Full wwPDB X-ray Structure Validation Report (i)

Mar 10, 2024 – 05:51 AM EDT

PDB ID	:	3WST
Title	:	Crystal structure of C.elegans PRMT7 in complex with SAH(P31)
Authors	:	Hasegawa, M.; Toma-fukai, S.; Shimizu, T.
Deposited on	:	2014-03-21
Resolution	:	2.39 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

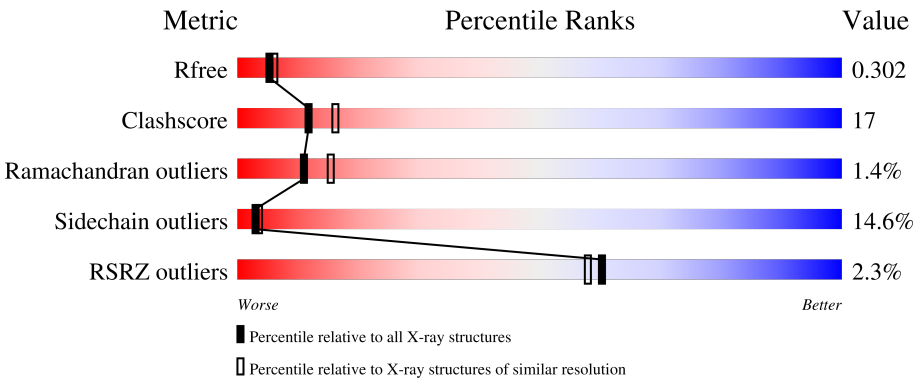
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.39 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	655	69% 23% 6% •
1	B	655	% 61% 29% 8% •
1	C	655	63% 30% • •
1	D	655	69% 24% • •
1	E	655	% 62% 27% 7% •

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Mol	Chain	Length	Quality of chain
1	F	655	2% 62% 28% 7%
1	G	655	2% 63% 29% 6%
1	H	655	65% 28%
1	I	655	% 63% 28% 7%
1	J	655	% 59% 32% 6%
1	K	655	% 53% 37% 8%
1	L	655	68% 25% 6%
1	M	655	5% 52% 36% 9%
1	N	655	% 54% 36% 7%
1	O	655	6% 53% 36% 7%
1	P	655	4% 61% 30% 6%
1	Q	655	7% 52% 36% 8%
1	R	655	9% 55% 35% 8%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 92645 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 Protein arginine N-methyltransferase 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	641	5106	3247	857	975	27	0	0	0
1	D	637	5078	3231	852	968	27	0	0	0
1	B	638	5084	3234	853	970	27	0	0	0
1	C	639	5091	3239	854	971	27	0	0	0
1	F	638	5084	3234	853	970	27	0	0	0
1	E	636	5069	3226	850	966	27	0	0	0
1	G	636	5070	3227	850	966	27	0	0	0
1	H	639	5091	3239	854	971	27	0	0	0
1	I	644	5122	3257	860	978	27	0	0	0
1	M	633	5049	3216	844	962	27	0	0	0
1	N	638	5084	3234	853	970	27	0	0	0
1	O	641	5106	3247	857	975	27	0	0	0
1	P	636	5069	3226	850	966	27	0	0	0
1	Q	632	5039	3209	845	958	27	0	0	0
1	R	638	5084	3234	853	970	27	0	0	0
1	J	644	5122	3257	860	978	27	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	K	641	5106	3247	857	975	27	0	0	0
			Total	C	N	O	S			
1	L	644	5122	3257	860	978	27	0	0	0

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	GLY	-	expression tag	UNP Q9XW42
A	-6	PRO	-	expression tag	UNP Q9XW42
A	-5	LEU	-	expression tag	UNP Q9XW42
A	-4	GLY	-	expression tag	UNP Q9XW42
A	-3	SER	-	expression tag	UNP Q9XW42
A	-2	GLY	-	expression tag	UNP Q9XW42
A	-1	ILE	-	expression tag	UNP Q9XW42
A	0	PRO	-	expression tag	UNP Q9XW42
D	-7	GLY	-	expression tag	UNP Q9XW42
D	-6	PRO	-	expression tag	UNP Q9XW42
D	-5	LEU	-	expression tag	UNP Q9XW42
D	-4	GLY	-	expression tag	UNP Q9XW42
D	-3	SER	-	expression tag	UNP Q9XW42
D	-2	GLY	-	expression tag	UNP Q9XW42
D	-1	ILE	-	expression tag	UNP Q9XW42
D	0	PRO	-	expression tag	UNP Q9XW42
B	-7	GLY	-	expression tag	UNP Q9XW42
B	-6	PRO	-	expression tag	UNP Q9XW42
B	-5	LEU	-	expression tag	UNP Q9XW42
B	-4	GLY	-	expression tag	UNP Q9XW42
B	-3	SER	-	expression tag	UNP Q9XW42
B	-2	GLY	-	expression tag	UNP Q9XW42
B	-1	ILE	-	expression tag	UNP Q9XW42
B	0	PRO	-	expression tag	UNP Q9XW42
C	-7	GLY	-	expression tag	UNP Q9XW42
C	-6	PRO	-	expression tag	UNP Q9XW42
C	-5	LEU	-	expression tag	UNP Q9XW42
C	-4	GLY	-	expression tag	UNP Q9XW42
C	-3	SER	-	expression tag	UNP Q9XW42
C	-2	GLY	-	expression tag	UNP Q9XW42
C	-1	ILE	-	expression tag	UNP Q9XW42
C	0	PRO	-	expression tag	UNP Q9XW42
F	-7	GLY	-	expression tag	UNP Q9XW42
F	-6	PRO	-	expression tag	UNP Q9XW42

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-5	LEU	-	expression tag	UNP Q9XW42
F	-4	GLY	-	expression tag	UNP Q9XW42
F	-3	SER	-	expression tag	UNP Q9XW42
F	-2	GLY	-	expression tag	UNP Q9XW42
F	-1	ILE	-	expression tag	UNP Q9XW42
F	0	PRO	-	expression tag	UNP Q9XW42
E	-7	GLY	-	expression tag	UNP Q9XW42
E	-6	PRO	-	expression tag	UNP Q9XW42
E	-5	LEU	-	expression tag	UNP Q9XW42
E	-4	GLY	-	expression tag	UNP Q9XW42
E	-3	SER	-	expression tag	UNP Q9XW42
E	-2	GLY	-	expression tag	UNP Q9XW42
E	-1	ILE	-	expression tag	UNP Q9XW42
E	0	PRO	-	expression tag	UNP Q9XW42
G	-7	GLY	-	expression tag	UNP Q9XW42
G	-6	PRO	-	expression tag	UNP Q9XW42
G	-5	LEU	-	expression tag	UNP Q9XW42
G	-4	GLY	-	expression tag	UNP Q9XW42
G	-3	SER	-	expression tag	UNP Q9XW42
G	-2	GLY	-	expression tag	UNP Q9XW42
G	-1	ILE	-	expression tag	UNP Q9XW42
G	0	PRO	-	expression tag	UNP Q9XW42
H	-7	GLY	-	expression tag	UNP Q9XW42
H	-6	PRO	-	expression tag	UNP Q9XW42
H	-5	LEU	-	expression tag	UNP Q9XW42
H	-4	GLY	-	expression tag	UNP Q9XW42
H	-3	SER	-	expression tag	UNP Q9XW42
H	-2	GLY	-	expression tag	UNP Q9XW42
H	-1	ILE	-	expression tag	UNP Q9XW42
H	0	PRO	-	expression tag	UNP Q9XW42
I	-7	GLY	-	expression tag	UNP Q9XW42
I	-6	PRO	-	expression tag	UNP Q9XW42
I	-5	LEU	-	expression tag	UNP Q9XW42
I	-4	GLY	-	expression tag	UNP Q9XW42
I	-3	SER	-	expression tag	UNP Q9XW42
I	-2	GLY	-	expression tag	UNP Q9XW42
I	-1	ILE	-	expression tag	UNP Q9XW42
I	0	PRO	-	expression tag	UNP Q9XW42
M	-7	GLY	-	expression tag	UNP Q9XW42
M	-6	PRO	-	expression tag	UNP Q9XW42
M	-5	LEU	-	expression tag	UNP Q9XW42
M	-4	GLY	-	expression tag	UNP Q9XW42

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Chain	Residue	Modelled	Actual	Comment	Reference
M	-3	SER	-	expression tag	UNP Q9XW42
M	-2	GLY	-	expression tag	UNP Q9XW42
M	-1	ILE	-	expression tag	UNP Q9XW42
M	0	PRO	-	expression tag	UNP Q9XW42
N	-7	GLY	-	expression tag	UNP Q9XW42
N	-6	PRO	-	expression tag	UNP Q9XW42
N	-5	LEU	-	expression tag	UNP Q9XW42
N	-4	GLY	-	expression tag	UNP Q9XW42
N	-3	SER	-	expression tag	UNP Q9XW42
N	-2	GLY	-	expression tag	UNP Q9XW42
N	-1	ILE	-	expression tag	UNP Q9XW42
N	0	PRO	-	expression tag	UNP Q9XW42
O	-7	GLY	-	expression tag	UNP Q9XW42
O	-6	PRO	-	expression tag	UNP Q9XW42
O	-5	LEU	-	expression tag	UNP Q9XW42
O	-4	GLY	-	expression tag	UNP Q9XW42
O	-3	SER	-	expression tag	UNP Q9XW42
O	-2	GLY	-	expression tag	UNP Q9XW42
O	-1	ILE	-	expression tag	UNP Q9XW42
O	0	PRO	-	expression tag	UNP Q9XW42
P	-7	GLY	-	expression tag	UNP Q9XW42
P	-6	PRO	-	expression tag	UNP Q9XW42
P	-5	LEU	-	expression tag	UNP Q9XW42
P	-4	GLY	-	expression tag	UNP Q9XW42
P	-3	SER	-	expression tag	UNP Q9XW42
P	-2	GLY	-	expression tag	UNP Q9XW42
P	-1	ILE	-	expression tag	UNP Q9XW42
P	0	PRO	-	expression tag	UNP Q9XW42
Q	-7	GLY	-	expression tag	UNP Q9XW42
Q	-6	PRO	-	expression tag	UNP Q9XW42
Q	-5	LEU	-	expression tag	UNP Q9XW42
Q	-4	GLY	-	expression tag	UNP Q9XW42
Q	-3	SER	-	expression tag	UNP Q9XW42
Q	-2	GLY	-	expression tag	UNP Q9XW42
Q	-1	ILE	-	expression tag	UNP Q9XW42
Q	0	PRO	-	expression tag	UNP Q9XW42
R	-7	GLY	-	expression tag	UNP Q9XW42
R	-6	PRO	-	expression tag	UNP Q9XW42
R	-5	LEU	-	expression tag	UNP Q9XW42
R	-4	GLY	-	expression tag	UNP Q9XW42
R	-3	SER	-	expression tag	UNP Q9XW42
R	-2	GLY	-	expression tag	UNP Q9XW42

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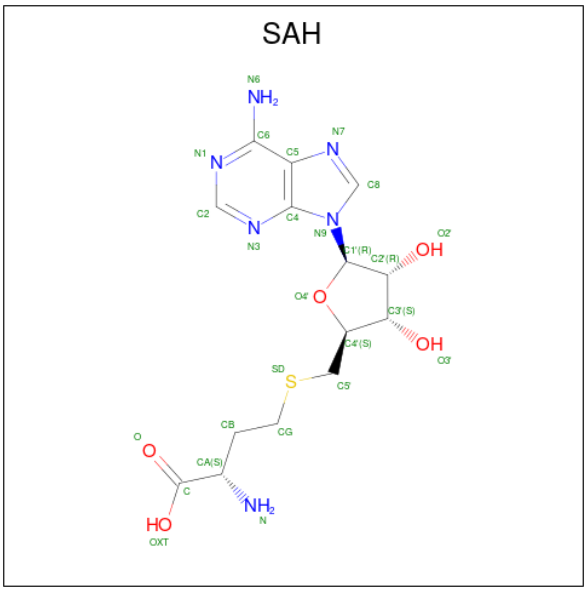
Chain	Residue	Modelled	Actual	Comment	Reference
R	-1	ILE	-	expression tag	UNP Q9XW42
R	0	PRO	-	expression tag	UNP Q9XW42
J	-7	GLY	-	expression tag	UNP Q9XW42
J	-6	PRO	-	expression tag	UNP Q9XW42
J	-5	LEU	-	expression tag	UNP Q9XW42
J	-4	GLY	-	expression tag	UNP Q9XW42
J	-3	SER	-	expression tag	UNP Q9XW42
J	-2	GLY	-	expression tag	UNP Q9XW42
J	-1	ILE	-	expression tag	UNP Q9XW42
J	0	PRO	-	expression tag	UNP Q9XW42
K	-7	GLY	-	expression tag	UNP Q9XW42
K	-6	PRO	-	expression tag	UNP Q9XW42
K	-5	LEU	-	expression tag	UNP Q9XW42
K	-4	GLY	-	expression tag	UNP Q9XW42
K	-3	SER	-	expression tag	UNP Q9XW42
K	-2	GLY	-	expression tag	UNP Q9XW42
K	-1	ILE	-	expression tag	UNP Q9XW42
K	0	PRO	-	expression tag	UNP Q9XW42
L	-7	GLY	-	expression tag	UNP Q9XW42
L	-6	PRO	-	expression tag	UNP Q9XW42
L	-5	LEU	-	expression tag	UNP Q9XW42
L	-4	GLY	-	expression tag	UNP Q9XW42
L	-3	SER	-	expression tag	UNP Q9XW42
L	-2	GLY	-	expression tag	UNP Q9XW42
L	-1	ILE	-	expression tag	UNP Q9XW42
L	0	PRO	-	expression tag	UNP Q9XW42

- Molecule 2 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: $C_{14}H_{20}N_6O_5S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
2	A	1	26	14	6	5	1	0	0
2	D	1	26	14	6	5	1	0	0
2	B	1	26	14	6	5	1	0	0
2	C	1	26	14	6	5	1	0	0
2	F	1	26	14	6	5	1	0	0
2	E	1	26	14	6	5	1	0	0
2	G	1	26	14	6	5	1	0	0
2	H	1	26	14	6	5	1	0	0
2	I	1	26	14	6	5	1	0	0
2	M	1	26	14	6	5	1	0	0
2	N	1	26	14	6	5	1	0	0
2	O	1	26	14	6	5	1	0	0
2	P	1	26	14	6	5	1	0	0
2	Q	1	26	14	6	5	1	0	0

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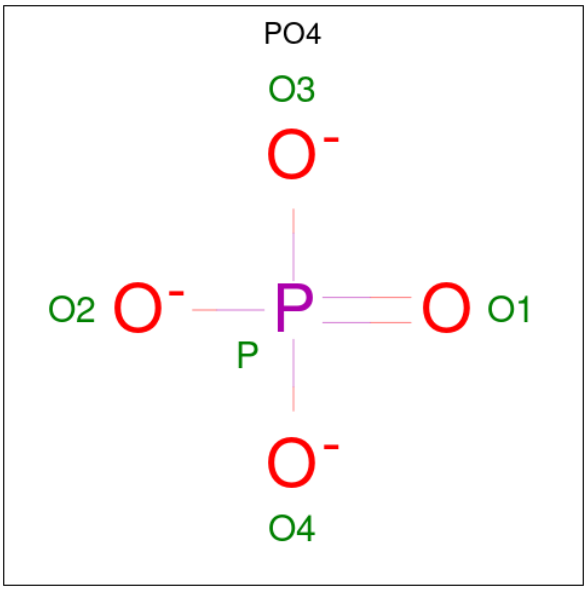
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
2	R	1	26	14	6	5	1	0	0
			Total	C	N	O	S		
2	J	1	26	14	6	5	1	0	0
			Total	C	N	O	S		
2	K	1	26	14	6	5	1	0	0
			Total	C	N	O	S		
2	L	1	26	14	6	5	1	0	0

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	P		
3	A	1	5	4	1	0	0
			Total	O	P		
3	D	1	5	4	1	0	0
			Total	O	P		
3	B	1	5	4	1	0	0
			Total	O	P		
3	C	1	5	4	1	0	0
			Total	O	P		
3	F	1	5	4	1	0	0
			Total	O	P		
3	E	1	5	4	1	0	0
			Total	O	P		
3	G	1	5	4	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	P		
3	H	1	5	4	1	0	0
3	I	1	5	4	1	0	0
3	M	1	5	4	1	0	0
3	N	1	5	4	1	0	0
3	O	1	5	4	1	0	0
3	P	1	5	4	1	0	0
3	Q	1	5	4	1	0	0
3	R	1	5	4	1	0	0
3	J	1	5	4	1	0	0
3	K	1	5	4	1	0	0
3	L	1	5	4	1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	105	105	105	0	0
4	D	93	93	93	0	0
4	B	26	26	26	0	0
4	C	16	16	16	0	0
4	F	12	12	12	0	0
4	E	41	41	41	0	0
4	G	19	19	19	0	0
4	H	59	59	59	0	0

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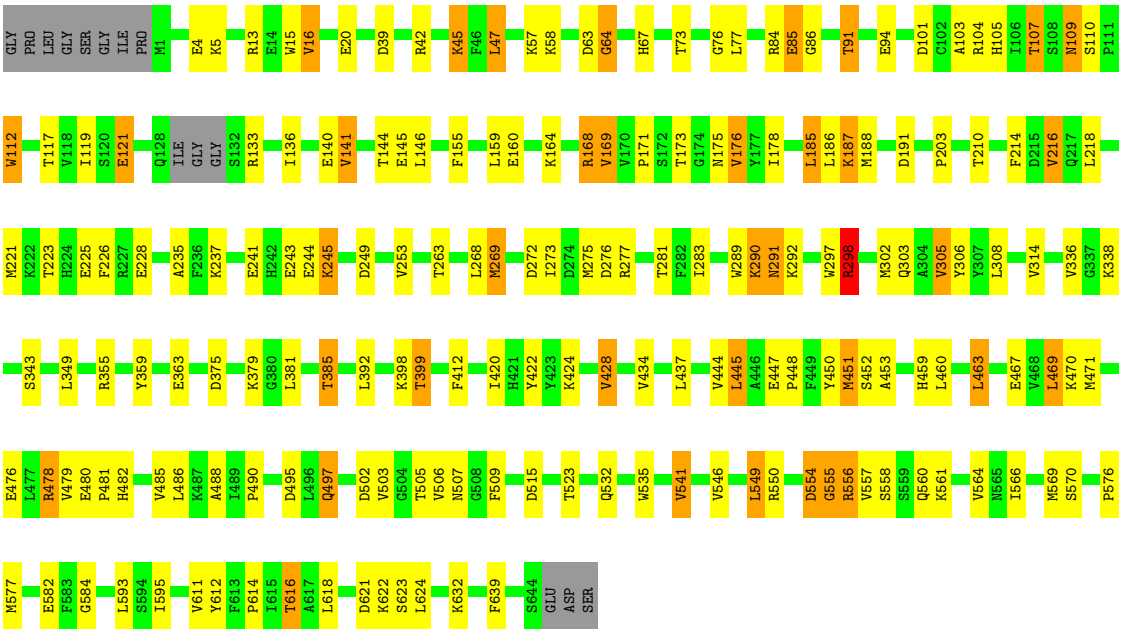
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	I	21	Total O 21 21	0	0
4	M	2	Total O 2 2	0	0
4	P	10	Total O 10 10	0	0
4	Q	2	Total O 2 2	0	0
4	R	2	Total O 2 2	0	0
4	J	12	Total O 12 12	0	0
4	K	6	Total O 6 6	0	0
4	L	85	Total O 85 85	0	0

3 Residue-property plots (i)

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

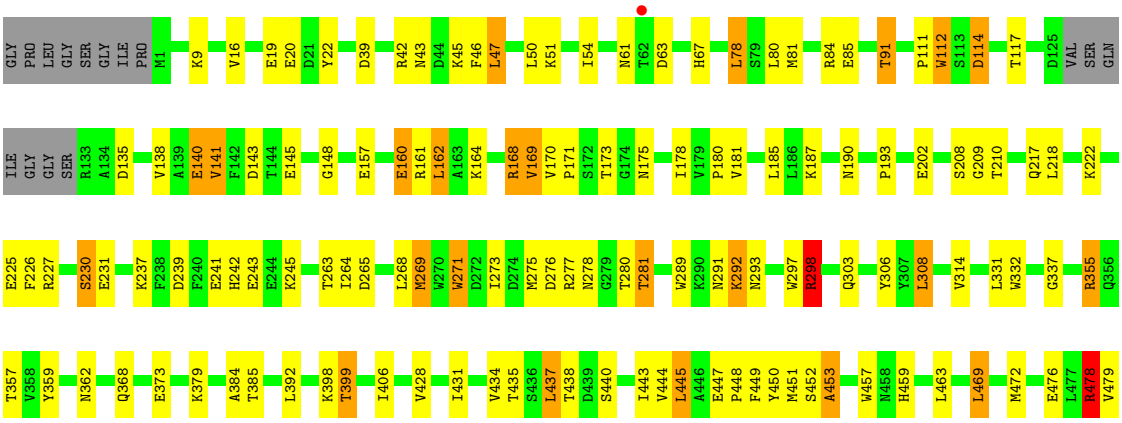
• Molecule 1: Protein arginine N-methyltransferase 7

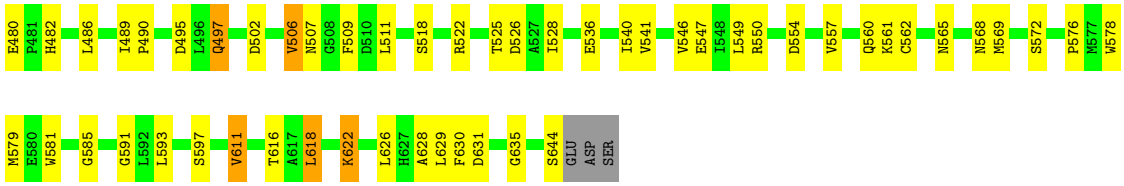
Chain A: 69% 23% 6%



• Molecule 1: Protein arginine N-methyltransferase 7

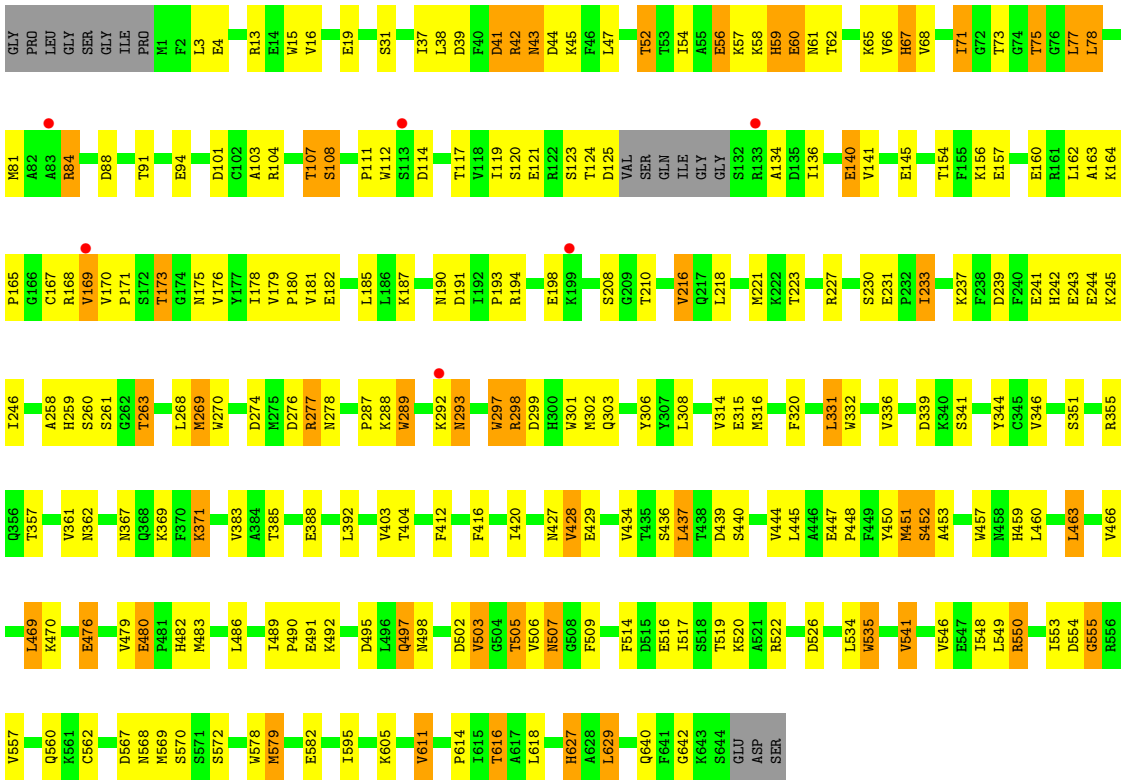
Chain D: 69% 24%





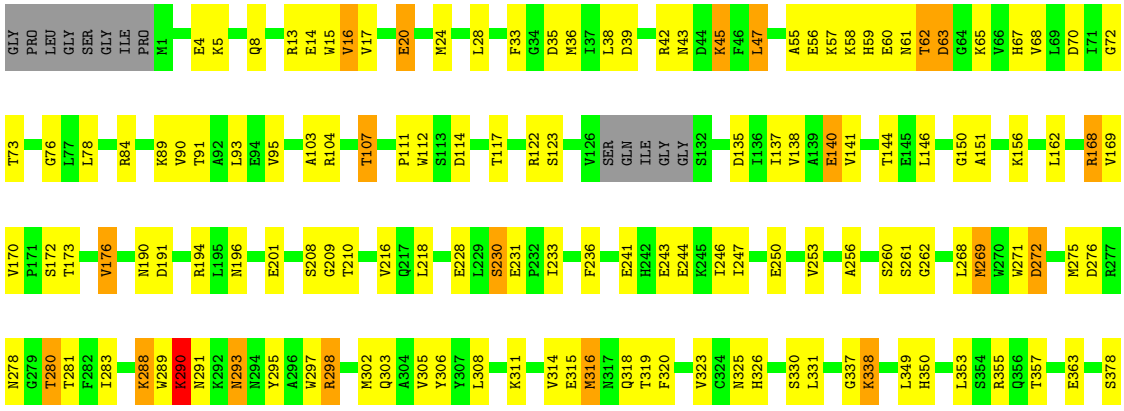
• Molecule 1: Protein arginine N-methyltransferase 7

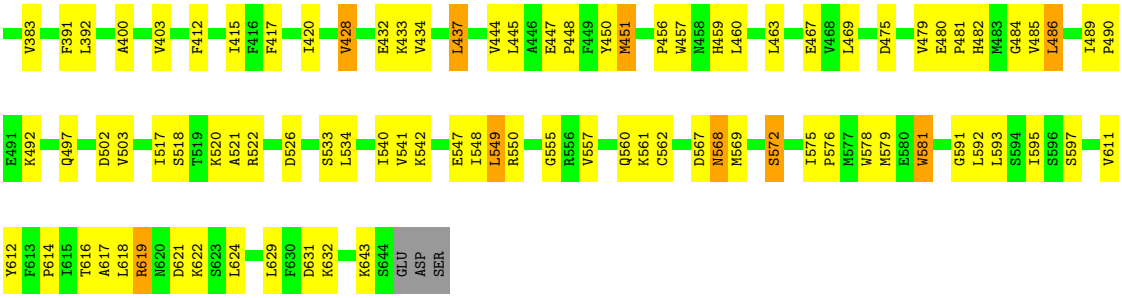
Chain B:



• Molecule 1: Protein arginine N-methyltransferase 7

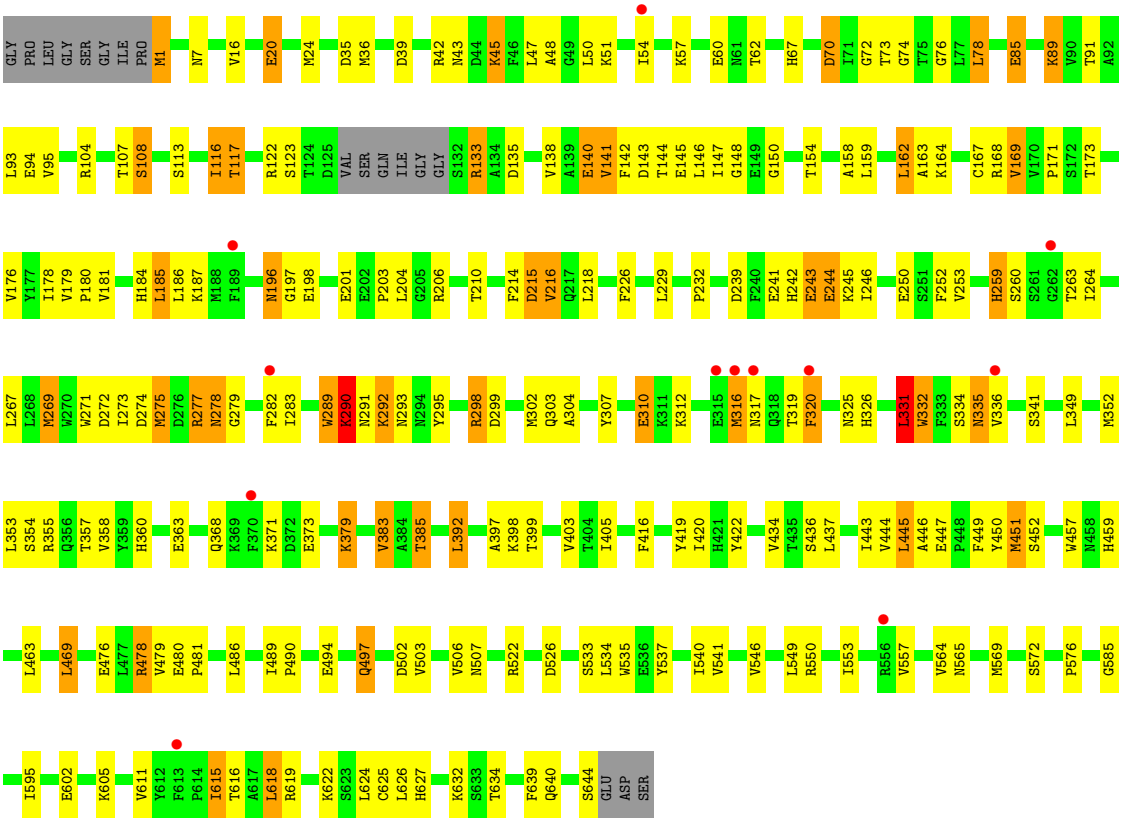
Chain C:





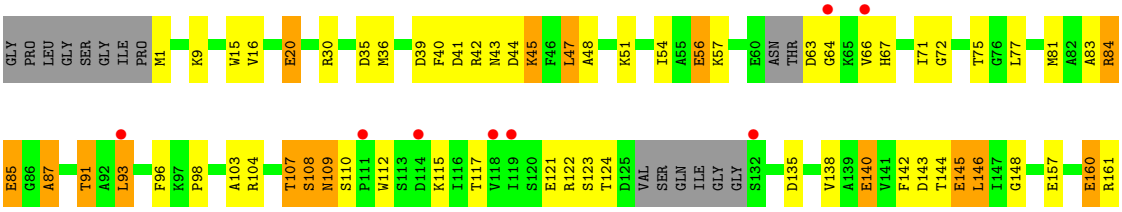
• Molecule 1: Protein arginine N-methyltransferase 7

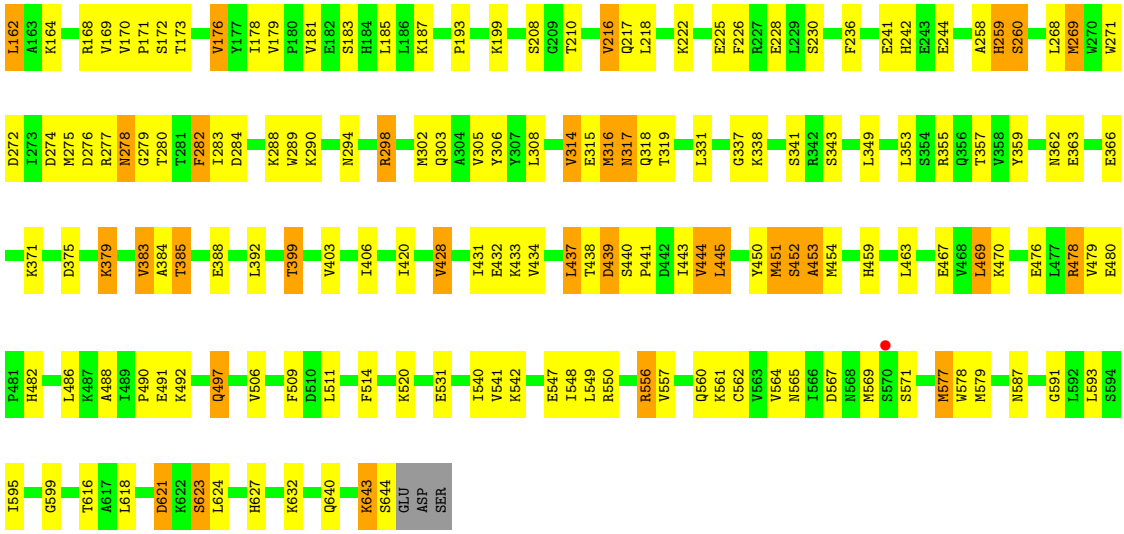
Chain F:



• Molecule 1: Protein arginine N-methyltransferase 7

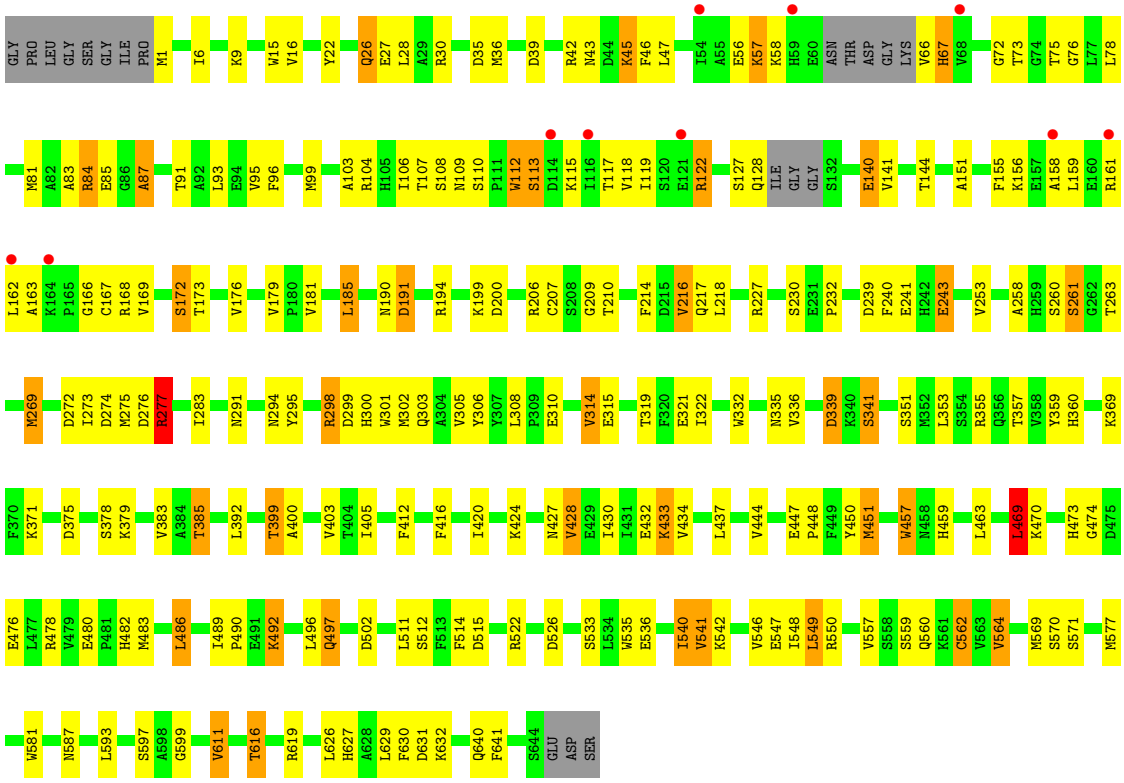
Chain E:





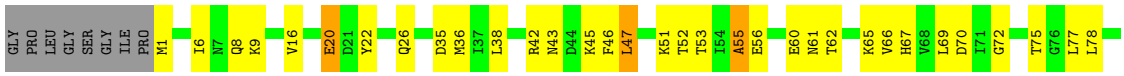
• Molecule 1: Protein arginine N-methyltransferase 7

Chain G:



• Molecule 1: Protein arginine N-methyltransferase 7

Chain H:



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L185 N190 G209 T210 A211 V216 Q217 L218 K222 P232 D239 F240 E241 H242 E243 E244 K245 E250 V253 A258 H259 S260 T263 L268 M269 I273 D274 M275 D276 R277 T281 F282 W289 K290 N291 K292 N293 W297 R298 W301 M302 Q303 A304

V305 Y306 Y307 L308 V314 E315 Q318 T319 H326 D327 W332 F333 V336 G337 K338 D339 K340 S341 R342 S343 G348 L349 H350 S351 M352 R355 Q368 V374 D375 S378 K379 V383 A384 T385 V386 G387 L392 K398 T399 A400 R411 I420 N427 V428

L437 V444 L445 F449 Y450 M451 S452 N455 P456 W457 N458 H459 L460 L463 L469 K470 D475 R478 V479 E480 P481 H482 V485 L486 P490 E491 K492 L496 Q497 N498 I499 D502 V503 G504 T505 F509 D510 L511 F514 T525 L534 W535 V541

V546 E547 I548 L549 R550 G555 R556 C562 V563 V564 M569 S570 A574 I575 P576 M577 W578 M579 E580 W581 G584 G591 L592 L593 E602 K605 V611 T616 A617 L618 D621 K622 S623 L624 C625 L626 H627 K632 S633 I637 G642 K643 S644 GLU ASP

SER

• Molecule 1: Protein arginine N-methyltransferase 7

Chain I:

GLY PRO LEU GLY SER GLY ILE PRO M1 F2 L3 V16 E19 Q26 R30 S31 R32 F33 G34 D35 R42 K45 F46 L47 K51 T52 T53 E56 D63 G64 K65 V66 H67 V68 L69 D70 I71 G72 T73 G76 L77 L78 E85 V90 T91 F96 K97

P98 R104 P111 W112 S113 D114 K115 I116 T117 V118 I129 G130 I136 I137 V138 A139 E140 V141 E145 L146 T154 F155 K156 E157 A158 L159 E160 R161 L162 C167 R168 V169 V170 P171 S172 T173 G174 N175 V176 Y177 I178 V181 L185 N190 D191 I192 P193 D200

G209 T210 L218 F226 R227 P232 I233 V234 A235 E241 H242 E243 E244 A256 S261 I264 D265 A266 L267 L268 M269 W270 W271 D272 I273 D274 M275 D276 R277 N278 G279 T280 T281 F282 I283 G286 P287 K290 N291 K292 N293 N294 Y295 A296 W297 R298 D299 H300 W301 Y306

Y307 L308 P309 K312 K313 V314 E315 M316 T319 V323 C324 N325 H326 S330 L331 W332 V336 G337 K340 S351 M352 L353 S354 R355 Q356 T357 N362 Q368 K369 D375 K379 V383 A384 T385 L392 K398 T399 V403 D414 I415 F416 F417 K418 Y419

I420 K424 L425 T426 N427 V428 V434 L437 T438 I443 V444 L445 A446 Y450 M451 S452 A453 M454 N455 P456 H459 L460 R461 F462 L463 Y464 D465 L469 K470 H473 E476 L477 R478 V479 E480 P481 H482 L486 I489 P490 E491 K492 D495 L496 Q497 D502

V506 N507 S533 L534 W535 G539 I540 V541 K542 G543 V546 L549 R550 I553 D554 G555 R556 V557 Q560 K561 V564 N565 I566 D567 N568 M569 S570 S571 S572 N573 P576 M577 W578 M579 N587 L592 L593 S594 I595 S596 S597 P601 V611 Y612 F613 P614 I615 T616

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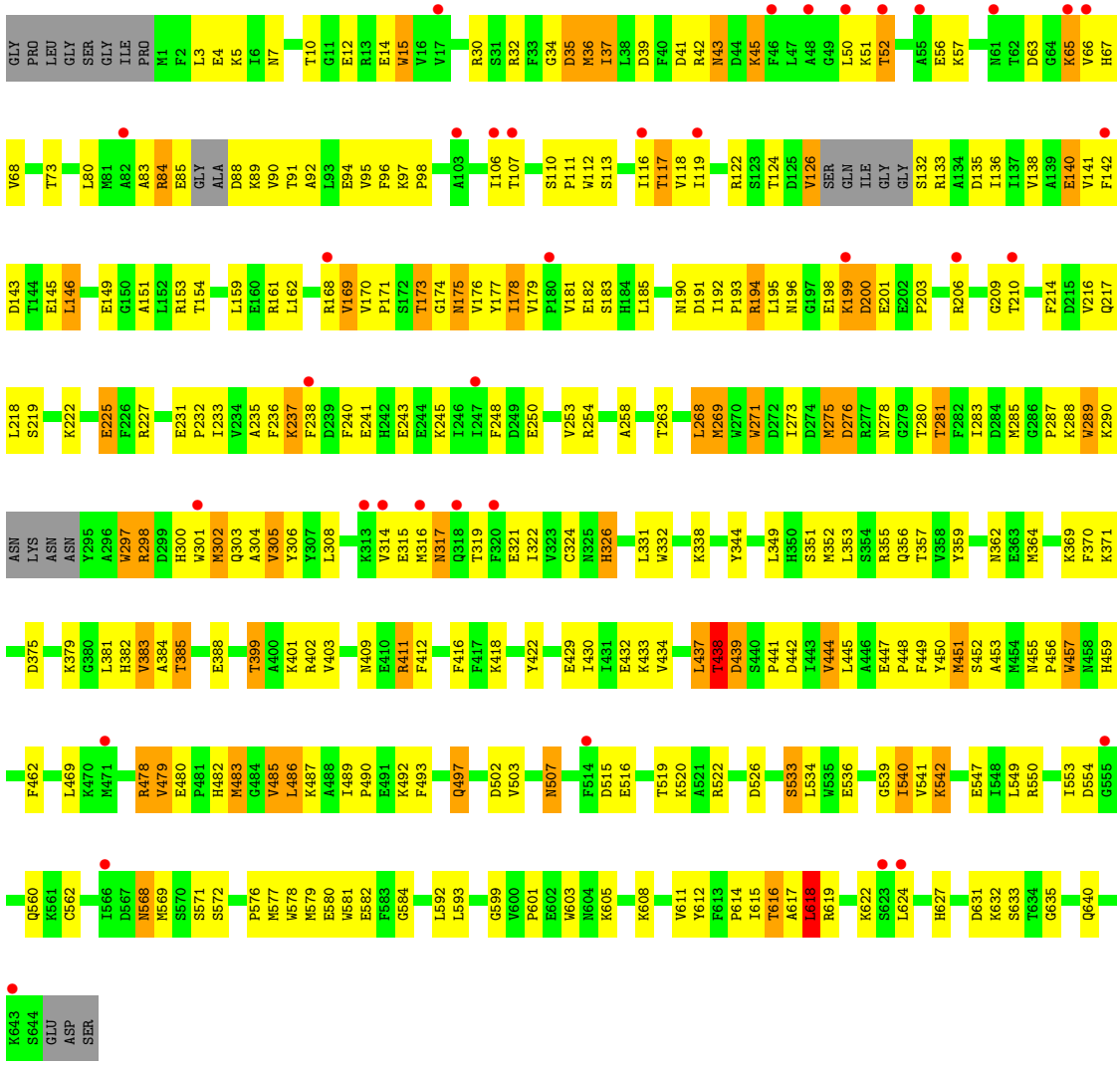
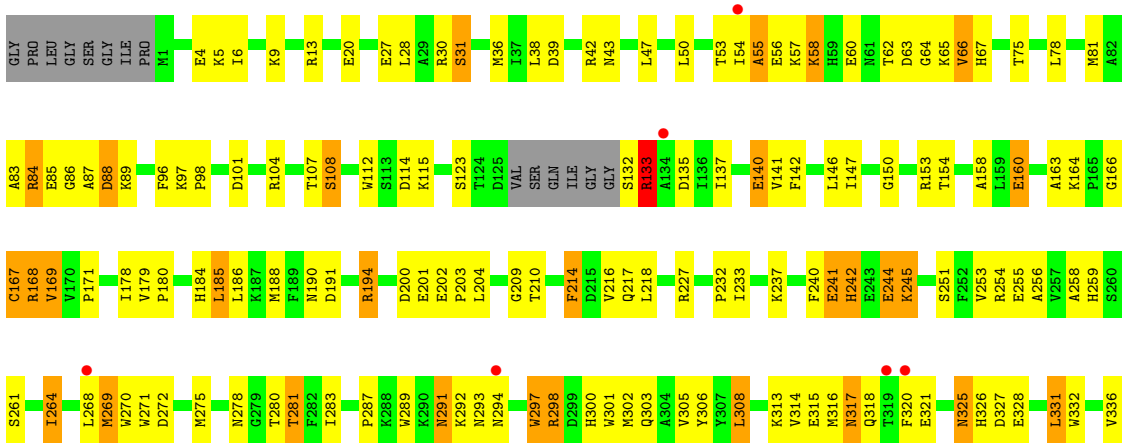
• Molecule 1: Protein arginine N-methyltransferase 7

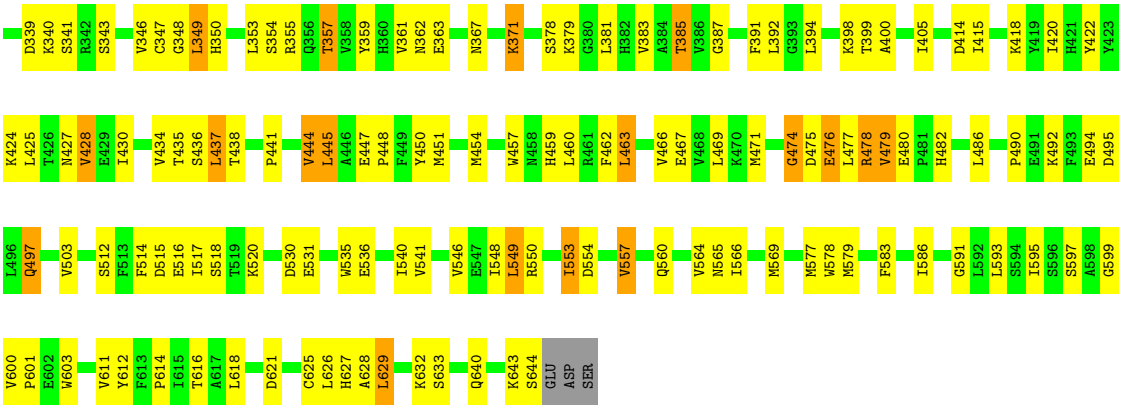
Chain M:



• Molecule 1: Protein arginine N-methyltransferase 7

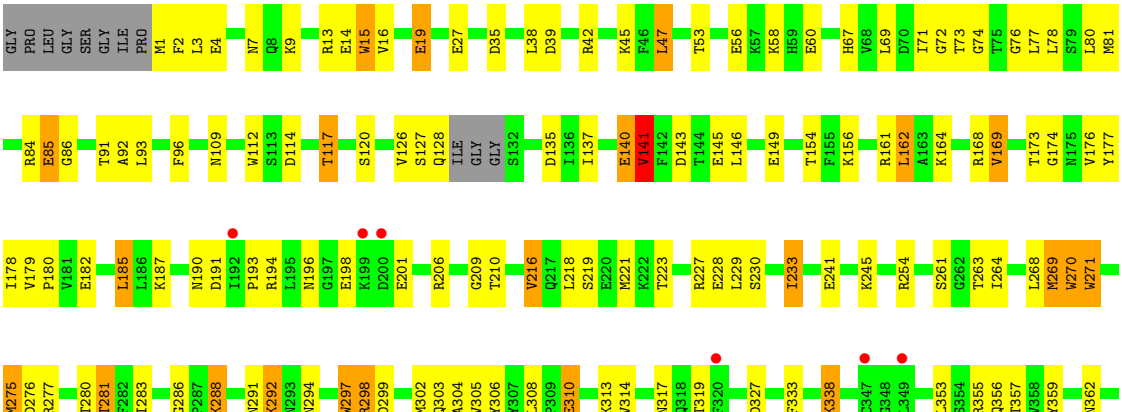
Chain N:





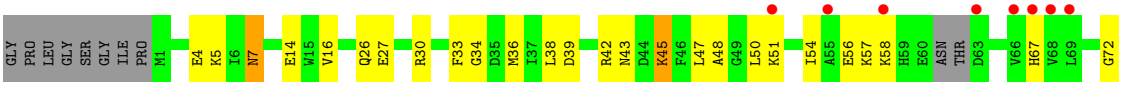
• Molecule 1: Protein arginine N-methyltransferase 7

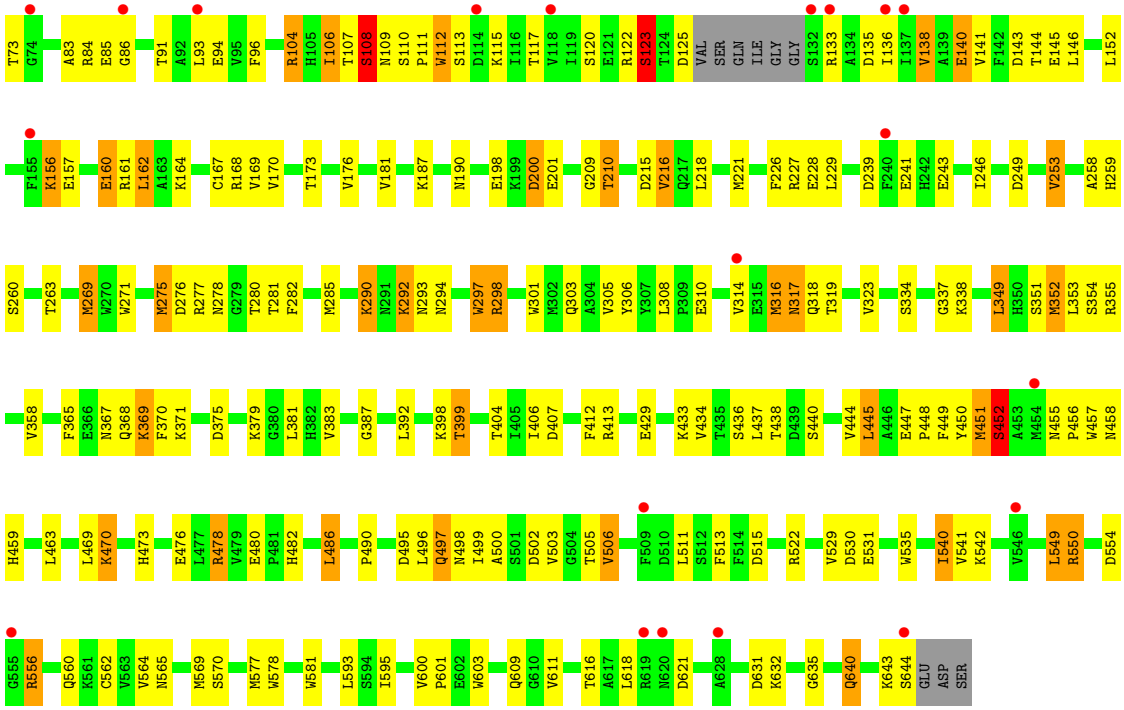
Chain O:



• Molecule 1: Protein arginine N-methyltransferase 7

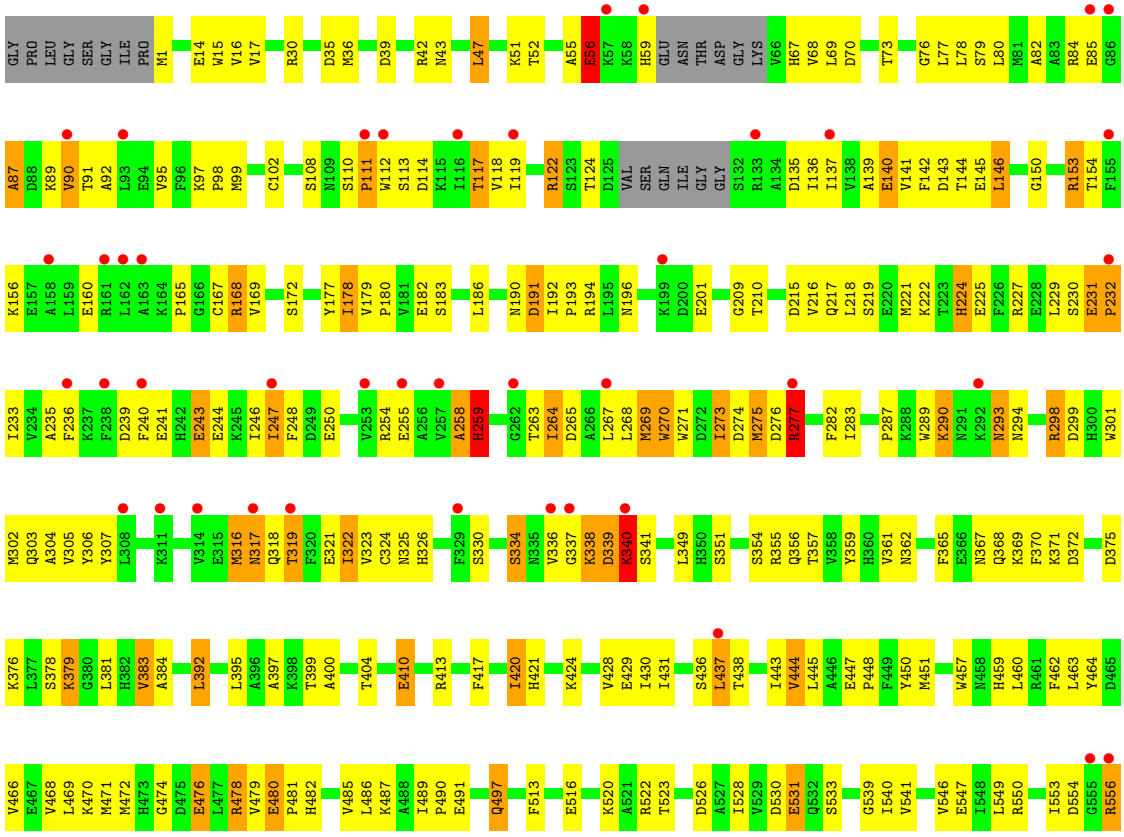
Chain P:

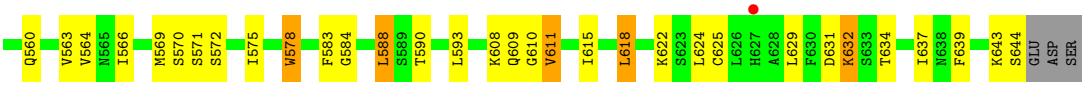




• Molecule 1: Protein arginine N-methyltransferase 7

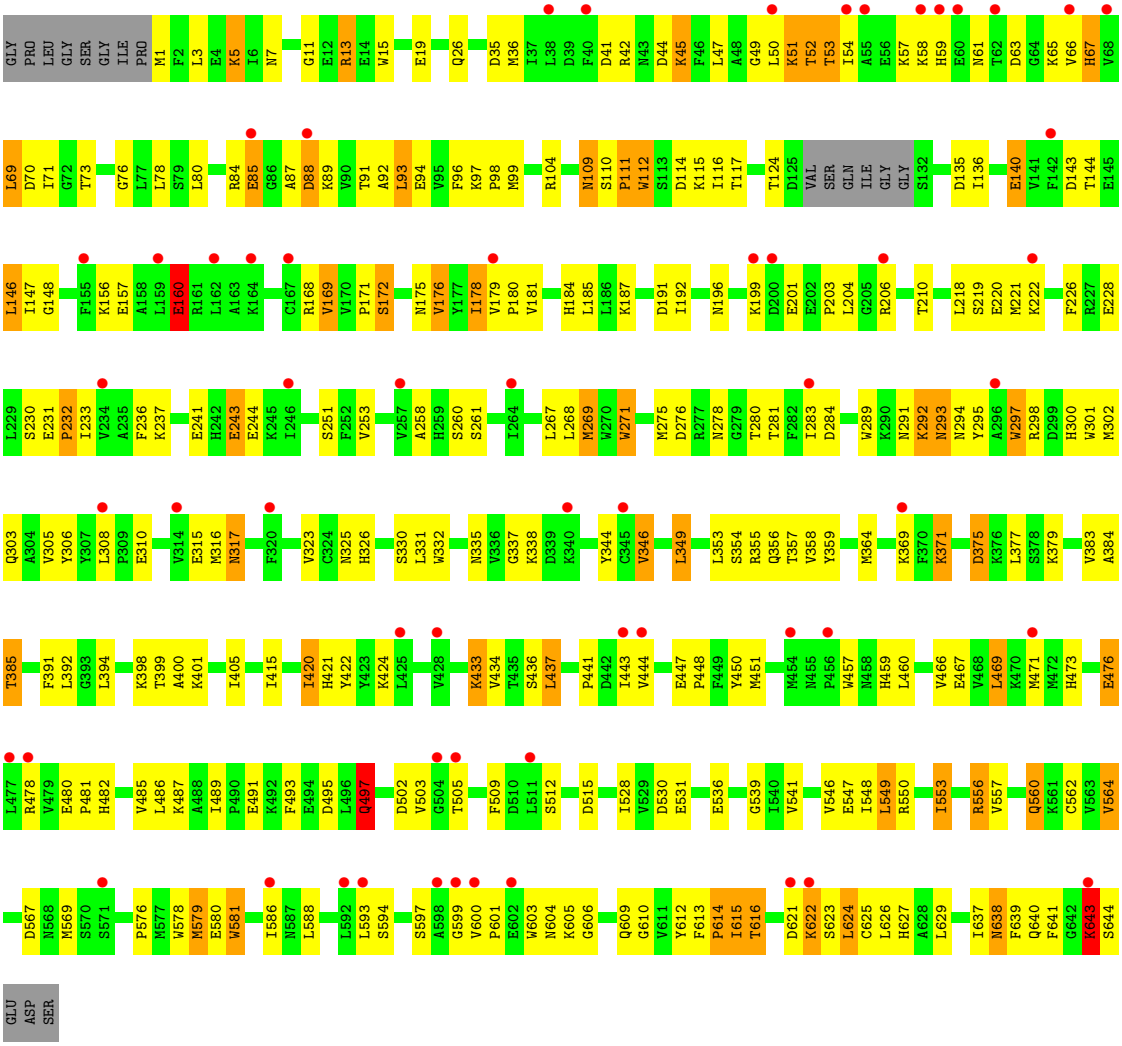
Chain Q:





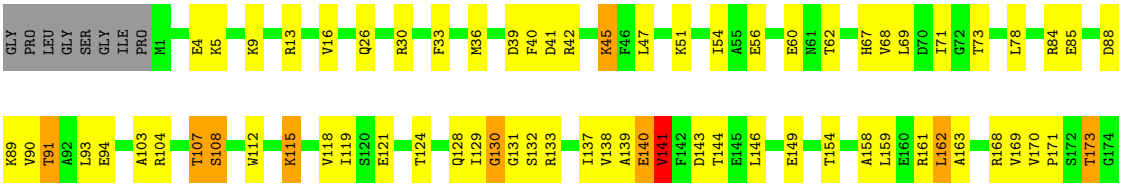
• Molecule 1: Protein arginine N-methyltransferase 7

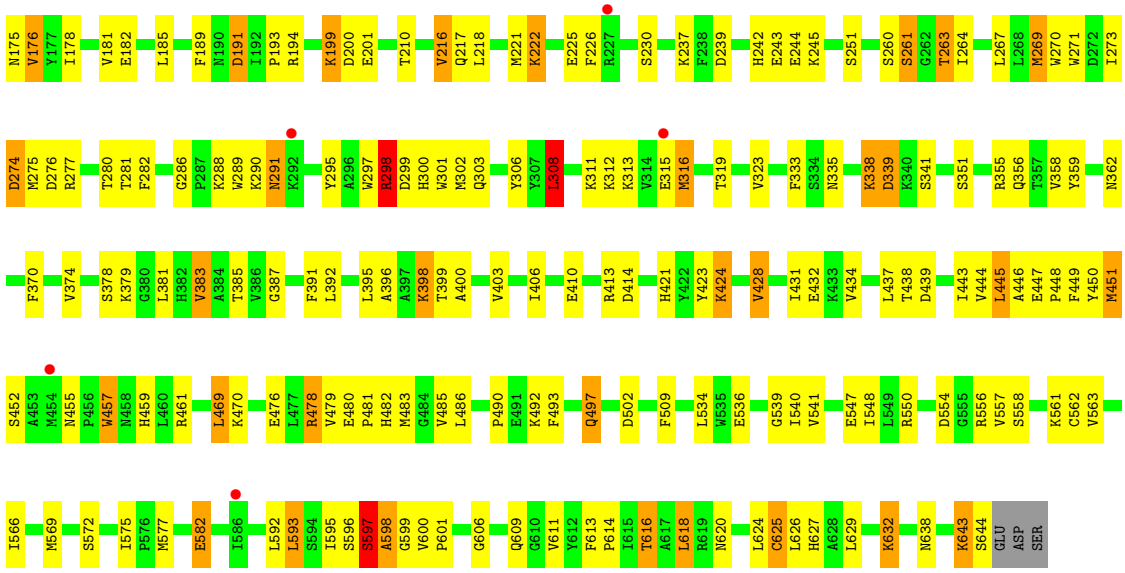
Chain R:



• Molecule 1: Protein arginine N-methyltransferase 7

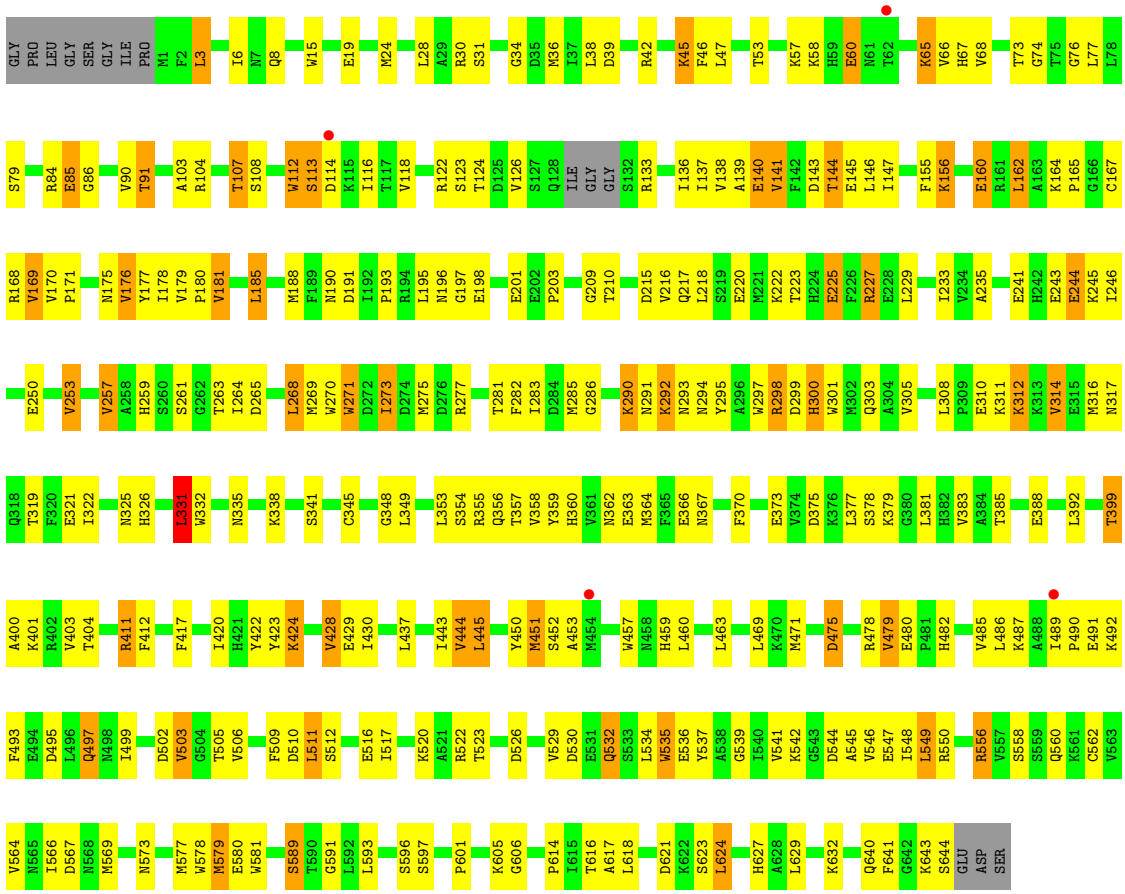
Chain J:





