



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:28 PM UTC

PDB ID : 1PV4 / pdb_00001pv4
Title : X-ray crystal structure of the Rho transcription termination factor in complex with single stranded DNA
Authors : Skordalakes, E.; Berger, J.M.
Deposited on : 2003-06-26
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

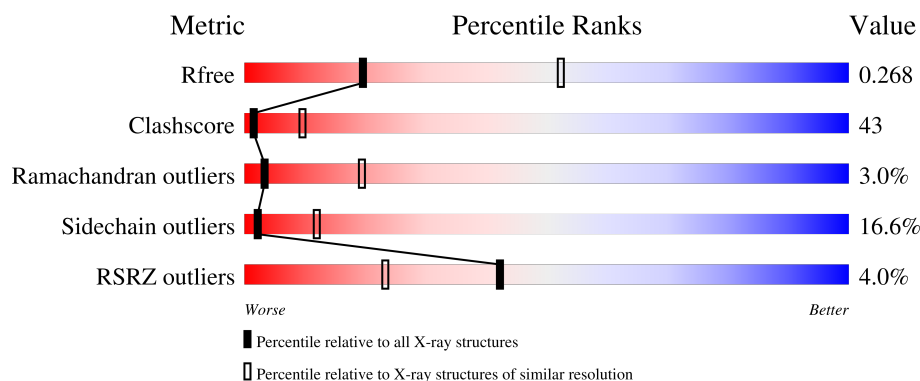
1 Overall quality at a glance

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	G	2	100%
1	H	2	50% 100%
1	J	2	50% 100%
1	K	2	50% 100%
1	L	2	50% 50%

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Mol	Chain	Length	Quality of chain
2	A	419	3% 41% 46% 10%
2	B	419	5% 37% 40% 8% 15%
2	C	419	2% 37% 45% 14%
2	D	419	3% 40% 45% 11%
2	E	419	4% 37% 47% 12%
2	F	419	4% 38% 50% 8%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 19077 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 DNA chain called 5'-D(P*CP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	2	Total	C	N	O	P	0	0	0
			38	18	6	12	2			
1	H	2	Total	C	N	O	P	0	0	0
			38	18	6	12	2			
1	J	2	Total	C	N	O	P	0	0	0
			38	18	6	12	2			
1	K	2	Total	C	N	O	P	0	0	0
			38	18	6	12	2			
1	L	2	Total	C	N	O	P	0	0	0
			38	18	6	12	2			

- Molecule 2 is a protein called Transcription termination factor rho.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	A	408	Total	C	N	O	S	Se	0	0	0
			3208	2025	562	604	1	16			
2	B	358	Total	C	N	O	S	Se	0	0	0
			2813	1776	494	529	1	13			
2	C	408	Total	C	N	O	S	Se	0	0	0
			3208	2025	562	604	1	16			
2	D	408	Total	C	N	O	S	Se	0	0	0
			3208	2025	562	604	1	16			
2	E	407	Total	C	N	O	S	Se	0	0	0
			3201	2020	561	603	1	16			
2	F	408	Total	C	N	O	S	Se	0	0	0
			3208	2025	562	604	1	16			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	modified residue	UNP P0AG30
A	21	MSE	MET	modified residue	UNP P0AG30
A	29	MSE	MET	modified residue	UNP P0AG30

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Chain	Residue	Modelled	Actual	Comment	Reference
A	147	MSE	MET	modified residue	UNP P0AG30
A	186	MSE	MET	modified residue	UNP P0AG30
A	205	MSE	MET	modified residue	UNP P0AG30
A	219	MSE	MET	modified residue	UNP P0AG30
A	245	MSE	MET	modified residue	UNP P0AG30
A	327	MSE	MET	modified residue	UNP P0AG30
A	341	MSE	MET	modified residue	UNP P0AG30
A	380	MSE	MET	modified residue	UNP P0AG30
A	390	MSE	MET	modified residue	UNP P0AG30
A	396	MSE	MET	modified residue	UNP P0AG30
A	405	MSE	MET	modified residue	UNP P0AG30
A	415	MSE	MET	modified residue	UNP P0AG30
A	416	MSE	MET	modified residue	UNP P0AG30
B	1	MSE	MET	modified residue	UNP P0AG30
B	21	MSE	MET	modified residue	UNP P0AG30
B	29	MSE	MET	modified residue	UNP P0AG30
B	147	MSE	MET	modified residue	UNP P0AG30
B	186	MSE	MET	modified residue	UNP P0AG30
B	205	MSE	MET	modified residue	UNP P0AG30
B	219	MSE	MET	modified residue	UNP P0AG30
B	245	MSE	MET	modified residue	UNP P0AG30
B	327	MSE	MET	modified residue	UNP P0AG30
B	341	MSE	MET	modified residue	UNP P0AG30
B	380	MSE	MET	modified residue	UNP P0AG30
B	390	MSE	MET	modified residue	UNP P0AG30
B	396	MSE	MET	modified residue	UNP P0AG30
B	405	MSE	MET	modified residue	UNP P0AG30
B	415	MSE	MET	modified residue	UNP P0AG30
B	416	MSE	MET	modified residue	UNP P0AG30
C	1	MSE	MET	modified residue	UNP P0AG30
C	21	MSE	MET	modified residue	UNP P0AG30
C	29	MSE	MET	modified residue	UNP P0AG30
C	147	MSE	MET	modified residue	UNP P0AG30
C	186	MSE	MET	modified residue	UNP P0AG30
C	205	MSE	MET	modified residue	UNP P0AG30
C	219	MSE	MET	modified residue	UNP P0AG30
C	245	MSE	MET	modified residue	UNP P0AG30
C	327	MSE	MET	modified residue	UNP P0AG30
C	341	MSE	MET	modified residue	UNP P0AG30
C	380	MSE	MET	modified residue	UNP P0AG30
C	390	MSE	MET	modified residue	UNP P0AG30
C	396	MSE	MET	modified residue	UNP P0AG30

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Chain	Residue	Modelled	Actual	Comment	Reference
C	405	MSE	MET	modified residue	UNP P0AG30
C	415	MSE	MET	modified residue	UNP P0AG30
C	416	MSE	MET	modified residue	UNP P0AG30
D	1	MSE	MET	modified residue	UNP P0AG30
D	21	MSE	MET	modified residue	UNP P0AG30
D	29	MSE	MET	modified residue	UNP P0AG30
D	147	MSE	MET	modified residue	UNP P0AG30
D	186	MSE	MET	modified residue	UNP P0AG30
D	205	MSE	MET	modified residue	UNP P0AG30
D	219	MSE	MET	modified residue	UNP P0AG30
D	245	MSE	MET	modified residue	UNP P0AG30
D	327	MSE	MET	modified residue	UNP P0AG30
D	341	MSE	MET	modified residue	UNP P0AG30
D	380	MSE	MET	modified residue	UNP P0AG30
D	390	MSE	MET	modified residue	UNP P0AG30
D	396	MSE	MET	modified residue	UNP P0AG30
D	405	MSE	MET	modified residue	UNP P0AG30
D	415	MSE	MET	modified residue	UNP P0AG30
D	416	MSE	MET	modified residue	UNP P0AG30
E	1	MSE	MET	modified residue	UNP P0AG30
E	21	MSE	MET	modified residue	UNP P0AG30
E	29	MSE	MET	modified residue	UNP P0AG30
E	147	MSE	MET	modified residue	UNP P0AG30
E	186	MSE	MET	modified residue	UNP P0AG30
E	205	MSE	MET	modified residue	UNP P0AG30
E	219	MSE	MET	modified residue	UNP P0AG30
E	245	MSE	MET	modified residue	UNP P0AG30
E	327	MSE	MET	modified residue	UNP P0AG30
E	341	MSE	MET	modified residue	UNP P0AG30
E	380	MSE	MET	modified residue	UNP P0AG30
E	390	MSE	MET	modified residue	UNP P0AG30
E	396	MSE	MET	modified residue	UNP P0AG30
E	405	MSE	MET	modified residue	UNP P0AG30
E	415	MSE	MET	modified residue	UNP P0AG30
E	416	MSE	MET	modified residue	UNP P0AG30
F	1	MSE	MET	modified residue	UNP P0AG30
F	21	MSE	MET	modified residue	UNP P0AG30
F	29	MSE	MET	modified residue	UNP P0AG30
F	147	MSE	MET	modified residue	UNP P0AG30
F	186	MSE	MET	modified residue	UNP P0AG30
F	205	MSE	MET	modified residue	UNP P0AG30
F	219	MSE	MET	modified residue	UNP P0AG30

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Chain	Residue	Modelled	Actual	Comment	Reference
F	245	MSE	MET	modified residue	UNP P0AG30
F	327	MSE	MET	modified residue	UNP P0AG30
F	341	MSE	MET	modified residue	UNP P0AG30
F	380	MSE	MET	modified residue	UNP P0AG30
F	390	MSE	MET	modified residue	UNP P0AG30
F	396	MSE	MET	modified residue	UNP P0AG30
F	405	MSE	MET	modified residue	UNP P0AG30
F	415	MSE	MET	modified residue	UNP P0AG30
F	416	MSE	MET	modified residue	UNP P0AG30

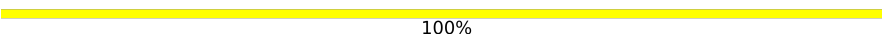
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	1	Total O 1 1	0	0
3	J	1	Total O 1 1	0	0
3	A	3	Total O 3 3	0	0
3	B	2	Total O 2 2	0	0
3	C	7	Total O 7 7	0	0
3	D	7	Total O 7 7	0	0
3	E	14	Total O 14 14	0	0
3	F	6	Total O 6 6	0	0

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: 5'-D(P*CP*C)-3'

Chain G:  100%

 C3 C4

- Molecule 1: 5'-D(P*CP*C)-3'

Chain H:  50% 100%

 C3 C4

- Molecule 1: 5'-D(P*CP*C)-3'

Chain J:  50% 100%

 C3 C4

- Molecule 1: 5'-D(P*CP*C)-3'

Chain K:  50% 100%

 C3 C4

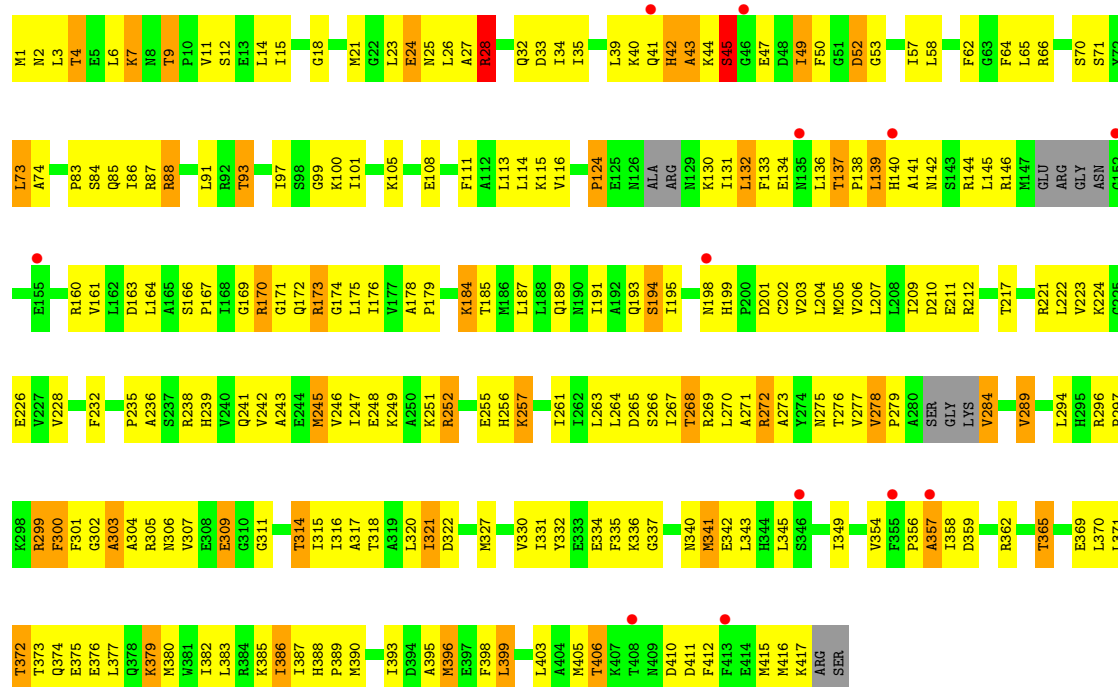
- Molecule 1: 5'-D(P*CP*C)-3'

