



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 06:14 AM UTC

PDB ID : 7WU7 / pdb_00007wu7
EMDB ID : EMD-32823
Title : Prefoldin-tubulin-TRiC complex
Authors : Gestaut, D.; Zhao, Y.; Park, J.; Ma, B.; Leitner, A.; Collier, M.; Pintilie, G.; Roh, S.-H.; Chiu, W.; Frydman, J.
Deposited on : 2022-02-07
Resolution : 3.85 Å(reported)
Based on initial model : 6NR8

This is a Full wwPDB EM 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/EMValidationReportHelp>
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:

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

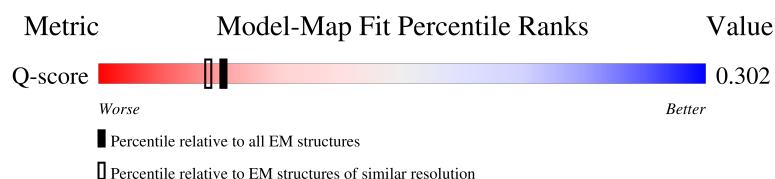
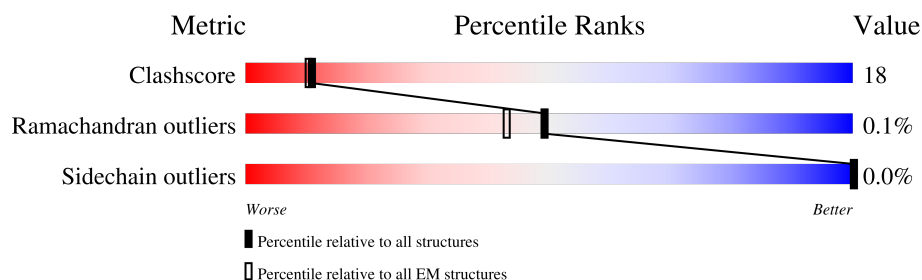
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.85 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)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	8989 (3.35 - 4.35)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1	122	19% 50% 38% 12%
2	2	154	19% 32% 21% 46%
3	3	197	7% 38% 21% 41%
4	4	140	13% 34% 29% 37%

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Mol	Chain	Length	Quality of chain
5	5	140	
6	6	129	
7	A	556	
7	I	556	
8	B	535	
8	J	535	
9	C	545	
9	K	545	
10	D	539	
10	L	539	
11	E	541	
11	M	541	
12	F	531	
12	N	531	
13	G	543	
13	O	543	
14	H	547	
14	P	547	

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 67031 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Prefoldin subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	107	Total	C	N	O	S	0	0
			873	546	150	172	5		

- Molecule 2 is a protein called Prefoldin subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	83	Total	C	N	O	S	0	0
			667	413	121	130	3		

- Molecule 3 is a protein called Prefoldin subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	116	Total	C	N	O	S	0	0
			956	607	157	186	6		

- Molecule 4 is a protein called Prefoldin subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	88	Total	C	N	O	S	0	0
			711	437	118	151	5		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4	135	HIS	-	expression tag	UNP Q9NQP4
4	136	HIS	-	expression tag	UNP Q9NQP4
4	137	HIS	-	expression tag	UNP Q9NQP4
4	138	HIS	-	expression tag	UNP Q9NQP4
4	139	HIS	-	expression tag	UNP Q9NQP4
4	140	HIS	-	expression tag	UNP Q9NQP4

- Molecule 5 is a protein called Prefoldin subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	5	127	Total	C	N	O	S	0	0
			1017	647	166	196	8		

- Molecule 6 is a protein called Prefoldin subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6	102	Total	C	N	O	S	0	0
			825	511	148	165	1		

- Molecule 7 is a protein called T-complex protein 1 subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A	516	Total	C	N	O	S	0	0
			3919	2456	685	755	23		
7	I	514	Total	C	N	O	S	0	0
			3903	2444	683	753	23		

- Molecule 8 is a protein called T-complex protein 1 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	B	497	Total	C	N	O	S	0	0
			3736	2339	655	723	19		
8	J	497	Total	C	N	O	S	0	0
			3736	2339	655	723	19		

- Molecule 9 is a protein called T-complex protein 1 subunit gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	C	505	Total	C	N	O	S	0	0
			3924	2448	690	756	30		
9	K	505	Total	C	N	O	S	0	0
			3924	2448	690	756	30		

- Molecule 10 is a protein called T-complex protein 1 subunit delta.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	D	511	Total	C	N	O	S	0	0
			3847	2409	665	750	23		
10	L	511	Total	C	N	O	S	0	0
			3847	2407	666	751	23		