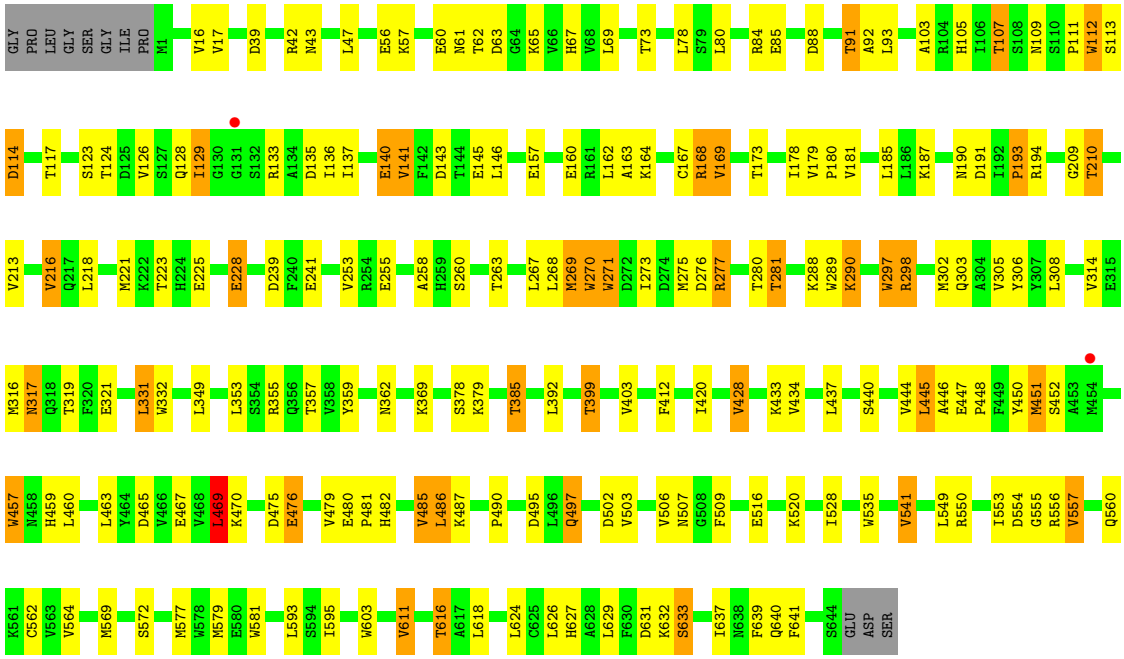
• Molecule 1: Protein arginine N-methyltransferase 7

Chain K:



• Molecule 1: Protein arginine N-methyltransferase 7

Chain L:


GLY PRO LEU GLY SER GLY ILE PRO M1 V16 V17 D39 R42 N43 L47 E56 K57 E60 N61 T62 D63 G64 K65 V66 H67 V68 L69 T73 L78 S79 L80 R84 E85 D88 T91 A92 L93 A103 R104 H105 I106 T107 S108 N109 S110 P111 W112 S113
D114 T117 S123 T124 D125 V126 S127 Q128 I129 G130 G131 S132 R133 A134 D135 I136 I137 E140 V141 F142 D143 T144 E145 L146 E157 E160 R161 L162 A163 K164 C167 R168 V169 T173 I178 V179 P180 V181 L185 L186 K187 N190 D191 I192 P193 R194 G209 T210
V213 V216 Q217 L218 M221 K222 T223 H224 E225 E228 D239 F240 E241 V253 R254 E255 A258 H259 S260 T263 L267 L268 M269 W270 W271 D272 I273 D274 M275 D276 R277 T280 T281 K288 W289 K290 W297 R298 M302 Q303 A304 V305 Y306 Y307 L308 V314 E315
M316 N317 Q318 T319 F320 E321 L331 W332 L349 L353 S354 R355 Q356 T357 V358 Y359 N362 K369 S378 K379 T385 L392 T399 V403 F412 I420 V428 K433 V434 L437 S440 V444 L445 A446 E447 P448 F449 Y450 M451 S452 A453 M454
W457 N458 H459 L460 L463 Y464 D465 V466 E467 V468 L469 K470 D475 E476 V479 E480 P481 H482 V485 L486 K487 P490 D495 L496 Q497 D502 V503 V506 N507 G508 F509 E516 K520 I528 W535 V541 L549 R550 I553 D554 G555 R556 V557 Q560
K561 C562 V563 V564 M569 S572 M577 W578 M579 E580 W581 L593 S594 I595 W603 V611 T616 A617 L618 L624 C625 L626 H627 A628 L629 F630 D631 K632 S633 I637 N638 F639 Q640 F641 S644 GLU ASP SER

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α, β, γ	190.70Å 190.70Å 373.09Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.41 – 2.39 47.41 – 2.39	Depositor EDS
% Data completeness (in resolution range)	98.9 (47.41-2.39) 98.9 (47.41-2.39)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	2.14 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.234 , 0.303 0.233 , 0.302	Depositor DCC
R_{free} test set	29764 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	44.9	Xtriage
Anisotropy	0.006	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 15.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.019 for -h,-k,l 0.069 for h,-h-k,-l 0.023 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	92645	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.30% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: SAH, PO4

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	0.85	4/5217 (0.1%)	0.95	5/7044 (0.1%)
1	B	0.79	7/5195 (0.1%)	0.88	0/7014
1	C	0.77	2/5202 (0.0%)	0.88	3/7024 (0.0%)
1	D	0.81	6/5189 (0.1%)	0.96	8/7006 (0.1%)
1	E	0.79	2/5179 (0.0%)	0.94	3/6990 (0.0%)
1	F	0.73	4/5195 (0.1%)	0.88	7/7014 (0.1%)
1	G	0.77	6/5180 (0.1%)	0.90	5/6993 (0.1%)
1	H	0.81	5/5202 (0.1%)	0.92	3/7024 (0.0%)
1	I	0.76	4/5234 (0.1%)	0.86	3/7068 (0.0%)
1	J	0.74	2/5234 (0.0%)	0.88	6/7068 (0.1%)
1	K	0.73	4/5217 (0.1%)	0.85	5/7044 (0.1%)
1	L	0.86	9/5234 (0.2%)	0.99	8/7068 (0.1%)
1	M	0.70	7/5158 (0.1%)	0.81	3/6962 (0.0%)
1	N	0.70	4/5195 (0.1%)	0.84	4/7014 (0.1%)
1	O	0.66	5/5217 (0.1%)	0.78	3/7044 (0.0%)
1	P	0.74	7/5179 (0.1%)	0.85	4/6990 (0.1%)
1	Q	0.68	5/5149 (0.1%)	0.81	1/6951 (0.0%)
1	R	0.65	8/5195 (0.2%)	0.77	0/7014
All	All	0.76	91/93571 (0.1%)	0.88	71/126332 (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	0	1
1	E	0	2
1	H	0	1
1	J	0	2
All	All	0	6

All (91) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	332	TRP	CD2-CE2	7.16	1.50	1.41
1	M	271	TRP	CD2-CE2	6.90	1.49	1.41
1	L	297	TRP	CD2-CE2	6.63	1.49	1.41
1	D	332	TRP	CD2-CE2	6.55	1.49	1.41
1	A	289	TRP	CD2-CE2	6.37	1.49	1.41
1	H	332	TRP	CD2-CE2	6.34	1.49	1.41
1	P	578	TRP	CD2-CE2	6.32	1.49	1.41
1	G	535	TRP	CD2-CE2	6.27	1.48	1.41
1	A	535	TRP	CD2-CE2	6.25	1.48	1.41
1	O	271	TRP	CD2-CE2	6.18	1.48	1.41
1	D	581	TRP	CD2-CE2	6.16	1.48	1.41
1	M	581	TRP	CD2-CE2	6.15	1.48	1.41
1	G	581	TRP	CD2-CE2	6.11	1.48	1.41
1	B	578	TRP	CD2-CE2	6.10	1.48	1.41
1	G	457	TRP	CD2-CE2	6.09	1.48	1.41
1	B	270	TRP	CD2-CE2	6.08	1.48	1.41
1	H	457	TRP	CD2-CE2	6.04	1.48	1.41
1	E	289	TRP	CD2-CE2	6.04	1.48	1.41
1	F	457	TRP	CD2-CE2	6.00	1.48	1.41
1	L	535	TRP	CD2-CE2	5.99	1.48	1.41
1	J	457	TRP	CD2-CE2	5.97	1.48	1.41
1	R	603	TRP	CD2-CE2	5.94	1.48	1.41
1	G	332	TRP	CD2-CE2	5.93	1.48	1.41
1	K	332	TRP	CD2-CE2	5.92	1.48	1.41
1	K	457	TRP	CD2-CE2	5.83	1.48	1.41
1	P	535	TRP	CD2-CE2	5.79	1.48	1.41
1	Q	578	TRP	CD2-CE2	5.79	1.48	1.41
1	B	289	TRP	CD2-CE2	5.79	1.48	1.41
1	B	332	TRP	CD2-CE2	5.78	1.48	1.41
1	D	289	TRP	CD2-CE2	5.76	1.48	1.41
1	P	457	TRP	CD2-CE2	5.74	1.48	1.41
1	N	270	TRP	CD2-CE2	5.73	1.48	1.41
1	N	603	TRP	CD2-CE2	5.68	1.48	1.41
1	P	603	TRP	CD2-CE2	5.65	1.48	1.41
1	L	112	TRP	CD2-CE2	5.65	1.48	1.41
1	M	457	TRP	CD2-CE2	5.64	1.48	1.41
1	N	457	TRP	CD2-CE2	5.62	1.48	1.41
1	L	289	TRP	CD2-CE2	5.60	1.48	1.41
1	R	581	TRP	CD2-CE2	5.57	1.48	1.41
1	K	581	TRP	CD2-CE2	5.56	1.48	1.41
1	F	332	TRP	CD2-CE2	5.55	1.48	1.41
1	Q	270	TRP	CD2-CE2	5.53	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	15	TRP	CD2-CE2	5.53	1.48	1.41
1	N	297	TRP	CD2-CE2	5.51	1.48	1.41
1	B	535	TRP	CD2-CE2	5.49	1.48	1.41
1	I	332	TRP	CD2-CE2	5.47	1.48	1.41
1	P	297	TRP	CD2-CE2	5.45	1.47	1.41
1	B	457	TRP	CD2-CE2	5.45	1.47	1.41
1	P	301	TRP	CD2-CE2	5.44	1.47	1.41
1	R	457	TRP	CD2-CE2	5.44	1.47	1.41
1	I	112	TRP	CD2-CE2	5.38	1.47	1.41
1	Q	301	TRP	CD2-CE2	5.38	1.47	1.41
1	M	297	TRP	CD2-CE2	5.36	1.47	1.41
1	H	301	TRP	CD2-CE2	5.34	1.47	1.41
1	R	112	TRP	CD2-CE2	5.34	1.47	1.41
1	L	271	TRP	CD2-CE2	5.34	1.47	1.41
1	G	112	TRP	CD2-CE2	5.33	1.47	1.41
1	M	603	TRP	CD2-CE2	5.33	1.47	1.41
1	H	581	TRP	CD2-CE2	5.32	1.47	1.41
1	G	15	TRP	CD2-CE2	5.31	1.47	1.41
1	P	581	TRP	CD2-CE2	5.31	1.47	1.41
1	A	112	TRP	CD2-CE2	5.30	1.47	1.41
1	Q	15	TRP	CD2-CE2	5.29	1.47	1.41
1	Q	457	TRP	CD2-CE2	5.28	1.47	1.41
1	F	271	TRP	CD2-CE2	5.28	1.47	1.41
1	O	297	TRP	CD2-CE2	5.23	1.47	1.41
1	D	271	TRP	CD2-CE2	5.22	1.47	1.41
1	I	535	TRP	CD2-CE2	5.22	1.47	1.41
1	E	112	TRP	CD2-CE2	5.21	1.47	1.41
1	R	289	TRP	CD2-CE2	5.21	1.47	1.41
1	M	332	TRP	CD2-CE2	5.21	1.47	1.41
1	K	271	TRP	CD2-CE2	5.18	1.47	1.41
1	R	271	TRP	CD2-CE2	5.18	1.47	1.41
1	I	271	TRP	CD2-CE2	5.16	1.47	1.41
1	O	15	TRP	CD2-CE2	5.16	1.47	1.41
1	J	271	TRP	CD2-CE2	5.16	1.47	1.41
1	R	297	TRP	CD2-CE2	5.15	1.47	1.41
1	M	15	TRP	CD2-CE2	5.15	1.47	1.41
1	H	289	TRP	CD2-CE2	5.13	1.47	1.41
1	C	297	TRP	CD2-CE2	5.13	1.47	1.41
1	C	581	TRP	CD2-CE2	5.12	1.47	1.41
1	F	289	TRP	CD2-CE2	5.12	1.47	1.41
1	L	457	TRP	CD2-CE2	5.12	1.47	1.41
1	O	270	TRP	CD2-CE2	5.09	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	112	TRP	CD2-CE2	5.09	1.47	1.41
1	L	603	TRP	CD2-CE2	5.07	1.47	1.41
1	O	578	TRP	CD2-CE2	5.05	1.47	1.41
1	L	270	TRP	CD2-CE2	5.05	1.47	1.41
1	B	297	TRP	CD2-CE2	5.04	1.47	1.41
1	D	457	TRP	CD2-CE2	5.03	1.47	1.41
1	R	332	TRP	CD2-CE2	5.03	1.47	1.41

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	277	ARG	NE-CZ-NH2	-9.40	115.60	120.30
1	F	331	LEU	CA-CB-CG	9.32	136.75	115.30
1	L	611	VAL	CB-CA-C	-8.32	95.60	111.40
1	L	277	ARG	NE-CZ-NH1	8.29	124.45	120.30
1	D	611	VAL	CB-CA-C	-7.93	96.34	111.40
1	K	331	LEU	CA-CB-CG	7.65	132.90	115.30
1	Q	611	VAL	CB-CA-C	-7.34	97.45	111.40
1	J	298	ARG	NE-CZ-NH2	-7.28	116.66	120.30
1	E	579	MET	CG-SD-CE	-7.25	88.59	100.20
1	C	437	LEU	CA-CB-CG	7.22	131.91	115.30
1	N	241	GLU	N-CA-C	7.17	130.36	111.00
1	H	611	VAL	CB-CA-C	-6.76	98.55	111.40
1	H	241	GLU	C-N-CA	6.58	138.16	121.70
1	O	624	LEU	CA-CB-CG	6.50	130.24	115.30
1	A	298	ARG	NE-CZ-NH2	-6.18	117.21	120.30
1	L	554	ASP	CB-CA-C	-6.05	98.30	110.40
1	D	579	MET	CG-SD-CE	-6.05	90.52	100.20
1	F	215	ASP	CB-CG-OD2	-5.99	112.91	118.30
1	K	549	LEU	CA-CB-CG	5.99	129.08	115.30
1	F	331	LEU	CB-CG-CD1	5.91	121.05	111.00
1	L	469	LEU	CA-CB-CG	5.88	128.81	115.30
1	P	215	ASP	CB-CG-OD1	5.87	123.58	118.30
1	P	486	LEU	CA-CB-CG	5.83	128.70	115.30
1	J	162	LEU	CA-CB-CG	5.76	128.54	115.30
1	I	185	LEU	CA-CB-CG	5.66	128.31	115.30
1	M	84	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	I	611	VAL	CB-CA-C	-5.60	100.76	111.40
1	G	486	LEU	CA-CB-CG	5.60	128.17	115.30
1	G	469	LEU	CA-CB-CG	5.59	128.17	115.30
1	G	611	VAL	CB-CA-C	-5.59	100.77	111.40
1	G	631	ASP	CB-CG-OD1	5.59	123.33	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	N	185	LEU	CA-CB-CG	5.56	128.09	115.30
1	A	86	GLY	N-CA-C	5.55	126.97	113.10
1	D	308	LEU	CB-CG-CD1	5.55	120.43	111.00
1	C	486	LEU	CA-CB-CG	5.52	128.00	115.30
1	H	241	GLU	CA-C-N	5.52	129.34	117.20
1	E	145	GLU	C-N-CA	5.47	135.37	121.70
1	N	629	LEU	CA-CB-CG	5.44	127.81	115.30
1	J	298	ARG	NE-CZ-NH1	5.43	123.01	120.30
1	M	84	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	A	549	LEU	CA-CB-CG	5.42	127.75	115.30
1	D	162	LEU	CA-CB-CG	5.40	127.72	115.30
1	D	208	SER	CB-CA-C	-5.40	99.84	110.10
1	K	215	ASP	CB-CG-OD1	5.37	123.14	118.30
1	L	486	LEU	CB-CG-CD2	5.34	120.08	111.00
1	F	611	VAL	CB-CA-C	-5.32	101.29	111.40
1	D	618	LEU	CB-CG-CD1	5.31	120.03	111.00
1	J	274	ASP	CB-CG-OD1	5.31	123.08	118.30
1	K	411	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	F	70	ASP	CB-CG-OD1	5.29	123.06	118.30
1	L	331	LEU	CA-CB-CG	5.28	127.44	115.30
1	D	298	ARG	NE-CZ-NH2	-5.27	117.66	120.30
1	A	47	LEU	CA-CB-CG	5.26	127.41	115.30
1	D	478	ARG	NE-CZ-NH2	5.26	122.93	120.30
1	C	331	LEU	CA-CB-CG	5.26	127.40	115.30
1	O	327	ASP	CB-CG-OD1	5.24	123.01	118.30
1	G	207	CYS	N-CA-C	-5.22	96.90	111.00
1	N	579	MET	CG-SD-CE	-5.20	91.88	100.20
1	J	308	LEU	CA-CB-CG	5.19	127.24	115.30
1	A	249	ASP	CB-CG-OD2	5.17	122.95	118.30
1	K	411	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	F	215	ASP	CB-CG-OD1	5.15	122.93	118.30
1	L	476	GLU	CB-CA-C	-5.13	100.13	110.40
1	J	387	GLY	N-CA-C	-5.13	100.28	113.10
1	F	272	ASP	CB-CG-OD1	5.11	122.90	118.30
1	I	465	ASP	CB-CG-OD2	5.06	122.85	118.30
1	E	375	ASP	CB-CG-OD2	5.05	122.85	118.30
1	M	618	LEU	CA-CB-CG	5.05	126.91	115.30
1	P	145	GLU	C-N-CA	5.02	134.25	121.70
1	P	162	LEU	CA-CB-CG	5.01	126.83	115.30
1	O	162	LEU	CA-CB-CG	5.01	126.81	115.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	85	GLU	Peptide
1	E	282	PHE	Peptide
1	E	316	MET	Peptide
1	H	282	PHE	Peptide
1	J	291	ASN	Peptide
1	J	597	SER	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	5106	0	4989	129	0
1	B	5084	0	4967	174	0
1	C	5091	0	4976	158	1
1	D	5078	0	4962	138	1
1	E	5069	0	4953	160	0
1	F	5084	0	4967	153	0
1	G	5070	0	4955	145	0
1	H	5091	0	4976	136	0
1	I	5122	0	5007	173	0
1	J	5122	0	5007	184	0
1	K	5106	0	4989	212	0
1	L	5122	0	5007	136	0
1	M	5049	0	4935	270	0
1	N	5084	0	4967	225	1
1	O	5106	0	4989	214	0
1	P	5069	0	4953	158	1
1	Q	5039	0	4927	233	0
1	R	5084	0	4967	202	0
2	A	26	0	19	0	0
2	B	26	0	19	2	0
2	C	26	0	19	1	0
2	D	26	0	19	0	0
2	E	26	0	19	3	0
2	F	26	0	19	2	0
2	G	26	0	19	2	0
2	H	26	0	19	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	I	26	0	19	1	0
2	J	26	0	19	0	0
2	K	26	0	19	3	0
2	L	26	0	19	0	0
2	M	26	0	19	2	0
2	N	26	0	19	1	0
2	O	26	0	19	0	0
2	P	26	0	19	3	0
2	Q	26	0	19	1	0
2	R	26	0	19	1	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
3	E	5	0	0	0	0
3	F	5	0	0	0	0
3	G	5	0	0	0	0
3	H	5	0	0	0	0
3	I	5	0	0	1	0
3	J	5	0	0	0	0
3	K	5	0	0	0	0
3	L	5	0	0	0	0
3	M	5	0	0	0	0
3	N	5	0	0	0	0
3	O	5	0	0	0	0
3	P	5	0	0	0	0
3	Q	5	0	0	1	0
3	R	5	0	0	0	0
4	A	105	0	0	0	0
4	B	26	0	0	0	0
4	C	16	0	0	1	0
4	D	93	0	0	3	0
4	E	41	0	0	0	0
4	F	12	0	0	1	0
4	G	19	0	0	1	0
4	H	59	0	0	1	0
4	I	21	0	0	3	0
4	J	12	0	0	1	0
4	K	6	0	0	0	0
4	L	85	0	0	4	0
4	M	2	0	0	2	0
4	P	10	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	Q	2	0	0	0	0
4	R	2	0	0	0	0
All	All	92645	0	89835	3158	2

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 17.