Chain L:  50% 50% 50%

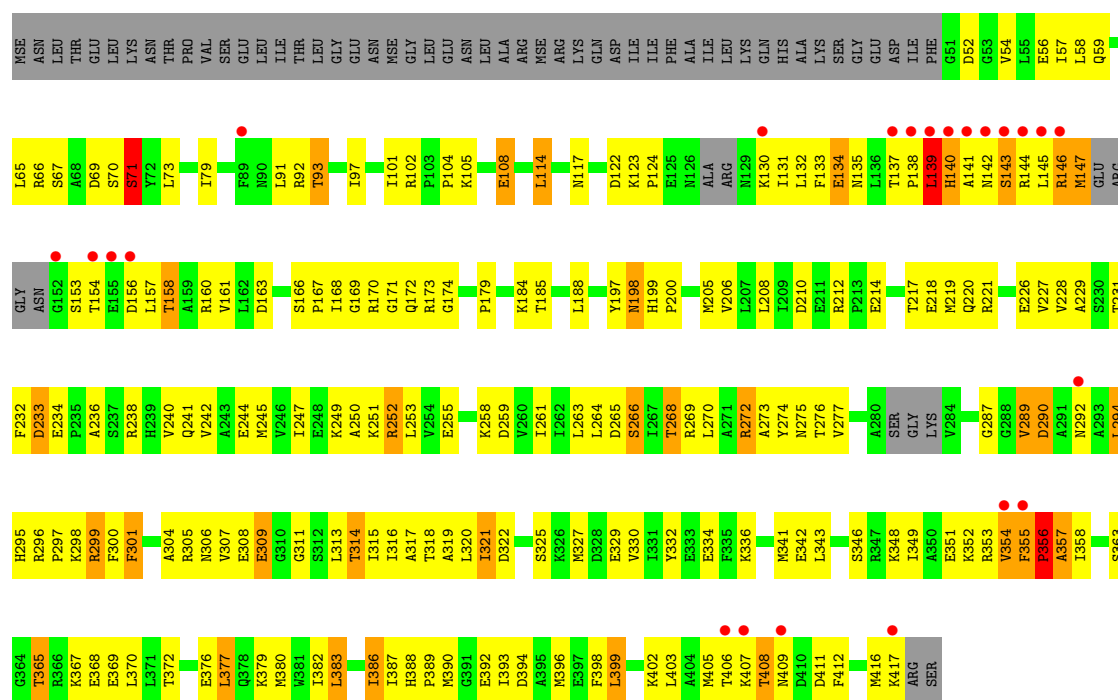
 C3 C4

- Molecule 2: Transcription termination factor rho

Chain A:  3% 41% 46% 10%

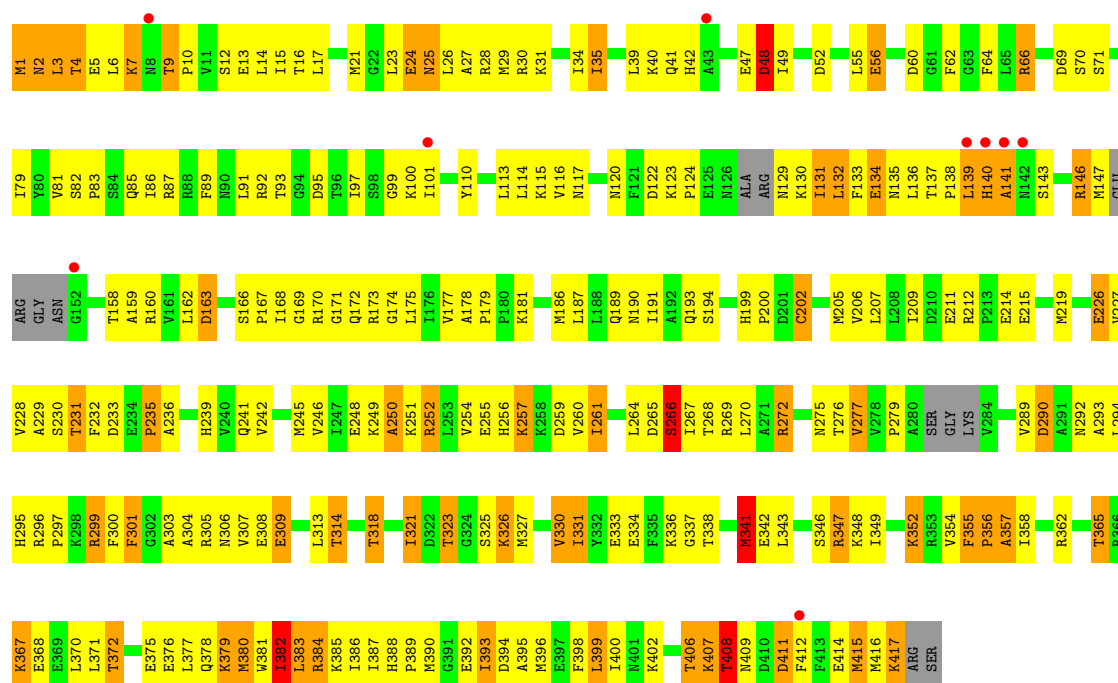


• Molecule 2: Transcription termination factor rho

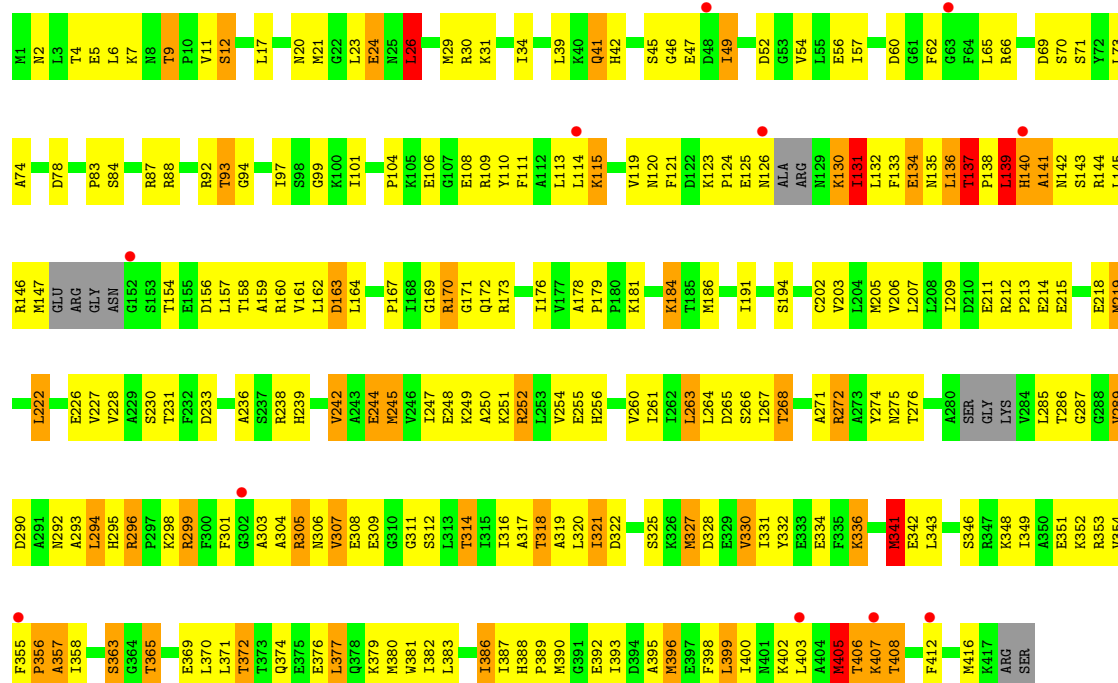


• Molecule 2: Transcription termination factor rho



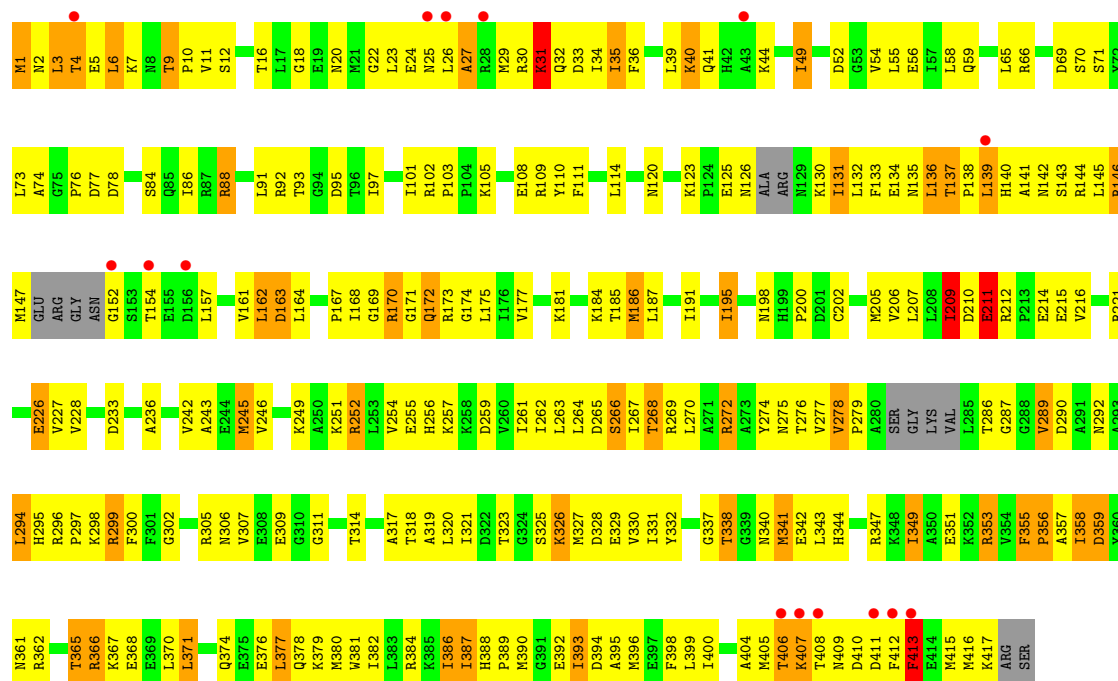


• Molecule 2: Transcription termination factor rho

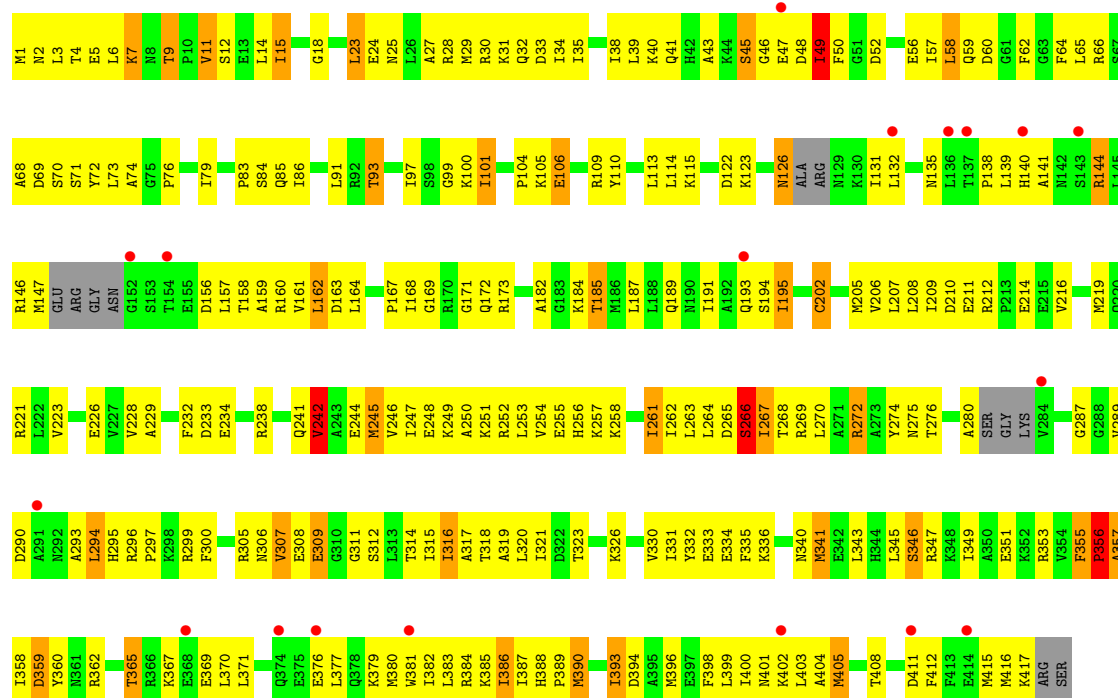


• Molecule 2: Transcription termination factor rho





• Molecule 2: Transcription termination factor rho



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	118.56Å 204.33Å 147.37Å 90.00° 95.86° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00 20.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	97.9 (20.00-3.00) 96.7 (20.00-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.270 , 0.296 0.244 , 0.268	Depositor DCC
R_{free} test set	3735 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	86.7	Xtriage
Anisotropy	0.162	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 89.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	19077	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.08% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	G	0.30	0/41	0.85	0/60
1	H	0.39	0/41	1.06	0/60
1	J	0.48	0/41	1.18	0/60
1	K	0.47	0/41	1.03	0/60
1	L	0.49	0/41	1.31	1/60 (1.7%)
2	A	0.70	0/3238	1.01	9/4334 (0.2%)
2	B	0.71	0/2841	1.02	4/3805 (0.1%)
2	C	0.97	4/3238 (0.1%)	1.17	10/4334 (0.2%)
2	D	0.94	2/3238 (0.1%)	1.14	8/4334 (0.2%)
2	E	0.89	0/3231	1.17	6/4324 (0.1%)
2	F	0.74	0/3238	1.02	3/4334 (0.1%)
All	All	0.83	6/19229 (0.0%)	1.09	41/25765 (0.2%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	341	MSE	SE-CE	-6.26	1.76	1.95
2	C	341	MSE	SE-CE	-6.15	1.76	1.95
2	D	186	MSE	SE-CE	5.81	2.12	1.95
2	C	21	MSE	CA-CB	-5.73	1.43	1.53
2	C	408	THR	CB-OG1	5.53	1.52	1.43
2	C	250	ALA	CA-CB	-5.24	1.45	1.53

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	323	THR	N-CA-C	-8.51	102.61	113.16
2	C	141	ALA	N-CA-C	-8.35	102.11	113.30
2	C	331	ILE	N-CA-C	-7.63	102.35	110.36
2	F	25	ASN	N-CA-C	7.25	120.50	110.35
2	A	43	ALA	N-CA-C	-7.10	104.70	113.15
2	D	131	ILE	N-CA-C	6.96	119.06	109.80
2	D	142	ASN	N-CA-C	-6.77	104.06	112.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	219	MSE	N-CA-C	-6.66	103.95	111.14
2	F	323	THR	N-CA-C	-6.54	105.27	113.18
2	D	307	VAL	N-CA-C	6.50	117.46	108.89
2	E	355	PHE	CA-CB-CG	-6.46	107.34	113.80
2	F	69	ASP	N-CA-C	-6.43	105.54	113.19
2	D	219	MSE	N-CA-C	-6.19	104.45	111.07
2	E	338	THR	N-CA-C	-6.18	104.44	112.23
2	C	330	VAL	CB-CA-C	-5.98	104.31	111.97
2	B	71	SER	N-CA-C	-5.96	103.44	111.54
2	C	382	ILE	N-CA-C	-5.93	104.85	110.42
2	A	267	ILE	N-CA-C	-5.91	103.71	111.09
2	E	186	MSE	N-CA-C	-5.85	104.90	111.28
2	D	203	VAL	CB-CA-C	-5.78	104.99	111.23
2	D	94	GLY	N-CA-C	-5.67	107.16	113.79
2	D	26	LEU	N-CA-C	-5.65	103.54	110.61
2	C	143	SER	N-CA-C	5.61	117.19	107.93
2	A	300	PHE	N-CA-C	-5.60	104.19	111.02
2	E	172	GLN	OE1-CD-NE2	-5.58	117.02	122.60
2	A	164	LEU	N-CA-C	-5.50	106.25	113.12
2	A	303	ALA	N-CA-C	-5.47	105.32	111.28
2	E	265	ASP	N-CA-C	5.43	116.97	109.15
1	L	3	DC	P-O3'-C3'	5.43	128.35	120.20
2	E	211	GLU	N-CA-C	5.41	118.43	110.59
2	A	49	ILE	N-CA-C	5.27	115.87	108.17
2	D	311	GLY	N-CA-C	-5.25	105.04	112.81
2	A	406	THR	N-CA-C	5.21	114.71	107.73
2	A	28	ARG	N-CA-C	5.17	116.72	111.14
2	C	270	LEU	N-CA-C	-5.16	104.92	111.11
2	A	278	VAL	N-CA-C	5.14	113.99	108.95
2	B	342	GLU	N-CA-C	5.14	117.44	108.76
2	C	261	ILE	CA-C-N	-5.09	116.88	123.19
2	C	261	ILE	C-N-CA	-5.09	116.88	123.19
2	B	315	ILE	N-CA-C	5.06	115.25	107.77
2	B	233	ASP	N-CA-C	5.02	117.40	111.33

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	38	0	23	2	0
1	H	38	0	23	3	0
1	J	38	0	23	5	0
1	K	38	0	23	5	0
1	L	38	0	23	7	0
2	A	3208	0	3284	284	0
2	B	2813	0	2870	239	0
2	C	3208	0	3284	324	0
2	D	3208	0	3284	277	0
2	E	3201	0	3275	314	0
2	F	3208	0	3284	268	0
3	A	3	0	0	2	0
3	B	2	0	0	2	0
3	C	7	0	0	1	0
3	D	7	0	0	3	0
3	E	14	0	0	6	0
3	F	6	0	0	3	0
3	G	1	0	0	0	0
3	J	1	0	0	0	0
All	All	19077	0	19396	1647	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 43.

