



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:29 PM UTC

PDB ID : 1YID / pdb_00001yid
Title : Crystal structure of tryptophanyl tRNA synthetase II from *Deinococcus radiodurans* in complex with ATP.
Authors : Buddha, M.R.; Crane, B.R.
Deposited on : 2005-01-11
Resolution : 2.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	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

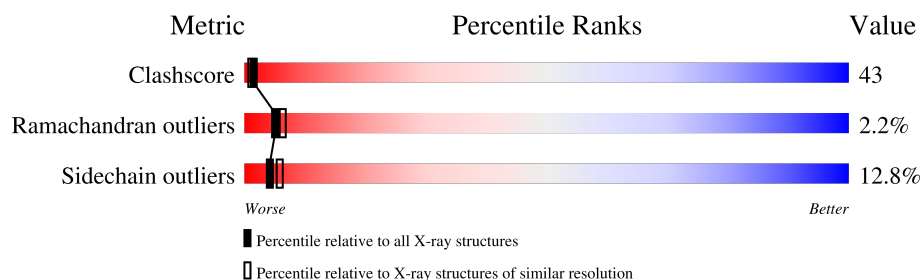
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	351	
1	B	351	
1	C	351	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 8016 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

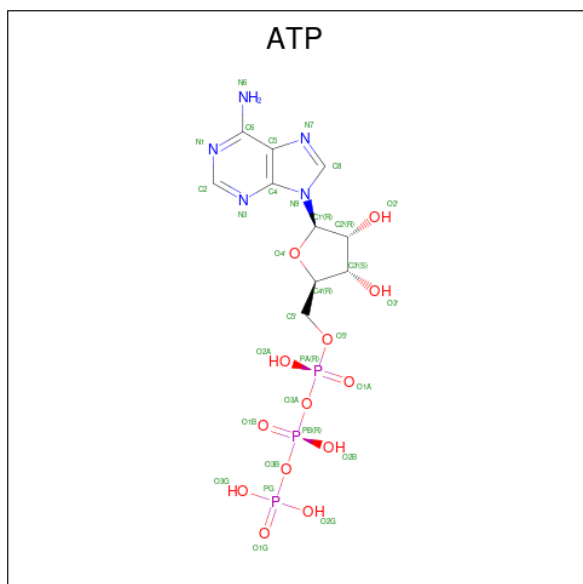
- Molecule 1 is a protein called tryptophanyl-tRNA synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	331	Total	C	N	O	S	2	0	0
			2544	1599	468	471	6			
1	A	331	Total	C	N	O	S	0	0	0
			2511	1581	457	467	6			
1	C	331	Total	C	N	O	S	0	0	0
			2532	1593	462	471	6			

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 4 is water.

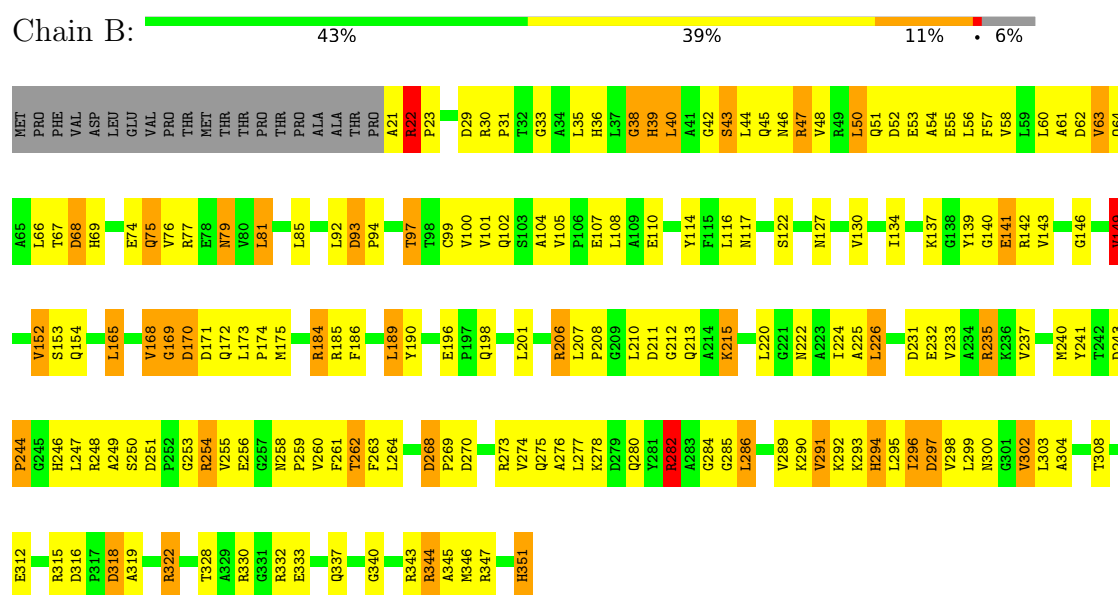
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	135	Total	O	0	0
			135	135		
4	A	132	Total	O	0	0
			132	132		
4	C	130	Total	O	0	0
			130	130		

3 Residue-property plots

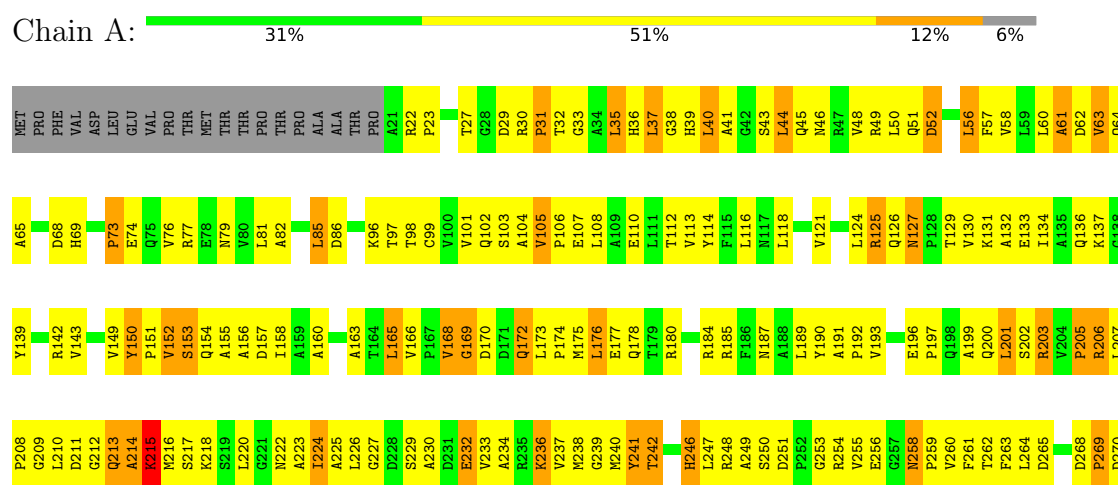
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

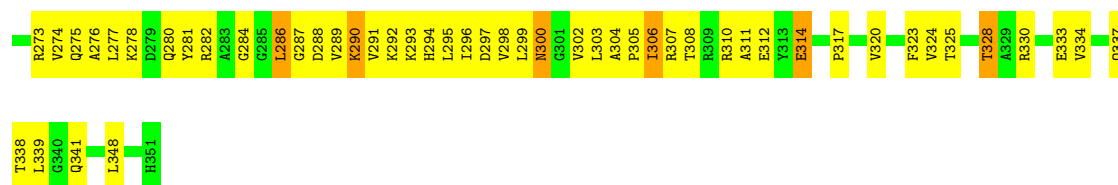
Note EDS was not executed.

• Molecule 1: tryptophanyl-tRNA synthetase



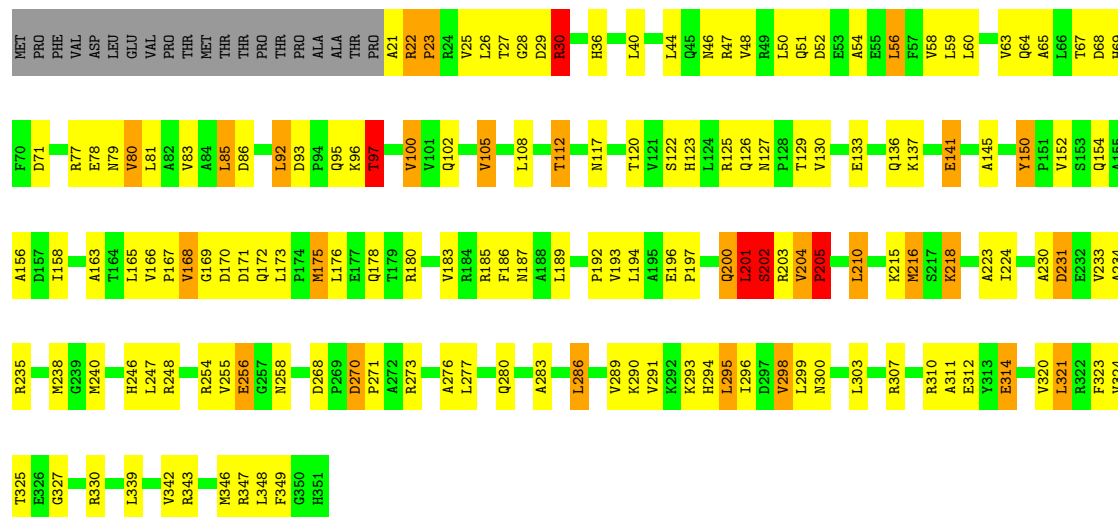
• Molecule 1: tryptophanyl-tRNA synthetase





• Molecule 1: tryptophanyl-tRNA synthetase

Chain C: 50% 36% 7% 6%



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	213.56Å 58.68Å 85.70Å 90.00° 96.60° 90.00°	Depositor
Resolution (Å)	30.00 – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) (30.00-2.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.260 , 0.280	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8016	wwPDB-VP
Average B, all atoms (Å ²)	69.0	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: MG, ATP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.54	0/2558	1.11	16/3478 (0.5%)
1	B	0.69	4/2591 (0.2%)	1.17	21/3519 (0.6%)
1	C	0.71	3/2579 (0.1%)	1.18	24/3505 (0.7%)
All	All	0.65	7/7728 (0.1%)	1.15	61/10502 (0.6%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	38	GLY	CA-C	-7.91	1.43	1.52
1	C	23	PRO	CA-CB	-7.05	1.46	1.54
1	B	39	HIS	N-CA	-6.28	1.39	1.46
1	B	76	VAL	CA-CB	5.54	1.60	1.54
1	C	342	VAL	CA-CB	5.10	1.60	1.54
1	B	39	HIS	C-N	5.06	1.40	1.33
1	C	216	MET	SD-CE	-5.05	1.67	1.79

