



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 10:22 AM UTC

PDB ID : 4UQV / pdb_00004uqv
Title : methanococcus jannaschii serine hydroxymethyl-transferase in complex with PLP
Authors : Saccoccia, F.; Angelucci, F.; Ilari, A.
Deposited on : 2014-06-25
Resolution : 3.00 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

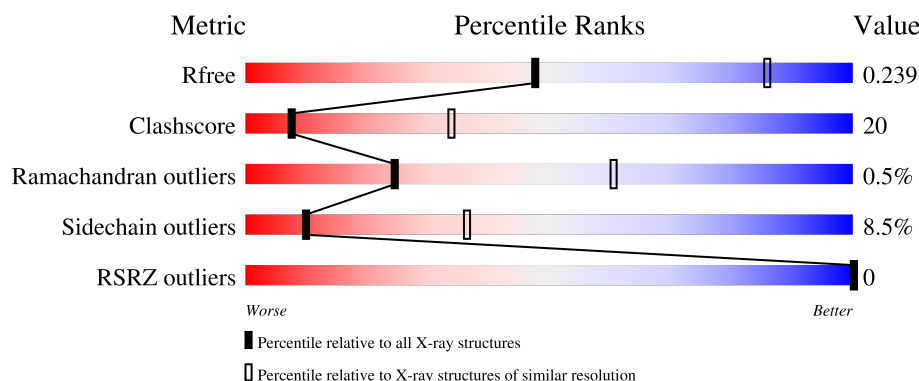
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

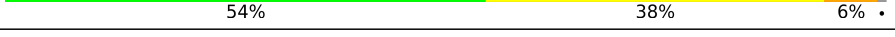
The reported resolution of this entry is 3.00 Å.

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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	429	 60% 34% . .
1	B	429	 59% 36% . .
1	C	429	 57% 37% . .
1	D	429	 54% 38% 6% .
1	E	429	 52% 43% .

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Mol	Chain	Length	Quality of chain
1	F	429	55%38%
1	G	429	56%39%5%
1	H	429	56%40%
1	I	429	58%38%
1	J	429	52%43%5%
1	K	429	52%41%5%
1	L	429	54%37%7%

2 Entry composition

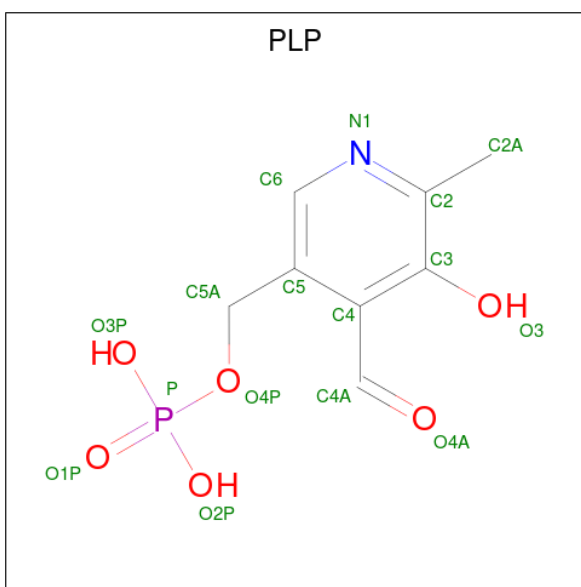
There are 2 unique types of molecules in this entry. The entry contains 40370 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 SERINE HYDROXYMETHYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	426	Total	C	N	O	S	0	0	0
			3362	2146	560	639	17			
1	B	424	Total	C	N	O	S	0	0	0
			3344	2133	558	636	17			
1	C	420	Total	C	N	O	S	0	0	0
			3308	2112	552	628	16			
1	D	425	Total	C	N	O	S	0	0	0
			3354	2141	559	638	16			
1	E	427	Total	C	N	O	S	0	0	0
			3369	2150	565	638	16			
1	F	418	Total	C	N	O	S	0	0	0
			3300	2107	554	623	16			
1	G	429	Total	C	N	O	S	0	0	0
			3386	2160	567	642	17			
1	H	427	Total	C	N	O	S	0	0	0
			3366	2146	564	639	17			
1	I	427	Total	C	N	O	S	0	0	0
			3369	2150	565	638	16			
1	J	429	Total	C	N	O	S	0	0	0
			3386	2160	567	642	17			
1	K	422	Total	C	N	O	S	0	0	0
			3329	2125	559	629	16			
1	L	420	Total	C	N	O	S	0	0	0
			3317	2122	555	624	16			

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: C₈H₁₀NO₆P).

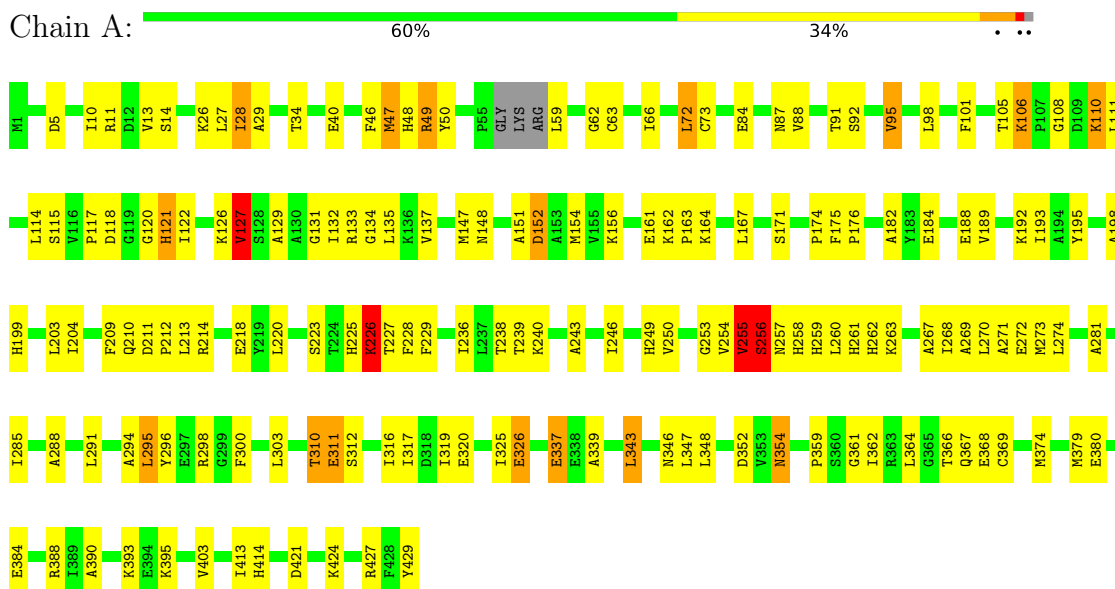


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	C	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	D	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	E	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	F	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	G	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	H	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	I	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	J	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	K	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	L	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

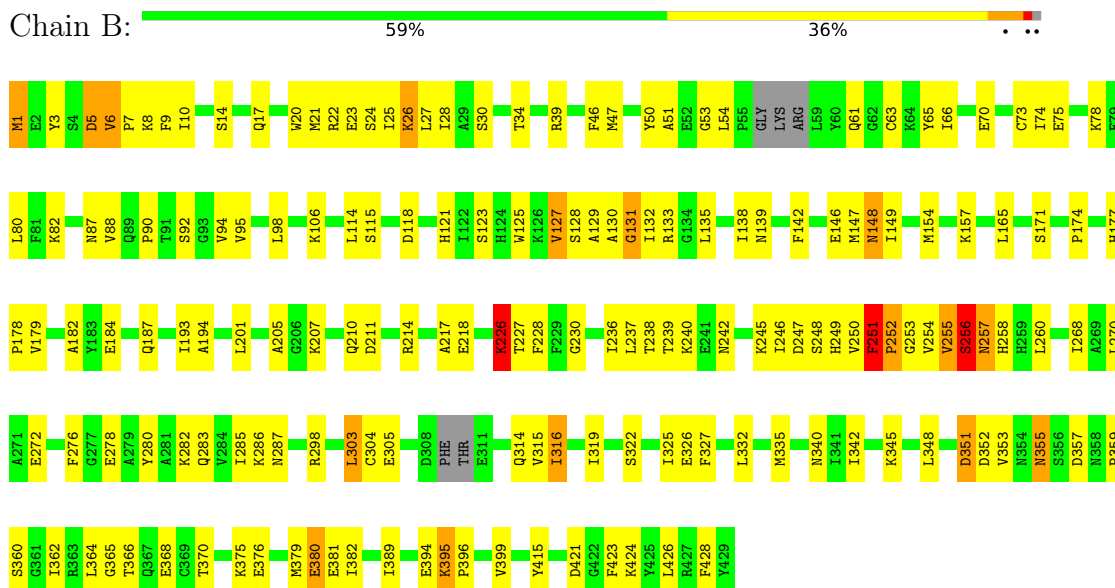
3 Residue-property plots

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: SERINE HYDROXYMETHYLTRANSFERASE

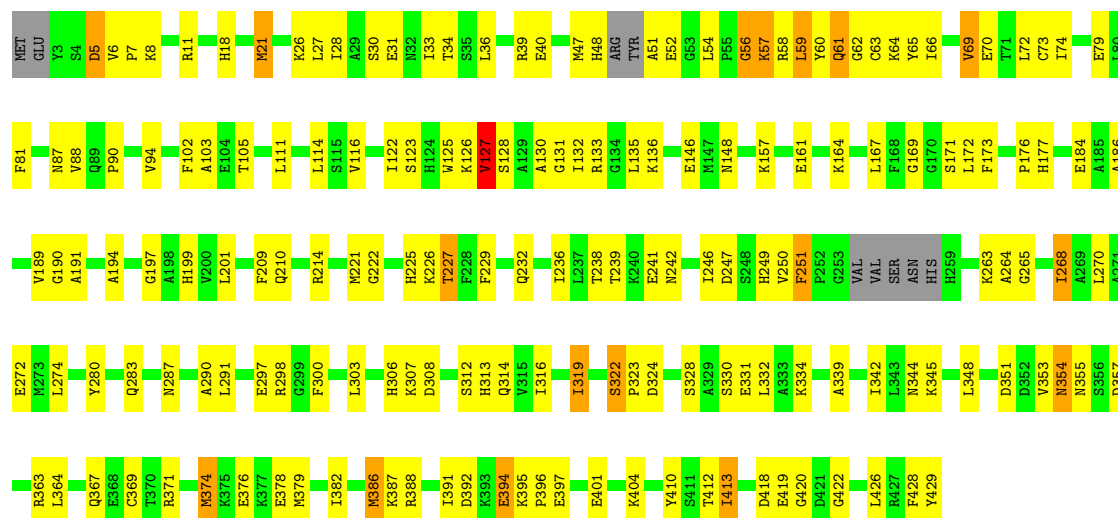


• Molecule 1: SERINE HYDROXYMETHYLTRANSFERASE



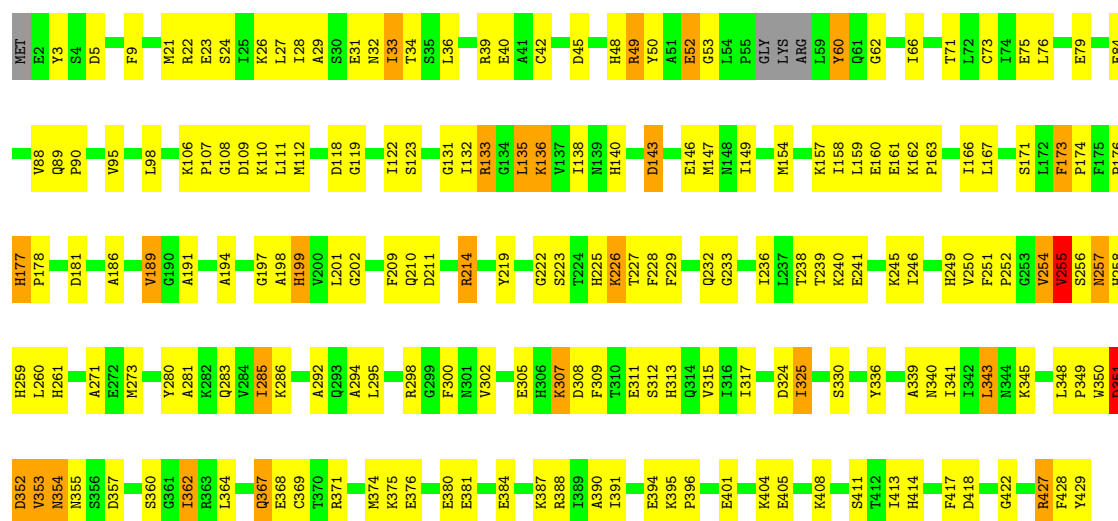
• Molecule 1: SERINE HYDROXYMETHYLTRANSFERASE

Chain C:  57% 37%



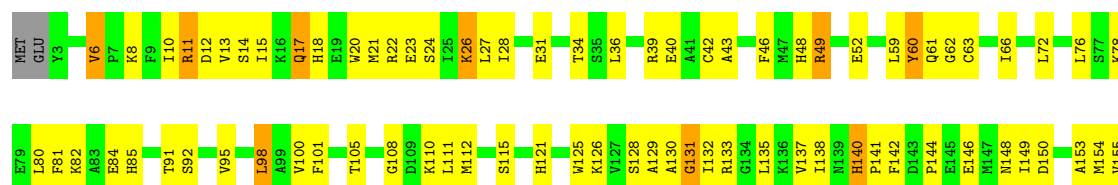
• Molecule 1: SERINE HYDROXYMETHYLTRANSFERASE

Chain D:  54% 38% 6%



• Molecule 1: SERINE HYDROXYMETHYLTRANSFERASE

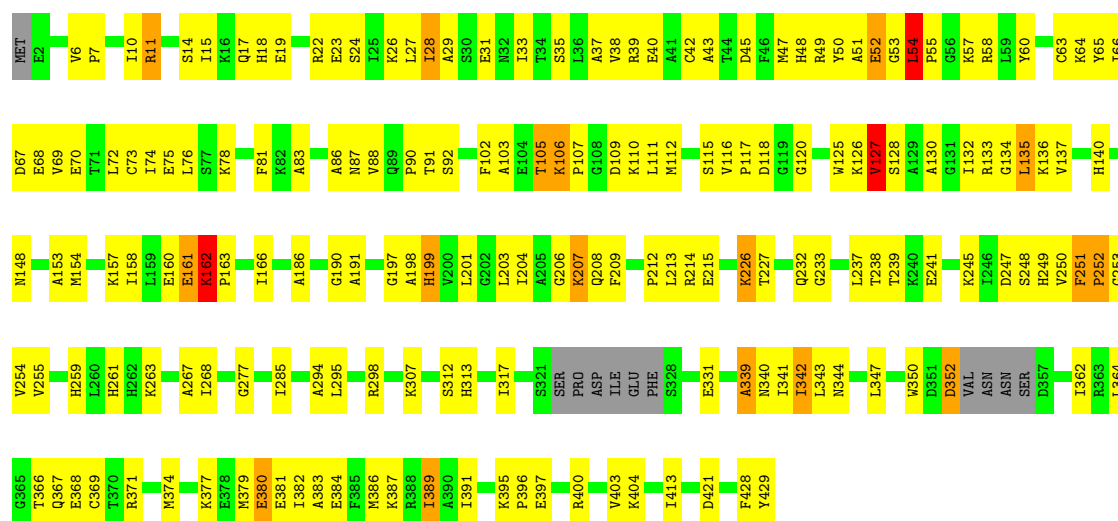
Chain E:  52% 43%





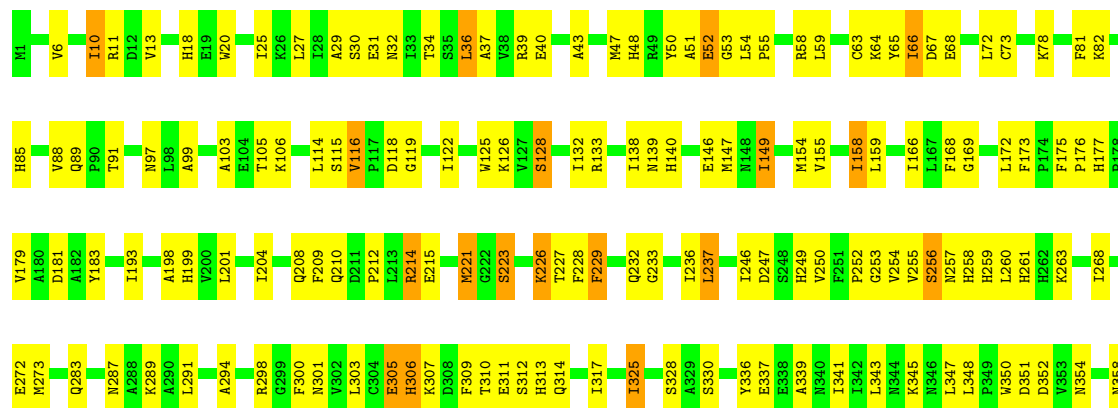
• Molecule 1: SERINE HYDROXYMETHYLTRANSFERASE

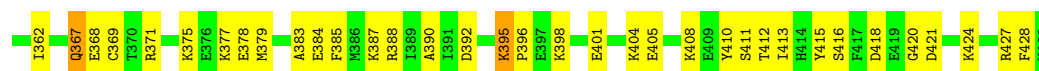
Chain F: 55% 38% . . .



• Molecule 1: SERINE HYDROXYMETHYLTRANSFERASE

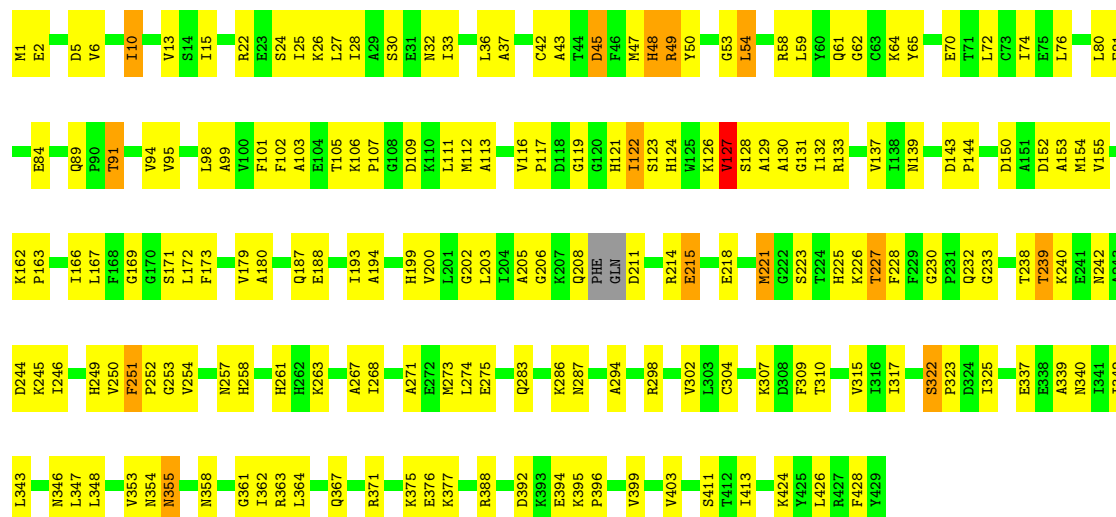
Chain G: 56% 39% 5%





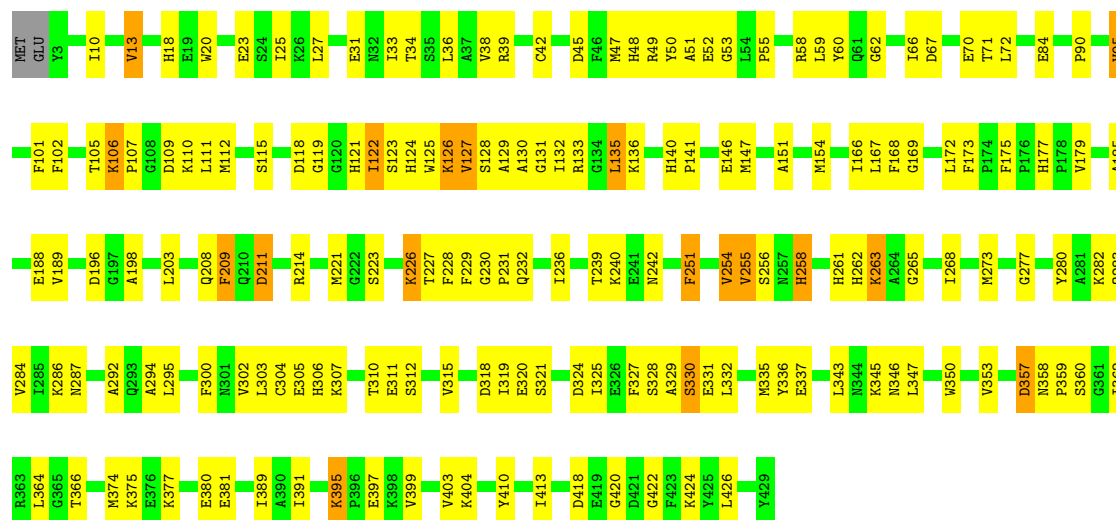
• Molecule 1: SERINE HYDROXYMETHYLTRANSFERASE

Chain H: 56% 40%



• Molecule 1: SERINE HYDROXYMETHYLTRANSFERASE

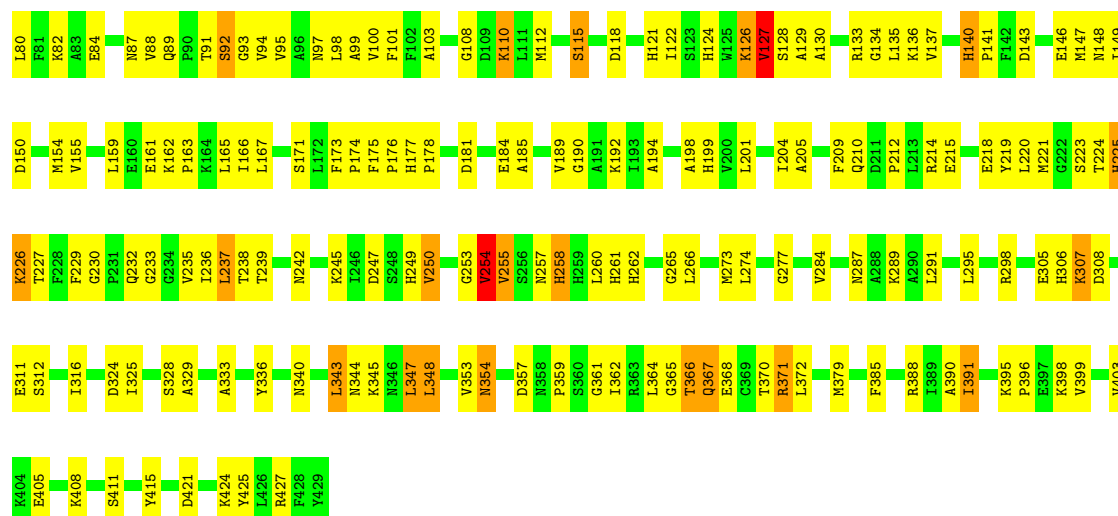
Chain I: 58% 38%



• Molecule 1: SERINE HYDROXYMETHYLTRANSFERASE

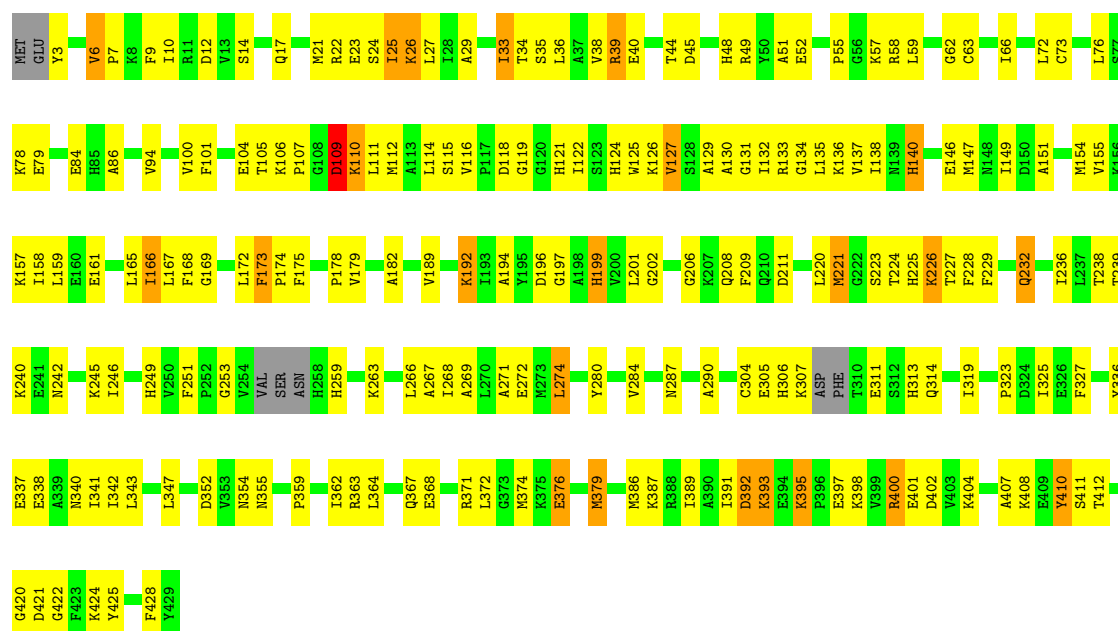
Chain J: 52% 43% 5%





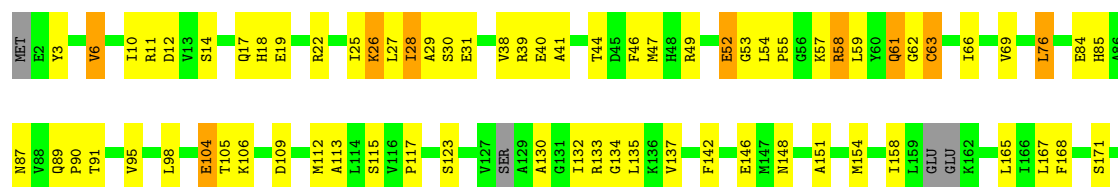
● Molecule 1: SERINE HYDROXYMETHYLTRANSFERASE

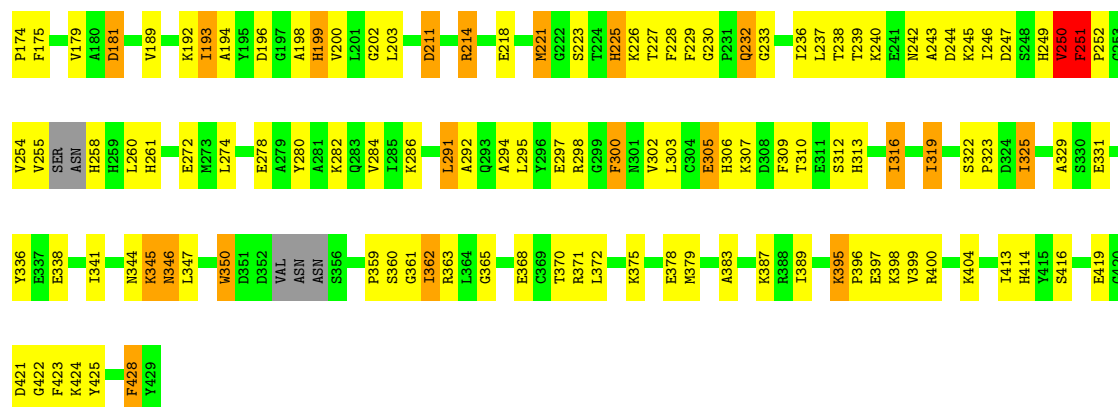
Chain K: 52% 41% 5% .