All (1647) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:355:PHE:HB3	2:F:356:PRO:CD	1.59	1.33
2:C:379:LYS:HG2	2:C:412:PHE:CD2	1.72	1.23
2:C:177:VAL:CG1	2:C:321:ILE:HD12	1.69	1.22
2:A:265:ASP:O	2:A:318:THR:HB	1.36	1.22
2:C:141:ALA:CB	2:C:370:LEU:HB2	1.72	1.19
2:E:152:GLY:HA2	2:E:407:LYS:HE3	1.20	1.17
2:E:356:PRO:HB2	2:E:396:MSE:HE2	1.28	1.14
2:E:141:ALA:CB	2:E:370:LEU:HB2	1.76	1.14
2:C:141:ALA:HA	2:C:371:LEU:CD2	1.79	1.13
2:C:141:ALA:HB3	2:C:370:LEU:CB	1.77	1.12
2:C:341:MSE:HE3	2:C:342:GLU:HA	1.26	1.11
2:E:272:ARG:HG3	2:E:272:ARG:HH11	1.06	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:412:PHE:CZ	2:C:416:MSE:SE	2.54	1.11
2:E:341:MSE:HE3	2:E:342:GLU:HA	1.26	1.10
2:B:390:MSE:HE1	2:B:398:PHE:HB2	1.11	1.10
2:A:272:ARG:HG3	2:A:272:ARG:HH11	1.04	1.09
2:B:272:ARG:HG3	2:B:272:ARG:HH11	0.95	1.09
2:D:390:MSE:HE3	2:D:395:ALA:HA	1.28	1.09
2:C:141:ALA:CB	2:C:370:LEU:CB	2.30	1.08
2:A:372:THR:HG23	2:A:376:GLU:HB3	1.34	1.07
2:C:177:VAL:HG13	2:C:321:ILE:CD1	1.84	1.07
2:A:226:GLU:OE2	2:A:249:LYS:HE2	1.53	1.07
2:E:341:MSE:HE3	2:E:341:MSE:C	1.81	1.06
2:C:390:MSE:HE1	2:C:398:PHE:HB2	1.34	1.05
2:F:390:MSE:HE1	2:F:398:PHE:CG	1.90	1.05
2:A:390:MSE:HE2	2:A:395:ALA:HA	1.38	1.04
2:C:141:ALA:HA	2:C:371:LEU:HD21	1.38	1.04
2:F:355:PHE:HB3	2:F:356:PRO:HD3	1.36	1.04
2:E:141:ALA:HB1	2:E:370:LEU:HB2	1.03	1.03
2:D:161:VAL:HG21	2:D:396:MSE:HE1	1.39	1.02
1:H:3:DC:H4'	1:H:4:DC:O5'	1.58	1.02
2:C:272:ARG:HG3	2:C:272:ARG:HH11	1.16	1.02
2:D:268:THR:HG21	2:D:320:LEU:H	1.24	1.02
2:C:356:PRO:O	2:C:358:ILE:HG13	1.60	1.02
2:C:83:PRO:O	2:C:87:ARG:HG3	1.59	1.01
2:D:341:MSE:CE	2:D:342:GLU:HA	1.90	1.01
2:E:341:MSE:HE3	2:E:342:GLU:CA	1.89	1.01
2:C:177:VAL:CG1	2:C:321:ILE:CD1	2.39	1.01
2:C:379:LYS:HZ2	2:C:412:PHE:HB2	1.26	1.01
2:D:289:VAL:HG11	2:D:330:VAL:HG11	1.41	1.01
2:F:202:CYS:SG	2:F:261:ILE:HD11	2.00	1.00
2:F:343:LEU:HD11	2:F:358:ILE:HD13	1.42	1.00
2:B:390:MSE:HE1	2:B:398:PHE:CB	1.90	1.00
2:C:23:LEU:HD21	2:C:41:GLN:HG3	1.42	1.00
2:A:245:MSE:HA	2:A:245:MSE:CE	1.91	1.00
2:E:169:GLY:H	2:E:172:GLN:HG2	1.27	1.00
2:C:79:ILE:HD13	2:C:101:ILE:HG21	1.39	1.00
2:C:141:ALA:HB3	2:C:370:LEU:HB3	1.40	1.00
2:E:140:HIS:CB	2:E:306:ASN:HB2	1.92	1.00
2:C:289:VAL:HG11	2:C:330:VAL:HG11	1.44	0.99
2:A:141:ALA:O	2:A:370:LEU:HB3	1.61	0.99
2:C:341:MSE:HE3	2:C:342:GLU:CA	1.93	0.98
2:F:355:PHE:CB	2:F:356:PRO:CD	2.40	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:141:ALA:HB1	2:E:370:LEU:CB	1.95	0.97
2:D:341:MSE:C	2:D:341:MSE:HE2	1.89	0.97
2:F:359:ASP:OD1	2:F:359:ASP:O	1.81	0.97
2:B:272:ARG:HG3	2:B:272:ARG:NH1	1.70	0.96
2:D:160:ARG:HD2	2:D:408:THR:CG2	1.95	0.96
2:A:1:MSE:HG3	2:A:2:ASN:H	1.31	0.96
2:A:4:THR:HG21	2:A:52:ASP:OD2	1.65	0.96
2:F:49:ILE:HG22	2:F:101:ILE:HD11	1.47	0.96
2:C:2:ASN:OD1	2:C:4:THR:HG22	1.67	0.95
2:D:341:MSE:HE3	2:D:342:GLU:CA	1.96	0.95
2:D:341:MSE:CE	2:D:342:GLU:CA	2.44	0.95
2:B:272:ARG:HH11	2:B:272:ARG:CG	1.78	0.95
2:D:131:ILE:HG21	2:D:133:PHE:HD2	1.32	0.95
2:C:177:VAL:HG13	2:C:321:ILE:HD12	0.97	0.95
2:A:341:MSE:HE3	2:A:341:MSE:O	1.66	0.94
2:D:131:ILE:CG2	2:D:133:PHE:HD2	1.80	0.94
2:D:236:ALA:HA	2:D:239:HIS:HD2	1.31	0.94
2:C:272:ARG:HD3	2:C:327:MSE:SE	2.17	0.94
2:C:379:LYS:NZ	2:C:412:PHE:HB2	1.83	0.94
2:E:141:ALA:HB3	2:E:370:LEU:CD1	1.98	0.94
2:B:269:ARG:HH11	2:B:272:ARG:NH1	1.65	0.93
2:E:396:MSE:O	2:E:400:ILE:HG13	1.68	0.93
2:F:169:GLY:H	2:F:172:GLN:HG3	1.32	0.93
2:B:140:HIS:HA	2:B:306:ASN:HB3	1.50	0.93
2:A:140:HIS:CB	2:A:306:ASN:HB3	1.99	0.92
2:A:272:ARG:HH11	2:A:272:ARG:CG	1.81	0.92
2:C:171:GLY:H	2:C:314:THR:CG2	1.82	0.92
2:C:205:MSE:HE3	2:C:226:GLU:OE1	1.69	0.92
2:D:167:PRO:O	2:D:365:THR:HG21	1.70	0.92
2:C:341:MSE:CE	2:C:341:MSE:O	2.18	0.92
2:C:356:PRO:HD2	2:C:400:ILE:HD11	1.52	0.92
2:E:272:ARG:HG3	2:E:272:ARG:NH1	1.80	0.91
2:B:269:ARG:HH11	2:B:272:ARG:HH12	0.98	0.91
2:E:132:LEU:HD22	2:E:251:LYS:HD3	1.48	0.91
2:A:161:VAL:HG11	2:A:396:MSE:HE1	1.51	0.91
2:A:132:LEU:HD22	2:A:251:LYS:HD3	1.51	0.91
2:F:4:THR:HB	2:F:52:ASP:OD1	1.70	0.91
2:E:23:LEU:HD21	2:E:41:GLN:HG3	1.52	0.91
2:E:141:ALA:CB	2:E:370:LEU:CB	2.48	0.90
2:B:321:ILE:HD11	2:B:332:TYR:CG	2.07	0.90
2:D:169:GLY:H	2:D:172:GLN:CG	1.84	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:269:ARG:HH11	2:C:272:ARG:HH12	1.17	0.90
2:F:390:MSE:HE2	2:F:398:PHE:HB2	1.53	0.90
2:F:141:ALA:HB1	2:F:370:LEU:HB2	1.52	0.90
2:C:379:LYS:HZ2	2:C:412:PHE:CB	1.84	0.89
2:D:169:GLY:H	2:D:172:GLN:HG2	1.36	0.89
2:D:341:MSE:HE3	2:D:342:GLU:C	1.98	0.89
2:D:238:ARG:O	2:D:242:VAL:HG23	1.73	0.89
2:E:356:PRO:CB	2:E:396:MSE:HE2	2.03	0.89
2:A:272:ARG:HG3	2:A:272:ARG:NH1	1.82	0.89
2:B:261:ILE:HG12	2:B:314:THR:CG2	2.02	0.89
2:E:169:GLY:H	2:E:172:GLN:CG	1.85	0.89
2:C:412:PHE:HZ	2:C:416:MSE:SE	2.06	0.88
2:D:131:ILE:HG22	2:D:133:PHE:H	1.38	0.88
2:B:269:ARG:NH1	2:B:272:ARG:HH12	1.71	0.88
2:E:275:ASN:ND2	2:E:327:MSE:HE1	1.89	0.88
2:A:140:HIS:HA	2:A:306:ASN:HD22	1.39	0.88
2:B:131:ILE:CG2	2:B:133:PHE:HD2	1.85	0.88
2:E:139:LEU:HD22	2:E:367:LYS:HD2	1.56	0.88
2:D:139:LEU:HD13	2:E:214:GLU:HG3	1.55	0.88
2:F:135:ASN:HB3	2:F:307:VAL:HG22	1.56	0.88
2:A:341:MSE:HE3	2:A:341:MSE:C	1.98	0.88
2:C:160:ARG:HG2	2:C:408:THR:HG23	1.55	0.88
2:A:372:THR:CG2	2:A:376:GLU:HB3	2.03	0.88
2:E:390:MSE:HE1	2:E:398:PHE:HB2	1.52	0.88
2:F:355:PHE:HB3	2:F:356:PRO:HD2	1.53	0.88
2:A:405:MSE:SE	2:A:415:MSE:CE	2.72	0.88
2:D:133:PHE:HB3	3:E:430:HOH:O	1.74	0.87
2:A:131:ILE:HG22	2:A:133:PHE:HD2	1.39	0.87
2:D:4:THR:HB	2:D:52:ASP:OD1	1.74	0.87
2:D:321:ILE:HD11	2:D:332:TYR:CD2	2.09	0.87
2:E:136:LEU:HD12	2:F:221:ARG:NH2	1.89	0.87
2:B:275:ASN:HD22	2:B:327:MSE:HE1	1.36	0.87
2:C:341:MSE:HE3	2:C:341:MSE:C	2.00	0.87
2:E:341:MSE:C	2:E:341:MSE:CE	2.47	0.87
2:D:137:THR:HG22	2:D:305:ARG:HB2	1.56	0.87
2:C:416:MSE:O	2:C:417:LYS:HB2	1.72	0.87
2:F:141:ALA:HB1	2:F:370:LEU:CB	2.05	0.87
2:D:136:LEU:O	2:D:138:PRO:HD3	1.74	0.86
2:A:385:LYS:HE2	2:B:353:ARG:HH12	1.40	0.86
2:C:294:LEU:CD1	2:C:334:GLU:HG3	2.05	0.86
2:C:379:LYS:HG2	2:C:412:PHE:CE2	2.10	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:144:ARG:HH11	2:A:146:ARG:HE	1.20	0.85
2:B:261:ILE:HG12	2:B:314:THR:HG23	1.57	0.85
2:C:167:PRO:HD2	2:C:365:THR:HG23	1.57	0.85
2:B:268:THR:HG21	2:B:320:LEU:H	1.40	0.85
2:C:341:MSE:O	2:C:341:MSE:HE2	1.77	0.85
2:E:205:MSE:HE3	2:E:226:GLU:OE1	1.76	0.85
2:F:207:LEU:HD11	2:F:242:VAL:CG1	2.07	0.85
2:E:132:LEU:HA	2:E:135:ASN:ND2	1.91	0.85
2:E:341:MSE:CE	2:E:341:MSE:O	2.24	0.85
2:E:152:GLY:CA	2:E:407:LYS:HE3	2.04	0.85
2:C:272:ARG:CD	2:C:327:MSE:SE	2.75	0.85
2:D:341:MSE:HE2	2:D:341:MSE:O	1.75	0.85
2:A:376:GLU:O	2:A:380:MSE:HG3	1.75	0.84
2:E:152:GLY:HA2	2:E:407:LYS:CE	2.04	0.84
2:C:390:MSE:HE1	2:C:398:PHE:CB	2.06	0.84
2:A:275:ASN:HD22	2:A:327:MSE:HE3	1.42	0.84
2:B:141:ALA:HB1	2:B:370:LEU:HB2	1.59	0.84
2:D:387:ILE:HG23	2:D:390:MSE:HE2	1.59	0.84
2:A:49:ILE:HG22	2:A:101:ILE:HG12	1.57	0.84
2:E:381:TRP:CZ3	2:F:353:ARG:HD3	2.12	0.84
2:A:144:ARG:HG3	2:A:145:LEU:N	1.92	0.84
2:B:174:GLY:HA3	2:B:341:MSE:HE3	1.59	0.84
2:E:366:ARG:HG3	2:E:366:ARG:HH11	1.41	0.84
2:A:24:GLU:O	2:A:26:LEU:HD23	1.77	0.84
2:A:169:GLY:H	2:A:172:GLN:CG	1.90	0.84
2:F:169:GLY:N	2:F:172:GLN:HG3	1.91	0.84
2:A:140:HIS:CB	2:A:306:ASN:CB	2.56	0.83
2:A:416:MSE:O	2:A:417:LYS:HB2	1.79	0.83
2:C:141:ALA:HA	2:C:371:LEU:HD23	1.58	0.83
2:E:359:ASP:OD1	2:E:359:ASP:O	1.97	0.83
2:D:405:MSE:O	2:D:406:THR:HG23	1.77	0.83
2:E:341:MSE:HE3	2:E:341:MSE:O	1.77	0.83
2:E:174:GLY:CA	2:E:341:MSE:HE2	2.08	0.83
2:C:379:LYS:CG	2:C:412:PHE:CD2	2.60	0.83
2:E:139:LEU:CD2	2:E:367:LYS:HG3	2.08	0.83
2:D:54:VAL:HG21	2:D:249:LYS:HD2	1.60	0.83
2:A:261:ILE:HG12	2:A:314:THR:HG23	1.61	0.82
2:C:379:LYS:HG2	2:C:412:PHE:CG	2.14	0.82
2:E:341:MSE:CE	2:E:342:GLU:HA	2.07	0.82
2:D:135:ASN:HB3	2:D:307:VAL:HG13	1.62	0.82
2:D:336:LYS:HD2	3:D:425:HOH:O	1.79	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:56:GLU:HG3	2:F:245:MSE:HE1	1.60	0.82
2:F:168:ILE:HG12	2:F:341:MSE:HE3	1.61	0.82
2:A:66:ARG:HH11	2:A:66:ARG:HG2	1.44	0.82
2:C:29:MSE:HG3	2:C:34:ILE:HG13	1.62	0.82
2:D:154:THR:O	2:D:157:LEU:HB2	1.79	0.82
2:A:245:MSE:HA	2:A:245:MSE:HE3	1.62	0.82
2:A:294:LEU:HD13	2:A:334:GLU:HG3	1.61	0.82
2:A:405:MSE:O	2:A:406:THR:HG23	1.79	0.82
2:A:236:ALA:HA	2:A:239:HIS:HD2	1.45	0.82
2:B:416:MSE:O	2:B:417:LYS:HB2	1.78	0.82
2:C:23:LEU:HD21	2:C:41:GLN:CG	2.08	0.82
2:E:416:MSE:O	2:E:417:LYS:HB2	1.78	0.82
2:B:228:VAL:CG1	2:B:242:VAL:HG13	2.09	0.82
2:C:140:HIS:CB	2:C:306:ASN:HB2	2.09	0.81
2:C:341:MSE:CE	2:C:341:MSE:C	2.54	0.81
2:C:355:PHE:HB2	2:C:356:PRO:HD3	1.61	0.81
2:E:407:LYS:HE2	3:E:428:HOH:O	1.80	0.81
2:B:132:LEU:HD22	2:B:251:LYS:HD3	1.60	0.81
2:D:147:MSE:HE1	2:D:191:ILE:HG23	1.63	0.81
2:E:386:ILE:HD11	2:E:398:PHE:CE2	2.15	0.81
2:C:171:GLY:H	2:C:314:THR:HG22	1.44	0.81
2:B:205:MSE:HE3	2:B:226:GLU:OE1	1.81	0.81
2:E:341:MSE:HE3	2:E:342:GLU:N	1.94	0.81
1:J:3:DC:H4'	1:J:4:DC:O5'	1.80	0.80
2:E:411:ASP:OD1	2:E:412:PHE:N	2.14	0.80
2:A:266:SER:HA	2:A:318:THR:O	1.79	0.80
2:C:23:LEU:CD2	2:C:41:GLN:HG3	2.12	0.80
2:E:356:PRO:HB2	2:E:396:MSE:CE	2.10	0.80
2:B:355:PHE:HB3	2:B:356:PRO:HD3	1.63	0.80
2:B:272:ARG:HD2	2:B:327:MSE:SE	2.31	0.80
2:E:141:ALA:HB3	2:E:370:LEU:HD12	1.63	0.80
2:A:174:GLY:HA2	2:A:341:MSE:HE2	1.63	0.80
2:E:209:ILE:HG22	2:E:210:ASP:N	1.97	0.79
2:F:390:MSE:CE	2:F:398:PHE:HB2	2.13	0.79
2:C:381:TRP:HB3	2:D:353:ARG:NH2	1.98	0.79
2:F:169:GLY:H	2:F:172:GLN:CG	1.95	0.79
2:C:79:ILE:CD1	2:C:101:ILE:HG21	2.13	0.79
2:B:140:HIS:CA	2:B:306:ASN:HB3	2.12	0.79
2:A:100:LYS:HD2	2:A:115:LYS:HD2	1.65	0.79
2:E:173:ARG:HH21	2:F:212:ARG:HD2	1.46	0.79
2:A:144:ARG:NH1	2:A:146:ARG:HE	1.79	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:5:GLU:O	2:E:9:THR:HG22	1.83	0.78
2:D:268:THR:HG21	2:D:320:LEU:N	1.99	0.78
2:D:289:VAL:CG1	2:D:330:VAL:HG11	2.13	0.78
2:B:140:HIS:HA	2:B:306:ASN:CB	2.12	0.78
2:D:236:ALA:HA	2:D:239:HIS:CD2	2.18	0.78
2:D:261:ILE:HG12	2:D:314:THR:HG23	1.66	0.78
2:D:268:THR:CG2	2:D:320:LEU:H	1.97	0.78
2:E:411:ASP:O	2:E:415:MSE:HG2	1.84	0.78
2:D:251:LYS:O	2:D:255:GLU:HG3	1.84	0.78
2:B:336:LYS:HE3	2:C:323:THR:O	1.84	0.77
2:D:160:ARG:HD2	2:D:408:THR:HG21	1.65	0.77
2:D:356:PRO:HB2	2:D:396:MSE:HE2	1.66	0.77
2:B:289:VAL:HG11	2:B:330:VAL:HG11	1.65	0.77
2:B:355:PHE:HB3	2:B:356:PRO:CD	2.15	0.77
2:C:272:ARG:HG3	2:C:272:ARG:NH1	1.86	0.77
2:E:141:ALA:CB	2:E:370:LEU:HD12	2.14	0.77
2:B:316:ILE:HD12	2:B:341:MSE:CE	2.15	0.77
2:A:49:ILE:HG22	2:A:101:ILE:CG1	2.15	0.77
2:B:251:LYS:O	2:B:255:GLU:HG3	1.83	0.76
2:E:206:VAL:HB	2:E:227:VAL:HG22	1.65	0.76
2:B:275:ASN:ND2	2:B:327:MSE:HE1	2.00	0.76
2:D:17:LEU:HD23	2:D:17:LEU:O	1.84	0.76
2:E:272:ARG:HE	2:E:327:MSE:SE	2.18	0.76
2:A:390:MSE:HE1	2:A:398:PHE:HB3	1.66	0.76
2:B:355:PHE:CB	2:B:356:PRO:CD	2.64	0.76
2:B:131:ILE:HD11	2:C:28:ARG:O	1.86	0.76
2:F:355:PHE:CB	2:F:356:PRO:HD2	2.11	0.76
2:D:341:MSE:HE2	2:D:342:GLU:HA	1.66	0.76
2:E:174:GLY:HA2	2:E:341:MSE:HE2	1.67	0.75
2:F:146:ARG:O	2:F:147:MSE:HG3	1.86	0.75
2:C:92:ARG:CZ	2:C:131:ILE:HD11	2.17	0.75
2:C:160:ARG:HG2	2:C:408:THR:CG2	2.15	0.75
2:A:275:ASN:HD22	2:A:327:MSE:CE	1.98	0.75
2:C:375:GLU:CD	2:C:375:GLU:H	1.94	0.75
2:C:29:MSE:HG3	2:C:34:ILE:CG1	2.17	0.75
2:C:91:LEU:HD13	2:C:97:ILE:HD11	1.68	0.75
2:C:139:LEU:O	2:C:140:HIS:CB	2.34	0.75
2:C:341:MSE:HE3	2:C:341:MSE:O	1.84	0.75
2:C:141:ALA:HB1	2:C:370:LEU:CB	2.15	0.75
2:D:294:LEU:O	2:D:298:LYS:HG3	1.87	0.75
2:C:415:MSE:HG2	2:C:415:MSE:O	1.85	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:341:MSE:CE	2:C:342:GLU:HA	2.14	0.74
2:F:252:ARG:HD3	2:F:255:GLU:OE1	1.87	0.74
2:E:275:ASN:HD22	2:E:327:MSE:HE1	1.49	0.74
2:F:60:ASP:HB2	2:F:62:PHE:CE2	2.22	0.74
2:A:245:MSE:HA	2:A:245:MSE:HE2	1.67	0.74
2:B:131:ILE:HG21	2:B:133:PHE:HD2	1.52	0.74
2:E:136:LEU:HD12	2:F:221:ARG:HH21	1.51	0.74
2:E:137:THR:CG2	2:E:305:ARG:HD3	2.18	0.74
2:D:346:SER:HB3	2:D:349:ILE:HG13	1.70	0.73
2:E:321:ILE:HD11	2:E:332:TYR:CD2	2.24	0.73
2:B:268:THR:CG2	2:B:320:LEU:H	2.02	0.73
2:F:268:THR:HG21	2:F:320:LEU:H	1.53	0.73
2:A:252:ARG:NH1	2:A:255:GLU:CD	2.47	0.73
2:B:295:HIS:NE2	2:C:235:PRO:HD3	2.03	0.73
2:C:4:THR:CG2	2:C:5:GLU:N	2.52	0.73
2:D:143:SER:OG	2:D:170:ARG:HD2	1.89	0.73
2:D:275:ASN:HD21	2:D:289:VAL:HA	1.54	0.73
2:E:186:MSE:HE2	2:E:355:PHE:CD2	2.24	0.73
2:B:131:ILE:CG2	2:B:133:PHE:CD2	2.70	0.73
2:E:386:ILE:HD11	2:E:398:PHE:HE2	1.53	0.73
2:A:173:ARG:HH22	2:B:214:GLU:CD	1.97	0.72
2:C:122:ASP:OD1	2:C:123:LYS:N	2.22	0.72
1:G:3:DC:H4'	1:G:4:DC:O5'	1.88	0.72
2:A:372:THR:HG23	2:A:376:GLU:CB	2.15	0.72
2:B:388:HIS:HB3	2:B:389:PRO:HD3	1.69	0.72
2:E:170:ARG:NH1	2:E:202:CYS:SG	2.62	0.72
2:E:390:MSE:HE1	2:E:398:PHE:CB	2.19	0.72
2:F:382:ILE:O	2:F:386:ILE:HG23	1.88	0.72
2:A:271:ALA:HB3	2:A:331:ILE:HD13	1.70	0.72
2:B:244:GLU:CD	2:B:296:ARG:HH21	1.96	0.72
2:D:144:ARG:HD3	2:D:146:ARG:HH21	1.53	0.72
2:F:272:ARG:CB	2:F:272:ARG:HH11	2.02	0.72
2:A:161:VAL:HG12	2:A:358:ILE:HD12	1.71	0.72
2:A:356:PRO:HB2	2:A:396:MSE:HE3	1.69	0.72
2:B:355:PHE:O	2:B:356:PRO:C	2.29	0.72
2:D:131:ILE:CG2	2:D:133:PHE:CD2	2.69	0.72
2:E:131:ILE:HG23	2:E:133:PHE:H	1.55	0.72
2:E:137:THR:HG23	2:E:305:ARG:HD3	1.72	0.72
2:A:261:ILE:HG12	2:A:314:THR:CG2	2.20	0.72
2:C:160:ARG:HE	2:C:408:THR:HG23	1.55	0.72
2:D:24:GLU:O	2:D:26:LEU:CD2	2.38	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:161:VAL:CG2	2:D:396:MSE:HE1	2.19	0.72
2:F:157:LEU:HD13	2:F:400:ILE:HG23	1.70	0.72
2:B:131:ILE:HG22	2:B:133:PHE:HD2	1.53	0.72
2:F:171:GLY:H	2:F:314:THR:HB	1.54	0.72
2:C:131:ILE:HG23	2:C:133:PHE:HD2	1.55	0.71
2:C:135:ASN:HB3	2:C:307:VAL:HG13	1.69	0.71
2:E:226:GLU:OE2	2:E:249:LYS:HE2	1.90	0.71
2:C:3:LEU:O	2:C:7:LYS:HG2	1.90	0.71
2:F:270:LEU:HD11	2:F:274:TYR:CE2	2.25	0.71
2:A:169:GLY:H	2:A:172:GLN:HG2	1.55	0.71
2:A:217:THR:O	2:A:221:ARG:HG3	1.91	0.71
2:F:65:LEU:HB2	2:F:79:ILE:HB	1.72	0.71
2:B:321:ILE:HD11	2:B:332:TYR:CD2	2.25	0.71
2:D:341:MSE:CE	2:D:341:MSE:C	2.63	0.71
2:A:369:GLU:HA	2:A:377:LEU:HD11	1.71	0.71
2:C:47:GLU:O	2:C:48:ASP:HB2	1.89	0.71
2:C:141:ALA:HB1	2:C:370:LEU:C	2.16	0.71
2:F:167:PRO:HD2	2:F:365:THR:CG2	2.21	0.71
2:B:131:ILE:HG22	2:B:133:PHE:CD2	2.25	0.71
2:B:169:GLY:H	2:B:172:GLN:HG3	1.56	0.71
2:B:170:ARG:HD3	2:B:259:ASP:OD2	1.91	0.71
2:B:228:VAL:HG12	2:B:242:VAL:HG13	1.73	0.71
2:C:269:ARG:NH1	2:C:272:ARG:HH12	1.87	0.71
2:D:60:ASP:HB2	2:D:62:PHE:CE2	2.26	0.71
2:F:268:THR:HG23	2:F:319:ALA:HA	1.72	0.71
2:F:369:GLU:HA	2:F:377:LEU:HD13	1.71	0.71
2:C:173:ARG:HD3	2:C:301:PHE:O	1.91	0.71
2:D:141:ALA:O	2:D:370:LEU:HB3	1.89	0.71
2:F:411:ASP:O	2:F:415:MSE:HB2	1.90	0.71
2:B:253:LEU:O	2:B:258:LYS:HB2	1.90	0.70
2:C:10:PRO:HG2	2:C:13:GLU:OE2	1.90	0.70
2:A:173:ARG:HB2	2:A:173:ARG:NH1	2.06	0.70
2:D:24:GLU:O	2:D:26:LEU:HD23	1.91	0.70
2:C:275:ASN:HD21	2:C:290:ASP:H	1.38	0.70
2:D:396:MSE:O	2:D:400:ILE:HG13	1.91	0.70
2:F:346:SER:HB3	2:F:349:ILE:HG13	1.71	0.70
2:A:86:ILE:HG23	2:A:91:LEU:HB2	1.73	0.70
2:C:167:PRO:HD2	2:C:365:THR:CG2	2.22	0.70
2:D:352:LYS:O	2:D:353:ARG:HB2	1.91	0.70
2:F:266:SER:HB2	2:F:269:ARG:H	1.55	0.70
2:D:66:ARG:HG2	2:D:66:ARG:HH11	1.54	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:390:MSE:CE	2:D:395:ALA:HA	2.16	0.70
2:E:211:GLU:HG3	2:E:212:ARG:H	1.56	0.70
2:C:356:PRO:HB2	2:C:396:MSE:HE2	1.73	0.69
2:E:18:GLY:O	2:E:23:LEU:HB2	1.92	0.69
2:B:158:THR:OG1	2:B:356:PRO:HG3	1.91	0.69
2:D:231:THR:OG1	2:D:233:ASP:HB2	1.91	0.69
2:E:139:LEU:HD22	2:E:367:LYS:CD	2.23	0.69
2:F:168:ILE:CG1	2:F:341:MSE:HE3	2.21	0.69
2:B:144:ARG:HG2	2:B:145:LEU:N	2.08	0.69
2:D:23:LEU:CG	2:D:41:GLN:HG3	2.22	0.69
2:A:184:LYS:HG2	2:A:185:THR:N	2.05	0.69
2:C:356:PRO:O	2:C:358:ILE:N	2.26	0.69
2:E:266:SER:H	2:E:318:THR:HG1	1.40	0.69
2:A:41:GLN:C	2:A:43:ALA:H	1.99	0.69
2:C:141:ALA:CA	2:C:371:LEU:HD23	2.22	0.69
2:A:405:MSE:SE	2:A:415:MSE:HE1	2.42	0.69
2:C:91:LEU:HD13	2:C:97:ILE:CD1	2.21	0.69
2:C:171:GLY:N	2:C:314:THR:HG22	2.08	0.69
2:D:372:THR:OG1	2:D:377:LEU:HD12	1.92	0.69
2:E:343:LEU:HD11	2:E:358:ILE:HG23	1.74	0.69
2:F:275:ASN:ND2	2:F:289:VAL:HA	2.08	0.69
2:A:140:HIS:HA	2:A:306:ASN:ND2	2.08	0.69
2:A:405:MSE:SE	2:A:415:MSE:HE2	2.41	0.69
2:D:272:ARG:HH11	2:D:272:ARG:CG	2.06	0.69
2:F:15:ILE:HD13	2:F:27:ALA:HA	1.74	0.69
2:A:173:ARG:HD2	2:A:301:PHE:O	1.92	0.69
2:B:139:LEU:O	2:B:141:ALA:N	2.26	0.68
2:D:130:LYS:HZ2	2:E:12:SER:HB3	1.58	0.68
2:A:131:ILE:CG2	2:A:133:PHE:HD2	2.06	0.68
2:A:265:ASP:O	2:A:318:THR:CB	2.30	0.68
2:B:210:ASP:OD1	2:B:232:PHE:HA	1.93	0.68
2:E:321:ILE:HD11	2:E:332:TYR:CG	2.28	0.68
2:C:236:ALA:HA	2:C:239:HIS:HD2	1.57	0.68
2:D:222:LEU:N	2:D:222:LEU:HD23	2.08	0.68
2:F:252:ARG:HA	2:F:255:GLU:OE1	1.93	0.68
2:F:382:ILE:O	2:F:386:ILE:CG2	2.41	0.68
2:C:252:ARG:NH1	2:C:255:GLU:OE2	2.26	0.68
2:D:131:ILE:HG21	2:D:133:PHE:CD2	2.23	0.68
2:E:272:ARG:HE	2:E:327:MSE:CG	2.06	0.68
2:F:402:LYS:NZ	2:F:415:MSE:HE1	2.07	0.68
2:B:105:LYS:O	2:B:108:GLU:HB2	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:141:ALA:CB	2:C:370:LEU:HB3	2.12	0.68
2:A:272:ARG:NE	2:A:327:MSE:SE	2.77	0.68
2:C:79:ILE:HD13	2:C:101:ILE:CG2	2.19	0.68
2:D:170:ARG:NH1	2:D:202:CYS:SG	2.66	0.68
2:E:141:ALA:HB3	2:E:370:LEU:CB	2.23	0.68
2:E:169:GLY:N	2:E:172:GLN:HG2	2.07	0.68
2:F:138:PRO:HD2	2:F:306:ASN:O	1.94	0.68
2:A:187:LEU:HD21	2:A:343:LEU:HD23	1.76	0.68
2:C:99:GLY:HA3	2:C:115:LYS:O	1.94	0.68
2:C:214:GLU:HG2	2:C:215:GLU:N	2.09	0.68
2:C:260:VAL:HG12	2:C:261:ILE:N	2.09	0.68
2:D:341:MSE:CE	2:D:342:GLU:N	2.56	0.68
2:B:137:THR:HG21	2:B:305:ARG:NH1	2.09	0.67
2:C:226:GLU:OE2	2:C:249:LYS:HE2	1.94	0.67
2:F:6:LEU:HD22	2:F:14:LEU:CD2	2.23	0.67
2:F:355:PHE:HA	3:F:420:HOH:O	1.94	0.67
2:D:136:LEU:N	2:D:136:LEU:HD23	2.07	0.67
2:D:184:LYS:NZ	2:D:265:ASP:OD2	2.28	0.67
2:E:337:GLY:O	2:F:212:ARG:NH1	2.26	0.67
2:C:275:ASN:ND2	2:C:290:ASP:H	1.92	0.67
2:D:402:LYS:O	2:D:405:MSE:HG2	1.94	0.67
2:F:18:GLY:O	2:F:23:LEU:HB2	1.94	0.67
2:B:143:SER:OG	2:B:170:ARG:HD2	1.95	0.67
2:C:236:ALA:HA	2:C:239:HIS:CD2	2.29	0.67
2:A:66:ARG:HG2	2:A:66:ARG:NH1	2.07	0.67
2:B:348:LYS:HD2	2:B:392:GLU:OE1	1.94	0.67
2:D:268:THR:O	2:D:272:ARG:HG2	1.94	0.67