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	201	LEU	N-CA-C	8.32	121.97	110.24
1	B	38	GLY	CA-C-O	7.91	129.05	120.66
1	A	43	SER	N-CA-C	7.69	119.44	111.14
1	C	105	VAL	CA-C-N	7.58	127.29	119.56
1	C	105	VAL	C-N-CA	7.58	127.29	119.56
1	A	241	TYR	N-CA-C	7.32	121.72	108.17
1	B	38	GLY	CA-C-N	-7.32	110.62	120.79
1	B	38	GLY	C-N-CA	-7.32	110.62	120.79
1	C	327	GLY	N-CA-C	-7.21	104.08	112.73
1	A	127	ASN	CA-C-N	7.07	126.33	118.97
1	A	127	ASN	C-N-CA	7.07	126.33	118.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	105	VAL	CA-C-N	6.93	126.63	119.56
1	A	105	VAL	C-N-CA	6.93	126.63	119.56
1	B	244	PRO	N-CA-C	-6.86	101.62	111.22
1	B	268	ASP	CA-C-N	6.80	126.76	119.28
1	B	268	ASP	C-N-CA	6.80	126.76	119.28
1	B	93	ASP	CA-C-N	6.79	127.35	119.47
1	B	93	ASP	C-N-CA	6.79	127.35	119.47
1	B	212	GLY	N-CA-C	-6.64	105.44	115.00
1	B	38	GLY	O-C-N	-6.57	115.82	122.19
1	B	39	HIS	CA-CB-CG	6.50	120.31	113.80
1	C	218	LYS	N-CA-C	-6.48	104.14	111.07
1	B	282	ARG	N-CA-C	-6.43	104.92	112.89
1	A	169	GLY	N-CA-C	-6.38	103.83	112.57
1	A	168	VAL	N-CA-C	6.35	116.65	107.88
1	C	324	VAL	N-CA-C	6.27	117.83	111.00
1	A	270	ASP	N-CA-C	6.26	117.53	109.65
1	C	303	LEU	N-CA-C	6.20	119.31	111.69
1	C	169	GLY	N-CA-C	-6.06	101.00	112.51
1	A	236	LYS	N-CA-C	-6.01	104.06	111.40
1	B	169	GLY	N-CA-C	-5.98	104.89	112.54
1	A	215	LYS	N-CA-C	5.90	123.37	110.80
1	B	291	VAL	N-CA-C	-5.85	104.62	110.30
1	C	202	SER	N-CA-C	5.79	123.14	110.80
1	A	155	ALA	N-CA-C	-5.73	105.04	111.28
1	A	314	GLU	N-CA-C	-5.69	105.08	111.28
1	C	173	LEU	CA-C-N	-5.58	113.93	119.56
1	C	173	LEU	C-N-CA	-5.58	113.93	119.56
1	C	175	MET	N-CA-C	-5.56	105.14	111.14
1	C	28	GLY	N-CA-C	5.49	118.77	110.75
1	A	44	LEU	N-CA-C	5.45	118.72	111.75
1	B	332	ARG	N-CA-C	-5.44	105.35	111.28
1	B	153	SER	N-CA-C	-5.44	105.35	111.28
1	C	141	GLU	CA-C-O	5.34	124.92	119.05
1	B	340	GLY	N-CA-C	-5.33	106.32	112.50
1	C	56	LEU	N-CA-C	5.28	118.23	109.46
1	C	97	THR	N-CA-C	5.27	118.07	109.59
1	B	100	VAL	N-CA-C	5.22	115.63	108.12
1	C	30	ARG	N-CA-C	-5.22	101.99	109.24
1	B	79	ASN	N-CA-C	5.17	119.44	113.18
1	B	63	VAL	N-CA-C	5.17	115.39	110.53
1	C	273	ARG	N-CA-C	-5.14	105.57	111.07
1	B	149	VAL	N-CA-C	5.13	117.91	112.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	215	LYS	N-CA-C	5.12	117.32	109.07
1	C	268	ASP	CA-C-N	5.11	125.15	119.32
1	C	268	ASP	C-N-CA	5.11	125.15	119.32
1	C	200	GLN	N-CA-C	-5.06	96.56	107.49
1	A	153	SER	N-CA-C	-5.05	106.37	112.54
1	C	270	ASP	CA-C-N	5.04	124.76	119.82
1	C	270	ASP	C-N-CA	5.04	124.76	119.82
1	A	178	GLN	N-CA-C	-5.03	105.89	112.23

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2511	0	2507	277	0
1	B	2544	0	2568	223	0
1	C	2532	0	2546	174	0
2	B	1	0	0	0	0
3	B	31	0	12	5	0
4	A	132	0	0	0	0
4	B	135	0	0	3	0
4	C	130	0	0	6	0
All	All	8016	0	7633	659	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 43.