All (3158) 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:L:490:PRO:HB3	1:L:569:MET:CE	1.55	1.36
1:G:490:PRO:HB3	1:G:569:MET:CE	1.58	1.32
1:F:490:PRO:HB3	1:F:569:MET:CE	1.60	1.28
1:M:569:MET:HG3	1:M:624:LEU:CD1	1.67	1.23
1:B:490:PRO:HB3	1:B:569:MET:CE	1.71	1.20
1:D:497:GLN:NE2	1:D:497:GLN:H	1.42	1.18
1:N:379:LYS:HA	1:N:399:THR:HG22	1.28	1.16
1:A:490:PRO:HB3	1:A:569:MET:CE	1.76	1.16
1:E:478:ARG:HH21	1:E:478:ARG:HG2	0.99	1.15
1:Q:375:ASP:HA	1:Q:399:THR:HG21	1.28	1.14
1:O:393:GLY:HA3	1:O:405:ILE:CD1	1.77	1.13
1:Q:153:ARG:HG3	1:Q:153:ARG:HH11	1.04	1.12
1:Q:218:LEU:H	1:Q:303:GLN:NE2	1.44	1.12
1:J:597:SER:HB2	1:J:598:ALA:HB2	1.32	1.12
1:O:627:HIS:HB2	1:O:640:GLN:HB2	1.13	1.11
1:H:490:PRO:HB3	1:H:569:MET:CE	1.81	1.11
1:L:67:HIS:CE1	1:L:91:THR:HG23	1.86	1.11
1:F:218:LEU:H	1:F:303:GLN:NE2	1.49	1.10
1:Q:68:VAL:HG13	1:Q:90:VAL:HG13	1.30	1.10
1:C:490:PRO:HB3	1:C:569:MET:CE	1.82	1.10
1:H:490:PRO:HB3	1:H:569:MET:HE2	1.30	1.10
1:J:490:PRO:HB3	1:J:569:MET:HE3	1.24	1.09
1:F:50:LEU:O	1:F:54:ILE:HD12	1.52	1.09
1:K:67:HIS:CE1	1:K:91:THR:HG22	1.85	1.09
1:L:67:HIS:HE1	1:L:91:THR:HG23	0.96	1.08
1:L:490:PRO:HB3	1:L:569:MET:HE1	1.27	1.08
1:C:169:VAL:HG22	1:C:241:GLU:HG2	1.14	1.08
1:I:26:GLN:HG2	1:I:30:ARG:HH12	1.12	1.08
1:M:280:THR:HG23	1:M:281:THR:HG22	1.35	1.08
1:J:490:PRO:HB3	1:J:569:MET:CE	1.84	1.08
1:G:169:VAL:HG12	1:G:241:GLU:HG3	1.25	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:490:PRO:HB3	1:A:569:MET:HE2	1.36	1.08
1:Q:264:ILE:O	1:Q:264:ILE:HG12	1.44	1.07
1:R:433:LYS:H	1:R:433:LYS:HE2	1.20	1.06
1:M:569:MET:HG3	1:M:624:LEU:HD12	1.32	1.06
1:N:54:ILE:CA	1:N:58:LYS:HZ3	1.69	1.06
1:O:227:ARG:NH2	1:O:261:SER:O	1.88	1.06
1:M:91:THR:HG22	1:M:117:THR:HG23	1.32	1.05
1:K:67:HIS:HE1	1:K:91:THR:HG22	0.94	1.05
1:Q:39:ASP:OD2	1:Q:298:ARG:HD3	1.56	1.05
1:C:168:ARG:HG2	1:C:168:ARG:HH11	0.90	1.05
1:H:273:ILE:HG13	1:H:275:MET:HE3	1.39	1.04
1:A:168:ARG:HG2	1:A:168:ARG:HH11	0.89	1.03
1:G:490:PRO:HB3	1:G:569:MET:HE3	1.36	1.03
1:N:55:ALA:N	1:N:58:LYS:HZ2	1.54	1.03
1:I:51:LYS:HE2	1:I:85:GLU:OE2	1.56	1.03
1:N:269:MET:HG2	1:N:306:TYR:HE1	1.24	1.03
1:Q:168:ARG:HH11	1:Q:168:ARG:HG2	1.24	1.03
1:K:67:HIS:HE1	1:K:91:THR:CG2	1.69	1.03
1:M:478:ARG:HH21	1:M:478:ARG:HG2	1.20	1.03
1:N:444:VAL:HG13	1:N:479:VAL:HB	1.40	1.03
1:A:103:ALA:O	1:A:107:THR:HB	1.57	1.02
1:N:54:ILE:HA	1:N:58:LYS:NZ	1.75	1.02
1:C:450:TYR:H	1:C:459:HIS:HD2	1.08	1.02
1:N:54:ILE:HA	1:N:58:LYS:HZ3	0.87	1.02
1:I:210:THR:HG21	4:I:809:HOH:O	1.60	1.02
1:N:63:ASP:HB2	1:N:65:LYS:H	1.23	1.02
1:D:490:PRO:HB3	1:D:569:MET:HE3	1.37	1.02
1:G:490:PRO:CB	1:G:569:MET:CE	2.38	1.01
1:H:547:GLU:OE2	1:H:550:ARG:NH1	1.92	1.01
1:I:497:GLN:HE21	1:I:497:GLN:N	1.56	1.01
1:F:490:PRO:HB3	1:F:569:MET:HE1	1.38	1.01
1:A:420:ILE:HD11	1:A:428:VAL:HG22	1.43	1.01
1:B:490:PRO:HB3	1:B:569:MET:HE1	1.42	1.00
1:C:168:ARG:HG2	1:C:168:ARG:NH1	1.72	1.00
1:I:67:HIS:HE1	1:I:91:THR:HG23	1.26	1.00
1:P:241:GLU:HG3	1:P:277:ARG:HH21	1.26	1.00
1:J:490:PRO:CB	1:J:569:MET:CE	2.39	1.00
1:Q:137:ILE:HG13	1:Q:169:VAL:HG12	1.44	1.00
1:K:68:VAL:HG22	1:K:136:ILE:HB	1.43	0.99
1:O:393:GLY:HA3	1:O:405:ILE:HD11	1.03	0.99
1:A:478:ARG:HG2	1:A:478:ARG:HH21	1.26	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:39:ASP:OD2	1:J:298:ARG:HD3	1.61	0.98
1:H:497:GLN:NE2	1:H:497:GLN:H	1.60	0.98
1:H:478:ARG:HH21	1:H:478:ARG:HG2	1.29	0.98
1:F:490:PRO:HB3	1:F:569:MET:HE3	1.44	0.98
1:H:497:GLN:H	1:H:497:GLN:HE21	1.09	0.98
1:Q:68:VAL:HG13	1:Q:90:VAL:CG1	1.94	0.98
1:I:26:GLN:HG2	1:I:30:ARG:NH1	1.76	0.98
1:R:450:TYR:H	1:R:459:HIS:CD2	1.82	0.97
1:K:67:HIS:CE1	1:K:91:THR:CG2	2.47	0.97
1:H:480:GLU:OE2	1:H:482:HIS:HD2	1.44	0.97
1:R:556:ARG:HH11	1:R:556:ARG:HG3	1.29	0.97
1:A:67:HIS:HE1	1:A:91:THR:CG2	1.77	0.96
1:C:169:VAL:CG2	1:C:241:GLU:HG2	1.95	0.96
1:A:168:ARG:HG2	1:A:168:ARG:NH1	1.69	0.96
1:I:497:GLN:H	1:I:497:GLN:NE2	1.63	0.96
1:R:450:TYR:H	1:R:459:HIS:HD2	1.04	0.96
1:E:317:ASN:HD22	1:E:317:ASN:H	0.99	0.96
1:M:478:ARG:HH21	1:M:478:ARG:CG	1.79	0.96
1:Q:42:ARG:NH1	1:Q:140:GLU:HG2	1.80	0.96
1:E:67:HIS:HE1	1:E:91:THR:HG23	1.30	0.96
1:J:597:SER:HB2	1:J:598:ALA:CB	1.94	0.96
1:A:497:GLN:NE2	1:A:497:GLN:H	1.63	0.95
1:N:438:THR:HG21	1:O:629:LEU:HD21	1.48	0.95
1:Q:218:LEU:N	1:Q:303:GLN:HE21	1.63	0.95
1:D:280:THR:HG23	1:D:281:THR:HG22	1.46	0.95
1:N:169:VAL:HG11	1:N:240:PHE:O	1.68	0.94
1:D:168:ARG:HG2	1:D:168:ARG:HH11	1.32	0.94
1:O:73:THR:HB	1:O:92:ALA:HB1	1.49	0.94
1:A:497:GLN:H	1:A:497:GLN:HE21	1.08	0.94
1:B:39:ASP:OD2	1:B:298:ARG:HD3	1.66	0.94
1:L:577:MET:HE3	1:L:641:PHE:HZ	1.30	0.94
1:A:502:ASP:OD2	1:A:616:THR:HG21	1.66	0.94
1:H:480:GLU:OE2	1:H:482:HIS:CD2	2.21	0.94
1:J:490:PRO:CB	1:J:569:MET:HE3	1.97	0.94
1:F:42:ARG:NH1	1:F:140:GLU:HG2	1.83	0.94
1:M:450:TYR:H	1:M:459:HIS:HD2	1.01	0.94
1:E:67:HIS:CE1	1:E:91:THR:HG23	2.03	0.93
1:P:450:TYR:H	1:P:459:HIS:HD2	1.07	0.93
1:D:497:GLN:HE21	1:D:497:GLN:N	1.64	0.93
1:D:490:PRO:HB3	1:D:569:MET:CE	1.97	0.93
1:J:158:ALA:HA	1:J:162:LEU:HD23	1.50	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:168:ARG:HG2	1:N:168:ARG:HH11	1.34	0.93
1:N:255:GLU:HG2	1:N:321:GLU:HG2	1.51	0.92
1:A:228:GLU:OE2	1:A:290:LYS:NZ	2.02	0.92
1:C:490:PRO:HB3	1:C:569:MET:HE3	1.47	0.92
1:J:168:ARG:HG2	1:J:168:ARG:HH11	1.33	0.92
1:B:450:TYR:H	1:B:459:HIS:HD2	0.99	0.92
1:E:259:HIS:HD2	1:E:260:SER:OG	1.51	0.92
1:P:157:GLU:HA	1:P:160:GLU:HG3	1.51	0.92
1:H:87:ALA:O	1:H:115:LYS:HE3	1.67	0.92
1:A:133:ARG:HB2	1:A:164:LYS:HG3	1.51	0.92
1:E:490:PRO:HB3	1:E:569:MET:CE	1.99	0.92
1:I:490:PRO:HB3	1:I:569:MET:HE2	1.52	0.92
1:O:218:LEU:H	1:O:303:GLN:NE2	1.68	0.92
1:E:169:VAL:HG12	1:E:241:GLU:HG2	1.52	0.92
1:J:497:GLN:H	1:J:497:GLN:HE21	1.16	0.92
1:D:478:ARG:HG2	1:D:478:ARG:HH21	1.35	0.91
1:E:478:ARG:HG2	1:E:478:ARG:NH2	1.79	0.91
1:L:42:ARG:NH1	1:L:140:GLU:HG2	1.85	0.91
1:L:490:PRO:CB	1:L:569:MET:HE1	2.00	0.91
1:D:168:ARG:NH2	1:D:276:ASP:O	2.03	0.91
1:F:218:LEU:H	1:F:303:GLN:HE21	1.13	0.91
1:E:42:ARG:NH1	1:E:140:GLU:HG2	1.84	0.91
1:H:117:THR:OG1	1:J:131:GLY:HA3	1.70	0.91
1:H:273:ILE:HG13	1:H:275:MET:CE	2.00	0.91
1:P:478:ARG:HH21	1:P:478:ARG:HG2	1.36	0.91
1:P:490:PRO:HB3	1:P:569:MET:CE	2.00	0.91
1:Q:180:PRO:HG2	1:Q:230:SER:HB3	1.52	0.91
1:D:497:GLN:H	1:D:497:GLN:HE21	0.97	0.91
1:C:137:ILE:HB	1:C:169:VAL:HG12	1.50	0.91
1:D:480:GLU:OE2	1:D:482:HIS:HD2	1.54	0.91
1:G:490:PRO:CB	1:G:569:MET:HE1	2.01	0.90
1:O:39:ASP:OD2	1:O:298:ARG:HD3	1.71	0.90
1:P:42:ARG:NH1	1:P:140:GLU:HG2	1.86	0.90
1:L:168:ARG:HG2	1:L:168:ARG:HH11	1.35	0.90
1:C:168:ARG:HH11	1:C:168:ARG:CG	1.81	0.90
1:M:91:THR:HG22	1:M:117:THR:CG2	2.02	0.90
1:O:497:GLN:HE21	1:O:497:GLN:H	1.14	0.90
1:L:169:VAL:HG13	1:L:241:GLU:HG2	1.52	0.90
1:R:196:ASN:HB2	1:R:201:GLU:OE2	1.71	0.90
1:M:497:GLN:NE2	1:M:497:GLN:H	1.68	0.90
1:D:434:VAL:CG1	1:D:469:LEU:HD13	2.02	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:42:ARG:HH11	1:M:140:GLU:HG3	1.36	0.90
1:P:490:PRO:HB3	1:P:569:MET:HE1	1.52	0.90
1:L:67:HIS:HE1	1:L:91:THR:CG2	1.81	0.90
1:D:42:ARG:HH11	1:D:140:GLU:HG2	1.34	0.90
1:L:379:LYS:HA	1:L:399:THR:HG23	1.53	0.90
1:I:450:TYR:H	1:I:459:HIS:HD2	1.12	0.89
1:K:123:SER:HB3	2:K:701:SAH:HN62	1.34	0.89
1:M:178:ILE:O	1:M:233:ILE:HG22	1.72	0.89
1:G:379:LYS:HA	1:G:399:THR:HG23	1.55	0.89
1:C:314:VAL:HG21	1:C:320:PHE:CD2	2.06	0.89
1:E:379:LYS:HA	1:E:399:THR:CG2	2.03	0.89
1:A:67:HIS:HE1	1:A:91:THR:HG22	1.37	0.89
1:A:168:ARG:HH11	1:A:168:ARG:CG	1.81	0.89
1:P:42:ARG:HH11	1:P:140:GLU:HG2	1.36	0.89
1:I:379:LYS:HA	1:I:399:THR:HG23	1.53	0.89
1:J:370:PHE:O	1:J:374:VAL:HG23	1.72	0.89
1:A:434:VAL:CG1	1:A:469:LEU:HD13	2.03	0.88
1:N:55:ALA:N	1:N:58:LYS:NZ	2.20	0.88
1:Q:196:ASN:HB2	1:Q:201:GLU:OE2	1.72	0.88
1:O:490:PRO:HB3	1:O:569:MET:CE	2.03	0.88
1:M:450:TYR:H	1:M:459:HIS:CD2	1.89	0.88
1:G:379:LYS:HA	1:G:399:THR:CG2	2.04	0.88
1:I:67:HIS:CE1	1:I:91:THR:HG23	2.08	0.88
1:F:497:GLN:HE21	1:F:497:GLN:H	1.19	0.88
1:O:643:LYS:H	1:O:643:LYS:HD2	1.37	0.88
1:R:291:ASN:HB3	1:R:295:TYR:HB2	1.56	0.88
1:Q:153:ARG:HG3	1:Q:153:ARG:NH1	1.74	0.88
1:J:194:ARG:HG2	1:J:201:GLU:HB2	1.54	0.87
1:R:547:GLU:OE2	1:R:550:ARG:NH2	2.07	0.87
1:Q:68:VAL:CG1	1:Q:90:VAL:HG13	2.03	0.87
1:D:379:LYS:HA	1:D:399:THR:HG23	1.56	0.87
1:M:497:GLN:H	1:M:497:GLN:HE21	1.19	0.87
1:O:373:GLU:O	1:O:377:LEU:HD12	1.75	0.87
1:H:450:TYR:H	1:H:459:HIS:HD2	1.22	0.87
1:M:68:VAL:HG22	1:M:136:ILE:HB	1.55	0.87
1:Q:450:TYR:H	1:Q:459:HIS:HD2	1.18	0.87
1:A:490:PRO:CB	1:A:569:MET:HE2	2.06	0.86
1:N:147:ILE:HD11	1:N:331:LEU:HD13	1.57	0.86
1:I:570:SER:HB3	1:I:622:LYS:HG2	1.54	0.86
1:B:550:ARG:H	1:B:560:GLN:HE22	1.23	0.86
1:N:478:ARG:HG2	1:N:478:ARG:HH21	1.39	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:379:LYS:HA	1:D:399:THR:CG2	2.06	0.86
1:E:57:LYS:O	1:E:66:VAL:HG21	1.75	0.86
1:F:379:LYS:HA	1:F:399:THR:HG22	1.57	0.86
1:P:146:LEU:HD23	1:P:146:LEU:H	1.40	0.86
1:K:42:ARG:NH1	1:K:140:GLU:HG2	1.89	0.86
1:M:379:LYS:HA	1:M:399:THR:CG2	2.06	0.86
1:J:483:MET:HB3	1:J:582:GLU:HG3	1.55	0.86
1:L:490:PRO:CB	1:L:569:MET:CE	2.50	0.86
1:M:181:VAL:HG21	1:M:268:LEU:HD11	1.57	0.86
1:F:39:ASP:OD2	1:F:298:ARG:HD3	1.76	0.85
1:O:393:GLY:CA	1:O:405:ILE:HD11	1.99	0.85
1:P:104:ARG:HB2	1:P:104:ARG:CZ	2.04	0.85
1:F:450:TYR:H	1:F:459:HIS:HD2	1.25	0.85
1:I:323:VAL:HG11	1:I:340:LYS:HD3	1.57	0.85
1:D:42:ARG:NH1	1:D:140:GLU:HG2	1.90	0.85
1:N:50:LEU:O	1:N:54:ILE:HG23	1.77	0.85
1:Q:153:ARG:HH11	1:Q:153:ARG:CG	1.89	0.85
1:L:168:ARG:NH1	1:L:241:GLU:OE2	2.08	0.85
1:F:218:LEU:HD12	1:F:303:GLN:CB	2.06	0.85
1:M:478:ARG:HG2	1:M:478:ARG:NH2	1.89	0.85
1:C:450:TYR:H	1:C:459:HIS:CD2	1.94	0.85
1:L:490:PRO:HB3	1:L:569:MET:HE3	1.57	0.85
1:M:379:LYS:HA	1:M:399:THR:HG23	1.57	0.85
1:N:58:LYS:HE2	1:N:66:VAL:HG21	1.57	0.85
1:K:569:MET:HG3	1:K:624:LEU:HD11	1.58	0.85
1:R:622:LYS:H	1:R:622:LYS:HD2	1.41	0.85
1:B:104:ARG:O	1:B:108:SER:HB3	1.77	0.84
1:K:169:VAL:HG13	1:K:241:GLU:HG2	1.57	0.84
1:F:565:ASN:HD21	1:F:644:SER:HB2	1.42	0.84
1:B:163:ALA:HB1	1:B:167:CYS:SG	2.17	0.84
1:O:528:ILE:H	1:O:528:ILE:HD12	1.41	0.84
1:J:438:THR:HG21	1:K:629:LEU:HD21	1.59	0.84
1:D:434:VAL:HG12	1:D:469:LEU:HD13	1.60	0.84
1:G:497:GLN:HE21	1:G:497:GLN:H	1.25	0.84
1:O:373:GLU:HG3	1:O:377:LEU:HD11	1.59	0.83
1:F:553:ILE:HG22	1:F:553:ILE:O	1.77	0.83
1:P:450:TYR:H	1:P:459:HIS:CD2	1.94	0.83
1:B:490:PRO:CB	1:B:569:MET:HE1	2.08	0.83
1:F:275:MET:HE1	1:F:283:ILE:HG13	1.59	0.83
1:E:87:ALA:O	1:E:115:LYS:HE2	1.78	0.83
1:R:51:LYS:HZ2	1:R:51:LYS:HB2	1.43	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:490:PRO:CB	1:D:569:MET:CE	2.56	0.83
1:A:67:HIS:CE1	1:A:91:THR:CG2	2.62	0.83
1:O:233:ILE:HD11	1:O:254:ARG:CB	2.08	0.83
1:R:66:VAL:HA	1:R:135:ASP:OD2	1.76	0.83
1:F:150:GLY:O	1:F:154:THR:OG1	1.96	0.83
1:N:379:LYS:HA	1:N:399:THR:CG2	2.08	0.83
1:N:480:GLU:OE2	1:N:482:HIS:HD2	1.60	0.83
1:R:379:LYS:HA	1:R:399:THR:CG2	2.08	0.83
1:Q:378:SER:HB2	1:Q:399:THR:HG23	1.60	0.82
1:K:550:ARG:H	1:K:560:GLN:HE22	1.24	0.82
1:N:27:GLU:OE2	1:N:96:PHE:CE1	2.32	0.82
1:N:254:ARG:O	1:N:321:GLU:HA	1.79	0.82
1:B:450:TYR:H	1:B:459:HIS:CD2	1.91	0.82
1:M:110:SER:HB2	1:M:111:PRO:HD2	1.62	0.82
1:Q:254:ARG:O	1:Q:321:GLU:HA	1.79	0.82
1:G:66:VAL:HG12	1:G:87:ALA:HA	1.62	0.82
1:O:450:TYR:H	1:O:459:HIS:HD2	1.27	0.82
1:K:379:LYS:HA	1:K:399:THR:HG23	1.60	0.82
1:K:388:GLU:OE1	1:K:452:SER:HB2	1.79	0.82
1:L:631:ASP:OD1	1:L:633:SER:HB2	1.80	0.82
1:A:506:VAL:HG12	1:A:507:ASN:HD22	1.45	0.82
1:L:577:MET:CE	1:L:641:PHE:HZ	1.92	0.82
1:P:104:ARG:O	1:P:108:SER:HB2	1.80	0.81
1:J:189:PHE:CD1	1:J:359:TYR:HB2	2.14	0.81
1:F:553:ILE:O	1:F:553:ILE:CG2	2.29	0.81
1:N:63:ASP:CB	1:N:65:LYS:H	1.93	0.81
1:K:42:ARG:HH12	1:K:140:GLU:HG2	1.45	0.81
1:B:490:PRO:HB3	1:B:569:MET:HE3	1.59	0.81
1:C:314:VAL:CG2	1:C:320:PHE:CD2	2.63	0.81
1:Q:183:SER:H	1:Q:265:ASP:HB2	1.46	0.81
1:Q:478:ARG:HG2	1:Q:478:ARG:HH21	1.45	0.81
1:H:42:ARG:HH11	1:H:140:GLU:HG2	1.46	0.81
1:J:243:GLU:OE1	1:J:243:GLU:N	2.12	0.81
1:P:259:HIS:HD2	1:P:260:SER:OG	1.62	0.81
1:C:480:GLU:OE2	1:C:482:HIS:HD2	1.64	0.81
1:G:169:VAL:CG1	1:G:241:GLU:HG3	2.09	0.81
1:M:50:LEU:HD23	1:M:170:VAL:HG21	1.62	0.81
1:N:269:MET:HG2	1:N:306:TYR:CE1	2.13	0.81
1:J:497:GLN:H	1:J:497:GLN:NE2	1.78	0.81
1:R:556:ARG:HH11	1:R:556:ARG:CG	1.93	0.81
1:B:216:VAL:O	1:B:302:MET:HG2	1.81	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:379:LYS:HA	1:E:399:THR:HG23	1.63	0.80
1:M:444:VAL:HG13	1:M:479:VAL:HB	1.61	0.80
1:D:450:TYR:H	1:D:459:HIS:HD2	1.27	0.80
1:Q:216:VAL:O	1:Q:302:MET:HG2	1.81	0.80
1:Q:264:ILE:HD11	1:Q:267:LEU:HD21	1.63	0.80
1:M:95:VAL:CG2	1:M:122:ARG:HG3	2.11	0.80
1:P:379:LYS:HA	1:P:399:THR:HG23	1.63	0.80
1:E:478:ARG:HH21	1:E:478:ARG:CG	1.90	0.80
1:Q:264:ILE:O	1:Q:264:ILE:CG1	2.29	0.80
1:E:258:ALA:HB3	1:E:315:GLU:O	1.82	0.79
1:E:317:ASN:H	1:E:317:ASN:ND2	1.79	0.79
1:R:379:LYS:HA	1:R:399:THR:HG21	1.64	0.79
1:R:567:ASP:HA	1:R:623:SER:HB2	1.64	0.79
1:B:140:GLU:HG3	1:B:140:GLU:O	1.82	0.79
1:M:39:ASP:OD2	1:M:298:ARG:HD2	1.81	0.79
1:J:450:TYR:H	1:J:459:HIS:HD2	1.31	0.79
1:J:596:SER:O	1:J:599:GLY:N	2.11	0.79
1:I:169:VAL:HG13	1:I:241:GLU:HG2	1.65	0.79
1:P:5:LYS:HA	1:R:420:ILE:HD11	1.65	0.79
1:D:169:VAL:HG13	1:D:241:GLU:HG2	1.63	0.79
1:F:50:LEU:O	1:F:54:ILE:CD1	2.31	0.79
1:B:39:ASP:O	1:B:43:ASN:ND2	2.16	0.79
1:N:242:HIS:HB3	1:N:245:LYS:HD3	1.64	0.79
1:K:141:VAL:HG13	1:K:141:VAL:O	1.81	0.79
1:L:210:THR:HB	4:L:815:HOH:O	1.83	0.79
1:G:158:ALA:HA	1:G:162:LEU:HD23	1.64	0.79
1:M:132:SER:N	1:P:104:ARG:NH2	2.31	0.79
1:M:569:MET:CG	1:M:624:LEU:CD1	2.58	0.78
1:Q:168:ARG:HH11	1:Q:168:ARG:CG	1.96	0.78
1:J:239:ASP:OD2	1:J:242:HIS:HD2	1.66	0.78
1:A:169:VAL:HG13	1:A:241:GLU:HG2	1.63	0.78
1:M:41:ASP:O	1:M:45:LYS:HB2	1.83	0.78
1:O:233:ILE:HD11	1:O:254:ARG:HB3	1.65	0.78
1:Q:218:LEU:N	1:Q:303:GLN:NE2	2.25	0.78
1:M:480:GLU:OE2	1:M:482:HIS:HD2	1.67	0.78
1:G:497:GLN:H	1:G:497:GLN:NE2	1.82	0.78
1:R:73:THR:OG1	1:R:76:GLY:HA2	1.83	0.78
1:O:42:ARG:NH1	1:O:140:GLU:HG2	1.98	0.78
1:K:76:GLY:O	1:K:79:SER:N	2.17	0.78
1:G:450:TYR:H	1:G:459:HIS:HD2	1.31	0.78
1:K:450:TYR:H	1:K:459:HIS:HD2	1.30	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:317:ASN:HD22	1:E:317:ASN:N	1.75	0.78
1:L:42:ARG:HH11	1:L:140:GLU:HG2	1.48	0.78
1:N:142:PHE:CD1	1:N:146:LEU:HD12	2.20	0.77
1:N:133:ARG:HB3	1:N:133:ARG:HH21	1.48	0.77
1:Q:178:ILE:HD13	1:Q:235:ALA:HB2	1.65	0.77
1:K:541:VAL:HG23	1:K:601:PRO:HG3	1.66	0.77
1:F:450:TYR:H	1:F:459:HIS:CD2	2.02	0.77
1:N:67:HIS:H	1:N:135:ASP:HB2	1.49	0.77
1:Q:232:PRO:HG2	1:Q:290:LYS:HE2	1.65	0.77
1:J:480:GLU:OE2	1:J:482:HIS:HD2	1.66	0.77
1:D:67:HIS:HE1	1:D:91:THR:CG2	1.96	0.77
1:C:490:PRO:CB	1:C:569:MET:CE	2.63	0.77
1:M:280:THR:HG23	1:M:281:THR:CG2	2.14	0.77
1:Q:247:ILE:HG12	1:Q:250:GLU:OE2	1.84	0.77
1:B:243:GLU:OE1	1:B:243:GLU:N	2.13	0.77
1:J:383:VAL:HG21	1:J:445:LEU:HD22	1.67	0.77
1:E:434:VAL:CG1	1:E:469:LEU:HD13	2.15	0.77
1:G:103:ALA:O	1:G:107:THR:HG23	1.84	0.77
1:Q:218:LEU:H	1:Q:303:GLN:HE21	0.78	0.77
1:B:179:VAL:HG12	1:B:180:PRO:O	1.85	0.77
1:F:104:ARG:O	1:F:108:SER:HB3	1.84	0.77
1:A:450:TYR:H	1:A:459:HIS:HD2	1.33	0.77
1:G:95:VAL:HG22	1:G:95:VAL:O	1.85	0.77
1:N:530:ASP:OD1	1:N:531:GLU:N	2.17	0.77
1:B:42:ARG:NH1	1:B:140:GLU:HG2	2.00	0.76
1:F:206:ARG:HH12	1:F:310:GLU:HG3	1.50	0.76
1:N:566:ILE:HG22	1:N:569:MET:CE	2.15	0.76
1:B:269:MET:HG2	1:B:306:TYR:HE2	1.50	0.76
1:C:489:ILE:O	1:C:576:PRO:HD2	1.86	0.76
1:H:450:TYR:H	1:H:459:HIS:CD2	2.04	0.76
1:O:411:ARG:O	1:O:415:ILE:HD12	1.84	0.76
1:R:450:TYR:N	1:R:459:HIS:HD2	1.80	0.76
1:A:67:HIS:CE1	1:A:91:THR:HG22	2.20	0.76
1:D:80:LEU:HB3	1:D:509:PHE:CE1	2.19	0.76
1:I:141:VAL:O	1:I:141:VAL:HG12	1.85	0.76
1:R:478:ARG:HH21	1:R:478:ARG:HG2	1.50	0.76
1:L:467:GLU:HG3	1:L:555:GLY:O	1.86	0.76
1:D:291:ASN:H	1:D:292:LYS:NZ	1.84	0.76
1:M:278:ASN:O	1:M:280:THR:HG22	1.85	0.76
1:I:273:ILE:HD12	1:I:275:MET:HE1	1.67	0.76
1:H:497:GLN:HE21	1:H:497:GLN:N	1.83	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:227:ARG:NH2	1:I:261:SER:O	2.19	0.75
1:M:222:LYS:O	1:M:225:GLU:HG2	1.86	0.75
1:K:480:GLU:OE2	1:K:482:HIS:HD2	1.67	0.75
1:F:218:LEU:HD12	1:F:303:GLN:HB3	1.67	0.75
1:C:4:GLU:OE2	1:C:13:ARG:HD3	1.86	0.75
1:Q:232:PRO:CG	1:Q:290:LYS:HE2	2.17	0.75
1:N:566:ILE:CG2	1:N:569:MET:HE3	2.16	0.75
1:Q:276:ASP:O	1:Q:277:ARG:HB2	1.87	0.75
1:I:568:ASN:O	1:I:572:SER:OG	2.03	0.75
1:M:412:PHE:HE2	1:M:451:MET:HG2	1.51	0.75
1:Q:480:GLU:HG3	1:Q:584:GLY:H	1.52	0.75
1:I:434:VAL:HG12	1:I:469:LEU:HD13	1.69	0.75
1:C:42:ARG:NH1	1:C:140:GLU:HG2	2.02	0.75
1:C:616:THR:O	1:C:619:ARG:HG2	1.85	0.75
1:H:478:ARG:HH21	1:H:478:ARG:CG	2.00	0.75
1:O:490:PRO:HB3	1:O:569:MET:HE3	1.69	0.75
1:O:442:ASP:O	1:O:478:ARG:HB2	1.87	0.75
1:I:275:MET:HA	1:I:275:MET:HE2	1.69	0.75
1:N:450:TYR:H	1:N:459:HIS:HD2	1.34	0.75
1:J:168:ARG:HG2	1:J:168:ARG:NH1	2.02	0.75
1:M:553:ILE:HG13	1:M:553:ILE:O	1.84	0.74
1:B:169:VAL:HG13	1:B:241:GLU:HG2	1.70	0.74
1:E:42:ARG:HH12	1:E:140:GLU:HG2	1.49	0.74
1:E:450:TYR:H	1:E:459:HIS:HD2	1.32	0.74
1:M:5:LYS:HA	1:O:420:ILE:HD11	1.69	0.74
1:M:615:ILE:O	1:M:617:ALA:N	2.20	0.74
1:C:4:GLU:OE2	1:C:13:ARG:CD	2.36	0.74
1:F:275:MET:CE	1:F:283:ILE:HG13	2.16	0.74
1:E:497:GLN:NE2	1:E:497:GLN:H	1.84	0.74
1:F:497:GLN:H	1:F:497:GLN:NE2	1.86	0.74
1:M:95:VAL:HG21	1:M:122:ARG:HG3	1.69	0.74
1:O:169:VAL:HG13	1:O:241:GLU:HG2	1.68	0.74
1:O:566:ILE:O	1:O:623:SER:HA	1.85	0.74
1:N:150:GLY:O	1:N:154:THR:OG1	2.06	0.74
1:R:371:LYS:O	1:R:375:ASP:OD1	2.06	0.74
1:D:67:HIS:HE1	1:D:91:THR:HG23	1.49	0.74
1:M:480:GLU:OE2	1:M:482:HIS:CD2	2.41	0.74
1:C:67:HIS:HE1	1:C:91:THR:HG22	1.53	0.74
1:O:4:GLU:OE2	1:O:13:ARG:HD3	1.88	0.74
1:R:51:LYS:HB2	1:R:51:LYS:NZ	2.02	0.73
1:H:66:VAL:N	1:H:88:ASP:OD2	2.21	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:590:THR:O	1:Q:609:GLN:NE2	2.20	0.73
1:R:384:ALA:HB3	1:R:444:VAL:HG12	1.70	0.73
1:B:314:VAL:HG22	1:B:315:GLU:H	1.53	0.73
1:M:450:TYR:N	1:M:459:HIS:HD2	1.81	0.73
1:O:382:HIS:CD2	1:O:441:PRO:HA	2.23	0.73
1:K:271:TRP:O	1:K:285:MET:HB2	1.88	0.73
1:N:566:ILE:HG21	1:N:569:MET:HE3	1.71	0.73
1:J:36:MET:HA	1:J:300:HIS:CD2	2.22	0.73
1:O:643:LYS:H	1:O:643:LYS:CD	1.99	0.73
1:L:273:ILE:HG13	1:L:275:MET:HE3	1.68	0.73
1:N:104:ARG:O	1:N:108:SER:OG	2.04	0.73
1:O:627:HIS:CB	1:O:640:GLN:HB2	2.08	0.73
1:K:550:ARG:N	1:K:560:GLN:HE22	1.87	0.73
1:L:103:ALA:O	1:L:107:THR:HB	1.89	0.73
1:Q:222:LYS:HB2	1:Q:225:GLU:HG2	1.71	0.73
1:L:378:SER:HB2	1:L:399:THR:HG22	1.71	0.73
1:I:278:ASN:O	1:I:280:THR:HG23	1.89	0.72
1:K:73:THR:OG1	1:K:76:GLY:HA2	1.89	0.72
1:H:42:ARG:NH1	1:H:140:GLU:HG2	2.04	0.72
1:H:490:PRO:CB	1:H:569:MET:CE	2.64	0.72
1:N:81:MET:O	1:N:84:ARG:O	2.07	0.72
1:B:218:LEU:H	1:B:303:GLN:NE2	1.87	0.72
1:B:392:LEU:HD23	1:B:392:LEU:O	1.89	0.72
1:M:42:ARG:NH1	1:M:140:GLU:HG3	2.04	0.72
1:M:245:LYS:HE3	1:R:337:GLY:HA2	1.70	0.72
1:B:43:ASN:H	1:B:43:ASN:HD22	1.38	0.72
1:M:412:PHE:CE2	1:M:451:MET:HG2	2.24	0.72
1:N:87:ALA:HA	1:N:88:ASP:HB2	1.69	0.72
1:D:39:ASP:OD2	1:D:298:ARG:HD3	1.88	0.72
1:H:549:LEU:HD23	1:H:637:ILE:HD13	1.70	0.72
1:M:126:VAL:H	1:M:161:ARG:NH2	1.86	0.72
1:O:190:ASN:HD21	1:O:209:GLY:HA3	1.53	0.72
1:O:497:GLN:H	1:O:497:GLN:NE2	1.87	0.72
1:P:365:PHE:O	1:P:371:LYS:CE	2.37	0.72
1:E:146:LEU:HB3	1:E:271:TRP:CD1	2.25	0.72
1:A:478:ARG:HH21	1:A:478:ARG:CG	2.03	0.72
1:Q:570:SER:HB2	1:Q:622:LYS:HD3	1.72	0.72
1:I:434:VAL:CG1	1:I:469:LEU:HD13	2.20	0.72
1:N:39:ASP:OD2	1:N:298:ARG:CD	2.38	0.72
1:E:41:ASP:C	1:E:41:ASP:OD1	2.27	0.72
1:L:497:GLN:HE21	1:L:497:GLN:H	1.35	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:203:PRO:HA	1:F:422:TYR:CD2	2.25	0.71
1:F:244:GLU:OE1	1:F:245:LYS:HG3	1.90	0.71
1:H:169:VAL:HG12	1:H:241:GLU:HG2	1.70	0.71
1:I:171:PRO:HB3	1:I:275:MET:HE2	1.70	0.71
1:Q:450:TYR:H	1:Q:459:HIS:CD2	2.07	0.71
1:F:616:THR:O	1:F:619:ARG:NH1	2.21	0.71
1:P:57:LYS:HE2	1:P:135:ASP:HB3	1.71	0.71
1:R:176:VAL:CG1	1:R:236:PHE:HB2	2.21	0.71
1:F:94:GLU:OE1	2:F:701:SAH:O2'	2.08	0.71
1:E:259:HIS:CD2	1:E:260:SER:OG	2.41	0.71
1:P:317:ASN:ND2	1:P:317:ASN:O	2.22	0.71
1:P:478:ARG:HH21	1:P:478:ARG:CG	2.03	0.71
1:Q:367:ASN:OD1	1:Q:370:PHE:HB2	1.90	0.71
1:M:91:THR:CG2	1:M:117:THR:HG23	2.14	0.71
1:N:133:ARG:HG3	1:N:164:LYS:HG3	1.73	0.71
1:E:550:ARG:H	1:E:560:GLN:HE22	1.37	0.71
1:I:450:TYR:H	1:I:459:HIS:CD2	2.03	0.71
1:M:45:LYS:O	1:M:275:MET:HG2	1.89	0.71
1:B:145:GLU:HG2	1:B:331:LEU:HD22	1.73	0.71
1:C:244:GLU:HA	1:C:244:GLU:OE2	1.91	0.71
1:M:145:GLU:HG3	1:M:331:LEU:HD13	1.72	0.71
1:I:443:ILE:HG12	1:I:445:LEU:HD13	1.73	0.71
1:Q:217:GLN:NE2	1:Q:298:ARG:O	2.14	0.71
1:N:55:ALA:HA	1:N:58:LYS:HD2	1.73	0.71
1:Q:169:VAL:HG21	1:Q:240:PHE:HB2	1.73	0.71
1:N:566:ILE:HG22	1:N:569:MET:HE2	1.70	0.70
1:J:173:THR:HG22	1:J:274:ASP:HB3	1.71	0.70
1:K:412:PHE:HE2	1:K:451:MET:HG2	1.56	0.70
1:E:595:ILE:CG2	1:E:599:GLY:HA2	2.21	0.70
1:K:420:ILE:HD11	1:K:428:VAL:HG22	1.72	0.70
1:K:547:GLU:OE2	1:K:550:ARG:NH1	2.20	0.70
1:A:490:PRO:HB3	1:A:569:MET:HE1	1.71	0.70
1:B:497:GLN:H	1:B:497:GLN:HE21	1.39	0.70
1:M:489:ILE:O	1:M:576:PRO:HD2	1.91	0.70
1:B:241:GLU:HB2	1:B:277:ARG:HH21	1.56	0.70
1:K:138:VAL:HG23	1:K:170:VAL:HB	1.71	0.70
1:M:321:GLU:O	1:M:322:ILE:HD12	1.90	0.70
1:R:291:ASN:C	1:R:292:LYS:HD2	2.12	0.70
1:B:450:TYR:N	1:B:459:HIS:HD2	1.82	0.70
1:R:489:ILE:O	1:R:576:PRO:HD2	1.91	0.70
1:I:490:PRO:HB3	1:I:569:MET:CE	2.21	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:269:MET:HG2	1:P:306:TYR:HE1	1.55	0.70
1:K:460:LEU:HB3	1:K:463:LEU:HD23	1.72	0.70
1:L:273:ILE:HG13	1:L:275:MET:CE	2.22	0.70
1:B:168:ARG:NH1	1:B:241:GLU:OE2	2.24	0.70
1:N:88:ASP:O	1:N:89:LYS:HG3	1.92	0.70
1:B:66:VAL:HG12	1:B:67:HIS:N	2.07	0.70
1:B:227:ARG:NH2	1:B:261:SER:O	2.25	0.70
1:C:95:VAL:HG21	1:C:122:ARG:HG3	1.72	0.70
1:G:39:ASP:OD2	1:G:298:ARG:HD3	1.91	0.70
1:R:269:MET:HG2	1:R:306:TYR:HE1	1.57	0.70
1:E:84:ARG:NH1	1:E:509:PHE:CZ	2.60	0.69
1:G:22:TYR:CE2	1:G:26:GLN:OE1	2.45	0.69
1:D:480:GLU:OE2	1:D:482:HIS:CD2	2.41	0.69
1:I:73:THR:OG1	1:I:76:GLY:HA2	1.92	0.69
1:R:349:LEU:HD12	1:R:415:ILE:HD13	1.74	0.69
1:G:547:GLU:OE2	1:G:550:ARG:NH2	2.24	0.69
1:H:169:VAL:CG1	1:H:241:GLU:HG2	2.22	0.69
1:I:550:ARG:H	1:I:560:GLN:HE22	1.38	0.69
1:O:233:ILE:HD11	1:O:254:ARG:HB2	1.74	0.69
1:K:169:VAL:HG13	1:K:241:GLU:CG	2.21	0.69
1:A:420:ILE:CD1	1:A:428:VAL:HG22	2.21	0.69
1:D:145:GLU:HA	1:D:269:MET:HE1	1.74	0.69
1:B:497:GLN:H	1:B:497:GLN:NE2	1.90	0.69
1:F:206:ARG:HH12	1:F:310:GLU:CG	2.06	0.69
1:J:193:PRO:HA	1:J:362:ASN:HD21	1.57	0.69
1:B:73:THR:HG22	1:B:94:GLU:HB2	1.72	0.69
1:P:278:ASN:HB2	1:P:280:THR:HG22	1.74	0.69
1:K:516:GLU:O	1:K:520:LYS:HG3	1.91	0.69
1:B:447:GLU:N	1:B:448:PRO:HA	2.08	0.69
1:G:27:GLU:HG2	1:G:96:PHE:CE1	2.26	0.69
1:H:269:MET:HG2	1:H:306:TYR:CE1	2.28	0.69
1:N:169:VAL:CG1	1:N:241:GLU:HG2	2.22	0.69
1:P:210:THR:HG21	4:P:810:HOH:O	1.93	0.69
1:J:67:HIS:HE1	1:J:91:THR:HG22	1.57	0.69
1:K:497:GLN:NE2	1:K:573:ASN:ND2	2.40	0.69
1:E:450:TYR:H	1:E:459:HIS:CD2	2.09	0.69
1:Q:42:ARG:HH12	1:Q:140:GLU:HG2	1.58	0.69
1:A:269:MET:HG2	1:A:306:TYR:HE1	1.58	0.69
1:I:210:THR:HB	4:I:807:HOH:O	1.92	0.69
1:M:51:LYS:HG2	1:M:85:GLU:HG2	1.73	0.69
1:N:87:ALA:CA	1:N:88:ASP:HB2	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:227:ARG:NH1	1:P:229:LEU:HD21	2.08	0.69
1:P:490:PRO:CB	1:P:569:MET:HE1	2.22	0.69
1:D:67:HIS:CE1	1:D:91:THR:HG23	2.28	0.69
1:H:51:LYS:CG	1:H:85:GLU:HG3	2.23	0.69
1:M:37:ILE:HG21	1:M:503:VAL:CG1	2.23	0.69
1:N:27:GLU:OE2	1:N:96:PHE:CD1	2.45	0.69
1:L:67:HIS:CE1	1:L:91:THR:CG2	2.66	0.69
1:A:434:VAL:HG12	1:A:469:LEU:HD13	1.74	0.69
1:C:39:ASP:OD2	1:C:298:ARG:HD3	1.93	0.69
1:N:566:ILE:CG2	1:N:569:MET:CE	2.70	0.69
1:C:140:GLU:HG3	1:C:140:GLU:O	1.92	0.68
1:Q:643:LYS:O	1:Q:644:SER:HB3	1.93	0.68
1:B:412:PHE:HE2	1:B:451:MET:HG2	1.58	0.68
1:G:412:PHE:HE2	1:G:451:MET:HG2	1.58	0.68
1:O:567:ASP:O	1:O:568:ASN:HB2	1.93	0.68
1:A:141:VAL:O	1:A:141:VAL:HG13	1.92	0.68
1:B:42:ARG:HH11	1:B:140:GLU:HG2	1.58	0.68
1:B:169:VAL:CG1	1:B:241:GLU:HG2	2.24	0.68
1:H:269:MET:HG2	1:H:306:TYR:HE1	1.58	0.68
2:M:701:SAH:HB1	2:M:701:SAH:H4'	1.76	0.68
1:M:145:GLU:CG	1:M:331:LEU:HD13	2.24	0.68
1:P:190:ASN:HD21	1:P:209:GLY:HA3	1.59	0.68
1:R:433:LYS:H	1:R:433:LYS:CE	2.03	0.68
1:K:84:ARG:O	1:K:85:GLU:HB2	1.93	0.68
1:K:580:GLU:HG2	1:K:589:SER:HB2	1.76	0.68
1:D:222:LYS:O	1:D:225:GLU:HB2	1.93	0.68
1:R:433:LYS:HE2	1:R:433:LYS:N	2.02	0.68
1:N:315:GLU:HB2	1:N:318:GLN:HG2	1.75	0.68
1:J:597:SER:CB	1:J:598:ALA:HB2	2.19	0.68
1:A:39:ASP:OD2	1:A:298:ARG:HD3	1.93	0.68
1:M:569:MET:HG3	1:M:624:LEU:HD11	1.74	0.68
1:Q:480:GLU:OE2	1:Q:482:HIS:HD2	1.77	0.68
1:J:42:ARG:NH1	1:J:140:GLU:HG2	2.09	0.68
1:J:480:GLU:OE2	1:J:482:HIS:CD2	2.46	0.68
1:L:280:THR:HG23	1:L:281:THR:HG22	1.74	0.68
1:D:502:ASP:OD2	1:D:616:THR:HG21	1.94	0.68
1:P:42:ARG:HH21	1:P:43:ASN:HD21	1.41	0.68
1:D:490:PRO:CB	1:D:569:MET:HE3	2.17	0.67
1:I:210:THR:CG2	4:I:809:HOH:O	2.29	0.67
1:M:522:ARG:O	1:M:526:ASP:HB2	1.94	0.67
1:N:147:ILE:HD11	1:N:331:LEU:CD1	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:264:ILE:HD11	1:Q:267:LEU:CD2	2.23	0.67
1:K:65:LYS:HA	1:K:65:LYS:HE3	1.76	0.67
1:I:177:TYR:O	1:I:269:MET:HA	1.93	0.67
1:A:497:GLN:HE21	1:A:497:GLN:N	1.87	0.67
1:B:168:ARG:HG2	1:B:168:ARG:HH11	1.59	0.67
1:H:244:GLU:CD	1:H:244:GLU:H	1.97	0.67
1:Q:137:ILE:CG1	1:Q:169:VAL:HG12	2.22	0.67
1:B:175:ASN:HD22	1:B:237:LYS:HG2	1.58	0.67
1:I:173:THR:HG22	1:I:274:ASP:HB3	1.76	0.67
1:Q:190:ASN:HD21	1:Q:209:GLY:HA3	1.59	0.67
1:A:480:GLU:CG	1:A:584:GLY:H	2.08	0.67
1:D:291:ASN:H	1:D:292:LYS:HZ3	1.41	0.67
1:C:95:VAL:CG2	1:C:122:ARG:HG3	2.25	0.67
1:M:258:ALA:HB2	1:M:314:VAL:HG13	1.77	0.67
1:D:522:ARG:O	1:D:526:ASP:HB2	1.95	0.67
1:D:497:GLN:NE2	1:D:497:GLN:N	2.25	0.67
1:D:550:ARG:H	1:D:560:GLN:HE22	1.43	0.67
1:C:618:LEU:HD23	1:C:624:LEU:HD22	1.75	0.67
1:H:478:ARG:HG2	1:H:478:ARG:NH2	2.04	0.67
1:M:214:PHE:CD2	1:M:305:VAL:HG22	2.30	0.67
1:N:63:ASP:HB2	1:N:65:LYS:N	2.05	0.67
1:O:506:VAL:O	1:O:509:PHE:HB2	1.95	0.67
1:P:152:LEU:HD22	1:P:246:ILE:HG23	1.76	0.67
1:E:565:ASN:HA	1:E:624:LEU:O	1.93	0.67
1:G:169:VAL:HG12	1:G:241:GLU:CG	2.16	0.67
1:D:42:ARG:NH1	1:D:140:GLU:CG	2.58	0.67
1:F:42:ARG:HH11	1:F:140:GLU:HG2	1.57	0.67
1:I:104:ARG:HG3	1:I:118:VAL:HB	1.76	0.67
1:M:490:PRO:HB3	1:M:569:MET:CE	2.25	0.67
1:N:497:GLN:HE21	1:N:497:GLN:H	1.41	0.67
1:F:141:VAL:O	1:F:141:VAL:HG12	1.94	0.66
1:O:444:VAL:HG13	1:O:479:VAL:HA	1.76	0.66
1:Q:480:GLU:OE2	1:Q:482:HIS:CD2	2.48	0.66
1:R:218:LEU:H	1:R:303:GLN:HE21	1.43	0.66
1:R:384:ALA:HB2	1:R:437:LEU:HD11	1.76	0.66
1:J:218:LEU:H	1:J:303:GLN:HE21	1.43	0.66
1:A:434:VAL:CG1	1:A:469:LEU:CD1	2.73	0.66
1:E:169:VAL:CG1	1:E:241:GLU:HG2	2.24	0.66
1:G:42:ARG:HH21	1:G:43:ASN:ND2	1.93	0.66
1:N:137:ILE:HD11	1:N:163:ALA:HB2	1.77	0.66
1:N:163:ALA:HB1	1:N:167:CYS:SG	2.35	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:50:LEU:O	1:R:54:ILE:HB	1.94	0.66
1:C:141:VAL:O	1:C:141:VAL:HG12	1.94	0.66
1:N:497:GLN:H	1:N:497:GLN:NE2	1.93	0.66
1:J:490:PRO:HB2	1:J:569:MET:CE	2.26	0.66
1:D:489:ILE:HG13	1:D:490:PRO:HD2	1.78	0.66
1:G:478:ARG:HH21	1:G:478:ARG:HG3	1.60	0.66
1:N:478:ARG:HH21	1:N:478:ARG:CG	2.09	0.66
1:P:506:VAL:HG23	1:P:511:LEU:HD12	1.78	0.66
1:Q:191:ASP:OD2	1:Q:194:ARG:NH1	2.29	0.66
1:R:460:LEU:HD11	1:R:637:ILE:HD11	1.78	0.66
1:J:239:ASP:OD2	1:J:242:HIS:CD2	2.49	0.66
1:E:318:GLN:OE1	1:H:368:GLN:HG2	1.96	0.66
1:I:414:ASP:O	1:I:418:LYS:HG3	1.96	0.66
1:Q:91:THR:HG22	1:Q:117:THR:HG23	1.77	0.66
1:D:193:PRO:HA	1:D:362:ASN:HD21	1.61	0.66
1:F:490:PRO:CB	1:F:569:MET:HE1	2.19	0.66
1:G:490:PRO:HB3	1:G:569:MET:HE2	1.72	0.66
1:J:490:PRO:CB	1:J:569:MET:HE2	2.26	0.66
1:I:541:VAL:HG23	1:I:601:PRO:HG3	1.78	0.66
1:M:83:ALA:HB1	1:M:112:TRP:CG	2.30	0.66
1:N:480:GLU:OE2	1:N:482:HIS:CD2	2.45	0.66
1:O:528:ILE:HD12	1:O:528:ILE:N	2.10	0.66
1:Q:69:LEU:HB3	1:Q:137:ILE:HG22	1.78	0.66
1:M:84:ARG:HD3	1:M:112:TRP:CH2	2.31	0.66
1:N:39:ASP:OD2	1:N:298:ARG:HD3	1.95	0.66
1:J:67:HIS:CE1	1:J:89:LYS:HD3	2.31	0.66
1:A:218:LEU:H	1:A:303:GLN:NE2	1.94	0.66
1:P:146:LEU:HB3	1:P:271:TRP:CD1	2.31	0.66
1:J:601:PRO:HD2	4:J:812:HOH:O	1.95	0.66
1:F:171:PRO:HB3	1:F:273:ILE:HD12	1.76	0.66
1:E:490:PRO:HB3	1:E:569:MET:HE3	1.77	0.66
1:K:349:LEU:HD11	1:K:353:LEU:HD12	1.78	0.66
1:G:559:SER:OG	1:G:632:LYS:HB2	1.95	0.65
1:N:242:HIS:O	1:N:245:LYS:HG2	1.94	0.65
1:A:141:VAL:O	1:A:141:VAL:CG1	2.44	0.65
1:A:269:MET:HG2	1:A:306:TYR:CE1	2.31	0.65
1:G:173:THR:HB	1:G:274:ASP:HB3	1.78	0.65
1:N:583:PHE:O	1:N:586:ILE:HG12	1.95	0.65
1:O:218:LEU:HD13	1:O:268:LEU:HD13	1.78	0.65
1:Q:85:GLU:O	1:Q:85:GLU:HG3	1.96	0.65
1:K:297:TRP:CD2	1:K:495:ASP:HB3	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:381:LEU:O	1:N:400:ALA:HB1	1.95	0.65
1:O:126:VAL:O	1:O:161:ARG:NH2	2.27	0.65
1:J:73:THR:HG22	1:J:94:GLU:HB2	1.77	0.65
1:D:67:HIS:CE1	1:D:91:THR:CG2	2.79	0.65
1:C:314:VAL:HG21	1:C:320:PHE:CE2	2.31	0.65
1:O:382:HIS:ND1	1:O:402:ARG:HD3	2.12	0.65
1:Q:84:ARG:O	1:Q:85:GLU:HB3	1.95	0.65
1:C:489:ILE:HD13	1:C:541:VAL:HG21	1.78	0.65
1:O:7:ASN:HD21	1:O:640:GLN:HE22	1.42	0.65
1:O:42:ARG:HH11	1:O:140:GLU:HG2	1.59	0.65
1:O:433:LYS:O	1:O:436:SER:HB2	1.97	0.65
1:Q:421:HIS:O	1:Q:424:LYS:HD3	1.97	0.65
1:R:597:SER:HA	1:R:599:GLY:H	1.62	0.65
1:D:42:ARG:HH11	1:D:140:GLU:CG	2.07	0.65
1:D:193:PRO:HA	1:D:362:ASN:ND2	2.11	0.65
1:L:168:ARG:NH2	1:L:276:ASP:O	2.28	0.65
1:A:480:GLU:OE2	1:A:482:HIS:CD2	2.49	0.65
1:C:262:GLY:O	1:C:314:VAL:HG12	1.96	0.65
1:H:623:SER:O	1:H:624:LEU:HD23	1.97	0.65
1:J:273:ILE:HG13	1:J:275:MET:HE3	1.79	0.65
1:K:250:GLU:HB2	1:K:326:HIS:NE2	2.12	0.65
1:G:42:ARG:HH21	1:G:43:ASN:HD21	1.44	0.65
1:K:283:ILE:HG23	1:K:298:ARG:HH21	1.62	0.65
1:D:616:THR:HG23	4:D:822:HOH:O	1.95	0.65
1:E:145:GLU:O	1:E:145:GLU:HG2	1.95	0.65
1:J:159:LEU:HA	1:J:163:ALA:HB3	1.79	0.65
1:K:217:GLN:HB2	1:K:536:GLU:HB3	1.78	0.65
1:D:169:VAL:HG22	1:D:171:PRO:O	1.97	0.64
1:C:314:VAL:CG2	1:C:320:PHE:HD2	2.10	0.64
1:F:368:GLN:NE2	1:F:371:LYS:HE3	2.12	0.64
1:M:359:TYR:CE2	1:M:605:LYS:HB2	2.32	0.64
1:Q:143:ASP:O	1:Q:145:GLU:N	2.30	0.64
1:R:168:ARG:NH1	1:R:241:GLU:OE2	2.29	0.64
1:D:629:LEU:HD21	1:E:438:THR:HG21	1.79	0.64
1:B:392:LEU:HD23	1:B:392:LEU:C	2.17	0.64
1:H:378:SER:HB3	1:H:383:VAL:HG11	1.79	0.64
1:H:502:ASP:OD2	1:H:616:THR:HG21	1.98	0.64
1:Q:323:VAL:HG11	1:Q:340:LYS:HE2	1.78	0.64
1:D:111:PRO:O	1:D:112:TRP:HB2	1.97	0.64
1:I:277:ARG:HG2	1:I:277:ARG:O	1.96	0.64
1:N:87:ALA:O	1:N:115:LYS:HE3	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:352:MET:HG2	1:P:412:PHE:CE2	2.32	0.64
1:P:478:ARG:HG2	1:P:478:ARG:NH2	2.11	0.64
1:N:39:ASP:OD2	1:N:298:ARG:HD2	1.98	0.64
1:Q:168:ARG:HG2	1:Q:168:ARG:NH1	2.02	0.64
1:L:317:ASN:H	1:L:317:ASN:HD22	1.44	0.64
1:A:63:ASP:OD1	1:A:63:ASP:O	2.16	0.64
1:F:565:ASN:ND2	1:F:644:SER:HB2	2.12	0.64
1:N:55:ALA:H	1:N:58:LYS:HZ2	1.45	0.64
1:N:550:ARG:H	1:N:560:GLN:HE22	1.45	0.64
1:R:280:THR:HG23	1:R:281:THR:H	1.63	0.64
1:H:61:ASN:ND2	1:H:65:LYS:O	2.28	0.64
1:N:50:LEU:O	1:N:54:ILE:CG2	2.46	0.64
1:P:4:GLU:O	1:R:420:ILE:HD11	1.98	0.64
1:K:218:LEU:HB2	1:K:303:GLN:HE21	1.62	0.64
1:G:45:LYS:O	1:G:275:MET:HG2	1.98	0.64
1:O:3:LEU:O	1:O:15:TRP:HA	1.98	0.64
1:N:462:PHE:O	1:N:466:VAL:HG23	1.98	0.64
1:B:4:GLU:OE2	1:B:13:ARG:HD3	1.98	0.64
1:C:42:ARG:HH21	1:C:43:ASN:HD21	1.46	0.64
1:G:218:LEU:H	1:G:303:GLN:NE2	1.96	0.64
1:G:474:GLY:HA3	1:G:476:GLU:OE2	1.98	0.64
1:R:176:VAL:HG13	1:R:236:PHE:HB2	1.80	0.64
1:J:218:LEU:H	1:J:303:GLN:NE2	1.96	0.64
1:A:218:LEU:HD12	1:A:303:GLN:HB2	1.80	0.63
1:P:38:LEU:HD13	1:P:498:ASN:HD22	1.63	0.63
1:P:375:ASP:O	1:P:399:THR:HG21	1.97	0.63
1:K:122:ARG:HD3	1:K:124:THR:OG1	1.98	0.63
1:C:269:MET:HG2	1:C:306:TYR:CE1	2.33	0.63
1:K:516:GLU:HG3	1:K:520:LYS:HE3	1.79	0.63
1:I:218:LEU:HD13	1:I:268:LEU:HD13	1.80	0.63
1:I:497:GLN:HE21	1:I:497:GLN:H	0.77	0.63
1:M:83:ALA:HB1	1:M:112:TRP:CB	2.28	0.63
1:P:141:VAL:O	1:P:141:VAL:HG12	1.96	0.63
1:L:450:TYR:H	1:L:459:HIS:HD2	1.45	0.63
1:L:168:ARG:HH11	1:L:168:ARG:CG	2.11	0.63
1:A:480:GLU:OE2	1:A:482:HIS:HD2	1.80	0.63
1:M:43:ASN:HD22	1:M:43:ASN:N	1.96	0.63
1:K:46:PHE:CE2	1:K:140:GLU:HB2	2.33	0.63
1:K:68:VAL:CG2	1:K:136:ILE:HB	2.26	0.63
1:E:103:ALA:O	1:E:107:THR:HB	1.97	0.63
1:H:84:ARG:O	1:H:85:GLU:HB2	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:ASN:HD22	1:A:109:ASN:N	1.96	0.63
1:I:543:GLY:HA3	1:I:568:ASN:ND2	2.14	0.63
1:O:218:LEU:H	1:O:303:GLN:HE21	1.43	0.63
1:R:497:GLN:HE21	1:R:497:GLN:H	1.44	0.63
1:K:624:LEU:H	1:K:624:LEU:HD12	1.64	0.63
1:B:41:ASP:O	1:B:44:ASP:N	2.30	0.63
1:H:156:LYS:O	1:H:160:GLU:HG2	1.98	0.63
1:M:434:VAL:CG1	1:M:469:LEU:HD13	2.28	0.63
1:Q:169:VAL:HG23	1:Q:172:SER:HA	1.79	0.63
1:Q:528:ILE:HD13	1:Q:639:PHE:O	1.99	0.63
1:L:577:MET:HE2	1:L:626:LEU:HD11	1.80	0.63
1:C:103:ALA:O	1:C:107:THR:HB	1.99	0.63
1:E:176:VAL:HG13	1:E:236:PHE:HB2	1.81	0.63
1:Q:73:THR:OG1	1:Q:76:GLY:HA2	1.98	0.63
1:K:169:VAL:HG22	1:K:171:PRO:O	1.99	0.63
1:I:193:PRO:HA	1:I:362:ASN:HD21	1.63	0.62
1:A:577:MET:HE1	1:A:639:PHE:CE1	2.33	0.62
1:I:171:PRO:HB3	1:I:275:MET:CE	2.29	0.62
1:K:141:VAL:O	1:K:141:VAL:CG1	2.47	0.62
1:C:353:LEU:HD22	1:C:357:THR:HG21	1.81	0.62
1:E:135:ASP:OD1	1:E:164:LYS:HD2	2.00	0.62
1:H:42:ARG:HH21	1:H:43:ASN:HD21	1.47	0.62
1:I:63:ASP:OD2	1:I:65:LYS:HB2	2.00	0.62
1:I:534:LEU:HD11	1:I:576:PRO:HB3	1.80	0.62
1:G:161:ARG:HB2	1:G:162:LEU:HD22	1.82	0.62
1:I:157:GLU:HA	1:I:160:GLU:HG2	1.81	0.62
1:K:510:ASP:OD2	1:K:512:SER:HB3	1.99	0.62
1:I:420:ILE:CD1	1:I:428:VAL:HG22	2.29	0.62
1:O:112:TRP:CZ3	1:O:509:PHE:HE1	2.18	0.62
1:C:191:ASP:OD2	1:C:194:ARG:NH1	2.32	0.62
1:G:72:GLY:O	2:G:701:SAH:N	2.31	0.62
1:I:178:ILE:HA	1:I:268:LEU:O	1.98	0.62
1:M:382:HIS:CD2	1:M:402:ARG:HG3	2.34	0.62
1:R:467:GLU:HG3	1:R:556:ARG:HD2	1.81	0.62
1:F:42:ARG:HH21	1:F:43:ASN:HD21	1.48	0.62
1:M:356:GLN:O	1:M:359:TYR:HB3	1.99	0.62
1:N:54:ILE:HD11	1:N:87:ALA:N	2.14	0.62
1:K:108:SER:O	1:K:113:SER:HB2	1.99	0.62
1:L:506:VAL:HG12	1:L:507:ASN:HD22	1.64	0.62
1:D:168:ARG:HG2	1:D:168:ARG:NH1	2.07	0.62
1:C:194:ARG:HB3	1:C:201:GLU:OE1	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:274:ASP:HA	1:E:282:PHE:HD1	1.64	0.62
1:H:51:LYS:HG3	1:H:85:GLU:HG3	1.81	0.62
1:R:356:GLN:O	1:R:606:GLY:HA2	2.00	0.62
1:I:26:GLN:CG	1:I:30:ARG:HH12	1.99	0.62
1:N:218:LEU:H	1:N:303:GLN:NE2	1.98	0.62
1:Q:97:LYS:HB2	1:Q:98:PRO:HD3	1.80	0.62
1:Q:379:LYS:HA	1:Q:399:THR:OG1	2.00	0.62
1:J:39:ASP:OD2	1:J:298:ARG:CD	2.43	0.62
1:D:622:LYS:HD3	1:D:622:LYS:H	1.64	0.62
1:I:176:VAL:HG22	1:I:235:ALA:HB3	1.82	0.62
1:I:292:LYS:HG2	1:I:293:ASN:HA	1.79	0.62
1:N:379:LYS:CA	1:N:399:THR:HG22	2.18	0.62
1:P:227:ARG:HH12	1:P:229:LEU:HD21	1.64	0.62
1:K:167:CYS:SG	1:K:168:ARG:N	2.73	0.62
1:G:108:SER:O	1:G:109:ASN:HB2	2.01	0.61
1:N:133:ARG:CG	1:N:164:LYS:HG3	2.29	0.61
1:L:379:LYS:CA	1:L:399:THR:HG23	2.28	0.61
1:C:337:GLY:O	1:C:338:LYS:HD2	2.00	0.61
1:F:259:HIS:HD2	1:F:260:SER:OG	1.83	0.61
1:E:497:GLN:H	1:E:497:GLN:HE21	1.46	0.61
1:I:480:GLU:OE2	1:I:482:HIS:HD2	1.83	0.61
1:N:565:ASN:ND2	1:N:644:SER:OG	2.32	0.61
1:K:250:GLU:HB2	1:K:326:HIS:CD2	2.33	0.61
1:D:622:LYS:HD3	1:D:622:LYS:N	2.15	0.61
1:F:243:GLU:HA	1:F:246:ILE:HD12	1.82	0.61
1:G:95:VAL:O	1:G:95:VAL:CG2	2.47	0.61
1:P:352:MET:HG2	1:P:412:PHE:CZ	2.35	0.61
1:J:563:VAL:HG13	1:J:625:CYS:SG	2.40	0.61
1:K:445:LEU:HD12	1:K:480:GLU:HB2	1.81	0.61
1:O:548:ILE:O	1:O:549:LEU:HD13	2.01	0.61
1:Q:417:PHE:CZ	1:Q:430:ILE:HB	2.36	0.61
1:J:470:LYS:HD2	1:J:554:ASP:O	2.00	0.61
1:L:577:MET:HE3	1:L:641:PHE:CZ	2.23	0.61
1:B:39:ASP:OD2	1:B:298:ARG:CD	2.45	0.61
1:M:3:LEU:HD22	1:O:418:LYS:HA	1.83	0.61
1:N:218:LEU:HD12	1:N:303:GLN:HB2	1.81	0.61
1:P:550:ARG:H	1:P:560:GLN:HE22	1.47	0.61
1:K:77:LEU:HD22	1:K:511:LEU:HD11	1.83	0.61
1:K:573:ASN:O	1:K:614:PRO:HD2	1.99	0.61
1:C:5:LYS:NZ	1:C:14:GLU:OE1	2.34	0.61
1:G:218:LEU:H	1:G:303:GLN:HE21	1.48	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:216:VAL:O	1:C:302:MET:HG2	2.00	0.61
1:M:42:ARG:HA	1:M:283:ILE:HD11	1.82	0.61
1:N:444:VAL:CG1	1:N:479:VAL:HB	2.24	0.61
1:K:475:ASP:OD1	1:K:475:ASP:N	2.33	0.61
1:O:587:ASN:HD22	1:O:588:LEU:N	1.98	0.61
1:Q:92:ALA:HB3	1:Q:118:VAL:HG23	1.83	0.61
1:Q:460:LEU:HB3	1:Q:463:LEU:HD23	1.81	0.61
1:R:275:MET:HE1	1:R:283:ILE:HG13	1.82	0.61
1:J:189:PHE:CE1	1:J:359:TYR:HB2	2.36	0.61
1:K:39:ASP:O	1:K:42:ARG:HB3	2.01	0.61
1:L:133:ARG:HB2	1:L:164:LYS:HG3	1.81	0.61
1:B:447:GLU:H	1:B:448:PRO:HA	1.64	0.61
1:E:241:GLU:HG3	1:E:277:ARG:HH21	1.65	0.61
1:M:196:ASN:HB2	1:M:201:GLU:OE2	2.01	0.61
1:Q:35:ASP:OD1	1:Q:299:ASP:HB3	2.01	0.61
1:J:67:HIS:HE1	1:J:91:THR:CG2	2.14	0.61
1:B:269:MET:HG2	1:B:306:TYR:CE2	2.35	0.60
1:F:218:LEU:N	1:F:303:GLN:NE2	2.34	0.60
1:H:190:ASN:HD21	1:H:209:GLY:HA3	1.66	0.60
1:Q:69:LEU:HD12	1:Q:91:THR:OG1	2.02	0.60
1:J:182:GLU:HG3	1:J:263:THR:O	2.01	0.60
1:A:480:GLU:HG3	1:A:481:PRO:HA	1.84	0.60
1:E:511:LEU:O	1:E:514:PHE:N	2.30	0.60
1:H:420:ILE:HD11	1:H:428:VAL:HG22	1.83	0.60
1:O:275:MET:HE1	1:O:283:ILE:H	1.66	0.60
1:P:5:LYS:NZ	1:P:14:GLU:OE1	2.34	0.60
1:R:146:LEU:HB2	1:R:271:TRP:CD1	2.35	0.60
1:I:273:ILE:CD1	1:I:275:MET:HE1	2.31	0.60
1:M:182:GLU:OE2	1:M:227:ARG:NH1	2.34	0.60
1:M:478:ARG:CG	1:M:478:ARG:NH2	2.50	0.60
1:K:241:GLU:HB2	1:K:277:ARG:HH21	1.65	0.60
1:A:291:ASN:H	1:A:292:LYS:NZ	1.99	0.60
1:C:460:LEU:HB3	1:C:463:LEU:HD23	1.83	0.60
1:E:72:GLY:HA3	2:E:701:SAH:O4'	2.01	0.60
1:E:258:ALA:O	1:E:317:ASN:HA	2.01	0.60
1:I:502:ASP:OD2	1:I:616:THR:HG21	2.01	0.60
1:P:365:PHE:O	1:P:371:LYS:HE3	2.01	0.60
1:R:562:CYS:SG	1:R:564:VAL:HG13	2.42	0.60
1:A:45:LYS:O	1:A:275:MET:HG2	2.02	0.60
1:F:196:ASN:O	1:F:198:GLU:N	2.33	0.60
1:M:143:ASP:HB3	1:M:149:GLU:OE1	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:114:ASP:HB3	1:B:65:LYS:NZ	2.16	0.60
1:A:185:LEU:O	1:A:188:MET:HB2	2.01	0.60
1:R:203:PRO:HA	1:R:422:TYR:CG	2.37	0.60
1:L:577:MET:CE	1:L:626:LEU:HD11	2.31	0.60
1:C:168:ARG:NH2	1:C:276:ASP:O	2.34	0.60
1:N:54:ILE:C	1:N:58:LYS:NZ	2.55	0.60
1:O:135:ASP:OD1	1:O:164:LYS:HD2	2.02	0.60
1:J:91:THR:HG21	1:J:129:ILE:CG2	2.32	0.60
1:J:597:SER:CB	1:J:598:ALA:CB	2.77	0.60
1:L:446:ALA:O	1:L:481:PRO:HD3	2.01	0.60
1:A:577:MET:CE	1:A:639:PHE:CE1	2.84	0.60
1:C:489:ILE:CD1	1:C:541:VAL:HG21	2.31	0.60
1:G:169:VAL:HG13	1:G:172:SER:HA	1.82	0.60
1:Q:95:VAL:HB	1:Q:122:ARG:HG3	1.84	0.60
1:Q:583:PHE:HB3	1:Q:588:LEU:HD12	1.82	0.60
1:J:141:VAL:HG13	1:J:141:VAL:O	2.00	0.60
1:D:622:LYS:H	1:D:622:LYS:CD	2.15	0.60
1:C:547:GLU:OE1	1:C:550:ARG:NH1	2.35	0.60
1:I:470:LYS:O	1:I:473:HIS:O	2.20	0.60
1:M:218:LEU:H	1:M:303:GLN:NE2	2.00	0.60
1:N:36:MET:HA	1:N:300:HIS:CD2	2.36	0.60
1:Q:480:GLU:CG	1:Q:584:GLY:H	2.14	0.60
1:B:66:VAL:HG12	1:B:67:HIS:H	1.66	0.59
1:B:480:GLU:OE2	1:B:482:HIS:HD2	1.86	0.59
1:P:84:ARG:C	1:P:86:GLY:H	2.05	0.59
1:J:243:GLU:H	1:J:243:GLU:CD	2.00	0.59
1:B:490:PRO:CB	1:B:569:MET:CE	2.60	0.59
1:K:373:GLU:OE1	1:K:373:GLU:HA	2.02	0.59
1:D:434:VAL:CG1	1:D:469:LEU:CD1	2.80	0.59
1:F:142:PHE:CD1	1:F:146:LEU:HD12	2.37	0.59
1:G:22:TYR:HE2	1:G:26:GLN:OE1	1.83	0.59
1:N:168:ARG:HG2	1:N:168:ARG:NH1	2.13	0.59
1:Q:77:LEU:HA	1:Q:80:LEU:HD12	1.83	0.59
1:Q:550:ARG:H	1:Q:560:GLN:HE21	1.50	0.59
1:B:54:ILE:O	1:B:58:LYS:HG2	2.03	0.59
1:G:434:VAL:CG1	1:G:469:LEU:HD13	2.32	0.59
1:M:492:LYS:HB2	1:M:572:SER:HA	1.84	0.59
1:P:310:GLU:OE2	1:P:338:LYS:HD2	2.02	0.59
1:Q:480:GLU:HG3	1:Q:584:GLY:N	2.18	0.59
1:R:175:ASN:HD21	1:R:237:LYS:HG2	1.66	0.59
1:D:143:ASP:OD2	1:D:148:GLY:HA3	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:379:LYS:CA	1:D:399:THR:CG2	2.80	0.59
1:C:291:ASN:HB3	1:C:295:TYR:HB2	1.83	0.59
1:F:451:MET:HG3	1:F:452:SER:N	2.18	0.59
1:M:84:ARG:HD3	1:M:112:TRP:HH2	1.66	0.59
1:P:190:ASN:ND2	1:P:209:GLY:HA3	2.17	0.59
1:Q:73:THR:O	2:Q:701:SAH:HA	2.02	0.59
1:L:126:VAL:HG11	1:L:129:ILE:HD13	1.85	0.59
1:A:67:HIS:HE1	1:A:91:THR:HG23	1.66	0.59
1:A:497:GLN:NE2	1:A:497:GLN:N	2.46	0.59
1:B:476:GLU:CD	1:B:476:GLU:H	2.05	0.59
1:I:269:MET:HG2	1:I:306:TYR:HE1	1.68	0.59
1:Q:231:GLU:O	1:Q:232:PRO:C	2.39	0.59
1:R:556:ARG:CG	1:R:556:ARG:NH1	2.62	0.59
1:H:52:THR:O	1:H:55:ALA:HB3	2.02	0.59
1:N:142:PHE:CD1	1:N:146:LEU:CD1	2.85	0.59
1:K:190:ASN:HD21	1:K:209:GLY:HA3	1.67	0.59
1:C:84:ARG:NH1	1:O:280:THR:HG23	2.18	0.59
1:F:42:ARG:HH12	1:F:140:GLU:HG2	1.62	0.59
1:N:275:MET:HE1	1:N:283:ILE:N	2.17	0.59
1:P:138:VAL:HG23	1:P:170:VAL:HB	1.83	0.59
1:P:156:LYS:O	1:P:160:GLU:HG2	2.02	0.59
1:B:41:ASP:O	1:B:42:ARG:C	2.41	0.59
1:I:35:ASP:OD1	1:I:300:HIS:HD2	1.86	0.59
1:M:84:ARG:HG2	1:M:85:GLU:OE1	2.01	0.59
1:M:141:VAL:O	1:M:141:VAL:HG12	2.02	0.59
1:N:54:ILE:HD11	1:N:87:ALA:H	1.67	0.59
1:Q:102:CYS:HA	1:Q:513:PHE:HE2	1.68	0.59
1:M:32:ARG:HG3	1:M:34:GLY:H	1.68	0.59
1:M:379:LYS:CA	1:M:399:THR:CG2	2.80	0.59
1:N:254:ARG:O	1:N:321:GLU:CA	2.49	0.59
1:O:67:HIS:HE1	1:O:91:THR:OG1	1.86	0.59
1:P:5:LYS:CA	1:R:420:ILE:HD11	2.33	0.59
1:Q:583:PHE:CB	1:Q:588:LEU:HD12	2.33	0.59
1:B:245:LYS:HE3	1:E:337:GLY:HA2	1.85	0.58
1:M:280:THR:HG23	1:M:281:THR:N	2.18	0.58
1:O:373:GLU:HG3	1:O:377:LEU:CD1	2.32	0.58
1:Q:258:ALA:O	1:Q:259:HIS:HB3	2.03	0.58
1:Q:365:PHE:O	1:Q:371:LYS:HE3	2.03	0.58
1:Q:375:ASP:HA	1:Q:399:THR:CG2	2.18	0.58
1:R:181:VAL:HG22	1:R:228:GLU:HA	1.85	0.58
1:K:53:THR:HG22	1:K:168:ARG:HE	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:486:LEU:HD12	1:C:548:ILE:HB	1.85	0.58
1:P:241:GLU:CG	1:P:277:ARG:HH21	2.10	0.58
1:P:367:ASN:OD1	1:P:369:LYS:HG2	2.02	0.58
1:R:491:GLU:HG2	1:R:493:PHE:CD2	2.38	0.58
1:J:4:GLU:OE2	1:J:13:ARG:HD3	2.02	0.58
1:L:497:GLN:H	1:L:497:GLN:NE2	2.01	0.58
1:A:434:VAL:HG12	1:A:469:LEU:CD1	2.34	0.58
1:M:37:ILE:HG21	1:M:503:VAL:HG11	1.85	0.58
1:M:176:VAL:HG21	1:M:236:PHE:HD2	1.68	0.58
1:B:140:GLU:OE1	1:B:301:TRP:HZ2	1.86	0.58
1:M:110:SER:HB2	1:M:111:PRO:CD	2.31	0.58
1:M:490:PRO:HB3	1:M:569:MET:HE2	1.85	0.58
1:N:490:PRO:HB3	1:N:569:MET:HE1	1.85	0.58
1:K:39:ASP:OD1	1:K:298:ARG:NH1	2.36	0.58
1:E:142:PHE:CD1	1:E:146:LEU:HD12	2.39	0.58
1:E:218:LEU:H	1:E:303:GLN:NE2	2.00	0.58
1:O:168:ARG:NH2	1:O:276:ASP:O	2.33	0.58
1:O:245:LYS:HD3	1:P:337:GLY:HA2	1.86	0.58
1:P:497:GLN:NE2	1:P:497:GLN:H	2.01	0.58
1:Q:497:GLN:NE2	1:Q:497:GLN:H	2.02	0.58
1:J:451:MET:HG3	1:J:452:SER:N	2.18	0.58
1:L:577:MET:CE	1:L:641:PHE:CZ	2.80	0.58
1:F:522:ARG:O	1:F:526:ASP:HB2	2.04	0.58
1:H:83:ALA:C	1:H:84:ARG:O	2.39	0.58
1:H:385:THR:HG22	4:H:820:HOH:O	2.04	0.58
1:N:184:HIS:O	1:N:188:MET:HG3	2.03	0.58
1:O:370:PHE:HE1	1:O:588:LEU:CD2	2.17	0.58
1:P:146:LEU:H	1:P:146:LEU:CD2	2.12	0.58
1:R:180:PRO:HD2	1:R:230:SER:HB3	1.84	0.58
1:E:383:VAL:HG21	1:E:445:LEU:HD22	1.84	0.58
1:M:169:VAL:HG11	1:M:241:GLU:HA	1.86	0.58
1:N:58:LYS:CE	1:N:66:VAL:HG21	2.31	0.58
1:Q:222:LYS:CB	1:Q:224:HIS:HB3	2.33	0.58
1:J:403:VAL:HB	1:J:428:VAL:HB	1.85	0.58
1:G:385:THR:HG21	1:G:405:ILE:HG23	1.86	0.58
1:H:141:VAL:HG13	1:H:141:VAL:O	2.04	0.58
1:N:53:THR:O	1:N:58:LYS:NZ	2.37	0.58
1:P:541:VAL:HG23	1:P:601:PRO:HG3	1.84	0.58
1:Q:39:ASP:OD2	1:Q:298:ARG:HB3	2.04	0.58
1:F:168:ARG:HA	1:F:241:GLU:OE2	2.04	0.58
1:F:206:ARG:NH1	1:F:310:GLU:HG3	2.17	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:36:MET:HB3	1:M:300:HIS:CG	2.39	0.58
1:N:354:SER:OG	1:N:357:THR:OG1	2.21	0.58
1:O:497:GLN:HE21	1:O:497:GLN:N	1.95	0.58
1:P:7:ASN:HD21	1:P:640:GLN:HE22	1.51	0.58
1:R:530:ASP:O	1:R:610:GLY:HA2	2.04	0.58
1:C:68:VAL:HB	1:C:90:VAL:HG22	1.85	0.58
1:F:373:GLU:OE2	1:F:585:GLY:N	2.26	0.58
1:E:317:ASN:ND2	1:E:317:ASN:N	2.41	0.58
1:G:66:VAL:CG1	1:G:87:ALA:HA	2.34	0.58
1:I:478:ARG:HH21	1:I:478:ARG:CG	2.16	0.58
1:O:112:TRP:HZ3	1:O:509:PHE:HE1	1.52	0.58
1:Q:110:SER:HB2	1:Q:111:PRO:CD	2.34	0.58
1:R:80:LEU:HB3	1:R:509:PHE:CD1	2.39	0.58
1:L:480:GLU:OE2	1:L:482:HIS:HD2	1.87	0.58
1:B:94:GLU:OE2	2:B:701:SAH:O3'	2.22	0.57
1:E:140:GLU:O	1:E:140:GLU:HG3	2.04	0.57
1:I:157:GLU:HA	1:I:160:GLU:CG	2.34	0.57
1:I:278:ASN:O	1:I:280:THR:N	2.37	0.57
1:M:37:ILE:HG21	1:M:503:VAL:HG13	1.85	0.57
1:N:242:HIS:HB3	1:N:245:LYS:CD	2.34	0.57
1:O:80:LEU:HB3	1:O:509:PHE:CZ	2.38	0.57
1:Q:122:ARG:HH21	1:Q:124:THR:HG21	1.69	0.57
1:B:480:GLU:OE2	1:B:482:HIS:CD2	2.57	0.57
1:M:67:HIS:CD2	1:M:133:ARG:O	2.56	0.57
1:O:194:ARG:HG2	1:O:201:GLU:CB	2.34	0.57
1:K:84:ARG:HB2	1:K:112:TRP:CE2	2.39	0.57
1:L:403:VAL:HB	1:L:428:VAL:HB	1.85	0.57
1:A:269:MET:CG	1:A:306:TYR:HE1	2.17	0.57
1:A:490:PRO:CB	1:A:569:MET:CE	2.64	0.57
1:E:383:VAL:HB	1:E:443:ILE:HG23	1.84	0.57
1:P:45:LYS:HG2	1:P:282:PHE:O	2.04	0.57
1:Q:150:GLY:O	1:Q:154:THR:OG1	2.22	0.57
1:J:144:THR:O	1:J:269:MET:CE	2.53	0.57
1:J:618:LEU:HG	1:J:624:LEU:HD22	1.86	0.57
1:K:179:VAL:HG21	1:K:270:TRP:CH2	2.39	0.57
1:D:50:LEU:O	1:D:54:ILE:HG13	2.05	0.57
1:D:373:GLU:OE2	1:D:585:GLY:N	2.26	0.57
1:C:288:LYS:O	1:C:290:LYS:N	2.37	0.57
1:G:81:MET:O	1:G:84:ARG:HB3	2.04	0.57
1:M:95:VAL:HG13	1:M:96:PHE:N	2.19	0.57
1:O:193:PRO:HA	1:O:362:ASN:HD21	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:253:VAL:CG2	1:P:253:VAL:O	2.52	0.57
1:L:434:VAL:CG1	1:L:469:LEU:HD13	2.35	0.57
1:L:541:VAL:HG11	1:L:595:ILE:HD13	1.86	0.57
1:A:155:PHE:O	1:A:159:LEU:HG	2.04	0.57
1:D:43:ASN:HB3	1:D:507:ASN:HD21	1.68	0.57
1:F:141:VAL:O	1:F:141:VAL:CG1	2.51	0.57
1:E:439:ASP:N	1:E:439:ASP:OD1	2.36	0.57
1:H:77:LEU:HD13	1:H:511:LEU:HD11	1.86	0.57
1:M:32:ARG:HG3	1:M:34:GLY:N	2.19	0.57
1:O:141:VAL:O	1:O:141:VAL:HG13	2.05	0.57
1:O:557:VAL:HG22	1:O:632:LYS:HB2	1.85	0.57
1:Q:239:ASP:OD1	1:Q:241:GLU:HB2	2.03	0.57
1:J:158:ALA:HA	1:J:162:LEU:CD2	2.30	0.57
1:J:274:ASP:OD2	1:J:277:ARG:HA	2.04	0.57
1:K:548:ILE:HG22	1:K:549:LEU:HD22	1.87	0.57
1:A:168:ARG:NH2	1:A:276:ASP:O	2.37	0.57
1:A:291:ASN:H	1:A:292:LYS:HZ3	1.53	0.57
1:A:379:LYS:HA	1:A:399:THR:HG23	1.86	0.57
1:I:169:VAL:HG22	1:I:171:PRO:O	2.04	0.57
1:O:419:TYR:O	1:O:420:ILE:C	2.42	0.57
1:Q:236:PHE:CZ	1:Q:324:CYS:HB3	2.40	0.57
1:J:497:GLN:NE2	1:J:497:GLN:N	2.51	0.57
1:L:187:LYS:O	1:L:191:ASP:HB2	2.03	0.57
1:L:239:ASP:OD1	1:L:277:ARG:NH2	2.36	0.57
1:C:269:MET:HG2	1:C:306:TYR:HE1	1.69	0.57
1:M:353:LEU:HD22	1:M:357:THR:HG21	1.87	0.57
1:M:493:PHE:HA	1:M:539:GLY:HA3	1.86	0.57
1:O:173:THR:CG2	1:O:174:GLY:N	2.68	0.57
1:P:123:SER:HB3	2:P:701:SAH:HN62	1.69	0.57
1:K:140:GLU:HG3	1:K:140:GLU:O	2.04	0.57
1:F:506:VAL:HG12	1:F:507:ASN:HD22	1.70	0.57
1:O:7:ASN:HB2	1:O:14:GLU:CD	2.24	0.57
1:O:420:ILE:HG13	1:O:421:HIS:N	2.19	0.57
1:P:221:MET:HG2	1:P:226:PHE:CD1	2.39	0.57
1:R:622:LYS:HD2	1:R:622:LYS:N	2.17	0.57
1:J:67:HIS:CE1	1:J:91:THR:CG2	2.87	0.57
1:J:129:ILE:O	1:J:130:GLY:C	2.43	0.57
1:L:56:GLU:OE1	1:L:168:ARG:HD2	2.04	0.57
1:M:192:ILE:O	1:M:194:ARG:HD3	2.05	0.57
1:M:541:VAL:CG2	1:M:601:PRO:HG3	2.35	0.57
1:O:56:GLU:O	1:O:60:GLU:HG2	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:77:LEU:HD13	1:O:511:LEU:HD11	1.86	0.57
1:O:485:VAL:HG21	1:O:547:GLU:HG2	1.87	0.57
1:Q:356:GLN:NE2	1:Q:608:LYS:HE3	2.20	0.57
1:J:67:HIS:HD2	1:J:133:ARG:O	1.86	0.57
1:D:111:PRO:O	1:D:112:TRP:CB	2.52	0.57
1:G:480:GLU:OE2	1:G:482:HIS:HD2	1.88	0.57
1:Q:447:GLU:N	1:Q:448:PRO:HA	2.20	0.57
1:L:193:PRO:HA	1:L:362:ASN:HD21	1.70	0.57
1:B:68:VAL:HG22	1:B:136:ILE:HD12	1.86	0.56
1:C:490:PRO:CB	1:C:569:MET:HE3	2.30	0.56
1:F:335:ASN:N	1:F:335:ASN:OD1	2.37	0.56
1:E:67:HIS:HE1	1:E:91:THR:CG2	2.11	0.56
1:N:140:GLU:OE1	1:N:301:TRP:HZ2	1.87	0.56
1:P:549:LEU:HD12	1:P:560:GLN:NE2	2.18	0.56
1:R:353:LEU:HD22	1:R:357:THR:HG21	1.87	0.56
1:K:283:ILE:HG23	1:K:298:ARG:NH2	2.20	0.56
1:K:356:GLN:O	1:K:359:TYR:HB3	2.04	0.56
1:L:460:LEU:HD21	1:L:579:MET:HE1	1.87	0.56
1:E:490:PRO:CB	1:E:569:MET:CE	2.79	0.56
1:R:622:LYS:H	1:R:622:LYS:CD	2.16	0.56
1:B:314:VAL:HG21	1:B:320:PHE:CD1	2.40	0.56
1:B:534:LEU:HD21	1:B:611:VAL:HG11	1.88	0.56
1:F:218:LEU:N	1:F:303:GLN:HE21	1.94	0.56
1:F:383:VAL:HG13	1:F:403:VAL:HG22	1.86	0.56
1:I:460:LEU:HB3	1:I:463:LEU:HD22	1.88	0.56
1:M:300:HIS:CE1	1:M:301:TRP:CD2	2.93	0.56
1:N:168:ARG:HH11	1:N:168:ARG:CG	2.13	0.56
1:N:280:THR:OG1	1:N:281:THR:HG22	2.04	0.56
1:Q:255:GLU:OE1	1:Q:319:THR:HG22	2.05	0.56
1:Q:289:TRP:O	1:Q:289:TRP:HE3	1.88	0.56
1:Q:491:GLU:OE1	1:Q:539:GLY:HA3	2.05	0.56
1:R:45:LYS:O	1:R:275:MET:HG2	2.05	0.56
1:R:52:THR:HG21	1:R:276:ASP:HB2	1.87	0.56
1:R:181:VAL:HG11	1:R:226:PHE:HB2	1.88	0.56
1:R:297:TRP:CE3	1:R:495:ASP:HB3	2.40	0.56
1:K:145:GLU:HG3	1:K:331:LEU:HD22	1.87	0.56
1:L:317:ASN:H	1:L:317:ASN:ND2	2.03	0.56
1:E:379:LYS:CA	1:E:399:THR:CG2	2.81	0.56
1:O:616:THR:OG1	1:O:617:ALA:N	2.39	0.56
1:Q:516:GLU:O	1:Q:520:LYS:HG3	2.05	0.56
1:R:80:LEU:HD13	1:R:509:PHE:HB3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:480:GLU:OE2	1:L:482:HIS:CD2	2.58	0.56
1:M:3:LEU:O	1:M:15:TRP:HA	2.05	0.56
1:M:37:ILE:CG2	1:M:503:VAL:HG13	2.36	0.56
1:M:169:VAL:CG1	1:M:241:GLU:HA	2.35	0.56
1:O:444:VAL:CG1	1:O:479:VAL:HA	2.35	0.56
1:O:624:LEU:HB2	1:O:643:LYS:HA	1.86	0.56
1:Q:356:GLN:HE22	1:Q:608:LYS:HE3	1.71	0.56
1:J:556:ARG:O	1:J:556:ARG:HG2	2.04	0.56
1:K:133:ARG:HB2	1:K:164:LYS:HG3	1.87	0.56
1:K:218:LEU:CD1	1:K:268:LEU:HD22	2.36	0.56
1:L:114:ASP:OD1	1:L:114:ASP:N	2.35	0.56
1:L:168:ARG:HH12	1:L:241:GLU:CD	2.08	0.56
1:C:288:LYS:C	1:C:290:LYS:H	2.08	0.56
1:F:145:GLU:HG2	1:F:331:LEU:HD22	1.87	0.56
1:I:141:VAL:O	1:I:141:VAL:CG1	2.52	0.56
1:N:179:VAL:HG22	1:N:232:PRO:HA	1.87	0.56
1:K:354:SER:O	1:K:358:VAL:HG23	2.05	0.56
1:A:73:THR:HG22	1:A:94:GLU:HB2	1.87	0.56
1:C:490:PRO:HB3	1:C:569:MET:HE2	1.84	0.56
1:C:522:ARG:O	1:C:526:ASP:HB2	2.05	0.56
1:M:7:ASN:HB2	1:M:14:GLU:OE1	2.05	0.56
1:R:310:GLU:OE1	1:R:338:LYS:HG3	2.06	0.56
1:R:437:LEU:O	1:R:473:HIS:NE2	2.38	0.56
1:J:273:ILE:HG13	1:J:275:MET:CE	2.36	0.56
1:K:30:ARG:NH1	1:K:526:ASP:OD1	2.39	0.56
1:K:502:ASP:CG	1:K:616:THR:HG21	2.25	0.56
1:A:218:LEU:H	1:A:303:GLN:HE21	1.52	0.56
1:C:517:ILE:HG13	1:C:518:SER:N	2.19	0.56
1:H:273:ILE:CG1	1:H:275:MET:CE	2.81	0.56
1:I:643:LYS:O	1:I:644:SER:CB	2.54	0.56
1:N:57:LYS:NZ	1:N:166:GLY:O	2.39	0.56
1:O:505:THR:HA	1:O:509:PHE:O	2.05	0.56
1:L:191:ASP:OD2	1:L:194:ARG:NH1	2.38	0.56
1:C:42:ARG:HH11	1:C:140:GLU:HG2	1.71	0.56
1:F:291:ASN:HB3	1:F:295:TYR:HB2	1.88	0.56
1:F:443:ILE:HG12	1:F:445:LEU:HD13	1.87	0.56
1:G:489:ILE:HD13	1:G:541:VAL:HG21	1.87	0.56
1:M:138:VAL:HG23	1:M:170:VAL:HB	1.88	0.56
1:K:241:GLU:HB2	1:K:277:ARG:NH2	2.21	0.56
1:A:39:ASP:OD2	1:A:298:ARG:CD	2.54	0.56
1:N:378:SER:HB3	1:N:400:ALA:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:69:LEU:HD12	1:R:70:ASP:N	2.20	0.56
1:F:163:ALA:HB1	1:F:167:CYS:SG	2.46	0.55
1:F:478:ARG:HG2	1:F:478:ARG:HH21	1.71	0.55
1:E:480:GLU:OE2	1:E:482:HIS:HD2	1.89	0.55
1:Q:569:MET:HE1	1:Q:575:ILE:HG12	1.88	0.55
1:F:35:ASP:O	1:F:36:MET:C	2.45	0.55
1:M:198:GLU:HB2	1:M:201:GLU:OE2	2.06	0.55
1:Q:370:PHE:HE2	1:Q:588:LEU:HD21	1.71	0.55
1:R:369:LYS:HE3	1:R:586:ILE:HG21	1.89	0.55
1:G:434:VAL:HG12	1:G:469:LEU:HD13	1.89	0.55
1:Q:222:LYS:HB2	1:Q:224:HIS:HB3	1.87	0.55
1:R:481:PRO:HG2	1:R:581:TRP:CE3	2.41	0.55
1:K:156:LYS:O	1:K:160:GLU:HG2	2.06	0.55
1:B:344:TYR:O	1:B:346:VAL:HG13	2.07	0.55
1:E:275:MET:HE1	1:E:283:ILE:HG13	1.88	0.55
1:M:66:VAL:O	1:M:88:ASP:HB2	2.06	0.55
1:M:126:VAL:H	1:M:161:ARG:HH22	1.51	0.55
1:N:58:LYS:N	1:N:58:LYS:HE3	2.21	0.55
1:N:348:GLY:O	1:N:415:ILE:HD11	2.07	0.55
1:O:615:ILE:O	1:O:616:THR:C	2.45	0.55
1:Q:180:PRO:CG	1:Q:230:SER:HB3	2.31	0.55
1:L:502:ASP:OD2	1:L:616:THR:HG21	2.07	0.55
1:D:180:PRO:HB3	1:D:264:ILE:HD13	1.89	0.55
1:B:38:LEU:HD21	1:B:503:VAL:HA	1.87	0.55
1:B:483:MET:HB3	1:B:582:GLU:HG3	1.87	0.55
1:E:72:GLY:CA	2:E:701:SAH:O4'	2.54	0.55
1:R:434:VAL:HG12	1:R:469:LEU:HD13	1.88	0.55
1:C:460:LEU:HD22	1:C:463:LEU:HD21	1.88	0.55
1:F:385:THR:HB	1:F:405:ILE:HA	1.88	0.55
1:G:36:MET:HA	1:G:300:HIS:CD2	2.41	0.55
1:I:478:ARG:HH21	1:I:478:ARG:HG2	1.70	0.55
1:N:123:SER:OG	2:N:701:SAH:N6	2.38	0.55
1:J:137:ILE:HD11	1:J:163:ALA:HB2	1.89	0.55
1:K:145:GLU:CG	1:K:331:LEU:HD22	2.37	0.55
1:A:379:LYS:HA	1:A:399:THR:CG2	2.36	0.55
1:B:506:VAL:O	1:B:507:ASN:C	2.44	0.55
1:F:218:LEU:H	1:F:303:GLN:HE22	1.48	0.55
1:O:643:LYS:HD2	1:O:643:LYS:N	2.14	0.55
1:P:210:THR:HB	4:P:804:HOH:O	2.05	0.55
1:Q:354:SER:HB2	3:Q:702:PO4:O3	2.07	0.55
1:K:38:LEU:HD21	1:K:503:VAL:HA	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:136:ILE:HA	1:L:168:ARG:O	2.07	0.55
1:L:627:HIS:HB2	1:L:640:GLN:HB2	1.88	0.55
1:B:239:ASP:OD2	1:B:242:HIS:HD2	1.89	0.55
1:G:412:PHE:CE2	1:G:451:MET:HG2	2.40	0.55
1:M:145:GLU:HG2	1:M:331:LEU:CD1	2.36	0.55
1:R:80:LEU:HB3	1:R:509:PHE:CE1	2.41	0.55
1:R:379:LYS:HA	1:R:399:THR:HG22	1.89	0.55
1:J:222:LYS:HB2	1:J:225:GLU:HG2	1.89	0.55
1:C:522:ARG:HG2	1:C:526:ASP:OD2	2.07	0.55
1:E:359:TYR:C	1:E:359:TYR:CD1	2.81	0.55
1:H:218:LEU:H	1:H:303:GLN:HE21	1.55	0.55
1:N:367:ASN:O	1:N:371:LYS:HD3	2.07	0.55
1:J:497:GLN:HE21	1:J:497:GLN:N	1.96	0.55
1:C:550:ARG:H	1:C:560:GLN:HE22	1.54	0.55
1:F:143:ASP:OD1	1:F:143:ASP:N	2.37	0.55
1:M:434:VAL:CG1	1:M:469:LEU:CD1	2.85	0.55
1:N:315:GLU:HB2	1:N:318:GLN:CG	2.35	0.55
1:Q:42:ARG:HH11	1:Q:140:GLU:HG2	1.67	0.55
1:J:383:VAL:CG2	1:J:445:LEU:HD22	2.37	0.55
1:D:42:ARG:HH21	1:D:43:ASN:HD21	1.54	0.54
1:D:157:GLU:HA	1:D:160:GLU:HG3	1.90	0.54
1:C:502:ASP:OD2	1:C:616:THR:CG2	2.55	0.54
1:M:568:ASN:HD22	1:M:568:ASN:N	2.05	0.54
1:N:132:SER:HB2	1:R:104:ARG:CZ	2.36	0.54
1:N:142:PHE:HD1	1:N:146:LEU:HD12	1.69	0.54
1:R:460:LEU:HD21	1:R:579:MET:CE	2.37	0.54
1:L:297:TRP:CD2	1:L:495:ASP:HB3	2.42	0.54
1:D:565:ASN:HD21	1:D:644:SER:HB3	1.71	0.54
1:B:241:GLU:HB2	1:B:277:ARG:NH2	2.21	0.54
1:B:550:ARG:H	1:B:560:GLN:NE2	1.99	0.54
1:B:554:ASP:O	1:B:555:GLY:O	2.26	0.54
1:C:84:ARG:NH1	1:O:280:THR:CG2	2.70	0.54
1:E:420:ILE:HD11	1:E:428:VAL:HG22	1.90	0.54
1:I:353:LEU:HD22	1:I:357:THR:HG21	1.88	0.54
1:M:402:ARG:NH2	1:M:429:GLU:OE1	2.28	0.54
1:B:218:LEU:H	1:B:303:GLN:HE21	1.52	0.54
1:B:534:LEU:HD11	1:B:611:VAL:HG13	1.90	0.54
1:E:39:ASP:OD2	1:E:298:ARG:HD3	2.07	0.54
1:M:486:LEU:HD22	1:M:578:TRP:O	2.07	0.54
1:R:156:LYS:HG3	1:R:157:GLU:N	2.22	0.54
1:J:71:ILE:HG21	1:J:154:THR:CG2	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:339:ASP:OD1	1:J:341:SER:HB2	2.06	0.54
1:I:534:LEU:CD1	1:I:576:PRO:HB3	2.37	0.54
1:M:485:VAL:HG13	1:M:487:LYS:HG3	1.88	0.54
1:O:180:PRO:HB2	1:O:264:ILE:HG12	1.89	0.54
1:O:182:GLU:OE1	1:O:263:THR:HG22	2.07	0.54
1:P:50:LEU:O	1:P:54:ILE:HB	2.06	0.54
1:P:470:LYS:O	1:P:473:HIS:O	2.26	0.54
1:K:578:TRP:CG	1:K:591:GLY:HA3	2.43	0.54
1:B:43:ASN:ND2	1:B:43:ASN:N	2.55	0.54
1:B:505:THR:HA	1:B:509:PHE:O	2.06	0.54
1:C:55:ALA:HB1	1:O:292:LYS:HE3	1.90	0.54
1:C:467:GLU:HG3	1:C:555:GLY:O	2.07	0.54
1:H:420:ILE:CD1	1:H:428:VAL:HG22	2.37	0.54
1:I:129:ILE:HG22	1:I:130:GLY:O	2.06	0.54
1:I:269:MET:HG2	1:I:306:TYR:CE1	2.42	0.54
1:N:169:VAL:CG1	1:N:240:PHE:O	2.51	0.54
1:P:5:LYS:HA	1:R:420:ILE:CD1	2.36	0.54
1:R:179:VAL:HG22	1:R:232:PRO:HA	1.88	0.54
1:K:485:VAL:HG13	1:K:487:LYS:HG3	1.90	0.54
1:K:556:ARG:H	1:K:556:ARG:CZ	2.20	0.54
1:E:216:VAL:HG23	1:E:217:GLN:N	2.21	0.54
1:G:432:GLU:HG2	1:G:433:LYS:HG3	1.89	0.54
1:I:497:GLN:CD	1:I:573:ASN:ND2	2.59	0.54
1:I:539:GLY:O	1:I:540:ILE:HD13	2.07	0.54
1:K:84:ARG:O	1:K:85:GLU:CB	2.56	0.54
1:B:123:SER:O	1:B:125:ASP:N	2.41	0.54
1:B:194:ARG:HD2	1:B:198:GLU:O	2.08	0.54
1:N:84:ARG:HB3	1:N:112:TRP:CZ2	2.43	0.54
1:P:379:LYS:HA	1:P:399:THR:CG2	2.37	0.54
1:M:169:VAL:HG11	1:M:240:PHE:O	2.08	0.54
1:P:33:PHE:HB2	1:P:36:MET:HE2	1.89	0.54
1:P:110:SER:HB2	1:P:112:TRP:CE3	2.43	0.54
1:A:245:LYS:HD3	1:D:337:GLY:HA2	1.90	0.54
1:D:46:PHE:CZ	1:D:140:GLU:HB2	2.42	0.54
1:D:291:ASN:O	1:D:292:LYS:HD3	2.08	0.54
1:M:190:ASN:HD21	1:M:209:GLY:HA3	1.73	0.54
1:M:533:SER:O	1:M:536:GLU:HB2	2.08	0.54
1:N:137:ILE:O	1:N:169:VAL:HA	2.08	0.54
1:O:417:PHE:CZ	1:O:430:ILE:HB	2.43	0.54
1:R:447:GLU:N	1:R:448:PRO:HA	2.23	0.54
1:L:168:ARG:HG2	1:L:168:ARG:NH1	2.15	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:45:LYS:O	1:C:275:MET:HG2	2.08	0.54
1:M:434:VAL:HG13	1:M:469:LEU:HD13	1.90	0.54
1:N:490:PRO:HB3	1:N:569:MET:CE	2.38	0.54
1:Q:178:ILE:CD1	1:Q:235:ALA:HB2	2.35	0.54
1:Q:276:ASP:O	1:Q:277:ARG:CB	2.56	0.54
1:K:179:VAL:HG21	1:K:270:TRP:HH2	1.72	0.54
1:I:489:ILE:O	1:I:576:PRO:HD2	2.08	0.53
1:Q:530:ASP:O	1:Q:610:GLY:HA2	2.09	0.53
1:J:592:LEU:HD21	1:J:595:ILE:HD11	1.90	0.53
1:B:297:TRP:CZ2	1:B:299:ASP:HB2	2.43	0.53
1:E:138:VAL:HG23	1:E:170:VAL:HB	1.89	0.53
1:I:42:ARG:HH11	1:I:140:GLU:HG3	1.72	0.53
1:O:4:GLU:OE2	1:O:13:ARG:NH1	2.42	0.53
1:O:73:THR:OG1	1:O:76:GLY:HA2	2.08	0.53
1:P:297:TRP:CE3	1:P:495:ASP:HB3	2.44	0.53
1:D:243:GLU:OE1	1:D:243:GLU:N	2.30	0.53
1:B:627:HIS:CD2	1:B:627:HIS:N	2.76	0.53
1:G:141:VAL:O	1:G:141:VAL:HG12	2.08	0.53
1:I:193:PRO:HA	1:I:362:ASN:ND2	2.23	0.53
1:O:229:LEU:HD13	1:O:314:VAL:HG12	1.89	0.53
1:J:88:ASP:O	1:J:115:LYS:HG2	2.08	0.53
1:A:176:VAL:HG22	1:A:235:ALA:HB3	1.90	0.53
1:D:242:HIS:HB2	1:D:245:LYS:HG3	1.90	0.53
1:F:91:THR:HG22	1:F:117:THR:HG22	1.89	0.53
1:M:132:SER:N	1:P:104:ARG:HH21	2.06	0.53
1:M:375:ASP:O	1:M:399:THR:HG21	2.09	0.53
1:Q:179:VAL:HG22	1:Q:232:PRO:HA	1.89	0.53
1:K:505:THR:HA	1:K:509:PHE:O	2.08	0.53
1:A:214:PHE:CD2	1:A:305:VAL:HG22	2.44	0.53
1:F:277:ARG:C	1:F:279:GLY:H	2.12	0.53
1:E:241:GLU:CG	1:E:277:ARG:HH21	2.20	0.53
1:E:274:ASP:HA	1:E:282:PHE:CD1	2.43	0.53
1:G:6:ILE:HG13	1:I:426:THR:HB	1.91	0.53
1:G:490:PRO:HB2	1:G:569:MET:HE1	1.84	0.53
1:I:68:VAL:O	1:I:90:VAL:HA	2.08	0.53
1:M:92:ALA:HB3	1:M:118:VAL:HG22	1.90	0.53
1:M:258:ALA:CB	1:M:314:VAL:HG13	2.38	0.53
1:N:55:ALA:CA	1:N:58:LYS:HZ2	2.22	0.53
1:R:489:ILE:HD11	1:R:541:VAL:HG11	1.91	0.53
1:K:36:MET:HA	1:K:300:HIS:CD2	2.43	0.53
1:L:528:ILE:HD13	1:L:639:PHE:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:250:GLU:HB2	1:H:326:HIS:NE2	2.23	0.53
1:P:198:GLU:HB2	1:P:201:GLU:HG3	1.90	0.53
1:Q:447:GLU:H	1:Q:448:PRO:HA	1.73	0.53
1:R:300:HIS:CE1	1:R:301:TRP:CD2	2.97	0.53
1:K:534:LEU:O	1:K:536:GLU:N	2.42	0.53
1:D:78:LEU:O	1:D:81:MET:HB2	2.09	0.53
1:D:178:ILE:HA	1:D:268:LEU:O	2.09	0.53
1:B:75:THR:HG22	1:B:77:LEU:H	1.73	0.53
1:E:434:VAL:HG13	1:E:469:LEU:HD13	1.91	0.53
1:I:379:LYS:HA	1:I:399:THR:CG2	2.33	0.53
1:N:450:TYR:H	1:N:459:HIS:CD2	2.22	0.53
1:R:144:THR:HG23	1:R:302:MET:O	2.09	0.53
1:K:122:ARG:O	1:K:123:SER:C	2.45	0.53
1:K:123:SER:HB3	2:K:701:SAH:N6	2.13	0.53
1:D:45:LYS:HB3	1:D:275:MET:HE3	1.91	0.53
1:D:490:PRO:CB	1:D:569:MET:HE1	2.38	0.53
1:E:627:HIS:HB2	1:E:640:GLN:HB2	1.90	0.53
1:J:264:ILE:HD12	1:J:312:LYS:HG3	1.90	0.53
1:L:258:ALA:CB	1:L:314:VAL:HG13	2.39	0.53
1:L:280:THR:HG23	1:L:281:THR:CG2	2.38	0.53
1:A:109:ASN:N	1:A:109:ASN:ND2	2.57	0.53
1:F:216:VAL:O	1:F:302:MET:HG2	2.09	0.53
1:G:190:ASN:HD21	1:G:209:GLY:HA3	1.73	0.53
1:I:168:ARG:HG2	1:I:168:ARG:HH11	1.72	0.53
1:M:84:ARG:O	1:M:85:GLU:HB2	2.09	0.53
1:O:387:GLY:HA2	1:O:450:TYR:CE1	2.43	0.53
1:P:496:LEU:O	1:P:499:ILE:HG12	2.09	0.53
1:Q:259:HIS:C	1:Q:259:HIS:CD2	2.82	0.53
1:Q:392:LEU:CD1	1:Q:445:LEU:HB3	2.38	0.53
1:L:553:ILE:HD11	1:L:581:TRP:HZ3	1.73	0.53
1:B:84:ARG:HB3	1:B:112:TRP:CH2	2.44	0.53
1:E:278:ASN:O	1:E:280:THR:N	2.40	0.53
1:M:409:ASN:OD1	1:M:411:ARG:HG2	2.09	0.53
1:M:615:ILE:HG13	1:M:618:LEU:HD22	1.90	0.53
1:N:87:ALA:CB	1:N:88:ASP:HB2	2.38	0.53
1:Q:410:GLU:HG3	1:Q:413:ARG:NH2	2.23	0.53
1:R:49:GLY:O	1:R:53:THR:OG1	2.27	0.53
1:R:178:ILE:HG13	1:R:267:LEU:HD22	1.90	0.53
1:R:184:HIS:HA	1:R:187:LYS:HD3	1.90	0.53
1:J:128:GLN:OE1	1:J:129:ILE:O	2.27	0.53
1:J:378:SER:HB3	1:J:400:ALA:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:126:VAL:HG12	1:K:162:LEU:HD11	1.90	0.53
1:K:143:ASP:O	1:K:146:LEU:N	2.32	0.53
1:L:490:PRO:HB3	1:L:569:MET:HE2	1.76	0.53
1:M:516:GLU:HG2	1:M:520:LYS:HE3	1.90	0.52
1:Q:218:LEU:HD22	1:Q:221:MET:HE2	1.92	0.52
1:R:157:GLU:O	1:R:160:GLU:HG2	2.09	0.52
1:J:410:GLU:OE2	1:K:19:GLU:HB3	2.09	0.52
1:K:485:VAL:O	1:K:579:MET:HG3	2.09	0.52
1:D:269:MET:HG2	1:D:306:TYR:HE1	1.73	0.52
1:D:445:LEU:HD12	1:D:480:GLU:HB2	1.91	0.52
1:B:567:ASP:O	1:B:568:ASN:HB2	2.09	0.52
1:F:239:ASP:OD2	1:F:242:HIS:HD2	1.92	0.52
1:E:35:ASP:O	1:E:36:MET:C	2.46	0.52
1:I:570:SER:HB3	1:I:622:LYS:HA	1.92	0.52
1:O:280:THR:HG22	1:O:281:THR:HG22	1.90	0.52
1:R:597:SER:HA	1:R:599:GLY:N	2.23	0.52
1:J:561:LYS:O	1:J:562:CYS:HB3	2.09	0.52
1:K:45:LYS:NZ	1:K:294:ASN:HD22	2.07	0.52
1:E:595:ILE:HG22	1:E:599:GLY:HA2	1.90	0.52
1:M:457:TRP:CD1	1:M:457:TRP:O	2.62	0.52
1:N:39:ASP:C	1:N:39:ASP:OD1	2.47	0.52
1:O:291:ASN:OD1	1:O:294:ASN:HB2	2.10	0.52
1:R:502:ASP:OD2	1:R:616:THR:HG21	2.08	0.52
1:B:163:ALA:CB	1:B:167:CYS:SG	2.95	0.52
1:G:540:ILE:HD11	1:G:542:LYS:HE2	1.91	0.52
1:R:593:LEU:O	1:R:594:SER:HB3	2.10	0.52
1:J:548:ILE:HD12	1:J:626:LEU:HD13	1.92	0.52
1:K:185:LEU:O	1:K:188:MET:HB2	2.10	0.52
1:K:379:LYS:CA	1:K:399:THR:HG23	2.38	0.52
1:L:57:LYS:HG2	1:L:135:ASP:HB3	1.91	0.52
1:A:273:ILE:HG13	1:A:275:MET:HE1	1.91	0.52
1:D:626:LEU:HD21	1:D:628:ALA:HB2	1.90	0.52
1:C:489:ILE:HG12	1:C:541:VAL:CG2	2.39	0.52
1:F:147:ILE:HD11	1:F:331:LEU:HD13	1.91	0.52
1:F:478:ARG:HH21	1:F:478:ARG:CG	2.22	0.52
1:E:218:LEU:H	1:E:303:GLN:HE21	1.55	0.52
1:E:506:VAL:N	1:E:509:PHE:O	2.37	0.52
1:I:275:MET:HA	1:I:275:MET:CE	2.39	0.52
1:N:169:VAL:HG13	1:N:241:GLU:HG2	1.89	0.52
1:O:506:VAL:HG12	1:O:507:ASN:HD22	1.74	0.52
1:J:478:ARG:HH21	1:J:478:ARG:HG2	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:297:TRP:CE3	1:L:495:ASP:HB3	2.45	0.52
1:A:541:VAL:HG11	1:A:595:ILE:HD13	1.91	0.52
1:D:630:PHE:CE1	1:D:635:GLY:HA2	2.44	0.52
1:G:73:THR:OG1	1:G:76:GLY:HA2	2.09	0.52
1:G:379:LYS:CA	1:G:399:THR:CG2	2.83	0.52
1:M:5:LYS:HD3	1:O:417:PHE:HE1	1.75	0.52
1:N:141:VAL:O	1:N:141:VAL:HG12	2.09	0.52
1:R:478:ARG:HG2	1:R:478:ARG:NH2	2.21	0.52
1:K:497:GLN:NE2	1:K:497:GLN:H	2.08	0.52
1:D:114:ASP:HB3	1:B:65:LYS:HZ1	1.73	0.52
1:G:104:ARG:HB3	1:G:118:VAL:HB	1.91	0.52
1:I:643:LYS:O	1:I:644:SER:HB2	2.10	0.52
1:P:7:ASN:HD21	1:P:640:GLN:NE2	2.08	0.52
1:J:91:THR:HG21	1:J:129:ILE:HG21	1.92	0.52
1:J:144:THR:O	1:J:269:MET:HE1	2.10	0.52
1:J:169:VAL:HG23	1:J:171:PRO:O	2.10	0.52
1:I:616:THR:O	1:I:619:ARG:HG2	2.10	0.52
1:R:35:ASP:OD2	1:R:300:HIS:HD2	1.93	0.52
1:R:291:ASN:CB	1:R:295:TYR:HB2	2.32	0.52
1:R:433:LYS:HE3	1:R:436:SER:OG	2.10	0.52
1:J:71:ILE:HG12	1:J:93:LEU:HD12	1.91	0.52
1:J:406:ILE:HG12	1:J:431:ILE:HD11	1.91	0.52
1:K:177:TYR:HA	1:K:233:ILE:O	2.09	0.52
1:K:529:VAL:HG12	1:K:530:ASP:O	2.10	0.52
1:D:547:GLU:OE2	1:D:550:ARG:NH1	2.37	0.52
1:B:218:LEU:HD12	1:B:303:GLN:HB3	1.92	0.52
1:C:73:THR:OG1	1:C:76:GLY:HA2	2.10	0.52
1:C:432:GLU:HG2	1:C:433:LYS:HG3	1.92	0.52
1:M:39:ASP:OD2	1:M:298:ARG:CD	2.57	0.52
1:Q:216:VAL:C	1:Q:302:MET:HG2	2.29	0.52
1:R:280:THR:HG23	1:R:281:THR:N	2.24	0.52
1:R:292:LYS:HA	1:R:293:ASN:HD22	1.75	0.52
1:D:135:ASP:OD1	1:D:164:LYS:HD2	2.09	0.52
1:B:460:LEU:HB3	1:B:463:LEU:HD22	1.91	0.52
1:F:259:HIS:C	1:F:259:HIS:CD2	2.83	0.52
1:G:27:GLU:HG2	1:G:96:PHE:CZ	2.45	0.52
1:M:542:LYS:HG3	1:M:571:SER:HB2	1.91	0.52
1:N:154:THR:O	1:N:158:ALA:HB2	2.09	0.52
1:P:94:GLU:O	1:P:120:SER:HA	2.10	0.52
1:J:483:MET:HG2	1:J:550:ARG:HH21	1.75	0.52
1:I:145:GLU:OE2	1:I:331:LEU:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:398:LYS:NZ	1:I:398:LYS:HB3	2.25	0.51
1:M:73:THR:HB	1:M:92:ALA:HB1	1.92	0.51
1:M:269:MET:HG2	1:M:306:TYR:HE2	1.75	0.51
1:J:217:GLN:HB2	1:J:536:GLU:HB3	1.93	0.51
1:B:43:ASN:O	1:B:81:MET:CE	2.58	0.51
1:C:67:HIS:HE1	1:C:91:THR:CG2	2.23	0.51
1:I:3:LEU:HB2	1:I:16:VAL:HG12	1.93	0.51
1:I:138:VAL:HG23	1:I:170:VAL:HB	1.92	0.51
1:I:337:GLY:HA2	1:K:245:LYS:HD3	1.92	0.51
1:M:178:ILE:HG13	1:M:233:ILE:HG23	1.93	0.51
1:M:550:ARG:H	1:M:560:GLN:HE22	1.58	0.51
1:N:171:PRO:O	1:N:240:PHE:HD2	1.93	0.51
1:P:450:TYR:N	1:P:459:HIS:HD2	1.92	0.51
1:K:139:ALA:HB3	1:K:155:PHE:CZ	2.45	0.51
1:B:41:ASP:O	1:B:43:ASN:N	2.43	0.51
1:C:111:PRO:HA	1:O:47:LEU:HD13	1.92	0.51
1:F:164:LYS:O	1:F:167:CYS:HB2	2.11	0.51
1:G:619:ARG:HG2	1:G:619:ARG:HH11	1.75	0.51
1:M:447:GLU:N	1:M:448:PRO:HA	2.26	0.51
1:M:492:LYS:O	1:M:540:ILE:N	2.38	0.51
1:N:595:ILE:CG2	1:N:599:GLY:HA2	2.40	0.51
1:O:229:LEU:HD13	1:O:314:VAL:CG1	2.40	0.51
1:O:535:TRP:CD2	1:O:605:LYS:HG2	2.45	0.51
1:O:632:LYS:HG3	1:O:633:SER:N	2.25	0.51
1:Q:275:MET:HE1	1:Q:283:ILE:H	1.75	0.51
1:K:57:LYS:HA	1:K:60:GLU:HB2	1.93	0.51
1:K:522:ARG:O	1:K:526:ASP:HB2	2.10	0.51
1:B:216:VAL:C	1:B:302:MET:HG2	2.30	0.51
1:F:181:VAL:HG11	1:F:226:PHE:HB2	1.92	0.51
1:G:626:LEU:HG	1:G:641:PHE:CE2	2.45	0.51
1:M:190:ASN:ND2	1:M:209:GLY:HA3	2.26	0.51
1:M:449:PHE:HA	1:M:459:HIS:CD2	2.46	0.51
1:N:217:GLN:NE2	1:N:298:ARG:O	2.31	0.51
1:N:517:ILE:HG13	1:N:518:SER:N	2.25	0.51
1:L:129:ILE:HG23	1:L:129:ILE:O	2.09	0.51
1:A:556:ARG:HG2	1:A:556:ARG:HH11	1.75	0.51
1:C:567:ASP:C	1:C:568:ASN:HD22	2.14	0.51
1:H:51:LYS:HG2	1:H:85:GLU:HG3	1.92	0.51
1:M:238:PHE:HB3	1:M:240:PHE:CE1	2.45	0.51
1:M:258:ALA:HB3	1:M:315:GLU:O	2.10	0.51
1:M:482:HIS:HA	1:M:553:ILE:HG12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:63:ASP:N	1:N:64:GLY:HA2	2.25	0.51
1:O:450:TYR:H	1:O:459:HIS:CD2	2.18	0.51
1:Q:232:PRO:HG3	1:Q:290:LYS:HE2	1.89	0.51
1:J:483:MET:HG2	1:J:550:ARG:NH2	2.26	0.51
1:K:68:VAL:O	1:K:90:VAL:HA	2.10	0.51
1:L:550:ARG:H	1:L:560:GLN:HE22	1.57	0.51
1:D:145:GLU:HA	1:D:269:MET:CE	2.41	0.51
1:D:271:TRP:CZ3	1:D:273:ILE:HG12	2.46	0.51
1:G:95:VAL:HB	1:G:122:ARG:HG3	1.92	0.51
1:M:83:ALA:HB2	1:M:116:ILE:HD11	1.92	0.51
1:M:203:PRO:HA	1:M:422:TYR:CG	2.45	0.51
1:M:356:GLN:NE2	1:M:608:LYS:HE3	2.25	0.51
1:M:379:LYS:HA	1:M:399:THR:HG22	1.90	0.51
1:O:2:PHE:CD2	1:O:520:LYS:HB3	2.46	0.51
1:Q:302:MET:HG2	1:Q:303:GLN:H	1.75	0.51
1:R:638:ASN:HD22	1:R:638:ASN:N	2.09	0.51
1:A:379:LYS:O	1:A:381:LEU:HG	2.11	0.51
1:D:269:MET:HG2	1:D:306:TYR:CE1	2.45	0.51
1:B:3:LEU:O	1:B:15:TRP:HA	2.11	0.51
1:H:626:LEU:HD23	1:H:627:HIS:N	2.25	0.51
1:M:385:THR:CG2	4:M:802:HOH:O	2.59	0.51
1:M:616:THR:O	1:M:619:ARG:HB2	2.11	0.51
1:O:194:ARG:HG2	1:O:201:GLU:HB3	1.93	0.51
1:O:441:PRO:O	1:O:477:LEU:HD11	2.11	0.51
1:Q:464:TYR:O	1:Q:468:VAL:HG23	2.11	0.51
1:D:478:ARG:HG2	1:D:478:ARG:NH2	2.13	0.51
1:B:94:GLU:O	1:B:120:SER:HA	2.10	0.51
1:F:1:MET:N	4:F:801:HOH:O	2.43	0.51
1:E:547:GLU:OE1	1:E:550:ARG:NH1	2.44	0.51
1:N:326:HIS:HB2	1:N:331:LEU:HD12	1.92	0.51
1:P:379:LYS:CA	1:P:399:THR:HG23	2.37	0.51
1:R:146:LEU:HD23	1:R:147:ILE:HG23	1.93	0.51
1:C:196:ASN:HB2	1:C:201:GLU:OE2	2.11	0.51
1:F:497:GLN:HE21	1:F:497:GLN:N	1.98	0.51
1:Q:243:GLU:HA	1:Q:246:ILE:HD12	1.92	0.51
1:Q:553:ILE:CG2	1:Q:553:ILE:O	2.59	0.51
1:J:103:ALA:O	1:J:107:THR:HB	2.11	0.51
1:L:412:PHE:HE2	1:L:451:MET:HG2	1.74	0.51
1:A:58:LYS:HD3	1:A:64:GLY:O	2.10	0.51
1:C:502:ASP:OD2	1:C:616:THR:HG21	2.11	0.51
1:E:157:GLU:O	1:E:160:GLU:HG3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:114:ASP:OD1	1:I:114:ASP:N	2.38	0.51
1:M:447:GLU:H	1:M:448:PRO:HA	1.75	0.51
1:O:173:THR:HG22	1:O:174:GLY:N	2.25	0.51
1:Q:231:GLU:C	1:Q:232:PRO:O	2.49	0.51
1:R:220:GLU:HG3	1:R:536:GLU:O	2.11	0.51
1:L:73:THR:HB	1:L:92:ALA:HB1	1.91	0.51
1:B:173:THR:HG22	1:B:274:ASP:HB3	1.93	0.50
1:C:233:ILE:HG12	1:C:256:ALA:HB2	1.94	0.50
1:C:569:MET:HA	1:C:572:SER:HB2	1.93	0.50
1:F:446:ALA:O	1:F:481:PRO:HD3	2.12	0.50
1:M:142:PHE:HD2	1:M:146:LEU:HD12	1.76	0.50
1:P:486:LEU:HD11	1:P:577:MET:HE2	1.92	0.50
1:K:273:ILE:HD12	1:K:275:MET:CE	2.40	0.50
1:L:39:ASP:OD2	1:L:298:ARG:CD	2.60	0.50
1:A:447:GLU:N	1:A:448:PRO:HA	2.26	0.50
1:E:107:THR:O	1:E:110:SER:OG	2.28	0.50
1:G:522:ARG:O	1:G:526:ASP:HB2	2.10	0.50
1:O:73:THR:HG23	1:O:74:GLY:N	2.26	0.50
1:O:91:THR:HG22	1:O:117:THR:HG23	1.93	0.50
1:O:194:ARG:HG2	1:O:201:GLU:HB2	1.93	0.50
1:P:26:GLN:O	1:P:30:ARG:CD	2.59	0.50
1:Q:82:ALA:O	1:Q:87:ALA:HB3	2.11	0.50
1:Q:550:ARG:H	1:Q:560:GLN:NE2	2.08	0.50
1:J:269:MET:HG2	1:J:306:TYR:HE1	1.76	0.50
1:A:101:ASP:O	1:A:105:HIS:HB2	2.11	0.50
1:C:35:ASP:O	1:C:38:LEU:N	2.44	0.50
1:C:42:ARG:NH2	1:C:43:ASN:HD21	2.09	0.50
1:F:289:TRP:O	1:F:290:LYS:HG2	2.11	0.50
1:I:627:HIS:HB2	1:I:640:GLN:HB2	1.94	0.50
1:M:541:VAL:HG22	1:M:601:PRO:HG3	1.92	0.50
1:N:203:PRO:HA	1:N:422:TYR:CD2	2.46	0.50
1:N:578:TRP:CB	1:N:591:GLY:HA3	2.41	0.50
1:J:300:HIS:CE1	1:J:301:TRP:CD2	2.99	0.50
1:K:65:LYS:HA	1:K:65:LYS:CE	2.41	0.50
1:K:556:ARG:H	1:K:556:ARG:NH1	2.09	0.50
1:L:84:ARG:HG3	1:L:112:TRP:CZ2	2.46	0.50
1:D:434:VAL:HG12	1:D:469:LEU:CD1	2.36	0.50
1:N:153:ARG:HB2	1:N:328:GLU:OE2	2.12	0.50
1:O:27:GLU:HB3	1:O:96:PHE:CZ	2.47	0.50
1:P:269:MET:HG2	1:P:306:TYR:CE1	2.40	0.50
1:R:218:LEU:HD13	1:R:268:LEU:HD13	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:217:GLN:HG3	1:K:537:TYR:CE1	2.46	0.50
1:K:356:GLN:HG2	1:K:357:THR:H	1.75	0.50
1:B:78:LEU:O	1:B:81:MET:HB2	2.12	0.50
1:E:42:ARG:HH11	1:E:140:GLU:HG2	1.72	0.50
1:G:457:TRP:HA	4:G:811:HOH:O	2.09	0.50
1:I:566:ILE:CG2	1:I:569:MET:HE3	2.42	0.50
1:M:269:MET:O	1:M:269:MET:HG3	2.11	0.50
1:O:39:ASP:OD2	1:O:298:ARG:CD	2.54	0.50
1:O:397:ALA:HA	1:O:403:VAL:HG21	1.93	0.50
1:K:103:ALA:O	1:K:107:THR:HB	2.11	0.50
1:K:143:ASP:O	1:K:144:THR:C	2.50	0.50
1:D:528:ILE:H	1:D:528:ILE:HD12	1.76	0.50
1:B:392:LEU:C	1:B:392:LEU:CD2	2.79	0.50
1:E:161:ARG:HB3	1:E:162:LEU:HD13	1.94	0.50
1:M:142:PHE:CD2	1:M:146:LEU:HD12	2.46	0.50
1:O:73:THR:CB	1:O:92:ALA:HB1	2.32	0.50
1:O:353:LEU:HB3	1:O:357:THR:HB	1.94	0.50
1:Q:14:GLU:HG2	1:Q:523:THR:HG21	1.93	0.50
1:Q:629:LEU:O	1:Q:637:ILE:HA	2.12	0.50
1:R:359:TYR:CZ	1:R:605:LYS:HB2	2.46	0.50
1:R:421:HIS:O	1:R:424:LYS:HE3	2.12	0.50
1:K:616:THR:C	1:K:618:LEU:H	2.15	0.50
1:D:379:LYS:CA	1:D:399:THR:HG23	2.37	0.50
1:B:486:LEU:HD12	1:B:548:ILE:HB	1.94	0.50
1:F:489:ILE:O	1:F:576:PRO:HD2	2.12	0.50