2:B:264:LEU:HD22	2:B:300:PHE:CE2	2.30	0.67
2:D:356:PRO:O	2:D:358:ILE:HG13	1.95	0.67
2:C:137:THR:HG22	2:D:214:GLU:HB3	1.75	0.67
2:D:136:LEU:O	2:D:138:PRO:CD	2.42	0.67
2:E:137:THR:HG22	2:E:305:ARG:HB2	1.77	0.67
2:E:252:ARG:NH1	2:E:255:GLU:OE2	2.28	0.67
2:F:367:LYS:HB3	2:F:370:LEU:HD12	1.76	0.67
2:F:212:ARG:O	2:F:216:VAL:HG23	1.95	0.66
2:A:207:LEU:HD23	2:A:264:LEU:HD13	1.77	0.66
2:B:173:ARG:HD3	2:B:304:ALA:HB3	1.76	0.66
2:B:356:PRO:HB2	2:B:396:MSE:HE2	1.77	0.66
2:C:141:ALA:HB1	2:C:370:LEU:HB2	1.69	0.66
2:C:341:MSE:HE3	2:C:342:GLU:N	2.09	0.66
2:C:398:PHE:CE1	2:C:402:LYS:HE3	2.30	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:329:GLU:OE1	2:B:329:GLU:HA	1.94	0.66
2:C:388:HIS:HB3	2:C:389:PRO:HD3	1.77	0.66
2:E:366:ARG:HG3	2:E:366:ARG:NH1	2.11	0.66
2:F:390:MSE:HE1	2:F:398:PHE:CD1	2.31	0.66
2:A:172:GLN:NE2	2:A:371:LEU:HD11	2.10	0.66
2:B:272:ARG:CD	2:B:327:MSE:SE	2.93	0.66
2:C:160:ARG:CG	2:C:408:THR:HG23	2.25	0.66
2:D:343:LEU:HA	2:D:363:SER:HB3	1.76	0.66
2:D:49:ILE:HG22	2:D:101:ILE:HD11	1.76	0.66
2:C:171:GLY:HA2	2:C:313:LEU:O	1.96	0.66
2:C:187:LEU:O	2:C:191:ILE:HG13	1.96	0.66
2:D:160:ARG:HD2	2:D:408:THR:HG23	1.78	0.66
2:B:141:ALA:HB3	2:B:370:LEU:HD12	1.76	0.66
2:A:296:ARG:HB2	2:A:297:PRO:HD3	1.77	0.66
2:E:289:VAL:HB	2:E:327:MSE:CE	2.27	0.66
2:A:50:PHE:CE1	2:A:100:LYS:HG2	2.31	0.65
2:D:341:MSE:HE2	2:D:342:GLU:CA	2.24	0.65
2:D:42:HIS:ND1	2:D:42:HIS:O	2.29	0.65
2:C:173:ARG:NH2	2:D:214:GLU:OE1	2.25	0.65
2:A:131:ILE:HG22	2:A:133:PHE:CD2	2.28	0.65
2:A:252:ARG:NH1	2:A:255:GLU:OE2	2.28	0.65
2:C:174:GLY:HA2	2:C:341:MSE:HE2	1.77	0.65
2:E:66:ARG:HG2	2:E:66:ARG:HH11	1.62	0.65
2:F:211:GLU:HG3	2:F:212:ARG:N	2.11	0.65
2:B:352:LYS:HG3	2:B:352:LYS:O	1.96	0.65
2:F:390:MSE:CE	2:F:398:PHE:CG	2.75	0.65
2:D:23:LEU:HG	2:D:41:GLN:HG3	1.79	0.65
2:C:290:ASP:OD1	2:C:290:ASP:C	2.39	0.65
2:E:49:ILE:CG2	2:E:101:ILE:HG13	2.26	0.65
2:A:171:GLY:H	2:A:314:THR:HB	1.60	0.65
2:C:89:PHE:HB2	2:C:91:LEU:HD21	1.79	0.65
2:D:6:LEU:O	2:D:9:THR:HG23	1.97	0.65
2:D:130:LYS:NZ	2:E:12:SER:HB3	2.12	0.65
2:D:377:LEU:HD23	2:D:381:TRP:CD1	2.32	0.65
2:F:381:TRP:O	2:F:385:LYS:HG3	1.96	0.65
2:F:160:ARG:HD2	2:F:408:THR:HB	1.79	0.65
2:F:390:MSE:CE	2:F:398:PHE:CB	2.75	0.65
2:B:289:VAL:CG1	2:B:330:VAL:HG11	2.28	0.64
2:C:251:LYS:O	2:C:255:GLU:HG3	1.97	0.64
2:E:7:LYS:HE2	2:E:77:ASP:OD1	1.97	0.64
2:A:379:LYS:HD3	2:A:412:PHE:HB2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:296:ARG:HB2	2:F:297:PRO:HD3	1.79	0.64
2:C:30:ARG:HG3	2:C:30:ARG:HH11	1.62	0.64
2:C:356:PRO:O	2:C:358:ILE:CG1	2.43	0.64
2:E:132:LEU:HA	2:E:135:ASN:HD22	1.61	0.64
2:A:144:ARG:HH21	2:A:167:PRO:HB3	1.63	0.64
2:C:169:GLY:H	2:C:172:GLN:CG	2.09	0.64
2:C:173:ARG:NH1	2:C:304:ALA:O	2.31	0.64
2:E:58:LEU:HD12	2:E:59:GLN:H	1.63	0.64
2:A:382:ILE:O	2:A:386:ILE:HG22	1.97	0.64
2:C:289:VAL:CG1	2:C:330:VAL:HG11	2.25	0.64
2:F:360:TYR:HE2	2:F:384:ARG:HE	1.44	0.64
2:D:130:LYS:HA	2:E:27:ALA:O	1.98	0.64
2:B:173:ARG:NH2	2:C:212:ARG:HB3	2.12	0.63
2:B:321:ILE:O	2:B:322:ASP:HB2	1.98	0.63
2:C:379:LYS:C	2:C:379:LYS:HD2	2.23	0.63
2:E:39:LEU:HB3	2:E:111:PHE:CZ	2.32	0.63
2:A:6:LEU:O	2:A:9:THR:HG23	1.98	0.63
2:B:167:PRO:HD2	2:B:365:THR:CG2	2.28	0.63
2:C:56:GLU:CD	2:C:66:ARG:HH11	2.06	0.63
2:C:228:VAL:CG1	2:C:242:VAL:HG13	2.28	0.63
2:A:144:ARG:NH2	2:A:167:PRO:HB3	2.13	0.63
2:B:131:ILE:HG21	2:B:133:PHE:CD2	2.32	0.63
2:B:320:LEU:HD12	3:B:421:HOH:O	1.98	0.63
2:D:272:ARG:HH11	2:D:272:ARG:CB	2.11	0.63
2:A:6:LEU:HD22	2:A:14:LEU:HD21	1.81	0.63
2:B:238:ARG:NH1	2:B:241:GLN:OE1	2.31	0.63
2:C:355:PHE:CB	2:C:356:PRO:HD3	2.27	0.63
2:E:268:THR:CG2	2:E:320:LEU:H	2.10	0.63
2:F:268:THR:CG2	2:F:320:LEU:H	2.10	0.63
2:A:236:ALA:HA	2:A:239:HIS:CD2	2.31	0.63
2:B:228:VAL:HG12	2:B:242:VAL:CG1	2.29	0.63
2:C:47:GLU:HG2	2:C:48:ASP:H	1.62	0.63
2:C:167:PRO:O	2:C:365:THR:HG21	1.99	0.63
2:E:137:THR:HG21	2:E:305:ARG:NH1	2.13	0.63
2:F:185:THR:HB	3:F:423:HOH:O	1.99	0.63
2:A:264:LEU:HD22	2:A:300:PHE:CE2	2.32	0.63
2:B:294:LEU:CD1	2:B:334:GLU:HG3	2.28	0.63
2:B:102:ARG:HB3	2:B:114:LEU:HD12	1.81	0.63
2:D:30:ARG:O	2:D:31:LYS:C	2.42	0.63
2:B:169:GLY:H	2:B:172:GLN:CG	2.12	0.62
2:D:135:ASN:HB3	2:D:307:VAL:CG1	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:138:PRO:HD2	2:E:306:ASN:O	1.98	0.62
2:B:104:PRO:HA	2:B:108:GLU:OE1	1.99	0.62
2:D:156:ASP:O	2:D:160:ARG:HG2	1.97	0.62
2:E:1:MSE:HG3	2:E:2:ASN:H	1.64	0.62
2:E:341:MSE:O	2:E:341:MSE:HE2	1.96	0.62
2:A:302:GLY:O	2:A:305:ARG:NH2	2.29	0.62
2:C:3:LEU:HD12	2:C:39:LEU:HD11	1.80	0.62
2:D:39:LEU:HB3	2:D:111:PHE:CZ	2.35	0.62
2:D:289:VAL:HG11	2:D:330:VAL:CG1	2.24	0.62
2:E:140:HIS:CA	2:E:306:ASN:HB2	2.28	0.62
2:E:381:TRP:CH2	2:F:353:ARG:HD3	2.35	0.62
2:C:356:PRO:HB2	2:C:396:MSE:CE	2.27	0.62
2:D:172:GLN:NE2	2:D:371:LEU:HD11	2.14	0.62
2:D:268:THR:HG22	2:D:319:ALA:HA	1.81	0.62
2:E:173:ARG:NH2	2:F:214:GLU:OE2	2.32	0.62
2:B:343:LEU:HD11	2:B:358:ILE:HG12	1.81	0.62
2:B:379:LYS:HD3	2:B:412:PHE:HB2	1.80	0.62
2:C:1:MSE:CG	2:C:2:ASN:H	2.13	0.62
2:C:140:HIS:CB	2:C:306:ASN:CB	2.77	0.62
2:C:269:ARG:HH11	2:C:272:ARG:NH1	1.94	0.62
2:F:274:TYR:CD2	2:F:297:PRO:HG3	2.35	0.62
2:D:139:LEU:HD13	2:E:214:GLU:CG	2.26	0.62
2:F:359:ASP:OD1	2:F:359:ASP:C	2.42	0.62
2:F:412:PHE:O	2:F:416:MSE:HG2	1.99	0.62
2:F:356:PRO:C	2:F:358:ILE:H	2.07	0.62
2:C:267:ILE:HG22	2:C:318:THR:O	2.00	0.62
2:A:145:LEU:HD21	2:A:170:ARG:HG3	1.81	0.62
2:A:341:MSE:O	2:A:341:MSE:CE	2.45	0.62
2:E:55:LEU:HB2	2:E:65:LEU:CD2	2.30	0.62
2:A:140:HIS:CB	2:A:306:ASN:HB2	2.29	0.61
2:A:266:SER:OG	2:A:269:ARG:HB2	1.99	0.61
2:E:207:LEU:HD11	2:E:242:VAL:HG12	1.82	0.61
2:F:353:ARG:HG3	2:F:353:ARG:HH11	1.65	0.61
2:A:49:ILE:CG2	2:A:101:ILE:CG1	2.77	0.61
2:F:173:ARG:N	2:F:340:ASN:OD1	2.30	0.61
2:A:166:SER:OG	2:A:343:LEU:HD13	2.01	0.61
2:C:136:LEU:O	2:C:138:PRO:HD3	2.00	0.61
2:D:330:VAL:HG12	2:D:331:ILE:N	2.15	0.61
2:A:174:GLY:CA	2:A:341:MSE:HE2	2.30	0.61
2:C:231:THR:C	2:C:233:ASP:H	2.06	0.61
2:A:261:ILE:CG1	2:A:314:THR:HG23	2.29	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:341:MSE:HE3	2:D:342:GLU:N	2.14	0.61
2:E:396:MSE:HE3	2:E:400:ILE:HD11	1.83	0.61
2:A:209:ILE:HD13	2:A:270:LEU:HD13	1.82	0.61
2:A:238:ARG:NH1	2:A:241:GLN:OE1	2.33	0.61
2:A:272:ARG:HD2	2:A:327:MSE:SE	2.51	0.61
2:C:4:THR:HG22	2:C:5:GLU:H	1.63	0.61
2:C:139:LEU:HD11	2:D:218:GLU:OE1	2.01	0.61
2:D:260:VAL:HG12	2:D:261:ILE:N	2.16	0.61
2:E:140:HIS:HA	2:E:306:ASN:CB	2.31	0.61
2:E:236:ALA:CB	2:E:277:VAL:HG23	2.31	0.61
2:C:352:LYS:HD2	2:C:393:ILE:HD12	1.83	0.61
2:F:268:THR:HG21	2:F:320:LEU:N	2.15	0.61
2:A:173:ARG:N	2:A:340:ASN:OD1	2.28	0.61
2:C:4:THR:HG23	2:C:5:GLU:N	2.16	0.60
2:C:47:GLU:HG2	2:C:48:ASP:N	2.16	0.60
2:C:383:LEU:O	2:C:387:ILE:HG13	2.00	0.60
2:D:54:VAL:CG2	2:D:249:LYS:HD2	2.30	0.60
2:E:327:MSE:O	2:E:328:ASP:C	2.44	0.60
2:F:191:ILE:O	2:F:195:ILE:HG13	2.01	0.60
2:F:169:GLY:H	2:F:172:GLN:CD	2.08	0.60
2:D:247:ILE:O	2:D:250:ALA:HB3	2.02	0.60
2:E:157:LEU:O	2:E:161:VAL:HG23	2.01	0.60
2:D:136:LEU:C	2:D:138:PRO:HD3	2.26	0.60
2:E:136:LEU:CD1	2:F:221:ARG:HH21	2.14	0.60
2:E:141:ALA:O	2:E:371:LEU:HG	2.02	0.60
2:A:209:ILE:HD11	2:A:243:ALA:HB2	1.83	0.60
2:A:275:ASN:HD21	2:A:289:VAL:HA	1.67	0.60
2:D:354:VAL:HG11	2:D:396:MSE:HB3	1.84	0.60
2:C:30:ARG:HG3	2:C:30:ARG:NH1	2.16	0.60
2:C:412:PHE:CE2	2:C:416:MSE:SE	3.04	0.60
2:F:6:LEU:O	2:F:9:THR:HG23	2.02	0.60
2:A:144:ARG:HH11	2:A:146:ARG:NE	1.97	0.60
2:C:272:ARG:HH11	2:C:272:ARG:CG	2.01	0.60
2:D:303:ALA:O	2:D:304:ALA:C	2.43	0.60
2:F:247:ILE:O	2:F:250:ALA:HB3	2.02	0.60
2:C:174:GLY:CA	2:C:341:MSE:HE2	2.31	0.60
2:D:132:LEU:HD13	2:D:251:LYS:HG2	1.83	0.60
2:B:245:MSE:HA	2:B:245:MSE:HE2	1.84	0.60
2:F:135:ASN:HB3	2:F:307:VAL:CG2	2.31	0.60
2:F:138:PRO:C	2:F:140:HIS:H	2.08	0.60
2:A:49:ILE:CG2	2:A:101:ILE:HG13	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:4:THR:CG2	2:C:5:GLU:H	2.15	0.59
2:D:245:MSE:HA	2:D:245:MSE:CE	2.32	0.59
2:D:386:ILE:O	2:D:386:ILE:HG13	2.01	0.59
2:E:268:THR:HG22	2:E:319:ALA:HA	1.84	0.59
2:A:1:MSE:CG	2:A:2:ASN:H	2.10	0.59
2:C:85:GLN:NE2	2:C:113:LEU:O	2.29	0.59
2:E:49:ILE:HG22	2:E:101:ILE:CG1	2.31	0.59
2:F:167:PRO:HD2	2:F:365:THR:HG22	1.84	0.59
2:D:136:LEU:HD12	2:E:221:ARG:NH2	2.17	0.59
2:D:252:ARG:HH11	2:D:255:GLU:CD	2.10	0.59
2:E:4:THR:HB	2:E:52:ASP:OD1	2.01	0.59
2:E:131:ILE:CG2	2:E:133:PHE:H	2.14	0.59
2:F:58:LEU:HD12	2:F:59:GLN:H	1.67	0.59
2:C:382:ILE:O	2:C:383:LEU:C	2.45	0.59
2:D:23:LEU:HD21	2:D:41:GLN:HG3	1.83	0.59
2:D:136:LEU:HD12	2:E:221:ARG:HH21	1.67	0.59
2:F:23:LEU:HG	2:F:41:GLN:HG3	1.84	0.59
2:F:68:ALA:C	2:F:70:SER:H	2.07	0.59
2:F:189:GLN:O	2:F:193:GLN:HG3	2.02	0.59
2:F:238:ARG:NH1	2:F:241:GLN:OE1	2.35	0.59
2:B:139:LEU:CD1	2:C:214:GLU:HG3	2.32	0.59
2:D:144:ARG:NH2	2:D:163:ASP:OD1	2.33	0.59
2:E:36:PHE:CE2	2:E:40:LYS:HD2	2.37	0.59
2:F:272:ARG:HH11	2:F:272:ARG:CG	2.14	0.59
2:A:411:ASP:O	2:A:415:MSE:HG3	2.02	0.59
2:B:407:LYS:HG2	2:B:408:THR:HG23	1.83	0.59
2:C:3:LEU:O	2:C:7:LYS:CG	2.50	0.59
2:C:56:GLU:HG3	2:C:245:MSE:SE	2.53	0.59
2:C:377:LEU:HA	2:C:380:MSE:HE2	1.85	0.59
2:B:407:LYS:CG	2:B:408:THR:HG23	2.32	0.59
2:C:379:LYS:CG	2:C:412:PHE:CG	2.82	0.59
2:D:377:LEU:HD23	2:D:381:TRP:HD1	1.64	0.59
2:E:268:THR:HG21	2:E:320:LEU:H	1.68	0.59
2:E:359:ASP:OD1	2:E:359:ASP:C	2.46	0.59
2:E:411:ASP:O	2:E:415:MSE:CG	2.50	0.59
2:A:167:PRO:O	2:A:365:THR:HG21	2.03	0.59
2:A:383:LEU:O	2:A:387:ILE:HG13	2.02	0.59
2:C:214:GLU:HG2	2:C:215:GLU:H	1.68	0.59
2:E:142:ASN:HD21	2:E:306:ASN:HD21	1.51	0.59
2:E:152:GLY:CA	2:E:407:LYS:CE	2.74	0.59
2:A:187:LEU:HD21	2:A:343:LEU:CD2	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:23:LEU:CD2	2:D:41:GLN:HG3	2.33	0.59
2:E:30:ARG:O	2:E:33:ASP:N	2.36	0.59
2:E:142:ASN:OD1	2:E:306:ASN:ND2	2.35	0.59
2:A:257:LYS:HD3	2:A:309:GLU:O	2.01	0.58
2:A:390:MSE:HE1	2:A:398:PHE:CB	2.32	0.58
2:B:161:VAL:HG21	2:B:396:MSE:HE1	1.84	0.58
2:C:56:GLU:CD	2:C:66:ARG:NH1	2.61	0.58
2:C:141:ALA:HB3	2:C:370:LEU:HB2	1.45	0.58
2:C:160:ARG:NE	2:C:408:THR:H	2.01	0.58
2:D:341:MSE:HE2	2:D:342:GLU:N	2.18	0.58
2:A:272:ARG:HE	2:A:327:MSE:SE	2.36	0.58
2:D:171:GLY:H	2:D:314:THR:HG22	1.68	0.58
2:F:294:LEU:O	2:F:297:PRO:HD2	2.03	0.58
2:A:1:MSE:HG3	2:A:2:ASN:N	2.11	0.58
2:B:266:SER:HA	2:B:318:THR:O	2.02	0.58
2:C:15:ILE:CD1	2:C:27:ALA:HA	2.33	0.58
2:C:160:ARG:HE	2:C:408:THR:H	1.52	0.58
2:F:402:LYS:HZ3	2:F:415:MSE:HE1	1.66	0.58
2:B:144:ARG:NH2	2:B:163:ASP:CG	2.62	0.58
2:D:137:THR:CG2	2:D:305:ARG:HB2	2.32	0.58
2:E:272:ARG:NE	2:E:327:MSE:SE	2.86	0.58
2:F:307:VAL:HG13	2:F:309:GLU:HG2	1.85	0.58
2:C:42:HIS:O	2:C:42:HIS:ND1	2.37	0.58
2:C:167:PRO:HG2	2:C:368:GLU:HG2	1.86	0.58
2:C:205:MSE:CE	2:C:246:VAL:HG13	2.33	0.58
1:H:4:DC:N3	2:C:66:ARG:NH2	2.52	0.58
2:A:390:MSE:CE	2:A:398:PHE:HB3	2.33	0.58
2:E:141:ALA:CB	2:E:370:LEU:CD1	2.73	0.58
2:F:2:ASN:OD1	2:F:4:THR:HG22	2.02	0.58
2:F:241:GLN:O	2:F:242:VAL:C	2.45	0.58
2:F:403:LEU:C	2:F:405:MSE:H	2.12	0.58
2:A:337:GLY:O	2:B:212:ARG:HD3	2.03	0.58
2:C:338:THR:O	2:D:212:ARG:HG2	2.04	0.58
2:F:376:GLU:O	2:F:380:MSE:HG3	2.03	0.58
2:C:169:GLY:H	2:C:172:GLN:HG3	1.68	0.58
2:E:137:THR:HG22	2:E:305:ARG:CB	2.33	0.58
2:B:298:LYS:NZ	2:B:334:GLU:O	2.36	0.58
2:C:375:GLU:OE1	2:C:375:GLU:N	2.29	0.58
2:F:211:GLU:HG3	2:F:212:ARG:H	1.67	0.58
2:A:385:LYS:CE	2:B:353:ARG:HH12	2.15	0.57
2:D:139:LEU:O	2:D:141:ALA:N	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:294:LEU:CD1	2:A:334:GLU:HG3	2.33	0.57
2:E:36:PHE:HE2	2:E:40:LYS:HD2	1.69	0.57
2:E:49:ILE:HG22	2:E:101:ILE:HG13	1.85	0.57
2:E:323:THR:OG1	2:E:325:SER:HB3	2.04	0.57
2:F:168:ILE:HD13	2:F:316:ILE:HD11	1.86	0.57
2:A:373:THR:HB	2:A:375:GLU:OE1	2.03	0.57
2:B:231:THR:OG1	2:B:233:ASP:HB2	2.04	0.57
2:D:144:ARG:HD2	2:D:371:LEU:O	2.03	0.57
2:E:268:THR:HB	2:E:331:ILE:HG21	1.86	0.57
2:B:307:VAL:HG12	2:B:309:GLU:H	1.69	0.57
2:B:407:LYS:O	2:B:408:THR:OG1	2.21	0.57
2:B:198:ASN:N	2:B:198:ASN:HD22	2.02	0.57
2:C:131:ILE:HG23	2:C:133:PHE:CD2	2.38	0.57
2:B:206:VAL:HB	2:B:227:VAL:HG22	1.85	0.57
2:B:341:MSE:C	2:B:341:MSE:SE	2.98	0.57
2:C:15:ILE:HD13	2:C:27:ALA:HA	1.85	0.57
2:C:131:ILE:HA	2:C:255:GLU:OE2	2.04	0.57
2:D:133:PHE:CB	3:E:430:HOH:O	2.42	0.57
2:E:173:ARG:NH2	2:F:212:ARG:HD2	2.19	0.57
2:E:254:VAL:CG1	2:E:307:VAL:HG21	2.34	0.57
2:F:30:ARG:O	2:F:33:ASP:N	2.38	0.57
2:D:230:SER:HB3	2:D:242:VAL:HG21	1.87	0.57
2:D:388:HIS:HB3	2:D:389:PRO:HD3	1.85	0.57
2:E:167:PRO:O	2:E:365:THR:HG21	2.04	0.57
2:F:294:LEU:HD11	2:F:334:GLU:HG3	1.86	0.57
2:C:139:LEU:CD1	2:D:218:GLU:OE1	2.53	0.57
2:D:275:ASN:HD22	2:D:289:VAL:HG23	1.69	0.57
2:F:100:LYS:O	2:F:114:LEU:HB3	2.05	0.57
2:A:140:HIS:CA	2:A:306:ASN:HB3	2.35	0.57
2:E:131:ILE:HG23	2:E:133:PHE:HD2	1.68	0.57
2:F:56:GLU:OE2	2:F:241:GLN:NE2	2.38	0.57
2:D:169:GLY:N	2:D:172:GLN:HG2	2.15	0.56
2:F:185:THR:O	2:F:189:GLN:HG3	2.04	0.56
2:F:268:THR:CG2	2:F:319:ALA:HA	2.35	0.56
2:B:290:ASP:C	2:B:290:ASP:OD1	2.46	0.56
2:E:95:ASP:OD2	2:F:28:ARG:NH1	2.31	0.56
2:E:146:ARG:NH2	2:E:376:GLU:OE1	2.38	0.56
2:F:274:TYR:HD2	2:F:297:PRO:HG3	1.69	0.56
2:A:1:MSE:N	3:A:420:HOH:O	2.37	0.56
2:E:195:ILE:HD13	2:E:261:ILE:HD12	1.87	0.56
2:A:161:VAL:HG22	2:A:399:LEU:HD13	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:172:GLN:HE22	2:A:371:LEU:HD11	1.68	0.56
2:B:261:ILE:HG12	2:B:314:THR:HG21	1.85	0.56
2:D:2:ASN:OD1	2:D:4:THR:HG22	2.05	0.56
2:F:68:ALA:C	2:F:70:SER:N	2.63	0.56
2:B:261:ILE:HA	2:B:314:THR:HG23	1.88	0.56
2:D:268:THR:CG2	2:D:319:ALA:HA	2.35	0.56
2:E:56:GLU:CD	2:E:66:ARG:HE	2.14	0.56
2:A:138:PRO:HD2	2:A:306:ASN:O	2.06	0.56
2:C:133:PHE:CB	3:D:422:HOH:O	2.52	0.56
2:C:141:ALA:CA	2:C:371:LEU:CD2	2.68	0.56
2:C:160:ARG:NE	2:C:408:THR:HG23	2.20	0.56
2:E:167:PRO:HD2	2:E:365:THR:CG2	2.35	0.56
2:E:174:GLY:HA3	2:E:341:MSE:HE2	1.87	0.56
2:F:264:LEU:HB3	2:F:317:ALA:HA	1.87	0.56
1:L:4:DC:H5	2:F:110:TYR:CZ	2.24	0.56
2:A:173:ARG:NH2	2:B:214:GLU:OE2	2.25	0.56
2:B:372:THR:HB	2:B:376:GLU:HB3	1.88	0.56
2:B:416:MSE:O	2:B:417:LYS:CB	2.51	0.56
2:D:272:ARG:NH1	2:D:272:ARG:HG3	2.20	0.56
2:A:169:GLY:H	2:A:172:GLN:HG3	1.68	0.56
2:F:245:MSE:HE2	2:F:245:MSE:HA	1.87	0.56
2:D:275:ASN:ND2	2:D:289:VAL:HA	2.21	0.56
2:E:92:ARG:NH2	2:E:131:ILE:HD11	2.21	0.56
2:E:139:LEU:HD22	2:E:367:LYS:CG	2.36	0.56
2:E:290:ASP:OD1	2:E:292:ASN:N	2.39	0.56
2:F:168:ILE:HD13	2:F:316:ILE:CD1	2.36	0.56
2:A:44:LYS:O	2:A:45:SER:HB2	2.06	0.56
2:B:316:ILE:HD12	2:B:341:MSE:HE2	1.87	0.56
2:E:31:LYS:O	2:E:35:ILE:HD12	2.06	0.56
2:B:355:PHE:O	2:B:357:ALA:N	2.39	0.55
2:C:416:MSE:O	2:C:417:LYS:CB	2.51	0.55
2:F:162:LEU:HD12	2:F:187:LEU:HD11	1.88	0.55
2:A:357:ALA:O	2:A:358:ILE:HG13	2.05	0.55
2:C:355:PHE:HB2	2:C:356:PRO:CD	2.34	0.55
2:E:289:VAL:HB	2:E:327:MSE:HE3	1.87	0.55
2:E:376:GLU:O	2:E:380:MSE:HG3	2.05	0.55
2:B:352:LYS:C	2:B:354:VAL:H	2.15	0.55
2:C:205:MSE:HE2	2:C:246:VAL:HG13	1.88	0.55
2:D:248:GLU:O	2:D:249:LYS:C	2.49	0.55
2:E:30:ARG:O	2:E:31:LYS:C	2.50	0.55
2:E:405:MSE:O	2:E:406:THR:HG23	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:341:MSE:C	2:A:341:MSE:CE	2.76	0.55
2:D:296:ARG:O	2:D:299:ARG:HB2	2.06	0.55
2:E:377:LEU:HD23	2:E:381:TRP:HE1	1.72	0.55
2:F:49:ILE:HG22	2:F:101:ILE:CD1	2.31	0.55
2:F:141:ALA:O	2:F:370:LEU:HB3	2.06	0.55
2:F:169:GLY:O	2:F:172:GLN:HG3	2.06	0.55
2:F:353:ARG:HG3	2:F:353:ARG:NH1	2.19	0.55
1:L:3:DC:O2	2:F:109:ARG:HB2	2.06	0.55
2:B:240:VAL:HG13	2:B:274:TYR:CZ	2.42	0.55
2:B:272:ARG:NE	2:B:327:MSE:SE	2.89	0.55
2:F:85:GLN:NE2	2:F:113:LEU:O	2.32	0.55
2:F:252:ARG:O	2:F:255:GLU:HB2	2.06	0.55
2:C:257:LYS:HE2	2:C:309:GLU:O	2.07	0.55
2:F:355:PHE:O	2:F:356:PRO:C	2.47	0.55
2:A:88:ARG:O	2:A:88:ARG:HG3	2.07	0.55
2:B:244:GLU:OE2	2:B:296:ARG:NH2	2.37	0.55
2:F:184:LYS:HD2	2:F:318:THR:HG21	1.88	0.55
2:B:154:THR:O	2:B:157:LEU:HB2	2.07	0.55
2:C:113:LEU:HD21	2:C:116:VAL:HG22	1.89	0.55
2:D:252:ARG:NH1	2:D:255:GLU:OE2	2.39	0.55
2:E:91:LEU:HD13	2:E:97:ILE:CD1	2.37	0.55
2:E:144:ARG:HG3	2:E:145:LEU:N	2.21	0.55
2:E:187:LEU:HG	2:E:191:ILE:HD11	1.89	0.55
2:B:206:VAL:HG22	2:B:263:LEU:HB2	1.89	0.55
2:B:245:MSE:HE2	2:B:245:MSE:CA	2.37	0.55
2:E:140:HIS:HA	2:E:306:ASN:HB2	1.88	0.55
2:F:60:ASP:CB	2:F:62:PHE:HE2	2.20	0.55
2:F:382:ILE:HD13	2:F:416:MSE:HE1	1.87	0.55
2:C:26:LEU:HB3	2:C:29:MSE:HG2	1.89	0.55
2:C:70:SER:O	2:C:71:SER:C	2.49	0.55
2:C:308:GLU:HB3	2:C:309:GLU:OE2	2.07	0.55
2:D:294:LEU:CD1	2:D:334:GLU:HG3	2.38	0.55
2:E:139:LEU:HD22	2:E:367:LYS:HG3	1.87	0.55
2:E:381:TRP:CD2	2:F:353:ARG:NH1	2.75	0.55
2:F:376:GLU:HA	2:F:379:LYS:HD2	1.88	0.55
2:B:139:LEU:C	2:B:141:ALA:N	2.64	0.54
2:C:1:MSE:HG3	2:C:2:ASN:N	2.22	0.54
2:F:160:ARG:O	2:F:164:LEU:HG	2.07	0.54
2:A:263:LEU:HD22	2:A:316:ILE:HB	1.88	0.54
2:A:390:MSE:CE	2:A:395:ALA:HA	2.24	0.54
2:D:139:LEU:CD1	2:E:214:GLU:HG3	2.32	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:173:ARG:HD3	2:D:301:PHE:O	2.06	0.54
2:E:141:ALA:HB3	2:E:370:LEU:HD13	1.84	0.54
2:F:275:ASN:HD21	2:F:289:VAL:HA	1.73	0.54
2:B:289:VAL:HG11	2:B:330:VAL:CG1	2.36	0.54
2:E:343:LEU:HD11	2:E:358:ILE:CG2	2.36	0.54
2:E:368:GLU:HA	2:E:371:LEU:HD12	1.89	0.54
2:F:264:LEU:HD23	2:F:317:ALA:HB1	1.88	0.54
2:B:139:LEU:HA	2:C:214:GLU:HB2	1.89	0.54
2:B:146:ARG:NH2	2:B:376:GLU:OE1	2.40	0.54
2:C:7:LYS:HA	2:C:35:ILE:HD11	1.90	0.54
2:E:140:HIS:CB	2:E:306:ASN:CB	2.78	0.54
2:F:60:ASP:CB	2:F:62:PHE:CE2	2.88	0.54
2:B:171:GLY:H	2:B:314:THR:HB	1.73	0.54
2:B:321:ILE:CD1	2:B:332:TYR:CG	2.88	0.54
2:C:296:ARG:HB2	2:C:297:PRO:HD3	1.90	0.54
2:D:147:MSE:HE1	2:D:191:ILE:HA	1.89	0.54
2:D:252:ARG:NH1	2:D:255:GLU:CD	2.65	0.54
2:A:7:LYS:HA	2:A:35:ILE:HD11	1.90	0.54
2:A:403:LEU:C	2:A:405:MSE:H	2.16	0.54
2:D:321:ILE:HD11	2:D:332:TYR:CE2	2.42	0.54
2:F:11:VAL:O	2:F:15:ILE:HG13	2.08	0.54
2:F:206:VAL:HG22	2:F:263:LEU:HD12	1.89	0.54
2:F:258:LYS:O	2:F:312:SER:N	2.40	0.54
2:C:309:GLU:OE2	2:C:309:GLU:N	2.41	0.54
2:D:272:ARG:HD2	2:D:327:MSE:SE	2.57	0.54
2:E:59:GLN:O	2:E:59:GLN:NE2	2.40	0.54
2:E:236:ALA:HB1	2:E:277:VAL:HG23	1.89	0.54
2:F:380:MSE:HG2	2:F:412:PHE:CZ	2.42	0.54
2:A:39:LEU:HD13	2:A:111:PHE:CZ	2.43	0.54
2:E:409:ASN:C	2:E:411:ASP:H	2.16	0.54
2:A:194:SER:O	2:A:198:ASN:HB2	2.08	0.54
