



Full wwPDB X-ray Structure Validation Report ⓘ

May 18, 2020 – 10:05 pm BST

PDB ID : 2GRE
Title : Crystal structure of Deblocking aminopeptidase from *Bacillus cereus*
Authors : Chang, C.; Wu, R.; Abdullah, J.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on : 2006-04-24
Resolution : 2.65 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

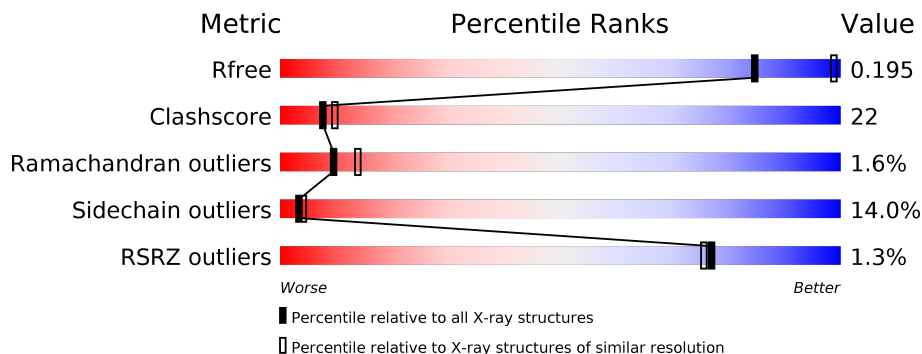
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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

Mol	Chain	Length	Quality of chain
1	A	349	 53% 27% 9% 10%
1	B	349	 54% 27% 8% 11%
1	C	349	 60% 23% 6% 12%
1	D	349	 53% 28% 6% 12%
1	E	349	 52% 29% 5% 12%
1	F	349	 56% 25% 7% 11%

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Mol	Chain	Length	Quality of chain
1	G	349	<p>%</p> <p>55% 26% 7% 11%</p>
1	H	349	<p>%</p> <p>56% 25% 6% 13%</p>
1	I	349	<p>%</p> <p>53% 27% 5% 14%</p>
1	J	349	<p>%</p> <p>56% 25% 7% 12%</p>
1	K	349	<p>%</p> <p>50% 32% 6% 13%</p>
1	L	349	<p>3%</p> <p>56% 26% 6% 11%</p>
1	M	349	<p>%</p> <p>56% 25% 7% 11%</p>
1	N	349	<p>2%</p> <p>53% 28% 7% 12%</p>
1	O	349	<p>2%</p> <p>56% 26% 5% 12%</p>
1	P	349	<p>%</p> <p>55% 25% 5% 13%</p>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 39559 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Deblocking aminopeptidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	313	Total 2441	C 1541	N 414	O 478	S 2	Se 6	0	0	0
1	B	312	Total 2431	C 1535	N 411	O 477	S 2	Se 6	0	0	0
1	C	308	Total 2413	C 1526	N 406	O 473	S 2	Se 6	0	0	0
1	D	306	Total 2398	C 1517	N 403	O 470	S 2	Se 6	0	0	0
1	E	306	Total 2393	C 1516	N 401	O 468	S 2	Se 6	0	0	0
1	F	310	Total 2426	C 1533	N 409	O 476	S 2	Se 6	0	0	0
1	G	309	Total 2413	C 1526	N 404	O 475	S 2	Se 6	0	0	0
1	H	305	Total 2394	C 1516	N 405	O 465	S 2	Se 6	0	0	0
1	I	299	Total 2364	C 1500	N 396	O 460	S 2	Se 6	0	0	0
1	J	307	Total 2399	C 1518	N 402	O 471	S 2	Se 6	0	0	0
1	K	304	Total 2389	C 1513	N 404	O 464	S 2	Se 6	0	0	0
1	L	310	Total 2421	C 1530	N 407	O 476	S 2	Se 6	0	0	0
1	M	309	Total 2422	C 1531	N 407	O 476	S 2	Se 6	0	0	0
1	N	307	Total 2407	C 1524	N 407	O 468	S 2	Se 6	0	0	0
1	O	308	Total 2404	C 1521	N 403	O 473	S 2	Se 5	0	0	0
1	P	305	Total 2382	C 1508	N 400	O 466	S 2	Se 6	0	0	0

There are 112 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	GB 29894598
A	9	MSE	MET	MODIFIED RESIDUE	GB 29894598
A	76	MSE	MET	MODIFIED RESIDUE	GB 29894598
A	90	MSE	MET	MODIFIED RESIDUE	GB 29894598
A	120	MSE	MET	MODIFIED RESIDUE	GB 29894598
A	242	MSE	MET	MODIFIED RESIDUE	GB 29894598
A	343	MSE	MET	MODIFIED RESIDUE	GB 29894598
B	1	MSE	MET	MODIFIED RESIDUE	GB 29894598
B	9	MSE	MET	MODIFIED RESIDUE	GB 29894598
B	76	MSE	MET	MODIFIED RESIDUE	GB 29894598
B	90	MSE	MET	MODIFIED RESIDUE	GB 29894598
B	120	MSE	MET	MODIFIED RESIDUE	GB 29894598
B	242	MSE	MET	MODIFIED RESIDUE	GB 29894598
B	343	MSE	MET	MODIFIED RESIDUE	GB 29894598
C	1	MSE	MET	MODIFIED RESIDUE	GB 29894598
C	9	MSE	MET	MODIFIED RESIDUE	GB 29894598
C	76	MSE	MET	MODIFIED RESIDUE	GB 29894598
C	90	MSE	MET	MODIFIED RESIDUE	GB 29894598
C	120	MSE	MET	MODIFIED RESIDUE	GB 29894598
C	242	MSE	MET	MODIFIED RESIDUE	GB 29894598
C	343	MSE	MET	MODIFIED RESIDUE	GB 29894598
D	1	MSE	MET	MODIFIED RESIDUE	GB 29894598
D	9	MSE	MET	MODIFIED RESIDUE	GB 29894598
D	76	MSE	MET	MODIFIED RESIDUE	GB 29894598
D	90	MSE	MET	MODIFIED RESIDUE	GB 29894598
D	120	MSE	MET	MODIFIED RESIDUE	GB 29894598
D	242	MSE	MET	MODIFIED RESIDUE	GB 29894598
D	343	MSE	MET	MODIFIED RESIDUE	GB 29894598
E	1	MSE	MET	MODIFIED RESIDUE	GB 29894598
E	9	MSE	MET	MODIFIED RESIDUE	GB 29894598
E	76	MSE	MET	MODIFIED RESIDUE	GB 29894598
E	90	MSE	MET	MODIFIED RESIDUE	GB 29894598
E	120	MSE	MET	MODIFIED RESIDUE	GB 29894598
E	242	MSE	MET	MODIFIED RESIDUE	GB 29894598
E	343	MSE	MET	MODIFIED RESIDUE	GB 29894598
F	1	MSE	MET	MODIFIED RESIDUE	GB 29894598
F	9	MSE	MET	MODIFIED RESIDUE	GB 29894598
F	76	MSE	MET	MODIFIED RESIDUE	GB 29894598
F	90	MSE	MET	MODIFIED RESIDUE	GB 29894598
F	120	MSE	MET	MODIFIED RESIDUE	GB 29894598
F	242	MSE	MET	MODIFIED RESIDUE	GB 29894598
F	343	MSE	MET	MODIFIED RESIDUE	GB 29894598

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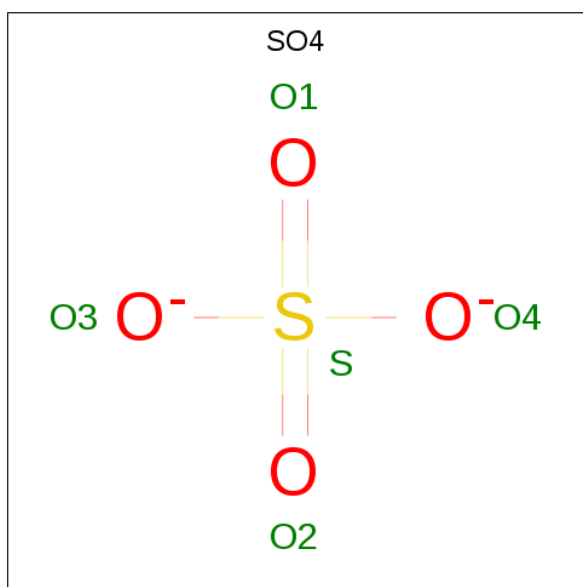
Chain	Residue	Modelled	Actual	Comment	Reference
G	1	MSE	MET	MODIFIED RESIDUE	GB 29894598
G	9	MSE	MET	MODIFIED RESIDUE	GB 29894598
G	76	MSE	MET	MODIFIED RESIDUE	GB 29894598
G	90	MSE	MET	MODIFIED RESIDUE	GB 29894598
G	120	MSE	MET	MODIFIED RESIDUE	GB 29894598
G	242	MSE	MET	MODIFIED RESIDUE	GB 29894598
G	343	MSE	MET	MODIFIED RESIDUE	GB 29894598
H	1	MSE	MET	MODIFIED RESIDUE	GB 29894598
H	9	MSE	MET	MODIFIED RESIDUE	GB 29894598
H	76	MSE	MET	MODIFIED RESIDUE	GB 29894598
H	90	MSE	MET	MODIFIED RESIDUE	GB 29894598
H	120	MSE	MET	MODIFIED RESIDUE	GB 29894598
H	242	MSE	MET	MODIFIED RESIDUE	GB 29894598
H	343	MSE	MET	MODIFIED RESIDUE	GB 29894598
I	1	MSE	MET	MODIFIED RESIDUE	GB 29894598
I	9	MSE	MET	MODIFIED RESIDUE	GB 29894598
I	76	MSE	MET	MODIFIED RESIDUE	GB 29894598
I	90	MSE	MET	MODIFIED RESIDUE	GB 29894598
I	120	MSE	MET	MODIFIED RESIDUE	GB 29894598
I	242	MSE	MET	MODIFIED RESIDUE	GB 29894598
I	343	MSE	MET	MODIFIED RESIDUE	GB 29894598
J	1	MSE	MET	MODIFIED RESIDUE	GB 29894598
J	9	MSE	MET	MODIFIED RESIDUE	GB 29894598
J	76	MSE	MET	MODIFIED RESIDUE	GB 29894598
J	90	MSE	MET	MODIFIED RESIDUE	GB 29894598
J	120	MSE	MET	MODIFIED RESIDUE	GB 29894598
J	242	MSE	MET	MODIFIED RESIDUE	GB 29894598
J	343	MSE	MET	MODIFIED RESIDUE	GB 29894598
K	1	MSE	MET	MODIFIED RESIDUE	GB 29894598
K	9	MSE	MET	MODIFIED RESIDUE	GB 29894598
K	76	MSE	MET	MODIFIED RESIDUE	GB 29894598
K	90	MSE	MET	MODIFIED RESIDUE	GB 29894598
K	120	MSE	MET	MODIFIED RESIDUE	GB 29894598
K	242	MSE	MET	MODIFIED RESIDUE	GB 29894598
K	343	MSE	MET	MODIFIED RESIDUE	GB 29894598
L	1	MSE	MET	MODIFIED RESIDUE	GB 29894598
L	9	MSE	MET	MODIFIED RESIDUE	GB 29894598
L	76	MSE	MET	MODIFIED RESIDUE	GB 29894598
L	90	MSE	MET	MODIFIED RESIDUE	GB 29894598
L	120	MSE	MET	MODIFIED RESIDUE	GB 29894598
L	242	MSE	MET	MODIFIED RESIDUE	GB 29894598
L	343	MSE	MET	MODIFIED RESIDUE	GB 29894598

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Chain	Residue	Modelled	Actual	Comment	Reference
M	1	MSE	MET	MODIFIED RESIDUE	GB 29894598
M	9	MSE	MET	MODIFIED RESIDUE	GB 29894598
M	76	MSE	MET	MODIFIED RESIDUE	GB 29894598
M	90	MSE	MET	MODIFIED RESIDUE	GB 29894598
M	120	MSE	MET	MODIFIED RESIDUE	GB 29894598
M	242	MSE	MET	MODIFIED RESIDUE	GB 29894598
M	343	MSE	MET	MODIFIED RESIDUE	GB 29894598
N	1	MSE	MET	MODIFIED RESIDUE	GB 29894598
N	9	MSE	MET	MODIFIED RESIDUE	GB 29894598
N	76	MSE	MET	MODIFIED RESIDUE	GB 29894598
N	90	MSE	MET	MODIFIED RESIDUE	GB 29894598
N	120	MSE	MET	MODIFIED RESIDUE	GB 29894598
N	242	MSE	MET	MODIFIED RESIDUE	GB 29894598
N	343	MSE	MET	MODIFIED RESIDUE	GB 29894598
O	1	MSE	MET	MODIFIED RESIDUE	GB 29894598
O	9	MSE	MET	MODIFIED RESIDUE	GB 29894598
O	76	MSE	MET	MODIFIED RESIDUE	GB 29894598
O	90	MSE	MET	MODIFIED RESIDUE	GB 29894598
O	120	MSE	MET	MODIFIED RESIDUE	GB 29894598
O	242	MSE	MET	MODIFIED RESIDUE	GB 29894598
O	343	MSE	MET	MODIFIED RESIDUE	GB 29894598
P	1	MSE	MET	MODIFIED RESIDUE	GB 29894598
P	9	MSE	MET	MODIFIED RESIDUE	GB 29894598
P	76	MSE	MET	MODIFIED RESIDUE	GB 29894598
P	90	MSE	MET	MODIFIED RESIDUE	GB 29894598
P	120	MSE	MET	MODIFIED RESIDUE	GB 29894598
P	242	MSE	MET	MODIFIED RESIDUE	GB 29894598
P	343	MSE	MET	MODIFIED RESIDUE	GB 29894598

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	A	1	5	4	1	0	0
2	B	1	5	4	1	0	0
2	C	1	5	4	1	0	0
2	D	1	5	4	1	0	0
2	E	1	5	4	1	0	0
2	F	1	5	4	1	0	0
2	G	1	5	4	1	0	0
2	H	1	5	4	1	0	0
2	I	1	5	4	1	0	0
2	J	1	5	4	1	0	0
2	K	1	5	4	1	0	0
2	L	1	5	4	1	0	0
2	M	1	5	4	1	0	0
2	N	1	5	4	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	O	1	Total	O	S	0	0
			5	4	1		
2	P	1	Total	O	S	0	0
			5	4	1		

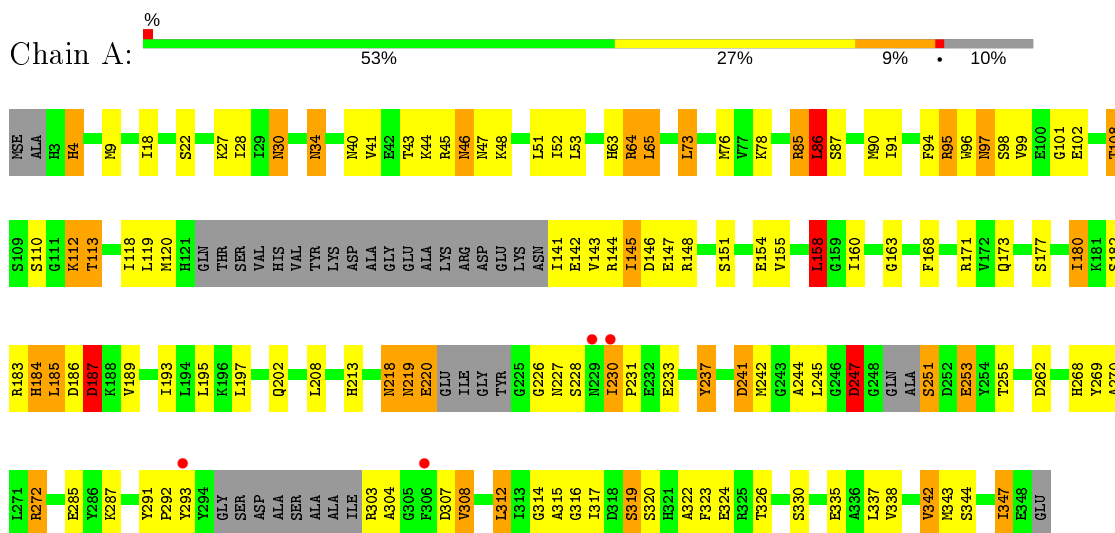
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	73	Total	O	0	0
			73	73		
3	B	71	Total	O	0	0
			71	71		
3	C	68	Total	O	0	0
			68	68		
3	D	57	Total	O	0	0
			57	57		
3	E	69	Total	O	0	0
			69	69		
3	F	57	Total	O	0	0
			57	57		
3	G	69	Total	O	0	0
			69	69		
3	H	61	Total	O	0	0
			61	61		
3	I	61	Total	O	0	0
			61	61		
3	J	57	Total	O	0	0
			57	57		
3	K	66	Total	O	0	0
			66	66		
3	L	54	Total	O	0	0
			54	54		
3	M	58	Total	O	0	0
			58	58		
3	N	67	Total	O	0	0
			67	67		
3	O	40	Total	O	0	0
			40	40		
3	P	54	Total	O	0	0
			54	54		

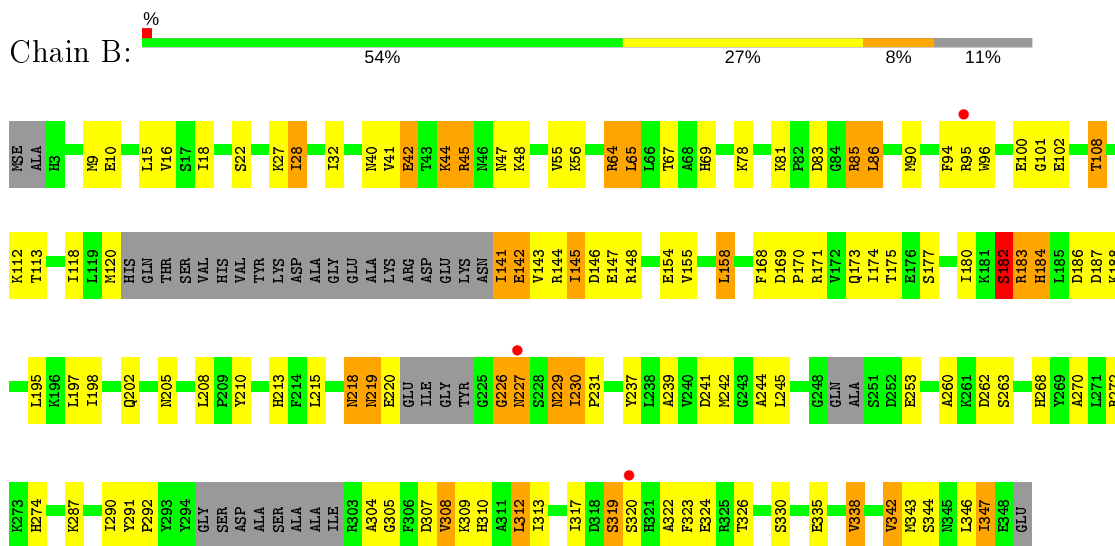
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Deblocking aminopeptidase