- Molecule 11 is a protein called T-complex protein 1 subunit epsilon.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	E	506	Total	C	N	O	S	0	0
			3883	2431	673	749	30		
11	M	506	Total	C	N	O	S	0	0
			3883	2431	673	749	30		

- Molecule 12 is a protein called T-complex protein 1 subunit zeta.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	F	508	Total	C	N	O	S	0	0
			3903	2454	681	748	20		
12	N	508	Total	C	N	O	S	0	0
			3903	2454	681	748	20		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	528	PHE	SER	conflict	UNP P40227
N	528	PHE	SER	conflict	UNP P40227

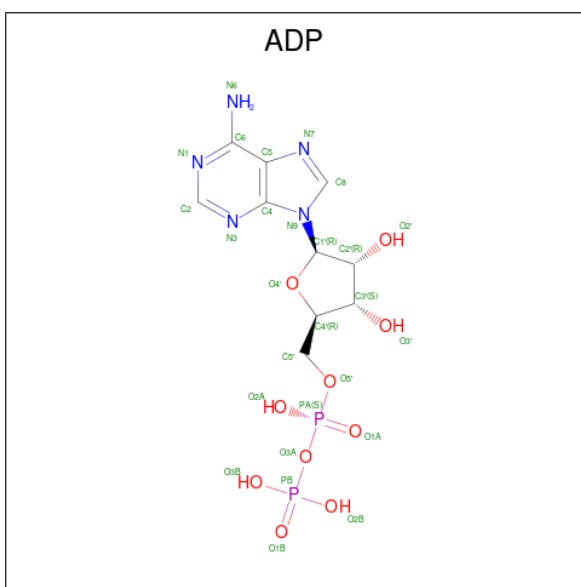
- Molecule 13 is a protein called T-complex protein 1 subunit eta.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	G	509	Total	C	N	O	S	0	0
			3910	2471	676	740	23		
13	O	509	Total	C	N	O	S	0	0
			3910	2471	676	740	23		

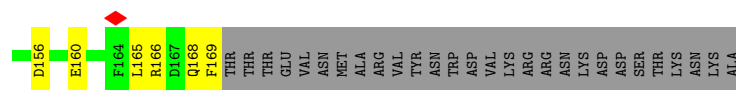
- Molecule 14 is a protein called T-complex protein 1 subunit theta.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	H	500	Total	C	N	O	S	0	0
			3816	2404	647	739	26		
14	P	502	Total	C	N	O	S	0	0
			3830	2413	650	741	26		

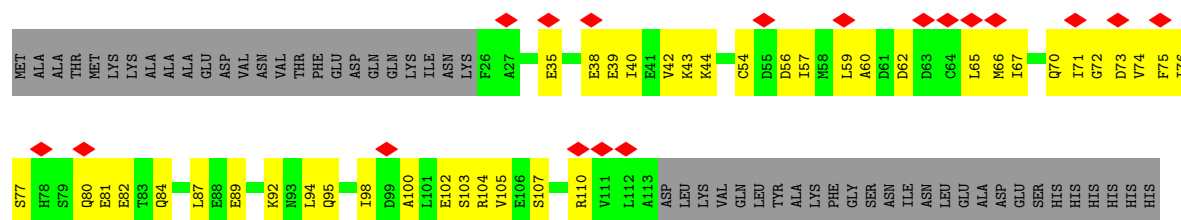
- Molecule 15 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).



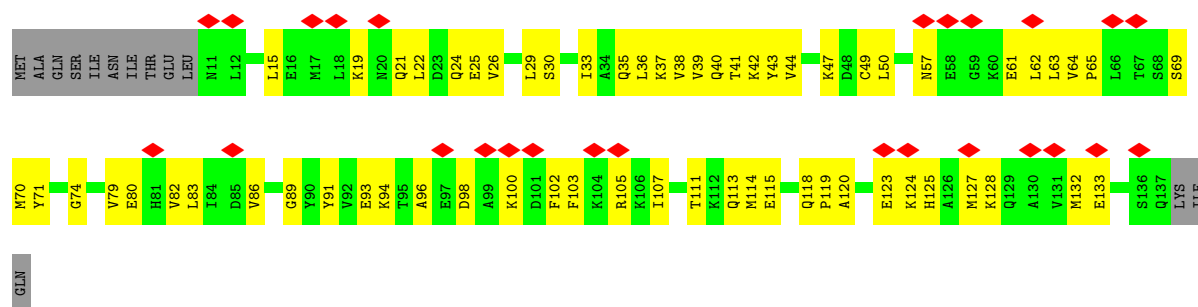
Mol	Chain	Residues	Atoms					AltConf
15	F	1	Total 27	C 10	N 5	O 10	P 2	0
15	H	1	Total 27	C 10	N 5	O 10	P 2	0
15	N	1	Total 27	C 10	N 5	O 10	P 2	0
15	P	1	Total 27	C 10	N 5	O 10	P 2	0