2:B:365:THR:HG23	2:B:368:GLU:HG2	1.89	0.54
2:C:294:LEU:HD12	2:C:334:GLU:HG3	1.90	0.54
1:L:3:DC:H4'	1:L:4:DC:O5'	2.08	0.53
2:A:187:LEU:O	2:A:191:ILE:HG13	2.08	0.53
2:C:381:TRP:HB3	2:D:353:ARG:HH21	1.71	0.53
2:C:402:LYS:HD3	2:C:415:MSE:HE1	1.89	0.53
2:D:119:VAL:O	2:D:120:ASN:HB2	2.07	0.53
2:E:65:LEU:HD21	2:E:97:ILE:HD12	1.89	0.53
2:F:253:LEU:O	2:F:258:LYS:HB2	2.08	0.53
2:A:161:VAL:HG11	2:A:396:MSE:CE	2.34	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:272:ARG:HE	2:B:327:MSE:CG	2.21	0.53
2:D:228:VAL:HG12	2:D:242:VAL:CG1	2.38	0.53
2:E:173:ARG:HH21	2:F:212:ARG:CD	2.19	0.53
2:F:280:ALA:HA	2:F:290:ASP:OD2	2.09	0.53
2:A:41:GLN:C	2:A:43:ALA:N	2.67	0.53
2:B:137:THR:CG2	2:B:305:ARG:HH11	2.21	0.53
2:C:132:LEU:HD22	2:C:251:LYS:HD3	1.90	0.53
2:C:169:GLY:H	2:C:172:GLN:HG2	1.74	0.53
2:F:219:MSE:HG3	2:F:223:VAL:HG23	1.91	0.53
2:B:67:SER:HB2	2:B:69:ASP:OD1	2.08	0.53
2:D:164:LEU:O	2:D:380:MSE:HE3	2.09	0.53
2:E:290:ASP:OD1	2:E:290:ASP:C	2.52	0.53
2:F:355:PHE:O	2:F:357:ALA:N	2.41	0.53
2:B:140:HIS:HA	2:B:306:ASN:HD22	1.74	0.53
2:B:173:ARG:HH22	2:C:214:GLU:CD	2.17	0.53
2:C:348:LYS:HD2	2:C:392:GLU:OE1	2.09	0.53
2:D:290:ASP:OD1	2:D:292:ASN:HB3	2.07	0.53
2:E:3:LEU:HD12	2:E:39:LEU:HD11	1.90	0.53
2:A:170:ARG:NH1	2:A:201:ASP:OD2	2.42	0.53
2:E:144:ARG:HH21	2:E:163:ASP:CG	2.16	0.53
2:E:298:LYS:O	2:E:302:GLY:N	2.27	0.53
2:A:252:ARG:HH11	2:A:255:GLU:CD	2.14	0.53
2:B:173:ARG:HH22	2:C:212:ARG:HB3	1.73	0.53
2:E:228:VAL:HG12	2:E:242:VAL:HG13	1.91	0.53
2:F:86:ILE:HA	2:F:91:LEU:HD12	1.90	0.53
1:J:3:DC:H4'	1:J:4:DC:C5'	2.38	0.53
2:B:173:ARG:HD2	2:B:301:PHE:O	2.08	0.53
2:E:272:ARG:NH1	2:E:272:ARG:CG	2.62	0.53
2:F:56:GLU:HG3	2:F:245:MSE:CE	2.36	0.53
2:B:91:LEU:HD22	2:B:97:ILE:HD11	1.89	0.53
2:C:173:ARG:NH2	2:D:213:PRO:HD2	2.24	0.53
2:D:171:GLY:H	2:D:314:THR:CG2	2.21	0.53
2:D:211:GLU:HG3	2:D:215:GLU:HB3	1.90	0.53
2:E:411:ASP:CG	2:E:412:PHE:N	2.67	0.53
2:F:15:ILE:CD1	2:F:27:ALA:HA	2.39	0.53
2:C:415:MSE:N	3:C:421:HOH:O	2.42	0.53
2:D:26:LEU:HB3	2:D:29:MSE:SE	2.59	0.53
2:E:140:HIS:CA	2:E:306:ASN:CB	2.87	0.53
2:C:375:GLU:CD	2:C:375:GLU:N	2.67	0.52
2:D:60:ASP:HB2	2:D:62:PHE:HE2	1.70	0.52
2:E:147:MSE:HE1	2:E:195:ILE:HG12	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:144:ARG:HD3	2:F:146:ARG:NE	2.24	0.52
2:F:162:LEU:CD1	2:F:187:LEU:HD11	2.39	0.52
2:A:136:LEU:HD13	2:B:221:ARG:HH21	1.74	0.52
2:A:387:ILE:HA	2:A:390:MSE:SE	2.59	0.52
2:B:144:ARG:HH21	2:B:163:ASP:CG	2.18	0.52
2:E:23:LEU:HD21	2:E:41:GLN:CG	2.33	0.52
2:F:382:ILE:CD1	2:F:416:MSE:HE1	2.38	0.52
2:A:62:PHE:HE1	2:A:64:PHE:HE2	1.57	0.52
2:B:240:VAL:HG13	2:B:274:TYR:CE1	2.44	0.52
2:B:245:MSE:HA	2:B:245:MSE:CE	2.39	0.52
2:B:307:VAL:HG12	2:B:309:GLU:N	2.22	0.52
2:E:187:LEU:HD21	2:E:343:LEU:HD23	1.91	0.52
2:A:166:SER:HA	2:A:365:THR:HG22	1.91	0.52
2:B:130:LYS:HZ3	2:C:12:SER:H	1.58	0.52
2:B:144:ARG:CG	2:B:145:LEU:N	2.71	0.52
2:B:173:ARG:CD	2:B:301:PHE:O	2.58	0.52
2:B:234:GLU:CD	2:B:238:ARG:HG2	2.33	0.52
2:D:275:ASN:ND2	2:D:289:VAL:HG23	2.24	0.52
2:E:266:SER:HB2	2:E:269:ARG:H	1.74	0.52
2:C:294:LEU:HD13	2:C:334:GLU:HG3	1.88	0.52
2:E:105:LYS:N	2:E:108:GLU:OE1	2.41	0.52
2:E:144:ARG:NH2	2:E:163:ASP:CG	2.67	0.52
2:A:406:THR:HB	2:A:410:ASP:HB2	1.91	0.52
2:B:356:PRO:C	2:B:358:ILE:H	2.17	0.52
2:C:141:ALA:O	2:C:370:LEU:O	2.27	0.52
2:D:5:GLU:O	2:D:9:THR:HG22	2.10	0.52
2:D:372:THR:HG22	2:D:376:GLU:CD	2.34	0.52
2:D:382:ILE:O	2:D:386:ILE:HG22	2.09	0.52
2:E:274:TYR:O	2:E:278:VAL:HB	2.09	0.52
2:F:52:ASP:HA	2:F:97:ILE:O	2.09	0.52
2:C:173:ARG:CD	2:C:301:PHE:O	2.57	0.52
2:E:55:LEU:HB2	2:E:65:LEU:HD23	1.91	0.52
2:C:30:ARG:O	2:C:31:LYS:C	2.52	0.52
2:C:268:THR:HA	2:C:331:ILE:HG21	1.92	0.52
2:C:343:LEU:HD11	2:C:358:ILE:HD13	1.92	0.52
2:E:170:ARG:HD3	2:E:259:ASP:OD2	2.09	0.52
2:E:214:GLU:HG2	2:E:215:GLU:N	2.24	0.52
2:E:294:LEU:C	2:E:297:PRO:HD2	2.35	0.52
2:E:378:GLN:O	2:E:382:ILE:HG13	2.10	0.52
2:A:173:ARG:CD	2:A:301:PHE:O	2.58	0.52
2:B:269:ARG:NH1	2:B:272:ARG:NH1	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:244:GLU:OE2	2:D:274:TYR:OH	2.25	0.52
2:B:141:ALA:CB	2:B:370:LEU:HB2	2.36	0.52
2:B:156:ASP:O	2:B:160:ARG:HB2	2.10	0.52
2:C:26:LEU:HD22	2:C:29:MSE:HE3	1.92	0.52
2:C:131:ILE:HG22	2:C:134:GLU:HG2	1.92	0.52
2:D:71:SER:HA	2:D:228:VAL:HG13	1.92	0.52
2:D:272:ARG:HH11	2:D:272:ARG:HG3	1.72	0.52
2:E:137:THR:HG21	2:E:305:ARG:CZ	2.40	0.52
2:E:264:LEU:HB3	2:E:317:ALA:HB2	1.92	0.52
2:F:132:LEU:HD13	2:F:251:LYS:HA	1.91	0.52
2:A:272:ARG:CD	2:A:327:MSE:SE	3.09	0.51
2:B:139:LEU:HD13	2:C:214:GLU:HG3	1.91	0.51
2:C:71:SER:OG	2:C:228:VAL:HA	2.10	0.51
1:J:4:DC:H5	2:D:110:TYR:CZ	2.28	0.51
2:B:355:PHE:HB2	2:B:356:PRO:HD2	1.92	0.51
2:C:6:LEU:O	2:C:9:THR:HG23	2.09	0.51
2:C:231:THR:C	2:C:233:ASP:N	2.69	0.51
2:A:266:SER:HG	2:A:269:ARG:H	1.55	0.51
2:B:316:ILE:HD12	2:B:341:MSE:HE3	1.92	0.51
2:C:265:ASP:O	2:C:266:SER:CB	2.58	0.51
2:E:321:ILE:HD11	2:E:332:TYR:CB	2.40	0.51
2:B:236:ALA:O	2:B:240:VAL:HG23	2.10	0.51
2:B:274:TYR:HE1	2:B:296:ARG:CZ	2.23	0.51
2:D:46:GLY:O	2:D:47:GLU:HB2	2.10	0.51
2:D:205:MSE:HE3	2:D:226:GLU:CD	2.35	0.51
2:F:39:LEU:HD23	3:F:425:HOH:O	2.10	0.51
2:F:72:TYR:CD2	2:F:245:MSE:HG2	2.46	0.51
2:F:160:ARG:CD	2:F:408:THR:HB	2.39	0.51
2:F:208:LEU:HB2	2:F:229:ALA:CB	2.40	0.51
2:F:356:PRO:C	2:F:358:ILE:N	2.69	0.51
1:L:3:DC:O2	2:F:109:ARG:N	2.40	0.51
2:B:299:ARG:O	2:B:300:PHE:C	2.54	0.51
2:E:168:ILE:HA	2:E:172:GLN:HG3	1.92	0.51
2:E:209:ILE:HG22	2:E:210:ASP:HB2	1.93	0.51
2:E:254:VAL:HG11	2:E:307:VAL:HG21	1.92	0.51
2:E:349:ILE:HD12	2:E:357:ALA:O	2.11	0.51
2:F:5:GLU:O	2:F:9:THR:HG22	2.10	0.51
2:F:266:SER:HA	2:F:318:THR:O	2.11	0.51
2:D:140:HIS:O	2:D:141:ALA:HB2	2.10	0.51
2:D:207:LEU:HD23	2:D:264:LEU:HD13	1.92	0.51
2:D:264:LEU:C	2:D:264:LEU:HD12	2.35	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:30:ARG:O	2:E:32:GLN:N	2.44	0.51
2:F:294:LEU:CD1	2:F:334:GLU:HG3	2.41	0.51
2:F:326:LYS:O	2:F:330:VAL:HG23	2.11	0.51
2:D:226:GLU:OE2	2:D:249:LYS:HE3	2.10	0.51
2:F:14:LEU:O	2:F:38:ILE:HD11	2.11	0.51
2:A:175:LEU:H	2:A:341:MSE:CE	2.23	0.51
2:B:137:THR:CG2	2:B:305:ARG:NH1	2.73	0.51
2:B:154:THR:HA	2:B:157:LEU:HG	1.91	0.51
2:C:47:GLU:HG3	2:C:100:LYS:HZ3	1.76	0.51
2:C:265:ASP:O	2:C:266:SER:HB2	2.09	0.51
2:E:173:ARG:HH22	2:F:214:GLU:CD	2.18	0.51
2:F:105:LYS:O	2:F:106:GLU:C	2.54	0.51
2:F:381:TRP:HB3	2:F:385:LYS:HE3	1.92	0.51
2:F:390:MSE:HE1	2:F:398:PHE:CB	2.34	0.51
2:C:170:ARG:HD3	2:C:259:ASP:OD2	2.10	0.51
2:C:260:VAL:CG1	2:C:261:ILE:N	2.73	0.51
2:E:92:ARG:O	2:E:95:ASP:HB2	2.11	0.51
2:A:405:MSE:O	2:A:406:THR:CG2	2.56	0.51
2:C:1:MSE:CG	2:C:2:ASN:N	2.74	0.51
2:C:130:LYS:HZ3	2:D:12:SER:H	1.59	0.51
2:D:308:GLU:CD	2:E:221:ARG:HH22	2.19	0.51
2:E:326:LYS:O	2:E:329:GLU:HB2	2.10	0.51
2:E:382:ILE:O	2:E:386:ILE:CG2	2.59	0.51
2:A:369:GLU:HG2	2:A:370:LEU:HD12	1.94	0.50
2:D:73:LEU:HB2	2:D:238:ARG:NH2	2.26	0.50
2:E:136:LEU:CD1	2:F:221:ARG:NH2	2.67	0.50
2:D:264:LEU:HD12	2:D:265:ASP:N	2.25	0.50
2:F:293:ALA:O	2:F:295:HIS:N	2.45	0.50
2:A:172:GLN:HA	2:A:340:ASN:HD21	1.76	0.50
2:A:236:ALA:CA	2:A:239:HIS:HD2	2.21	0.50
2:A:390:MSE:CE	2:A:398:PHE:CB	2.90	0.50
2:B:71:SER:OG	2:B:229:ALA:N	2.41	0.50
2:B:402:LYS:HD3	2:B:405:MSE:CE	2.41	0.50
2:C:23:LEU:CG	2:C:41:GLN:HG3	2.41	0.50
2:E:130:LYS:HE2	2:F:11:VAL:HB	1.92	0.50
2:E:382:ILE:O	2:E:386:ILE:HG23	2.12	0.50
2:C:406:THR:OG1	2:C:411:ASP:N	2.45	0.50
2:C:415:MSE:O	2:C:415:MSE:CG	2.53	0.50
2:A:42:HIS:CE1	3:A:420:HOH:O	2.63	0.50
2:A:141:ALA:O	2:A:370:LEU:C	2.55	0.50
2:B:376:GLU:O	2:B:380:MSE:HG3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:390:MSE:HE2	2:B:394:ASP:HB3	1.93	0.50
2:F:64:PHE:HA	2:F:79:ILE:O	2.11	0.50
2:F:380:MSE:HG2	2:F:412:PHE:HZ	1.76	0.50
2:D:132:LEU:HB3	2:D:251:LYS:HD3	1.93	0.50
2:F:356:PRO:HB2	2:F:396:MSE:HE2	1.93	0.50
2:B:409:ASN:C	2:B:411:ASP:H	2.20	0.50
2:C:186:MSE:O	2:C:187:LEU:C	2.54	0.50
2:C:356:PRO:O	2:C:357:ALA:C	2.53	0.50
2:C:91:LEU:N	2:C:91:LEU:HD23	2.27	0.50
2:C:177:VAL:CG1	2:C:321:ILE:HD13	2.38	0.50
2:C:377:LEU:HD12	2:C:380:MSE:HE2	1.94	0.50
2:D:65:LEU:HD11	2:D:97:ILE:HB	1.93	0.50
2:D:205:MSE:HE3	2:D:226:GLU:OE2	2.10	0.50
2:D:369:GLU:HA	2:D:377:LEU:CD1	2.41	0.50
2:E:92:ARG:CZ	2:E:131:ILE:HD11	2.42	0.50
2:E:132:LEU:HD22	2:E:251:LYS:CD	2.32	0.50
2:F:46:GLY:C	2:F:48:ASP:H	2.20	0.50
2:F:141:ALA:HB3	2:F:370:LEU:HD13	1.93	0.50
2:A:50:PHE:HE1	2:A:100:LYS:HG2	1.74	0.50
2:C:137:THR:HG23	2:C:305:ARG:HB2	1.94	0.50
2:C:138:PRO:HD2	2:C:306:ASN:O	2.12	0.50
2:D:120:ASN:O	2:D:121:PHE:HB2	2.12	0.50
2:D:123:LYS:HB2	2:D:126:ASN:CG	2.37	0.50
2:E:103:PRO:HA	2:E:111:PHE:CD1	2.47	0.50
2:E:123:LYS:O	2:E:126:ASN:N	2.44	0.50
2:A:137:THR:HG22	2:A:305:ARG:HD3	1.93	0.49
2:B:268:THR:HG21	2:B:320:LEU:N	2.20	0.49
2:B:352:LYS:HB3	2:B:354:VAL:HG23	1.93	0.49
2:C:347:ARG:O	2:C:348:LYS:C	2.54	0.49
2:A:307:VAL:HB	2:A:311:GLY:O	2.11	0.49
2:E:152:GLY:N	2:E:407:LYS:CE	2.75	0.49
2:A:268:THR:O	2:A:272:ARG:HG2	2.12	0.49
2:B:227:VAL:HG12	2:B:227:VAL:O	2.13	0.49
2:C:131:ILE:O	2:C:132:LEU:C	2.55	0.49
2:D:123:LYS:O	2:D:125:GLU:N	2.46	0.49
2:D:169:GLY:O	2:D:172:GLN:HG2	2.13	0.49
2:D:254:VAL:C	2:D:256:HIS:H	2.20	0.49
2:D:260:VAL:CG1	2:D:261:ILE:N	2.75	0.49
2:D:399:LEU:O	2:D:403:LEU:HD12	2.11	0.49
2:E:91:LEU:HD13	2:E:97:ILE:HD11	1.93	0.49
2:F:144:ARG:HD3	2:F:146:ARG:HE	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:267:ILE:HG22	2:F:318:THR:O	2.13	0.49
2:C:139:LEU:HD13	2:C:367:LYS:HD2	1.93	0.49
2:C:275:ASN:ND2	2:C:289:VAL:HA	2.27	0.49
2:D:405:MSE:HE2	2:D:405:MSE:HA	1.95	0.49
2:E:252:ARG:NH1	2:E:255:GLU:CD	2.70	0.49
2:E:343:LEU:CD1	2:E:358:ILE:HG23	2.43	0.49
2:F:141:ALA:HB1	2:F:370:LEU:HB3	1.88	0.49
2:F:399:LEU:HD22	2:F:403:LEU:HD11	1.95	0.49
2:B:52:ASP:HA	2:B:97:ILE:O	2.12	0.49
2:E:211:GLU:HG3	2:E:212:ARG:N	2.27	0.49
2:F:331:ILE:O	2:F:332:TYR:C	2.53	0.49
2:B:160:ARG:CZ	2:B:407:LYS:HA	2.42	0.49
2:D:348:LYS:HD2	2:D:392:GLU:OE1	2.12	0.49
2:F:182:ALA:HB1	2:F:345:LEU:HB3	1.94	0.49
2:A:44:LYS:O	2:A:45:SER:CB	2.60	0.49
2:B:268:THR:CG2	2:B:319:ALA:HA	2.43	0.49
2:C:250:ALA:O	2:C:254:VAL:HG23	2.13	0.49
2:C:254:VAL:HG21	2:C:313:LEU:HB2	1.94	0.49
2:C:378:GLN:O	2:C:382:ILE:HD12	2.13	0.49
2:E:49:ILE:CG2	2:E:101:ILE:CG1	2.91	0.49
2:E:66:ARG:HG2	2:E:66:ARG:NH1	2.28	0.49
2:F:254:VAL:C	2:F:256:HIS:N	2.71	0.49
2:A:198:ASN:HB3	2:A:199:HIS:CD2	2.48	0.49
2:A:228:VAL:HG12	2:A:242:VAL:CG1	2.43	0.49
2:B:382:ILE:O	2:B:386:ILE:HG22	2.12	0.49
2:C:158:THR:O	2:C:162:LEU:HB2	2.12	0.49
2:C:346:SER:HB3	2:C:349:ILE:HG13	1.95	0.49
2:E:207:LEU:HD13	2:E:246:VAL:HG21	1.93	0.49
2:E:338:THR:O	2:F:212:ARG:HD3	2.13	0.49
2:F:73:LEU:O	2:F:74:ALA:C	2.51	0.49
2:A:57:ILE:HG13	2:A:93:THR:HG22	1.94	0.48
2:A:86:ILE:HA	2:A:91:LEU:HD12	1.94	0.48
2:A:146:ARG:NH2	2:A:376:GLU:OE1	2.46	0.48
2:A:189:GLN:O	2:A:193:GLN:HG3	2.12	0.48
2:B:238:ARG:NH1	2:B:242:VAL:HG23	2.28	0.48
2:B:321:ILE:HD11	2:B:332:TYR:CB	2.43	0.48
2:C:55:LEU:HD12	2:C:64:PHE:O	2.13	0.48
2:C:71:SER:OG	2:C:229:ALA:N	2.39	0.48
2:E:355:PHE:CD2	3:E:424:HOH:O	2.55	0.48
2:F:184:LYS:HZ3	2:F:265:ASP:CG	2.21	0.48
2:F:207:LEU:HD11	2:F:242:VAL:HG12	1.89	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:303:ALA:O	2:A:305:ARG:NE	2.39	0.48
2:B:58:LEU:HD12	2:B:59:GLN:H	1.77	0.48
2:C:167:PRO:CD	2:C:365:THR:CG2	2.90	0.48
2:D:206:VAL:HG22	2:D:263:LEU:HB2	1.95	0.48
2:D:261:ILE:HG12	2:D:314:THR:CG2	2.39	0.48
2:A:321:ILE:HD11	2:A:332:TYR:CD2	2.47	0.48
2:D:156:ASP:OD1	2:D:160:ARG:HG2	2.13	0.48
2:E:73:LEU:O	2:E:74:ALA:C	2.54	0.48
2:E:131:ILE:HG22	2:E:134:GLU:HG2	1.95	0.48
2:F:1:MSE:HG3	2:F:2:ASN:H	1.79	0.48
2:B:306:ASN:OD1	2:B:306:ASN:C	2.56	0.48
2:D:74:ALA:HA	2:D:78:ASP:OD2	2.12	0.48
2:E:236:ALA:HB3	2:E:277:VAL:HG23	1.95	0.48
2:F:6:LEU:O	2:F:9:THR:CG2	2.61	0.48
2:A:275:ASN:ND2	2:A:289:VAL:HA	2.27	0.48
2:C:167:PRO:N	2:C:365:THR:HG21	2.29	0.48
2:D:355:PHE:C	2:D:357:ALA:N	2.71	0.48
2:F:264:LEU:HD23	2:F:317:ALA:CB	2.44	0.48
2:F:335:PHE:O	2:F:336:LYS:C	2.55	0.48
2:F:359:ASP:OD1	2:F:362:ARG:HB2	2.14	0.48
2:A:289:VAL:CG1	2:A:330:VAL:HG11	2.43	0.48
2:A:372:THR:HG21	2:A:380:MSE:HE2	1.96	0.48
2:C:120:ASN:HB3	2:C:256:HIS:CD2	2.48	0.48
2:D:184:LYS:HG3	2:D:318:THR:HG21	1.95	0.48
2:D:390:MSE:HE1	2:D:398:PHE:CD2	2.49	0.48
2:E:356:PRO:CB	2:E:396:MSE:CE	2.82	0.48
2:D:57:ILE:H	2:D:93:THR:HB	1.78	0.48
2:D:147:MSE:CE	2:D:191:ILE:HG23	2.41	0.48
2:E:252:ARG:NH1	2:E:252:ARG:N	2.62	0.48
2:F:46:GLY:O	2:F:47:GLU:HB2	2.13	0.48
2:A:39:LEU:O	2:A:49:ILE:HD11	2.14	0.48
2:A:245:MSE:HE3	2:A:245:MSE:CA	2.40	0.48
2:D:206:VAL:HB	2:D:227:VAL:HG22	1.96	0.48
2:F:138:PRO:O	2:F:140:HIS:N	2.47	0.48
2:C:294:LEU:C	2:C:297:PRO:HD2	2.39	0.48
1:K:3:DC:H4'	1:K:4:DC:O5'	2.13	0.48
2:A:91:LEU:HD22	2:A:97:ILE:HD11	1.94	0.48
2:C:187:LEU:O	2:C:187:LEU:HD12	2.14	0.48
2:E:1:MSE:CG	2:E:2:ASN:H	2.26	0.48
2:E:278:VAL:O	2:E:279:PRO:C	2.57	0.48
2:A:170:ARG:NH1	2:A:202:CYS:SG	2.87	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:272:ARG:HE	2:B:327:MSE:SE	2.47	0.47
2:C:355:PHE:CB	2:C:356:PRO:CD	2.92	0.47
2:D:271:ALA:HB3	2:D:331:ILE:HD13	1.96	0.47
2:E:137:THR:CG2	2:E:305:ARG:CD	2.90	0.47
2:A:178:ALA:HB2	2:A:345:LEU:HD12	1.96	0.47
2:B:139:LEU:O	2:B:140:HIS:C	2.57	0.47
2:C:207:LEU:HD11	2:C:242:VAL:HG12	1.96	0.47
2:E:123:LYS:O	2:E:125:GLU:N	2.47	0.47
2:E:245:MSE:HE2	2:E:245:MSE:HA	1.96	0.47
2:E:393:ILE:H	2:E:393:ILE:HG12	1.37	0.47
2:F:254:VAL:O	2:F:257:LYS:N	2.47	0.47
2:F:257:LYS:HD3	2:F:309:GLU:O	2.14	0.47
1:L:4:DC:H42	2:F:66:ARG:HH12	1.62	0.47
2:C:146:ARG:NH2	2:C:376:GLU:OE1	2.42	0.47
2:D:131:ILE:HG22	2:D:132:LEU:N	2.28	0.47
2:D:131:ILE:HG22	2:D:133:PHE:N	2.18	0.47
2:E:366:ARG:NH1	2:E:366:ARG:CG	2.74	0.47
2:F:2:ASN:HD22	2:F:50:PHE:HB2	1.79	0.47
2:A:137:THR:HG21	2:A:305:ARG:NH1	2.29	0.47
2:A:144:ARG:NH1	2:A:163:ASP:OD1	2.47	0.47
2:A:266:SER:OG	2:A:269:ARG:CB	2.63	0.47
2:A:296:ARG:HB2	2:A:297:PRO:CD	2.44	0.47
2:B:70:SER:HB3	2:B:73:LEU:HB3	1.95	0.47
2:A:26:LEU:O	2:A:27:ALA:C	2.56	0.47
2:A:173:ARG:NH2	2:B:212:ARG:HB3	2.30	0.47
2:A:175:LEU:N	2:A:341:MSE:CE	2.78	0.47
2:C:406:THR:OG1	2:C:407:LYS:N	2.47	0.47
2:D:23:LEU:HD21	2:D:41:GLN:CG	2.44	0.47
2:D:141:ALA:HB1	2:D:371:LEU:HG	1.95	0.47
2:D:144:ARG:NH1	2:D:376:GLU:OE2	2.48	0.47
2:E:49:ILE:HG22	2:E:101:ILE:HG12	1.96	0.47
2:E:175:LEU:H	2:E:341:MSE:CE	2.28	0.47
2:A:49:ILE:HG22	2:A:101:ILE:O	2.15	0.47
2:A:145:LEU:HD21	2:A:170:ARG:CG	2.44	0.47
2:E:131:ILE:HG23	2:E:133:PHE:CD2	2.49	0.47
1:K:4:DC:N4	2:E:78:ASP:OD2	2.48	0.47
2:A:144:ARG:CG	2:A:145:LEU:N	2.64	0.47
2:C:137:THR:HG22	2:D:214:GLU:CB	2.44	0.47
2:C:177:VAL:HG11	2:C:321:ILE:CD1	2.36	0.47
2:C:228:VAL:HG12	2:C:242:VAL:HG13	1.94	0.47
2:D:60:ASP:CB	2:D:62:PHE:HE2	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:66:ARG:HG2	2:D:66:ARG:NH1	2.27	0.47
2:D:134:GLU:OE2	2:E:29:MSE:O	2.32	0.47
2:D:293:ALA:O	2:D:295:HIS:N	2.47	0.47
2:D:294:LEU:HD13	2:D:334:GLU:HG3	1.95	0.47
2:E:157:LEU:HD13	2:E:400:ILE:HG23	1.97	0.47
2:B:70:SER:O	2:B:71:SER:C	2.58	0.47
2:B:173:ARG:CD	2:B:304:ALA:HB3	2.43	0.47
2:C:140:HIS:HA	2:C:306:ASN:HD22	1.79	0.47
2:C:377:LEU:HD12	2:C:380:MSE:CE	2.45	0.47
2:E:169:GLY:O	2:E:171:GLY:N	2.48	0.47
2:E:205:MSE:O	2:E:262:ILE:HA	2.15	0.47
2:E:390:MSE:HE2	2:E:395:ALA:N	2.30	0.47
2:F:393:ILE:O	2:F:394:ASP:C	2.58	0.47
2:A:284:VAL:HG12	2:A:284:VAL:O	2.15	0.47
2:B:54:VAL:HG21	2:B:249:LYS:HD2	1.97	0.47
2:B:387:ILE:HG22	2:B:387:ILE:O	2.13	0.47
2:C:264:LEU:HD22	2:C:300:PHE:CE2	2.50	0.47
2:D:267:ILE:HG23	2:D:268:THR:N	2.30	0.47
2:E:20:ASN:C	2:E:22:GLY:H	2.21	0.47
2:E:23:LEU:CD2	2:E:41:GLN:HG3	2.33	0.47
2:B:102:ARG:HB3	2:B:114:LEU:CD1	2.45	0.47
2:B:139:LEU:C	2:B:141:ALA:H	2.22	0.47
2:B:140:HIS:CB	2:B:306:ASN:HB3	2.44	0.47
2:B:402:LYS:HD3	2:B:405:MSE:HE2	1.97	0.47
2:C:56:GLU:CG	2:C:245:MSE:HE1	2.45	0.47
2:C:296:ARG:O	2:C:299:ARG:HB2	2.15	0.47
2:D:169:GLY:H	2:D:172:GLN:HG3	1.74	0.47
2:E:416:MSE:O	2:E:417:LYS:CB	2.55	0.47
2:A:105:LYS:HG3	2:A:108:GLU:OE1	2.16	0.46
2:A:228:VAL:CG1	2:A:242:VAL:HG13	2.45	0.46
2:B:250:ALA:HB1	2:B:313:LEU:CD1	2.45	0.46
2:C:1:MSE:HG3	2:C:2:ASN:H	1.79	0.46
2:C:4:THR:O	2:C:7:LYS:HG3	2.15	0.46
2:E:409:ASN:O	2:E:411:ASP:N	2.49	0.46
2:B:247:ILE:O	2:B:251:LYS:HG3	2.15	0.46
2:B:270:LEU:O	2:B:273:ALA:HB3	2.15	0.46
2:C:206:VAL:HB	2:C:227:VAL:HG22	1.98	0.46
2:C:356:PRO:C	2:C:358:ILE:N	2.73	0.46
2:D:131:ILE:HA	2:D:255:GLU:OE2	2.15	0.46
2:F:191:ILE:O	2:F:195:ILE:CG1	2.62	0.46
2:A:139:LEU:HA	2:B:214:GLU:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:144:ARG:HH11	2:A:146:ARG:HG3	1.81	0.46
2:A:175:LEU:HD13	2:A:301:PHE:CZ	2.48	0.46
2:A:205:MSE:HE2	2:A:246:VAL:HG13	1.97	0.46
2:B:130:LYS:HZ3	2:C:12:SER:N	2.13	0.46
2:C:159:ALA:O	2:C:163:ASP:HB2	2.15	0.46
2:C:175:LEU:H	2:C:341:MSE:CE	2.28	0.46
2:C:266:SER:OG	2:C:269:ARG:HG2	2.16	0.46
2:C:387:ILE:CG2	2:C:395:ALA:HB1	2.45	0.46
2:F:248:GLU:O	2:F:249:LYS:C	2.57	0.46
2:A:160:ARG:HD3	2:A:403:LEU:HD22	1.97	0.46
2:A:184:LYS:HD2	2:A:318:THR:HG21	1.97	0.46
2:A:411:ASP:O	2:A:415:MSE:CG	2.64	0.46
2:C:303:ALA:O	2:C:304:ALA:C	2.58	0.46
2:E:88:ARG:O	2:E:88:ARG:HG3	2.15	0.46
2:E:347:ARG:O	2:E:351:GLU:HG2	2.14	0.46
2:F:30:ARG:O	2:F:31:LYS:C	2.59	0.46
2:A:264:LEU:HB3	2:A:317:ALA:CB	2.45	0.46
2:C:349:ILE:HG22	2:C:354:VAL:HB	1.97	0.46
2:D:2:ASN:OD1	2:D:2:ASN:C	2.57	0.46
2:D:139:LEU:O	2:D:140:HIS:C	2.58	0.46
2:E:66:ARG:NH1	2:E:74:ALA:HA	2.30	0.46
2:E:267:ILE:HG22	2:E:318:THR:O	2.15	0.46
2:F:403:LEU:C	2:F:405:MSE:N	2.74	0.46
2:A:173:ARG:HB2	2:A:173:ARG:HH11	1.79	0.46
2:D:254:VAL:C	2:D:256:HIS:N	2.73	0.46
2:E:162:LEU:CD1	2:E:187:LEU:HD11	2.46	0.46
2:E:294:LEU:HA	2:E:297:PRO:HG2	1.96	0.46
2:F:264:LEU:HB3	2:F:317:ALA:CB	2.45	0.46
2:F:379:LYS:HB3	2:F:412:PHE:CD1	2.51	0.46
1:K:3:DC:O2	2:E:109:ARG:HB2	2.15	0.46
2:A:24:GLU:O	2:A:26:LEU:CD2	2.55	0.46
2:A:73:LEU:O	2:A:74:ALA:C	2.57	0.46
2:A:100:LYS:O	2:A:114:LEU:N	2.42	0.46
2:B:296:ARG:O	2:B:297:PRO:C	2.57	0.46
2:C:248:GLU:O	2:C:249:LYS:C	2.58	0.46
2:D:17:LEU:HD23	2:D:17:LEU:C	2.41	0.46
2:E:136:LEU:N	2:E:136:LEU:HD23	2.30	0.46
2:F:7:LYS:HA	2:F:35:ILE:HD11	1.98	0.46