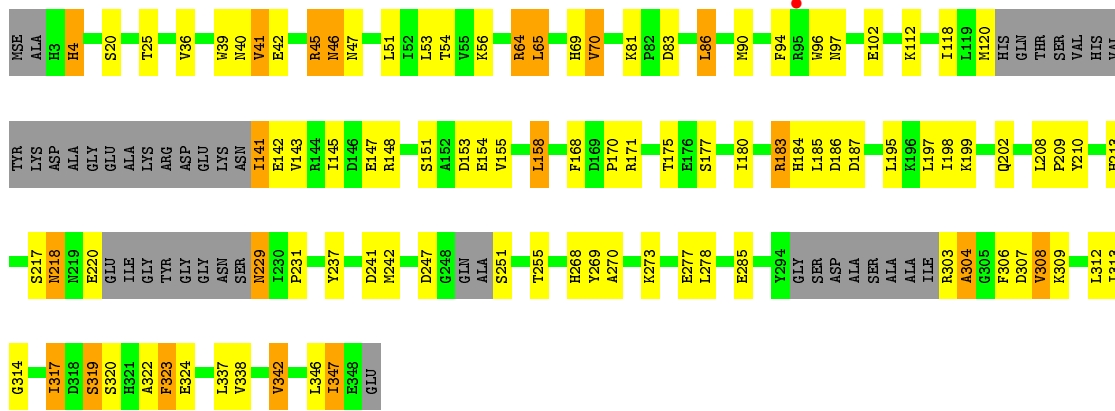


- Molecule 1: Deblocking aminopeptidase

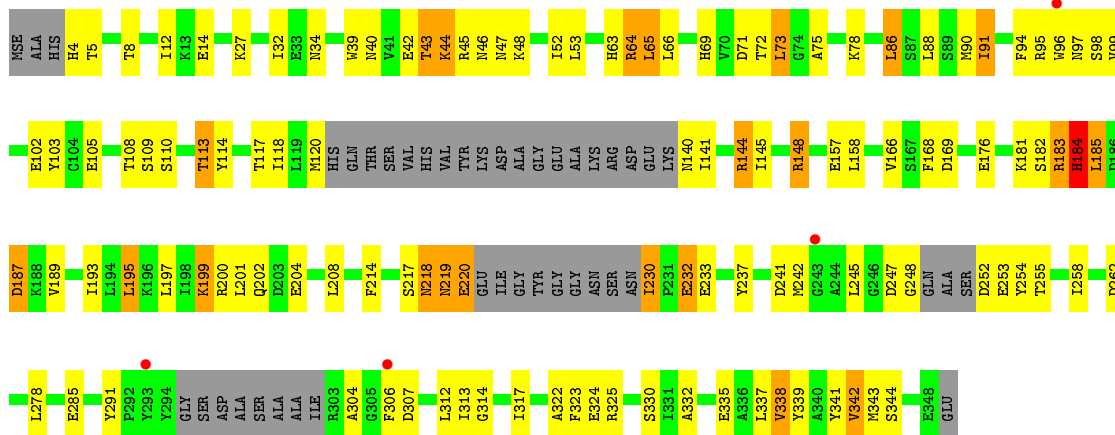


- Molecule 1: Deblocking aminopeptidase

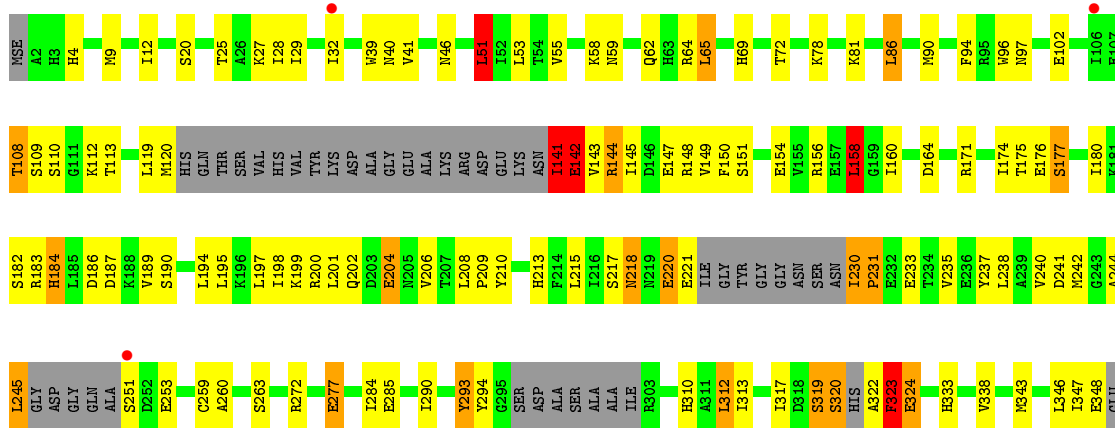




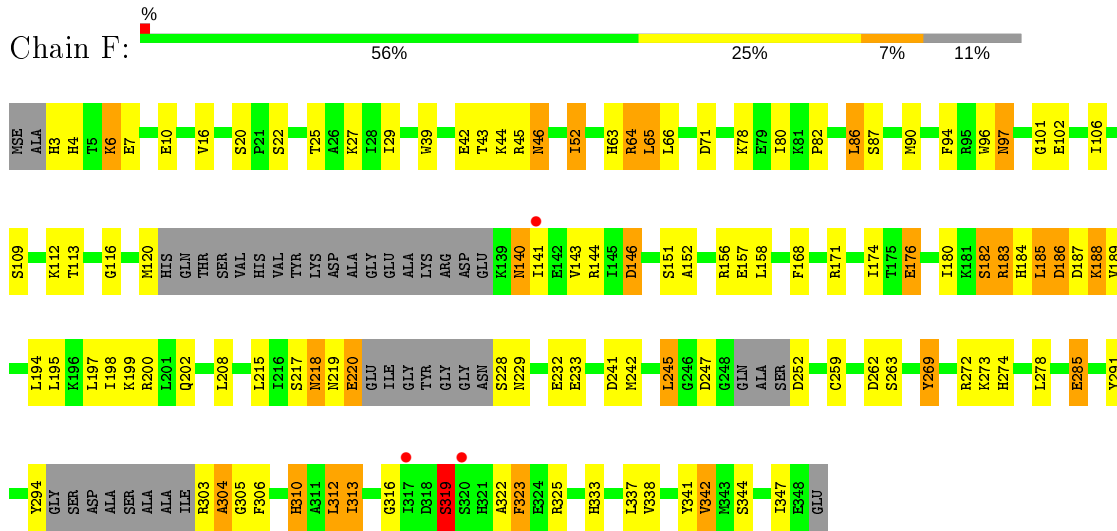
● Molecule 1: Deblocking aminopeptidase



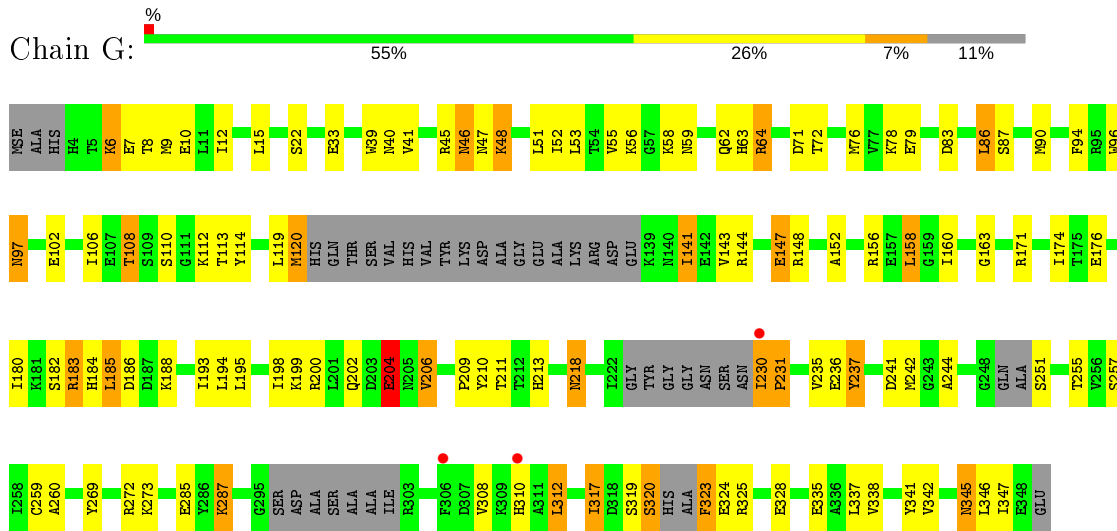
● Molecule 1: Deblocking aminopeptidase



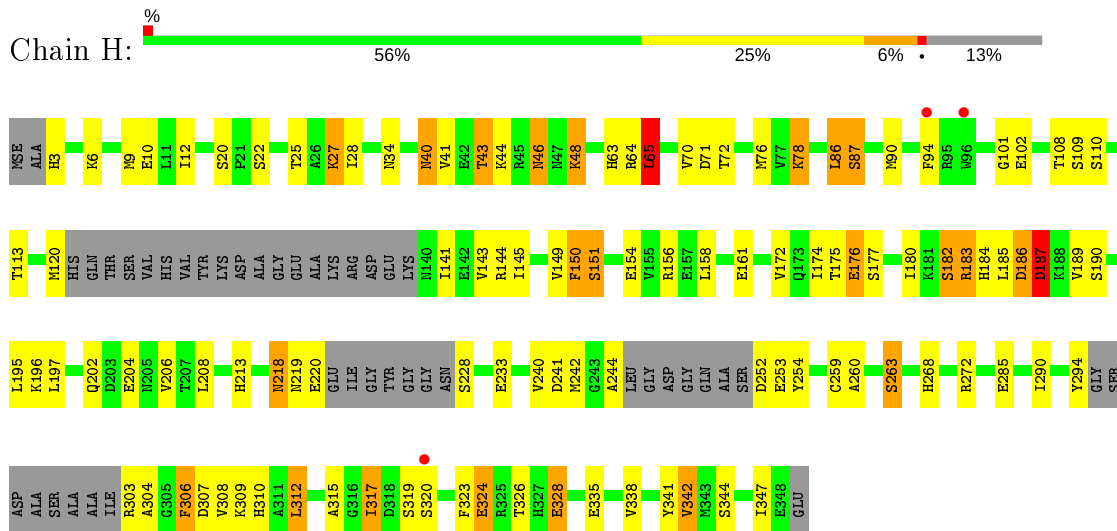
● Molecule 1: Deblocking aminopeptidase



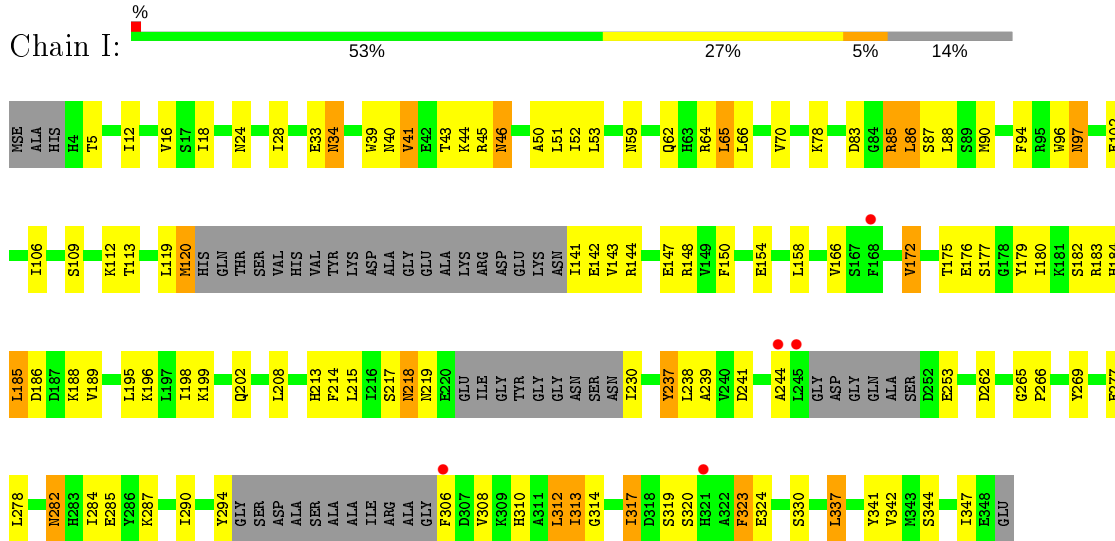
• Molecule 1: Deblocking aminopeptidase



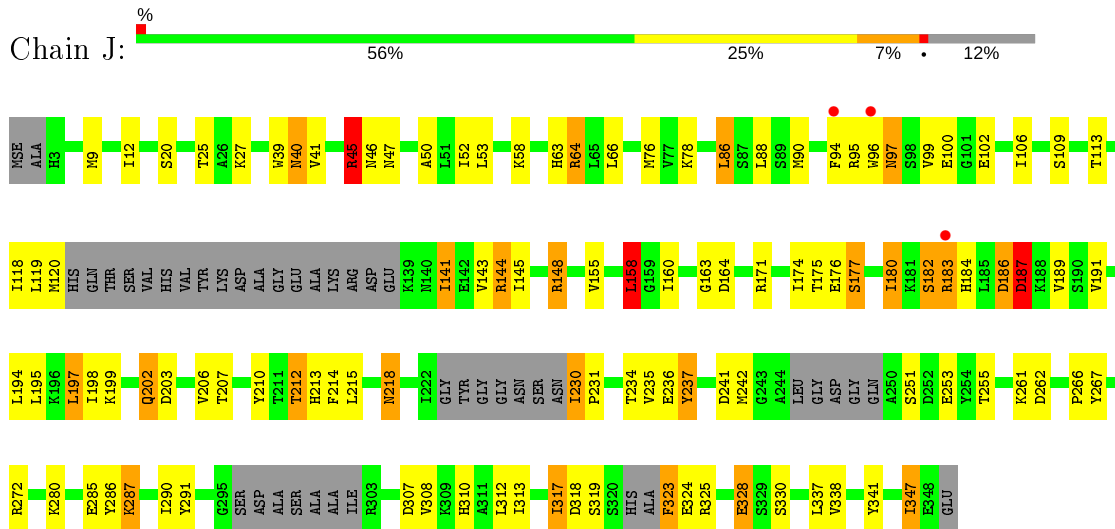
• Molecule 1: Deblocking aminopeptidase



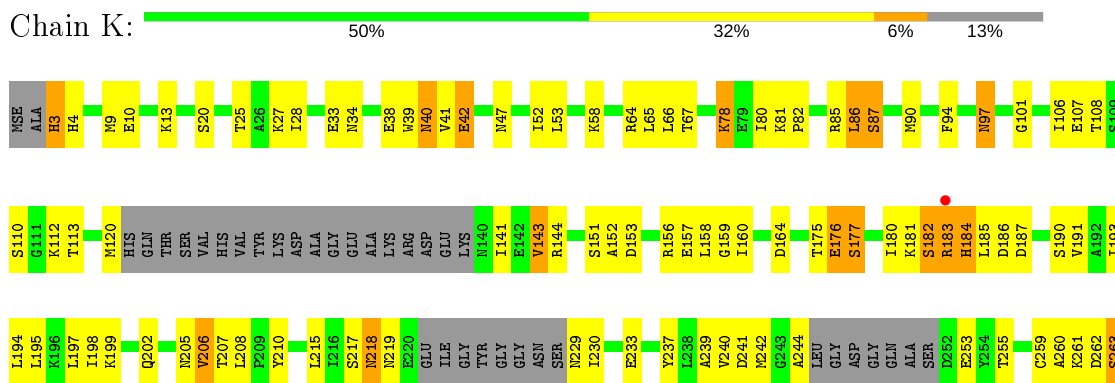
- Molecule 1: Deblocking aminopeptidase



- Molecule 1: Deblocking aminopeptidase

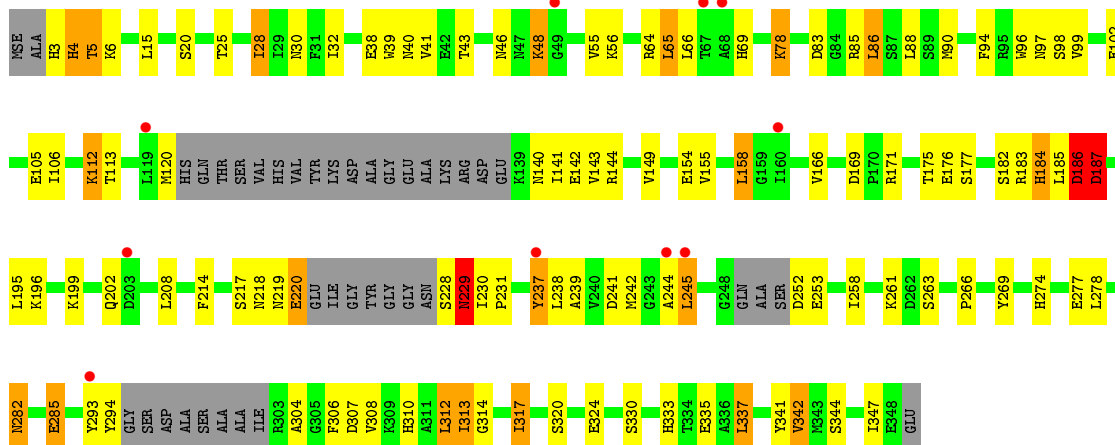


- Molecule 1: Deblocking aminopeptidase

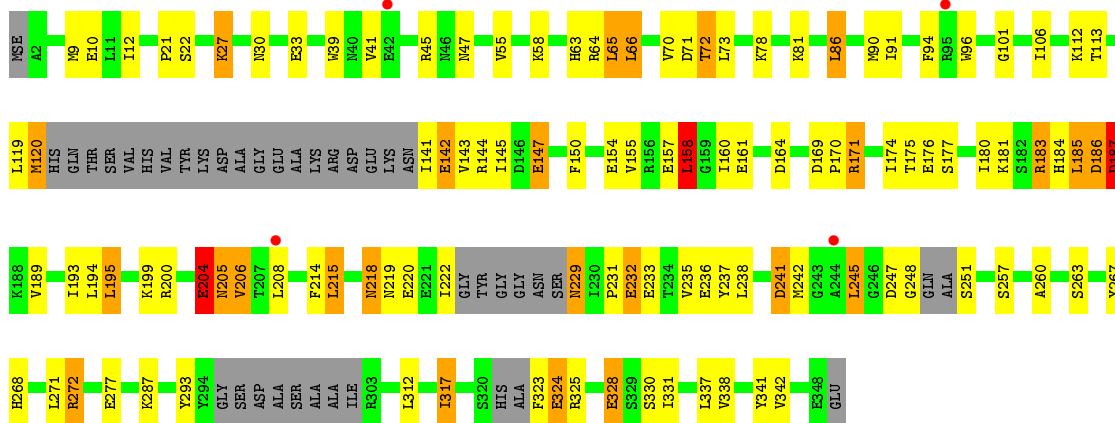




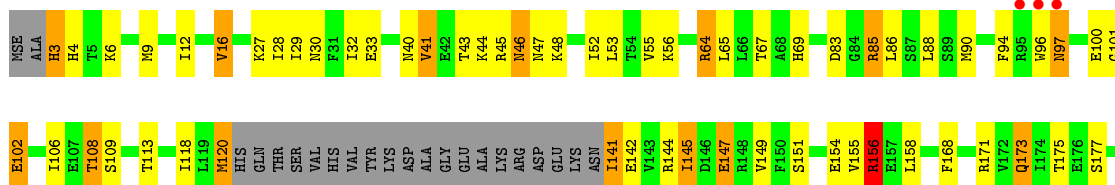
● Molecule 1: Deblocking aminopeptidase

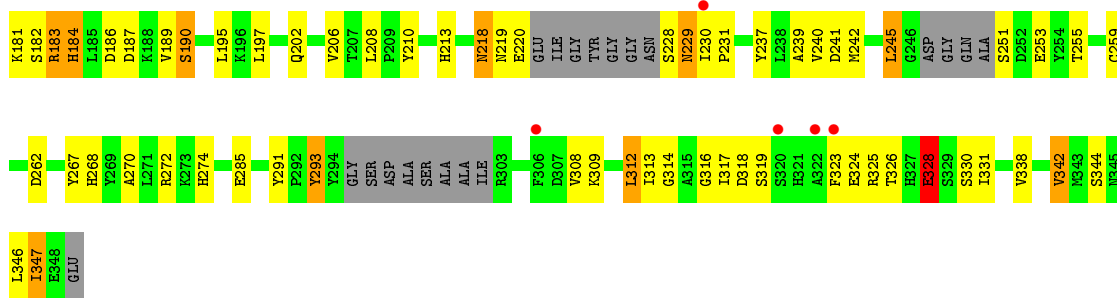


● Molecule 1: Deblocking aminopeptidase

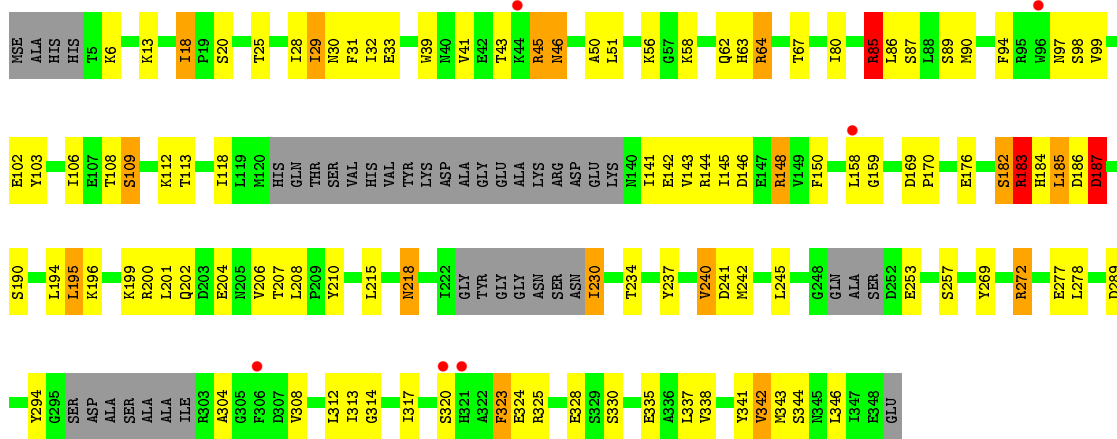


● Molecule 1: Deblocking aminopeptidase

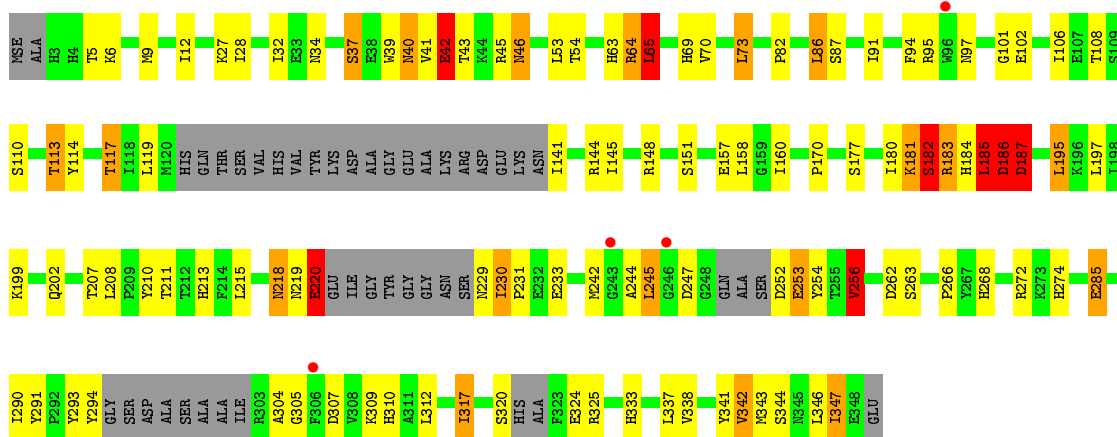




• Molecule 1: Deblocking aminopeptidase



• Molecule 1: Deblocking aminopeptidase



4 Data and refinement statistics i

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	240.92Å 240.92Å 294.82Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.65 47.25 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-2.65) 99.4 (47.25-2.55)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.61 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.194 , 0.264 0.197 , 0.195	Depositor DCC
R_{free} test set	10380 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	48.7	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 47.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.021 for $-2/3^*h-1/3^*k+2/3^*l,-1/3^*h-2/3^*k-2/3^*l,2/3^*h-2/3^*k+1/3^*l$ 0.019 for $-h,1/3^*h-1/3^*k+2/3^*l,2/3^*h+4/3^*k+1/3^*l$ 0.019 for $-1/3^*h+1/3^*k-2/3^*l,-k,-4/3^*h-2/3^*k+1/3^*l$ 0.477 for $-h,2/3^*h+1/3^*k-2/3^*l,-2/3^*h-4/3^*k-1/3^*l$ 0.477 for $1/3^*h+2/3^*k+2/3^*l,-k,4/3^*h+2/3^*k-1/3^*l$ 0.478 for $-1/3^*h-2/3^*k-2/3^*l,-2/3^*h-1/3^*k+2/3^*l,-2/3^*h+2/3^*k-1/3^*l$ 0.020 for $h,-h-k,-l$	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	39559	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.05% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

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

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.92	0/2477	1.03	11/3339 (0.3%)
1	B	0.92	0/2466	0.97	3/3324 (0.1%)
1	C	0.91	1/2448 (0.0%)	1.00	5/3300 (0.2%)
1	D	0.75	0/2433	0.85	1/3281 (0.0%)
1	E	0.85	0/2426	0.91	8/3269 (0.2%)
1	F	0.87	2/2461 (0.1%)	0.92	3/3318 (0.1%)
1	G	0.83	0/2446	0.87	4/3295 (0.1%)
1	H	0.85	0/2430	0.91	2/3277 (0.1%)
1	I	0.74	0/2399	0.84	0/3234
1	J	0.85	1/2432 (0.0%)	0.90	4/3277 (0.1%)
1	K	0.89	0/2425	0.91	1/3270 (0.0%)
1	L	0.75	0/2455	0.86	2/3310 (0.1%)
1	M	0.88	2/2456 (0.1%)	0.95	9/3309 (0.3%)
1	N	0.93	2/2443 (0.1%)	0.96	6/3294 (0.2%)
1	O	0.79	1/2438 (0.0%)	0.88	3/3287 (0.1%)
1	P	0.89	3/2415 (0.1%)	0.96	5/3254 (0.2%)
All	All	0.85	12/39050 (0.0%)	0.92	67/52638 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	0
1	B	0	1
1	C	0	1
1	D	0	2
1	E	0	1
1	F	0	2
1	G	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	J	0	3
1	K	0	1
1	L	1	0
1	N	0	1
1	O	1	0
1	P	0	4
All	All	3	18

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	161	GLU	CG-CD	10.39	1.67	1.51
1	P	253	GLU	CG-CD	7.05	1.62	1.51
1	F	342	VAL	CB-CG1	-6.18	1.39	1.52
1	J	328	GLU	CG-CD	5.99	1.60	1.51
1	M	328	GLU	CG-CD	5.88	1.60	1.51
1	N	293	TYR	CD2-CE2	5.82	1.48	1.39
1	P	42	GLU	CG-CD	5.81	1.60	1.51
1	P	220	GLU	CB-CG	5.71	1.62	1.52
1	C	277	GLU	CG-CD	5.42	1.60	1.51
1	N	328	GLU	CB-CG	-5.39	1.42	1.52
1	O	176	GLU	CB-CG	5.31	1.62	1.52
1	F	176	GLU	CG-CD	5.23	1.59	1.51

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	187	ASP	N-CA-C	8.37	133.60	111.00
1	A	148	ARG	NE-CZ-NH1	-7.49	116.56	120.30
1	A	272	ARG	NE-CZ-NH1	7.49	124.05	120.30
1	E	144	ARG	NE-CZ-NH2	-7.45	116.58	120.30
1	A	272	ARG	NE-CZ-NH2	-7.37	116.61	120.30
1	C	64	ARG	NE-CZ-NH2	-7.29	116.66	120.30
1	E	156	ARG	NE-CZ-NH2	-7.18	116.71	120.30
1	L	187	ASP	N-CA-C	7.17	130.37	111.00
1	N	156	ARG	NE-CZ-NH1	6.70	123.65	120.30
1	E	144	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	N	64	ARG	NE-CZ-NH2	-6.43	117.09	120.30
1	A	184	HIS	CB-CA-C	6.38	123.16	110.40
1	M	144	ARG	NE-CZ-NH1	6.37	123.49	120.30
1	A	73	LEU	CA-CB-CG	6.37	129.95	115.30
1	E	215	LEU	CA-CB-CG	6.34	129.88	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	144	ARG	NE-CZ-NH2	-6.26	117.17	120.30
1	A	86	LEU	CA-CB-CG	6.25	129.67	115.30
1	A	65	LEU	CA-CB-CG	6.25	129.67	115.30
1	O	187	ASP	N-CA-C	6.23	127.82	111.00
1	A	187	ASP	N-CA-C	6.15	127.60	111.00
1	N	272	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	J	215	LEU	CA-CB-CG	6.14	129.42	115.30
1	F	241	ASP	CB-CG-OD1	6.14	123.83	118.30
1	M	65	LEU	CA-CB-CG	6.12	129.37	115.30
1	P	256	VAL	CB-CA-C	-6.11	99.80	111.40
1	P	182	SER	N-CA-C	6.10	127.46	111.00
1	C	65	LEU	CA-CB-CG	6.09	129.32	115.30
1	H	65	LEU	CA-CB-CG	6.05	129.22	115.30
1	G	144	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	C	64	ARG	NE-CZ-NH1	6.01	123.30	120.30
1	A	187	ASP	CB-CG-OD2	-6.00	112.90	118.30
1	F	342	VAL	CG1-CB-CG2	-5.94	101.40	110.90
1	M	186	ASP	CB-CG-OD1	5.90	123.61	118.30
1	J	144	ARG	NE-CZ-NH1	5.87	123.23	120.30
1	J	158	LEU	CA-CB-CG	5.84	128.72	115.30
1	E	65	LEU	CA-CB-CG	5.72	128.46	115.30
1	C	83	ASP	CB-CG-OD2	5.72	123.45	118.30
1	E	158	LEU	CA-CB-CG	5.71	128.43	115.30
1	B	272	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	N	46	ASN	CB-CA-C	5.48	121.36	110.40
1	N	85	ARG	NE-CZ-NH2	5.47	123.04	120.30
1	M	27	LYS	CD-CE-NZ	5.47	124.28	111.70
1	G	158	LEU	CA-CB-CG	5.46	127.87	115.30
1	B	64	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	G	83	ASP	CB-CG-OD1	5.46	123.21	118.30
1	A	241	ASP	CB-CG-OD1	5.44	123.19	118.30
1	H	187	ASP	N-CA-C	5.42	125.64	111.00
1	N	272	ARG	NE-CZ-NH1	5.41	123.01	120.30
1	P	65	LEU	CA-CB-CG	5.34	127.59	115.30
1	L	245	LEU	CA-CB-CG	5.33	127.56	115.30
1	E	51	LEU	CA-CB-CG	5.33	127.55	115.30
1	F	156	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	M	272	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	D	144	ARG	CG-CD-NE	5.30	122.93	111.80
1	O	85	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	M	158	LEU	CB-CG-CD2	-5.23	102.11	111.00
1	J	187	ASP	CB-CG-OD2	-5.17	113.65	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	142	GLU	N-CA-C	5.17	124.95	111.00
1	M	215	LEU	CA-CB-CG	5.16	127.17	115.30
1	P	182	SER	CA-C-N	-5.15	105.87	117.20
1	C	70	VAL	CB-CA-C	-5.11	101.69	111.40
1	B	219	ASN	N-CA-C	5.09	124.74	111.00
1	M	241	ASP	CB-CG-OD1	5.07	122.86	118.30
1	K	143	VAL	CB-CA-C	-5.05	101.80	111.40
1	G	144	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	A	158	LEU	CA-CB-CG	5.03	126.86	115.30
1	O	64	ARG	NE-CZ-NH2	-5.00	117.80	120.30

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	187	ASP	CA
1	L	187	ASP	CA
1	O	187	ASP	CA

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	182	SER	Peptide
1	C	229	ASN	Peptide
1	D	182	SER	Peptide
1	D	185	LEU	Peptide
1	E	141	ILE	Peptide
1	F	182	SER	Peptide
1	F	304	ALA	Peptide
1	G	182	SER	Peptide
1	G	251	SER	Peptide
1	J	182	SER	Peptide
1	J	186	ASP	Peptide
1	J	45	ARG	Peptide
1	K	182	SER	Peptide
1	N	3	HIS	Peptide
1	P	181	LYS	Peptide
1	P	185	LEU	Peptide
1	P	186	ASP	Peptide
1	P	305	GLY	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2441	0	2395	134	0
1	B	2431	0	2388	137	0
1	C	2413	0	2375	102	0
1	D	2398	0	2357	91	0
1	E	2393	0	2361	132	0
1	F	2426	0	2383	102	0
1	G	2413	0	2369	108	0
1	H	2394	0	2354	105	0
1	I	2364	0	2342	94	0
1	J	2399	0	2355	123	0
1	K	2389	0	2352	121	0
1	L	2421	0	2378	113	0
1	M	2422	0	2380	109	0
1	N	2407	0	2371	108	0
1	O	2404	0	2361	78	0
1	P	2382	0	2340	117	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
2	E	5	0	0	0	0
2	F	5	0	0	0	0
2	G	5	0	0	0	0
2	H	5	0	0	0	0
2	I	5	0	0	0	0
2	J	5	0	0	0	0
2	K	5	0	0	0	0
2	L	5	0	0	0	0
2	M	5	0	0	0	0
2	N	5	0	0	0	0
2	O	5	0	0	0	0
2	P	5	0	0	0	0
3	A	73	0	0	23	0
3	B	71	0	0	23	0
3	C	68	0	0	19	0
3	D	57	0	0	9	0
3	E	69	0	0	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	57	0	0	28	0
3	G	69	0	0	6	0
3	H	61	0	0	16	0
3	I	61	0	0	12	0
3	J	57	0	0	12	0
3	K	66	0	0	18	0
3	L	54	0	0	23	0
3	M	58	0	0	21	0
3	N	67	0	0	14	0
3	O	40	0	0	8	0
3	P	54	0	0	24	0
All	All	39559	0	37861	1685	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 22.