All (659) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:VAL:HG23	1:A:172:GLN:HB2	1.11	1.11
1:C:204:VAL:HG12	1:C:205:PRO:HD2	1.32	1.08
1:B:240:MET:HE3	1:B:260:VAL:HG12	1.37	1.06
1:C:120:THR:HG23	1:C:123:HIS:H	1.19	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:LEU:HD11	1:A:86:ASP:HB3	1.41	1.00
1:C:180:ARG:HG3	1:C:180:ARG:HH11	1.26	1.00
1:B:51:GLN:HE21	1:B:97:THR:HG22	1.25	0.99
1:C:22:ARG:HB2	1:C:23:PRO:HD3	1.46	0.98
1:B:254:ARG:HD3	1:B:256:GLU:HG2	1.46	0.97
1:A:226:LEU:HB3	1:A:306:ILE:HD11	1.46	0.96
1:B:47:ARG:HA	1:B:50:LEU:HG	1.50	0.93
1:C:51:GLN:HE22	1:C:93:ASP:H	1.06	0.93
1:B:51:GLN:HE22	1:B:93:ASP:N	1.68	0.91
1:A:218:LYS:HA	1:A:218:LYS:HE2	1.54	0.89
1:B:51:GLN:HE22	1:B:93:ASP:H	0.89	0.89
1:C:254:ARG:HD3	1:C:256:GLU:HG2	1.54	0.88
1:A:193:VAL:HG21	1:A:341:GLN:HB3	1.54	0.88
1:B:168:VAL:HG23	1:B:172:GLN:HB2	1.55	0.87
1:C:77:ARG:O	1:C:80:VAL:HG12	1.72	0.87
1:B:50:LEU:HD11	1:B:56:LEU:HD13	1.55	0.86
1:C:26:LEU:HD23	1:C:158:ILE:HD13	1.55	0.86
1:A:168:VAL:CG2	1:A:172:GLN:HB2	2.02	0.85
1:A:207:LEU:HD23	1:A:216:MET:HE1	1.55	0.85
1:B:36:HIS:HD2	1:B:38:GLY:H	1.23	0.85
1:B:280:GLN:HB2	1:B:286:LEU:HD12	1.59	0.84
1:A:169:GLY:H	1:A:172:GLN:HG3	1.43	0.83
1:A:73:PRO:O	1:A:76:VAL:HG12	1.78	0.83
1:A:207:LEU:HD12	1:A:208:PRO:HD2	1.61	0.82
1:C:311:ALA:HA	1:C:314:GLU:HG3	1.62	0.82
1:A:35:LEU:CD1	1:A:86:ASP:HB3	2.10	0.82
1:A:254:ARG:HH11	1:A:256:GLU:HB2	1.43	0.81
1:C:51:GLN:HE21	1:C:97:THR:HG22	1.44	0.81
1:B:277:LEU:HD12	1:B:286:LEU:HD11	1.60	0.81
1:B:68:ASP:HB3	1:B:69:HIS:HD2	1.45	0.80
1:A:127:ASN:HB3	1:A:130:VAL:HG12	1.63	0.80
1:B:36:HIS:H	1:B:39:HIS:HD2	1.29	0.80
1:B:295:LEU:O	1:B:298:VAL:HG12	1.82	0.80
1:B:51:GLN:NE2	1:B:93:ASP:H	1.75	0.79
1:B:44:LEU:O	1:B:48:VAL:HG23	1.83	0.79
1:A:52:ASP:HB3	1:A:96:LYS:NZ	1.98	0.79
1:A:63:VAL:HG13	1:A:102:GLN:HG2	1.65	0.78
1:A:229:SER:OG	1:A:232:GLU:HB2	1.83	0.78
1:B:51:GLN:HE21	1:B:97:THR:CG2	1.96	0.78
1:C:216:MET:HE3	1:C:223:ALA:HB1	1.65	0.78
1:C:93:ASP:HB3	1:C:96:LYS:HB2	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:322:ARG:HG2	1:B:322:ARG:HH21	1.50	0.77
1:A:168:VAL:HG22	1:A:169:GLY:O	1.84	0.77
1:A:207:LEU:CD1	1:A:208:PRO:HD2	2.14	0.77
1:A:226:LEU:HD12	1:A:226:LEU:H	1.49	0.76
1:A:60:LEU:O	1:A:62:ASP:N	2.18	0.76
1:A:168:VAL:HG23	1:A:172:GLN:CB	2.06	0.76
1:A:254:ARG:HH11	1:A:256:GLU:CB	1.99	0.76
1:B:127:ASN:HB3	1:B:130:VAL:CG1	2.16	0.76
1:B:29:ASP:OD2	3:B:3000:ATP:H4'	1.86	0.75
1:C:180:ARG:HG3	1:C:180:ARG:NH1	2.00	0.75
1:B:127:ASN:HB3	1:B:130:VAL:HG12	1.67	0.75
1:C:123:HIS:CD2	1:C:178:GLN:HE21	2.04	0.75
1:C:204:VAL:HG12	1:C:205:PRO:CD	2.15	0.74
1:B:206:ARG:HG3	3:B:3000:ATP:N1	2.02	0.74
1:A:112:THR:O	1:A:116:LEU:HG	1.89	0.73
1:A:303:LEU:O	1:A:307:ARG:HB2	1.88	0.72
1:A:333:GLU:O	1:A:337:GLN:HG2	1.89	0.72
1:A:291:VAL:HG13	1:A:292:LYS:N	2.04	0.72
1:A:201:LEU:HD23	1:A:202:SER:H	1.53	0.72
1:B:36:HIS:H	1:B:39:HIS:CD2	2.08	0.72
1:A:216:MET:HG3	1:A:223:ALA:HA	1.71	0.72
1:A:288:ASP:HA	1:A:291:VAL:HG12	1.69	0.71
1:B:273:ARG:O	1:B:276:ALA:HB3	1.90	0.71
1:A:305:PRO:HG2	1:A:306:ILE:H	1.56	0.71
1:A:230:ALA:HB1	1:A:300:ASN:HD21	1.55	0.71
1:C:166:VAL:HG23	1:C:166:VAL:O	1.90	0.71
1:B:289:VAL:O	1:B:293:LYS:HG3	1.91	0.71
1:A:229:SER:O	1:A:233:VAL:HG23	1.91	0.71
1:B:213:GLN:OE1	1:B:220:LEU:HD13	1.91	0.70
1:A:85:LEU:HD13	1:A:310:ARG:HH22	1.56	0.70
1:B:184:ARG:HG2	1:B:184:ARG:HH21	1.54	0.70
1:C:56:LEU:HD11	1:C:58:VAL:HG13	1.74	0.70
1:B:254:ARG:HD3	1:B:256:GLU:CG	2.21	0.69
1:A:85:LEU:HD13	1:A:310:ARG:NH2	2.07	0.69
1:C:290:LYS:HE2	1:C:290:LYS:HA	1.74	0.69
1:B:39:HIS:O	1:B:42:GLY:N	2.25	0.69
1:B:254:ARG:CD	1:B:256:GLU:HG2	2.21	0.69
1:A:101:VAL:O	1:A:104:ALA:HB3	1.92	0.69
1:B:122:SER:OG	1:C:141:GLU:HB3	1.93	0.69
1:A:269:PRO:HD2	1:A:273:ARG:NH1	2.08	0.69
1:C:180:ARG:HD3	1:C:197:PRO:O	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:LEU:HA	1:A:44:LEU:HB3	1.73	0.69
1:B:68:ASP:OD1	1:B:137:LYS:HE2	1.92	0.69
1:A:112:THR:HG22	1:A:153:SER:HA	1.75	0.69
1:A:291:VAL:HG13	1:A:292:LYS:H	1.57	0.69
1:B:51:GLN:NE2	1:B:97:THR:HG22	2.05	0.69
1:A:253:GLY:O	1:A:282:ARG:HA	1.92	0.69
1:C:36:HIS:CG	1:C:216:MET:HE2	2.27	0.69
1:A:173:LEU:N	1:A:174:PRO:HD2	2.07	0.68
1:C:22:ARG:HB2	1:C:23:PRO:CD	2.20	0.68
1:C:51:GLN:HE22	1:C:93:ASP:N	1.87	0.68
1:A:184:ARG:HD2	1:A:196:GLU:OE1	1.93	0.68
1:A:259:PRO:HA	1:A:262:THR:CG2	2.24	0.68
1:A:201:LEU:CD2	1:A:202:SER:H	2.06	0.68
1:A:30:ARG:HH22	1:A:68:ASP:HB3	1.58	0.68
1:A:254:ARG:HD2	1:A:256:GLU:HB2	1.74	0.68
1:C:123:HIS:CD2	1:C:178:GLN:NE2	2.62	0.68
1:A:127:ASN:HB3	1:A:130:VAL:CG1	2.23	0.68
1:A:133:GLU:O	1:A:137:LYS:HG3	1.94	0.68
1:C:254:ARG:CD	1:C:256:GLU:HG2	2.23	0.68
1:B:22:ARG:CG	1:B:23:PRO:HD3	2.24	0.67
1:A:277:LEU:HD12	1:A:286:LEU:HD11	1.75	0.67
1:C:168:VAL:HG22	1:C:172:GLN:HB2	1.77	0.67
1:A:108:LEU:O	1:A:112:THR:HG23	1.93	0.67
1:A:139:TYR:O	1:A:142:ARG:HG3	1.95	0.67
1:A:237:VAL:O	1:A:240:MET:N	2.28	0.67
1:C:187:ASN:HB3	1:C:192:PRO:HA	1.75	0.67
1:B:168:VAL:HG22	1:B:169:GLY:O	1.94	0.67
1:A:110:GLU:O	1:A:113:VAL:HG12	1.94	0.67
1:A:44:LEU:O	1:A:48:VAL:HG23	1.95	0.67
1:B:22:ARG:HH21	1:B:53:GLU:HG3	1.59	0.67
1:A:112:THR:HG22	1:A:156:ALA:CB	2.25	0.67
1:A:291:VAL:CG1	1:A:292:LYS:H	2.07	0.67
1:B:22:ARG:CB	1:B:23:PRO:HD3	2.26	0.67
1:B:255:VAL:HG21	1:B:278:LYS:HG3	1.77	0.67
1:C:168:VAL:CG2	1:C:172:GLN:HB2	2.25	0.66
1:A:27:THR:O	1:A:58:VAL:HA	1.96	0.66
1:A:180:ARG:O	1:A:184:ARG:HD3	1.94	0.66
1:A:302:VAL:O	1:A:305:PRO:HD2	1.95	0.66
1:C:92:LEU:HG	1:C:97:THR:HG21	1.78	0.66
1:C:95:GLN:HA	1:C:95:GLN:NE2	2.11	0.66
1:C:294:HIS:O	1:C:298:VAL:HG12	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:233:VAL:O	1:B:237:VAL:HG23	1.95	0.65
1:A:226:LEU:HD23	1:A:306:ILE:CD1	2.26	0.65
1:B:259:PRO:HA	1:B:262:THR:CG2	2.26	0.65
1:C:175:MET:SD	1:C:175:MET:C	2.80	0.65
1:A:220:LEU:C	1:A:222:ASN:H	2.04	0.65
1:B:240:MET:CE	1:B:260:VAL:HG12	2.23	0.65
1:B:68:ASP:HB3	1:B:69:HIS:CD2	2.30	0.64
1:A:232:GLU:O	1:A:236:LYS:HB2	1.97	0.64
1:C:166:VAL:HG21	1:C:176:LEU:HD23	1.79	0.64
1:B:64:GLN:H	1:B:102:GLN:HE22	1.43	0.64
1:A:202:SER:OG	1:A:205:PRO:HB3	1.96	0.64
1:A:250:SER:O	1:A:284:GLY:HA2	1.97	0.64
1:A:294:HIS:HA	1:A:297:ASP:OD2	1.98	0.64
1:B:35:LEU:HD13	1:B:44:LEU:HD11	1.79	0.64
1:B:36:HIS:CD2	1:B:38:GLY:H	2.11	0.64
1:A:273:ARG:O	1:A:277:LEU:HD23	1.97	0.64
1:B:43:SER:O	1:B:46:ASN:N	2.31	0.63
1:A:168:VAL:HG11	1:A:199:ALA:HB1	1.81	0.63
1:C:127:ASN:HB3	1:C:130:VAL:HG22	1.80	0.63
1:A:130:VAL:O	1:A:134:ILE:HG13	1.98	0.63
1:B:277:LEU:CD1	1:B:286:LEU:HD11	2.29	0.63
1:B:146:GLY:HA3	1:C:117:ASN:ND2	2.13	0.63
1:B:237:VAL:HG13	1:B:240:MET:HE1	1.81	0.63
1:B:127:ASN:CB	1:B:130:VAL:HG12	2.28	0.62
1:B:74:GLU:OE1	1:C:347:ARG:NH1	2.31	0.62
1:A:256:GLU:H	1:A:256:GLU:CD	2.07	0.62
1:A:317:PRO:O	1:A:320:VAL:HG12	1.99	0.62
1:B:137:LYS:HD3	1:B:139:TYR:CE2	2.35	0.62
1:B:146:GLY:HA3	1:C:117:ASN:HD22	1.64	0.62
1:B:351:HIS:N	1:B:351:HIS:CD2	2.67	0.62
1:C:56:LEU:CD1	1:C:58:VAL:HG13	2.29	0.62
1:C:108:LEU:O	1:C:112:THR:HG23	2.00	0.62
1:C:133:GLU:O	1:C:136:GLN:HG3	2.00	0.62
1:C:238:MET:HE2	1:C:238:MET:HA	1.81	0.62
1:A:180:ARG:HG2	1:A:196:GLU:HG2	1.82	0.62
1:A:304:ALA:N	1:A:305:PRO:HD2	2.14	0.62
1:C:238:MET:HE3	1:C:296:ILE:HD11	1.80	0.62
1:A:207:LEU:CG	1:A:208:PRO:HD2	2.31	0.61
1:A:108:LEU:HD13	1:A:157:ASP:OD1	2.01	0.61
1:A:241:TYR:O	1:A:259:PRO:HD2	2.00	0.61
1:A:254:ARG:HB2	1:A:256:GLU:OE1	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:268:ASP:OD2	1:B:274:VAL:HG23	1.99	0.61
1:A:105:VAL:HG13	1:A:108:LEU:HG	1.83	0.61
1:C:40:LEU:HA	1:C:44:LEU:HD12	1.81	0.61
1:B:22:ARG:HH21	1:B:53:GLU:CG	2.13	0.61
1:B:23:PRO:HD2	1:B:54:ALA:HB2	1.81	0.61
1:A:180:ARG:HG2	1:A:197:PRO:HD2	1.80	0.61
1:A:259:PRO:O	1:A:263:PHE:HB2	2.00	0.61
1:A:210:LEU:HB2	1:A:222:ASN:OD1	2.00	0.61
1:C:52:ASP:OD2	1:C:96:LYS:NZ	2.33	0.61
1:C:51:GLN:NE2	1:C:97:THR:HG22	2.16	0.61
1:B:63:VAL:H	1:B:102:GLN:HE21	1.49	0.60
1:A:220:LEU:C	1:A:222:ASN:N	2.57	0.60
1:C:51:GLN:NE2	1:C:93:ASP:H	1.88	0.60
1:B:255:VAL:HG13	1:B:261:PHE:CD2	2.36	0.60
1:A:291:VAL:CG1	1:A:292:LYS:N	2.63	0.60
1:B:66:LEU:C	1:B:68:ASP:H	2.08	0.60
1:A:296:ILE:HG13	1:A:297:ASP:N	2.16	0.60
1:A:255:VAL:HG22	1:A:261:PHE:CE1	2.36	0.60
1:A:134:ILE:HD13	1:A:143:VAL:HG21	1.83	0.60
1:B:105:VAL:HG12	1:B:108:LEU:HG	1.84	0.60
1:C:51:GLN:NE2	1:C:97:THR:CG2	2.64	0.60
1:C:123:HIS:HD2	1:C:178:GLN:HE21	1.47	0.59
1:B:22:ARG:HB2	1:B:23:PRO:HD3	1.83	0.59
1:A:36:HIS:H	1:A:39:HIS:HD2	1.50	0.59
1:A:58:VAL:HG13	1:A:58:VAL:O	2.00	0.59
1:A:205:PRO:O	1:A:206:ARG:C	2.44	0.59
1:C:175:MET:HB2	4:C:1003:HOH:O	2.02	0.59
1:C:187:ASN:CB	1:C:192:PRO:HA	2.32	0.59
1:C:256:GLU:H	1:C:256:GLU:CD	2.08	0.59
1:C:295:LEU:HD22	1:C:299:LEU:HG	1.84	0.59
1:A:41:ALA:CB	1:A:207:LEU:HD22	2.33	0.59
1:B:40:LEU:O	1:B:45:GLN:HG2	2.01	0.59
1:C:56:LEU:HD12	1:C:97:THR:HB	1.83	0.59
1:B:33:GLY:HA2	1:B:79:ASN:OD1	2.03	0.59
1:B:173:LEU:N	1:B:174:PRO:HD2	2.18	0.59
1:A:226:LEU:HD12	1:A:226:LEU:N	2.17	0.59
1:B:53:GLU:OE1	1:B:53:GLU:HA	2.03	0.59
1:B:101:VAL:HG13	1:B:104:ALA:HB3	1.85	0.59
1:A:139:TYR:CD2	1:A:143:VAL:HG13	2.37	0.59
1:C:36:HIS:ND1	1:C:216:MET:HE2	2.18	0.59
1:A:142:ARG:O	1:A:142:ARG:HD3	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:64:GLN:H	1:C:102:GLN:HE22	1.51	0.58
1:B:75:GLN:O	1:B:79:ASN:ND2	2.36	0.58
1:A:288:ASP:CA	1:A:291:VAL:HG12	2.34	0.58
1:A:295:LEU:O	1:A:299:LEU:HG	2.03	0.58
1:A:52:ASP:OD2	1:A:52:ASP:N	2.32	0.58
1:C:286:LEU:HD12	1:C:291:VAL:HG23	1.85	0.58
1:B:40:LEU:HA	1:B:44:LEU:HB2	1.84	0.58
1:A:190:TYR:O	1:A:191:ALA:C	2.45	0.58
1:A:288:ASP:HA	1:A:291:VAL:CG1	2.33	0.58
1:C:63:VAL:H	1:C:102:GLN:HE21	1.52	0.58