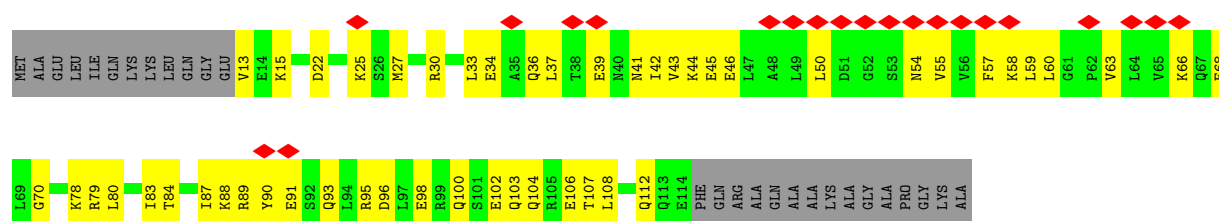
- Molecule 4: Prefoldin subunit 4



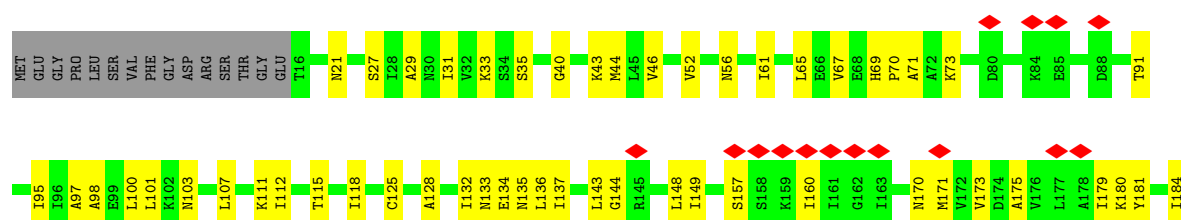
- Molecule 5: Prefoldin subunit 5

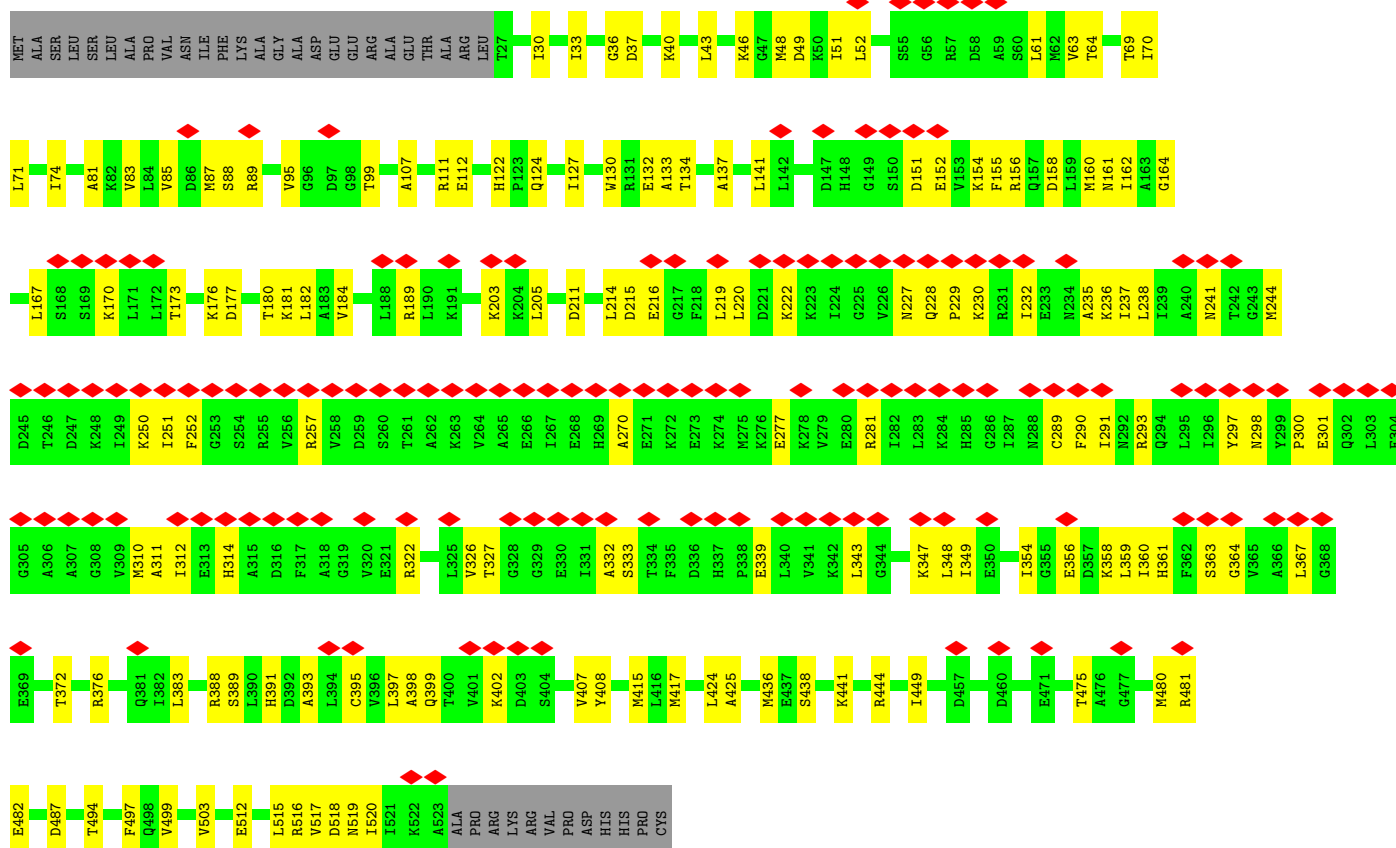