2:A:32:GLN:O	2:A:33:ASP:C	2.58	0.46
2:B:134:GLU:OE1	2:C:31:LYS:N	2.41	0.46
2:B:217:THR:O	2:B:218:GLU:C	2.59	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:6:LEU:HD23	2:E:6:LEU:HA	1.80	0.46
2:A:172:GLN:OE1	2:A:340:ASN:ND2	2.49	0.46
2:D:161:VAL:HG21	2:D:396:MSE:CE	2.28	0.46
2:E:139:LEU:O	2:E:140:HIS:CB	2.63	0.46
2:F:184:LYS:NZ	2:F:265:ASP:OD2	2.49	0.46
2:F:347:ARG:O	2:F:351:GLU:HG2	2.16	0.46
2:A:299:ARG:O	2:A:300:PHE:C	2.58	0.46
2:B:356:PRO:HB2	2:B:396:MSE:CE	2.44	0.46
2:C:60:ASP:HB3	2:C:62:PHE:CE2	2.51	0.46
2:C:189:GLN:O	2:C:193:GLN:HG3	2.16	0.46
2:D:140:HIS:HA	2:D:306:ASN:CB	2.45	0.46
2:D:245:MSE:HA	2:D:245:MSE:HE3	1.97	0.46
2:A:42:HIS:C	2:A:44:LYS:H	2.22	0.45
2:B:135:ASN:HB3	2:B:307:VAL:HG13	1.98	0.45
2:B:231:THR:C	2:B:233:ASP:N	2.72	0.45
2:C:24:GLU:O	2:C:25:ASN:C	2.58	0.45
2:C:261:ILE:HG12	2:C:314:THR:HG23	1.97	0.45
2:F:131:ILE:O	2:F:132:LEU:C	2.58	0.45
2:F:146:ARG:C	2:F:147:MSE:HG3	2.40	0.45
2:F:159:ALA:O	2:F:163:ASP:HB2	2.15	0.45
2:F:207:LEU:HD12	2:F:228:VAL:O	2.16	0.45
2:F:210:ASP:OD1	2:F:232:PHE:HA	2.16	0.45
2:B:71:SER:OG	2:B:228:VAL:HA	2.16	0.45
2:B:168:ILE:HD11	2:B:341:MSE:HE2	1.97	0.45
2:B:308:GLU:HB3	2:B:309:GLU:OE2	2.16	0.45
2:C:348:LYS:O	2:C:349:ILE:C	2.59	0.45
2:D:66:ARG:HH11	2:D:66:ARG:CG	2.26	0.45
2:D:160:ARG:CD	2:D:408:THR:CG2	2.82	0.45
2:E:269:ARG:O	2:E:270:LEU:C	2.59	0.45
2:F:135:ASN:CB	2:F:307:VAL:HG22	2.37	0.45
2:F:383:LEU:HD23	2:F:383:LEU:C	2.41	0.45
2:F:390:MSE:HE1	2:F:398:PHE:CD2	2.49	0.45
2:A:248:GLU:O	2:A:249:LYS:C	2.58	0.45
2:C:390:MSE:HB3	2:C:394:ASP:HB3	1.99	0.45
2:D:160:ARG:CD	2:D:408:THR:HG23	2.45	0.45
2:F:207:LEU:HD11	2:F:242:VAL:HG13	1.94	0.45
2:F:355:PHE:HB2	2:F:356:PRO:HD2	1.92	0.45
2:A:195:ILE:HG21	2:A:204:LEU:HD13	1.98	0.45
2:A:226:GLU:CD	2:A:249:LYS:HE2	2.37	0.45
2:B:346:SER:HB3	2:B:349:ILE:HD12	1.98	0.45
2:D:272:ARG:HH11	2:D:272:ARG:HB3	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:293:ALA:C	2:D:295:HIS:H	2.24	0.45
2:E:393:ILE:O	2:E:394:ASP:C	2.59	0.45
2:F:294:LEU:C	2:F:297:PRO:HD2	2.41	0.45
2:B:65:LEU:HB2	2:B:79:ILE:HB	1.97	0.45
2:C:114:LEU:HD21	2:C:115:LYS:NZ	2.30	0.45
2:D:304:ALA:O	2:D:305:ARG:HB3	2.16	0.45
2:D:381:TRP:CE3	2:E:353:ARG:HD3	2.52	0.45
2:E:252:ARG:HA	2:E:252:ARG:HH11	1.81	0.45
2:A:141:ALA:O	2:A:370:LEU:O	2.35	0.45
2:A:251:LYS:O	2:A:252:ARG:C	2.59	0.45
2:E:95:ASP:OD1	2:E:120:ASN:ND2	2.38	0.45
2:E:161:VAL:HG21	2:E:396:MSE:HE1	1.99	0.45
2:E:295:HIS:CD2	2:F:233:ASP:O	2.70	0.45
2:E:390:MSE:HE2	2:E:395:ALA:HA	1.98	0.45
2:F:57:ILE:HB	2:F:93:THR:HG22	1.97	0.45
2:F:158:THR:HA	2:F:356:PRO:HG2	1.98	0.45
2:A:178:ALA:HA	2:A:179:PRO:HD3	1.74	0.45
2:A:304:ALA:O	2:A:305:ARG:HB3	2.16	0.45
2:B:173:ARG:CG	2:B:304:ALA:HB3	2.47	0.45
2:C:15:ILE:O	2:C:16:THR:C	2.60	0.45
2:C:277:VAL:O	2:C:279:PRO:HD3	2.17	0.45
2:E:6:LEU:O	2:E:9:THR:HG23	2.15	0.45
2:F:32:GLN:HB3	2:F:76:PRO:HD2	1.98	0.45
2:A:116:VAL:HG12	2:A:124:PRO:HG3	1.98	0.45
2:A:266:SER:HB2	2:A:320:LEU:HG	1.98	0.45
2:A:385:LYS:HE2	2:B:353:ARG:NH1	2.22	0.45
2:C:289:VAL:HG11	2:C:330:VAL:CG1	2.30	0.45
2:C:349:ILE:HA	2:C:393:ILE:HD13	1.98	0.45
2:C:379:LYS:HD3	2:C:412:PHE:CD1	2.52	0.45
2:D:144:ARG:CG	2:D:145:LEU:N	2.79	0.45
2:E:26:LEU:HD22	2:E:29:MSE:SE	2.67	0.45
2:F:138:PRO:C	2:F:140:HIS:N	2.73	0.45
2:F:247:ILE:HB	2:F:300:PHE:CE1	2.52	0.45
2:A:294:LEU:C	2:A:297:PRO:HD2	2.42	0.45
2:B:274:TYR:HE1	2:B:296:ARG:NH2	2.15	0.45
2:D:49:ILE:HG22	2:D:101:ILE:CD1	2.44	0.45
2:D:238:ARG:NH1	2:D:242:VAL:HG22	2.32	0.45
2:D:267:ILE:HG22	2:D:318:THR:O	2.17	0.45
2:A:388:HIS:HB3	2:A:389:PRO:HD3	1.99	0.45
2:D:219:MSE:HE2	2:D:219:MSE:HB2	1.91	0.45
2:E:266:SER:N	2:E:318:THR:HG1	2.11	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:208:LEU:HB2	2:F:229:ALA:HB2	1.98	0.45
2:D:52:ASP:HA	2:D:97:ILE:O	2.18	0.44
2:E:211:GLU:HG2	2:E:215:GLU:HB3	1.99	0.44
2:C:133:PHE:HB2	3:D:422:HOH:O	2.16	0.44
2:C:137:THR:HG22	2:C:137:THR:O	2.17	0.44
2:D:29:MSE:HG3	2:D:34:ILE:HG12	1.99	0.44
2:D:104:PRO:HB3	2:D:108:GLU:HB2	1.98	0.44
2:F:156:ASP:OD1	2:F:159:ALA:HB3	2.16	0.44
2:B:173:ARG:HG3	2:B:304:ALA:HB3	2.00	0.44
2:B:272:ARG:O	2:B:273:ALA:C	2.60	0.44
2:B:294:LEU:HD11	2:B:334:GLU:HG3	1.99	0.44
2:B:399:LEU:HD13	2:B:403:LEU:CD1	2.47	0.44
2:C:232:PHE:CD1	2:C:232:PHE:C	2.95	0.44
2:E:252:ARG:O	2:E:255:GLU:HB2	2.18	0.44
2:F:71:SER:HB3	2:F:228:VAL:HG13	1.99	0.44
2:F:369:GLU:OE2	2:F:370:LEU:HG	2.17	0.44
2:C:231:THR:O	2:C:233:ASP:N	2.50	0.44
2:C:390:MSE:HE2	2:C:394:ASP:C	2.43	0.44
2:E:9:THR:HA	2:E:10:PRO:HD3	1.86	0.44
2:E:56:GLU:HB3	2:E:66:ARG:HE	1.82	0.44
2:F:79:ILE:HD13	2:F:101:ILE:HG21	1.99	0.44
2:F:402:LYS:HZ2	2:F:415:MSE:HE1	1.78	0.44
2:A:4:THR:HA	2:A:7:LYS:HG3	1.99	0.44
2:A:39:LEU:CD1	2:A:111:PHE:CZ	3.01	0.44
2:A:140:HIS:HA	2:A:306:ASN:CB	2.48	0.44
2:A:304:ALA:HB2	2:A:315:ILE:HG13	2.00	0.44
2:C:117:ASN:O	2:C:124:PRO:CG	2.65	0.44
2:D:158:THR:O	2:D:159:ALA:C	2.59	0.44
2:F:41:GLN:C	2:F:43:ALA:H	2.26	0.44
2:F:293:ALA:C	2:F:295:HIS:N	2.74	0.44
2:F:416:MSE:O	2:F:417:LYS:HB2	2.17	0.44
2:A:49:ILE:CG2	2:A:101:ILE:O	2.65	0.44
2:C:385:LYS:NZ	2:D:353:ARG:NH2	2.65	0.44
2:D:26:LEU:O	2:D:29:MSE:HG2	2.17	0.44
2:D:49:ILE:HG22	2:D:101:ILE:CG1	2.48	0.44
2:D:178:ALA:HA	2:D:179:PRO:HD3	1.71	0.44
2:D:383:LEU:O	2:D:386:ILE:HG23	2.18	0.44
2:E:376:GLU:O	2:E:377:LEU:C	2.61	0.44
2:D:99:GLY:HA3	2:D:115:LYS:O	2.18	0.44
2:D:209:ILE:HD13	2:D:209:ILE:HA	1.70	0.44
2:E:252:ARG:HH11	2:E:252:ARG:CA	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:359:ASP:OD1	2:E:362:ARG:HB2	2.16	0.44
2:E:387:ILE:O	2:E:388:HIS:C	2.61	0.44
2:C:385:LYS:HE3	2:C:385:LYS:HB2	1.68	0.44
2:E:207:LEU:HD21	2:E:243:ALA:HA	2.00	0.44
1:J:3:DC:O2	2:D:109:ARG:N	2.49	0.44
2:B:122:ASP:OD1	2:B:123:LYS:N	2.47	0.44
2:B:268:THR:HG21	3:B:420:HOH:O	2.17	0.44
2:B:351:GLU:C	2:B:353:ARG:H	2.26	0.44
2:C:228:VAL:HG12	2:C:242:VAL:CG1	2.48	0.44
2:E:175:LEU:N	2:E:341:MSE:CE	2.81	0.44
2:F:48:ASP:C	2:F:49:ILE:HG13	2.42	0.44
2:F:268:THR:O	2:F:272:ARG:HG2	2.18	0.44
2:A:247:ILE:O	2:A:251:LYS:HG3	2.18	0.43
2:A:294:LEU:HD21	2:A:331:ILE:HG12	1.99	0.43
2:C:417:LYS:C	2:C:417:LYS:HD2	2.43	0.43
2:A:205:MSE:CE	2:A:249:LYS:HD3	2.48	0.43
2:B:57:ILE:HG13	2:B:93:THR:HG22	2.00	0.43
2:B:143:SER:OG	2:B:143:SER:O	2.36	0.43
2:B:259:ASP:OD1	2:B:311:GLY:HA2	2.17	0.43
2:C:47:GLU:O	2:C:48:ASP:CB	2.64	0.43
2:C:81:VAL:HG12	2:C:86:ILE:HG13	1.99	0.43
2:C:175:LEU:N	2:C:341:MSE:CE	2.81	0.43
2:C:275:ASN:OD1	2:C:275:ASN:C	2.61	0.43
2:E:268:THR:HG21	2:E:320:LEU:N	2.31	0.43
2:F:356:PRO:O	2:F:358:ILE:N	2.52	0.43
2:A:169:GLY:O	2:A:172:GLN:HG2	2.18	0.43
2:A:206:VAL:HG21	2:A:223:VAL:HG11	1.99	0.43
2:A:252:ARG:O	2:A:255:GLU:HB2	2.18	0.43
2:A:271:ALA:CB	2:A:331:ILE:HD13	2.45	0.43
2:D:147:MSE:HE1	2:D:191:ILE:CG2	2.41	0.43
1:H:4:DC:H5	2:C:110:TYR:CZ	2.35	0.43
2:A:49:ILE:O	2:A:100:LYS:HA	2.18	0.43
2:A:137:THR:CG2	2:A:305:ARG:HD3	2.48	0.43
2:A:252:ARG:HA	2:A:252:ARG:HD3	1.70	0.43
2:D:83:PRO:O	2:D:87:ARG:HG3	2.18	0.43
2:D:327:MSE:O	2:D:328:ASP:C	2.61	0.43
2:E:330:VAL:O	2:E:330:VAL:CG1	2.66	0.43
2:F:104:PRO:HG3	2:F:110:TYR:C	2.42	0.43
2:F:123:LYS:HB2	2:F:126:ASN:HB2	1.99	0.43
2:F:141:ALA:CB	2:F:370:LEU:HD13	2.49	0.43
2:F:388:HIS:HB3	2:F:389:PRO:HD3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:4:DC:H5	2:F:110:TYR:OH	2.00	0.43
2:A:205:MSE:HE3	2:A:249:LYS:HD3	2.00	0.43
2:B:272:ARG:NH1	2:B:272:ARG:CG	2.49	0.43
2:B:399:LEU:HD13	2:B:403:LEU:HD11	1.99	0.43
2:C:141:ALA:HB1	2:C:370:LEU:CA	2.49	0.43
2:E:355:PHE:HA	3:E:424:HOH:O	2.17	0.43
2:E:361:ASN:ND2	2:E:388:HIS:O	2.51	0.43
2:A:3:LEU:C	2:A:3:LEU:HD23	2.42	0.43
2:F:272:ARG:CG	2:F:272:ARG:NH1	2.77	0.43
2:A:6:LEU:HD23	2:A:6:LEU:HA	1.90	0.43
2:A:374:GLN:HA	2:A:377:LEU:HD12	2.00	0.43
2:B:228:VAL:HG11	2:B:242:VAL:HG13	1.94	0.43
2:B:273:ALA:O	2:B:277:VAL:HG23	2.17	0.43
2:C:293:ALA:C	2:C:295:HIS:N	2.76	0.43
2:D:387:ILE:O	2:D:387:ILE:HG22	2.18	0.43
2:F:234:GLU:HB3	2:F:238:ARG:HG2	2.01	0.43
2:A:161:VAL:HG12	2:A:161:VAL:O	2.18	0.43
2:B:356:PRO:O	2:B:396:MSE:HE2	2.18	0.43
2:C:95:ASP:OD1	2:C:120:ASN:ND2	2.49	0.43
2:D:173:ARG:CD	2:D:301:PHE:O	2.67	0.43
2:E:169:GLY:H	2:E:172:GLN:HG3	1.75	0.43
2:B:383:LEU:O	2:B:386:ILE:HG23	2.18	0.43
2:C:56:GLU:HG3	2:C:245:MSE:HE1	2.01	0.43
2:D:379:LYS:HG3	2:D:412:PHE:CG	2.54	0.43
2:E:186:MSE:O	2:E:187:LEU:C	2.62	0.43
2:F:400:ILE:O	2:F:401:ASN:C	2.62	0.43
1:J:4:DC:H5	2:D:110:TYR:HH	1.60	0.43
2:A:53:GLY:HA3	2:A:65:LEU:HB3	2.01	0.43
2:C:139:LEU:HD22	2:C:367:LYS:HG3	2.00	0.43
2:C:333:GLU:OE1	2:D:325:SER:HB2	2.18	0.43
2:C:356:PRO:HD2	2:C:400:ILE:CD1	2.37	0.43
2:D:405:MSE:O	2:D:406:THR:CG2	2.59	0.43
2:E:132:LEU:HA	2:E:135:ASN:HD21	1.78	0.43
2:E:272:ARG:HH11	2:E:272:ARG:CG	1.97	0.43
2:F:144:ARG:HB2	2:F:371:LEU:HB3	2.00	0.43
2:A:26:LEU:HD12	2:A:34:ILE:HG23	2.01	0.42
2:B:166:SER:HA	2:B:365:THR:HG22	2.00	0.42
2:C:252:ARG:HA	2:C:252:ARG:HD3	1.65	0.42
2:D:381:TRP:CD2	2:E:353:ARG:HD3	2.54	0.42
2:F:161:VAL:HG12	2:F:358:ILE:HD12	2.00	0.42
2:B:146:ARG:C	2:B:147:MSE:HG2	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:244:GLU:CD	2:B:296:ARG:NH2	2.73	0.42
2:B:407:LYS:HG3	2:B:408:THR:HG23	2.01	0.42
2:C:120:ASN:HB2	2:C:256:HIS:NE2	2.34	0.42
2:C:211:GLU:HG3	2:C:212:ARG:N	2.34	0.42
2:C:338:THR:O	2:D:212:ARG:CD	2.67	0.42
2:E:355:PHE:CG	3:E:424:HOH:O	2.72	0.42
2:F:144:ARG:NH2	2:F:163:ASP:O	2.51	0.42
2:F:205:MSE:HE2	2:F:246:VAL:HG13	2.01	0.42
2:F:257:LYS:C	2:F:311:GLY:HA3	2.44	0.42
2:A:372:THR:HG23	2:A:376:GLU:CG	2.49	0.42
2:E:23:LEU:HD23	2:E:23:LEU:HA	1.87	0.42
2:A:28:ARG:HD3	2:A:28:ARG:HA	1.62	0.42
2:A:256:HIS:O	2:A:257:LYS:HB2	2.18	0.42
2:A:272:ARG:CG	2:A:272:ARG:NH1	2.53	0.42
2:A:321:ILE:O	2:A:322:ASP:HB2	2.18	0.42
2:A:373:THR:O	2:A:374:GLN:C	2.62	0.42
2:C:252:ARG:HH11	2:C:255:GLU:CD	2.27	0.42
2:D:226:GLU:OE2	2:D:249:LYS:CE	2.67	0.42
2:E:186:MSE:HE2	2:E:355:PHE:HD2	1.80	0.42
2:F:247:ILE:HG23	2:F:248:GLU:N	2.34	0.42
2:A:264:LEU:HB3	2:A:317:ALA:HB2	2.02	0.42
2:A:341:MSE:HE2	2:A:341:MSE:HB3	1.86	0.42
2:B:137:THR:HG22	2:B:305:ARG:HD3	2.01	0.42
2:C:5:GLU:O	2:C:9:THR:HG22	2.20	0.42
2:D:21:MSE:HE2	2:D:41:GLN:HB3	2.00	0.42
2:E:70:SER:O	2:E:71:SER:HB2	2.20	0.42
2:E:102:ARG:HD3	2:E:114:LEU:HD13	2.02	0.42
2:E:131:ILE:HG21	2:E:131:ILE:HD13	1.76	0.42
2:F:383:LEU:HD23	2:F:383:LEU:O	2.19	0.42
1:G:4:DC:O2	2:A:66:ARG:NH2	2.52	0.42
2:A:2:ASN:OD1	2:A:4:THR:HG23	2.20	0.42
2:A:207:LEU:HD13	2:A:246:VAL:HG21	2.02	0.42
2:A:228:VAL:CG1	2:A:242:VAL:CG1	2.97	0.42
2:B:117:ASN:O	2:B:124:PRO:HD3	2.19	0.42
2:C:226:GLU:CD	2:C:249:LYS:HE2	2.45	0.42
2:D:176:ILE:HG21	2:D:176:ILE:HD13	1.77	0.42
2:D:341:MSE:HE3	2:D:343:LEU:N	2.31	0.42
2:A:21:MSE:HE2	2:A:41:GLN:HB3	2.01	0.42
2:B:184:LYS:HE2	2:B:320:LEU:HD21	2.00	0.42
2:B:252:ARG:HA	2:B:252:ARG:HD3	1.65	0.42
2:B:264:LEU:O	2:B:317:ALA:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:54:VAL:O	2:E:65:LEU:HA	2.20	0.42
2:E:388:HIS:HB3	2:E:389:PRO:HD3	2.02	0.42
1:L:4:DC:C5	2:F:110:TYR:OH	2.70	0.42
2:A:268:THR:HA	2:A:331:ILE:HG21	2.01	0.42
2:B:188:LEU:HD23	2:B:188:LEU:HA	1.90	0.42
2:D:138:PRO:HD3	2:D:308:GLU:HB2	2.02	0.42
2:E:4:THR:CB	2:E:52:ASP:OD1	2.68	0.42
2:A:41:GLN:O	2:A:43:ALA:N	2.52	0.42
2:A:278:VAL:HA	2:A:279:PRO:HD3	1.84	0.42
2:B:231:THR:O	2:B:232:PHE:C	2.63	0.42
2:B:369:GLU:HA	2:B:377:LEU:HD13	2.02	0.42
2:E:33:ASP:OD1	2:E:76:PRO:HG2	2.20	0.42
2:E:58:LEU:HD12	2:E:59:GLN:N	2.32	0.42
2:E:186:MSE:HE2	2:E:355:PHE:CE2	2.54	0.42
2:E:344:HIS:O	2:E:358:ILE:HA	2.20	0.42
2:A:85:GLN:NE2	2:A:113:LEU:O	2.38	0.42
2:A:140:HIS:CA	2:A:306:ASN:CB	2.96	0.42
2:A:211:GLU:HG3	2:A:212:ARG:N	2.35	0.42
2:B:139:LEU:HD21	2:B:367:LYS:HG3	2.02	0.42
2:B:219:MSE:O	2:B:220:GLN:C	2.63	0.42
2:B:390:MSE:HE2	2:B:394:ASP:C	2.45	0.42
2:C:382:ILE:C	2:C:384:ARG:N	2.76	0.42
2:D:212:ARG:HB3	2:D:214:GLU:OE2	2.20	0.42
2:E:296:ARG:HA	2:E:299:ARG:HB2	2.02	0.42
2:E:390:MSE:CE	2:E:395:ALA:HA	2.50	0.42
2:A:40:LYS:HB3	2:A:40:LYS:HE3	1.70	0.41
2:A:50:PHE:CD1	2:A:100:LYS:HG2	2.54	0.41
2:A:266:SER:OG	2:A:269:ARG:N	2.40	0.41
2:A:403:LEU:C	2:A:405:MSE:N	2.78	0.41
2:C:113:LEU:HD21	2:C:116:VAL:CG2	2.49	0.41
2:C:326:LYS:O	2:C:327:MSE:C	2.62	0.41
2:C:379:LYS:HZ1	2:C:412:PHE:HB2	1.79	0.41
2:D:137:THR:CG2	2:D:305:ARG:NH1	2.83	0.41
2:D:247:ILE:HD12	2:D:247:ILE:HA	1.89	0.41
2:F:56:GLU:CD	2:F:66:ARG:HE	2.28	0.41
2:F:141:ALA:CB	2:F:370:LEU:HB3	2.50	0.41
2:F:270:LEU:CD1	2:F:274:TYR:CE2	3.01	0.41
2:A:83:PRO:O	2:A:87:ARG:HG3	2.20	0.41
2:A:169:GLY:O	2:A:171:GLY:N	2.53	0.41
2:A:309:GLU:H	2:A:309:GLU:CD	2.28	0.41
2:A:359:ASP:OD2	2:A:362:ARG:HD2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:179:PRO:HA	2:B:321:ILE:O	2.20	0.41
2:C:409:ASN:OD1	2:C:409:ASN:C	2.63	0.41
2:E:29:MSE:HG3	2:E:34:ILE:HG13	2.02	0.41
2:E:71:SER:HA	2:E:228:VAL:HG13	2.02	0.41
2:E:198:ASN:C	2:E:200:PRO:HD3	2.45	0.41
2:E:210:ASP:HB2	2:E:269:ARG:HB3	2.01	0.41
2:E:294:LEU:O	2:E:297:PRO:HD2	2.20	0.41
2:E:412:PHE:O	2:E:413:PHE:C	2.62	0.41
2:F:234:GLU:CD	2:F:238:ARG:HG2	2.44	0.41
2:A:62:PHE:HE1	2:A:64:PHE:CE2	2.35	0.41
2:C:209:ILE:HA	2:C:209:ILE:HD13	1.64	0.41
2:D:42:HIS:O	2:D:42:HIS:CG	2.72	0.41
2:D:154:THR:O	2:D:157:LEU:CB	2.59	0.41
2:E:137:THR:CG2	2:E:305:ARG:NH1	2.81	0.41
2:E:264:LEU:HD22	2:E:300:PHE:CE2	2.56	0.41
2:F:122:ASP:OD1	2:F:123:LYS:N	2.48	0.41
1:K:4:DC:H5	2:E:110:TYR:CZ	2.38	0.41
2:A:57:ILE:CG1	2:A:93:THR:HG22	2.51	0.41
2:A:261:ILE:HA	2:A:314:THR:O	2.20	0.41
2:A:349:ILE:HG23	2:A:354:VAL:HB	2.02	0.41
2:B:247:ILE:HD12	2:B:247:ILE:HA	1.86	0.41
2:C:199:HIS:HB3	2:C:202:CYS:SG	2.60	0.41
2:C:294:LEU:HA	2:C:297:PRO:HG2	2.01	0.41
2:D:252:ARG:HD3	2:D:252:ARG:HA	1.82	0.41
2:E:56:GLU:CD	2:E:66:ARG:NE	2.77	0.41
2:E:131:ILE:CG2	2:E:133:PHE:HD2	2.33	0.41
2:A:142:ASN:OD1	2:A:306:ASN:ND2	2.54	0.41
2:A:247:ILE:HD11	2:A:303:ALA:CB	2.51	0.41
2:B:138:PRO:HD2	2:B:306:ASN:O	2.20	0.41
2:D:147:MSE:C	2:D:159:ALA:HB1	2.45	0.41
2:D:396:MSE:HE3	2:D:400:ILE:HD11	2.01	0.41
2:F:169:GLY:O	2:F:172:GLN:CG	2.68	0.41
2:A:235:PRO:O	2:A:236:ALA:C	2.63	0.41
2:B:199:HIS:N	2:B:200:PRO:HD3	2.35	0.41
2:C:60:ASP:CB	2:C:62:PHE:CE2	3.03	0.41
2:D:131:ILE:HG22	2:D:133:PHE:CD2	2.51	0.41
2:D:264:LEU:O	2:D:317:ALA:HA	2.21	0.41
2:E:206:VAL:HG22	2:E:263:LEU:HD12	2.01	0.41
2:F:99:GLY:HA3	2:F:115:LYS:O	2.21	0.41
2:F:387:ILE:HG12	2:F:390:MSE:SE	2.70	0.41
2:D:17:LEU:C	2:D:17:LEU:CD2	2.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:66:ARG:NH1	2:D:78:ASP:OD2	2.54	0.41
2:F:6:LEU:HD22	2:F:14:LEU:HD21	2.02	0.41
2:A:161:VAL:CG1	2:A:358:ILE:HD12	2.47	0.41
2:B:144:ARG:NH1	2:B:372:THR:HG22	2.36	0.41
2:B:197:TYR:HD2	2:B:198:ASN:ND2	2.19	0.41
2:B:252:ARG:O	2:B:255:GLU:HB2	2.21	0.41
2:C:337:GLY:O	2:D:212:ARG:NH1	2.44	0.41
2:D:355:PHE:O	2:D:357:ALA:N	2.54	0.41
2:E:307:VAL:HB	2:E:311:GLY:O	2.21	0.41
2:F:264:LEU:HB3	2:F:317:ALA:CA	2.49	0.41
1:K:4:DC:H5	2:E:110:TYR:HH	1.67	0.41
2:A:210:ASP:OD1	2:A:232:PHE:HA	2.20	0.41
2:A:273:ALA:O	2:A:277:VAL:HG23	2.21	0.41
2:A:386:ILE:HD11	2:A:398:PHE:CZ	2.56	0.41
2:A:387:ILE:O	2:A:388:HIS:C	2.62	0.41
2:A:393:ILE:H	2:A:393:ILE:HG13	1.75	0.41
2:B:139:LEU:HD23	2:B:367:LYS:HD2	2.01	0.41
2:B:144:ARG:HH11	2:B:372:THR:HG22	1.85	0.41
2:B:184:LYS:NZ	2:B:265:ASP:OD2	2.54	0.41
2:C:272:ARG:HD2	2:C:327:MSE:SE	2.67	0.41
2:D:26:LEU:HB3	2:D:29:MSE:HE3	2.03	0.41
2:D:56:GLU:HB2	2:D:245:MSE:SE	2.70	0.41
2:D:176:ILE:O	2:D:318:THR:HA	2.20	0.41
2:E:400:ILE:O	2:E:404:ALA:HB2	2.21	0.41
2:E:406:THR:HB	2:E:407:LYS:H	1.68	0.41
2:F:62:PHE:HB3	2:F:83:PRO:HD3	2.02	0.41
2:F:144:ARG:HA	2:F:169:GLY:HA2	2.03	0.41
2:F:320:LEU:N	2:F:320:LEU:HD23	2.36	0.41
2:F:332:TYR:O	2:F:333:GLU:C	2.64	0.41
2:F:341:MSE:HA	2:F:365:THR:HA	2.03	0.41
2:F:399:LEU:O	2:F:403:LEU:HD12	2.21	0.41
2:A:296:ARG:O	2:A:297:PRO:C	2.64	0.41
2:B:269:ARG:HH12	2:B:272:ARG:HH22	1.69	0.41
2:C:166:SER:HA	2:C:365:THR:HG22	2.03	0.41
2:C:330:VAL:O	2:C:331:ILE:C	2.62	0.41
2:C:341:MSE:HA	2:C:365:THR:HA	2.02	0.41
2:D:140:HIS:HA	2:D:306:ASN:HB2	2.03	0.41
2:D:157:LEU:HD23	2:D:157:LEU:HA	1.93	0.41
2:D:369:GLU:HA	2:D:377:LEU:HD13	2.02	0.41
2:A:3:LEU:HD23	2:A:3:LEU:O	2.21	0.40
2:B:234:GLU:HB3	2:B:238:ARG:HG2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:17:LEU:O	2:D:21:MSE:HG3	2.22	0.40
2:D:113:LEU:HA	2:D:113:LEU:HD12	1.87	0.40
2:A:18:GLY:O	2:A:23:LEU:HB2	2.22	0.40
2:A:161:VAL:O	2:A:161:VAL:CG1	2.69	0.40
2:A:297:PRO:HB2	2:A:335:PHE:HZ	1.86	0.40
2:B:92:ARG:O	2:B:93:THR:C	2.63	0.40
2:B:138:PRO:C	2:B:140:HIS:H	2.30	0.40
2:B:356:PRO:O	2:B:358:ILE:N	2.47	0.40
2:C:9:THR:OG1	2:C:14:LEU:HG	2.22	0.40
2:C:55:LEU:HD13	2:C:81:VAL:HG21	2.02	0.40
2:C:355:PHE:O	2:C:357:ALA:N	2.53	0.40
2:C:372:THR:HG22	2:C:376:GLU:CD	2.46	0.40
2:E:102:ARG:HG2	2:E:114:LEU:HD13	2.04	0.40
2:E:209:ILE:HA	2:E:209:ILE:HD13	1.61	0.40
2:F:254:VAL:C	2:F:256:HIS:H	2.29	0.40
2:F:369:GLU:HG2	2:F:370:LEU:N	2.36	0.40
2:A:173:ARG:HD3	2:A:304:ALA:HB3	2.03	0.40
2:A:309:GLU:OE2	2:A:309:GLU:N	2.46	0.40
2:B:352:LYS:HB3	2:B:354:VAL:CG2	2.52	0.40
2:C:399:LEU:HD23	2:C:399:LEU:HA	1.93	0.40
2:A:321:ILE:CG2	2:A:322:ASP:N	2.85	0.40
2:C:178:ALA:HA	2:C:179:PRO:HD3	1.96	0.40
2:C:199:HIS:N	2:C:200:PRO:HD3	2.36	0.40
2:C:241:GLN:O	2:C:242:VAL:C	2.64	0.40
2:D:351:GLU:OE1	2:D:351:GLU:HA	2.21	0.40
2:E:256:HIS:O	2:E:257:LYS:HB2	2.20	0.40
2:E:274:TYR:CD2	2:E:297:PRO:HD3	2.57	0.40
2:F:205:MSE:HE3	2:F:226:GLU:OE1	2.21	0.40
2:F:262:ILE:HB	2:F:315:ILE:HG12	2.03	0.40
2:A:99:GLY:HA3	2:A:115:LYS:O	2.22	0.40
2:D:66:ARG:NH1	2:D:66:ARG:CG	2.84	0.40
2:E:4:THR:CG2	2:E:52:ASP:OD1	2.70	0.40
2:E:55:LEU:CB	2:E:65:LEU:HD23	2.51	0.40
2:E:137:THR:O	2:F:214:GLU:HA	2.21	0.40
2:E:173:ARG:N	2:E:340:ASN:OD1	2.40	0.40
2:F:29:MSE:HG3	2:F:34:ILE:HG12	2.03	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	
2	A	400/419 (96%)	363 (91%)	30 (8%)	7 (2%)	6	31
2	B	350/419 (84%)	306 (87%)	31 (9%)	13 (4%)	2	15
2	C	400/419 (96%)	354 (88%)	37 (9%)	9 (2%)	5	25
2	D	400/419 (96%)	352 (88%)	33 (8%)	15 (4%)	2	15
2	E	399/419 (95%)	346 (87%)	39 (10%)	14 (4%)	3	16
2	F	400/419 (96%)	352 (88%)	35 (9%)	13 (3%)	3	17
All	All	2349/2514 (93%)	2073 (88%)	205 (9%)	71 (3%)	3	19

