



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:28 PM UTC

PDB ID : 1IVS / pdb_00001ivs
Title : CRYSTAL STRUCTURE OF THERMUS THERMOPHILUS VALYL-
TRNA SYNTHETASE COMPLEXED WITH TRNA(VAL) AND VALYL-
ADENYLATE ANALOGUE
Authors : Fukai, S.; Nureki, O.; Sekine, S.-I.; Shimada, A.; Vassilyev, D.G.; Yokoyama,
S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2002-03-29
Resolution : 2.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtrriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

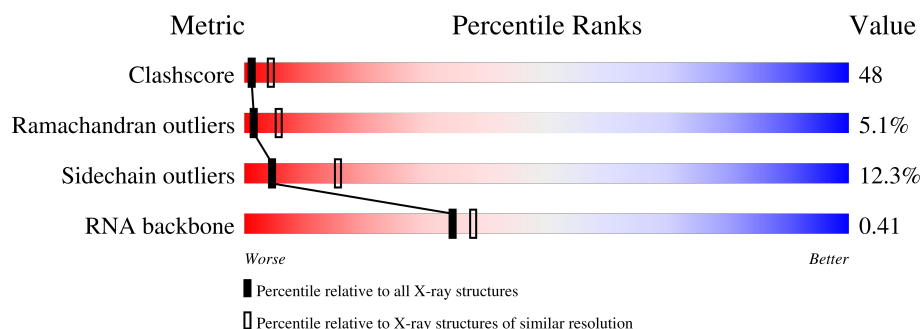
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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))
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RNA backbone	3983	1120 (3.10-2.70)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	C	75	29% 40% 23% 8%
1	D	75	20% 53% 21% 5%
2	A	862	36% 51% 11% .
2	B	862	34% 52% 13% .

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 17424 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.

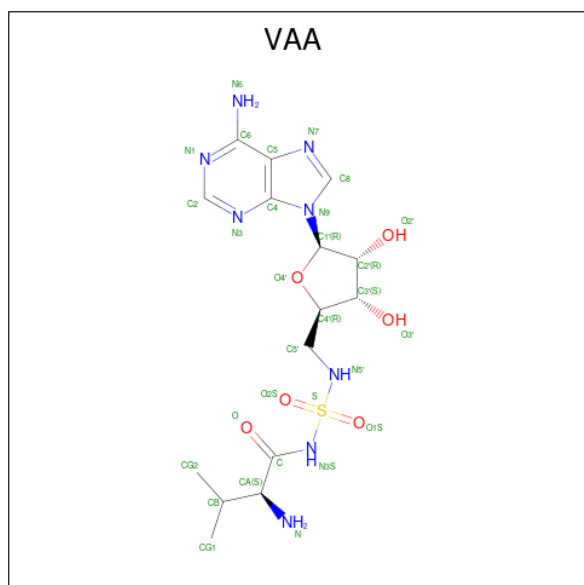
- Molecule 1 is a RNA chain called tRNA (Val).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	75	Total	C	N	O	P	0	0	0
			1603	714	293	521	75			
1	D	75	Total	C	N	O	P	0	0	0
			1603	714	293	521	75			

- Molecule 2 is a protein called Valyl-tRNA synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	862	Total	C	N	O	S	0	0	0
			6970	4449	1228	1266	27			
2	B	862	Total	C	N	O	S	0	0	0
			6970	4449	1228	1266	27			

- Molecule 3 is N-[VALINYL]-N'-[ADENOSYL]-DIAMINOSUFONE (CCD ID: VAA) (formula: $C_{15}H_{24}N_8O_6S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			30	15	8	6	1		
3	B	1	Total	C	N	O	S	0	0
			30	15	8	6	1		

- Molecule 4 is water.

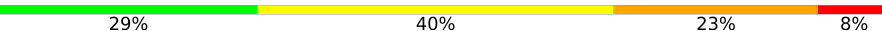
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	29	Total	O	0	0
			29	29		
4	D	13	Total	O	0	0
			13	13		
4	A	101	Total	O	0	0
			101	101		
4	B	75	Total	O	0	0
			75	75		

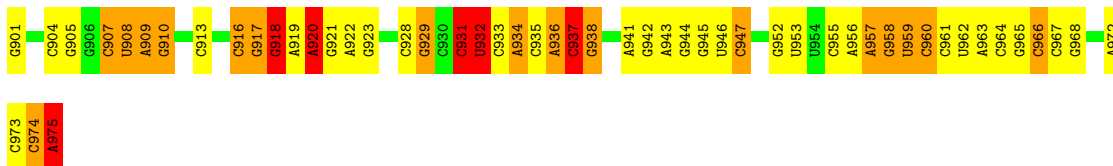
3 Residue-property plots

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

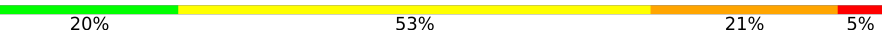
Note EDS was not executed.

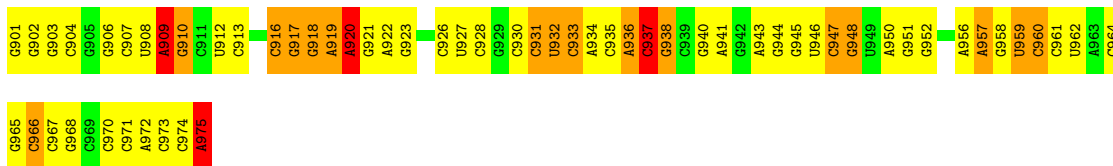
• Molecule 1: tRNA (Val)

Chain C: 



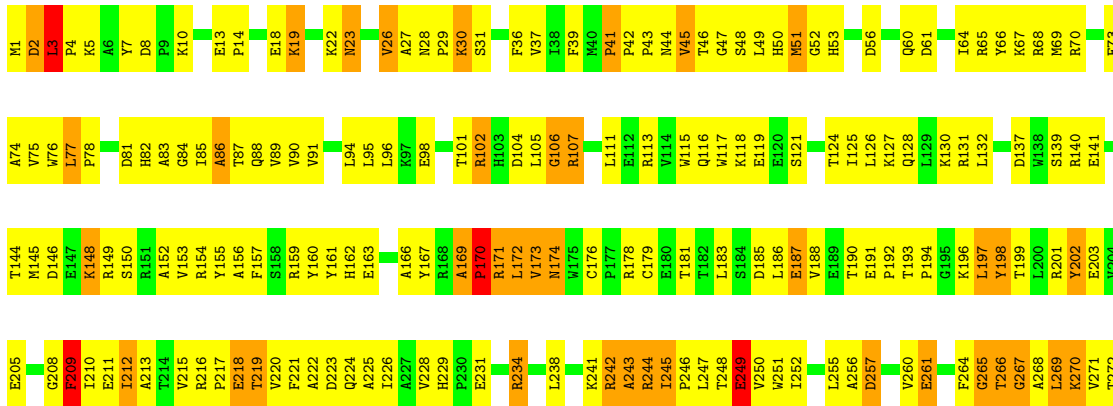
• Molecule 1: tRNA (Val)

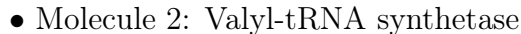
Chain D: 



• Molecule 2: Valyl-tRNA synthetase

Chain A: 





I402 S403 R404 Q405 L406 W407 W408 G409	Y337 T338 T339 A340 L341 W407 T343 T344	D276 P277 L278 D279 Y280 E281 L282 G283	I212 T213 T214 V215 R216 P217 E218 T219	D146 E147 L148 R149 S150 T151 E152 V153	W76 L77 P78 T79 G80 D81 H82 A83	M1 D2 L3 P4 K5 A6 Y7																																																
							R346 C347 G348 T349 P350 L351 E352 Y353 A354 L355 F356 T357 C358 W359 W360 L361 R362 M363 R364 A365 L366 W367 Y368 E369 V370 L371 K372 G373 L374 D378	D276 P277 L278 D279 Y280 E281 L282 G283	I212 T213 T214 V215 R216 P217 E218 T219	D146 E147 L148 R149 S150 T151 E152 V153	W76 L77 P78 T79 G80 D81 H82 A83	M1 D2 L3 P4 K5 A6 Y7																																										
													R346 C347 G348 T349 P350 L351 E352 Y353 A354 L355 F356 T357 C358 W359 W360 L361 R362 M363 R364 A365 L366 W367 Y368 E369 V370 L371 K372 G373 L374 D378	D276 P277 L278 D279 Y280 E281 L282 G283	I212 T213 T214 V215 R216 P217 E218 T219	D146 E147 L148 R149 S150 T151 E152 V153	W76 L77 P78 T79 G80 D81 H82 A83	M1 D2 L3 P4 K5 A6 Y7																																				
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																									R346 C347 G348 T349 P350 L351 E352 Y353 A354 L355 F356 T357 C358 W359 W360 L361 R362 M363 R364 A365 L366 W367 Y368 E369 V370 L371 K372 G373 L374 D378	D276 P277 L278 D279 Y280 E281 L282 G283	I212 T213 T214 V215 R216 P217 E218 T219	D146 E147 L148 R149 S150 T151 E152 V153	W76 L77 P78 T79 G80 D81 H82 A83	M1 D2 L3 P4 K5 A6 Y7																								
																															R346 C347 G348 T349 P350 L351 E352 Y353 A354 L355 F356 T357 C358 W359 W360 L361 R362 M363 R364 A365 L366 W367 Y368 E369 V370 L371 K372 G373 L374 D378	D276 P277 L278 D279 Y280 E281 L282 G283	I212 T213 T214 V215 R216 P217 E218 T219	D146 E147 L148 R149 S150 T151 E152 V153	W76 L77 P78 T79 G80 D81 H82 A83	M1 D2 L3 P4 K5 A6 Y7																		
																																					R346 C347 G348 T349 P350 L351 E352 Y353 A354 L355 F356 T357 C358 W359 W360 L361 R362 M363 R364 A365 L366 W367 Y368 E369 V370 L371 K372 G373 L374 D378	D276 P277 L278 D279 Y280 E281 L282 G283	I212 T213 T214 V215 R216 P217 E218 T219	D146 E147 L148 R149 S150 T151 E152 V153	W76 L77 P78 T79 G80 D81 H82 A83	M1 D2 L3 P4 K5 A6 Y7												
																																											R346 C347 G348 T349 P350 L351 E352 Y353 A354 L355 F356 T357 C358 W359 W360 L361 R362 M363 R364 A365 L366 W367 Y368 E369 V370 L371 K372 G373 L374 D378	D276 P277 L278 D279 Y280 E281 L282 G283	I212 T213 T214 V215 R216 P217 E218 T219	D146 E147 L148 R149 S150 T151 E152 V153	W76 L77 P78 T79 G80 D81 H82 A83	M1 D2 L3 P4 K5 A6 Y7						
																																																	R346 C347 G348 T349 P350 L351 E352 Y353 A354 L355 F356 T357 C358 W359 W360 L361 R362 M363 R364 A365 L366 W367 Y368 E369 V370 L371 K372 G373 L374 D378	D276 P277 L278 D279 Y280 E281 L282 G283	I212 T213 T214 V215 R216 P217 E218 T219	D146 E147 L148 R149 S150 T151 E152 V153	W76 L77 P78 T79 G80 D81 H82 A83	M1 D2 L3 P4 K5 A6 Y7



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α , β , γ	411.81Å 411.81Å 81.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.90	Depositor
% Data completeness (in resolution range)	96.5 (40.00-2.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.248 , 0.282	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	17424	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	C	0.40	0/1791	0.88	9/2789 (0.3%)
1	D	0.40	0/1791	0.87	4/2789 (0.1%)
2	A	0.54	0/7143	1.05	45/9678 (0.5%)
2	B	0.54	0/7143	1.09	53/9678 (0.5%)
All	All	0.51	0/17868	1.03	111/24934 (0.4%)

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	C	0	1

There are no bond length outliers.

All (111) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	975	A	C4'-C3'-O3'	11.97	127.36	109.40
2	B	382	VAL	CA-C-N	-11.00	106.09	119.84
2	B	382	VAL	C-N-CA	-11.00	106.09	119.84
2	A	244	ARG	N-CA-C	-9.27	96.79	110.23
1	D	937	C	C2'-C3'-O3'	9.10	123.14	109.50
2	B	475	ASP	N-CA-C	-8.52	101.68	110.97
1	C	937	C	C2'-C3'-O3'	8.22	121.83	109.50
2	B	469	TRP	CA-C-N	-8.07	109.75	119.84
2	B	469	TRP	C-N-CA	-8.07	109.75	119.84
1	D	975	A	C4'-C3'-O3'	8.03	121.44	109.40
2	A	266	THR	N-CA-C	-7.99	98.70	110.52
2	A	638	TYR	N-CA-C	-7.82	102.71	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	705	TRP	CA-C-N	7.72	127.71	119.76
2	B	705	TRP	C-N-CA	7.72	127.71	119.76
2	B	810	LYS	N-CA-C	-7.57	102.97	111.07
2	A	469	TRP	CA-C-N	-7.43	110.85	119.47
2	A	469	TRP	C-N-CA	-7.43	110.85	119.47
2	A	382	VAL	CA-C-N	-7.38	110.92	119.47
2	A	382	VAL	C-N-CA	-7.38	110.92	119.47
1	C	907	C	C2'-C3'-O3'	-7.20	102.90	113.70
2	B	202	TYR	N-CA-C	7.17	119.97	109.07
2	A	328	ALA	N-CA-C	-7.13	104.45	113.72
2	B	309	LEU	N-CA-C	-7.08	104.51	113.43
2	A	23	ASN	CA-C-N	7.07	128.67	119.84
2	A	23	ASN	C-N-CA	7.07	128.67	119.84
2	A	202	TYR	N-CA-C	6.94	119.62	109.07
2	B	3	LEU	N-CA-C	6.91	125.08	109.81
2	A	249	GLU	N-CA-C	-6.91	102.28	113.19
2	B	248	THR	CA-C-O	6.90	121.94	117.94
2	B	276	ASP	CA-C-N	6.90	126.60	119.56
2	B	276	ASP	C-N-CA	6.90	126.60	119.56
1	C	931	C	C2'-C3'-O3'	6.81	119.71	109.50
2	B	683	MET	CA-C-N	6.79	126.04	118.97
2	B	683	MET	C-N-CA	6.79	126.04	118.97
2	A	209	PHE	N-CA-C	6.78	120.33	108.75
2	B	245	ILE	CA-C-N	6.70	128.21	119.84
2	B	245	ILE	C-N-CA	6.70	128.21	119.84
2	B	248	THR	CB-CA-C	-6.61	107.55	117.07
2	A	642	TRP	N-CA-C	6.57	118.23	111.14
2	A	286	HIS	N-CA-C	-6.54	102.94	111.71
1	D	920	A	C4'-C3'-O3'	-6.53	103.20	113.00
2	A	42	PRO	N-CA-C	6.50	118.63	110.70
2	B	385	ARG	N-CA-C	-6.42	104.55	112.38
2	B	285	ARG	N-CA-C	-6.36	104.97	114.64
2	B	332	VAL	N-CA-C	6.36	119.27	113.10
2	B	839	ALA	N-CA-C	-6.32	105.58	113.55
2	A	470	PRO	N-CA-C	-6.32	104.65	113.81
2	A	226	ILE	N-CA-C	-6.30	99.05	108.12
2	A	276	ASP	CA-C-N	6.27	126.17	119.28
2	A	276	ASP	C-N-CA	6.27	126.17	119.28
2	A	234	ARG	N-CA-C	-6.23	105.16	112.89
2	B	270	LYS	N-CA-C	-6.17	102.82	110.41
1	C	975	A	C2'-C3'-O3'	6.15	118.73	109.50
2	A	541	GLU	N-CA-C	-6.14	104.14	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	471	GLU	CB-CA-C	-6.14	107.51	116.53
2	B	659	ALA	N-CA-C	-6.12	105.80	113.20
2	A	3	LEU	N-CA-C	6.10	123.29	109.81
2	B	286	HIS	N-CA-C	-6.09	103.56	113.19
2	B	646	CYS	N-CA-C	6.05	117.75	111.03
2	A	579	ALA	N-CA-C	-5.98	104.67	111.07
1	C	920	A	C4'-C3'-O3'	-5.97	104.04	113.00
2	A	107	ARG	N-CA-C	-5.96	105.31	113.30
2	B	480	TYR	CA-C-N	-5.95	112.40	119.84
2	B	480	TYR	C-N-CA	-5.95	112.40	119.84
2	B	297	GLU	N-CA-C	-5.94	105.99	113.18
2	B	339	ILE	N-CA-C	5.85	117.16	109.21
1	C	920	A	N9-C1'-C2'	5.84	120.76	112.00
2	B	400	TRP	N-CA-C	5.83	118.23	108.73
2	B	176	CYS	CA-C-N	5.80	126.20	119.47
2	B	176	CYS	C-N-CA	5.80	126.20	119.47
2	B	314	ARG	N-CA-C	-5.79	105.89	113.12
2	A	173	VAL	N-CA-C	5.72	116.72	108.48
2	B	280	TYR	N-CA-C	-5.72	105.13	111.36
2	B	572	LEU	N-CA-C	-5.71	105.14	111.36
2	B	409	GLY	N-CA-C	5.69	126.67	113.18
2	B	292	SER	N-CA-C	5.65	118.28	109.52
2	B	412	ILE	CA-C-N	5.65	128.92	120.96
2	B	412	ILE	C-N-CA	5.65	128.92	120.96
2	A	806	GLU	N-CA-C	-5.64	106.11	112.87
2	B	346	ARG	N-CA-C	5.64	118.28	111.40
2	A	843	ARG	N-CA-C	-5.63	104.77	111.69
2	A	297	GLU	N-CA-C	-5.61	106.41	113.20
2	B	840	GLU	N-CA-C	-5.61	105.16	112.23
1	C	947	C	N1-C1'-C2'	5.59	122.38	114.00
2	B	173	VAL	N-CA-C	5.57	116.76	108.46
2	A	316	GLU	N-CA-C	-5.55	105.71	113.37
2	A	573	GLU	N-CA-C	-5.51	105.19	111.14
2	B	26	VAL	N-CA-C	5.37	116.34	109.30
1	C	932	U	N1-C1'-C2'	5.37	120.06	112.00
2	A	26	VAL	N-CA-C	5.35	117.16	109.51
2	A	780	VAL	N-CA-C	5.34	116.16	108.48
2	A	649	TYR	N-CA-C	5.33	116.78	110.97
2	B	244	ARG	N-CA-C	-5.32	103.12	110.35
2	B	638	TYR	N-CA-C	-5.31	104.73	111.11
1	D	909	A	C4'-C3'-O3'	5.30	117.36	109.40
2	A	409	GLY	N-CA-C	5.30	125.73	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	212	ILE	N-CA-C	5.29	116.34	108.46
2	B	579	ALA	N-CA-C	-5.23	105.23	111.03
2	A	528	LYS	N-CA-C	5.22	117.67	110.35
2	A	475	ASP	N-CA-C	-5.22	105.28	110.97
2	A	346	ARG	N-CA-C	5.16	119.54	112.88
2	B	648	TRP	N-CA-C	5.16	119.03	112.12
2	A	720	GLU	N-CA-C	-5.15	105.75	111.36
2	A	443	SER	CA-C-N	5.10	126.22	119.84
2	A	443	SER	C-N-CA	5.10	126.22	119.84
2	B	226	ILE	N-CA-C	-5.09	100.19	107.78
2	A	480	TYR	CA-C-N	-5.09	113.48	119.84
2	A	480	TYR	C-N-CA	-5.09	113.48	119.84
2	A	41	PRO	N-CA-C	-5.09	104.50	110.70
2	B	248	THR	N-CA-C	5.02	112.90	108.78
2	A	615	SER	N-CA-C	-5.02	105.81	111.28

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	918	G	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1603	0	816	65	0
1	D	1603	0	816	58	0
2	A	6970	0	6949	719	1
2	B	6970	0	6949	765	0
3	A	30	0	24	5	0
3	B	30	0	24	1	0
4	A	101	0	0	16	0
4	B	75	0	0	12	0
4	C	29	0	0	1	0
4	D	13	0	0	1	0
All	All	17424	0	15578	1570	1

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 48.