All (1685) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:102:GLU:HG3	1:D:183:ARG:NH2	1.25	1.46
1:J:45:ARG:HB2	1:J:45:ARG:NH1	1.18	1.42
1:P:208:LEU:HD23	1:P:343:MSE:CE	1.50	1.39
1:L:102:GLU:HG3	1:L:183:ARG:NH1	1.31	1.37
1:J:102:GLU:HG3	1:J:183:ARG:NH2	1.39	1.35
1:M:81:LYS:NZ	1:M:142:GLU:HG2	1.43	1.33
1:P:41:VAL:HB	3:P:395:HOH:O	1.21	1.33
1:G:102:GLU:HG3	1:G:183:ARG:NH1	1.42	1.30
1:A:9:MSE:CE	1:A:180:ILE:HB	1.62	1.30
1:K:208:LEU:HD23	1:K:343:MSE:CE	1.61	1.28
1:C:347:ILE:HB	3:C:402:HOH:O	1.23	1.28
1:F:252:ASP:HA	3:F:397:HOH:O	1.25	1.27
1:D:102:GLU:CG	1:D:183:ARG:HH22	1.48	1.25
3:B:417:HOH:O	1:J:177:SER:HB2	1.37	1.25
1:P:41:VAL:HG12	3:P:353:HOH:O	1.36	1.22
1:J:45:ARG:NH1	1:J:45:ARG:CB	2.04	1.20
1:D:183:ARG:O	1:D:184:HIS:HB2	1.40	1.19
1:B:347:ILE:HB	3:B:397:HOH:O	1.42	1.18
1:H:219:ASN:O	1:H:220:GLU:HB2	1.44	1.17
1:A:9:MSE:HE2	1:A:180:ILE:HB	1.24	1.16
1:E:39:TRP:HB3	1:E:202:GLN:HE22	1.09	1.14
1:F:197:LEU:HD22	1:F:338:VAL:HG12	1.29	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:102:GLU:CG	1:G:183:ARG:HH12	1.61	1.13
1:B:183:ARG:NH2	1:B:184:HIS:HB2	1.64	1.13
1:A:183:ARG:HA	3:A:393:HOH:O	1.48	1.12
1:L:220:GLU:HA	3:L:397:HOH:O	1.48	1.12
1:G:244:ALA:HB2	1:G:320:SER:HB2	1.30	1.10
1:J:45:ARG:HH11	1:J:45:ARG:CB	1.63	1.10
1:B:154:GLU:HB2	3:B:378:HOH:O	1.52	1.10
1:E:183:ARG:O	1:E:184:HIS:HB2	1.31	1.09
1:G:184:HIS:HB3	3:G:411:HOH:O	1.49	1.08
1:N:9:MSE:HE2	1:N:331:ILE:HD12	1.27	1.08
1:B:183:ARG:HH21	1:B:184:HIS:HB2	1.09	1.08
1:G:76:MSE:HE1	1:H:260:ALA:CB	1.84	1.07
1:P:184:HIS:HB3	3:P:362:HOH:O	1.52	1.07
1:M:171:ARG:HD3	1:N:171:ARG:HD3	1.38	1.05
1:O:294:TYR:HA	3:O:363:HOH:O	1.54	1.05
1:N:142:GLU:HA	3:N:404:HOH:O	1.56	1.05
1:H:197:LEU:HD22	1:H:338:VAL:HG12	1.37	1.05
1:A:76:MSE:HE1	1:B:260:ALA:HB3	1.35	1.04
1:K:208:LEU:HD23	1:K:343:MSE:HE1	1.06	1.04
1:A:208:LEU:HD23	1:A:343:MSE:HE2	1.38	1.04
1:L:102:GLU:HG3	1:L:183:ARG:CZ	1.86	1.04
1:P:208:LEU:CD2	1:P:343:MSE:CE	2.34	1.04
1:M:175:THR:HB	3:M:368:HOH:O	0.88	1.04
1:P:197:LEU:HD22	1:P:338:VAL:HG12	1.38	1.04
1:M:186:ASP:HB2	3:M:360:HOH:O	1.57	1.04
1:I:102:GLU:HG3	1:I:183:ARG:HH12	1.22	1.03
1:P:208:LEU:HD23	1:P:343:MSE:HE1	1.03	1.03
1:B:208:LEU:HD23	1:B:343:MSE:CE	1.89	1.03
1:P:184:HIS:O	1:P:186:ASP:HA	1.58	1.03
1:N:9:MSE:CE	1:N:331:ILE:HD12	1.89	1.02
1:G:76:MSE:HE1	1:H:260:ALA:HB3	1.39	1.02
1:J:76:MSE:HE1	1:K:260:ALA:HB3	1.40	1.02
1:C:185:LEU:N	3:C:408:HOH:O	1.91	1.02
1:K:183:ARG:O	1:K:183:ARG:HG3	1.58	1.01
1:C:183:ARG:HB3	1:C:183:ARG:NH1	1.75	1.01
1:K:197:LEU:HD22	1:K:338:VAL:HG12	1.41	1.01
1:C:183:ARG:HB3	1:C:183:ARG:HH11	1.23	1.01
1:P:9:MSE:HE3	1:P:180:ILE:HB	1.40	1.00
1:N:9:MSE:HE2	1:N:331:ILE:CD1	1.89	1.00
1:A:76:MSE:HE2	1:B:290:ILE:HD11	1.44	0.99
1:J:76:MSE:HE1	1:K:260:ALA:CB	1.92	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:76:MSE:CE	1:H:260:ALA:HB3	1.92	0.98
1:C:171:ARG:HE	1:C:183:ARG:HH22	1.04	0.98
1:F:183:ARG:NH1	1:F:323:PHE:HD2	1.62	0.98
1:F:189:VAL:HB	1:F:242:MSE:HE1	1.40	0.98
1:J:76:MSE:CE	1:K:260:ALA:HB3	1.93	0.98
1:C:347:ILE:HD11	3:C:418:HOH:O	1.64	0.98
1:L:102:GLU:CG	1:L:183:ARG:HH12	1.76	0.98
1:F:197:LEU:HD22	1:F:338:VAL:CG1	1.94	0.97
1:G:338:VAL:O	1:G:342:VAL:HG23	1.62	0.97
1:K:183:ARG:O	1:K:184:HIS:HB2	1.64	0.97
1:L:102:GLU:CG	1:L:183:ARG:NH1	2.28	0.97
1:B:183:ARG:O	1:B:184:HIS:HB3	1.64	0.96
1:M:9:MSE:HE3	1:M:180:ILE:HB	1.47	0.96
1:D:183:ARG:HG2	1:D:322:ALA:O	1.66	0.96
1:E:120:MSE:HG2	1:E:141:ILE:HG13	1.46	0.96
1:L:277:GLU:HG2	3:L:398:HOH:O	1.66	0.96
1:A:76:MSE:HE3	1:A:163:GLY:HA2	1.48	0.96
1:B:184:HIS:CD2	1:B:186:ASP:OD2	2.18	0.96
1:C:102:GLU:HG2	1:C:183:ARG:HH21	1.32	0.95
1:C:45:ARG:HH11	1:C:45:ARG:HG3	1.32	0.95
1:H:34:ASN:HB2	3:H:401:HOH:O	1.65	0.95
1:A:90:MSE:HA	3:A:421:HOH:O	1.67	0.94
1:L:252:ASP:HA	3:L:399:HOH:O	1.68	0.94
1:K:208:LEU:CD2	1:K:343:MSE:CE	2.45	0.94
1:M:147:GLU:HG3	3:M:365:HOH:O	1.66	0.93
1:F:10:GLU:HG3	3:F:407:HOH:O	1.67	0.93
1:B:320:SER:HB2	3:B:403:HOH:O	1.66	0.93
1:A:208:LEU:CD2	1:A:342:VAL:HG13	1.99	0.93
1:M:81:LYS:HZ1	1:M:142:GLU:HG2	1.17	0.92
1:G:97:ASN:ND2	1:G:97:ASN:H	1.68	0.92
1:C:4:HIS:H	1:C:4:HIS:CD2	1.76	0.92
1:A:171:ARG:HD2	1:G:171:ARG:HD3	1.52	0.92
1:B:242:MSE:HE1	3:B:411:HOH:O	1.69	0.92
1:I:172:VAL:HG23	1:I:182:SER:HB2	1.50	0.92
1:P:108:THR:HG22	1:P:110:SER:H	1.33	0.92
1:B:242:MSE:SE	1:B:317:ILE:HD11	2.21	0.91
1:B:208:LEU:HD23	1:B:343:MSE:HE2	1.50	0.91
1:I:175:THR:HG22	1:I:177:SER:H	1.35	0.91
1:H:303:ARG:O	3:H:410:HOH:O	1.89	0.91
1:A:208:LEU:HD21	1:A:342:VAL:HG13	1.51	0.91
1:P:253:GLU:HG2	3:P:404:HOH:O	1.69	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:102:GLU:HG3	3:H:402:HOH:O	1.70	0.90
1:O:208:LEU:HD23	1:O:343:MSE:CE	2.00	0.90
1:G:97:ASN:HD22	1:G:97:ASN:N	1.70	0.90
1:J:76:MSE:HE2	1:K:290:ILE:HG12	1.53	0.90
1:E:141:ILE:HG12	3:E:417:HOH:O	1.70	0.90
1:G:97:ASN:HD22	1:G:97:ASN:H	0.91	0.89
1:B:41:VAL:HG21	1:B:198:ILE:CG2	2.01	0.89
1:J:102:GLU:CG	1:J:183:ARG:HH21	1.84	0.89
1:B:45:ARG:HG3	1:B:45:ARG:HH11	1.37	0.89
1:P:229:ASN:HA	3:P:397:HOH:O	1.72	0.89
1:M:81:LYS:HZ3	1:M:142:GLU:HG2	1.17	0.89
1:M:141:ILE:N	3:M:390:HOH:O	2.06	0.89
1:E:183:ARG:O	1:E:184:HIS:CB	2.17	0.88
1:A:208:LEU:HD23	1:A:343:MSE:CE	2.02	0.88
1:B:102:GLU:CD	1:B:183:ARG:HD2	1.94	0.88
1:O:272:ARG:HG3	1:O:272:ARG:HH11	1.38	0.88
1:E:81:LYS:NZ	1:E:142:GLU:HG2	1.88	0.88
1:I:102:GLU:HG3	1:I:183:ARG:NH1	1.87	0.88
1:D:102:GLU:CG	1:D:183:ARG:NH2	2.19	0.88
1:K:208:LEU:CD2	1:K:343:MSE:HE1	1.99	0.88
3:D:393:HOH:O	1:H:319:SER:HB3	1.74	0.88
1:K:263:SER:HB2	1:K:294:TYR:N	1.89	0.88
1:B:184:HIS:HD2	1:B:186:ASP:OD2	1.54	0.87
1:E:183:ARG:NH1	1:E:323:PHE:CE2	2.41	0.87
1:F:20:SER:HB2	1:F:25:THR:HG22	1.53	0.87
1:F:200:ARG:HB3	3:F:398:HOH:O	1.73	0.87
1:N:102:GLU:OE2	1:N:183:ARG:HD2	1.74	0.87
1:G:185:LEU:HB2	1:G:324:GLU:OE2	1.75	0.87
1:P:54:THR:OG1	1:P:213:HIS:HD2	1.57	0.86
1:J:317:ILE:HD11	1:J:324:GLU:HB3	1.58	0.86
1:F:120:MSE:HB2	3:F:404:HOH:O	1.76	0.86
1:G:141:ILE:HD13	1:G:141:ILE:O	1.76	0.85
1:F:310:HIS:CD2	3:F:384:HOH:O	2.29	0.84
1:E:175:THR:CG2	1:E:177:SER:HB2	2.07	0.84
1:A:185:LEU:N	3:A:407:HOH:O	2.10	0.84
1:J:184:HIS:O	1:J:324:GLU:OE2	1.94	0.84
1:L:3:HIS:O	1:L:6:LYS:HB3	1.77	0.84
1:B:208:LEU:HD23	1:B:343:MSE:HE1	1.60	0.84
1:O:183:ARG:HG2	3:O:387:HOH:O	1.77	0.84
1:E:183:ARG:HH11	1:E:323:PHE:HE2	1.25	0.84
1:L:182:SER:C	3:L:404:HOH:O	2.15	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:310:HIS:HB2	3:L:385:HOH:O	1.77	0.84
1:H:189:VAL:HB	1:H:242:MSE:HE1	1.60	0.83
1:I:102:GLU:CG	1:I:183:ARG:HH12	1.91	0.83
1:P:145:ILE:HG12	3:P:356:HOH:O	1.78	0.83
1:L:242:MSE:SE	1:L:317:ILE:HG21	2.28	0.83
1:E:108:THR:HG22	1:E:112:LYS:H	1.44	0.83
1:O:184:HIS:O	1:O:186:ASP:N	2.10	0.83
1:O:183:ARG:CG	3:O:387:HOH:O	2.27	0.83
1:I:120:MSE:HG2	1:I:141:ILE:HD13	1.60	0.82
1:B:171:ARG:HD3	1:J:171:ARG:HD3	1.61	0.82
1:J:9:MSE:CE	1:J:174:ILE:HG23	2.10	0.82
1:E:277:GLU:OE2	1:E:277:GLU:HA	1.77	0.82
1:J:97:ASN:H	1:J:97:ASN:ND2	1.73	0.82
1:K:317:ILE:O	1:K:317:ILE:HG23	1.78	0.82
1:N:40:ASN:H	1:N:202:GLN:NE2	1.78	0.82
1:N:102:GLU:HG3	3:N:412:HOH:O	1.79	0.81
1:A:76:MSE:SE	3:A:416:HOH:O	2.48	0.81
1:K:184:HIS:CD2	1:K:186:ASP:OD2	2.33	0.81
3:O:380:HOH:O	1:P:119:LEU:HD13	1.81	0.81
1:H:184:HIS:HA	1:H:186:ASP:HB2	1.62	0.81
1:A:76:MSE:CE	1:B:260:ALA:HB3	2.09	0.81
1:M:183:ARG:HB3	1:M:183:ARG:HH11	1.46	0.81
1:A:76:MSE:HE1	1:B:260:ALA:CB	2.10	0.81
1:E:39:TRP:HB3	1:E:202:GLN:NE2	1.93	0.81
1:F:183:ARG:NH1	1:F:323:PHE:CD2	2.49	0.81
1:G:241:ASP:OD1	3:G:392:HOH:O	1.97	0.81
1:H:9:MSE:HE3	1:H:180:ILE:HB	1.62	0.80
1:M:81:LYS:NZ	1:M:142:GLU:CG	2.36	0.80
1:B:41:VAL:HG23	3:B:400:HOH:O	1.81	0.80
1:J:45:ARG:HB2	1:J:45:ARG:CZ	2.10	0.80
1:P:317:ILE:O	1:P:317:ILE:HG23	1.80	0.80
1:A:322:ALA:O	3:A:393:HOH:O	1.99	0.80
1:M:218:ASN:HD22	1:M:218:ASN:H	1.27	0.80
1:B:197:LEU:HD22	1:B:338:VAL:CG1	2.12	0.80
1:D:183:ARG:HB3	1:D:183:ARG:HH11	1.47	0.80
1:E:220:GLU:O	1:E:220:GLU:HG3	1.82	0.80
1:B:208:LEU:CD2	1:B:343:MSE:HE2	2.12	0.79
1:E:175:THR:HG22	1:E:177:SER:H	1.47	0.79
1:E:230:ILE:HG13	1:E:230:ILE:O	1.79	0.79
1:A:76:MSE:HE2	1:B:290:ILE:CD1	2.11	0.79
1:E:208:LEU:HD23	1:E:343:MSE:CE	2.12	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:183:ARG:HG2	3:I:389:HOH:O	1.82	0.79
1:F:184:HIS:HB3	3:F:386:HOH:O	1.81	0.79
1:I:185:LEU:HB2	1:I:324:GLU:OE1	1.83	0.79
1:J:102:GLU:CG	1:J:183:ARG:NH2	2.35	0.79
1:J:45:ARG:CZ	1:J:45:ARG:CB	2.61	0.79
1:F:228:SER:HA	3:F:399:HOH:O	1.83	0.79
1:N:41:VAL:HG23	1:N:55:VAL:HG22	1.64	0.79
1:J:141:ILE:HD13	1:J:141:ILE:O	1.83	0.78
1:P:117:THR:CG2	3:P:379:HOH:O	2.30	0.78
1:I:310:HIS:HB2	3:I:400:HOH:O	1.82	0.78
1:F:313:ILE:C	1:F:313:ILE:HD13	2.02	0.78
1:G:76:MSE:HE3	1:G:163:GLY:HA2	1.64	0.78
1:M:317:ILE:HD13	1:M:317:ILE:O	1.83	0.78
1:I:144:ARG:NH2	3:K:390:HOH:O	2.17	0.78
1:E:183:ARG:HA	3:E:410:HOH:O	1.82	0.78
1:J:76:MSE:CE	1:K:260:ALA:CB	2.57	0.78
1:E:241:ASP:OD1	3:E:376:HOH:O	2.01	0.78
1:N:9:MSE:HE1	1:N:328:GLU:HA	1.65	0.78
1:F:174:ILE:HD11	1:F:180:ILE:HD12	1.66	0.77
1:G:76:MSE:CE	1:H:260:ALA:CB	2.56	0.77
1:P:197:LEU:HD22	1:P:338:VAL:CG1	2.15	0.77
1:I:144:ARG:HD3	1:K:325:ARG:CZ	2.13	0.77
1:L:102:GLU:HG3	1:L:183:ARG:HH12	0.97	0.77
1:F:197:LEU:CD2	1:F:338:VAL:HG12	2.13	0.77
1:G:171:ARG:HD2	3:G:401:HOH:O	1.83	0.77
1:G:269:TYR:CE2	1:G:273:LYS:HE3	2.20	0.77
1:B:41:VAL:HG21	1:B:198:ILE:HG23	1.67	0.77
1:C:185:LEU:O	1:C:242:MSE:CE	2.33	0.77
1:J:97:ASN:H	1:J:97:ASN:HD22	1.31	0.77
1:A:34:ASN:HB3	3:A:412:HOH:O	1.84	0.77
1:E:120:MSE:CG	1:E:141:ILE:HG13	2.14	0.77
1:E:208:LEU:HD23	1:E:343:MSE:HE1	1.64	0.77
1:D:183:ARG:O	1:D:184:HIS:CB	2.27	0.76
1:N:184:HIS:HD2	1:N:186:ASP:OD2	1.68	0.76
1:J:102:GLU:HG3	1:J:183:ARG:HH21	0.95	0.76
1:P:119:LEU:CB	3:P:396:HOH:O	2.31	0.76
1:P:95:ARG:HD2	1:P:97:ASN:ND2	2.00	0.76
1:F:189:VAL:HB	1:F:242:MSE:CE	2.15	0.76
1:K:229:ASN:HB2	3:K:395:HOH:O	1.84	0.76
1:I:41:VAL:O	3:I:410:HOH:O	2.04	0.76
1:C:45:ARG:HH11	1:C:45:ARG:CG	1.97	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:230:ILE:HG23	3:E:375:HOH:O	1.86	0.76
1:H:184:HIS:HD2	1:H:186:ASP:OD2	1.69	0.76
1:H:197:LEU:HD22	1:H:338:VAL:CG1	2.14	0.76
1:H:86:LEU:HD22	1:H:145:ILE:HD11	1.68	0.76
1:C:183:ARG:O	1:C:183:ARG:HG2	1.86	0.76
1:E:218:ASN:HD22	1:E:218:ASN:H	1.34	0.76
1:G:76:MSE:HE2	1:H:290:ILE:HG12	1.68	0.76
1:M:142:GLU:HB2	3:M:394:HOH:O	1.87	0.75
1:B:183:ARG:CZ	1:B:184:HIS:HB2	2.16	0.75
1:C:171:ARG:NE	1:C:183:ARG:HH22	1.84	0.75
1:D:185:LEU:HB2	1:D:324:GLU:OE2	1.86	0.75
1:E:220:GLU:O	1:E:221:GLU:HG3	1.87	0.75
1:H:149:VAL:HB	3:H:373:HOH:O	1.85	0.75
1:L:64:ARG:NH2	1:L:344:SER:O	2.19	0.75
1:H:185:LEU:O	1:H:187:ASP:N	2.20	0.75
1:K:208:LEU:HD23	1:K:343:MSE:HE2	1.66	0.75
1:A:197:LEU:HD22	1:A:338:VAL:HG12	1.69	0.74
1:E:41:VAL:HG12	1:E:55:VAL:HG22	1.69	0.74
1:P:208:LEU:CD2	1:P:343:MSE:HE1	2.00	0.74
1:F:116:GLY:HA2	1:F:146:ASP:OD1	1.86	0.74
1:I:218:ASN:H	1:I:218:ASN:HD22	1.34	0.74
1:C:171:ARG:HD3	1:E:171:ARG:HD3	1.69	0.74
1:O:204:GLU:HG3	3:O:383:HOH:O	1.88	0.74
1:P:293:TYR:O	1:P:294:TYR:O	2.05	0.74
1:A:40:ASN:H	1:A:202:GLN:NE2	1.86	0.74
1:B:108:THR:HG23	3:B:392:HOH:O	1.87	0.74
1:C:40:ASN:H	1:C:202:GLN:HE22	1.36	0.74
1:E:102:GLU:OE1	1:E:183:ARG:HD2	1.87	0.74
1:F:310:HIS:CD2	1:F:310:HIS:H	2.06	0.74
1:F:325:ARG:CZ	1:L:144:ARG:HD3	2.17	0.74
1:F:184:HIS:O	1:F:185:LEU:C	2.24	0.74
1:J:237:TYR:HB2	1:J:308:VAL:HG11	1.68	0.74
1:L:237:TYR:HB2	1:L:308:VAL:HG11	1.70	0.74
1:D:120:MSE:HG2	1:D:141:ILE:HD12	1.70	0.74
1:O:185:LEU:HB2	1:O:324:GLU:OE2	1.87	0.74
1:A:242:MSE:SE	1:A:317:ILE:HG13	2.38	0.73
1:B:85:ARG:HA	3:B:356:HOH:O	1.88	0.73
1:L:182:SER:HB3	3:L:404:HOH:O	1.89	0.73
1:A:186:ASP:N	3:A:407:HOH:O	2.22	0.73
1:K:197:LEU:HD22	1:K:338:VAL:CG1	2.14	0.73
1:M:72:THR:HG23	1:M:73:LEU:O	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:185:LEU:CA	3:C:408:HOH:O	2.34	0.73
1:L:15:LEU:HD22	1:L:28:ILE:HD11	1.69	0.73
1:M:81:LYS:HZ1	1:M:142:GLU:CG	1.96	0.73
1:N:251:SER:HB3	3:N:409:HOH:O	1.87	0.73
1:E:206:VAL:HG22	3:E:407:HOH:O	1.88	0.73
1:M:21:PRO:HA	1:M:72:THR:HG22	1.70	0.73
1:A:208:LEU:CD2	1:A:343:MSE:HE2	2.18	0.73
1:C:120:MSE:HA	3:C:388:HOH:O	1.89	0.73
1:B:65:LEU:HD12	1:B:230:ILE:HG21	1.70	0.73
1:E:320:SER:HB3	3:E:414:HOH:O	1.89	0.73
1:G:230:ILE:HG13	1:G:230:ILE:O	1.89	0.73
1:F:52:ILE:CG1	3:F:402:HOH:O	2.36	0.72
1:H:197:LEU:CD2	1:H:338:VAL:HG12	2.18	0.72
1:N:9:MSE:CE	1:N:328:GLU:HA	2.19	0.72
1:H:10:GLU:HG3	3:H:411:HOH:O	1.89	0.72
1:I:112:LYS:HE2	3:I:403:HOH:O	1.88	0.72
1:L:335:GLU:HG2	3:L:403:HOH:O	1.88	0.72
1:M:72:THR:HG21	3:M:354:HOH:O	1.87	0.72
1:D:71:ASP:OD2	1:D:219:ASN:HA	1.89	0.72
1:C:102:GLU:HG2	1:C:183:ARG:NH2	2.04	0.72
1:F:183:ARG:HH12	1:F:323:PHE:HD2	1.36	0.72
1:G:269:TYR:CZ	1:G:273:LYS:HE3	2.25	0.72
1:M:9:MSE:HE2	1:M:174:ILE:HG23	1.72	0.72
1:B:220:GLU:N	1:B:220:GLU:OE1	2.22	0.72
1:B:230:ILE:HG22	1:B:231:PRO:HD2	1.71	0.72
1:J:47:ASN:HB2	1:K:307:ASP:CG	2.09	0.72
1:A:242:MSE:SE	1:A:317:ILE:CG1	2.87	0.71
1:M:171:ARG:HE	1:M:183:ARG:HH12	1.36	0.71
1:P:197:LEU:CD2	1:P:338:VAL:HG12	2.16	0.71
1:H:184:HIS:C	1:H:186:ASP:N	2.36	0.71
1:N:197:LEU:HD22	1:N:338:VAL:HG12	1.70	0.71
1:P:310:HIS:HB2	3:P:369:HOH:O	1.89	0.71
1:J:186:ASP:HA	1:J:242:MSE:HE3	1.72	0.71
1:K:206:VAL:HG12	3:K:407:HOH:O	1.90	0.71
1:F:338:VAL:O	1:F:342:VAL:HG23	1.90	0.71
1:M:171:ARG:CD	1:N:171:ARG:HD3	2.19	0.71
1:E:175:THR:HG22	1:E:177:SER:HB2	1.71	0.71
1:B:183:ARG:HH21	1:B:184:HIS:CB	1.95	0.71
1:C:4:HIS:H	1:C:4:HIS:HD2	1.31	0.71
1:D:72:THR:HB	1:D:184:HIS:HE1	1.55	0.71
1:G:48:LYS:HE3	1:H:304:ALA:HB1	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:72:THR:HB	1:D:184:HIS:CE1	2.26	0.71
1:E:175:THR:HG22	1:E:177:SER:N	2.06	0.71
1:E:9:MSE:CE	1:E:174:ILE:HG23	2.21	0.71
1:E:186:ASP:O	1:E:242:MSE:HE3	1.91	0.70
1:L:86:LEU:O	1:L:142:GLU:HA	1.91	0.70
1:M:268:HIS:HD2	1:M:271:LEU:H	1.35	0.70
1:N:184:HIS:CD2	1:N:186:ASP:OD2	2.44	0.70
1:G:186:ASP:O	1:G:242:MSE:HE3	1.91	0.70
1:J:76:MSE:HE2	1:K:290:ILE:CG1	2.20	0.70
1:P:102:GLU:HG2	1:P:183:ARG:NH2	2.06	0.70
1:E:171:ARG:NH2	1:E:183:ARG:HE	1.90	0.70
1:H:64:ARG:NH2	1:H:344:SER:O	2.24	0.70
1:O:190:SER:HB3	1:O:240:VAL:HG22	1.73	0.70
1:L:175:THR:HG22	1:L:177:SER:H	1.57	0.70
1:N:181:LYS:HB3	1:N:325:ARG:HG3	1.72	0.70
1:P:184:HIS:O	1:P:186:ASP:N	2.25	0.70
1:E:81:LYS:HZ1	1:E:142:GLU:HG2	1.54	0.70
1:I:184:HIS:ND1	1:I:186:ASP:OD1	2.23	0.70
1:J:46:ASN:HB3	1:J:50:ALA:H	1.55	0.70
1:K:194:LEU:O	1:K:198:ILE:HG12	1.90	0.70
3:M:392:HOH:O	1:N:175:THR:HG23	1.92	0.70
1:N:45:ARG:HD2	3:N:406:HOH:O	1.90	0.70
1:B:81:LYS:NZ	1:B:142:GLU:HG2	2.07	0.70
1:G:108:THR:HG22	1:G:112:LYS:N	2.06	0.70
1:H:184:HIS:HA	1:H:186:ASP:CB	2.22	0.70
1:I:219:ASN:HA	3:I:404:HOH:O	1.92	0.70
1:M:200:ARG:O	1:M:204:GLU:HB2	1.92	0.70
1:A:9:MSE:HE2	1:A:180:ILE:CB	2.15	0.70
1:P:54:THR:OG1	1:P:213:HIS:CD2	2.44	0.69
1:A:185:LEU:C	3:A:407:HOH:O	2.31	0.69
1:B:102:GLU:OE1	1:B:183:ARG:HD2	1.91	0.69
1:D:108:THR:HG22	1:D:110:SER:H	1.56	0.69
1:E:220:GLU:O	1:E:221:GLU:CG	2.41	0.69
1:F:319:SER:HB2	3:F:365:HOH:O	1.93	0.69
1:D:90:MSE:HB2	1:D:96:TRP:CZ2	2.27	0.69
1:P:184:HIS:O	1:P:186:ASP:CA	2.39	0.69
1:D:230:ILE:O	1:D:230:ILE:HG13	1.92	0.69
1:K:208:LEU:CD2	1:K:342:VAL:HG13	2.21	0.69
1:L:102:GLU:CG	1:L:183:ARG:CZ	2.70	0.69
1:E:183:ARG:NH1	1:E:323:PHE:HE2	1.85	0.69
1:P:46:ASN:HD22	1:P:46:ASN:C	1.94	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:197:LEU:CD2	1:F:338:VAL:CG1	2.70	0.69
1:H:317:ILE:HD11	1:H:324:GLU:HB3	1.74	0.69
1:I:184:HIS:O	1:I:186:ASP:N	2.26	0.69
1:P:119:LEU:HB2	3:P:396:HOH:O	1.91	0.69
1:A:43:THR:CG2	3:A:391:HOH:O	2.41	0.69
1:O:230:ILE:O	1:O:230:ILE:HG23	1.92	0.69
1:A:97:ASN:ND2	1:A:97:ASN:H	1.91	0.69
1:G:108:THR:HG22	1:G:112:LYS:H	1.58	0.69
1:G:194:LEU:O	1:G:198:ILE:HG12	1.92	0.68
1:F:65:LEU:C	1:F:65:LEU:HD12	2.13	0.68
1:H:184:HIS:CD2	1:H:186:ASP:OD2	2.47	0.68
1:A:112:LYS:HD2	1:A:113:THR:H	1.58	0.68
1:D:255:THR:HG22	1:D:285:GLU:HB3	1.75	0.68
1:H:108:THR:HG22	1:H:110:SER:H	1.57	0.68
1:P:184:HIS:C	1:P:186:ASP:N	2.45	0.68
1:B:347:ILE:CB	3:B:397:HOH:O	2.15	0.68
1:A:141:ILE:HA	3:A:408:HOH:O	1.93	0.68
1:N:175:THR:HG22	1:N:177:SER:H	1.57	0.68
1:O:99:VAL:HG12	1:O:183:ARG:HH12	1.57	0.68
1:D:5:THR:HG21	1:D:332:ALA:HB2	1.75	0.68
1:G:200:ARG:O	1:G:204:GLU:HB2	1.93	0.68
1:P:253:GLU:HG2	3:P:389:HOH:O	1.93	0.68
1:C:185:LEU:O	1:C:242:MSE:HE1	1.94	0.67
1:K:208:LEU:HD22	1:K:342:VAL:HG13	1.76	0.67
1:D:12:ILE:HD13	1:D:189:VAL:HG22	1.76	0.67
1:E:9:MSE:HE3	1:E:180:ILE:HB	1.76	0.67
1:K:317:ILE:O	1:K:317:ILE:CG2	2.42	0.67
1:A:303:ARG:N	3:A:405:HOH:O	2.27	0.67
1:N:40:ASN:H	1:N:202:GLN:HE22	1.42	0.67
1:G:317:ILE:HD11	1:G:324:GLU:HB3	1.76	0.67
1:J:186:ASP:OD1	3:J:387:HOH:O	2.11	0.67
1:K:244:ALA:HB3	3:K:396:HOH:O	1.94	0.67
1:C:185:LEU:O	1:C:242:MSE:HE3	1.95	0.67
1:C:40:ASN:H	1:C:202:GLN:NE2	1.91	0.67
1:A:9:MSE:HE3	1:A:180:ILE:HB	1.71	0.67
1:C:197:LEU:HD22	1:C:338:VAL:CG1	2.25	0.67
1:I:172:VAL:HG23	1:I:182:SER:CB	2.22	0.66
1:A:319:SER:OG	3:A:369:HOH:O	2.13	0.66
1:B:183:ARG:O	1:B:184:HIS:CB	2.39	0.66
1:E:253:GLU:HG2	3:E:389:HOH:O	1.94	0.66
1:I:102:GLU:CD	1:I:183:ARG:HH22	1.98	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:184:HIS:CD2	3:F:386:HOH:O	2.47	0.66
1:P:42:GLU:O	3:P:353:HOH:O	2.13	0.66
1:H:183:ARG:HA	1:H:324:GLU:HG3	1.76	0.66
1:K:323:PHE:O	3:K:390:HOH:O	2.13	0.66
1:A:208:LEU:HD21	1:A:342:VAL:CG1	2.23	0.66
1:A:197:LEU:HD22	1:A:338:VAL:CG1	2.25	0.66
1:C:141:ILE:N	1:C:141:ILE:HD13	2.11	0.66
1:A:173:GLN:NE2	3:A:423:HOH:O	2.28	0.65
1:H:228:SER:CB	3:H:408:HOH:O	2.43	0.65
1:P:244:ALA:HB2	1:P:320:SER:HB3	1.78	0.65
1:B:41:VAL:HG21	1:B:198:ILE:HG21	1.77	0.65
1:G:319:SER:HB3	1:G:323:PHE:O	1.96	0.65
1:B:183:ARG:O	1:B:183:ARG:HG3	1.95	0.65
1:C:90:MSE:HG3	1:C:94:PHE:CE1	2.31	0.65
1:J:90:MSE:HG3	1:J:94:PHE:CE1	2.31	0.65
1:P:141:ILE:N	3:P:390:HOH:O	2.30	0.65
1:G:102:GLU:CG	1:G:183:ARG:NH1	2.38	0.65
1:C:251:SER:N	3:C:391:HOH:O	2.29	0.65
1:B:242:MSE:SE	1:B:317:ILE:CD1	2.94	0.65
1:M:204:GLU:O	1:M:205:ASN:HB2	1.94	0.65
1:B:144:ARG:HD2	3:B:360:HOH:O	1.96	0.65
1:G:120:MSE:HG2	1:G:141:ILE:HB	1.79	0.65
1:H:186:ASP:O	3:H:369:HOH:O	2.14	0.65
1:L:102:GLU:CG	1:L:183:ARG:NH2	2.60	0.65
1:H:145:ILE:HG12	3:H:380:HOH:O	1.96	0.64
1:J:187:ASP:OD2	1:J:241:ASP:HA	1.96	0.64
1:P:54:THR:N	3:P:353:HOH:O	2.29	0.64
1:C:4:HIS:N	1:C:4:HIS:CD2	2.58	0.64
1:E:183:ARG:HD3	1:E:323:PHE:HD2	1.63	0.64
1:E:347:ILE:HD12	1:E:348:GLU:H	1.62	0.64
1:M:242:MSE:SE	1:M:317:ILE:CG2	2.96	0.64
1:O:32:ILE:HG23	1:O:195:LEU:HD21	1.80	0.64
1:B:41:VAL:HG22	1:B:55:VAL:HG22	1.80	0.64
1:D:183:ARG:NH1	1:D:183:ARG:HB3	2.13	0.64
1:B:9:MSE:CE	1:B:174:ILE:HG23	2.27	0.64
1:D:148:ARG:HD2	1:H:254:TYR:CE2	2.32	0.64
1:G:76:MSE:HE1	1:H:260:ALA:HB1	1.76	0.64
1:A:208:LEU:CD2	1:A:343:MSE:CE	2.74	0.64
1:K:9:MSE:HE3	1:K:180:ILE:HB	1.79	0.64
1:B:65:LEU:CD1	1:B:230:ILE:HG21	2.28	0.64
1:L:183:ARG:HG2	3:L:389:HOH:O	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:MSE:HG3	1:B:94:PHE:CE1	2.33	0.64
1:I:102:GLU:CG	1:I:183:ARG:HH22	2.10	0.64
1:A:268:HIS:HE1	1:A:270:ALA:HB3	1.63	0.63
1:B:208:LEU:CD2	1:B:343:MSE:CE	2.68	0.63
1:E:174:ILE:HG12	1:E:180:ILE:HD12	1.80	0.63
1:J:213:HIS:CE1	1:J:231:PRO:HG3	2.33	0.63
1:L:282:ASN:N	1:L:282:ASN:HD22	1.96	0.63
1:B:9:MSE:HE2	1:B:174:ILE:HG23	1.80	0.63
1:H:20:SER:HB2	1:H:25:THR:HG22	1.79	0.63
1:I:175:THR:HG22	1:I:177:SER:N	2.11	0.63
1:L:238:LEU:HD11	1:L:313:ILE:HD13	1.79	0.63
1:E:108:THR:HG23	1:E:110:SER:H	1.63	0.63
1:H:244:ALA:HB2	1:H:320:SER:HB3	1.80	0.63
1:I:262:ASP:HB2	1:I:294:TYR:CB	2.28	0.63
1:P:208:LEU:HD23	1:P:343:MSE:HE2	1.70	0.63
1:P:317:ILE:HD11	1:P:324:GLU:HB3	1.81	0.63
1:A:46:ASN:HB3	1:A:48:LYS:H	1.63	0.63
1:B:183:ARG:HE	1:B:184:HIS:CB	2.11	0.63
1:D:200:ARG:O	1:D:204:GLU:HG2	1.99	0.63
1:G:287:LYS:HA	1:G:287:LYS:HE2	1.80	0.63
1:P:170:PRO:HB3	1:P:184:HIS:HD2	1.63	0.63
1:A:184:HIS:C	1:A:186:ASP:H	2.02	0.63
1:C:171:ARG:HD3	1:E:171:ARG:CD	2.27	0.63
1:C:229:ASN:CB	3:C:370:HOH:O	2.46	0.63
1:O:277:GLU:HB3	3:O:376:HOH:O	1.97	0.63
1:K:184:HIS:HD2	1:K:186:ASP:OD2	1.82	0.63
1:B:208:LEU:CD2	1:B:342:VAL:HG13	2.28	0.63
1:C:90:MSE:HB2	1:C:96:TRP:CZ2	2.33	0.63
1:E:81:LYS:HZ3	1:E:142:GLU:HG2	1.61	0.63
1:M:169:ASP:O	1:M:183:ARG:NE	2.32	0.63
1:F:63:HIS:CE1	1:F:233:GLU:HG3	2.34	0.62
1:E:12:ILE:HD13	1:E:189:VAL:HG22	1.80	0.62
1:L:182:SER:CA	3:L:404:HOH:O	2.47	0.62
1:M:81:LYS:HZ3	1:M:142:GLU:CG	2.03	0.62
1:B:268:HIS:HE1	1:B:270:ALA:HB3	1.64	0.62
1:B:81:LYS:HZ3	1:B:142:GLU:HG2	1.63	0.62
1:C:186:ASP:N	3:C:408:HOH:O	2.33	0.62
1:F:184:HIS:O	1:F:185:LEU:O	2.16	0.62
1:F:252:ASP:CA	3:F:397:HOH:O	2.03	0.62
1:B:187:ASP:OD2	1:B:242:MSE:HE2	1.99	0.62
1:B:45:ARG:CG	1:B:45:ARG:HH11	2.10	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:171:ARG:HE	1:C:183:ARG:NH2	1.87	0.62
1:C:255:THR:HG22	1:C:285:GLU:HB3	1.82	0.62
1:N:184:HIS:HA	1:N:324:GLU:OE1	1.99	0.62
1:E:197:LEU:HB2	3:E:415:HOH:O	2.00	0.62
1:K:4:HIS:HE1	1:K:335:GLU:OE2	1.82	0.62
1:L:90:MSE:HB2	1:L:96:TRP:CZ2	2.35	0.62
1:A:245:LEU:HD12	1:A:251:SER:HB2	1.82	0.62
1:L:102:GLU:HG3	1:L:183:ARG:NH2	2.15	0.62
1:M:187:ASP:OD2	1:M:241:ASP:HA	2.00	0.62
1:A:9:MSE:CE	1:A:180:ILE:CB	2.58	0.62
1:B:229:ASN:HA	3:B:406:HOH:O	1.98	0.62
1:E:183:ARG:CA	3:E:410:HOH:O	2.42	0.62
1:G:90:MSE:HG3	1:G:94:PHE:CE1	2.35	0.62
1:E:39:TRP:CB	1:E:202:GLN:HE22	2.00	0.62
1:B:45:ARG:NH1	1:B:45:ARG:HG3	2.14	0.62
1:C:218:ASN:HD22	1:C:218:ASN:H	1.45	0.62
1:J:313:ILE:HD11	1:J:338:VAL:HG12	1.80	0.62
1:F:252:ASP:N	3:F:397:HOH:O	2.28	0.61
1:F:6:LYS:HG3	1:F:7:GLU:N	2.14	0.61
1:O:45:ARG:HG3	1:O:51:LEU:HD23	1.82	0.61
1:B:197:LEU:HD22	1:B:338:VAL:HG12	1.82	0.61
1:M:208:LEU:HD22	1:M:342:VAL:HG12	1.82	0.61
1:G:184:HIS:O	1:G:324:GLU:CD	2.38	0.61
1:L:102:GLU:HG2	1:L:183:ARG:HH22	1.63	0.61
1:M:90:MSE:HB2	1:M:96:TRP:CZ2	2.35	0.61
1:A:155:VAL:O	1:A:158:LEU:HB2	1.99	0.61
1:E:218:ASN:HD22	1:E:218:ASN:N	1.98	0.61
1:I:218:ASN:ND2	1:I:218:ASN:H	1.97	0.61
1:P:317:ILE:O	1:P:317:ILE:CG2	2.47	0.61
1:G:287:LYS:HG2	3:G:386:HOH:O	2.00	0.61
1:B:120:MSE:SE	3:B:398:HOH:O	2.68	0.61
1:G:102:GLU:HG2	1:G:183:ARG:HH22	1.65	0.61
1:M:91:ILE:HD12	1:P:266:PRO:HG3	1.82	0.61
1:A:65:LEU:HG	1:A:230:ILE:HG21	1.82	0.61
1:K:65:LEU:C	1:K:65:LEU:HD23	2.20	0.61
1:C:317:ILE:C	1:C:317:ILE:HD13	2.21	0.61
1:K:113:THR:HG22	3:K:403:HOH:O	2.01	0.61
1:J:9:MSE:SE	1:J:328:GLU:HB3	2.52	0.60
1:L:182:SER:CB	3:L:404:HOH:O	2.45	0.60
1:M:245:LEU:N	1:M:245:LEU:HD12	2.16	0.60
1:C:269:TYR:CZ	1:C:273:LYS:HE2	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:255:THR:HG22	1:N:285:GLU:HB3	1.83	0.60
1:O:28:ILE:O	1:O:31:PHE:HB3	2.01	0.60
1:B:155:VAL:O	1:B:158:LEU:HB2	2.01	0.60
1:K:9:MSE:CE	1:K:180:ILE:HB	2.31	0.60
1:O:253:GLU:O	1:O:330:SER:HB2	2.01	0.60
1:G:184:HIS:O	1:G:324:GLU:OE2	2.19	0.60
1:K:120:MSE:HG2	1:K:141:ILE:HG22	1.84	0.60
1:B:120:MSE:HA	3:B:390:HOH:O	2.00	0.60
1:B:304:ALA:HA	3:B:391:HOH:O	2.02	0.60
1:B:262:ASP:HA	1:B:291:TYR:O	2.02	0.60
1:F:52:ILE:HG13	3:F:402:HOH:O	1.98	0.60
1:N:208:LEU:CD2	1:N:342:VAL:HG13	2.31	0.60
1:O:144:ARG:HD3	1:P:325:ARG:CZ	2.31	0.60
1:O:184:HIS:O	1:O:185:LEU:C	2.40	0.60
1:B:213:HIS:NE2	1:B:231:PRO:HG2	2.16	0.60
1:C:155:VAL:O	1:C:158:LEU:HB2	2.01	0.60
1:G:108:THR:HG23	1:G:110:SER:H	1.67	0.60
1:I:34:ASN:HD22	1:I:34:ASN:N	1.99	0.60
1:D:75:ALA:HA	1:D:91:ILE:HD13	1.82	0.60
1:F:3:HIS:HA	1:F:6:LYS:HG2	1.83	0.60
1:N:90:MSE:HB2	1:N:96:TRP:CZ2	2.36	0.60
1:G:102:GLU:HG3	1:G:183:ARG:CZ	2.25	0.60
1:I:39:TRP:CH2	1:I:199:LYS:HB2	2.37	0.60
1:P:34:ASN:O	1:P:37:SER:HB2	2.02	0.59
1:E:40:ASN:H	1:E:202:GLN:NE2	2.00	0.59
1:F:64:ARG:HD2	1:F:341:TYR:OH	2.02	0.59
1:G:317:ILE:CD1	1:G:324:GLU:HB3	2.32	0.59
1:A:307:ASP:CG	1:C:47:ASN:HB2	2.23	0.59
1:F:184:HIS:CG	3:F:386:HOH:O	2.55	0.59
1:F:16:VAL:HA	1:F:188:LYS:HE3	1.84	0.59
1:K:4:HIS:CE1	1:K:335:GLU:OE2	2.56	0.59
1:O:317:ILE:HD11	1:O:324:GLU:HB3	1.84	0.59
1:A:242:MSE:SE	1:A:317:ILE:HD11	2.52	0.59
1:A:183:ARG:CA	3:A:393:HOH:O	2.26	0.59
1:F:313:ILE:O	1:F:313:ILE:HD13	2.02	0.59
1:J:230:ILE:O	1:J:230:ILE:HG13	2.02	0.59
1:A:317:ILE:CD1	1:A:326:THR:HB	2.32	0.59
1:O:208:LEU:HD23	1:O:343:MSE:HE3	1.81	0.59
1:I:44:LYS:HG2	1:I:45:ARG:H	1.68	0.59
1:J:76:MSE:HE3	1:K:260:ALA:HB3	1.82	0.59
1:D:47:ASN:HD21	1:E:235:VAL:HG22	1.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:64:ARG:NH2	1:F:344:SER:O	2.36	0.59
1:J:317:ILE:CD1	1:J:324:GLU:HB3	2.31	0.59
1:L:41:VAL:CG2	1:L:55:VAL:HG22	2.32	0.59
1:B:218:ASN:HD22	1:B:218:ASN:H	1.51	0.59