1:E:222:LYS:O	1:E:225:GLU:HG2	2.12	0.50
1:I:168:ARG:HG2	1:I:168:ARG:NH1	2.24	0.50
1:I:375:ASP:O	1:I:399:THR:HG21	2.12	0.50
1:O:477:LEU:O	1:O:479:VAL:HG12	2.12	0.50
1:P:143:ASP:O	1:P:146:LEU:HA	2.12	0.50
1:L:65:LYS:HA	1:L:88:ASP:OD2	2.12	0.50
1:D:230:SER:OG	1:D:231:GLU:O	2.28	0.50
1:B:339:ASP:OD1	1:B:341:SER:HB2	2.12	0.50
1:G:273:ILE:HG13	1:G:273:ILE:O	2.10	0.50
1:N:359:TYR:CD1	1:N:359:TYR:C	2.85	0.50
1:P:503:VAL:H	1:P:515:ASP:CG	2.15	0.50
1:J:168:ARG:NH2	1:J:276:ASP:O	2.43	0.50
1:J:625:CYS:SG	1:J:627:HIS:CD2	3.05	0.50
1:K:84:ARG:HB2	1:K:112:TRP:NE1	2.27	0.50
1:K:487:LYS:HE3	1:K:547:GLU:HG2	1.94	0.50
1:C:244:GLU:OE2	1:C:244:GLU:CA	2.60	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:56:GLU:HG3	1:E:57:LYS:N	2.25	0.50
1:E:168:ARG:HH22	1:E:276:ASP:C	2.15	0.50
1:N:4:GLU:OE2	1:N:13:ARG:HD3	2.11	0.50
1:O:77:LEU:O	1:O:81:MET:HG3	2.11	0.50
1:Q:367:ASN:HD21	1:Q:369:LYS:HG2	1.77	0.50
1:R:41:ASP:O	1:R:45:LYS:HB2	2.12	0.50
1:R:556:ARG:HG3	1:R:556:ARG:NH1	2.09	0.50
1:R:612:TYR:OH	1:R:615:ILE:HD12	2.11	0.50
1:J:26:GLN:O	1:J:30:ARG:HD2	2.12	0.50
1:A:273:ILE:HD11	1:A:283:ILE:HD12	1.93	0.49
1:D:489:ILE:CG1	1:D:490:PRO:HD2	2.40	0.49
1:B:67:HIS:C	1:B:67:HIS:ND1	2.64	0.49
1:B:452:SER:O	1:B:453:ALA:C	2.51	0.49
1:C:485:VAL:CG2	1:C:547:GLU:HG3	2.42	0.49
1:F:299:ASP:OD1	1:F:537:TYR:OH	2.15	0.49
1:H:222:LYS:NZ	1:H:602:GLU:OE2	2.44	0.49
1:I:278:ASN:O	1:I:280:THR:CG2	2.58	0.49
1:N:87:ALA:HB1	1:N:88:ASP:HB2	1.94	0.49
1:O:356:GLN:O	1:O:359:TYR:HB3	2.12	0.49
1:Q:141:VAL:O	1:Q:141:VAL:HG12	2.12	0.49
1:R:7:ASN:O	1:R:11:GLY:N	2.40	0.49
1:R:218:LEU:O	1:R:220:GLU:N	2.44	0.49
1:J:406:ILE:HG21	1:J:434:VAL:HG22	1.94	0.49
1:L:253:VAL:HG22	1:L:253:VAL:O	2.10	0.49
1:A:221:MET:HE3	1:A:226:PHE:CD1	2.47	0.49
1:A:550:ARG:H	1:A:560:GLN:NE2	2.10	0.49
1:B:141:VAL:HG12	1:B:141:VAL:O	2.12	0.49
1:E:403:VAL:HB	1:E:428:VAL:HB	1.94	0.49
1:R:626:LEU:HD21	1:R:639:PHE:HD2	1.77	0.49
1:J:69:LEU:HD12	1:J:91:THR:O	2.12	0.49
1:J:563:VAL:CG1	1:J:625:CYS:SG	3.00	0.49
1:L:557:VAL:HG23	1:L:632:LYS:HB2	1.95	0.49
1:B:37:ILE:O	1:B:37:ILE:HG22	2.13	0.49
1:B:629:LEU:O	1:B:629:LEU:HG	2.12	0.49
1:C:67:HIS:CE1	1:C:91:THR:HG22	2.42	0.49
1:C:612:TYR:CE2	1:C:614:PRO:HA	2.47	0.49
1:F:144:THR:HG21	1:F:215:ASP:HB3	1.93	0.49
1:F:218:LEU:HD12	1:F:303:GLN:HB2	1.90	0.49
1:E:315:GLU:HB3	1:E:318:GLN:HG3	1.93	0.49
1:H:618:LEU:HD21	1:H:642:GLY:HA2	1.95	0.49
1:I:256:ALA:O	1:I:319:THR:HA	2.10	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:136:ILE:HA	1:M:168:ARG:O	2.11	0.49
1:O:196:ASN:HB2	1:O:201:GLU:OE2	2.12	0.49
1:P:146:LEU:HB3	1:P:271:TRP:NE1	2.26	0.49
1:P:354:SER:O	1:P:358:VAL:HG23	2.12	0.49
1:Q:114:ASP:OD1	1:Q:114:ASP:N	2.44	0.49
1:Q:186:LEU:O	1:Q:307:TYR:OH	2.17	0.49
1:Q:269:MET:SD	1:Q:270:TRP:N	2.85	0.49
1:R:51:LYS:NZ	1:R:51:LYS:CB	2.74	0.49
1:R:261:SER:OG	1:R:316:MET:N	2.43	0.49
1:J:67:HIS:CE1	1:J:91:THR:HG22	2.43	0.49
1:K:137:ILE:O	1:K:169:VAL:HA	2.12	0.49
1:L:218:LEU:H	1:L:303:GLN:HE21	1.60	0.49
1:E:39:ASP:OD2	1:E:298:ARG:CD	2.60	0.49
1:H:138:VAL:HG23	1:H:170:VAL:HB	1.94	0.49
1:H:379:LYS:HA	1:H:399:THR:HG23	1.94	0.49
1:O:194:ARG:HD2	1:O:198:GLU:O	2.13	0.49
1:Q:153:ARG:NH1	1:Q:248:PHE:CZ	2.80	0.49
1:R:143:ASP:OD2	1:R:148:GLY:HA3	2.13	0.49
1:R:297:TRP:CD2	1:R:495:ASP:HB3	2.48	0.49
1:J:42:ARG:HH11	1:J:140:GLU:HG2	1.76	0.49
1:F:626:LEU:HD23	1:F:626:LEU:C	2.32	0.49
1:G:239:ASP:OD2	1:G:277:ARG:NH2	2.45	0.49
1:M:434:VAL:HG12	1:M:469:LEU:CD1	2.42	0.49
1:K:326:HIS:HB3	1:K:331:LEU:HD12	1.93	0.49
1:L:218:LEU:H	1:L:303:GLN:NE2	2.09	0.49
1:A:375:ASP:O	1:A:399:THR:HG21	2.13	0.49
1:F:67:HIS:ND1	1:F:89:LYS:HB3	2.27	0.49
1:G:405:ILE:HB	1:G:430:ILE:HG12	1.93	0.49
1:I:634:THR:OG1	1:I:636:ASP:HB2	2.12	0.49
1:O:190:ASN:ND2	1:O:209:GLY:HA3	2.26	0.49
1:P:451:MET:HG3	1:P:452:SER:N	2.28	0.49
1:D:406:ILE:HG12	1:D:431:ILE:HD11	1.95	0.49
1:C:480:GLU:HA	1:C:481:PRO:C	2.33	0.49
1:G:272:ASP:HA	1:G:283:ILE:O	2.12	0.49
1:H:42:ARG:NH2	1:H:43:ASN:HD21	2.09	0.49
1:I:35:ASP:OD1	1:I:300:HIS:CD2	2.65	0.49
1:O:624:LEU:HB2	1:O:642:GLY:O	2.11	0.49
1:P:292:LYS:HB3	1:P:293:ASN:OD1	2.12	0.49
1:P:349:LEU:HD11	1:P:353:LEU:HD12	1.94	0.49
1:R:553:ILE:HD12	1:R:553:ILE:H	1.77	0.49
1:R:567:ASP:HA	1:R:623:SER:CB	2.37	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:493:PHE:HA	1:K:539:GLY:HA2	1.94	0.49
1:L:241:GLU:HB2	1:L:277:ARG:NH2	2.27	0.49
1:F:45:LYS:HE2	1:F:282:PHE:O	2.12	0.49
1:H:273:ILE:HG13	1:H:275:MET:HE1	1.90	0.49
1:I:69:LEU:HD23	1:I:137:ILE:HG12	1.95	0.49
1:M:569:MET:HG3	1:M:624:LEU:HD13	1.83	0.49
1:N:255:GLU:HA	1:N:320:PHE:O	2.13	0.49
1:O:460:LEU:C	1:O:462:PHE:N	2.65	0.49
1:Q:139:ALA:O	1:Q:142:PHE:CE1	2.65	0.49
1:R:87:ALA:O	1:R:88:ASP:C	2.51	0.49
1:R:109:ASN:HD22	1:R:109:ASN:N	2.10	0.49
1:R:172:SER:HB3	1:R:241:GLU:OE2	2.12	0.49
1:L:39:ASP:OD2	1:L:298:ARG:HD3	2.13	0.49
1:F:171:PRO:CB	1:F:273:ILE:HD12	2.43	0.49
1:F:353:LEU:HD22	1:F:357:THR:HG21	1.95	0.49
1:H:273:ILE:CG1	1:H:275:MET:HE3	2.28	0.49
1:I:497:GLN:N	1:I:497:GLN:NE2	2.38	0.49
1:M:35:ASP:O	1:M:37:ILE:N	2.45	0.49
1:N:28:LEU:O	1:N:31:SER:HB2	2.13	0.49
1:Q:443:ILE:HG13	1:Q:478:ARG:O	2.13	0.49
1:R:42:ARG:HH11	1:R:140:GLU:HG2	1.78	0.49
1:R:218:LEU:HD22	1:R:221:MET:HE2	1.94	0.49
1:D:355:ARG:HD3	4:D:806:HOH:O	2.11	0.49
1:B:447:GLU:N	1:B:448:PRO:CA	2.76	0.49
1:C:15:TRP:CD2	1:C:520:LYS:HG2	2.48	0.49
1:C:168:ARG:NH1	1:C:241:GLU:OE2	2.46	0.49
1:C:378:SER:HB3	1:C:400:ALA:HB2	1.95	0.49
1:G:470:LYS:O	1:G:473:HIS:O	2.30	0.49
1:H:42:ARG:HH11	1:H:140:GLU:CG	2.22	0.49
1:M:214:PHE:HD2	1:M:305:VAL:HG22	1.75	0.49
1:M:569:MET:CG	1:M:624:LEU:HD12	2.22	0.49
1:P:168:ARG:HH22	1:P:276:ASP:C	2.16	0.49
1:Q:643:LYS:O	1:Q:644:SER:CB	2.61	0.49
1:J:443:ILE:HG12	1:J:445:LEU:HD13	1.95	0.49
1:F:145:GLU:CG	1:F:331:LEU:HD22	2.42	0.48
1:G:353:LEU:HD22	1:G:357:THR:HG21	1.94	0.48
1:I:175:ASN:O	1:I:271:TRP:HA	2.13	0.48
1:M:278:ASN:O	1:M:280:THR:N	2.44	0.48
1:O:467:GLU:OE1	1:O:467:GLU:HA	2.13	0.48
1:O:535:TRP:CD1	1:O:605:LYS:HA	2.48	0.48
1:Q:275:MET:HE1	1:Q:283:ILE:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:169:VAL:HG23	1:R:171:PRO:O	2.13	0.48
1:R:284:ASP:HB3	1:R:291:ASN:HD21	1.78	0.48
1:K:90:VAL:HB	1:K:116:ILE:HG12	1.94	0.48
1:K:299:ASP:O	1:K:301:TRP:N	2.46	0.48
1:A:218:LEU:HD12	1:A:303:GLN:CB	2.42	0.48
1:D:80:LEU:HD13	1:D:509:PHE:CD1	2.48	0.48
1:C:218:LEU:HD13	1:C:268:LEU:HD13	1.95	0.48
1:I:273:ILE:CG1	1:I:275:MET:HE1	2.43	0.48
1:R:175:ASN:ND2	1:R:237:LYS:HG2	2.28	0.48
1:J:490:PRO:HB2	1:J:569:MET:HE2	1.90	0.48
1:K:316:MET:HG2	1:K:317:ASN:N	2.27	0.48
1:L:193:PRO:HA	1:L:362:ASN:ND2	2.28	0.48
1:B:66:VAL:CG1	1:B:67:HIS:N	2.76	0.48
1:C:218:LEU:H	1:C:303:GLN:HE21	1.61	0.48
1:E:41:ASP:O	1:E:42:ARG:C	2.51	0.48
1:N:188:MET:O	1:N:362:ASN:OD1	2.31	0.48
1:P:106:ILE:HD11	1:P:513:PHE:HB3	1.96	0.48
1:P:141:VAL:O	1:P:141:VAL:CG1	2.61	0.48
1:P:500:ALA:HB1	1:P:522:ARG:HH22	1.78	0.48
1:R:539:GLY:O	1:R:601:PRO:HD2	2.13	0.48
1:K:444:VAL:HG13	1:K:479:VAL:HB	1.95	0.48
1:B:218:LEU:HD12	1:B:303:GLN:CB	2.43	0.48
1:C:57:LYS:HE2	1:C:135:ASP:HB3	1.95	0.48
1:C:62:THR:N	1:C:63:ASP:HB3	2.29	0.48
1:I:45:LYS:NZ	1:I:282:PHE:O	2.45	0.48
1:I:291:ASN:ND2	1:I:295:TYR:HA	2.29	0.48
1:M:89:LYS:HZ2	1:M:89:LYS:HB3	1.78	0.48
1:M:111:PRO:C	1:M:113:SER:H	2.17	0.48
1:N:56:GLU:OE1	1:N:168:ARG:HD2	2.14	0.48
1:O:599:GLY:O	1:O:601:PRO:HD3	2.13	0.48
1:Q:269:MET:HG2	1:Q:306:TYR:HE1	1.79	0.48
1:R:218:LEU:C	1:R:220:GLU:H	2.16	0.48
1:J:242:HIS:O	1:J:245:LYS:HB2	2.12	0.48
1:C:280:THR:HG23	1:C:281:THR:HG23	1.95	0.48
1:E:36:MET:SD	2:E:701:SAH:HG1	2.54	0.48
1:E:168:ARG:HA	1:E:241:GLU:OE2	2.13	0.48
1:M:550:ARG:O	1:M:560:GLN:OE1	2.31	0.48
1:O:297:TRP:CD2	1:O:495:ASP:HB3	2.48	0.48
1:O:467:GLU:OE2	1:O:556:ARG:HA	2.13	0.48
1:O:569:MET:HA	1:O:572:SER:HB2	1.95	0.48
1:P:280:THR:HG23	1:P:281:THR:HG23	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:631:ASP:O	1:P:635:GLY:N	2.41	0.48
1:Q:570:SER:CB	1:Q:622:LYS:HD3	2.40	0.48
1:H:51:LYS:HG3	1:H:85:GLU:CG	2.43	0.48
1:I:136:ILE:HA	1:I:168:ARG:O	2.13	0.48
1:O:548:ILE:O	1:O:562:CYS:SG	2.67	0.48
1:Q:51:LYS:HA	1:Q:85:GLU:CD	2.33	0.48
1:R:36:MET:HA	1:R:300:HIS:CD2	2.48	0.48
1:K:273:ILE:HD12	1:K:275:MET:HE3	1.95	0.48
1:L:253:VAL:O	1:L:253:VAL:CG2	2.61	0.48
1:L:420:ILE:HD11	1:L:428:VAL:HG22	1.94	0.48
1:D:528:ILE:HD12	1:D:528:ILE:N	2.28	0.48
1:B:178:ILE:HA	1:B:268:LEU:O	2.14	0.48
1:C:484:GLY:HA3	1:C:581:TRP:CZ3	2.49	0.48
1:E:226:PHE:N	1:E:226:PHE:CD1	2.81	0.48
1:E:275:MET:HE1	1:E:283:ILE:H	1.78	0.48
1:I:543:GLY:HA3	1:I:568:ASN:HD22	1.77	0.48
1:I:587:ASN:ND2	1:I:587:ASN:C	2.67	0.48
1:N:84:ARG:HD2	1:N:85:GLU:HG2	1.95	0.48
1:O:535:TRP:O	1:O:535:TRP:CE3	2.67	0.48
1:J:169:VAL:CG2	1:J:171:PRO:O	2.62	0.48
1:J:308:LEU:HD13	1:J:333:PHE:O	2.13	0.48
1:L:290:LYS:O	1:L:290:LYS:HG2	2.13	0.48
1:A:467:GLU:CD	1:A:557:VAL:HG12	2.34	0.48
1:D:489:ILE:O	1:D:576:PRO:HD2	2.13	0.48
1:E:75:THR:O	1:E:103:ALA:HA	2.13	0.48
1:N:42:ARG:NH1	1:N:140:GLU:HG2	2.28	0.48
1:N:84:ARG:O	1:N:85:GLU:HB2	2.14	0.48
1:N:387:GLY:HA2	1:N:450:TYR:CE2	2.48	0.48
1:O:553:ILE:HG13	1:O:554:ASP:H	1.79	0.48
1:P:228:GLU:OE2	1:P:290:LYS:NZ	2.47	0.48
1:P:455:ASN:HB2	1:P:458:ASN:HB2	1.96	0.48
1:R:338:LYS:HA	1:R:338:LYS:HD3	1.52	0.48
1:J:193:PRO:HA	1:J:362:ASN:ND2	2.26	0.48
1:B:218:LEU:HD13	1:B:268:LEU:HD13	1.96	0.48
1:B:460:LEU:HD21	1:B:579:MET:CE	2.44	0.48
1:E:388:GLU:OE1	1:E:452:SER:HB2	2.13	0.48
1:H:38:LEU:HD21	1:H:503:VAL:HA	1.96	0.48
1:I:273:ILE:HG13	1:I:283:ILE:HB	1.96	0.48
1:M:159:LEU:HD13	1:M:243:GLU:N	2.29	0.48
1:M:300:HIS:CE1	1:M:301:TRP:CE2	3.02	0.48
1:N:405:ILE:HB	1:N:430:ILE:HG12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:143:ASP:C	1:Q:145:GLU:H	2.17	0.48
1:Q:356:GLN:O	1:Q:359:TYR:HB3	2.13	0.48
1:R:548:ILE:HG22	1:R:549:LEU:HD22	1.95	0.48
1:K:145:GLU:HG3	1:K:331:LEU:CD2	2.44	0.48
1:K:218:LEU:HD13	1:K:268:LEU:HD22	1.95	0.48
1:K:220:GLU:HG3	1:K:536:GLU:O	2.13	0.48
1:D:443:ILE:HG13	1:D:478:ARG:HB3	1.95	0.48
1:C:293:ASN:OD1	1:C:293:ASN:N	2.46	0.48
1:G:56:GLU:C	1:G:58:LYS:H	2.16	0.48
1:O:382:HIS:HD2	1:O:441:PRO:HA	1.73	0.48
1:O:522:ARG:O	1:O:526:ASP:HB2	2.14	0.48
1:K:297:TRP:CE3	1:K:495:ASP:HB3	2.48	0.48
1:A:612:TYR:CE2	1:A:614:PRO:HA	2.49	0.47
1:D:578:TRP:CG	1:D:591:GLY:HA3	2.49	0.47
1:C:323:VAL:HG12	1:C:325:ASN:HD21	1.79	0.47
1:F:497:GLN:NE2	1:F:497:GLN:N	2.59	0.47
1:H:20:GLU:H	1:H:20:GLU:HG3	1.52	0.47
1:I:615:ILE:O	1:I:616:THR:C	2.52	0.47
1:M:271:TRP:O	1:M:285:MET:HB2	2.14	0.47
1:N:67:HIS:HB3	1:N:135:ASP:H	1.79	0.47
1:N:339:ASP:HA	1:Q:244:GLU:HG3	1.96	0.47
1:O:375:ASP:HB3	1:O:399:THR:OG1	2.14	0.47
1:P:72:GLY:O	2:P:701:SAH:N	2.42	0.47
1:P:531:GLU:HA	1:P:609:GLN:O	2.14	0.47
1:Q:489:ILE:HG22	1:Q:578:TRP:HZ3	1.79	0.47
1:K:291:ASN:HB3	1:K:295:TYR:HB2	1.96	0.47
1:D:22:TYR:CE2	1:D:525:THR:HG22	2.50	0.47
1:D:67:HIS:HE1	1:D:91:THR:HG22	1.77	0.47
1:D:202:GLU:HA	4:D:852:HOH:O	2.14	0.47
1:D:239:ASP:OD2	1:D:242:HIS:HD2	1.96	0.47
1:D:435:THR:HA	1:D:472:MET:SD	2.54	0.47
1:M:497:GLN:HE21	1:M:497:GLN:N	1.99	0.47
1:N:84:ARG:CB	1:N:112:TRP:CZ2	2.97	0.47
1:N:180:PRO:HB2	1:N:264:ILE:HG12	1.96	0.47
1:O:85:GLU:OE1	1:O:85:GLU:HA	2.14	0.47
1:Q:236:PHE:CE2	1:Q:326:HIS:HD2	2.32	0.47
1:L:385:THR:HG22	4:L:825:HOH:O	2.13	0.47
1:A:76:GLY:O	1:A:77:LEU:C	2.53	0.47
1:B:491:GLU:HG3	1:B:492:LYS:N	2.29	0.47
1:C:28:LEU:HD23	1:C:521:ALA:HB2	1.95	0.47
1:C:480:GLU:OE2	1:C:482:HIS:CD2	2.55	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:140:GLU:HG3	1:F:140:GLU:O	2.14	0.47
1:G:489:ILE:HG13	1:G:490:PRO:HD2	1.95	0.47
1:H:51:LYS:NZ	1:H:51:LYS:CB	2.78	0.47
1:H:218:LEU:HD13	1:H:268:LEU:HD13	1.96	0.47
1:M:111:PRO:HG2	1:M:112:TRP:CE3	2.48	0.47
1:M:250:GLU:HB2	1:M:326:HIS:CD2	2.49	0.47
1:M:507:ASN:HD22	1:M:507:ASN:N	2.11	0.47
1:O:218:LEU:H	1:O:303:GLN:HE22	1.57	0.47
1:Q:357:THR:O	1:Q:361:VAL:HG23	2.15	0.47
1:R:291:ASN:O	1:R:292:LYS:HD2	2.12	0.47
1:J:270:TRP:CE2	1:J:286:GLY:HA2	2.49	0.47
1:J:356:GLN:O	1:J:606:GLY:HA2	2.14	0.47
1:K:353:LEU:HD22	1:K:357:THR:HG21	1.95	0.47
1:K:532:GLN:HE21	1:K:532:GLN:HB2	1.45	0.47
1:L:317:ASN:ND2	1:L:317:ASN:N	2.63	0.47
1:A:243:GLU:HG2	1:A:244:GLU:OE1	2.14	0.47
1:B:535:TRP:CE3	1:B:605:LYS:HE3	2.49	0.47
1:F:42:ARG:HH21	1:F:43:ASN:ND2	2.11	0.47
1:E:157:GLU:HA	1:E:160:GLU:CG	2.45	0.47
1:E:284:ASP:HB3	1:E:294:ASN:HB2	1.96	0.47
1:G:478:ARG:NH2	1:G:480:GLU:OE1	2.47	0.47
1:O:146:LEU:HB2	1:O:271:TRP:CD1	2.49	0.47
1:O:168:ARG:HG2	1:O:241:GLU:OE2	2.14	0.47
1:R:643:LYS:O	1:R:644:SER:HB3	2.15	0.47
1:J:450:TYR:H	1:J:459:HIS:CD2	2.20	0.47
1:K:193:PRO:HA	1:K:362:ASN:ND2	2.28	0.47
1:K:196:ASN:HB2	1:K:201:GLU:OE2	2.15	0.47
1:K:412:PHE:CE2	1:K:451:MET:HG2	2.44	0.47
1:K:489:ILE:HD12	1:K:545:ALA:HB2	1.95	0.47
1:B:507:ASN:HD22	1:B:507:ASN:N	2.13	0.47
1:F:250:GLU:OE2	1:F:252:PHE:CE2	2.68	0.47
1:H:277:ARG:O	1:H:277:ARG:HG2	2.13	0.47
1:R:218:LEU:N	1:R:303:GLN:HE21	2.11	0.47
1:J:490:PRO:HB2	1:J:572:SER:OG	2.14	0.47
1:A:623:SER:O	1:A:624:LEU:HD23	2.15	0.47
1:B:470:LYS:NZ	1:B:553:ILE:O	2.47	0.47
1:E:567:ASP:OD1	1:E:623:SER:OG	2.29	0.47
1:G:112:TRP:HD1	1:G:115:LYS:HD2	1.78	0.47
1:I:420:ILE:HD11	1:I:428:VAL:HG22	1.95	0.47
1:N:625:CYS:HB2	1:N:643:LYS:O	2.13	0.47
1:O:556:ARG:O	1:O:558:SER:OG	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:243:GLU:H	1:R:243:GLU:CD	2.16	0.47
1:R:437:LEU:HD13	1:R:441:PRO:HD3	1.95	0.47
1:R:548:ILE:HD12	1:R:564:VAL:HG21	1.96	0.47
1:J:143:ASP:HB3	1:J:149:GLU:HG3	1.95	0.47
1:L:61:ASN:O	1:L:63:ASP:O	2.33	0.47
1:A:452:SER:O	1:A:453:ALA:C	2.53	0.47
1:A:480:GLU:HA	1:A:481:PRO:C	2.34	0.47
1:A:556:ARG:HG2	1:A:556:ARG:NH1	2.29	0.47
1:D:218:LEU:H	1:D:303:GLN:HE21	1.62	0.47
1:D:379:LYS:HA	1:D:399:THR:HG22	1.92	0.47
1:B:258:ALA:O	1:B:316:MET:HA	2.14	0.47
1:C:35:ASP:O	1:C:36:MET:C	2.53	0.47
1:C:261:SER:OG	1:C:316:MET:N	2.47	0.47
1:F:316:MET:HA	1:F:317:ASN:HA	1.63	0.47
1:E:71:ILE:HG23	1:E:93:LEU:HD12	1.96	0.47
1:E:108:SER:O	1:E:110:SER:N	2.47	0.47
1:E:451:MET:HG3	1:E:452:SER:N	2.28	0.47
1:H:450:TYR:N	1:H:459:HIS:HD2	2.02	0.47
1:H:497:GLN:NE2	1:H:497:GLN:N	2.43	0.47
1:I:137:ILE:O	1:I:169:VAL:HA	2.15	0.47
1:I:297:TRP:CD2	1:I:495:ASP:HB3	2.50	0.47
1:M:179:VAL:HG22	1:M:232:PRO:HA	1.96	0.47
1:M:181:VAL:HG21	1:M:268:LEU:CD1	2.37	0.47
1:M:540:ILE:HD12	1:M:542:LYS:HE2	1.97	0.47
1:M:568:ASN:N	1:M:568:ASN:ND2	2.62	0.47
1:N:325:ASN:HB2	1:N:332:TRP:CE2	2.50	0.47
1:O:177:TYR:O	1:O:269:MET:HA	2.14	0.47
1:O:539:GLY:O	1:O:601:PRO:HD2	2.14	0.47
1:O:587:ASN:HD22	1:O:587:ASN:C	2.18	0.47
1:P:387:GLY:HA2	1:P:450:TYR:CE1	2.50	0.47
1:Q:438:THR:HG21	1:R:629:LEU:HD21	1.97	0.47
1:R:13:ARG:NH1	1:R:13:ARG:HB2	2.30	0.47
1:R:69:LEU:HD11	1:R:71:ILE:HG12	1.97	0.47
1:R:375:ASP:OD1	1:R:375:ASP:N	2.48	0.47
1:J:444:VAL:HG13	1:J:479:VAL:HB	1.96	0.47
1:D:278:ASN:HB2	1:D:280:THR:HG22	1.95	0.47
1:B:78:LEU:HD22	2:B:701:SAH:HN2	1.80	0.47
1:E:45:LYS:O	1:E:275:MET:HG2	2.15	0.47
1:M:95:VAL:CB	1:M:122:ARG:HG3	2.44	0.47
1:N:43:ASN:N	1:N:43:ASN:HD22	2.12	0.47
1:P:367:ASN:HD21	1:P:369:LYS:HD3	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:478:ARG:HH21	1:Q:478:ARG:CG	2.20	0.47
1:R:604:ASN:OD1	1:R:606:GLY:N	2.33	0.47
1:F:416:PHE:O	1:F:420:ILE:HG13	2.15	0.47
1:G:375:ASP:O	1:G:399:THR:HG21	2.14	0.47
1:I:177:TYR:HA	1:I:233:ILE:O	2.14	0.47
1:N:57:LYS:HB3	1:N:66:VAL:HG11	1.97	0.47
1:N:275:MET:H	1:N:275:MET:HE2	1.79	0.47
1:R:84:ARG:O	1:R:85:GLU:HB2	2.15	0.47
1:R:354:SER:O	1:R:358:VAL:HG23	2.14	0.47
1:R:578:TRP:HE1	1:R:580:GLU:HG3	1.80	0.47
1:K:168:ARG:HG2	1:K:168:ARG:HH11	1.80	0.47
1:A:241:GLU:HG3	1:A:277:ARG:HH21	1.79	0.47
1:D:292:LYS:HA	1:D:293:ASN:HA	1.53	0.47
1:B:416:PHE:O	1:B:420:ILE:HG13	2.15	0.47
1:F:57:LYS:HG2	1:F:135:ASP:HB3	1.97	0.47
1:G:179:VAL:HG22	1:G:232:PRO:HA	1.96	0.47
1:I:298:ARG:HD2	1:I:301:TRP:HE3	1.80	0.47
1:I:566:ILE:HG22	1:I:569:MET:HE3	1.97	0.47
1:M:111:PRO:HG2	1:M:112:TRP:CZ3	2.50	0.47
1:M:615:ILE:O	1:M:615:ILE:HG13	2.14	0.47
1:N:514:PHE:O	1:N:518:SER:CB	2.63	0.47
1:P:529:VAL:HG12	1:P:530:ASP:O	2.15	0.47
1:Q:222:LYS:HB3	1:Q:224:HIS:HB3	1.96	0.47
1:R:35:ASP:O	1:R:36:MET:C	2.53	0.47
1:R:97:LYS:HB2	1:R:98:PRO:HD3	1.96	0.47
1:J:129:ILE:O	1:J:131:GLY:N	2.47	0.47
1:K:181:VAL:HG21	1:K:268:LEU:HD11	1.97	0.47
1:B:59:HIS:O	1:B:60:GLU:C	2.52	0.46
1:B:516:GLU:HG2	1:B:517:ILE:N	2.30	0.46
1:C:73:THR:O	2:C:701:SAH:HA	2.15	0.46
1:F:259:HIS:CD2	1:F:259:HIS:O	2.68	0.46
1:F:449:PHE:CD1	1:F:449:PHE:C	2.89	0.46
1:E:84:ARG:HG3	1:E:85:GLU:N	2.31	0.46
1:E:216:VAL:O	1:E:302:MET:HG2	2.16	0.46
1:G:57:LYS:NZ	1:G:166:GLY:O	2.48	0.46
1:G:483:MET:SD	1:G:550:ARG:HG3	2.55	0.46
1:G:492:LYS:HB2	1:G:571:SER:O	2.14	0.46
1:H:137:ILE:O	1:H:169:VAL:HA	2.15	0.46
1:I:146:LEU:HB2	1:I:271:TRP:CD1	2.50	0.46
1:N:512:SER:O	1:N:515:ASP:HB2	2.15	0.46
1:N:595:ILE:HG22	1:N:599:GLY:HA2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:269:MET:HG3	1:O:304:ALA:HB3	1.97	0.46
1:P:285:MET:O	1:P:303:GLN:OE1	2.33	0.46
1:P:407:ASP:O	1:P:413:ARG:HD3	2.15	0.46
1:Q:179:VAL:HG21	1:Q:270:TRP:CH2	2.51	0.46
1:Q:460:LEU:HD22	1:Q:463:LEU:HD21	1.97	0.46
1:R:580:GLU:HA	1:R:588:LEU:O	2.15	0.46
1:K:180:PRO:O	1:K:181:VAL:HG23	2.16	0.46
1:L:412:PHE:CE2	1:L:451:MET:HG2	2.49	0.46
1:B:297:TRP:CE3	1:B:298:ARG:HA	2.50	0.46
1:B:434:VAL:HG12	1:B:469:LEU:HD13	1.97	0.46
1:F:198:GLU:O	1:F:201:GLU:HG3	2.16	0.46
1:E:179:VAL:HG11	1:E:228:GLU:HG2	1.97	0.46
1:E:258:ALA:HB2	1:E:314:VAL:HG13	1.98	0.46
1:E:406:ILE:HG12	1:E:431:ILE:HD11	1.97	0.46
1:N:27:GLU:HB3	1:N:96:PHE:CE1	2.50	0.46
1:N:56:GLU:O	1:N:60:GLU:HG3	2.14	0.46
1:O:419:TYR:O	1:O:422:TYR:N	2.44	0.46
1:R:53:THR:HB	1:R:136:ILE:HD13	1.96	0.46
1:J:381:LEU:HD23	1:J:381:LEU:HA	1.73	0.46
1:K:104:ARG:HA	1:K:107:THR:HG22	1.98	0.46
1:C:70:ASP:HA	1:C:138:VAL:O	2.14	0.46
1:C:168:ARG:NH1	1:C:168:ARG:CG	2.52	0.46
1:F:107:THR:HG21	1:F:116:ILE:HG21	1.97	0.46
1:F:360:HIS:NE2	1:F:447:GLU:OE2	2.40	0.46
1:E:242:HIS:HB3	1:E:244:GLU:OE2	2.15	0.46
1:G:75:THR:O	1:G:106:ILE:HD12	2.15	0.46
1:G:550:ARG:H	1:G:560:GLN:HE22	1.64	0.46
1:H:178:ILE:HA	1:H:268:LEU:O	2.15	0.46
1:I:271:TRP:HZ3	1:I:283:ILE:HG22	1.79	0.46
1:I:398:LYS:HB3	1:I:398:LYS:HZ3	1.81	0.46
1:M:94:GLU:OE2	2:M:701:SAH:H1'	2.15	0.46
1:M:381:LEU:HB3	1:M:442:ASP:HB2	1.97	0.46
1:N:160:GLU:H	1:N:160:GLU:HG2	1.55	0.46
1:N:549:LEU:HD12	1:N:560:GLN:NE2	2.30	0.46
1:N:553:ILE:HD12	1:N:553:ILE:HA	1.72	0.46
1:O:84:ARG:HG3	1:O:112:TRP:CZ2	2.50	0.46
1:R:181:VAL:CG1	1:R:226:PHE:HB2	2.45	0.46
1:R:480:GLU:OE2	1:R:482:HIS:HD2	1.97	0.46
1:J:51:LYS:HG3	1:J:85:GLU:CD	2.34	0.46
1:K:218:LEU:HD11	1:K:268:LEU:HD22	1.98	0.46
1:C:144:THR:O	1:C:271:TRP:CD1	2.68	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:250:GLU:HB2	1:H:326:HIS:CD2	2.51	0.46
1:I:555:GLY:HA3	1:I:556:ARG:O	2.14	0.46
1:M:175:ASN:HD21	1:M:237:LYS:NZ	2.13	0.46
1:M:193:PRO:HA	1:M:362:ASN:HD21	1.81	0.46
1:O:38:LEU:HD21	1:O:503:VAL:HA	1.96	0.46
1:O:410:GLU:O	1:O:410:GLU:HG3	2.14	0.46
1:O:498:ASN:HA	1:O:501:SER:OG	2.15	0.46
1:Q:254:ARG:O	1:Q:321:GLU:CA	2.59	0.46
1:Q:392:LEU:HD12	1:Q:445:LEU:HB3	1.97	0.46
1:Q:522:ARG:O	1:Q:526:ASP:HB2	2.14	0.46
1:R:553:ILE:HD12	1:R:553:ILE:N	2.29	0.46
1:J:175:ASN:ND2	1:J:237:LYS:HG2	2.31	0.46
1:K:28:LEU:HD11	1:K:517:ILE:HD12	1.98	0.46
1:A:244:GLU:H	1:A:244:GLU:CD	2.18	0.46
1:F:73:THR:O	1:F:74:GLY:C	2.54	0.46
1:F:169:VAL:HG22	1:F:241:GLU:HG2	1.97	0.46
1:G:144:THR:HG23	1:G:302:MET:O	2.16	0.46
1:G:258:ALA:HB3	1:G:315:GLU:O	2.15	0.46
1:H:218:LEU:H	1:H:303:GLN:NE2	2.12	0.46
1:M:483:MET:HE3	1:M:550:ARG:HG2	1.96	0.46
1:N:349:LEU:HD23	1:N:350:HIS:N	2.30	0.46
1:P:45:LYS:HZ1	1:P:294:ASN:HD22	1.61	0.46
1:P:157:GLU:O	1:P:161:ARG:HB2	2.15	0.46
1:P:447:GLU:N	1:P:448:PRO:HA	2.30	0.46
1:Q:420:ILE:HD11	1:R:5:LYS:HA	1.98	0.46
1:R:140:GLU:HG3	1:R:140:GLU:O	2.16	0.46
1:R:258:ALA:C	1:R:260:SER:H	2.19	0.46
1:B:71:ILE:HG21	1:B:154:THR:HG23	1.98	0.46
1:C:56:GLU:OE1	1:C:168:ARG:HD2	2.16	0.46
1:E:67:HIS:CE1	1:E:91:THR:CG2	2.88	0.46
1:G:559:SER:HA	1:G:630:PHE:O	2.16	0.46
1:H:258:ALA:HB2	1:H:314:VAL:CG2	2.46	0.46
1:M:218:LEU:H	1:M:303:GLN:HE21	1.62	0.46
1:N:379:LYS:CA	1:N:399:THR:CG2	2.86	0.46
1:N:627:HIS:HB2	1:N:640:GLN:HB2	1.98	0.46
1:O:621:ASP:N	1:O:621:ASP:OD1	2.46	0.46
1:Q:339:ASP:C	1:Q:341:SER:H	2.19	0.46
1:J:323:VAL:HG23	1:J:335:ASN:HA	1.96	0.46
1:J:421:HIS:HB2	1:K:3:LEU:HB3	1.97	0.46
1:K:34:GLY:C	1:K:499:ILE:HA	2.36	0.46
1:K:335:ASN:O	1:K:338:LYS:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:145:GLU:HG3	1:L:213:VAL:HG21	1.96	0.46
1:L:146:LEU:HB2	1:L:271:TRP:CD1	2.49	0.46
1:L:179:VAL:HG21	1:L:270:TRP:CH2	2.50	0.46
1:L:190:ASN:HD21	1:L:209:GLY:HA3	1.81	0.46
1:A:168:ARG:NH1	1:A:241:GLU:OE2	2.49	0.46
1:A:169:VAL:HG22	1:A:171:PRO:O	2.15	0.46
1:A:175:ASN:ND2	1:A:237:LYS:HG2	2.30	0.46
1:D:452:SER:O	1:D:453:ALA:C	2.54	0.46
1:D:506:VAL:O	1:D:507:ASN:C	2.53	0.46
1:B:156:LYS:HE2	1:B:246:ILE:O	2.16	0.46
1:C:190:ASN:ND2	1:C:209:GLY:HA3	2.31	0.46
1:C:631:ASP:C	1:C:631:ASP:OD1	2.54	0.46
1:F:480:GLU:HA	1:F:481:PRO:C	2.35	0.46
1:E:143:ASP:O	1:E:146:LEU:HA	2.16	0.46
1:G:502:ASP:OD2	1:G:616:THR:HG21	2.16	0.46
1:H:478:ARG:CG	1:H:478:ARG:NH2	2.70	0.46
1:I:478:ARG:HG2	1:I:478:ARG:NH2	2.30	0.46
1:N:385:THR:HA	1:N:445:LEU:O	2.15	0.46
1:P:216:VAL:HG22	1:P:218:LEU:HD23	1.98	0.46
1:P:253:VAL:O	1:P:253:VAL:HG23	2.15	0.46
1:Q:139:ALA:O	1:Q:142:PHE:HE1	1.99	0.46
1:J:502:ASP:OD2	1:J:616:THR:HG21	2.16	0.46
1:K:123:SER:CB	2:K:701:SAH:HN62	2.17	0.46
1:A:145:GLU:O	1:A:146:LEU:HB3	2.16	0.46
1:A:272:ASP:C	1:A:272:ASP:OD1	2.54	0.46
1:C:16:VAL:HG22	4:C:811:HOH:O	2.16	0.46
1:C:314:VAL:HG23	1:C:320:PHE:CD2	2.50	0.46
1:F:7:ASN:ND2	1:F:640:GLN:OE1	2.45	0.46
1:G:93:LEU:CD2	1:G:119:ILE:HB	2.46	0.46
1:G:151:ALA:O	1:G:155:PHE:HD2	1.99	0.46
1:I:379:LYS:CA	1:I:399:THR:HG23	2.36	0.46
1:M:67:HIS:HD2	1:M:133:ARG:O	1.98	0.46
1:M:218:LEU:N	1:M:303:GLN:NE2	2.64	0.46
1:M:280:THR:CG2	1:M:281:THR:N	2.79	0.46
1:N:327:ASP:OD1	1:N:328:GLU:N	2.49	0.46
1:P:73:THR:O	2:P:701:SAH:HA	2.15	0.46
1:Q:42:ARG:HE	1:Q:43:ASN:ND2	2.14	0.46
1:J:274:ASP:OD2	1:J:277:ARG:CA	2.63	0.46
1:A:554:ASP:O	1:A:555:GLY:O	2.34	0.46
1:D:626:LEU:CD2	1:D:628:ALA:HB2	2.45	0.46
1:F:203:PRO:HA	1:F:422:TYR:CG	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:42:ARG:HE	1:E:43:ASN:HD21	1.64	0.46
1:E:385:THR:HA	1:E:445:LEU:O	2.16	0.46
1:G:156:LYS:HA	1:G:243:GLU:HB3	1.97	0.46
1:G:190:ASN:ND2	1:G:209:GLY:HA3	2.31	0.46
1:H:67:HIS:CE1	1:H:89:LYS:HE3	2.51	0.46
1:H:242:HIS:O	1:H:245:LYS:HB2	2.16	0.46
1:I:298:ARG:O	1:I:301:TRP:O	2.34	0.46
1:I:492:LYS:HA	1:I:573:ASN:OD1	2.16	0.46
1:M:364:MET:HG3	1:M:370:PHE:CE2	2.51	0.46
1:P:406:ILE:HD13	1:P:434:VAL:HA	1.97	0.46
1:K:257:VAL:HG12	1:K:257:VAL:O	2.14	0.46
1:D:138:VAL:HG23	1:D:170:VAL:HB	1.97	0.46
1:C:140:GLU:O	1:C:140:GLU:CG	2.61	0.46
1:F:48:ALA:O	1:F:51:LYS:N	2.48	0.46
1:F:73:THR:O	1:F:76:GLY:N	2.49	0.46
1:G:35:ASP:OD1	1:G:35:ASP:N	2.48	0.46
1:H:133:ARG:HG3	1:H:164:LYS:HG2	1.98	0.46
1:H:239:ASP:OD1	1:H:242:HIS:HB2	2.16	0.46
1:H:460:LEU:HD21	1:H:579:MET:CE	2.46	0.46
1:M:289:TRP:O	1:M:290:LYS:HG2	2.16	0.46
1:M:418:LYS:HE3	1:M:418:LYS:HB2	1.79	0.46
1:P:502:ASP:OD2	1:P:616:THR:HB	2.15	0.46
1:J:216:VAL:O	1:J:302:MET:HG2	2.16	0.46
1:K:367:ASN:OD1	1:K:370:PHE:N	2.48	0.46
1:D:45:LYS:O	1:D:275:MET:HG2	2.15	0.45
1:C:61:ASN:HD22	1:C:61:ASN:N	2.14	0.45
1:C:247:ILE:HB	1:C:250:GLU:OE2	2.16	0.45
1:G:217:GLN:HB2	1:G:536:GLU:HB3	1.98	0.45
1:M:483:MET:CE	1:M:550:ARG:HG2	2.46	0.45
1:O:412:PHE:HE2	1:O:451:MET:HG2	1.81	0.45
1:P:164:LYS:O	1:P:167:CYS:HB2	2.16	0.45
1:Q:99:MET:O	1:Q:102:CYS:HB3	2.16	0.45
1:R:243:GLU:OE1	1:R:243:GLU:N	2.43	0.45
1:R:316:MET:HA	1:R:317:ASN:HA	1.69	0.45
1:R:353:LEU:HD22	1:R:357:THR:CG2	2.46	0.45
1:J:291:ASN:HB3	1:J:295:TYR:HB2	1.98	0.45
1:K:360:HIS:HB2	1:K:606:GLY:HA3	1.98	0.45
1:K:404:THR:HG23	1:K:429:GLU:HG3	1.99	0.45
1:L:353:LEU:HD22	1:L:357:THR:HG21	1.97	0.45
1:A:84:ARG:HG3	1:A:112:TRP:CZ2	2.50	0.45
1:A:385:THR:HA	1:A:445:LEU:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:466:VAL:HG11	1:B:553:ILE:CG2	2.46	0.45
1:B:569:MET:HA	1:B:572:SER:HB2	1.97	0.45
1:F:502:ASP:OD2	1:F:616:THR:HG21	2.17	0.45
1:E:48:ALA:HA	1:E:51:LYS:HB2	1.98	0.45
1:E:490:PRO:CB	1:E:569:MET:HE1	2.46	0.45
1:G:478:ARG:HH21	1:G:478:ARG:CG	2.29	0.45
1:G:489:ILE:HG12	1:G:541:VAL:HG22	1.99	0.45
1:N:566:ILE:HG21	1:N:569:MET:CE	2.42	0.45
1:O:143:ASP:HB3	1:O:149:GLU:HG3	1.98	0.45
1:O:427:ASN:OD1	1:O:427:ASN:N	2.49	0.45
1:P:39:ASP:OD2	1:P:298:ARG:HD3	2.16	0.45
1:Q:218:LEU:HA	1:Q:218:LEU:HD23	1.42	0.45
1:Q:287:PRO:HG2	1:Q:289:TRP:CZ2	2.50	0.45
1:Q:395:LEU:C	1:Q:397:ALA:H	2.18	0.45
1:Q:468:VAL:O	1:Q:472:MET:HG3	2.16	0.45
1:J:144:THR:O	1:J:144:THR:CG2	2.64	0.45
1:J:218:LEU:N	1:J:303:GLN:NE2	2.62	0.45
1:K:179:VAL:CG2	1:K:270:TRP:CH2	2.99	0.45
1:K:193:PRO:HA	1:K:362:ASN:HD21	1.82	0.45
1:L:447:GLU:N	1:L:448:PRO:HA	2.32	0.45
1:A:447:GLU:H	1:A:448:PRO:HA	1.82	0.45
1:B:119:ILE:HG22	1:B:121:GLU:HG2	1.99	0.45
1:B:190:ASN:O	1:B:190:ASN:ND2	2.50	0.45
1:B:297:TRP:CE3	1:B:495:ASP:HB3	2.51	0.45
1:B:357:THR:O	1:B:361:VAL:HG23	2.16	0.45
1:C:456:PRO:HD2	1:C:457:TRP:CE3	2.51	0.45
1:C:592:LEU:HD21	1:C:595:ILE:HD11	1.97	0.45
1:F:72:GLY:CA	2:F:701:SAH:O4'	2.65	0.45
1:G:540:ILE:HB	1:G:599:GLY:O	2.15	0.45
1:H:47:LEU:HD22	1:H:51:LYS:CD	2.46	0.45
1:H:269:MET:CG	1:H:306:TYR:HE1	2.27	0.45
1:M:35:ASP:HB3	1:M:300:HIS:H	1.80	0.45
1:M:174:GLY:HA2	1:M:273:ILE:HA	1.98	0.45
1:N:315:GLU:CB	1:N:318:GLN:HG2	2.44	0.45
1:O:460:LEU:HD11	1:O:637:ILE:HD11	1.98	0.45
1:P:110:SER:HB2	1:P:112:TRP:CZ3	2.51	0.45
1:K:292:LYS:HA	1:K:293:ASN:HB3	1.98	0.45
1:L:157:GLU:HA	1:L:160:GLU:HG2	1.97	0.45
1:A:4:GLU:OE2	1:A:13:ARG:NH1	2.50	0.45
1:A:480:GLU:HG2	1:A:584:GLY:H	1.79	0.45
1:B:43:ASN:O	1:B:81:MET:HE1	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:287:PRO:O	1:B:289:TRP:N	2.50	0.45
1:B:534:LEU:HD11	1:B:611:VAL:CG1	2.46	0.45
1:B:535:TRP:CG	1:B:605:LYS:HG2	2.51	0.45
1:F:179:VAL:HG22	1:F:232:PRO:HA	1.98	0.45
1:F:214:PHE:O	1:F:304:ALA:HA	2.17	0.45
1:G:258:ALA:CB	1:G:314:VAL:HG13	2.47	0.45
1:I:72:GLY:O	2:I:701:SAH:N	2.50	0.45
1:I:420:ILE:HD11	1:I:428:VAL:CG2	2.46	0.45
1:M:385:THR:HG22	4:M:802:HOH:O	2.15	0.45
1:N:287:PRO:O	1:N:291:ASN:HB3	2.16	0.45
1:K:181:VAL:O	1:K:265:ASP:N	2.49	0.45
1:L:137:ILE:HB	1:L:169:VAL:HB	1.97	0.45
1:A:488:ALA:HA	1:A:576:PRO:O	2.16	0.45
1:B:56:GLU:O	1:B:59:HIS:HB2	2.17	0.45
1:B:193:PRO:HA	1:B:362:ASN:ND2	2.32	0.45
1:C:349:LEU:HD11	1:C:391:PHE:HZ	1.82	0.45
1:E:83:ALA:O	1:E:84:ARG:C	2.55	0.45
1:I:111:PRO:HB2	1:I:112:TRP:CE3	2.52	0.45
1:I:612:TYR:CZ	1:I:614:PRO:HA	2.51	0.45
1:M:42:ARG:HH11	1:M:140:GLU:CG	2.20	0.45
1:M:67:HIS:N	1:M:135:ASP:OD2	2.36	0.45
1:N:577:MET:CE	1:N:626:LEU:HD11	2.47	0.45
1:O:567:ASP:O	1:O:568:ASN:CB	2.62	0.45
1:P:258:ALA:O	1:P:317:ASN:HA	2.17	0.45
1:Q:480:GLU:HA	1:Q:481:PRO:C	2.36	0.45
1:J:45:LYS:O	1:J:275:MET:HG3	2.17	0.45
1:D:550:ARG:H	1:D:560:GLN:NE2	2.11	0.45
1:B:567:ASP:O	1:B:568:ASN:CB	2.64	0.45
1:C:349:LEU:HD12	1:C:415:ILE:HD13	1.99	0.45
1:F:95:VAL:HG23	1:F:122:ARG:HB2	1.98	0.45
1:F:269:MET:HE3	1:F:304:ALA:HB3	1.99	0.45
1:E:161:ARG:HB3	1:E:162:LEU:CD1	2.46	0.45
1:E:241:GLU:HG3	1:E:277:ARG:NH2	2.31	0.45
1:E:275:MET:CE	1:E:283:ILE:HG13	2.46	0.45
1:E:443:ILE:HG12	1:E:445:LEU:HD13	1.99	0.45
1:E:452:SER:O	1:E:453:ALA:C	2.54	0.45
1:M:63:ASP:OD2	1:M:65:LYS:HB2	2.16	0.45
1:M:432:GLU:HG2	1:M:433:LYS:HG3	1.98	0.45
1:O:470:LYS:HE3	1:O:554:ASP:HA	1.98	0.45
1:Q:35:ASP:O	1:Q:36:MET:C	2.53	0.45
1:J:597:SER:HB2	1:J:598:ALA:HB3	1.91	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:188:MET:O	1:K:359:TYR:HA	2.16	0.45
1:K:203:PRO:HA	1:K:422:TYR:CG	2.52	0.45
1:L:216:VAL:O	1:L:302:MET:HG2	2.17	0.45
1:A:84:ARG:O	1:A:85:GLU:HB2	2.17	0.45
1:B:292:LYS:HA	1:B:293:ASN:HA	1.75	0.45
1:C:323:VAL:HG12	1:C:325:ASN:ND2	2.31	0.45
1:E:258:ALA:CB	1:E:314:VAL:HG13	2.47	0.45
1:H:56:GLU:O	1:H:60:GLU:HG2	2.17	0.45
1:H:258:ALA:HB2	1:H:314:VAL:HG22	1.97	0.45
1:M:169:VAL:HG22	1:M:171:PRO:O	2.16	0.45
1:M:485:VAL:HG12	1:M:580:GLU:HB2	1.98	0.45
1:N:146:LEU:HB2	1:N:271:TRP:CD1	2.52	0.45
1:N:268:LEU:HD12	1:N:289:TRP:HH2	1.82	0.45
1:O:277:ARG:HG2	1:O:277:ARG:O	2.17	0.45
1:P:168:ARG:HE	1:P:168:ARG:HB3	1.67	0.45
1:P:368:GLN:O	1:P:369:LYS:C	2.55	0.45
1:Q:68:VAL:HG13	1:Q:90:VAL:HG12	1.90	0.45
1:Q:68:VAL:HG23	1:Q:136:ILE:HB	1.99	0.45
1:Q:437:LEU:HD23	1:Q:437:LEU:HA	1.87	0.45
1:J:199:LYS:HA	1:J:200:ASP:HA	1.71	0.45
1:K:491:GLU:OE1	1:K:539:GLY:HA3	2.16	0.45
1:A:104:ARG:HA	1:A:107:THR:HG22	1.99	0.45
1:A:178:ILE:HA	1:A:268:LEU:O	2.17	0.45
1:B:412:PHE:CE2	1:B:451:MET:HG2	2.44	0.45
1:F:158:ALA:HA	1:F:162:LEU:HB2	1.98	0.45
1:F:275:MET:HE1	1:F:283:ILE:CG1	2.39	0.45
1:H:61:ASN:O	1:H:62:THR:C	2.55	0.45
1:M:379:LYS:CA	1:M:399:THR:HG23	2.38	0.45
1:M:447:GLU:HB2	1:M:449:PHE:N	2.32	0.45
1:N:297:TRP:CD2	1:N:495:ASP:HB3	2.52	0.45
1:N:549:LEU:HD21	1:N:628:ALA:HB1	1.98	0.45
1:P:241:GLU:HG3	1:P:277:ARG:NH2	2.10	0.45
1:Q:95:VAL:CB	1:Q:122:ARG:HG3	2.46	0.45
1:Q:316:MET:HA	1:Q:317:ASN:HA	1.70	0.45
1:Q:321:GLU:O	1:Q:322:ILE:HD12	2.17	0.45
1:Q:381:LEU:O	1:Q:400:ALA:HB1	2.17	0.45
1:Q:466:VAL:CG1	1:Q:470:LYS:HE2	2.46	0.45
1:R:344:TYR:O	1:R:346:VAL:HG13	2.17	0.45
1:K:373:GLU:O	1:K:377:LEU:HD12	2.17	0.45
1:L:16:VAL:CG1	1:L:17:VAL:N	2.79	0.45
1:L:629:LEU:O	1:L:637:ILE:HA	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:20:GLU:H	1:F:20:GLU:HG3	1.62	0.45
1:E:84:ARG:NH1	1:E:509:PHE:CE2	2.85	0.45
1:I:200:ASP:OD1	1:I:200:ASP:N	2.39	0.45
1:M:141:VAL:O	1:M:141:VAL:CG1	2.65	0.45
1:M:382:HIS:HD2	1:M:402:ARG:HG3	1.80	0.45
1:M:450:TYR:HE1	1:M:462:PHE:HB2	1.82	0.45
1:M:542:LYS:CG	1:M:571:SER:HB2	2.46	0.45
1:N:178:ILE:HG13	1:N:233:ILE:HB	1.99	0.45
1:N:414:ASP:O	1:N:418:LYS:HG3	2.17	0.45
1:O:19:GLU:O	1:O:19:GLU:HG2	2.14	0.45
1:O:292:LYS:HD2	1:O:292:LYS:HA	1.54	0.45
1:P:317:ASN:HD22	1:P:317:ASN:C	2.16	0.45
1:J:534:LEU:HG	1:J:609:GLN:HB2	1.98	0.45
1:K:168:ARG:HG2	1:K:168:ARG:NH1	2.32	0.45
1:K:176:VAL:HG22	1:K:235:ALA:HB3	1.99	0.45
1:A:225:GLU:HA	1:A:225:GLU:OE1	2.17	0.45
1:B:157:GLU:HA	1:B:160:GLU:HG2	1.98	0.45
1:F:325:ASN:HB3	1:F:332:TRP:CE2	2.52	0.45
1:M:95:VAL:HG13	1:M:96:PHE:H	1.80	0.45
1:M:493:PHE:HA	1:M:539:GLY:CA	2.47	0.45
1:M:632:LYS:HG3	1:M:633:SER:N	2.32	0.45
1:O:72:GLY:N	1:O:93:LEU:O	2.48	0.45
1:Q:431:ILE:HD12	1:Q:436:SER:HB2	1.99	0.45
1:Q:631:ASP:HB3	1:Q:634:THR:OG1	2.16	0.45
1:J:414:ASP:OD2	1:K:19:GLU:HG2	2.17	0.45
1:K:143:ASP:O	1:K:145:GLU:N	2.50	0.45
1:B:123:SER:C	1:B:125:ASP:H	2.18	0.44
1:B:427:ASN:HA	1:C:8:GLN:HE22	1.81	0.44
1:E:432:GLU:HG2	1:E:433:LYS:HG2	1.99	0.44
1:G:420:ILE:HD11	1:G:428:VAL:HG22	1.99	0.44
1:I:181:VAL:HG21	1:I:226:PHE:HB2	1.98	0.44
1:M:569:MET:CG	1:M:624:LEU:HD11	2.39	0.44
1:N:54:ILE:HG13	1:N:58:LYS:HD3	1.99	0.44
1:O:480:GLU:HG3	1:O:481:PRO:HA	1.99	0.44
1:O:512:SER:O	1:O:515:ASP:HB2	2.17	0.44
1:P:26:GLN:O	1:P:30:ARG:HD2	2.17	0.44
1:P:136:ILE:HA	1:P:168:ARG:O	2.16	0.44
1:P:365:PHE:O	1:P:371:LYS:NZ	2.50	0.44
1:Q:480:GLU:CG	1:Q:584:GLY:N	2.78	0.44
1:R:476:GLU:H	1:R:476:GLU:CD	2.20	0.44
1:R:505:THR:HA	1:R:509:PHE:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:600:VAL:HA	1:J:601:PRO:HD3	1.86	0.44
1:D:218:LEU:H	1:D:303:GLN:NE2	2.15	0.44
1:F:319:THR:O	1:F:320:PHE:HB3	2.17	0.44
1:H:632:LYS:HG2	1:H:633:SER:N	2.31	0.44
1:M:231:GLU:H	1:M:231:GLU:HG2	1.58	0.44
1:M:276:ASP:OD1	1:M:278:ASN:HB2	2.16	0.44
1:M:316:MET:HA	1:M:317:ASN:HA	1.78	0.44
1:O:353:LEU:HD22	1:O:357:THR:HG21	1.98	0.44
1:O:483:MET:CG	1:O:550:ARG:HH21	2.30	0.44
1:O:541:VAL:N	1:O:599:GLY:O	2.41	0.44
1:O:623:SER:O	1:O:624:LEU:HB3	2.17	0.44
1:L:228:GLU:OE2	1:L:290:LYS:HE2	2.17	0.44
1:L:631:ASP:OD1	1:L:633:SER:N	2.47	0.44
1:A:67:HIS:CE1	1:A:91:THR:HG23	2.47	0.44
1:C:447:GLU:N	1:C:448:PRO:HA	2.33	0.44
1:E:492:LYS:HB2	1:E:542:LYS:HE2	1.99	0.44
1:G:450:TYR:H	1:G:459:HIS:CD2	2.22	0.44
1:M:287:PRO:O	1:M:288:LYS:C	2.56	0.44
1:N:460:LEU:HB3	1:N:463:LEU:HD22	1.99	0.44
1:P:48:ALA:HA	1:P:51:LYS:HD2	1.99	0.44
1:Q:569:MET:CE	1:Q:575:ILE:HG12	2.47	0.44
1:J:300:HIS:HE1	1:J:301:TRP:CE3	2.35	0.44
1:K:378:SER:HB2	1:K:399:THR:HG22	1.99	0.44
1:B:519:THR:O	1:B:520:LYS:C	2.54	0.44
1:F:159:LEU:HB3	1:F:243:GLU:HG2	1.98	0.44
1:E:20:GLU:H	1:E:20:GLU:HG3	1.21	0.44
1:E:488:ALA:HB2	1:E:577:MET:HE3	1.98	0.44
1:G:67:HIS:HE1	1:G:91:THR:HG23	1.81	0.44
1:G:385:THR:CG2	1:G:405:ILE:HG23	2.47	0.44
1:H:190:ASN:ND2	1:H:209:GLY:HA3	2.31	0.44
1:I:190:ASN:O	1:I:190:ASN:CG	2.56	0.44
1:I:452:SER:O	1:I:453:ALA:C	2.56	0.44
1:I:507:ASN:N	1:I:507:ASN:ND2	2.65	0.44
1:M:68:VAL:HA	1:M:136:ILE:O	2.17	0.44
1:N:353:LEU:HB3	1:N:357:THR:HB	1.99	0.44
1:O:145:GLU:HA	1:O:269:MET:HE1	2.00	0.44
1:O:395:LEU:HD23	1:O:395:LEU:HA	1.75	0.44
1:P:26:GLN:O	1:P:30:ARG:HD3	2.16	0.44
1:P:42:ARG:NH2	1:P:43:ASN:HD21	2.09	0.44
1:Q:583:PHE:CB	1:Q:588:LEU:CD1	2.96	0.44
1:R:192:ILE:HG23	1:R:204:LEU:HD12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:379:LYS:CA	1:R:399:THR:HG21	2.42	0.44
1:J:178:ILE:HB	1:J:267:LEU:HD22	1.99	0.44
1:J:300:HIS:CE1	1:J:301:TRP:CE3	3.05	0.44
1:K:169:VAL:CG1	1:K:241:GLU:HG2	2.39	0.44
1:K:375:ASP:O	1:K:399:THR:HG21	2.17	0.44
1:L:516:GLU:O	1:L:520:LYS:HG3	2.18	0.44
1:F:51:LYS:HG3	1:F:85:GLU:HG3	1.98	0.44
1:G:28:LEU:O	1:G:28:LEU:HG	2.17	0.44
1:I:31:SER:O	1:I:33:PHE:CD2	2.71	0.44
1:I:156:LYS:NZ	1:I:243:GLU:O	2.51	0.44
1:M:80:LEU:HD21	1:M:107:THR:HG22	2.00	0.44
1:M:269:MET:HG2	1:M:306:TYR:CE2	2.51	0.44
1:M:502:ASP:OD1	1:M:616:THR:HG21	2.17	0.44
1:N:218:LEU:HD12	1:N:303:GLN:CB	2.47	0.44
1:N:387:GLY:HA2	1:N:450:TYR:CZ	2.53	0.44
1:N:460:LEU:C	1:N:462:PHE:N	2.70	0.44
1:O:550:ARG:HD2	1:O:550:ARG:HA	1.80	0.44
1:Q:216:VAL:HG13	1:Q:218:LEU:HG	2.00	0.44
1:Q:460:LEU:C	1:Q:462:PHE:N	2.71	0.44
1:L:143:ASP:O	1:L:146:LEU:N	2.43	0.44
1:D:50:LEU:O	1:D:54:ILE:CG1	2.65	0.44
1:B:43:ASN:HD22	1:B:43:ASN:N	2.07	0.44
1:F:392:LEU:O	1:F:392:LEU:HD22	2.17	0.44
1:E:362:ASN:O	1:E:366:GLU:HG2	2.18	0.44
1:G:403:VAL:HB	1:G:428:VAL:HB	1.99	0.44
1:M:269:MET:HG3	1:M:304:ALA:HB3	2.00	0.44
1:M:316:MET:HG3	1:M:316:MET:O	2.17	0.44
1:N:168:ARG:NH1	1:N:241:GLU:OE2	2.51	0.44
1:Q:108:SER:HA	1:Q:113:SER:HB2	1.99	0.44
1:Q:375:ASP:CA	1:Q:399:THR:HG21	2.21	0.44
1:Q:404:THR:HG23	1:Q:429:GLU:HG3	2.00	0.44
1:Q:490:PRO:HB2	1:Q:572:SER:OG	2.18	0.44
1:A:412:PHE:HE2	1:A:451:MET:HG2	1.82	0.44
1:D:140:GLU:C	1:D:140:GLU:OE1	2.56	0.44
1:B:489:ILE:HD13	1:B:541:VAL:HG22	1.99	0.44
1:F:277:ARG:O	1:F:279:GLY:N	2.51	0.44
1:H:211:ALA:HB2	1:H:343:SER:O	2.17	0.44
1:I:51:LYS:HG3	1:I:85:GLU:HG2	2.00	0.44
1:I:185:LEU:O	1:I:185:LEU:HD22	2.18	0.44
1:N:201:GLU:HA	1:N:422:TYR:OH	2.17	0.44
1:P:497:GLN:H	1:P:497:GLN:HE21	1.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:52:THR:O	1:Q:55:ALA:HB3	2.17	0.44
1:Q:235:ALA:HB1	1:Q:324:CYS:SG	2.58	0.44
1:Q:383:VAL:HG23	1:Q:384:ALA:N	2.33	0.44
1:Q:566:ILE:HG22	1:Q:569:MET:HE2	2.00	0.44
1:R:94:GLU:OE2	2:R:701:SAH:H1'	2.18	0.44
1:J:56:GLU:OE1	1:J:168:ARG:HD2	2.18	0.44
1:J:395:LEU:O	1:J:398:LYS:HB2	2.18	0.44
1:J:449:PHE:CD1	1:J:449:PHE:C	2.91	0.44
1:L:359:TYR:CD1	1:L:359:TYR:C	2.90	0.44
1:A:434:VAL:HG13	1:A:469:LEU:CD1	2.47	0.44
1:C:57:LYS:HG2	1:C:135:ASP:HB3	1.99	0.44
1:F:186:LEU:O	1:F:307:TYR:OH	2.21	0.44
1:F:264:ILE:HB	1:F:312:LYS:HB3	2.00	0.44
1:I:145:GLU:HG3	1:I:331:LEU:HD22	2.00	0.44
1:M:383:VAL:HG13	1:M:403:VAL:HG22	2.00	0.44
1:O:145:GLU:HA	1:O:269:MET:CE	2.48	0.44
1:O:233:ILE:CD1	1:O:254:ARG:HB3	2.42	0.44
1:P:84:ARG:O	1:P:85:GLU:HB2	2.18	0.44
1:P:110:SER:O	1:P:113:SER:HB3	2.18	0.44
1:Q:146:LEU:HD13	1:Q:271:TRP:CD2	2.53	0.44
1:Q:168:ARG:CG	1:Q:168:ARG:NH1	2.65	0.44
1:R:69:LEU:HD13	1:R:91:THR:HG23	1.99	0.44
1:R:201:GLU:C	1:R:203:PRO:HD3	2.37	0.44
1:J:490:PRO:HB3	1:J:569:MET:HE2	1.81	0.44
1:J:593:LEU:HD12	1:J:593:LEU:HA	1.91	0.44
1:K:244:GLU:H	1:K:244:GLU:CD	2.19	0.44
1:A:103:ALA:O	1:A:107:THR:CB	2.47	0.44
1:D:297:TRP:CE3	1:D:495:ASP:HB3	2.53	0.44
1:B:231:GLU:O	1:B:233:ILE:HG22	2.18	0.44
1:F:292:LYS:HD2	1:F:292:LYS:HA	1.74	0.44
1:G:42:ARG:HG3	1:G:301:TRP:CH2	2.53	0.44
1:G:107:THR:O	1:G:110:SER:OG	2.35	0.44
1:M:68:VAL:HB	1:M:90:VAL:HG22	2.00	0.44
1:M:235:ALA:HA	1:M:254:ARG:HG3	2.00	0.44
1:M:269:MET:CG	1:M:304:ALA:HB3	2.48	0.44
1:O:297:TRP:CE3	1:O:495:ASP:HB3	2.52	0.44
1:Q:169:VAL:HG22	1:Q:241:GLU:HG2	2.00	0.44
1:R:67:HIS:CE1	1:R:89:LYS:HG2	2.53	0.44
1:R:168:ARG:HG2	1:R:241:GLU:OE1	2.18	0.44
1:R:550:ARG:CZ	1:R:550:ARG:HB2	2.47	0.44
1:K:147:ILE:HD11	1:K:331:LEU:HD13	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:80:LEU:HB3	1:L:509:PHE:CE1	2.53	0.44
1:B:169:VAL:HG22	1:B:171:PRO:O	2.17	0.43
1:C:275:MET:HE1	1:C:283:ILE:H	1.82	0.43
1:C:338:LYS:N	1:F:244:GLU:HG3	2.32	0.43
1:F:625:CYS:HB2	1:F:644:SER:HA	2.00	0.43
1:E:63:ASP:CG	1:E:64:GLY:H	2.21	0.43
1:E:480:GLU:OE2	1:E:482:HIS:CD2	2.69	0.43
1:G:497:GLN:NE2	1:G:497:GLN:N	2.60	0.43
1:I:63:ASP:OD1	1:I:63:ASP:N	2.48	0.43
1:O:219:SER:HB3	1:O:288:LYS:HB2	2.00	0.43
1:O:404:THR:HG21	1:O:437:LEU:HD23	2.00	0.43
1:O:442:ASP:O	1:O:478:ARG:CB	2.62	0.43
1:O:451:MET:HG3	1:O:452:SER:N	2.32	0.43
1:Q:274:ASP:OD2	1:Q:277:ARG:N	2.50	0.43
1:Q:513:PHE:O	1:Q:516:GLU:HB3	2.18	0.43
1:R:35:ASP:OD1	1:R:300:HIS:N	2.47	0.43
1:J:191:ASP:OD2	1:J:194:ARG:NH1	2.51	0.43
1:K:510:ASP:C	1:K:512:SER:H	2.22	0.43
1:D:518:SER:O	1:D:522:ARG:HG3	2.18	0.43
1:B:168:ARG:NH1	1:B:168:ARG:HG2	2.31	0.43
1:C:146:LEU:HD13	1:C:271:TRP:CG	2.53	0.43
1:C:230:SER:OG	1:C:231:GLU:O	2.36	0.43
1:C:288:LYS:HG3	1:C:295:TYR:CE2	2.53	0.43
1:C:403:VAL:HB	1:C:428:VAL:HB	2.00	0.43
1:C:578:TRP:CB	1:C:591:GLY:HA3	2.48	0.43
1:N:251:SER:OG	1:N:340:LYS:HD3	2.18	0.43
1:N:258:ALA:HB3	1:N:315:GLU:O	2.18	0.43
1:O:414:ASP:O	1:O:418:LYS:HG3	2.17	0.43
1:Q:67:HIS:O	1:Q:135:ASP:N	2.47	0.43
1:R:178:ILE:HA	1:R:268:LEU:O	2.18	0.43
1:J:54:ILE:HD13	1:J:85:GLU:HB3	1.99	0.43
1:K:171:PRO:HB3	1:K:275:MET:HE1	1.99	0.43
1:K:348:GLY:CA	1:K:411:ARG:HH22	2.31	0.43
1:L:190:ASN:ND2	1:L:209:GLY:HA3	2.33	0.43
1:B:218:LEU:HD22	1:B:221:MET:CE	2.48	0.43
1:B:514:PHE:HA	1:B:517:ILE:HG12	1.99	0.43
1:F:178:ILE:HB	1:F:267:LEU:HD22	1.99	0.43
1:E:623:SER:O	1:E:624:LEU:HD23	2.18	0.43
1:H:70:ASP:HA	1:H:138:VAL:O	2.18	0.43
1:H:455:ASN:HB3	1:H:457:TRP:CE2	2.53	0.43
1:I:451:MET:HE2	1:I:452:SER:HA	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:593:LEU:HD12	1:I:593:LEU:HA	1.73	0.43
1:M:349:LEU:HD11	1:M:353:LEU:HD12	1.99	0.43
1:N:339:ASP:OD1	1:N:340:LYS:N	2.51	0.43
1:N:447:GLU:N	1:N:448:PRO:HA	2.32	0.43
1:N:474:GLY:HA3	1:N:476:GLU:OE2	2.18	0.43
1:O:198:GLU:O	1:O:201:GLU:HB2	2.17	0.43
1:O:548:ILE:HD12	1:O:626:LEU:HD13	2.01	0.43
1:P:83:ALA:HB1	1:P:112:TRP:CG	2.53	0.43
1:P:156:LYS:O	1:P:160:GLU:CG	2.65	0.43
1:Q:67:HIS:HA	1:Q:89:LYS:O	2.17	0.43
1:R:218:LEU:HD23	1:R:218:LEU:HA	1.72	0.43
1:R:485:VAL:HA	1:R:549:LEU:O	2.19	0.43
1:R:512:SER:O	1:R:515:ASP:HB2	2.18	0.43
1:J:124:THR:O	1:J:161:ARG:NH2	2.51	0.43
1:J:194:ARG:HG2	1:J:201:GLU:CB	2.37	0.43
1:K:229:LEU:CD1	1:K:314:VAL:HG12	2.48	0.43
1:K:641:PHE:N	1:K:641:PHE:CD1	2.85	0.43
1:L:84:ARG:HG3	1:L:112:TRP:HZ2	1.83	0.43
1:L:141:VAL:CG1	1:L:141:VAL:O	2.66	0.43
1:A:297:TRP:CE3	1:A:495:ASP:HB3	2.53	0.43
1:D:622:LYS:N	1:D:622:LYS:CD	2.79	0.43
1:B:111:PRO:HG2	1:B:112:TRP:CH2	2.53	0.43
1:E:643:LYS:O	1:E:644:SER:OG	2.27	0.43
1:N:190:ASN:HD21	1:N:209:GLY:HA3	1.83	0.43
1:O:178:ILE:HG21	1:O:333:PHE:CZ	2.53	0.43
1:O:367:ASN:O	1:O:371:LYS:HD3	2.18	0.43
1:O:466:VAL:HA	1:O:469:LEU:HB2	1.99	0.43
1:O:483:MET:HB3	1:O:582:GLU:HG2	1.99	0.43
1:Q:140:GLU:HG3	1:Q:140:GLU:O	2.17	0.43
1:R:52:THR:HG21	1:R:276:ASP:CB	2.46	0.43
1:R:69:LEU:HD12	1:R:69:LEU:C	2.39	0.43
1:R:466:VAL:HG11	1:R:553:ILE:HG21	2.00	0.43
1:J:68:VAL:O	1:J:90:VAL:HA	2.18	0.43
1:J:93:LEU:HD23	1:J:119:ILE:HB	2.01	0.43
1:J:226:PHE:CZ	1:J:289:TRP:CZ2	3.06	0.43
1:J:261:SER:OG	1:J:316:MET:N	2.52	0.43
1:A:144:THR:O	1:A:269:MET:HE1	2.17	0.43
1:A:359:TYR:CD1	1:A:359:TYR:C	2.92	0.43
1:B:388:GLU:OE1	1:B:452:SER:HB2	2.19	0.43
1:F:143:ASP:O	1:F:146:LEU:N	2.34	0.43
1:F:368:GLN:NE2	1:F:371:LYS:CE	2.80	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:42:ARG:HG3	1:G:301:TRP:CZ3	2.53	0.43
1:G:378:SER:O	1:G:400:ALA:HA	2.18	0.43
1:H:375:ASP:O	1:H:399:THR:HG21	2.19	0.43
1:M:111:PRO:C	1:M:113:SER:N	2.72	0.43
1:M:480:GLU:CG	1:M:584:GLY:H	2.32	0.43
1:N:55:ALA:CA	1:N:58:LYS:HD2	2.47	0.43
1:N:612:TYR:CE2	1:N:614:PRO:HA	2.53	0.43
1:P:600:VAL:HA	1:P:601:PRO:HD3	1.86	0.43
1:Q:1:MET:O	1:Q:17:VAL:HG12	2.19	0.43
1:Q:143:ASP:C	1:Q:145:GLU:N	2.71	0.43
1:R:136:ILE:HG23	1:R:168:ARG:O	2.18	0.43
1:R:487:LYS:HE3	1:R:547:GLU:HG2	2.00	0.43
1:J:290:LYS:HD3	1:J:290:LYS:HA	1.92	0.43
1:K:492:LYS:HD3	1:K:542:LYS:NZ	2.33	0.43
1:K:534:LEU:C	1:K:536:GLU:H	2.22	0.43
1:A:216:VAL:O	1:A:302:MET:HG2	2.18	0.43
1:C:176:VAL:HG13	1:C:236:PHE:HB2	1.99	0.43
1:E:269:MET:HG2	1:E:306:TYR:CE1	2.54	0.43
1:E:384:ALA:O	1:E:444:VAL:HA	2.18	0.43
1:H:449:PHE:HA	1:H:459:HIS:CD2	2.54	0.43
1:I:264:ILE:HD12	1:I:312:LYS:HG2	2.00	0.43
1:I:550:ARG:HH11	1:I:550:ARG:CG	2.30	0.43
1:M:4:GLU:O	1:O:420:ILE:HD11	2.19	0.43
1:M:515:ASP:O	1:M:519:THR:HB	2.18	0.43
1:N:437:LEU:HD11	1:N:441:PRO:HD3	2.00	0.43
1:P:480:GLU:OE2	1:P:482:HIS:HD2	2.01	0.43
1:R:297:TRP:CZ3	1:R:495:ASP:HB3	2.54	0.43
1:K:253:VAL:O	1:K:253:VAL:CG2	2.66	0.43
1:K:264:ILE:HD12	1:K:312:LYS:HG3	2.01	0.43
1:K:550:ARG:O	1:K:560:GLN:OE1	2.36	0.43
1:K:616:THR:O	1:K:618:LEU:N	2.52	0.43
1:L:569:MET:HA	1:L:572:SER:HB2	2.00	0.43
1:A:460:LEU:HD22	1:A:463:LEU:HD22	2.00	0.43
1:A:480:GLU:HG2	1:A:584:GLY:N	2.34	0.43
1:D:47:LEU:HD22	1:D:51:LYS:HE2	2.01	0.43
1:D:84:ARG:HG3	1:D:112:TRP:CZ2	2.54	0.43
1:D:190:ASN:ND2	1:D:209:GLY:HA3	2.33	0.43
1:B:476:GLU:CD	1:B:476:GLU:N	2.72	0.43
1:C:489:ILE:HG12	1:C:541:VAL:HG22	1.99	0.43
1:G:427:ASN:HA	1:H:8:GLN:OE1	2.18	0.43
1:G:489:ILE:CD1	1:G:541:VAL:HG21	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:480:GLU:HG3	1:H:584:GLY:H	1.84	0.43
1:I:570:SER:CB	1:I:622:LYS:HG2	2.38	0.43
1:M:151:ALA:O	1:M:154:THR:HG22	2.18	0.43
1:M:615:ILE:CG1	1:M:618:LEU:HD22	2.48	0.43
1:N:169:VAL:HG12	1:N:241:GLU:HG2	2.00	0.43
1:N:214:PHE:CD1	1:N:214:PHE:C	2.91	0.43
1:O:7:ASN:HD21	1:O:640:GLN:NE2	2.14	0.43
1:O:269:MET:HG2	1:O:306:TYR:CE1	2.54	0.43
1:P:161:ARG:HB3	1:P:162:LEU:HD13	2.01	0.43
1:P:218:LEU:H	1:P:303:GLN:HE21	1.66	0.43
1:A:203:PRO:HA	1:A:422:TYR:CG	2.54	0.43
1:D:78:LEU:HD12	1:D:78:LEU:HA	1.82	0.43
1:B:111:PRO:HG2	1:B:112:TRP:CZ3	2.54	0.43
1:C:315:GLU:HB3	1:C:318:GLN:HG3	1.99	0.43
1:C:403:VAL:O	1:C:428:VAL:HA	2.19	0.43
1:F:534:LEU:HD23	1:F:534:LEU:HA	1.88	0.43
1:E:54:ILE:HD13	1:E:87:ALA:H	1.83	0.43
1:E:176:VAL:CG1	1:E:236:PHE:HB2	2.49	0.43
1:G:35:ASP:O	1:G:36:MET:C	2.56	0.43
1:G:269:MET:HG2	1:G:306:TYR:CE1	2.53	0.43
1:I:291:ASN:HD21	1:I:295:TYR:HA	1.84	0.43
1:O:534:LEU:C	1:O:536:GLU:H	2.22	0.43
1:R:385:THR:HG21	1:R:405:ILE:HG23	2.01	0.43
1:R:569:MET:HG3	1:R:624:LEU:HG	2.00	0.43
1:J:138:VAL:HG23	1:J:170:VAL:HB	2.00	0.43
1:J:423:TYR:O	1:J:424:LYS:C	2.57	0.43
1:L:69:LEU:HD12	1:L:91:THR:O	2.18	0.43
1:L:163:ALA:HB1	1:L:167:CYS:SG	2.58	0.43
1:L:258:ALA:O	1:L:317:ASN:HA	2.18	0.43
1:D:569:MET:HA	1:D:572:SER:HB2	2.01	0.43
1:B:103:ALA:O	1:B:107:THR:HB	2.19	0.43
1:B:170:VAL:HA	1:B:171:PRO:HA	1.85	0.43
1:B:367:ASN:O	1:B:371:LYS:HD3	2.18	0.43
1:E:170:VAL:HA	1:E:171:PRO:HA	1.92	0.43
1:H:67:HIS:CE1	1:H:91:THR:HG22	2.53	0.43
1:H:92:ALA:HB3	1:H:118:VAL:HG22	2.00	0.43
1:I:502:ASP:OD2	1:I:616:THR:CG2	2.65	0.43
1:M:43:ASN:N	1:M:43:ASN:ND2	2.64	0.43
1:M:96:PHE:CD2	1:M:98:PRO:HD2	2.54	0.43
1:M:176:VAL:CG2	1:M:236:PHE:HD2	2.31	0.43
1:N:63:ASP:CB	1:N:65:LYS:N	2.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:327:ASP:OD1	1:N:327:ASP:C	2.58	0.43
1:O:35:ASP:CG	1:O:299:ASP:H	2.22	0.43
1:Q:215:ASP:HA	1:Q:304:ALA:HA	2.00	0.43
1:R:359:TYR:CD1	1:R:359:TYR:C	2.91	0.43
1:C:20:GLU:H	1:C:20:GLU:HG3	1.40	0.43
1:G:118:VAL:C	1:G:119:ILE:HD12	2.39	0.43
1:G:339:ASP:OD1	1:G:341:SER:HB2	2.18	0.43
1:G:357:THR:O	1:G:360:HIS:HB3	2.19	0.43
1:H:97:LYS:N	1:H:98:PRO:CD	2.82	0.43
1:H:178:ILE:HG21	1:H:333:PHE:CZ	2.54	0.43
1:N:254:ARG:O	1:N:321:GLU:HB3	2.19	0.43
1:N:535:TRP:CE2	1:N:536:GLU:HG3	2.54	0.43
1:O:71:ILE:HG21	1:O:154:THR:CG2	2.49	0.43
1:Q:566:ILE:CG2	1:Q:569:MET:CE	2.97	0.43
1:R:110:SER:C	1:R:112:TRP:H	2.23	0.43
1:J:274:ASP:HB2	1:J:282:PHE:CE1	2.54	0.43
1:J:547:GLU:OE2	1:J:550:ARG:CG	2.66	0.43
1:A:550:ARG:NH1	1:A:550:ARG:HB2	2.33	0.42
1:A:577:MET:HE2	1:A:639:PHE:CE1	2.54	0.42
1:D:490:PRO:HB2	1:D:569:MET:CE	2.45	0.42
1:D:506:VAL:HG21	1:D:511:LEU:HD12	2.00	0.42
1:B:502:ASP:OD2	1:B:616:THR:HG21	2.19	0.42
1:E:169:VAL:HG13	1:E:172:SER:HA	2.01	0.42
1:E:621:ASP:OD1	1:E:621:ASP:N	2.52	0.42
1:G:159:LEU:HB2	1:G:243:GLU:HG3	2.01	0.42
1:G:291:ASN:HB3	1:G:295:TYR:HB2	2.01	0.42
1:H:563:VAL:HG22	1:H:627:HIS:CG	2.54	0.42
1:H:578:TRP:CG	1:H:591:GLY:HA3	2.54	0.42
1:I:77:LEU:HD11	1:I:506:VAL:HG12	2.00	0.42
1:I:162:LEU:HD13	1:I:162:LEU:N	2.34	0.42
1:M:627:HIS:HB2	1:M:640:GLN:HB2	2.01	0.42
1:N:65:LYS:HA	1:N:88:ASP:OD2	2.19	0.42
1:O:275:MET:CE	1:O:283:ILE:H	2.31	0.42
1:O:379:LYS:O	1:O:381:LEU:N	2.52	0.42
1:Q:547:GLU:CD	1:Q:550:ARG:HH11	2.23	0.42
1:J:51:LYS:HG3	1:J:85:GLU:OE2	2.19	0.42
1:J:146:LEU:HD22	1:J:176:VAL:HG12	2.01	0.42
1:D:180:PRO:CB	1:D:264:ILE:HD13	2.50	0.42
1:C:138:VAL:HG23	1:C:170:VAL:HB	2.01	0.42
1:F:142:PHE:HD1	1:F:146:LEU:HD12	1.80	0.42
1:F:615:ILE:CG1	1:F:618:LEU:HD22	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:548:ILE:HD12	1:E:564:VAL:HG21	2.00	0.42
1:H:496:LEU:O	1:H:499:ILE:HG12	2.19	0.42
1:I:416:PHE:O	1:I:420:ILE:HG13	2.18	0.42
1:I:615:ILE:HG12	1:I:618:LEU:HD22	2.01	0.42
1:M:10:THR:C	1:M:12:GLU:H	2.22	0.42
1:M:95:VAL:HB	1:M:122:ARG:HG3	2.02	0.42
1:M:599:GLY:O	1:M:601:PRO:HD3	2.19	0.42
1:N:245:LYS:HE3	1:Q:337:GLY:O	2.18	0.42
1:N:308:LEU:HD12	1:N:308:LEU:HA	1.91	0.42
1:O:490:PRO:HG2	1:O:543:GLY:HA3	2.01	0.42
1:P:239:ASP:OD1	1:P:277:ARG:NH2	2.52	0.42
1:Q:553:ILE:O	1:Q:553:ILE:HG23	2.19	0.42
1:R:231:GLU:O	1:R:232:PRO:C	2.57	0.42
1:K:253:VAL:O	1:K:253:VAL:HG23	2.19	0.42
1:K:490:PRO:HG3	1:K:566:ILE:HG22	2.01	0.42
1:K:534:LEU:C	1:K:536:GLU:N	2.72	0.42
1:L:42:ARG:HH12	1:L:140:GLU:HG2	1.75	0.42
1:L:470:LYS:HG2	1:L:475:ASP:HA	1.99	0.42
1:A:470:LYS:NZ	1:A:554:ASP:HA	2.34	0.42
1:A:503:VAL:HB	1:A:515:ASP:OD1	2.19	0.42
1:G:46:PHE:CZ	1:G:140:GLU:HB3	2.54	0.42
1:H:69:LEU:CD1	1:H:91:THR:HG23	2.49	0.42
1:H:72:GLY:O	2:H:701:SAH:N	2.53	0.42
1:H:563:VAL:HA	1:H:626:LEU:O	2.19	0.42
1:M:51:LYS:HD3	1:M:85:GLU:OE2	2.19	0.42
1:N:38:LEU:HD21	1:N:503:VAL:HA	2.00	0.42
1:N:391:PHE:O	1:N:394:LEU:HB2	2.19	0.42
1:N:550:ARG:O	1:N:560:GLN:OE1	2.37	0.42
1:O:423:TYR:HB2	1:O:425:LEU:HG	2.01	0.42
1:O:440:SER:HA	1:O:441:PRO:HD3	1.86	0.42
1:O:483:MET:HB3	1:O:582:GLU:CG	2.49	0.42
1:P:323:VAL:HB	1:P:334:SER:OG	2.19	0.42
1:Q:273:ILE:O	1:Q:282:PHE:HA	2.19	0.42
1:R:578:TRP:NE1	1:R:580:GLU:HG3	2.34	0.42
1:K:53:THR:HG22	1:K:168:ARG:NE	2.34	0.42
1:L:210:THR:HG21	4:L:809:HOH:O	2.18	0.42
1:D:190:ASN:HD21	1:D:209:GLY:HA3	1.84	0.42
1:D:217:GLN:HB2	1:D:536:GLU:HB3	2.00	0.42
1:D:550:ARG:O	1:D:560:GLN:OE1	2.37	0.42
1:C:463:LEU:H	1:C:463:LEU:HD22	1.83	0.42
1:G:627:HIS:HB2	1:G:640:GLN:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:82:ALA:O	1:H:84:ARG:O	2.37	0.42
1:H:491:GLU:HG3	1:H:492:LYS:N	2.34	0.42
1:I:145:GLU:CG	1:I:331:LEU:HD22	2.49	0.42
1:N:516:GLU:O	1:N:520:LYS:HG3	2.20	0.42
1:O:491:GLU:HG3	1:O:492:LYS:N	2.34	0.42
1:P:56:GLU:O	1:P:56:GLU:HG2	2.19	0.42
1:P:84:ARG:C	1:P:86:GLY:N	2.73	0.42
1:R:613:PHE:HA	1:R:614:PRO:HD2	1.93	0.42
1:J:107:THR:HG22	1:J:108:SER:N	2.35	0.42
1:J:480:GLU:HA	1:J:481:PRO:C	2.39	0.42
1:L:178:ILE:HA	1:L:268:LEU:O	2.18	0.42
1:L:241:GLU:HB2	1:L:277:ARG:HH21	1.85	0.42
1:A:577:MET:HE2	1:A:639:PHE:CZ	2.54	0.42
1:C:288:LYS:HG3	1:C:295:TYR:CZ	2.54	0.42
1:G:67:HIS:CE1	1:G:91:THR:HG23	2.54	0.42
1:G:514:PHE:O	1:G:515:ASP:C	2.57	0.42
1:H:75:THR:HG22	1:H:514:PHE:CD1	2.55	0.42
1:H:123:SER:C	1:H:125:ASP:H	2.22	0.42
1:M:217:GLN:C	1:M:219:SER:H	2.22	0.42
1:N:55:ALA:H	1:N:58:LYS:NZ	2.05	0.42
1:N:420:ILE:CD1	1:N:428:VAL:HG22	2.50	0.42
1:N:477:LEU:O	1:N:479:VAL:HG12	2.20	0.42
1:O:618:LEU:HB3	1:O:624:LEU:HD11	2.01	0.42
1:P:292:LYS:HA	1:P:292:LYS:NZ	2.34	0.42
1:Q:182:GLU:HG3	1:Q:263:THR:O	2.20	0.42
1:Q:182:GLU:HB2	1:Q:229:LEU:HD11	2.02	0.42
1:R:326:HIS:HA	1:R:330:SER:O	2.20	0.42
1:R:627:HIS:HB2	1:R:640:GLN:HB2	2.00	0.42
1:K:325:ASN:O	1:K:331:LEU:HA	2.19	0.42
1:L:485:VAL:HG22	1:L:487:LYS:HG3	2.01	0.42
1:B:541:VAL:HG11	1:B:595:ILE:HD13	2.02	0.42
1:C:169:VAL:HG23	1:C:172:SER:HA	2.01	0.42
1:C:272:ASP:C	1:C:272:ASP:OD1	2.58	0.42
1:C:542:LYS:HD3	1:C:542:LYS:HA	1.78	0.42
1:F:133:ARG:HB2	1:F:164:LYS:HG3	2.02	0.42
1:F:399:THR:HG22	1:F:399:THR:O	2.19	0.42
1:E:77:LEU:O	1:E:81:MET:HG3	2.20	0.42
1:E:434:VAL:HG13	1:E:469:LEU:CD1	2.49	0.42
1:G:112:TRP:O	1:G:113:SER:C	2.58	0.42
1:G:416:PHE:O	1:G:420:ILE:HG13	2.19	0.42
1:H:22:TYR:CE1	1:H:525:THR:HG22	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:158:ALA:HA	1:I:162:LEU:HD22	2.00	0.42
1:I:379:LYS:N	1:I:399:THR:CG2	2.83	0.42
1:M:91:THR:CG2	1:M:117:THR:CG2	2.86	0.42
1:M:194:ARG:O	1:M:195:LEU:C	2.58	0.42
1:Q:177:TYR:N	1:Q:177:TYR:CD1	2.88	0.42
1:R:497:GLN:H	1:R:497:GLN:NE2	2.11	0.42
1:K:195:LEU:HB3	1:K:423:TYR:CZ	2.54	0.42
1:K:423:TYR:O	1:K:424:LYS:C	2.58	0.42
1:L:269:MET:HG3	1:L:306:TYR:HE1	1.85	0.42
1:D:218:LEU:HD13	1:D:268:LEU:HD13	2.02	0.42
1:B:182:GLU:OE2	1:B:227:ARG:NH1	2.52	0.42
1:C:534:LEU:HD21	1:C:611:VAL:HG11	2.02	0.42
1:F:93:LEU:HD13	1:F:123:SER:HA	2.02	0.42
1:F:158:ALA:O	1:F:162:LEU:N	2.52	0.42
1:F:397:ALA:O	1:F:399:THR:N	2.52	0.42
1:E:44:ASP:O	1:E:47:LEU:HB3	2.20	0.42
1:E:445:LEU:HD12	1:E:480:GLU:HB2	2.01	0.42
1:G:96:PHE:HD2	1:G:99:MET:HG2	1.84	0.42
1:G:619:ARG:HG2	1:G:619:ARG:NH1	2.34	0.42
1:H:35:ASP:O	1:H:36:MET:C	2.57	0.42
1:I:592:LEU:HD21	1:I:595:ILE:HD11	2.02	0.42
1:I:616:THR:C	1:I:618:LEU:H	2.22	0.42
1:M:181:VAL:HG12	1:M:183:SER:HB3	2.02	0.42
1:N:27:GLU:HB3	1:N:96:PHE:CZ	2.55	0.42
1:N:96:PHE:CD2	1:N:98:PRO:HD2	2.54	0.42
1:N:316:MET:HA	1:N:317:ASN:HA	1.65	0.42
1:Q:323:VAL:HG23	1:Q:334:SER:O	2.20	0.42
1:Q:395:LEU:C	1:Q:397:ALA:N	2.72	0.42
1:R:391:PHE:O	1:R:394:LEU:HB2	2.20	0.42
1:K:45:LYS:HE2	1:K:282:PHE:O	2.19	0.42
1:L:269:MET:CG	1:L:306:TYR:HE1	2.32	0.42
1:A:57:LYS:HD2	1:A:57:LYS:HA	1.82	0.42
1:A:612:TYR:CZ	1:A:614:PRO:HA	2.55	0.42
1:C:190:ASN:HD21	1:C:209:GLY:HA3	1.85	0.42
1:C:490:PRO:CB	1:C:569:MET:HE1	2.47	0.42
1:F:73:THR:HG22	1:F:94:GLU:HB2	2.01	0.42
1:F:184:HIS:O	1:F:185:LEU:C	2.58	0.42
1:F:229:LEU:HD23	1:F:229:LEU:HA	1.63	0.42
1:F:354:SER:O	1:F:358:VAL:HG23	2.19	0.42
1:E:269:MET:HG2	1:E:306:TYR:HE1	1.84	0.42
1:E:491:GLU:HG3	1:E:540:ILE:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:119:ILE:HD12	1:G:119:ILE:N	2.35	0.42
1:G:447:GLU:N	1:G:448:PRO:HA	2.35	0.42
1:H:119:ILE:HG23	1:J:128:GLN:HG2	2.02	0.42
1:H:169:VAL:HG11	1:H:240:PHE:O	2.20	0.42
1:O:58:LYS:NZ	1:O:86:GLY:O	2.45	0.42
1:O:481:PRO:HB3	1:O:583:PHE:HD1	1.85	0.42
1:P:379:LYS:O	1:P:381:LEU:HG	2.20	0.42
1:Q:55:ALA:O	1:Q:56:GLU:C	2.58	0.42
1:J:141:VAL:O	1:J:141:VAL:CG1	2.68	0.42
1:J:168:ARG:HH22	1:J:277:ARG:HB2	1.84	0.42
1:K:532:GLN:HG2	1:K:537:TYR:HE2	1.85	0.42
1:A:566:ILE:O	1:A:623:SER:HA	2.20	0.42
1:C:320:PHE:CD1	1:C:320:PHE:C	2.93	0.42
1:C:349:LEU:O	1:C:350:HIS:C	2.58	0.42
1:F:91:THR:HG22	1:F:117:THR:CG2	2.50	0.42
1:G:269:MET:HG2	1:G:306:TYR:HE1	1.84	0.42
1:H:6:ILE:O	1:H:8:GLN:NE2	2.50	0.42
1:H:51:LYS:NZ	1:H:51:LYS:HB3	2.35	0.42
1:H:53:THR:HG22	1:H:168:ARG:HE	1.85	0.42
1:H:574:ALA:C	1:H:575:ILE:HG13	2.40	0.42
1:I:403:VAL:HB	1:I:428:VAL:HB	2.00	0.42
1:I:577:MET:HA	1:I:578:TRP:CE3	2.55	0.42
1:M:301:TRP:O	1:M:302:MET:HB3	2.20	0.42
1:M:384:ALA:O	1:M:444:VAL:HA	2.19	0.42
1:M:451:MET:HE2	1:M:451:MET:HB2	1.93	0.42
1:N:467:GLU:OE1	1:N:557:VAL:HG13	2.20	0.42
1:P:144:THR:O	1:P:269:MET:HE1	2.20	0.42
1:Q:190:ASN:ND2	1:Q:209:GLY:HA3	2.29	0.42
1:R:3:LEU:O	1:R:15:TRP:HA	2.20	0.42
1:J:51:LYS:HA	1:J:85:GLU:HG2	2.02	0.42
1:L:631:ASP:CG	1:L:633:SER:HB2	2.40	0.42
1:B:339:ASP:OD1	1:B:341:SER:N	2.45	0.42
1:C:412:PHE:HE2	1:C:451:MET:HG2	1.85	0.42
1:C:569:MET:SD	1:C:575:ILE:HD11	2.60	0.42
1:E:146:LEU:HD23	1:E:146:LEU:H	1.85	0.42
1:I:550:ARG:HH11	1:I:550:ARG:HB2	1.85	0.42
1:M:66:VAL:HA	1:M:135:ASP:OD2	2.20	0.42
1:M:275:MET:HB2	1:M:275:MET:HE3	1.74	0.42
1:M:455:ASN:HA	1:M:456:PRO:HD3	1.87	0.42
1:N:227:ARG:NH2	1:N:261:SER:O	2.53	0.42
1:Q:186:LEU:HD11	1:Q:268:LEU:HD21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:193:PRO:HA	1:Q:362:ASN:HD21	1.84	0.42
1:Q:618:LEU:HG	1:Q:624:LEU:HD22	2.01	0.42
1:R:57:LYS:O	1:R:61:ASN:ND2	2.52	0.42
1:R:323:VAL:HG12	1:R:325:ASN:HD21	1.85	0.42
1:R:550:ARG:O	1:R:560:GLN:NE2	2.48	0.42
1:J:434:VAL:HG12	1:J:469:LEU:HD13	2.01	0.42
1:J:563:VAL:HG22	1:J:627:HIS:CD2	2.55	0.42
1:K:310:GLU:OE2	1:K:338:LYS:HG2	2.20	0.42
1:K:403:VAL:HB	1:K:428:VAL:HB	2.02	0.42
1:A:505:THR:HA	1:A:509:PHE:O	2.20	0.41
1:B:59:HIS:O	1:B:61:ASN:N	2.52	0.41
1:B:134:ALA:HB3	1:B:163:ALA:HA	2.01	0.41
1:B:522:ARG:O	1:B:526:ASP:HB2	2.19	0.41
1:C:295:TYR:CD2	1:C:295:TYR:C	2.93	0.41
1:F:535:TRP:CG	1:F:605:LYS:HG2	2.54	0.41
1:G:191:ASP:OD2	1:G:194:ARG:NH1	2.42	0.41
1:G:369:LYS:HE3	1:G:369:LYS:HB3	1.93	0.41
1:G:490:PRO:CB	1:G:569:MET:HE3	2.23	0.41
1:H:84:ARG:O	1:H:85:GLU:CB	2.62	0.41
1:H:97:LYS:HB2	1:H:98:PRO:HD3	2.02	0.41
1:H:374:VAL:O	1:H:378:SER:OG	2.37	0.41
1:M:416:PHE:HB2	1:M:430:ILE:HD13	2.00	0.41
1:M:612:TYR:CE2	1:M:614:PRO:HA	2.55	0.41
1:O:179:VAL:HG11	1:O:228:GLU:HG2	2.00	0.41
1:O:216:VAL:C	1:O:302:MET:HG2	2.40	0.41
1:Q:169:VAL:HG21	1:Q:240:PHE:C	2.41	0.41
1:Q:191:ASP:O	1:Q:192:ILE:C	2.58	0.41
1:R:267:LEU:C	1:R:268:LEU:HD23	2.41	0.41
1:J:447:GLU:N	1:J:448:PRO:HA	2.35	0.41
1:K:178:ILE:HA	1:K:268:LEU:O	2.20	0.41
1:K:359:TYR:CZ	1:K:605:LYS:HB2	2.55	0.41
1:L:39:ASP:OD2	1:L:298:ARG:HD2	2.20	0.41
1:A:570:SER:HB3	1:A:622:LYS:HG3	2.02	0.41
1:B:66:VAL:CG1	1:B:67:HIS:H	2.32	0.41
1:B:403:VAL:HB	1:B:428:VAL:HB	2.01	0.41
1:B:437:LEU:HD22	1:B:439:ASP:O	2.19	0.41
1:E:96:PHE:CZ	1:E:98:PRO:HG2	2.55	0.41
1:E:550:ARG:H	1:E:560:GLN:NE2	2.13	0.41
1:G:169:VAL:HG11	1:G:240:PHE:C	2.41	0.41
1:H:178:ILE:HG21	1:H:333:PHE:CE2	2.55	0.41
1:H:179:VAL:HG22	1:H:232:PRO:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:387:GLY:HA2	1:H:450:TYR:CE2	2.55	0.41
1:I:478:ARG:CG	1:I:478:ARG:NH2	2.83	0.41
1:M:52:THR:HG21	1:M:278:ASN:HD21	1.85	0.41
1:Q:231:GLU:H	1:Q:231:GLU:HG2	1.68	0.41
1:Q:269:MET:HG2	1:Q:306:TYR:CE1	2.54	0.41
1:R:54:ILE:HD13	1:R:54:ILE:HA	1.90	0.41
1:R:385:THR:CG2	1:R:405:ILE:HG23	2.49	0.41
1:J:391:PHE:O	1:J:392:LEU:C	2.58	0.41
1:J:478:ARG:HH21	1:J:478:ARG:CG	2.33	0.41
1:K:198:GLU:O	1:K:201:GLU:HG3	2.19	0.41
1:L:280:THR:HG23	1:L:281:THR:N	2.35	0.41
1:A:502:ASP:CG	1:A:616:THR:HG21	2.34	0.41
1:D:291:ASN:H	1:D:292:LYS:HZ1	1.64	0.41
1:D:357:THR:HG21	1:D:449:PHE:CZ	2.54	0.41
1:B:182:GLU:HG3	1:B:263:THR:O	2.19	0.41
1:C:47:LEU:HD23	1:C:47:LEU:HA	1.83	0.41
1:C:228:GLU:OE2	1:C:290:LYS:NZ	2.51	0.41
1:H:348:GLY:O	1:H:352:MET:HG2	2.20	0.41
1:H:449:PHE:CD1	1:H:449:PHE:C	2.94	0.41
1:I:495:ASP:C	1:I:497:GLN:NE2	2.74	0.41
1:I:576:PRO:HA	1:I:611:VAL:HA	2.02	0.41
1:M:631:ASP:O	1:M:635:GLY:N	2.50	0.41
1:N:27:GLU:OE2	1:N:96:PHE:HE1	1.96	0.41
1:N:133:ARG:HH21	1:N:133:ARG:CB	2.25	0.41
1:N:275:MET:HE1	1:N:283:ILE:HG13	2.01	0.41
1:N:514:PHE:O	1:N:518:SER:HB3	2.20	0.41
1:N:548:ILE:O	1:N:549:LEU:HD13	2.21	0.41
1:O:385:THR:HB	1:O:405:ILE:HD13	2.01	0.41
1:O:597:SER:HB3	1:O:598:ALA:H	1.73	0.41
1:Q:70:ASP:HB3	1:Q:79:SER:OG	2.20	0.41
1:Q:190:ASN:ND2	1:Q:190:ASN:O	2.54	0.41
1:Q:216:VAL:N	1:Q:302:MET:SD	2.93	0.41
1:R:84:ARG:O	1:R:85:GLU:CB	2.68	0.41
1:K:6:ILE:O	1:K:8:GLN:NE2	2.53	0.41
1:K:136:ILE:HA	1:K:168:ARG:O	2.20	0.41
1:A:273:ILE:HG13	1:A:275:MET:CE	2.49	0.41
1:B:427:ASN:HA	1:C:8:GLN:NE2	2.35	0.41
1:F:42:ARG:HH11	1:F:140:GLU:CG	2.30	0.41
1:F:264:ILE:N	1:F:312:LYS:O	2.54	0.41
1:F:569:MET:HA	1:F:572:SER:HB2	2.01	0.41
1:E:143:ASP:OD2	1:E:148:GLY:HA3	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:379:LYS:HA	1:E:399:THR:HG22	1.93	0.41
1:E:467:GLU:OE1	1:E:556:ARG:HG3	2.21	0.41
1:G:9:LYS:HD2	1:G:9:LYS:HA	1.72	0.41
1:G:83:ALA:HA	1:G:87:ALA:HB3	2.01	0.41
1:G:562:CYS:SG	1:G:564:VAL:HG22	2.60	0.41
1:H:400:ALA:O	1:H:427:ASN:ND2	2.50	0.41
1:H:535:TRP:CE3	1:H:605:LYS:HE3	2.55	0.41
1:M:153:ARG:HB2	1:M:248:PHE:CZ	2.54	0.41
1:M:173:THR:HG23	1:M:174:GLY:N	2.35	0.41
1:M:173:THR:CG2	1:M:174:GLY:N	2.83	0.41
1:M:199:LYS:HA	1:M:200:ASP:HA	1.34	0.41
1:M:235:ALA:HB1	1:M:324:CYS:HB3	2.03	0.41
1:M:382:HIS:ND1	1:M:441:PRO:HA	2.35	0.41
1:N:54:ILE:CA	1:N:58:LYS:NZ	2.51	0.41
1:O:53:THR:HG22	1:O:168:ARG:HE	1.84	0.41
1:O:513:PHE:O	1:O:516:GLU:HB3	2.21	0.41
1:P:39:ASP:OD2	1:P:298:ARG:CD	2.68	0.41
1:P:107:THR:C	1:P:109:ASN:N	2.74	0.41
1:P:540:ILE:HG22	1:P:542:LYS:HE3	2.03	0.41
1:J:104:ARG:HA	1:J:118:VAL:HG21	2.02	0.41
1:J:613:PHE:HA	1:J:614:PRO:HD2	1.89	0.41
1:K:417:PHE:CZ	1:K:430:ILE:HB	2.55	0.41
1:K:443:ILE:HG13	1:K:478:ARG:HB3	2.03	0.41
1:B:164:LYS:O	1:B:167:CYS:HB2	2.20	0.41
1:B:549:LEU:HD12	1:B:549:LEU:HA	1.93	0.41
1:F:180:PRO:HB2	1:F:229:LEU:HB2	2.03	0.41
1:E:84:ARG:HD3	1:O:620:ASN:HD21	1.84	0.41
1:H:109:ASN:HD22	1:H:109:ASN:N	2.18	0.41
1:H:141:VAL:O	1:H:141:VAL:CG1	2.69	0.41
1:I:129:ILE:HG22	1:I:130:GLY:N	2.36	0.41
1:M:68:VAL:HG22	1:M:136:ILE:CB	2.40	0.41
1:M:176:VAL:HG22	1:M:236:PHE:HB2	2.01	0.41
1:M:297:TRP:CE3	1:M:298:ARG:HA	2.55	0.41
1:N:42:ARG:HH11	1:N:140:GLU:HG2	1.85	0.41
1:N:216:VAL:HG13	1:N:218:LEU:HG	2.03	0.41
1:P:111:PRO:HD2	1:P:112:TRP:CZ3	2.54	0.41
1:R:639:PHE:HB3	1:R:641:PHE:CE1	2.55	0.41
1:J:643:LYS:HG3	1:J:644:SER:H	1.86	0.41
1:K:104:ARG:NH1	1:K:118:VAL:HG12	2.34	0.41
1:K:218:LEU:HB2	1:K:303:GLN:NE2	2.31	0.41
1:K:616:THR:C	1:K:618:LEU:N	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:290:LYS:HZ2	1:L:290:LYS:HG3	1.76	0.41
1:A:16:VAL:HG11	1:C:417:PHE:CG	2.55	0.41
1:B:444:VAL:O	1:B:445:LEU:HD12	2.21	0.41
1:C:84:ARG:HG3	1:C:112:TRP:CZ2	2.55	0.41
1:I:616:THR:C	1:I:618:LEU:N	2.74	0.41
1:N:36:MET:HA	1:N:300:HIS:NE2	2.35	0.41
1:N:85:GLU:N	1:N:86:GLY:HA2	2.36	0.41
1:O:386:VAL:HG23	1:O:446:ALA:HB2	2.02	0.41
1:O:390:SER:OG	1:O:447:GLU:OE1	2.33	0.41
1:O:632:LYS:HG3	1:O:633:SER:H	1.86	0.41
1:P:259:HIS:CD2	1:P:260:SER:OG	2.54	0.41
1:P:316:MET:HA	1:P:317:ASN:HA	1.71	0.41
1:Q:110:SER:HB2	1:Q:111:PRO:HD2	2.01	0.41
1:J:618:LEU:O	1:J:620:ASN:N	2.53	0.41
1:K:143:ASP:C	1:K:145:GLU:N	2.73	0.41
1:K:312:LYS:HA	1:K:312:LYS:HD3	1.87	0.41
1:L:93:LEU:CD1	1:L:123:SER:HA	2.50	0.41
1:B:314:VAL:HG22	1:B:315:GLU:N	2.30	0.41
1:E:437:LEU:HD11	1:E:441:PRO:HG3	2.01	0.41
1:G:108:SER:O	1:G:109:ASN:CB	2.67	0.41
1:G:163:ALA:HB1	1:G:167:CYS:SG	2.61	0.41
1:G:239:ASP:OD1	1:G:277:ARG:NH2	2.54	0.41
1:I:355:ARG:NE	3:I:702:PO4:O1	2.45	0.41
1:I:553:ILE:H	1:I:553:ILE:HD12	1.86	0.41
1:M:218:LEU:HB2	1:M:303:GLN:HE21	1.86	0.41
1:M:222:LYS:O	1:M:225:GLU:CG	2.64	0.41
1:N:378:SER:O	1:N:379:LYS:C	2.59	0.41
1:P:27:GLU:HB3	1:P:96:PHE:CZ	2.56	0.41
1:P:45:LYS:O	1:P:275:MET:HG2	2.21	0.41
1:P:67:HIS:HE1	1:P:91:THR:HG23	1.85	0.41
1:P:297:TRP:CD2	1:P:495:ASP:HB3	2.55	0.41
1:P:369:LYS:CG	1:P:370:PHE:N	2.82	0.41
1:Q:137:ILE:O	1:Q:169:VAL:HA	2.21	0.41
1:Q:378:SER:HB2	1:Q:399:THR:CG2	2.41	0.41
1:Q:556:ARG:HE	1:Q:556:ARG:HB2	1.67	0.41
1:J:84:ARG:HG3	1:J:112:TRP:CZ2	2.56	0.41
1:J:263:THR:HA	1:J:313:LYS:HA	2.02	0.41
1:K:156:LYS:HG3	1:K:246:ILE:HB	2.02	0.41
1:K:381:LEU:O	1:K:400:ALA:HB1	2.20	0.41
1:K:535:TRP:O	1:K:535:TRP:CE3	2.74	0.41
1:L:180:PRO:HA	1:L:267:LEU:HD23	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:629:LEU:CD2	1:E:438:THR:HG21	2.48	0.41
1:C:150:GLY:O	1:C:151:ALA:C	2.59	0.41
1:E:57:LYS:O	1:E:66:VAL:CG2	2.58	0.41
1:E:216:VAL:CG2	1:E:217:GLN:N	2.83	0.41
1:E:595:ILE:HG23	1:E:599:GLY:HA2	2.02	0.41
1:G:168:ARG:NH2	1:G:276:ASP:O	2.54	0.41
1:I:71:ILE:HG21	1:I:154:THR:HG23	2.02	0.41
1:I:445:LEU:HD12	1:I:480:GLU:HB2	2.02	0.41
1:I:446:ALA:HB3	1:I:462:PHE:CE1	2.56	0.41
1:M:177:TYR:HA	1:M:233:ILE:O	2.21	0.41
1:M:534:LEU:C	1:M:536:GLU:N	2.72	0.41
1:N:58:LYS:CE	1:N:58:LYS:N	2.84	0.41
1:N:186:LEU:HD23	1:N:186:LEU:HA	1.95	0.41
1:O:7:ASN:HB2	1:O:14:GLU:OE1	2.21	0.41
1:O:182:GLU:HB2	1:O:229:LEU:HD21	2.03	0.41
1:O:185:LEU:C	1:O:185:LEU:HD23	2.41	0.41
1:O:410:GLU:HB2	1:O:413:ARG:NH2	2.35	0.41
1:O:443:ILE:HA	1:O:478:ARG:O	2.20	0.41
1:O:447:GLU:H	1:O:448:PRO:HA	1.85	0.41
1:P:45:LYS:HZ1	1:P:294:ASN:ND2	2.19	0.41
1:P:554:ASP:C	1:P:556:ARG:H	2.24	0.41
1:Q:485:VAL:HG12	1:Q:487:LYS:HG3	2.02	0.41
1:R:471:MET:HG3	1:R:556:ARG:NH2	2.35	0.41
1:J:493:PHE:HA	1:J:539:GLY:HA3	2.03	0.41
1:K:112:TRP:O	1:K:114:ASP:N	2.54	0.41
1:K:164:LYS:O	1:K:165:PRO:C	2.59	0.41
1:L:255:GLU:HG2	1:L:321:GLU:HG2	2.03	0.41
1:L:288:LYS:HB3	1:L:288:LYS:HE2	1.63	0.41
1:A:186:LEU:O	1:A:187:LYS:C	2.59	0.41
1:A:478:ARG:CG	1:A:478:ARG:NH2	2.70	0.41
1:D:437:LEU:HD22	1:D:437:LEU:C	2.41	0.41
1:B:38:LEU:HD13	1:B:498:ASN:HD22	1.86	0.41
1:C:141:VAL:O	1:C:141:VAL:CG1	2.65	0.41
1:C:616:THR:C	1:C:618:LEU:H	2.24	0.41
1:F:60:GLU:O	1:F:60:GLU:HG3	2.21	0.41
1:F:70:ASP:HA	1:F:138:VAL:O	2.20	0.41
1:F:627:HIS:O	1:F:639:PHE:HA	2.21	0.41
1:E:15:TRP:NE1	1:E:520:LYS:HE2	2.36	0.41
1:E:42:ARG:HE	1:E:43:ASN:ND2	2.18	0.41
1:E:316:MET:HA	1:E:317:ASN:HA	1.86	0.41
1:E:353:LEU:HD22	1:E:357:THR:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:169:VAL:HG11	1:G:240:PHE:O	2.21	0.41
1:G:185:LEU:HD23	1:G:359:TYR:HE2	1.86	0.41
1:G:448:PRO:O	1:G:448:PRO:HG2	2.21	0.41
1:H:46:PHE:CZ	1:H:140:GLU:HB2	2.56	0.41
1:H:268:LEU:HD12	1:H:289:TRP:HH2	1.85	0.41
1:H:327:ASP:OD1	1:H:327:ASP:C	2.60	0.41
1:I:96:PHE:CZ	1:I:98:PRO:HG2	2.56	0.41
1:I:190:ASN:HD21	1:I:209:GLY:HA3	1.86	0.41
1:I:243:GLU:HG2	1:I:244:GLU:N	2.34	0.41
1:I:275:MET:HE2	1:I:275:MET:CA	2.43	0.41
1:I:326:HIS:HA	1:I:330:SER:O	2.21	0.41
1:I:455:ASN:HA	1:I:456:PRO:HD2	1.65	0.41
1:M:52:THR:HG21	1:M:278:ASN:ND2	2.36	0.41
1:M:57:LYS:HD3	1:M:57:LYS:HA	1.96	0.41
1:M:437:LEU:HD23	1:M:437:LEU:HA	1.88	0.41
1:M:482:HIS:CE1	1:M:582:GLU:HB3	2.56	0.41
1:M:487:LYS:O	1:M:577:MET:HA	2.21	0.41
1:N:302:MET:HG2	1:N:303:GLN:H	1.86	0.41
1:N:427:ASN:N	1:N:427:ASN:OD1	2.53	0.41
1:P:449:PHE:HA	1:P:459:HIS:CD2	2.56	0.41
1:R:96:PHE:HD2	1:R:99:MET:HG2	1.85	0.41
1:R:550:ARG:H	1:R:560:GLN:NE2	2.18	0.41
1:J:119:ILE:HG22	1:J:121:GLU:HG3	2.02	0.41
1:J:413:ARG:NH1	1:J:432:GLU:HG3	2.36	0.41
1:J:446:ALA:O	1:J:481:PRO:HD3	2.21	0.41
1:J:547:GLU:OE2	1:J:550:ARG:HD2	2.21	0.41
1:K:478:ARG:NH2	1:K:480:GLU:OE1	2.54	0.41
1:K:516:GLU:CG	1:K:520:LYS:HE3	2.50	0.41
1:K:623:SER:O	1:K:644:SER:OG	2.30	0.41
1:L:42:ARG:HH21	1:L:43:ASN:HD21	1.68	0.41
1:L:105:HIS:O	1:L:109:ASN:ND2	2.46	0.41
1:A:119:ILE:HG22	1:A:121:GLU:HG2	2.02	0.41
1:D:226:PHE:CD1	1:D:226:PHE:N	2.89	0.41
1:D:447:GLU:N	1:D:448:PRO:HA	2.35	0.41
1:B:164:LYS:O	1:B:165:PRO:C	2.58	0.41
1:B:460:LEU:HD21	1:B:579:MET:HE2	2.02	0.41
1:C:420:ILE:HD11	1:C:428:VAL:HG22	2.02	0.41
1:C:549:LEU:HD12	1:C:549:LEU:HA	1.68	0.41
1:F:434:VAL:CG1	1:F:469:LEU:HD13	2.52	0.41
1:E:383:VAL:HB	1:E:443:ILE:CG2	2.51	0.41
1:G:216:VAL:CG2	1:G:217:GLN:N	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:292:LYS:HA	1:H:293:ASN:HA	1.93	0.41
1:H:505:THR:HA	1:H:509:PHE:O	2.20	0.41
1:N:292:LYS:HD2	1:N:293:ASN:ND2	2.37	0.41
1:N:600:VAL:HA	1:N:601:PRO:HD3	1.85	0.41
1:P:445:LEU:HD12	1:P:480:GLU:HB2	2.03	0.41
1:Q:323:VAL:HB	1:Q:334:SER:OG	2.21	0.41
1:Q:531:GLU:HG2	1:Q:531:GLU:O	2.21	0.41
1:J:358:VAL:O	1:J:359:TYR:C	2.59	0.41
1:J:455:ASN:HB3	1:J:457:TRP:CE2	2.56	0.41
1:K:227:ARG:NH2	1:K:261:SER:O	2.53	0.41
1:L:168:ARG:NH1	1:L:168:ARG:CG	2.75	0.41
1:D:157:GLU:HB3	1:D:161:ARG:NH1	2.36	0.40
1:B:37:ILE:O	1:B:37:ILE:CG2	2.68	0.40
1:B:57:LYS:HG3	1:B:57:LYS:O	2.21	0.40
1:B:489:ILE:HD13	1:B:541:VAL:CG2	2.51	0.40
1:B:553:ILE:O	1:B:553:ILE:HG22	2.21	0.40
1:C:16:VAL:HG13	1:C:17:VAL:N	2.36	0.40
1:C:72:GLY:N	1:C:93:LEU:O	2.53	0.40
1:F:78:LEU:HD12	1:F:78:LEU:HA	1.83	0.40
1:F:274:ASP:OD1	1:F:277:ARG:N	2.45	0.40
1:E:178:ILE:HA	1:E:268:LEU:O	2.21	0.40
1:H:342:ARG:HH11	1:H:342:ARG:HD3	1.69	0.40
1:H:534:LEU:CD1	1:H:576:PRO:HB3	2.51	0.40
1:I:427:ASN:OD1	1:I:427:ASN:N	2.54	0.40
1:O:69:LEU:HD23	1:O:137:ILE:HG12	2.03	0.40
1:O:270:TRP:CE2	1:O:286:GLY:HA2	2.57	0.40
1:P:404:THR:HG23	1:P:429:GLU:HG3	2.03	0.40
1:P:447:GLU:H	1:P:448:PRO:HA	1.87	0.40
1:Q:566:ILE:CG2	1:Q:569:MET:HE2	2.51	0.40
1:J:71:ILE:HB	1:J:139:ALA:HB2	2.02	0.40
1:J:566:ILE:HG21	1:J:575:ILE:HD13	2.04	0.40
1:K:222:LYS:HB2	1:K:225:GLU:CG	2.51	0.40
1:D:175:ASN:ND2	1:D:237:LYS:HG2	2.37	0.40
1:D:359:TYR:CD1	1:D:359:TYR:C	2.94	0.40
1:C:59:HIS:HD2	1:C:60:GLU:HG3	1.85	0.40
1:C:547:GLU:OE2	1:C:550:ARG:NH1	2.52	0.40
1:F:204:LEU:HD21	1:F:419:TYR:CE1	2.56	0.40
1:G:321:GLU:O	1:G:322:ILE:HD13	2.21	0.40
1:M:194:ARG:HB3	1:M:201:GLU:OE1	2.21	0.40
1:M:344:TYR:CD1	1:M:344:TYR:N	2.89	0.40
1:M:438:THR:HB	1:M:439:ASP:OD1	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:198:GLU:HB3	1:P:200:ASP:HB2	2.04	0.40
1:P:541:VAL:HG11	1:P:595:ILE:HD13	2.03	0.40
1:Q:216:VAL:CA	1:Q:302:MET:SD	3.10	0.40
1:Q:287:PRO:HG2	1:Q:289:TRP:CH2	2.56	0.40
1:Q:460:LEU:HD22	1:Q:463:LEU:CD2	2.51	0.40
1:Q:474:GLY:C	1:Q:476:GLU:N	2.74	0.40
1:R:92:ALA:C	1:R:93:LEU:HD23	2.42	0.40
1:R:460:LEU:HD21	1:R:579:MET:HE1	2.03	0.40
1:J:40:PHE:CD1	1:J:41:ASP:N	2.90	0.40
1:J:144:THR:O	1:J:144:THR:HG22	2.20	0.40
1:J:297:TRP:CZ2	1:J:299:ASP:HB2	2.56	0.40
1:J:338:LYS:HD2	1:J:338:LYS:HA	1.90	0.40
1:K:277:ARG:O	1:K:277:ARG:HG2	2.21	0.40
1:K:299:ASP:C	1:K:301:TRP:N	2.75	0.40
1:L:63:ASP:OD1	1:L:63:ASP:N	2.36	0.40
1:L:445:LEU:HD12	1:L:480:GLU:HB2	2.03	0.40
1:L:457:TRP:HA	4:L:831:HOH:O	2.20	0.40
1:L:465:ASP:O	1:L:469:LEU:HD22	2.21	0.40
1:L:631:ASP:OD1	1:L:631:ASP:C	2.59	0.40
1:A:136:ILE:HA	1:A:168:ARG:O	2.21	0.40
1:D:631:ASP:OD1	1:D:631:ASP:C	2.59	0.40
1:B:618:LEU:HD21	1:B:642:GLY:HA2	2.03	0.40
1:E:578:TRP:CG	1:E:591:GLY:HA3	2.57	0.40
1:G:548:ILE:HG22	1:G:549:LEU:HD22	2.02	0.40
1:H:297:TRP:CE3	1:H:298:ARG:HA	2.56	0.40
1:M:434:VAL:HG12	1:M:469:LEU:HD12	2.03	0.40
1:N:140:GLU:OE1	1:N:301:TRP:CZ2	2.71	0.40
1:N:194:ARG:HB3	1:N:201:GLU:HG3	2.04	0.40
1:O:185:LEU:HD23	1:O:185:LEU:O	2.21	0.40
1:O:549:LEU:HD12	1:O:549:LEU:HA	1.81	0.40
1:O:612:TYR:CG	1:O:613:PHE:N	2.88	0.40
1:P:122:ARG:O	1:P:125:ASP:HB2	2.22	0.40
1:Q:47:LEU:O	1:Q:51:LYS:HB2	2.21	0.40
1:Q:179:VAL:HA	1:Q:180:PRO:HD2	1.88	0.40
1:Q:372:ASP:O	1:Q:376:LYS:HB2	2.21	0.40
1:R:612:TYR:OH	1:R:615:ILE:CD1	2.70	0.40
1:J:261:SER:OG	1:J:315:GLU:HA	2.21	0.40
1:J:392:LEU:HD23	1:J:392:LEU:HA	1.90	0.40
1:K:58:LYS:NZ	1:K:86:GLY:O	2.45	0.40
1:K:175:ASN:O	1:K:271:TRP:HA	2.22	0.40
1:K:549:LEU:HD12	1:K:560:GLN:HB3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:269:MET:HG2	1:L:306:TYR:CE1	2.56	0.40
1:D:181:VAL:O	1:D:265:ASP:N	2.54	0.40
1:B:91:THR:HG23	1:B:119:ILE:CD1	2.52	0.40
1:C:275:MET:CE	1:C:283:ILE:H	2.34	0.40
1:E:122:ARG:O	1:E:124:THR:N	2.55	0.40
1:G:35:ASP:OD2	1:G:299:ASP:N	2.40	0.40
1:G:227:ARG:NH2	1:G:261:SER:O	2.55	0.40
1:G:310:GLU:OE1	1:G:335:ASN:OD1	2.40	0.40
1:G:448:PRO:O	1:G:448:PRO:CG	2.69	0.40
1:H:315:GLU:HB3	1:H:318:GLN:HB2	2.03	0.40
1:H:460:LEU:HD21	1:H:579:MET:HE3	2.03	0.40
1:H:470:LYS:HD2	1:H:555:GLY:HA3	2.04	0.40
1:I:181:VAL:HG12	1:I:266:ALA:O	2.22	0.40
1:M:280:THR:CG2	1:M:281:THR:HG22	2.26	0.40
1:M:388:GLU:HB3	1:M:450:TYR:HA	2.03	0.40
1:N:114:ASP:N	1:N:114:ASP:OD1	2.55	0.40
1:N:233:ILE:HG12	1:N:256:ALA:HB2	2.04	0.40
1:N:346:VAL:O	1:N:347:CYS:C	2.60	0.40
1:N:420:ILE:HA	1:N:425:LEU:HD12	2.03	0.40
1:O:375:ASP:HA	1:O:399:THR:OG1	2.21	0.40
1:P:455:ASN:HA	1:P:456:PRO:HD3	1.89	0.40
1:R:111:PRO:HD2	1:R:112:TRP:CZ3	2.57	0.40
1:R:531:GLU:HA	1:R:609:GLN:O	2.21	0.40
1:K:497:GLN:H	1:K:497:GLN:CD	2.25	0.40
1:D:384:ALA:O	1:D:444:VAL:HA	2.21	0.40
1:D:565:ASN:ND2	1:D:644:SER:HB3	2.37	0.40
1:B:168:ARG:NH2	1:B:276:ASP:O	2.55	0.40
1:B:404:THR:HG23	1:B:429:GLU:HG3	2.03	0.40
1:C:156:LYS:NZ	1:C:246:ILE:O	2.46	0.40
1:F:39:ASP:C	1:F:39:ASP:OD1	2.60	0.40
1:F:259:HIS:CD2	1:F:260:SER:OG	2.70	0.40
1:E:193:PRO:HA	1:E:362:ASN:ND2	2.36	0.40
1:G:73:THR:HA	2:G:701:SAH:N	2.36	0.40
1:I:162:LEU:N	1:I:162:LEU:CD1	2.85	0.40
1:I:619:ARG:HG2	1:I:619:ARG:HH11	1.86	0.40
1:M:96:PHE:CE2	1:M:98:PRO:HD2	2.56	0.40
1:M:145:GLU:O	1:M:146:LEU:HB3	2.21	0.40
1:M:174:GLY:HA3	1:M:273:ILE:HG22	2.03	0.40
1:M:388:GLU:HG2	1:M:451:MET:HG3	2.04	0.40
1:N:141:VAL:O	1:N:141:VAL:CG1	2.69	0.40
1:N:242:HIS:HB3	1:N:245:LYS:CG	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:357:THR:O	1:N:361:VAL:HG23	2.22	0.40
1:O:310:GLU:OE2	1:O:338:LYS:HG2	2.22	0.40
1:O:557:VAL:CG2	1:O:632:LYS:HB2	2.49	0.40
1:Q:410:GLU:HG3	1:Q:413:ARG:HH22	1.87	0.40
1:Q:443:ILE:CG1	1:Q:444:VAL:N	2.85	0.40
1:Q:468:VAL:O	1:Q:471:MET:HB3	2.21	0.40
1:R:278:ASN:HB2	1:R:280:THR:HG22	2.01	0.40
1:R:377:LEU:HB3	1:R:443:ILE:HD13	2.03	0.40
1:R:600:VAL:HA	1:R:601:PRO:HD2	1.82	0.40
1:J:264:ILE:HD12	1:J:312:LYS:CG	2.52	0.40
1:K:627:HIS:HB2	1:K:640:GLN:HB2	2.03	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:554:ASP:OD1	1:C:550:ARG:NH2[3_554]	2.01	0.19
1:N:554:ASP:OD1	1:P:550:ARG:NH2[3_654]	2.09	0.11