All (1570) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:382:VAL:HG23	2:B:383:PRO:CD	1.71	1.20
2:B:448:ARG:HD3	2:B:448:ARG:H	1.05	1.18
2:A:282:ILE:HA	2:A:285:ARG:HD3	1.31	1.13
2:A:777:LYS:H	2:A:777:LYS:HD3	0.98	1.12
2:B:382:VAL:HG23	2:B:383:PRO:HD3	1.29	1.12
2:A:382:VAL:HG23	2:A:383:PRO:CD	1.78	1.12
2:A:28:ASN:HD21	2:A:30:LYS:HG2	1.15	1.11
2:A:855:ARG:HH22	2:B:810:LYS:HE2	1.18	1.08
2:B:777:LYS:HE3	2:B:777:LYS:H	1.09	1.08
2:A:448:ARG:H	2:A:448:ARG:HD3	0.92	1.07
2:B:412:ILE:HD12	2:B:413:PRO:HD2	1.35	1.06
2:A:494:LEU:HD23	2:A:494:LEU:H	1.13	1.05
2:A:382:VAL:HG23	2:A:383:PRO:HD3	1.06	1.05
2:A:171:ARG:HH22	2:A:364:ARG:NH2	1.55	1.04
2:B:225:ALA:HA	2:B:252:ILE:HG23	1.42	1.01
2:A:540:LEU:HA	2:A:543:VAL:HG12	1.40	1.00
2:B:382:VAL:CG2	2:B:516:LEU:HA	1.91	1.00
2:A:224:GLN:HE22	2:A:304:ARG:NH2	1.58	1.00
2:A:810:LYS:HE3	2:B:855:ARG:HH22	1.26	0.99
1:C:928:C:H2'	1:C:929:G:H5''	1.41	0.99
2:A:448:ARG:HD3	2:A:448:ARG:N	1.76	0.98
2:A:37:VAL:HG21	2:A:479:PHE:HB2	1.45	0.97
2:A:382:VAL:CG2	2:A:383:PRO:HD3	1.95	0.97
2:B:282:ILE:HA	2:B:285:ARG:HD3	1.48	0.96
2:B:745:ARG:HH11	2:B:745:ARG:HB3	1.31	0.96
2:A:777:LYS:HD3	2:A:777:LYS:N	1.81	0.95
2:A:186:LEU:HD12	2:A:186:LEU:H	1.30	0.95
2:B:448:ARG:HD3	2:B:448:ARG:N	1.80	0.95
2:A:225:ALA:HA	2:A:252:ILE:HG23	1.48	0.94
2:A:358:GLN:HE22	2:A:405:GLN:HE22	1.10	0.94
2:B:382:VAL:HG22	2:B:516:LEU:HA	1.48	0.94
2:B:494:LEU:HD23	2:B:494:LEU:H	1.31	0.94
2:A:448:ARG:H	2:A:448:ARG:CD	1.82	0.93
2:A:159:ARG:O	2:A:163:GLU:HB2	1.69	0.93
2:A:382:VAL:HG21	2:A:516:LEU:HD12	1.46	0.92
2:A:224:GLN:HE22	2:A:304:ARG:HH22	1.01	0.92
2:B:220:VAL:HG12	2:B:270:LYS:HZ1	1.34	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:805:GLN:H	2:B:805:GLN:HE21	1.17	0.92
2:B:248:THR:HG23	2:B:249:GLU:N	1.84	0.92
2:A:50:HIS:HD2	2:A:52:GLY:H	1.16	0.91
1:D:918:G:O6	2:B:833:PRO:HD2	1.70	0.91
2:B:201:ARG:HE	2:B:211:GLU:HB3	1.36	0.91
2:B:248:THR:HG23	2:B:250:VAL:H	1.33	0.91
1:D:932:U:HO2'	1:D:933:C:H5	1.13	0.91
2:B:210:ILE:HD13	2:B:238:LEU:HD13	1.53	0.91
2:A:220:VAL:HG12	2:A:270:LYS:HZ1	1.34	0.90
2:B:245:ILE:HB	2:B:248:THR:CG2	2.00	0.90
2:A:777:LYS:H	2:A:777:LYS:CD	1.84	0.90
2:B:245:ILE:HB	2:B:248:THR:HG21	1.53	0.90
2:B:246:PRO:O	2:B:247:LEU:HB2	1.71	0.90
2:B:522:LEU:HD11	2:B:564:ASP:HB3	1.54	0.90
2:A:171:ARG:HH22	2:A:364:ARG:HH22	1.19	0.89
2:A:855:ARG:NH2	2:B:810:LYS:HE2	1.86	0.89
1:C:928:C:C2'	1:C:929:G:H5''	2.03	0.88
2:B:295:ASN:HD21	2:B:299:ARG:HB2	1.39	0.88
2:A:224:GLN:NE2	2:A:304:ARG:HH22	1.72	0.88
2:A:388:LYS:H	2:A:388:LYS:HZ2	0.91	0.88
2:B:5:LYS:H	2:B:5:LYS:HD2	1.36	0.88
2:B:421:GLN:HE21	2:B:421:GLN:N	1.71	0.88
2:B:382:VAL:CG2	2:B:383:PRO:HD3	2.04	0.87
2:B:388:LYS:H	2:B:388:LYS:HD2	1.37	0.87
2:A:529:MET:HE2	2:A:536:VAL:HA	1.54	0.87
2:B:248:THR:HG23	2:B:249:GLU:H	1.38	0.87
2:A:201:ARG:HG2	2:A:211:GLU:HB3	1.55	0.86
2:B:789:ARG:HB2	2:B:789:ARG:HH11	1.37	0.86
2:B:248:THR:OG1	2:B:250:VAL:HG23	1.76	0.86
2:A:245:ILE:O	2:A:248:THR:HG22	1.76	0.86
2:B:101:THR:HG22	2:B:104:ASP:OD2	1.75	0.86
2:B:777:LYS:H	2:B:777:LYS:CE	1.88	0.86
2:A:83:ALA:HB1	2:A:86:ALA:HB3	1.58	0.86
2:A:352:GLU:HG2	2:A:353:TYR:H	1.41	0.85
2:B:307:GLU:C	2:B:309:LEU:H	1.82	0.85
2:A:5:LYS:H	2:A:5:LYS:HD2	1.40	0.85
2:B:358:GLN:HE22	2:B:405:GLN:HE22	1.19	0.85
2:B:98:GLU:HG3	2:B:99:GLY:H	1.42	0.85
2:A:382:VAL:CG2	2:A:516:LEU:HA	2.06	0.84
2:A:178:ARG:HG2	2:A:347:CYS:SG	2.18	0.84
2:B:201:ARG:NE	2:B:211:GLU:HB3	1.91	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:494:LEU:H	2:A:494:LEU:CD2	1.90	0.84
2:B:361:LEU:HD12	2:B:402:ILE:HD11	1.58	0.83
2:A:751:GLU:HB2	2:A:785:ARG:HH21	1.41	0.83
2:B:823:LEU:HD12	2:B:829:ARG:NH1	1.93	0.83
2:A:171:ARG:HD2	4:A:1088:HOH:O	1.79	0.83
2:A:277:PRO:HD3	2:A:353:TYR:CE2	2.12	0.83
2:A:486:VAL:HG22	2:A:516:LEU:HD23	1.60	0.83
1:D:936:A:H4'	1:D:937:C:O5'	1.78	0.83
2:A:388:LYS:H	2:A:388:LYS:NZ	1.75	0.83
2:B:312:LEU:HG	2:B:313:ASP:H	1.41	0.83
2:B:201:ARG:HH11	2:B:332:VAL:HG11	1.44	0.82
2:A:593:ARG:HG3	2:A:593:ARG:HH11	1.45	0.82
2:B:789:ARG:HB2	2:B:789:ARG:NH1	1.94	0.82
2:B:777:LYS:HE3	2:B:777:LYS:N	1.92	0.82
2:B:324:LEU:H	2:B:324:LEU:HD22	1.44	0.82
2:B:516:LEU:HD12	2:B:628:LEU:HD13	1.62	0.82
2:A:499:MET:CE	2:A:512:PHE:HE2	1.93	0.81
2:B:277:PRO:HD3	2:B:353:TYR:CE2	2.16	0.81
2:A:176:CYS:SG	2:A:178:ARG:HB3	2.20	0.81
2:A:28:ASN:ND2	2:A:30:LYS:HG2	1.95	0.81
1:C:936:A:H4'	1:C:937:C:O5'	1.81	0.81
2:B:100:LYS:HB3	2:B:104:ASP:OD2	1.82	0.80
2:B:201:ARG:HD3	2:B:332:VAL:HG21	1.62	0.80
2:A:171:ARG:HH12	2:A:364:ARG:HH21	1.28	0.80
2:B:202:TYR:HE1	2:B:330:HIS:ND1	1.80	0.80
2:B:304:ARG:HG3	2:B:304:ARG:HH11	1.46	0.80
2:B:374:LEU:HD12	2:B:374:LEU:H	1.47	0.80
1:C:964:C:H2'	1:C:965:G:H8	1.48	0.79
2:A:382:VAL:HG22	2:A:516:LEU:HA	1.64	0.79
2:B:202:TYR:HE1	2:B:330:HIS:CG	1.99	0.79
2:A:540:LEU:HA	2:A:543:VAL:CG1	2.12	0.79
2:A:45:VAL:HG23	2:A:81:ASP:O	1.83	0.79
2:A:281:GLU:O	2:A:285:ARG:HG3	1.83	0.79
2:A:436:THR:HA	4:A:1040:HOH:O	1.82	0.79
2:B:361:LEU:HD21	2:B:366:LEU:HD11	1.65	0.79
2:B:388:LYS:HD2	2:B:388:LYS:N	1.98	0.78
2:B:352:GLU:HG2	2:B:353:TYR:H	1.48	0.78
2:A:248:THR:HG23	2:A:250:VAL:H	1.49	0.78
2:B:118:LYS:HD3	2:B:143:PHE:CZ	2.18	0.78
2:B:248:THR:CG2	2:B:250:VAL:H	1.95	0.78
2:A:82:HIS:CD2	2:A:145:MET:HE2	2.18	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:426:PRO:HG3	2:A:435:PRO:HD3	1.66	0.78
2:A:503:GLY:HA3	2:A:511:PRO:HG3	1.65	0.78
2:A:326:ARG:HG3	2:A:327:GLU:N	1.99	0.77
2:B:438:CYS:SG	2:B:441:CYS:HB3	2.24	0.77
2:B:522:LEU:HD12	2:B:522:LEU:N	1.99	0.77
2:B:677:LYS:HD2	2:B:706:PRO:HG3	1.66	0.77
2:B:680:HIS:HD2	2:B:687:THR:CG2	1.98	0.77
2:A:438:CYS:SG	2:A:440:ALA:HB3	2.25	0.77
2:A:210:ILE:HD13	2:A:238:LEU:HD13	1.66	0.76
2:A:245:ILE:HG12	2:A:248:THR:CG2	2.15	0.76
2:B:1:MET:HE1	2:B:690:LEU:HD23	1.67	0.76
2:B:382:VAL:HG21	2:B:516:LEU:HA	1.65	0.76
2:B:805:GLN:HE21	2:B:805:GLN:N	1.81	0.76
2:A:416:TYR:CE2	2:A:423:VAL:HG12	2.20	0.76
2:A:343:THR:HB	2:A:348:GLY:O	1.86	0.76
2:B:68:ARG:HB2	2:B:74:ALA:HB2	1.67	0.76
2:B:819:SER:O	2:B:823:LEU:HD23	1.85	0.76
2:A:169:ALA:O	2:A:357:PRO:HA	1.85	0.76
2:B:201:ARG:HG3	2:B:332:VAL:HG11	1.67	0.75
2:B:225:ALA:HA	2:B:252:ILE:CG2	2.14	0.75
2:B:358:GLN:NE2	2:B:405:GLN:HE22	1.85	0.75
2:A:557:TYR:CE1	2:A:635:ARG:HB3	2.21	0.75
2:B:496:VAL:O	2:B:500:GLU:HG3	1.86	0.75
2:A:275:HIS:CE1	2:A:294:ILE:HG12	2.22	0.75
2:A:304:ARG:HG3	2:A:304:ARG:HH11	1.51	0.75
2:A:733:LYS:NZ	2:A:767:ARG:HB3	2.01	0.75
2:A:320:LYS:O	2:A:324:LEU:HD23	1.86	0.75
2:B:257:ASP:OD1	2:B:282:ILE:HG12	1.87	0.75
2:A:171:ARG:NH2	2:A:364:ARG:NH2	2.33	0.75
2:B:361:LEU:HB2	2:B:402:ILE:HD11	1.68	0.74
2:A:614:LEU:HD22	2:A:671:VAL:HG13	1.69	0.74
2:A:476:LEU:HD23	2:A:476:LEU:O	1.88	0.74
2:B:680:HIS:HA	2:B:687:THR:HG21	1.68	0.74
2:A:245:ILE:CG2	2:A:252:ILE:HD13	2.16	0.74
2:A:473:THR:HG23	2:A:476:LEU:H	1.52	0.74
2:A:201:ARG:HG2	2:A:211:GLU:CB	2.15	0.74
2:A:371:LEU:HD21	2:A:394:LEU:HB2	1.68	0.74
2:B:242:ARG:HE	2:B:251:TRP:HB3	1.52	0.74
2:A:362:ARG:NH2	4:A:1068:HOH:O	2.21	0.74
2:B:113:ARG:HH11	2:B:113:ARG:HB2	1.52	0.74
2:A:188:VAL:HG23	2:A:343:THR:O	1.88	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:202:TYR:O	2:A:210:ILE:HG22	1.87	0.73
2:B:382:VAL:HG23	2:B:383:PRO:HD2	1.65	0.73
2:A:202:TYR:HE1	2:A:330:HIS:CE1	2.07	0.73
2:A:412:ILE:HA	2:A:453:PHE:HE1	1.53	0.73
1:D:932:U:O2'	1:D:933:C:H5	1.70	0.73
2:B:469:TRP:CD1	2:B:507:MET:HE3	2.23	0.73
2:B:818:ARG:HA	2:B:821:ARG:HH12	1.54	0.73
2:A:680:HIS:HA	2:A:687:THR:HG21	1.70	0.73
2:A:388:LYS:HZ2	2:A:388:LYS:N	1.77	0.73
2:B:480:TYR:O	2:B:482:GLY:N	2.21	0.73
2:A:806:GLU:HA	2:A:858:LEU:HD21	1.70	0.73
2:B:161:TYR:CD1	2:B:425:VAL:HB	2.23	0.73
2:A:126:LEU:O	2:A:130:LYS:HG2	1.89	0.72
2:B:201:ARG:CD	2:B:211:GLU:HB3	2.18	0.72
2:B:613:ARG:HH21	2:B:640:LEU:HD13	1.54	0.72
1:C:975:A:H3'	2:A:215:VAL:HG23	1.70	0.72
2:A:496:VAL:O	2:A:500:GLU:HG3	1.89	0.72
2:A:724:GLN:HE22	2:A:785:ARG:H	1.35	0.72
2:A:808:ARG:NH2	2:A:812:LEU:HD21	2.04	0.72
2:A:220:VAL:HG12	2:A:270:LYS:NZ	2.05	0.72
2:A:222:ALA:HB2	2:A:293:VAL:HG13	1.69	0.72
2:A:462:TRP:H	2:A:463:PRO:HD2	1.53	0.72
2:A:332:VAL:HG22	2:A:333:LYS:N	2.02	0.72
2:A:785:ARG:HG3	4:A:1060:HOH:O	1.89	0.72
2:B:245:ILE:O	2:B:247:LEU:N	2.23	0.72
2:B:753:ALA:HB3	2:B:754:PRO:HD3	1.70	0.72
2:A:818:ARG:HA	2:A:821:ARG:HH12	1.55	0.72
2:B:90:VAL:O	2:B:94:LEU:HG	1.90	0.72
2:A:315:PHE:C	2:A:317:ALA:H	1.97	0.72
2:A:448:ARG:HD2	4:A:1082:HOH:O	1.89	0.72
2:A:468:GLY:C	2:A:470:PRO:HD2	2.14	0.71
2:B:202:TYR:O	2:B:210:ILE:HG22	1.90	0.71
2:B:529:MET:HE2	2:B:537:ILE:N	2.05	0.71
1:D:937:C:O2'	1:D:938:G:OP1	2.05	0.71
2:A:289:LYS:H	2:A:289:LYS:HD3	1.54	0.71
2:B:584:ASN:HA	2:B:587:ARG:HB3	1.72	0.71
2:B:83:ALA:HB1	2:B:86:ALA:HB3	1.71	0.71
2:A:50:HIS:CD2	2:A:52:GLY:H	2.05	0.71
2:B:448:ARG:H	2:B:448:ARG:CD	1.94	0.71
2:A:543:VAL:HG23	2:A:548:ALA:N	2.06	0.71
2:A:714:GLU:HG3	2:A:715:ALA:H	1.54	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:293:VAL:HA	2:B:301:GLU:O	1.91	0.70
2:A:118:LYS:HD2	2:A:118:LYS:O	1.90	0.70
2:A:680:HIS:HD2	2:A:684:PRO:HA	1.55	0.70
2:B:382:VAL:HG11	2:B:516:LEU:HD12	1.72	0.70
2:A:244:ARG:NH2	4:A:1055:HOH:O	2.14	0.70
2:B:153:VAL:HG23	2:B:154:ARG:N	2.05	0.70
2:B:305:VAL:HG13	2:B:310:ARG:HD3	1.71	0.70
2:A:242:ARG:O	2:A:243:ALA:HB2	1.92	0.70
2:B:818:ARG:HA	2:B:821:ARG:NH1	2.06	0.70
2:A:50:HIS:HD2	2:A:52:GLY:N	1.88	0.70
2:B:751:GLU:HB2	2:B:785:ARG:HH21	1.55	0.70
2:A:313:ASP:O	2:A:317:ALA:HB2	1.92	0.70
2:A:387:LYS:HG2	2:A:391:MET:HE2	1.71	0.70
2:A:431:TYR:CE1	2:A:432:LEU:HD12	2.27	0.70
2:B:383:PRO:HB2	2:B:386:TRP:CD1	2.27	0.70
2:B:416:TYR:HA	2:B:422:ALA:O	1.91	0.70
2:A:733:LYS:HZ1	2:A:767:ARG:HB3	1.57	0.70
2:A:460:ALA:HB2	2:A:498:ARG:HB3	1.74	0.69
2:B:149:ARG:HG3	2:B:465:SER:OG	1.91	0.69
2:B:242:ARG:O	2:B:243:ALA:HB2	1.91	0.69
2:B:7:TYR:CZ	2:B:686:LEU:HD13	2.26	0.69
2:A:45:VAL:HG11	2:A:118:LYS:HA	1.75	0.69
2:A:522:LEU:HB3	2:A:528:LYS:HA	1.73	0.69
2:A:834:LYS:H	2:A:834:LYS:HD2	1.57	0.69
2:A:201:ARG:CG	2:A:211:GLU:HB3	2.22	0.69
2:A:358:GLN:NE2	2:A:405:GLN:HE22	1.88	0.69
1:D:973:C:H1'	2:B:278:LEU:HB2	1.73	0.69
2:A:224:GLN:NE2	2:A:291:VAL:HG11	2.08	0.69
2:B:170:PRO:O	2:B:355:ILE:HG23	1.93	0.69
1:C:957:A:H4'	1:C:958:G:OP1	1.92	0.69
2:A:306:PRO:HG2	2:A:309:LEU:HB3	1.73	0.69
2:B:322:VAL:O	2:B:325:PHE:HB2	1.92	0.69
2:B:361:LEU:HB2	2:B:402:ILE:CD1	2.22	0.69
2:B:372:LYS:NZ	2:B:372:LYS:HA	2.07	0.69
2:B:802:ARG:HB2	2:B:802:ARG:HH11	1.58	0.69
2:A:7:TYR:HB2	2:A:583:TYR:CD2	2.27	0.69
2:A:304:ARG:HG3	2:A:304:ARG:NH1	2.07	0.69
2:A:610:MET:HG2	2:A:649:TYR:CD2	2.27	0.69
2:A:205:GLU:HB2	2:A:242:ARG:HB2	1.72	0.69
2:A:43:PRO:HB2	2:A:125:ILE:HD13	1.75	0.68
2:B:680:HIS:CD2	2:B:684:PRO:HA	2.28	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:312:LEU:HD21	2:A:316:GLU:HG2	1.75	0.68
2:B:248:THR:CG2	2:B:249:GLU:H	1.97	0.68
2:B:464:LEU:HB3	2:B:469:TRP:CB	2.24	0.68
2:A:807:LYS:O	2:A:811:GLU:HG3	1.92	0.68
2:B:145:MET:HG3	2:B:410:HIS:CD2	2.27	0.68
2:B:201:ARG:HD2	2:B:211:GLU:HB3	1.75	0.68
2:A:394:LEU:O	2:A:397:VAL:HG23	1.92	0.68
2:A:680:HIS:CD2	2:A:684:PRO:HA	2.28	0.68
2:B:307:GLU:C	2:B:309:LEU:N	2.51	0.68
2:B:352:GLU:HG2	2:B:353:TYR:N	2.06	0.68
2:B:745:ARG:HB3	2:B:745:ARG:NH1	2.06	0.68
2:A:412:ILE:HA	2:A:453:PHE:CE1	2.27	0.68
2:A:549:ASP:HB3	2:A:683:MET:HE2	1.74	0.68
2:A:593:ARG:HG3	2:A:593:ARG:NH1	2.07	0.68
2:B:421:GLN:HE21	2:B:421:GLN:H	1.40	0.68
2:A:712:ASP:HB3	2:A:715:ALA:HB3	1.75	0.68
2:B:295:ASN:ND2	2:B:299:ARG:HB2	2.09	0.68
2:B:420:CYS:SG	2:B:422:ALA:HB2	2.32	0.68
2:B:462:TRP:H	2:B:463:PRO:CD	2.07	0.68
2:A:300:MET:HB2	2:A:311:GLY:H	1.57	0.68
2:A:540:LEU:CA	2:A:543:VAL:HG12	2.21	0.68
2:B:13:GLU:HA	2:B:685:PHE:HD2	1.59	0.68
2:A:492:LEU:O	2:A:492:LEU:HG	1.92	0.68
2:B:1:MET:HE3	2:B:693:ALA:CB	2.24	0.68
2:B:245:ILE:HB	2:B:248:THR:HG22	1.76	0.68
2:B:421:GLN:HE21	2:B:421:GLN:CA	2.06	0.68
2:B:783:MET:HE3	2:B:783:MET:HA	1.76	0.68
2:A:171:ARG:NH1	2:A:364:ARG:HH21	1.90	0.68
2:B:47:GLY:H	2:B:117:TRP:HZ2	1.39	0.68
2:B:464:LEU:HB3	2:B:469:TRP:HB3	1.75	0.68
2:A:216:ARG:HB3	2:A:219:THR:HG23	1.76	0.67
2:A:845:LYS:O	2:A:849:GLU:HG3	1.93	0.67
2:B:409:GLY:HA3	2:B:452:VAL:CG1	2.24	0.67
2:A:401:ASN:HD22	2:A:402:ILE:N	1.92	0.67
2:B:7:TYR:HB2	2:B:583:TYR:CD2	2.28	0.67
2:B:387:LYS:HG2	2:B:388:LYS:HE2	1.75	0.67
2:A:170:PRO:HA	2:A:356:PHE:O	1.94	0.67
2:B:802:ARG:O	2:B:806:GLU:HB2	1.95	0.67
2:A:183:LEU:HD21	2:A:344:CYS:SG	2.35	0.67
2:A:297:GLU:N	2:A:297:GLU:OE1	2.28	0.67
2:A:382:VAL:HG21	2:A:516:LEU:HA	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:415:TRP:HA	2:B:447:LYS:O	1.95	0.67
2:B:529:MET:HE2	2:B:536:VAL:HA	1.76	0.67
2:A:591:LEU:O	2:A:594:GLU:HB2	1.94	0.66
2:B:415:TRP:O	2:B:424:ASN:N	2.24	0.66
2:B:593:ARG:HB2	2:B:665:LEU:HD21	1.76	0.66
2:B:830:GLU:C	2:B:831:LYS:HE3	2.20	0.66
2:A:225:ALA:HA	2:A:252:ILE:CG2	2.25	0.66
2:B:304:ARG:HG3	2:B:304:ARG:NH1	2.08	0.66
2:B:372:LYS:HA	2:B:372:LYS:HZ3	1.58	0.66
2:A:162:HIS:NE2	2:A:425:VAL:O	2.20	0.66
2:B:501:VAL:HG13	2:B:502:SER:N	2.10	0.66
2:A:167:TYR:CE2	2:A:360:TRP:HB2	2.30	0.66
2:B:221:PHE:O	2:B:304:ARG:NH1	2.28	0.66
2:A:383:PRO:HB2	2:A:386:TRP:CD1	2.30	0.66
2:B:312:LEU:HG	2:B:313:ASP:N	2.10	0.66
2:B:382:VAL:CG2	2:B:383:PRO:CD	2.62	0.66
2:B:303:GLU:OE2	2:B:303:GLU:HA	1.94	0.66
2:B:778:ALA:HB1	2:B:790:MET:O	1.95	0.66
2:A:833:PRO:C	2:A:835:GLU:H	2.04	0.66
2:A:224:GLN:HE21	2:A:291:VAL:HG11	1.61	0.66
2:A:494:LEU:HD23	2:A:494:LEU:N	1.97	0.66
1:C:918:G:O6	2:A:833:PRO:HD3	1.96	0.66
2:A:157:PHE:HD2	2:A:413:PRO:HG2	1.60	0.66
2:B:41:PRO:HD2	2:B:60:GLN:HE22	1.60	0.66
2:A:316:GLU:OE1	2:A:319:ARG:HD2	1.96	0.66
2:B:193:THR:CG2	2:B:194:PRO:HD2	2.26	0.66
2:B:169:ALA:O	2:B:357:PRO:HA	1.96	0.65
2:B:388:LYS:HB3	4:B:1032:HOH:O	1.96	0.65
2:B:473:THR:HG23	2:B:476:LEU:H	1.61	0.65
2:B:771:LEU:HD13	2:B:772:PRO:HD2	1.77	0.65
2:A:855:ARG:HD3	2:B:813:LEU:HD12	1.79	0.65
2:B:167:TYR:CE2	2:B:360:TRP:HB2	2.31	0.65
2:B:494:LEU:H	2:B:494:LEU:CD2	2.05	0.65
2:A:23:ASN:HB3	4:A:1005:HOH:O	1.97	0.65
2:A:86:ALA:HA	2:A:346:ARG:HD3	1.77	0.65
2:A:289:LYS:HD3	2:A:289:LYS:N	2.12	0.65
2:A:401:ASN:HD22	2:A:401:ASN:C	2.03	0.65
2:B:260:VAL:HG22	2:B:269:LEU:CD2	2.25	0.65
2:B:529:MET:HE2	2:B:537:ILE:H	1.61	0.65
2:B:349:THR:HG23	2:B:350:PRO:HD2	1.79	0.65
2:B:651:GLU:OE1	2:B:654:LYS:HE3	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:522:LEU:HD12	2:A:566:ARG:HA	1.79	0.65
2:B:371:LEU:HD21	2:B:394:LEU:HB2	1.76	0.65
2:A:153:VAL:HG23	2:A:154:ARG:N	2.10	0.65
2:A:358:GLN:HE22	2:A:405:GLN:NE2	1.90	0.65
2:B:188:VAL:HG23	2:B:343:THR:O	1.97	0.65
2:B:468:GLY:C	2:B:470:PRO:HD2	2.21	0.65
2:A:429:GLU:CD	2:A:429:GLU:H	2.04	0.64
2:B:190:THR:HG22	2:B:342:ALA:HB2	1.78	0.64
2:B:414:ALA:HA	2:B:425:VAL:HG22	1.79	0.64
2:B:480:TYR:O	2:B:481:PRO:C	2.39	0.64
2:A:47:GLY:H	2:A:117:TRP:HZ2	1.45	0.64
2:A:242:ARG:NH1	2:A:251:TRP:HB3	2.12	0.64
2:B:415:TRP:CE3	2:B:448:ARG:HB3	2.32	0.64
2:B:480:TYR:HB3	2:B:481:PRO:HD3	1.80	0.64
2:B:272:THR:H	2:B:279:ASP:HB3	1.62	0.64
2:A:186:LEU:H	2:A:186:LEU:CD1	2.09	0.64
2:B:50:HIS:HD2	2:B:52:GLY:H	1.45	0.64
2:B:306:PRO:HD2	2:B:309:LEU:HD23	1.78	0.64
2:B:588:PHE:CD2	2:B:650:LEU:HD11	2.32	0.64
2:A:154:ARG:HD2	4:A:1058:HOH:O	1.98	0.64
2:A:294:ILE:HG22	2:A:300:MET:SD	2.37	0.64
2:B:201:ARG:NH1	2:B:332:VAL:HG11	2.13	0.64
2:B:275:HIS:HE1	2:B:294:ILE:HB	1.63	0.64
2:B:220:VAL:HA	2:B:223:ASP:OD2	1.97	0.64
2:B:161:TYR:C	2:B:163:GLU:H	2.06	0.64
2:B:179:CYS:O	2:B:181:THR:HG22	1.95	0.64
2:B:415:TRP:CZ3	2:B:448:ARG:HB3	2.33	0.64
2:A:245:ILE:HG22	2:A:252:ILE:HD13	1.79	0.64
1:D:918:G:H21	1:D:956:A:H1'	1.64	0.63
2:A:66:TYR:O	2:A:70:ARG:HB2	1.97	0.63
2:A:326:ARG:HB3	2:A:331:LEU:HD23	1.80	0.63
2:B:488:GLY:O	2:B:490:ASP:N	2.31	0.63
2:B:278:LEU:O	2:B:281:GLU:HB3	1.98	0.63
2:B:307:GLU:O	2:B:309:LEU:N	2.31	0.63
2:A:248:THR:CG2	2:A:250:VAL:H	2.11	0.63
2:B:398:LYS:HD2	2:B:398:LYS:N	2.14	0.63
1:D:959:U:H5''	1:D:960:C:OP2	1.99	0.63
2:A:160:TYR:HB3	2:A:166:ALA:HB2	1.80	0.63
2:A:416:TYR:HE2	2:A:423:VAL:HG12	1.62	0.63
2:A:810:LYS:HG3	2:B:855:ARG:NH2	2.14	0.63
2:B:50:HIS:HD2	2:B:52:GLY:N	1.96	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:83:ALA:HB3	2:B:87:THR:OG1	1.99	0.63
2:B:651:GLU:OE1	2:B:651:GLU:HA	1.99	0.63
2:A:256:ALA:O	2:A:257:ASP:HB2	1.99	0.63
2:A:726:VAL:O	2:A:730:ARG:HG2	1.98	0.63
3:A:990:VAA:O	3:A:990:VAA:H5'1	1.98	0.63
1:C:937:C:O2'	1:C:938:G:OP1	2.09	0.63
2:B:50:HIS:CD2	2:B:52:GLY:H	2.16	0.63
2:B:198:TYR:N	2:B:198:TYR:CD2	2.66	0.63
2:B:272:THR:N	2:B:279:ASP:HB3	2.14	0.63
2:B:49:LEU:HD21	2:B:125:ILE:HG23	1.80	0.63
2:B:220:VAL:O	2:B:223:ASP:HB2	1.99	0.62
1:C:928:C:C3'	1:C:929:G:H5''	2.28	0.62
2:A:155:TYR:HD1	2:A:431:TYR:CD2	2.17	0.62
2:B:277:PRO:HD3	2:B:353:TYR:CD2	2.34	0.62
2:B:545:ARG:HB3	2:B:546:TYR:CD1	2.34	0.62
2:B:834:LYS:O	2:B:838:GLU:HG2	2.00	0.62
2:A:497:SER:HA	2:A:500:GLU:OE1	2.00	0.62
2:B:178:ARG:HG3	2:B:179:CYS:SG	2.39	0.62
2:B:374:LEU:HD12	2:B:374:LEU:N	2.15	0.62
2:B:469:TRP:N	2:B:470:PRO:HD2	2.14	0.62
2:A:87:THR:O	2:A:91:VAL:HG23	1.99	0.62
2:B:654:LYS:HB2	2:B:655:PRO:HD3	1.81	0.62