- Molecule 6: Prefoldin subunit 6

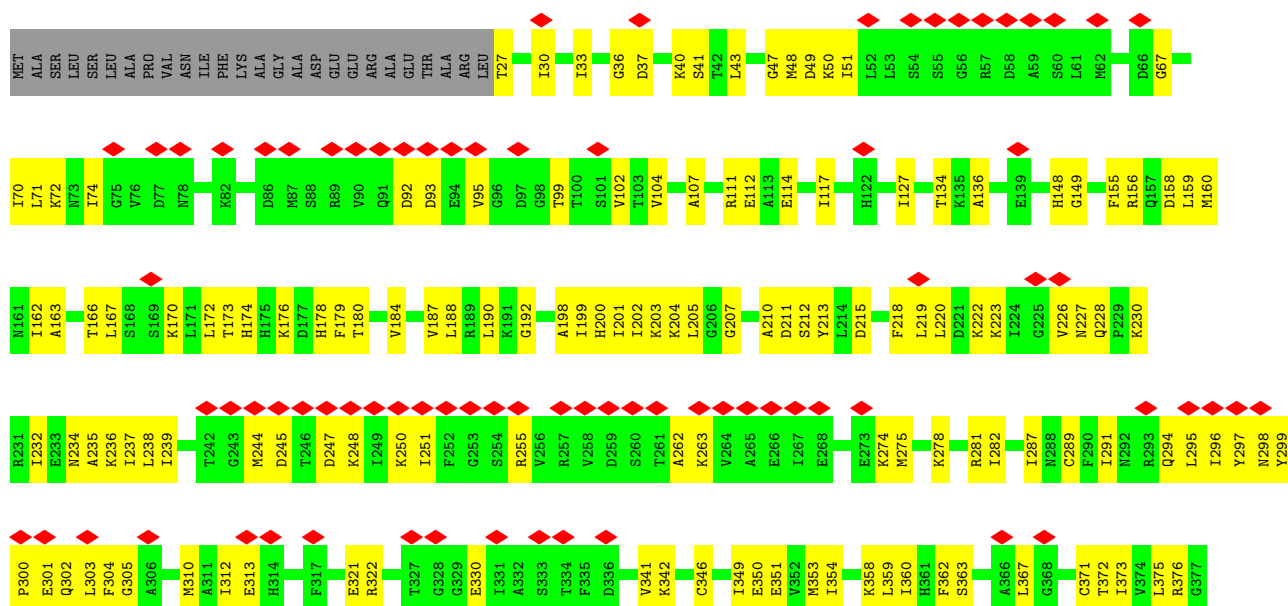


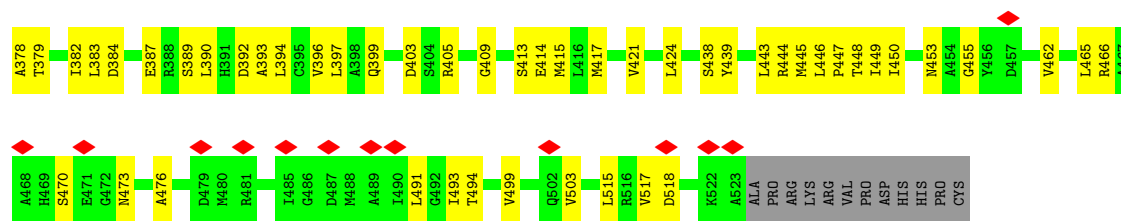
- Molecule 7: T-complex protein 1 subunit alpha