All (71) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	357	ALA
2	B	140	HIS
2	B	355	PHE
2	C	140	HIS
2	C	408	THR
2	D	45	SER
2	D	137	THR
2	D	140	HIS
2	D	266	SER
2	E	408	THR
2	F	355	PHE
2	A	25	ASN
2	A	170	ARG
2	C	25	ASN
2	C	266	SER
2	C	292	ASN
2	C	357	ALA
2	D	139	LEU
2	D	141	ALA
2	D	294	LEU

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Mol	Chain	Res	Type
2	D	357	ALA
2	D	407	LYS
2	E	25	ASN
2	E	31	LYS
2	E	170	ARG
2	E	294	LEU
2	E	392	GLU
2	E	410	ASP
2	F	139	LEU
2	F	242	VAL
2	F	266	SER
2	F	357	ALA
2	F	404	ALA
2	A	42	HIS
2	A	45	SER
2	A	47	GLU
2	B	153	SER
2	B	266	SER
2	B	287	GLY
2	B	408	THR
2	C	355	PHE
2	E	27	ALA
2	E	154	THR
2	E	287	GLY
2	E	358	ILE
2	F	45	SER
2	F	356	PRO
2	B	139	LEU
2	B	142	ASN
2	B	143	SER
2	B	292	ASN
2	D	20	ASN
2	D	405	MSE
2	E	413	PHE
2	F	23	LEU
2	F	341	MSE
2	B	356	PRO
2	B	357	ALA
2	C	48	ASP
2	D	106	GLU
2	E	266	SER
2	F	294	LEU

