



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:27 PM UTC

PDB ID : 1T8W / pdb_00001t8w
Title : Crystal Structure of E. coli AMP Nucleosidase
Authors : Zhang, Y.; Cottet, S.E.; Ealick, S.E.
Deposited on : 2004-05-13
Resolution : 2.80 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
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

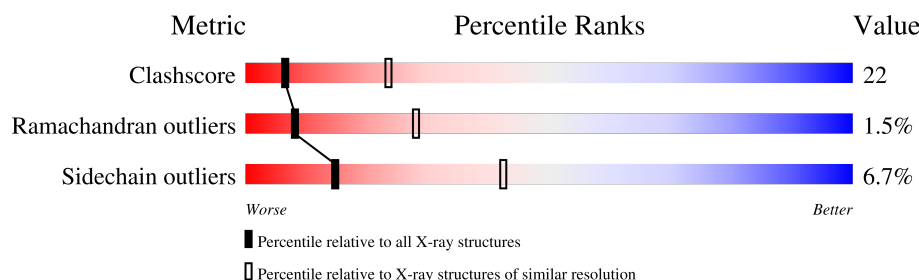
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)

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	484	
1	B	484	
1	C	484	
1	D	484	
1	E	484	
1	F	484	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 22064 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 AMP nucleosidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	461	Total	C	N	O	S	Se	0	0	0
			3648	2317	641	681	5	4			
1	B	461	Total	C	N	O	S	Se	0	0	0
			3648	2317	641	681	5	4			
1	C	461	Total	C	N	O	S	Se	0	0	0
			3648	2317	641	681	5	4			
1	D	461	Total	C	N	O	S	Se	0	0	0
			3648	2317	641	681	5	4			
1	E	461	Total	C	N	O	S	Se	0	0	0
			3648	2317	641	681	5	4			
1	F	461	Total	C	N	O	S	Se	0	0	0
			3648	2317	641	681	5	4			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	138	MSE	MET	modified residue	UNP P15272
A	260	MSE	MET	modified residue	UNP P15272
A	302	MSE	MET	modified residue	UNP P15272
A	404	MSE	MET	modified residue	UNP P15272
B	138	MSE	MET	modified residue	UNP P15272
B	260	MSE	MET	modified residue	UNP P15272
B	302	MSE	MET	modified residue	UNP P15272
B	404	MSE	MET	modified residue	UNP P15272
C	138	MSE	MET	modified residue	UNP P15272
C	260	MSE	MET	modified residue	UNP P15272
C	302	MSE	MET	modified residue	UNP P15272
C	404	MSE	MET	modified residue	UNP P15272
D	138	MSE	MET	modified residue	UNP P15272
D	260	MSE	MET	modified residue	UNP P15272
D	302	MSE	MET	modified residue	UNP P15272
D	404	MSE	MET	modified residue	UNP P15272
E	138	MSE	MET	modified residue	UNP P15272

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Chain	Residue	Modelled	Actual	Comment	Reference
E	260	MSE	MET	modified residue	UNP P15272
E	302	MSE	MET	modified residue	UNP P15272
E	404	MSE	MET	modified residue	UNP P15272
F	138	MSE	MET	modified residue	UNP P15272
F	260	MSE	MET	modified residue	UNP P15272
F	302	MSE	MET	modified residue	UNP P15272
F	404	MSE	MET	modified residue	UNP P15272

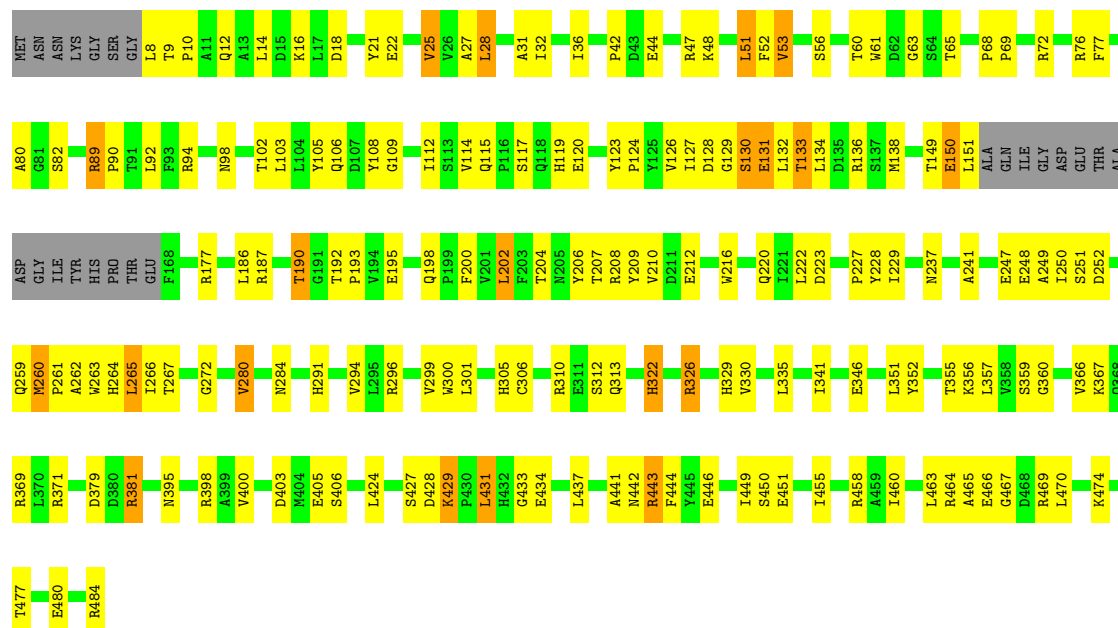
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	22	Total O 22 22	0	0
2	B	37	Total O 37 37	0	0
2	C	33	Total O 33 33	0	0
2	D	30	Total O 30 30	0	0
2	E	24	Total O 24 24	0	0
2	F	30	Total O 30 30	0	0



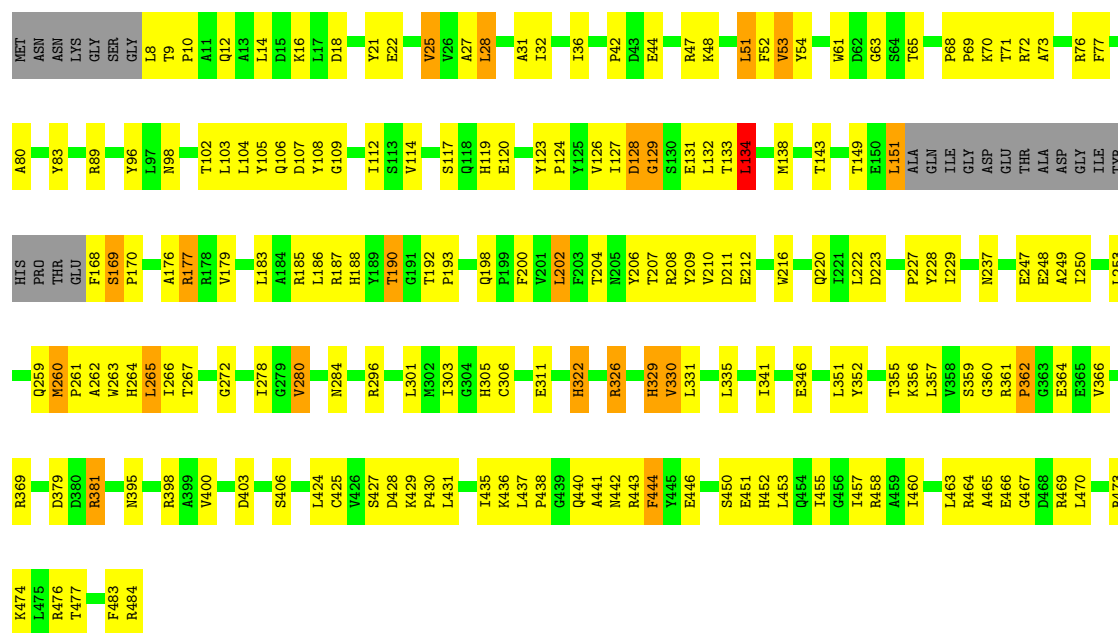
• Molecule 1: AMP nucleosidase

Chain C: 58% 33% 5%



• Molecule 1: AMP nucleosidase

Chain D: 56% 34% 5%

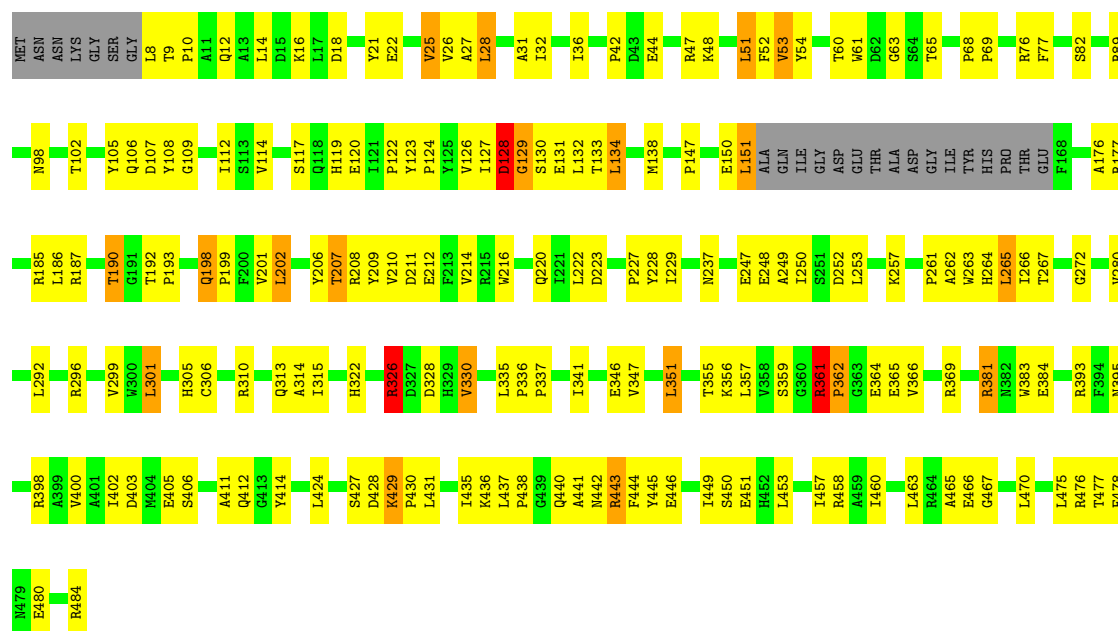


• Molecule 1: AMP nucleosidase

Age Group	Percentage
18-24	56%
25-34	34%
35-44	5%
45-54	5%



Response	Percentage
Yes	57%
No	34%
Don't know	5%



4 Data and refinement statistics

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

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α , β , γ	271.80 Å 271.80 Å 113.40 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.93 – 2.80	Depositor
% Data completeness (in resolution range)	93.7 (25.93-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.223 , 0.245	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	22064	wwPDB-VP
Average B, all atoms (Å ²)	91.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.49	0/3738	0.95	11/5088 (0.2%)
1	B	0.54	0/3738	0.94	9/5088 (0.2%)
1	C	0.56	0/3738	0.98	15/5088 (0.3%)
1	D	0.53	0/3738	0.96	11/5088 (0.2%)
1	E	0.50	0/3738	0.98	18/5088 (0.4%)
1	F	0.50	0/3738	0.95	9/5088 (0.2%)
All	All	0.52	0/22428	0.96	73/30528 (0.2%)

There are no bond length outliers.