1:J:76:MSE:HE3	1:J:163:GLY:HA2	1.84	0.59
1:P:117:THR:HG23	3:P:379:HOH:O	1.97	0.59
1:B:241:ASP:HB3	1:B:312:LEU:HD21	1.83	0.58
1:L:144:ARG:HD2	3:L:357:HOH:O	2.03	0.58
1:C:184:HIS:O	1:C:185:LEU:HB2	2.03	0.58
1:C:197:LEU:HD22	1:C:338:VAL:HG12	1.85	0.58
1:D:185:LEU:HD12	1:D:317:ILE:HD11	1.84	0.58
1:M:171:ARG:HD3	1:N:171:ARG:CD	2.24	0.58
1:M:186:ASP:CB	3:M:360:HOH:O	2.32	0.58
1:A:76:MSE:CE	1:B:260:ALA:CB	2.77	0.58
1:B:40:ASN:H	1:B:202:GLN:NE2	2.00	0.58
1:C:185:LEU:O	1:C:187:ASP:HA	2.03	0.58
1:C:41:VAL:HG21	1:C:198:ILE:HG21	1.85	0.58
1:G:90:MSE:HB2	1:G:96:TRP:CZ2	2.38	0.58
1:L:261:LYS:HB2	1:L:266:PRO:HA	1.85	0.58
1:M:186:ASP:HB3	3:M:407:HOH:O	2.04	0.58
1:A:185:LEU:CA	3:A:407:HOH:O	2.50	0.58
1:B:141:ILE:HG13	1:B:141:ILE:O	2.03	0.58
1:C:304:ALA:HA	3:C:394:HOH:O	2.03	0.58
1:J:158:LEU:HD23	1:J:160:ILE:HD12	1.86	0.58
1:A:4:HIS:CG	3:A:395:HOH:O	2.55	0.58
1:C:229:ASN:HB2	3:C:370:HOH:O	2.02	0.58
1:H:175:THR:CG2	1:H:177:SER:HB2	2.34	0.58
1:H:184:HIS:CA	1:H:186:ASP:HB2	2.32	0.58
1:H:185:LEU:HG	1:H:324:GLU:HB2	1.85	0.58
1:J:9:MSE:HE2	1:J:174:ILE:HG23	1.85	0.58
1:L:88:LEU:CD2	1:L:166:VAL:HG21	2.34	0.58
1:D:317:ILE:HD12	1:D:325:ARG:O	2.04	0.58
1:L:304:ALA:N	3:L:396:HOH:O	2.35	0.58
1:J:47:ASN:HB2	1:K:307:ASP:OD2	2.03	0.58
1:O:272:ARG:HG3	1:O:272:ARG:NH1	2.15	0.58
1:A:102:GLU:OE1	1:A:168:PHE:HB3	2.04	0.58
1:B:183:ARG:HE	1:B:184:HIS:HB3	1.69	0.58
1:A:76:MSE:HE2	1:B:290:ILE:CG1	2.33	0.58
1:E:69:HIS:CE1	1:E:220:GLU:HG2	2.39	0.58
1:L:102:GLU:CG	1:L:183:ARG:HH22	2.17	0.58
1:L:285:GLU:HG3	3:L:381:HOH:O	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:308:VAL:HG12	1:B:310:HIS:CE1	2.39	0.58
1:D:43:THR:HG23	1:D:53:LEU:HD11	1.83	0.58
1:H:263:SER:HB2	1:H:294:TYR:HA	1.86	0.58
1:N:9:MSE:HE1	1:N:328:GLU:CA	2.33	0.58
1:F:313:ILE:CD1	1:F:313:ILE:C	2.72	0.57
1:D:218:ASN:HD22	1:D:218:ASN:H	1.52	0.57
1:D:252:ASP:N	3:D:398:HOH:O	2.36	0.57
1:J:120:MSE:HG3	1:J:141:ILE:HB	1.86	0.57
1:K:197:LEU:CD2	1:K:338:VAL:HG12	2.27	0.57
1:M:323:PHE:N	3:M:405:HOH:O	2.37	0.57
1:E:120:MSE:C	3:E:398:HOH:O	2.43	0.57
1:G:41:VAL:HG11	1:G:198:ILE:CG2	2.35	0.57
1:K:3:HIS:CG	1:K:4:HIS:H	2.23	0.57
1:E:90:MSE:HB2	1:E:96:TRP:CZ2	2.40	0.57
1:G:8:THR:O	1:G:12:ILE:HG13	2.04	0.57
1:H:120:MSE:SE	1:H:141:ILE:HG22	2.55	0.57
1:K:183:ARG:O	1:K:184:HIS:CB	2.40	0.57
1:L:185:LEU:HB2	1:L:324:GLU:OE1	2.05	0.57
1:A:241:ASP:O	1:A:314:GLY:HA3	2.05	0.57
1:B:242:MSE:SE	1:B:317:ILE:CG1	3.02	0.57
1:M:170:PRO:HA	1:M:183:ARG:HD2	1.87	0.57
1:P:40:ASN:H	1:P:202:GLN:NE2	2.03	0.57
1:L:258:ILE:HD11	1:L:337:LEU:HD11	1.85	0.57
1:J:78:LYS:HA	1:K:290:ILE:HD12	1.86	0.57
1:M:184:HIS:O	1:M:324:GLU:OE1	2.23	0.57
1:E:175:THR:HG22	1:E:177:SER:CB	2.35	0.56
1:I:86:LEU:HB2	1:I:143:VAL:HB	1.86	0.56
1:J:90:MSE:HB2	1:J:96:TRP:CZ2	2.40	0.56
1:K:64:ARG:NH2	1:K:344:SER:O	2.38	0.56
1:I:282:ASN:HD22	1:I:282:ASN:N	2.04	0.56
1:N:183:ARG:HH21	1:N:184:HIS:HB3	1.70	0.56
1:P:220:GLU:C	1:P:220:GLU:OE2	2.43	0.56
1:E:171:ARG:HH21	1:E:183:ARG:HE	1.53	0.56
1:E:213:HIS:NE2	1:E:231:PRO:HG2	2.20	0.56
1:G:141:ILE:HD13	1:G:141:ILE:C	2.24	0.56
1:I:278:LEU:CD1	1:I:341:TYR:HA	2.35	0.56
1:P:117:THR:HG22	3:P:379:HOH:O	1.99	0.56
1:B:83:ASP:OD1	1:B:85:ARG:HB2	2.05	0.56
1:F:310:HIS:HD2	3:F:384:HOH:O	1.75	0.56
1:J:183:ARG:CG	1:J:183:ARG:HH11	2.18	0.56
1:E:208:LEU:HD23	1:E:343:MSE:HE2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:208:LEU:HD22	1:I:342:VAL:CG1	2.36	0.56
1:J:235:VAL:HG12	1:J:236:GLU:HG3	1.87	0.56
1:N:9:MSE:HE2	1:N:331:ILE:HD13	1.85	0.56
1:E:245:LEU:HD23	1:E:245:LEU:N	2.19	0.56
1:G:41:VAL:HG12	1:G:55:VAL:HG22	1.87	0.56
1:E:260:ALA:HA	1:E:272:ARG:HD2	1.88	0.56
1:F:184:HIS:CB	3:F:386:HOH:O	2.48	0.56
1:G:147:GLU:HG3	3:G:395:HOH:O	2.04	0.56
1:G:97:ASN:ND2	1:G:97:ASN:N	2.35	0.56
1:H:182:SER:OG	1:H:183:ARG:N	2.35	0.56
1:I:285:GLU:HA	3:I:381:HOH:O	2.06	0.56
1:J:100:GLU:HG3	3:J:397:HOH:O	2.06	0.56
1:J:97:ASN:ND2	1:J:97:ASN:N	2.49	0.56
1:K:183:ARG:C	3:K:404:HOH:O	2.44	0.56
1:M:22:SER:HB2	1:M:71:ASP:OD2	2.05	0.56
1:A:218:ASN:H	1:A:218:ASN:HD22	1.53	0.56
1:A:63:HIS:NE2	1:A:233:GLU:HG3	2.21	0.56
1:D:117:THR:OG1	1:D:144:ARG:NH1	2.39	0.56
1:L:228:SER:O	1:L:229:ASN:HB2	2.06	0.56
1:C:242:MSE:SE	1:C:317:ILE:CG2	3.03	0.56
1:E:108:THR:HG22	1:E:112:LYS:N	2.17	0.56
1:E:171:ARG:NH2	1:E:183:ARG:NE	2.54	0.56
1:F:218:ASN:HD22	1:F:218:ASN:H	1.54	0.56
1:J:218:ASN:HD22	1:J:218:ASN:H	1.54	0.56
1:L:112:LYS:HD2	1:L:113:THR:H	1.71	0.56
1:L:253:GLU:O	1:L:330:SER:HB2	2.05	0.56
1:J:290:ILE:HD12	1:L:78:LYS:HB3	1.88	0.56
1:C:242:MSE:SE	1:C:317:ILE:HG23	2.56	0.56
1:E:244:ALA:HB2	1:E:320:SER:OG	2.05	0.56
1:L:4:HIS:C	1:L:4:HIS:CD2	2.80	0.56
1:N:210:TYR:CZ	1:N:346:LEU:HG	2.41	0.56
1:P:268:HIS:CE1	1:P:309:LYS:HD3	2.41	0.56
1:D:197:LEU:CD1	1:D:338:VAL:HB	2.36	0.56
1:F:52:ILE:HG12	3:F:402:HOH:O	1.98	0.56
1:G:39:TRP:CE2	1:G:199:LYS:HD3	2.41	0.56
1:G:47:ASN:HB2	1:H:307:ASP:OD1	2.06	0.56
1:M:186:ASP:HA	3:M:398:HOH:O	2.05	0.56
1:M:204:GLU:HA	1:M:204:GLU:OE2	2.06	0.56
1:N:88:LEU:HG	3:N:404:HOH:O	2.06	0.56
1:P:208:LEU:CD2	1:P:343:MSE:HE3	2.33	0.56
1:G:235:VAL:HG12	1:G:236:GLU:HG3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:102:GLU:HG3	1:I:183:ARG:CZ	2.36	0.55
1:I:253:GLU:O	1:I:330:SER:HB2	2.06	0.55
1:A:102:GLU:OE2	1:A:183:ARG:CZ	2.54	0.55
1:B:229:ASN:C	1:B:230:ILE:HG13	2.26	0.55
1:D:69:HIS:HB3	1:D:220:GLU:HB2	1.87	0.55
1:G:76:MSE:HE2	1:H:290:ILE:CG1	2.35	0.55
1:J:261:LYS:HB3	1:J:266:PRO:HA	1.87	0.55
1:M:9:MSE:SE	1:M:328:GLU:HB3	2.57	0.55
1:N:197:LEU:HD22	1:N:338:VAL:CG1	2.34	0.55
1:A:184:HIS:O	1:A:186:ASP:N	2.39	0.55
1:K:218:ASN:H	1:K:218:ASN:HD22	1.55	0.55
1:M:9:MSE:CE	1:M:174:ILE:HG23	2.36	0.55
1:B:183:ARG:NE	1:B:184:HIS:HB2	2.21	0.55
1:C:42:GLU:HG3	1:C:54:THR:HB	1.88	0.55
1:E:277:GLU:OE2	1:E:277:GLU:CA	2.53	0.55
1:K:262:ASP:HA	1:K:291:TYR:O	2.06	0.55
1:M:47:ASN:HB2	1:P:307:ASP:CG	2.27	0.55
1:E:9:MSE:HE2	1:E:174:ILE:HG23	1.88	0.55
1:F:208:LEU:HD22	1:F:342:VAL:HG12	1.89	0.55
1:I:278:LEU:HD13	1:I:341:TYR:HA	1.88	0.55
1:M:120:MSE:HB2	3:M:390:HOH:O	2.06	0.55
1:P:208:LEU:HA	1:P:343:MSE:HE1	1.87	0.55
1:B:9:MSE:HE3	1:B:180:ILE:HB	1.87	0.55
1:D:64:ARG:NH2	1:D:344:SER:O	2.39	0.55
1:H:335:GLU:HG2	3:H:404:HOH:O	2.07	0.55
1:J:9:MSE:HE1	1:J:174:ILE:HG23	1.85	0.55
1:N:251:SER:N	3:N:397:HOH:O	2.40	0.55
1:P:63:HIS:CD2	1:P:211:THR:HB	2.42	0.55
1:E:204:GLU:OE2	1:E:204:GLU:HA	2.06	0.55
1:G:40:ASN:H	1:G:202:GLN:NE2	2.04	0.55
1:J:183:ARG:HH11	1:J:183:ARG:HG2	1.72	0.55
1:M:86:LEU:HD22	1:M:145:ILE:HD11	1.89	0.55
1:M:229:ASN:HB2	3:M:396:HOH:O	2.06	0.55
1:B:102:GLU:OE2	1:B:183:ARG:HD2	2.06	0.55
1:B:64:ARG:NH2	1:B:344:SER:O	2.38	0.55
1:N:316:GLY:O	1:N:326:THR:OG1	2.13	0.55
1:C:241:ASP:O	1:C:314:GLY:HA3	2.07	0.55
1:E:86:LEU:O	1:E:142:GLU:HB3	2.06	0.55
1:L:278:LEU:HD13	1:L:341:TYR:HA	1.89	0.55
1:N:145:ILE:HD11	1:N:147:GLU:HB2	1.89	0.55
1:O:218:ASN:H	1:O:218:ASN:HD22	1.55	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:335:GLU:HG2	3:B:409:HOH:O	2.07	0.54
1:H:78:LYS:HG2	1:H:87:SER:HB3	1.89	0.54
1:I:238:LEU:HD11	1:I:313:ILE:HD13	1.89	0.54
1:I:43:THR:O	1:I:43:THR:HG23	2.07	0.54
1:L:238:LEU:HD11	1:L:313:ILE:CD1	2.37	0.54
1:O:190:SER:CB	1:O:240:VAL:HG22	2.37	0.54
1:C:183:ARG:CB	1:C:183:ARG:HH11	2.08	0.54
1:F:194:LEU:O	1:F:198:ILE:HG12	2.07	0.54
1:K:39:TRP:CE2	1:K:199:LYS:HD3	2.42	0.54
1:K:310:HIS:HB2	3:K:376:HOH:O	2.06	0.54
1:C:175:THR:CG2	1:C:177:SER:OG	2.55	0.54
1:F:171:ARG:HD3	1:L:171:ARG:HH11	1.72	0.54
1:L:64:ARG:HD2	1:L:341:TYR:OH	2.07	0.54
1:M:63:HIS:CD2	1:M:233:GLU:HG3	2.42	0.54
1:P:9:MSE:CE	1:P:180:ILE:HB	2.26	0.54
1:B:183:ARG:O	1:B:183:ARG:CG	2.55	0.54
1:B:219:ASN:O	1:B:226:GLY:HA2	2.07	0.54
1:H:189:VAL:HB	1:H:242:MSE:CE	2.34	0.54
1:J:237:TYR:HB2	1:J:308:VAL:CG1	2.38	0.54
1:M:66:LEU:CD1	1:M:238:LEU:HB3	2.38	0.54
1:O:242:MSE:HE3	1:O:317:ILE:HD12	1.89	0.54
1:P:69:HIS:CE1	1:P:187:ASP:HB2	2.42	0.54
1:P:97:ASN:ND2	1:P:97:ASN:H	2.04	0.54
1:A:63:HIS:CE1	1:A:233:GLU:HG3	2.42	0.54
1:C:45:ARG:CG	1:C:45:ARG:NH1	2.68	0.54
1:F:39:TRP:HB3	1:F:202:GLN:HE22	1.72	0.54
1:A:173:GLN:NE2	3:A:409:HOH:O	2.41	0.54
1:G:33:GLU:HG3	1:G:51:LEU:HD21	1.89	0.54
1:N:237:TYR:HB2	1:N:308:VAL:HG11	1.90	0.54
1:A:262:ASP:HA	1:A:291:TYR:O	2.07	0.54
1:A:47:ASN:HB2	1:B:307:ASP:CG	2.28	0.54
1:D:39:TRP:CZ2	1:D:199:LYS:HG2	2.43	0.54
1:H:63:HIS:CE1	1:H:233:GLU:HG3	2.43	0.54
1:H:90:MSE:HG3	1:H:94:PHE:CE1	2.43	0.54
1:K:108:THR:HG22	1:K:110:SER:H	1.73	0.54
1:F:80:ILE:CG2	1:F:152:ALA:HA	2.38	0.54
1:H:184:HIS:C	1:H:186:ASP:H	2.12	0.54
1:H:263:SER:HB2	1:H:294:TYR:CA	2.38	0.54
1:K:197:LEU:CD2	1:K:338:VAL:CG1	2.85	0.54
1:P:210:TYR:CZ	1:P:346:LEU:HG	2.43	0.54
1:C:86:LEU:HB2	1:C:143:VAL:HB	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:185:LEU:O	1:F:186:ASP:C	2.45	0.53
1:G:48:LYS:CE	1:H:304:ALA:HB1	2.38	0.53
1:I:51:LEU:HD21	1:I:53:LEU:HD21	1.89	0.53
1:B:171:ARG:CD	1:J:171:ARG:HD3	2.36	0.53
1:E:86:LEU:HD22	1:E:145:ILE:HD11	1.90	0.53
1:F:174:ILE:N	1:F:174:ILE:HD12	2.22	0.53
1:F:319:SER:OG	1:F:322:ALA:O	2.26	0.53
1:H:175:THR:HG22	1:H:177:SER:H	1.74	0.53
1:I:12:ILE:HD13	1:I:189:VAL:HG22	1.90	0.53
1:I:144:ARG:HD2	3:I:356:HOH:O	2.09	0.53
1:N:175:THR:HG21	1:N:177:SER:OG	2.08	0.53
1:O:64:ARG:NH2	1:O:344:SER:O	2.34	0.53
1:J:148:ARG:NH2	3:J:398:HOH:O	2.41	0.53
1:J:40:ASN:H	1:J:202:GLN:HE21	1.56	0.53
1:A:90:MSE:HG3	1:A:94:PHE:CE1	2.43	0.53
1:F:310:HIS:CD2	1:F:310:HIS:N	2.76	0.53
1:I:284:ILE:O	3:I:387:HOH:O	2.18	0.53
1:O:218:ASN:N	1:O:218:ASN:HD22	2.06	0.53
1:A:185:LEU:O	1:A:187:ASP:N	2.42	0.53
1:A:48:LYS:HZ3	1:A:227:ASN:ND2	2.07	0.53
1:C:347:ILE:HG12	3:C:384:HOH:O	2.09	0.53
1:G:120:MSE:HB3	1:G:141:ILE:HA	1.90	0.53
1:G:120:MSE:CG	1:G:141:ILE:HB	2.37	0.53
1:G:9:MSE:HE3	1:G:174:ILE:HG12	1.91	0.53
1:M:66:LEU:HD23	1:M:214:PHE:CE2	2.43	0.53
1:D:63:HIS:CE1	1:D:233:GLU:HG3	2.43	0.53
1:G:310:HIS:HB2	3:G:387:HOH:O	2.07	0.53
1:O:46:ASN:HB2	1:O:50:ALA:H	1.73	0.53
1:E:238:LEU:HD11	1:E:313:ILE:HG23	1.90	0.53
1:H:40:ASN:H	1:H:202:GLN:NE2	2.07	0.53
1:H:22:SER:OG	1:H:71:ASP:OD2	2.27	0.53
1:P:119:LEU:HB3	3:P:396:HOH:O	2.01	0.53
1:B:175:THR:HG22	1:B:177:SER:H	1.74	0.53
1:B:244:ALA:HB2	1:B:320:SER:OG	2.08	0.53
1:H:208:LEU:CD2	1:H:342:VAL:HG13	2.39	0.53
1:L:171:ARG:HD2	3:L:400:HOH:O	2.08	0.53
1:H:182:SER:O	1:H:183:ARG:HG3	2.07	0.53
1:I:40:ASN:HD22	1:I:202:GLN:HG3	1.74	0.53
1:I:90:MSE:HG3	1:I:94:PHE:CE1	2.44	0.53
1:N:173:GLN:NE2	3:N:416:HOH:O	2.32	0.53
1:O:97:ASN:O	1:O:99:VAL:N	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:140:ASN:HB2	3:D:407:HOH:O	2.08	0.53
1:F:229:ASN:HB2	3:F:369:HOH:O	2.09	0.53
1:J:58:LYS:HD3	1:J:207:THR:HG21	1.91	0.53
1:B:317:ILE:HD13	1:B:326:THR:HB	1.91	0.52
1:D:78:LYS:HA	1:E:290:ILE:HD12	1.90	0.52
1:E:171:ARG:HH21	1:E:183:ARG:NE	2.07	0.52
1:I:88:LEU:CD2	1:I:166:VAL:HG21	2.39	0.52
1:K:82:PRO:O	1:K:151:SER:HA	2.09	0.52
1:L:184:HIS:C	1:L:185:LEU:O	2.44	0.52
1:N:9:MSE:HE1	1:N:331:ILE:HD12	1.85	0.52
1:P:218:ASN:HD22	1:P:218:ASN:H	1.57	0.52
1:B:144:ARG:HD3	1:J:325:ARG:CZ	2.38	0.52
1:E:263:SER:OG	1:E:294:TYR:CB	2.57	0.52
1:E:41:VAL:CG1	1:E:55:VAL:HG22	2.36	0.52
1:J:45:ARG:HB2	1:J:45:ARG:HH11	0.70	0.52
1:L:242:MSE:SE	1:L:317:ILE:CG2	3.04	0.52
1:M:33:GLU:OE2	1:M:45:ARG:HD3	2.09	0.52
1:A:108:THR:HG22	1:A:110:SER:H	1.73	0.52
1:C:313:ILE:HD11	1:C:338:VAL:HG23	1.91	0.52
1:F:310:HIS:HD2	1:F:310:HIS:H	1.50	0.52
1:G:230:ILE:CG1	1:G:230:ILE:O	2.57	0.52
1:J:253:GLU:HG2	3:J:392:HOH:O	2.09	0.52
1:N:175:THR:CG2	1:N:177:SER:OG	2.57	0.52
1:A:244:ALA:HB2	1:A:320:SER:HB3	1.91	0.52
1:A:43:THR:HG22	3:A:391:HOH:O	2.05	0.52
1:B:183:ARG:HA	3:B:401:HOH:O	2.09	0.52
1:G:6:LYS:O	1:G:10:GLU:HG2	2.10	0.52
1:K:183:ARG:CA	3:K:404:HOH:O	2.58	0.52
1:M:241:ASP:OD1	3:M:369:HOH:O	2.19	0.52
1:G:345:ASN:HD22	1:G:345:ASN:N	2.08	0.52
1:I:102:GLU:HG3	1:I:183:ARG:HH22	1.74	0.52
1:I:64:ARG:NH2	1:I:344:SER:O	2.40	0.52
1:L:219:ASN:O	1:L:220:GLU:O	2.27	0.52
1:P:73:LEU:HG	1:P:94:PHE:CD1	2.44	0.52
1:A:65:LEU:HD23	1:A:213:HIS:HB2	1.91	0.52
1:D:183:ARG:HD2	1:D:183:ARG:O	2.10	0.52
1:D:317:ILE:HD11	1:D:324:GLU:HB3	1.90	0.52
1:H:76:MSE:HE1	1:I:266:PRO:HB3	1.92	0.52
1:K:317:ILE:HD11	1:K:324:GLU:HB3	1.92	0.52
1:K:64:ARG:HD2	1:K:341:TYR:OH	2.10	0.52
1:N:262:ASP:HA	1:N:291:TYR:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:204:GLU:HB2	1:O:206:VAL:HG22	1.92	0.52
1:A:113:THR:HG22	3:A:379:HOH:O	2.10	0.52
1:B:183:ARG:HA	1:B:323:PHE:HA	1.90	0.52
1:C:208:LEU:CD2	1:C:342:VAL:HG13	2.39	0.52
1:E:149:VAL:HB	3:E:373:HOH:O	2.10	0.52
1:F:144:ARG:HD2	3:F:356:HOH:O	2.10	0.52
1:H:175:THR:HG22	1:H:177:SER:HB2	1.91	0.52
1:J:41:VAL:HG21	1:J:198:ILE:CG2	2.40	0.52
1:M:64:ARG:HD2	1:M:341:TYR:OH	2.10	0.52
1:N:85:ARG:HH21	1:N:144:ARG:HG3	1.74	0.52
1:N:69:HIS:HE1	3:N:410:HOH:O	1.93	0.52
1:O:18:ILE:HB	1:O:28:ILE:HD12	1.91	0.52
1:G:39:TRP:CZ2	1:G:199:LYS:HD3	2.45	0.52
1:J:47:ASN:HB2	1:K:307:ASP:OD1	2.09	0.52
1:K:208:LEU:CD2	1:K:343:MSE:HE2	2.31	0.52
1:L:184:HIS:O	1:L:324:GLU:OE1	2.28	0.52
1:O:208:LEU:CD2	1:O:342:VAL:HG13	2.40	0.52
1:A:113:THR:CG2	3:A:379:HOH:O	2.56	0.52
1:B:268:HIS:CE1	1:B:270:ALA:HB3	2.45	0.52
1:D:219:ASN:ND2	1:D:219:ASN:N	2.57	0.52
1:I:102:GLU:HG3	1:I:183:ARG:NH2	2.25	0.52
1:J:12:ILE:HD13	1:J:189:VAL:HG22	1.91	0.52
1:N:102:GLU:OE2	1:N:183:ARG:NH1	2.37	0.52
1:P:108:THR:HG22	1:P:110:SER:N	2.15	0.52
1:P:46:ASN:ND2	1:P:46:ASN:C	2.62	0.52
1:C:218:ASN:HD22	1:C:218:ASN:N	2.03	0.52
1:K:144:ARG:HD2	3:K:356:HOH:O	2.09	0.52
1:K:183:ARG:HA	3:K:404:HOH:O	2.09	0.52
1:M:242:MSE:SE	1:M:317:ILE:HG21	2.59	0.52
1:O:182:SER:OG	1:O:183:ARG:N	2.41	0.52
1:C:268:HIS:HE1	1:C:270:ALA:HB3	1.73	0.51
1:K:52:ILE:HG13	1:K:215:LEU:HD13	1.92	0.51
1:P:63:HIS:CE1	1:P:233:GLU:HG3	2.45	0.51
1:A:219:ASN:ND2	1:A:226:GLY:HA2	2.25	0.51
1:E:9:MSE:HE1	1:E:174:ILE:HG23	1.90	0.51
1:M:78:LYS:HA	1:P:290:ILE:HD12	1.93	0.51
1:D:95:ARG:HH21	1:D:97:ASN:HD22	1.57	0.51
1:O:272:ARG:C	1:O:272:ARG:HD2	2.30	0.51
1:D:44:LYS:HD2	1:D:45:ARG:H	1.73	0.51
1:E:183:ARG:HD3	1:E:323:PHE:CD2	2.43	0.51
1:K:190:SER:O	1:K:191:VAL:C	2.49	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:67:THR:HG22	1:K:239:ALA:HA	1.93	0.51
1:M:218:ASN:N	1:M:218:ASN:HD22	1.96	0.51
1:D:181:LYS:HB3	1:D:325:ARG:HG3	1.93	0.51
1:G:102:GLU:HG3	1:G:183:ARG:HH12	0.66	0.51
1:L:182:SER:OG	1:L:183:ARG:N	2.44	0.51
1:O:102:GLU:HG2	1:O:183:ARG:NH2	2.26	0.51
1:F:219:ASN:O	1:F:220:GLU:O	2.27	0.51
1:M:41:VAL:HG23	1:M:55:VAL:HG22	1.92	0.51
1:K:90:MSE:HG3	1:K:94:PHE:CE1	2.45	0.51
1:M:184:HIS:O	1:M:324:GLU:CD	2.49	0.51
1:D:144:ARG:NH1	3:D:356:HOH:O	2.38	0.51
1:F:259:CYS:HB3	1:F:312:LEU:HB3	1.93	0.51
1:G:63:HIS:CD2	1:G:211:THR:HB	2.46	0.51
1:A:86:LEU:HB2	1:A:143:VAL:HB	1.93	0.51
1:B:242:MSE:SE	1:B:317:ILE:HG13	2.61	0.51
1:J:76:MSE:HE1	1:K:260:ALA:HB1	1.88	0.51
1:K:141:ILE:HD12	1:K:141:ILE:C	2.31	0.51
1:L:186:ASP:H	1:L:242:MSE:CE	2.23	0.51
1:N:151:SER:OG	1:N:154:GLU:HG3	2.12	0.51
1:P:102:GLU:HG2	1:P:183:ARG:CZ	2.40	0.51
1:F:263:SER:HB3	1:F:294:TYR:CB	2.41	0.50
1:H:183:ARG:HB3	3:H:405:HOH:O	2.10	0.50
1:B:101:GLY:HA3	1:J:323:PHE:CE2	2.46	0.50
1:O:6:LYS:HG2	3:O:390:HOH:O	2.11	0.50
1:B:253:GLU:O	1:B:330:SER:HB2	2.11	0.50
1:C:142:GLU:HA	3:C:409:HOH:O	2.10	0.50
1:C:185:LEU:C	3:C:408:HOH:O	2.50	0.50
1:C:309:LYS:HE3	1:C:347:ILE:HG23	1.94	0.50
1:D:86:LEU:CD1	1:D:145:ILE:HD11	2.41	0.50
1:D:65:LEU:HD23	1:D:66:LEU:N	2.26	0.50
1:G:79:GLU:HB3	1:G:87:SER:HB3	1.92	0.50
1:I:106:ILE:O	1:I:113:THR:HA	2.11	0.50
1:I:183:ARG:CG	3:I:389:HOH:O	2.49	0.50
1:I:41:VAL:HG21	1:I:198:ILE:HG21	1.93	0.50
1:J:86:LEU:HB2	1:J:143:VAL:HB	1.93	0.50
1:J:97:ASN:HD22	1:J:97:ASN:N	2.03	0.50
1:P:95:ARG:HD2	1:P:97:ASN:HD22	1.75	0.50
1:B:67:THR:HG22	1:B:239:ALA:HA	1.92	0.50
1:E:285:GLU:HB2	1:E:333:HIS:CE1	2.47	0.50
1:F:319:SER:CB	3:F:396:HOH:O	2.58	0.50
1:J:106:ILE:O	1:J:113:THR:HA	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:193:ILE:HD11	1:M:331:ILE:HG23	1.92	0.50
1:E:187:ASP:OD2	1:E:241:ASP:HA	2.11	0.50
1:H:190:SER:HB3	1:H:240:VAL:HG12	1.92	0.50
1:J:183:ARG:O	1:J:183:ARG:HG2	2.11	0.50
1:L:244:ALA:HB2	1:L:320:SER:HB3	1.93	0.50
1:M:169:ASP:O	1:M:183:ARG:CZ	2.60	0.50
1:B:175:THR:CG2	1:B:177:SER:OG	2.59	0.50
1:B:322:ALA:O	1:B:323:PHE:CG	2.64	0.50
1:D:307:ASP:HB2	3:F:369:HOH:O	2.11	0.50
1:E:194:LEU:O	1:E:198:ILE:HG13	2.12	0.50
1:I:90:MSE:HB2	1:I:96:TRP:CZ2	2.47	0.50
1:J:267:TYR:HB3	3:J:359:HOH:O	2.11	0.50
1:J:90:MSE:HE3	1:J:96:TRP:CE2	2.46	0.50
1:K:253:GLU:HG2	1:K:326:THR:HA	1.93	0.50
1:L:32:ILE:HG23	1:L:195:LEU:HD21	1.94	0.50
1:L:65:LEU:HD12	1:L:66:LEU:C	2.32	0.50
1:P:213:HIS:CE1	1:P:231:PRO:HG2	2.46	0.50
1:H:175:THR:HG22	1:H:177:SER:N	2.26	0.50
1:J:9:MSE:HE2	1:J:174:ILE:CG2	2.41	0.50
1:N:190:SER:HB3	1:N:240:VAL:HG12	1.93	0.50
1:N:218:ASN:HD22	1:N:218:ASN:H	1.58	0.50
1:O:90:MSE:HE1	1:O:94:PHE:O	2.12	0.50
1:B:90:MSE:HB2	1:B:96:TRP:CZ2	2.46	0.50
1:G:260:ALA:HA	1:G:272:ARG:HD2	1.93	0.50
1:K:210:TYR:CZ	1:K:346:LEU:HG	2.47	0.50
1:L:186:ASP:HA	1:L:242:MSE:HE2	1.92	0.50
1:L:285:GLU:H	1:L:333:HIS:CD2	2.30	0.50
1:B:183:ARG:NE	1:B:184:HIS:CB	2.74	0.50
1:C:45:ARG:HG3	1:C:45:ARG:NH1	2.12	0.50
1:G:259:CYS:HB3	1:G:312:LEU:HB3	1.92	0.50
1:G:79:GLU:HA	1:G:79:GLU:OE1	2.11	0.50
1:H:154:GLU:HB2	3:H:373:HOH:O	2.10	0.50
1:F:262:ASP:HA	1:F:291:TYR:O	2.12	0.50
1:G:106:ILE:O	1:G:113:THR:HA	2.12	0.50
1:G:59:ASN:HD21	1:G:62:GLN:HE21	1.60	0.50
1:H:303:ARG:O	1:H:306:PHE:CZ	2.65	0.50
1:I:119:LEU:O	1:I:142:GLU:N	2.38	0.50
1:J:184:HIS:O	1:J:324:GLU:CD	2.50	0.50
1:K:183:ARG:HB3	3:K:410:HOH:O	2.12	0.50
1:M:235:VAL:HG12	1:M:236:GLU:HG3	1.94	0.50
1:M:39:TRP:CH2	1:M:199:LYS:HB2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:208:LEU:HD22	1:N:342:VAL:HG13	1.93	0.50
1:N:313:ILE:HD11	1:N:338:VAL:HG23	1.94	0.50
1:E:230:ILE:N	3:E:375:HOH:O	2.45	0.49
1:E:28:ILE:O	1:E:32:ILE:HG12	2.12	0.49
1:G:22:SER:OG	1:G:71:ASP:OD2	2.30	0.49
1:H:184:HIS:HA	1:H:186:ASP:OD2	2.11	0.49
1:I:241:ASP:HB3	1:I:312:LEU:HD21	1.93	0.49
1:K:183:ARG:HG2	3:K:410:HOH:O	2.12	0.49
1:K:97:ASN:OD1	1:K:97:ASN:N	2.43	0.49
1:L:304:ALA:HA	3:L:396:HOH:O	2.12	0.49
1:A:177:SER:N	3:A:413:HOH:O	2.43	0.49
1:J:39:TRP:CH2	1:J:199:LYS:HB2	2.47	0.49
1:K:193:ILE:HD12	1:K:335:GLU:HG2	1.93	0.49
1:C:175:THR:HG22	1:C:177:SER:H	1.76	0.49
1:F:269:TYR:CZ	1:F:273:LYS:HE3	2.47	0.49
1:P:252:ASP:N	3:P:370:HOH:O	2.44	0.49
1:C:90:MSE:HG3	1:C:94:PHE:CZ	2.46	0.49
1:K:80:ILE:CG2	1:K:152:ALA:HA	2.42	0.49
1:N:28:ILE:O	1:N:32:ILE:HG13	2.12	0.49
1:N:64:ARG:NH2	1:N:344:SER:O	2.38	0.49
1:P:182:SER:OG	1:P:183:ARG:N	2.45	0.49
1:C:184:HIS:O	1:C:185:LEU:CB	2.54	0.49
1:J:76:MSE:CE	1:K:260:ALA:HB1	2.41	0.49
1:L:83:ASP:OD1	1:L:85:ARG:HG3	2.12	0.49
1:O:39:TRP:CE2	1:O:199:LYS:HD2	2.48	0.49
1:B:208:LEU:HD22	1:B:342:VAL:HG13	1.93	0.49
1:C:268:HIS:CE1	1:C:270:ALA:HB3	2.48	0.49
1:E:201:LEU:HD13	1:E:208:LEU:HD21	1.93	0.49
1:E:183:ARG:NH1	1:E:323:PHE:CD2	2.81	0.49
1:F:86:LEU:HB2	1:F:143:VAL:HB	1.94	0.49
1:H:151:SER:O	3:H:373:HOH:O	2.20	0.49
1:H:187:ASP:HA	1:H:242:MSE:HE3	1.94	0.49
1:K:190:SER:HA	1:K:193:ILE:HG12	1.95	0.49
1:K:41:VAL:HG21	1:K:198:ILE:HG22	1.94	0.49
1:M:160:ILE:HA	1:M:164:ASP:OD2	2.13	0.49
1:M:220:GLU:C	1:M:222:ILE:H	2.16	0.49
1:P:114:TYR:CD1	1:P:160:ILE:HD11	2.47	0.49
1:A:184:HIS:C	1:A:186:ASP:N	2.65	0.49
1:F:63:HIS:NE2	1:F:233:GLU:HG3	2.27	0.49
1:G:152:ALA:HB1	1:G:156:ARG:NH2	2.28	0.49
1:H:218:ASN:H	1:H:218:ASN:HD22	1.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:GLU:OE2	1:A:183:ARG:HG3	2.12	0.49
1:A:78:LYS:HB3	1:B:290:ILE:HD12	1.95	0.49
1:C:141:ILE:CD1	1:C:141:ILE:N	2.75	0.49
1:C:171:ARG:CD	1:E:171:ARG:HD3	2.42	0.49
1:E:230:ILE:CG1	1:E:230:ILE:O	2.56	0.49
1:J:183:ARG:NH1	1:J:183:ARG:HB3	2.28	0.49
1:K:259:CYS:HB3	1:K:312:LEU:HB3	1.95	0.49
1:K:20:SER:HB2	1:K:25:THR:HG22	1.95	0.49
1:N:208:LEU:HD21	1:N:342:VAL:HG13	1.94	0.49
1:P:82:PRO:O	1:P:151:SER:HA	2.13	0.49
1:H:259:CYS:HB3	1:H:312:LEU:HB3	1.94	0.49
1:K:244:ALA:C	3:K:398:HOH:O	2.51	0.49
1:M:247:ASP:O	3:M:402:HOH:O	2.20	0.49
1:M:101:GLY:HA3	1:N:323:PHE:CD2	2.48	0.49
1:O:325:ARG:CZ	1:P:144:ARG:HD3	2.42	0.49
1:E:175:THR:HG21	1:E:177:SER:HB2	1.94	0.48
1:E:245:LEU:CD2	1:E:245:LEU:N	2.76	0.48
1:F:102:GLU:OE2	1:F:168:PHE:HB3	2.13	0.48
1:J:63:HIS:HB2	1:J:234:THR:HA	1.95	0.48
1:L:102:GLU:CB	1:L:183:ARG:HH12	2.26	0.48
1:N:41:VAL:HG23	1:N:55:VAL:CG2	2.41	0.48
1:O:335:GLU:HG2	3:O:365:HOH:O	2.13	0.48
1:C:183:ARG:HB3	1:C:183:ARG:CZ	2.38	0.48
1:J:323:PHE:N	1:J:323:PHE:CD1	2.80	0.48
1:K:237:TYR:HB2	1:K:308:VAL:HG11	1.95	0.48
1:M:9:MSE:HE2	1:M:174:ILE:CG2	2.43	0.48
1:O:210:TYR:CZ	1:O:346:LEU:HG	2.47	0.48
1:A:151:SER:OG	1:A:154:GLU:HG3	2.12	0.48
1:A:219:ASN:HD22	1:A:219:ASN:C	2.16	0.48
1:G:218:ASN:HD22	1:G:218:ASN:H	1.61	0.48
1:H:304:ALA:HA	3:H:410:HOH:O	2.13	0.48
1:J:155:VAL:O	1:J:158:LEU:HB2	2.14	0.48
1:J:86:LEU:HD13	1:J:145:ILE:HD11	1.96	0.48
1:J:9:MSE:HE3	1:J:174:ILE:HG12	1.94	0.48
1:P:262:ASP:HA	1:P:291:TYR:O	2.13	0.48
1:B:15:LEU:HB3	1:B:188:LYS:HD2	1.96	0.48
1:D:247:ASP:OD2	1:D:248:GLY:N	2.45	0.48
1:E:158:LEU:HD23	1:E:160:ILE:HD12	1.96	0.48
1:F:101:GLY:O	1:L:171:ARG:NH2	2.40	0.48
1:G:210:TYR:CZ	1:G:346:LEU:HG	2.48	0.48
1:I:52:ILE:HG13	1:I:215:LEU:HD13	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:251:SER:HB3	3:J:406:HOH:O	2.13	0.48
1:M:90:MSE:HE3	1:M:96:TRP:CE2	2.48	0.48
1:O:313:ILE:HD11	1:O:338:VAL:HG22	1.94	0.48
1:O:148:ARG:HD2	1:P:254:TYR:CE2	2.48	0.48
1:B:18:ILE:HB	1:B:28:ILE:HD12	1.94	0.48
1:C:65:LEU:HD12	1:C:237:TYR:CD2	2.49	0.48
1:D:43:THR:HG23	1:D:53:LEU:CD1	2.43	0.48
1:K:106:ILE:HG21	1:K:160:ILE:HD12	1.96	0.48
1:B:41:VAL:CG2	1:B:198:ILE:HG23	2.42	0.48
1:K:261:LYS:HB2	1:K:266:PRO:HA	1.95	0.48
1:C:175:THR:HG22	1:C:177:SER:N	2.29	0.48
1:E:175:THR:CG2	1:E:177:SER:H	2.22	0.48
1:A:144:ARG:HD3	1:G:325:ARG:CZ	2.43	0.48
1:K:183:ARG:HA	1:K:323:PHE:HA	1.96	0.48
1:M:219:ASN:C	1:M:220:GLU:O	2.51	0.48
1:G:237:TYR:HB2	1:G:308:VAL:HG11	1.95	0.48
3:D:393:HOH:O	1:H:319:SER:CB	2.47	0.48
1:I:46:ASN:HB2	1:I:50:ALA:HB3	1.95	0.48
1:I:59:ASN:C	1:I:59:ASN:OD1	2.52	0.48
1:M:86:LEU:HB2	1:M:143:VAL:HB	1.95	0.48
1:O:184:HIS:C	1:O:186:ASP:N	2.66	0.48
1:O:323:PHE:CE2	1:P:101:GLY:HA3	2.49	0.48
1:O:85:ARG:HG3	1:O:143:VAL:O	2.14	0.48
1:P:113:THR:HB	3:P:360:HOH:O	2.13	0.48
1:E:317:ILE:HD11	1:E:324:GLU:HB3	1.95	0.48
1:F:174:ILE:N	1:F:174:ILE:CD1	2.76	0.48
1:G:176:GLU:O	1:G:176:GLU:HG2	2.14	0.48
1:N:168:PHE:O	1:N:184:HIS:HE1	1.97	0.48
1:A:51:LEU:HD22	1:A:53:LEU:CD1	2.43	0.48
1:E:323:PHE:N	3:E:410:HOH:O	2.47	0.48
1:F:65:LEU:C	1:F:65:LEU:CD1	2.81	0.48
1:I:182:SER:C	3:I:409:HOH:O	2.52	0.48
1:I:323:PHE:CE2	1:K:101:GLY:HA3	2.49	0.48
1:L:65:LEU:HD12	1:L:66:LEU:N	2.29	0.48
1:M:204:GLU:HB3	1:M:206:VAL:HG22	1.95	0.48
1:M:245:LEU:H	1:M:245:LEU:HD12	1.77	0.48
1:A:253:GLU:O	1:A:330:SER:HB2	2.14	0.47
1:H:78:LYS:HA	1:I:290:ILE:HD12	1.95	0.47
1:I:317:ILE:O	1:I:317:ILE:HD13	2.14	0.47
1:J:197:LEU:HD13	1:J:338:VAL:HG23	1.96	0.47
1:P:9:MSE:HA	1:P:12:ILE:HD12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:ILE:HD12	1:A:347:ILE:HA	1.61	0.47
1:D:73:LEU:HG	1:D:94:PHE:CD1	2.49	0.47
1:F:120:MSE:HB3	1:F:140:ASN:HB2	1.95	0.47
1:O:323:PHE:CE1	1:P:119:LEU:HD12	2.49	0.47
1:F:39:TRP:CE2	1:F:199:LYS:HD3	2.49	0.47
1:G:9:MSE:SE	1:G:328:GLU:HB3	2.64	0.47
1:A:118:ILE:CD1	1:A:168:PHE:CE2	2.97	0.47
1:E:53:LEU:N	1:E:53:LEU:HD12	2.29	0.47
1:F:182:SER:OG	1:F:183:ARG:N	2.46	0.47
1:J:118:ILE:HD13	1:J:143:VAL:HG22	1.96	0.47
1:K:229:ASN:CB	3:K:395:HOH:O	2.53	0.47
1:L:20:SER:HB2	1:L:25:THR:HG22	1.95	0.47
1:N:102:GLU:CD	1:N:183:ARG:HD2	2.34	0.47
1:N:309:LYS:HE3	3:N:403:HOH:O	2.13	0.47
1:O:45:ARG:CG	1:O:51:LEU:HD23	2.45	0.47
1:A:335:GLU:HG2	3:A:402:HOH:O	2.13	0.47
1:E:184:HIS:ND1	1:E:186:ASP:OD2	2.39	0.47
1:F:319:SER:HB2	3:F:396:HOH:O	2.14	0.47
1:H:303:ARG:N	3:H:407:HOH:O	2.47	0.47
1:J:39:TRP:CE2	1:J:199:LYS:HD3	2.49	0.47
1:L:182:SER:HB3	1:L:185:LEU:HG	1.95	0.47
1:M:66:LEU:HD12	1:M:238:LEU:HB3	1.96	0.47
1:O:240:VAL:HA	1:O:313:ILE:O	2.15	0.47
1:O:278:LEU:HD13	1:O:341:TYR:HA	1.97	0.47
1:C:177:SER:N	3:C:401:HOH:O	2.41	0.47
1:E:200:ARG:O	1:E:204:GLU:HB2	2.14	0.47
1:G:53:LEU:HD12	1:G:53:LEU:N	2.29	0.47
1:H:242:MSE:HG2	1:H:315:ALA:O	2.14	0.47
1:H:86:LEU:HD22	1:H:145:ILE:CD1	2.42	0.47
1:K:152:ALA:HB1	1:K:156:ARG:NH2	2.29	0.47
1:P:43:THR:HG22	1:P:53:LEU:HG	1.97	0.47
1:B:81:LYS:HZ1	1:B:142:GLU:HG2	1.80	0.47
1:C:317:ILE:HD13	1:C:317:ILE:O	2.14	0.47
1:D:323:PHE:CE2	1:H:101:GLY:HA3	2.50	0.47
1:D:339:TYR:CE2	1:D:343:MSE:HE3	2.50	0.47