2:A:346:ARG:NH1	2:A:346:ARG:HB2	2.14	0.62
2:A:810:LYS:HE3	2:B:855:ARG:NH2	2.08	0.62
2:B:201:ARG:HH11	2:B:201:ARG:HG3	1.63	0.62
2:B:312:LEU:CG	2:B:313:ASP:H	2.09	0.62
2:B:397:VAL:C	2:B:398:LYS:HD2	2.25	0.62
2:B:501:VAL:HG13	2:B:502:SER:H	1.65	0.62
2:B:374:LEU:H	2:B:374:LEU:CD1	2.13	0.62
2:B:198:TYR:N	2:B:198:TYR:HD2	1.98	0.62
2:B:358:GLN:NE2	2:B:403:SER:HB2	2.15	0.62
2:A:169:ALA:HB1	2:A:170:PRO:CD	2.29	0.62
2:B:159:ARG:O	2:B:163:GLU:HB2	2.00	0.62
2:B:802:ARG:HG3	2:B:803:ARG:N	2.13	0.62
1:C:918:G:N2	1:C:956:A:H1'	2.15	0.62
2:A:714:GLU:HG3	2:A:715:ALA:N	2.14	0.62
2:B:220:VAL:HG21	2:B:325:PHE:HZ	1.64	0.62
2:B:733:LYS:NZ	2:B:733:LYS:HB3	2.15	0.62
2:B:65:ARG:O	2:B:69:MET:HG2	2.00	0.62
2:B:229:HIS:CD2	2:B:231:GLU:H	2.18	0.62
2:B:469:TRP:O	2:B:470:PRO:C	2.39	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:789:ARG:HH11	2:B:789:ARG:CB	2.12	0.62
2:B:44:ASN:HB3	2:B:83:ALA:HB2	1.80	0.61
2:B:82:HIS:HB2	2:B:408:TRP:NE1	2.15	0.61
2:A:845:LYS:NZ	2:B:820:GLN:HE22	1.97	0.61
2:B:370:VAL:HG12	2:B:374:LEU:HD11	1.81	0.61
2:B:591:LEU:O	2:B:594:GLU:HB2	1.99	0.61
2:B:611:ARG:HH22	2:B:666:ARG:HH21	1.48	0.61
2:A:352:GLU:HG2	2:A:353:TYR:N	2.12	0.61
2:A:473:THR:CG2	2:A:476:LEU:H	2.12	0.61
2:A:592:SER:C	2:A:594:GLU:H	2.08	0.61
2:B:3:LEU:HD21	2:B:590:LEU:HD12	1.81	0.61
2:A:732:LEU:HD13	2:A:781:LYS:HB2	1.80	0.61
1:C:973:C:O2	2:A:278:LEU:HD13	2.00	0.61
1:D:931:C:H5''	1:D:932:U:OP2	1.99	0.61
2:B:171:ARG:HH12	2:B:364:ARG:NH2	1.98	0.61
1:D:964:C:H2'	1:D:965:G:H8	1.65	0.61
2:A:198:TYR:N	2:A:198:TYR:CD2	2.68	0.61
2:B:680:HIS:CD2	2:B:687:THR:CG2	2.81	0.61
1:D:933:C:H3'	1:D:933:C:H6	1.65	0.61
2:B:153:VAL:CG2	2:B:154:ARG:N	2.64	0.61
2:A:66:TYR:OH	2:A:70:ARG:NH1	2.34	0.61
2:B:556:ILE:HD12	2:B:682:MET:HG2	1.83	0.61
2:B:805:GLN:N	2:B:805:GLN:NE2	2.47	0.61
1:D:940:G:O2'	1:D:941:A:H5'	2.01	0.61
2:A:244:ARG:HB2	2:A:251:TRP:CZ2	2.36	0.61
1:C:929:G:H5'	1:C:929:G:H8	1.66	0.60
2:A:1:MET:HE2	2:A:693:ALA:CB	2.31	0.60
2:A:94:LEU:O	2:A:98:GLU:HG3	2.01	0.60
2:A:666:ARG:HH11	2:A:666:ARG:HG3	1.65	0.60
2:B:341:LEU:HD13	2:B:341:LEU:C	2.27	0.60
2:A:153:VAL:HG21	2:A:410:HIS:ND1	2.15	0.60
2:A:221:PHE:CD2	2:A:306:PRO:HD3	2.36	0.60
2:A:326:ARG:HG3	2:A:327:GLU:H	1.64	0.60
2:B:162:HIS:NE2	2:B:425:VAL:O	2.31	0.60
2:B:222:ALA:HB2	2:B:293:VAL:HG22	1.82	0.60
2:B:270:LYS:NZ	2:B:270:LYS:CB	2.64	0.60
2:A:171:ARG:HH12	2:A:364:ARG:NH2	1.96	0.60
2:A:95:LEU:O	2:A:98:GLU:HB2	2.01	0.60
2:A:499:MET:HE3	2:A:512:PHE:HE2	1.65	0.60
2:B:540:LEU:O	2:B:543:VAL:HG22	2.01	0.60
2:A:316:GLU:HA	2:A:319:ARG:HH11	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:124:THR:O	2:B:128:GLN:HG3	2.02	0.60
2:B:150:SER:O	2:B:153:VAL:HG22	2.00	0.60
2:B:324:LEU:HD22	2:B:324:LEU:N	2.16	0.60
2:A:248:THR:HG23	2:A:250:VAL:N	2.16	0.60
2:A:401:ASN:C	2:A:401:ASN:ND2	2.60	0.60
2:A:744:VAL:HG11	2:A:790:MET:HE2	1.83	0.60
1:C:961:C:O2'	1:C:962:U:H5'	2.02	0.60
2:A:85:ILE:O	2:A:89:VAL:HG23	2.02	0.60
2:A:201:ARG:CD	2:A:211:GLU:HB3	2.32	0.60
2:A:412:ILE:HB	2:A:453:PHE:CE1	2.36	0.60
1:D:975:A:H3'	2:B:215:VAL:HG23	1.82	0.60
2:B:625:TYR:OH	2:B:682:MET:HE2	2.02	0.60
2:A:245:ILE:HG23	2:A:248:THR:HG21	1.82	0.60
2:A:468:GLY:C	2:A:470:PRO:CD	2.74	0.60
2:B:242:ARG:NE	2:B:251:TRP:HB3	2.16	0.60
2:B:613:ARG:NH2	2:B:640:LEU:HD13	2.16	0.60
1:D:922:A:H2'	1:D:923:G:C8	2.37	0.60
2:A:844:LEU:O	2:A:848:LEU:HD23	2.01	0.60
2:B:248:THR:HG23	2:B:250:VAL:N	2.13	0.60
2:B:326:ARG:HG3	2:B:327:GLU:N	2.17	0.60
2:A:28:ASN:ND2	2:A:30:LYS:H	1.99	0.59
2:A:198:TYR:N	2:A:198:TYR:HD2	1.99	0.59
2:A:387:LYS:HB3	2:A:388:LYS:NZ	2.16	0.59
2:A:498:ARG:HG2	2:A:498:ARG:HH11	1.67	0.59
2:A:529:MET:HE2	2:A:536:VAL:CA	2.31	0.59
2:A:680:HIS:HD2	2:A:687:THR:CG2	2.15	0.59
2:B:469:TRP:C	2:B:471:GLU:N	2.58	0.59
2:B:161:TYR:CE1	2:B:425:VAL:HB	2.37	0.59
2:B:289:LYS:H	2:B:289:LYS:HD2	1.66	0.59
2:B:126:LEU:O	2:B:130:LYS:HG2	2.01	0.59
2:B:1:MET:HE1	2:B:690:LEU:HA	1.84	0.59
2:B:382:VAL:O	2:B:383:PRO:C	2.39	0.59
2:A:4:PRO:HD2	2:A:583:TYR:OH	2.02	0.59
2:B:172:LEU:HD23	2:B:354:ALA:O	2.02	0.59
2:A:46:THR:HG22	2:A:90:VAL:HG21	1.85	0.59
2:A:124:THR:O	2:A:128:GLN:HG3	2.02	0.59
2:B:40:MET:HA	2:B:60:GLN:HE22	1.68	0.59
2:B:238:LEU:O	2:B:254:ILE:HG21	2.02	0.59
2:B:383:PRO:HB2	2:B:386:TRP:HD1	1.67	0.59
1:D:927:U:O2'	1:D:928:C:H5'	2.02	0.59
2:A:153:VAL:CG2	2:A:154:ARG:N	2.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:228:VAL:O	2:B:256:ALA:HA	2.03	0.59
1:C:935:C:H1'	2:A:584:ASN:ND2	2.17	0.59
2:B:88:GLN:HG3	2:B:406:LEU:HD22	1.85	0.59
2:B:346:ARG:HB2	2:B:346:ARG:CZ	2.33	0.59
2:A:495:TRP:NE1	3:A:990:VAA:HG21	2.17	0.59
2:B:383:PRO:HG2	4:B:1003:HOH:O	2.02	0.59
2:A:245:ILE:H	2:A:248:THR:CG2	2.16	0.58
2:A:855:ARG:HG3	2:B:809:LEU:CD1	2.33	0.58
2:B:409:GLY:HA3	2:B:452:VAL:HG13	1.84	0.58
2:B:617:GLY:HA3	2:B:640:LEU:HD22	1.84	0.58
2:A:264:PHE:CD2	2:A:265:GLY:N	2.71	0.58
2:A:314:ARG:NH2	2:A:352:GLU:HG3	2.18	0.58
2:A:364:ARG:HD2	4:A:1056:HOH:O	2.02	0.58
2:B:738:LEU:HD23	2:B:744:VAL:HG11	1.84	0.58
2:B:13:GLU:HA	2:B:685:PHE:CD2	2.37	0.58
1:D:918:G:O6	2:B:833:PRO:CD	2.46	0.58
2:A:145:MET:HG2	2:A:410:HIS:CD2	2.38	0.58
2:B:201:ARG:HG3	2:B:201:ARG:NH1	2.18	0.58
2:B:366:LEU:HB3	2:B:501:VAL:CG2	2.33	0.58
2:A:220:VAL:HA	2:A:270:LYS:HE3	1.85	0.58
2:B:246:PRO:O	2:B:247:LEU:CB	2.48	0.58
2:B:202:TYR:CE1	2:B:330:HIS:CG	2.87	0.58
2:B:315:PHE:C	2:B:317:ALA:H	2.10	0.58
2:B:391:MET:O	2:B:395:GLU:HB2	2.04	0.58
2:B:837:VAL:O	2:B:841:GLU:HG3	2.02	0.58
2:A:202:TYR:HE1	2:A:330:HIS:ND1	2.00	0.58
2:A:469:TRP:O	2:A:470:PRO:C	2.40	0.58
2:B:324:LEU:H	2:B:324:LEU:CD2	2.15	0.58
2:A:28:ASN:HD22	2:A:28:ASN:C	2.11	0.58
2:A:293:VAL:HG23	2:A:294:ILE:HG23	1.85	0.58
2:B:109:LYS:O	2:B:112:GLU:HB2	2.03	0.58
2:B:151:ARG:HG2	2:B:151:ARG:HH11	1.68	0.58
2:B:666:ARG:NH2	4:B:1047:HOH:O	2.33	0.58
2:B:170:PRO:HA	2:B:356:PHE:O	2.04	0.58
2:A:398:LYS:O	2:A:399:ASP:C	2.47	0.58
2:B:197:LEU:HB2	2:B:337:TYR:HB2	1.85	0.58
2:B:281:GLU:O	2:B:285:ARG:HG3	2.03	0.58
2:B:522:LEU:HD12	2:B:522:LEU:H	1.68	0.58
2:A:684:PRO:O	2:A:687:THR:HG22	2.03	0.57
2:A:3:LEU:HD21	2:A:590:LEU:HD12	1.85	0.57
2:A:170:PRO:O	2:A:355:ILE:HG23	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:315:PHE:C	2:A:317:ALA:N	2.63	0.57
2:A:462:TRP:C	2:A:464:LEU:H	2.11	0.57
2:A:680:HIS:CD2	2:A:687:THR:HG21	2.38	0.57
2:B:456:TRP:CE3	2:B:494:LEU:O	2.57	0.57
2:B:600:GLU:HG2	2:B:601:ASP:N	2.20	0.57
2:B:412:ILE:HA	2:B:453:PHE:CE1	2.40	0.57
2:A:131:ARG:HD2	2:A:131:ARG:O	2.05	0.57
2:A:248:THR:OG1	2:A:250:VAL:HG23	2.05	0.57
2:B:312:LEU:O	2:B:313:ASP:O	2.23	0.57
2:B:454:ASP:O	2:B:457:PHE:N	2.31	0.57
2:A:280:TYR:O	2:A:284:GLU:HG2	2.04	0.57
2:A:714:GLU:CG	2:A:715:ALA:H	2.17	0.57
2:B:245:ILE:O	2:B:248:THR:HG22	2.04	0.57
2:B:371:LEU:HD21	2:B:394:LEU:CB	2.34	0.57
2:B:492:LEU:HD12	2:B:496:VAL:HB	1.87	0.57
2:A:202:TYR:OH	2:A:244:ARG:NH2	2.38	0.57
2:A:282:ILE:HA	2:A:285:ARG:CD	2.21	0.57
2:A:395:GLU:HA	2:A:395:GLU:OE2	2.04	0.57
2:B:245:ILE:HG13	2:B:252:ILE:HD13	1.85	0.57
2:B:266:THR:O	2:B:268:ALA:N	2.38	0.57
2:A:5:LYS:HD2	2:A:5:LYS:N	2.16	0.57
2:A:169:ALA:HB1	2:A:170:PRO:HD2	1.87	0.57
2:A:188:VAL:HG21	2:A:351:ILE:HD13	1.86	0.57
2:B:36:PHE:CD1	2:B:67:LYS:HG3	2.39	0.57
2:B:69:MET:HE1	2:B:680:HIS:ND1	2.20	0.57
2:B:148:LYS:HD2	2:B:468:GLY:HA2	1.87	0.57
2:B:473:THR:HG22	2:B:476:LEU:HB3	1.86	0.57
2:B:151:ARG:HG2	2:B:151:ARG:NH1	2.20	0.56
2:B:759:LEU:CD1	2:B:763:ARG:HE	2.18	0.56
2:A:289:LYS:H	2:A:289:LYS:CD	2.18	0.56
2:A:415:TRP:CE3	2:A:448:ARG:HB3	2.40	0.56
2:A:456:TRP:HB3	2:A:498:ARG:HH12	1.70	0.56
2:B:9:PRO:C	2:B:11:SER:H	2.14	0.56
2:B:51:MET:HE2	2:B:537:ILE:HB	1.87	0.56
2:B:172:LEU:HB2	2:B:280:TYR:CD1	2.41	0.56
2:B:230:PRO:HG2	2:B:258:PRO:HG3	1.86	0.56
2:B:382:VAL:C	2:B:384:GLU:N	2.63	0.56
2:B:823:LEU:HD11	2:B:841:GLU:HG2	1.87	0.56
2:A:4:PRO:O	2:A:587:ARG:NE	2.38	0.56
2:A:415:TRP:O	2:A:424:ASN:N	2.36	0.56
2:B:270:LYS:HZ3	2:B:270:LYS:HB3	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:473:THR:CG2	2:B:476:LEU:H	2.17	0.56
2:A:13:GLU:OE2	2:A:548:ALA:HB3	2.06	0.56
2:B:260:VAL:HG22	2:B:269:LEU:HD21	1.87	0.56
2:B:382:VAL:HG21	2:B:516:LEU:CA	2.36	0.56
2:A:157:PHE:HD2	2:A:413:PRO:CG	2.18	0.56
2:B:7:TYR:CE2	2:B:686:LEU:HD13	2.39	0.56
2:A:84:GLY:HA3	2:A:455:THR:OG1	2.04	0.56
2:A:107:ARG:HA	2:A:407:TRP:CZ3	2.40	0.56
2:A:467:LEU:O	2:A:473:THR:CG2	2.54	0.56
2:A:777:LYS:O	2:A:778:ALA:HB2	2.06	0.56
2:B:680:HIS:HB3	2:B:681:PRO:HD3	1.88	0.56
2:B:777:LYS:HD2	2:B:777:LYS:O	2.05	0.56
2:A:65:ARG:O	2:A:69:MET:HG2	2.05	0.56
2:A:317:ALA:O	2:A:321:ALA:HB2	2.06	0.56
2:B:724:GLN:HB3	2:B:783:MET:HG2	1.87	0.56
2:A:157:PHE:CD2	2:A:413:PRO:HG2	2.41	0.56
2:A:199:THR:HA	2:A:212:ILE:O	2.07	0.56
1:D:975:A:H8	2:B:213:ALA:O	1.89	0.55
2:A:105:LEU:O	2:A:106:GLY:O	2.24	0.55
2:A:245:ILE:HG12	2:A:248:THR:HB	1.88	0.55
2:A:855:ARG:HG3	2:B:809:LEU:HD12	1.88	0.55
2:B:217:PRO:HD2	2:B:318:ARG:HE	1.71	0.55
2:A:260:VAL:HG22	2:A:269:LEU:HD21	1.88	0.55
2:A:408:TRP:O	2:A:409:GLY:O	2.24	0.55
2:A:579:ALA:HB2	2:A:683:MET:HE1	1.88	0.55
1:D:917:G:H4'	1:D:918:G:OP1	2.06	0.55
1:D:922:A:H2'	1:D:923:G:H8	1.72	0.55
2:B:201:ARG:CD	2:B:332:VAL:HG21	2.33	0.55
2:B:714:GLU:O	2:B:717:ARG:HB3	2.05	0.55
2:A:170:PRO:O	2:A:171:ARG:O	2.24	0.55
2:A:202:TYR:OH	2:A:244:ARG:CZ	2.53	0.55
2:A:343:THR:HA	2:A:350:PRO:HA	1.88	0.55
2:A:412:ILE:HG13	2:A:413:PRO:HD2	1.88	0.55
2:A:424:ASN:ND2	2:A:446:LEU:HD21	2.21	0.55
2:A:480:TYR:HB3	2:A:481:PRO:HD3	1.89	0.55
2:A:557:TYR:O	2:A:635:ARG:NH2	2.36	0.55
2:B:306:PRO:O	2:B:309:LEU:HB3	2.05	0.55
2:B:462:TRP:C	2:B:464:LEU:H	2.15	0.55
2:A:96:LEU:C	2:A:98:GLU:H	2.14	0.55
2:A:307:GLU:C	2:A:309:LEU:H	2.14	0.55
2:A:747:TYR:CE2	2:A:749:GLU:HG2	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:114:VAL:HG11	2:B:408:TRP:CE3	2.42	0.55
2:B:202:TYR:CE1	2:B:330:HIS:ND1	2.69	0.55
2:B:445:ARG:HB2	4:B:1037:HOH:O	2.06	0.55
2:A:146:ASP:OD1	2:A:149:ARG:HB2	2.06	0.55
1:C:965:G:H2'	1:C:966:C:C6	2.42	0.55
2:A:172:LEU:HD23	2:A:354:ALA:O	2.07	0.55
2:A:711:ARG:HG2	2:A:711:ARG:HH11	1.72	0.55
2:B:805:GLN:H	2:B:805:GLN:NE2	1.96	0.55
2:B:830:GLU:HG2	2:B:831:LYS:NZ	2.22	0.55
2:A:467:LEU:O	2:A:473:THR:HG21	2.07	0.55
2:A:837:VAL:HG13	2:A:838:GLU:N	2.21	0.55
2:B:2:ASP:O	2:B:4:PRO:HD3	2.06	0.55
2:B:146:ASP:OD1	2:B:149:ARG:HB2	2.07	0.55
2:B:153:VAL:CG2	2:B:154:ARG:H	2.20	0.55
2:A:221:PHE:CE2	2:A:306:PRO:HD3	2.42	0.54
2:A:307:GLU:CD	2:A:307:GLU:H	2.15	0.54
2:A:680:HIS:CD2	2:A:687:THR:CG2	2.90	0.54
2:B:416:TYR:CD2	2:B:423:VAL:HG22	2.42	0.54
1:C:931:C:H2'	1:C:931:C:O2	2.08	0.54
2:A:49:LEU:HG	2:A:128:GLN:OE1	2.07	0.54
2:A:51:MET:HE3	2:A:537:ILE:HB	1.88	0.54
2:A:282:ILE:CA	2:A:285:ARG:HD3	2.22	0.54
2:A:759:LEU:HD12	2:A:763:ARG:HD2	1.89	0.54
2:B:35:PRO:HA	2:B:73:GLU:HB2	1.88	0.54
2:B:242:ARG:HH21	2:B:251:TRP:HB2	1.72	0.54
2:A:462:TRP:C	2:A:464:LEU:N	2.64	0.54
2:B:270:LYS:CB	2:B:270:LYS:HZ3	2.20	0.54
2:B:462:TRP:H	2:B:463:PRO:HD2	1.71	0.54
1:C:964:C:H2'	1:C:965:G:C8	2.36	0.54
2:B:179:CYS:C	2:B:180:GLU:HG2	2.31	0.54
2:A:27:ALA:O	2:A:140:ARG:NH2	2.41	0.54
2:A:196:LYS:HB3	2:A:198:TYR:CE2	2.42	0.54
2:A:228:VAL:HG22	2:A:268:ALA:HB2	1.89	0.54
2:A:242:ARG:O	2:A:243:ALA:CB	2.56	0.54
2:A:242:ARG:HH11	2:A:251:TRP:HB3	1.72	0.54
2:A:358:GLN:HB2	2:A:360:TRP:HE1	1.73	0.54
2:A:460:ALA:HA	2:A:499:MET:HG3	1.89	0.54
2:B:143:PHE:HB3	2:B:146:ASP:HB3	1.90	0.54
2:B:161:TYR:O	2:B:163:GLU:N	2.40	0.54
2:B:245:ILE:CB	2:B:248:THR:HG22	2.38	0.54
2:B:341:LEU:CD1	2:B:343:THR:HG23	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:498:ARG:O	2:B:501:VAL:HG12	2.07	0.54
1:C:916:C:C6	1:C:916:C:OP2	2.60	0.54
2:A:248:THR:HG23	2:A:249:GLU:N	2.22	0.54
2:A:250:VAL:HG21	2:A:304:ARG:HD2	1.89	0.54
2:A:501:VAL:HG12	2:A:502:SER:N	2.22	0.54
2:B:452:VAL:HG12	2:B:453:PHE:O	2.07	0.54
2:B:714:GLU:O	2:B:717:ARG:N	2.41	0.54
2:A:473:THR:OG1	2:A:474:GLU:N	2.41	0.54
2:B:201:ARG:HD2	2:B:211:GLU:CB	2.37	0.54
2:B:454:ASP:O	2:B:455:THR:C	2.50	0.54
2:B:680:HIS:CD2	2:B:687:THR:HG21	2.43	0.54
2:B:814:ALA:O	2:B:818:ARG:HG3	2.07	0.54
2:A:61:ASP:OD1	2:A:65:ARG:HG3	2.08	0.54
2:A:82:HIS:HD2	2:A:145:MET:HE2	1.72	0.54
2:A:376:ARG:HH11	2:A:376:ARG:HB2	1.73	0.54
2:A:448:ARG:O	2:A:448:ARG:NH1	2.40	0.54
2:B:107:ARG:HA	2:B:407:TRP:CE3	2.43	0.54
2:B:118:LYS:HD3	2:B:143:PHE:CE1	2.43	0.54
2:B:467:LEU:O	2:B:473:THR:HG21	2.07	0.54
2:A:221:PHE:HA	2:A:245:ILE:HD11	1.88	0.54
2:A:349:THR:HG23	2:A:350:PRO:HD2	1.90	0.54
2:A:364:ARG:N	2:A:365:PRO:HD2	2.23	0.54
2:A:593:ARG:HH11	2:A:593:ARG:CG	2.19	0.54
2:B:153:VAL:HG11	2:B:410:HIS:ND1	2.23	0.54
2:A:242:ARG:NH1	2:A:251:TRP:CB	2.71	0.53
2:A:593:ARG:HB2	2:A:665:LEU:HD21	1.90	0.53
2:A:382:VAL:O	2:A:383:PRO:C	2.49	0.53
2:A:416:TYR:CD2	2:A:423:VAL:HG12	2.43	0.53
2:A:613:ARG:NH2	2:A:644:GLU:HG3	2.24	0.53
2:A:845:LYS:HE3	2:B:820:GLN:OE1	2.09	0.53
2:B:155:TYR:HD1	2:B:431:TYR:CD2	2.27	0.53
2:B:525:LYS:HD2	2:B:525:LYS:N	2.23	0.53
2:A:271:VAL:HG12	2:A:273:PRO:HD3	1.89	0.53
2:A:277:PRO:HD3	2:A:353:TYR:CD2	2.44	0.53
2:B:178:ARG:HG2	2:B:347:CYS:SG	2.48	0.53
2:B:255:LEU:HD12	2:B:255:LEU:O	2.08	0.53
2:B:277:PRO:O	2:B:281:GLU:HB2	2.08	0.53
2:B:795:LEU:O	2:B:796:LEU:HD23	2.08	0.53
1:C:904:C:H2'	1:C:905:G:H8	1.73	0.53
2:A:456:TRP:HB3	2:A:498:ARG:NH1	2.23	0.53
2:B:87:THR:O	2:B:91:VAL:HG23	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:527:GLN:HE21	2:B:533:LYS:HE2	1.72	0.53
2:A:37:VAL:CG2	2:A:479:PHE:HB2	2.28	0.53
2:A:404:ARG:HG2	2:A:406:LEU:HD12	1.90	0.53
2:A:431:TYR:HE1	2:A:432:LEU:HD12	1.74	0.53
2:A:747:TYR:CZ	2:A:774:ARG:HB2	2.44	0.53
2:B:69:MET:CE	2:B:680:HIS:ND1	2.71	0.53
2:B:172:LEU:HB2	2:B:280:TYR:CE1	2.42	0.53
2:B:280:TYR:C	2:B:280:TYR:CD2	2.86	0.53
2:A:217:PRO:O	2:A:220:VAL:HG13	2.09	0.53
2:A:593:ARG:O	2:A:593:ARG:HG2	2.08	0.53
2:B:217:PRO:O	2:B:220:VAL:HG22	2.09	0.53
2:A:85:ILE:O	2:A:88:GLN:HB3	2.09	0.53
2:A:234:ARG:HH21	2:A:267:GLY:HA3	1.73	0.53
1:C:922:A:H2'	1:C:923:G:H8	1.74	0.53
2:A:218:GLU:CD	2:A:318:ARG:HB3	2.34	0.53
2:A:346:ARG:HB2	2:A:346:ARG:HH11	1.72	0.53
2:B:152:ALA:HB2	2:B:470:PRO:HD3	1.89	0.53
2:B:242:ARG:HE	2:B:251:TRP:CB	2.22	0.53
2:B:359:TRP:HB2	2:B:403:SER:OG	2.09	0.53
2:B:430:ARG:O	2:B:432:LEU:N	2.42	0.53
2:A:171:ARG:HB2	4:A:1088:HOH:O	2.09	0.53
2:A:522:LEU:CD1	2:A:566:ARG:HA	2.39	0.53
2:B:98:GLU:HG3	2:B:99:GLY:N	2.18	0.53
2:A:771:LEU:HD11	2:A:791:PRO:HG2	1.91	0.53
2:B:86:ALA:O	2:B:90:VAL:HG23	2.08	0.53
2:B:160:TYR:HE2	2:B:505:HIS:CD2	2.27	0.53
2:B:388:LYS:N	2:B:388:LYS:CD	2.72	0.53
2:A:476:LEU:HD23	2:A:476:LEU:C	2.34	0.52
2:A:774:ARG:HG3	2:A:774:ARG:HH11	1.74	0.52
2:B:405:GLN:CD	2:B:405:GLN:N	2.67	0.52
1:C:922:A:H2'	1:C:923:G:C8	2.45	0.52
1:D:909:A:H4'	1:D:910:G:OP1	2.08	0.52
2:A:229:HIS:CD2	2:A:231:GLU:H	2.28	0.52
2:B:193:THR:HG23	2:B:194:PRO:HD2	1.89	0.52
2:B:302:GLY:O	2:B:310:ARG:NH1	2.38	0.52
2:B:361:LEU:CD1	2:B:402:ILE:HD11	2.34	0.52
2:A:64:ILE:HG23	2:A:74:ALA:HB1	1.91	0.52
2:A:245:ILE:HG12	2:A:248:THR:CB	2.39	0.52
2:A:469:TRP:O	2:A:469:TRP:CG	2.62	0.52
2:A:499:MET:CE	2:A:512:PHE:CE2	2.83	0.52
2:A:665:LEU:O	2:A:669:GLU:HG3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:753:ALA:HB3	2:A:754:PRO:HD3	1.90	0.52
2:B:807:LYS:O	2:B:811:GLU:HG3	2.08	0.52
2:B:834:LYS:H	2:B:834:LYS:HD2	1.73	0.52
2:A:430:ARG:HB3	2:A:433:GLU:OE2	2.10	0.52
2:B:93:ARG:O	2:B:97:LYS:HG3	2.10	0.52
2:B:244:ARG:NH2	4:B:992:HOH:O	2.17	0.52
2:B:326:ARG:HB3	2:B:331:LEU:HD23	1.91	0.52
2:B:416:TYR:N	2:B:447:LYS:O	2.38	0.52
1:C:920:A:H2'	1:C:945:G:O6	2.10	0.52
1:C:967:C:O2'	1:C:968:G:H5'	2.10	0.52
2:A:78:PRO:HG2	2:A:141:GLU:HA	1.91	0.52
2:A:341:LEU:HD21	2:A:350:PRO:HB3	1.92	0.52
2:A:382:VAL:HG11	2:A:516:LEU:CD1	2.40	0.52
2:A:469:TRP:N	2:A:470:PRO:CD	2.71	0.52
2:B:1:MET:HE3	2:B:693:ALA:HB2	1.91	0.52
2:B:217:PRO:HD2	2:B:318:ARG:NE	2.24	0.52
2:B:297:GLU:OE2	2:B:297:GLU:N	2.43	0.52
2:B:299:ARG:NH2	2:B:312:LEU:HD12	2.25	0.52
2:B:516:LEU:CD1	2:B:628:LEU:HD13	2.38	0.52
1:D:901:G:N2	1:D:972:A:H1'	2.25	0.52
2:B:724:GLN:HE22	2:B:785:ARG:H	1.57	0.52
2:B:736:ALA:CB	2:B:738:LEU:HD13	2.40	0.52
2:A:101:THR:O	2:A:104:ASP:HB2	2.10	0.52
2:A:431:TYR:CD1	2:A:431:TYR:C	2.87	0.52
2:A:529:MET:HG3	2:A:535:ASN:O	2.10	0.52
2:B:363:MET:HE3	2:B:363:MET:HA	1.92	0.52
2:B:382:VAL:HG11	2:B:516:LEU:CD1	2.40	0.52
2:B:429:GLU:O	2:B:430:ARG:HG2	2.10	0.52
2:A:520:LEU:HA	3:A:990:VAA:N1	2.25	0.52
2:B:51:MET:HE1	2:B:567:LEU:HD13	1.92	0.52
2:B:233:GLU:C	2:B:235:TYR:H	2.17	0.52
2:B:280:TYR:C	2:B:280:TYR:HD2	2.17	0.52
2:B:593:ARG:HG3	2:B:593:ARG:NH1	2.24	0.52
2:A:216:ARG:HG2	2:A:218:GLU:OE1	2.09	0.52
2:A:306:PRO:HG2	2:A:309:LEU:CB	2.39	0.52
2:A:453:PHE:CD2	2:A:457:PHE:CD2	2.98	0.52
2:B:82:HIS:O	2:B:87:THR:OG1	2.17	0.52
2:B:618:VAL:HG12	2:B:708:PRO:HG3	1.92	0.52
2:B:724:GLN:HE22	2:B:785:ARG:HB2	1.74	0.52
1:D:932:U:O2'	1:D:933:C:C5	2.45	0.52
1:D:947:C:HO2'	1:D:948:G:P	2.33	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:221:PHE:HB2	2:A:293:VAL:HG11	1.91	0.52
2:A:278:LEU:O	2:A:282:ILE:HG12	2.10	0.52
2:A:651:GLU:OE2	2:A:651:GLU:HA	2.10	0.52
2:B:820:GLN:NE2	2:B:821:ARG:N	2.57	0.52