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	169	SER	CA-C-N	8.48	129.01	119.93
1	E	169	SER	C-N-CA	8.48	129.01	119.93
1	C	429	LYS	CA-C-N	8.33	128.82	119.32
1	C	429	LYS	C-N-CA	8.33	128.82	119.32
1	B	429	LYS	CA-C-N	8.05	128.49	119.32
1	B	429	LYS	C-N-CA	8.05	128.49	119.32
1	E	429	LYS	CA-C-N	7.65	127.70	119.28
1	E	429	LYS	C-N-CA	7.65	127.70	119.28
1	C	444	PHE	N-CA-C	7.30	121.94	112.89
1	A	429	LYS	CA-C-N	7.29	127.63	119.32
1	A	429	LYS	C-N-CA	7.29	127.63	119.32
1	D	429	LYS	CA-C-N	7.18	127.51	119.32
1	D	429	LYS	C-N-CA	7.18	127.51	119.32
1	D	198	GLN	CA-C-N	7.06	127.04	119.28
1	D	198	GLN	C-N-CA	7.06	127.04	119.28
1	F	128	ASP	N-CA-C	7.04	118.84	111.03
1	F	429	LYS	CA-C-N	6.88	127.16	119.32
1	F	429	LYS	C-N-CA	6.88	127.16	119.32
1	E	53	VAL	N-CA-C	6.80	118.40	108.53
1	C	449	ILE	N-CA-C	6.66	117.35	110.36
1	D	444	PHE	N-CA-C	6.58	118.53	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	198	GLN	CA-C-N	6.51	126.21	119.56
1	A	198	GLN	C-N-CA	6.51	126.21	119.56
1	E	129	GLY	N-CA-C	6.42	122.06	111.59
1	D	53	VAL	N-CA-C	6.41	118.63	108.89
1	D	169	SER	CA-C-N	6.28	126.61	119.83
1	D	169	SER	C-N-CA	6.28	126.61	119.83
1	C	133	THR	CA-C-N	-6.21	112.90	122.09
1	C	133	THR	C-N-CA	-6.21	112.90	122.09
1	C	198	GLN	CA-C-N	6.19	126.09	119.28
1	C	198	GLN	C-N-CA	6.19	126.09	119.28
1	F	53	VAL	N-CA-C	6.11	118.18	108.89
1	E	260	MSE	CA-C-N	6.08	126.02	119.76
1	E	260	MSE	C-N-CA	6.08	126.02	119.76
1	F	198	GLN	CA-C-N	6.08	126.53	119.47
1	F	198	GLN	C-N-CA	6.08	126.53	119.47
1	E	444	PHE	N-CA-C	6.03	120.37	112.89
1	C	480	GLU	CA-C-N	6.03	124.06	119.66
1	C	480	GLU	C-N-CA	6.03	124.06	119.66
1	B	53	VAL	N-CA-C	6.00	118.02	108.89
1	B	326	ARG	N-CA-C	5.97	119.45	108.58
1	D	326	ARG	N-CA-C	5.95	119.40	108.58
1	A	260	MSE	CA-C-N	5.93	125.95	119.90
1	A	260	MSE	C-N-CA	5.93	125.95	119.90
1	C	260	MSE	CA-C-N	5.83	125.76	119.76
1	C	260	MSE	C-N-CA	5.83	125.76	119.76
1	E	434	GLU	N-CA-C	5.82	118.78	108.24
1	A	444	PHE	N-CA-C	5.68	121.21	113.37
1	E	326	ARG	N-CA-C	5.59	118.76	108.58
1	F	326	ARG	N-CA-C	5.54	118.66	108.58
1	B	260	MSE	CA-C-N	5.53	125.45	119.76
1	B	260	MSE	C-N-CA	5.53	125.45	119.76
1	C	326	ARG	N-CA-C	5.51	118.60	108.58
1	E	480	GLU	CA-C-N	5.49	123.67	119.66
1	E	480	GLU	C-N-CA	5.49	123.67	119.66
1	C	53	VAL	N-CA-C	5.47	117.21	108.89
1	B	198	GLN	CA-C-N	5.44	125.27	119.28
1	B	198	GLN	C-N-CA	5.44	125.27	119.28
1	A	326	ARG	N-CA-C	5.44	118.48	108.58
1	E	198	GLN	CA-C-N	5.43	125.26	119.28
1	E	198	GLN	C-N-CA	5.43	125.26	119.28
1	A	53	VAL	N-CA-C	5.43	117.14	108.89
1	A	361	ARG	CA-C-N	5.36	126.54	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	361	ARG	C-N-CA	5.36	126.54	119.84
1	E	39	GLY	N-CA-C	-5.23	107.83	115.63
1	F	480	GLU	CA-C-N	5.19	123.45	119.66
1	F	480	GLU	C-N-CA	5.19	123.45	119.66
1	C	433	GLY	N-CA-C	5.14	122.21	115.47
1	E	340	PRO	N-CA-C	5.14	118.57	110.50
1	D	260	MSE	CA-C-N	5.09	125.00	119.76
1	D	260	MSE	C-N-CA	5.09	125.00	119.76
1	E	413	GLY	N-CA-C	-5.05	106.64	112.50
1	B	128	ASP	N-CA-C	5.00	121.46	110.80

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	3648	0	3576	175	0
1	B	3648	0	3576	178	0
1	C	3648	0	3576	159	0
1	D	3648	0	3576	168	0
1	E	3648	0	3576	170	0
1	F	3648	0	3576	175	0
2	A	22	0	0	1	0
2	B	37	0	0	3	0
2	C	33	0	0	3	0
2	D	30	0	0	3	0
2	E	24	0	0	2	0
2	F	30	0	0	2	0
All	All	22064	0	21456	944	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 22.