● Molecule 1: SERINE HYDROXYMETHYLTRANSFERASE

Chain L: 54% 37% 7% .





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	123.13Å 47.16Å 344.08Å 90.00° 90.02° 90.00°	Depositor
Resolution (Å)	49.15 – 3.00 49.15 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.15-3.00) 90.7 (49.15-3.00)	Depositor EDS
R_{merge}	0.28	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.85 (at 3.01Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: DEV_1702)	Depositor
R, R_{free}	0.198 , 0.243 0.202 , 0.239	Depositor DCC
R_{free} test set	4050 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	47.6	Xtriage
Anisotropy	0.350	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 15.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.438 for h,-k,-l	Xtriage
Reported twinning fraction	0.500 for -h,-k,l	Depositor
Outliers	0 of 80986 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	40370	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.90% 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 ⓘ

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

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	0.32	0/3437	0.81	3/4635 (0.1%)
1	B	0.36	2/3417 (0.1%)	0.92	21/4606 (0.5%)
1	C	0.34	0/3380	0.85	9/4554 (0.2%)
1	D	0.35	0/3429	0.89	11/4625 (0.2%)
1	E	0.33	0/3445	0.91	8/4646 (0.2%)
1	F	0.35	0/3372	0.87	6/4542 (0.1%)
1	G	0.33	0/3462	0.83	3/4668 (0.1%)
1	H	0.33	0/3440	0.86	10/4637 (0.2%)
1	I	0.35	1/3445 (0.0%)	0.90	9/4646 (0.2%)
1	J	0.37	0/3462	0.91	8/4668 (0.2%)
1	K	0.35	0/3402	0.86	12/4584 (0.3%)
1	L	0.33	0/3389	0.82	11/4563 (0.2%)
All	All	0.34	3/41080 (0.0%)	0.87	111/55374 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	2
1	C	0	5
1	D	0	3
1	E	0	2
1	F	0	2
1	G	0	1
1	I	0	3
1	J	0	1
1	K	0	3
1	L	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	27

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	251	PHE	C-N	6.29	1.41	1.34
1	I	226	LYS	CA-C	-5.63	1.47	1.53
1	B	252	PRO	N-CD	5.28	1.55	1.47

All (111) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	226	LYS	N-CA-C	16.87	137.19	111.04
1	E	226	LYS	N-CA-C	12.17	136.72	110.80
1	B	226	LYS	N-CA-C	11.80	135.94	110.80
1	I	226	LYS	N-CA-C	11.76	133.38	110.56
1	B	255	VAL	CB-CA-C	10.35	125.57	110.98
1	F	251	PHE	CA-C-N	-9.73	107.68	119.84
1	F	251	PHE	C-N-CA	-9.73	107.68	119.84
1	J	226	LYS	CB-CA-C	-9.32	96.57	111.39
1	C	226	LYS	N-CA-C	9.15	125.22	111.04
1	E	131	GLY	N-CA-C	-8.98	103.52	114.66
1	J	254	VAL	CB-CA-C	-8.84	96.79	111.29
1	I	226	LYS	CB-CA-C	-8.52	96.75	112.00
1	E	358	ASN	CA-C-N	-8.40	111.99	120.98
1	E	358	ASN	C-N-CA	-8.40	111.99	120.98
1	J	258	HIS	N-CA-C	8.37	122.80	112.59
1	H	251	PHE	CA-C-N	-8.27	110.06	120.23
1	H	251	PHE	C-N-CA	-8.27	110.06	120.23
1	B	255	VAL	N-CA-C	-8.14	96.58	108.71
1	B	257	ASN	N-CA-C	-8.11	97.42	108.86
1	H	54	LEU	CB-CA-C	6.96	123.87	110.17
1	B	395	LYS	CA-C-N	6.91	126.72	119.05
1	B	395	LYS	C-N-CA	6.91	126.72	119.05
1	J	129	ALA	N-CA-C	6.89	117.08	108.19
1	F	54	LEU	CB-CA-C	6.84	123.65	110.17
1	H	162	LYS	CA-C-N	6.83	128.38	119.84
1	H	162	LYS	C-N-CA	6.83	128.38	119.84
1	I	277	GLY	N-CA-C	6.80	120.87	112.64
1	D	351	ASP	N-CA-C	6.71	119.46	109.59
1	G	395	LYS	CA-C-N	6.67	126.18	119.24
1	G	395	LYS	C-N-CA	6.67	126.18	119.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	251	PHE	CA-C-N	6.59	128.08	119.84
1	L	251	PHE	C-N-CA	6.59	128.08	119.84
1	L	6	VAL	CA-C-N	-6.58	112.92	119.56
1	L	6	VAL	C-N-CA	-6.58	112.92	119.56
1	B	51	ALA	N-CA-C	6.55	117.69	108.00
1	B	352	ASP	N-CA-C	6.37	116.64	108.24
1	B	226	LYS	CB-CA-C	-6.35	97.79	110.42
1	K	109	ASP	CB-CA-C	-6.34	107.46	116.34
1	C	226	LYS	CB-CA-C	-6.27	101.43	111.39
1	E	226	LYS	CB-CA-C	-6.26	97.97	110.42
1	B	251	PHE	CA-C-N	-6.23	113.39	119.87
1	B	251	PHE	C-N-CA	-6.23	113.39	119.87
1	K	395	LYS	CA-C-N	6.14	125.36	118.97
1	K	395	LYS	C-N-CA	6.14	125.36	118.97
1	B	6	VAL	CB-CA-C	-6.11	107.88	114.35
1	D	211	ASP	CA-C-N	6.10	125.50	118.85
1	D	211	ASP	C-N-CA	6.10	125.50	118.85
1	K	392	ASP	N-CA-C	6.06	123.70	110.80
1	B	131	GLY	N-CA-C	-6.01	105.66	115.46
1	J	190	GLY	N-CA-C	-5.94	106.53	115.32
1	F	6	VAL	CA-C-N	-5.94	112.38	118.85
1	F	6	VAL	C-N-CA	-5.94	112.38	118.85
1	G	198	ALA	CB-CA-C	-5.84	109.82	116.54
1	D	352	ASP	N-CA-C	5.82	117.15	108.31
1	C	319	ILE	N-CA-C	5.76	116.41	110.82
1	A	253	GLY	N-CA-C	5.76	119.44	112.48
1	L	211	ASP	CA-C-N	5.70	124.90	118.97
1	L	211	ASP	C-N-CA	5.70	124.90	118.97
1	C	322	SER	CA-C-N	5.67	124.86	118.97
1	C	322	SER	C-N-CA	5.67	124.86	118.97
1	F	277	GLY	N-CA-C	5.61	119.43	112.64
1	K	109	ASP	N-CA-C	5.60	116.29	108.00
1	C	61	GLN	N-CA-C	5.58	116.26	108.00
1	J	92	SER	CB-CA-C	-5.52	110.22	116.63
1	I	211	ASP	CA-C-N	5.52	124.98	119.24
1	I	211	ASP	C-N-CA	5.52	124.98	119.24
1	K	121	HIS	CA-C-N	-5.51	115.59	122.48
1	K	121	HIS	C-N-CA	-5.51	115.59	122.48
1	E	256	SER	CB-CA-C	-5.50	110.26	116.63
1	H	322	SER	CA-C-N	5.43	124.62	118.97
1	H	322	SER	C-N-CA	5.43	124.62	118.97
1	A	354	ASN	N-CA-C	5.41	117.22	108.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	249	HIS	CA-C-N	-5.38	116.28	123.17
1	L	249	HIS	C-N-CA	-5.38	116.28	123.17
1	K	392	ASP	CB-CA-C	-5.37	99.72	110.42
1	E	216	GLY	N-CA-C	5.36	121.46	115.08
1	I	395	LYS	CA-C-N	5.35	125.43	119.87
1	I	395	LYS	C-N-CA	5.35	125.43	119.87
1	D	353	VAL	N-CA-C	5.33	116.73	111.67
1	B	380	GLU	N-CA-C	-5.30	105.58	111.36
1	D	62	GLY	N-CA-C	-5.29	106.93	115.08
1	C	222	GLY	N-CA-C	5.28	117.71	110.69
1	E	309	PHE	CB-CA-C	-5.27	99.94	110.42
1	C	56	GLY	N-CA-C	-5.25	107.42	114.25
1	L	361	GLY	N-CA-C	5.25	119.09	112.79
1	D	49	ARG	N-CA-C	5.24	118.94	112.54
1	K	110	LYS	N-CA-C	5.24	118.07	110.42
1	B	230	GLY	CA-C-N	5.22	125.20	120.03
1	B	230	GLY	C-N-CA	5.22	125.20	120.03
1	H	124	HIS	N-CA-C	-5.20	106.71	113.16
1	L	395	LYS	CA-C-N	5.15	124.94	119.28
1	L	395	LYS	C-N-CA	5.15	124.94	119.28
1	C	357	ASP	N-CA-C	-5.14	107.01	113.28
1	H	230	GLY	CA-C-N	5.13	126.25	119.84
1	H	230	GLY	C-N-CA	5.13	126.25	119.84
1	I	135	LEU	CB-CA-C	-5.13	109.16	116.34
1	A	209	PHE	CB-CA-C	-5.12	110.26	117.23
1	B	211	ASP	CA-C-N	5.12	124.74	119.05
1	B	211	ASP	C-N-CA	5.12	124.74	119.05
1	K	209	PHE	CB-CA-C	-5.12	110.26	117.23
1	B	227	THR	N-CA-C	-5.11	107.17	113.41
1	D	143	ASP	CA-C-N	5.11	124.77	119.56
1	D	143	ASP	C-N-CA	5.11	124.77	119.56
1	J	225	HIS	N-CA-C	5.09	119.64	113.38
1	D	255	VAL	CA-C-N	-5.08	115.26	123.23
1	D	255	VAL	C-N-CA	-5.08	115.26	123.23
1	I	389	ILE	N-CA-C	5.03	115.25	110.53
1	K	211	ASP	CA-C-N	5.03	124.47	119.24
1	K	211	ASP	C-N-CA	5.03	124.47	119.24
1	B	226	LYS	CA-C-N	5.02	131.08	122.09
1	B	226	LYS	C-N-CA	5.02	131.08	122.09

There are no chirality outliers.

All (27) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	254	VAL	Peptide
1	A	255	VAL	Peptide
1	A	256	SER	Peptide
1	B	226	LYS	Peptide
1	B	256	SER	Peptide
1	C	251	PHE	Peptide
1	C	308	ASP	Peptide
1	C	354	ASN	Peptide
1	C	355	ASN	Peptide
1	C	56	GLY	Peptide
1	D	257	ASN	Peptide
1	D	350	TRP	Peptide
1	D	351	ASP	Peptide
1	E	226	LYS	Peptide
1	E	356	SER	Peptide
1	F	339	ALA	Peptide
1	F	52	GLU	Peptide
1	G	253	GLY	Peptide
1	I	126	LYS	Peptide
1	I	251	PHE	Peptide
1	I	254	VAL	Peptide
1	J	128	SER	Peptide
1	K	107	PRO	Peptide
1	K	109	ASP	Peptide
1	K	354	ASN	Peptide
1	L	250	VAL	Peptide
1	L	251	PHE	Peptide

5.2 Too-close contacts [i](#)

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	3362	0	3304	136	0
1	B	3344	0	3288	152	0
1	C	3308	0	3257	138	0
1	D	3354	0	3292	189	0
1	E	3369	0	3316	159	0
1	F	3300	0	3252	142	0
1	G	3386	0	3334	159	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	3366	0	3316	135	0
1	I	3369	0	3316	152	0
1	J	3386	0	3335	144	0
1	K	3329	0	3281	147	0
1	L	3317	0	3269	140	0
2	A	15	0	7	2	0
2	B	15	0	7	1	0
2	C	15	0	7	1	0
2	D	15	0	7	0	0
2	E	15	0	7	3	0
2	F	15	0	7	2	0
2	G	15	0	7	2	0
2	H	15	0	7	0	0
2	I	15	0	7	0	0
2	J	15	0	7	1	0
2	K	15	0	7	1	0
2	L	15	0	7	0	0
All	All	40370	0	39644	1612	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 20.