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Mol	Chain	Res	Type
2	A	124	PRO
2	B	294	LEU
2	D	287	GLY
2	F	49	ILE
2	F	287	GLY
2	D	49	ILE
2	D	124	PRO
2	E	209	ILE
2	C	356	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	A	350/343 (102%)	300 (86%)	50 (14%)	3	16
2	B	306/343 (89%)	269 (88%)	37 (12%)	5	21
2	C	350/343 (102%)	278 (79%)	72 (21%)	1	7
2	D	350/343 (102%)	282 (81%)	68 (19%)	1	8
2	E	349/343 (102%)	281 (80%)	68 (20%)	1	8
2	F	350/343 (102%)	304 (87%)	46 (13%)	4	19
All	All	2055/2058 (100%)	1714 (83%)	341 (17%)	2	12

All (341) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	4	THR
2	A	7	LYS
2	A	9	THR
2	A	11	VAL
2	A	12	SER
2	A	15	ILE
2	A	24	GLU
2	A	28	ARG
2	A	45	SER

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Mol	Chain	Res	Type
2	A	52	ASP
2	A	58	LEU
2	A	70	SER
2	A	71	SER
2	A	73	LEU
2	A	84	SER
2	A	88	ARG
2	A	93	THR
2	A	130	LYS
2	A	132	LEU
2	A	134	GLU
2	A	137	THR
2	A	139	LEU
2	A	173	ARG
2	A	176	ILE
2	A	184	LYS
2	A	194	SER
2	A	203	VAL
2	A	222	LEU
2	A	224	LYS
2	A	245	MSE
2	A	252	ARG
2	A	257	LYS
2	A	268	THR
2	A	272	ARG
2	A	276	THR
2	A	284	VAL
2	A	289	VAL
2	A	299	ARG
2	A	309	GLU
2	A	314	THR
2	A	321	ILE
2	A	336	LYS
2	A	341	MSE
2	A	342	GLU
2	A	365	THR
2	A	372	THR
2	A	379	LYS
2	A	386	ILE
2	A	396	MSE
2	A	399	LEU
2	B	56	GLU

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Mol	Chain	Res	Type
2	B	66	ARG
2	B	71	SER
2	B	93	THR
2	B	101	ILE
2	B	108	GLU
2	B	114	LEU
2	B	134	GLU
2	B	139	LEU
2	B	146	ARG
2	B	147	MSE
2	B	158	THR
2	B	185	THR
2	B	198	ASN
2	B	208	LEU
2	B	252	ARG
2	B	268	THR
2	B	272	ARG
2	B	276	THR
2	B	289	VAL
2	B	290	ASP
2	B	299	ARG
2	B	301	PHE
2	B	309	GLU
2	B	314	THR
2	B	321	ILE
2	B	325	SER
2	B	354	VAL
2	B	356	PRO
2	B	363	SER
2	B	365	THR
2	B	377	LEU
2	B	383	LEU
2	B	386	ILE
2	B	393	ILE
2	B	399	LEU
2	B	406	THR
2	C	1	MSE
2	C	2	ASN
2	C	3	LEU
2	C	4	THR
2	C	7	LYS
2	C	9	THR

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Mol	Chain	Res	Type
2	C	17	LEU
2	C	24	GLU
2	C	35	ILE
2	C	40	LYS
2	C	48	ASP
2	C	49	ILE
2	C	52	ASP
2	C	56	GLU
2	C	66	ARG
2	C	69	ASP
2	C	82	SER
2	C	93	THR
2	C	129	ASN
2	C	131	ILE
2	C	132	LEU
2	C	134	GLU
2	C	139	LEU
2	C	146	ARG
2	C	147	MSE
2	C	163	ASP
2	C	168	ILE
2	C	181	LYS
2	C	190	ASN
2	C	194	SER
2	C	202	CYS
2	C	226	GLU
2	C	230	SER
2	C	231	THR
2	C	235	PRO
2	C	252	ARG
2	C	257	LYS
2	C	266	SER
2	C	272	ARG
2	C	276	THR
2	C	277	VAL
2	C	290	ASP
2	C	299	ARG
2	C	301	PHE
2	C	309	GLU
2	C	314	THR
2	C	318	THR
2	C	321	ILE

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Mol	Chain	Res	Type
2	C	325	SER
2	C	326	LYS
2	C	336	LYS
2	C	341	MSE
2	C	347	ARG
2	C	352	LYS
2	C	362	ARG
2	C	365	THR
2	C	367	LYS
2	C	372	THR
2	C	379	LYS
2	C	380	MSE
2	C	382	ILE
2	C	383	LEU
2	C	384	ARG
2	C	386	ILE
2	C	393	ILE
2	C	399	LEU
2	C	406	THR
2	C	407	LYS
2	C	411	ASP
2	C	414	GLU
2	C	415	MSE
2	C	417	LYS
2	D	7	LYS
2	D	9	THR
2	D	11	VAL
2	D	12	SER
2	D	24	GLU
2	D	26	LEU
2	D	41	GLN
2	D	69	ASP
2	D	70	SER
2	D	84	SER
2	D	88	ARG
2	D	92	ARG
2	D	93	THR
2	D	114	LEU
2	D	115	LYS
2	D	130	LYS
2	D	131	ILE
2	D	134	GLU

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Mol	Chain	Res	Type
2	D	136	LEU
2	D	137	THR
2	D	139	LEU
2	D	162	LEU
2	D	163	ASP
2	D	170	ARG
2	D	181	LYS
2	D	184	LYS
2	D	194	SER
2	D	222	LEU
2	D	242	VAL
2	D	244	GLU
2	D	245	MSE
2	D	252	ARG
2	D	263	LEU
2	D	268	THR
2	D	272	ARG
2	D	276	THR
2	D	285	LEU
2	D	286	THR
2	D	289	VAL
2	D	296	ARG
2	D	299	ARG
2	D	305	ARG
2	D	309	GLU
2	D	312	SER
2	D	314	THR
2	D	316	ILE
2	D	318	THR
2	D	321	ILE
2	D	322	ASP
2	D	327	MSE
2	D	330	VAL
2	D	336	LYS
2	D	341	MSE
2	D	356	PRO
2	D	363	SER
2	D	365	THR
2	D	372	THR
2	D	374	GLN
2	D	377	LEU
2	D	386	ILE

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Mol	Chain	Res	Type
2	D	393	ILE
2	D	396	MSE
2	D	399	LEU
2	D	405	MSE
2	D	406	THR
2	D	407	LYS
2	D	408	THR
2	D	416	MSE
2	E	1	MSE
2	E	3	LEU
2	E	4	THR
2	E	6	LEU
2	E	9	THR
2	E	11	VAL
2	E	16	THR
2	E	24	GLU
2	E	31	LYS
2	E	35	ILE
2	E	40	LYS
2	E	44	LYS
2	E	49	ILE
2	E	69	ASP
2	E	84	SER
2	E	86	ILE
2	E	88	ARG
2	E	93	THR
2	E	131	ILE
2	E	136	LEU
2	E	137	THR
2	E	139	LEU
2	E	143	SER
2	E	146	ARG
2	E	162	LEU
2	E	163	ASP
2	E	164	LEU
2	E	177	VAL
2	E	181	LYS
2	E	184	LYS
2	E	185	THR
2	E	195	ILE
2	E	209	ILE
2	E	211	GLU

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Mol	Chain	Res	Type
2	E	216	VAL
2	E	226	GLU
2	E	233	ASP
2	E	245	MSE
2	E	252	ARG
2	E	268	THR
2	E	272	ARG
2	E	276	THR
2	E	278	VAL
2	E	286	THR
2	E	289	VAL
2	E	299	ARG
2	E	309	GLU
2	E	314	THR
2	E	326	LYS
2	E	341	MSE
2	E	349	ILE
2	E	353	ARG
2	E	356	PRO
2	E	359	ASP
2	E	365	THR
2	E	366	ARG
2	E	371	LEU
2	E	374	GLN
2	E	377	LEU
2	E	379	LYS
2	E	384	ARG
2	E	386	ILE
2	E	387	ILE
2	E	393	ILE
2	E	399	LEU
2	E	406	THR
2	E	407	LYS
2	E	413	PHE
2	F	3	LEU
2	F	7	LYS
2	F	9	THR
2	F	11	VAL
2	F	12	SER
2	F	15	ILE
2	F	24	GLU
2	F	40	LYS

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Mol	Chain	Res	Type
2	F	45	SER
2	F	49	ILE
2	F	58	LEU
2	F	84	SER
2	F	93	THR
2	F	101	ILE
2	F	106	GLU
2	F	126	ASN
2	F	144	ARG
2	F	162	LEU
2	F	185	THR
2	F	194	SER
2	F	195	ILE
2	F	202	CYS
2	F	209	ILE
2	F	242	VAL
2	F	244	GLU
2	F	245	MSE
2	F	261	ILE
2	F	266	SER
2	F	267	ILE
2	F	272	ARG
2	F	276	THR
2	F	299	ARG
2	F	305	ARG
2	F	307	VAL
2	F	308	GLU
2	F	309	GLU
2	F	316	ILE
2	F	321	ILE
2	F	346	SER
2	F	356	PRO
2	F	359	ASP
2	F	365	THR
2	F	386	ILE
2	F	390	MSE
2	F	393	ILE
2	F	405	MSE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	42	HIS
2	A	198	ASN
2	A	199	HIS
2	A	275	ASN
2	A	306	ASN
2	B	198	ASN
2	B	199	HIS
2	B	275	ASN
2	C	41	GLN
2	C	190	ASN
2	C	275	ASN
2	C	292	ASN
2	C	306	ASN
2	D	41	GLN
2	D	120	ASN
2	D	129	ASN
2	D	172	GLN
2	D	193	GLN
2	D	256	HIS
2	D	275	ASN
2	D	292	ASN
2	E	59	GLN
2	E	129	ASN
2	E	135	ASN
2	E	190	ASN
2	E	275	ASN
2	E	295	HIS
2	E	306	ASN
2	F	193	GLN
2	F	198	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 [i](#)

There are no ligands in this entry.

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	G	2/2 (100%)	1.49	0 100 100	150, 150, 150, 150	0
1	H	2/2 (100%)	1.89	1 (50%) 0 0	150, 150, 150, 150	0
1	J	2/2 (100%)	1.94	1 (50%) 0 0	150, 150, 150, 150	0
1	K	2/2 (100%)	1.98	1 (50%) 0 0	150, 150, 150, 150	0
1	L	2/2 (100%)	2.01	1 (50%) 0 0	150, 150, 150, 150	0
2	A	392/419 (93%)	0.18	12 (3%) 51 30	35, 69, 121, 127	0
2	B	345/419 (82%)	0.22	23 (6%) 24 12	30, 69, 114, 127	0
2	C	392/419 (93%)	-0.15	9 (2%) 61 38	18, 44, 96, 113	0
2	D	392/419 (93%)	-0.19	11 (2%) 55 32	14, 45, 77, 126	0
2	E	391/419 (93%)	-0.10	15 (3%) 44 24	18, 47, 87, 126	0
2	F	392/419 (93%)	0.15	18 (4%) 37 20	36, 67, 114, 124	0
All	All	2314/2524 (91%)	0.02	92 (3%) 42 23	14, 57, 110, 150	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	139	LEU	5.5
2	D	355	PHE	5.5
2	F	140	HIS	4.7
2	A	152	GLY	4.6
2	B	141	ALA	4.4
2	C	152	GLY	4.2
2	A	346	SER	4.1
2	B	144	ARG	4.1
2	B	140	HIS	4.1
2	C	139	LEU	4.0
2	A	140	HIS	3.8
2	E	152	GLY	3.8

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Mol	Chain	Res	Type	RSRZ
2	C	412	PHE	3.8
2	F	381	TRP	3.7
2	B	156	ASP	3.7
2	B	145	LEU	3.6
2	B	143	SER	3.6
2	B	355	PHE	3.4
2	F	284	VAL	3.4
2	A	355	PHE	3.3
2	F	132	LEU	3.3
2	E	407	LYS	3.3
2	E	408	THR	3.3
2	B	407	LYS	3.2
2	B	152	GLY	3.1
2	D	403	LEU	3.0
2	B	406	THR	3.0
2	B	138	PRO	3.0
2	F	136	LEU	3.0
2	E	156	ASP	3.0
2	E	406	THR	3.0
2	B	142	ASN	2.9
2	E	25	ASN	2.9
2	E	26	LEU	2.9
2	A	41	GLN	2.9
2	A	46	GLY	2.9
2	B	154	THR	2.8
2	F	137	THR	2.8
2	D	63	GLY	2.8
2	A	357	ALA	2.7
2	B	354	VAL	2.7
2	F	143	SER	2.7
2	D	412	PHE	2.7
2	A	155	GLU	2.7
2	F	368	GLU	2.6
2	E	139	LEU	2.6
2	E	28	ARG	2.6
2	D	126	ASN	2.5
2	E	413	PHE	2.5
2	E	43	ALA	2.5
2	F	411	ASP	2.5
2	F	414	GLU	2.4
2	C	140	HIS	2.4
2	C	141	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	130	LYS	2.4
2	E	154	THR	2.3
2	F	152	GLY	2.3
2	A	198	ASN	2.3
2	D	48	ASP	2.3
1	H	3	DC	2.3
2	D	407	LYS	2.3
2	A	413	PHE	2.3
2	F	402	LYS	2.3
2	E	412	PHE	2.3
2	F	374	GLN	2.3
2	A	408	THR	2.3
2	B	137	THR	2.3
2	C	101	ILE	2.3
2	D	140	HIS	2.3
2	B	146	ARG	2.3
2	E	411	ASP	2.2
2	D	152	GLY	2.2
2	F	47	GLU	2.2
1	L	3	DC	2.2
2	B	89	PHE	2.2
2	E	4	THR	2.2
2	F	193	GLN	2.2
2	B	409	ASN	2.2
2	C	142	ASN	2.2
2	C	43	ALA	2.1
2	C	8	ASN	2.1
2	F	376	GLU	2.1
2	D	302	GLY	2.1
2	F	291	ALA	2.1
2	A	135	ASN	2.1
2	D	114	LEU	2.1
2	B	292	ASN	2.0
1	J	4	DC	2.0
2	F	154	THR	2.0
2	B	417	LYS	2.0
1	K	4	DC	2.0
2	B	155	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.