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	637/655 (97%)	600 (94%)	34 (5%)	3 (0%)	29	41
1	B	634/655 (97%)	561 (88%)	62 (10%)	11 (2%)	9	11
1	C	635/655 (97%)	578 (91%)	47 (7%)	10 (2%)	9	13
1	D	633/655 (97%)	595 (94%)	34 (5%)	4 (1%)	25	36
1	E	630/655 (96%)	569 (90%)	53 (8%)	8 (1%)	12	17
1	F	634/655 (97%)	563 (89%)	62 (10%)	9 (1%)	11	15
1	G	630/655 (96%)	575 (91%)	50 (8%)	5 (1%)	19	29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	635/655 (97%)	590 (93%)	39 (6%)	6 (1%)	17	25
1	I	642/655 (98%)	572 (89%)	58 (9%)	12 (2%)	8	10
1	J	642/655 (98%)	578 (90%)	54 (8%)	10 (2%)	9	13
1	K	637/655 (97%)	570 (90%)	53 (8%)	14 (2%)	6	7
1	L	642/655 (98%)	607 (94%)	34 (5%)	1 (0%)	47	62
1	M	625/655 (95%)	551 (88%)	65 (10%)	9 (1%)	11	15
1	N	634/655 (97%)	558 (88%)	67 (11%)	9 (1%)	11	15
1	O	637/655 (97%)	567 (89%)	61 (10%)	9 (1%)	11	15
1	P	630/655 (96%)	576 (91%)	48 (8%)	6 (1%)	15	23
1	Q	626/655 (96%)	526 (84%)	81 (13%)	19 (3%)	4	3
1	R	634/655 (97%)	567 (89%)	52 (8%)	15 (2%)	6	6
All	All	11417/11790 (97%)	10303 (90%)	954 (8%)	160 (1%)	11	15