All (944) 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:192:THR:HG21	1:A:264:HIS:NE2	1.74	1.02
1:F:361:ARG:HB2	1:F:365:GLU:HG2	1.42	1.00
1:C:190:THR:CG2	1:C:192:THR:HB	1.91	1.00
1:A:190:THR:CG2	1:A:192:THR:HB	1.93	0.99
1:D:190:THR:CG2	1:D:192:THR:HB	1.92	0.98
1:C:192:THR:HG21	1:C:264:HIS:NE2	1.78	0.98
1:B:192:THR:HG21	1:B:264:HIS:NE2	1.80	0.96
1:B:190:THR:CG2	1:B:192:THR:HB	1.93	0.96
1:D:192:THR:HG21	1:D:264:HIS:NE2	1.78	0.96
1:F:192:THR:HG21	1:F:264:HIS:NE2	1.82	0.95
1:E:190:THR:CG2	1:E:192:THR:HB	1.96	0.95
1:F:190:THR:CG2	1:F:192:THR:HB	1.97	0.93
1:E:192:THR:HG21	1:E:264:HIS:NE2	1.83	0.92
1:D:190:THR:HG22	1:D:192:THR:HB	1.50	0.91
1:C:190:THR:HG22	1:C:192:THR:HB	1.51	0.91
1:A:202:LEU:HD13	1:A:460:ILE:HD11	1.54	0.90
1:C:18:ASP:O	1:C:22:GLU:HG2	1.73	0.89
1:A:190:THR:HG22	1:A:192:THR:HB	1.53	0.89
1:A:131:GLU:HB2	1:B:441:ALA:HB3	1.54	0.88
1:A:477:THR:HB	1:F:395:ASN:HD21	1.39	0.87
1:B:192:THR:HG21	1:B:264:HIS:HE2	1.37	0.87
1:A:437:LEU:HD12	1:A:437:LEU:H	1.40	0.86
1:B:18:ASP:O	1:B:22:GLU:HG2	1.75	0.86
1:B:32:ILE:HD11	1:B:123:TYR:HB2	1.58	0.86
1:A:18:ASP:O	1:A:22:GLU:HG2	1.76	0.85
1:B:192:THR:HG21	1:B:264:HIS:CD2	2.09	0.85
1:F:192:THR:HG21	1:F:264:HIS:CD2	2.12	0.84
1:A:441:ALA:HB3	1:B:131:GLU:HB2	1.60	0.84
1:A:132:LEU:HB3	1:A:134:LEU:HD13	1.57	0.84
1:E:18:ASP:O	1:E:22:GLU:HG2	1.79	0.83
1:A:395:ASN:HD21	1:F:477:THR:HB	1.43	0.83
1:F:326:ARG:HG2	1:F:326:ARG:HH11	1.45	0.81
1:E:192:THR:HG21	1:E:264:HIS:CD2	2.14	0.81
1:A:32:ILE:HD11	1:A:123:TYR:HB2	1.63	0.81
1:F:18:ASP:O	1:F:22:GLU:HG2	1.80	0.80
1:E:190:THR:HG22	1:E:192:THR:HB	1.63	0.80
1:D:18:ASP:O	1:D:22:GLU:HG2	1.81	0.80
1:E:202:LEU:HD13	1:E:460:ILE:HD11	1.66	0.78
1:D:190:THR:HG23	1:D:262:ALA:HB3	1.66	0.78
1:A:435:ILE:HG21	1:B:185:ARG:HH22	1.46	0.78
1:F:8:LEU:HD12	1:F:12:GLN:HE21	1.49	0.78
1:F:190:THR:HG22	1:F:192:THR:HB	1.63	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:ARG:HG2	1:A:326:ARG:HH11	1.48	0.77
1:B:190:THR:HG22	1:B:192:THR:HB	1.66	0.77
1:C:192:THR:HG21	1:C:264:HIS:CD2	2.18	0.77
1:D:192:THR:HG21	1:D:264:HIS:CD2	2.19	0.77
1:C:32:ILE:HD11	1:C:123:TYR:HB2	1.65	0.77
1:A:192:THR:HG21	1:A:264:HIS:CD2	2.18	0.77
1:B:134:LEU:HD23	1:B:138:MSE:HB3	1.66	0.77
1:D:127:ILE:HD13	1:D:132:LEU:HG	1.67	0.77
1:E:135:ASP:HA	1:F:443:ARG:HH21	1.49	0.77
1:F:32:ILE:HD11	1:F:123:TYR:HB2	1.65	0.77
1:B:202:LEU:HD13	1:B:460:ILE:HD11	1.65	0.77
1:F:134:LEU:HD23	1:F:138:MSE:HB3	1.65	0.77
1:A:356:LYS:HG2	1:A:366:VAL:HG11	1.66	0.77
1:B:132:LEU:HB3	1:B:134:LEU:HD13	1.67	0.76
1:E:326:ARG:HH11	1:E:326:ARG:HG2	1.50	0.76
1:B:361:ARG:HB3	1:B:365:GLU:CD	2.11	0.76
1:E:134:LEU:HD23	1:E:138:MSE:HB3	1.68	0.76
1:F:356:LYS:HG2	1:F:366:VAL:HG11	1.68	0.76
1:D:134:LEU:HD23	1:D:138:MSE:HB3	1.67	0.76
1:D:32:ILE:HD11	1:D:123:TYR:HB2	1.68	0.75
1:F:132:LEU:HB3	1:F:134:LEU:HD13	1.68	0.75
1:A:8:LEU:HD12	1:A:12:GLN:NE2	2.01	0.75
1:F:202:LEU:HD13	1:F:460:ILE:HD11	1.66	0.75
1:F:190:THR:HG23	1:F:262:ALA:HB3	1.69	0.75
1:D:395:ASN:HD22	1:E:478:PHE:HD1	1.35	0.74
1:F:8:LEU:HD12	1:F:12:GLN:NE2	2.01	0.74
1:A:8:LEU:HD12	1:A:12:GLN:HE21	1.53	0.74
1:E:32:ILE:HD11	1:E:123:TYR:HB2	1.70	0.73
1:E:44:GLU:O	1:E:48:LYS:HG2	1.88	0.73
1:B:186:LEU:O	1:B:190:THR:HB	1.87	0.73
1:C:44:GLU:O	1:C:48:LYS:HG2	1.89	0.73
1:F:430:PRO:HA	1:F:435:ILE:HG12	1.68	0.73
1:F:131:GLU:CD	1:F:131:GLU:H	1.97	0.73
1:C:241:ALA:HB2	2:C:489:HOH:O	1.88	0.73
1:D:9:THR:H	1:D:12:GLN:HE21	1.36	0.73
1:A:435:ILE:CG2	1:B:185:ARG:HH22	2.01	0.72
1:B:326:ARG:HG2	1:B:326:ARG:HH11	1.54	0.72
1:B:477:THR:HB	1:C:395:ASN:HD21	1.54	0.72
1:A:190:THR:HG23	1:A:262:ALA:HB3	1.70	0.71
1:C:8:LEU:HD12	1:C:12:GLN:NE2	2.05	0.71
1:E:190:THR:HG23	1:E:262:ALA:HB3	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:395:ASN:HD21	1:C:477:THR:HB	1.56	0.71
1:B:69:PRO:O	1:B:76:ARG:HD2	1.89	0.71
1:D:186:LEU:O	1:D:190:THR:HB	1.91	0.71
1:F:127:ILE:HD13	1:F:132:LEU:HG	1.73	0.71
1:A:134:LEU:HD23	1:A:138:MSE:HB3	1.72	0.70
1:B:361:ARG:HB3	1:B:365:GLU:OE2	1.91	0.70
1:D:356:LYS:HG2	1:D:366:VAL:HG11	1.73	0.70
1:D:44:GLU:O	1:D:48:LYS:HG2	1.91	0.70
1:E:8:LEU:HD12	1:E:12:GLN:HE21	1.57	0.70
1:A:186:LEU:O	1:A:190:THR:HB	1.91	0.70
1:F:65:THR:HB	1:F:68:PRO:HG3	1.73	0.70
1:F:134:LEU:HB3	1:F:138:MSE:CB	2.21	0.70
1:B:8:LEU:HD12	1:B:12:GLN:NE2	2.06	0.70
1:B:364:GLU:HG2	1:C:469:ARG:NH2	2.06	0.70
1:C:65:THR:HB	1:C:68:PRO:HG3	1.73	0.70
1:C:8:LEU:HD12	1:C:12:GLN:HE21	1.56	0.69
1:F:151:LEU:HD13	1:F:151:LEU:H	1.57	0.69
1:A:44:GLU:O	1:A:48:LYS:HG2	1.92	0.69
1:B:356:LYS:HG2	1:B:366:VAL:HG11	1.73	0.69
1:A:360:GLY:O	1:A:362:PRO:HD3	1.92	0.69
1:C:127:ILE:HG22	1:C:129:GLY:O	1.92	0.69
1:E:190:THR:HG21	1:E:192:THR:HB	1.73	0.69
1:E:65:THR:HB	1:E:68:PRO:HG3	1.75	0.69
1:B:44:GLU:O	1:B:48:LYS:HG2	1.92	0.68
1:B:132:LEU:HB3	1:B:134:LEU:CD1	2.22	0.68
1:C:28:LEU:HD13	1:C:126:VAL:HG21	1.75	0.68
1:C:326:ARG:HH11	1:C:326:ARG:HG2	1.57	0.68
1:A:185:ARG:HH22	1:B:435:ILE:HG21	1.59	0.68
1:E:8:LEU:HD12	1:E:12:GLN:NE2	2.09	0.68
1:B:134:LEU:HB3	1:B:138:MSE:HB2	1.76	0.68
1:B:134:LEU:HB3	1:B:138:MSE:CB	2.24	0.67
1:D:326:ARG:HG2	1:D:326:ARG:HH11	1.59	0.67
1:C:190:THR:HG21	1:C:192:THR:HB	1.76	0.67
1:E:356:LYS:HB3	1:E:362:PRO:HB3	1.77	0.67
1:A:228:TYR:CG	1:A:265:LEU:HD13	2.30	0.67
1:E:28:LEU:HD13	1:E:126:VAL:HG21	1.76	0.67
1:F:44:GLU:O	1:F:48:LYS:HG2	1.95	0.67
1:C:186:LEU:O	1:C:190:THR:HB	1.94	0.67
1:D:8:LEU:HD12	1:D:12:GLN:NE2	2.09	0.67
1:E:134:LEU:HB3	1:E:138:MSE:CB	2.24	0.67
1:B:356:LYS:HE2	1:B:363:GLY:O	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:190:THR:HG23	1:C:262:ALA:HB3	1.75	0.67
1:D:9:THR:H	1:D:12:GLN:NE2	1.92	0.67
1:A:443:ARG:HD3	1:B:133:THR:HG22	1.76	0.67
1:E:119:HIS:ND1	1:E:177:ARG:NH2	2.43	0.67
1:E:442:ASN:ND2	1:E:445:TYR:HB3	2.10	0.66
1:E:69:PRO:O	1:E:76:ARG:HD2	1.95	0.66
1:C:69:PRO:O	1:C:76:ARG:HD2	1.94	0.66
1:D:134:LEU:HB3	1:D:138:MSE:CB	2.25	0.66
1:F:296:ARG:HD3	1:F:484:ARG:OXT	1.94	0.66
1:D:65:THR:HB	1:D:68:PRO:HG3	1.78	0.66
1:D:477:THR:HB	1:E:395:ASN:HD21	1.59	0.66
1:E:356:LYS:HE2	1:E:363:GLY:O	1.96	0.66
1:B:9:THR:H	1:B:12:GLN:HE21	1.44	0.66
1:B:364:GLU:HG2	1:C:469:ARG:HH21	1.59	0.66
1:E:305:HIS:HB2	1:E:427:SER:HB3	1.77	0.65
1:A:65:THR:HB	1:A:68:PRO:HG3	1.78	0.65
1:C:134:LEU:HD23	1:C:138:MSE:HB3	1.78	0.65
1:B:352:TYR:CE2	1:B:356:LYS:HE3	2.30	0.65
1:A:134:LEU:HB3	1:A:138:MSE:CB	2.26	0.65
1:A:443:ARG:HG2	1:A:444:PHE:CE1	2.30	0.65
1:B:8:LEU:HD12	1:B:12:GLN:HE21	1.61	0.65
1:C:36:ILE:HA	1:C:138:MSE:HE1	1.79	0.65
1:E:9:THR:H	1:E:12:GLN:HE21	1.44	0.65
1:F:69:PRO:O	1:F:76:ARG:HD2	1.97	0.65
1:A:69:PRO:O	1:A:76:ARG:HD2	1.96	0.64
1:B:65:THR:HB	1:B:68:PRO:HG3	1.80	0.64
1:A:463:LEU:HD22	1:A:470:LEU:HD13	1.79	0.64
1:C:202:LEU:HD13	1:C:460:ILE:HD11	1.79	0.64
1:B:310:ARG:H	1:B:313:GLN:NE2	1.96	0.64
1:D:69:PRO:O	1:D:76:ARG:HD2	1.98	0.64
1:F:105:TYR:O	1:F:109:GLY:HA2	1.97	0.64
1:E:135:ASP:HA	1:F:443:ARG:NH2	2.13	0.63
1:F:190:THR:HG21	1:F:192:THR:HB	1.80	0.63
1:A:280:VAL:HG11	1:A:381:ARG:NH1	2.13	0.63
1:E:186:LEU:O	1:E:190:THR:HB	1.99	0.63
1:E:72:ARG:NH1	1:E:103:LEU:HD22	2.12	0.63
1:D:437:LEU:HD13	1:D:440:GLN:OE1	1.99	0.63
1:D:202:LEU:HD13	1:D:460:ILE:HD11	1.79	0.63
1:D:335:LEU:HD21	1:D:341:ILE:HD11	1.80	0.63
1:E:9:THR:H	1:E:12:GLN:NE2	1.96	0.63
1:B:105:TYR:O	1:B:109:GLY:HA2	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:206:TYR:HB3	1:F:209:TYR:HD2	1.64	0.62
1:A:132:LEU:HB3	1:A:134:LEU:CD1	2.29	0.62
1:F:128:ASP:O	1:F:129:GLY:O	2.17	0.62
1:F:134:LEU:HB3	1:F:138:MSE:HB2	1.82	0.62
1:A:356:LYS:HB3	1:A:362:PRO:HB3	1.81	0.62
1:F:186:LEU:O	1:F:190:THR:HB	1.99	0.62
1:C:356:LYS:HG2	1:C:366:VAL:HG11	1.80	0.62
1:D:128:ASP:O	1:D:129:GLY:O	2.17	0.62
1:E:250:ILE:HG22	1:E:250:ILE:O	1.99	0.62
1:D:437:LEU:HB2	1:D:440:GLN:CD	2.24	0.62
1:D:228:TYR:CG	1:D:265:LEU:HD13	2.34	0.62
1:D:105:TYR:O	1:D:109:GLY:HA2	2.00	0.62
1:B:237:ASN:HD21	1:B:248:GLU:HB2	1.64	0.61
1:A:9:THR:H	1:A:12:GLN:HE21	1.48	0.61
1:A:305:HIS:HB2	1:A:427:SER:HB3	1.81	0.61
1:C:9:THR:H	1:C:12:GLN:HE21	1.48	0.61
1:C:237:ASN:HD21	1:C:248:GLU:HB2	1.65	0.61
1:D:77:PHE:CE2	1:D:104:LEU:HD22	2.34	0.61
1:E:27:ALA:HB1	1:E:51:LEU:CD2	2.30	0.61
1:E:105:TYR:O	1:E:109:GLY:HA2	2.00	0.61
1:E:355:THR:O	1:E:359:SER:HB3	2.00	0.61
1:A:477:THR:HB	1:F:395:ASN:ND2	2.12	0.61
1:C:187:ARG:HH11	1:C:187:ARG:HG3	1.66	0.61
1:C:465:ALA:C	1:C:467:GLY:H	2.06	0.61
1:E:36:ILE:HG23	1:E:138:MSE:HE1	1.82	0.61
1:A:105:TYR:O	1:A:109:GLY:HA2	2.00	0.61
1:E:228:TYR:CG	1:E:265:LEU:HD13	2.35	0.61
1:D:237:ASN:HD21	1:D:248:GLU:HB2	1.65	0.61
1:F:187:ARG:HG3	1:F:187:ARG:HH11	1.66	0.61
1:B:16:LYS:HD3	1:B:114:VAL:HB	1.81	0.61
1:B:9:THR:H	1:B:12:GLN:NE2	1.99	0.61
1:F:27:ALA:HB1	1:F:51:LEU:HD22	1.83	0.61
1:D:477:THR:HG22	1:E:398:ARG:HD3	1.83	0.60
1:F:355:THR:O	1:F:359:SER:HB3	2.02	0.60
1:A:190:THR:HG21	1:A:192:THR:HB	1.78	0.60
1:E:465:ALA:C	1:E:467:GLY:H	2.08	0.60
1:A:237:ASN:HD21	1:A:248:GLU:HB2	1.67	0.60
1:E:16:LYS:HD3	1:E:114:VAL:HB	1.83	0.60
1:B:28:LEU:HD13	1:B:126:VAL:HG21	1.83	0.60
1:D:52:PHE:O	1:D:120:GLU:HA	2.02	0.60
1:D:190:THR:HG21	1:D:192:THR:HB	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:206:TYR:HB3	1:F:209:TYR:CD2	2.37	0.60
1:B:361:ARG:HH11	1:B:361:ARG:HB2	1.67	0.60
1:E:268:ALA:HB3	2:E:493:HOH:O	2.02	0.60
1:A:465:ALA:C	1:A:467:GLY:H	2.10	0.59
1:B:463:LEU:HD22	1:B:470:LEU:HD13	1.84	0.59
1:B:250:ILE:HG22	1:B:250:ILE:O	2.02	0.59
1:C:463:LEU:HD22	1:C:470:LEU:HD13	1.83	0.59
1:D:430:PRO:HA	1:D:435:ILE:HG12	1.83	0.59
1:B:465:ALA:C	1:B:467:GLY:H	2.09	0.59
1:C:296:ARG:HD3	1:C:484:ARG:OXT	2.03	0.59
1:D:190:THR:HG22	1:D:192:THR:CB	2.28	0.59
1:E:42:PRO:HA	2:E:497:HOH:O	2.02	0.59
1:F:253:LEU:HD21	1:F:257:LYS:NZ	2.18	0.59
1:A:61:TRP:CZ3	1:A:63:GLY:HA2	2.38	0.59
1:A:185:ARG:NH2	1:B:435:ILE:HG21	2.17	0.59
1:E:134:LEU:HB3	1:E:138:MSE:HB3	1.84	0.59
1:A:9:THR:H	1:A:12:GLN:NE2	2.01	0.58
1:D:8:LEU:HD12	1:D:12:GLN:HE21	1.67	0.58
1:F:305:HIS:HB2	1:F:427:SER:HB3	1.84	0.58
1:C:190:THR:HG22	1:C:192:THR:CB	2.30	0.58
1:B:72:ARG:NH1	1:B:103:LEU:HD22	2.19	0.58
1:D:134:LEU:HB3	1:D:138:MSE:HB2	1.84	0.58
1:C:250:ILE:HG22	1:C:250:ILE:O	2.03	0.58
1:C:150:GLU:O	1:C:151:LEU:HB2	2.03	0.58
1:F:250:ILE:O	1:F:250:ILE:HG22	2.03	0.58
1:F:306:CYS:HB3	1:F:424:LEU:HD13	1.85	0.58
1:A:296:ARG:HD3	1:A:484:ARG:OXT	2.03	0.58
1:A:346:GLU:H	1:A:346:GLU:CD	2.12	0.58
1:F:346:GLU:H	1:F:346:GLU:CD	2.11	0.58
1:A:36:ILE:HA	1:A:138:MSE:HE1	1.86	0.58
1:E:151:LEU:HD21	1:F:430:PRO:O	2.04	0.58