All (1612) 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:I:52:GLU:HG2	1:I:60:TYR:CD1	1.70	1.24
1:D:351:ASP:HB2	1:D:352:ASP:OD1	1.44	1.16
1:A:147:MET:HB2	1:A:175:PHE:HE2	1.08	1.09
1:C:47:MET:CE	1:D:34:THR:HG21	1.83	1.08
1:A:310:THR:HG23	1:A:311:GLU:N	1.55	1.05
1:A:310:THR:CG2	1:A:311:GLU:H	1.69	1.04
1:C:47:MET:HE1	1:D:34:THR:HG21	1.06	1.04
1:A:147:MET:HB2	1:A:175:PHE:CE2	1.97	0.99
1:A:310:THR:HG23	1:A:311:GLU:H	0.82	0.98
1:D:351:ASP:CB	1:D:352:ASP:OD1	2.12	0.97
1:I:52:GLU:CG	1:I:60:TYR:CD1	2.47	0.96
1:A:310:THR:CG2	1:A:311:GLU:N	2.25	0.96
1:I:52:GLU:CD	1:I:60:TYR:HD1	1.77	0.93
1:B:251:PHE:HB3	1:B:252:PRO:HD3	1.51	0.91
1:A:310:THR:CG2	1:A:312:SER:H	1.84	0.89
1:C:48:HIS:NE2	1:D:34:THR:HG22	1.88	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:353:VAL:O	1:D:354:ASN:ND2	2.07	0.88
1:C:290:ALA:HB3	1:C:379:MET:HE3	1.54	0.88
1:A:310:THR:HG23	1:A:312:SER:H	1.36	0.88
1:C:287:ASN:HA	1:C:379:MET:HE1	1.55	0.88
1:K:59:LEU:HB3	1:L:345:LYS:HE2	1.56	0.87
1:A:50:TYR:CD2	1:B:30:SER:HB3	2.09	0.86
1:C:47:MET:HE1	1:D:34:THR:CG2	2.01	0.84
1:K:135:LEU:HB3	1:K:136:LYS:HG2	1.59	0.84
1:E:289:LYS:HB3	1:E:310:THR:HG22	1.59	0.84
1:I:127:VAL:HG13	1:I:128:SER:H	1.43	0.82
1:B:251:PHE:O	1:B:255:VAL:HG12	1.78	0.82
1:I:52:GLU:CG	1:I:60:TYR:HD1	1.90	0.82
1:L:198:ALA:HA	1:L:223:SER:H	1.44	0.81
1:E:289:LYS:HB3	1:E:310:THR:CG2	2.10	0.81
1:K:290:ALA:HB3	1:K:379:MET:HE1	1.61	0.80
1:H:353:VAL:HG12	1:H:355:ASN:H	1.46	0.79
1:K:251:PHE:N	1:K:253:GLY:H	1.81	0.78
1:B:250:VAL:O	1:B:255:VAL:HB	1.83	0.78
1:B:251:PHE:HB3	1:B:252:PRO:CD	2.13	0.78
1:K:7:PRO:HA	1:K:10:ILE:HD12	1.65	0.78
1:A:147:MET:CB	1:A:175:PHE:HE2	1.94	0.78
1:E:10:ILE:HD12	1:F:268:ILE:HG13	1.64	0.78
1:C:40:GLU:HG3	1:D:428:PHE:HD1	1.49	0.77
1:J:287:ASN:HB3	1:J:366:THR:HG21	1.65	0.77
1:D:202:GLY:HA3	1:D:227:THR:O	1.85	0.77
1:D:33:ILE:HB	1:D:368:GLU:HG3	1.67	0.77
1:D:251:PHE:H	1:D:254:VAL:HG12	1.50	0.77
1:G:388:ARG:HA	1:G:392:ASP:HB2	1.65	0.76
1:C:127:VAL:O	1:D:252:PRO:HB2	1.84	0.76
1:I:101:PHE:HD2	1:I:129:ALA:O	1.68	0.76
1:L:38:VAL:HG11	1:L:230:GLY:HA2	1.67	0.76
1:A:133:ARG:HB2	1:B:132:ILE:HG23	1.67	0.75
1:I:324:ASP:HB3	1:I:391:ILE:HG23	1.68	0.75
1:A:198:ALA:HA	1:A:223:SER:H	1.52	0.75
1:F:160:GLU:O	1:F:161:GLU:HG3	1.87	0.74
1:A:203:LEU:HG	1:A:227:THR:HG21	1.69	0.74
1:B:251:PHE:HA	1:B:255:VAL:HG11	1.70	0.74
1:D:199:HIS:HA	1:D:226:LYS:HD2	1.68	0.74
1:D:325:ILE:HB	1:D:391:ILE:HA	1.70	0.74
1:B:248:SER:HA	1:B:252:PRO:HD2	1.71	0.73
1:E:23:GLU:HB2	1:E:404:LYS:HG3	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:51:ALA:O	1:I:52:GLU:HG3	1.87	0.73
1:L:49:ARG:NH2	1:L:62:GLY:O	2.22	0.73
1:C:21:MET:HE2	1:D:49:ARG:HD2	1.71	0.73
1:J:100:VAL:HG21	1:J:221:MET:HE2	1.70	0.73
1:B:53:GLY:H	1:B:251:PHE:HE2	1.34	0.73
1:B:87:ASN:ND2	1:B:250:VAL:HG21	2.04	0.73
1:D:23:GLU:HG2	1:D:408:LYS:HD3	1.71	0.73
1:F:400:ARG:HE	1:F:404:LYS:HZ1	1.37	0.72
1:E:255:VAL:HG12	1:E:256:SER:N	2.04	0.72
1:K:100:VAL:HG11	1:K:221:MET:HG2	1.70	0.72
1:L:194:ALA:HB1	1:L:221:MET:HE1	1.72	0.72
1:G:36:LEU:HD11	1:G:420:GLY:HA3	1.72	0.71
1:B:87:ASN:HD21	1:B:250:VAL:HG21	1.54	0.71
1:D:371:ARG:NH1	1:D:414:HIS:O	2.23	0.71
1:H:50:TYR:CE1	1:H:257:ASN:HB3	2.26	0.71
1:K:39:ARG:NH1	1:K:422:GLY:O	2.23	0.71
1:E:130:ALA:O	1:E:135:LEU:N	2.23	0.70
1:A:199:HIS:HA	1:A:226:LYS:HG2	1.72	0.70
1:J:146:GLU:HG3	1:J:307:LYS:HD2	1.73	0.70
1:I:319:ILE:HD13	1:I:332:LEU:HD23	1.74	0.70
1:B:348:LEU:H	1:B:351:ASP:HB2	1.54	0.70
1:F:11:ARG:NH2	1:F:429:TYR:O	2.25	0.70
1:G:73:CYS:HB3	1:G:88:VAL:HG11	1.74	0.70
1:I:13:VAL:HG13	1:J:65:TYR:HB3	1.73	0.70
1:I:52:GLU:CD	1:I:60:TYR:CD1	2.65	0.70
1:K:337:GLU:OE1	1:L:61:GLN:NE2	2.25	0.70
1:C:40:GLU:HG3	1:D:428:PHE:CD1	2.26	0.70
1:A:110:LYS:HB3	1:A:163:PRO:HA	1.73	0.69
1:F:33:ILE:H	1:F:368:GLU:HG3	1.55	0.69
1:K:51:ALA:O	1:K:58:ARG:NH1	2.25	0.69
1:E:92:SER:HB3	1:E:95:VAL:HG13	1.74	0.69
1:I:51:ALA:C	1:I:52:GLU:HG3	2.18	0.69
1:B:50:TYR:CE1	1:B:257:ASN:HB3	2.28	0.69
1:B:251:PHE:HD1	1:B:252:PRO:CD	2.05	0.69
1:E:428:PHE:HB2	1:F:40:GLU:HB2	1.74	0.69
1:I:251:PHE:CD2	1:I:251:PHE:O	2.46	0.69
1:G:133:ARG:NH1	1:H:132:ILE:O	2.26	0.68
1:I:101:PHE:CD2	1:I:129:ALA:O	2.46	0.68
1:C:388:ARG:HA	1:C:392:ASP:HB2	1.75	0.68
1:I:51:ALA:HB1	1:I:58:ARG:NH1	2.08	0.68
1:J:78:LYS:NZ	1:J:84:GLU:O	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:34:THR:HG23	1:D:39:ARG:HG3	1.74	0.68
1:F:27:LEU:HB3	1:F:364:LEU:HD22	1.76	0.68
1:A:256:SER:H	1:B:94:VAL:HG21	1.58	0.68
1:E:255:VAL:HG12	1:E:256:SER:H	1.58	0.67
1:C:26:LYS:HA	1:C:342:ILE:HB	1.74	0.67
1:L:39:ARG:NH2	1:L:422:GLY:O	2.28	0.67
1:I:258:HIS:O	1:I:263:LYS:NZ	2.28	0.67
1:C:229:PHE:HE1	1:C:272:GLU:HG3	1.59	0.67
1:E:251:PHE:O	1:E:251:PHE:CD2	2.48	0.67
1:I:231:PRO:HB2	1:I:262:HIS:HD2	1.60	0.67
1:K:325:ILE:HG22	1:K:327:PHE:H	1.60	0.67
1:F:110:LYS:HB3	1:F:163:PRO:HA	1.76	0.67
1:G:105:THR:O	1:G:133:ARG:NH2	2.28	0.67
1:G:58:ARG:NH2	1:G:67:ASP:OD2	2.28	0.67
1:K:130:ALA:HA	1:K:134:GLY:H	1.60	0.67
1:E:111:LEU:HB3	1:E:137:VAL:HG12	1.77	0.66
1:E:31:GLU:O	1:E:367:GLN:NE2	2.28	0.66
1:A:298:ARG:NH1	1:A:384:GLU:OE1	2.29	0.66
1:E:330:SER:OG	1:E:334:LYS:NZ	2.28	0.66
1:A:225:HIS:NE2	2:A:1430:PLP:O3P	2.21	0.66
1:C:87:ASN:ND2	1:C:247:ASP:OD1	2.28	0.66
1:E:252:PRO:O	1:E:255:VAL:CG2	2.44	0.66
1:H:84:GLU:HB3	1:H:240:LYS:HG3	1.78	0.66
1:D:258:HIS:O	1:D:259:HIS:ND1	2.29	0.65
1:D:251:PHE:N	1:D:254:VAL:HG12	2.11	0.65
1:B:139:ASN:OD1	1:B:157:LYS:NZ	2.30	0.65
1:I:121:HIS:ND1	1:I:122:ILE:O	2.29	0.65
1:H:45:ASP:OD2	1:H:49:ARG:NE	2.29	0.65
1:H:123:SER:HB2	1:H:129:ALA:HB3	1.77	0.65
1:L:261:HIS:HD1	1:L:261:HIS:H	1.43	0.65
1:B:251:PHE:HA	1:B:255:VAL:CG1	2.27	0.65
1:F:395:LYS:NZ	1:F:397:GLU:OE1	2.30	0.65
1:A:50:TYR:CE1	1:A:257:ASN:HB3	2.33	0.65
1:G:50:TYR:HD1	1:G:256:SER:HB2	1.61	0.65
1:A:325:ILE:HG12	1:A:390:ALA:HB1	1.79	0.64
1:B:246:ILE:O	1:B:250:VAL:HG12	1.96	0.64
1:E:14:SER:O	1:E:18:HIS:ND1	2.23	0.64
1:A:310:THR:HG23	1:A:312:SER:N	2.11	0.64
1:G:81:PHE:O	1:G:214:ARG:NH2	2.30	0.64
1:G:119:GLY:HA2	1:G:172:LEU:HD13	1.78	0.64
1:I:52:GLU:OE2	1:I:59:LEU:N	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:73:CYS:HB3	1:D:88:VAL:HG11	1.78	0.64
1:D:228:PHE:HA	1:D:273:MET:HE3	1.79	0.64
1:H:395:LYS:HD2	1:H:396:PRO:HD2	1.80	0.64
1:J:42:CYS:HA	1:J:261:HIS:HB2	1.80	0.64
1:B:247:ASP:HA	1:B:250:VAL:HG12	1.80	0.64
1:F:247:ASP:HA	1:F:250:VAL:HG12	1.78	0.64
1:I:345:LYS:NZ	1:I:357:ASP:O	2.31	0.64
1:A:319:ILE:HD11	1:A:362:ILE:HG13	1.80	0.64
1:G:212:PRO:HA	1:G:215:GLU:HB2	1.80	0.64
1:A:147:MET:CB	1:A:175:PHE:CE2	2.76	0.63
1:A:152:ASP:N	1:A:152:ASP:OD1	2.31	0.63
1:B:27:LEU:HG	1:B:364:LEU:HD23	1.80	0.63
1:B:353:VAL:HG23	1:B:355:ASN:H	1.62	0.63
1:H:194:ALA:HB1	1:H:221:MET:HE1	1.79	0.63
1:H:200:VAL:HG13	1:H:203:LEU:HD12	1.81	0.63
1:I:310:THR:O	1:I:311:GLU:OE2	2.16	0.63
1:G:226:LYS:NZ	1:H:50:TYR:HE2	1.96	0.63
1:L:319:ILE:HD11	1:L:362:ILE:HB	1.80	0.63
1:D:112:MET:HE2	1:D:140:HIS:HD2	1.62	0.63
1:D:283:GLN:HG2	1:D:375:LYS:HD2	1.79	0.63
1:G:255:VAL:HG22	1:H:94:VAL:HG11	1.79	0.63
1:D:300:PHE:HZ	1:D:390:ALA:HB3	1.62	0.63
1:E:28:ILE:HD13	1:F:60:TYR:HD2	1.64	0.63
1:C:401:GLU:HA	1:C:404:LYS:HD2	1.81	0.63
1:K:17:GLN:OE1	1:L:49:ARG:NH1	2.31	0.63
1:E:10:ILE:HD11	1:F:267:ALA:HB3	1.81	0.63
1:E:49:ARG:NH2	1:E:62:GLY:O	2.28	0.62
1:L:84:GLU:HB3	1:L:240:LYS:HB3	1.81	0.62
1:B:254:VAL:O	1:B:254:VAL:HG22	1.99	0.62
1:D:295:LEU:HD13	1:D:317:ILE:HD11	1.80	0.62
1:F:35:SER:OG	1:F:371:ARG:NH2	2.33	0.62
1:J:405:GLU:HA	1:J:408:LYS:HB2	1.80	0.62
1:K:34:THR:O	1:K:39:ARG:NH2	2.32	0.62
1:K:376:GLU:HA	1:K:379:MET:HE3	1.81	0.62
1:E:411:SER:O	1:E:422:GLY:N	2.32	0.62
1:D:95:VAL:HG11	1:D:254:VAL:HG23	1.80	0.62
1:D:336:TYR:HB3	1:D:341:ILE:HB	1.80	0.62
1:F:58:ARG:NE	1:F:67:ASP:OD1	2.28	0.62
1:A:148:ASN:ND2	1:A:176:PRO:O	2.32	0.62
1:D:351:ASP:CA	1:D:352:ASP:OD1	2.47	0.62
1:J:162:LYS:HG2	1:J:189:VAL:HG22	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:29:ALA:HA	1:D:367:GLN:HE22	1.64	0.62
1:D:177:HIS:HB2	1:D:178:PRO:HD2	1.82	0.62
1:D:251:PHE:CD2	1:D:251:PHE:O	2.52	0.62
1:C:51:ALA:O	1:C:58:ARG:NH1	2.33	0.62
1:G:66:ILE:HG21	1:G:260:LEU:HD13	1.82	0.62
1:G:115:SER:HB3	1:G:118:ASP:HB2	1.82	0.62
1:K:38:VAL:HG11	1:K:269:ALA:HB2	1.82	0.62
1:B:251:PHE:CD1	1:B:252:PRO:HD3	2.34	0.61
1:F:340:ASN:HB2	1:F:403:VAL:CG2	2.29	0.61
1:G:227:THR:O	1:G:228:PHE:C	2.42	0.61
1:I:282:LYS:HE3	1:I:286:LYS:HE2	1.81	0.61
1:B:325:ILE:HG23	1:B:326:GLU:H	1.64	0.61
1:F:14:SER:O	1:F:18:HIS:ND1	2.25	0.61
1:J:46:PHE:HB3	1:J:260:LEU:HB2	1.82	0.61
1:E:112:MET:HE3	1:E:163:PRO:HG3	1.80	0.61
1:K:38:VAL:HG12	1:K:268:ILE:HB	1.82	0.61
1:B:27:LEU:O	1:B:365:GLY:N	2.33	0.61
1:C:6:VAL:HB	1:D:271:ALA:HB2	1.82	0.61
1:J:121:HIS:ND1	1:J:122:ILE:O	2.33	0.61
1:J:324:ASP:HB3	1:J:391:ILE:HD12	1.82	0.61
1:K:25:ILE:HG22	1:K:407:ALA:HB2	1.83	0.61
1:B:256:SER:OG	1:B:257:ASN:N	2.27	0.61
1:C:73:CYS:HB3	1:C:88:VAL:HG11	1.82	0.61
1:E:319:ILE:HG13	1:E:320:GLU:H	1.64	0.61
1:G:50:TYR:CD1	1:G:256:SER:HB2	2.35	0.61
1:C:270:LEU:O	1:C:274:LEU:HB2	2.01	0.61
1:H:187:GLN:HG2	1:K:137:VAL:HG12	1.83	0.61
1:G:306:HIS:HD2	1:G:307:LYS:HG3	1.65	0.60
1:J:254:VAL:O	1:J:254:VAL:HG12	2.01	0.60
1:D:313:HIS:HD2	1:D:367:GLN:HE21	1.48	0.60
1:F:340:ASN:HB2	1:F:403:VAL:HG23	1.82	0.60
1:B:73:CYS:HB3	1:B:88:VAL:HG11	1.84	0.60
1:F:91:THR:HG23	1:F:255:VAL:HG13	1.82	0.60
1:G:29:ALA:HA	1:G:367:GLN:HE22	1.66	0.60
1:C:291:LEU:HA	1:C:379:MET:HB3	1.83	0.60
1:E:209:PHE:HE1	1:E:312:SER:HB2	1.66	0.60
1:J:91:THR:O	1:J:94:VAL:HG22	2.01	0.60
1:D:353:VAL:HG22	1:D:355:ASN:H	1.66	0.60
1:G:229:PHE:CE1	1:G:272:GLU:HG3	2.36	0.60
1:K:367:GLN:N	1:K:367:GLN:OE1	2.32	0.60
1:L:272:GLU:OE2	1:L:371:ARG:NH2	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:ALA:HA	1:A:274:LEU:HB2	1.84	0.60
1:E:24:SER:O	1:E:26:LYS:NZ	2.35	0.60
1:G:339:ALA:HB2	1:G:396:PRO:HB3	1.82	0.60
1:H:89:GLN:HB2	1:H:250:VAL:HG11	1.82	0.60
1:L:250:VAL:HG23	1:L:254:VAL:H	1.67	0.60
1:D:24:SER:HA	1:D:340:ASN:HB3	1.83	0.60
1:G:132:ILE:HG22	1:H:133:ARG:HB2	1.83	0.60
1:L:255:VAL:O	1:L:258:HIS:N	2.34	0.60
1:C:39:ARG:NH1	1:C:422:GLY:O	2.35	0.60
1:I:33:ILE:HA	1:J:48:HIS:HD2	1.66	0.60
1:K:206:GLY:O	1:K:208:GLN:NE2	2.31	0.60
1:A:59:LEU:HA	1:B:345:LYS:HE3	1.84	0.59
1:E:252:PRO:O	1:E:255:VAL:HG23	2.02	0.59
1:H:28:ILE:HG22	1:H:30:SER:H	1.65	0.59
1:L:345:LYS:O	1:L:346:ASN:ND2	2.29	0.59
1:J:130:ALA:O	1:J:135:LEU:N	2.31	0.59
1:K:374:MET:HE2	1:K:410:TYR:HE2	1.68	0.59
1:G:255:VAL:HG21	1:H:121:HIS:NE2	2.16	0.59
1:J:273:MET:HE3	1:J:277:GLY:HA2	1.83	0.59
1:K:126:LYS:HA	1:K:131:GLY:HA3	1.83	0.59
1:D:45:ASP:OD2	1:D:49:ARG:NE	2.35	0.59
1:E:219:TYR:HA	1:E:238:THR:HG22	1.85	0.59
1:G:236:ILE:HG21	1:G:246:ILE:HG12	1.85	0.59
1:H:348:LEU:HD21	1:H:361:GLY:HA3	1.85	0.59
1:I:53:GLY:O	1:I:58:ARG:NH1	2.36	0.59
1:K:271:ALA:HB3	1:L:6:VAL:HG21	1.84	0.59
1:E:356:SER:HB3	1:E:358:ASN:N	2.17	0.59
1:F:54:LEU:HB3	1:F:55:PRO:CD	2.32	0.59
1:G:10:ILE:HA	1:G:13:VAL:HB	1.85	0.59
1:G:43:ALA:HB2	1:H:43:ALA:HB2	1.85	0.59
1:G:85:HIS:NE2	1:G:247:ASP:OD1	2.28	0.59
1:I:50:TYR:HE2	1:I:256:SER:HB3	1.67	0.59
1:J:221:MET:HB2	1:J:236:ILE:HG12	1.84	0.59
1:I:105:THR:HG23	1:I:109:ASP:HB2	1.85	0.59
1:I:126:LYS:O	1:I:127:VAL:HG12	2.02	0.59
1:K:104:GLU:OE1	1:K:192:LYS:NZ	2.31	0.59
1:B:351:ASP:CG	1:B:360:SER:H	2.10	0.59
1:H:304:CYS:HB3	1:H:307:LYS:HB2	1.85	0.59
1:I:10:ILE:HA	1:I:13:VAL:HB	1.85	0.59
1:I:268:ILE:HD11	1:J:10:ILE:HD11	1.85	0.59
1:J:82:LYS:O	1:J:214:ARG:NH2	2.31	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:10:ILE:O	1:L:14:SER:N	2.36	0.59
1:B:283:GLN:HG2	1:B:375:LYS:HZ3	1.67	0.58
1:E:101:PHE:O	1:E:105:THR:OG1	2.21	0.58
1:F:78:LYS:HB3	1:F:86:ALA:HB2	1.84	0.58
1:F:111:LEU:HB2	1:F:135:LEU:HD22	1.84	0.58
1:I:127:VAL:HG13	1:I:128:SER:N	2.17	0.58
1:L:26:LYS:HB2	1:L:368:GLU:OE1	2.03	0.58
1:B:251:PHE:CD1	1:B:252:PRO:CD	2.86	0.58
1:E:284:VAL:HG22	1:E:370:THR:HG21	1.83	0.58
1:G:176:PRO:HD3	1:G:209:PHE:CE1	2.39	0.58
1:E:52:GLU:HB3	1:E:251:PHE:CE1	2.38	0.58
1:F:162:LYS:HB3	1:F:163:PRO:HD3	1.85	0.58
1:K:24:SER:O	1:K:26:LYS:NZ	2.36	0.58
1:J:80:LEU:HD13	1:J:274:LEU:HA	1.83	0.58
1:J:95:VAL:HG22	1:J:99:ALA:HB2	1.85	0.58
1:A:111:LEU:HD21	1:A:167:LEU:HD12	1.84	0.58
1:F:115:SER:HB2	1:F:118:ASP:HB2	1.85	0.58
1:A:228:PHE:HA	1:A:273:MET:HE1	1.85	0.58
1:B:345:LYS:NZ	1:B:357:ASP:O	2.27	0.58
1:E:13:VAL:HG13	1:F:65:TYR:HB3	1.85	0.58
1:G:227:THR:HG23	1:G:228:PHE:H	1.68	0.58
1:H:53:GLY:HA3	1:H:258:HIS:NE2	2.18	0.58
1:I:90:PRO:HB3	1:I:95:VAL:HG12	1.85	0.58
1:K:172:LEU:HD23	1:K:363:ARG:HD3	1.86	0.58
1:C:280:TYR:HE1	1:C:371:ARG:HG2	1.68	0.58
1:D:261:HIS:HD1	1:D:261:HIS:H	1.50	0.58
1:E:289:LYS:CB	1:E:310:THR:HG22	2.31	0.58
1:J:345:LYS:NZ	1:J:357:ASP:OD2	2.33	0.58
1:K:167:LEU:HD23	1:K:194:ALA:HB3	1.85	0.58
1:B:82:LYS:HB2	1:B:214:ARG:HH22	1.69	0.58
1:D:23:GLU:HB3	1:D:404:LYS:HB2	1.86	0.58
1:G:183:TYR:HA	1:G:193:ILE:HD11	1.84	0.58
1:A:114:LEU:HD23	1:A:114:LEU:H	1.69	0.57
1:B:26:LYS:HA	1:B:342:ILE:HB	1.85	0.57
1:B:177:HIS:O	1:B:210:GLN:NE2	2.37	0.57
1:E:312:SER:OG	1:E:313:HIS:N	2.36	0.57
1:G:37:ALA:HB1	1:G:268:ILE:HD13	1.85	0.57
1:G:268:ILE:HD11	1:H:10:ILE:HD11	1.86	0.57
1:B:282:LYS:HG2	1:B:286:LYS:HE2	1.86	0.57
1:E:259:HIS:HB3	1:E:261:HIS:CE1	2.40	0.57
1:L:306:HIS:CD2	1:L:307:LYS:HG3	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:187:GLN:HG2	1:E:126:LYS:HE2	1.86	0.57
1:F:106:LYS:HA	1:F:133:ARG:HH12	1.69	0.57
1:G:30:SER:HB2	1:H:50:TYR:CD2	2.39	0.57
1:G:65:TYR:HB3	1:H:13:VAL:HG13	1.85	0.57
1:G:208:GLN:O	1:G:209:PHE:HB3	2.04	0.57
1:H:30:SER:OG	1:H:363:ARG:NH1	2.37	0.57
1:G:32:ASN:HD22	1:G:229:PHE:HA	1.69	0.57
1:C:47:MET:CE	1:D:34:THR:CG2	2.70	0.57
1:G:18:HIS:HE1	1:G:39:ARG:HH22	1.51	0.57
1:K:25:ILE:HG12	1:K:341:ILE:HG22	1.87	0.57
1:L:19:GLU:HA	1:L:22:ARG:HE	1.69	0.57
1:A:354:ASN:HA	1:D:135:LEU:HD13	1.87	0.57
1:C:11:ARG:NH2	1:C:429:TYR:O	2.38	0.57
1:K:49:ARG:NH1	1:K:62:GLY:O	2.38	0.57
1:K:197:GLY:O	1:K:201:LEU:N	2.38	0.57
1:D:42:CYS:HA	1:D:261:HIS:HB2	1.86	0.57
1:G:313:HIS:HD2	1:G:367:GLN:HE21	1.52	0.57
1:I:306:HIS:CD2	1:I:307:LYS:HG2	2.40	0.57
1:J:357:ASP:O	1:J:359:PRO:HD3	2.04	0.57
1:G:405:GLU:HA	1:G:408:LYS:HB2	1.87	0.57
1:I:232:GLN:OE1	1:J:257:ASN:ND2	2.37	0.57
1:B:24:SER:O	1:B:26:LYS:NZ	2.38	0.57
1:I:111:LEU:HD21	1:I:167:LEU:HD12	1.86	0.57
1:E:209:PHE:CE1	1:E:312:SER:HB2	2.39	0.57
1:F:7:PRO:O	1:F:10:ILE:HG13	2.05	0.57
1:G:268:ILE:O	1:G:272:GLU:HG2	2.05	0.57
1:I:319:ILE:HD11	1:I:362:ILE:HG12	1.87	0.57
1:J:24:SER:OG	1:J:340:ASN:ND2	2.33	0.57
1:L:223:SER:HB3	1:L:225:HIS:CD2	2.39	0.57
1:C:111:LEU:HD11	1:C:167:LEU:HG	1.87	0.56
1:G:30:SER:HB2	1:H:50:TYR:HD2	1.69	0.56
1:E:395:LYS:HE3	1:E:397:GLU:HB2	1.87	0.56
1:F:153:ALA:O	1:F:157:LYS:HB2	2.05	0.56
1:C:36:LEU:HB3	1:D:428:PHE:HB2	1.87	0.56
1:J:54:LEU:HB2	1:J:57:LYS:HG3	1.88	0.56
1:K:238:THR:OG1	1:K:239:THR:N	2.37	0.56
1:C:36:LEU:HD12	1:D:429:TYR:HB3	1.87	0.56
1:G:328:SER:HB3	1:G:358:ASN:HD21	1.70	0.56
1:D:351:ASP:HB2	1:D:352:ASP:CG	2.25	0.56
1:E:382:ILE:HG22	1:E:386:MET:HE2	1.88	0.56
1:G:428:PHE:HB3	1:H:36:LEU:HD22	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:249:HIS:O	1:F:253:GLY:HA3	2.06	0.56
1:D:351:ASP:C	1:D:352:ASP:OD1	2.49	0.56
1:G:54:LEU:HD12	1:G:55:PRO:HD2	1.88	0.56
1:I:119:GLY:HA2	1:I:172:LEU:HD13	1.86	0.56
1:K:101:PHE:O	1:K:105:THR:N	2.38	0.56
1:E:196:ASP:HB2	1:E:221:MET:HE3	1.87	0.56
1:E:319:ILE:HG13	1:E:320:GLU:N	2.19	0.56
1:F:186:ALA:O	1:F:190:GLY:N	2.32	0.56
1:K:79:GLU:OE2	1:L:3:TYR:OH	2.23	0.56
1:L:175:PHE:HZ	1:L:307:LYS:HB3	1.71	0.56
1:A:271:ALA:HB3	1:B:6:VAL:HG21	1.86	0.56
1:F:295:LEU:HD21	1:F:317:ILE:HG13	1.87	0.56
1:H:25:ILE:HG13	1:H:403:VAL:HG13	1.87	0.56
1:A:48:HIS:HE1	1:B:39:ARG:HE	1.52	0.55
1:B:278:GLU:N	1:B:278:GLU:OE1	2.35	0.55
1:C:52:GLU:HB3	1:C:251:PHE:CZ	2.41	0.55
1:C:172:LEU:HD11	1:C:316:ILE:HG12	1.87	0.55
1:D:39:ARG:NH2	1:D:422:GLY:O	2.39	0.55
1:B:251:PHE:CB	1:B:252:PRO:HD3	2.30	0.55
1:D:246:ILE:O	1:D:250:VAL:HG12	2.06	0.55
1:F:74:ILE:HD13	1:F:88:VAL:HG13	1.87	0.55
1:F:83:ALA:HB2	1:F:213:LEU:HD13	1.88	0.55
1:H:211:ASP:OD1	1:H:214:ARG:NH2	2.39	0.55
1:J:204:ILE:HG21	1:J:220:LEU:HD11	1.88	0.55
1:L:47:MET:HG2	1:L:261:HIS:CG	2.42	0.55
1:D:36:LEU:HD11	1:D:422:GLY:HA2	1.87	0.55
1:F:368:GLU:HA	1:F:371:ARG:HB3	1.88	0.55
1:F:395:LYS:HZ2	1:F:397:GLU:H	1.53	0.55
1:I:45:ASP:HB2	1:J:18:HIS:CE1	2.41	0.55
1:I:239:THR:OG1	1:I:242:ASN:OD1	2.22	0.55
1:K:49:ARG:HD2	1:K:66:ILE:HD11	1.88	0.55
1:K:73:CYS:HB3	1:K:267:ALA:HB2	1.89	0.55
1:K:154:MET:HE3	1:K:182:ALA:HB2	1.88	0.55
1:B:114:LEU:O	1:B:125:TRP:NE1	2.33	0.55
1:C:265:GLY:HA2	1:C:268:ILE:HD12	1.88	0.55
1:D:71:THR:O	1:D:75:GLU:HG2	2.06	0.55
1:D:107:PRO:HG3	1:D:133:ARG:HH12	1.70	0.55
1:G:72:LEU:HD21	1:H:6:VAL:HG13	1.89	0.55
2:A:1430:PLP:O1P	1:B:256:SER:HB2	2.06	0.55
1:B:179:VAL:HG13	1:B:193:ILE:HG21	1.88	0.55
1:G:252:PRO:HB2	1:H:128:SER:HB3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:23:GLU:HB3	1:I:404:LYS:HG2	1.88	0.55
1:I:112:MET:HB3	1:I:166:ILE:HA	1.87	0.55
1:K:21:MET:O	1:K:26:LYS:NZ	2.31	0.55
1:D:119:GLY:O	1:D:171:SER:N	2.40	0.55
1:E:49:ARG:NH1	1:F:17:GLN:OE1	2.40	0.55
1:J:95:VAL:HB	1:J:254:VAL:HB	1.88	0.55
1:K:40:GLU:HB2	1:L:428:PHE:HB2	1.89	0.55
1:G:289:LYS:NZ	1:G:310:THR:O	2.29	0.55
1:B:245:LYS:O	1:B:249:HIS:ND1	2.39	0.55
1:E:259:HIS:HB2	1:E:262:HIS:HB2	1.88	0.55
1:I:25:ILE:HD11	1:I:403:VAL:HB	1.89	0.55
1:I:55:PRO:HG2	1:I:71:THR:HG23	1.88	0.55
1:I:332:LEU:HD13	1:I:335:MET:HE2	1.89	0.55
1:K:127:VAL:O	1:L:252:PRO:HB2	2.07	0.55
1:A:236:ILE:HG21	1:A:246:ILE:HD13	1.89	0.55
1:D:34:THR:HG22	1:D:39:ARG:HH11	1.72	0.55
1:E:48:HIS:HB3	1:F:33:ILE:HA	1.89	0.55
1:J:199:HIS:HA	1:J:226:LYS:HG2	1.89	0.55
1:D:257:ASN:HB3	1:D:258:HIS:O	2.07	0.55
1:H:375:LYS:HG3	1:H:376:GLU:H	1.72	0.55