2:A:28:ASN:ND2	2:A:28:ASN:C	2.68	0.51
2:A:83:ALA:HB3	2:A:87:THR:OG1	2.10	0.51
2:A:201:ARG:NH2	2:A:332:VAL:HG21	2.25	0.51
2:A:202:TYR:CD2	2:A:203:GLU:N	2.78	0.51
2:A:361:LEU:O	2:A:363:MET:N	2.42	0.51
2:B:101:THR:HG23	2:B:104:ASP:H	1.74	0.51
2:B:401:ASN:C	2:B:401:ASN:ND2	2.68	0.51
2:B:467:LEU:O	2:B:473:THR:CG2	2.58	0.51
2:B:489:TYR:HA	2:B:517:LEU:HD22	1.90	0.51
2:B:778:ALA:HB3	2:B:789:ARG:HG2	1.93	0.51
2:A:304:ARG:O	2:A:305:VAL:C	2.51	0.51
2:A:369:GLU:OE2	2:A:505:HIS:HA	2.09	0.51
2:A:529:MET:HE1	2:A:537:ILE:HG13	1.93	0.51
2:A:759:LEU:HD12	2:A:763:ARG:CD	2.40	0.51
2:B:200:LEU:HD21	2:B:325:PHE:CE1	2.45	0.51
2:B:202:TYR:OH	2:B:244:ARG:CZ	2.59	0.51
2:B:362:ARG:O	2:B:365:PRO:HD2	2.10	0.51
2:B:462:TRP:C	2:B:464:LEU:N	2.67	0.51
2:B:751:GLU:HB2	2:B:785:ARG:NH2	2.25	0.51
1:C:934:A:N3	2:A:584:ASN:HB3	2.25	0.51
1:D:973:C:C2	2:B:278:LEU:HD13	2.46	0.51
2:A:279:ASP:HA	2:A:282:ILE:CG1	2.40	0.51
2:B:181:THR:OG1	2:B:404:ARG:HG3	2.10	0.51
2:B:434:ASP:O	2:B:435:PRO:C	2.53	0.51
2:A:197:LEU:HD21	2:A:213:ALA:HB1	1.93	0.51
2:A:818:ARG:HA	2:A:821:ARG:NH1	2.22	0.51
1:C:918:G:O6	2:A:833:PRO:CD	2.57	0.51
2:A:388:LYS:N	2:A:388:LYS:HD3	2.26	0.51
2:A:469:TRP:C	2:A:471:GLU:N	2.66	0.51
2:B:69:MET:HB2	2:B:703:GLU:O	2.11	0.51
2:B:161:TYR:HD1	2:B:425:VAL:HB	1.70	0.51
2:B:593:ARG:HG3	2:B:593:ARG:HH11	1.75	0.51
1:D:902:G:O6	1:D:970:C:N3	2.44	0.51
2:A:64:ILE:HG13	2:A:76:TRP:HB2	1.93	0.51
2:A:212:ILE:HD11	2:A:268:ALA:C	2.36	0.51
2:A:802:ARG:NH2	2:A:861:ILE:HG22	2.25	0.51
2:A:260:VAL:HG13	2:A:269:LEU:HD23	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:279:ASP:HA	2:A:282:ILE:HG12	1.93	0.51
2:B:362:ARG:C	2:B:365:PRO:HD2	2.36	0.51
1:D:964:C:H2'	1:D:965:G:C8	2.44	0.51
2:B:412:ILE:HD12	2:B:413:PRO:CD	2.24	0.51
2:B:724:GLN:NE2	2:B:785:ARG:HB2	2.25	0.51
2:A:5:LYS:H	2:A:5:LYS:CD	2.18	0.51
2:A:522:LEU:HD12	2:A:522:LEU:O	2.11	0.51
2:B:370:VAL:HG12	2:B:374:LEU:CD1	2.41	0.51
2:B:544:GLU:C	2:B:544:GLU:CD	2.78	0.51
1:C:933:C:H6	1:C:933:C:O5'	1.94	0.50
1:D:967:C:O2'	1:D:968:G:H5'	2.11	0.50
2:A:19:LYS:HE3	2:A:699:GLU:OE2	2.11	0.50
2:A:51:MET:CE	2:A:537:ILE:HB	2.41	0.50
2:B:149:ARG:CD	2:B:465:SER:OG	2.59	0.50
2:B:494:LEU:HD23	2:B:494:LEU:N	2.13	0.50
2:B:745:ARG:HH11	2:B:745:ARG:CB	2.14	0.50
2:B:748:LEU:CD1	2:B:755:VAL:HG21	2.41	0.50
2:A:498:ARG:HG2	2:A:498:ARG:NH1	2.26	0.50
2:B:266:THR:C	2:B:268:ALA:H	2.18	0.50
2:B:349:THR:CG2	2:B:350:PRO:HD2	2.41	0.50
2:B:428:PRO:C	2:B:430:ARG:H	2.19	0.50
1:C:932:U:H2'	1:C:932:U:O2	2.09	0.50
2:A:201:ARG:CZ	2:A:211:GLU:OE1	2.60	0.50
2:A:518:HIS:CD2	2:A:519:GLY:O	2.65	0.50
2:B:529:MET:HA	2:B:535:ASN:OD1	2.10	0.50
2:B:565:ILE:HG22	2:B:565:ILE:O	2.11	0.50
2:A:1:MET:HE2	2:A:693:ALA:HB2	1.92	0.50
2:A:145:MET:HE1	2:A:408:TRP:CD2	2.46	0.50
2:A:203:GLU:O	2:A:243:ALA:HA	2.10	0.50
2:A:417:CYS:C	2:A:419:ASP:H	2.20	0.50
2:B:613:ARG:HH21	2:B:640:LEU:CD1	2.24	0.50
2:A:150:SER:O	2:A:153:VAL:HG22	2.11	0.50
2:A:153:VAL:HG11	2:A:410:HIS:CE1	2.46	0.50
2:A:224:GLN:O	2:A:225:ALA:HB2	2.10	0.50
2:A:460:ALA:CB	2:A:498:ARG:HB3	2.42	0.50
2:B:220:VAL:HG12	2:B:270:LYS:NZ	2.17	0.50
2:B:322:VAL:HG13	2:B:323:GLU:N	2.27	0.50
2:A:26:VAL:HG22	2:A:139:SER:HB3	1.94	0.50
2:A:46:THR:CG2	2:A:90:VAL:HG21	2.40	0.50
2:A:148:LYS:NZ	4:A:1063:HOH:O	2.45	0.50
2:A:152:ALA:HB2	2:A:470:PRO:HG3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:85:ILE:HG23	2:B:86:ALA:N	2.27	0.50
2:B:224:GLN:O	2:B:225:ALA:HB2	2.11	0.50
2:B:487:THR:O	2:B:517:LEU:HA	2.11	0.50
2:A:155:TYR:OH	2:A:159:ARG:HD2	2.12	0.50
2:A:362:ARG:C	2:A:365:PRO:HD2	2.37	0.50
2:B:424:ASN:ND2	2:B:446:LEU:HD21	2.26	0.50
2:B:501:VAL:CG1	2:B:502:SER:H	2.25	0.50
2:B:683:MET:O	2:B:687:THR:CG2	2.59	0.50
2:A:714:GLU:O	2:A:715:ALA:C	2.55	0.50
2:B:846:GLU:HA	2:B:849:GLU:HB2	1.92	0.50
2:A:196:LYS:CB	2:A:198:TYR:HE2	2.25	0.50
2:A:387:LYS:HB3	2:A:388:LYS:CE	2.42	0.50
2:A:518:HIS:HD2	2:A:519:GLY:O	1.95	0.50
2:B:221:PHE:C	2:B:223:ASP:H	2.20	0.50
1:C:932:U:OP1	1:C:933:C:OP2	2.30	0.49
1:D:933:C:H3'	1:D:933:C:C6	2.46	0.49
2:A:260:VAL:HG22	2:A:269:LEU:CD2	2.42	0.49
2:A:592:SER:C	2:A:594:GLU:N	2.70	0.49
2:B:165:LEU:HD13	2:B:366:LEU:HD21	1.94	0.49
2:B:415:TRP:HB2	2:B:424:ASN:HB2	1.94	0.49
2:A:69:MET:HB2	2:A:703:GLU:O	2.11	0.49
2:A:276:ASP:OD1	2:A:278:LEU:N	2.45	0.49
2:A:382:VAL:HG11	2:A:516:LEU:HD13	1.93	0.49
2:A:666:ARG:HH11	2:A:666:ARG:CG	2.25	0.49
2:B:205:GLU:HB2	2:B:242:ARG:HB2	1.92	0.49
2:A:250:VAL:HG12	2:A:252:ILE:HD12	1.93	0.49
2:A:488:GLY:O	2:A:490:ASP:N	2.45	0.49
2:A:744:VAL:CG1	2:A:745:ARG:N	2.75	0.49
2:A:171:ARG:NH2	2:A:364:ARG:HH21	2.11	0.49
2:A:246:PRO:O	2:A:247:LEU:HB2	2.11	0.49
2:A:385:ARG:HB3	4:A:1038:HOH:O	2.11	0.49
2:A:387:LYS:HB3	2:A:388:LYS:HZ1	1.75	0.49
2:B:409:GLY:HA3	2:B:452:VAL:HG11	1.92	0.49
2:B:469:TRP:O	2:B:469:TRP:CG	2.66	0.49
2:A:218:GLU:OE1	2:A:218:GLU:N	2.38	0.49
2:A:373:GLY:O	2:A:376:ARG:N	2.45	0.49
2:A:500:GLU:HA	2:A:511:PRO:HG2	1.93	0.49
2:B:64:ILE:HG23	2:B:74:ALA:HB1	1.94	0.49
2:B:499:MET:HE3	2:B:512:PHE:CE2	2.47	0.49
2:A:198:TYR:CE1	2:A:322:VAL:HG21	2.48	0.49
2:B:272:THR:H	2:B:279:ASP:CB	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:294:ILE:CD1	2:B:300:MET:SD	3.00	0.49
2:B:415:TRP:HZ3	4:B:1022:HOH:O	1.95	0.49
2:B:501:VAL:CG1	2:B:502:SER:N	2.75	0.49
2:B:587:ARG:CG	2:B:587:ARG:HH11	2.25	0.49
2:A:611:ARG:NH1	4:A:1004:HOH:O	2.45	0.49
2:B:149:ARG:CG	2:B:465:SER:OG	2.60	0.49
2:B:242:ARG:O	2:B:243:ALA:CB	2.57	0.49
2:B:248:THR:CG2	2:B:249:GLU:N	2.52	0.49
2:B:326:ARG:HE	2:B:331:LEU:HD23	1.76	0.49
2:B:172:LEU:CD2	2:B:354:ALA:H	2.26	0.49
2:B:352:GLU:HA	4:B:1010:HOH:O	2.12	0.49
2:B:498:ARG:HG2	2:B:498:ARG:HH11	1.78	0.49
2:B:529:MET:HE1	2:B:537:ILE:HB	1.94	0.49
2:B:579:ALA:HB2	2:B:683:MET:HE1	1.93	0.49
1:C:959:U:H5''	1:C:960:C:OP2	2.12	0.49
2:A:412:ILE:HG13	2:A:413:PRO:CD	2.42	0.49
2:A:680:HIS:HD2	2:A:687:THR:HG21	1.74	0.49
2:A:753:ALA:O	2:A:757:GLU:HG3	2.13	0.49
2:B:487:THR:HG23	2:B:517:LEU:HD23	1.94	0.49
2:B:540:LEU:HA	2:B:543:VAL:HG22	1.95	0.49
2:A:358:GLN:NE2	2:A:403:SER:HB2	2.28	0.49
2:A:711:ARG:HG2	2:A:711:ARG:NH1	2.27	0.49
2:B:401:ASN:C	2:B:401:ASN:HD22	2.19	0.49
2:B:582:LEU:O	2:B:583:TYR:C	2.55	0.49
2:B:680:HIS:HD2	2:B:687:THR:HG21	1.74	0.49
2:A:36:PHE:CD1	2:A:67:LYS:HD3	2.48	0.48
2:A:245:ILE:H	2:A:248:THR:HG22	1.77	0.48
2:A:839:ALA:C	2:A:841:GLU:H	2.19	0.48
2:B:1:MET:HE3	2:B:693:ALA:HB3	1.95	0.48
2:B:85:ILE:HG23	2:B:86:ALA:H	1.78	0.48
2:B:745:ARG:HB2	2:B:771:LEU:CD2	2.43	0.48
2:B:755:VAL:HG12	2:B:762:PHE:CG	2.47	0.48
2:A:68:ARG:C	2:A:70:ARG:H	2.20	0.48
2:A:155:TYR:CD1	2:A:431:TYR:CD2	3.00	0.48
2:A:401:ASN:ND2	2:A:403:SER:H	2.10	0.48
2:A:573:GLU:O	2:A:574:MET:C	2.56	0.48
2:B:106:GLY:C	2:B:108:GLU:N	2.69	0.48
2:B:153:VAL:HG21	2:B:410:HIS:ND1	2.27	0.48
2:B:322:VAL:HG13	2:B:323:GLU:OE1	2.13	0.48
2:A:31:SER:HB3	2:A:73:GLU:HG3	1.96	0.48
2:A:829:ARG:HH21	2:B:829:ARG:NH1	2.11	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:78:PRO:HG2	2:B:141:GLU:HA	1.95	0.48
2:B:101:THR:HG22	2:B:104:ASP:CG	2.38	0.48
2:B:175:TRP:O	2:B:177:PRO:HD3	2.13	0.48
2:B:429:GLU:C	2:B:430:ARG:HG2	2.37	0.48
2:A:31:SER:CB	2:A:73:GLU:HG3	2.43	0.48
2:A:216:ARG:HG3	2:A:318:ARG:NH2	2.28	0.48
2:B:4:PRO:HD2	2:B:583:TYR:OH	2.13	0.48
2:B:63:LEU:O	2:B:67:LYS:HB2	2.14	0.48
2:B:82:HIS:HB2	2:B:408:TRP:HE1	1.78	0.48
2:B:338:THR:HG23	2:B:338:THR:O	2.13	0.48
2:B:808:ARG:HG2	2:B:854:ILE:CD1	2.44	0.48
2:B:831:LYS:HE3	2:B:831:LYS:CA	2.44	0.48
2:B:46:THR:HG22	2:B:90:VAL:HG21	1.94	0.48
2:A:181:THR:OG1	2:A:404:ARG:HG3	2.13	0.48
2:A:193:THR:HG23	2:A:194:PRO:HD2	1.96	0.48
2:A:412:ILE:HG13	2:A:413:PRO:N	2.27	0.48
2:A:845:LYS:HZ1	2:B:820:GLN:HE22	1.59	0.48
2:B:736:ALA:HB3	2:B:738:LEU:HD13	1.95	0.48
1:C:946:U:C6	1:C:946:U:H3'	2.48	0.48
1:C:973:C:C2	2:A:278:LEU:HD13	2.48	0.48
1:D:965:G:H2'	1:D:966:C:C6	2.48	0.48
2:A:839:ALA:C	2:A:841:GLU:N	2.71	0.48
2:B:333:LYS:HE2	2:B:335:GLU:OE1	2.13	0.48
2:A:18:GLU:HG3	2:A:22:LYS:HD3	1.96	0.48
2:A:400:TRP:O	2:A:402:ILE:HD12	2.13	0.48
2:A:429:GLU:CD	2:A:429:GLU:N	2.70	0.48
2:B:7:TYR:CD1	2:B:8:ASP:N	2.81	0.48
2:B:145:MET:HE1	2:B:408:TRP:CZ3	2.48	0.48
2:B:298:GLY:O	2:B:314:ARG:HB3	2.14	0.48
2:B:684:PRO:HG2	2:B:685:PHE:CD1	2.49	0.48
2:B:710:GLY:O	2:B:711:ARG:HB3	2.13	0.48
2:B:806:GLU:HA	2:B:858:LEU:HD11	1.96	0.48
2:A:255:LEU:HD12	2:A:255:LEU:C	2.38	0.48
2:A:714:GLU:O	2:A:717:ARG:N	2.46	0.48
2:A:810:LYS:HG3	2:B:855:ARG:CZ	2.44	0.48
2:B:274:ALA:HB3	2:B:291:VAL:O	2.13	0.48
2:B:358:GLN:HE22	2:B:405:GLN:NE2	2.00	0.48
2:B:488:GLY:O	2:B:490:ASP:OD1	2.31	0.48
2:A:19:LYS:HE3	2:A:699:GLU:CD	2.39	0.48
2:A:51:MET:HE1	2:A:537:ILE:CG2	2.43	0.48
2:A:362:ARG:O	2:A:365:PRO:HG2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:397:VAL:HG12	2:A:398:LYS:N	2.29	0.48
2:A:632:GLN:O	2:A:633:ALA:C	2.56	0.48
2:A:833:PRO:HD2	2:A:836:VAL:CG1	2.44	0.48
2:B:99:GLY:C	2:B:100:LYS:HD2	2.39	0.48
2:B:592:SER:C	2:B:594:GLU:H	2.20	0.48
2:B:712:ASP:O	2:B:716:GLU:HG3	2.13	0.48
1:C:917:G:H5'	1:C:959:U:O2	2.13	0.47
2:A:373:GLY:O	2:A:374:LEU:C	2.55	0.47
2:A:383:PRO:HB2	2:A:386:TRP:HD1	1.76	0.47
2:B:233:GLU:C	2:B:235:TYR:N	2.71	0.47
1:C:961:C:C2'	1:C:962:U:H5'	2.43	0.47
1:C:973:C:H1'	2:A:278:LEU:HB2	1.95	0.47
2:A:197:LEU:CD2	2:A:213:ALA:HB1	2.44	0.47
2:B:46:THR:CG2	2:B:90:VAL:HG21	2.45	0.47
2:B:161:TYR:C	2:B:163:GLU:N	2.71	0.47
2:B:730:ARG:HH12	2:B:765:LEU:HB3	1.79	0.47
2:B:839:ALA:O	2:B:843:ARG:HG3	2.14	0.47
1:C:941:A:H2'	1:C:942:G:O5'	2.14	0.47
1:D:957:A:H4'	1:D:959:U:H5	1.80	0.47
2:A:405:GLN:N	2:A:405:GLN:CD	2.72	0.47
2:A:408:TRP:HA	2:A:408:TRP:CE3	2.49	0.47
2:A:456:TRP:CE3	2:A:494:LEU:O	2.67	0.47
2:A:538:ASP:OD1	2:A:539:PRO:HD2	2.14	0.47
2:A:729:VAL:HG11	2:A:766:SER:HB2	1.96	0.47
2:B:199:THR:HA	2:B:212:ILE:O	2.15	0.47
2:B:361:LEU:HD21	2:B:366:LEU:CD1	2.40	0.47
2:B:783:MET:HB2	2:B:786:VAL:O	2.13	0.47
2:A:1:MET:CE	2:A:690:LEU:HD23	2.44	0.47
2:A:76:TRP:O	2:A:78:PRO:HD3	2.15	0.47
2:A:225:ALA:CA	2:A:252:ILE:HG23	2.31	0.47
2:A:289:LYS:N	2:A:289:LYS:CD	2.77	0.47
2:A:416:TYR:HA	2:A:422:ALA:O	2.14	0.47
2:B:179:CYS:O	2:B:180:GLU:C	2.56	0.47
2:B:193:THR:HG22	2:B:194:PRO:HD2	1.94	0.47
2:B:305:VAL:CG1	2:B:310:ARG:HD3	2.41	0.47
2:B:433:GLU:HA	4:B:1046:HOH:O	2.13	0.47
2:B:827:GLY:O	2:B:828:PHE:C	2.58	0.47
2:A:667:THR:O	2:A:671:VAL:HG23	2.14	0.47
2:B:393:TRP:CE3	2:B:394:LEU:HD23	2.49	0.47
2:B:510:ARG:HH11	2:B:510:ARG:HG3	1.78	0.47
2:B:524:GLU:OE2	2:B:524:GLU:N	2.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:185:ASP:O	2:A:188:VAL:HG12	2.14	0.47
2:A:371:LEU:HD21	2:A:394:LEU:CB	2.41	0.47
2:A:382:VAL:CG2	2:A:383:PRO:CD	2.70	0.47
2:A:480:TYR:O	2:A:482:GLY:N	2.47	0.47
2:A:613:ARG:HH21	2:A:644:GLU:HG3	1.78	0.47
2:A:772:PRO:HG2	2:A:773:GLU:H	1.79	0.47
2:B:160:TYR:CE2	2:B:505:HIS:CD2	3.02	0.47
2:B:282:ILE:CA	2:B:285:ARG:HD3	2.34	0.47
2:B:537:ILE:HD12	2:B:567:LEU:HD22	1.97	0.47
2:A:13:GLU:N	2:A:14:PRO:HD2	2.29	0.47
2:A:160:TYR:CE2	2:A:505:HIS:CD2	3.03	0.47
2:A:215:VAL:HG11	2:A:339:ILE:HG21	1.97	0.47
2:A:245:ILE:N	2:A:248:THR:HG22	2.29	0.47
2:A:408:TRP:HA	2:A:408:TRP:HE3	1.80	0.47
2:B:50:HIS:CD2	2:B:50:HIS:C	2.93	0.47
2:B:477:LYS:HD2	2:B:477:LYS:O	2.15	0.47
2:B:831:LYS:HE3	2:B:831:LYS:N	2.30	0.47
2:B:833:PRO:HG2	2:B:836:VAL:HB	1.97	0.47
1:C:932:U:O2	1:C:932:U:C2'	2.62	0.47
1:D:916:C:H5''	1:D:917:G:OP1	2.14	0.47
2:A:2:ASP:O	2:A:4:PRO:HD3	2.14	0.47
2:A:210:ILE:CD1	2:A:238:LEU:HD13	2.42	0.47
2:A:430:ARG:NE	2:A:433:GLU:OE2	2.48	0.47
2:B:695:THR:OG1	2:B:697:LYS:HG2	2.14	0.47
2:B:733:LYS:HB3	2:B:733:LYS:HZ2	1.80	0.47
2:B:3:LEU:HB3	2:B:587:ARG:HD3	1.97	0.47
2:B:383:PRO:O	2:B:384:GLU:HB3	2.14	0.47
1:D:917:G:O2'	1:D:918:G:O4'	2.32	0.47
1:D:971:C:H6	1:D:971:C:O5'	1.98	0.47
2:A:364:ARG:CD	4:A:1056:HOH:O	2.63	0.47
2:A:393:TRP:CE3	2:A:394:LEU:HD23	2.48	0.47
2:B:224:GLN:OE1	2:B:291:VAL:HG11	2.15	0.47
2:B:244:ARG:HB2	2:B:251:TRP:CZ2	2.50	0.47
2:B:270:LYS:NZ	2:B:270:LYS:HB2	2.30	0.47
2:B:422:ALA:HA	4:B:1017:HOH:O	2.13	0.47
2:B:469:TRP:HD1	2:B:507:MET:HE3	1.78	0.47
1:C:901:G:N2	1:C:972:A:H1'	2.30	0.46
2:A:220:VAL:HG23	2:A:221:PHE:N	2.30	0.46
2:A:507:MET:HE3	2:A:507:MET:HB3	1.70	0.46
2:B:13:GLU:HB2	2:B:14:PRO:HD3	1.97	0.46
2:B:200:LEU:HD21	2:B:325:PHE:CD1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:186:LEU:HD12	2:A:186:LEU:N	2.14	0.46
2:A:312:LEU:O	2:A:313:ASP:O	2.33	0.46
2:A:367:ALA:O	2:A:371:LEU:HG	2.15	0.46
2:B:121:SER:O	2:B:125:ILE:HG13	2.16	0.46
2:B:221:PHE:O	2:B:304:ARG:HG3	2.15	0.46
2:B:275:HIS:CE1	2:B:294:ILE:HB	2.49	0.46
2:B:323:GLU:C	2:B:325:PHE:H	2.23	0.46
1:D:956:A:H5'	1:D:957:A:OP1	2.15	0.46
2:A:153:VAL:CG2	2:A:154:ARG:H	2.28	0.46
2:A:397:VAL:HG12	2:A:398:LYS:H	1.80	0.46
2:A:683:MET:O	2:A:687:THR:CG2	2.63	0.46
2:B:318:ARG:C	2:B:320:LYS:H	2.23	0.46
2:B:447:LYS:NZ	2:B:447:LYS:HA	2.30	0.46
2:B:482:GLY:O	2:B:513:LYS:HG3	2.15	0.46
2:B:731:ALA:O	2:B:734:ALA:HB3	2.16	0.46
2:B:801:TRP:CH2	2:B:858:LEU:HD23	2.50	0.46
2:B:833:PRO:O	2:B:834:LYS:C	2.57	0.46
1:D:916:C:H4'	1:D:917:G:O5'	2.15	0.46
2:A:275:HIS:HE1	2:A:294:ILE:HG12	1.76	0.46
2:A:699:GLU:OE1	2:A:699:GLU:HA	2.14	0.46
2:B:66:TYR:CE2	2:B:70:ARG:HD3	2.50	0.46
2:A:45:VAL:HG12	2:A:121:SER:HB3	1.97	0.46
2:A:216:ARG:HG2	2:A:218:GLU:CD	2.41	0.46
2:A:452:VAL:CG1	2:A:453:PHE:N	2.78	0.46
2:A:521:VAL:HA	2:A:565:ILE:O	2.16	0.46
2:A:855:ARG:CZ	2:B:810:LYS:HE2	2.43	0.46
2:B:364:ARG:N	2:B:365:PRO:HD2	2.30	0.46
2:B:408:TRP:O	2:B:409:GLY:O	2.33	0.46
2:B:603:PRO:HG3	2:B:663:HIS:ND1	2.31	0.46
2:B:786:VAL:HG22	2:B:787:THR:N	2.31	0.46
2:A:255:LEU:H	2:A:255:LEU:HG	1.61	0.46
2:A:279:ASP:HA	2:A:282:ILE:HD11	1.98	0.46
2:A:409:GLY:HA3	2:A:452:VAL:HG13	1.98	0.46
2:A:637:VAL:HG21	2:A:679:LEU:CD2	2.46	0.46
2:B:343:THR:HG22	2:B:350:PRO:HA	1.97	0.46
2:B:471:GLU:O	4:B:1041:HOH:O	2.21	0.46
2:B:487:THR:HG23	2:B:517:LEU:CD2	2.46	0.46
2:B:489:TYR:CD1	2:B:489:TYR:C	2.93	0.46
2:A:170:PRO:C	2:A:171:ARG:O	2.57	0.46
2:A:196:LYS:CB	2:A:198:TYR:CE2	2.99	0.46
2:A:307:GLU:O	2:A:309:LEU:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:153:VAL:HG11	2:B:410:HIS:CE1	2.50	0.46
2:B:370:VAL:O	2:B:373:GLY:N	2.46	0.46
2:B:745:ARG:NH1	2:B:745:ARG:CB	2.76	0.46
1:C:908:U:H6	1:C:908:U:O5'	1.99	0.46
2:A:156:ALA:CB	2:A:461:LEU:HD21	2.45	0.46
2:A:382:VAL:CG2	2:A:517:LEU:H	2.28	0.46
2:B:1:MET:HE2	2:B:689:GLU:HG3	1.98	0.46
2:B:117:TRP:O	2:B:118:LYS:C	2.59	0.46
2:B:145:MET:HE1	2:B:408:TRP:CE3	2.51	0.46
2:B:159:ARG:HG3	2:B:159:ARG:HH11	1.80	0.46
2:B:393:TRP:HB2	2:B:493:PHE:CE2	2.51	0.46
2:A:161:TYR:C	2:A:163:GLU:H	2.24	0.46
2:A:245:ILE:HG12	2:A:248:THR:HG21	1.97	0.46
2:A:39:PHE:CE2	2:A:463:PRO:HA	2.51	0.46
2:A:272:THR:H	2:A:279:ASP:HB3	1.81	0.46
2:A:441:CYS:SG	2:A:443:SER:CB	3.04	0.46
2:B:366:LEU:O	2:B:369:GLU:HB2	2.16	0.46
1:C:929:G:H5'	1:C:929:G:C8	2.48	0.45
1:D:933:C:C6	1:D:933:C:C3'	2.99	0.45
1:D:947:C:O2'	1:D:948:G:OP2	2.33	0.45
2:A:145:MET:HG2	2:A:410:HIS:NE2	2.31	0.45
2:A:201:ARG:HG2	2:A:211:GLU:CA	2.46	0.45
2:A:382:VAL:C	2:A:384:GLU:N	2.72	0.45
2:A:727:THR:HA	2:A:730:ARG:CG	2.47	0.45
2:B:363:MET:C	2:B:365:PRO:HD2	2.41	0.45
2:B:420:CYS:HG	2:B:441:CYS:HB3	1.80	0.45
2:B:469:TRP:N	2:B:470:PRO:CD	2.77	0.45
2:A:77:LEU:N	2:A:77:LEU:HD22	2.32	0.45
2:A:212:ILE:CD1	2:A:268:ALA:O	2.65	0.45
2:A:318:ARG:HA	2:A:321:ALA:HB3	1.98	0.45
2:A:830:GLU:CD	2:A:830:GLU:N	2.74	0.45
2:A:845:LYS:HE3	2:A:845:LYS:HA	1.98	0.45
2:B:5:LYS:H	2:B:5:LYS:CD	2.08	0.45
2:B:211:GLU:C	2:B:266:THR:HG21	2.41	0.45
2:B:473:THR:HG22	2:B:476:LEU:CB	2.44	0.45
2:B:624:LEU:HD12	2:B:633:ALA:HA	1.98	0.45
2:B:746:VAL:C	2:B:771:LEU:HB2	2.40	0.45
2:B:763:ARG:HH12	2:B:769:ASP:CG	2.23	0.45
2:A:231:GLU:OE1	2:A:231:GLU:HA	2.16	0.45
2:A:501:VAL:O	2:A:502:SER:C	2.59	0.45
2:A:684:PRO:C	2:A:687:THR:HG22	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:148:LYS:HD2	2:B:468:GLY:CA	2.45	0.45
2:B:190:THR:HG22	2:B:342:ALA:CB	2.46	0.45
2:B:710:GLY:O	2:B:711:ARG:CB	2.64	0.45
2:A:247:LEU:N	2:A:247:LEU:HD22	2.31	0.45
2:A:274:ALA:HB2	2:A:291:VAL:H	1.80	0.45
2:A:820:GLN:HG2	2:B:844:LEU:HD23	1.99	0.45
2:B:101:THR:HG23	2:B:103:HIS:N	2.32	0.45
2:B:229:HIS:HD2	2:B:231:GLU:H	1.61	0.45
2:B:250:VAL:HG12	2:B:252:ILE:HD12	1.98	0.45
1:D:934:A:C6	1:D:935:C:N4	2.85	0.45
2:A:495:TRP:CD1	3:A:990:VAA:HG21	2.52	0.45
2:B:323:GLU:C	2:B:325:PHE:N	2.71	0.45
2:B:361:LEU:CD2	2:B:366:LEU:HD11	2.43	0.45
2:B:759:LEU:HD13	2:B:763:ARG:HE	1.82	0.45
2:A:224:GLN:NE2	2:A:304:ARG:NH2	2.41	0.45
2:A:830:GLU:CD	2:A:830:GLU:H	2.25	0.45
2:B:49:LEU:HB2	2:B:128:GLN:OE1	2.16	0.45
1:D:957:A:H4'	1:D:959:U:C5	2.52	0.45
2:A:49:LEU:HA	2:A:53:HIS:ND1	2.32	0.45
2:A:70:ARG:HA	2:A:70:ARG:HD2	1.68	0.45
2:A:111:LEU:O	2:A:111:LEU:HD13	2.16	0.45
2:A:128:GLN:O	2:A:132:LEU:HG	2.16	0.45
2:A:202:TYR:CE1	2:A:330:HIS:CE1	2.96	0.45
2:A:261:GLU:OE1	2:A:261:GLU:HA	2.17	0.45
2:A:401:ASN:ND2	2:A:403:SER:N	2.64	0.45
2:A:833:PRO:C	2:A:835:GLU:N	2.71	0.45
2:B:195:GLY:HA3	2:B:339:ILE:HD11	1.99	0.45
2:B:585:ALA:O	2:B:589:VAL:HG23	2.17	0.45
1:C:955:C:H1'	2:A:828:PHE:HA	1.99	0.45
2:A:56:ASP:O	2:A:60:GLN:HG3	2.17	0.45
2:A:326:ARG:O	2:A:329:GLY:N	2.49	0.45