1:C:254:ARG:CG	1:C:256:GLU:HG2	2.33	0.58
1:A:160:ALA:HA	1:A:338:THR:HG21	1.85	0.58
1:A:289:VAL:O	1:A:293:LYS:HB2	2.04	0.58
1:A:56:LEU:HD13	1:A:97:THR:HG23	1.86	0.58
1:A:112:THR:HG22	1:A:156:ALA:HB3	1.86	0.58
1:C:254:ARG:HD2	1:C:256:GLU:O	2.04	0.58
1:C:216:MET:HE3	1:C:223:ALA:CB	2.32	0.58
1:C:234:ALA:O	1:C:238:MET:HG2	2.04	0.58
1:B:40:LEU:HD23	1:B:226:LEU:HD21	1.85	0.57
1:A:288:ASP:O	1:A:291:VAL:HG12	2.03	0.57
1:A:56:LEU:HD22	1:A:57:PHE:N	2.19	0.57
1:A:99:CYS:SG	1:A:324:VAL:HG12	2.43	0.57
1:B:273:ARG:NH2	1:B:294:HIS:NE2	2.52	0.57
1:A:52:ASP:HB3	1:A:96:LYS:HZ3	1.68	0.57
1:A:30:ARG:HD2	1:A:65:ALA:HA	1.84	0.57
1:C:295:LEU:O	1:C:298:VAL:HG13	2.05	0.57
1:A:52:ASP:HB3	1:A:96:LYS:HZ1	1.68	0.57
1:C:36:HIS:HB2	1:C:216:MET:HE2	1.86	0.57
1:A:259:PRO:HA	1:A:262:THR:HG22	1.86	0.57
1:B:278:LYS:HG2	1:B:282:ARG:NH2	2.19	0.57
1:A:185:ARG:HD2	1:A:189:LEU:HD22	1.86	0.57
1:B:259:PRO:HA	1:B:262:THR:HG23	1.86	0.56
1:A:216:MET:HA	1:A:222:ASN:O	2.05	0.56
1:C:216:MET:HE3	1:C:224:ILE:H	1.69	0.56
1:B:260:VAL:HG23	1:B:261:PHE:N	2.19	0.56
1:C:233:VAL:HG21	1:C:307:ARG:HH21	1.69	0.56
1:B:127:ASN:CG	1:B:130:VAL:HG12	2.30	0.56
1:B:270:ASP:O	1:B:273:ARG:HB3	2.06	0.56
1:A:30:ARG:HH22	1:A:68:ASP:CB	2.18	0.56
1:A:173:LEU:O	1:A:177:GLU:HB2	2.06	0.56
1:C:77:ARG:O	1:C:80:VAL:CG1	2.50	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:SER:C	1:B:47:ARG:HD2	2.31	0.56
1:C:127:ASN:OD1	1:C:129:THR:HG22	2.06	0.56
1:C:79:ASN:O	1:C:83:VAL:HG22	2.04	0.56
1:A:208:PRO:HG2	1:A:263:PHE:CE2	2.40	0.56
1:B:23:PRO:O	1:B:54:ALA:HB1	2.06	0.56
1:B:296:ILE:HD12	1:B:300:ASN:ND2	2.20	0.56
1:A:248:ARG:HD3	1:A:248:ARG:N	2.21	0.56
1:C:112:THR:HG22	1:C:156:ALA:CB	2.36	0.56
1:C:258:ASN:C	1:C:258:ASN:HD22	2.13	0.56
1:B:316:ASP:OD2	1:B:319:ALA:HB2	2.06	0.55
1:A:112:THR:CG2	1:A:153:SER:HA	2.36	0.55
1:A:212:GLY:O	1:A:213:GLN:C	2.49	0.55
1:C:171:ASP:HB2	1:C:172:GLN:NE2	2.21	0.55
1:B:296:ILE:HG13	1:B:297:ASP:N	2.20	0.55
1:B:248:ARG:HD3	1:B:248:ARG:N	2.22	0.55
1:A:136:GLN:O	1:A:136:GLN:HG3	2.06	0.55
1:C:51:GLN:HE21	1:C:97:THR:CG2	2.15	0.55
1:C:105:VAL:O	1:C:105:VAL:HG13	2.06	0.55
1:A:98:THR:CG2	1:A:330:ARG:HD2	2.36	0.55
1:A:240:MET:CE	1:A:259:PRO:HB2	2.37	0.55
1:C:36:HIS:HB2	1:C:216:MET:CE	2.37	0.55
1:A:35:LEU:O	1:A:226:LEU:CD1	2.54	0.55
1:A:79:ASN:HA	1:A:82:ALA:HB3	1.88	0.55
1:A:218:LYS:HA	1:A:218:LYS:CE	2.34	0.55
1:A:32:THR:HG22	1:A:32:THR:O	2.06	0.55
1:C:133:GLU:O	1:C:137:LYS:HD3	2.06	0.55
1:A:234:ALA:HA	1:A:296:ILE:CG2	2.37	0.55
1:C:339:LEU:O	1:C:343:ARG:HG3	2.07	0.55
1:B:36:HIS:N	1:B:39:HIS:HD2	2.00	0.54
1:A:207:LEU:HG	1:A:208:PRO:HD2	1.89	0.54
1:B:35:LEU:HD22	1:B:39:HIS:CD2	2.43	0.54
1:A:205:PRO:HG2	1:A:206:ARG:H	1.72	0.54
1:B:330:ARG:O	1:B:333:GLU:HB3	2.08	0.54
1:A:68:ASP:OD2	1:A:137:LYS:NZ	2.41	0.54
1:A:193:VAL:HG21	1:A:341:GLN:CB	2.33	0.54
1:B:296:ILE:CD1	1:B:300:ASN:ND2	2.71	0.54
1:A:170:ASP:OD1	1:A:203:ARG:NH2	2.40	0.54
1:A:76:VAL:HG13	1:A:77:ARG:N	2.22	0.54
1:A:99:CYS:HB2	1:A:323:PHE:CZ	2.43	0.54
1:A:150:TYR:CE2	1:A:154:GLN:NE2	2.76	0.54
1:A:277:LEU:HA	1:A:280:GLN:NE2	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:MET:CG	1:A:223:ALA:HA	2.38	0.53
1:B:23:PRO:HD2	1:B:54:ALA:CB	2.37	0.53
1:B:248:ARG:HD3	1:B:248:ARG:H	1.72	0.53
1:A:261:PHE:CE1	1:A:278:LYS:HG2	2.42	0.53
1:C:180:ARG:HE	1:C:196:GLU:CD	2.15	0.53
1:A:215:LYS:NZ	1:A:217:SER:OG	2.41	0.53
1:A:250:SER:O	1:A:284:GLY:CA	2.56	0.53
1:A:254:ARG:CD	1:A:256:GLU:HB2	2.39	0.53
1:B:255:VAL:HG22	1:B:261:PHE:CE2	2.43	0.53
1:B:277:LEU:HD22	1:B:277:LEU:H	1.73	0.53
1:C:21:ALA:HB2	4:C:1133:HOH:O	2.08	0.53
1:A:242:THR:HB	1:A:258:ASN:HD21	1.73	0.53
1:A:288:ASP:C	1:A:291:VAL:HG12	2.34	0.53
1:A:260:VAL:HG13	1:A:295:LEU:HD22	1.89	0.53
1:C:254:ARG:HG2	1:C:255:VAL:N	2.22	0.53
1:B:64:GLN:HE22	1:B:154:GLN:CG	2.22	0.53
1:A:36:HIS:HD2	1:A:38:GLY:H	1.55	0.53
1:A:37:LEU:HG	1:A:224:ILE:HG12	1.90	0.53
1:C:210:LEU:HD12	1:C:240:MET:CG	2.39	0.53
1:B:333:GLU:OE2	1:B:333:GLU:HA	2.09	0.53
1:A:136:GLN:O	1:A:136:GLN:CG	2.56	0.53
1:A:125:ARG:HG3	1:A:125:ARG:HH21	1.74	0.53
1:A:176:LEU:O	1:A:176:LEU:HD13	2.09	0.53
1:C:51:GLN:HB2	1:C:96:LYS:HB3	1.90	0.52
1:B:66:LEU:C	1:B:68:ASP:N	2.68	0.52
1:B:264:LEU:HG	1:B:295:LEU:HD12	1.92	0.52
1:B:74:GLU:CD	1:C:347:ARG:NH1	2.67	0.52
1:B:149:VAL:O	1:B:149:VAL:CG1	2.57	0.52
1:A:35:LEU:HD12	1:A:226:LEU:HD13	1.91	0.52
1:B:29:ASP:O	1:B:31:PRO:HD3	2.10	0.52
1:A:208:PRO:HG3	1:A:262:THR:HG23	1.91	0.52
1:A:288:ASP:O	1:A:292:LYS:HG3	2.09	0.52
1:A:246:HIS:NE2	1:A:251:ASP:O	2.35	0.52
1:C:30:ARG:HD2	1:C:64:GLN:HE21	1.75	0.52
1:C:201:LEU:HD23	1:C:202:SER:H	1.75	0.52
1:B:116:LEU:O	1:C:145:ALA:HB3	2.10	0.52
1:B:292:LYS:O	1:B:296:ILE:HG23	2.10	0.52
1:A:41:ALA:HB2	1:A:207:LEU:HD22	1.91	0.52
1:C:180:ARG:NH1	1:C:180:ARG:CG	2.70	0.52
1:C:203:ARG:C	1:C:204:VAL:HG23	2.35	0.52
1:B:263:PHE:HB3	1:B:295:LEU:HD11	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:322:ARG:HG2	1:B:322:ARG:NH2	2.20	0.51
1:A:211:ASP:C	1:A:213:GLN:H	2.18	0.51
1:C:295:LEU:CD2	1:C:299:LEU:HG	2.40	0.51
1:B:315:ARG:O	1:B:315:ARG:HG2	2.10	0.51
1:A:255:VAL:HG21	1:A:278:LYS:HD3	1.92	0.51
1:A:261:PHE:CD1	1:A:278:LYS:HG2	2.45	0.51
1:A:273:ARG:O	1:A:276:ALA:HB3	2.11	0.51
1:C:123:HIS:HD2	1:C:178:GLN:NE2	2.05	0.51
1:C:311:ALA:CA	1:C:314:GLU:HG3	2.38	0.51
1:B:58:VAL:HG23	1:B:99:CYS:HA	1.92	0.51
1:A:49:ARG:O	1:A:52:ASP:OD2	2.29	0.51
1:B:30:ARG:HH22	1:B:68:ASP:HB2	1.74	0.51
1:B:274:VAL:C	1:B:276:ALA:N	2.68	0.51
1:A:260:VAL:HG13	1:A:295:LEU:CD2	2.41	0.51
1:C:166:VAL:O	1:C:166:VAL:CG2	2.58	0.51
1:B:43:SER:O	1:B:47:ARG:HD2	2.11	0.51
1:A:98:THR:OG1	1:A:330:ARG:HD2	2.11	0.51
1:A:299:LEU:O	1:A:303:LEU:HD13	2.10	0.51
1:C:120:THR:CG2	1:C:123:HIS:H	2.08	0.51
1:B:22:ARG:HE	1:B:53:GLU:HG3	1.76	0.51
1:B:140:GLY:O	1:B:143:VAL:HG23	2.11	0.51
1:C:122:SER:O	1:C:126:GLN:HG3	2.10	0.51
1:C:78:GLU:HA	1:C:78:GLU:OE2	2.11	0.51
1:B:292:LYS:O	1:B:296:ILE:CG2	2.59	0.51
1:A:158:ILE:HG23	1:A:163:ALA:HB3	1.93	0.51
1:B:22:ARG:NH2	1:B:53:GLU:HG3	2.25	0.50
1:B:101:VAL:HG13	1:B:101:VAL:O	2.12	0.50
1:A:277:LEU:HD13	1:A:280:GLN:NE2	2.26	0.50
1:C:56:LEU:HD11	1:C:58:VAL:CG1	2.40	0.50
1:B:21:ALA:HA	1:B:54:ALA:HA	1.92	0.50
1:A:193:VAL:HG22	1:A:193:VAL:O	2.12	0.50
1:A:234:ALA:HA	1:A:296:ILE:HG22	1.93	0.50
1:A:237:VAL:HG13	1:A:295:LEU:HD23	1.93	0.50
1:B:299:LEU:HA	1:B:302:VAL:HG12	1.94	0.50
1:A:46:ASN:ND2	1:A:50:LEU:HG	2.25	0.50
1:A:305:PRO:HG2	1:A:306:ILE:HG22	1.93	0.50
1:C:40:LEU:HD12	1:C:44:LEU:HB2	1.92	0.50
1:C:187:ASN:CG	1:C:192:PRO:HA	2.37	0.50
1:A:277:LEU:O	1:A:281:TYR:N	2.45	0.50
1:A:185:ARG:O	1:A:189:LEU:HB2	2.12	0.50
1:A:256:GLU:CD	1:A:256:GLU:N	2.70	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:LEU:HB3	1:A:307:ARG:NH2	2.27	0.50
1:B:38:GLY:O	1:B:39:HIS:C	2.49	0.50
1:B:186:PHE:CD1	1:B:186:PHE:C	2.90	0.50
1:C:185:ARG:HH11	1:C:189:LEU:HD22	1.76	0.50
1:A:253:GLY:HA3	1:A:281:TYR:CE2	2.47	0.49
1:B:184:ARG:HE	1:B:196:GLU:CD	2.20	0.49
1:C:127:ASN:HB3	1:C:130:VAL:CG2	2.42	0.49
1:C:85:LEU:CD1	1:C:310:ARG:CZ	2.91	0.49
1:C:180:ARG:CD	1:C:197:PRO:O	2.61	0.49
1:B:189:LEU:CD2	1:C:71:ASP:HA	2.42	0.49
1:B:211:ASP:OD1	1:B:213:GLN:NE2	2.44	0.49
1:A:149:VAL:O	1:A:152:VAL:HG13	2.13	0.49
1:C:22:ARG:CB	1:C:23:PRO:HD3	2.31	0.49
1:B:344:ARG:HG3	1:B:344:ARG:HH11	1.78	0.49
1:A:260:VAL:O	1:A:264:LEU:HB2	2.13	0.49
1:C:120:THR:HG23	1:C:123:HIS:N	2.04	0.49
1:C:216:MET:CE	1:C:224:ILE:H	2.25	0.49
1:B:175:MET:SD	1:B:175:MET:C	2.96	0.49
1:B:237:VAL:HG13	1:B:240:MET:CE	2.42	0.49
1:B:344:ARG:HG3	1:B:344:ARG:NH1	2.28	0.49
1:B:210:LEU:HD21	1:B:224:ILE:HG13	1.93	0.49
1:B:254:ARG:HH11	1:B:256:GLU:CG	2.25	0.49
1:B:268:ASP:OD1	1:B:273:ARG:NH2	2.46	0.49
1:B:134:ILE:HD13	1:B:143:VAL:HG21	1.95	0.49
1:A:32:THR:HG23	1:A:69:HIS:HE1	1.77	0.49
1:B:58:VAL:HG23	1:B:58:VAL:O	2.12	0.48
1:B:215:LYS:HG2	1:B:220:LEU:CD1	2.43	0.48
1:B:295:LEU:O	1:B:295:LEU:HD23	2.13	0.48
1:B:116:LEU:HD23	1:B:152:VAL:HG21	1.95	0.48
1:A:63:VAL:HG13	1:A:102:GLN:CG	2.40	0.48
1:B:316:ASP:OD1	1:B:318:ASP:OD2	2.32	0.48
1:C:325:THR:HG21	4:C:1339:HOH:O	2.14	0.48
1:A:226:LEU:HD23	1:A:306:ILE:HD12	1.95	0.48
1:C:36:HIS:CB	1:C:216:MET:HE2	2.44	0.48
1:B:110:GLU:OE1	1:B:343:ARG:HD3	2.14	0.48
1:B:254:ARG:NH1	1:B:256:GLU:HG3	2.28	0.48
1:B:295:LEU:HD23	1:B:295:LEU:C	2.39	0.48
1:A:240:MET:HE1	1:A:259:PRO:HB2	1.95	0.48
1:C:68:ASP:OD2	1:C:69:HIS:HD2	1.97	0.48
1:C:65:ALA:O	1:C:69:HIS:HB2	2.13	0.48
1:C:85:LEU:HD13	1:C:310:ARG:NH2	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:210:LEU:HD12	1:C:240:MET:HG2	1.96	0.48
1:C:321:LEU:HD22	1:C:325:THR:HG23	1.95	0.48
1:B:67:THR:HG22	1:C:117:ASN:HD21	1.79	0.47
1:B:260:VAL:CG2	1:B:261:PHE:N	2.76	0.47
1:A:32:THR:HG23	1:A:69:HIS:CE1	2.49	0.47
1:C:127:ASN:OD1	1:C:129:THR:CG2	2.62	0.47
1:C:210:LEU:HD12	1:C:240:MET:SD	2.53	0.47
1:B:38:GLY:HA2	1:B:207:LEU:HD23	1.96	0.47
1:B:141:GLU:O	1:C:122:SER:HB2	2.13	0.47
1:B:247:LEU:HB2	1:B:248:ARG:HH21	1.77	0.47
1:B:263:PHE:CB	1:B:295:LEU:HD11	2.45	0.47
1:A:208:PRO:HG2	1:A:263:PHE:HE2	1.76	0.47
1:C:63:VAL:HB	1:C:102:GLN:NE2	2.28	0.47
1:A:149:VAL:O	1:A:149:VAL:HG12	2.15	0.47
1:A:116:LEU:HD23	1:A:152:VAL:HG21	1.96	0.47
1:C:204:VAL:CG1	1:C:205:PRO:HD2	2.23	0.47
1:C:40:LEU:HA	1:C:44:LEU:HB2	1.97	0.47
1:A:232:GLU:HA	1:A:232:GLU:OE1	2.14	0.47
1:C:218:LYS:HG2	4:C:1293:HOH:O	2.15	0.47
1:B:74:GLU:OE2	1:C:347:ARG:NH1	2.48	0.47
1:B:207:LEU:HD12	1:B:208:PRO:HD2	1.97	0.47
1:B:274:VAL:C	1:B:276:ALA:H	2.22	0.47
1:A:255:VAL:HG22	1:A:261:PHE:CD1	2.50	0.47
1:A:293:LYS:HD2	1:A:293:LYS:HA	1.75	0.47
1:C:246:HIS:C	1:C:247:LEU:HD12	2.40	0.47
1:B:130:VAL:O	1:B:134:ILE:HG13	2.15	0.47
1:A:30:ARG:O	1:A:32:THR:N	2.47	0.47