1:L:338:GLU:OE2	1:L:400:ARG:NH1	2.40	0.55
1:L:421:ASP:HB3	1:L:424:LYS:HB2	1.90	0.55
1:F:91:THR:O	1:F:233:GLY:HA2	2.07	0.54
1:G:88:VAL:O	1:G:263:LYS:NZ	2.27	0.54
1:F:52:GLU:HB3	1:F:251:PHE:HE1	1.72	0.54
1:I:169:GLY:H	1:I:177:HIS:CD2	2.25	0.54
1:B:34:THR:O	1:B:39:ARG:NH2	2.40	0.54
1:B:87:ASN:ND2	1:B:90:PRO:HD3	2.22	0.54
1:L:105:THR:HG23	1:L:109:ASP:HB2	1.89	0.54
1:L:345:LYS:HG2	1:L:359:PRO:HG3	1.90	0.54
1:A:48:HIS:CE1	1:B:39:ARG:HE	2.25	0.54
1:B:74:ILE:HD13	1:B:88:VAL:HG13	1.89	0.54
1:G:313:HIS:CD2	1:G:367:GLN:HE21	2.25	0.54
1:B:421:ASP:HB2	1:B:424:LYS:HG3	1.88	0.54
1:D:343:LEU:HB2	1:D:362:ILE:HD11	1.89	0.54
1:F:112:MET:HB3	1:F:166:ILE:HG23	1.90	0.54
1:G:31:GLU:HG2	1:H:50:TYR:H	1.71	0.54
1:L:52:GLU:OE1	1:L:58:ARG:NH1	2.41	0.54
1:L:193:ILE:HG23	1:L:218:GLU:H	1.72	0.54
1:A:29:ALA:O	1:A:367:GLN:NE2	2.41	0.54
1:F:387:LYS:HG3	1:F:391:ILE:HD12	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:376:GLU:O	1:C:379:MET:HG2	2.07	0.54
1:D:52:GLU:HG3	1:D:251:PHE:CZ	2.43	0.54
1:J:159:LEU:O	1:J:162:LYS:NZ	2.40	0.54
1:L:292:ALA:HB1	1:L:309:PHE:CD2	2.43	0.54
1:L:305:GLU:H	1:L:305:GLU:CD	2.16	0.54
1:L:344:ASN:O	1:L:362:ILE:HG13	2.07	0.54
1:L:372:LEU:HA	1:L:413:ILE:HA	1.89	0.54
1:H:283:GLN:O	1:H:287:ASN:ND2	2.41	0.54
1:J:27:LEU:O	1:J:365:GLY:N	2.41	0.54
1:B:98:LEU:HB3	1:B:254:VAL:HG11	1.90	0.54
1:E:27:LEU:O	1:E:365:GLY:N	2.39	0.54
1:E:61:GLN:HB3	1:F:342:ILE:HG22	1.89	0.54
1:E:63:CYS:O	1:E:66:ILE:HG13	2.08	0.54
1:F:75:GLU:HA	1:F:78:LYS:HE2	1.90	0.54
1:I:48:HIS:CD2	1:J:34:THR:H	2.25	0.54
1:I:169:GLY:HA2	1:I:173:PHE:CE2	2.43	0.54
1:L:298:ARG:HG2	1:L:387:LYS:HG3	1.89	0.54
1:B:327:PHE:HB3	1:B:332:LEU:HG	1.90	0.53
1:K:154:MET:HE1	1:K:178:PRO:HG2	1.89	0.53
1:L:27:LEU:O	1:L:365:GLY:N	2.38	0.53
1:A:46:PHE:HB3	1:A:260:LEU:HB2	1.89	0.53
1:B:80:LEU:HD11	1:B:205:ALA:HB1	1.89	0.53
1:E:344:ASN:HD21	1:F:60:TYR:HA	1.74	0.53
1:I:34:THR:H	1:J:48:HIS:CD2	2.25	0.53
1:A:133:ARG:NH1	1:B:131:GLY:O	2.42	0.53
1:A:369:CYS:HB3	1:A:379:MET:HE1	1.89	0.53
1:C:40:GLU:CG	1:D:428:PHE:HD1	2.20	0.53
1:H:238:THR:HG21	1:H:246:ILE:HG21	1.90	0.53
1:I:305:GLU:OE1	1:I:305:GLU:N	2.37	0.53
1:J:58:ARG:O	1:J:59:LEU:HB2	2.07	0.53
1:A:13:VAL:HG13	1:B:65:TYR:HD1	1.73	0.53
1:B:218:GLU:OE2	1:B:242:ASN:ND2	2.40	0.53
1:B:251:PHE:HD1	1:B:252:PRO:HD3	1.73	0.53
1:C:48:HIS:CE1	1:D:33:ILE:HG13	2.43	0.53
1:C:148:ASN:ND2	1:C:176:PRO:O	2.41	0.53
1:E:128:SER:HA	1:F:252:PRO:O	2.08	0.53
1:F:102:PHE:HB3	1:F:249:HIS:HB3	1.90	0.53
1:F:107:PRO:HA	1:F:134:GLY:O	2.08	0.53
1:F:212:PRO:HA	1:F:215:GLU:HB2	1.90	0.53
1:J:305:GLU:H	1:J:305:GLU:CD	2.15	0.53
1:L:89:GLN:N	1:L:90:PRO:HD2	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:LYS:HA	1:A:243:ALA:HB2	1.90	0.53
1:B:25:ILE:O	1:B:342:ILE:N	2.27	0.53
1:C:31:GLU:O	1:C:367:GLN:NE2	2.40	0.53
1:C:209:PHE:HE1	1:C:312:SER:HB3	1.74	0.53
1:D:52:GLU:HG2	1:D:53:GLY:N	2.24	0.53
1:G:416:SER:OG	1:G:418:ASP:O	2.24	0.53
1:H:126:LYS:O	1:H:127:VAL:HG22	2.08	0.53
1:I:105:THR:CG2	1:I:109:ASP:HB2	2.38	0.53
1:J:284:VAL:HG12	1:J:370:THR:HB	1.91	0.53
1:L:142:PHE:CD1	1:L:148:ASN:O	2.62	0.53
1:E:421:ASP:HB3	1:E:424:LYS:HB2	1.90	0.53
1:G:228:PHE:CD2	1:G:273:MET:HG3	2.44	0.53
1:G:412:THR:HA	1:G:420:GLY:O	2.08	0.53
1:I:209:PHE:CE1	1:I:312:SER:HB3	2.44	0.53
1:L:395:LYS:HB2	1:L:398:LYS:HG2	1.91	0.53
1:A:63:CYS:HA	1:A:66:ILE:HD12	1.90	0.53
1:A:151:ALA:HA	1:A:154:MET:HE2	1.91	0.53
1:G:128:SER:HA	1:H:253:GLY:HA3	1.91	0.53
1:G:176:PRO:HB2	1:G:210:GLN:NE2	2.24	0.53
1:K:168:PHE:CG	1:K:179:VAL:HG12	2.44	0.53
1:K:239:THR:OG1	1:K:242:ASN:OD1	2.21	0.53
1:G:32:ASN:ND2	1:G:227:THR:O	2.42	0.53
1:H:112:MET:HB2	1:H:163:PRO:HB2	1.91	0.53
1:H:227:THR:O	1:H:228:PHE:C	2.52	0.53
1:J:140:HIS:HE1	1:J:166:ILE:HG23	1.73	0.53
1:K:35:SER:OG	1:K:371:ARG:NH2	2.41	0.53
1:K:45:ASP:O	1:K:48:HIS:HB2	2.09	0.53
1:C:298:ARG:HD2	1:C:387:LYS:HD3	1.91	0.53
1:C:328:SER:HB3	1:C:331:GLU:HG2	1.90	0.53
1:G:283:GLN:O	1:G:287:ASN:ND2	2.42	0.53
1:H:99:ALA:HA	1:H:254:VAL:HG21	1.91	0.53
1:L:303:LEU:HD11	1:L:350:TRP:HZ2	1.73	0.53
1:A:84:GLU:HB2	1:A:239:THR:HA	1.91	0.53
1:B:319:ILE:HG12	1:B:332:LEU:HD12	1.90	0.53
1:D:27:LEU:HD12	1:D:364:LEU:HB3	1.90	0.53
1:D:75:GLU:O	1:D:79:GLU:HG3	2.09	0.53
1:A:115:SER:O	1:A:120:GLY:N	2.36	0.52
1:C:251:PHE:O	1:C:251:PHE:CD2	2.62	0.52
1:D:325:ILE:HD12	1:D:390:ALA:HB1	1.89	0.52
1:G:147:MET:HG3	1:G:303:LEU:HD23	1.89	0.52
1:I:115:SER:HA	1:I:125:TRP:NE1	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:169:GLY:HA2	1:E:173:PHE:CE2	2.44	0.52
1:J:209:PHE:CE1	1:J:312:SER:HB3	2.45	0.52
1:K:94:VAL:HG11	1:L:254:VAL:HG13	1.91	0.52
1:D:201:LEU:HD22	1:D:222:GLY:HA3	1.91	0.52
1:D:381:GLU:O	1:D:384:GLU:HG2	2.09	0.52
1:J:87:ASN:ND2	1:J:247:ASP:OD1	2.42	0.52
1:G:325:ILE:HG21	1:G:390:ALA:HB1	1.91	0.52
1:H:80:LEU:HD21	1:H:205:ALA:HB1	1.90	0.52
1:I:48:HIS:HD2	1:J:33:ILE:HA	1.73	0.52
1:K:229:PHE:HB2	1:K:269:ALA:HB1	1.92	0.52
1:L:322:SER:OG	1:L:323:PRO:HD2	2.10	0.52
1:E:28:ILE:HG13	1:E:342:ILE:HG22	1.92	0.52
1:E:105:THR:C	1:E:133:ARG:HH12	2.18	0.52
1:L:171:SER:OG	1:L:363:ARG:NH1	2.43	0.52
1:D:34:THR:CG2	1:D:39:ARG:HH11	2.23	0.52
1:G:229:PHE:HE1	1:G:272:GLU:HG3	1.74	0.52
1:I:58:ARG:NH2	1:I:70:GLU:OE1	2.31	0.52
1:K:236:ILE:HG21	1:K:246:ILE:HG12	1.92	0.52
1:K:268:ILE:HD11	1:L:10:ILE:HG12	1.90	0.52
1:A:10:ILE:O	1:A:14:SER:N	2.34	0.52
1:D:194:ALA:HA	1:D:219:TYR:HB2	1.92	0.52
1:D:245:LYS:O	1:D:249:HIS:ND1	2.39	0.52
1:D:315:VAL:HB	1:D:364:LEU:HB2	1.90	0.52
1:E:91:THR:O	1:E:233:GLY:HA2	2.10	0.52
1:E:280:TYR:O	1:E:284:VAL:HG23	2.10	0.52
1:H:45:ASP:C	1:H:47:MET:H	2.17	0.52
1:I:329:ALA:HB1	1:I:362:ILE:HG23	1.90	0.52
1:J:224:THR:HG21	1:J:266:LEU:HD13	1.92	0.52
1:K:287:ASN:HA	1:K:379:MET:HE2	1.90	0.52
1:L:146:GLU:HG3	1:L:306:HIS:NE2	2.25	0.52
1:E:108:GLY:H	1:E:135:LEU:HD22	1.75	0.52
1:E:244:ASP:HA	1:E:247:ASP:HB2	1.91	0.52
1:G:421:ASP:HB3	1:G:424:LYS:HB2	1.92	0.52
1:K:340:ASN:OD1	1:K:400:ARG:NH1	2.43	0.52
1:A:195:TYR:HD2	1:A:220:LEU:HD13	1.75	0.52
1:C:199:HIS:O	1:C:227:THR:CG2	2.58	0.52
1:C:246:ILE:O	1:C:250:VAL:HG12	2.10	0.52
1:C:426:LEU:HB2	1:D:428:PHE:CE2	2.44	0.52
1:E:340:ASN:HB2	1:E:403:VAL:HG21	1.92	0.52
1:K:101:PHE:CD2	1:K:130:ALA:HB2	2.44	0.52
1:K:114:LEU:HD21	1:K:149:ILE:HD11	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:251:PHE:H	1:K:253:GLY:H	1.57	0.52
1:B:142:PHE:HB3	1:B:149:ILE:HA	1.92	0.52
1:D:429:TYR:OXT	1:K:392:ASP:HB3	2.10	0.52
1:E:243:ALA:O	1:E:246:ILE:HG22	2.10	0.52
1:H:315:VAL:HB	1:H:364:LEU:HB2	1.92	0.52
1:K:26:LYS:HE2	1:K:372:LEU:HD11	1.91	0.52
1:L:52:GLU:HB3	1:L:58:ARG:HA	1.92	0.52
1:C:297:GLU:OE2	1:C:298:ARG:NH2	2.43	0.51
1:F:22:ARG:NH2	1:F:421:ASP:OD2	2.42	0.51
1:F:352:ASP:OD1	1:F:352:ASP:N	2.43	0.51
1:I:122:ILE:C	1:I:124:HIS:H	2.17	0.51
1:B:247:ASP:HA	1:B:250:VAL:CG1	2.39	0.51
1:F:339:ALA:HA	1:F:400:ARG:HG3	1.91	0.51
1:L:319:ILE:N	1:L:360:SER:O	2.32	0.51
1:E:142:PHE:O	1:E:144:PRO:HD3	2.10	0.51
1:G:232:GLN:HG3	1:H:261:HIS:HE1	1.76	0.51
1:I:115:SER:HB2	1:I:118:ASP:HB2	1.92	0.51
1:L:196:ASP:HA	1:L:221:MET:HG2	1.93	0.51
1:B:228:PHE:HZ	1:B:270:LEU:HD12	1.74	0.51
1:C:330:SER:HA	1:C:345:LYS:HD3	1.92	0.51
1:D:401:GLU:HA	1:D:404:LYS:HG2	1.93	0.51
1:F:106:LYS:N	1:F:109:ASP:OD2	2.39	0.51
1:L:319:ILE:O	1:L:325:ILE:HG21	2.11	0.51
1:D:143:ASP:HB3	1:D:146:GLU:O	2.10	0.51
1:E:240:LYS:HA	1:E:243:ALA:HB2	1.91	0.51
1:I:315:VAL:HB	1:I:364:LEU:HB2	1.92	0.51
1:D:209:PHE:CD2	1:D:210:GLN:HG2	2.46	0.51
1:E:158:ILE:HD12	1:E:185:ALA:HB3	1.93	0.51
1:E:296:TYR:HA	1:E:300:PHE:O	2.11	0.51
1:F:24:SER:O	1:F:26:LYS:NZ	2.32	0.51
1:F:251:PHE:HD2	1:F:252:PRO:HD3	1.75	0.51
1:I:203:LEU:HG	1:I:227:THR:HG21	1.92	0.51
1:I:343:LEU:HD13	1:I:362:ILE:HD13	1.92	0.51
1:K:130:ALA:O	1:K:135:LEU:N	2.42	0.51
1:K:23:GLU:HB3	1:K:404:LYS:HB2	1.91	0.51
1:K:45:ASP:HB2	1:L:18:HIS:CD2	2.46	0.51
1:L:113:ALA:HB2	1:L:167:LEU:HD12	1.91	0.51
1:B:28:ILE:HG22	1:B:30:SER:H	1.75	0.51
1:C:324:ASP:HB3	1:C:391:ILE:HG23	1.93	0.51
1:F:58:ARG:HH22	1:F:70:GLU:CD	2.19	0.51
1:I:283:GLN:NE2	1:I:375:LYS:HD3	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:94:VAL:HG23	1:J:95:VAL:H	1.75	0.51
1:D:280:TYR:HE2	1:D:371:ARG:HD3	1.76	0.51
1:E:336:TYR:HE1	1:E:389:ILE:HB	1.76	0.51
1:G:25:ILE:HD11	1:G:341:ILE:HG23	1.93	0.51
1:J:27:LEU:HD22	1:J:364:LEU:HD22	1.92	0.51
1:J:250:VAL:HA	1:J:253:GLY:O	2.11	0.51
1:A:192:LYS:NZ	1:A:218:GLU:OE2	2.42	0.51
1:A:320:GLU:HB2	1:D:138:ILE:HD12	1.93	0.51
1:D:198:ALA:HA	1:D:223:SER:H	1.76	0.51
1:G:6:VAL:HG13	1:H:72:LEU:HD21	1.93	0.51
1:G:51:ALA:HB1	1:G:58:ARG:HH12	1.75	0.51
1:I:131:GLY:HA2	1:I:135:LEU:HG	1.93	0.51
1:I:229:PHE:CZ	1:I:273:MET:HB3	2.46	0.51
1:K:391:ILE:O	1:K:392:ASP:HB2	2.10	0.51
1:A:295:LEU:HG	1:A:300:PHE:HD2	1.75	0.50
1:B:379:MET:HA	1:B:382:ILE:HB	1.93	0.50
1:C:238:THR:OG1	1:C:239:THR:N	2.44	0.50
1:G:305:GLU:HA	1:G:309:PHE:CE1	2.46	0.50
1:H:251:PHE:HB3	1:H:252:PRO:HD3	1.93	0.50
1:L:47:MET:HG2	1:L:261:HIS:CD2	2.46	0.50
1:A:347:LEU:HG	1:A:359:PRO:HB3	1.93	0.50
1:E:304:CYS:HB3	1:E:307:LYS:HB2	1.93	0.50
1:H:42:CYS:HA	1:H:261:HIS:HB2	1.93	0.50
1:I:45:ASP:HB2	1:J:18:HIS:NE2	2.26	0.50
1:L:66:ILE:HA	1:L:69:VAL:HG12	1.92	0.50
1:D:226:LYS:C	1:D:228:PHE:H	2.19	0.50
1:E:110:LYS:HB3	1:E:163:PRO:HA	1.93	0.50
1:J:141:PRO:HB2	1:J:150:ASP:HB3	1.93	0.50
1:J:224:THR:HG22	1:J:230:GLY:HA3	1.92	0.50
1:C:132:ILE:HG23	1:D:133:ARG:HD2	1.92	0.50
1:C:199:HIS:O	1:C:227:THR:HG23	2.12	0.50
1:G:18:HIS:CE1	1:G:39:ARG:HH22	2.28	0.50
1:H:1:MET:HG3	1:H:5:ASP:HB2	1.93	0.50
1:I:357:ASP:N	1:I:357:ASP:OD1	2.44	0.50
1:J:140:HIS:CE1	1:J:166:ILE:HG23	2.46	0.50
1:K:151:ALA:HA	1:K:154:MET:HE2	1.93	0.50
1:L:53:GLY:HA2	1:L:89:GLN:HE22	1.75	0.50
1:L:371:ARG:O	1:L:414:HIS:N	2.43	0.50
1:A:269:ALA:HA	1:A:272:GLU:HB2	1.94	0.50
1:D:285:ILE:HG13	1:D:311:GLU:O	2.11	0.50
1:K:48:HIS:NE2	1:L:368:GLU:OE1	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:146:GLU:HB3	1:L:307:LYS:NZ	2.26	0.50
1:B:251:PHE:CB	1:B:252:PRO:CD	2.87	0.50
1:C:146:GLU:HG3	1:C:306:HIS:CE1	2.46	0.50
1:G:401:GLU:HA	1:G:404:LYS:HD3	1.94	0.50
1:J:94:VAL:HG23	1:J:95:VAL:N	2.27	0.50
1:A:50:TYR:CD2	1:B:30:SER:CB	2.90	0.50
1:D:162:LYS:HG3	1:D:189:VAL:HG22	1.94	0.50
1:D:388:ARG:HH22	1:I:375:LYS:HD2	1.76	0.50
1:I:280:TYR:O	1:I:284:VAL:HG23	2.12	0.50
1:B:6:VAL:HG23	1:B:7:PRO:HD3	1.93	0.50
1:F:259:HIS:HB3	1:F:261:HIS:CE1	2.47	0.50
1:H:346:ASN:OD1	1:H:363:ARG:HB2	2.12	0.50
1:I:51:ALA:HB2	1:I:66:ILE:HG21	1.93	0.50
1:K:49:ARG:HA	1:L:31:GLU:CD	2.37	0.50
1:A:175:PHE:CD1	1:A:310:THR:OG1	2.53	0.50
1:C:58:ARG:NH2	1:C:70:GLU:OE1	2.45	0.50
1:E:251:PHE:O	1:E:251:PHE:CG	2.64	0.50
1:J:333:ALA:HA	1:J:343:LEU:HD11	1.92	0.50
1:L:295:LEU:HD12	1:L:387:LYS:NZ	2.27	0.50
1:B:193:ILE:HB	1:B:217:ALA:HA	1.92	0.49
1:C:81:PHE:O	1:C:214:ARG:NH2	2.45	0.49
1:D:21:MET:HE3	1:D:26:LYS:HG2	1.94	0.49
1:I:126:LYS:HE2	1:I:135:LEU:HB3	1.94	0.49
1:I:129:ALA:H	1:I:132:ILE:HG13	1.77	0.49
1:J:223:SER:HB2	1:J:225:HIS:CE1	2.46	0.49
1:D:197:GLY:O	1:D:201:LEU:N	2.43	0.49
1:D:209:PHE:CE1	1:D:312:SER:HB3	2.48	0.49
1:E:259:HIS:O	1:E:263:LYS:HG2	2.12	0.49
1:G:63:CYS:O	1:G:64:LYS:HD2	2.11	0.49
1:A:154:MET:HE3	1:A:182:ALA:HB2	1.94	0.49
1:A:213:LEU:HB2	1:A:214:ARG:NH1	2.27	0.49
1:B:298:ARG:HH21	1:B:380:GLU:HG3	1.77	0.49
1:F:186:ALA:HB1	1:F:191:ALA:O	2.12	0.49
1:F:199:HIS:HA	1:F:226:LYS:HD2	1.93	0.49
1:F:312:SER:OG	1:F:313:HIS:N	2.44	0.49
1:G:352:ASP:HB3	1:J:136:LYS:N	2.26	0.49
1:K:135:LEU:HD13	1:L:133:ARG:NH1	2.27	0.49
1:A:10:ILE:HD11	1:B:268:ILE:HD11	1.94	0.49
1:B:389:ILE:HA	1:B:394:GLU:HB3	1.93	0.49
1:E:291:LEU:O	1:E:295:LEU:HB2	2.13	0.49
1:I:255:VAL:HG22	1:I:256:SER:H	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:223:SER:HB2	1:K:225:HIS:CE1	2.47	0.49
1:B:63:CYS:HA	1:B:66:ILE:HD13	1.94	0.49
1:D:28:ILE:HB	1:D:31:GLU:HG2	1.94	0.49
1:D:294:ALA:O	1:D:298:ARG:HG2	2.13	0.49
1:F:110:LYS:HE2	1:F:136:LYS:HD2	1.94	0.49
1:G:146:GLU:HG2	1:G:306:HIS:NE2	2.27	0.49
1:J:70:GLU:OE2	1:J:89:GLN:NE2	2.44	0.49
1:K:225:HIS:ND1	1:K:232:GLN:HA	2.28	0.49
1:K:280:TYR:O	1:K:284:VAL:HG23	2.13	0.49
1:K:304:CYS:HB3	1:K:307:LYS:HD2	1.93	0.49
1:A:110:LYS:NZ	1:C:241:GLU:OE1	2.41	0.49
1:C:103:ALA:HA	1:C:249:HIS:CD2	2.47	0.49
1:E:36:LEU:HD12	1:E:39:ARG:HH12	1.77	0.49
1:E:154:MET:HA	1:E:157:LYS:NZ	2.28	0.49
1:E:395:LYS:HD2	1:E:396:PRO:HD2	1.94	0.49
1:F:248:SER:O	1:F:252:PRO:HD2	2.12	0.49
1:F:249:HIS:C	1:F:253:GLY:HA3	2.38	0.49
1:L:112:MET:O	1:L:167:LEU:N	2.45	0.49
1:L:203:LEU:HD13	1:L:227:THR:HB	1.95	0.49
1:C:7:PRO:HG3	1:D:417:PHE:CD2	2.48	0.49
1:D:178:PRO:HB2	1:D:181:ASP:HB2	1.93	0.49
1:F:245:LYS:O	1:F:249:HIS:ND1	2.43	0.49
1:G:378:GLU:HG2	1:G:410:TYR:OH	2.12	0.49
1:H:27:LEU:HB2	1:H:342:ILE:O	2.12	0.49
1:H:91:THR:H	1:H:95:VAL:HG11	1.77	0.49
1:I:49:ARG:NH1	1:J:21:MET:HG3	2.28	0.49
1:I:112:MET:HG3	1:I:140:HIS:CE1	2.48	0.49
1:J:51:ALA:HB2	1:J:260:LEU:HD11	1.94	0.49
1:C:176:PRO:HB3	1:C:210:GLN:HB2	1.95	0.49
2:C:1430:PLP:O1P	1:D:255:VAL:HG22	2.12	0.49
1:E:157:LYS:HB3	1:E:157:LYS:HE2	1.49	0.49
1:F:383:ALA:HA	1:F:386:MET:HE3	1.95	0.49
1:H:238:THR:OG1	1:H:239:THR:N	2.45	0.49
1:I:330:SER:OG	1:I:358:ASN:OD1	2.26	0.49
1:J:176:PRO:HB3	1:J:210:GLN:HB2	1.93	0.49
1:K:165:LEU:HD13	1:K:192:LYS:HB2	1.93	0.49
1:K:199:HIS:HA	1:K:226:LYS:HD2	1.94	0.49
1:B:345:LYS:HD2	1:B:359:PRO:HD2	1.95	0.49
1:D:106:LYS:HG2	1:D:109:ASP:CG	2.38	0.49
1:K:355:ASN:OD1	1:K:355:ASN:N	2.46	0.49
1:A:288:ALA:HA	1:A:366:THR:HG21	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:59:LEU:HA	1:D:345:LYS:HD3	1.94	0.48
1:C:369:CYS:O	1:C:374:MET:HB2	2.13	0.48
1:D:32:ASN:HA	1:D:368:GLU:HB2	1.94	0.48
1:E:416:SER:OG	1:E:417:PHE:N	2.46	0.48
1:F:197:GLY:O	1:F:201:LEU:N	2.46	0.48
1:G:175:PHE:CD1	1:G:311:GLU:HG2	2.47	0.48
1:H:388:ARG:HA	1:H:392:ASP:HB2	1.94	0.48
1:I:31:GLU:OE1	1:J:49:ARG:NH1	2.46	0.48
1:L:76:LEU:HD12	1:L:274:LEU:HD11	1.95	0.48
1:L:225:HIS:CE1	1:L:232:GLN:HG3	2.48	0.48
1:F:73:CYS:HB3	1:F:88:VAL:HG11	1.94	0.48
1:G:78:LYS:O	1:G:82:LYS:N	2.47	0.48
1:H:167:LEU:HD23	1:H:194:ALA:HB3	1.94	0.48
1:A:47:MET:HB2	1:A:261:HIS:CG	2.48	0.48
1:E:43:ALA:HB2	1:F:43:ALA:HB2	1.95	0.48
1:G:175:PHE:HD1	1:G:311:GLU:HG2	1.79	0.48
1:G:345:LYS:HA	1:G:362:ILE:HD13	1.95	0.48
1:H:169:GLY:HA2	1:H:173:PHE:CE2	2.48	0.48
1:H:245:LYS:O	1:H:249:HIS:ND1	2.45	0.48
1:I:102:PHE:CZ	1:J:127:VAL:HA	2.48	0.48
1:J:126:LYS:O	1:J:127:VAL:HG22	2.13	0.48
1:J:148:ASN:OD1	1:J:149:ILE:N	2.46	0.48
1:J:348:LEU:HD13	1:J:361:GLY:HA3	1.94	0.48
1:B:345:LYS:HA	1:B:362:ILE:HD13	1.95	0.48
1:C:376:GLU:HA	1:C:379:MET:HE2	1.95	0.48
1:F:162:LYS:HB3	1:F:163:PRO:CD	2.42	0.48
1:G:34:THR:H	1:H:48:HIS:CE1	2.31	0.48
1:A:27:LEU:HB2	1:A:343:LEU:HB3	1.96	0.48
1:D:89:GLN:HG2	1:D:258:HIS:NE2	2.28	0.48
1:F:72:LEU:O	1:F:76:LEU:HB2	2.13	0.48
1:F:105:THR:O	1:F:133:ARG:NH1	2.45	0.48
1:H:32:ASN:ND2	1:H:227:THR:O	2.46	0.48
1:I:38:VAL:HG13	1:I:265:GLY:HA3	1.93	0.48
1:I:231:PRO:HB2	1:I:262:HIS:CD2	2.44	0.48
1:J:371:ARG:NH2	1:J:415:TYR:O	2.46	0.48
1:K:342:ILE:HG21	1:L:62:GLY:HA3	1.95	0.48
1:A:62:GLY:HA2	1:B:20:TRP:CH2	2.48	0.48
1:C:62:GLY:O	1:C:66:ILE:HD13	2.13	0.48
1:C:319:ILE:HD13	1:C:332:LEU:HD23	1.96	0.48
1:G:32:ASN:O	1:H:48:HIS:HB3	2.13	0.48
1:G:228:PHE:CE2	1:G:273:MET:HG3	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:272:GLU:OE2	1:G:371:ARG:NH2	2.45	0.48
1:H:32:ASN:ND2	1:H:367:GLN:HB2	2.29	0.48
1:H:37:ALA:HB1	1:H:268:ILE:HD13	1.95	0.48
1:J:122:ILE:C	1:J:124:HIS:H	2.21	0.48
1:A:303:LEU:HD11	1:A:348:LEU:HD13	1.96	0.48
1:D:281:ALA:O	1:D:285:ILE:HG22	2.14	0.48
1:E:354:ASN:OD1	1:E:354:ASN:N	2.44	0.48
1:G:50:TYR:CE1	1:G:257:ASN:HB2	2.48	0.48
1:H:271:ALA:HA	1:H:274:LEU:HD12	1.94	0.48
1:I:105:THR:HG22	1:I:106:LYS:O	2.13	0.48
1:I:287:ASN:ND2	1:I:374:MET:O	2.45	0.48
1:K:146:GLU:HG3	1:K:307:LYS:NZ	2.29	0.48
1:B:94:VAL:HG13	2:B:1430:PLP:O2P	2.13	0.48
1:C:94:VAL:HG21	1:D:255:VAL:HA	1.95	0.48
1:C:169:GLY:HA2	1:C:173:PHE:CE1	2.49	0.48
1:D:427:ARG:NH1	1:K:392:ASP:OD1	2.47	0.48
1:F:374:MET:HE3	1:F:374:MET:HB3	1.74	0.48
1:L:291:LEU:HD13	1:L:379:MET:HB3	1.95	0.48
1:B:115:SER:HB2	1:B:118:ASP:HB2	1.95	0.48
1:D:50:TYR:OH	1:D:256:SER:O	2.30	0.48
1:E:46:PHE:HB3	1:E:260:LEU:CB	2.44	0.48
1:F:377:LYS:O	1:F:380:GLU:HB3	2.13	0.48
1:L:41:ALA:O	1:L:44:THR:OG1	2.27	0.48
1:A:339:ALA:O	1:A:403:VAL:HG11	2.13	0.48
1:C:70:GLU:O	1:C:74:ILE:HG12	2.14	0.48
1:D:36:LEU:O	1:D:40:GLU:HG3	2.14	0.48
1:D:285:ILE:HG23	1:D:286:LYS:HD2	1.95	0.48
1:F:317:ILE:HB	1:F:362:ILE:HG13	1.95	0.48
1:G:32:ASN:HA	1:G:368:GLU:HB2	1.95	0.48
1:J:73:CYS:HB3	1:J:88:VAL:HG11	1.96	0.48
1:L:63:CYS:O	1:L:66:ILE:N	2.46	0.48
1:L:244:ASP:HA	1:L:247:ASP:HB2	1.96	0.48
1:L:251:PHE:CZ	1:L:258:HIS:HB2	2.49	0.48
1:B:26:LYS:HD3	1:B:368:GLU:HG3	1.96	0.47
1:C:114:LEU:O	1:C:125:TRP:NE1	2.43	0.47
1:C:157:LYS:O	1:C:161:GLU:HB2	2.14	0.47
1:D:140:HIS:CG	1:D:149:ILE:HG12	2.49	0.47
1:D:225:HIS:CD2	1:D:232:GLN:HG3	2.49	0.47
1:K:44:THR:HG21	1:L:14:SER:HB3	1.96	0.47
1:A:126:LYS:O	1:A:127:VAL:HG22	2.15	0.47
1:A:162:LYS:HG2	1:A:189:VAL:HG13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:348:LEU:HD11	1:E:361:GLY:HA3	1.96	0.47
1:F:203:LEU:HD13	1:F:285:ILE:HD11	1.95	0.47
1:G:13:VAL:HG13	1:H:65:TYR:HB3	1.96	0.47
1:J:210:GLN:NE2	1:J:215:GLU:OE1	2.43	0.47
1:K:202:GLY:HA3	1:K:227:THR:O	2.13	0.47
1:K:421:ASP:HB3	1:K:424:LYS:HB2	1.96	0.47
1:C:344:ASN:HD21	1:C:363:ARG:HE	1.60	0.47
1:D:225:HIS:HD2	1:D:233:GLY:H	1.60	0.47
1:G:176:PRO:HB2	1:G:210:GLN:HE21	1.80	0.47
1:I:115:SER:HA	1:I:125:TRP:HE1	1.79	0.47
1:I:292:ALA:HB1	1:I:302:VAL:HG11	1.95	0.47
1:L:310:THR:OG1	1:L:312:SER:N	2.38	0.47
1:L:319:ILE:HG21	1:L:329:ALA:HA	1.96	0.47
1:B:165:LEU:HD11	1:B:194:ALA:HB2	1.97	0.47
1:C:52:GLU:O	1:C:58:ARG:HB2	2.13	0.47
1:C:133:ARG:NH1	1:D:131:GLY:O	2.43	0.47
1:D:250:VAL:HG23	1:D:254:VAL:HB	1.96	0.47