2:A:332:VAL:HG13	2:A:333:LYS:H	1.82	0.45
2:A:469:TRP:HB2	2:A:476:LEU:HD12	1.98	0.45
2:A:680:HIS:CA	2:A:687:THR:HG21	2.43	0.45
2:A:714:GLU:CG	2:A:715:ALA:N	2.75	0.45
2:B:713:GLU:CD	2:B:713:GLU:H	2.25	0.45
2:B:808:ARG:HG2	2:B:854:ILE:HD13	1.99	0.45
1:D:961:C:O2'	1:D:962:U:H5'	2.17	0.45
2:A:425:VAL:O	2:A:426:PRO:C	2.59	0.45
2:B:44:ASN:ND2	3:B:991:VAA:N3S	2.65	0.45
2:B:50:HIS:CD2	2:B:52:GLY:N	2.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:171:ARG:HH12	2:B:364:ARG:HH21	1.64	0.45
2:B:264:PHE:O	2:B:265:GLY:C	2.59	0.45
2:B:759:LEU:HD11	2:B:763:ARG:HE	1.82	0.45
2:A:13:GLU:HA	2:A:685:PHE:CD2	2.52	0.45
2:A:674:VAL:O	2:A:677:LYS:HB2	2.16	0.45
2:B:173:VAL:HG12	2:B:360:TRP:HZ2	1.82	0.45
2:B:218:GLU:CD	2:B:218:GLU:H	2.24	0.45
2:B:593:ARG:O	2:B:593:ARG:HG2	2.17	0.45
2:A:101:THR:O	2:A:102:ARG:C	2.59	0.44
2:A:245:ILE:HG21	2:A:252:ILE:HD13	1.96	0.44
2:A:312:LEU:HG	2:A:313:ASP:N	2.32	0.44
2:A:482:GLY:O	2:A:513:LYS:HG3	2.17	0.44
2:A:722:LEU:O	2:A:723:LYS:C	2.59	0.44
2:A:795:LEU:HD13	2:A:795:LEU:C	2.42	0.44
2:B:148:LYS:HE2	4:B:1061:HOH:O	2.17	0.44
2:B:225:ALA:HB1	2:B:255:LEU:HD21	1.99	0.44
2:B:812:LEU:HD22	2:B:847:ASN:O	2.17	0.44
2:B:831:LYS:HE3	2:B:831:LYS:HA	1.98	0.44
2:A:28:ASN:HD22	2:A:29:PRO:N	2.13	0.44
2:A:759:LEU:HD12	2:A:763:ARG:HG3	1.99	0.44
2:A:800:GLU:HA	2:A:800:GLU:OE1	2.17	0.44
2:B:59:LEU:O	2:B:63:LEU:HD23	2.18	0.44
2:B:257:ASP:OD1	2:B:282:ILE:HG23	2.17	0.44
2:B:280:TYR:O	2:B:284:GLU:HG2	2.17	0.44
2:B:294:ILE:HD13	2:B:300:MET:SD	2.57	0.44
1:D:947:C:O2'	1:D:948:G:P	2.75	0.44
2:A:443:SER:OG	2:A:444:PRO:HD2	2.17	0.44
2:A:494:LEU:CD2	2:A:494:LEU:N	2.63	0.44
2:A:549:ASP:OD1	2:A:683:MET:HA	2.17	0.44
2:A:678:LEU:O	2:A:681:PRO:HD2	2.18	0.44
2:A:746:VAL:HG13	2:A:747:TYR:N	2.33	0.44
2:A:806:GLU:CA	2:A:858:LEU:HD21	2.42	0.44
2:A:808:ARG:HD2	2:A:808:ARG:HA	1.84	0.44
2:B:283:GLY:HA2	2:B:288:LEU:HG	1.99	0.44
1:C:962:U:H2'	1:C:963:A:C8	2.52	0.44
2:A:41:PRO:O	2:A:43:PRO:HD3	2.17	0.44
2:A:221:PHE:HA	2:A:245:ILE:CD1	2.47	0.44
2:A:789:ARG:HG2	2:A:789:ARG:HH11	1.82	0.44
2:B:170:PRO:C	2:B:171:ARG:O	2.60	0.44
2:B:172:LEU:HD21	2:B:353:TYR:HB3	1.97	0.44
2:B:221:PHE:HB2	2:B:293:VAL:HG11	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:277:PRO:CD	2:B:353:TYR:CE2	2.94	0.44
2:B:393:TRP:CZ3	2:B:394:LEU:HD23	2.52	0.44
2:A:201:ARG:NE	2:A:332:VAL:HG11	2.32	0.44
2:A:814:ALA:O	2:A:818:ARG:HG3	2.17	0.44
2:B:341:LEU:HD13	2:B:342:ALA:N	2.32	0.44
2:B:398:LYS:N	2:B:398:LYS:CD	2.81	0.44
2:B:543:VAL:HG23	2:B:544:GLU:N	2.32	0.44
2:B:779:LEU:HD22	2:B:790:MET:HE2	1.99	0.44
2:A:170:PRO:O	2:A:171:ARG:C	2.60	0.44
2:A:774:ARG:HD3	2:A:774:ARG:C	2.43	0.44
2:B:61:ASP:CG	2:B:552:ARG:HH22	2.26	0.44
2:B:201:ARG:HH11	2:B:332:VAL:CG1	2.22	0.44
2:B:418:GLU:HG3	2:B:445:ARG:O	2.17	0.44
2:B:684:PRO:O	2:B:687:THR:HG22	2.17	0.44
2:B:722:LEU:O	2:B:726:VAL:HG23	2.17	0.44
2:A:2:ASP:C	2:A:4:PRO:HD3	2.43	0.44
2:A:266:THR:C	2:A:268:ALA:H	2.25	0.44
2:B:202:TYR:HE1	2:B:330:HIS:CE1	2.34	0.44
2:B:202:TYR:HE2	2:B:244:ARG:HD3	1.83	0.44
2:B:606:ALA:HB1	2:B:649:TYR:CD1	2.53	0.44
1:C:932:U:HO2'	1:C:933:C:H5	1.61	0.44
1:C:955:C:O2	2:A:832:ALA:HB2	2.17	0.44
1:D:935:C:H1'	2:B:584:ASN:ND2	2.32	0.44
2:A:201:ARG:HG2	2:A:211:GLU:HA	2.00	0.44
2:A:837:VAL:CG1	2:A:838:GLU:N	2.81	0.44
2:B:7:TYR:HB2	2:B:583:TYR:CG	2.53	0.44
2:B:223:ASP:HB2	2:B:245:ILE:HD13	2.00	0.44
2:B:305:VAL:HG22	2:B:310:ARG:HB2	1.99	0.44
1:C:941:A:C2'	1:C:942:G:O5'	2.66	0.44
1:D:912:U:H2'	1:D:913:C:O5'	2.18	0.44
2:A:44:ASN:C	2:A:46:THR:H	2.26	0.44
2:A:85:ILE:HG23	2:A:86:ALA:N	2.32	0.44
2:A:115:TRP:O	2:A:116:GLN:C	2.61	0.44
2:A:173:VAL:HG12	2:A:360:TRP:HZ2	1.83	0.44
2:A:572:LEU:HD23	2:A:572:LEU:HA	1.81	0.44
2:A:774:ARG:HG3	2:A:774:ARG:NH1	2.33	0.44
2:B:51:MET:HE2	2:B:537:ILE:CB	2.47	0.44
2:B:202:TYR:OH	2:B:244:ARG:NH2	2.51	0.44
2:B:223:ASP:HB2	2:B:245:ILE:CD1	2.48	0.44
2:B:416:TYR:CE2	2:B:423:VAL:HG22	2.53	0.44
2:B:421:GLN:CA	2:B:421:GLN:NE2	2.76	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:448:ARG:NH1	2:B:448:ARG:HG2	2.33	0.44
1:C:975:A:OP2	2:A:337:TYR:OH	2.29	0.43
1:D:923:G:N2	2:B:570:ARG:NH2	2.66	0.43
2:A:171:ARG:CZ	2:A:364:ARG:HH21	2.31	0.43
2:A:190:THR:HG22	2:A:342:ALA:HB2	1.99	0.43
2:A:576:ARG:NH1	2:A:577:ASN:OD1	2.51	0.43
2:A:641:VAL:O	2:A:645:PHE:HB3	2.18	0.43
2:B:201:ARG:HH11	2:B:201:ARG:CG	2.31	0.43
2:B:202:TYR:O	2:B:203:GLU:O	2.36	0.43
2:B:274:ALA:HB1	2:B:292:SER:OG	2.17	0.43
2:B:378:ASP:OD2	2:B:504:TYR:OH	2.36	0.43
1:C:931:C:O4'	1:C:936:A:N6	2.52	0.43
2:A:279:ASP:O	2:A:283:GLY:N	2.43	0.43
2:B:12:VAL:O	2:B:16:TRP:HD1	2.01	0.43
2:B:364:ARG:H	2:B:364:ARG:HG2	1.53	0.43
2:B:469:TRP:HA	2:B:476:LEU:HD22	1.99	0.43
2:B:510:ARG:HG3	2:B:510:ARG:NH1	2.32	0.43
2:A:7:TYR:HB2	2:A:583:TYR:CG	2.53	0.43
2:A:489:TYR:CD1	2:A:489:TYR:C	2.96	0.43
2:A:766:SER:O	2:A:767:ARG:CB	2.66	0.43
2:B:176:CYS:SG	2:B:347:CYS:SG	3.16	0.43
2:B:225:ALA:CA	2:B:252:ILE:CG2	2.92	0.43
2:B:261:GLU:OE2	2:B:261:GLU:HA	2.18	0.43
2:B:627:ALA:O	2:B:628:LEU:HB2	2.18	0.43
2:B:738:LEU:HD23	2:B:744:VAL:CG1	2.47	0.43
2:A:8:ASP:OD1	2:A:10:LYS:HB2	2.18	0.43
2:A:96:LEU:C	2:A:98:GLU:N	2.77	0.43
2:A:199:THR:HB	2:A:332:VAL:HG13	1.99	0.43
2:A:312:LEU:CD2	2:A:316:GLU:HG2	2.44	0.43
2:A:382:VAL:CG2	2:A:516:LEU:HD12	2.33	0.43
2:B:157:PHE:O	2:B:160:TYR:N	2.52	0.43
2:B:170:PRO:O	2:B:171:ARG:C	2.61	0.43
2:B:592:SER:C	2:B:594:GLU:N	2.76	0.43
2:B:778:ALA:HA	2:B:792:LEU:HB2	2.01	0.43
2:A:1:MET:HE1	2:A:690:LEU:HD23	2.00	0.43
2:A:68:ARG:C	2:A:70:ARG:N	2.77	0.43
2:A:202:TYR:HE1	2:A:330:HIS:CG	2.36	0.43
2:A:211:GLU:O	2:A:212:ILE:HD12	2.19	0.43
2:A:255:LEU:HD12	2:A:255:LEU:O	2.19	0.43
2:A:441:CYS:SG	2:A:443:SER:HB2	2.59	0.43
2:B:412:ILE:HG23	2:B:451:ASP:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:486:VAL:HG22	2:B:516:LEU:HD22	2.00	0.43
1:C:918:G:N2	1:C:956:A:C1'	2.81	0.43
2:A:326:ARG:CG	2:A:327:GLU:N	2.74	0.43
2:B:428:PRO:O	2:B:430:ARG:N	2.50	0.43
1:D:936:A:O4'	1:D:938:G:C8	2.72	0.43
1:D:943:A:H2'	1:D:944:G:O4'	2.18	0.43
2:A:28:ASN:HD22	2:A:29:PRO:CD	2.32	0.43
2:A:196:LYS:HB2	2:A:198:TYR:HE2	1.84	0.43
2:A:241:LYS:HB3	2:A:242:ARG:H	1.61	0.43
2:A:683:MET:O	2:A:687:THR:HB	2.18	0.43
2:A:718:ALA:O	2:A:721:ALA:HB3	2.18	0.43
2:A:844:LEU:HD23	2:B:820:GLN:HG2	2.01	0.43
2:B:245:ILE:CA	2:B:248:THR:HG22	2.48	0.43
2:A:452:VAL:HG12	2:A:453:PHE:N	2.33	0.43
2:A:743:GLU:O	2:A:744:VAL:HG23	2.19	0.43
2:A:759:LEU:HD12	2:A:763:ARG:CG	2.49	0.43
2:B:9:PRO:C	2:B:11:SER:N	2.77	0.43
2:B:126:LEU:HD23	2:B:126:LEU:HA	1.84	0.43
2:B:160:TYR:HB3	2:B:166:ALA:HB2	2.01	0.43
2:B:290:PRO:C	2:B:291:VAL:HG12	2.44	0.43
2:B:587:ARG:HH11	2:B:587:ARG:HG3	1.83	0.43
2:B:610:MET:HG2	2:B:649:TYR:CD2	2.53	0.43
2:A:304:ARG:HH11	2:A:304:ARG:CG	2.25	0.43
2:A:820:GLN:CD	2:A:820:GLN:C	2.86	0.43
2:B:145:MET:HG3	2:B:410:HIS:NE2	2.34	0.43
2:B:363:MET:HE3	2:B:363:MET:CA	2.49	0.43
2:B:639:GLU:O	2:B:640:LEU:C	2.60	0.43
2:B:771:LEU:HD12	2:B:773:GLU:H	1.84	0.43
2:A:73:GLU:O	2:A:75:VAL:HG23	2.19	0.43
2:A:216:ARG:HB3	2:A:219:THR:CG2	2.47	0.43
2:A:469:TRP:HB2	2:A:476:LEU:CD1	2.49	0.43
2:A:608:ARG:NH2	4:A:1057:HOH:O	2.52	0.43
2:A:828:PHE:CE2	2:A:837:VAL:HG23	2.54	0.43
2:B:216:ARG:HA	2:B:318:ARG:NH2	2.33	0.43
2:B:225:ALA:CA	2:B:252:ILE:HG23	2.31	0.43
2:B:448:ARG:HG2	2:B:448:ARG:HH11	1.82	0.43
2:B:714:GLU:O	2:B:715:ALA:C	2.62	0.43
2:B:774:ARG:HG2	2:B:774:ARG:HH11	1.84	0.43
2:B:778:ALA:HB1	2:B:790:MET:C	2.44	0.43
1:C:913:C:OP1	2:A:566:ARG:HB3	2.19	0.42
1:D:906:G:N2	1:D:967:C:C2	2.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:932:U:H3'	1:D:932:U:OP1	2.19	0.42
2:A:637:VAL:CG2	2:A:679:LEU:CD2	2.97	0.42
2:B:130:LYS:HE3	2:B:138:TRP:CD1	2.54	0.42
2:B:210:ILE:CD1	2:B:238:LEU:HD13	2.36	0.42
2:B:830:GLU:O	2:B:831:LYS:HE3	2.19	0.42
2:A:45:VAL:CG1	2:A:118:LYS:HA	2.47	0.42
2:A:178:ARG:HG3	2:A:179:CYS:N	2.33	0.42
2:A:242:ARG:HB3	2:A:251:TRP:HE3	1.83	0.42
2:A:247:LEU:HD23	2:A:325:PHE:CE1	2.54	0.42
2:A:535:ASN:O	2:A:535:ASN:CG	2.61	0.42
2:B:3:LEU:HD21	2:B:590:LEU:CD1	2.47	0.42
2:B:41:PRO:HD2	2:B:60:GLN:NE2	2.30	0.42
2:B:220:VAL:HG21	2:B:325:PHE:CZ	2.50	0.42
2:B:412:ILE:CG2	2:B:451:ASP:O	2.66	0.42
2:B:480:TYR:HE2	2:B:509:GLU:HG3	1.83	0.42
2:A:152:ALA:CA	2:A:470:PRO:HG3	2.49	0.42
2:A:160:TYR:HE2	2:A:505:HIS:CD2	2.37	0.42
2:A:170:PRO:HB2	2:A:355:ILE:HG22	2.01	0.42
2:A:515:VAL:HG12	2:A:517:LEU:HD13	2.00	0.42
2:A:672:LEU:O	2:A:676:LEU:HG	2.19	0.42
2:B:136:ALA:O	2:B:138:TRP:N	2.52	0.42
2:B:390:ASN:C	2:B:392:ASP:H	2.27	0.42
2:B:404:ARG:HH12	2:B:454:ASP:CG	2.27	0.42
2:B:557:TYR:CE1	2:B:635:ARG:HB3	2.53	0.42
2:B:754:PRO:O	2:B:755:VAL:C	2.62	0.42
1:C:918:G:C2	1:C:956:A:N3	2.87	0.42
2:A:228:VAL:O	2:A:229:HIS:C	2.63	0.42
2:A:247:LEU:HD23	2:A:325:PHE:HE1	1.85	0.42
2:A:310:ARG:HG3	2:A:310:ARG:O	2.18	0.42
2:A:371:LEU:O	2:A:375:ARG:HB2	2.19	0.42
2:A:805:GLN:C	2:A:807:LYS:N	2.78	0.42
2:B:212:ILE:HD12	2:B:268:ALA:O	2.19	0.42
2:B:221:PHE:HB3	2:B:304:ARG:HB2	2.01	0.42
2:B:297:GLU:HB2	2:B:299:ARG:HG2	2.01	0.42
1:D:920:A:H2'	1:D:945:G:O6	2.20	0.42
2:A:2:ASP:O	2:A:4:PRO:CD	2.68	0.42
2:A:209:PHE:O	2:A:238:LEU:HD21	2.20	0.42
2:A:245:ILE:HG12	2:A:248:THR:HG22	1.98	0.42
2:A:272:THR:N	2:A:279:ASP:HB3	2.34	0.42
2:A:766:SER:O	2:A:767:ARG:HB2	2.19	0.42
2:B:372:LYS:NZ	2:B:372:LYS:CA	2.80	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:738:LEU:HA	2:B:739:PRO:HD3	1.89	0.42
1:C:918:G:H21	1:C:956:A:H1'	1.83	0.42
1:D:960:C:O2'	1:D:961:C:H5'	2.19	0.42
2:A:438:CYS:C	2:A:440:ALA:H	2.28	0.42
2:A:746:VAL:CG1	2:A:747:TYR:N	2.79	0.42
2:A:755:VAL:HG13	2:A:762:PHE:CG	2.54	0.42
2:A:825:SER:OG	2:A:826:PRO:HD2	2.18	0.42
2:A:833:PRO:HD2	2:A:836:VAL:HG11	2.02	0.42
2:B:361:LEU:CD2	2:B:366:LEU:CD1	2.97	0.42
2:B:462:TRP:N	2:B:463:PRO:CD	2.77	0.42
2:B:529:MET:HE2	2:B:536:VAL:CA	2.47	0.42
1:C:943:A:H2'	1:C:944:G:O4'	2.19	0.42
1:C:946:U:H3'	1:C:946:U:H6	1.84	0.42
2:A:88:GLN:OE1	2:A:406:LEU:HD22	2.19	0.42
2:A:145:MET:HE1	2:A:408:TRP:CE2	2.54	0.42
2:A:286:HIS:O	2:A:287:GLY:C	2.62	0.42
2:A:417:CYS:SG	2:A:441:CYS:SG	3.17	0.42
2:B:482:GLY:O	2:B:512:PHE:HA	2.20	0.42
2:B:683:MET:O	2:B:687:THR:HG22	2.19	0.42
2:B:721:ALA:HB3	2:B:754:PRO:HG2	2.01	0.42
2:B:830:GLU:N	2:B:830:GLU:CD	2.76	0.42
2:A:456:TRP:CB	2:A:498:ARG:HH12	2.33	0.42
2:A:674:VAL:HA	2:A:677:LYS:HG3	2.02	0.42
2:B:339:ILE:H	2:B:339:ILE:HG13	1.67	0.42
2:B:802:ARG:HB2	2:B:802:ARG:NH1	2.32	0.42
1:C:931:C:O2'	1:C:932:U:P	2.78	0.42
2:A:140:ARG:HH12	2:A:479:PHE:HZ	1.67	0.42
2:A:412:ILE:HB	2:A:453:PHE:CZ	2.55	0.42
2:B:19:LYS:HE2	2:B:699:GLU:OE2	2.20	0.42
2:B:190:THR:HA	2:B:342:ALA:HA	2.01	0.42
2:B:217:PRO:CG	2:B:318:ARG:HG3	2.49	0.42
2:A:220:VAL:HA	2:A:223:ASP:OD2	2.20	0.42
2:A:249:GLU:OE1	2:A:249:GLU:HA	2.20	0.42
2:A:372:LYS:O	2:A:372:LYS:NZ	2.47	0.42
2:B:233:GLU:O	2:B:235:TYR:N	2.53	0.42
2:B:294:ILE:HD11	2:B:300:MET:SD	2.60	0.42
2:B:382:VAL:O	2:B:384:GLU:N	2.53	0.42
2:B:453:PHE:CD2	2:B:457:PHE:CD2	3.08	0.42
2:B:529:MET:HG3	2:B:535:ASN:O	2.20	0.42
1:D:904:C:H1'	4:D:171:HOH:O	2.20	0.41
2:A:202:TYR:CE1	2:A:330:HIS:ND1	2.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:216:ARG:HD2	2:A:219:THR:CG2	2.50	0.41
2:A:273:PRO:HG3	2:A:283:GLY:HA3	2.02	0.41
2:B:94:LEU:O	2:B:98:GLU:HG2	2.20	0.41
2:B:178:ARG:CG	2:B:347:CYS:SG	3.08	0.41
2:B:326:ARG:CG	2:B:327:GLU:N	2.82	0.41
1:C:952:G:O2'	1:C:953:U:H5'	2.20	0.41
2:A:178:ARG:HG3	2:A:179:CYS:SG	2.60	0.41
2:B:397:VAL:HG12	2:B:398:LYS:H	1.84	0.41
2:B:431:TYR:CZ	2:B:432:LEU:HD23	2.55	0.41
2:B:469:TRP:C	2:B:471:GLU:H	2.28	0.41
2:B:488:GLY:C	2:B:490:ASP:N	2.78	0.41
2:A:51:MET:HE3	2:A:51:MET:HB2	1.92	0.41
2:A:82:HIS:CG	2:A:145:MET:HE2	2.55	0.41
2:A:221:PHE:O	2:A:304:ARG:HG3	2.19	0.41
2:A:428:PRO:HB2	2:A:429:GLU:OE1	2.20	0.41
2:A:747:TYR:CE2	2:A:774:ARG:HB2	2.56	0.41
2:B:201:ARG:HD2	2:B:211:GLU:HA	2.02	0.41
2:B:210:ILE:HD12	2:B:210:ILE:HA	1.89	0.41
2:B:255:LEU:HD12	2:B:255:LEU:C	2.44	0.41
2:B:692:GLN:HA	2:B:697:LYS:O	2.20	0.41
2:B:821:ARG:HH11	2:B:821:ARG:CB	2.33	0.41
2:B:830:GLU:CG	2:B:831:LYS:NZ	2.83	0.41
1:C:946:U:C6	1:C:946:U:C3'	3.03	0.41
1:C:974:C:H3'	1:C:974:C:H6	1.85	0.41
1:C:975:A:H8	2:A:213:ALA:O	2.03	0.41
1:D:957:A:HO2'	1:D:959:U:P	2.43	0.41
2:A:422:ALA:HB1	4:A:1000:HOH:O	2.20	0.41
2:A:624:LEU:HD13	2:A:633:ALA:N	2.35	0.41
2:A:779:LEU:HD13	2:A:792:LEU:CD2	2.49	0.41
2:B:293:VAL:CA	2:B:301:GLU:O	2.66	0.41
2:B:420:CYS:HG	2:B:438:CYS:HG	1.65	0.41
2:B:738:LEU:HD12	2:B:738:LEU:N	2.35	0.41
2:A:417:CYS:SG	2:A:419:ASP:HB2	2.61	0.41
2:B:51:MET:HE2	2:B:537:ILE:CG2	2.50	0.41
2:B:363:MET:O	2:B:364:ARG:C	2.63	0.41
2:B:370:VAL:HG22	2:B:501:VAL:HA	2.02	0.41
1:C:955:C:C2'	1:C:956:A:H5'	2.51	0.41
4:C:178:HOH:O	2:A:783:MET:HE1	2.20	0.41
2:A:127:LYS:O	2:A:128:GLN:C	2.63	0.41
2:A:313:ASP:CG	2:A:314:ARG:N	2.79	0.41
2:B:84:GLY:HA2	2:B:408:TRP:HD1	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:276:ASP:HA	2:B:277:PRO:HD2	1.86	0.41
2:B:527:GLN:O	2:B:528:LYS:C	2.62	0.41
2:B:609:PHE:O	2:B:610:MET:C	2.62	0.41
2:B:779:LEU:CD1	2:B:792:LEU:HD13	2.51	0.41
1:C:929:G:H8	1:C:929:G:C5'	2.33	0.41
2:A:101:THR:O	2:A:104:ASP:N	2.54	0.41
2:A:220:VAL:HG12	2:A:270:LYS:CE	2.51	0.41
2:A:362:ARG:O	2:A:365:PRO:HD2	2.20	0.41
2:B:42:PRO:HB2	2:B:80:THR:C	2.45	0.41
2:B:252:ILE:HG23	2:B:253:PRO:HD2	2.03	0.41
2:B:280:TYR:CD2	2:B:284:GLU:HG2	2.55	0.41
2:B:425:VAL:O	2:B:426:PRO:C	2.64	0.41
2:B:473:THR:CG2	2:B:476:LEU:HB3	2.51	0.41
1:C:909:A:O2'	1:C:910:G:N7	2.45	0.41
1:C:952:G:H2'	1:C:953:U:C6	2.56	0.41
2:A:228:VAL:O	2:A:256:ALA:HA	2.21	0.41
2:B:462:TRP:HB3	2:B:463:PRO:HD3	2.02	0.41
2:B:537:ILE:HD12	2:B:567:LEU:CD2	2.51	0.41
2:B:678:LEU:HD23	2:B:705:TRP:CZ2	2.56	0.41
1:D:918:G:HO2'	1:D:919:A:P	2.44	0.41
1:D:931:C:O5'	1:D:931:C:C6	2.74	0.41
1:D:950:A:H2'	1:D:951:G:O4'	2.21	0.41
2:A:153:VAL:HG11	2:A:410:HIS:ND1	2.35	0.41
2:A:193:THR:CG2	2:A:194:PRO:HD2	2.51	0.41
2:A:264:PHE:O	2:A:265:GLY:C	2.64	0.41
2:A:280:TYR:CE1	2:A:355:ILE:HD11	2.55	0.41
2:A:462:TRP:O	2:A:464:LEU:N	2.53	0.41
2:A:472:GLU:HG2	2:A:472:GLU:O	2.20	0.41
2:A:779:LEU:HD13	2:A:792:LEU:HD21	2.02	0.41
2:A:829:ARG:NH2	2:A:841:GLU:OE2	2.53	0.41
2:B:9:PRO:O	2:B:11:SER:N	2.54	0.41
2:B:61:ASP:OD1	2:B:65:ARG:NE	2.53	0.41
2:B:107:ARG:HH11	2:B:107:ARG:HB3	1.85	0.41
2:B:188:VAL:HG21	2:B:351:ILE:HD13	2.03	0.41
2:B:225:ALA:CB	2:B:255:LEU:HD21	2.51	0.41
2:B:248:THR:OG1	2:B:249:GLU:N	2.50	0.41
2:B:270:LYS:HB2	2:B:270:LYS:HZ2	1.86	0.41
2:B:362:ARG:HH11	2:B:362:ARG:HG2	1.85	0.41
2:B:425:VAL:HA	2:B:426:PRO:HD2	1.86	0.41
2:B:680:HIS:HD2	2:B:684:PRO:HA	1.79	0.41
2:B:724:GLN:O	2:B:725:ALA:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:780:VAL:HG22	2:B:789:ARG:HG3	2.03	0.41
2:A:45:VAL:HG12	2:A:45:VAL:O	2.20	0.41
2:A:245:ILE:O	2:A:246:PRO:C	2.64	0.41
2:A:341:LEU:HD23	2:A:343:THR:HG23	2.03	0.41
2:B:242:ARG:HA	2:B:252:ILE:O	2.21	0.41
2:B:488:GLY:C	2:B:490:ASP:H	2.29	0.41
2:B:745:ARG:H	2:B:745:ARG:HG2	1.79	0.41
1:C:921:G:O2'	1:C:922:A:H5'	2.21	0.40
1:D:909:A:O2'	1:D:910:G:N7	2.37	0.40
2:A:174:ASN:OD1	2:A:174:ASN:N	2.53	0.40
2:A:185:ASP:C	2:A:187:GLU:N	2.79	0.40
2:A:305:VAL:CG1	2:A:310:ARG:HB3	2.52	0.40
2:A:362:ARG:O	2:A:365:PRO:CG	2.69	0.40
2:A:424:ASN:HD22	2:A:446:LEU:CD2	2.32	0.40
2:A:467:LEU:O	2:A:473:THR:HG22	2.19	0.40
2:A:616:ARG:HH12	2:A:711:ARG:HB2	1.86	0.40
2:B:68:ARG:C	2:B:70:ARG:N	2.78	0.40
2:B:149:ARG:O	2:B:152:ALA:N	2.52	0.40
2:B:366:LEU:HB3	2:B:501:VAL:HG21	2.02	0.40
2:B:367:ALA:O	2:B:371:LEU:HG	2.21	0.40
2:B:485:LEU:HD22	2:B:512:PHE:CE2	2.57	0.40
2:B:546:TYR:HE2	2:B:573:GLU:HG2	1.87	0.40
2:B:558:LEU:HB2	2:B:565:ILE:HD13	2.03	0.40
2:B:700:LEU:N	4:B:1006:HOH:O	2.53	0.40
1:C:904:C:H2'	1:C:905:G:C8	2.54	0.40
2:A:44:ASN:HB3	2:A:83:ALA:HB2	2.03	0.40
2:A:257:ASP:OD1	2:A:257:ASP:C	2.64	0.40
2:A:593:ARG:O	2:A:594:GLU:O	2.40	0.40
2:B:87:THR:O	2:B:88:GLN:C	2.64	0.40
2:B:313:ASP:HB3	2:B:316:GLU:HB2	2.03	0.40
2:B:382:VAL:HG11	2:B:516:LEU:CG	2.51	0.40
2:B:748:LEU:HD12	2:B:755:VAL:HG21	2.02	0.40
2:A:349:THR:CG2	2:A:350:PRO:HD2	2.52	0.40
2:A:721:ALA:HB3	2:A:754:PRO:HG2	2.03	0.40
2:A:727:THR:HA	2:A:730:ARG:HG2	2.02	0.40
2:B:38:ILE:HG22	2:B:76:TRP:CD1	2.56	0.40
2:B:67:LYS:O	2:B:70:ARG:HB3	2.20	0.40
2:B:173:VAL:HG12	2:B:360:TRP:CZ2	2.55	0.40
2:B:494:LEU:CD2	2:B:494:LEU:N	2.79	0.40
2:B:738:LEU:N	2:B:738:LEU:CD1	2.84	0.40
2:B:832:ALA:HB1	2:B:833:PRO:HD2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:916:C:H4'	1:C:959:U:O2	2.22	0.40
2:A:313:ASP:HB3	2:A:316:GLU:HB3	2.03	0.40
2:A:393:TRP:HE3	2:A:394:LEU:HD23	1.87	0.40
2:A:415:TRP:HB2	2:A:424:ASN:HB2	2.03	0.40
2:A:429:GLU:N	2:A:429:GLU:OE1	2.54	0.40
2:A:559:ALA:O	2:A:631:ALA:HB2	2.21	0.40
2:B:130:LYS:HD3	2:B:138:TRP:CZ2	2.56	0.40
2:B:326:ARG:HG3	2:B:327:GLU:H	1.86	0.40
1:C:960:C:O2'	1:C:961:C:H5'	2.21	0.40
1:D:926:C:O2'	1:D:927:U:H5'	2.21	0.40
1:D:934:A:C6	2:B:650:LEU:HD23	2.55	0.40
2:A:44:ASN:ND2	3:A:990:VAA:N3S	2.69	0.40
2:A:270:LYS:CB	2:A:270:LYS:HZ3	2.35	0.40
2:A:700:LEU:HA	2:A:703:GLU:HG2	2.04	0.40
2:A:717:ARG:NH1	2:A:717:ARG:HB2	2.37	0.40
2:B:170:PRO:O	2:B:171:ARG:O	2.40	0.40

