F	139	LEU	2.2
1	G	188	LEU	2.2
1	J	373	GLY	2.2
1	E	375	ASP	2.2
1	I	77	TYR	2.2
1	L	81	GLN	2.2
1	K	301	ALA	2.2
1	E	109	GLY	2.2
1	J	350	GLY	2.2
1	G	185	CYS	2.2
1	C	199	PHE	2.2
1	B	365	TYR	2.1
1	H	186	LEU	2.1
1	K	38	LEU	2.1
1	D	264	MET	2.1
1	D	233	ARG	2.1
1	H	24	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	262	TRP	2.1
1	J	85	HIS	2.1
1	G	198	THR	2.1
1	H	340	THR	2.1
1	H	77	TYR	2.1
1	E	56	LEU	2.1
1	G	222	LEU	2.1
1	K	178	MET	2.1
1	B	230	ALA	2.1
1	L	160	SER	2.1
1	K	262	TRP	2.1
1	J	107	TYR	2.1
1	A	236	GLY	2.1
1	K	111	GLU	2.1
1	H	206	SER	2.1
1	J	195	ASN	2.1
1	B	321	VAL	2.1
1	J	184	VAL	2.1
1	A	189	HIS	2.1
1	B	337	ASP	2.1
1	E	304	LEU	2.1
1	G	186	LEU	2.1
1	F	365	TYR	2.1
1	G	288	ALA	2.1
1	D	26	GLY	2.1
1	E	184	VAL	2.1
1	B	368	THR	2.1
1	F	136	MET	2.1
1	D	73	TYR	2.1
1	K	30	TYR	2.1
1	A	137	ALA	2.1
1	C	230	ALA	2.1
1	E	65	PHE	2.1
1	E	238	LEU	2.0
1	K	146	ILE	2.0
1	K	286	LEU	2.0
1	D	230	ALA	2.0
1	G	112	CYS	2.0
1	B	369	GLN	2.0
1	L	109	GLY	2.0
1	K	246	ASN	2.0
1	E	337	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	169	PHE	2.0
1	G	86	PHE	2.0
1	A	152	PRO	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.