1:C:290:LYS:HG3	4:C:1228:HOH:O	2.14	0.47
1:A:209:GLY:O	1:A:210:LEU:C	2.58	0.46
1:C:27:THR:HG22	1:C:167:PRO:HD2	1.97	0.46
1:B:68:ASP:OD1	1:B:137:LYS:CE	2.63	0.46
1:B:255:VAL:HG22	1:B:261:PHE:CD2	2.51	0.46
1:B:278:LYS:HG2	1:B:282:ARG:HH22	1.77	0.46
1:B:333:GLU:HG3	1:B:337:GLN:HE21	1.80	0.46
1:A:213:GLN:O	1:A:214:ALA:C	2.58	0.46
1:C:59:LEU:HD12	1:C:100:VAL:HG22	1.97	0.46
1:C:230:ALA:HB1	1:C:300:ASN:HD21	1.81	0.46
1:B:215:LYS:HG2	1:B:220:LEU:HD11	1.98	0.46
1:B:253:GLY:O	1:B:282:ARG:HA	2.16	0.46
1:B:299:LEU:HA	1:B:302:VAL:CG1	2.46	0.46
1:A:62:ASP:H	1:A:102:GLN:HB3	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:LEU:N	1:A:174:PRO:CD	2.78	0.46
1:C:310:ARG:O	1:C:314:GLU:HG2	2.15	0.46
1:B:62:ASP:O	1:B:66:LEU:HD23	2.16	0.46
1:B:244:PRO:C	1:B:246:HIS:H	2.23	0.46
1:A:247:LEU:HD23	1:A:248:ARG:NH2	2.30	0.46
1:A:308:THR:HG22	1:A:312:GLU:OE2	2.16	0.46
1:B:243:ASP:OD1	1:B:244:PRO:O	2.33	0.46
1:A:193:VAL:CG2	1:A:341:GLN:HE21	2.28	0.46
1:C:25:VAL:HG13	1:C:167:PRO:HD3	1.97	0.46
1:C:105:VAL:O	1:C:105:VAL:HG22	2.14	0.46
1:C:270:ASP:HA	1:C:271:PRO:HD2	1.79	0.46
1:B:44:LEU:HA	1:B:47:ARG:CD	2.45	0.46
1:A:58:VAL:O	1:A:58:VAL:CG1	2.64	0.46
1:A:116:LEU:HD21	1:A:149:VAL:HG11	1.97	0.46
1:C:183:VAL:HG13	1:C:194:LEU:HB2	1.98	0.46
1:B:36:HIS:HA	1:B:225:ALA:HA	1.98	0.46
1:B:39:HIS:CE1	3:B:3000:ATP:O4'	2.68	0.46
1:A:76:VAL:CG1	1:A:77:ARG:N	2.79	0.46
1:A:193:VAL:HG21	1:A:341:GLN:HE21	1.80	0.46
1:A:290:LYS:HE2	1:A:290:LYS:N	2.31	0.46
1:A:296:ILE:O	1:A:300:ASN:HB2	2.15	0.46
1:B:60:LEU:O	1:B:62:ASP:N	2.37	0.46
1:A:302:VAL:O	1:A:305:PRO:CD	2.63	0.46
1:B:211:ASP:HB3	1:B:213:GLN:HG3	1.98	0.46
1:A:201:LEU:CD2	1:A:202:SER:N	2.75	0.46
1:C:150:TYR:C	1:C:150:TYR:CD2	2.94	0.46
1:B:114:TYR:CE1	1:B:346:MET:HE1	2.52	0.45
1:C:120:THR:HG22	1:C:123:HIS:HB3	1.97	0.45
1:C:202:SER:HB2	4:C:1161:HOH:O	2.15	0.45
1:C:166:VAL:HG21	1:C:176:LEU:CD2	2.43	0.45
1:B:101:VAL:HG12	1:B:328:THR:OG1	2.16	0.45
1:B:184:ARG:HG2	1:B:184:ARG:NH2	2.26	0.45
1:A:129:THR:O	1:A:132:ALA:HB3	2.17	0.45
1:A:226:LEU:H	1:A:226:LEU:CD1	2.26	0.45
1:A:61:ALA:HB1	1:A:64:GLN:HB3	1.98	0.45
1:A:262:THR:O	1:A:265:ASP:OD1	2.34	0.45
1:B:232:GLU:O	1:B:233:VAL:C	2.57	0.45
1:C:254:ARG:HD3	1:C:256:GLU:CG	2.36	0.45
1:B:249:ALA:O	1:B:250:SER:C	2.60	0.45
1:B:296:ILE:HD12	1:B:296:ILE:O	2.15	0.45
1:A:98:THR:HG23	1:A:330:ARG:HD2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:324:VAL:HG23	1:A:325:THR:N	2.32	0.45
1:B:22:ARG:CB	1:B:23:PRO:CD	2.95	0.45
1:B:39:HIS:ND1	3:B:3000:ATP:O4'	2.49	0.45
1:B:278:LYS:HE3	1:B:278:LYS:HB2	1.74	0.45
1:B:50:LEU:C	1:B:50:LEU:HD12	2.42	0.45
1:B:189:LEU:HD21	1:C:71:ASP:HA	1.98	0.45
1:B:298:VAL:O	1:B:302:VAL:HG12	2.17	0.45
1:A:170:ASP:OD1	1:A:203:ARG:CZ	2.65	0.45
1:C:63:VAL:H	1:C:102:GLN:NE2	2.13	0.45
1:B:255:VAL:HG13	1:B:261:PHE:CG	2.52	0.45
1:A:130:VAL:CG1	1:A:131:LYS:N	2.79	0.45
1:A:255:VAL:HG21	1:A:278:LYS:HB3	1.98	0.45
1:A:294:HIS:HD2	1:A:297:ASP:OD2	1.99	0.45
1:C:92:LEU:HD12	1:C:92:LEU:HA	1.75	0.44
1:C:203:ARG:C	1:C:204:VAL:O	2.60	0.44
1:B:351:HIS:HB3	4:B:1088:HOH:O	2.16	0.44
1:A:293:LYS:HD2	1:A:296:ILE:HD11	1.98	0.44
1:C:56:LEU:HD13	1:C:56:LEU:C	2.42	0.44
1:C:154:GLN:O	1:C:158:ILE:HG12	2.18	0.44
1:B:105:VAL:CG1	1:B:108:LEU:HG	2.46	0.44
1:B:255:VAL:HG13	1:B:261:PHE:CB	2.46	0.44
1:B:344:ARG:HH11	1:B:344:ARG:CG	2.30	0.44
1:A:242:THR:HG23	1:A:292:LYS:HE2	1.99	0.44
1:A:305:PRO:HG2	1:A:306:ILE:N	2.28	0.44
1:C:258:ASN:C	1:C:258:ASN:ND2	2.76	0.44
1:B:190:TYR:HB3	1:B:345:ALA:O	2.16	0.44
1:C:58:VAL:O	1:C:58:VAL:HG23	2.16	0.44
1:B:77:ARG:NE	1:C:347:ARG:NH2	2.65	0.44
1:A:110:GLU:O	1:A:113:VAL:CG1	2.64	0.44
1:A:237:VAL:O	1:A:239:GLY:N	2.51	0.44
1:B:206:ARG:HG3	3:B:3000:ATP:C2	2.53	0.44
1:A:35:LEU:O	1:A:226:LEU:HD12	2.16	0.44
1:B:169:GLY:HA3	4:B:1288:HOH:O	2.17	0.44
1:B:241:TYR:O	1:B:259:PRO:HG2	2.17	0.44
1:A:45:GLN:O	1:A:48:VAL:HB	2.18	0.44
1:A:130:VAL:HG13	1:A:131:LYS:N	2.32	0.44
1:B:22:ARG:HG3	1:B:23:PRO:HD3	1.98	0.44
1:B:36:HIS:C	1:B:226:LEU:HD13	2.43	0.44
1:A:62:ASP:OD1	1:A:103:SER:HB2	2.18	0.44
1:B:51:GLN:NE2	1:B:97:THR:CG2	2.72	0.43
1:B:211:ASP:OD1	1:B:222:ASN:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:GLU:HB3	1:A:339:LEU:HG	2.00	0.43
1:A:150:TYR:O	1:A:154:GLN:HG3	2.17	0.43
1:B:237:VAL:O	1:B:240:MET:HE2	2.18	0.43
1:A:105:VAL:HG13	1:A:105:VAL:O	2.17	0.43
1:C:60:LEU:HD22	1:C:83:VAL:CG2	2.48	0.43
1:B:35:LEU:CD1	1:B:44:LEU:HD11	2.47	0.43
1:B:308:THR:O	1:B:312:GLU:HG3	2.17	0.43
1:C:60:LEU:HD22	1:C:83:VAL:HG21	2.01	0.43
1:C:180:ARG:HD2	1:C:196:GLU:HG3	2.01	0.43
1:B:22:ARG:HB2	1:B:23:PRO:CD	2.48	0.43
1:B:268:ASP:HA	1:B:269:PRO:HD2	1.87	0.43
1:A:241:TYR:O	1:A:241:TYR:CD1	2.72	0.43
1:C:26:LEU:HB2	1:C:163:ALA:HB2	2.00	0.43
1:B:273:ARG:O	1:B:277:LEU:HD22	2.19	0.43
1:A:32:THR:CG2	1:A:69:HIS:HE1	2.31	0.43
1:A:33:GLY:HA2	1:A:79:ASN:ND2	2.34	0.43
1:B:55:GLU:HG2	1:B:57:PHE:HE2	1.84	0.43
1:B:184:ARG:HH21	1:B:184:ARG:CG	2.27	0.43
1:A:209:GLY:CA	1:A:215:LYS:O	2.67	0.43
1:A:290:LYS:HE2	1:A:290:LYS:CA	2.49	0.43
1:C:21:ALA:HA	1:C:54:ALA:C	2.44	0.43
1:C:171:ASP:HB2	1:C:172:GLN:HE22	1.82	0.43
1:A:104:ALA:HB1	1:A:328:THR:HG21	2.01	0.43
1:A:110:GLU:HG2	1:A:114:TYR:CE1	2.54	0.43
1:A:50:LEU:O	1:A:51:GLN:C	2.62	0.43
1:A:125:ARG:HG3	1:A:125:ARG:NH2	2.34	0.43
1:B:38:GLY:O	1:B:39:HIS:O	2.36	0.42
1:B:248:ARG:NE	1:B:251:ASP:OD2	2.52	0.42
1:A:230:ALA:CB	1:A:300:ASN:HD21	2.26	0.42
1:C:112:THR:HG22	1:C:156:ALA:HB3	2.01	0.42
1:B:165:LEU:HD23	1:B:198:GLN:O	2.19	0.42
1:A:121:VAL:O	1:A:125:ARG:HB2	2.19	0.42
1:B:58:VAL:CG2	1:B:99:CYS:HA	2.48	0.42
1:B:93:ASP:OD2	1:B:94:PRO:HD2	2.19	0.42
1:C:320:VAL:O	1:C:323:PHE:HB3	2.19	0.42
1:B:35:LEU:HA	1:B:39:HIS:CD2	2.54	0.42
1:B:274:VAL:O	1:B:276:ALA:N	2.52	0.42
1:A:249:ALA:HB2	1:A:287:GLY:HA3	2.00	0.42
1:A:304:ALA:N	1:A:305:PRO:CD	2.80	0.42
1:B:274:VAL:HG12	1:B:275:GLN:N	2.33	0.42
1:A:40:LEU:HA	1:A:44:LEU:CB	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:25:VAL:HG11	1:C:50:LEU:HD13	2.01	0.42
1:B:142:ARG:HA	1:C:120:THR:OG1	2.19	0.42
1:B:211:ASP:CB	1:B:213:GLN:HG3	2.50	0.42
1:A:214:ALA:C	1:A:215:LYS:HG3	2.44	0.42
1:B:30:ARG:HH22	1:B:68:ASP:CB	2.33	0.42
1:B:303:LEU:O	1:B:304:ALA:C	2.62	0.42
1:A:22:ARG:N	1:A:23:PRO:CD	2.83	0.42
1:A:253:GLY:O	1:A:282:ARG:CA	2.66	0.42
1:A:255:VAL:HG13	1:A:261:PHE:CD1	2.55	0.42
1:A:269:PRO:HD2	1:A:273:ARG:HH12	1.79	0.42
1:C:60:LEU:HD13	1:C:80:VAL:HG23	2.02	0.42
1:C:48:VAL:O	1:C:51:GLN:HG2	2.20	0.42
1:B:258:ASN:O	1:B:262:THR:HG22	2.19	0.42
1:A:298:VAL:O	1:A:302:VAL:HG12	2.19	0.42
1:C:30:ARG:HD2	1:C:64:GLN:NE2	2.34	0.42
1:C:346:MET:O	1:C:347:ARG:HB2	2.20	0.42
1:B:149:VAL:O	1:B:149:VAL:HG13	2.20	0.42
1:B:322:ARG:NH2	1:B:322:ARG:CG	2.80	0.42
1:A:46:ASN:O	1:A:50:LEU:N	2.38	0.42
1:A:29:ASP:O	1:A:31:PRO:HD3	2.20	0.41
1:A:249:ALA:CB	1:A:287:GLY:HA3	2.50	0.41
1:C:276:ALA:O	1:C:280:GLN:HG3	2.19	0.41
1:A:241:TYR:O	1:A:259:PRO:CD	2.66	0.41
1:C:171:ASP:CB	1:C:172:GLN:NE2	2.83	0.41
1:C:348:LEU:O	1:C:349:PHE:C	2.63	0.41
1:B:184:ARG:HD3	1:B:196:GLU:OE2	2.21	0.41
1:A:302:VAL:C	1:A:305:PRO:HD2	2.44	0.41
1:B:39:HIS:O	1:B:42:GLY:CA	2.69	0.41
1:B:117:ASN:ND2	1:C:67:THR:HA	2.34	0.41
1:A:150:TYR:N	1:A:151:PRO:CD	2.84	0.41
1:A:303:LEU:CB	1:A:307:ARG:NH2	2.83	0.41
1:B:81:LEU:HD13	1:C:349:PHE:CZ	2.55	0.41
1:B:107:GLU:HA	4:B:1214:HOH:O	2.19	0.41
1:A:242:THR:HG23	1:A:292:LYS:CE	2.50	0.41
1:A:165:LEU:HD22	1:A:166:VAL:N	2.36	0.41
1:A:187:ASN:OD1	1:A:192:PRO:HA	2.21	0.41
1:A:242:THR:HB	1:A:258:ASN:ND2	2.33	0.41
1:A:269:PRO:HD2	1:A:273:ARG:HH11	1.83	0.41
1:A:334:VAL:HA	1:A:337:GLN:HG3	2.01	0.41
1:C:29:ASP:OD2	1:C:47:ARG:NH2	2.48	0.41
1:C:125:ARG:O	1:C:125:ARG:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:170:ASP:OD1	1:C:170:ASP:N	2.52	0.41
1:C:289:VAL:O	1:C:293:LYS:HB2	2.20	0.41
1:B:286:LEU:HD22	1:B:291:VAL:HG23	2.01	0.41
1:B:63:VAL:H	1:B:102:GLN:NE2	2.16	0.41
1:A:175:MET:SD	1:A:175:MET:C	3.04	0.41
1:A:211:ASP:C	1:A:213:GLN:N	2.79	0.41
1:A:225:ALA:C	1:A:227:GLY:H	2.28	0.41
1:A:261:PHE:C	1:A:263:PHE:N	2.76	0.41
1:B:60:LEU:HD23	1:B:60:LEU:HA	1.84	0.41
1:B:81:LEU:HA	1:B:81:LEU:HD12	1.81	0.41
1:A:105:VAL:HA	1:A:106:PRO:HD2	1.80	0.41
1:A:149:VAL:C	1:A:151:PRO:HD2	2.46	0.41
1:A:209:GLY:HA2	1:A:215:LYS:O	2.21	0.41
1:A:261:PHE:O	1:A:262:THR:C	2.64	0.41
1:A:305:PRO:CG	1:A:306:ILE:H	2.28	0.41
1:C:30:ARG:HE	1:C:64:GLN:HG2	1.86	0.41
1:C:270:ASP:O	1:C:270:ASP:CG	2.63	0.41
1:B:258:ASN:HA	1:B:259:PRO:HD2	1.99	0.41
1:A:40:LEU:C	1:A:40:LEU:CD2	2.93	0.41
1:A:69:HIS:CD2	1:A:69:HIS:N	2.88	0.40
1:A:299:LEU:O	1:A:303:LEU:HD22	2.21	0.40
1:C:255:VAL:O	1:C:258:ASN:HB3	2.21	0.40
1:A:310:ARG:HG2	1:A:314:GLU:CD	2.46	0.40
1:C:231:ASP:OD1	1:C:235:ARG:NE	2.54	0.40
1:B:169:GLY:O	1:B:170:ASP:C	2.64	0.40
1:B:231:ASP:O	1:B:235:ARG:HG3	2.22	0.40
1:B:254:ARG:NH1	1:B:256:GLU:CG	2.83	0.40
1:A:33:GLY:HA2	1:A:79:ASN:CG	2.46	0.40
1:A:113:VAL:HG13	1:A:114:TYR:N	2.35	0.40
1:A:118:LEU:HB3	1:A:185:ARG:HG2	2.03	0.40
1:A:293:LYS:HD2	1:A:296:ILE:CD1	2.51	0.40
1:C:86:ASP:OD1	1:C:310:ARG:NH2	2.50	0.40
1:B:127:ASN:HB3	1:B:130:VAL:HG11	2.01	0.40
1:A:274:VAL:C	1:A:276:ALA:H	2.29	0.40
1:B:286:LEU:HD22	1:B:291:VAL:CG2	2.51	0.40
1:A:211:ASP:O	1:A:213:GLN:N	2.50	0.40
1:A:260:VAL:HA	1:A:295:LEU:HD22	2.03	0.40
1:A:275:GLN:HG3	1:A:275:GLN:O	2.21	0.40
1:A:308:THR:O	1:A:311:ALA:HB3	2.21	0.40
1:C:186:PHE:C	1:C:186:PHE:CD1	2.99	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	329/351 (94%)	280 (85%)	37 (11%)	12 (4%)	2	2
1	B	329/351 (94%)	297 (90%)	26 (8%)	6 (2%)	6	9
1	C	329/351 (94%)	309 (94%)	16 (5%)	4 (1%)	10	16
All	All	987/1053 (94%)	886 (90%)	79 (8%)	22 (2%)	5	6