1:B:151:LEU:HD23	2:B:490:HOH:O	2.03	0.58
1:D:465:ALA:C	1:D:467:GLY:H	2.12	0.58
1:B:266:ILE:H	1:B:266:ILE:HD12	1.69	0.58
1:E:237:ASN:HD21	1:E:248:GLU:HB2	1.69	0.57
1:F:237:ASN:HD21	1:F:248:GLU:HB2	1.68	0.57
1:F:310:ARG:H	1:F:313:GLN:NE2	2.01	0.57
1:B:313:GLN:HB2	1:B:429:LYS:NZ	2.19	0.57
1:E:359:SER:HA	1:E:451:GLU:OE1	2.04	0.57
1:B:206:TYR:HB3	1:B:209:TYR:HD2	1.69	0.57
1:B:237:ASN:ND2	1:B:248:GLU:HB2	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:355:THR:O	1:C:359:SER:HB3	2.04	0.57
1:D:36:ILE:HG23	1:D:138:MSE:HE1	1.87	0.57
1:F:465:ALA:C	1:F:467:GLY:H	2.12	0.57
1:B:359:SER:HA	1:B:451:GLU:OE1	2.03	0.57
1:C:21:TYR:O	1:C:25:VAL:HG12	2.05	0.57
1:E:335:LEU:HD21	1:E:341:ILE:HD11	1.86	0.57
1:F:313:GLN:HB2	1:F:429:LYS:NZ	2.19	0.57
1:A:134:LEU:HB3	1:A:138:MSE:HB2	1.86	0.57
1:B:206:TYR:HB3	1:B:209:TYR:CD2	2.38	0.57
1:C:335:LEU:HD21	1:C:341:ILE:HD11	1.87	0.57
1:D:187:ARG:HG3	1:D:187:ARG:HH11	1.69	0.57
1:F:266:ILE:HD12	1:F:266:ILE:H	1.69	0.57
1:C:52:PHE:O	1:C:120:GLU:HA	2.04	0.57
1:B:478:PHE:HD1	1:C:395:ASN:HD22	1.52	0.57
1:C:306:CYS:HB3	1:C:424:LEU:HD13	1.85	0.57
1:A:21:TYR:O	1:A:25:VAL:HG12	2.04	0.57
1:A:22:GLU:O	1:A:26:VAL:HG23	2.05	0.57
1:B:52:PHE:O	1:B:120:GLU:HA	2.05	0.57
1:C:61:TRP:CZ3	1:C:63:GLY:HA2	2.40	0.57
1:B:357:LEU:HD13	1:B:458:ARG:NH1	2.19	0.57
1:D:134:LEU:CD1	1:D:134:LEU:H	2.18	0.57
1:A:131:GLU:CD	1:A:131:GLU:H	2.13	0.56
1:D:208:ARG:HD3	1:D:446:GLU:OE1	2.05	0.56
1:C:131:GLU:CB	1:D:441:ALA:HB1	2.35	0.56
1:B:36:ILE:HA	1:B:138:MSE:HE1	1.87	0.56
1:F:326:ARG:HG2	1:F:326:ARG:NH1	2.19	0.56
1:E:36:ILE:HG23	1:E:138:MSE:CE	2.35	0.56
1:A:52:PHE:O	1:A:120:GLU:HA	2.05	0.56
1:A:77:PHE:CE2	1:A:104:LEU:HD22	2.40	0.56
1:C:105:TYR:O	1:C:109:GLY:HA2	2.06	0.56
1:D:237:ASN:ND2	1:D:248:GLU:HB2	2.20	0.56
1:D:355:THR:O	1:D:359:SER:HB3	2.06	0.56
1:A:250:ILE:O	1:A:250:ILE:HG22	2.06	0.56
1:B:190:THR:HG22	1:B:192:THR:N	2.20	0.56
1:E:356:LYS:HG2	1:E:366:VAL:HG11	1.88	0.56
1:A:355:THR:O	1:A:359:SER:HB3	2.06	0.56
1:B:127:ILE:HD13	1:B:132:LEU:HG	1.87	0.56
1:A:469:ARG:HG2	1:A:469:ARG:HH11	1.71	0.56
1:B:187:ARG:HG3	1:B:187:ARG:HH11	1.71	0.56
1:D:305:HIS:HB2	1:D:427:SER:HB3	1.87	0.56
1:A:151:LEU:HD22	1:A:151:LEU:N	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:ARG:NH1	1:A:449:ILE:HD12	2.20	0.55
1:A:228:TYR:CD1	1:A:265:LEU:HD13	2.40	0.55
1:B:430:PRO:HA	1:B:435:ILE:HG12	1.87	0.55
1:C:130:SER:HB2	1:D:441:ALA:HB2	1.88	0.55
1:D:28:LEU:HD13	1:D:126:VAL:HG21	1.87	0.55
1:F:31:ALA:HB1	1:F:42:PRO:HG3	1.86	0.55
1:A:395:ASN:HD22	1:F:478:PHE:HD1	1.54	0.55
1:F:36:ILE:HA	1:F:138:MSE:HE1	1.88	0.55
1:E:296:ARG:HD3	1:E:484:ARG:OXT	2.06	0.55
1:F:16:LYS:HD3	1:F:114:VAL:HB	1.89	0.55
1:D:14:LEU:HD11	1:D:98:ASN:HB2	1.89	0.55
1:D:61:TRP:CZ3	1:D:63:GLY:HA2	2.42	0.55
1:D:83:TYR:HA	1:D:169:SER:O	2.06	0.55
1:D:250:ILE:O	1:D:250:ILE:HG22	2.06	0.55
1:D:119:HIS:ND1	1:D:177:ARG:NH2	2.53	0.55
1:E:134:LEU:HB3	1:E:138:MSE:HB2	1.88	0.55
1:E:266:ILE:HD12	1:E:266:ILE:H	1.70	0.55
1:F:305:HIS:CE1	1:F:438:PRO:HG2	2.41	0.55
1:A:190:THR:HG22	1:A:192:THR:CB	2.32	0.55
1:D:395:ASN:HD21	1:E:477:THR:HB	1.71	0.55
1:E:52:PHE:O	1:E:120:GLU:HA	2.05	0.55
1:E:228:TYR:CD1	1:E:265:LEU:HD13	2.42	0.55
1:C:14:LEU:HD11	1:C:98:ASN:HB2	1.88	0.55
1:B:27:ALA:HB1	1:B:51:LEU:HD22	1.89	0.55
1:B:364:GLU:CG	1:C:469:ARG:NH2	2.70	0.55
1:E:280:VAL:HG11	1:E:381:ARG:NH1	2.22	0.55
1:F:227:PRO:O	1:F:229:ILE:HG23	2.06	0.55
1:D:346:GLU:CD	1:D:346:GLU:H	2.15	0.55
1:B:123:TYR:CG	1:B:124:PRO:HD3	2.42	0.55
1:D:296:ARG:HD3	1:D:484:ARG:OXT	2.07	0.54
1:E:310:ARG:H	1:E:313:GLN:NE2	2.05	0.54
1:B:14:LEU:HD11	1:B:98:ASN:HB2	1.90	0.54
1:C:9:THR:H	1:C:12:GLN:NE2	2.03	0.54
1:C:357:LEU:HD13	1:C:458:ARG:NH1	2.23	0.54
1:F:436:LYS:C	1:F:437:LEU:HD12	2.32	0.54
1:C:208:ARG:HD3	1:C:446:GLU:OE1	2.07	0.54
1:E:21:TYR:O	1:E:25:VAL:HG12	2.07	0.54
1:C:441:ALA:HB3	1:D:131:GLU:HB2	1.89	0.54
1:D:127:ILE:HD13	1:D:132:LEU:CG	2.36	0.54
1:F:61:TRP:CZ3	1:F:63:GLY:HA2	2.43	0.54
1:F:208:ARG:HD3	1:F:446:GLU:OE1	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:ALA:O	1:B:476:ARG:HD2	2.08	0.54
1:C:31:ALA:HB1	1:C:42:PRO:HG3	1.90	0.54
1:D:469:ARG:NH2	1:E:364:GLU:HB2	2.22	0.54
1:B:266:ILE:HG22	1:B:267:THR:N	2.22	0.54
1:C:53:VAL:HG11	1:C:117:SER:O	2.08	0.54
1:C:123:TYR:CG	1:C:124:PRO:HD3	2.42	0.54
1:C:346:GLU:CD	1:C:346:GLU:H	2.15	0.54
1:D:21:TYR:O	1:D:25:VAL:HG12	2.08	0.54
1:D:436:LYS:C	1:D:437:LEU:HD12	2.32	0.54
1:C:237:ASN:ND2	1:C:248:GLU:HB2	2.22	0.54
1:E:190:THR:HG22	1:E:192:THR:N	2.22	0.54
1:E:313:GLN:HB2	1:E:429:LYS:NZ	2.23	0.54
1:F:228:TYR:CG	1:F:265:LEU:HD13	2.42	0.54
1:B:21:TYR:O	1:B:25:VAL:HG12	2.06	0.54
1:E:427:SER:O	1:E:428:ASP:HB3	2.07	0.54
1:B:122:PRO:HA	1:B:147:PRO:O	2.07	0.54
1:B:305:HIS:HB2	1:B:427:SER:HB3	1.89	0.54
1:B:190:THR:HG23	1:B:262:ALA:HB3	1.89	0.54
1:B:437:LEU:HD12	1:B:440:GLN:OE1	2.07	0.54
1:C:27:ALA:HB1	1:C:51:LEU:HD22	1.90	0.54
1:D:427:SER:O	1:D:428:ASP:HB3	2.08	0.54
1:E:134:LEU:HD12	1:E:134:LEU:N	2.23	0.54
1:E:237:ASN:ND2	1:E:248:GLU:HB2	2.22	0.54
1:F:237:ASN:ND2	1:F:248:GLU:HB2	2.23	0.54
1:B:355:THR:O	1:B:359:SER:HB3	2.08	0.53
1:E:22:GLU:O	1:E:26:VAL:HG23	2.08	0.53
1:A:36:ILE:HG23	1:A:138:MSE:CE	2.37	0.53
1:C:16:LYS:HD3	1:C:114:VAL:HB	1.89	0.53
1:B:335:LEU:HD21	1:B:341:ILE:HD11	1.89	0.53
1:D:395:ASN:ND2	1:E:478:PHE:H	2.06	0.53
1:F:356:LYS:CG	1:F:366:VAL:HG11	2.38	0.53
1:A:16:LYS:HD3	1:A:114:VAL:HB	1.91	0.53
1:C:56:SER:HB2	1:C:117:SER:HB3	1.90	0.53
1:C:305:HIS:HB2	1:C:427:SER:HB3	1.90	0.53
1:D:132:LEU:HB3	1:D:134:LEU:HD13	1.90	0.53
1:A:335:LEU:HD21	1:A:341:ILE:HD11	1.90	0.53
1:A:361:ARG:CD	1:A:361:ARG:H	2.21	0.53
1:B:478:PHE:H	1:C:395:ASN:ND2	2.06	0.53
1:D:73:ALA:O	1:D:476:ARG:HD2	2.09	0.53
1:F:52:PHE:O	1:F:120:GLU:HA	2.08	0.53
1:F:362:PRO:O	1:F:365:GLU:HB3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:437:LEU:HD12	1:F:437:LEU:N	2.23	0.53
1:B:296:ARG:HD3	1:B:484:ARG:OXT	2.08	0.53
1:C:228:TYR:HB3	1:C:265:LEU:HD22	1.89	0.53
1:D:360:GLY:O	1:D:362:PRO:HD3	2.09	0.53
1:F:27:ALA:HB1	1:F:51:LEU:CD2	2.38	0.53
1:F:60:THR:HG23	1:F:82:SER:OG	2.09	0.53
1:A:28:LEU:HD13	1:A:126:VAL:HG21	1.90	0.53
1:D:357:LEU:HD13	1:D:458:ARG:NH1	2.23	0.53
1:A:227:PRO:O	1:A:229:ILE:HG23	2.08	0.53
1:C:131:GLU:CD	1:D:443:ARG:HB2	2.34	0.53
1:F:427:SER:O	1:F:428:ASP:HB3	2.09	0.53
1:A:27:ALA:HB1	1:A:51:LEU:CD2	2.39	0.53
1:A:237:ASN:ND2	1:A:248:GLU:HB2	2.23	0.53
1:E:123:TYR:O	1:E:126:VAL:HG22	2.09	0.53
1:F:216:TRP:O	1:F:220:GLN:HG2	2.09	0.53
1:C:251:SER:HA	2:C:501:HOH:O	2.09	0.52
1:D:31:ALA:HB1	1:D:42:PRO:HG3	1.91	0.52
1:E:190:THR:HG22	1:E:192:THR:CB	2.35	0.52
1:E:208:ARG:NH2	1:E:212:GLU:OE1	2.42	0.52
1:A:53:VAL:HG13	1:A:117:SER:OG	2.09	0.52
1:A:134:LEU:HB3	1:A:138:MSE:HB3	1.91	0.52
1:A:352:TYR:CE2	1:A:356:LYS:HE3	2.45	0.52
1:D:352:TYR:CE2	1:D:356:LYS:HE3	2.45	0.52
1:F:53:VAL:HG13	1:F:117:SER:OG	2.09	0.52
1:D:51:LEU:HD13	1:D:52:PHE:CE2	2.45	0.52
1:C:151:LEU:HD21	1:D:430:PRO:O	2.09	0.52
1:F:359:SER:HA	1:F:451:GLU:OE1	2.09	0.52
1:F:28:LEU:HD13	1:F:126:VAL:HG21	1.91	0.52
1:F:305:HIS:HB3	1:F:445:TYR:CZ	2.45	0.52
1:A:398:ARG:HD2	1:F:476:ARG:O	2.10	0.52
1:B:356:LYS:CG	1:B:366:VAL:HG11	2.39	0.52
1:A:395:ASN:ND2	1:F:477:THR:HB	2.19	0.52
1:E:133:THR:C	1:E:134:LEU:HD12	2.34	0.52
1:B:70:LYS:HB3	1:C:312:SER:HB2	1.92	0.52
1:C:465:ALA:C	1:C:467:GLY:N	2.68	0.52
1:D:72:ARG:NH1	1:D:103:LEU:HD22	2.24	0.52
1:A:119:HIS:ND1	1:A:177:ARG:NH2	2.57	0.52
1:A:231:LEU:HD12	1:A:264:HIS:O	2.10	0.52
1:D:27:ALA:HB1	1:D:51:LEU:HD22	1.91	0.52
1:E:14:LEU:HD11	1:E:98:ASN:HB2	1.92	0.52
1:E:53:VAL:HG13	1:E:117:SER:OG	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:83:TYR:HA	1:E:169:SER:O	2.10	0.51
1:F:134:LEU:HB3	1:F:138:MSE:HB3	1.92	0.51
1:F:347:VAL:O	1:F:351:LEU:HD22	2.11	0.51
1:B:261:PRO:HB2	1:B:263:TRP:CZ3	2.44	0.51
1:E:208:ARG:HD3	1:E:446:GLU:OE1	2.10	0.51
1:E:442:ASN:ND2	1:E:445:TYR:CB	2.74	0.51
1:E:465:ALA:C	1:E:467:GLY:N	2.69	0.51
1:B:357:LEU:HD13	1:B:458:ARG:HH11	1.75	0.51
1:D:425:CYS:HB2	1:D:452:HIS:CE1	2.45	0.51
1:E:53:VAL:HG11	1:E:117:SER:O	2.11	0.51
1:A:27:ALA:HB1	1:A:51:LEU:HD22	1.91	0.51
1:A:187:ARG:HG3	1:A:187:ARG:HH11	1.75	0.51
1:A:437:LEU:HD12	1:A:437:LEU:N	2.17	0.51
1:A:451:GLU:O	1:A:455:ILE:HG13	2.10	0.51
1:B:51:LEU:HD13	1:B:52:PHE:CE2	2.46	0.51
1:B:477:THR:HB	1:C:395:ASN:ND2	2.22	0.51
1:C:119:HIS:ND1	1:C:177:ARG:NH2	2.59	0.51
1:D:71:THR:CG2	1:E:367:LYS:HB3	2.40	0.51
1:A:185:ARG:HH22	1:B:435:ILE:CG2	2.24	0.51
1:D:71:THR:HG23	1:E:367:LYS:HB3	1.93	0.51
1:F:119:HIS:ND1	1:F:177:ARG:NH2	2.58	0.51
1:A:326:ARG:HG2	1:A:326:ARG:NH1	2.22	0.51
1:B:227:PRO:O	1:B:229:ILE:HG23	2.11	0.51
1:B:477:THR:HG22	1:C:398:ARG:HD3	1.92	0.50
1:E:463:LEU:HD22	1:E:470:LEU:HD13	1.92	0.50
1:B:119:HIS:ND1	1:B:177:ARG:NH2	2.59	0.50
1:F:190:THR:HG22	1:F:192:THR:N	2.24	0.50
1:B:228:TYR:CG	1:B:265:LEU:HD13	2.46	0.50
1:A:359:SER:HA	1:A:451:GLU:OE1	2.10	0.50
1:D:131:GLU:CD	1:D:131:GLU:H	2.20	0.50
1:D:306:CYS:HB3	1:D:424:LEU:HD13	1.93	0.50
1:E:123:TYR:CG	1:E:124:PRO:HD3	2.47	0.50
1:E:202:LEU:HD13	1:E:460:ILE:CD1	2.40	0.50
1:E:326:ARG:NH2	1:E:335:LEU:O	2.44	0.50
1:E:346:GLU:CD	1:E:346:GLU:H	2.18	0.50
1:F:9:THR:H	1:F:12:GLN:NE2	2.10	0.50
1:B:465:ALA:C	1:B:467:GLY:N	2.70	0.50
1:C:72:ARG:NH1	1:C:103:LEU:HD22	2.26	0.50
1:D:36:ILE:HG23	1:D:138:MSE:CE	2.41	0.50
1:D:227:PRO:O	1:D:229:ILE:HG23	2.12	0.50
1:D:260:MSE:HG2	1:D:278:ILE:HA	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:122:PRO:HA	1:F:147:PRO:O	2.12	0.50
1:C:51:LEU:HD13	1:C:52:PHE:CE2	2.47	0.50
1:C:356:LYS:CG	1:C:366:VAL:HG11	2.42	0.50
1:F:151:LEU:HD13	1:F:151:LEU:N	2.23	0.50
1:D:453:LEU:O	1:D:457:ILE:HG13	2.11	0.50
1:E:216:TRP:O	1:E:220:GLN:HG2	2.11	0.50
1:F:280:VAL:HG11	1:F:381:ARG:NH1	2.26	0.50
1:A:134:LEU:CD1	1:A:134:LEU:H	2.25	0.50
1:B:27:ALA:HB1	1:B:51:LEU:CD2	2.42	0.50
1:C:280:VAL:HG11	1:C:381:ARG:NH1	2.26	0.50
1:F:357:LEU:HD13	1:F:458:ARG:NH1	2.27	0.50
1:A:437:LEU:H	1:A:437:LEU:CD1	2.20	0.49
1:E:313:GLN:HB2	1:E:429:LYS:HZ1	1.75	0.49
1:E:357:LEU:HD13	1:E:458:ARG:NH1	2.27	0.49
1:F:190:THR:HG22	1:F:192:THR:CB	2.37	0.49
1:B:190:THR:HG21	1:B:192:THR:HB	1.86	0.49
1:B:346:GLU:CD	1:B:346:GLU:H	2.20	0.49
1:C:60:THR:HG23	1:C:82:SER:OG	2.12	0.49
1:E:187:ARG:HG3	1:E:187:ARG:HH11	1.77	0.49
1:F:463:LEU:HD22	1:F:470:LEU:HD13	1.94	0.49
1:A:120:GLU:OE1	1:A:147:PRO:HG3	2.12	0.49
1:A:266:ILE:HG22	1:A:267:THR:N	2.28	0.49
1:C:131:GLU:HB3	1:D:441:ALA:HB1	1.92	0.49