All (160) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	63	ASP
1	B	59	HIS
1	B	60	GLU
1	B	278	ASN
1	F	290	LYS
1	G	87	ALA
1	I	279	GLY
1	M	35	ASP
1	M	36	MET
1	M	438	THR
1	M	616	THR
1	N	88	ASP
1	O	568	ASN
1	P	438	THR
1	Q	144	THR
1	Q	259	HIS
1	Q	336	VAL
1	R	88	ASP
1	R	219	SER
1	R	400	ALA
1	J	141	VAL
1	K	300	HIS

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Mol	Chain	Res	Type
1	A	555	GLY
1	D	277	ARG
1	D	453	ALA
1	B	77	LEU
1	B	288	LYS
1	B	555	GLY
1	C	63	ASP
1	C	289	TRP
1	C	290	LYS
1	C	617	ALA
1	F	197	GLY
1	F	278	ASN
1	F	398	LYS
1	E	87	ALA
1	E	109	ASN
1	E	123	SER
1	E	183	SER
1	H	113	SER
1	I	286	GLY
1	I	453	ALA
1	M	146	LEU
1	N	264	ILE
1	N	291	ASN
1	N	474	GLY
1	O	141	VAL
1	O	380	GLY
1	O	461	ARG
1	O	478	ARG
1	O	617	ALA
1	P	108	SER
1	P	123	SER
1	P	452	SER
1	Q	56	GLU
1	Q	219	SER
1	Q	258	ALA
1	Q	277	ARG
1	R	346	VAL
1	J	130	GLY
1	J	396	ALA
1	J	598	ALA
1	K	85	GLU
1	K	113	SER

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Mol	Chain	Res	Type
1	K	286	GLY
1	K	535	TRP
1	B	41	ASP
1	B	42	ARG
1	B	124	THR
1	C	243	GLU
1	F	148	GLY
1	G	113	SER
1	G	496	LEU
1	H	242	HIS
1	I	111	PRO
1	I	533	SER
1	M	276	ASP
1	M	289	TRP
1	Q	224	HIS
1	Q	227	ARG
1	Q	232	PRO
1	Q	340	LYS
1	R	614	PRO
1	J	597	SER
1	J	632	LYS
1	J	643	LYS
1	K	144	THR
1	K	345	CYS
1	K	453	ALA
1	K	511	LEU
1	A	291	ASN
1	B	277	ARG
1	C	33	PHE
1	C	278	ASN
1	C	316	MET
1	C	475	ASP
1	F	185	LEU
1	E	288	LYS
1	E	453	ALA
1	G	277	ARG
1	H	84	ARG
1	H	277	ARG
1	I	277	ARG
1	I	594	SER
1	I	616	THR
1	M	302	MET

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Mol	Chain	Res	Type
1	M	453	ALA
1	N	55	ALA
1	N	83	ALA
1	N	133	ARG
1	O	616	THR
1	Q	87	ALA
1	Q	243	GLU
1	Q	293	ASN
1	Q	338	LYS
1	R	52	THR
1	R	85	GLU
1	R	160	GLU
1	R	497	GLN
1	R	643	LYS
1	J	316	MET
1	K	74	GLY
1	K	617	ALA
1	B	52	THR
1	C	632	LYS
1	F	379	LYS
1	E	108	SER
1	G	57	LYS
1	H	55	ALA
1	I	556	ARG
1	P	7	ASN
1	Q	146	LEU
1	Q	632	LYS
1	R	26	GLN
1	R	243	GLU
1	J	424	LYS
1	K	290	LYS
1	K	523	THR
1	H	350	HIS
1	I	309	PRO
1	N	242	HIS
1	N	244	GLU
1	O	441	PRO
1	O	614	PRO
1	R	557	VAL
1	J	33	PHE
1	A	64	GLY
1	E	279	GLY

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Mol	Chain	Res	Type
1	R	111	PRO
1	L	111	PRO
1	D	141	VAL
1	F	615	ILE
1	P	34	GLY
1	K	197	GLY
1	F	141	VAL
1	I	553	ILE
1	R	232	PRO
1	I	232	PRO
1	Q	111	PRO
1	Q	165	PRO

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	556/569 (98%)	479 (86%)	77 (14%)	3 4
1	B	553/569 (97%)	474 (86%)	79 (14%)	3 4
1	C	554/569 (97%)	484 (87%)	70 (13%)	4 5
1	D	552/569 (97%)	488 (88%)	64 (12%)	5 7
1	E	551/569 (97%)	459 (83%)	92 (17%)	2 2
1	F	553/569 (97%)	471 (85%)	82 (15%)	3 3
1	G	552/569 (97%)	473 (86%)	79 (14%)	3 4
1	H	554/569 (97%)	481 (87%)	73 (13%)	4 4
1	I	557/569 (98%)	476 (86%)	81 (14%)	3 3
1	J	557/569 (98%)	481 (86%)	76 (14%)	3 4
1	K	556/569 (98%)	465 (84%)	91 (16%)	2 2
1	L	557/569 (98%)	483 (87%)	74 (13%)	4 4
1	M	550/569 (97%)	470 (86%)	80 (14%)	3 3
1	N	553/569 (97%)	455 (82%)	98 (18%)	2 2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	O	556/569 (98%)	472 (85%)	84 (15%)	3 3
1	P	551/569 (97%)	469 (85%)	82 (15%)	3 3
1	Q	548/569 (96%)	465 (85%)	83 (15%)	3 3
1	R	553/569 (97%)	467 (84%)	86 (16%)	2 3
All	All	9963/10242 (97%)	8512 (85%)	1451 (15%)	3 3

All (1451) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LYS
1	A	16	VAL
1	A	20	GLU
1	A	42	ARG
1	A	45	LYS
1	A	47	LEU
1	A	91	THR
1	A	107	THR
1	A	109	ASN
1	A	110	SER
1	A	117	THR
1	A	121	GLU
1	A	140	GLU
1	A	141	VAL
1	A	160	GLU
1	A	168	ARG
1	A	169	VAL
1	A	173	THR
1	A	176	VAL
1	A	185	LEU
1	A	187	LYS
1	A	191	ASP
1	A	210	THR
1	A	216	VAL
1	A	223	THR
1	A	245	LYS
1	A	253	VAL
1	A	263	THR
1	A	269	MET
1	A	281	THR
1	A	290	LYS
1	A	298	ARG

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Mol	Chain	Res	Type
1	A	305	VAL
1	A	308	LEU
1	A	314	VAL
1	A	336	VAL
1	A	338	LYS
1	A	343	SER
1	A	349	LEU
1	A	355	ARG
1	A	363	GLU
1	A	385	THR
1	A	392	LEU
1	A	398	LYS
1	A	399	THR
1	A	424	LYS
1	A	428	VAL
1	A	437	LEU
1	A	444	VAL
1	A	445	LEU
1	A	451	MET
1	A	463	LEU
1	A	469	LEU
1	A	471	MET
1	A	476	GLU
1	A	478	ARG
1	A	479	VAL
1	A	485	VAL
1	A	486	LEU
1	A	497	GLN
1	A	523	THR
1	A	532	GLN
1	A	541	VAL
1	A	546	VAL
1	A	549	LEU
1	A	554	ASP
1	A	556	ARG
1	A	558	SER
1	A	561	LYS
1	A	564	VAL
1	A	582	GLU
1	A	593	LEU
1	A	611	VAL
1	A	616	THR

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Mol	Chain	Res	Type
1	A	618	LEU
1	A	621	ASP
1	A	632	LYS
1	D	9	LYS
1	D	16	VAL
1	D	19	GLU
1	D	20	GLU
1	D	47	LEU
1	D	61	ASN
1	D	78	LEU
1	D	85	GLU
1	D	91	THR
1	D	114	ASP
1	D	117	THR
1	D	140	GLU
1	D	141	VAL
1	D	160	GLU
1	D	162	LEU
1	D	168	ARG
1	D	169	VAL
1	D	173	THR
1	D	185	LEU
1	D	187	LYS
1	D	210	THR
1	D	227	ARG
1	D	230	SER
1	D	263	THR
1	D	269	MET
1	D	281	THR
1	D	292	LYS
1	D	298	ARG
1	D	308	LEU
1	D	314	VAL
1	D	331	LEU
1	D	355	ARG
1	D	368	GLN
1	D	385	THR
1	D	392	LEU
1	D	398	LYS
1	D	399	THR
1	D	428	VAL
1	D	437	LEU

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Mol	Chain	Res	Type
1	D	438	THR
1	D	440	SER
1	D	445	LEU
1	D	451	MET
1	D	463	LEU
1	D	469	LEU
1	D	476	GLU
1	D	478	ARG
1	D	479	VAL
1	D	486	LEU
1	D	497	GLN
1	D	506	VAL
1	D	540	ILE
1	D	541	VAL
1	D	546	VAL
1	D	549	LEU
1	D	557	VAL
1	D	561	LYS
1	D	562	CYS
1	D	568	ASN
1	D	593	LEU
1	D	597	SER
1	D	611	VAL
1	D	618	LEU
1	D	622	LYS
1	B	16	VAL
1	B	19	GLU
1	B	31	SER
1	B	43	ASN
1	B	45	LYS
1	B	47	LEU
1	B	52	THR
1	B	56	GLU
1	B	62	THR
1	B	67	HIS
1	B	71	ILE
1	B	75	THR
1	B	78	LEU
1	B	84	ARG
1	B	88	ASP
1	B	101	ASP
1	B	107	THR

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Mol	Chain	Res	Type
1	B	108	SER
1	B	114	ASP
1	B	117	THR
1	B	140	GLU
1	B	162	LEU
1	B	169	VAL
1	B	173	THR
1	B	176	VAL
1	B	181	VAL
1	B	185	LEU
1	B	187	LYS
1	B	191	ASP
1	B	208	SER
1	B	210	THR
1	B	216	VAL
1	B	223	THR
1	B	230	SER
1	B	233	ILE
1	B	244	GLU
1	B	259	HIS
1	B	260	SER
1	B	263	THR
1	B	269	MET
1	B	293	ASN
1	B	298	ARG
1	B	308	LEU
1	B	331	LEU
1	B	336	VAL
1	B	351	SER
1	B	355	ARG
1	B	369	LYS
1	B	371	LYS
1	B	383	VAL
1	B	385	THR
1	B	428	VAL
1	B	436	SER
1	B	437	LEU
1	B	440	SER
1	B	451	MET
1	B	452	SER
1	B	463	LEU
1	B	469	LEU

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Mol	Chain	Res	Type
1	B	476	GLU
1	B	479	VAL
1	B	480	GLU
1	B	497	GLN
1	B	503	VAL
1	B	505	THR
1	B	507	ASN
1	B	541	VAL
1	B	546	VAL
1	B	550	ARG
1	B	557	VAL
1	B	562	CYS
1	B	570	SER
1	B	579	MET
1	B	611	VAL
1	B	614	PRO
1	B	616	THR
1	B	627	HIS
1	B	629	LEU
1	B	640	GLN
1	C	16	VAL
1	C	20	GLU
1	C	24	MET
1	C	45	LYS
1	C	47	LEU
1	C	58	LYS
1	C	62	THR
1	C	65	LYS
1	C	78	LEU
1	C	89	LYS
1	C	104	ARG
1	C	107	THR
1	C	114	ASP
1	C	117	THR
1	C	123	SER
1	C	140	GLU
1	C	162	LEU
1	C	168	ARG
1	C	173	THR
1	C	176	VAL
1	C	208	SER
1	C	210	THR

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Mol	Chain	Res	Type
1	C	230	SER
1	C	253	VAL
1	C	260	SER
1	C	269	MET
1	C	272	ASP
1	C	280	THR
1	C	288	LYS
1	C	290	LYS
1	C	293	ASN
1	C	298	ARG
1	C	305	VAL
1	C	308	LEU
1	C	311	LYS
1	C	319	THR
1	C	326	HIS
1	C	330	SER
1	C	338	LYS
1	C	355	ARG
1	C	363	GLU
1	C	383	VAL
1	C	392	LEU
1	C	428	VAL
1	C	434	VAL
1	C	437	LEU
1	C	444	VAL
1	C	445	LEU
1	C	451	MET
1	C	469	LEU
1	C	479	VAL
1	C	492	LYS
1	C	497	GLN
1	C	503	VAL
1	C	533	SER
1	C	540	ILE
1	C	549	LEU
1	C	557	VAL
1	C	561	LYS
1	C	562	CYS
1	C	568	ASN
1	C	572	SER
1	C	579	MET
1	C	593	LEU

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Mol	Chain	Res	Type
1	C	597	SER
1	C	619	ARG
1	C	621	ASP
1	C	622	LYS
1	C	629	LEU
1	C	643	LYS
1	F	1	MET
1	F	16	VAL
1	F	20	GLU
1	F	24	MET
1	F	45	LYS
1	F	47	LEU
1	F	62	THR
1	F	78	LEU
1	F	85	GLU
1	F	89	LYS
1	F	108	SER
1	F	113	SER
1	F	116	ILE
1	F	117	THR
1	F	133	ARG
1	F	140	GLU
1	F	162	LEU
1	F	169	VAL
1	F	173	THR
1	F	176	VAL
1	F	187	LYS
1	F	196	ASN
1	F	210	THR
1	F	216	VAL
1	F	243	GLU
1	F	244	GLU
1	F	253	VAL
1	F	259	HIS
1	F	263	THR
1	F	269	MET
1	F	275	MET
1	F	277	ARG
1	F	278	ASN
1	F	290	LYS
1	F	292	LYS
1	F	293	ASN

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Mol	Chain	Res	Type
1	F	298	ARG
1	F	310	GLU
1	F	316	MET
1	F	320	PHE
1	F	326	HIS
1	F	331	LEU
1	F	334	SER
1	F	335	ASN
1	F	336	VAL
1	F	341	SER
1	F	349	LEU
1	F	352	MET
1	F	355	ARG
1	F	363	GLU
1	F	383	VAL
1	F	385	THR
1	F	392	LEU
1	F	436	SER
1	F	437	LEU
1	F	444	VAL
1	F	445	LEU
1	F	451	MET
1	F	463	LEU
1	F	469	LEU
1	F	476	GLU
1	F	478	ARG
1	F	479	VAL
1	F	486	LEU
1	F	494	GLU
1	F	497	GLN
1	F	503	VAL
1	F	533	SER
1	F	540	ILE
1	F	541	VAL
1	F	546	VAL
1	F	549	LEU
1	F	550	ARG
1	F	557	VAL
1	F	564	VAL
1	F	595	ILE
1	F	602	GLU
1	F	618	LEU

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Mol	Chain	Res	Type
1	F	622	LYS
1	F	624	LEU
1	F	632	LYS
1	F	634	THR
1	E	1	MET
1	E	9	LYS
1	E	16	VAL
1	E	20	GLU
1	E	30	ARG
1	E	40	PHE
1	E	45	LYS
1	E	47	LEU
1	E	56	GLU
1	E	84	ARG
1	E	85	GLU
1	E	91	THR
1	E	93	LEU
1	E	104	ARG
1	E	107	THR
1	E	109	ASN
1	E	117	THR
1	E	121	GLU
1	E	140	GLU
1	E	144	THR
1	E	146	LEU
1	E	160	GLU
1	E	162	LEU
1	E	173	THR
1	E	176	VAL
1	E	181	VAL
1	E	185	LEU
1	E	187	LYS
1	E	199	LYS
1	E	208	SER
1	E	210	THR
1	E	216	VAL
1	E	230	SER
1	E	259	HIS
1	E	260	SER
1	E	269	MET
1	E	272	ASP
1	E	278	ASN

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Mol	Chain	Res	Type
1	E	290	LYS
1	E	298	ARG
1	E	305	VAL
1	E	308	LEU
1	E	314	VAL
1	E	317	ASN
1	E	319	THR
1	E	331	LEU
1	E	338	LYS
1	E	341	SER
1	E	343	SER
1	E	349	LEU
1	E	355	ARG
1	E	363	GLU
1	E	371	LYS
1	E	379	LYS
1	E	383	VAL
1	E	385	THR
1	E	392	LEU
1	E	399	THR
1	E	428	VAL
1	E	437	LEU
1	E	439	ASP
1	E	440	SER
1	E	444	VAL
1	E	445	LEU
1	E	451	MET
1	E	452	SER
1	E	454	MET
1	E	463	LEU
1	E	469	LEU
1	E	470	LYS
1	E	476	GLU
1	E	478	ARG
1	E	479	VAL
1	E	486	LEU
1	E	497	GLN
1	E	531	GLU
1	E	541	VAL
1	E	549	LEU
1	E	556	ARG
1	E	557	VAL

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Mol	Chain	Res	Type
1	E	561	LYS
1	E	562	CYS
1	E	571	SER
1	E	577	MET
1	E	587	ASN
1	E	593	LEU
1	E	616	THR
1	E	618	LEU
1	E	621	ASP
1	E	623	SER
1	E	632	LYS
1	E	643	LYS
1	G	1	MET
1	G	16	VAL
1	G	26	GLN
1	G	30	ARG
1	G	45	LYS
1	G	47	LEU
1	G	67	HIS
1	G	78	LEU
1	G	84	ARG
1	G	85	GLU
1	G	117	THR
1	G	122	ARG
1	G	127	SER
1	G	128	GLN
1	G	140	GLU
1	G	172	SER
1	G	176	VAL
1	G	181	VAL
1	G	185	LEU
1	G	191	ASP
1	G	199	LYS
1	G	200	ASP
1	G	206	ARG
1	G	210	THR
1	G	214	PHE
1	G	216	VAL
1	G	230	SER
1	G	243	GLU
1	G	253	VAL
1	G	260	SER

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Mol	Chain	Res	Type
1	G	261	SER
1	G	263	THR
1	G	269	MET
1	G	277	ARG
1	G	294	ASN
1	G	298	ARG
1	G	305	VAL
1	G	308	LEU
1	G	314	VAL
1	G	319	THR
1	G	336	VAL
1	G	339	ASP
1	G	341	SER
1	G	351	SER
1	G	355	ARG
1	G	371	LYS
1	G	383	VAL
1	G	385	THR
1	G	392	LEU
1	G	399	THR
1	G	424	LYS
1	G	428	VAL
1	G	433	LYS
1	G	437	LEU
1	G	444	VAL
1	G	451	MET
1	G	463	LEU
1	G	469	LEU
1	G	486	LEU
1	G	492	LYS
1	G	497	GLN
1	G	511	LEU
1	G	512	SER
1	G	533	SER
1	G	540	ILE
1	G	541	VAL
1	G	546	VAL
1	G	549	LEU
1	G	557	VAL
1	G	562	CYS
1	G	564	VAL
1	G	570	SER

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Mol	Chain	Res	Type
1	G	577	MET
1	G	587	ASN
1	G	593	LEU
1	G	597	SER
1	G	611	VAL
1	G	616	THR
1	G	629	LEU
1	H	1	MET
1	H	9	LYS
1	H	16	VAL
1	H	20	GLU
1	H	26	GLN
1	H	45	LYS
1	H	47	LEU
1	H	78	LEU
1	H	85	GLU
1	H	110	SER
1	H	114	ASP
1	H	117	THR
1	H	140	GLU
1	H	141	VAL
1	H	173	THR
1	H	181	VAL
1	H	185	LEU
1	H	210	THR
1	H	216	VAL
1	H	243	GLU
1	H	244	GLU
1	H	253	VAL
1	H	260	SER
1	H	263	THR
1	H	269	MET
1	H	281	THR
1	H	290	LYS
1	H	292	LYS
1	H	293	ASN
1	H	298	ARG
1	H	305	VAL
1	H	308	LEU
1	H	319	THR
1	H	336	VAL
1	H	338	LYS

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Mol	Chain	Res	Type
1	H	339	ASP
1	H	341	SER
1	H	351	SER
1	H	355	ARG
1	H	378	SER
1	H	385	THR
1	H	392	LEU
1	H	398	LYS
1	H	411	ARG
1	H	428	VAL
1	H	437	LEU
1	H	444	VAL
1	H	445	LEU
1	H	452	SER
1	H	463	LEU
1	H	469	LEU
1	H	475	ASP
1	H	478	ARG
1	H	479	VAL
1	H	485	VAL
1	H	486	LEU
1	H	490	PRO
1	H	497	GLN
1	H	541	VAL
1	H	546	VAL
1	H	549	LEU
1	H	556	ARG
1	H	562	CYS
1	H	564	VAL
1	H	570	SER
1	H	593	LEU
1	H	611	VAL
1	H	616	THR
1	H	618	LEU
1	H	621	ASP
1	H	632	LYS
1	H	643	LYS
1	H	644	SER
1	I	16	VAL
1	I	19	GLU
1	I	30	ARG
1	I	31	SER

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Mol	Chain	Res	Type
1	I	47	LEU
1	I	53	THR
1	I	56	GLU
1	I	63	ASP
1	I	78	LEU
1	I	85	GLU
1	I	97	LYS
1	I	104	ARG
1	I	114	ASP
1	I	115	LYS
1	I	117	THR
1	I	140	GLU
1	I	162	LEU
1	I	167	CYS
1	I	168	ARG
1	I	169	VAL
1	I	172	SER
1	I	173	THR
1	I	176	VAL
1	I	185	LEU
1	I	191	ASP
1	I	210	THR
1	I	243	GLU
1	I	261	SER
1	I	269	MET
1	I	277	ARG
1	I	278	ASN
1	I	280	THR
1	I	287	PRO
1	I	290	LYS
1	I	293	ASN
1	I	298	ARG
1	I	308	LEU
1	I	314	VAL
1	I	316	MET
1	I	325	ASN
1	I	331	LEU
1	I	336	VAL
1	I	351	SER
1	I	355	ARG
1	I	368	GLN
1	I	369	LYS

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Mol	Chain	Res	Type
1	I	383	VAL
1	I	385	THR
1	I	392	LEU
1	I	398	LYS
1	I	399	THR
1	I	424	LYS
1	I	428	VAL
1	I	437	LEU
1	I	438	THR
1	I	445	LEU
1	I	451	MET
1	I	463	LEU
1	I	469	LEU
1	I	476	GLU
1	I	478	ARG
1	I	479	VAL
1	I	486	LEU
1	I	497	GLN
1	I	541	VAL
1	I	546	VAL
1	I	549	LEU
1	I	550	ARG
1	I	554	ASP
1	I	556	ARG
1	I	557	VAL
1	I	561	LYS
1	I	564	VAL
1	I	568	ASN
1	I	572	SER
1	I	579	MET
1	I	587	ASN
1	I	593	LEU
1	I	597	SER
1	I	618	LEU
1	I	624	LEU
1	M	30	ARG
1	M	37	ILE
1	M	43	ASN
1	M	45	LYS
1	M	52	THR
1	M	56	GLU
1	M	65	LYS

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Mol	Chain	Res	Type
1	M	97	LYS
1	M	106	ILE
1	M	117	THR
1	M	119	ILE
1	M	124	THR
1	M	126	VAL
1	M	140	GLU
1	M	162	LEU
1	M	169	VAL
1	M	173	THR
1	M	175	ASN
1	M	178	ILE
1	M	185	LEU
1	M	191	ASP
1	M	194	ARG
1	M	199	LYS
1	M	200	ASP
1	M	206	ARG
1	M	210	THR
1	M	216	VAL
1	M	225	GLU
1	M	237	LYS
1	M	253	VAL
1	M	263	THR
1	M	268	LEU
1	M	269	MET
1	M	275	MET
1	M	281	THR
1	M	298	ARG
1	M	305	VAL
1	M	308	LEU
1	M	317	ASN
1	M	319	THR
1	M	326	HIS
1	M	338	LYS
1	M	351	SER
1	M	352	MET
1	M	355	ARG
1	M	369	LYS
1	M	371	LYS
1	M	383	VAL
1	M	385	THR

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Mol	Chain	Res	Type
1	M	399	THR
1	M	401	LYS
1	M	411	ARG
1	M	437	LEU
1	M	438	THR
1	M	439	ASP
1	M	444	VAL
1	M	445	LEU
1	M	451	MET
1	M	452	SER
1	M	478	ARG
1	M	479	VAL
1	M	483	MET
1	M	485	VAL
1	M	486	LEU
1	M	497	GLN
1	M	507	ASN
1	M	533	SER
1	M	540	ILE
1	M	542	LYS
1	M	547	GLU
1	M	549	LEU
1	M	554	ASP
1	M	562	CYS
1	M	568	ASN
1	M	579	MET
1	M	592	LEU
1	M	593	LEU
1	M	611	VAL
1	M	618	LEU
1	M	622	LYS
1	N	5	LYS
1	N	6	ILE
1	N	9	LYS
1	N	20	GLU
1	N	30	ARG
1	N	31	SER
1	N	47	LEU
1	N	58	LYS
1	N	62	THR
1	N	66	VAL
1	N	75	THR

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Mol	Chain	Res	Type
1	N	78	LEU
1	N	84	ARG
1	N	97	LYS
1	N	101	ASP
1	N	107	THR
1	N	108	SER
1	N	133	ARG
1	N	140	GLU
1	N	160	GLU
1	N	167	CYS
1	N	168	ARG
1	N	169	VAL
1	N	185	LEU
1	N	191	ASP
1	N	194	ARG
1	N	200	ASP
1	N	202	GLU
1	N	204	LEU
1	N	210	THR
1	N	214	PHE
1	N	237	LYS
1	N	244	GLU
1	N	245	LYS
1	N	253	VAL
1	N	259	HIS
1	N	269	MET
1	N	272	ASP
1	N	278	ASN
1	N	281	THR
1	N	294	ASN
1	N	298	ARG
1	N	305	VAL
1	N	308	LEU
1	N	313	LYS
1	N	314	VAL
1	N	317	ASN
1	N	325	ASN
1	N	331	LEU
1	N	336	VAL
1	N	341	SER
1	N	343	SER
1	N	349	LEU

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Mol	Chain	Res	Type
1	N	355	ARG
1	N	357	THR
1	N	363	GLU
1	N	371	LYS
1	N	383	VAL
1	N	385	THR
1	N	392	LEU
1	N	398	LYS
1	N	424	LYS
1	N	428	VAL
1	N	434	VAL
1	N	435	THR
1	N	436	SER
1	N	437	LEU
1	N	444	VAL
1	N	445	LEU
1	N	451	MET
1	N	454	MET
1	N	463	LEU
1	N	469	LEU
1	N	471	MET
1	N	475	ASP
1	N	476	GLU
1	N	478	ARG
1	N	479	VAL
1	N	486	LEU
1	N	492	LYS
1	N	494	GLU
1	N	497	GLN
1	N	540	ILE
1	N	541	VAL
1	N	546	VAL
1	N	549	LEU
1	N	553	ILE
1	N	557	VAL
1	N	564	VAL
1	N	593	LEU
1	N	597	SER
1	N	611	VAL
1	N	616	THR
1	N	618	LEU
1	N	621	ASP

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Mol	Chain	Res	Type
1	N	629	LEU
1	N	632	LYS
1	N	633	SER
1	O	1	MET
1	O	9	LYS
1	O	16	VAL
1	O	19	GLU
1	O	45	LYS
1	O	47	LEU
1	O	78	LEU
1	O	85	GLU
1	O	109	ASN
1	O	114	ASP
1	O	117	THR
1	O	120	SER
1	O	127	SER
1	O	128	GLN
1	O	140	GLU
1	O	141	VAL
1	O	156	LYS
1	O	162	LEU
1	O	169	VAL
1	O	176	VAL
1	O	185	LEU
1	O	187	LYS
1	O	191	ASP
1	O	206	ARG
1	O	210	THR
1	O	216	VAL
1	O	221	MET
1	O	223	THR
1	O	230	SER
1	O	233	ILE
1	O	269	MET
1	O	275	MET
1	O	281	THR
1	O	288	LYS
1	O	292	LYS
1	O	298	ARG
1	O	305	VAL
1	O	308	LEU
1	O	310	GLU

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Mol	Chain	Res	Type
1	O	313	LYS
1	O	317	ASN
1	O	319	THR
1	O	338	LYS
1	O	355	ARG
1	O	375	ASP
1	O	377	LEU
1	O	382	HIS
1	O	385	THR
1	O	399	THR
1	O	401	LYS
1	O	420	ILE
1	O	426	THR
1	O	436	SER
1	O	438	THR
1	O	445	LEU
1	O	451	MET
1	O	463	LEU
1	O	472	MET
1	O	478	ARG
1	O	486	LEU
1	O	487	LYS
1	O	497	GLN
1	O	501	SER
1	O	528	ILE
1	O	541	VAL
1	O	544	ASP
1	O	546	VAL
1	O	549	LEU
1	O	550	ARG
1	O	556	ARG
1	O	558	SER
1	O	559	SER
1	O	563	VAL
1	O	567	ASP
1	O	577	MET
1	O	579	MET
1	O	587	ASN
1	O	588	LEU
1	O	597	SER
1	O	602	GLU
1	O	621	ASP

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Mol	Chain	Res	Type
1	O	623	SER
1	O	624	LEU
1	O	643	LYS
1	P	16	VAL
1	P	45	LYS
1	P	47	LEU
1	P	58	LYS
1	P	93	LEU
1	P	104	ARG
1	P	106	ILE
1	P	108	SER
1	P	112	TRP
1	P	115	LYS
1	P	117	THR
1	P	123	SER
1	P	133	ARG
1	P	138	VAL
1	P	140	GLU
1	P	156	LYS
1	P	160	GLU
1	P	169	VAL
1	P	173	THR
1	P	176	VAL
1	P	181	VAL
1	P	187	LYS
1	P	200	ASP
1	P	210	THR
1	P	216	VAL
1	P	243	GLU
1	P	249	ASP
1	P	253	VAL
1	P	263	THR
1	P	269	MET
1	P	275	MET
1	P	290	LYS
1	P	292	LYS
1	P	298	ARG
1	P	305	VAL
1	P	308	LEU
1	P	314	VAL
1	P	316	MET
1	P	317	ASN

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Mol	Chain	Res	Type
1	P	318	GLN
1	P	319	THR
1	P	349	LEU
1	P	351	SER
1	P	352	MET
1	P	355	ARG
1	P	369	LYS
1	P	383	VAL
1	P	392	LEU
1	P	398	LYS
1	P	399	THR
1	P	433	LYS
1	P	436	SER
1	P	437	LEU
1	P	440	SER
1	P	444	VAL
1	P	445	LEU
1	P	451	MET
1	P	452	SER
1	P	463	LEU
1	P	469	LEU
1	P	470	LYS
1	P	476	GLU
1	P	478	ARG
1	P	497	GLN
1	P	505	THR
1	P	506	VAL
1	P	540	ILE
1	P	549	LEU
1	P	550	ARG
1	P	556	ARG
1	P	562	CYS
1	P	564	VAL
1	P	565	ASN
1	P	570	SER
1	P	593	LEU
1	P	611	VAL
1	P	618	LEU
1	P	621	ASP
1	P	632	LYS
1	P	640	GLN
1	P	643	LYS

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Mol	Chain	Res	Type
1	P	644	SER
1	Q	16	VAL
1	Q	30	ARG
1	Q	47	LEU
1	Q	56	GLU
1	Q	59	HIS
1	Q	78	LEU
1	Q	90	VAL
1	Q	112	TRP
1	Q	117	THR
1	Q	119	ILE
1	Q	122	ARG
1	Q	140	GLU
1	Q	153	ARG
1	Q	156	LYS
1	Q	160	GLU
1	Q	167	CYS
1	Q	168	ARG
1	Q	178	ILE
1	Q	191	ASP
1	Q	210	THR
1	Q	231	GLU
1	Q	233	ILE
1	Q	247	ILE
1	Q	259	HIS
1	Q	264	ILE
1	Q	269	MET
1	Q	273	ILE
1	Q	275	MET
1	Q	277	ARG
1	Q	290	LYS
1	Q	293	ASN
1	Q	294	ASN
1	Q	298	ARG
1	Q	305	VAL
1	Q	316	MET
1	Q	317	ASN
1	Q	318	GLN
1	Q	319	THR
1	Q	322	ILE
1	Q	325	ASN
1	Q	330	SER

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Mol	Chain	Res	Type
1	Q	334	SER
1	Q	338	LYS
1	Q	339	ASP
1	Q	340	LYS
1	Q	349	LEU
1	Q	351	SER
1	Q	355	ARG
1	Q	368	GLN
1	Q	379	LYS
1	Q	383	VAL
1	Q	392	LEU
1	Q	410	GLU
1	Q	420	ILE
1	Q	428	VAL
1	Q	437	LEU
1	Q	444	VAL
1	Q	451	MET
1	Q	469	LEU
1	Q	476	GLU
1	Q	478	ARG
1	Q	479	VAL
1	Q	480	GLU
1	Q	486	LEU
1	Q	497	GLN
1	Q	531	GLU
1	Q	533	SER
1	Q	540	ILE
1	Q	541	VAL
1	Q	546	VAL
1	Q	549	LEU
1	Q	554	ASP
1	Q	556	ARG
1	Q	563	VAL
1	Q	564	VAL
1	Q	571	SER
1	Q	588	LEU
1	Q	593	LEU
1	Q	611	VAL
1	Q	615	ILE
1	Q	618	LEU
1	Q	625	CYS
1	Q	632	LYS

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Mol	Chain	Res	Type
1	R	1	MET
1	R	5	LYS
1	R	13	ARG
1	R	19	GLU
1	R	44	ASP
1	R	45	LYS
1	R	47	LEU
1	R	51	LYS
1	R	53	THR
1	R	58	LYS
1	R	59	HIS
1	R	63	ASP
1	R	65	LYS
1	R	67	HIS
1	R	69	LEU
1	R	78	LEU
1	R	93	LEU
1	R	109	ASN
1	R	114	ASP
1	R	115	LYS
1	R	116	ILE
1	R	117	THR
1	R	124	THR
1	R	140	GLU
1	R	146	LEU
1	R	160	GLU
1	R	169	VAL
1	R	172	SER
1	R	176	VAL
1	R	178	ILE
1	R	185	LEU
1	R	191	ASP
1	R	199	LYS
1	R	206	ARG
1	R	210	THR
1	R	222	LYS
1	R	233	ILE
1	R	244	GLU
1	R	251	SER
1	R	253	VAL
1	R	269	MET
1	R	292	LYS

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Mol	Chain	Res	Type
1	R	293	ASN
1	R	294	ASN
1	R	298	ARG
1	R	305	VAL
1	R	308	LEU
1	R	315	GLU
1	R	317	ASN
1	R	331	LEU
1	R	335	ASN
1	R	349	LEU
1	R	355	ARG
1	R	364	MET
1	R	371	LYS
1	R	375	ASP
1	R	383	VAL
1	R	385	THR
1	R	392	LEU
1	R	398	LYS
1	R	401	LYS
1	R	420	ILE
1	R	433	LYS
1	R	437	LEU
1	R	451	MET
1	R	469	LEU
1	R	476	GLU
1	R	486	LEU
1	R	497	GLN
1	R	503	VAL
1	R	528	ILE
1	R	546	VAL
1	R	549	LEU
1	R	553	ILE
1	R	556	ARG
1	R	560	GLN
1	R	564	VAL
1	R	579	MET
1	R	615	ILE
1	R	616	THR
1	R	621	ASP
1	R	622	LYS
1	R	624	LEU
1	R	625	CYS

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Mol	Chain	Res	Type
1	R	638	ASN
1	R	643	LYS
1	J	5	LYS
1	J	9	LYS
1	J	16	VAL
1	J	45	LYS
1	J	47	LEU
1	J	60	GLU
1	J	62	THR
1	J	78	LEU
1	J	91	THR
1	J	107	THR
1	J	108	SER
1	J	115	LYS
1	J	132	SER
1	J	140	GLU
1	J	141	VAL
1	J	173	THR
1	J	176	VAL
1	J	181	VAL
1	J	185	LEU
1	J	191	ASP
1	J	199	LYS
1	J	210	THR
1	J	216	VAL
1	J	221	MET
1	J	222	LYS
1	J	230	SER
1	J	244	GLU
1	J	251	SER
1	J	260	SER
1	J	261	SER
1	J	263	THR
1	J	269	MET
1	J	280	THR
1	J	281	THR
1	J	288	LYS
1	J	298	ARG
1	J	308	LEU
1	J	311	LYS
1	J	319	THR
1	J	338	LYS

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Mol	Chain	Res	Type
1	J	339	ASP
1	J	351	SER
1	J	355	ARG
1	J	379	LYS
1	J	383	VAL
1	J	385	THR
1	J	398	LYS
1	J	399	THR
1	J	428	VAL
1	J	437	LEU
1	J	439	ASP
1	J	445	LEU
1	J	451	MET
1	J	461	ARG
1	J	469	LEU
1	J	476	GLU
1	J	478	ARG
1	J	485	VAL
1	J	486	LEU
1	J	492	LYS
1	J	497	GLN
1	J	509	PHE
1	J	540	ILE
1	J	541	VAL
1	J	557	VAL
1	J	558	SER
1	J	577	MET
1	J	582	GLU
1	J	593	LEU
1	J	611	VAL
1	J	616	THR
1	J	618	LEU
1	J	625	CYS
1	J	629	LEU
1	J	632	LYS
1	J	638	ASN
1	K	3	LEU
1	K	15	TRP
1	K	24	MET
1	K	31	SER
1	K	45	LYS
1	K	47	LEU

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Mol	Chain	Res	Type
1	K	60	GLU
1	K	65	LYS
1	K	66	VAL
1	K	91	THR
1	K	107	THR
1	K	112	TRP
1	K	140	GLU
1	K	141	VAL
1	K	156	LYS
1	K	160	GLU
1	K	162	LEU
1	K	169	VAL
1	K	176	VAL
1	K	181	VAL
1	K	185	LEU
1	K	191	ASP
1	K	210	THR
1	K	216	VAL
1	K	223	THR
1	K	225	GLU
1	K	227	ARG
1	K	243	GLU
1	K	244	GLU
1	K	253	VAL
1	K	257	VAL
1	K	259	HIS
1	K	263	THR
1	K	268	LEU
1	K	269	MET
1	K	273	ILE
1	K	281	THR
1	K	290	LYS
1	K	292	LYS
1	K	298	ARG
1	K	305	VAL
1	K	308	LEU
1	K	311	LYS
1	K	312	LYS
1	K	314	VAL
1	K	319	THR
1	K	321	GLU
1	K	322	ILE

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Mol	Chain	Res	Type
1	K	331	LEU
1	K	341	SER
1	K	355	ARG
1	K	363	GLU
1	K	364	MET
1	K	366	GLU
1	K	383	VAL
1	K	385	THR
1	K	392	LEU
1	K	399	THR
1	K	401	LYS
1	K	424	LYS
1	K	428	VAL
1	K	437	LEU
1	K	444	VAL
1	K	445	LEU
1	K	451	MET
1	K	469	LEU
1	K	471	MET
1	K	475	ASP
1	K	479	VAL
1	K	486	LEU
1	K	497	GLN
1	K	503	VAL
1	K	506	VAL
1	K	532	GLN
1	K	544	ASP
1	K	546	VAL
1	K	556	ARG
1	K	558	SER
1	K	562	CYS
1	K	564	VAL
1	K	567	ASP
1	K	577	MET
1	K	579	MET
1	K	589	SER
1	K	593	LEU
1	K	596	SER
1	K	597	SER
1	K	621	ASP
1	K	624	LEU
1	K	632	LYS

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Mol	Chain	Res	Type
1	K	643	LYS
1	L	47	LEU
1	L	60	GLU
1	L	62	THR
1	L	78	LEU
1	L	85	GLU
1	L	91	THR
1	L	107	THR
1	L	113	SER
1	L	114	ASP
1	L	117	THR
1	L	124	THR
1	L	128	GLN
1	L	129	ILE
1	L	140	GLU
1	L	141	VAL
1	L	162	LEU
1	L	168	ARG
1	L	169	VAL
1	L	173	THR
1	L	181	VAL
1	L	185	LEU
1	L	193	PRO
1	L	210	THR
1	L	216	VAL
1	L	221	MET
1	L	223	THR
1	L	225	GLU
1	L	228	GLU
1	L	260	SER
1	L	263	THR
1	L	269	MET
1	L	281	THR
1	L	290	LYS
1	L	298	ARG
1	L	305	VAL
1	L	308	LEU
1	L	316	MET
1	L	317	ASN
1	L	319	THR
1	L	331	LEU
1	L	349	LEU