1:G:176:PRO:HD3	1:G:209:PHE:HE1	1.77	0.47
1:J:176:PRO:HD3	1:J:209:PHE:CE1	2.49	0.47
1:K:305:GLU:OE1	1:K:305:GLU:N	2.45	0.47
1:D:300:PHE:CZ	1:D:390:ALA:HB3	2.47	0.47
1:F:379:MET:HA	1:F:382:ILE:HB	1.96	0.47
1:G:99:ALA:HB1	1:G:250:VAL:HG22	1.96	0.47
1:G:199:HIS:HE2	2:G:1430:PLP:HO3	1.59	0.47
1:H:199:HIS:O	1:H:227:THR:OG1	2.29	0.47
1:I:95:VAL:HG13	1:I:254:VAL:HG21	1.97	0.47
1:K:259:HIS:ND1	1:L:232:GLN:HG2	2.29	0.47
1:A:132:ILE:HG22	1:B:132:ILE:HG22	1.96	0.47
1:A:246:ILE:HA	1:A:249:HIS:HB2	1.97	0.47
1:A:259:HIS:HB2	1:A:262:HIS:HB2	1.97	0.47
1:D:108:GLY:HA2	1:D:135:LEU:O	2.15	0.47
1:E:100:VAL:HG21	1:E:221:MET:SD	2.54	0.47
1:E:144:PRO:C	1:E:146:GLU:H	2.23	0.47
1:J:178:PRO:HB2	1:J:181:ASP:HB2	1.97	0.47
1:A:227:THR:HG22	1:A:227:THR:O	2.13	0.47
1:B:366:THR:O	1:B:370:THR:N	2.40	0.47
1:C:130:ALA:O	1:C:135:LEU:N	2.48	0.47
1:C:418:ASP:HB2	1:D:429:TYR:CG	2.50	0.47
1:D:22:ARG:NE	1:D:411:SER:HB2	2.30	0.47
1:E:129:ALA:C	1:E:131:GLY:H	2.22	0.47
1:F:112:MET:HG2	1:F:140:HIS:CE1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:31:GLU:HG2	1:H:50:TYR:N	2.29	0.47
1:G:66:ILE:HG22	1:G:260:LEU:HD22	1.95	0.47
1:G:312:SER:OG	1:G:313:HIS:N	2.47	0.47
1:H:206:GLY:O	1:H:208:GLN:NE2	2.38	0.47
1:H:294:ALA:O	1:H:298:ARG:HG2	2.15	0.47
1:I:84:GLU:CD	1:I:240:LYS:H	2.23	0.47
1:I:102:PHE:HZ	1:J:127:VAL:HA	1.79	0.47
1:I:110:LYS:HE2	1:I:136:LYS:NZ	2.30	0.47
1:I:132:ILE:HA	1:J:133:ARG:HD3	1.96	0.47
1:I:146:GLU:HA	1:I:304:CYS:SG	2.55	0.47
1:I:325:ILE:HG22	1:I:327:PHE:HB2	1.97	0.47
1:J:95:VAL:HA	1:J:98:LEU:HB2	1.97	0.47
1:K:411:SER:HB2	1:K:421:ASP:OD1	2.14	0.47
1:L:181:ASP:OD1	1:L:181:ASP:N	2.47	0.47
1:L:202:GLY:HA3	1:L:227:THR:O	2.15	0.47
1:L:305:GLU:HA	1:L:309:PHE:CE1	2.50	0.47
1:B:23:GLU:HG3	1:B:340:ASN:ND2	2.30	0.47
1:F:58:ARG:HH21	1:F:67:ASP:HA	1.80	0.47
1:G:32:ASN:ND2	1:G:229:PHE:HA	2.29	0.47
1:I:123:SER:HA	1:I:128:SER:O	2.15	0.47
1:K:323:PRO:C	1:K:325:ILE:H	2.23	0.47
1:A:126:LYS:HA	1:A:131:GLY:HA3	1.95	0.47
1:D:149:ILE:H	1:D:149:ILE:HD12	1.79	0.47
1:D:163:PRO:HG2	1:D:166:ILE:HD11	1.97	0.47
1:F:51:ALA:O	1:F:58:ARG:HD2	2.15	0.47
1:F:53:GLY:HA2	1:F:251:PHE:CE1	2.50	0.47
1:H:101:PHE:CD2	1:H:130:ALA:HB2	2.50	0.47
1:I:151:ALA:HA	1:I:154:MET:HE2	1.97	0.47
1:J:53:GLY:O	1:J:89:GLN:NE2	2.45	0.47
1:J:155:VAL:HG13	1:J:185:ALA:HB1	1.96	0.47
1:A:121:HIS:HB2	1:A:171:SER:HB3	1.97	0.47
1:B:315:VAL:HB	1:B:364:LEU:HB2	1.97	0.47
1:E:92:SER:O	1:E:95:VAL:HG22	2.15	0.47
1:F:238:THR:OG1	1:F:239:THR:N	2.48	0.47
1:F:339:ALA:O	1:F:341:ILE:N	2.48	0.47
1:G:53:GLY:HA3	1:G:89:GLN:CD	2.39	0.47
1:I:167:LEU:HD21	1:I:221:MET:HE1	1.96	0.47
1:I:318:ASP:OD1	1:I:360:SER:OG	2.25	0.47
1:J:165:LEU:HD11	1:J:194:ALA:HB2	1.97	0.47
1:J:232:GLN:HB2	1:J:262:HIS:CE1	2.50	0.47
1:K:78:LYS:HE2	1:K:86:ALA:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:ASP:HB3	1:B:142:PHE:HE1	1.80	0.46
1:C:127:VAL:HG13	1:D:252:PRO:HG2	1.97	0.46
1:D:122:ILE:O	1:D:123:SER:OG	2.27	0.46
1:G:81:PHE:HB2	1:G:237:LEU:HD22	1.98	0.46
1:G:169:GLY:HA2	1:G:173:PHE:CE2	2.50	0.46
1:G:257:ASN:C	1:G:259:HIS:H	2.22	0.46
1:J:5:ASP:OD1	1:J:5:ASP:N	2.42	0.46
1:D:405:GLU:HB3	1:I:286:LYS:NZ	2.30	0.46
1:G:47:MET:O	1:H:232:GLN:NE2	2.49	0.46
1:G:47:MET:HA	1:G:261:HIS:HD2	1.79	0.46
1:G:50:TYR:CE2	1:H:30:SER:HB3	2.49	0.46
1:G:336:TYR:HB3	1:G:341:ILE:O	2.15	0.46
1:A:174:PRO:O	1:A:310:THR:OG1	2.34	0.46
1:A:268:ILE:HD11	1:B:10:ILE:HD11	1.97	0.46
1:E:72:LEU:HD13	1:E:267:ALA:HB1	1.95	0.46
1:G:223:SER:OG	2:G:1430:PLP:O1P	2.33	0.46
1:H:106:LYS:N	1:H:109:ASP:OD2	2.42	0.46
1:J:154:MET:HG3	1:J:155:VAL:H	1.80	0.46
1:A:101:PHE:CE1	1:A:167:LEU:HD11	2.50	0.46
1:B:147:MET:HE3	1:B:303:LEU:HD23	1.95	0.46
1:B:238:THR:OG1	1:B:239:THR:N	2.47	0.46
1:E:82:LYS:HB2	1:E:214:ARG:NH2	2.30	0.46
1:E:141:PRO:HG3	1:E:157:LYS:HD3	1.97	0.46
1:F:102:PHE:HD1	1:F:133:ARG:HH21	1.62	0.46
1:I:328:SER:HB3	1:I:331:GLU:HG2	1.96	0.46
1:J:143:ASP:HB3	1:J:146:GLU:O	2.16	0.46
1:L:295:LEU:HD12	1:L:387:LYS:HZ3	1.80	0.46
1:D:49:ARG:HB2	1:D:260:LEU:HD12	1.97	0.46
1:D:174:PRO:O	1:D:311:GLU:N	2.47	0.46
1:E:158:ILE:HG22	1:E:189:VAL:HG21	1.97	0.46
1:F:111:LEU:HB2	1:F:135:LEU:CD2	2.45	0.46
1:H:28:ILE:HG23	1:H:363:ARG:HD2	1.97	0.46
1:H:72:LEU:O	1:H:76:LEU:HB2	2.16	0.46
1:H:154:MET:HE2	1:H:154:MET:HB3	1.83	0.46
1:I:51:ALA:HB3	1:I:258:HIS:NE2	2.30	0.46
1:L:104:GLU:O	1:L:105:THR:OG1	2.23	0.46
1:B:1:MET:HG2	1:B:5:ASP:OD1	2.15	0.46
1:C:102:PHE:CD1	1:D:132:ILE:HG12	2.50	0.46
1:C:306:HIS:HB3	1:E:306:HIS:HB3	1.98	0.46
1:D:336:TYR:CD2	1:D:343:LEU:HD21	2.51	0.46
1:G:140:HIS:CG	1:G:149:ILE:HD12	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:303:LEU:HD21	1:I:350:TRP:CH2	2.51	0.46
1:J:238:THR:OG1	1:J:239:THR:N	2.49	0.46
1:K:40:GLU:OE2	1:L:425:TYR:OH	2.30	0.46
1:K:155:VAL:O	1:K:159:LEU:HB2	2.16	0.46
1:K:226:LYS:C	1:K:228:PHE:H	2.23	0.46
1:K:393:LYS:HE2	1:K:393:LYS:HB3	1.64	0.46
1:A:91:THR:HG23	1:A:255:VAL:HG23	1.96	0.46
1:B:46:PHE:HB3	1:B:260:LEU:HB3	1.98	0.46
1:C:135:LEU:HB3	1:C:136:LYS:H	1.55	0.46
1:E:371:ARG:NH2	1:E:416:SER:HB2	2.30	0.46
1:F:105:THR:HG22	1:F:133:ARG:NH1	2.31	0.46
1:H:32:ASN:HB2	1:H:367:GLN:HG3	1.98	0.46
1:I:55:PRO:HG3	1:I:58:ARG:HH21	1.80	0.46
1:D:214:ARG:HH11	1:D:214:ARG:H	1.63	0.46
1:D:225:HIS:CG	1:D:232:GLN:HG3	2.51	0.46
1:E:198:ALA:HA	1:E:223:SER:H	1.81	0.46
1:G:294:ALA:O	1:G:298:ARG:HG2	2.15	0.46
1:H:27:LEU:HD22	1:H:343:LEU:HD22	1.98	0.46
1:H:49:ARG:HA	1:H:49:ARG:HD3	1.72	0.46
1:I:169:GLY:HA2	1:I:173:PHE:HE2	1.80	0.46
1:J:227:THR:HG22	1:J:367:GLN:HG2	1.98	0.46
1:K:132:ILE:HD13	1:L:98:LEU:HD11	1.97	0.46
1:B:26:LYS:HB2	1:B:368:GLU:HG2	1.98	0.46
1:D:136:LYS:HD3	1:D:136:LYS:HA	1.73	0.46
1:D:367:GLN:CD	1:D:367:GLN:H	2.23	0.46
1:E:150:ASP:OD1	1:E:153:ALA:N	2.46	0.46
1:G:36:LEU:HD21	1:G:421:ASP:H	1.81	0.46
1:H:246:ILE:O	1:H:250:VAL:HG23	2.15	0.46
1:J:97:ASN:HB3	1:J:101:PHE:CE2	2.51	0.46
1:J:367:GLN:H	1:J:367:GLN:HG3	1.55	0.46
1:A:50:TYR:HD2	1:B:30:SER:HB3	1.75	0.46
1:A:246:ILE:O	1:A:250:VAL:HG22	2.15	0.46
1:C:57:LYS:NZ	1:C:61:GLN:HA	2.31	0.46
1:F:81:PHE:HB2	1:F:237:LEU:HD22	1.98	0.46
1:F:117:PRO:HA	1:F:347:LEU:HB3	1.98	0.46
1:I:39:ARG:NH2	1:I:424:LYS:O	2.49	0.46
1:I:122:ILE:HG22	1:I:123:SER:H	1.80	0.46
1:I:319:ILE:HB	1:I:329:ALA:HB2	1.97	0.46
1:K:428:PHE:N	1:L:40:GLU:OE2	2.44	0.46
1:C:34:THR:HG23	1:D:48:HIS:CD2	2.52	0.45
1:D:336:TYR:HA	1:D:339:ALA:HB3	1.96	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:257:ASN:OD1	1:E:257:ASN:N	2.50	0.45
1:F:106:LYS:NZ	1:F:109:ASP:OD1	2.27	0.45
1:F:154:MET:O	1:F:158:ILE:HG13	2.16	0.45
1:G:10:ILE:HD12	1:H:267:ALA:HB3	1.98	0.45
1:G:291:LEU:HD22	1:G:379:MET:HE2	1.98	0.45
1:I:36:LEU:HD13	1:I:422:GLY:HA2	1.98	0.45
1:J:194:ALA:HB1	1:J:221:MET:HE1	1.99	0.45
1:L:91:THR:H	1:L:95:VAL:HG11	1.81	0.45
1:A:267:ALA:HA	1:A:270:LEU:HD12	1.98	0.45
1:C:374:MET:HE3	1:C:374:MET:HB3	1.76	0.45
1:C:388:ARG:HD3	1:C:394:GLU:HG3	1.98	0.45
1:D:52:GLU:HB3	1:D:60:TYR:HE2	1.80	0.45
1:D:84:GLU:HB2	1:D:239:THR:HA	1.99	0.45
1:E:40:GLU:HB2	1:F:428:PHE:HB2	1.98	0.45
1:G:301:ASN:O	1:G:317:ILE:HG23	2.15	0.45
1:H:54:LEU:HD23	1:H:54:LEU:HA	1.86	0.45
1:I:377:LYS:O	1:I:381:GLU:HG2	2.17	0.45
1:A:10:ILE:HG13	1:A:11:ARG:N	2.31	0.45
1:C:69:VAL:HG11	1:C:264:ALA:HA	1.98	0.45
1:C:94:VAL:HB	1:D:255:VAL:HG23	1.98	0.45
1:C:209:PHE:CE1	1:C:312:SER:HB3	2.52	0.45
1:D:254:VAL:HG13	1:D:255:VAL:N	2.31	0.45
1:E:156:LYS:HA	1:E:159:LEU:HD12	1.97	0.45
1:E:165:LEU:HD21	1:E:194:ALA:HB3	1.97	0.45
1:F:63:CYS:HA	1:F:66:ILE:HD12	1.99	0.45
1:G:347:LEU:HD11	1:G:354:ASN:HA	1.97	0.45
1:J:93:GLY:N	2:J:1430:PLP:O1P	2.49	0.45
1:J:110:LYS:HE2	1:J:161:GLU:HB2	1.99	0.45
1:K:33:ILE:HB	1:K:368:GLU:HG3	1.99	0.45
1:K:109:ASP:HA	1:K:136:LYS:HB3	1.98	0.45
1:K:259:HIS:O	1:K:263:LYS:HG2	2.16	0.45
1:L:52:GLU:H	1:L:58:ARG:HG2	1.81	0.45
1:C:72:LEU:HD11	1:D:9:PHE:CD2	2.51	0.45
1:G:64:LYS:NZ	1:H:337:GLU:OE2	2.44	0.45
1:G:352:ASP:HB3	1:J:136:LYS:CA	2.47	0.45
1:J:173:PHE:HE1	1:J:177:HIS:CE1	2.33	0.45
1:K:126:LYS:HE3	1:K:135:LEU:HD12	1.98	0.45
1:K:169:GLY:HA2	1:K:173:PHE:CE2	2.52	0.45
1:L:383:ALA:O	1:L:387:LYS:HG2	2.16	0.45
1:C:225:HIS:HE1	1:D:50:TYR:CE2	2.34	0.45
1:C:322:SER:HA	1:C:323:PRO:HD3	1.75	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:378:GLU:OE2	1:C:410:TYR:OH	2.33	0.45
1:C:428:PHE:CD1	1:D:40:GLU:HG2	2.52	0.45
1:E:84:GLU:OE1	1:E:240:LYS:HG2	2.17	0.45
1:F:339:ALA:HB2	1:F:396:PRO:O	2.15	0.45
1:G:34:THR:HG23	1:H:48:HIS:ND1	2.32	0.45
1:I:20:TRP:CZ3	1:J:62:GLY:HA2	2.51	0.45
1:I:42:CYS:HA	1:I:261:HIS:HB2	1.98	0.45
1:I:126:LYS:HE2	1:I:136:LYS:H	1.81	0.45
1:J:253:GLY:O	1:J:255:VAL:N	2.50	0.45
1:K:14:SER:O	1:K:17:GLN:HB3	2.16	0.45
1:K:138:ILE:HG21	1:K:157:LYS:NZ	2.31	0.45
1:L:95:VAL:HG13	1:L:254:VAL:HG21	1.99	0.45
1:L:174:PRO:HB3	1:L:316:ILE:HD11	1.99	0.45
1:L:280:TYR:O	1:L:284:VAL:HG23	2.16	0.45
1:A:211:ASP:OD2	1:A:214:ARG:NH1	2.49	0.45
1:C:51:ALA:HA	1:C:63:CYS:SG	2.57	0.45
1:C:79:GLU:OE2	1:D:3:TYR:OH	2.25	0.45
1:C:171:SER:O	1:C:314:GLN:NE2	2.42	0.45
1:G:385:PHE:O	1:G:388:ARG:HG2	2.16	0.45
1:G:395:LYS:HA	1:G:396:PRO:HD3	1.84	0.45
1:I:287:ASN:C	1:I:366:THR:HG21	2.42	0.45
1:K:49:ARG:NE	1:L:17:GLN:HE22	2.15	0.45
1:K:271:ALA:CB	1:L:6:VAL:HG21	2.45	0.45
1:A:49:ARG:NH2	1:B:368:GLU:OE2	2.49	0.45
1:E:46:PHE:HA	1:E:49:ARG:HG2	1.98	0.45
1:E:133:ARG:HD3	1:F:132:ILE:O	2.16	0.45
1:G:303:LEU:HD21	1:G:350:TRP:HH2	1.82	0.45
1:H:1:MET:HG2	1:H:2:GLU:O	2.17	0.45
1:H:32:ASN:OD1	1:H:33:ILE:N	2.50	0.45
1:H:395:LYS:HG3	1:H:396:PRO:O	2.17	0.45
1:J:192:LYS:HD2	1:J:218:GLU:HG3	1.99	0.45
1:K:3:TYR:CE1	1:L:274:LEU:HD22	2.52	0.45
1:L:282:LYS:O	1:L:286:LYS:HG2	2.17	0.45
1:A:296:TYR:HA	1:A:300:PHE:O	2.17	0.45
1:B:50:TYR:HA	1:B:257:ASN:HD22	1.80	0.45
1:B:123:SER:HA	1:B:128:SER:HG	1.81	0.45
1:B:251:PHE:HD1	1:B:252:PRO:CG	2.29	0.45
1:D:34:THR:O	1:D:39:ARG:NH1	2.50	0.45
1:D:49:ARG:HA	1:D:49:ARG:HD3	1.64	0.45
1:D:343:LEU:HD13	1:D:362:ILE:HD11	1.97	0.45
1:E:252:PRO:HB2	1:F:127:VAL:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:11:ARG:O	1:F:15:ILE:HG13	2.16	0.45
1:F:88:VAL:O	1:F:263:LYS:NZ	2.33	0.45
1:F:214:ARG:HA	1:F:214:ARG:HD3	1.85	0.45
1:G:32:ASN:HD21	1:G:229:PHE:HB3	1.81	0.45
1:G:168:PHE:CD1	1:G:177:HIS:HB3	2.51	0.45
1:H:58:ARG:HH12	1:H:64:LYS:NZ	2.15	0.45
1:H:91:THR:C	1:H:233:GLY:HA2	2.41	0.45
1:I:251:PHE:O	1:I:251:PHE:CG	2.69	0.45
1:J:201:LEU:HD22	1:J:223:SER:O	2.16	0.45
1:A:271:ALA:HA	1:A:274:LEU:HD12	1.98	0.45
1:B:335:MET:HB3	1:B:396:PRO:HG3	1.98	0.45
1:C:197:GLY:O	1:C:201:LEU:N	2.50	0.45
1:E:98:LEU:HD13	1:E:98:LEU:HA	1.85	0.45
1:E:132:ILE:O	1:F:133:ARG:HD3	2.17	0.45
1:F:126:LYS:C	1:F:128:SER:H	2.25	0.45
1:F:367:GLN:HG2	1:F:368:GLU:N	2.32	0.45
1:G:125:TRP:HH2	1:G:139:ASN:HB3	1.81	0.45
1:G:411:SER:HB3	1:G:421:ASP:OD1	2.17	0.45
1:K:29:ALA:HB1	1:K:199:HIS:CE1	2.52	0.45
1:I:125:TRP:C	1:I:130:ALA:HB3	2.42	0.45
1:K:347:LEU:HD23	1:K:359:PRO:HB3	1.99	0.45
1:L:242:ASN:O	1:L:245:LYS:HB3	2.16	0.45
1:L:294:ALA:O	1:L:297:GLU:HG2	2.17	0.45
1:B:171:SER:O	1:B:314:GLN:NE2	2.49	0.44
1:C:413:ILE:HG22	1:C:420:GLY:O	2.18	0.44
1:D:388:ARG:NH2	1:I:375:LYS:HD2	2.33	0.44
1:F:90:PRO:HA	1:F:255:VAL:HG21	1.98	0.44
1:G:313:HIS:CE1	1:G:314:GLN:HG3	2.52	0.44
1:A:66:ILE:HD13	1:A:260:LEU:HD13	1.99	0.44
1:D:176:PRO:HB3	1:D:210:GLN:HB3	2.00	0.44
1:D:351:ASP:C	1:D:352:ASP:CG	2.85	0.44
1:E:424:LYS:HA	1:E:424:LYS:HD2	1.86	0.44
1:F:241:GLU:OE1	1:F:241:GLU:N	2.41	0.44
1:L:10:ILE:HG13	1:L:11:ARG:N	2.30	0.44
1:A:229:PHE:CE2	1:A:273:MET:HE2	2.53	0.44
1:D:118:ASP:HA	1:D:349:PRO:HB3	1.98	0.44
1:F:103:ALA:HA	1:F:249:HIS:CG	2.52	0.44
1:G:20:TRP:CH2	1:H:62:GLY:HA2	2.52	0.44
1:G:125:TRP:CE3	1:G:126:LYS:HE3	2.53	0.44
1:L:302:VAL:HB	1:L:309:PHE:CE1	2.53	0.44
1:A:174:PRO:O	1:A:310:THR:HG21	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:26:LYS:H	1:B:26:LYS:HD2	1.83	0.44
1:B:46:PHE:HB3	1:B:260:LEU:CB	2.47	0.44
1:B:123:SER:HA	1:B:128:SER:OG	2.17	0.44
1:C:298:ARG:HB2	1:C:300:PHE:HD1	1.83	0.44
1:E:18:HIS:NE2	1:F:45:ASP:HB2	2.33	0.44
1:E:111:LEU:O	1:E:138:ILE:HG12	2.18	0.44
1:H:309:PHE:O	1:H:310:THR:HB	2.17	0.44
1:I:228:PHE:HD1	1:I:230:GLY:H	1.65	0.44
1:J:28:ILE:HA	1:J:344:ASN:HD21	1.82	0.44
1:L:58:ARG:HD3	1:L:59:LEU:H	1.81	0.44
1:B:50:TYR:CD1	1:B:257:ASN:HB3	2.52	0.44
1:C:6:VAL:HB	1:D:271:ALA:CB	2.46	0.44
1:D:27:LEU:HB3	1:D:364:LEU:HD12	2.00	0.44
1:F:116:VAL:HA	1:F:120:GLY:O	2.18	0.44
1:F:340:ASN:O	1:F:341:ILE:HG13	2.17	0.44
1:G:226:LYS:H	1:G:226:LYS:HG2	1.55	0.44
1:H:102:PHE:O	1:H:133:ARG:NH1	2.50	0.44
1:I:198:ALA:HA	1:I:223:SER:H	1.82	0.44
1:K:158:ILE:O	1:K:189:VAL:HG21	2.18	0.44
1:K:428:PHE:HD2	1:L:40:GLU:HG3	1.83	0.44
1:A:105:THR:O	1:A:133:ARG:NE	2.41	0.44
1:A:256:SER:H	1:B:94:VAL:CG2	2.29	0.44
1:B:22:ARG:NH1	1:B:423:PHE:HB2	2.33	0.44
1:D:255:VAL:HG13	1:D:257:ASN:N	2.32	0.44
1:D:292:ALA:HB1	1:D:302:VAL:HG11	1.99	0.44
1:E:101:PHE:CD2	1:E:130:ALA:HB2	2.53	0.44
1:E:378:GLU:O	1:E:382:ILE:HG13	2.17	0.44
1:F:207:LYS:O	1:F:207:LYS:HG3	2.18	0.44
1:F:294:ALA:O	1:F:298:ARG:HG2	2.18	0.44
1:I:318:ASP:OD2	1:I:321:SER:HB2	2.18	0.44
1:J:159:LEU:O	1:J:162:LYS:HG3	2.17	0.44
1:J:421:ASP:HB3	1:J:424:LYS:HG3	2.00	0.44
1:K:115:SER:HB3	1:K:118:ASP:HB2	2.00	0.44
1:B:114:LEU:HD11	1:B:142:PHE:CE1	2.53	0.44
1:B:128:SER:OG	1:B:129:ALA:N	2.50	0.44
1:B:276:PHE:HB3	1:B:415:TYR:HD1	1.82	0.44
1:C:27:LEU:HD13	1:C:364:LEU:HD23	1.99	0.44
1:E:371:ARG:HH22	1:E:416:SER:HB2	1.82	0.44
1:I:62:GLY:HA2	1:J:20:TRP:CZ3	2.53	0.44
1:I:101:PHE:CZ	1:I:167:LEU:HD11	2.52	0.44
1:I:251:PHE:N	1:I:254:VAL:O	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:47:MET:HE3	1:J:47:MET:HB2	1.92	0.44
1:K:76:LEU:HD21	1:K:271:ALA:HB2	1.99	0.44
1:K:130:ALA:HA	1:K:133:ARG:HB3	1.99	0.44
1:K:173:PHE:H	1:K:314:GLN:CD	2.25	0.44
1:L:22:ARG:HB3	1:L:423:PHE:CG	2.53	0.44
1:C:122:ILE:O	1:C:123:SER:OG	2.26	0.44
1:E:255:VAL:CG1	1:E:256:SER:N	2.73	0.44
1:E:271:ALA:HA	1:E:274:LEU:HB2	2.00	0.44
1:I:303:LEU:HD21	1:I:350:TRP:HH2	1.82	0.44
1:J:38:VAL:HG13	1:J:265:GLY:HA3	2.00	0.44
1:J:175:PHE:CE2	1:J:311:GLU:HB2	2.53	0.44
1:C:59:LEU:HB2	1:C:60:TYR:HD1	1.83	0.44
1:C:306:HIS:CD2	1:C:307:LYS:HG3	2.53	0.44
1:D:90:PRO:HG2	1:D:236:ILE:HG13	2.00	0.44
1:D:225:HIS:HB3	1:D:232:GLN:HA	1.99	0.44
1:E:27:LEU:HD13	1:E:341:ILE:HG23	2.00	0.44
1:E:72:LEU:O	1:E:76:LEU:HB2	2.18	0.44
1:E:115:SER:HA	1:E:125:TRP:NE1	2.33	0.44
1:F:28:ILE:HG22	1:F:344:ASN:HD21	1.83	0.44
1:G:226:LYS:O	1:G:227:THR:C	2.61	0.44
1:H:22:ARG:NH2	1:H:411:SER:OG	2.50	0.44
1:L:211:ASP:OD1	1:L:214:ARG:HD2	2.18	0.44
1:L:319:ILE:HD12	1:L:329:ALA:HB1	2.00	0.44
1:A:421:ASP:HB3	1:A:424:LYS:HE3	2.00	0.43
1:A:427:ARG:HB3	1:A:427:ARG:HH11	1.83	0.43
1:B:201:LEU:HB3	1:B:228:PHE:HB2	2.00	0.43
1:B:325:ILE:HG13	1:B:327:PHE:H	1.83	0.43
1:E:8:LYS:HE3	1:E:8:LYS:HB2	1.87	0.43
1:E:212:PRO:HB2	1:E:217:ALA:HB3	1.98	0.43
1:G:82:LYS:HE3	1:G:214:ARG:HH21	1.82	0.43
1:I:133:ARG:HD2	1:I:133:ARG:HA	1.66	0.43
1:J:103:ALA:HA	1:J:249:HIS:CE1	2.53	0.43
1:K:9:PHE:O	1:K:12:ASP:HB3	2.17	0.43
1:A:108:GLY:H	1:A:135:LEU:H	1.66	0.43
1:C:314:GLN:HA	1:C:364:LEU:O	2.18	0.43
1:D:186:ALA:O	1:D:191:ALA:N	2.41	0.43
1:D:305:GLU:HA	1:D:309:PHE:CE1	2.53	0.43
1:E:66:ILE:HG21	1:E:260:LEU:HD13	2.00	0.43
1:E:112:MET:HG2	1:E:140:HIS:CD2	2.54	0.43
1:F:340:ASN:HB2	1:F:403:VAL:HG21	2.00	0.43
1:G:27:LEU:HB2	1:G:343:LEU:HD23	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:50:TYR:HH	1:H:225:HIS:CD2	2.34	0.43
1:G:50:TYR:OH	1:H:225:HIS:NE2	2.41	0.43
1:G:337:GLU:CD	1:H:61:GLN:HG3	2.43	0.43
1:J:173:PHE:CE2	1:J:209:PHE:HE2	2.36	0.43
1:K:199:HIS:O	1:K:313:HIS:NE2	2.51	0.43
1:K:387:LYS:HE2	1:K:387:LYS:HB3	1.83	0.43
1:D:110:LYS:HG3	1:D:136:LYS:HB3	2.00	0.43
1:G:11:ARG:NH2	1:G:427:ARG:HB3	2.32	0.43
1:I:282:LYS:O	1:I:286:LYS:HG2	2.18	0.43
1:I:295:LEU:HD22	1:I:300:PHE:CD2	2.54	0.43
1:L:85:HIS:CD2	1:L:243:ALA:HA	2.53	0.43
1:A:73:CYS:HB3	1:A:88:VAL:HG11	1.99	0.43
1:C:128:SER:HB2	1:D:252:PRO:HB3	1.99	0.43
1:C:169:GLY:H	1:C:177:HIS:CE1	2.36	0.43
1:C:268:ILE:O	1:C:272:GLU:HG2	2.18	0.43
1:D:198:ALA:HA	1:D:222:GLY:HA2	2.00	0.43
1:D:336:TYR:HD2	1:D:343:LEU:HD21	1.84	0.43
1:E:8:LYS:HA	1:E:11:ARG:HB2	2.00	0.43
1:E:18:HIS:CE1	1:E:425:TYR:HD1	2.35	0.43
1:E:80:LEU:O	1:E:82:LYS:NZ	2.32	0.43
1:E:81:PHE:HB2	1:E:237:LEU:HD22	2.01	0.43
1:E:256:SER:HA	2:F:1430:PLP:O2P	2.19	0.43
1:E:428:PHE:CB	1:F:40:GLU:HB2	2.46	0.43
1:J:253:GLY:C	1:J:255:VAL:H	2.26	0.43
1:L:29:ALA:HA	1:L:365:GLY:HA3	2.00	0.43
1:A:92:SER:HB2	1:A:95:VAL:HB	2.00	0.43
1:C:5:ASP:OD1	1:C:5:ASP:N	2.51	0.43
1:C:28:ILE:HB	1:C:31:GLU:HB2	2.00	0.43
1:D:367:GLN:C	1:D:369:CYS:H	2.27	0.43
1:F:154:MET:HA	1:F:157:LYS:HB2	2.00	0.43
1:G:298:ARG:HB2	1:G:300:PHE:HD1	1.84	0.43
1:G:384:GLU:HA	1:G:387:LYS:HD3	2.01	0.43
1:H:187:GLN:HB3	1:K:126:LYS:HG3	2.01	0.43
1:I:124:HIS:CG	1:I:167:LEU:HD13	2.54	0.43
1:I:395:LYS:HG3	1:I:397:GLU:H	1.84	0.43
1:J:58:ARG:HG2	1:J:59:LEU:H	1.83	0.43
1:K:112:MET:HE2	1:K:140:HIS:HD2	1.82	0.43
1:K:165:LEU:HD12	1:K:166:ILE:H	1.83	0.43
1:K:175:PHE:CD1	1:K:307:LYS:HD3	2.53	0.43
1:K:368:GLU:O	1:K:372:LEU:HG	2.18	0.43
1:A:256:SER:HG	1:A:257:ASN:H	1.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:339:ALA:HB2	1:C:396:PRO:HB3	2.00	0.43
1:C:354:ASN:OD1	1:C:354:ASN:N	2.47	0.43
1:D:312:SER:OG	1:D:313:HIS:N	2.51	0.43
1:E:42:CYS:HA	1:E:261:HIS:HB2	2.00	0.43
1:E:343:LEU:HD23	1:E:364:LEU:HD11	2.00	0.43
1:F:54:LEU:HB3	1:F:55:PRO:HD2	2.00	0.43
1:F:366:THR:O	1:F:366:THR:OG1	2.36	0.43
1:I:72:LEU:HD21	1:J:6:VAL:HG13	1.99	0.43
1:I:211:ASP:CG	1:I:214:ARG:HE	2.27	0.43
1:J:112:MET:O	1:J:167:LEU:HB2	2.17	0.43
1:J:306:HIS:CD2	1:J:307:LYS:HG2	2.53	0.43
1:J:325:ILE:HG23	1:J:390:ALA:HB1	2.01	0.43
1:K:6:VAL:N	1:K:7:PRO:HD2	2.34	0.43
1:K:272:GLU:OE1	1:K:371:ARG:NH2	2.51	0.43
1:C:90:PRO:HG3	1:C:250:VAL:HG21	2.00	0.43