1:G:102:GLU:CG	1:G:183:ARG:HH22	2.26	0.47
1:H:172:VAL:HA	1:H:182:SER:HB2	1.97	0.47
1:N:145:ILE:CD1	1:N:147:GLU:HB2	2.44	0.47
1:A:291:TYR:CE2	1:A:312:LEU:HD13	2.50	0.47
1:B:313:ILE:HD11	1:B:338:VAL:HG23	1.96	0.47
1:C:269:TYR:CE2	1:C:273:LYS:HE2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:204:GLU:HG2	1:G:206:VAL:HG22	1.96	0.47
1:I:175:THR:HB	1:I:179:TYR:H	1.80	0.47
1:K:263:SER:HB2	1:K:294:TYR:H	1.75	0.47
1:M:86:LEU:CD2	1:M:145:ILE:HD11	2.44	0.47
1:N:9:MSE:CE	1:N:328:GLU:CA	2.92	0.47
1:A:98:SER:O	1:A:183:ARG:NH2	2.48	0.47
1:A:307:ASP:OD1	1:C:47:ASN:HB2	2.15	0.47
1:A:242:MSE:SE	1:A:317:ILE:CD1	3.12	0.47
1:B:28:ILE:O	1:B:32:ILE:HG13	2.15	0.47
1:D:262:ASP:HA	1:D:291:TYR:O	2.14	0.47
1:P:208:LEU:CD2	1:P:343:MSE:HE2	2.32	0.47
1:P:304:ALA:HB2	3:P:392:HOH:O	2.14	0.47
1:C:142:GLU:CA	3:C:409:HOH:O	2.63	0.47
1:C:151:SER:OG	1:C:154:GLU:HG3	2.15	0.47
1:M:183:ARG:HB3	1:M:183:ARG:NH1	2.23	0.47
1:C:213:HIS:NE2	1:C:231:PRO:HG2	2.29	0.46
1:J:171:ARG:HD2	3:J:399:HOH:O	2.15	0.46
1:J:45:ARG:CZ	1:J:45:ARG:HB3	2.43	0.46
1:L:230:ILE:HA	1:L:231:PRO:HD2	1.74	0.46
1:P:106:ILE:HD12	1:P:114:TYR:O	2.15	0.46
1:E:20:SER:HB2	1:E:25:THR:HG22	1.97	0.46
1:K:13:LYS:HE3	3:K:412:HOH:O	2.15	0.46
1:M:90:MSE:HG3	1:M:94:PHE:CE1	2.50	0.46
1:A:102:GLU:OE2	1:A:183:ARG:NE	2.49	0.46
1:A:184:HIS:O	1:A:185:LEU:HB2	2.16	0.46
1:A:317:ILE:HD13	1:A:326:THR:HB	1.95	0.46
1:D:322:ALA:HB1	1:D:323:PHE:CD1	2.50	0.46
1:E:59:ASN:HD21	1:E:62:GLN:HE21	1.63	0.46
1:G:213:HIS:CE1	1:G:231:PRO:HG3	2.51	0.46
1:I:97:ASN:N	1:I:97:ASN:OD1	2.32	0.46
1:L:120:MSE:HG2	1:L:141:ILE:HD13	1.98	0.46
1:L:184:HIS:O	1:L:185:LEU:HB2	2.15	0.46
1:L:239:ALA:O	1:L:312:LEU:HA	2.15	0.46
1:N:33:GLU:OE1	1:N:45:ARG:HD2	2.16	0.46
1:C:320:SER:HA	1:C:324:GLU:HG2	1.97	0.46
1:F:63:HIS:CE1	1:F:233:GLU:CG	2.99	0.46
1:H:48:LYS:HE3	1:I:306:PHE:O	2.16	0.46
1:I:44:LYS:HG2	1:I:45:ARG:N	2.29	0.46
1:L:306:PHE:HD1	3:L:396:HOH:O	1.98	0.46
1:N:253:GLU:O	1:N:330:SER:HB2	2.15	0.46
1:P:184:HIS:ND1	1:P:186:ASP:OD2	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:ILE:HD11	1:B:147:GLU:HB2	1.98	0.46
1:D:241:ASP:O	1:D:314:GLY:HA3	2.15	0.46
1:F:303:ARG:O	3:F:387:HOH:O	2.21	0.46
1:I:83:ASP:OD1	1:I:85:ARG:HG3	2.16	0.46
1:L:69:HIS:CE1	1:L:187:ASP:HB2	2.49	0.46
1:O:169:ASP:HA	1:O:170:PRO:HD3	1.71	0.46
1:C:142:GLU:C	3:C:409:HOH:O	2.54	0.46
1:H:176:GLU:N	1:H:176:GLU:CD	2.69	0.46
1:J:76:MSE:HE3	1:K:260:ALA:CB	2.42	0.46
1:L:293:TYR:O	1:L:294:TYR:CB	2.63	0.46
1:M:150:PHE:N	1:M:154:GLU:OE1	2.37	0.46
1:M:175:THR:HG22	1:M:177:SER:H	1.79	0.46
1:P:253:GLU:CG	3:P:404:HOH:O	2.44	0.46
1:C:20:SER:HB2	1:C:25:THR:HG22	1.97	0.46
1:G:9:MSE:CE	1:G:174:ILE:HG23	2.45	0.46
1:H:268:HIS:CE1	1:H:309:LYS:HD3	2.50	0.46
1:J:141:ILE:C	1:J:141:ILE:HD13	2.35	0.46
1:K:41:VAL:HG21	1:K:198:ILE:CG2	2.46	0.46
1:L:186:ASP:H	1:L:242:MSE:HE1	1.79	0.46
1:N:90:MSE:HG3	1:N:94:PHE:CE1	2.50	0.46
1:D:193:ILE:HG12	1:D:335:GLU:HG3	1.96	0.46
1:E:319:SER:CB	3:E:365:HOH:O	2.64	0.46
1:G:76:MSE:HE3	1:H:260:ALA:HB3	1.88	0.46
1:K:218:ASN:HD22	1:K:218:ASN:N	2.13	0.46
1:L:220:GLU:HG2	3:L:393:HOH:O	2.16	0.46
1:M:39:TRP:HB3	3:M:357:HOH:O	2.16	0.46
1:N:156:ARG:HH11	1:N:156:ARG:HG2	1.81	0.46
1:B:170:PRO:O	1:B:182:SER:HB3	2.16	0.46
1:D:102:GLU:HG3	1:D:183:ARG:HH21	1.56	0.46
1:E:39:TRP:CE2	1:E:199:LYS:HD3	2.51	0.46
1:F:97:ASN:N	1:F:97:ASN:OD1	2.47	0.46
1:H:156:ARG:HD3	1:H:161:GLU:OE2	2.16	0.46
1:J:218:ASN:HD22	1:J:218:ASN:N	2.12	0.46
1:J:46:ASN:HB2	1:J:50:ALA:O	2.15	0.46
1:K:181:LYS:HB3	1:K:325:ARG:HG3	1.98	0.46
1:E:293:TYR:HD1	3:E:401:HOH:O	1.99	0.46
1:E:322:ALA:HB1	1:E:323:PHE:CZ	2.51	0.46
1:J:46:ASN:HB3	1:J:50:ALA:N	2.28	0.46
1:L:187:ASP:OD2	1:L:241:ASP:HA	2.16	0.46
1:N:259:CYS:HB3	1:N:312:LEU:HB3	1.97	0.46
1:E:313:ILE:HD11	1:E:338:VAL:HG22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:160:ILE:HA	1:J:164:ASP:OD2	2.16	0.45
1:M:187:ASP:H	1:M:242:MSE:HE2	1.79	0.45
1:A:213:HIS:NE2	1:A:231:PRO:HG2	2.31	0.45
1:A:97:ASN:HD22	1:A:97:ASN:H	1.62	0.45
1:D:72:THR:CB	1:D:184:HIS:CE1	2.98	0.45
1:E:151:SER:OG	1:E:154:GLU:HG3	2.16	0.45
1:E:90:MSE:HG3	1:E:94:PHE:CE1	2.51	0.45
1:G:56:LYS:HE2	1:G:56:LYS:HB3	1.81	0.45
1:I:237:TYR:HB2	1:I:308:VAL:HG11	1.98	0.45
1:K:278:LEU:HD13	1:K:341:TYR:HA	1.99	0.45
1:J:307:ASP:HA	1:L:48:LYS:HZ1	1.81	0.45
1:P:86:LEU:HD22	1:P:145:ILE:HD11	1.97	0.45
1:E:69:HIS:ND1	1:E:220:GLU:HG2	2.31	0.45
1:F:102:GLU:CD	1:F:183:ARG:HE	2.20	0.45
1:F:65:LEU:HD12	1:F:66:LEU:N	2.32	0.45
1:I:218:ASN:N	1:I:218:ASN:HD22	2.01	0.45
1:L:65:LEU:C	1:L:65:LEU:HD12	2.37	0.45
1:N:189:VAL:HB	1:N:242:MSE:CE	2.47	0.45
1:O:187:ASP:OD2	1:O:241:ASP:HA	2.16	0.45
1:E:175:THR:HG22	1:E:177:SER:CA	2.47	0.45
1:E:323:PHE:N	1:E:323:PHE:CD2	2.82	0.45
1:F:218:ASN:HD22	1:F:218:ASN:N	2.11	0.45
1:J:287:LYS:HG2	3:J:381:HOH:O	2.16	0.45
1:L:304:ALA:CA	3:L:396:HOH:O	2.64	0.45
1:M:155:VAL:O	1:M:158:LEU:HB2	2.15	0.45
1:M:66:LEU:HA	1:M:66:LEU:HD12	1.73	0.45
1:A:102:GLU:CD	1:A:183:ARG:NH2	2.70	0.45
1:B:324:GLU:N	3:B:414:HOH:O	2.49	0.45
1:E:86:LEU:HB2	1:E:143:VAL:HB	1.99	0.45
1:E:293:TYR:O	1:E:293:TYR:CD1	2.70	0.45
1:I:244:ALA:HB2	1:I:320:SER:HB3	1.96	0.45
1:I:33:GLU:OE1	1:I:45:ARG:NH1	2.50	0.45
1:N:175:THR:HG22	3:N:392:HOH:O	2.17	0.45
1:N:241:ASP:O	1:N:314:GLY:HA3	2.16	0.45
1:B:177:SER:N	3:B:395:HOH:O	2.50	0.45
1:C:319:SER:HB3	1:C:323:PHE:O	2.16	0.45
1:C:210:TYR:CZ	1:C:346:LEU:HG	2.52	0.45
1:D:99:VAL:HG12	1:D:183:ARG:HH21	1.81	0.45
1:D:88:LEU:CD2	1:D:166:VAL:HG21	2.47	0.45
1:E:183:ARG:C	3:E:410:HOH:O	2.54	0.45
1:N:149:VAL:HG11	1:N:155:VAL:CG2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:HIS:CD2	1:A:4:HIS:H	2.20	0.45
1:B:230:ILE:HG22	1:B:231:PRO:CD	2.45	0.45
1:B:42:GLU:OE1	1:B:44:LYS:NZ	2.50	0.45
1:C:65:LEU:HD23	1:C:213:HIS:HB2	1.98	0.45
1:D:113:THR:HG22	3:D:373:HOH:O	2.16	0.45
1:D:66:LEU:O	1:D:214:PHE:HA	2.17	0.45
1:E:187:ASP:HA	1:E:242:MSE:CE	2.46	0.45
1:G:39:TRP:CD1	1:G:39:TRP:N	2.83	0.45
1:I:24:ASN:HA	3:I:370:HOH:O	2.17	0.45
1:J:255:THR:HG22	1:J:285:GLU:HB3	1.99	0.45
1:K:219:ASN:HB2	3:K:406:HOH:O	2.16	0.45
1:L:263:SER:HB2	1:L:294:TYR:O	2.17	0.45
1:A:95:ARG:O	1:A:98:SER:OG	2.27	0.45
1:D:197:LEU:C	1:D:197:LEU:HD23	2.37	0.45
1:H:65:LEU:HD22	1:H:213:HIS:HB2	1.99	0.45
1:N:291:TYR:CE2	1:N:312:LEU:HD13	2.51	0.45
1:O:90:MSE:HE2	1:O:94:PHE:CD2	2.52	0.45
1:O:103:TYR:OH	1:P:182:SER:HB3	2.17	0.45
1:P:64:ARG:NH2	1:P:344:SER:O	2.50	0.45
1:A:317:ILE:HD12	1:A:326:THR:HB	1.98	0.45
1:B:120:MSE:HG3	3:B:398:HOH:O	2.17	0.45
1:B:322:ALA:O	1:B:323:PHE:CD2	2.70	0.45
1:K:182:SER:HB2	1:K:185:LEU:HD23	1.99	0.45
1:K:255:THR:HG22	1:K:285:GLU:HB3	1.99	0.45
1:P:208:LEU:CD2	1:P:342:VAL:HG13	2.47	0.45
1:J:182:SER:OG	1:J:183:ARG:N	2.50	0.45
1:K:107:GLU:O	1:K:164:ASP:HB3	2.16	0.45
1:K:187:ASP:OD2	1:K:242:MSE:CE	2.65	0.45
1:K:40:ASN:HA	1:K:40:ASN:HD22	1.58	0.45
1:N:213:HIS:NE2	1:N:231:PRO:HG2	2.32	0.45
1:N:83:ASP:OD1	1:N:85:ARG:HB2	2.16	0.45
1:K:3:HIS:N	1:K:3:HIS:HD1	2.14	0.44
1:N:228:SER:O	1:N:229:ASN:HB2	2.17	0.44
1:N:65:LEU:HD22	1:N:237:TYR:CE2	2.53	0.44
1:G:108:THR:CG2	1:G:112:LYS:H	2.28	0.44
1:I:317:ILE:HD13	1:I:317:ILE:H	1.82	0.44
1:J:9:MSE:HE3	1:J:180:ILE:HB	2.00	0.44
1:P:39:TRP:CE2	1:P:199:LYS:HD3	2.52	0.44
1:B:118:ILE:HD11	1:B:168:PHE:CD2	2.52	0.44
1:B:208:LEU:HD21	1:B:342:VAL:HG13	1.99	0.44
1:H:184:HIS:HA	1:H:186:ASP:CG	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:190:SER:HB3	1:N:240:VAL:CG1	2.48	0.44
1:P:181:LYS:HB3	1:P:325:ARG:HG3	1.99	0.44
1:P:69:HIS:CE1	1:P:220:GLU:HG3	2.52	0.44
1:C:81:LYS:CE	1:C:142:GLU:HG2	2.47	0.44
1:D:103:TYR:HB2	1:D:169:ASP:OD2	2.18	0.44
1:H:43:THR:HG22	1:H:43:THR:O	2.16	0.44
1:I:66:LEU:O	1:I:214:PHE:HA	2.18	0.44
1:K:233:GLU:OE2	1:K:233:GLU:N	2.51	0.44
1:L:105:GLU:O	1:L:166:VAL:HA	2.18	0.44
1:M:229:ASN:CB	3:M:396:HOH:O	2.62	0.44
1:M:242:MSE:SE	1:M:317:ILE:HG23	2.67	0.44
1:N:118:ILE:CD1	1:N:168:PHE:CE2	3.00	0.44
1:N:41:VAL:HG11	1:N:53:LEU:HD23	1.99	0.44
1:O:234:THR:O	1:O:308:VAL:HG12	2.17	0.44
1:A:108:THR:HG22	1:A:110:SER:N	2.33	0.44
1:A:253:GLU:HB3	1:A:326:THR:HA	1.99	0.44
1:M:251:SER:N	3:M:402:HOH:O	2.49	0.44
1:O:148:ARG:HG3	1:O:150:PHE:CZ	2.53	0.44
1:B:171:ARG:HD3	1:J:171:ARG:CD	2.42	0.44
1:B:16:VAL:HA	1:B:188:LYS:HE3	1.99	0.44
1:E:86:LEU:CD2	1:E:145:ILE:HD11	2.47	0.44
1:E:160:ILE:HA	1:E:164:ASP:OD2	2.17	0.44
1:F:25:THR:O	1:F:29:ILE:HD12	2.18	0.44
1:G:209:PRO:HB2	1:G:210:TYR:CD1	2.52	0.44
1:I:262:ASP:O	1:I:265:GLY:N	2.46	0.44
1:C:209:PRO:HG2	1:C:210:TYR:CD1	2.53	0.44
1:D:90:MSE:HE2	1:D:94:PHE:CE2	2.53	0.44
1:G:53:LEU:N	1:G:53:LEU:CD1	2.81	0.44
1:I:239:ALA:O	1:I:312:LEU:HD23	2.18	0.44
1:I:59:ASN:HD21	1:I:62:GLN:NE2	2.16	0.44
1:L:237:TYR:HB2	1:L:308:VAL:CG1	2.43	0.44
1:M:175:THR:CB	3:M:368:HOH:O	1.79	0.44
1:M:267:TYR:HB3	3:M:382:HOH:O	2.17	0.44
1:O:106:ILE:O	1:O:113:THR:HA	2.17	0.44
1:A:158:LEU:HD23	1:A:160:ILE:HD12	1.99	0.44
1:A:30:ASN:ND2	1:A:45:ARG:HH22	2.15	0.44
1:B:85:ARG:HG3	3:B:356:HOH:O	2.18	0.44
1:E:201:LEU:CD1	1:E:208:LEU:HD21	2.47	0.44
1:F:174:ILE:CD1	1:F:180:ILE:HD12	2.43	0.44
1:F:252:ASP:O	1:F:316:GLY:HA3	2.18	0.44
1:M:277:GLU:OE1	1:M:277:GLU:HA	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:145:ILE:C	1:N:145:ILE:HD13	2.38	0.44
1:O:39:TRP:N	1:O:39:TRP:CD1	2.86	0.44
1:B:274:HIS:HE1	1:B:344:SER:OG	2.01	0.44
1:E:29:ILE:HG23	1:E:51:LEU:HD22	2.00	0.44
1:J:66:LEU:HD22	1:J:214:PHE:CE2	2.53	0.44
1:J:317:ILE:CG2	1:J:317:ILE:O	2.66	0.44
1:J:90:MSE:O	1:K:261:LYS:HE3	2.17	0.44
1:L:184:HIS:CD2	3:L:389:HOH:O	2.70	0.44
1:M:73:LEU:HG	3:M:407:HOH:O	2.17	0.44
1:N:268:HIS:HE1	1:N:270:ALA:HB3	1.83	0.44
1:A:303:ARG:CA	3:A:405:HOH:O	2.66	0.43
1:B:319:SER:HB3	1:B:323:PHE:O	2.18	0.43
1:C:41:VAL:HG11	1:C:53:LEU:HB3	1.98	0.43
1:D:140:ASN:ND2	3:D:395:HOH:O	2.50	0.43
1:D:254:TYR:CE1	1:H:150:PHE:HE2	2.36	0.43
1:F:200:ARG:NE	3:F:398:HOH:O	2.50	0.43
1:F:22:SER:OG	1:F:71:ASP:OD2	2.35	0.43
1:G:15:LEU:HB3	1:G:188:LYS:HD3	1.99	0.43
1:K:10:GLU:HA	1:K:10:GLU:OE1	2.18	0.43
1:K:40:ASN:H	1:K:202:GLN:NE2	2.16	0.43
1:N:67:THR:HG22	1:N:239:ALA:HA	2.00	0.43
1:O:323:PHE:CD1	1:P:119:LEU:HD12	2.53	0.43
1:B:9:MSE:HE2	1:B:174:ILE:CG2	2.48	0.43
1:I:120:MSE:CG	1:I:141:ILE:HD13	2.41	0.43
1:I:64:ARG:HD2	1:I:341:TYR:OH	2.18	0.43
1:J:310:HIS:HB2	3:J:382:HOH:O	2.18	0.43
1:M:231:PRO:O	1:M:233:GLU:N	2.51	0.43
1:M:245:LEU:N	1:M:245:LEU:CD1	2.80	0.43
1:O:30:ASN:O	1:O:33:GLU:HB3	2.17	0.43
1:B:69:HIS:HE1	3:B:381:HOH:O	2.01	0.43
1:E:209:PRO:HB2	1:E:210:TYR:CD1	2.53	0.43
1:F:186:ASP:HA	1:F:187:ASP:HA	1.49	0.43
1:F:319:SER:CB	3:F:365:HOH:O	2.59	0.43
1:I:241:ASP:O	1:I:314:GLY:HA3	2.17	0.43
1:L:196:LYS:HD3	1:L:196:LYS:HA	1.79	0.43
1:O:194:LEU:HD21	1:O:240:VAL:HG11	2.01	0.43
1:A:184:HIS:O	1:A:324:GLU:OE2	2.36	0.43
1:D:105:GLU:HA	1:D:114:TYR:O	2.18	0.43
1:F:64:ARG:NH1	3:F:358:HOH:O	2.51	0.43
1:I:16:VAL:HA	1:I:188:LYS:HD2	2.01	0.43
1:L:241:ASP:O	1:L:314:GLY:HA3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:242:MSE:SE	1:N:317:ILE:HD13	2.68	0.43
1:N:65:LEU:HD22	1:N:237:TYR:CD2	2.53	0.43
1:O:39:TRP:CZ2	1:O:199:LYS:HD2	2.53	0.43
1:B:210:TYR:CZ	1:B:346:LEU:HG	2.52	0.43
1:D:141:ILE:HG23	1:D:141:ILE:O	2.17	0.43
1:F:44:LYS:HE3	1:F:44:LYS:HB2	1.89	0.43
1:H:219:ASN:O	1:H:220:GLU:CB	2.30	0.43
1:O:146:ASP:HA	1:P:325:ARG:NH1	2.34	0.43
1:O:99:VAL:HG23	1:O:118:ILE:HG21	1.99	0.43
1:B:118:ILE:HD11	1:B:168:PHE:CE2	2.54	0.43
1:D:8:THR:O	1:D:12:ILE:HG13	2.18	0.43
1:F:102:GLU:OE1	1:F:183:ARG:NE	2.51	0.43
1:F:319:SER:HA	3:F:396:HOH:O	2.17	0.43
1:H:9:MSE:HE2	1:H:174:ILE:HG23	1.99	0.43
1:I:120:MSE:HG2	1:I:141:ILE:CD1	2.42	0.43
1:J:20:SER:HB2	1:J:25:THR:HG22	2.00	0.43
1:O:29:ILE:HG22	1:O:30:ASN:N	2.34	0.43
1:B:218:ASN:N	1:B:218:ASN:HD22	2.10	0.43
1:C:170:PRO:HB3	1:C:184:HIS:CD2	2.54	0.43
1:C:303:ARG:CB	1:C:306:PHE:HD1	2.31	0.43
1:J:175:THR:C	1:J:177:SER:H	2.22	0.43
1:K:347:ILE:HD12	1:K:348:GLU:H	1.83	0.43
1:P:114:TYR:HD1	1:P:160:ILE:HD11	1.83	0.43
1:P:182:SER:C	1:P:184:HIS:H	2.22	0.43
1:P:184:HIS:O	1:P:185:LEU:C	2.57	0.43
1:D:232:GLU:HG3	1:D:232:GLU:H	1.69	0.43
1:G:64:ARG:HD2	1:G:341:TYR:OH	2.19	0.43
1:K:80:ILE:HG21	1:K:152:ALA:HA	2.01	0.43
1:K:240:VAL:HA	1:K:313:ILE:O	2.19	0.43
1:L:39:TRP:CH2	1:L:199:LYS:HB2	2.54	0.43
1:A:268:HIS:CE1	1:A:270:ALA:HB3	2.47	0.43
1:D:86:LEU:HD11	1:D:145:ILE:HD11	2.01	0.43
1:D:75:ALA:CA	1:D:91:ILE:HD13	2.47	0.43
1:E:182:SER:OG	1:E:183:ARG:N	2.52	0.43
1:K:42:GLU:O	1:K:53:LEU:HA	2.19	0.43
1:N:253:GLU:OE1	1:N:318:ASP:HB2	2.19	0.43
1:P:64:ARG:HD2	1:P:341:TYR:OH	2.19	0.43
1:D:338:VAL:O	1:D:342:VAL:HB	2.19	0.43
1:G:114:TYR:CD1	1:G:160:ILE:HD11	2.52	0.42
1:H:317:ILE:HG23	1:H:317:ILE:O	2.17	0.42
1:K:274:HIS:HE1	1:K:344:SER:OG	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:81:LYS:HB2	1:K:85:ARG:O	2.19	0.42
3:J:385:HOH:O	1:L:229:ASN:HB3	2.19	0.42
1:P:32:ILE:HD12	1:P:195:LEU:HD21	2.01	0.42
1:A:118:ILE:HD11	1:A:168:PHE:CE2	2.55	0.42
1:B:145:ILE:HD12	1:B:146:ASP:N	2.33	0.42
1:I:90:MSE:HE2	1:I:94:PHE:CE2	2.53	0.42
1:K:176:GLU:HA	1:K:176:GLU:OE2	2.18	0.42
1:K:183:ARG:HH11	1:K:183:ARG:HG3	1.85	0.42
1:K:230:ILE:N	1:K:230:ILE:HD13	2.34	0.42
1:K:241:ASP:O	1:K:314:GLY:HA3	2.20	0.42
1:M:175:THR:HG22	1:M:176:GLU:N	2.34	0.42
1:M:323:PHE:CE2	1:N:101:GLY:HA3	2.54	0.42
1:O:208:LEU:HD23	1:O:343:MSE:HE1	1.95	0.42
1:A:120:MSE:HG2	1:A:141:ILE:CG2	2.50	0.42
1:A:247:ASP:HB3	3:C:417:HOH:O	2.18	0.42
1:A:316:GLY:O	1:A:317:ILE:HD13	2.19	0.42
1:D:258:ILE:HA	1:D:313:ILE:HG22	2.01	0.42
1:K:78:LYS:HG3	1:K:87:SER:HB3	2.01	0.42
1:L:183:ARG:CG	3:L:389:HOH:O	2.62	0.42
1:L:40:ASN:H	1:L:202:GLN:NE2	2.17	0.42
1:M:195:LEU:HD12	1:M:195:LEU:HA	1.94	0.42
1:N:30:ASN:ND2	3:N:406:HOH:O	2.52	0.42
1:N:317:ILE:HA	1:N:317:ILE:HD12	1.76	0.42
1:A:319:SER:HB3	1:A:323:PHE:O	2.18	0.42
1:B:323:PHE:CE1	1:J:100:GLU:HG2	2.55	0.42
1:G:86:LEU:HB2	1:G:143:VAL:HB	2.00	0.42
1:I:78:LYS:HG2	1:I:87:SER:HB3	2.01	0.42
1:L:90:MSE:HE2	1:L:94:PHE:CE2	2.54	0.42
1:M:39:TRP:N	1:M:39:TRP:CD1	2.87	0.42
1:O:186:ASP:HA	1:O:242:MSE:CE	2.48	0.42
1:A:145:ILE:HG12	1:A:146:ASP:N	2.33	0.42
1:C:218:ASN:ND2	1:C:218:ASN:N	2.68	0.42
1:E:9:MSE:HE2	1:E:174:ILE:CG2	2.49	0.42
1:I:208:LEU:CD2	1:I:342:VAL:CG1	2.97	0.42
1:K:303:ARG:C	3:K:416:HOH:O	2.58	0.42
1:M:106:ILE:O	1:M:113:THR:HA	2.19	0.42
1:O:257:SER:OG	1:O:289:ASP:OD2	2.29	0.42
1:O:241:ASP:O	1:O:314:GLY:HA3	2.19	0.42
1:P:256:VAL:HG23	1:P:285:GLU:O	2.20	0.42
1:A:323:PHE:N	1:A:323:PHE:CD1	2.87	0.42
1:A:52:ILE:N	1:A:52:ILE:HD12	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:LEU:HB2	1:B:143:VAL:HB	2.02	0.42
1:C:229:ASN:HB3	3:C:370:HOH:O	2.14	0.42
1:D:40:ASN:H	1:D:202:GLN:HE22	1.66	0.42
1:E:346:LEU:HD23	1:E:346:LEU:HA	1.88	0.42
1:E:40:ASN:HA	1:E:40:ASN:HD22	1.70	0.42
1:H:204:GLU:HB2	1:H:206:VAL:HG23	2.00	0.42
1:H:253:GLU:HG2	1:H:326:THR:HA	2.00	0.42
1:J:210:TYR:O	1:J:212:THR:HG23	2.20	0.42
1:J:64:ARG:HD2	1:J:341:TYR:OH	2.20	0.42
1:L:141:ILE:HA	1:L:141:ILE:HD13	1.91	0.42
1:L:208:LEU:CD2	1:L:342:VAL:HG13	2.50	0.42
1:L:220:GLU:HB2	3:L:393:HOH:O	2.19	0.42
1:L:41:VAL:HG21	1:L:55:VAL:HG22	2.01	0.42
1:M:21:PRO:CA	1:M:72:THR:HG22	2.45	0.42
1:N:237:TYR:HB2	1:N:308:VAL:CG1	2.49	0.42
1:N:43:THR:CG2	3:N:414:HOH:O	2.67	0.42
1:P:304:ALA:CA	3:P:392:HOH:O	2.67	0.42
1:E:213:HIS:CE1	1:E:231:PRO:HG2	2.53	0.42
1:F:171:ARG:HH11	1:L:171:ARG:HD3	1.84	0.42
1:G:41:VAL:HG11	1:G:198:ILE:HG23	2.00	0.42
1:J:194:LEU:HA	1:J:194:LEU:HD23	1.85	0.42
1:L:66:LEU:O	1:L:214:PHE:HA	2.19	0.42
1:M:45:ARG:HB2	1:M:45:ARG:HH11	1.85	0.42
1:N:108:THR:HG23	3:N:363:HOH:O	2.19	0.42
1:P:256:VAL:HG22	1:P:333:HIS:HB3	2.02	0.42
1:P:65:LEU:HD22	1:P:213:HIS:HB2	2.01	0.42
1:B:15:LEU:O	1:B:188:LYS:HE3	2.19	0.42
1:D:253:GLU:O	1:D:330:SER:HB2	2.20	0.42
1:E:171:ARG:HH21	1:E:183:ARG:HG3	1.84	0.42
1:F:96:TRP:HB3	1:F:141:ILE:HD11	2.02	0.42
1:H:197:LEU:CD2	1:H:338:VAL:CG1	2.91	0.42
1:I:186:ASP:O	3:I:371:HOH:O	2.22	0.42
1:I:337:LEU:HD23	1:I:337:LEU:HA	1.79	0.42
1:L:86:LEU:HB2	1:L:143:VAL:HB	2.02	0.42
1:L:282:ASN:N	1:L:282:ASN:ND2	2.66	0.42
1:B:186:ASP:O	3:B:411:HOH:O	2.22	0.42
1:E:310:HIS:HB2	3:E:378:HOH:O	2.20	0.42
1:E:317:ILE:CG2	1:E:317:ILE:O	2.68	0.42
1:F:10:GLU:CG	3:F:407:HOH:O	2.44	0.42
1:F:274:HIS:CE1	1:F:278:LEU:HD11	2.54	0.42
1:G:269:TYR:O	1:G:273:LYS:HG2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:GLY:HA3	1:G:323:PHE:CE2	2.55	0.42
1:H:12:ILE:HG12	1:H:189:VAL:HA	2.02	0.42
1:I:150:PHE:N	1:I:154:GLU:OE2	2.45	0.42
1:I:196:LYS:HD2	1:I:196:LYS:HA	1.79	0.42
1:J:241:ASP:OD1	3:J:387:HOH:O	2.21	0.42
1:N:12:ILE:O	1:N:16:VAL:HG13	2.19	0.42
1:N:85:ARG:NH2	1:N:144:ARG:HG3	2.34	0.42
1:O:20:SER:HB2	1:O:25:THR:HG22	2.02	0.42
1:O:64:ARG:HD2	1:O:341:TYR:OH	2.20	0.42
1:P:184:HIS:O	1:P:324:GLU:OE1	2.37	0.42
1:A:262:ASP:HB2	1:A:293:TYR:O	2.20	0.42
1:A:96:TRP:O	1:A:99:VAL:HG22	2.20	0.42
1:E:120:MSE:HG2	1:E:141:ILE:CG1	2.33	0.42
1:F:78:LYS:HB2	1:F:78:LYS:HE3	1.69	0.42
1:H:218:ASN:N	1:H:218:ASN:HD22	2.17	0.42
1:J:175:THR:C	1:J:177:SER:N	2.71	0.42
1:M:245:LEU:H	1:M:245:LEU:CD1	2.33	0.42
1:M:73:LEU:HD22	1:M:94:PHE:HD1	1.85	0.42
1:O:196:LYS:HD3	1:O:196:LYS:HA	1.82	0.42
1:P:218:ASN:HD22	1:P:218:ASN:N	2.15	0.42
1:P:41:VAL:H	1:P:41:VAL:HG23	1.15	0.42
1:A:40:ASN:H	1:A:202:GLN:HE22	1.61	0.41
1:A:48:LYS:HZ3	1:A:227:ASN:CG	2.23	0.41
1:B:170:PRO:O	1:B:182:SER:CB	2.68	0.41
1:C:118:ILE:HD11	1:C:168:PHE:CD2	2.55	0.41
1:F:106:ILE:O	1:F:113:THR:HA	2.20	0.41
1:G:230:ILE:HA	1:G:231:PRO:HD2	1.91	0.41
1:H:241:ASP:HB3	1:H:312:LEU:HD21	2.01	0.41
1:I:218:ASN:N	1:I:218:ASN:ND2	2.61	0.41
1:J:99:VAL:HG12	1:J:183:ARG:NH2	2.35	0.41
1:J:262:ASP:HA	1:J:291:TYR:O	2.20	0.41
1:F:325:ARG:NH1	1:L:144:ARG:HD3	2.33	0.41
1:L:183:ARG:N	3:L:404:HOH:O	2.46	0.41
1:L:39:TRP:CD1	1:L:39:TRP:N	2.86	0.41
1:N:208:LEU:HD21	1:N:342:VAL:CG1	2.50	0.41
1:N:9:MSE:CE	1:N:328:GLU:HB3	2.50	0.41
1:P:185:LEU:O	1:P:242:MSE:HE1	2.20	0.41
1:A:18:ILE:HB	1:A:28:ILE:HD12	2.02	0.41
1:A:255:THR:HG22	1:A:285:GLU:HB3	2.02	0.41
1:L:120:MSE:HG2	1:L:141:ILE:CD1	2.50	0.41
1:L:220:GLU:CG	3:L:393:HOH:O	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:TYR:HB2	1:A:308:VAL:HG11	2.02	0.41
1:C:183:ARG:O	1:C:183:ARG:CG	2.64	0.41
1:C:36:VAL:HG12	1:C:39:TRP:CZ3	2.55	0.41
1:C:81:LYS:HE2	1:C:142:GLU:HG2	2.01	0.41
1:D:195:LEU:HD12	1:D:195:LEU:HA	1.88	0.41
1:D:278:LEU:CD1	1:D:341:TYR:HA	2.50	0.41
1:E:259:CYS:HB3	1:E:312:LEU:HB3	2.03	0.41
1:H:9:MSE:SE	1:H:328:GLU:HB2	2.69	0.41
1:I:65:LEU:HD23	1:I:213:HIS:O	2.20	0.41
1:J:218:ASN:ND2	1:J:218:ASN:N	2.69	0.41
1:J:318:ASP:O	1:J:324:GLU:HA	2.20	0.41
1:K:180:ILE:HG23	1:K:180:ILE:O	2.20	0.41
1:K:183:ARG:CG	1:K:183:ARG:O	2.44	0.41
1:L:149:VAL:HG12	1:L:154:GLU:HB3	2.02	0.41
1:M:325:ARG:CZ	1:N:144:ARG:HD3	2.49	0.41
1:N:86:LEU:HD11	1:N:106:ILE:HD13	2.03	0.41
1:P:186:ASP:HB3	3:P:354:HOH:O	2.19	0.41
1:P:187:ASP:HA	1:P:242:MSE:CE	2.51	0.41
1:M:47:ASN:HB2	1:P:307:ASP:OD1	2.19	0.41
1:A:182:SER:HB3	1:A:185:LEU:HG	2.00	0.41
1:B:187:ASP:HA	1:B:242:MSE:CE	2.50	0.41
1:C:278:LEU:HD23	1:C:278:LEU:HA	1.90	0.41
1:D:144:ARG:HB3	3:D:356:HOH:O	2.21	0.41
1:I:239:ALA:O	1:I:312:LEU:HA	2.19	0.41
1:I:85:ARG:HD2	1:I:142:GLU:OE1	2.20	0.41
1:J:261:LYS:CB	1:J:266:PRO:HA	2.50	0.41
1:N:274:HIS:CG	1:N:347:ILE:HD11	2.55	0.41
1:N:88:LEU:HD12	1:N:141:ILE:HD11	2.01	0.41
1:O:108:THR:HG23	1:O:159:GLY:O	2.21	0.41
1:A:64:ARG:NH2	1:A:344:SER:O	2.46	0.41
1:A:22:SER:HB2	1:A:91:ILE:CG2	2.51	0.41
1:B:226:GLY:O	1:B:227:ASN:HB3	2.20	0.41
1:C:255:THR:HG22	1:C:285:GLU:CB	2.49	0.41
1:C:237:TYR:HB2	1:C:308:VAL:CG1	2.50	0.41
1:I:34:ASN:ND2	1:I:34:ASN:N	2.66	0.41
1:L:274:HIS:HE1	1:L:344:SER:OG	2.03	0.41
1:L:39:TRP:HA	1:L:202:GLN:HE22	1.85	0.41
1:N:118:ILE:HD11	1:N:168:PHE:CE2	2.56	0.41
1:N:141:ILE:O	1:N:141:ILE:HG13	2.20	0.41
1:N:218:ASN:HD22	1:N:218:ASN:N	2.15	0.41
1:B:175:THR:HG22	1:B:177:SER:N	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:317:ILE:HD11	1:C:320:SER:HB3	2.02	0.41
1:E:72:THR:HB	1:E:184:HIS:HE1	1.86	0.41
1:E:190:SER:HB3	1:E:240:VAL:HB	2.03	0.41
1:F:80:ILE:HG22	1:F:152:ALA:HA	2.02	0.41
1:G:52:ILE:C	1:G:53:LEU:HD12	2.41	0.41
1:H:27:LYS:HB3	1:H:27:LYS:HE2	1.61	0.41
1:I:40:ASN:ND2	1:I:202:GLN:HG3	2.35	0.41
1:L:64:ARG:HH22	1:L:344:SER:C	2.23	0.41
1:M:30:ASN:HD22	1:M:30:ASN:HA	1.71	0.41
1:N:208:LEU:HA	1:N:208:LEU:HD23	1.72	0.41
1:N:189:VAL:HB	1:N:242:MSE:HE1	2.02	0.41
1:A:85:ARG:NH2	1:A:144:ARG:HG3	2.36	0.41
1:A:63:HIS:CD2	1:A:233:GLU:HG3	2.56	0.41
1:E:284:ILE:HG12	3:E:364:HOH:O	2.21	0.41
1:G:198:ILE:H	1:G:198:ILE:HG12	1.67	0.41
1:J:88:LEU:HD11	1:J:143:VAL:CG2	2.51	0.41
1:K:108:THR:HG23	1:K:159:GLY:O	2.19	0.41
1:K:47:ASN:H	1:L:307:ASP:CG	2.23	0.41
1:K:86:LEU:HB2	1:K:143:VAL:HB	2.03	0.41
1:N:245:LEU:HG	1:N:251:SER:HA	2.02	0.41
1:O:108:THR:HG22	1:O:109:SER:N	2.36	0.41
1:O:45:ARG:HG3	1:O:51:LEU:CD2	2.49	0.41
1:P:86:LEU:CD1	1:P:86:LEU:N	2.83	0.41
1:B:47:ASN:HB2	1:C:307:ASP:CG	2.40	0.41
1:C:69:HIS:HE1	3:C:410:HOH:O	2.03	0.41
1:F:90:MSE:HG3	1:F:94:PHE:CE1	2.56	0.41
1:G:76:MSE:HG2	1:H:290:ILE:HD11	2.01	0.41
1:H:86:LEU:HB2	1:H:143:VAL:HB	2.03	0.41
1:M:12:ILE:HD13	1:M:189:VAL:HG22	2.03	0.41
1:N:149:VAL:HG11	1:N:155:VAL:HG22	2.01	0.41
1:P:304:ALA:N	3:P:392:HOH:O	2.53	0.41
1:B:309:LYS:HE3	3:B:405:HOH:O	2.19	0.41
1:F:285:GLU:HB2	1:F:333:HIS:CD2	2.56	0.41
1:G:230:ILE:O	1:G:231:PRO:O	2.39	0.41
1:G:255:THR:HG22	1:G:285:GLU:HB3	2.03	0.41
1:G:193:ILE:HG23	1:G:335:GLU:HG2	2.03	0.41
1:I:18:ILE:HB	1:I:28:ILE:HD12	2.03	0.41
1:O:145:ILE:HG13	1:O:145:ILE:H	1.63	0.41
1:P:230:ILE:HA	1:P:231:PRO:HD3	1.91	0.41
1:D:278:LEU:HD13	1:D:341:TYR:HA	2.03	0.41
1:D:337:LEU:HD23	1:D:337:LEU:HA	1.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:252:ASP:HA	3:H:386:HOH:O	2.21	0.41
1:G:78:LYS:HB2	1:H:290:ILE:HD12	2.02	0.41
1:O:85:ARG:HG2	1:O:142:GLU:CD	2.42	0.41
1:P:274:HIS:HB2	1:P:347:ILE:HD11	2.03	0.41
1:P:338:VAL:O	1:P:342:VAL:HB	2.21	0.41
1:B:47:ASN:HB2	1:C:307:ASP:OD1	2.21	0.41
1:D:96:TRP:O	1:D:97:ASN:C	2.59	0.41
1:E:150:PHE:N	1:E:154:GLU:OE2	2.54	0.41
1:E:208:LEU:CD2	1:E:343:MSE:HE2	2.50	0.41
1:J:197:LEU:HD13	1:J:338:VAL:CG2	2.51	0.41
1:J:347:ILE:HD12	1:J:347:ILE:H	1.86	0.41
1:J:52:ILE:C	1:J:53:LEU:HD12	2.42	0.41
1:K:65:LEU:HD23	1:K:66:LEU:N	2.36	0.41
1:M:248:GLY:HA3	1:M:251:SER:N	2.36	0.41
1:A:242:MSE:HG2	1:A:315:ALA:O	2.21	0.40
1:D:40:ASN:H	1:D:202:GLN:NE2	2.19	0.40
1:D:208:LEU:N	3:D:355:HOH:O	2.52	0.40
1:E:144:ARG:CD	3:E:356:HOH:O	2.69	0.40
1:G:209:PRO:HB2	1:G:210:TYR:CE1	2.55	0.40
1:G:72:THR:HB	1:G:186:ASP:OD2	2.21	0.40
1:M:260:ALA:HA	1:M:272:ARG:HD2	2.03	0.40
1:P:197:LEU:CD2	1:P:338:VAL:CG1	2.89	0.40
1:C:208:LEU:HD21	1:C:342:VAL:HG13	2.03	0.40
1:E:144:ARG:HD2	3:E:356:HOH:O	2.20	0.40
1:F:82:PRO:O	1:F:151:SER:HA	2.21	0.40
1:H:196:LYS:NZ	3:H:367:HOH:O	2.48	0.40
1:H:208:LEU:HD21	1:H:342:VAL:HG13	2.03	0.40
1:M:194:LEU:HA	1:M:194:LEU:HD23	1.84	0.40
1:M:338:VAL:O	1:M:342:VAL:HG23	2.21	0.40
1:P:63:HIS:ND1	1:P:213:HIS:HE1	2.19	0.40
1:P:274:HIS:HE1	1:P:344:SER:OG	2.04	0.40
1:P:63:HIS:CE1	1:P:233:GLU:CG	3.04	0.40
1:A:9:MSE:HE1	1:A:180:ILE:HB	1.80	0.40
1:A:189:VAL:O	1:A:193:ILE:HG12	2.21	0.40
1:A:220:GLU:C	1:A:220:GLU:CD	2.80	0.40
1:A:46:ASN:HB3	1:A:48:LYS:N	2.31	0.40
1:D:187:ASP:OD2	1:D:241:ASP:HA	2.21	0.40
1:D:187:ASP:H	1:D:242:MSE:HE2	1.86	0.40
1:J:187:ASP:O	1:J:191:VAL:HG23	2.20	0.40
1:K:190:SER:O	1:K:193:ILE:N	2.54	0.40
1:L:155:VAL:O	1:L:158:LEU:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:267:TYR:O	1:N:268:HIS:C	2.60	0.40
1:A:90:MSE:HG3	1:A:94:PHE:CZ	2.57	0.40
1:D:118:ILE:CD1	1:D:168:PHE:CE2	3.04	0.40
1:D:72:THR:CB	1:D:184:HIS:HE1	2.28	0.40
1:D:218:ASN:ND2	1:D:219:ASN:HD21	2.19	0.40
1:F:64:ARG:HD2	1:F:341:TYR:CZ	2.56	0.40
1:H:72:THR:HB	1:H:184:HIS:CD2	2.57	0.40
1:H:64:ARG:HD2	1:H:341:TYR:OH	2.19	0.40
1:J:144:ARG:HD2	3:J:356:HOH:O	2.22	0.40
1:J:280:LYS:HE2	1:J:286:TYR:OH	2.21	0.40
1:L:69:HIS:O	1:L:187:ASP:HB3	2.22	0.40
1:N:120:MSE:HA	3:N:391:HOH:O	2.21	0.40
1:N:230:ILE:HD13	1:N:230:ILE:N	2.35	0.40
1:O:186:ASP:HA	1:O:242:MSE:HE2	2.04	0.40
1:O:62:GLN:C	1:O:63:HIS:HD2	2.24	0.40
1:A:119:LEU:HD21	1:A:144:ARG:NH2	2.36	0.40
1:D:201:LEU:HD22	1:D:343:MSE:CE	2.52	0.40
1:D:32:ILE:HG23	1:D:195:LEU:HD21	2.03	0.40
1:L:40:ASN:HD22	1:L:202:GLN:HG3	1.86	0.40
1:L:96:TRP:O	1:L:99:VAL:HG22	2.22	0.40
1:M:185:LEU:HB2	1:M:324:GLU:OE1	2.22	0.40
1:N:187:ASP:HA	1:N:242:MSE:HE3	2.04	0.40
1:N:347:ILE:HA	1:N:347:ILE:HD12	1.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [\(i\)](#)