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	22	ARG
1	B	61	ALA
1	A	61	ALA
1	C	202	SER
1	C	205	PRO
1	B	284	GLY
1	A	238	MET
1	B	43	SER
1	A	37	LEU
1	A	205	PRO
1	A	206	ARG
1	A	213	GLN
1	A	242	THR
1	A	269	PRO
1	C	22	ARG
1	A	31	PRO
1	A	214	ALA
1	C	283	ALA
1	B	294	HIS
1	A	73	PRO
1	A	258	ASN
1	B	285	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	
1	A	256/282 (91%)	226 (88%)	30 (12%)	5	7
1	B	264/282 (94%)	225 (85%)	39 (15%)	3	4
1	C	262/282 (93%)	231 (88%)	31 (12%)	5	7
All	All	782/846 (92%)	682 (87%)	100 (13%)	4	6

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	22	ARG
1	B	40	LEU
1	B	47	ARG
1	B	50	LEU
1	B	52	ASP
1	B	68	ASP
1	B	75	GLN
1	B	81	LEU
1	B	85	LEU
1	B	92	LEU
1	B	97	THR
1	B	141	GLU
1	B	149	VAL
1	B	152	VAL
1	B	165	LEU
1	B	168	VAL
1	B	170	ASP
1	B	171	ASP
1	B	184	ARG
1	B	185	ARG
1	B	189	LEU
1	B	201	LEU
1	B	206	ARG
1	B	215	LYS
1	B	226	LEU
1	B	235	ARG