1:C:348:LEU:N	1:C:351:ASP:OD2	2.40	0.43
1:E:289:LYS:HB3	1:E:310:THR:HG23	1.95	0.43
1:F:28:ILE:HG13	1:F:31:GLU:HB3	2.01	0.43
1:G:114:LEU:O	1:G:125:TRP:NE1	2.38	0.43
1:G:375:LYS:NZ	1:G:415:TYR:OH	2.51	0.43
1:H:119:GLY:HA3	1:H:172:LEU:HB2	2.00	0.43
1:I:228:PHE:HA	1:I:273:MET:HE1	2.01	0.43
1:J:154:MET:HG3	1:J:155:VAL:N	2.33	0.43
1:J:368:GLU:O	1:J:372:LEU:HG	2.19	0.43
1:K:398:LYS:HE2	1:K:398:LYS:HB3	1.82	0.43
1:L:371:ARG:NH2	1:L:416:SER:HB2	2.34	0.43
1:A:50:TYR:CZ	1:A:257:ASN:HB3	2.52	0.43
1:B:394:GLU:HG2	1:B:395:LYS:H	1.84	0.43
1:D:307:LYS:O	1:D:308:ASP:HB2	2.19	0.43
1:D:404:LYS:O	1:D:408:LYS:HB2	2.19	0.43
1:E:78:LYS:HE2	1:E:85:HIS:HA	1.99	0.43
1:G:82:LYS:HB2	1:G:214:ARG:NH2	2.33	0.43
1:G:155:VAL:O	1:G:159:LEU:HB2	2.19	0.43
1:G:246:ILE:O	1:G:250:VAL:HG23	2.19	0.43
1:I:141:PRO:HG2	1:I:154:MET:HA	2.00	0.43
1:I:294:ALA:HB2	1:I:380:GLU:HG2	2.00	0.43
1:J:97:ASN:HB3	1:J:101:PHE:HE2	1.83	0.43
1:L:238:THR:OG1	1:L:239:THR:N	2.51	0.43
1:A:326:GLU:HG2	1:D:157:LYS:HA	1.99	0.43
1:C:419:GLU:O	1:K:398:LYS:NZ	2.52	0.43
1:F:206:GLY:C	1:F:208:GLN:H	2.27	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:399:VAL:O	1:H:403:VAL:HG23	2.19	0.43
1:I:185:ALA:O	1:I:189:VAL:HG23	2.19	0.43
1:J:212:PRO:HG2	1:J:220:LEU:HD12	2.01	0.43
1:K:386:MET:HE3	1:K:386:MET:HB3	1.93	0.43
1:L:19:GLU:HA	1:L:22:ARG:NE	2.32	0.43
1:B:325:ILE:HG23	1:B:326:GLU:N	2.31	0.43
1:B:379:MET:HB2	1:B:379:MET:HE3	1.69	0.43
1:D:374:MET:HE3	1:D:374:MET:HB2	1.95	0.43
1:E:34:THR:HG22	1:F:48:HIS:NE2	2.34	0.43
1:E:429:TYR:CD1	1:F:37:ALA:HA	2.54	0.43
1:H:116:VAL:HG21	1:H:122:ILE:HG23	2.01	0.43
1:J:291:LEU:HB2	1:J:379:MET:HB3	1.99	0.43
1:J:399:VAL:O	1:J:403:VAL:HG13	2.18	0.43
1:L:134:GLY:C	1:L:135:LEU:HD12	2.43	0.43
1:L:199:HIS:O	1:L:313:HIS:NE2	2.48	0.43
1:A:193:ILE:O	1:A:218:GLU:N	2.46	0.42
1:B:268:ILE:O	1:B:272:GLU:HG3	2.19	0.42
1:C:6:VAL:HG21	1:D:76:LEU:HD21	2.01	0.42
1:C:186:ALA:O	1:C:191:ALA:N	2.38	0.42
1:C:242:ASN:O	1:C:246:ILE:HG22	2.19	0.42
1:D:254:VAL:HG13	1:D:255:VAL:H	1.84	0.42
1:E:256:SER:HB3	1:F:92:SER:HB2	2.01	0.42
1:E:336:TYR:HB3	1:E:343:LEU:HD11	2.01	0.42
1:F:339:ALA:O	1:F:340:ASN:C	2.61	0.42
1:F:386:MET:HA	1:F:389:ILE:HD11	2.01	0.42
1:I:169:GLY:HA3	1:I:196:ASP:O	2.19	0.42
1:K:109:ASP:OD1	1:K:110:LYS:N	2.47	0.42
1:K:147:MET:HB2	1:K:174:PRO:HG2	2.01	0.42
1:A:226:LYS:HB3	1:A:227:THR:H	1.51	0.42
1:A:348:LEU:HG	1:A:361:GLY:HA3	2.01	0.42
1:C:225:HIS:CD2	1:C:225:HIS:H	2.36	0.42
1:D:251:PHE:HA	1:D:252:PRO:HA	1.84	0.42
1:D:330:SER:HB2	1:D:357:ASP:O	2.18	0.42
1:D:395:LYS:HA	1:D:396:PRO:HD3	1.85	0.42
1:E:22:ARG:HA	1:E:423:PHE:CE1	2.54	0.42
1:E:49:ARG:HA	1:F:31:GLU:HG3	2.00	0.42
1:G:158:ILE:HG13	1:G:166:ILE:HG12	2.01	0.42
1:H:111:LEU:HB3	1:H:137:VAL:HG13	2.01	0.42
1:H:122:ILE:H	1:H:122:ILE:HG12	1.63	0.42
1:H:283:GLN:HA	1:H:286:LYS:HB2	2.02	0.42
1:K:412:THR:HA	1:K:420:GLY:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:75:GLU:HA	1:B:78:LYS:HB2	2.01	0.42
1:C:394:GLU:OE1	1:C:395:LYS:N	2.33	0.42
1:H:105:THR:O	1:H:133:ARG:NH1	2.53	0.42
1:H:202:GLY:H	1:H:227:THR:HB	1.84	0.42
1:L:14:SER:O	1:L:17:GLN:HB3	2.19	0.42
1:L:151:ALA:HA	1:L:154:MET:HE2	2.01	0.42
1:A:27:LEU:HD13	1:A:364:LEU:HD22	2.01	0.42
1:A:72:LEU:HD22	1:A:72:LEU:HA	1.84	0.42
1:C:58:ARG:NH2	1:C:66:ILE:HG22	2.34	0.42
1:C:374:MET:SD	1:C:378:GLU:HG2	2.60	0.42
1:D:147:MET:HB2	1:D:174:PRO:HG3	2.01	0.42
1:E:39:ARG:HE	1:F:48:HIS:CE1	2.37	0.42
1:F:58:ARG:NH2	1:F:70:GLU:OE1	2.48	0.42
1:G:383:ALA:O	1:G:387:LYS:HB3	2.19	0.42
1:I:336:TYR:CD2	1:I:343:LEU:HD21	2.54	0.42
1:J:198:ALA:O	1:J:226:LYS:HB2	2.20	0.42
1:K:17:GLN:HE22	1:K:21:MET:HE2	1.85	0.42
1:K:133:ARG:HB2	1:L:132:ILE:HG23	2.01	0.42
1:K:224:THR:HG21	1:K:266:LEU:HD13	2.00	0.42
1:K:395:LYS:HB3	1:K:398:LYS:HE2	2.01	0.42
1:L:175:PHE:CZ	1:L:307:LYS:HB3	2.53	0.42
1:A:211:ASP:HA	1:A:212:PRO:HD2	1.88	0.42
1:E:121:HIS:HB2	2:E:1430:PLP:H2A2	2.01	0.42
1:F:29:ALA:HA	1:F:367:GLN:HE22	1.85	0.42
1:F:42:CYS:HA	1:F:261:HIS:HB2	2.02	0.42
1:G:298:ARG:HB3	1:G:387:LYS:HB2	2.02	0.42
1:H:152:ASP:HB3	1:L:245:LYS:HD2	2.01	0.42
1:J:11:ARG:HG3	1:J:425:TYR:OH	2.19	0.42
1:J:219:TYR:OH	1:J:242:ASN:HB3	2.20	0.42
1:K:36:LEU:HD12	1:K:420:GLY:HA3	2.01	0.42
1:L:175:PHE:CZ	1:L:307:LYS:HD3	2.53	0.42
1:L:236:ILE:HG21	1:L:246:ILE:HG12	2.00	0.42
1:A:46:PHE:HB3	1:A:260:LEU:CB	2.48	0.42
1:C:283:GLN:NE2	1:C:287:ASN:OD1	2.42	0.42
1:D:111:LEU:HD11	1:D:167:LEU:HB2	2.02	0.42
1:D:163:PRO:O	1:D:191:ALA:HB2	2.20	0.42
1:E:252:PRO:HA	1:E:255:VAL:HG22	2.02	0.42
1:E:405:GLU:O	1:E:409:GLU:HG2	2.19	0.42
1:I:18:HIS:CD2	1:J:45:ASP:HB2	2.54	0.42
1:K:55:PRO:O	1:K:57:LYS:NZ	2.52	0.42
1:K:271:ALA:HA	1:K:274:LEU:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:ALA:O	1:A:285:ILE:HG13	2.20	0.42
1:B:70:GLU:O	1:B:74:ILE:HG12	2.19	0.42
1:B:250:VAL:O	1:B:255:VAL:CB	2.61	0.42
1:C:123:SER:HA	1:C:128:SER:HB3	2.02	0.42
1:D:154:MET:O	1:D:158:ILE:HG13	2.19	0.42
1:D:238:THR:OG1	1:D:239:THR:N	2.49	0.42
1:D:307:LYS:HE3	1:D:307:LYS:HB3	1.69	0.42
1:J:92:SER:H	1:J:233:GLY:CA	2.32	0.42
1:J:130:ALA:HB1	1:J:134:GLY:HA3	2.02	0.42
1:K:132:ILE:HG21	1:L:98:LEU:HD11	2.02	0.42
1:K:245:LYS:O	1:K:249:HIS:HD2	2.03	0.42
1:A:106:LYS:H	1:A:164:LYS:HZ3	1.68	0.42
1:A:238:THR:OG1	1:A:239:THR:N	2.49	0.42
1:E:244:ASP:O	1:E:248:SER:N	2.53	0.42
1:E:344:ASN:ND2	1:F:60:TYR:HA	2.34	0.42
1:F:54:LEU:HA	1:F:54:LEU:HD23	1.50	0.42
1:F:87:ASN:OD1	1:F:90:PRO:HD3	2.20	0.42
1:H:171:SER:HB2	1:H:363:ARG:NH2	2.34	0.42
1:A:50:TYR:CE2	1:B:30:SER:HB3	2.54	0.42
1:A:115:SER:OG	1:A:117:PRO:HD2	2.19	0.42
1:A:263:LYS:HD3	1:A:263:LYS:HA	1.78	0.42
1:A:316:ILE:HA	1:A:362:ILE:O	2.20	0.42
1:B:236:ILE:HD12	1:B:246:ILE:HD11	2.01	0.42
1:E:195:TYR:HE2	1:E:210:GLN:HE21	1.66	0.42
1:H:107:PRO:O	1:I:188:GLU:HG3	2.19	0.42
1:H:218:GLU:OE2	1:H:242:ASN:ND2	2.40	0.42
1:H:322:SER:HA	1:H:323:PRO:HD3	1.77	0.42
1:I:55:PRO:HA	1:I:58:ARG:HE	1.85	0.42
1:I:110:LYS:HA	1:I:136:LYS:O	2.20	0.42
1:J:80:LEU:HD21	1:J:205:ALA:HB1	2.01	0.42
1:J:245:LYS:O	1:J:249:HIS:HD2	2.02	0.42
1:K:22:ARG:CZ	1:K:411:SER:HB3	2.49	0.42
1:K:63:CYS:HA	1:K:66:ILE:HD12	2.02	0.42
1:K:84:GLU:OE1	1:K:240:LYS:HE3	2.20	0.42
1:K:425:TYR:OH	1:L:40:GLU:OE1	2.33	0.42
1:L:389:ILE:HD11	1:L:399:VAL:HG11	2.02	0.42
1:C:330:SER:O	1:C:334:LYS:HB2	2.20	0.42
1:D:186:ALA:HA	1:D:189:VAL:HG12	2.01	0.42
1:E:381:GLU:HG2	1:E:406:PHE:CE1	2.54	0.42
1:G:125:TRP:HE3	1:G:126:LYS:HE3	1.85	0.42
1:I:320:GLU:HG3	1:I:321:SER:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:110:LYS:HE3	1:J:110:LYS:HB2	1.84	0.42
1:K:115:SER:HA	1:K:125:TRP:CZ2	2.54	0.42
1:L:39:ARG:NH1	1:L:424:LYS:O	2.53	0.42
1:L:154:MET:O	1:L:158:ILE:HG13	2.20	0.42
1:A:174:PRO:C	1:A:310:THR:OG1	2.63	0.41
1:B:149:ILE:O	1:B:178:PRO:HG3	2.19	0.41
1:B:251:PHE:CD1	1:B:252:PRO:N	2.88	0.41
1:B:332:LEU:HD23	1:B:332:LEU:HA	1.83	0.41
1:B:348:LEU:H	1:B:351:ASP:CB	2.30	0.41
1:C:388:ARG:O	1:C:394:GLU:N	2.53	0.41
1:D:171:SER:HA	1:D:199:HIS:HD2	1.85	0.41
1:E:154:MET:HE1	1:E:178:PRO:HG2	2.02	0.41
1:G:348:LEU:H	1:G:351:ASP:HB2	1.85	0.41
1:I:345:LYS:HA	1:I:362:ILE:HG22	2.02	0.41
1:J:289:LYS:NZ	1:J:308:ASP:OD1	2.43	0.41
1:J:347:LEU:HD21	1:J:354:ASN:CG	2.45	0.41
1:K:140:HIS:NE2	1:K:154:MET:SD	2.94	0.41
1:K:337:GLU:HA	1:K:342:ILE:HG13	2.02	0.41
1:L:146:GLU:HB3	1:L:307:LYS:HZ2	1.84	0.41
1:A:294:ALA:HB2	1:A:380:GLU:HG2	2.03	0.41
1:B:14:SER:O	1:B:17:GLN:HB3	2.20	0.41
1:C:64:LYS:HE3	1:C:65:TYR:CE2	2.55	0.41
1:D:107:PRO:HG3	1:D:133:ARG:NH1	2.34	0.41
1:D:348:LEU:HD13	1:D:360:SER:HB2	2.01	0.41
1:D:376:GLU:O	1:D:380:GLU:N	2.52	0.41
1:D:429:TYR:OXT	1:D:429:TYR:CD2	2.73	0.41
1:F:53:GLY:HA2	1:F:251:PHE:CD1	2.55	0.41
1:G:34:THR:HG22	1:G:229:PHE:O	2.19	0.41
1:H:227:THR:HB	1:H:228:PHE:H	1.48	0.41
1:J:77:SER:HB2	1:J:237:LEU:HD21	2.02	0.41
1:K:111:LEU:HD23	1:K:124:HIS:HB3	2.02	0.41
1:L:28:ILE:HG12	1:L:31:GLU:CD	2.45	0.41
1:L:174:PRO:HB2	1:L:175:PHE:HD1	1.85	0.41
1:A:72:LEU:HG	1:B:9:PHE:CE2	2.54	0.41
1:B:8:LYS:HB2	1:B:8:LYS:HE3	1.74	0.41
1:C:126:LYS:HA	1:C:131:GLY:HA3	2.02	0.41
1:C:232:GLN:NE2	1:D:257:ASN:OD1	2.53	0.41
1:E:15:ILE:HG12	1:E:425:TYR:CG	2.55	0.41
1:E:20:TRP:O	1:E:23:GLU:HG2	2.21	0.41
1:E:298:ARG:HG3	1:E:387:LYS:HD2	2.02	0.41
1:G:11:ARG:CZ	1:G:427:ARG:HD2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:27:LEU:HD12	1:I:364:LEU:HB3	2.01	0.41
1:J:121:HIS:HB2	1:J:171:SER:H	1.85	0.41
1:K:129:ALA:C	1:K:131:GLY:H	2.28	0.41
1:A:114:LEU:HD12	1:A:118:ASP:O	2.20	0.41
1:A:274:LEU:HD13	1:B:3:TYR:HE1	1.85	0.41
1:A:388:ARG:O	1:A:393:LYS:N	2.54	0.41
1:B:129:ALA:O	1:B:130:ALA:HB3	2.20	0.41
1:B:146:GLU:HA	1:B:304:CYS:SG	2.60	0.41
1:B:426:LEU:HD12	1:B:426:LEU:HA	1.89	0.41
1:C:33:ILE:HG13	1:D:48:HIS:CE1	2.55	0.41
1:E:17:GLN:HE21	1:E:17:GLN:HB2	1.64	0.41
1:F:23:GLU:O	1:F:340:ASN:OD1	2.38	0.41
1:F:226:LYS:HD3	1:F:226:LYS:HA	1.93	0.41
1:G:154:MET:HB3	1:G:154:MET:HE2	1.81	0.41
1:I:413:ILE:N	1:I:420:GLY:O	2.52	0.41
1:J:51:ALA:HB3	1:J:258:HIS:NE2	2.35	0.41
1:A:40:GLU:HB2	1:B:428:PHE:HB2	2.02	0.41
1:A:317:ILE:HB	1:A:362:ILE:HB	2.03	0.41
1:B:118:ASP:HB3	1:B:142:PHE:CE1	2.55	0.41
1:B:251:PHE:HD1	1:B:252:PRO:HG3	1.85	0.41
1:E:95:VAL:O	1:E:254:VAL:HG11	2.21	0.41
1:E:111:LEU:O	1:E:138:ILE:N	2.49	0.41
1:E:388:ARG:HH21	1:E:399:VAL:HG22	1.85	0.41
1:E:428:PHE:CG	1:F:40:GLU:HB2	2.56	0.41
1:G:103:ALA:HA	1:G:249:HIS:ND1	2.35	0.41
1:H:180:ALA:HB3	1:L:106:LYS:NZ	2.34	0.41
1:A:34:THR:HG22	1:A:229:PHE:O	2.21	0.41
1:B:26:LYS:HD3	1:B:368:GLU:CG	2.50	0.41
1:C:90:PRO:HG2	1:C:236:ILE:HG13	2.01	0.41
1:D:110:LYS:HD2	1:D:138:ILE:HD11	2.03	0.41
1:E:256:SER:HA	2:F:1430:PLP:O1P	2.19	0.41
1:F:198:ALA:C	1:F:226:LYS:HG3	2.45	0.41
1:G:65:TYR:O	1:G:68:GLU:HB2	2.20	0.41
1:H:117:PRO:HB3	1:H:354:ASN:OD1	2.20	0.41
1:I:38:VAL:HG11	1:I:231:PRO:HD3	2.03	0.41
1:J:130:ALA:O	1:J:134:GLY:N	2.53	0.41
1:A:204:ILE:HD12	1:A:210:GLN:O	2.20	0.41
1:B:92:SER:HB3	1:B:95:VAL:HG23	2.02	0.41
1:B:121:HIS:ND1	1:B:123:SER:OG	2.40	0.41
1:B:148:ASN:OD1	1:B:178:PRO:HD3	2.21	0.41
1:B:154:MET:SD	1:B:182:ALA:HB2	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:376:GLU:HA	1:B:379:MET:HE2	2.01	0.41
1:D:173:PHE:HZ	1:D:177:HIS:CE1	2.39	0.41
1:G:52:GLU:HG3	1:G:59:LEU:HD13	2.01	0.41
1:G:149:ILE:HD11	1:G:154:MET:SD	2.60	0.41
1:G:352:ASP:OD1	1:G:352:ASP:N	2.52	0.41
1:H:211:ASP:O	1:H:215:GLU:HB2	2.20	0.41
1:I:208:GLN:HG3	1:I:209:PHE:H	1.85	0.41
1:I:300:PHE:CD1	1:I:325:ILE:HD11	2.56	0.41
1:K:119:GLY:HA2	1:K:172:LEU:HB2	2.01	0.41
1:L:322:SER:HB3	1:L:325:ILE:HG12	2.02	0.41
1:A:337:GLU:HG3	1:B:61:GLN:HB3	2.02	0.41
1:B:174:PRO:HB3	1:B:316:ILE:HD11	2.02	0.41
1:C:59:LEU:O	1:C:60:TYR:HB2	2.19	0.41
1:C:194:ALA:HB1	1:C:221:MET:HE2	2.02	0.41
1:C:225:HIS:HE1	1:D:50:TYR:HE2	1.69	0.41
1:D:34:THR:HG23	1:D:39:ARG:CG	2.48	0.41
1:E:282:LYS:O	1:E:286:LYS:HD3	2.21	0.41
1:F:35:SER:O	1:F:39:ARG:HG3	2.20	0.41
1:G:10:ILE:H	1:G:10:ILE:HG12	1.54	0.41
1:G:63:CYS:C	1:G:64:LYS:HD2	2.45	0.41
1:G:64:LYS:O	1:G:68:GLU:HG3	2.20	0.41
1:G:97:ASN:HA	1:G:221:MET:HE2	2.03	0.41
1:H:101:PHE:CE1	1:H:167:LEU:HD11	2.56	0.41
1:H:302:VAL:HG22	1:H:317:ILE:HG22	2.02	0.41
1:H:339:ALA:HB2	1:H:396:PRO:HB3	2.03	0.41
1:H:388:ARG:HB3	1:H:394:GLU:OE1	2.20	0.41
1:I:47:MET:HG2	1:I:261:HIS:HB3	2.03	0.41
1:I:107:PRO:HD3	1:I:133:ARG:NH2	2.36	0.41
1:J:175:PHE:CD2	1:J:176:PRO:HD2	2.56	0.41
1:J:329:ALA:O	1:J:362:ILE:HD11	2.20	0.41
1:K:168:PHE:CD2	1:K:179:VAL:HG12	2.55	0.41
1:A:5:ASP:N	1:A:5:ASP:OD1	2.54	0.41
1:B:21:MET:O	1:B:26:LYS:NZ	2.45	0.41
1:B:30:SER:HA	1:B:226:LYS:HD2	2.02	0.41
1:B:125:TRP:O	1:B:128:SER:HB3	2.21	0.41
1:B:280:TYR:HA	1:B:415:TYR:CZ	2.56	0.41
1:B:287:ASN:HA	1:B:379:MET:HE1	2.02	0.41
1:B:319:ILE:HD12	1:B:319:ILE:HA	1.99	0.41
1:B:389:ILE:HD11	1:B:399:VAL:HG21	2.03	0.41
1:C:18:HIS:HE1	1:C:39:ARG:NH2	2.19	0.41
1:C:28:ILE:HG22	1:C:30:SER:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:66:ILE:HG21	1:D:260:LEU:HD13	2.02	0.41
1:D:300:PHE:HE1	1:D:387:LYS:HA	1.85	0.41
1:D:371:ARG:NH1	1:D:413:ILE:HG12	2.35	0.41
1:E:105:THR:OG1	1:E:133:ARG:NH1	2.54	0.41
1:E:155:VAL:O	1:E:159:LEU:HG	2.21	0.41
1:E:198:ALA:HB3	2:E:1430:PLP:C2	2.50	0.41
1:F:54:LEU:O	1:F:58:ARG:NH2	2.53	0.41
1:G:201:LEU:O	1:G:204:ILE:HB	2.21	0.41
1:H:112:MET:HB3	1:H:166:ILE:HA	2.02	0.41
1:H:129:ALA:C	1:H:131:GLY:H	2.29	0.41
1:H:150:ASP:HB2	1:H:153:ALA:HB3	2.03	0.41
1:H:424:LYS:HE3	1:H:426:LEU:HD11	2.02	0.41
1:I:48:HIS:HD2	1:J:34:THR:H	1.66	0.41
1:I:168:PHE:CE2	1:I:179:VAL:HA	2.55	0.41
1:J:57:LYS:HE3	1:J:57:LYS:HB3	1.87	0.41
1:J:110:LYS:HB2	1:J:163:PRO:HA	2.03	0.41
1:K:319:ILE:HD13	1:K:362:ILE:HG13	2.03	0.41
1:K:336:TYR:CD1	1:K:389:ILE:HD12	2.56	0.41
1:L:123:SER:O	1:L:130:ALA:HB2	2.20	0.41
1:L:168:PHE:CE2	1:L:179:VAL:HA	2.56	0.41
1:A:274:LEU:HD13	1:B:3:TYR:CE1	2.56	0.41
1:A:295:LEU:HG	1:A:300:PHE:CD2	2.53	0.41
1:C:146:GLU:HG3	1:C:306:HIS:HE1	1.86	0.41
1:D:84:GLU:HB3	1:D:240:LYS:HG2	2.03	0.41
1:E:72:LEU:HD22	1:E:76:LEU:HD22	2.03	0.41
1:F:369:CYS:HB3	1:F:374:MET:HG3	2.01	0.41
1:G:40:GLU:HB2	1:H:428:PHE:HB2	2.03	0.41
1:G:214:ARG:H	1:G:214:ARG:HG2	1.49	0.41
1:G:227:THR:HG23	1:G:228:PHE:N	2.32	0.41
1:G:330:SER:HA	1:G:345:LYS:HD3	2.03	0.41
1:H:113:ALA:O	1:H:139:ASN:HA	2.21	0.41
1:H:150:ASP:O	1:H:154:MET:HB2	2.21	0.41
1:H:193:ILE:O	1:H:218:GLU:N	2.54	0.41
1:H:286:LYS:HB3	1:H:376:GLU:OE2	2.21	0.41
1:I:347:LEU:HD12	1:I:359:PRO:HB3	2.02	0.41
1:J:115:SER:OG	1:J:118:ASP:HB2	2.21	0.41
1:L:25:ILE:HG13	1:L:341:ILE:HG23	2.03	0.41
1:L:115:SER:OG	1:L:117:PRO:HD2	2.20	0.41
1:L:336:TYR:HB3	1:L:341:ILE:HB	2.02	0.41
1:A:28:ILE:H	1:A:28:ILE:HG12	1.63	0.40
1:A:110:LYS:HE2	1:A:110:LYS:HB2	1.80	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:LEU:HD11	1:C:190:GLY:HA2	2.03	0.40
1:C:40:GLU:CD	1:D:427:ARG:HA	2.46	0.40
1:C:229:PHE:CD2	1:C:371:ARG:HD3	2.55	0.40
1:E:60:TYR:HD1	1:E:60:TYR:HA	1.67	0.40
1:E:174:PRO:HA	1:E:312:SER:HB3	2.02	0.40
1:F:103:ALA:HA	1:F:249:HIS:CD2	2.56	0.40
1:F:381:GLU:O	1:F:384:GLU:HB3	2.20	0.40
1:J:214:ARG:N	1:J:214:ARG:HD2	2.37	0.40
1:L:30:SER:OG	1:L:363:ARG:NH2	2.54	0.40
1:L:87:ASN:ND2	1:L:247:ASP:OD1	2.54	0.40
1:A:87:ASN:HB3	1:A:236:ILE:HB	2.04	0.40
1:A:108:GLY:H	1:A:134:GLY:HA2	1.85	0.40
1:A:110:LYS:HE3	1:A:161:GLU:O	2.21	0.40
1:A:129:ALA:HA	1:A:132:ILE:HG13	2.03	0.40
1:A:131:GLY:O	1:B:133:ARG:NH1	2.53	0.40
1:C:114:LEU:HD23	1:C:114:LEU:HA	1.91	0.40
1:D:110:LYS:NZ	1:D:161:GLU:HB3	2.36	0.40
1:E:6:VAL:O	1:E:10:ILE:HG13	2.21	0.40
1:G:116:VAL:HG22	1:G:125:TRP:CD1	2.57	0.40
1:H:70:GLU:O	1:H:74:ILE:HG13	2.21	0.40
1:H:81:PHE:CZ	1:H:205:ALA:HB2	2.56	0.40
1:H:123:SER:N	1:H:128:SER:OG	2.54	0.40
1:H:143:ASP:HA	1:H:144:PRO:HD3	1.81	0.40
1:H:322:SER:HB3	1:H:325:ILE:HD13	2.04	0.40
1:J:385:PHE:HD1	1:J:388:ARG:HD2	1.84	0.40
1:L:46:PHE:HB3	1:L:260:LEU:HB3	2.03	0.40
1:L:395:LYS:HA	1:L:396:PRO:HD3	1.82	0.40
1:A:184:GLU:O	1:A:188:GLU:HG3	2.22	0.40
1:A:291:LEU:HB2	1:A:379:MET:HB3	2.03	0.40
1:B:240:LYS:HB2	1:B:240:LYS:HE3	1.85	0.40
1:C:102:PHE:HA	1:C:133:ARG:HG2	2.03	0.40
1:C:297:GLU:HG3	1:C:298:ARG:NH1	2.37	0.40
1:F:37:ALA:HB1	1:F:268:ILE:HD13	2.02	0.40
1:F:204:ILE:HG23	1:F:212:PRO:HD2	2.02	0.40
1:G:91:THR:O	1:G:233:GLY:HA2	2.22	0.40
1:H:103:ALA:HA	1:H:249:HIS:CD2	2.56	0.40
1:H:228:PHE:HA	1:H:273:MET:HE3	2.03	0.40
1:J:56:GLY:H	1:J:67:ASP:CG	2.29	0.40
1:J:147:MET:HE2	1:J:174:PRO:HG3	2.04	0.40
1:K:196:ASP:OD2	2:K:1430:PLP:H2A3	2.22	0.40
1:L:295:LEU:O	1:L:300:PHE:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:184:GLU:H	1:B:184:GLU:HG2	1.71	0.40
1:B:305:GLU:OE1	1:B:305:GLU:N	2.52	0.40
1:C:87:ASN:OD1	1:C:90:PRO:HD3	2.21	0.40
1:C:386:MET:HB3	1:C:386:MET:HE3	1.85	0.40
1:D:229:PHE:CD2	1:D:273:MET:HE2	2.56	0.40
1:D:353:VAL:HG13	1:D:354:ASN:N	2.36	0.40
1:E:21:MET:HE3	1:F:49:ARG:HD3	2.04	0.40
1:E:356:SER:HB3	1:E:358:ASN:H	1.84	0.40
2:E:1430:PLP:O3P	1:F:50:TYR:OH	2.39	0.40
1:F:125:TRP:O	1:F:130:ALA:HB3	2.21	0.40
1:G:54:LEU:HD12	1:G:55:PRO:CD	2.51	0.40
1:H:24:SER:HA	1:H:340:ASN:HB3	2.03	0.40
1:H:91:THR:O	1:H:233:GLY:HA2	2.21	0.40
1:H:258:HIS:O	1:H:263:LYS:NZ	2.48	0.40
1:I:328:SER:OG	1:I:358:ASN:OD1	2.38	0.40
1:J:14:SER:O	1:J:18:HIS:HD2	2.04	0.40
1:J:108:GLY:N	1:J:135:LEU:HD12	2.36	0.40
1:J:395:LYS:HA	1:J:396:PRO:HD3	1.94	0.40
1:K:114:LEU:HD23	1:K:140:HIS:HB3	2.03	0.40
1:K:135:LEU:HD23	1:K:136:LYS:HE2	2.03	0.40
1:L:225:HIS:CE1	1:L:233:GLY:H	2.40	0.40
1:L:303:LEU:HB2	1:L:316:ILE:O	2.22	0.40
1:A:427:ARG:NH1	1:A:429:TYR:OXT	2.50	0.40
1:D:157:LYS:HG3	1:D:161:GLU:HG3	2.04	0.40
1:E:149:ILE:HD12	1:E:168:PHE:HE1	1.85	0.40
1:E:305:GLU:HA	1:E:309:PHE:CE1	2.57	0.40
1:H:89:GLN:HE21	1:H:258:HIS:CE1	2.40	0.40
1:I:51:ALA:O	1:I:58:ARG:HD2	2.22	0.40
1:I:55:PRO:HB3	1:I:67:ASP:HB3	2.03	0.40
1:I:105:THR:HG23	1:I:109:ASP:CB	2.50	0.40
1:I:169:GLY:H	1:I:177:HIS:HD2	1.68	0.40
1:I:413:ILE:HG22	1:I:420:GLY:O	2.21	0.40
1:J:45:ASP:O	1:J:48:HIS:ND1	2.49	0.40
1:J:175:PHE:CZ	1:J:307:LYS:HB3	2.57	0.40
1:J:336:TYR:CD2	1:J:343:LEU:HD21	2.56	0.40
1:J:398:LYS:HA	1:J:398:LYS:HD2	1.86	0.40
1:K:340:ASN:CG	1:K:400:ARG:HD3	2.47	0.40
1:L:284:VAL:HG22	1:L:370:THR:HG21	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	422/429 (98%)	391 (93%)	28 (7%)	3 (1%)	18	53
1	B	418/429 (97%)	382 (91%)	32 (8%)	4 (1%)	12	45
1	C	414/429 (96%)	375 (91%)	38 (9%)	1 (0%)	43	76
1	D	421/429 (98%)	375 (89%)	44 (10%)	2 (0%)	24	60
1	E	425/429 (99%)	380 (89%)	43 (10%)	2 (0%)	24	60
1	F	412/429 (96%)	368 (89%)	38 (9%)	6 (2%)	8	35
1	G	427/429 (100%)	394 (92%)	33 (8%)	0	100	100
1	H	423/429 (99%)	378 (89%)	44 (10%)	1 (0%)	43	76
1	I	425/429 (99%)	398 (94%)	26 (6%)	1 (0%)	43	76
1	J	427/429 (100%)	383 (90%)	41 (10%)	3 (1%)	18	53
1	K	416/429 (97%)	377 (91%)	38 (9%)	1 (0%)	43	76
1	L	410/429 (96%)	368 (90%)	40 (10%)	2 (0%)	24	60
All	All	5040/5148 (98%)	4569 (91%)	445 (9%)	26 (0%)	24	60