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Mol	Chain	Res	Type
1	L	355	ARG
1	L	369	LYS
1	L	385	THR
1	L	392	LEU
1	L	399	THR
1	L	428	VAL
1	L	433	LYS
1	L	437	LEU
1	L	440	SER
1	L	444	VAL
1	L	445	LEU
1	L	451	MET
1	L	452	SER
1	L	463	LEU
1	L	469	LEU
1	L	476	GLU
1	L	479	VAL
1	L	485	VAL
1	L	486	LEU
1	L	497	GLN
1	L	503	VAL
1	L	541	VAL
1	L	549	LEU
1	L	556	ARG
1	L	557	VAL
1	L	562	CYS
1	L	564	VAL
1	L	593	LEU
1	L	611	VAL
1	L	616	THR
1	L	618	LEU
1	L	624	LEU
1	L	633	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (309) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	ASN
1	A	67	HIS
1	A	109	ASN
1	A	175	ASN
1	A	242	HIS

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Mol	Chain	Res	Type
1	A	259	HIS
1	A	294	ASN
1	A	303	GLN
1	A	335	ASN
1	A	362	ASN
1	A	459	HIS
1	A	482	HIS
1	A	497	GLN
1	A	498	ASN
1	A	507	ASN
1	A	587	ASN
1	D	43	ASN
1	D	67	HIS
1	D	175	ASN
1	D	190	ASN
1	D	242	HIS
1	D	259	HIS
1	D	293	ASN
1	D	303	GLN
1	D	335	ASN
1	D	362	ASN
1	D	459	HIS
1	D	482	HIS
1	D	497	GLN
1	D	507	ASN
1	D	560	GLN
1	D	565	ASN
1	B	175	ASN
1	B	190	ASN
1	B	242	HIS
1	B	259	HIS
1	B	291	ASN
1	B	294	ASN
1	B	303	GLN
1	B	335	ASN
1	B	362	ASN
1	B	455	ASN
1	B	459	HIS
1	B	482	HIS
1	B	497	GLN
1	B	498	ASN
1	B	507	ASN

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Mol	Chain	Res	Type
1	B	560	GLN
1	C	43	ASN
1	C	59	HIS
1	C	61	ASN
1	C	67	HIS
1	C	109	ASN
1	C	190	ASN
1	C	242	HIS
1	C	259	HIS
1	C	294	ASN
1	C	303	GLN
1	C	335	ASN
1	C	362	ASN
1	C	459	HIS
1	C	482	HIS
1	C	497	GLN
1	C	498	ASN
1	C	507	ASN
1	C	560	GLN
1	C	568	ASN
1	F	43	ASN
1	F	61	ASN
1	F	242	HIS
1	F	259	HIS
1	F	278	ASN
1	F	303	GLN
1	F	362	ASN
1	F	368	GLN
1	F	455	ASN
1	F	459	HIS
1	F	482	HIS
1	F	497	GLN
1	F	507	ASN
1	F	565	ASN
1	F	587	ASN
1	F	620	ASN
1	E	43	ASN
1	E	67	HIS
1	E	109	ASN
1	E	175	ASN
1	E	259	HIS
1	E	278	ASN

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Mol	Chain	Res	Type
1	E	303	GLN
1	E	317	ASN
1	E	335	ASN
1	E	362	ASN
1	E	459	HIS
1	E	482	HIS
1	E	497	GLN
1	E	507	ASN
1	E	560	GLN
1	E	587	ASN
1	E	638	ASN
1	G	43	ASN
1	G	67	HIS
1	G	109	ASN
1	G	190	ASN
1	G	259	HIS
1	G	293	ASN
1	G	294	ASN
1	G	300	HIS
1	G	303	GLN
1	G	335	ASN
1	G	362	ASN
1	G	459	HIS
1	G	482	HIS
1	G	497	GLN
1	G	560	GLN
1	G	587	ASN
1	H	26	GLN
1	H	43	ASN
1	H	67	HIS
1	H	109	ASN
1	H	175	ASN
1	H	190	ASN
1	H	224	HIS
1	H	294	ASN
1	H	303	GLN
1	H	335	ASN
1	H	362	ASN
1	H	459	HIS
1	H	482	HIS
1	H	497	GLN
1	H	507	ASN

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Mol	Chain	Res	Type
1	I	26	GLN
1	I	43	ASN
1	I	67	HIS
1	I	190	ASN
1	I	242	HIS
1	I	259	HIS
1	I	278	ASN
1	I	294	ASN
1	I	300	HIS
1	I	303	GLN
1	I	335	ASN
1	I	362	ASN
1	I	459	HIS
1	I	482	HIS
1	I	497	GLN
1	I	498	ASN
1	I	507	ASN
1	I	560	GLN
1	I	568	ASN
1	I	587	ASN
1	I	640	GLN
1	M	43	ASN
1	M	67	HIS
1	M	109	ASN
1	M	175	ASN
1	M	190	ASN
1	M	259	HIS
1	M	278	ASN
1	M	303	GLN
1	M	335	ASN
1	M	362	ASN
1	M	459	HIS
1	M	482	HIS
1	M	497	GLN
1	M	507	ASN
1	M	560	GLN
1	M	568	ASN
1	N	26	GLN
1	N	43	ASN
1	N	175	ASN
1	N	190	ASN
1	N	259	HIS

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Mol	Chain	Res	Type
1	N	291	ASN
1	N	293	ASN
1	N	294	ASN
1	N	303	GLN
1	N	335	ASN
1	N	362	ASN
1	N	459	HIS
1	N	482	HIS
1	N	497	GLN
1	N	498	ASN
1	N	507	ASN
1	N	560	GLN
1	N	565	ASN
1	O	43	ASN
1	O	67	HIS
1	O	109	ASN
1	O	175	ASN
1	O	190	ASN
1	O	303	GLN
1	O	335	ASN
1	O	362	ASN
1	O	459	HIS
1	O	497	GLN
1	O	498	ASN
1	O	507	ASN
1	O	560	GLN
1	O	565	ASN
1	O	587	ASN
1	O	620	ASN
1	O	638	ASN
1	O	640	GLN
1	P	43	ASN
1	P	67	HIS
1	P	175	ASN
1	P	190	ASN
1	P	259	HIS
1	P	294	ASN
1	P	303	GLN
1	P	317	ASN
1	P	362	ASN
1	P	459	HIS
1	P	482	HIS

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Mol	Chain	Res	Type
1	P	497	GLN
1	P	498	ASN
1	P	507	ASN
1	P	560	GLN
1	P	565	ASN
1	P	587	ASN
1	P	640	GLN
1	Q	43	ASN
1	Q	67	HIS
1	Q	175	ASN
1	Q	190	ASN
1	Q	196	ASN
1	Q	224	HIS
1	Q	242	HIS
1	Q	259	HIS
1	Q	291	ASN
1	Q	293	ASN
1	Q	300	HIS
1	Q	303	GLN
1	Q	335	ASN
1	Q	362	ASN
1	Q	455	ASN
1	Q	459	HIS
1	Q	482	HIS
1	Q	497	GLN
1	Q	498	ASN
1	Q	532	GLN
1	Q	560	GLN
1	Q	568	ASN
1	R	43	ASN
1	R	61	ASN
1	R	109	ASN
1	R	175	ASN
1	R	190	ASN
1	R	224	HIS
1	R	242	HIS
1	R	259	HIS
1	R	293	ASN
1	R	294	ASN
1	R	300	HIS
1	R	303	GLN
1	R	362	ASN

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Mol	Chain	Res	Type
1	R	459	HIS
1	R	482	HIS
1	R	497	GLN
1	R	498	ASN
1	R	560	GLN
1	R	638	ASN
1	J	43	ASN
1	J	67	HIS
1	J	175	ASN
1	J	190	ASN
1	J	242	HIS
1	J	300	HIS
1	J	303	GLN
1	J	362	ASN
1	J	459	HIS
1	J	482	HIS
1	J	497	GLN
1	J	498	ASN
1	J	627	HIS
1	K	43	ASN
1	K	67	HIS
1	K	190	ASN
1	K	259	HIS
1	K	294	ASN
1	K	303	GLN
1	K	335	ASN
1	K	362	ASN
1	K	459	HIS
1	K	482	HIS
1	K	497	GLN
1	K	498	ASN
1	K	532	GLN
1	K	560	GLN
1	K	587	ASN
1	L	26	GLN
1	L	43	ASN
1	L	61	ASN
1	L	67	HIS
1	L	175	ASN
1	L	190	ASN
1	L	242	HIS
1	L	259	HIS

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Mol	Chain	Res	Type
1	L	294	ASN
1	L	303	GLN
1	L	317	ASN
1	L	335	ASN
1	L	362	ASN
1	L	459	HIS
1	L	482	HIS
1	L	497	GLN
1	L	507	ASN
1	L	560	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

36 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	$\#\|Z\| > 2$
3	PO4	B	702	-	4,4,4	0.82	0	6,6,6	1.08	0
2	SAH	C	701	-	24,28,28	1.20	2 (8%)	25,40,40	1.39	6 (24%)
2	SAH	P	701	-	24,28,28	1.21	3 (12%)	25,40,40	1.58	6 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	SAH	G	701	-	24,28,28	1.27	4 (16%)	25,40,40	1.58	6 (24%)
3	PO4	I	702	-	4,4,4	1.13	0	6,6,6	1.46	2 (33%)
3	PO4	P	702	-	4,4,4	0.87	0	6,6,6	0.98	0
3	PO4	R	702	-	4,4,4	0.68	0	6,6,6	0.78	0
2	SAH	H	701	-	24,28,28	1.41	4 (16%)	25,40,40	1.56	4 (16%)
3	PO4	H	702	-	4,4,4	0.69	0	6,6,6	1.47	1 (16%)
2	SAH	M	701	-	24,28,28	1.52	5 (20%)	25,40,40	1.72	6 (24%)
3	PO4	Q	702	-	4,4,4	0.96	0	6,6,6	0.55	0
3	PO4	N	702	-	4,4,4	0.96	0	6,6,6	0.71	0
3	PO4	E	702	-	4,4,4	0.66	0	6,6,6	0.91	0
2	SAH	I	701	-	24,28,28	1.19	3 (12%)	25,40,40	2.17	10 (40%)
2	SAH	D	701	-	24,28,28	1.23	4 (16%)	25,40,40	1.78	7 (28%)
3	PO4	A	702	-	4,4,4	0.67	0	6,6,6	1.31	1 (16%)
3	PO4	C	702	-	4,4,4	0.74	0	6,6,6	1.15	1 (16%)
2	SAH	J	701	-	24,28,28	0.97	2 (8%)	25,40,40	1.53	5 (20%)
2	SAH	L	701	-	24,28,28	1.35	3 (12%)	25,40,40	1.84	9 (36%)
3	PO4	G	702	-	4,4,4	1.05	0	6,6,6	0.97	0
2	SAH	O	701	-	24,28,28	1.15	3 (12%)	25,40,40	1.55	5 (20%)
2	SAH	F	701	-	24,28,28	1.13	3 (12%)	25,40,40	1.58	5 (20%)
2	SAH	K	701	-	24,28,28	1.23	2 (8%)	25,40,40	1.61	6 (24%)
3	PO4	K	702	-	4,4,4	0.93	0	6,6,6	0.60	0
2	SAH	R	701	-	24,28,28	1.05	2 (8%)	25,40,40	1.64	6 (24%)
2	SAH	N	701	-	24,28,28	1.26	4 (16%)	25,40,40	1.72	7 (28%)
2	SAH	Q	701	-	24,28,28	1.03	1 (4%)	25,40,40	1.52	5 (20%)
3	PO4	D	702	-	4,4,4	1.04	0	6,6,6	1.69	2 (33%)
3	PO4	J	702	-	4,4,4	1.02	0	6,6,6	0.76	0
2	SAH	E	701	-	24,28,28	1.13	1 (4%)	25,40,40	1.66	7 (28%)
3	PO4	O	702	-	4,4,4	0.81	0	6,6,6	0.39	0
3	PO4	F	702	-	4,4,4	0.99	0	6,6,6	1.39	1 (16%)
3	PO4	L	702	-	4,4,4	1.07	0	6,6,6	0.89	0
2	SAH	A	701	-	24,28,28	1.25	3 (12%)	25,40,40	1.64	7 (28%)
2	SAH	B	701	-	24,28,28	1.02	1 (4%)	25,40,40	1.56	6 (24%)
3	PO4	M	702	-	4,4,4	0.76	0	6,6,6	0.80	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SAH	H	701	-	-	3/11/31/31	0/3/3/3
2	SAH	C	701	-	-	1/11/31/31	0/3/3/3
2	SAH	I	701	-	-	1/11/31/31	0/3/3/3
2	SAH	G	701	-	-	2/11/31/31	0/3/3/3
2	SAH	P	701	-	-	2/11/31/31	0/3/3/3
2	SAH	R	701	-	-	2/11/31/31	0/3/3/3
2	SAH	N	701	-	-	5/11/31/31	0/3/3/3
2	SAH	J	701	-	-	1/11/31/31	0/3/3/3
2	SAH	K	701	-	-	0/11/31/31	0/3/3/3
2	SAH	L	701	-	-	2/11/31/31	0/3/3/3
2	SAH	M	701	-	-	4/11/31/31	0/3/3/3
2	SAH	Q	701	-	-	2/11/31/31	0/3/3/3
2	SAH	E	701	-	-	0/11/31/31	0/3/3/3
2	SAH	D	701	-	-	0/11/31/31	0/3/3/3
2	SAH	O	701	-	-	0/11/31/31	0/3/3/3
2	SAH	A	701	-	-	0/11/31/31	0/3/3/3
2	SAH	B	701	-	-	1/11/31/31	0/3/3/3
2	SAH	F	701	-	-	2/11/31/31	0/3/3/3

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	701	SAH	C2-N3	3.85	1.38	1.32
2	L	701	SAH	O4'-C1'	3.83	1.46	1.41
2	C	701	SAH	O4'-C1'	3.74	1.46	1.41
2	K	701	SAH	C2'-C1'	-3.40	1.48	1.53
2	M	701	SAH	C4-N3	3.17	1.40	1.35
2	N	701	SAH	O4'-C1'	3.13	1.45	1.41
2	M	701	SAH	O4'-C1'	3.11	1.45	1.41
2	M	701	SAH	C5-C4	2.95	1.48	1.40
2	P	701	SAH	C5-C4	2.86	1.48	1.40
2	M	701	SAH	C2-N3	2.77	1.36	1.32
2	I	701	SAH	C2'-C1'	-2.77	1.49	1.53
2	G	701	SAH	C5-C4	2.72	1.48	1.40
2	L	701	SAH	C5-C4	2.66	1.48	1.40
2	A	701	SAH	C5-C4	2.65	1.47	1.40
2	N	701	SAH	C4-N3	2.62	1.39	1.35
2	K	701	SAH	O4'-C1'	2.58	1.44	1.41
2	R	701	SAH	C5-C4	2.55	1.47	1.40
2	O	701	SAH	O4'-C1'	2.51	1.44	1.41
2	H	701	SAH	C2'-C1'	-2.48	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	701	SAH	C5-C4	2.44	1.47	1.40
2	F	701	SAH	C2-N3	2.42	1.36	1.32
2	F	701	SAH	OXT-C	-2.41	1.22	1.30
2	A	701	SAH	C2'-C1'	-2.39	1.50	1.53
2	E	701	SAH	C5-C4	2.38	1.47	1.40
2	D	701	SAH	C2-N3	2.34	1.35	1.32
2	H	701	SAH	C5-C4	2.34	1.47	1.40
2	G	701	SAH	C2'-C1'	-2.31	1.50	1.53
2	B	701	SAH	C5-C4	2.29	1.47	1.40
2	L	701	SAH	C2'-C1'	-2.27	1.50	1.53
2	J	701	SAH	C5-C4	2.27	1.46	1.40
2	N	701	SAH	C5-C4	2.25	1.46	1.40
2	O	701	SAH	C5-C4	2.20	1.46	1.40
2	I	701	SAH	C5-C4	2.17	1.46	1.40
2	Q	701	SAH	C5-C4	2.15	1.46	1.40
2	G	701	SAH	OXT-C	-2.15	1.23	1.30
2	I	701	SAH	O4'-C4'	-2.15	1.40	1.45
2	D	701	SAH	C2'-C1'	-2.14	1.50	1.53
2	D	701	SAH	OXT-C	-2.10	1.23	1.30
2	R	701	SAH	OXT-C	-2.07	1.23	1.30
2	F	701	SAH	O4'-C1'	2.07	1.44	1.41
2	C	701	SAH	OXT-C	-2.06	1.23	1.30
2	P	701	SAH	C2-N3	2.05	1.35	1.32
2	H	701	SAH	O4'-C4'	-2.04	1.40	1.45
2	N	701	SAH	OXT-C	-2.04	1.23	1.30
2	M	701	SAH	C2-N1	2.03	1.37	1.33
2	O	701	SAH	C2-N3	2.03	1.35	1.32
2	G	701	SAH	O4'-C1'	2.01	1.43	1.41
2	A	701	SAH	C2-N3	2.01	1.35	1.32
2	J	701	SAH	O4'-C1'	2.00	1.43	1.41
2	P	701	SAH	OXT-C	-2.00	1.24	1.30

All (121) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	N	701	SAH	N3-C2-N1	-4.37	121.85	128.68
2	I	701	SAH	N3-C2-N1	-4.34	121.90	128.68
2	I	701	SAH	C1'-N9-C4	-4.22	119.23	126.64
2	L	701	SAH	N3-C2-N1	-4.04	122.36	128.68
2	O	701	SAH	N3-C2-N1	-4.00	122.42	128.68
2	M	701	SAH	N3-C2-N1	-3.86	122.64	128.68
2	Q	701	SAH	N3-C2-N1	-3.79	122.75	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	701	SAH	OXT-C-O	-3.79	115.48	124.09
2	M	701	SAH	N6-C6-N1	3.72	126.30	118.57
2	H	701	SAH	N3-C2-N1	-3.71	122.88	128.68
2	R	701	SAH	N3-C2-N1	-3.71	122.88	128.68
2	F	701	SAH	N3-C2-N1	-3.69	122.92	128.68
2	E	701	SAH	N3-C2-N1	-3.64	123.00	128.68
2	P	701	SAH	N3-C2-N1	-3.59	123.06	128.68
2	R	701	SAH	OXT-C-O	-3.59	115.94	124.09
2	I	701	SAH	OXT-C-CA	3.53	125.41	113.38
2	K	701	SAH	N3-C2-N1	-3.49	123.22	128.68
2	G	701	SAH	N3-C2-N1	-3.48	123.24	128.68
2	D	701	SAH	O4'-C1'-C2'	-3.42	101.93	106.93
2	B	701	SAH	N3-C2-N1	-3.40	123.36	128.68
2	C	701	SAH	N3-C2-N1	-3.38	123.39	128.68
2	P	701	SAH	C1'-N9-C4	-3.35	120.75	126.64
2	I	701	SAH	OXT-C-O	-3.33	116.53	124.09
2	A	701	SAH	N3-C2-N1	-3.27	123.57	128.68
2	K	701	SAH	C1'-N9-C4	-3.25	120.92	126.64
2	A	701	SAH	O3'-C3'-C4'	-3.14	101.96	111.05
2	G	701	SAH	C4-C5-N7	-3.09	106.18	109.40
2	E	701	SAH	C3'-C2'-C1'	3.06	105.59	100.98
2	L	701	SAH	C4-C5-N7	-2.99	106.28	109.40
2	I	701	SAH	CB-CG-SD	-2.97	106.64	113.31
2	L	701	SAH	O2'-C2'-C1'	-2.96	99.93	110.85
2	I	701	SAH	C2'-C3'-C4'	2.95	108.38	102.64
2	O	701	SAH	C2'-C3'-C4'	2.94	108.36	102.64
2	I	701	SAH	C4-C5-N7	-2.94	106.34	109.40
2	D	701	SAH	CB-CG-SD	-2.94	106.72	113.31
3	H	702	PO4	O4-P-O2	2.93	117.39	107.97
2	J	701	SAH	N3-C2-N1	-2.91	124.13	128.68
2	D	701	SAH	O3'-C3'-C4'	-2.87	102.76	111.05
2	H	701	SAH	O4'-C1'-C2'	-2.86	102.75	106.93
2	G	701	SAH	CB-CG-SD	-2.82	106.99	113.31
2	D	701	SAH	OXT-C-CA	2.77	122.83	113.38
2	E	701	SAH	C4'-C5'-SD	-2.73	103.99	113.78
2	N	701	SAH	CB-CA-N	2.69	117.21	110.17
2	A	701	SAH	OXT-C-CA	2.68	122.52	113.38
2	N	701	SAH	C2-N1-C6	2.67	123.33	118.75
2	I	701	SAH	O3'-C3'-C4'	-2.67	103.33	111.05
2	D	701	SAH	N3-C2-N1	-2.65	124.54	128.68
2	L	701	SAH	C1'-N9-C4	-2.64	122.01	126.64
2	L	701	SAH	CB-CG-SD	-2.62	107.42	113.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	701	SAH	O3'-C3'-C4'	-2.62	103.47	111.05
2	B	701	SAH	O3'-C3'-C2'	-2.61	103.38	111.82
3	D	702	PO4	O4-P-O3	2.60	116.31	107.97
2	J	701	SAH	C1'-N9-C4	-2.59	122.08	126.64
2	L	701	SAH	OXT-C-CA	2.58	122.17	113.38
2	L	701	SAH	O3'-C3'-C4'	-2.58	103.60	111.05
2	F	701	SAH	C2'-C3'-C4'	2.57	107.63	102.64
2	E	701	SAH	O3'-C3'-C4'	-2.56	103.65	111.05
2	F	701	SAH	C1'-N9-C4	-2.55	122.16	126.64
2	B	701	SAH	C2'-C3'-C4'	2.54	107.58	102.64
2	N	701	SAH	N6-C6-N1	2.54	123.84	118.57
2	H	701	SAH	CB-CG-SD	-2.52	107.66	113.31
2	C	701	SAH	C4-C5-N7	-2.51	106.79	109.40
2	B	701	SAH	OXT-C-O	-2.49	118.44	124.09
2	N	701	SAH	C1'-N9-C4	-2.48	122.29	126.64
3	A	702	PO4	O4-P-O3	2.48	115.91	107.97
2	C	701	SAH	O3'-C3'-C4'	-2.47	103.91	111.05
2	I	701	SAH	C2-N1-C6	2.46	122.97	118.75
2	F	701	SAH	CB-CA-N	2.45	116.60	110.17
2	M	701	SAH	O4'-C1'-C2'	-2.45	103.34	106.93
2	R	701	SAH	C2-N1-C6	2.45	122.95	118.75
3	D	702	PO4	O3-P-O1	-2.44	101.97	110.89
2	G	701	SAH	C2-N1-C6	2.43	122.92	118.75
2	A	701	SAH	C1'-N9-C4	-2.43	122.36	126.64
2	B	701	SAH	OXT-C-CA	2.43	121.66	113.38
2	P	701	SAH	C2'-C3'-C4'	2.42	107.34	102.64
2	H	701	SAH	C4-C5-N7	-2.42	106.88	109.40
2	J	701	SAH	C2'-C3'-C4'	2.40	107.31	102.64
2	M	701	SAH	C3'-C2'-C1'	2.40	104.59	100.98
2	P	701	SAH	C4-C5-N7	-2.39	106.90	109.40
2	M	701	SAH	C2-N1-C6	2.39	122.85	118.75
2	L	701	SAH	O4'-C1'-C2'	-2.39	103.44	106.93
2	A	701	SAH	OXT-C-O	-2.38	118.68	124.09
2	B	701	SAH	C4-C5-N7	-2.38	106.92	109.40
2	K	701	SAH	OXT-C-CA	2.36	121.41	113.38
2	M	701	SAH	C5-C6-N6	-2.36	116.77	120.35
2	G	701	SAH	OXT-C-O	-2.35	118.75	124.09
2	R	701	SAH	OXT-C-CA	2.34	121.37	113.38
2	E	701	SAH	C1'-N9-C4	-2.34	122.52	126.64
2	E	701	SAH	C4-C5-N7	-2.34	106.96	109.40
2	A	701	SAH	C2'-C3'-C4'	2.33	107.18	102.64
2	K	701	SAH	N6-C6-N1	2.31	123.37	118.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	701	SAH	O4'-C1'-C2'	-2.29	103.58	106.93
2	I	701	SAH	C5'-SD-CG	-2.27	95.46	102.27
2	R	701	SAH	CB-CG-SD	-2.26	108.24	113.31
2	K	701	SAH	C2-N1-C6	2.25	122.60	118.75
2	P	701	SAH	O3'-C3'-C4'	-2.24	104.57	111.05
2	Q	701	SAH	N6-C6-N1	2.23	123.20	118.57
2	N	701	SAH	OXT-C-O	-2.21	119.07	124.09
2	K	701	SAH	C2'-C3'-C4'	2.21	106.93	102.64
2	P	701	SAH	C2-N1-C6	2.19	122.51	118.75
3	I	702	PO4	O4-P-O1	2.19	118.92	110.89
2	J	701	SAH	C4-C5-N7	-2.18	107.12	109.40
2	O	701	SAH	N6-C6-N1	2.18	123.11	118.57
2	O	701	SAH	CB-CG-SD	-2.17	108.44	113.31
2	E	701	SAH	OXT-C-O	-2.17	119.17	124.09
2	Q	701	SAH	C3'-C2'-C1'	2.16	104.24	100.98
2	A	701	SAH	C2-N1-C6	2.16	122.44	118.75
3	F	702	PO4	O4-P-O2	2.14	114.83	107.97
2	Q	701	SAH	CB-CG-SD	-2.13	108.53	113.31
2	N	701	SAH	CB-CG-SD	-2.13	108.54	113.31
2	G	701	SAH	OXT-C-CA	2.13	120.62	113.38
3	I	702	PO4	O2-P-O1	-2.07	103.32	110.89
2	O	701	SAH	C1'-N9-C4	-2.07	123.01	126.64
2	D	701	SAH	C4-C5-N7	-2.06	107.25	109.40
2	C	701	SAH	C2'-C3'-C4'	2.05	106.63	102.64
2	L	701	SAH	C2-N1-C6	2.05	122.26	118.75
2	F	701	SAH	C4-C5-N7	-2.04	107.28	109.40
2	R	701	SAH	C4-C5-N7	-2.03	107.28	109.40
2	C	701	SAH	OXT-C-O	-2.01	119.53	124.09
2	Q	701	SAH	CB-CA-N	2.01	115.44	110.17
3	C	702	PO4	O4-P-O2	2.01	114.41	107.97

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	701	SAH	O4'-C4'-C5'-SD
2	G	701	SAH	O4'-C4'-C5'-SD
2	G	701	SAH	C3'-C4'-C5'-SD
2	N	701	SAH	O-C-CA-N
2	N	701	SAH	O4'-C4'-C5'-SD
2	N	701	SAH	C3'-C4'-C5'-SD
2	P	701	SAH	O4'-C4'-C5'-SD

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Mol	Chain	Res	Type	Atoms
2	P	701	SAH	C3'-C4'-C5'-SD
2	Q	701	SAH	O4'-C4'-C5'-SD
2	Q	701	SAH	C3'-C4'-C5'-SD
2	R	701	SAH	O4'-C4'-C5'-SD
2	R	701	SAH	C3'-C4'-C5'-SD
2	H	701	SAH	C-CA-CB-CG
2	M	701	SAH	C-CA-CB-CG
2	N	701	SAH	OXT-C-CA-N
2	H	701	SAH	N-CA-CB-CG
2	F	701	SAH	C3'-C4'-C5'-SD
2	L	701	SAH	C3'-C4'-C5'-SD
2	M	701	SAH	O4'-C4'-C5'-SD
2	L	701	SAH	O4'-C4'-C5'-SD
2	H	701	SAH	CB-CG-SD-C5'
2	I	701	SAH	C-CA-CB-CG
2	J	701	SAH	CB-CG-SD-C5'
2	M	701	SAH	N-CA-CB-CG
2	B	701	SAH	C3'-C4'-C5'-SD
2	C	701	SAH	C3'-C4'-C5'-SD
2	M	701	SAH	C3'-C4'-C5'-SD
2	N	701	SAH	CB-CG-SD-C5'

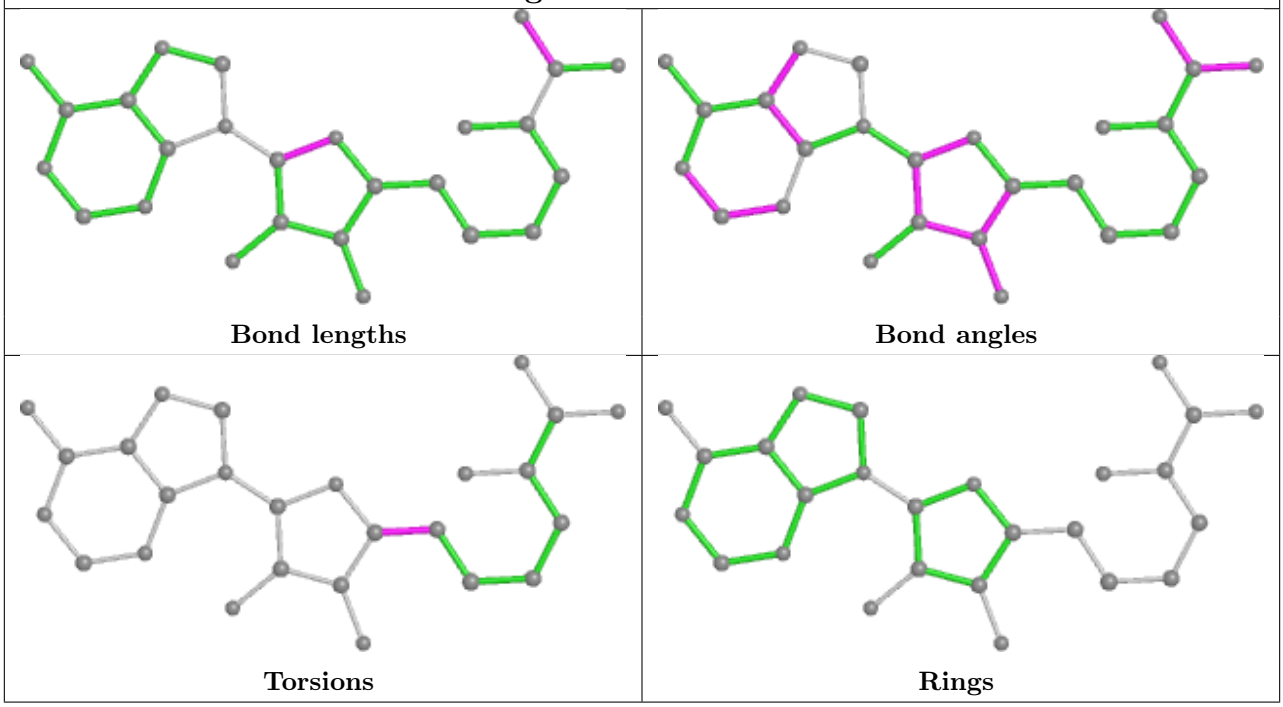
There are no ring outliers.

15 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	701	SAH	1	0
2	P	701	SAH	3	0
2	G	701	SAH	2	0
3	I	702	PO4	1	0
2	H	701	SAH	1	0
2	M	701	SAH	2	0
3	Q	702	PO4	1	0
2	I	701	SAH	1	0
2	F	701	SAH	2	0
2	K	701	SAH	3	0
2	R	701	SAH	1	0
2	N	701	SAH	1	0
2	Q	701	SAH	1	0
2	E	701	SAH	3	0
2	B	701	SAH	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand SAH C 701



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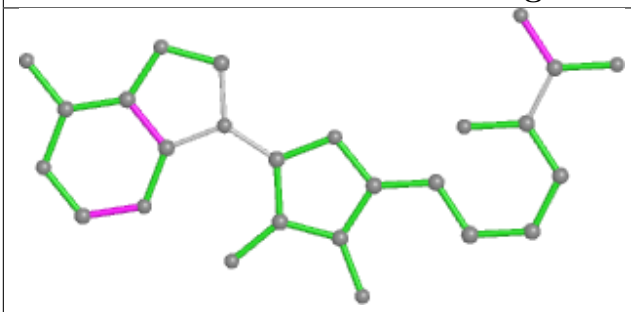
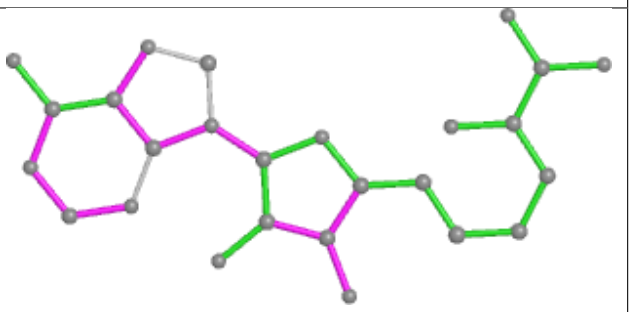
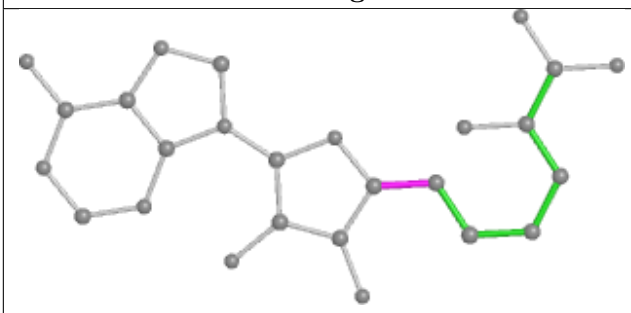
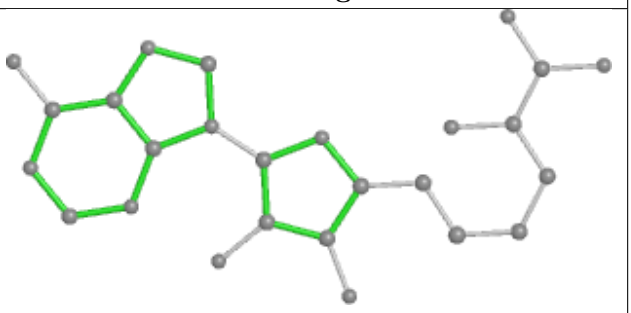
 Bond lengths	 Bond angles
 Torsions	 Rings

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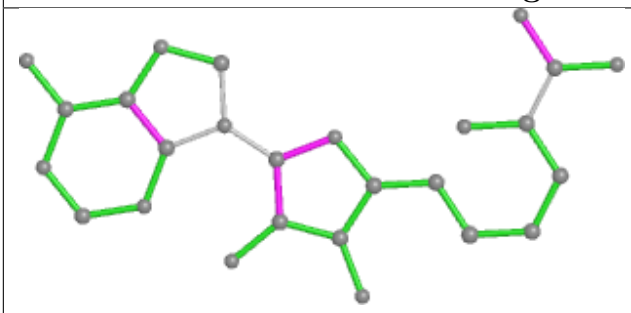
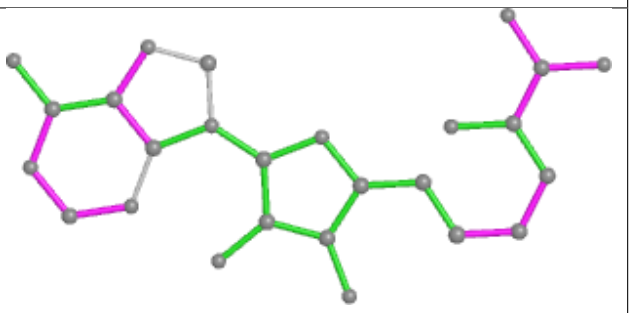
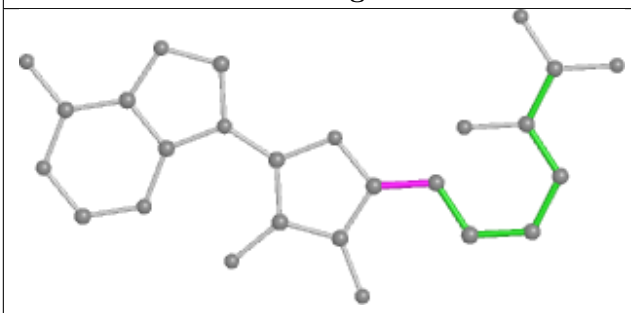
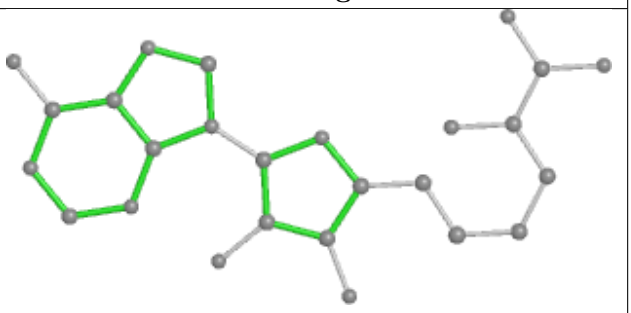
 Bond lengths	 Bond angles
 Torsions	 Rings

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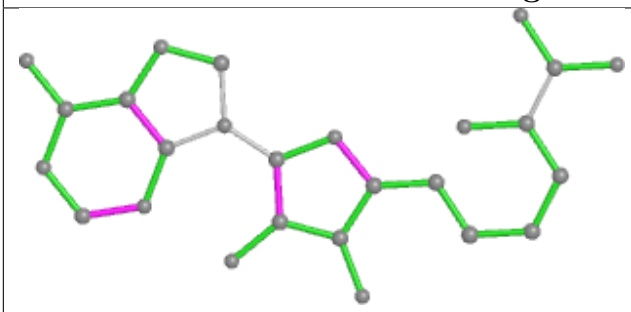
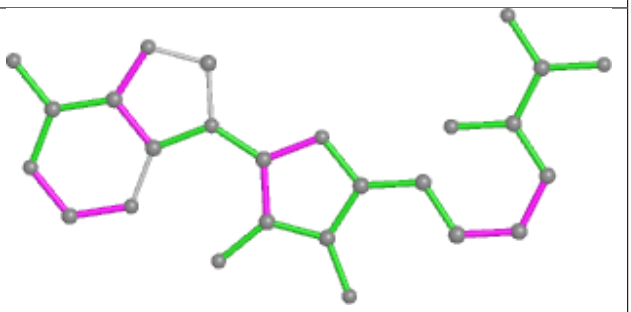
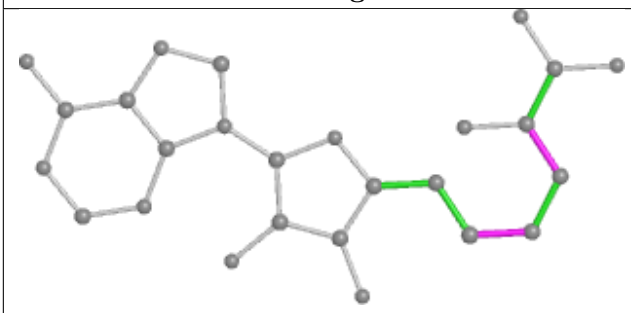
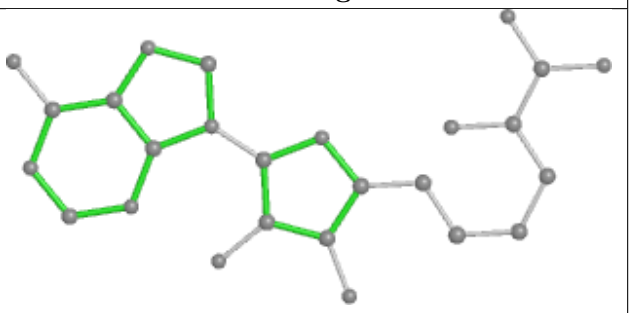
 Bond lengths	 Bond angles
 Torsions	 Rings

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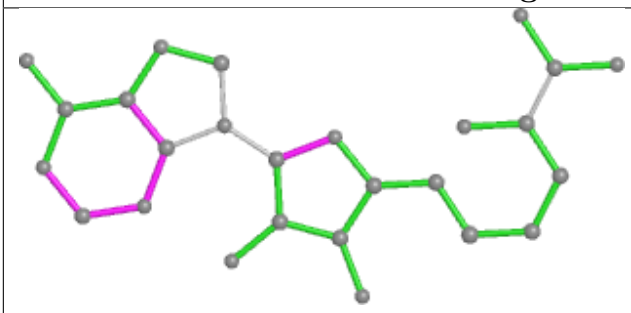
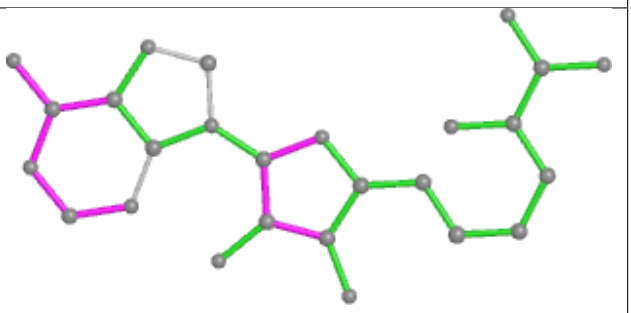
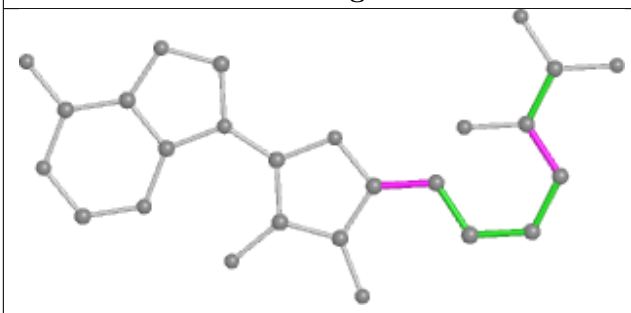
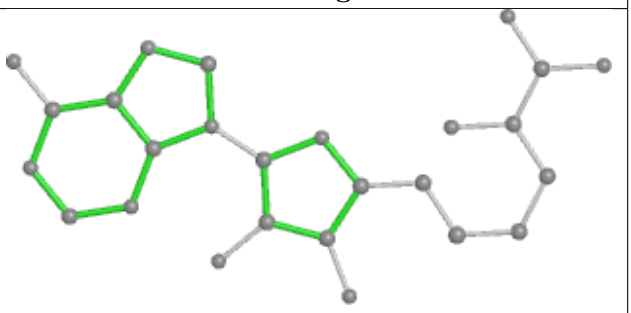
 Bond lengths	 Bond angles
 Torsions	 Rings

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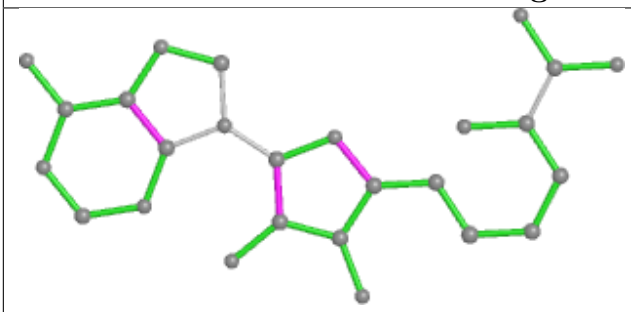
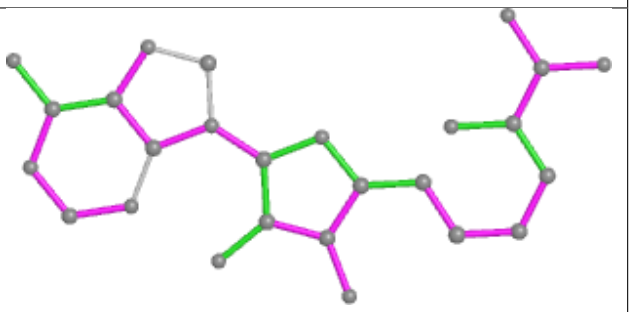
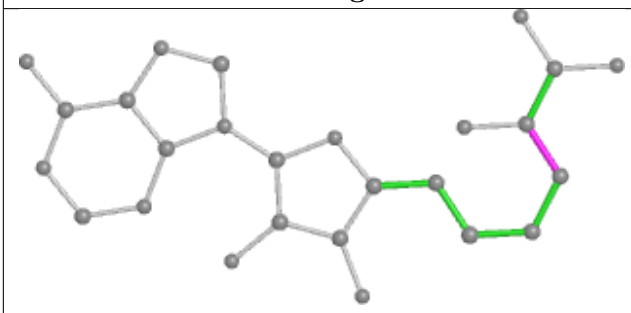
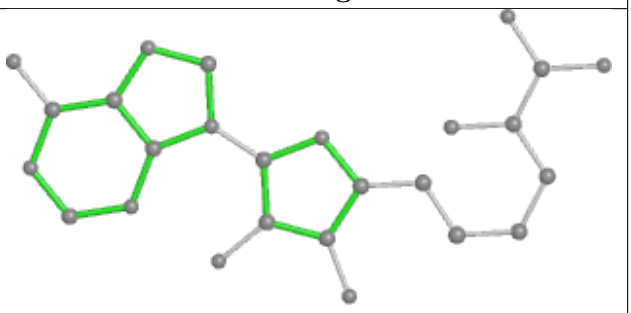
 Bond lengths	 Bond angles
 Torsions	 Rings

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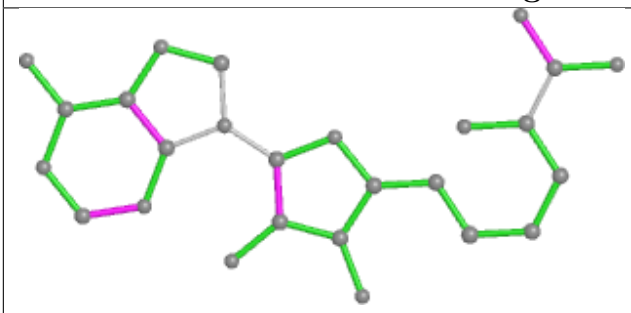
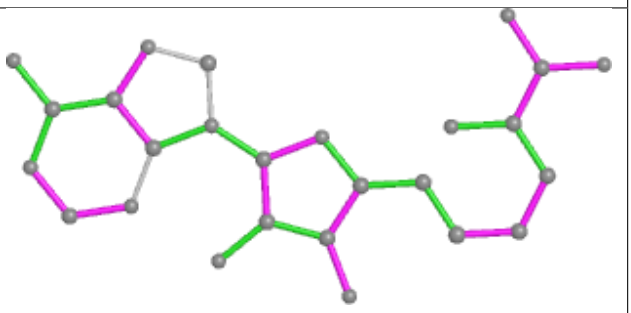
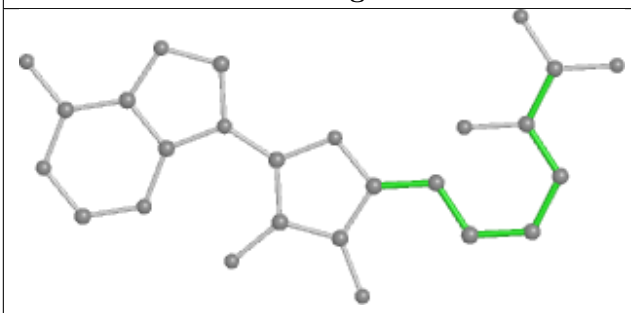
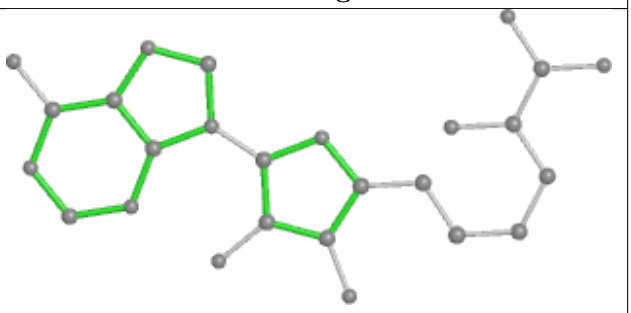
 Bond lengths	 Bond angles
 Torsions	 Rings

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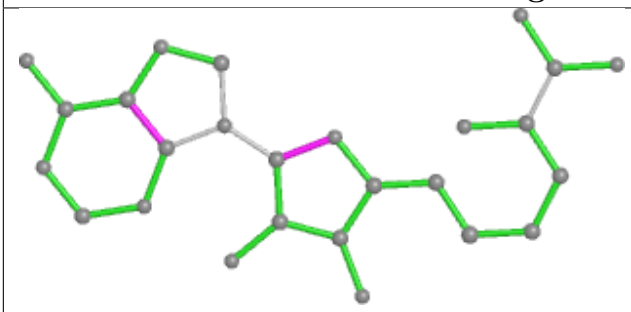
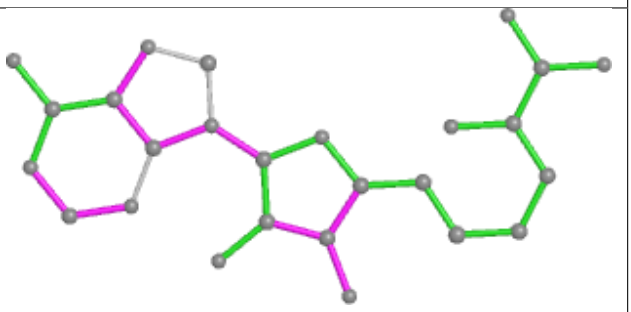
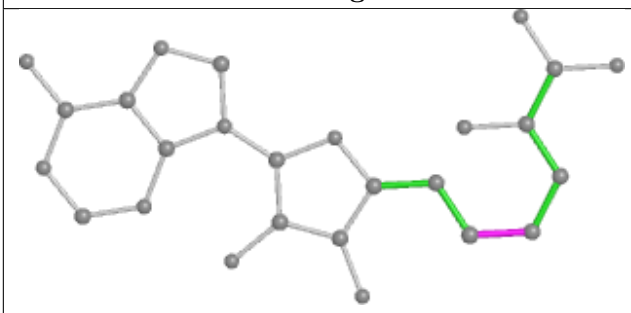
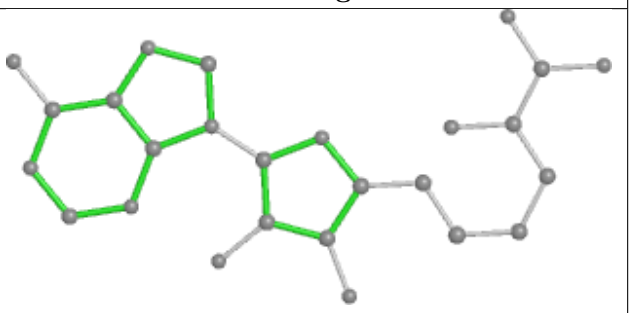
 Bond lengths	 Bond angles
 Torsions	 Rings

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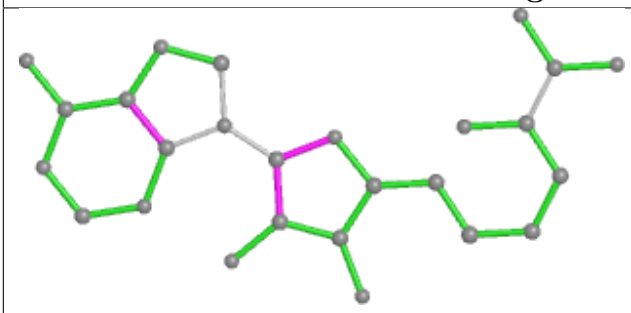
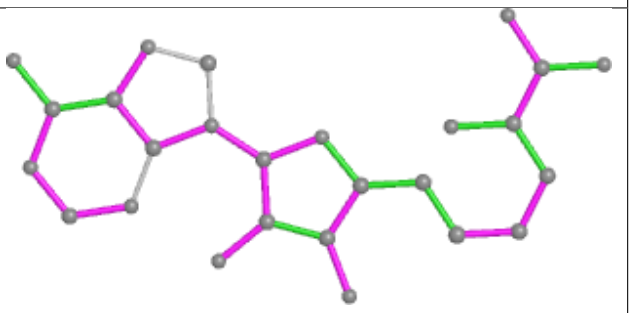
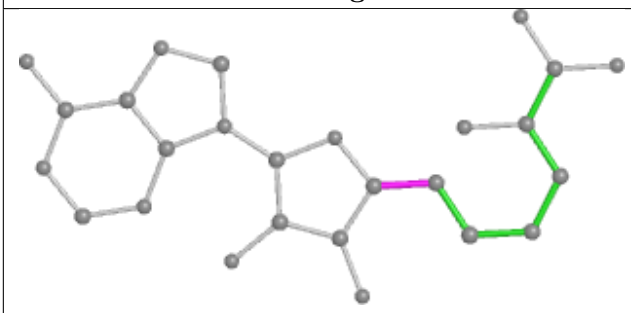
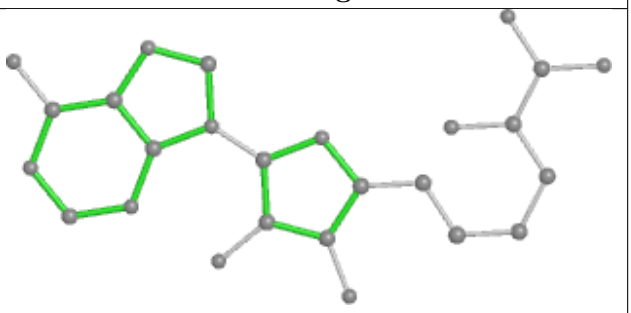
 Bond lengths	 Bond angles
 Torsions	 Rings

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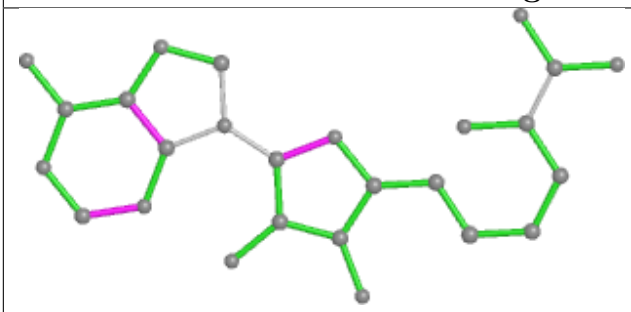
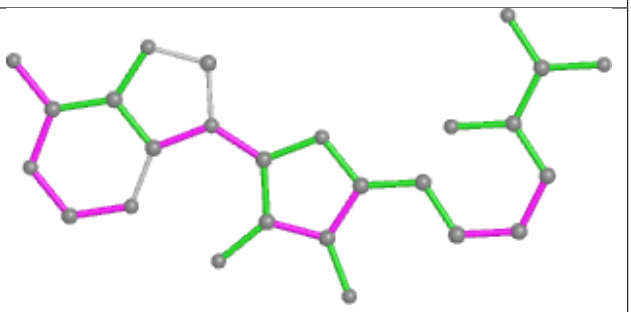
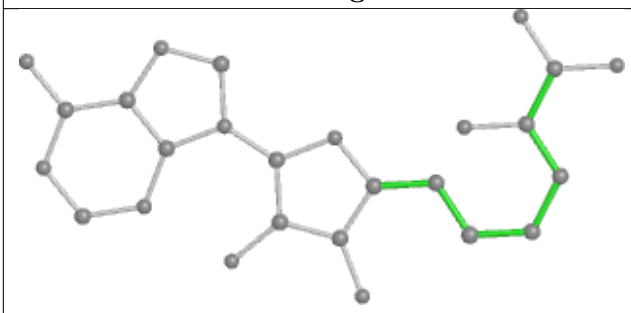
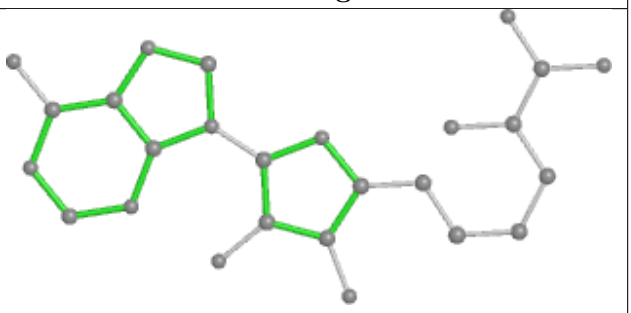
 Bond lengths	 Bond angles
 Torsions	 Rings

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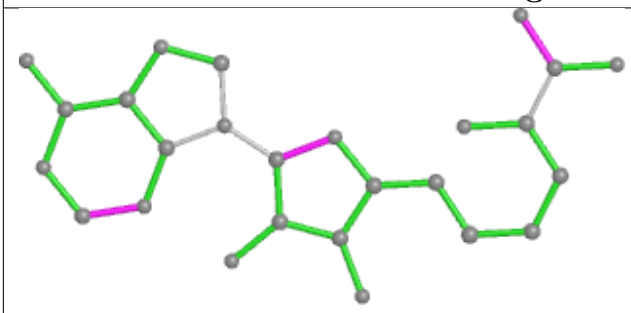
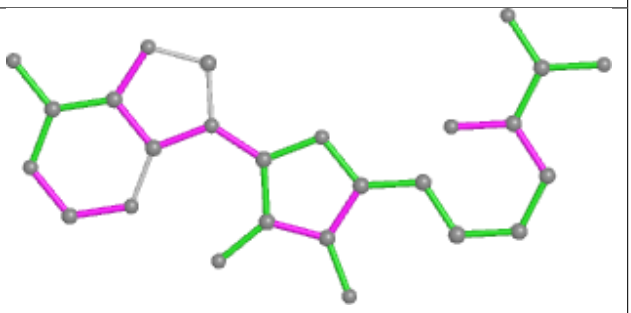
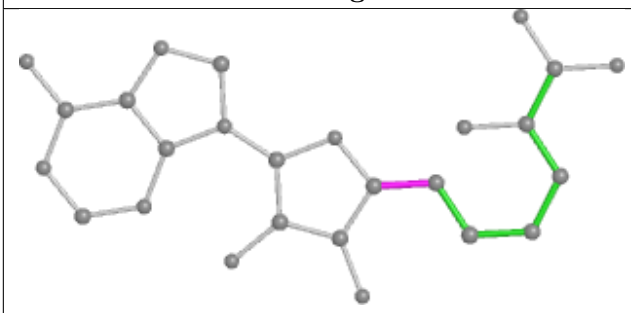
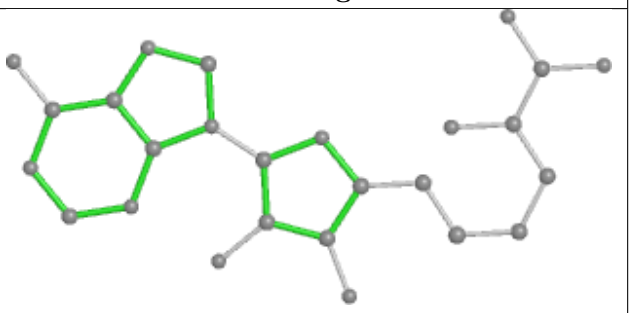
 Bond lengths	 Bond angles
 Torsions	 Rings

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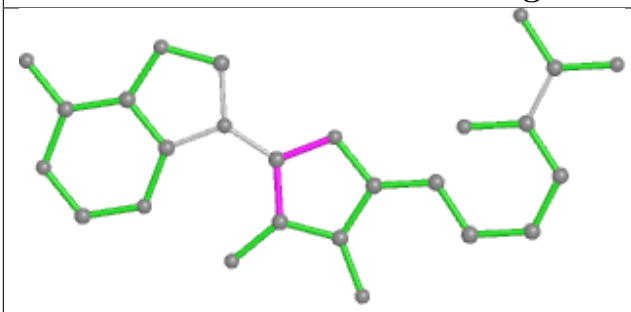
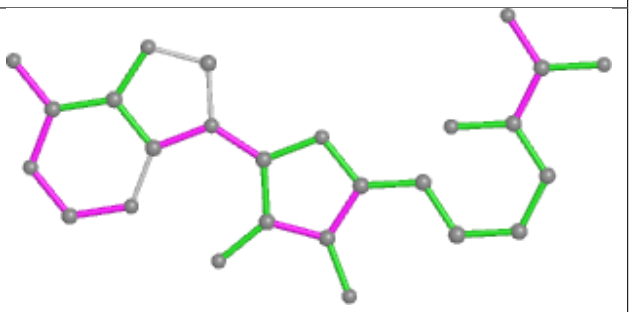
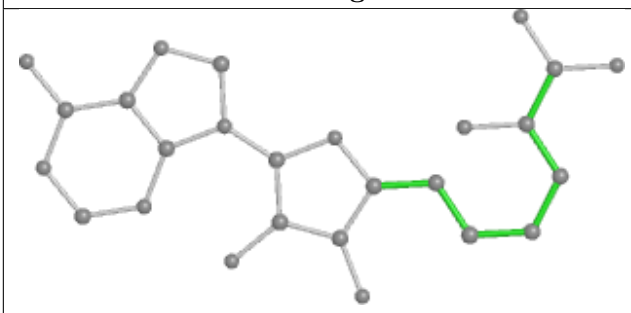
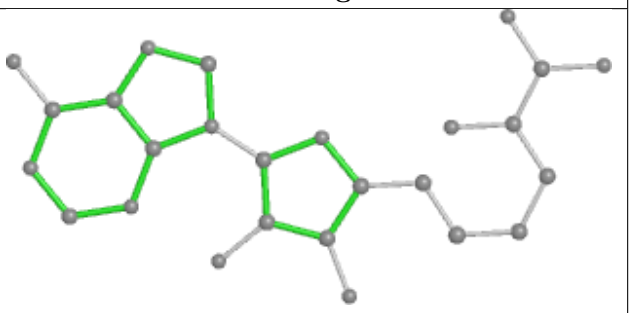
 Bond lengths	 Bond angles
 Torsions	 Rings

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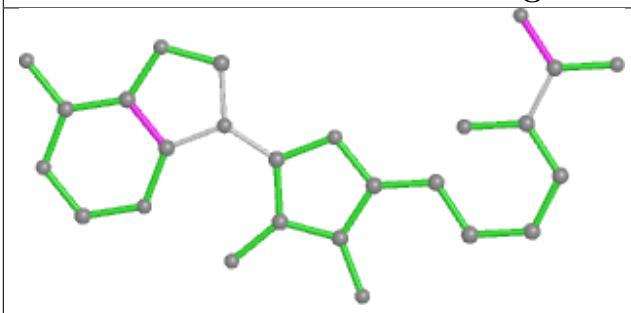
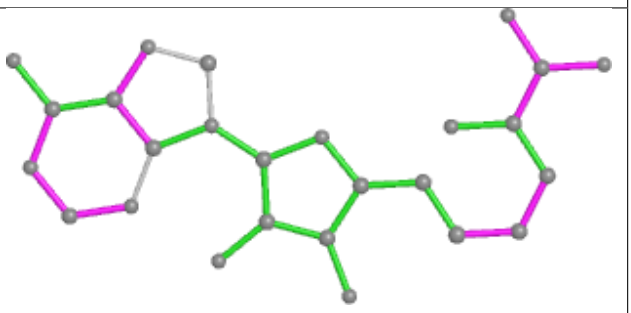
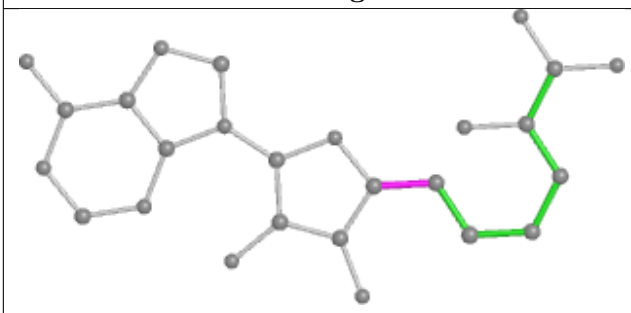
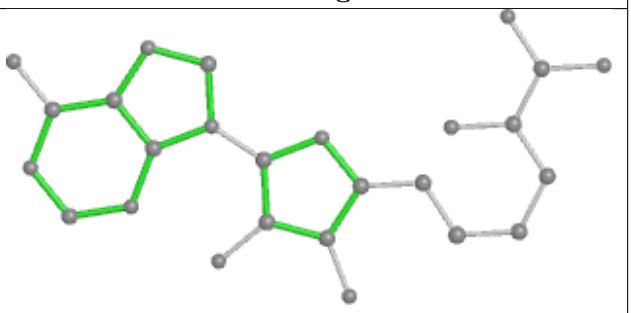
 Bond lengths	 Bond angles
 Torsions	 Rings