All (1) 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)
2:A:742:GLN:OE1	2:A:742:GLN:OE1[7_555]	2.19	0.01

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	A	860/862 (100%)	683 (79%)	141 (16%)	36 (4%)	2 9
2	B	860/862 (100%)	670 (78%)	139 (16%)	51 (6%)	1 4
All	All	1720/1724 (100%)	1353 (79%)	280 (16%)	87 (5%)	1 6

All (87) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	106	GLY
2	A	171	ARG
2	A	243	ALA
2	A	257	ASP
2	A	312	LEU
2	A	313	ASP
2	A	362	ARG
2	A	409	GLY
2	A	473	THR
2	A	594	GLU
2	B	162	HIS
2	B	165	LEU
2	B	203	GLU
2	B	243	ALA
2	B	246	PRO
2	B	247	LEU
2	B	249	GLU
2	B	312	LEU
2	B	313	ASP
2	B	409	GLY
2	B	431	TYR
2	B	489	TYR
2	B	594	GLU
2	B	711	ARG
2	A	45	VAL
2	A	102	ARG
2	A	332	VAL
2	A	451	ASP
2	A	489	TYR
2	B	2	ASP
2	B	10	LYS
2	B	45	VAL
2	B	267	GLY
2	B	307	GLU
2	B	429	GLU
2	B	435	PRO
2	B	462	TRP
2	B	473	THR
2	B	627	ALA
2	B	710	GLY
2	A	86	ALA
2	A	170	PRO