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	127	VAL
1	B	127	VAL
1	C	127	VAL
1	F	54	LEU
1	F	127	VAL
1	H	127	VAL
1	I	127	VAL
1	J	127	VAL
1	A	226	LYS
1	B	251	PHE
1	E	255	VAL
1	F	252	PRO

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Mol	Chain	Res	Type
1	L	55	PRO
1	A	256	SER
1	B	351	ASP
1	D	255	VAL
1	E	243	ALA
1	F	226	LYS
1	D	133	ARG
1	F	162	LYS
1	B	253	GLY
1	J	353	VAL
1	J	254	VAL
1	L	251	PHE
1	F	254	VAL
1	K	127	VAL

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	357/359 (99%)	326 (91%)	31 (9%)	9	35
1	B	355/359 (99%)	335 (94%)	20 (6%)	19	52
1	C	350/359 (98%)	324 (93%)	26 (7%)	13	42
1	D	356/359 (99%)	328 (92%)	28 (8%)	11	39
1	E	357/359 (99%)	327 (92%)	30 (8%)	10	37
1	F	348/359 (97%)	317 (91%)	31 (9%)	9	34
1	G	359/359 (100%)	328 (91%)	31 (9%)	10	36
1	H	357/359 (99%)	328 (92%)	29 (8%)	11	38
1	I	357/359 (99%)	336 (94%)	21 (6%)	18	50
1	J	359/359 (100%)	328 (91%)	31 (9%)	10	36
1	K	352/359 (98%)	315 (90%)	37 (10%)	6	27
1	L	350/359 (98%)	303 (87%)	47 (13%)	4	18
All	All	4257/4308 (99%)	3895 (92%)	362 (8%)	10	36