5.3.1 Protein backbone [\(i\)](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	303/349 (87%)	278 (92%)	21 (7%)	4 (1%)	12 18
1	B	302/349 (86%)	278 (92%)	19 (6%)	5 (2%)	9 13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	298/349 (85%)	274 (92%)	20 (7%)	4 (1%)	12	18
1	D	296/349 (85%)	268 (90%)	25 (8%)	3 (1%)	15	23
1	E	294/349 (84%)	273 (93%)	15 (5%)	6 (2%)	7	10
1	F	300/349 (86%)	271 (90%)	20 (7%)	9 (3%)	4	5
1	G	297/349 (85%)	276 (93%)	17 (6%)	4 (1%)	12	18
1	H	295/349 (84%)	276 (94%)	13 (4%)	6 (2%)	7	10
1	I	289/349 (83%)	268 (93%)	18 (6%)	3 (1%)	15	23
1	J	295/349 (84%)	273 (92%)	20 (7%)	2 (1%)	22	33
1	K	294/349 (84%)	267 (91%)	25 (8%)	2 (1%)	22	33
1	L	300/349 (86%)	269 (90%)	24 (8%)	7 (2%)	6	8
1	M	297/349 (85%)	271 (91%)	21 (7%)	5 (2%)	9	13
1	N	297/349 (85%)	276 (93%)	17 (6%)	4 (1%)	12	18
1	O	298/349 (85%)	270 (91%)	21 (7%)	7 (2%)	6	8
1	P	293/349 (84%)	269 (92%)	19 (6%)	5 (2%)	9	13
All	All	4748/5584 (85%)	4357 (92%)	315 (7%)	76 (2%)	9	14