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Mol	Chain	Res	Type
1	B	254	ARG
1	B	262	THR
1	B	282	ARG
1	B	286	LEU
1	B	290	LYS
1	B	296	ILE
1	B	297	ASP
1	B	302	VAL
1	B	318	ASP
1	B	322	ARG
1	B	344	ARG
1	B	347	ARG
1	B	351	HIS
1	A	35	LEU
1	A	40	LEU
1	A	52	ASP
1	A	56	LEU
1	A	63	VAL
1	A	74	GLU
1	A	81	LEU
1	A	85	LEU
1	A	124	LEU
1	A	125	ARG
1	A	126	GLN
1	A	150	TYR
1	A	152	VAL
1	A	165	LEU
1	A	172	GLN
1	A	176	LEU
1	A	200	GLN
1	A	201	LEU
1	A	203	ARG
1	A	215	LYS
1	A	224	ILE
1	A	232	GLU
1	A	246	HIS
1	A	268	ASP
1	A	286	LEU
1	A	290	LYS
1	A	300	ASN
1	A	306	ILE
1	A	328	THR

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Mol	Chain	Res	Type
1	A	348	LEU
1	C	30	ARG
1	C	46	ASN
1	C	80	VAL
1	C	81	LEU
1	C	85	LEU
1	C	92	LEU
1	C	97	THR
1	C	100	VAL
1	C	112	THR
1	C	150	TYR
1	C	152	VAL
1	C	165	LEU
1	C	168	VAL
1	C	193	VAL
1	C	200	GLN
1	C	201	LEU
1	C	202	SER
1	C	204	VAL
1	C	205	PRO
1	C	210	LEU
1	C	231	ASP
1	C	248	ARG
1	C	256	GLU
1	C	277	LEU
1	C	286	LEU
1	C	295	LEU
1	C	298	VAL
1	C	312	GLU
1	C	314	GLU
1	C	321	LEU
1	C	330	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	36	HIS
1	B	39	HIS
1	B	46	ASN
1	B	51	GLN
1	B	64	GLN
1	B	69	HIS