1:C:190:THR:HG22	1:C:192:THR:N	2.28	0.49
1:D:206:TYR:HB3	1:D:209:TYR:HD2	1.77	0.49
1:E:36:ILE:HA	1:E:138:MSE:HE1	1.94	0.49
1:D:16:LYS:HD3	1:D:114:VAL:HB	1.94	0.49
1:E:31:ALA:HB1	1:E:42:PRO:HG3	1.93	0.49
1:A:411:ALA:O	1:A:414:TYR:HB3	2.11	0.49
1:D:357:LEU:HD13	1:D:458:ARG:HH11	1.78	0.49
1:E:206:TYR:HB3	1:E:209:TYR:CD2	2.48	0.49
1:F:335:LEU:HD21	1:F:341:ILE:HD11	1.94	0.49
1:A:14:LEU:HD11	1:A:98:ASN:HB2	1.95	0.49
1:A:356:LYS:CG	1:A:366:VAL:HG11	2.40	0.49
1:D:228:TYR:CD1	1:D:265:LEU:HD13	2.47	0.49
1:D:477:THR:HB	1:E:395:ASN:ND2	2.26	0.49
1:B:280:VAL:HG11	1:B:381:ARG:NH1	2.28	0.49
1:B:398:ARG:HD3	1:C:477:THR:HG22	1.94	0.49
1:C:150:GLU:OE1	1:C:150:GLU:HA	2.12	0.49
1:E:9:THR:HG23	1:E:12:GLN:NE2	2.28	0.49
1:E:352:TYR:CE2	1:E:356:LYS:HE3	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:266:ILE:HG22	1:F:267:THR:N	2.27	0.49
1:F:313:GLN:HB2	1:F:429:LYS:HZ1	1.77	0.49
1:A:36:ILE:HG23	1:A:138:MSE:HE1	1.93	0.49
1:E:27:ALA:HB1	1:E:51:LEU:HD22	1.94	0.49
1:F:192:THR:HG23	1:F:193:PRO:HD2	1.95	0.49
1:A:265:LEU:O	1:A:272:GLY:HA3	2.13	0.49
1:A:326:ARG:NH2	1:A:335:LEU:O	2.46	0.49
1:A:437:LEU:HD13	1:A:440:GLN:HG3	1.93	0.49
1:B:200:PHE:CZ	1:B:464:ARG:HG3	2.47	0.49
1:D:9:THR:HG23	1:D:12:GLN:NE2	2.28	0.49
1:D:123:TYR:CG	1:D:124:PRO:HD3	2.48	0.49
1:F:261:PRO:HB2	1:F:263:TRP:CZ3	2.48	0.49
1:A:206:TYR:HB3	1:A:209:TYR:HD2	1.78	0.48
1:C:27:ALA:HB1	1:C:51:LEU:CD2	2.43	0.48
1:C:437:LEU:HD11	1:D:185:ARG:NH2	2.28	0.48
1:E:261:PRO:HB2	1:E:263:TRP:CZ3	2.47	0.48
1:E:411:ALA:O	1:E:414:TYR:HB3	2.13	0.48
1:D:361:ARG:HG3	1:D:361:ARG:HH11	1.77	0.48
1:F:9:THR:H	1:F:12:GLN:HE21	1.60	0.48
1:A:248:GLU:HA	2:A:503:HOH:O	2.13	0.48
1:B:360:GLY:O	1:B:361:ARG:C	2.55	0.48
1:D:322:HIS:HD2	1:E:474:LYS:HD3	1.78	0.48
1:E:206:TYR:HB3	1:E:209:TYR:HD2	1.78	0.48
1:E:231:LEU:HD12	1:E:264:HIS:O	2.13	0.48
1:F:51:LEU:HD13	1:F:52:PHE:CE2	2.48	0.48
1:F:134:LEU:H	1:F:134:LEU:CD1	2.27	0.48
1:F:228:TYR:HB3	1:F:265:LEU:HD22	1.95	0.48
1:B:123:TYR:CD2	1:B:124:PRO:HD3	2.49	0.48
1:F:119:HIS:HA	2:F:498:HOH:O	2.12	0.48
1:C:28:LEU:HD13	1:C:126:VAL:CG2	2.43	0.48
1:D:398:ARG:HD2	1:E:476:ARG:O	2.14	0.48
1:E:8:LEU:HB3	1:E:112:ILE:O	2.14	0.48
1:A:369:ARG:HG2	1:A:369:ARG:HH11	1.78	0.48
1:D:266:ILE:HG22	1:D:267:THR:N	2.28	0.48
1:E:61:TRP:CZ3	1:E:63:GLY:HA2	2.48	0.48
1:E:266:ILE:HG22	1:E:267:THR:N	2.29	0.48
1:A:206:TYR:HB3	1:A:209:TYR:CD2	2.48	0.48
1:A:465:ALA:C	1:A:467:GLY:N	2.70	0.48
1:B:31:ALA:HB1	1:B:42:PRO:HG3	1.95	0.48
1:B:61:TRP:CZ3	1:B:63:GLY:HA2	2.48	0.48
1:D:266:ILE:HD12	1:D:266:ILE:H	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:369:ARG:HH11	1:D:369:ARG:HG2	1.79	0.48
1:E:151:LEU:CD1	1:F:384:GLU:HB3	2.43	0.48
1:F:14:LEU:HD11	1:F:98:ASN:HB2	1.96	0.48
1:F:414:TYR:HA	1:F:475:LEU:HD22	1.96	0.48
1:B:151:LEU:N	1:B:151:LEU:HD22	2.29	0.48
1:B:326:ARG:NH2	1:B:335:LEU:O	2.47	0.48
1:D:27:ALA:HB1	1:D:51:LEU:CD2	2.43	0.48
1:B:474:LYS:HD3	1:C:322:HIS:CD2	2.49	0.48
1:E:72:ARG:HH12	1:E:103:LEU:HD22	1.76	0.48
1:B:474:LYS:HD3	1:C:322:HIS:HD2	1.78	0.48
1:C:123:TYR:CD2	1:C:124:PRO:HD3	2.48	0.48
1:F:393:ARG:HG2	1:F:393:ARG:HH11	1.79	0.48
1:C:437:LEU:HD23	1:D:188:HIS:CD2	2.49	0.47
1:D:206:TYR:HB3	1:D:209:TYR:CD2	2.49	0.47
1:A:77:PHE:HD2	1:A:108:TYR:CD2	2.32	0.47
1:A:261:PRO:HB2	1:A:263:TRP:CZ3	2.49	0.47
1:C:261:PRO:HB2	1:C:263:TRP:CZ3	2.49	0.47
1:E:390:SER:HB3	1:E:394:PHE:CE1	2.49	0.47
1:F:357:LEU:CD1	1:F:458:ARG:HH11	2.27	0.47
1:A:208:ARG:HH11	1:A:449:ILE:HD12	1.79	0.47
1:A:427:SER:O	1:A:428:ASP:HB3	2.13	0.47
1:E:169:SER:HA	1:E:170:PRO:HD3	1.69	0.47
1:E:228:TYR:HB3	1:E:265:LEU:HD22	1.97	0.47
1:F:211:ASP:HA	1:F:250:ILE:CD1	2.44	0.47
1:F:326:ARG:NH1	2:F:485:HOH:O	2.46	0.47
1:A:202:LEU:CD1	1:A:460:ILE:HD11	2.35	0.47
1:B:443:ARG:HG3	1:B:444:PHE:N	2.30	0.47
1:C:329:HIS:HD2	1:C:379:ASP:OD2	1.97	0.47
1:C:131:GLU:HG3	1:C:132:LEU:N	2.29	0.47
1:D:70:LYS:CE	2:D:496:HOH:O	2.63	0.47
1:F:127:ILE:HD13	1:F:132:LEU:CG	2.42	0.47
1:A:51:LEU:HD13	1:A:52:PHE:CE2	2.50	0.47
1:A:223:ASP:C	1:A:223:ASP:OD2	2.58	0.47
1:A:291:HIS:O	1:A:294:VAL:HG22	2.14	0.47
1:C:265:LEU:O	1:C:272:GLY:HA3	2.15	0.47
1:C:266:ILE:HG22	1:C:267:THR:N	2.29	0.47
1:C:310:ARG:H	1:C:313:GLN:NE2	2.13	0.47
1:C:326:ARG:HG2	1:C:326:ARG:NH1	2.28	0.47
1:C:356:LYS:HG2	1:C:366:VAL:CG1	2.44	0.47
1:E:151:LEU:N	1:E:151:LEU:HD22	2.29	0.47
1:F:465:ALA:C	1:F:467:GLY:N	2.72	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:313:GLN:HB2	1:C:429:LYS:HZ1	1.80	0.47
1:D:356:LYS:CG	1:D:366:VAL:HG11	2.41	0.47
1:A:430:PRO:HA	1:A:435:ILE:HG12	1.97	0.47
1:A:469:ARG:HG2	1:A:469:ARG:NH1	2.29	0.47
1:D:134:LEU:CD1	1:D:134:LEU:N	2.78	0.47
1:E:441:ALA:HB3	1:F:131:GLU:HB2	1.97	0.47
1:F:21:TYR:O	1:F:25:VAL:HG12	2.15	0.47
1:F:299:VAL:HG22	1:F:301:LEU:HD13	1.97	0.47
1:F:411:ALA:O	1:F:414:TYR:HB3	2.15	0.47
1:D:329:HIS:HD2	1:D:379:ASP:OD2	1.97	0.47
1:E:253:LEU:HD13	1:F:252:ASP:OD1	2.15	0.47
1:F:223:ASP:C	1:F:223:ASP:OD2	2.57	0.47
1:A:476:ARG:O	1:F:398:ARG:HD2	2.15	0.46
1:C:247:GLU:C	1:C:249:ALA:H	2.23	0.46
1:D:280:VAL:HG11	1:D:381:ARG:NH1	2.30	0.46
1:E:28:LEU:HD13	1:E:126:VAL:CG2	2.43	0.46
1:F:123:TYR:CG	1:F:124:PRO:HD3	2.50	0.46
1:A:266:ILE:HD12	1:A:266:ILE:H	1.80	0.46
1:C:369:ARG:HG2	1:C:369:ARG:HH11	1.80	0.46
1:A:31:ALA:HB1	1:A:42:PRO:HG3	1.97	0.46
1:A:395:ASN:ND2	1:F:478:PHE:H	2.13	0.46
1:B:469:ARG:HH11	1:B:469:ARG:HG2	1.80	0.46
1:F:36:ILE:HG23	1:F:138:MSE:CE	2.45	0.46
1:D:190:THR:HG22	1:D:192:THR:N	2.30	0.46
1:D:212:GLU:HG2	1:D:450:SER:HA	1.98	0.46
1:E:77:PHE:HD2	1:E:108:TYR:CD2	2.33	0.46
1:A:357:LEU:HD13	1:A:458:ARG:NH1	2.31	0.46
1:C:130:SER:HB2	1:D:441:ALA:CB	2.45	0.46
1:C:228:TYR:CG	1:C:265:LEU:HD13	2.50	0.46
1:A:53:VAL:HG11	1:A:117:SER:N	2.31	0.46
1:B:150:GLU:C	1:B:151:LEU:HD22	2.40	0.46
1:B:192:THR:HG23	1:B:193:PRO:HD2	1.98	0.46
1:B:259:GLN:C	1:B:260:MSE:HG3	2.40	0.46
1:C:77:PHE:HD2	1:C:108:TYR:CD2	2.33	0.46
1:C:129:GLY:O	1:C:130:SER:O	2.33	0.46
1:E:89:ARG:N	1:E:90:PRO:HD3	2.31	0.46
1:E:173:HIS:HE1	1:E:480:GLU:OE2	1.99	0.46
1:F:356:LYS:HG2	1:F:366:VAL:CG1	2.41	0.46
1:A:284:ASN:ND2	1:B:381:ARG:HH21	2.14	0.46
1:A:356:LYS:HG2	1:A:366:VAL:CG1	2.41	0.46
1:D:71:THR:OG1	1:E:368:GLN:HG2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:360:GLY:HA3	2:D:514:HOH:O	2.15	0.46
1:E:87:ILE:HG22	1:E:88:THR:N	2.31	0.46
1:B:223:ASP:OD2	1:B:223:ASP:C	2.58	0.46
1:D:326:ARG:HG2	1:D:326:ARG:NH1	2.27	0.46
1:D:326:ARG:NH2	1:D:335:LEU:O	2.49	0.46
1:B:134:LEU:HB3	1:B:138:MSE:HB3	1.96	0.46
1:B:357:LEU:CD1	1:B:458:ARG:HH11	2.28	0.46
1:C:200:PHE:CZ	1:C:464:ARG:HG3	2.50	0.46
1:F:216:TRP:CZ3	1:F:265:LEU:HD12	2.51	0.46
1:A:151:LEU:HD11	1:B:384:GLU:HB3	1.97	0.45
1:A:444:PHE:CD2	1:B:136:ARG:NH2	2.84	0.45
1:B:71:THR:CG2	1:C:367:LYS:HB3	2.46	0.45
1:B:208:ARG:HD3	1:B:446:GLU:OE1	2.16	0.45
1:A:313:GLN:HB2	1:A:429:LYS:NZ	2.31	0.45
1:C:123:TYR:O	1:C:126:VAL:HG22	2.16	0.45
1:D:465:ALA:C	1:D:467:GLY:N	2.72	0.45
1:E:36:ILE:HD13	1:E:132:LEU:HD22	1.98	0.45
1:F:36:ILE:HG23	1:F:138:MSE:HE1	1.98	0.45
1:B:442:ASN:ND2	1:B:445:TYR:HB3	2.31	0.45
1:C:134:LEU:HD12	1:C:134:LEU:N	2.31	0.45
1:D:8:LEU:HB3	1:D:112:ILE:O	2.16	0.45
1:D:211:ASP:HA	1:D:250:ILE:CD1	2.47	0.45
1:D:469:ARG:HG2	1:D:469:ARG:HH11	1.80	0.45
1:E:63:GLY:HA3	1:E:80:ALA:HB2	1.99	0.45
1:A:47:ARG:HA	1:A:51:LEU:HB2	1.97	0.45
1:A:53:VAL:HG11	1:A:117:SER:O	2.16	0.45
1:A:127:ILE:HD13	1:A:132:LEU:HG	1.97	0.45
1:A:280:VAL:HG11	1:A:381:ARG:CZ	2.47	0.45
1:B:134:LEU:CD1	1:B:134:LEU:H	2.29	0.45
1:B:228:TYR:HB3	1:B:265:LEU:HD22	1.98	0.45
1:B:259:GLN:O	1:B:260:MSE:HG3	2.16	0.45
1:B:427:SER:O	1:B:428:ASP:HB3	2.16	0.45
1:C:56:SER:HB3	1:C:115:GLN:O	2.17	0.45
1:E:51:LEU:HD13	1:E:52:PHE:CE2	2.52	0.45
1:E:231:LEU:HA	1:E:264:HIS:O	2.17	0.45
1:F:131:GLU:CD	1:F:131:GLU:N	2.72	0.45
1:B:123:TYR:O	1:B:126:VAL:HG22	2.17	0.45
1:B:22:GLU:O	1:B:26:VAL:HG23	2.16	0.45
1:B:322:HIS:HD2	1:C:474:LYS:HD3	1.82	0.45
1:C:8:LEU:HB3	1:C:112:ILE:O	2.16	0.45
1:C:131:GLU:HB2	1:D:441:ALA:HB1	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:326:ARG:NH2	1:C:335:LEU:O	2.50	0.45
1:C:352:TYR:CE2	1:C:356:LYS:HE3	2.52	0.45
1:E:451:GLU:O	1:E:455:ILE:HG13	2.17	0.45
1:F:53:VAL:HG11	1:F:117:SER:O	2.16	0.45
1:F:437:LEU:HD13	1:F:440:GLN:OE1	2.17	0.45
1:A:76:ARG:HH11	1:A:76:ARG:HB3	1.82	0.45
1:A:190:THR:HG22	1:A:192:THR:N	2.31	0.45
1:B:247:GLU:C	1:B:249:ALA:H	2.23	0.45
1:F:202:LEU:HD13	1:F:460:ILE:CD1	2.43	0.45
1:F:214:VAL:HG21	1:F:250:ILE:HG12	1.98	0.45
1:A:305:HIS:CE1	1:A:438:PRO:HG2	2.52	0.45
1:C:442:ASN:O	1:C:443:ARG:C	2.60	0.45
1:C:469:ARG:HG2	1:C:469:ARG:HH11	1.81	0.45
1:D:463:LEU:HD22	1:D:470:LEU:HD13	1.99	0.45
1:E:56:SER:HB3	1:E:115:GLN:O	2.17	0.45
1:C:47:ARG:HA	1:C:51:LEU:HB2	1.99	0.45
1:E:223:ASP:OD2	1:E:223:ASP:C	2.59	0.45
1:E:443:ARG:HG2	1:E:444:PHE:CE1	2.52	0.45
1:F:8:LEU:HB3	1:F:112:ILE:O	2.16	0.45
1:F:47:ARG:HA	1:F:51:LEU:HB2	1.99	0.45
1:B:186:LEU:HD23	1:B:186:LEU:HA	1.88	0.45
1:B:212:GLU:HG2	1:B:450:SER:HA	1.98	0.45
1:B:356:LYS:HG2	1:B:366:VAL:CG1	2.44	0.45
1:C:357:LEU:HD13	1:C:458:ARG:HH11	1.81	0.45
1:E:135:ASP:CA	1:F:443:ARG:HH21	2.23	0.45
1:E:265:LEU:O	1:E:272:GLY:HA3	2.16	0.45
1:F:253:LEU:HD21	1:F:257:LYS:HZ1	1.79	0.45
1:B:72:ARG:HH12	1:B:103:LEU:HD22	1.81	0.44
1:C:89:ARG:N	1:C:90:PRO:HD3	2.31	0.44
1:D:123:TYR:O	1:D:126:VAL:HG22	2.17	0.44
1:D:237:ASN:HD21	1:D:248:GLU:CB	2.30	0.44
1:F:265:LEU:HD23	1:F:265:LEU:HA	1.87	0.44
1:B:133:THR:HG22	1:B:133:THR:O	2.17	0.44
1:D:204:THR:HG22	1:D:303:ILE:O	2.17	0.44
1:F:364:GLU:O	1:F:364:GLU:HG2	2.17	0.44
1:F:369:ARG:HG2	1:F:369:ARG:HH11	1.81	0.44
1:C:223:ASP:OD2	1:C:223:ASP:C	2.60	0.44
1:D:134:LEU:HB3	1:D:138:MSE:HB3	1.99	0.44
1:D:265:LEU:HD23	1:D:265:LEU:HA	1.77	0.44
1:E:435:ILE:HG21	1:F:185:ARG:HH22	1.83	0.44
1:A:122:PRO:HA	1:A:147:PRO:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:VAL:HG12	1:A:54:TYR:O	2.17	0.44
1:A:216:TRP:O	1:A:220:GLN:HG2	2.17	0.44
1:B:89:ARG:N	1:B:90:PRO:HD3	2.33	0.44
1:D:200:PHE:CZ	1:D:464:ARG:HG3	2.53	0.44
1:F:265:LEU:O	1:F:272:GLY:HA3	2.17	0.44
1:A:8:LEU:HD11	1:A:12:GLN:HB3	1.99	0.44
1:A:61:TRP:CE3	1:A:63:GLY:HA2	2.53	0.44
1:B:70:LYS:HD3	1:B:76:ARG:NH1	2.33	0.44
1:B:260:MSE:HG2	1:B:278:ILE:HA	1.98	0.44
1:C:187:ARG:HG3	1:C:187:ARG:NH1	2.30	0.44
1:E:260:MSE:HG2	1:E:278:ILE:HA	1.98	0.44
1:E:357:LEU:HD13	1:E:458:ARG:HH11	1.83	0.44
1:F:77:PHE:HD2	1:F:108:TYR:CD2	2.35	0.44
1:F:383:TRP:CE2	1:F:402:ILE:HD13	2.52	0.44
1:E:247:GLU:C	1:E:249:ALA:H	2.25	0.44