All (362) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	LYS
1	A	28	ILE
1	A	47	MET
1	A	49	ARG
1	A	72	LEU
1	A	95	VAL
1	A	98	LEU
1	A	106	LYS
1	A	110	LYS
1	A	121	HIS
1	A	122	ILE
1	A	127	VAL
1	A	137	VAL
1	A	152	ASP
1	A	156	LYS
1	A	226	LYS
1	A	255	VAL
1	A	258	HIS
1	A	295	LEU
1	A	310	THR
1	A	311	GLU
1	A	326	GLU
1	A	337	GLU
1	A	343	LEU
1	A	346	ASN
1	A	352	ASP
1	A	368	GLU
1	A	374	MET
1	A	395	LYS
1	A	413	ILE
1	A	414	HIS
1	B	1	MET
1	B	5	ASP
1	B	26	LYS
1	B	47	MET
1	B	54	LEU
1	B	106	LYS
1	B	127	VAL
1	B	135	LEU
1	B	138	ILE
1	B	148	ASN
1	B	207	LYS

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Mol	Chain	Res	Type
1	B	237	LEU
1	B	256	SER
1	B	258	HIS
1	B	285	ILE
1	B	303	LEU
1	B	316	ILE
1	B	322	SER
1	B	355	ASN
1	B	381	GLU
1	C	5	ASP
1	C	8	LYS
1	C	21	MET
1	C	54	LEU
1	C	57	LYS
1	C	59	LEU
1	C	69	VAL
1	C	105	THR
1	C	116	VAL
1	C	127	VAL
1	C	164	LYS
1	C	184	GLU
1	C	189	VAL
1	C	227	THR
1	C	263	LYS
1	C	268	ILE
1	C	303	LEU
1	C	313	HIS
1	C	353	VAL
1	C	374	MET
1	C	382	ILE
1	C	386	MET
1	C	394	GLU
1	C	397	GLU
1	C	412	THR
1	C	413	ILE
1	D	5	ASP
1	D	33	ILE
1	D	52	GLU
1	D	60	TYR
1	D	98	LEU
1	D	135	LEU
1	D	136	LYS

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Mol	Chain	Res	Type
1	D	159	LEU
1	D	160	GLU
1	D	173	PHE
1	D	177	HIS
1	D	189	VAL
1	D	199	HIS
1	D	214	ARG
1	D	226	LYS
1	D	241	GLU
1	D	254	VAL
1	D	285	ILE
1	D	307	LYS
1	D	324	ASP
1	D	325	ILE
1	D	343	LEU
1	D	354	ASN
1	D	362	ILE
1	D	367	GLN
1	D	394	GLU
1	D	418	ASP
1	D	427	ARG
1	E	6	VAL
1	E	11	ARG
1	E	12	ASP
1	E	17	GLN
1	E	26	LYS
1	E	49	ARG
1	E	59	LEU
1	E	60	TYR
1	E	98	LEU
1	E	140	HIS
1	E	148	ASN
1	E	157	LYS
1	E	183	TYR
1	E	188	GLU
1	E	199	HIS
1	E	215	GLU
1	E	226	LYS
1	E	256	SER
1	E	315	VAL
1	E	325	ILE
1	E	336	TYR

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Mol	Chain	Res	Type
1	E	343	LEU
1	E	346	ASN
1	E	354	ASN
1	E	355	ASN
1	E	362	ILE
1	E	363	ARG
1	E	377	LYS
1	E	385	PHE
1	E	428	PHE
1	F	11	ARG
1	F	19	GLU
1	F	28	ILE
1	F	38	VAL
1	F	47	MET
1	F	57	LYS
1	F	64	LYS
1	F	68	GLU
1	F	69	VAL
1	F	105	THR
1	F	106	LYS
1	F	127	VAL
1	F	135	LEU
1	F	137	VAL
1	F	148	ASN
1	F	161	GLU
1	F	162	LYS
1	F	199	HIS
1	F	207	LYS
1	F	209	PHE
1	F	227	THR
1	F	232	GLN
1	F	307	LYS
1	F	331	GLU
1	F	342	ILE
1	F	343	LEU
1	F	350	TRP
1	F	352	ASP
1	F	380	GLU
1	F	389	ILE
1	F	413	ILE
1	G	10	ILE
1	G	36	LEU

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Mol	Chain	Res	Type
1	G	48	HIS
1	G	52	GLU
1	G	66	ILE
1	G	106	LYS
1	G	116	VAL
1	G	122	ILE
1	G	128	SER
1	G	138	ILE
1	G	149	ILE
1	G	158	ILE
1	G	179	VAL
1	G	181	ASP
1	G	214	ARG
1	G	221	MET
1	G	223	SER
1	G	226	LYS
1	G	229	PHE
1	G	237	LEU
1	G	254	VAL
1	G	256	SER
1	G	258	HIS
1	G	305	GLU
1	G	306	HIS
1	G	325	ILE
1	G	367	GLN
1	G	369	CYS
1	G	377	LYS
1	G	398	LYS
1	G	413	ILE
1	H	10	ILE
1	H	15	ILE
1	H	26	LYS
1	H	45	ASP
1	H	48	HIS
1	H	49	ARG
1	H	59	LEU
1	H	91	THR
1	H	98	LEU
1	H	122	ILE
1	H	127	VAL
1	H	155	VAL
1	H	179	VAL

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Mol	Chain	Res	Type
1	H	188	GLU
1	H	215	GLU
1	H	221	MET
1	H	223	SER
1	H	226	LYS
1	H	227	THR
1	H	239	THR
1	H	244	ASP
1	H	275	GLU
1	H	347	LEU
1	H	355	ASN
1	H	358	ASN
1	H	362	ILE
1	H	371	ARG
1	H	377	LYS
1	H	413	ILE
1	I	13	VAL
1	I	95	VAL
1	I	106	LYS
1	I	122	ILE
1	I	147	MET
1	I	175	PHE
1	I	209	PHE
1	I	226	LYS
1	I	236	ILE
1	I	255	VAL
1	I	258	HIS
1	I	263	LYS
1	I	330	SER
1	I	337	GLU
1	I	346	ASN
1	I	353	VAL
1	I	357	ASP
1	I	399	VAL
1	I	410	TYR
1	I	418	ASP
1	I	426	LEU
1	J	13	VAL
1	J	16	LYS
1	J	52	GLU
1	J	69	VAL
1	J	110	LYS

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Mol	Chain	Res	Type
1	J	115	SER
1	J	126	LYS
1	J	127	VAL
1	J	137	VAL
1	J	140	HIS
1	J	184	GLU
1	J	229	PHE
1	J	235	VAL
1	J	237	LEU
1	J	250	VAL
1	J	255	VAL
1	J	295	LEU
1	J	298	ARG
1	J	307	LYS
1	J	316	ILE
1	J	328	SER
1	J	343	LEU
1	J	347	LEU
1	J	348	LEU
1	J	354	ASN
1	J	366	THR
1	J	367	GLN
1	J	371	ARG
1	J	391	ILE
1	J	411	SER
1	J	427	ARG
1	K	6	VAL
1	K	25	ILE
1	K	26	LYS
1	K	27	LEU
1	K	33	ILE
1	K	39	ARG
1	K	52	GLU
1	K	72	LEU
1	K	106	LYS
1	K	116	VAL
1	K	122	ILE
1	K	140	HIS
1	K	161	GLU
1	K	166	ILE
1	K	173	PHE
1	K	192	LYS

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Mol	Chain	Res	Type
1	K	199	HIS
1	K	220	LEU
1	K	221	MET
1	K	226	LYS
1	K	232	GLN
1	K	274	LEU
1	K	306	HIS
1	K	311	GLU
1	K	338	GLU
1	K	343	LEU
1	K	352	ASP
1	K	364	LEU
1	K	376	GLU
1	K	379	MET
1	K	393	LYS
1	K	397	GLU
1	K	400	ARG
1	K	401	GLU
1	K	402	ASP
1	K	408	LYS
1	K	410	TYR
1	L	12	ASP
1	L	26	LYS
1	L	28	ILE
1	L	52	GLU
1	L	54	LEU
1	L	57	LYS
1	L	58	ARG
1	L	61	GLN
1	L	63	CYS
1	L	76	LEU
1	L	104	GLU
1	L	137	VAL
1	L	165	LEU
1	L	181	ASP
1	L	189	VAL
1	L	192	LYS
1	L	193	ILE
1	L	199	HIS
1	L	200	VAL
1	L	214	ARG
1	L	221	MET

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Mol	Chain	Res	Type
1	L	225	HIS
1	L	226	LYS
1	L	228	PHE
1	L	229	PHE
1	L	232	GLN
1	L	237	LEU
1	L	250	VAL
1	L	278	GLU
1	L	291	LEU
1	L	300	PHE
1	L	305	GLU
1	L	316	ILE
1	L	319	ILE
1	L	325	ILE
1	L	331	GLU
1	L	345	LYS
1	L	346	ASN
1	L	347	LEU
1	L	350	TRP
1	L	362	ILE
1	L	375	LYS
1	L	378	GLU
1	L	397	GLU
1	L	404	LYS
1	L	419	GLU
1	L	428	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	HIS
1	A	199	HIS
1	A	232	GLN
1	A	242	ASN
1	B	87	ASN
1	B	89	GLN
1	B	262	HIS
1	B	301	ASN
1	B	340	ASN
1	B	355	ASN
1	B	414	HIS
1	C	17	GLN

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Mol	Chain	Res	Type
1	C	199	HIS
1	C	225	HIS
1	C	313	HIS
1	D	140	HIS
1	D	301	ASN
1	D	367	GLN
1	D	414	HIS
1	E	48	HIS
1	E	89	GLN
1	E	242	ASN
1	E	261	HIS
1	E	262	HIS
1	E	344	ASN
1	F	283	GLN
1	F	340	ASN
1	F	414	HIS
1	G	32	ASN
1	G	210	GLN
1	G	258	HIS
1	G	358	ASN
1	G	367	GLN
1	H	87	ASN
1	H	89	GLN
1	H	199	HIS
1	H	259	HIS
1	I	17	GLN
1	I	18	HIS
1	J	140	HIS
1	J	187	GLN
1	J	257	ASN
1	J	340	ASN
1	J	367	GLN
1	K	89	GLN
1	K	97	ASN
1	K	210	GLN
1	K	301	ASN
1	K	344	ASN
1	L	208	GLN
1	L	225	HIS
1	L	262	HIS
1	L	358	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

12 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	PLP	B	1430	1	15,15,16	1.05	1 (6%)	21,22,23	1.61	2 (9%)
2	PLP	A	1430	1	15,15,16	1.06	2 (13%)	21,22,23	1.45	3 (14%)
2	PLP	F	1430	1	15,15,16	1.01	1 (6%)	21,22,23	1.67	2 (9%)
2	PLP	H	1430	1	15,15,16	1.00	1 (6%)	21,22,23	1.44	2 (9%)
2	PLP	J	1430	1	15,15,16	1.03	2 (13%)	21,22,23	1.58	2 (9%)
2	PLP	I	1430	1	15,15,16	1.04	1 (6%)	21,22,23	1.65	2 (9%)
2	PLP	G	1430	1	15,15,16	1.03	1 (6%)	21,22,23	1.58	2 (9%)
2	PLP	L	1430	1	15,15,16	1.01	1 (6%)	21,22,23	1.62	2 (9%)
2	PLP	D	1430	1	15,15,16	1.12	1 (6%)	21,22,23	1.72	3 (14%)
2	PLP	E	1430	1	15,15,16	1.17	1 (6%)	21,22,23	2.28	4 (19%)
2	PLP	K	1430	1	15,15,16	1.03	2 (13%)	21,22,23	1.48	2 (9%)
2	PLP	C	1430	1	15,15,16	1.01	1 (6%)	21,22,23	1.81	2 (9%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.
'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PLP	B	1430	1	-	3/6/6/8	0/1/1/1
2	PLP	A	1430	1	-	0/6/6/8	0/1/1/1
2	PLP	F	1430	1	-	1/6/6/8	0/1/1/1
2	PLP	H	1430	1	-	3/6/6/8	0/1/1/1
2	PLP	J	1430	1	-	2/6/6/8	0/1/1/1
2	PLP	I	1430	1	-	3/6/6/8	0/1/1/1
2	PLP	G	1430	1	-	2/6/6/8	0/1/1/1
2	PLP	L	1430	1	-	3/6/6/8	0/1/1/1
2	PLP	D	1430	1	-	0/6/6/8	0/1/1/1
2	PLP	E	1430	1	-	2/6/6/8	0/1/1/1
2	PLP	K	1430	1	-	3/6/6/8	0/1/1/1
2	PLP	C	1430	1	-	4/6/6/8	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1430	PLP	C3-C2	-3.15	1.37	1.41
2	E	1430	PLP	C3-C2	-3.07	1.37	1.41
2	K	1430	PLP	C3-C2	-2.65	1.38	1.41
2	B	1430	PLP	C3-C2	-2.60	1.38	1.41
2	G	1430	PLP	C3-C2	-2.59	1.38	1.41
2	A	1430	PLP	C3-C2	-2.59	1.38	1.41
2	J	1430	PLP	C3-C2	-2.59	1.38	1.41
2	I	1430	PLP	C3-C2	-2.55	1.38	1.41
2	F	1430	PLP	C3-C2	-2.37	1.38	1.41
2	L	1430	PLP	C3-C2	-2.35	1.38	1.41
2	C	1430	PLP	C3-C2	-2.33	1.38	1.41
2	H	1430	PLP	C3-C2	-2.28	1.38	1.41
2	A	1430	PLP	O4P-C5A	-2.15	1.37	1.44
2	J	1430	PLP	O4P-C5A	-2.01	1.37	1.44
2	K	1430	PLP	O4P-C5A	-2.01	1.37	1.44

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1430	PLP	O4P-C5A-C5	6.98	122.44	109.36
2	C	1430	PLP	O4P-C5A-C5	6.58	121.68	109.36
2	F	1430	PLP	O4P-C5A-C5	6.02	120.64	109.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1430	PLP	C4A-C4-C5	5.71	126.83	120.94
2	D	1430	PLP	O4P-C5A-C5	5.67	119.98	109.36
2	I	1430	PLP	O4P-C5A-C5	5.45	119.57	109.36
2	J	1430	PLP	O4P-C5A-C5	5.44	119.55	109.36
2	L	1430	PLP	O4P-C5A-C5	5.25	119.20	109.36
2	B	1430	PLP	O4P-C5A-C5	5.20	119.10	109.36
2	H	1430	PLP	O4P-C5A-C5	4.87	118.48	109.36
2	K	1430	PLP	O4P-C5A-C5	4.86	118.47	109.36
2	G	1430	PLP	O4P-C5A-C5	4.84	118.43	109.36
2	A	1430	PLP	O4P-C5A-C5	4.56	117.90	109.36
2	L	1430	PLP	C4A-C4-C5	3.37	124.41	120.94
2	D	1430	PLP	C4A-C4-C5	3.24	124.28	120.94
2	I	1430	PLP	C4A-C4-C5	3.21	124.25	120.94
2	G	1430	PLP	C4A-C4-C5	3.08	124.12	120.94
2	E	1430	PLP	C4A-C4-C3	-2.97	115.56	120.52
2	K	1430	PLP	C4A-C4-C5	2.95	123.98	120.94
2	B	1430	PLP	C4A-C4-C5	2.94	123.97	120.94
2	C	1430	PLP	C4A-C4-C5	2.84	123.87	120.94
2	F	1430	PLP	C4A-C4-C5	2.72	123.74	120.94
2	H	1430	PLP	C4A-C4-C5	2.43	123.44	120.94
2	A	1430	PLP	C5-C6-N1	-2.24	120.19	123.83
2	A	1430	PLP	C6-C5-C4	2.14	119.85	118.10
2	E	1430	PLP	C5A-C5-C6	-2.11	115.93	119.36
2	J	1430	PLP	C5-C6-N1	-2.10	120.42	123.83
2	D	1430	PLP	C2A-C2-C3	-2.06	118.39	120.80

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1430	PLP	C5A-O4P-P-O2P
2	B	1430	PLP	C5A-O4P-P-O3P
2	C	1430	PLP	C4-C5-C5A-O4P
2	C	1430	PLP	C6-C5-C5A-O4P
2	C	1430	PLP	C5A-O4P-P-O2P
2	C	1430	PLP	C5A-O4P-P-O3P
2	E	1430	PLP	C4-C5-C5A-O4P
2	E	1430	PLP	C6-C5-C5A-O4P
2	G	1430	PLP	C5A-O4P-P-O2P
2	G	1430	PLP	C5A-O4P-P-O3P
2	H	1430	PLP	C5A-O4P-P-O2P
2	H	1430	PLP	C5A-O4P-P-O3P

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Mol	Chain	Res	Type	Atoms
2	I	1430	PLP	C5A-O4P-P-O2P
2	I	1430	PLP	C5A-O4P-P-O3P
2	J	1430	PLP	C5A-O4P-P-O1P
2	K	1430	PLP	C5A-O4P-P-O1P
2	K	1430	PLP	C5A-O4P-P-O2P
2	K	1430	PLP	C5A-O4P-P-O3P
2	L	1430	PLP	C5A-O4P-P-O2P
2	B	1430	PLP	C5A-O4P-P-O1P
2	H	1430	PLP	C5A-O4P-P-O1P
2	I	1430	PLP	C5A-O4P-P-O1P
2	L	1430	PLP	C5A-O4P-P-O3P
2	L	1430	PLP	C5A-O4P-P-O1P
2	F	1430	PLP	C5A-O4P-P-O2P
2	J	1430	PLP	C5A-O4P-P-O2P

There are no ring outliers.

8 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1430	PLP	1	0
2	A	1430	PLP	2	0
2	F	1430	PLP	2	0
2	J	1430	PLP	1	0
2	G	1430	PLP	2	0
2	E	1430	PLP	3	0
2	K	1430	PLP	1	0
2	C	1430	PLP	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	426/429 (99%)	-1.72	0 100 100	30, 45, 66, 73	0
1	B	424/429 (98%)	-1.71	0 100 100	31, 47, 68, 80	0
1	C	420/429 (97%)	-1.69	0 100 100	34, 52, 67, 79	0
1	D	425/429 (99%)	-1.60	0 100 100	33, 61, 78, 85	0
1	E	427/429 (99%)	-1.64	0 100 100	40, 62, 80, 95	0
1	F	418/429 (97%)	-1.64	0 100 100	43, 62, 76, 93	0
1	G	429/429 (100%)	-1.72	0 100 100	30, 45, 61, 71	0
1	H	427/429 (99%)	-1.70	0 100 100	29, 47, 71, 79	0
1	I	427/429 (99%)	-1.71	0 100 100	33, 48, 64, 71	0
1	J	429/429 (100%)	-1.67	0 100 100	37, 53, 72, 78	0
1	K	422/429 (98%)	-1.65	0 100 100	45, 62, 76, 91	0
1	L	420/429 (97%)	-1.62	0 100 100	51, 66, 79, 93	0
All	All	5094/5148 (98%)	-1.67	0 100 100	29, 55, 74, 95	0

There are no RSRZ outliers to report.

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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	PLP	C	1430	15/16	0.99	0.03	45,46,46,47	0
2	PLP	D	1430	15/16	0.99	0.03	53,56,59,60	0
2	PLP	F	1430	15/16	0.99	0.03	51,54,56,57	0
2	PLP	I	1430	15/16	0.99	0.03	41,42,42,43	0
2	PLP	J	1430	15/16	0.99	0.03	47,47,47,48	0
2	PLP	L	1430	15/16	0.99	0.03	65,66,66,66	0
2	PLP	G	1430	15/16	1.00	0.03	37,37,39,39	0
2	PLP	H	1430	15/16	1.00	0.03	42,44,45,46	0
2	PLP	B	1430	15/16	1.00	0.03	41,43,44,44	0
2	PLP	E	1430	15/16	1.00	0.02	43,44,46,47	0
2	PLP	K	1430	15/16	1.00	0.03	58,59,59,60	0
2	PLP	A	1430	15/16	1.00	0.02	36,37,39,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.