All (76) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	228	SER
1	A	247	ASP
1	C	41	VAL
1	D	184	HIS
1	D	304	ALA
1	E	184	HIS
1	F	46	ASN
1	F	185	LEU
1	F	186	ASP
1	F	306	PHE
1	G	46	ASN
1	G	231	PRO
1	H	46	ASN
1	H	182	SER
1	H	186	ASP
1	H	187	ASP
1	J	187	ASP
1	K	177	SER

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Mol	Chain	Res	Type
1	K	184	HIS
1	L	187	ASP
1	L	229	ASN
1	M	232	GLU
1	N	184	HIS
1	N	229	ASN
1	O	183	ARG
1	O	185	LEU
1	O	187	ASP
1	P	182	SER
1	P	185	LEU
1	P	186	ASP
1	B	226	GLY
1	B	227	ASN
1	C	46	ASN
1	C	304	ALA
1	E	319	SER
1	F	109	SER
1	F	245	LEU
1	F	319	SER
1	G	185	LEU
1	G	204	GLU
1	H	183	ARG
1	H	328	GLU
1	I	5	THR
1	L	5	THR
1	L	98	SER
1	M	185	LEU
1	M	204	GLU
1	O	98	SER
1	O	201	LEU
1	P	245	LEU
1	A	292	PRO
1	A	304	ALA
1	B	184	HIS
1	C	322	ALA
1	D	98	SER
1	E	46	ASN
1	I	185	LEU
1	L	186	ASP
1	M	263	SER
1	N	4	HIS