1:F:22:GLU:O	1:F:26:VAL:HG23	2.18	0.44
1:A:123:TYR:CG	1:A:124:PRO:HD3	2.52	0.44
1:B:266:ILE:CG2	1:B:267:THR:N	2.81	0.44
1:D:169:SER:HA	1:D:170:PRO:HD3	1.83	0.44
1:D:216:TRP:O	1:D:220:GLN:HG2	2.18	0.44
1:D:364:GLU:H	1:D:364:GLU:CD	2.26	0.44
1:E:200:PHE:CZ	1:E:464:ARG:HG3	2.53	0.44
1:E:216:TRP:CZ3	1:E:265:LEU:HD12	2.53	0.44
1:B:47:ARG:HA	1:B:51:LEU:HB2	1.99	0.44
1:C:53:VAL:HG13	1:C:117:SER:OG	2.18	0.44
1:C:63:GLY:HA3	1:C:80:ALA:HB2	1.99	0.44
1:F:253:LEU:HD21	1:F:257:LYS:CE	2.48	0.44
1:B:83:TYR:HA	1:B:169:SER:O	2.18	0.43
1:B:313:GLN:HB2	1:B:429:LYS:HZ3	1.83	0.43
1:E:381:ARG:O	1:E:381:ARG:HG3	2.17	0.43
1:F:357:LEU:HD13	1:F:458:ARG:HH11	1.83	0.43
1:A:134:LEU:N	1:A:134:LEU:HD12	2.33	0.43
1:F:187:ARG:HG3	1:F:187:ARG:NH1	2.32	0.43
1:F:190:THR:CG2	1:F:262:ALA:HB3	2.45	0.43
1:F:214:VAL:HG21	1:F:250:ILE:CG1	2.48	0.43
1:A:131:GLU:CD	1:A:131:GLU:N	2.74	0.43
1:A:357:LEU:HD13	1:A:458:ARG:HH11	1.83	0.43
1:B:53:VAL:HG13	1:B:117:SER:OG	2.18	0.43
1:B:63:GLY:HA3	1:B:80:ALA:HB2	2.00	0.43
1:C:136:ARG:CZ	1:D:444:PHE:CD2	3.00	0.43
1:C:428:ASP:HB2	1:C:434:GLU:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:47:ARG:HA	1:D:51:LEU:HB2	1.99	0.43
1:E:214:VAL:HG21	1:E:250:ILE:HG12	1.99	0.43
1:E:306:CYS:HB3	1:E:424:LEU:HD13	2.00	0.43
1:E:326:ARG:HG2	1:E:326:ARG:NH1	2.23	0.43
1:F:54:TYR:CD2	1:F:176:ALA:HB1	2.54	0.43
1:F:280:VAL:HA	1:F:405:GLU:OE2	2.18	0.43
1:A:72:ARG:NH1	1:A:103:LEU:HD22	2.33	0.43
1:A:275:LEU:C	1:A:275:LEU:HD23	2.43	0.43
1:A:442:ASN:O	1:A:443:ARG:C	2.62	0.43
1:B:473:ARG:CZ	1:C:371:ARG:HD3	2.49	0.43
1:C:381:ARG:HD2	2:C:510:HOH:O	2.17	0.43
1:D:322:HIS:CD2	1:E:474:LYS:HD3	2.53	0.43
1:F:453:LEU:O	1:F:457:ILE:HG13	2.18	0.43
1:A:330:VAL:HG13	1:A:331:LEU:HG	2.00	0.43
1:B:9:THR:HG23	1:B:12:GLN:NE2	2.33	0.43
1:B:326:ARG:HH11	1:B:326:ARG:CG	2.28	0.43
1:B:428:ASP:HB3	1:B:436:LYS:HB2	2.00	0.43
1:C:208:ARG:NH2	1:C:212:GLU:OE1	2.52	0.43
1:D:134:LEU:N	1:D:134:LEU:HD12	2.34	0.43
1:F:326:ARG:NH2	1:F:335:LEU:O	2.52	0.43
1:B:53:VAL:CG1	1:B:117:SER:H	2.32	0.43
1:E:57:LEU:HD21	1:E:101:LEU:HD21	1.98	0.43
1:A:201:VAL:HG12	1:A:202:LEU:N	2.33	0.43
1:A:280:VAL:HA	1:A:405:GLU:OE2	2.19	0.43
1:E:53:VAL:HG11	1:E:117:SER:N	2.34	0.43
1:E:136:ARG:CZ	1:F:444:PHE:CD2	3.02	0.43
1:E:356:LYS:HB3	1:E:362:PRO:CB	2.48	0.43
1:C:434:GLU:HG3	1:D:143:THR:HG21	2.00	0.43
1:E:146:PHE:HB3	1:E:147:PRO:CD	2.49	0.43
1:E:212:GLU:HG2	1:E:450:SER:HA	2.01	0.43
1:F:130:SER:O	1:F:131:GLU:C	2.62	0.43
1:F:208:ARG:NH2	1:F:212:GLU:OE1	2.52	0.43
1:A:443:ARG:HG2	1:A:444:PHE:CD1	2.53	0.43
1:E:226:SER:HA	1:E:227:PRO:HD3	1.92	0.43
1:A:211:ASP:HA	1:A:250:ILE:CD1	2.49	0.43
1:A:231:LEU:HA	1:A:264:HIS:O	2.19	0.43
1:B:248:GLU:HA	2:B:496:HOH:O	2.18	0.43
1:C:227:PRO:O	1:C:229:ILE:HG23	2.19	0.43
1:D:442:ASN:O	1:D:443:ARG:C	2.62	0.43
1:E:75:GLY:HA2	1:E:482:PRO:O	2.19	0.43
1:F:436:LYS:HG3	1:F:442:ASN:ND2	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:216:TRP:O	1:C:220:GLN:HG2	2.18	0.42
1:C:280:VAL:HA	1:C:405:GLU:OE2	2.19	0.42
1:D:247:GLU:C	1:D:249:ALA:H	2.26	0.42
1:D:473:ARG:CZ	1:E:371:ARG:HD3	2.49	0.42
1:E:28:LEU:O	1:E:32:ILE:HG13	2.19	0.42
1:E:296:ARG:N	1:E:297:PRO:HD3	2.34	0.42
1:F:102:THR:O	1:F:106:GLN:HG3	2.19	0.42
1:B:53:VAL:HG11	1:B:117:SER:O	2.19	0.42
1:B:326:ARG:HG2	1:B:326:ARG:NH1	2.26	0.42
1:B:364:GLU:C	1:B:366:VAL:H	2.27	0.42
1:B:411:ALA:O	1:B:414:TYR:HB3	2.19	0.42
1:C:61:TRP:CE3	1:C:63:GLY:HA2	2.54	0.42
1:F:247:GLU:C	1:F:249:ALA:H	2.26	0.42
1:C:252:ASP:OD1	1:D:253:LEU:HD13	2.19	0.42
1:A:361:ARG:HD2	1:A:361:ARG:O	2.18	0.42
1:B:322:HIS:HB2	2:B:519:HOH:O	2.18	0.42
1:D:102:THR:O	1:D:106:GLN:HG3	2.20	0.42
1:D:237:ASN:ND2	1:D:248:GLU:CB	2.82	0.42
1:F:53:VAL:HG11	1:F:117:SER:N	2.34	0.42
1:A:8:LEU:HB3	1:A:112:ILE:O	2.20	0.42
1:B:453:LEU:O	1:B:457:ILE:HG13	2.20	0.42
1:D:77:PHE:HD2	1:D:108:TYR:CD2	2.38	0.42
1:E:8:LEU:HD11	1:E:12:GLN:HB3	2.02	0.42
1:E:356:LYS:CG	1:E:366:VAL:HG11	2.48	0.42
1:F:132:LEU:HB3	1:F:134:LEU:CD1	2.45	0.42
1:F:192:THR:HG23	1:F:193:PRO:CD	2.50	0.42
1:A:53:VAL:CG1	1:A:117:SER:H	2.32	0.42
1:B:87:ILE:HG22	1:B:88:THR:N	2.34	0.42
1:B:228:TYR:CD1	1:B:265:LEU:HD13	2.54	0.42
1:D:61:TRP:CE3	1:D:63:GLY:HA2	2.55	0.42
1:F:212:GLU:HG2	1:F:450:SER:HA	2.02	0.42
1:A:329:HIS:HD2	1:A:379:ASP:OD2	2.02	0.42
1:B:190:THR:HG22	1:B:192:THR:H	1.83	0.42
1:D:474:LYS:HD3	1:E:322:HIS:CD2	2.54	0.42
1:A:56:SER:HB2	1:A:117:SER:HB3	2.01	0.42
1:A:437:LEU:CD1	1:A:440:GLN:HG3	2.49	0.42
1:B:53:VAL:HG11	1:B:117:SER:N	2.35	0.42
1:C:259:GLN:C	1:C:260:MSE:HG3	2.45	0.42
1:F:336:PRO:HA	1:F:337:PRO:HD3	1.84	0.42
1:A:74:PHE:CD2	1:A:484:ARG:HD3	2.55	0.42
1:B:68:PRO:HA	1:B:69:PRO:HD3	1.96	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:102:THR:O	1:C:106:GLN:HG3	2.20	0.42
1:C:381:ARG:HH21	1:D:284:ASN:ND2	2.18	0.42
1:E:192:THR:HG23	1:E:193:PRO:HD2	2.02	0.42
1:F:198:GLN:HA	1:F:199:PRO:HD3	1.91	0.42
1:A:207:THR:CG2	1:A:208:ARG:N	2.82	0.42
1:B:369:ARG:HG2	1:B:369:ARG:HH11	1.84	0.42
1:B:414:TYR:HA	1:B:475:LEU:HD22	2.02	0.42
1:C:127:ILE:CG2	1:C:129:GLY:O	2.64	0.42
1:C:291:HIS:O	1:C:294:VAL:HG22	2.19	0.42
1:C:381:ARG:HH12	1:D:259:GLN:CD	2.25	0.42
1:C:427:SER:O	1:C:428:ASP:HB3	2.20	0.42
1:E:465:ALA:O	1:E:467:GLY:N	2.53	0.42
1:F:25:VAL:HG23	1:F:126:VAL:HB	2.02	0.42
1:A:356:LYS:O	1:A:362:PRO:HG3	2.20	0.41
1:D:469:ARG:HG2	1:D:469:ARG:NH1	2.35	0.41
1:E:259:GLN:C	1:E:260:MSE:HG3	2.45	0.41
1:A:200:PHE:CZ	1:A:464:ARG:HG3	2.55	0.41
1:A:256:LYS:HD2	1:B:255:TRP:CZ3	2.55	0.41
1:B:299:VAL:HG22	1:B:301:LEU:HD13	2.02	0.41
1:C:192:THR:HA	1:C:193:PRO:HD3	1.90	0.41
1:C:206:TYR:HB3	1:C:209:TYR:CD2	2.55	0.41
1:C:356:LYS:O	1:C:360:GLY:N	2.51	0.41
1:F:361:ARG:HD3	1:F:361:ARG:N	2.36	0.41
1:A:76:ARG:HB3	1:A:76:ARG:NH1	2.34	0.41
1:B:237:ASN:HD21	1:B:248:GLU:CB	2.33	0.41
1:C:204:THR:HG21	1:C:209:TYR:HB3	2.01	0.41
1:C:299:VAL:HG22	1:C:300:TRP:N	2.34	0.41
1:C:451:GLU:O	1:C:455:ILE:HG13	2.19	0.41
1:D:223:ASP:OD2	1:D:223:ASP:C	2.63	0.41
1:F:328:ASP:OD1	1:F:328:ASP:N	2.54	0.41
1:A:87:ILE:HG22	1:A:88:THR:N	2.36	0.41
1:A:478:PHE:H	1:F:395:ASN:ND2	2.18	0.41
1:C:206:TYR:HB3	1:C:209:TYR:HD2	1.84	0.41
1:C:431:LEU:HD12	1:D:151:LEU:HD22	2.01	0.41
1:C:465:ALA:O	1:C:467:GLY:N	2.53	0.41
1:D:96:TYR:OH	1:D:483:PHE:HB3	2.20	0.41
1:D:179:VAL:O	1:D:183:LEU:HG	2.20	0.41
1:B:211:ASP:HA	1:B:250:ILE:CD1	2.50	0.41
1:B:310:ARG:O	1:B:429:LYS:NZ	2.41	0.41
1:C:8:LEU:HD11	1:C:12:GLN:HB3	2.02	0.41
1:C:14:LEU:HD13	1:C:94:ARG:HD3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:92:LEU:HD13	1:C:195:GLU:HG3	2.03	0.41
1:C:228:TYR:CD1	1:C:265:LEU:HD13	2.54	0.41
1:D:261:PRO:HB2	1:D:263:TRP:CZ3	2.55	0.41
1:E:56:SER:HB2	1:E:117:SER:HB3	2.01	0.41
1:E:481:PRO:HA	1:E:482:PRO:HD3	1.92	0.41
1:F:206:TYR:HE2	1:F:449:ILE:HD11	1.85	0.41
1:F:292:LEU:HD12	1:F:292:LEU:HA	1.91	0.41
1:F:314:ALA:O	1:F:315:ILE:C	2.63	0.41
1:A:199:PRO:HB3	1:A:298:ASP:OD2	2.20	0.41
1:C:72:ARG:HH12	1:C:103:LEU:HD22	1.85	0.41
1:C:212:GLU:HG2	1:C:450:SER:HA	2.02	0.41
1:D:70:LYS:HE2	2:D:496:HOH:O	2.20	0.41
1:D:330:VAL:HG13	1:D:331:LEU:HG	2.01	0.41
1:D:381:ARG:O	1:D:381:ARG:HG3	2.19	0.41
1:D:451:GLU:O	1:D:455:ILE:HG13	2.21	0.41
1:E:211:ASP:HA	1:E:250:ILE:CD1	2.51	0.41
1:F:313:GLN:O	1:F:429:LYS:HE2	2.21	0.41
1:A:214:VAL:HB	1:A:250:ILE:HD11	2.02	0.41
1:B:306:CYS:HB3	1:B:424:LEU:HD13	2.01	0.41
1:B:469:ARG:HG2	1:B:469:ARG:NH1	2.36	0.41
1:C:469:ARG:HG2	1:C:469:ARG:NH1	2.36	0.41
1:D:359:SER:HA	1:D:451:GLU:OE1	2.21	0.41
1:E:237:ASN:HD21	1:E:248:GLU:CB	2.33	0.41
1:F:216:TRP:HZ3	1:F:265:LEU:HD12	1.86	0.41
1:A:212:GLU:HG2	1:A:450:SER:HA	2.02	0.41
1:A:260:MSE:HG2	1:A:278:ILE:HA	2.01	0.41
1:A:265:LEU:HD23	1:A:265:LEU:HA	1.84	0.41
1:B:14:LEU:HD13	1:B:94:ARG:HD3	2.02	0.41
1:D:177:ARG:NH1	1:D:177:ARG:HG3	2.36	0.41
1:D:187:ARG:HG3	1:D:187:ARG:NH1	2.35	0.41
1:F:253:LEU:HD21	1:F:257:LYS:HE3	2.01	0.41
1:A:281:GLY:HA2	1:A:282:PRO:HD3	1.96	0.41
1:B:192:THR:HG23	1:B:193:PRO:CD	2.51	0.41
1:C:313:GLN:HB2	1:C:429:LYS:NZ	2.35	0.41
1:D:53:VAL:HG13	1:D:117:SER:OG	2.21	0.41
1:D:123:TYR:CD2	1:D:124:PRO:HD3	2.56	0.41
1:D:437:LEU:HD22	1:D:440:GLN:OE1	2.20	0.41
1:E:68:PRO:HA	1:E:69:PRO:HD3	1.99	0.41
1:E:134:LEU:N	1:E:134:LEU:CD1	2.84	0.41
1:E:237:ASN:ND2	1:E:248:GLU:CB	2.84	0.41
1:F:123:TYR:O	1:F:126:VAL:HG22	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:412:GLN:OE1	1:F:412:GLN:HA	2.20	0.41
1:A:247:GLU:C	1:A:249:ALA:H	2.28	0.41
1:A:398:ARG:HD3	1:F:477:THR:HG22	2.03	0.41
1:A:440:GLN:NE2	1:B:131:GLU:OE2	2.51	0.41
1:B:134:LEU:N	1:B:134:LEU:HD12	2.36	0.41
1:B:481:PRO:HA	1:B:482:PRO:HD3	1.90	0.41
1:E:32:ILE:O	1:E:36:ILE:HG13	2.20	0.41
1:E:47:ARG:HA	1:E:51:LEU:HB2	2.03	0.41
1:E:336:PRO:HA	1:E:337:PRO:HD3	1.87	0.41
1:F:201:VAL:HG12	1:F:202:LEU:N	2.35	0.41
1:B:190:THR:HG22	1:B:192:THR:CB	2.44	0.40
1:B:192:THR:HA	1:B:193:PRO:HD3	1.92	0.40
1:B:423:LEU:CD2	1:B:455:ILE:HG21	2.51	0.40
1:C:284:ASN:ND2	1:D:381:ARG:HH21	2.19	0.40
1:D:54:TYR:CD2	1:D:176:ALA:HB1	2.57	0.40
1:D:63:GLY:HA3	1:D:80:ALA:HB2	2.03	0.40
1:D:192:THR:HA	1:D:193:PRO:HD3	1.93	0.40
1:E:207:THR:CG2	1:E:208:ARG:N	2.83	0.40
1:E:442:ASN:O	1:E:443:ARG:C	2.64	0.40
1:F:186:LEU:HD23	1:F:186:LEU:HA	1.85	0.40
1:F:207:THR:CG2	1:F:208:ARG:N	2.82	0.40
1:A:414:TYR:HA	1:A:475:LEU:HD22	2.04	0.40
1:A:429:LYS:HA	1:A:430:PRO:HD3	1.88	0.40
1:B:28:LEU:HD13	1:B:126:VAL:CG2	2.49	0.40
1:B:187:ARG:HG3	1:B:187:ARG:NH1	2.36	0.40
1:D:72:ARG:HH12	1:D:103:LEU:HD22	1.83	0.40
1:E:53:VAL:CG1	1:E:117:SER:H	2.35	0.40
1:E:412:GLN:HA	1:E:412:GLN:OE1	2.21	0.40
1:A:102:THR:O	1:A:106:GLN:HG3	2.21	0.40
1:B:322:HIS:CD2	1:C:474:LYS:HD3	2.57	0.40
1:D:131:GLU:CD	1:D:131:GLU:N	2.79	0.40
1:F:61:TRP:CE3	1:F:63:GLY:HA2	2.56	0.40
1:A:9:THR:HG23	1:A:12:GLN:NE2	2.37	0.40
1:A:75:GLY:HA2	1:A:482:PRO:O	2.21	0.40
1:D:204:THR:HG21	1:D:209:TYR:HB3	2.04	0.40
1:D:265:LEU:O	1:D:272:GLY:HA3	2.21	0.40
1:A:56:SER:HB3	1:A:115:GLN:O	2.21	0.40
1:B:77:PHE:CE2	1:B:104:LEU:HD22	2.56	0.40
1:C:68:PRO:HA	1:C:69:PRO:HD3	1.97	0.40
1:C:237:ASN:HD21	1:C:248:GLU:CB	2.32	0.40
1:F:53:VAL:CG1	1:F:117:SER:H	2.34	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	457/484 (94%)	408 (89%)	43 (9%)	6 (1%)	9	31
1	B	457/484 (94%)	413 (90%)	38 (8%)	6 (1%)	9	31
1	C	457/484 (94%)	410 (90%)	43 (9%)	4 (1%)	14	41
1	D	457/484 (94%)	409 (90%)	39 (8%)	9 (2%)	6	21
1	E	457/484 (94%)	414 (91%)	38 (8%)	5 (1%)	11	36
1	F	457/484 (94%)	409 (90%)	37 (8%)	11 (2%)	4	17
All	All	2742/2904 (94%)	2463 (90%)	238 (9%)	41 (2%)	8	28