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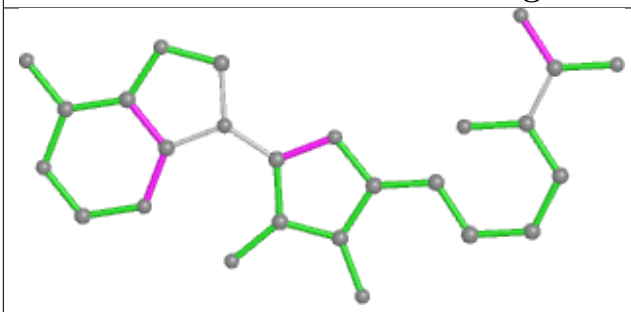
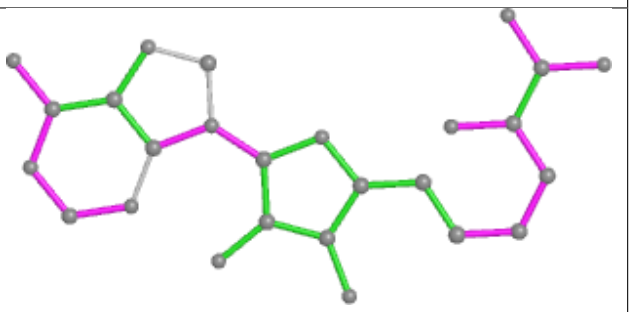
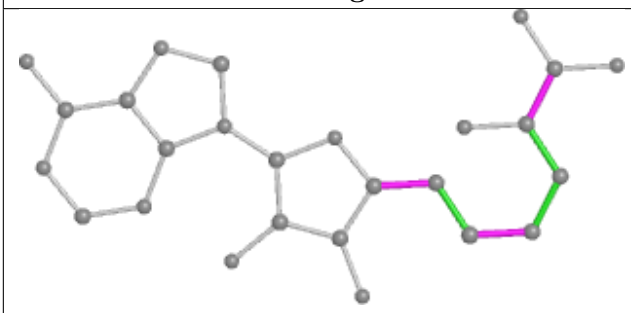
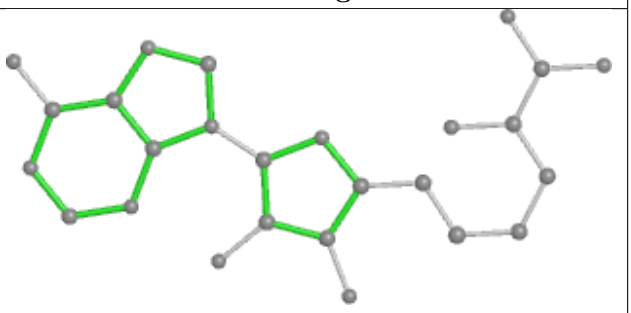
 Bond lengths	 Bond angles
 Torsions	 Rings

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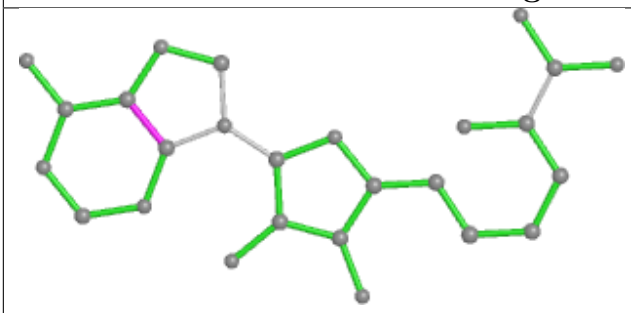
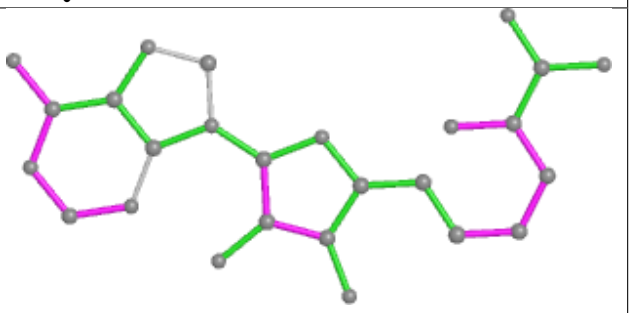
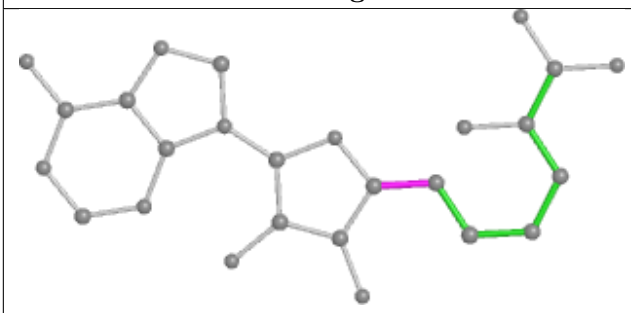
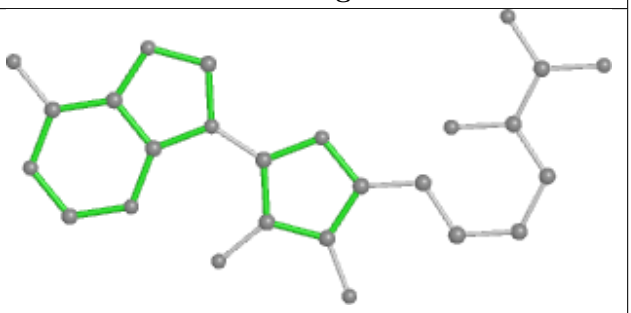
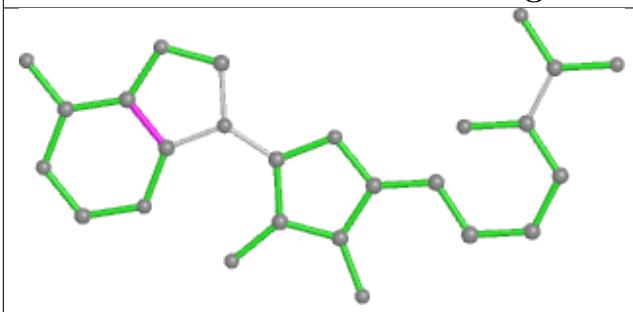
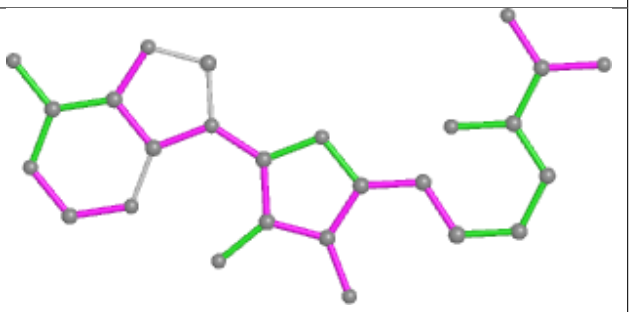
 Bond lengths	 Bond angles
 Torsions	 Rings

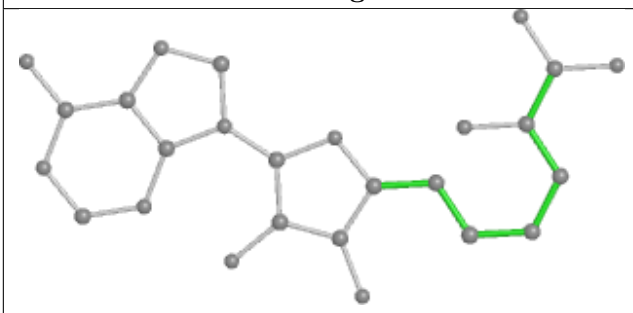
Ligand SAH E 701



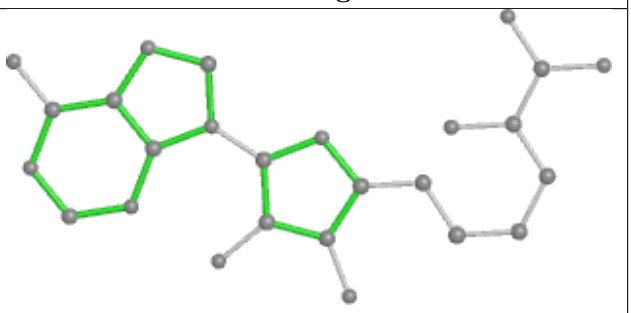
Bond lengths



Bond angles

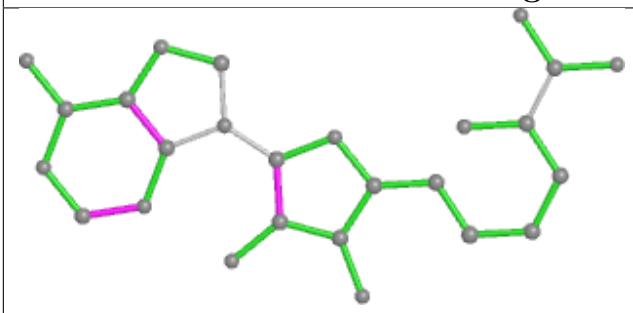


Torsions

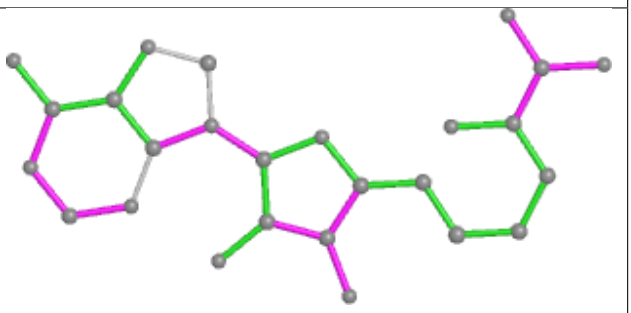


Rings

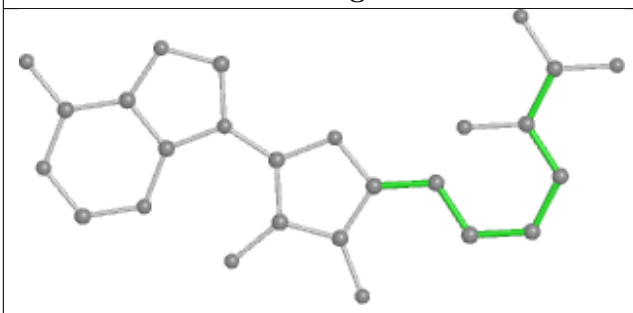
Ligand SAH A 701



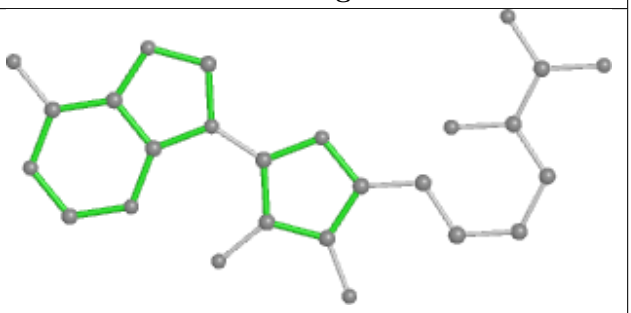
Bond lengths



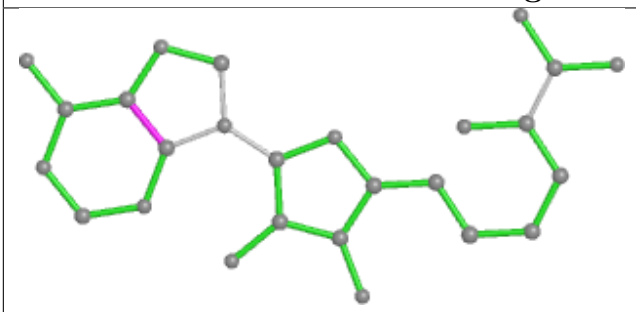
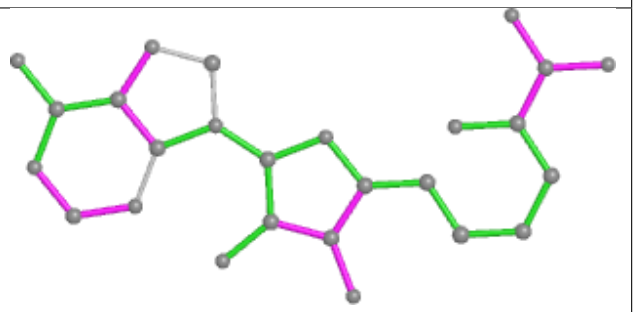
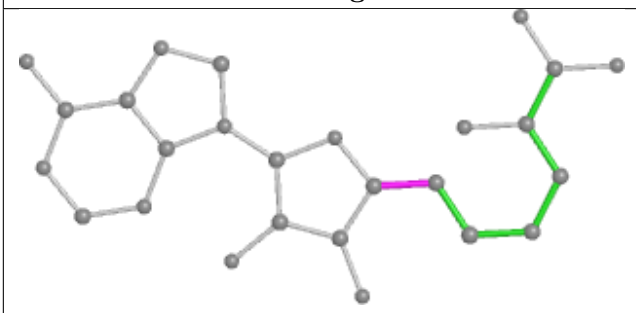
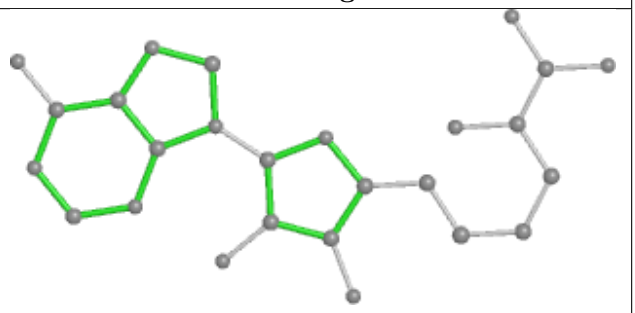
Bond angles



Torsions



Rings

Ligand SAH B 701	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	641/655 (97%)	-0.01	0	100	100	16, 33, 57, 83	0
1	B	638/655 (97%)	0.10	6 (0%)	84	82	24, 43, 74, 103	0
1	C	639/655 (97%)	0.03	0	100	100	26, 44, 68, 100	0
1	D	637/655 (97%)	-0.02	1 (0%)	95	94	19, 34, 56, 101	0
1	E	636/655 (97%)	0.15	9 (1%)	75	73	21, 41, 80, 124	0
1	F	638/655 (97%)	0.15	12 (1%)	66	64	27, 48, 75, 120	0
1	G	636/655 (97%)	0.10	10 (1%)	72	70	23, 43, 81, 129	0
1	H	639/655 (97%)	-0.02	1 (0%)	95	94	18, 38, 60, 91	0
1	I	644/655 (98%)	-0.00	4 (0%)	89	88	28, 44, 68, 94	0
1	J	644/655 (98%)	0.09	5 (0%)	86	84	29, 47, 69, 92	0
1	K	641/655 (97%)	0.13	4 (0%)	89	88	26, 52, 77, 99	0
1	L	644/655 (98%)	-0.03	2 (0%)	94	93	19, 33, 55, 78	0
1	M	633/655 (96%)	0.40	36 (5%)	23	22	38, 61, 84, 110	0
1	N	638/655 (97%)	0.15	6 (0%)	84	82	36, 55, 75, 93	0
1	O	641/655 (97%)	0.43	39 (6%)	21	20	39, 64, 96, 127	0
1	P	636/655 (97%)	0.19	28 (4%)	34	33	30, 51, 82, 105	0
1	Q	632/655 (96%)	0.46	43 (6%)	17	15	37, 62, 99, 124	0
1	R	638/655 (97%)	0.59	59 (9%)	9	8	44, 69, 99, 131	0
All	All	11495/11790 (97%)	0.16	265 (2%)	60	58	16, 48, 82, 131	0

All (265) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	586	ILE	8.7
1	E	64	GLY	6.6
1	E	119	ILE	5.5

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Mol	Chain	Res	Type	RSRZ
1	O	644	SER	5.4
1	Q	116	ILE	5.3
1	Q	86	GLY	5.0
1	O	553	ILE	5.0
1	R	54	ILE	4.9
1	R	68	VAL	4.8
1	G	114	ASP	4.6
1	R	598	ALA	4.6
1	Q	155	PHE	4.5
1	M	107	THR	4.5
1	R	599	GLY	4.4
1	R	264	ILE	4.3
1	O	377	LEU	4.3
1	Q	329	PHE	4.2
1	R	199	LYS	4.2
1	F	317	ASN	4.2
1	R	60	GLU	4.2
1	O	595	ILE	4.2
1	O	583	PHE	4.1
1	R	40	PHE	4.1
1	M	106	ILE	4.1
1	Q	340	LYS	4.0
1	R	257	VAL	4.0
1	P	136	ILE	3.9
1	O	557	VAL	3.9
1	R	66	VAL	3.9
1	F	315	GLU	3.8
1	G	164	LYS	3.8
1	Q	311	LYS	3.8
1	Q	257	VAL	3.8
1	Q	437	LEU	3.7
1	D	62	THR	3.7
1	R	222	LYS	3.7
1	Q	236	PHE	3.6
1	R	320	PHE	3.6
1	R	162	LEU	3.6
1	N	54	ILE	3.5
1	E	118	VAL	3.5
1	R	50	LEU	3.5
1	M	66	VAL	3.5
1	M	316	MET	3.5
1	M	48	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
1	F	262	GLY	3.5
1	O	633	SER	3.5
1	R	593	LEU	3.4
1	G	121	GLU	3.4
1	Q	262	GLY	3.4
1	P	55	ALA	3.4
1	O	564	VAL	3.4
1	R	200	ASP	3.4
1	O	577	MET	3.4
1	P	137	ILE	3.4
1	E	66	VAL	3.4
1	O	620	ASN	3.4
1	M	566	ILE	3.3
1	O	426	THR	3.3
1	K	62	THR	3.3
1	P	86	GLY	3.2
1	O	566	ILE	3.2
1	R	428	VAL	3.2
1	Q	336	VAL	3.2
1	M	514	PHE	3.2
1	M	555	GLY	3.2
1	P	114	ASP	3.2
1	M	301	TRP	3.2
1	Q	119	ILE	3.1
1	R	602	GLU	3.1
1	O	517	ILE	3.1
1	R	477	LEU	3.1
1	F	336	VAL	3.1
1	Q	59	HIS	3.1
1	R	55	ALA	3.1
1	O	199	LYS	3.1
1	P	66	VAL	3.1
1	I	622	LYS	3.0
1	I	129	ILE	3.0
1	M	82	ALA	3.0
1	P	555	GLY	3.0
1	R	58	LYS	3.0
1	R	155	PHE	3.0
1	Q	90	VAL	3.0
1	J	292	LYS	3.0
1	R	88	ASP	3.0
1	P	93	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	R	444	VAL	3.0
1	K	489	ILE	3.0
1	Q	317	ASN	3.0
1	P	74	GLY	2.9
1	N	320	PHE	2.9
1	M	643	LYS	2.9
1	P	118	VAL	2.9
1	Q	308	LEU	2.9
1	M	238	PHE	2.9
1	I	66	VAL	2.8
1	P	454	MET	2.8
1	P	155	PHE	2.8
1	E	93	LEU	2.8
1	P	132	SER	2.8
1	E	114	ASP	2.8
1	K	454	MET	2.8
1	Q	337	GLY	2.8
1	F	189	PHE	2.8
1	M	50	LEU	2.8
1	M	180	PRO	2.8
1	R	159	LEU	2.8
1	O	379	LYS	2.8
1	P	67	HIS	2.8
1	O	585	GLY	2.8
1	Q	93	LEU	2.8
1	Q	555	GLY	2.8
1	O	483	MET	2.7
1	Q	247	ILE	2.7
1	M	314	VAL	2.7
1	O	320	PHE	2.7
1	Q	253	VAL	2.7
1	J	454	MET	2.7
1	Q	137	ILE	2.7
1	O	584	GLY	2.7
1	L	131	GLY	2.7
1	O	629	LEU	2.7
1	M	52	THR	2.7
1	F	556	ARG	2.7
1	M	206	ARG	2.7
1	F	320	PHE	2.7
1	R	234	VAL	2.7
1	P	546	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	R	425	LEU	2.6
1	R	471	MET	2.6
1	E	570	SER	2.6
1	E	111	PRO	2.6
1	O	347	CYS	2.6
1	R	246	ILE	2.6
1	P	240	PHE	2.6
1	Q	240	PHE	2.6
1	R	179	VAL	2.6
1	Q	556	ARG	2.6
1	F	316	MET	2.6
1	M	318	GLN	2.6
1	R	478	ARG	2.5
1	G	162	LEU	2.5
1	Q	158	ALA	2.5
1	R	296	ALA	2.5
1	Q	162	LEU	2.5
1	P	314	VAL	2.5
1	L	454	MET	2.5
1	J	227	ARG	2.5
1	N	134	ALA	2.5
1	K	114	ASP	2.5
1	O	489	ILE	2.5
1	O	540	ILE	2.5
1	M	46	PHE	2.5
1	O	565	ASN	2.5
1	R	308	LEU	2.5
1	P	68	VAL	2.4
1	Q	314	VAL	2.4
1	M	210	THR	2.4
1	Q	112	TRP	2.4
1	R	622	LYS	2.4
1	M	119	ILE	2.4
1	M	247	ILE	2.4
1	O	486	LEU	2.4
1	O	551	PHE	2.4
1	Q	238	PHE	2.4
1	Q	319	THR	2.4
1	R	85	GLU	2.4
1	Q	292	LYS	2.4
1	P	509	PHE	2.4
1	M	61	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	133	ARG	2.4
1	M	103	ALA	2.4
1	Q	627	HIS	2.4
1	R	167	CYS	2.4
1	J	315	GLU	2.4
1	B	292	LYS	2.4
1	Q	277	ARG	2.4
1	Q	255	GLU	2.4
1	M	624	LEU	2.3
1	Q	111	PRO	2.3
1	M	65	LYS	2.3
1	G	116	ILE	2.3
1	O	545	ALA	2.3
1	Q	161	ARG	2.3
1	R	505	THR	2.3
1	R	59	HIS	2.3
1	O	192	ILE	2.3
1	I	292	LYS	2.3
1	R	142	PHE	2.3
1	R	643	LYS	2.3
1	N	294	ASN	2.3
1	B	83	ALA	2.3
1	R	511	LEU	2.3
1	F	370	PHE	2.3
1	F	613	PHE	2.3
1	O	428	VAL	2.3
1	Q	57	LYS	2.3
1	N	268	LEU	2.3
1	O	561	LYS	2.3
1	R	164	LYS	2.3
1	Q	163	ALA	2.3
1	R	62	THR	2.2
1	G	68	VAL	2.2
1	M	320	PHE	2.2
1	B	113	SER	2.2
1	Q	85	GLU	2.2
1	R	369	LYS	2.2
1	P	63	ASP	2.2
1	Q	133	ARG	2.2
1	B	199	LYS	2.2
1	J	586	ILE	2.2
1	P	133	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	132	SER	2.2
1	F	282	PHE	2.2
1	N	319	THR	2.2
1	F	54	ILE	2.2
1	O	443	ILE	2.2
1	M	623	SER	2.2
1	Q	199	LYS	2.2
1	O	399	THR	2.2
1	R	504	GLY	2.2
1	G	161	ARG	2.1
1	O	403	VAL	2.1
1	R	443	ILE	2.1
1	O	349	LEU	2.1
1	O	477	LEU	2.1
1	P	58	LYS	2.1
1	R	571	SER	2.1
1	O	200	ASP	2.1
1	G	54	ILE	2.1
1	R	600	VAL	2.1
1	P	620	ASN	2.1
1	P	69	LEU	2.1
1	Q	267	LEU	2.1
1	R	456	PRO	2.1
1	G	59	HIS	2.1
1	O	567	ASP	2.1
1	G	158	ALA	2.1
1	R	283	ILE	2.1
1	R	38	LEU	2.1
1	R	592	LEU	2.1
1	M	471	MET	2.1
1	R	621	ASP	2.1
1	R	206	ARG	2.1
1	M	55	ALA	2.1
1	P	628	ALA	2.1
1	B	169	VAL	2.1
1	P	51	LYS	2.1
1	P	644	SER	2.1
1	M	313	LYS	2.1
1	O	622	LYS	2.1
1	R	314	VAL	2.1
1	M	116	ILE	2.0
1	P	619	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
1	M	199	LYS	2.0
1	R	340	LYS	2.0
1	M	17	VAL	2.0
1	H	556	ARG	2.0
1	M	142	PHE	2.0
1	M	168	ARG	2.0
1	Q	232	PRO	2.0
1	R	345	CYS	2.0
1	R	586	ILE	2.0
1	R	454	MET	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 monosaccharides 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	SAH	M	701	26/26	0.89	0.16	36,61,74,79	0
2	SAH	N	701	26/26	0.90	0.12	40,53,58,58	0
2	SAH	R	701	26/26	0.91	0.17	47,56,92,99	0
3	PO4	M	702	5/5	0.91	0.13	70,71,74,78	0
2	SAH	Q	701	26/26	0.92	0.14	48,64,75,76	0
2	SAH	P	701	26/26	0.93	0.11	43,53,63,65	0
2	SAH	G	701	26/26	0.93	0.14	46,63,72,72	0
2	SAH	K	701	26/26	0.94	0.13	37,41,47,51	0
2	SAH	E	701	26/26	0.95	0.13	43,53,63,65	0
2	SAH	D	701	26/26	0.95	0.15	32,37,45,46	0
2	SAH	C	701	26/26	0.95	0.14	36,48,57,59	0
2	SAH	F	701	26/26	0.95	0.14	35,46,61,64	0
2	SAH	O	701	26/26	0.95	0.10	37,41,47,52	0

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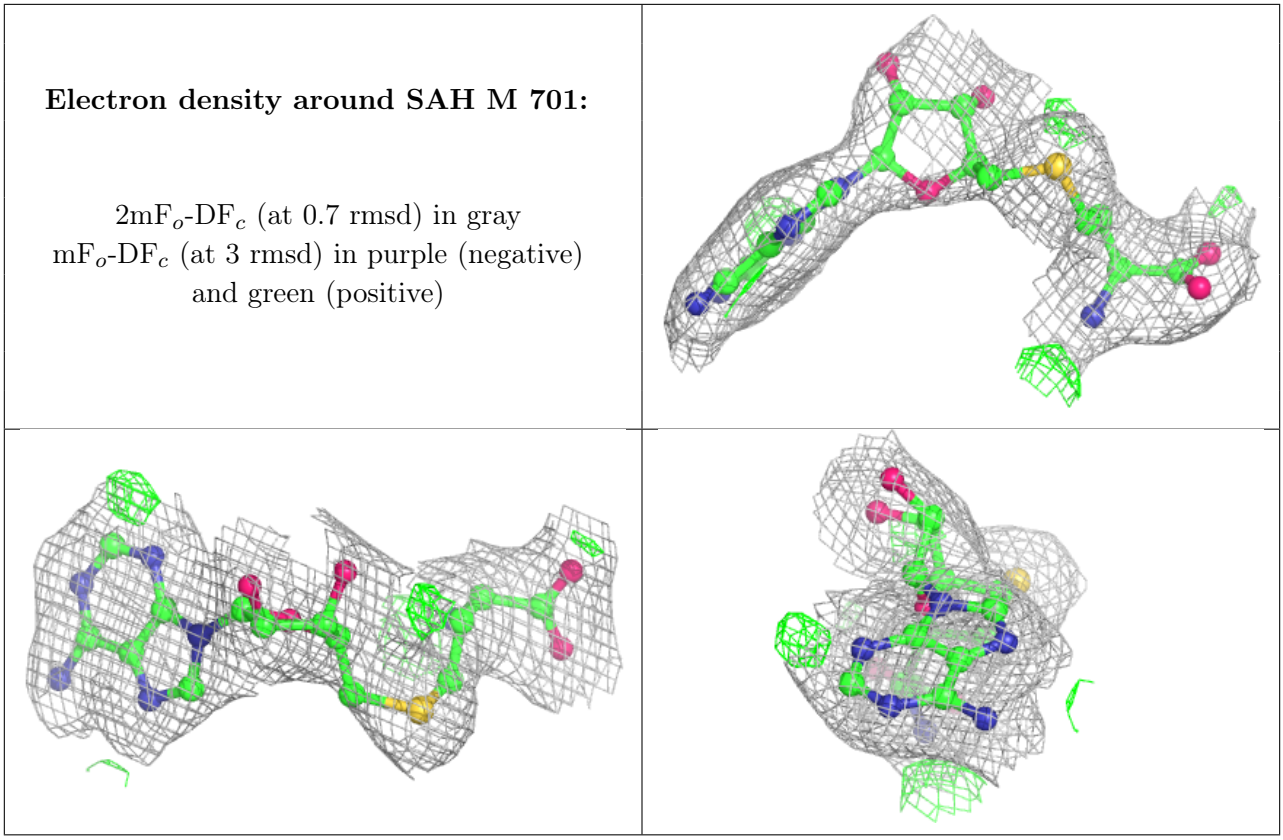
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SAH	A	701	26/26	0.96	0.13	27,33,38,38	0
2	SAH	B	701	26/26	0.96	0.12	36,43,57,58	0
2	SAH	J	701	26/26	0.96	0.11	34,38,44,46	0
2	SAH	H	701	26/26	0.96	0.12	24,29,33,34	0
2	SAH	I	701	26/26	0.96	0.12	35,38,45,47	0
3	PO4	Q	702	5/5	0.96	0.12	59,63,72,72	0
3	PO4	R	702	5/5	0.96	0.09	52,55,59,61	0
3	PO4	N	702	5/5	0.97	0.09	52,57,62,66	0
3	PO4	O	702	5/5	0.97	0.07	57,58,70,72	0
3	PO4	I	702	5/5	0.97	0.14	36,37,44,49	0
2	SAH	L	701	26/26	0.97	0.12	27,33,36,39	0
3	PO4	C	702	5/5	0.98	0.09	37,41,44,44	0
3	PO4	F	702	5/5	0.98	0.08	38,42,49,56	0
3	PO4	E	702	5/5	0.98	0.10	36,40,43,47	0
3	PO4	P	702	5/5	0.98	0.12	43,43,45,47	0
3	PO4	H	702	5/5	0.98	0.09	28,34,36,37	0
3	PO4	B	702	5/5	0.98	0.13	36,39,45,48	0
3	PO4	J	702	5/5	0.98	0.11	45,46,49,51	0
3	PO4	K	702	5/5	0.98	0.09	43,45,46,51	0
3	PO4	D	702	5/5	0.99	0.12	31,35,36,37	0
3	PO4	G	702	5/5	0.99	0.11	42,42,49,50	0
3	PO4	A	702	5/5	0.99	0.12	31,32,37,39	0
3	PO4	L	702	5/5	0.99	0.12	32,32,35,37	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

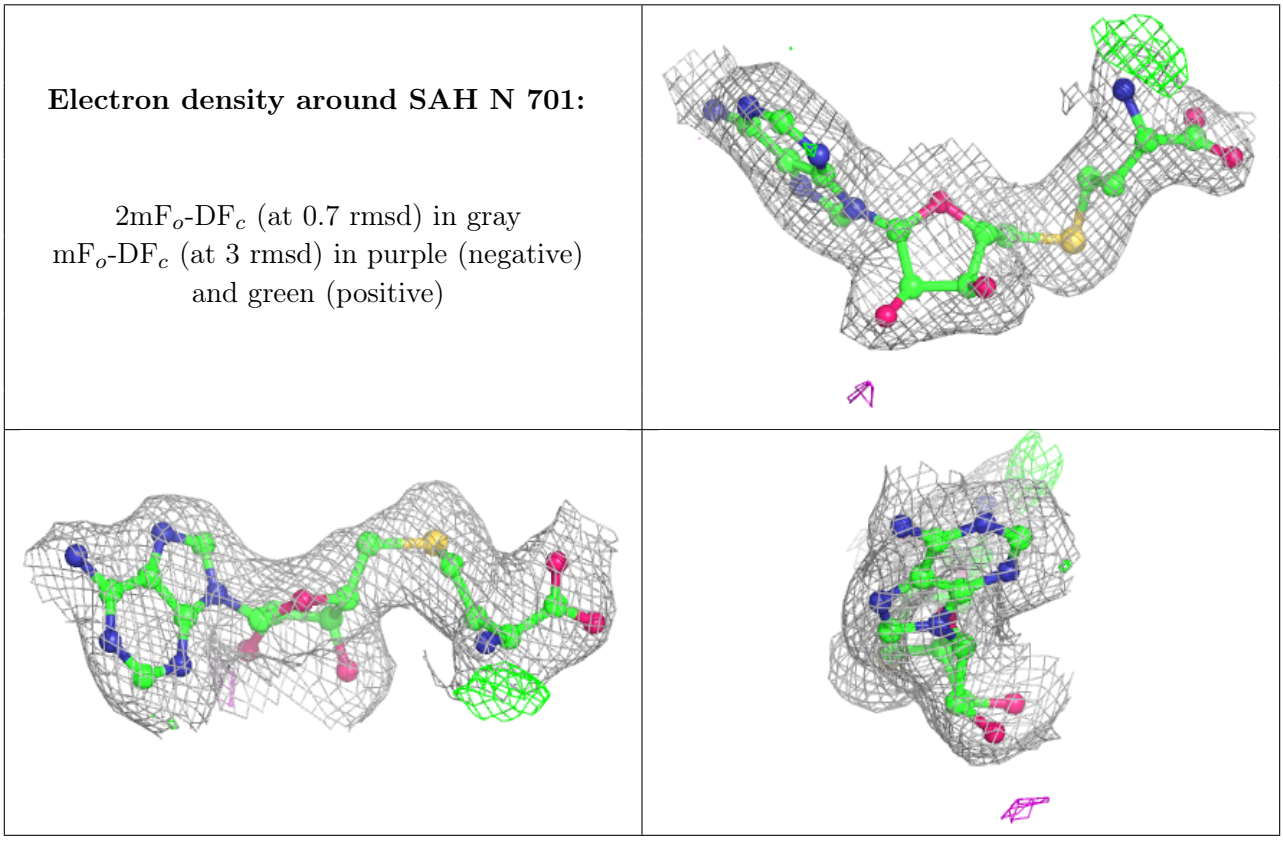
Electron density around SAH M 701:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



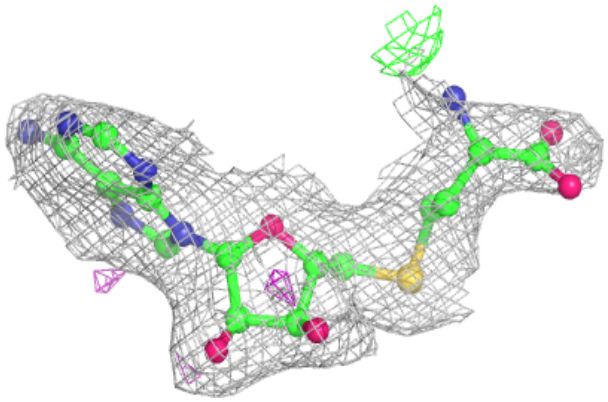
Electron density around SAH N 701:

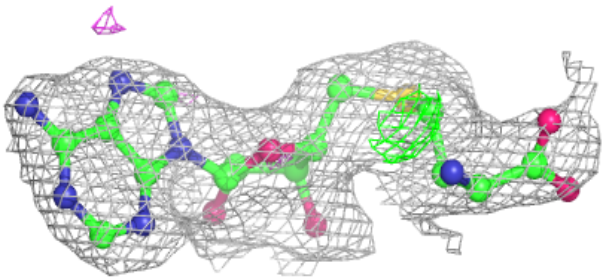
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

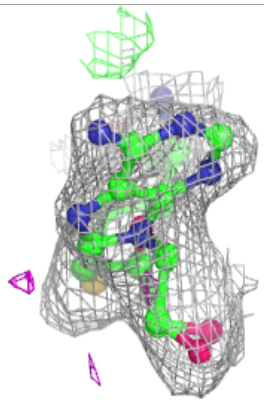


Electron density around SAH R 701:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

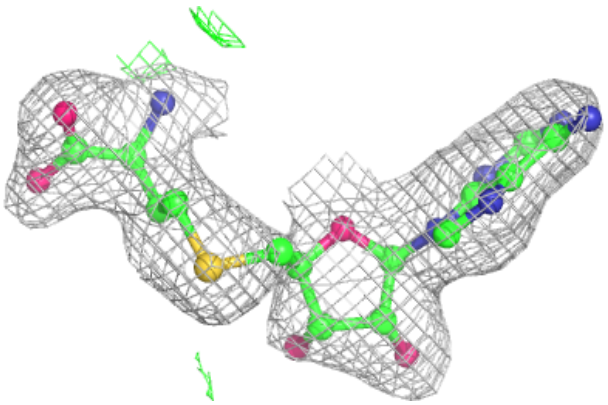


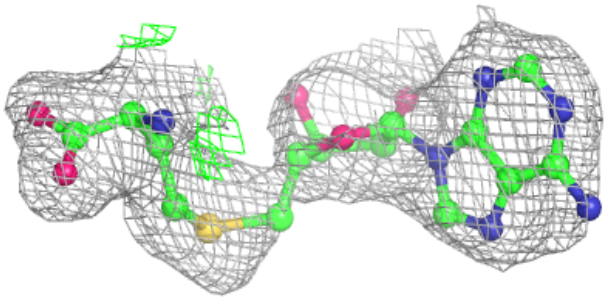


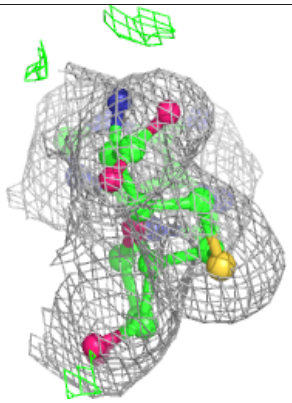


Electron density around SAH Q 701:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

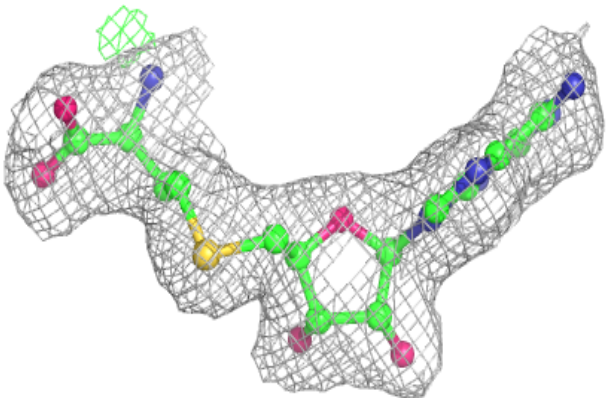


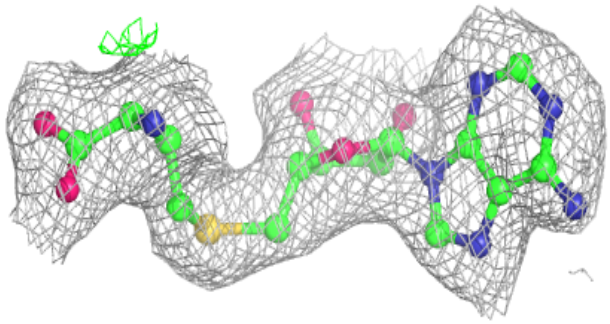


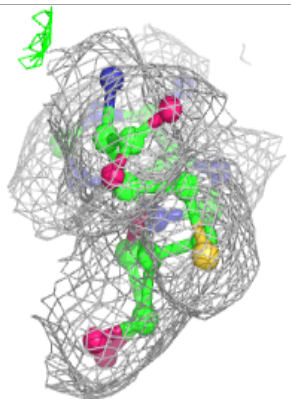


Electron density around SAH P 701:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

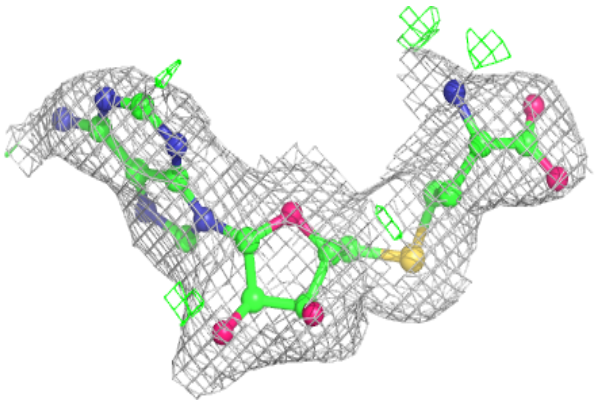


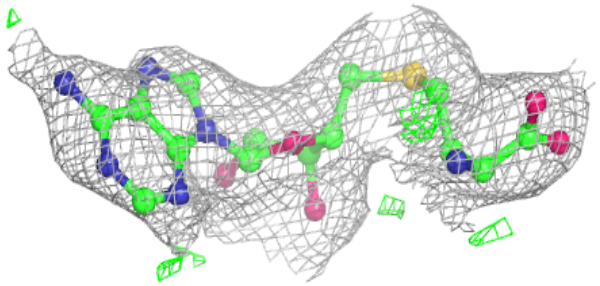


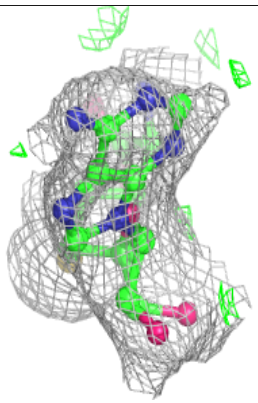


Electron density around SAH G 701:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

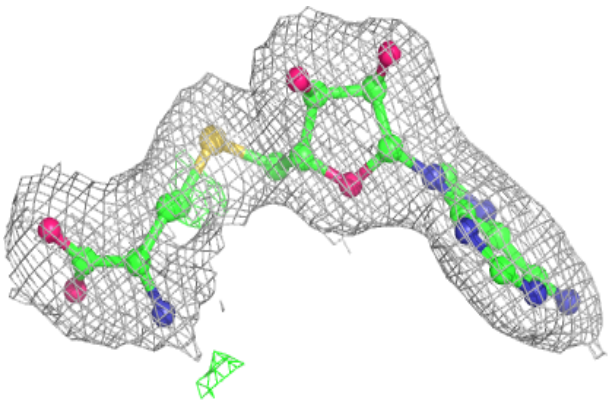


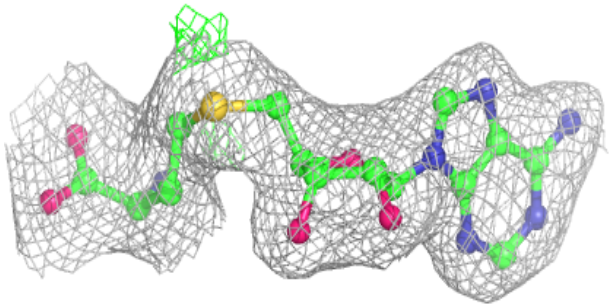


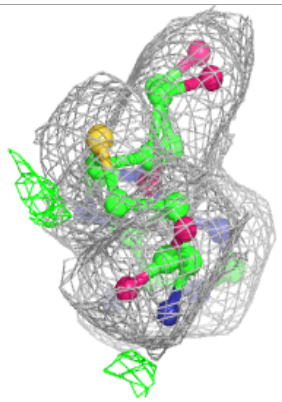


Electron density around SAH K 701:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

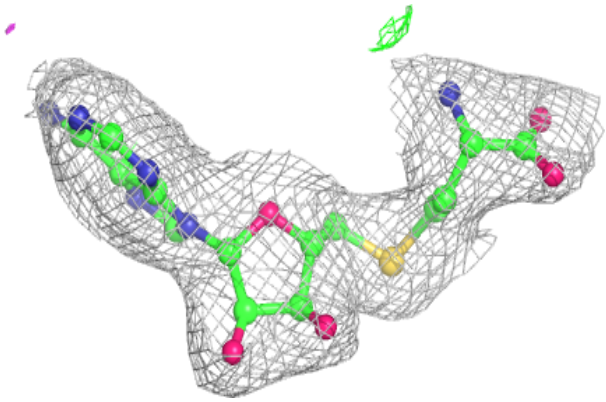


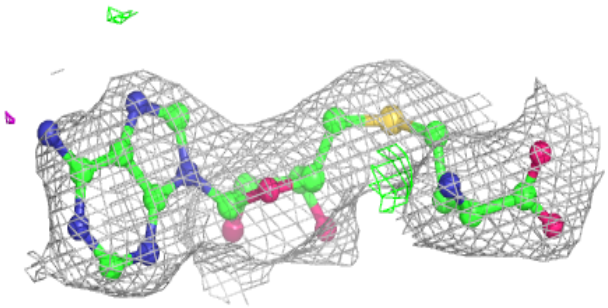


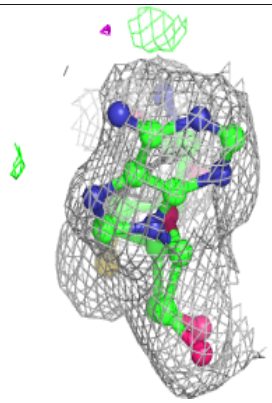


Electron density around SAH E 701:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

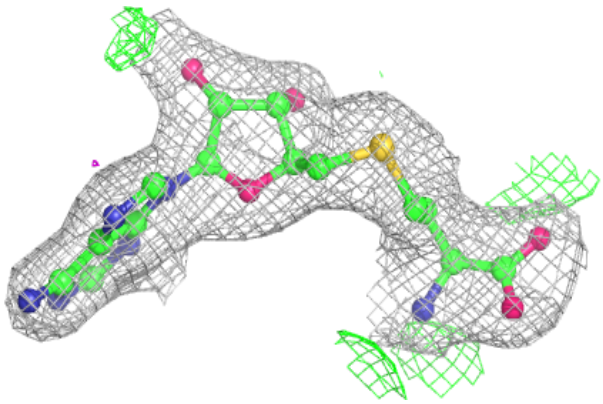


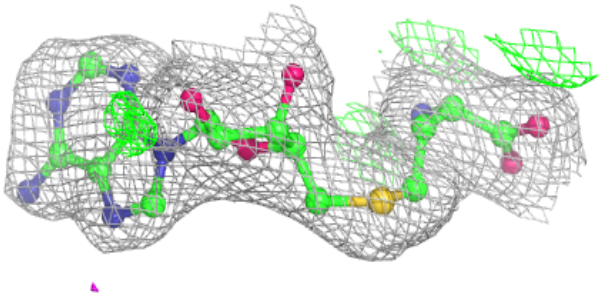


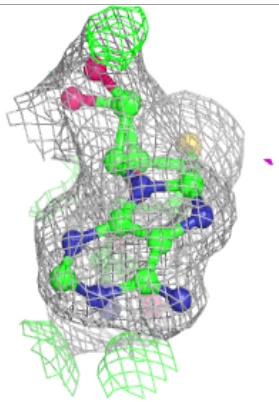


Electron density around SAH D 701:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

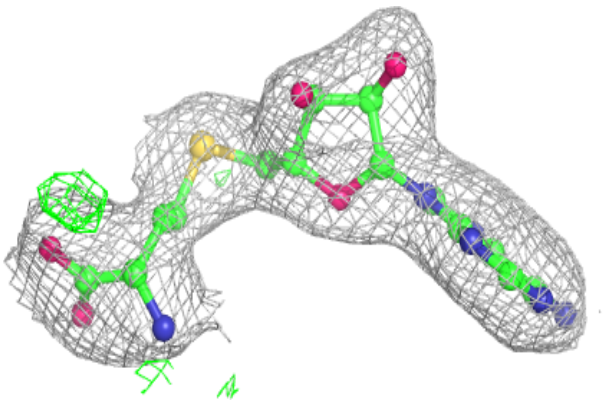


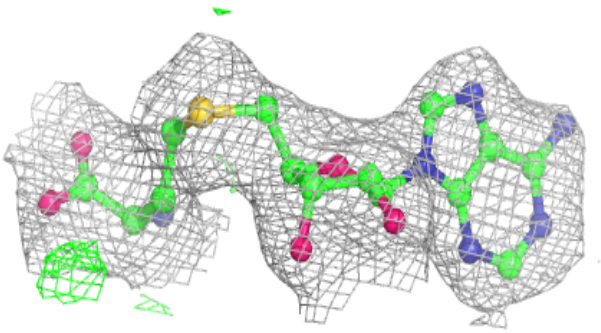


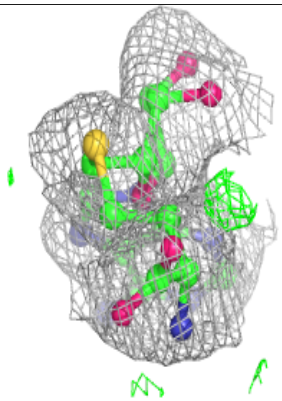


Electron density around SAH C 701:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

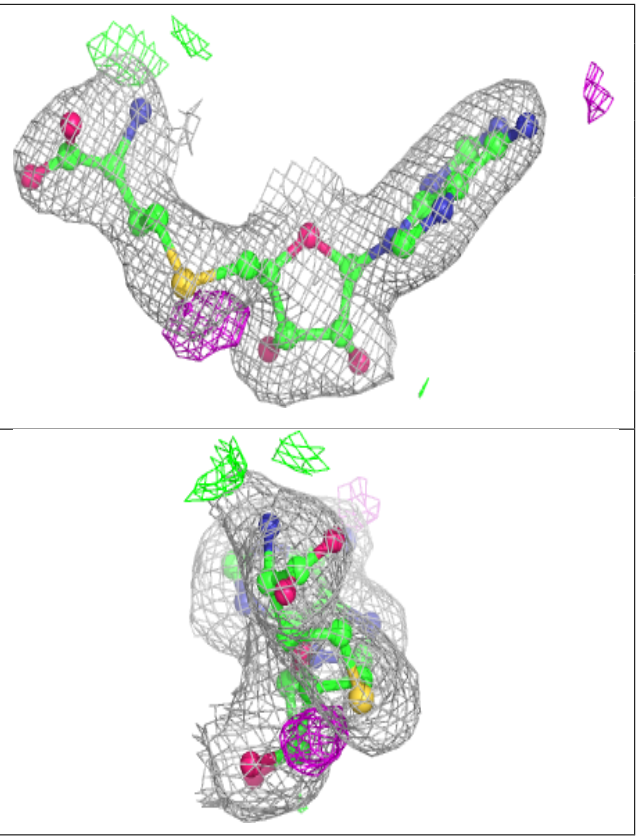






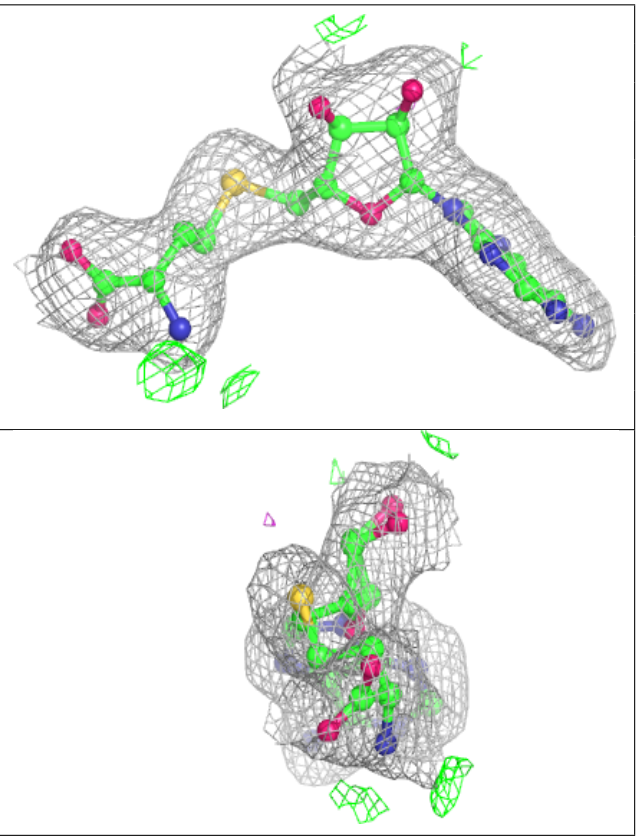
Electron density around SAH F 701:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



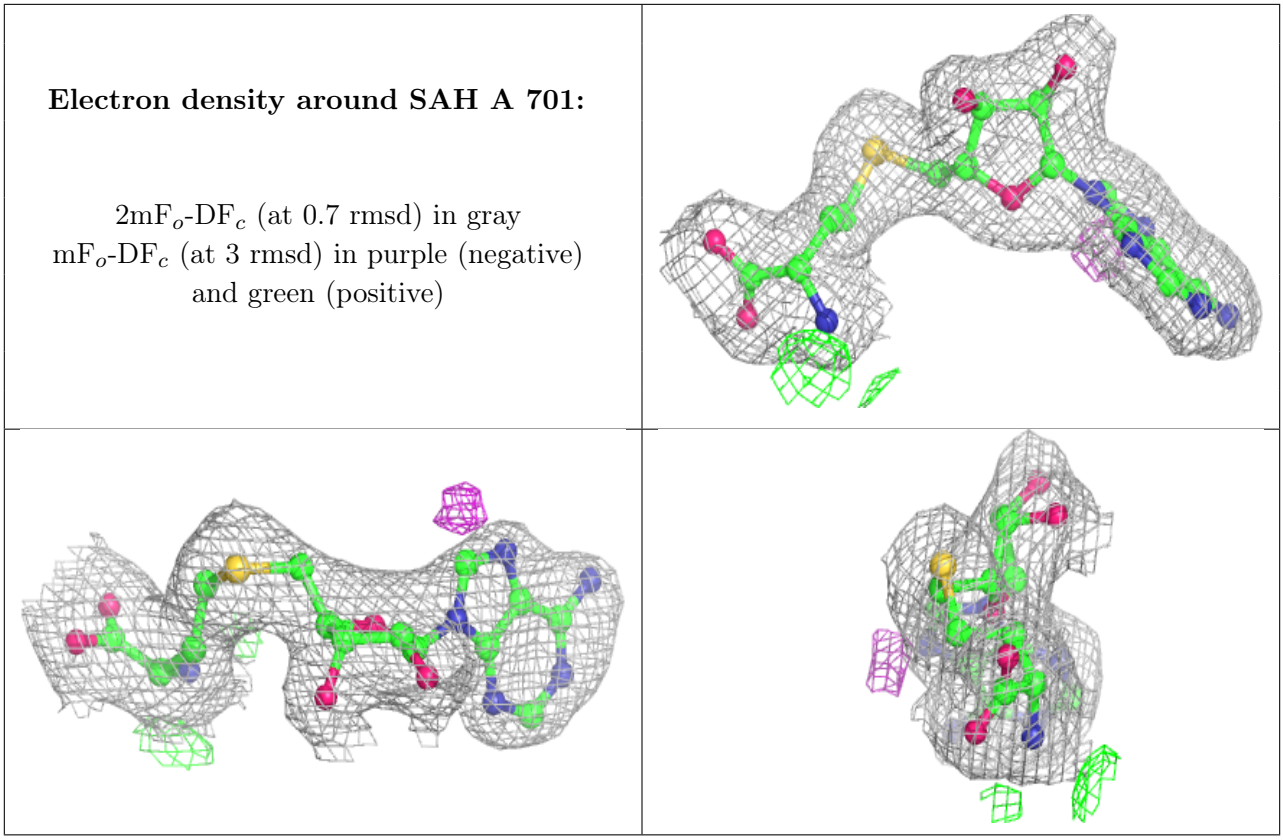
Electron density around SAH O 701:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



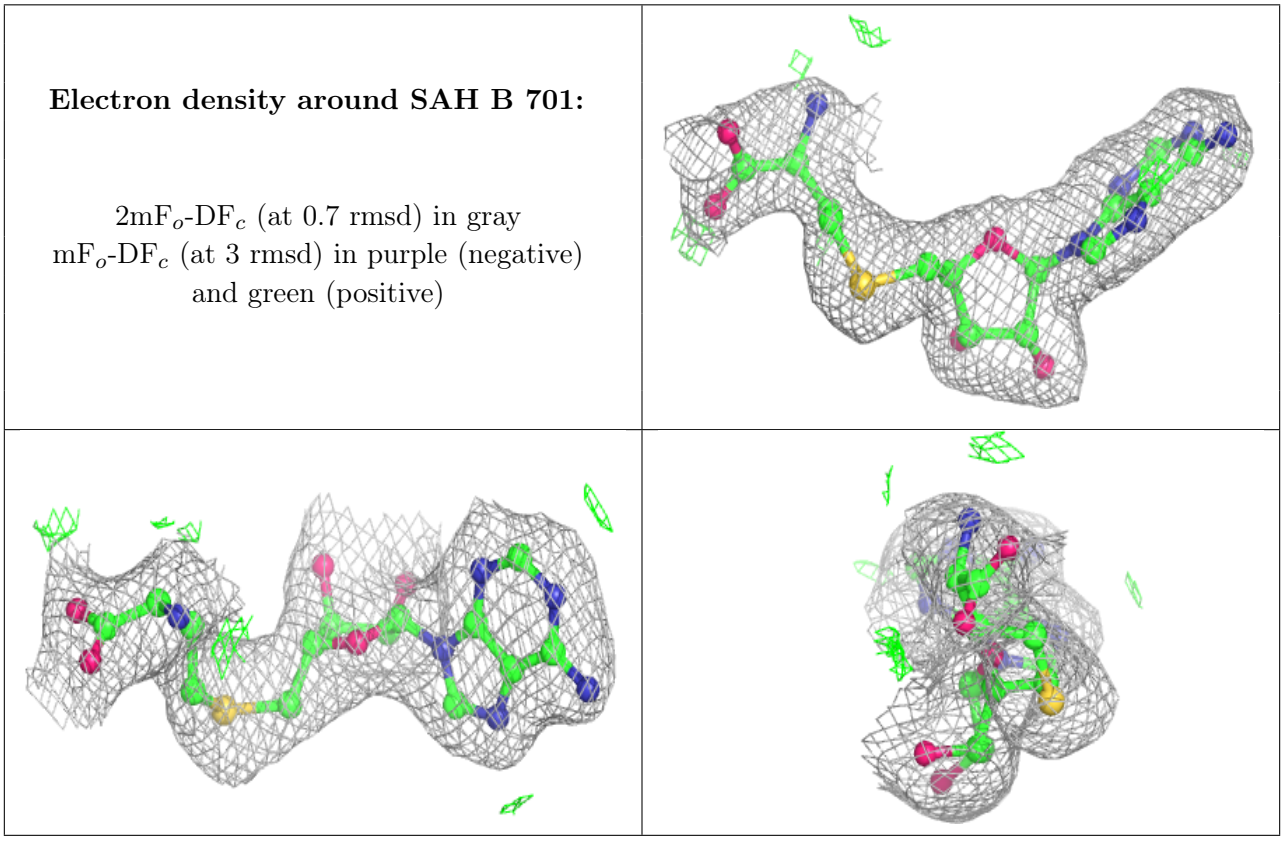
Electron density around SAH A 701:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around SAH B 701:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around SAH J 701:

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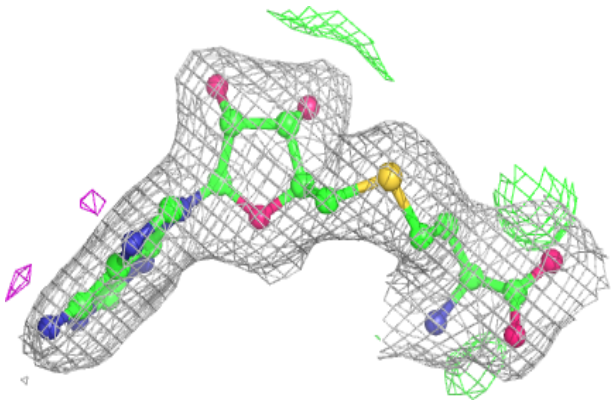
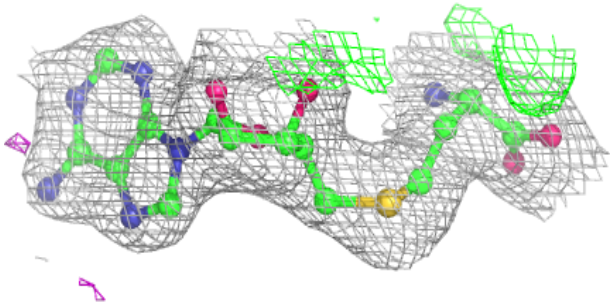
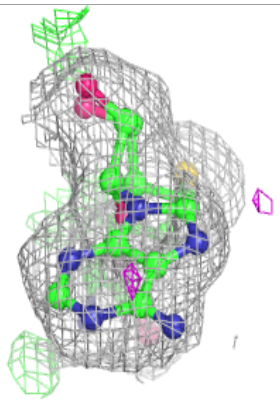
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

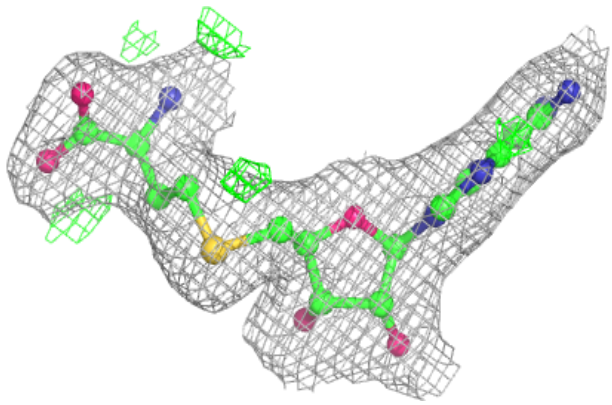


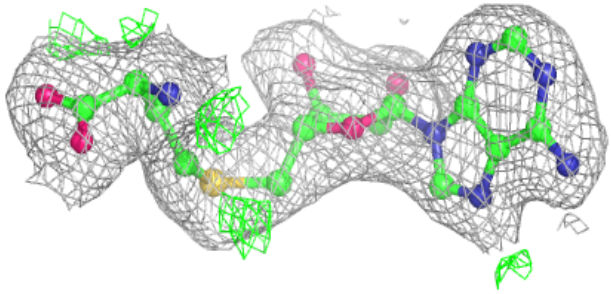


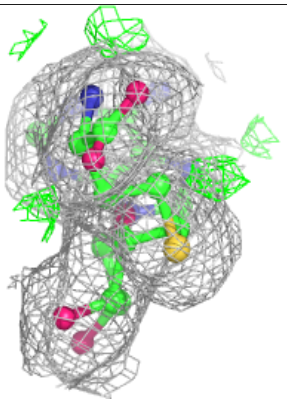


Electron density around SAH H 701:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

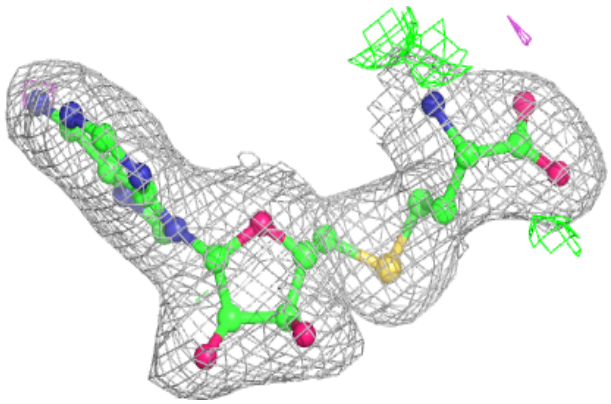


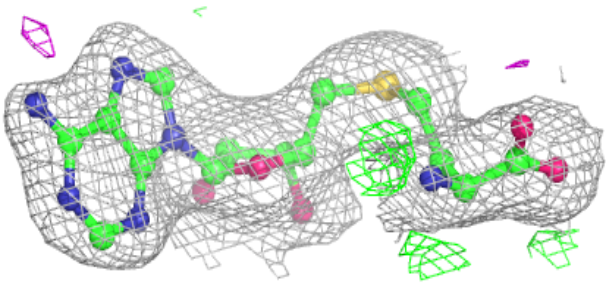


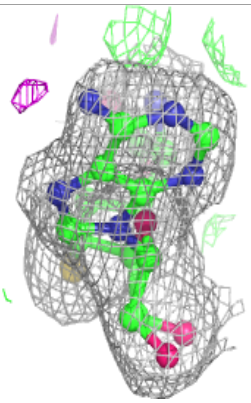


Electron density around SAH I 701:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

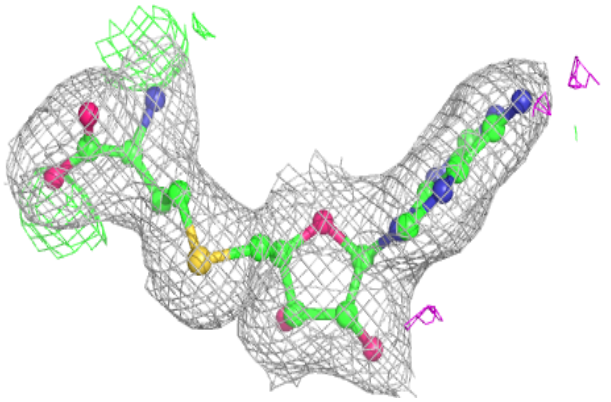


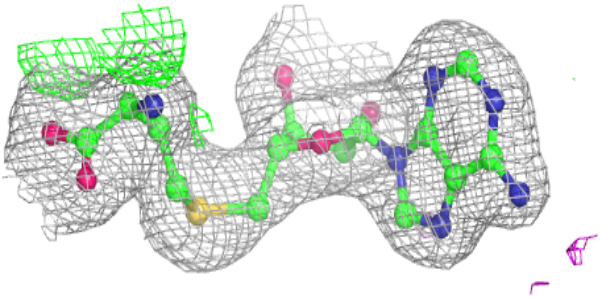


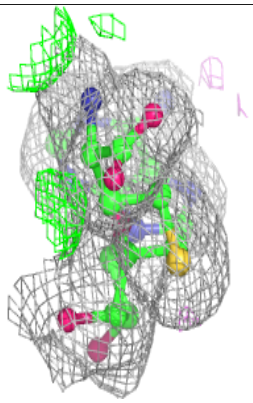


Electron density around SAH L 701:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







6.5 Other polymers (i)

There are no such residues in this entry.