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Mol	Chain	Res	Type
1	O	182	SER
1	O	304	ALA
1	B	305	GLY
1	E	148	ARG
1	E	323	PHE
1	F	304	ALA
1	I	148	ARG
1	L	140	ASN
1	L	184	HIS
1	J	203	ASP
1	M	187	ASP
1	N	97	ASN
1	P	177	SER
1	B	292	PRO
1	E	231	PRO
1	F	305	GLY

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	267/291 (92%)	225 (84%)	42 (16%)	2	2
1	B	266/291 (91%)	223 (84%)	43 (16%)	2	2
1	C	265/291 (91%)	233 (88%)	32 (12%)	5	6
1	D	263/291 (90%)	225 (86%)	38 (14%)	3	3
1	E	262/291 (90%)	227 (87%)	35 (13%)	4	5
1	F	266/291 (91%)	227 (85%)	39 (15%)	3	3
1	G	264/291 (91%)	231 (88%)	33 (12%)	4	6
1	H	262/291 (90%)	225 (86%)	37 (14%)	3	4
1	I	262/291 (90%)	231 (88%)	31 (12%)	5	7
1	J	262/291 (90%)	228 (87%)	34 (13%)	4	5
1	K	262/291 (90%)	226 (86%)	36 (14%)	3	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	265/291 (91%)	231 (87%)	34 (13%)	4	5
1	M	266/291 (91%)	229 (86%)	37 (14%)	3	4
1	N	264/291 (91%)	224 (85%)	40 (15%)	3	3
1	O	262/291 (90%)	223 (85%)	39 (15%)	3	3
1	P	260/291 (89%)	218 (84%)	42 (16%)	2	2
All	All	4218/4656 (91%)	3626 (86%)	592 (14%)	3	4

All (592) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	HIS
1	A	27	LYS
1	A	30	ASN
1	A	34	ASN
1	A	41	VAL
1	A	44	LYS
1	A	46	ASN
1	A	64	ARG
1	A	73	LEU
1	A	85	ARG
1	A	86	LEU
1	A	87	SER
1	A	95	ARG
1	A	97	ASN
1	A	108	THR
1	A	112	LYS
1	A	113	THR
1	A	142	GLU
1	A	145	ILE
1	A	147	GLU
1	A	158	LEU
1	A	180	ILE
1	A	185	LEU
1	A	187	ASP
1	A	195	LEU
1	A	218	ASN
1	A	219	ASN
1	A	220	GLU
1	A	230	ILE
1	A	237	TYR

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Mol	Chain	Res	Type
1	A	247	ASP
1	A	251	SER
1	A	253	GLU
1	A	269	TYR
1	A	272	ARG
1	A	287	LYS
1	A	308	VAL
1	A	312	LEU
1	A	319	SER
1	A	337	LEU
1	A	342	VAL
1	A	347	ILE
1	B	10	GLU
1	B	22	SER
1	B	27	LYS
1	B	28	ILE
1	B	42	GLU
1	B	44	LYS
1	B	45	ARG
1	B	48	LYS
1	B	56	LYS
1	B	65	LEU
1	B	78	LYS
1	B	85	ARG
1	B	86	LEU
1	B	95	ARG
1	B	100	GLU
1	B	108	THR
1	B	112	LYS
1	B	113	THR
1	B	141	ILE
1	B	142	GLU
1	B	145	ILE
1	B	148	ARG
1	B	158	LEU
1	B	169	ASP
1	B	173	GLN
1	B	182	SER
1	B	183	ARG
1	B	195	LEU
1	B	205	ASN
1	B	215	LEU

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Mol	Chain	Res	Type
1	B	218	ASN
1	B	229	ASN
1	B	230	ILE
1	B	237	TYR
1	B	245	LEU
1	B	263	SER
1	B	287	LYS
1	B	308	VAL
1	B	312	LEU
1	B	319	SER
1	B	338	VAL
1	B	342	VAL
1	B	347	ILE
1	C	4	HIS
1	C	45	ARG
1	C	46	ASN
1	C	51	LEU
1	C	56	LYS
1	C	64	ARG
1	C	70	VAL
1	C	86	LEU
1	C	97	ASN
1	C	112	LYS
1	C	141	ILE
1	C	145	ILE
1	C	147	GLU
1	C	148	ARG
1	C	153	ASP
1	C	158	LEU
1	C	180	ILE
1	C	183	ARG
1	C	195	LEU
1	C	199	LYS
1	C	217	SER
1	C	218	ASN
1	C	220	GLU
1	C	247	ASP
1	C	308	VAL
1	C	312	LEU
1	C	317	ILE
1	C	319	SER
1	C	323	PHE

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Mol	Chain	Res	Type
1	C	337	LEU
1	C	342	VAL
1	C	347	ILE
1	D	4	HIS
1	D	14	GLU
1	D	27	LYS
1	D	34	ASN
1	D	42	GLU
1	D	43	THR
1	D	44	LYS
1	D	46	ASN
1	D	48	LYS
1	D	52	ILE
1	D	64	ARG
1	D	65	LEU
1	D	73	LEU
1	D	86	LEU
1	D	91	ILE
1	D	109	SER
1	D	113	THR
1	D	148	ARG
1	D	157	GLU
1	D	158	LEU
1	D	176	GLU
1	D	183	ARG
1	D	184	HIS
1	D	187	ASP
1	D	195	LEU
1	D	199	LYS
1	D	217	SER
1	D	218	ASN
1	D	219	ASN
1	D	220	GLU
1	D	230	ILE
1	D	232	GLU
1	D	237	TYR
1	D	245	LEU
1	D	306	PHE
1	D	312	LEU
1	D	338	VAL
1	D	342	VAL
1	E	4	HIS

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Mol	Chain	Res	Type
1	E	27	LYS
1	E	51	LEU
1	E	58	LYS
1	E	64	ARG
1	E	65	LEU
1	E	78	LYS
1	E	86	LEU
1	E	97	ASN
1	E	108	THR
1	E	109	SER
1	E	113	THR
1	E	119	LEU
1	E	141	ILE
1	E	142	GLU
1	E	147	GLU
1	E	158	LEU
1	E	176	GLU
1	E	177	SER
1	E	195	LEU
1	E	204	GLU
1	E	217	SER
1	E	218	ASN
1	E	220	GLU
1	E	230	ILE
1	E	233	GLU
1	E	237	TYR
1	E	245	LEU
1	E	251	SER
1	E	277	GLU
1	E	293	TYR
1	E	312	LEU
1	E	320	SER
1	E	323	PHE
1	E	324	GLU
1	F	4	HIS
1	F	6	LYS
1	F	27	LYS
1	F	42	GLU
1	F	43	THR
1	F	45	ARG
1	F	46	ASN
1	F	52	ILE

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Mol	Chain	Res	Type
1	F	64	ARG
1	F	65	LEU
1	F	86	LEU
1	F	87	SER
1	F	97	ASN
1	F	112	LYS
1	F	140	ASN
1	F	146	ASP
1	F	157	GLU
1	F	158	LEU
1	F	176	GLU
1	F	183	ARG
1	F	188	LYS
1	F	195	LEU
1	F	215	LEU
1	F	217	SER
1	F	218	ASN
1	F	220	GLU
1	F	232	GLU
1	F	245	LEU
1	F	247	ASP
1	F	269	TYR
1	F	272	ARG
1	F	285	GLU
1	F	310	HIS
1	F	312	LEU
1	F	313	ILE
1	F	319	SER
1	F	323	PHE
1	F	337	LEU
1	F	347	ILE
1	G	6	LYS
1	G	7	GLU
1	G	45	ARG
1	G	46	ASN
1	G	48	LYS
1	G	58	LYS
1	G	64	ARG
1	G	86	LEU
1	G	97	ASN
1	G	108	THR
1	G	119	LEU

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Mol	Chain	Res	Type
1	G	120	MSE
1	G	141	ILE
1	G	147	GLU
1	G	148	ARG
1	G	158	LEU
1	G	180	ILE
1	G	183	ARG
1	G	195	LEU
1	G	204	GLU
1	G	206	VAL
1	G	218	ASN
1	G	230	ILE
1	G	237	TYR
1	G	257	SER
1	G	287	LYS
1	G	312	LEU
1	G	317	ILE
1	G	320	SER
1	G	323	PHE
1	G	337	LEU
1	G	345	ASN
1	G	347	ILE
1	H	3	HIS
1	H	6	LYS
1	H	27	LYS
1	H	28	ILE
1	H	40	ASN
1	H	41	VAL
1	H	43	THR
1	H	44	LYS
1	H	46	ASN
1	H	48	LYS
1	H	65	LEU
1	H	70	VAL
1	H	78	LYS
1	H	86	LEU
1	H	87	SER
1	H	109	SER
1	H	113	THR
1	H	144	ARG
1	H	150	PHE
1	H	151	SER

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Mol	Chain	Res	Type
1	H	158	LEU
1	H	176	GLU
1	H	187	ASP
1	H	195	LEU
1	H	218	ASN
1	H	263	SER
1	H	272	ARG
1	H	285	GLU
1	H	306	PHE
1	H	308	VAL
1	H	310	HIS
1	H	312	LEU
1	H	317	ILE
1	H	323	PHE
1	H	324	GLU
1	H	342	VAL
1	H	347	ILE
1	I	34	ASN
1	I	41	VAL
1	I	46	ASN
1	I	65	LEU
1	I	70	VAL
1	I	85	ARG
1	I	86	LEU
1	I	97	ASN
1	I	109	SER
1	I	120	MSE
1	I	147	GLU
1	I	158	LEU
1	I	172	VAL
1	I	176	GLU
1	I	180	ILE
1	I	195	LEU
1	I	217	SER
1	I	218	ASN
1	I	230	ILE
1	I	237	TYR
1	I	269	TYR
1	I	277	GLU
1	I	282	ASN
1	I	287	LYS
1	I	312	LEU

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Mol	Chain	Res	Type
1	I	313	ILE
1	I	317	ILE
1	I	319	SER
1	I	323	PHE
1	I	337	LEU
1	I	347	ILE
1	J	27	LYS
1	J	40	ASN
1	J	45	ARG
1	J	64	ARG
1	J	86	LEU
1	J	95	ARG
1	J	97	ASN
1	J	109	SER
1	J	119	LEU
1	J	141	ILE
1	J	148	ARG
1	J	158	LEU
1	J	176	GLU
1	J	177	SER
1	J	180	ILE
1	J	183	ARG
1	J	187	ASP
1	J	195	LEU
1	J	197	LEU
1	J	202	GLN
1	J	206	VAL
1	J	212	THR
1	J	218	ASN
1	J	230	ILE
1	J	237	TYR
1	J	272	ARG
1	J	287	LYS
1	J	312	LEU
1	J	317	ILE
1	J	319	SER
1	J	323	PHE
1	J	330	SER
1	J	337	LEU
1	J	347	ILE
1	K	3	HIS
1	K	27	LYS

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Mol	Chain	Res	Type
1	K	28	ILE
1	K	33	GLU
1	K	34	ASN
1	K	38	GLU
1	K	40	ASN
1	K	42	GLU
1	K	58	LYS
1	K	78	LYS
1	K	86	LEU
1	K	87	SER
1	K	97	ASN
1	K	112	LYS
1	K	153	ASP
1	K	157	GLU
1	K	158	LEU
1	K	175	THR
1	K	176	GLU
1	K	177	SER
1	K	183	ARG
1	K	195	LEU
1	K	205	ASN
1	K	206	VAL
1	K	207	THR
1	K	217	SER
1	K	218	ASN
1	K	263	SER
1	K	264	SER
1	K	272	ARG
1	K	308	VAL
1	K	310	HIS
1	K	312	LEU
1	K	319	SER
1	K	328	GLU
1	K	342	VAL
1	L	4	HIS
1	L	5	THR
1	L	28	ILE
1	L	30	ASN
1	L	38	GLU
1	L	43	THR
1	L	46	ASN
1	L	48	LYS

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Mol	Chain	Res	Type
1	L	56	LYS
1	L	65	LEU
1	L	78	LYS
1	L	86	LEU
1	L	97	ASN
1	L	106	ILE
1	L	112	LYS
1	L	158	LEU
1	L	169	ASP
1	L	176	GLU
1	L	186	ASP
1	L	217	SER
1	L	218	ASN
1	L	220	GLU
1	L	229	ASN
1	L	237	TYR
1	L	245	LEU
1	L	269	TYR
1	L	282	ASN
1	L	285	GLU
1	L	312	LEU
1	L	313	ILE
1	L	317	ILE
1	L	337	LEU
1	L	342	VAL
1	L	347	ILE
1	M	10	GLU
1	M	27	LYS
1	M	58	LYS
1	M	65	LEU
1	M	66	LEU
1	M	70	VAL
1	M	72	THR
1	M	86	LEU
1	M	112	LYS
1	M	119	LEU
1	M	120	MSE
1	M	142	GLU
1	M	147	GLU
1	M	157	GLU
1	M	158	LEU
1	M	171	ARG

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Mol	Chain	Res	Type
1	M	181	LYS
1	M	183	ARG
1	M	187	ASP
1	M	195	LEU
1	M	204	GLU
1	M	205	ASN
1	M	206	VAL
1	M	215	LEU
1	M	218	ASN
1	M	229	ASN
1	M	232	GLU
1	M	237	TYR
1	M	245	LEU
1	M	257	SER
1	M	287	LYS
1	M	293	TYR
1	M	312	LEU
1	M	317	ILE
1	M	324	GLU
1	M	330	SER
1	M	337	LEU
1	N	3	HIS
1	N	6	LYS
1	N	16	VAL
1	N	27	LYS
1	N	29	ILE
1	N	41	VAL
1	N	44	LYS
1	N	46	ASN
1	N	47	ASN
1	N	48	LYS
1	N	52	ILE
1	N	56	LYS
1	N	97	ASN
1	N	100	GLU
1	N	102	GLU
1	N	108	THR
1	N	109	SER
1	N	113	THR
1	N	120	MSE
1	N	141	ILE
1	N	145	ILE

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Mol	Chain	Res	Type
1	N	147	GLU
1	N	156	ARG
1	N	158	LEU
1	N	173	GLN
1	N	182	SER
1	N	183	ARG
1	N	190	SER
1	N	195	LEU
1	N	206	VAL
1	N	218	ASN
1	N	219	ASN
1	N	220	GLU
1	N	245	LEU
1	N	293	TYR
1	N	312	LEU
1	N	319	SER
1	N	328	GLU
1	N	342	VAL
1	N	347	ILE
1	O	13	LYS
1	O	18	ILE
1	O	29	ILE
1	O	41	VAL
1	O	43	THR
1	O	45	ARG
1	O	46	ASN
1	O	56	LYS
1	O	58	LYS
1	O	67	THR
1	O	80	ILE
1	O	85	ARG
1	O	86	LEU
1	O	87	SER
1	O	89	SER
1	O	109	SER
1	O	112	LYS
1	O	141	ILE
1	O	148	ARG
1	O	158	LEU
1	O	183	ARG
1	O	195	LEU
1	O	200	ARG

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Mol	Chain	Res	Type
1	O	202	GLN
1	O	207	THR
1	O	215	LEU
1	O	218	ASN
1	O	230	ILE
1	O	237	TYR
1	O	240	VAL
1	O	245	LEU
1	O	269	TYR
1	O	272	ARG
1	O	312	LEU
1	O	320	SER
1	O	323	PHE
1	O	328	GLU
1	O	337	LEU
1	O	342	VAL
1	P	5	THR
1	P	6	LYS
1	P	27	LYS
1	P	28	ILE
1	P	37	SER
1	P	40	ASN
1	P	42	GLU
1	P	45	ARG
1	P	46	ASN
1	P	64	ARG
1	P	65	LEU
1	P	70	VAL
1	P	73	LEU
1	P	86	LEU
1	P	87	SER
1	P	91	ILE
1	P	113	THR
1	P	117	THR
1	P	148	ARG
1	P	157	GLU
1	P	158	LEU
1	P	183	ARG
1	P	186	ASP
1	P	187	ASP
1	P	195	LEU
1	P	207	THR

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Mol	Chain	Res	Type
1	P	215	LEU
1	P	218	ASN
1	P	219	ASN
1	P	220	GLU
1	P	230	ILE
1	P	245	LEU
1	P	247	ASP
1	P	256	VAL
1	P	263	SER
1	P	272	ARG
1	P	285	GLU
1	P	312	LEU
1	P	317	ILE
1	P	337	LEU
1	P	342	VAL
1	P	347	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (127) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	HIS
1	A	30	ASN
1	A	40	ASN
1	A	46	ASN
1	A	69	HIS
1	A	97	ASN
1	A	202	GLN
1	A	218	ASN
1	A	219	ASN
1	A	227	ASN
1	B	47	ASN
1	B	69	HIS
1	B	184	HIS
1	B	202	GLN
1	B	218	ASN
1	B	229	ASN
1	B	274	HIS
1	B	310	HIS
1	C	4	HIS
1	C	30	ASN
1	C	34	ASN
1	C	46	ASN

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Mol	Chain	Res	Type
1	C	69	HIS
1	C	97	ASN
1	C	202	GLN
1	C	218	ASN
1	D	34	ASN
1	D	46	ASN
1	D	62	GLN
1	D	97	ASN
1	D	184	HIS
1	D	202	GLN
1	D	218	ASN
1	D	219	ASN
1	E	40	ASN
1	E	47	ASN
1	E	62	GLN
1	E	69	HIS
1	E	173	GLN
1	E	202	GLN
1	E	218	ASN
1	F	46	ASN
1	F	69	HIS
1	F	140	ASN
1	F	173	GLN
1	F	202	GLN
1	F	218	ASN
1	F	310	HIS
1	G	40	ASN
1	G	46	ASN
1	G	62	GLN
1	G	97	ASN
1	G	173	GLN
1	G	202	GLN
1	G	218	ASN
1	G	274	HIS
1	G	345	ASN
1	H	40	ASN
1	H	46	ASN
1	H	47	ASN
1	H	69	HIS
1	H	173	GLN
1	H	184	HIS
1	H	202	GLN

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Mol	Chain	Res	Type
1	H	218	ASN
1	H	274	HIS
1	I	34	ASN
1	I	40	ASN
1	I	46	ASN
1	I	62	GLN
1	I	218	ASN
1	I	274	HIS
1	I	282	ASN
1	J	40	ASN
1	J	46	ASN
1	J	62	GLN
1	J	97	ASN
1	J	173	GLN
1	J	202	GLN
1	J	205	ASN
1	J	218	ASN
1	J	274	HIS
1	K	4	HIS
1	K	40	ASN
1	K	47	ASN
1	K	69	HIS
1	K	184	HIS
1	K	202	GLN
1	K	218	ASN
1	L	40	ASN
1	L	62	GLN
1	L	69	HIS
1	L	140	ASN
1	L	173	GLN
1	L	202	GLN
1	L	205	ASN
1	L	218	ASN
1	L	219	ASN
1	L	274	HIS
1	L	282	ASN
1	L	333	HIS
1	M	30	ASN
1	M	69	HIS
1	M	173	GLN
1	M	218	ASN
1	M	229	ASN

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Mol	Chain	Res	Type
1	M	268	HIS
1	N	3	HIS
1	N	30	ASN
1	N	46	ASN
1	N	69	HIS
1	N	184	HIS
1	N	202	GLN
1	N	218	ASN
1	N	229	ASN
1	N	274	HIS
1	O	173	GLN
1	O	218	ASN
1	O	274	HIS
1	P	40	ASN
1	P	46	ASN
1	P	69	HIS
1	P	97	ASN
1	P	202	GLN
1	P	213	HIS
1	P	218	ASN
1	P	274	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

16 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	D	350	-	4,4,4	0.16	0	6,6,6	0.54	0
2	SO4	N	350	-	4,4,4	0.15	0	6,6,6	0.84	0
2	SO4	H	350	-	4,4,4	0.16	0	6,6,6	0.48	0
2	SO4	B	350	-	4,4,4	0.22	0	6,6,6	0.51	0
2	SO4	L	350	-	4,4,4	0.19	0	6,6,6	0.40	0
2	SO4	A	350	-	4,4,4	0.23	0	6,6,6	0.54	0
2	SO4	C	350	-	4,4,4	0.10	0	6,6,6	0.53	0
2	SO4	P	350	-	4,4,4	0.15	0	6,6,6	0.33	0
2	SO4	E	350	-	4,4,4	0.20	0	6,6,6	0.10	0
2	SO4	J	350	-	4,4,4	0.15	0	6,6,6	0.10	0
2	SO4	G	350	-	4,4,4	0.16	0	6,6,6	0.11	0
2	SO4	I	350	-	4,4,4	0.14	0	6,6,6	0.41	0
2	SO4	K	350	-	4,4,4	0.17	0	6,6,6	0.33	0
2	SO4	M	350	-	4,4,4	0.12	0	6,6,6	0.15	0
2	SO4	O	350	-	4,4,4	0.12	0	6,6,6	0.38	0
2	SO4	F	350	-	4,4,4	0.12	0	6,6,6	0.30	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	A	307/349 (87%)	0.14	4 (1%) 77 75	47, 57, 85, 106	0
1	B	306/349 (87%)	0.06	3 (0%) 82 81	51, 60, 88, 111	0
1	C	302/349 (86%)	0.04	1 (0%) 94 95	45, 55, 79, 93	0
1	D	300/349 (85%)	0.09	4 (1%) 77 75	39, 53, 71, 91	0
1	E	300/349 (85%)	0.05	3 (1%) 82 81	39, 55, 74, 87	0
1	F	304/349 (87%)	0.11	3 (0%) 82 81	48, 57, 80, 98	0
1	G	303/349 (86%)	0.12	3 (0%) 82 81	40, 54, 72, 98	0
1	H	299/349 (85%)	0.00	3 (1%) 82 81	47, 56, 77, 91	0
1	I	293/349 (83%)	0.12	5 (1%) 70 67	42, 53, 67, 78	0
1	J	301/349 (86%)	0.20	3 (0%) 82 81	43, 59, 75, 86	0
1	K	298/349 (85%)	0.13	1 (0%) 94 95	45, 56, 78, 97	0
1	L	304/349 (87%)	0.28	10 (3%) 46 43	45, 56, 75, 88	0
1	M	303/349 (86%)	0.11	4 (1%) 77 75	27, 41, 63, 83	0
1	N	301/349 (86%)	0.16	8 (2%) 54 50	35, 44, 68, 81	0
1	O	302/349 (86%)	0.18	6 (1%) 65 60	15, 33, 54, 67	0
1	P	299/349 (85%)	0.07	4 (1%) 77 75	27, 38, 61, 75	0
All	All	4822/5584 (86%)	0.12	65 (1%) 77 75	15, 54, 75, 111	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	94	PHE	3.9
1	O	321	HIS	3.9
1	F	317	ILE	3.7
1	O	44	LYS	3.7
1	H	96	TRP	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	306	PHE	3.3
1	G	306	PHE	3.3
1	A	306	PHE	3.3
1	D	293	TYR	3.2
1	L	293	TYR	3.1
1	N	96	TRP	3.1
1	H	320	SER	3.0
1	J	96	TRP	3.0
1	O	96	TRP	2.9
1	N	230	ILE	2.8
1	L	203	ASP	2.8
1	G	230	ILE	2.8
1	N	322	ALA	2.8
1	K	183	ARG	2.7
1	I	245	LEU	2.7
1	O	306	PHE	2.7
1	E	32	ILE	2.7
1	F	320	SER	2.6
1	A	230	ILE	2.6
1	J	183	ARG	2.6
1	L	245	LEU	2.6
1	O	158	LEU	2.6
1	N	306	PHE	2.6
1	P	246	GLY	2.6
1	L	244	ALA	2.5
1	L	160	ILE	2.5
1	M	208	LEU	2.5
1	I	321	HIS	2.5
1	M	42	GLU	2.5
1	C	95	ARG	2.5
1	E	251	SER	2.4
1	A	229	ASN	2.4
1	L	68	ALA	2.4
1	N	323	PHE	2.4
1	P	243	GLY	2.4
1	M	244	ALA	2.4
1	P	306	PHE	2.4
1	A	293	TYR	2.4
1	N	97	ASN	2.3
1	I	168	PHE	2.3
1	P	96	TRP	2.3
1	B	227	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	106	ILE	2.3
1	B	320	SER	2.3
1	I	306	PHE	2.3
1	M	95	ARG	2.3
1	F	141	ILE	2.2
1	L	67	THR	2.2
1	H	94	PHE	2.2
1	G	310	HIS	2.2
1	L	237	TYR	2.1
1	D	243	GLY	2.1
1	N	95	ARG	2.1
1	O	320	SER	2.1
1	L	49	GLY	2.1
1	I	244	ALA	2.1
1	D	96	TRP	2.1
1	N	320	SER	2.1
1	B	95	ARG	2.0
1	L	119	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SO4	E	350	5/5	0.83	0.24	128,129,129,129	0
2	SO4	J	350	5/5	0.90	0.52	145,145,145,146	0
2	SO4	G	350	5/5	0.90	0.30	124,125,125,126	0
2	SO4	O	350	5/5	0.94	0.23	74,75,77,78	0
2	SO4	A	350	5/5	0.96	0.16	58,59,60,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	SO4	D	350	5/5	0.96	0.21	75,78,80,80	0
2	SO4	N	350	5/5	0.96	0.13	53,54,56,57	0
2	SO4	H	350	5/5	0.96	0.19	69,69,71,72	0
2	SO4	I	350	5/5	0.96	0.14	86,87,89,90	0
2	SO4	B	350	5/5	0.96	0.15	54,56,58,59	0
2	SO4	K	350	5/5	0.97	0.14	63,64,64,65	0
2	SO4	M	350	5/5	0.97	0.20	130,130,131,131	0
2	SO4	L	350	5/5	0.97	0.14	75,76,77,78	0
2	SO4	F	350	5/5	0.97	0.18	69,70,71,73	0
2	SO4	C	350	5/5	0.98	0.11	50,50,52,54	0
2	SO4	P	350	5/5	0.98	0.24	67,68,70,70	0

6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.