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Mol	Chain	Res	Type
1	B	75	GLN
1	B	102	GLN
1	B	117	ASN
1	B	136	GLN
1	B	200	GLN
1	B	300	ASN
1	B	337	GLN
1	B	351	HIS
1	A	36	HIS
1	A	45	GLN
1	A	46	ASN
1	A	69	HIS
1	A	79	ASN
1	A	154	GLN
1	A	172	GLN
1	A	200	GLN
1	A	280	GLN
1	A	294	HIS
1	A	300	ASN
1	A	341	GLN
1	C	51	GLN
1	C	64	GLN
1	C	69	HIS
1	C	95	GLN
1	C	102	GLN
1	C	117	ASN
1	C	123	HIS
1	C	126	GLN
1	C	178	GLN
1	C	213	GLN
1	C	246	HIS
1	C	258	ASN
1	C	300	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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	ATP	B	3000	2	32,33,33	4.27	7 (21%)	48,52,52	1.20	6 (12%)

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	ATP	B	3000	2	-	4/22/38/38	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	3000	ATP	PB-O3B	21.37	1.82	1.59
3	B	3000	ATP	PB-O3A	6.80	1.66	1.59
3	B	3000	ATP	PA-O3A	5.19	1.65	1.59
3	B	3000	ATP	PG-O1G	3.74	1.62	1.50
3	B	3000	ATP	PG-O2G	2.72	1.64	1.54
3	B	3000	ATP	PG-O3G	-2.35	1.46	1.54
3	B	3000	ATP	C4-N3	2.29	1.38	1.34

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	3000	ATP	O2A-PA-O3A	2.88	115.05	107.27
3	B	3000	ATP	O5'-C5'-C4'	2.47	117.39	108.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	3000	ATP	O3B-PB-O1B	2.31	117.65	110.70
3	B	3000	ATP	O4'-C1'-N9	2.28	112.46	108.09
3	B	3000	ATP	O3G-PG-O3B	2.11	111.71	104.64
3	B	3000	ATP	O2G-PG-O3B	-2.07	97.71	104.64

There are no chirality outliers.

All (4) torsion outliers are listed below:

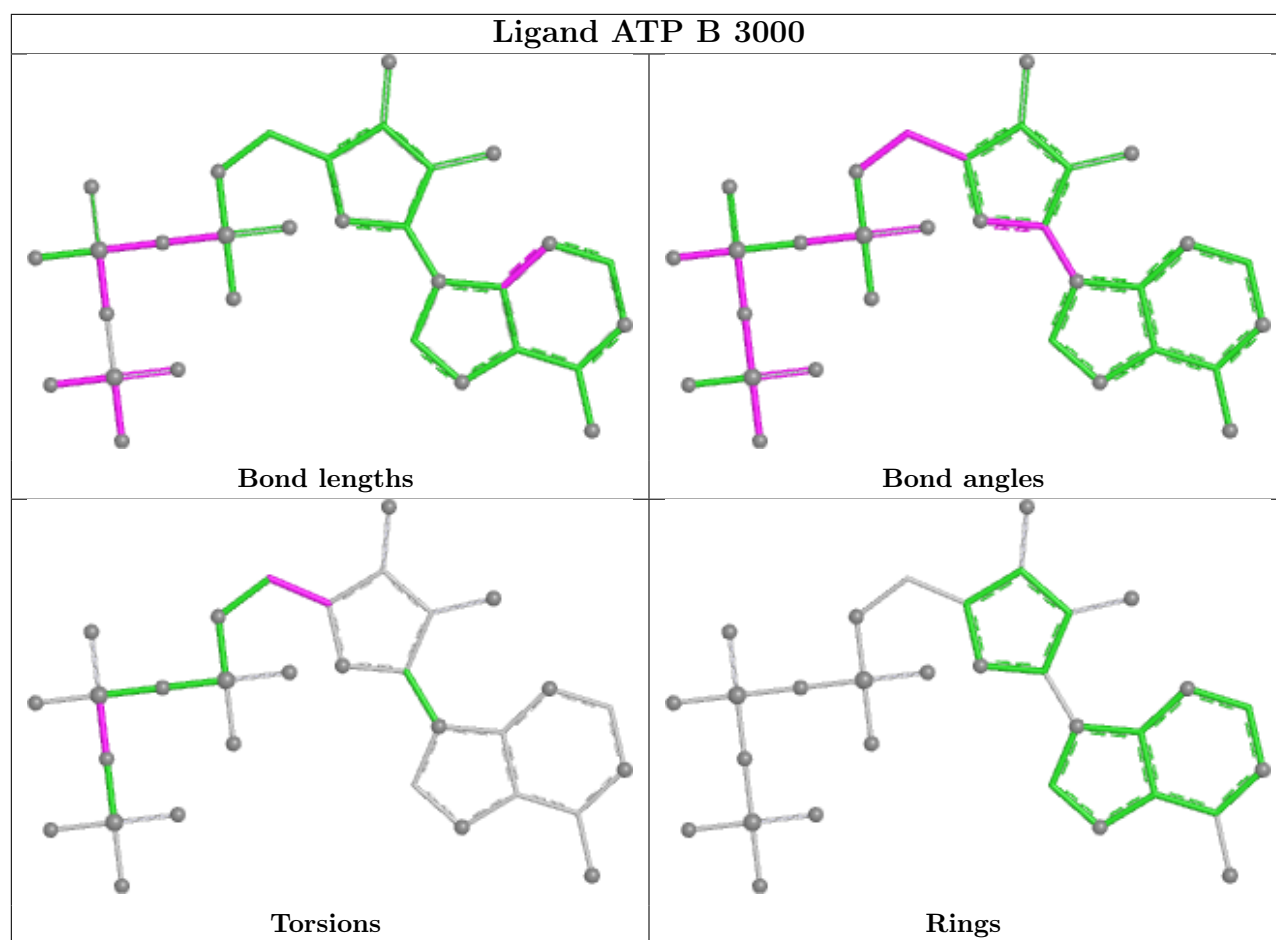
Mol	Chain	Res	Type	Atoms
3	B	3000	ATP	O4'-C4'-C5'-O5'
3	B	3000	ATP	C3'-C4'-C5'-O5'
3	B	3000	ATP	PG-O3B-PB-O1B
3	B	3000	ATP	PG-O3B-PB-O2B

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	3000	ATP	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.