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Mol	Chain	Res	Type
2	A	287	GLY
2	A	429	GLU
2	A	711	ARG
2	B	3	LEU
2	B	99	GLY
2	B	137	ASP
2	B	161	TYR
2	B	180	GLU
2	B	208	GLY
2	B	308	ALA
2	B	362	ARG
2	B	569	LEU
2	A	3	LEU
2	A	169	ALA
2	A	308	ALA
2	A	523	ASP
2	B	171	ARG
2	B	714	GLU
2	B	754	PRO
2	A	137	ASP
2	A	431	TYR
2	A	462	TRP
2	A	713	GLU
2	B	170	PRO
2	B	391	MET
2	B	480	TYR
2	B	481	PRO
2	B	600	GLU
2	B	673	ALA
2	B	719	PHE
2	A	144	THR
2	A	267	GLY
2	A	834	LYS
2	B	234	ARG
2	B	767	ARG
2	A	428	PRO
2	A	709	GLY
2	B	428	PRO
2	B	24	PRO
2	B	382	VAL
2	B	426	PRO
2	A	208	GLY

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Mol	Chain	Res	Type
2	A	265	GLY
2	A	784	PRO
2	B	265	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	A	724/724 (100%)	641 (88%)	83 (12%)	5	18
2	B	724/724 (100%)	629 (87%)	95 (13%)	4	13
All	All	1448/1448 (100%)	1270 (88%)	178 (12%)	4	15