All (41) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	362	PRO
1	C	130	SER
1	D	129	GLY
1	F	129	GLY
1	B	129	GLY
1	A	134	LEU
1	B	365	GLU
1	C	466	GLU
1	D	10	PRO
1	D	134	LEU
1	D	329	HIS
1	D	406	SER
1	E	362	PRO
1	E	466	GLU
1	F	330	VAL
1	F	361	ARG
1	F	441	ALA

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Mol	Chain	Res	Type
1	A	10	PRO
1	A	107	ASP
1	A	443	ARG
1	B	10	PRO
1	C	10	PRO
1	D	362	PRO
1	E	10	PRO
1	E	406	SER
1	F	443	ARG
1	A	330	VAL
1	B	361	ARG
1	B	406	SER
1	C	406	SER
1	D	466	GLU
1	F	10	PRO
1	F	107	ASP
1	F	134	LEU
1	F	362	PRO
1	F	406	SER
1	F	466	GLU
1	B	466	GLU
1	D	107	ASP
1	D	438	PRO
1	E	330	VAL

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	390/403 (97%)	363 (93%)	27 (7%)	14	41
1	B	390/403 (97%)	363 (93%)	27 (7%)	14	41
1	C	390/403 (97%)	365 (94%)	25 (6%)	16	44
1	D	390/403 (97%)	363 (93%)	27 (7%)	14	41
1	E	390/403 (97%)	364 (93%)	26 (7%)	15	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	390/403 (97%)	366 (94%)	24 (6%)	16	45
All	All	2340/2418 (97%)	2184 (93%)	156 (7%)	15	42

All (156) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	VAL
1	A	28	LEU
1	A	51	LEU
1	A	89	ARG
1	A	128	ASP
1	A	148	THR
1	A	175	ASP
1	A	177	ARG
1	A	190	THR
1	A	202	LEU
1	A	207	THR
1	A	210	VAL
1	A	219	SER
1	A	222	LEU
1	A	265	LEU
1	A	280	VAL
1	A	301	LEU
1	A	311	GLU
1	A	322	HIS
1	A	330	VAL
1	A	351	LEU
1	A	361	ARG
1	A	381	ARG
1	A	403	ASP
1	A	431	LEU
1	A	437	LEU
1	A	443	ARG
1	B	25	VAL
1	B	28	LEU
1	B	30	ASN
1	B	51	LEU
1	B	89	ARG
1	B	128	ASP
1	B	148	THR
1	B	190	THR
1	B	202	LEU

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Mol	Chain	Res	Type
1	B	207	THR
1	B	210	VAL
1	B	222	LEU
1	B	265	LEU
1	B	280	VAL
1	B	294	VAL
1	B	301	LEU
1	B	311	GLU
1	B	322	HIS
1	B	330	VAL
1	B	351	LEU
1	B	361	ARG
1	B	365	GLU
1	B	381	ARG
1	B	400	VAL
1	B	403	ASP
1	B	431	LEU
1	B	443	ARG
1	C	25	VAL
1	C	28	LEU
1	C	51	LEU
1	C	89	ARG
1	C	128	ASP
1	C	131	GLU
1	C	133	THR
1	C	149	THR
1	C	150	GLU
1	C	190	THR
1	C	202	LEU
1	C	207	THR
1	C	210	VAL
1	C	222	LEU
1	C	265	LEU
1	C	280	VAL
1	C	301	LEU
1	C	322	HIS
1	C	330	VAL
1	C	351	LEU
1	C	381	ARG
1	C	400	VAL
1	C	403	ASP
1	C	431	LEU

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Mol	Chain	Res	Type
1	C	443	ARG
1	D	25	VAL
1	D	28	LEU
1	D	51	LEU
1	D	89	ARG
1	D	128	ASP
1	D	133	THR
1	D	134	LEU
1	D	149	THR
1	D	151	LEU
1	D	168	PHE
1	D	177	ARG
1	D	190	THR
1	D	202	LEU
1	D	207	THR
1	D	210	VAL
1	D	222	LEU
1	D	265	LEU
1	D	280	VAL
1	D	301	LEU
1	D	311	GLU
1	D	322	HIS
1	D	330	VAL
1	D	351	LEU
1	D	381	ARG
1	D	400	VAL
1	D	403	ASP
1	D	431	LEU
1	E	25	VAL
1	E	28	LEU
1	E	30	ASN
1	E	51	LEU
1	E	89	ARG
1	E	128	ASP
1	E	151	LEU
1	E	175	ASP
1	E	177	ARG
1	E	190	THR
1	E	202	LEU
1	E	207	THR
1	E	210	VAL
1	E	222	LEU

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Mol	Chain	Res	Type
1	E	265	LEU
1	E	301	LEU
1	E	322	HIS
1	E	326	ARG
1	E	330	VAL
1	E	351	LEU
1	E	364	GLU
1	E	381	ARG
1	E	400	VAL
1	E	403	ASP
1	E	431	LEU
1	E	443	ARG
1	F	25	VAL
1	F	28	LEU
1	F	51	LEU
1	F	89	ARG
1	F	128	ASP
1	F	133	THR
1	F	150	GLU
1	F	151	LEU
1	F	190	THR
1	F	202	LEU
1	F	207	THR
1	F	210	VAL
1	F	222	LEU
1	F	265	LEU
1	F	301	LEU
1	F	322	HIS
1	F	326	ARG
1	F	330	VAL
1	F	351	LEU
1	F	361	ARG
1	F	381	ARG
1	F	400	VAL
1	F	403	ASP
1	F	431	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (63) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	173	HIS

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Mol	Chain	Res	Type
1	A	188	HIS
1	A	237	ASN
1	A	284	ASN
1	A	313	GLN
1	A	329	HIS
1	A	348	GLN
1	A	395	ASN
1	A	440	GLN
1	B	12	GLN
1	B	173	HIS
1	B	237	ASN
1	B	277	ASN
1	B	284	ASN
1	B	313	GLN
1	B	322	HIS
1	B	329	HIS
1	B	368	GLN
1	B	395	ASN
1	B	442	ASN
1	C	12	GLN
1	C	173	HIS
1	C	188	HIS
1	C	237	ASN
1	C	284	ASN
1	C	313	GLN
1	C	322	HIS
1	C	329	HIS
1	C	348	GLN
1	C	395	ASN
1	C	440	GLN
1	D	12	GLN
1	D	173	HIS
1	D	188	HIS
1	D	237	ASN
1	D	284	ASN
1	D	305	HIS
1	D	313	GLN
1	D	322	HIS
1	D	329	HIS
1	D	395	ASN
1	E	12	GLN
1	E	173	HIS

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Mol	Chain	Res	Type
1	E	237	ASN
1	E	284	ASN
1	E	305	HIS
1	E	313	GLN
1	E	329	HIS
1	E	348	GLN
1	E	395	ASN
1	F	12	GLN
1	F	188	HIS
1	F	220	GLN
1	F	237	ASN
1	F	284	ASN
1	F	305	HIS
1	F	313	GLN
1	F	322	HIS
1	F	329	HIS
1	F	348	GLN
1	F	368	GLN
1	F	395	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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.