All (178) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	2	ASP
2	A	19	LYS
2	A	30	LYS
2	A	48	SER
2	A	51	MET
2	A	77	LEU
2	A	113	ARG
2	A	119	GLU
2	A	148	LYS
2	A	170	PRO
2	A	172	LEU
2	A	174	ASN
2	A	187	GLU
2	A	191	GLU
2	A	192	PRO
2	A	197	LEU
2	A	198	TYR
2	A	209	PHE
2	A	212	ILE
2	A	218	GLU

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Mol	Chain	Res	Type
2	A	219	THR
2	A	242	ARG
2	A	245	ILE
2	A	249	GLU
2	A	261	GLU
2	A	269	LEU
2	A	270	LYS
2	A	276	ASP
2	A	291	VAL
2	A	292	SER
2	A	301	GLU
2	A	307	GLU
2	A	323	GLU
2	A	332	VAL
2	A	339	ILE
2	A	347	CYS
2	A	356	PHE
2	A	372	LYS
2	A	382	VAL
2	A	388	LYS
2	A	396	ASN
2	A	397	VAL
2	A	401	ASN
2	A	404	ARG
2	A	408	TRP
2	A	412	ILE
2	A	420	CYS
2	A	421	GLN
2	A	429	GLU
2	A	431	TYR
2	A	432	LEU
2	A	448	ARG
2	A	461	LEU
2	A	479	PHE
2	A	494	LEU
2	A	501	VAL
2	A	512	PHE
2	A	521	VAL
2	A	522	LEU
2	A	541	GLU
2	A	560	THR
2	A	570	ARG

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Mol	Chain	Res	Type
2	A	592	SER
2	A	593	ARG
2	A	604	THR
2	A	679	LEU
2	A	707	GLU
2	A	727	THR
2	A	732	LEU
2	A	738	LEU
2	A	740	PRO
2	A	743	GLU
2	A	746	VAL
2	A	759	LEU
2	A	767	ARG
2	A	777	LYS
2	A	779	LEU
2	A	783	MET
2	A	800	GLU
2	A	805	GLN
2	A	830	GLU
2	A	834	LYS
2	A	845	LYS
2	B	2	ASP
2	B	5	LYS
2	B	30	LYS
2	B	37	VAL
2	B	63	LEU
2	B	75	VAL
2	B	77	LEU
2	B	88	GLN
2	B	107	ARG
2	B	113	ARG
2	B	118	LYS
2	B	127	LYS
2	B	147	GLU
2	B	151	ARG
2	B	172	LEU
2	B	178	ARG
2	B	180	GLU
2	B	181	THR
2	B	191	GLU
2	B	192	PRO
2	B	198	TYR

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Mol	Chain	Res	Type
2	B	201	ARG
2	B	202	TYR
2	B	205	GLU
2	B	209	PHE
2	B	211	GLU
2	B	212	ILE
2	B	218	GLU
2	B	228	VAL
2	B	246	PRO
2	B	247	LEU
2	B	255	LEU
2	B	266	THR
2	B	270	LYS
2	B	280	TYR
2	B	284	GLU
2	B	291	VAL
2	B	301	GLU
2	B	339	ILE
2	B	356	PHE
2	B	372	LYS
2	B	383	PRO
2	B	388	LYS
2	B	397	VAL
2	B	404	ARG
2	B	412	ILE
2	B	413	PRO
2	B	420	CYS
2	B	421	GLN
2	B	429	GLU
2	B	430	ARG
2	B	432	LEU
2	B	435	PRO
2	B	441	CYS
2	B	447	LYS
2	B	448	ARG
2	B	461	LEU
2	B	477	LYS
2	B	494	LEU
2	B	507	MET
2	B	510	ARG
2	B	512	PHE
2	B	521	VAL

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Mol	Chain	Res	Type
2	B	522	LEU
2	B	545	ARG
2	B	552	ARG
2	B	560	THR
2	B	580	ASN
2	B	587	ARG
2	B	593	ARG
2	B	600	GLU
2	B	604	THR
2	B	608	ARG
2	B	679	LEU
2	B	727	THR
2	B	730	ARG
2	B	732	LEU
2	B	745	ARG
2	B	755	VAL
2	B	767	ARG
2	B	769	ASP
2	B	770	LEU
2	B	771	LEU
2	B	777	LYS
2	B	783	MET
2	B	802	ARG
2	B	805	GLN
2	B	808	ARG
2	B	809	LEU
2	B	820	GLN
2	B	830	GLU
2	B	831	LYS
2	B	836	VAL
2	B	860	GLN
2	B	861	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	28	ASN
2	A	50	HIS
2	A	224	GLN
2	A	229	HIS
2	A	286	HIS
2	A	358	GLN

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Mol	Chain	Res	Type
2	A	390	ASN
2	A	401	ASN
2	A	424	ASN
2	A	505	HIS
2	A	518	HIS
2	A	563	GLN
2	A	580	ASN
2	A	584	ASN
2	A	680	HIS
2	A	692	GLN
2	A	724	GLN
2	A	860	GLN
2	B	50	HIS
2	B	57	ASN
2	B	60	GLN
2	B	116	GLN
2	B	229	HIS
2	B	237	HIS
2	B	275	HIS
2	B	358	GLN
2	B	421	GLN
2	B	424	ASN
2	B	505	HIS
2	B	518	HIS
2	B	527	GLN
2	B	580	ASN
2	B	584	ASN
2	B	680	HIS
2	B	692	GLN
2	B	724	GLN
2	B	805	GLN
2	B	820	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	C	74/75 (98%)	22 (29%)	9 (12%)
1	D	74/75 (98%)	28 (37%)	9 (12%)
All	All	148/150 (98%)	50 (33%)	18 (12%)

All (50) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	C	907	C
1	C	908	U
1	C	910	G
1	C	916	C
1	C	917	G
1	C	918	G
1	C	919	A
1	C	920	A
1	C	929	G
1	C	931	C
1	C	932	U
1	C	934	A
1	C	936	A
1	C	937	C
1	C	938	G
1	C	947	C
1	C	958	G
1	C	959	U
1	C	960	C
1	C	966	C
1	C	974	C
1	C	975	A
1	D	903	G
1	D	908	U
1	D	909	A
1	D	910	G
1	D	916	C
1	D	917	G
1	D	918	G
1	D	919	A
1	D	920	A
1	D	921	G
1	D	930	C
1	D	931	C
1	D	932	U
1	D	933	C
1	D	936	A
1	D	937	C
1	D	938	G
1	D	946	U
1	D	947	C
1	D	948	G
1	D	952	G

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Mol	Chain	Res	Type
1	D	957	A
1	D	958	G
1	D	959	U
1	D	960	C
1	D	966	C
1	D	974	C
1	D	975	A

All (18) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	C	907	C
1	C	909	A
1	C	917	G
1	C	931	C
1	C	936	A
1	C	937	C
1	C	947	C
1	C	957	A
1	C	959	U
1	D	907	C
1	D	909	A
1	D	916	C
1	D	917	G
1	D	936	A
1	D	937	C
1	D	947	C
1	D	957	A
1	D	959	U

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

2 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	VAA	B	991	-	31,32,32	3.23	9 (29%)	42,48,48	1.86	7 (16%)
3	VAA	A	990	-	31,32,32	3.21	10 (32%)	42,48,48	1.66	8 (19%)

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
3	VAA	B	991	-	-	5/23/39/39	0/3/3/3
3	VAA	A	990	-	-	1/23/39/39	0/3/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	990	VAA	C5'-N5'	-9.41	1.32	1.47
3	B	991	VAA	S-N5'	9.24	1.72	1.61
3	B	991	VAA	C5'-N5'	-9.14	1.33	1.47
3	B	991	VAA	O1S-S	7.33	1.53	1.43
3	A	990	VAA	O1S-S	7.15	1.53	1.43
3	A	990	VAA	S-N5'	6.78	1.69	1.61
3	A	990	VAA	S-N3S	5.99	1.74	1.63
3	B	991	VAA	S-N3S	5.69	1.74	1.63
3	A	990	VAA	C5'-C4'	-4.81	1.41	1.52
3	A	990	VAA	C4-N3	3.44	1.40	1.34
3	A	990	VAA	C4-N9	3.37	1.44	1.37
3	B	991	VAA	C4-N3	3.36	1.40	1.34
3	A	990	VAA	O2S-S	3.01	1.47	1.43
3	B	991	VAA	C4-N9	2.90	1.43	1.37
3	B	991	VAA	O4'-C1'	2.61	1.48	1.42
3	A	990	VAA	O4'-C1'	2.41	1.47	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	991	VAA	C6-N1	2.23	1.42	1.35
3	A	990	VAA	C3'-C2'	-2.16	1.47	1.53
3	B	991	VAA	C3'-C2'	-2.10	1.47	1.53

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	991	VAA	O2S-S-O1S	-7.19	109.75	120.34
3	A	990	VAA	O2S-S-O1S	-6.11	111.34	120.34
3	B	991	VAA	O4'-C1'-N9	4.47	116.67	108.09
3	B	991	VAA	C1'-N9-C8	3.97	135.90	127.09
3	A	990	VAA	C1'-N9-C8	3.27	134.36	127.09
3	A	990	VAA	O-C-CA	-2.75	118.49	120.66
3	B	991	VAA	C4-N9-C1'	-2.68	120.36	126.63
3	A	990	VAA	C4'-C5'-N5'	-2.65	107.48	112.53
3	B	991	VAA	N3S-S-N5'	2.38	116.40	110.59
3	A	990	VAA	C4-N9-C8	-2.37	103.25	105.74
3	A	990	VAA	O1S-S-N5'	-2.28	102.80	106.77
3	B	991	VAA	O2S-S-N5'	-2.28	102.80	106.77
3	B	991	VAA	C6-C5-C4	-2.17	114.22	117.18
3	A	990	VAA	C6-C5-C4	-2.14	114.26	117.18
3	A	990	VAA	C-CA-N	2.13	113.45	110.31

There are no chirality outliers.

All (6) torsion outliers are listed below:

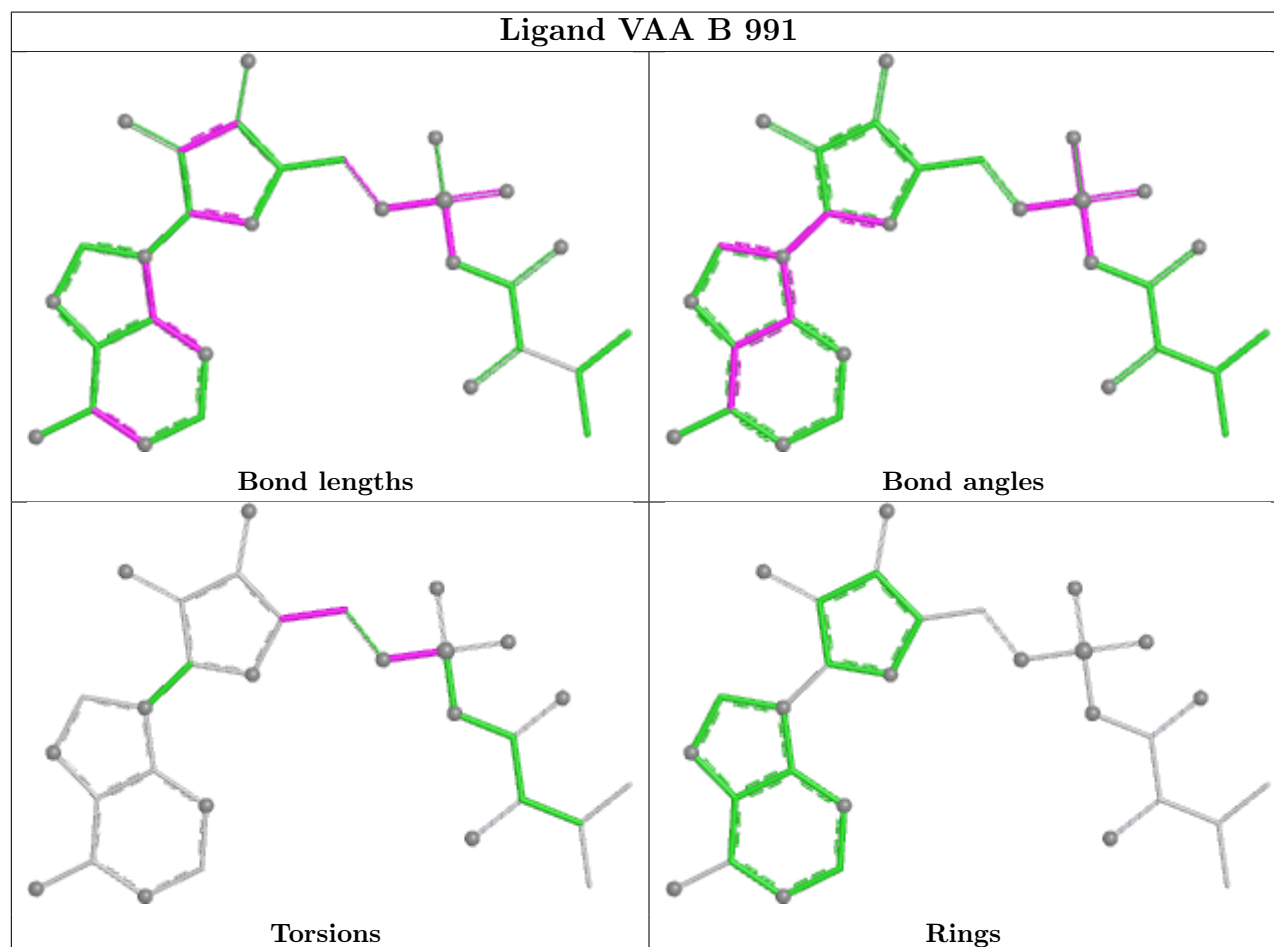
Mol	Chain	Res	Type	Atoms
3	B	991	VAA	C5'-N5'-S-O1S
3	B	991	VAA	C5'-N5'-S-N3S
3	B	991	VAA	O4'-C4'-C5'-N5'
3	B	991	VAA	C5'-N5'-S-O2S
3	A	990	VAA	C5'-N5'-S-O1S
3	B	991	VAA	C3'-C4'-C5'-N5'

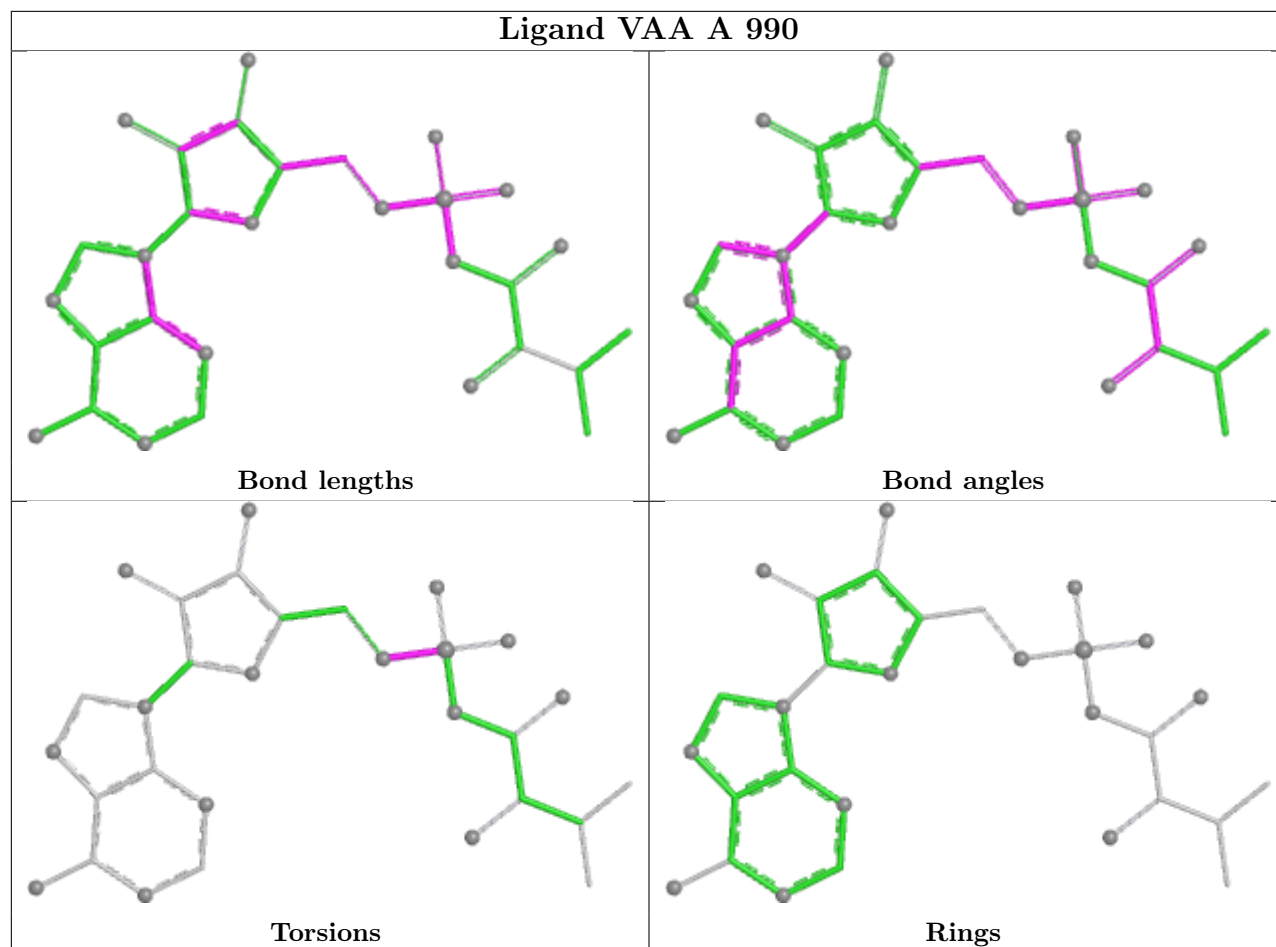
There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	991	VAA	1	0
3	A	990	VAA	5	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 than 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.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.