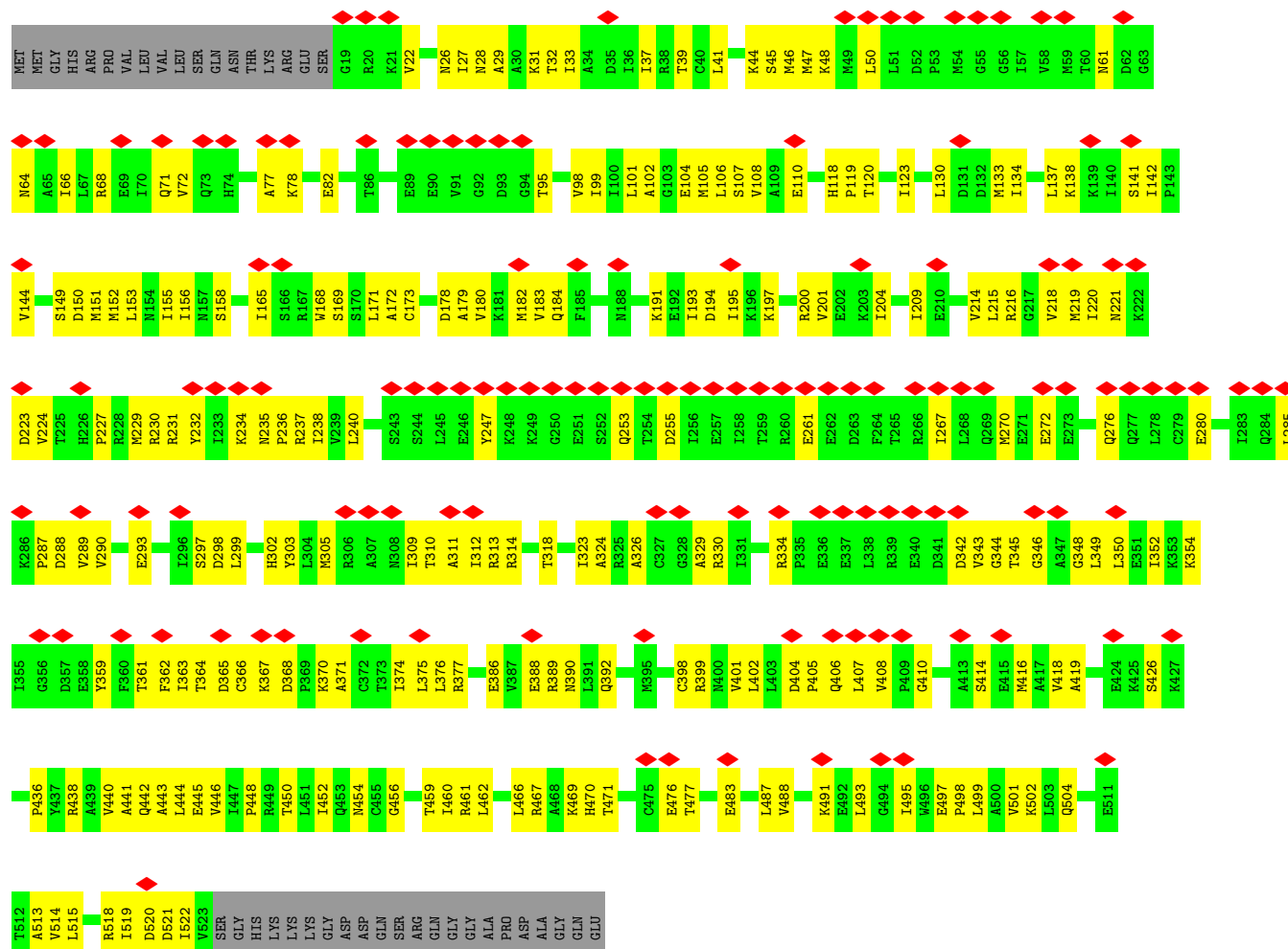


• Molecule 8: T-complex protein 1 subunit beta



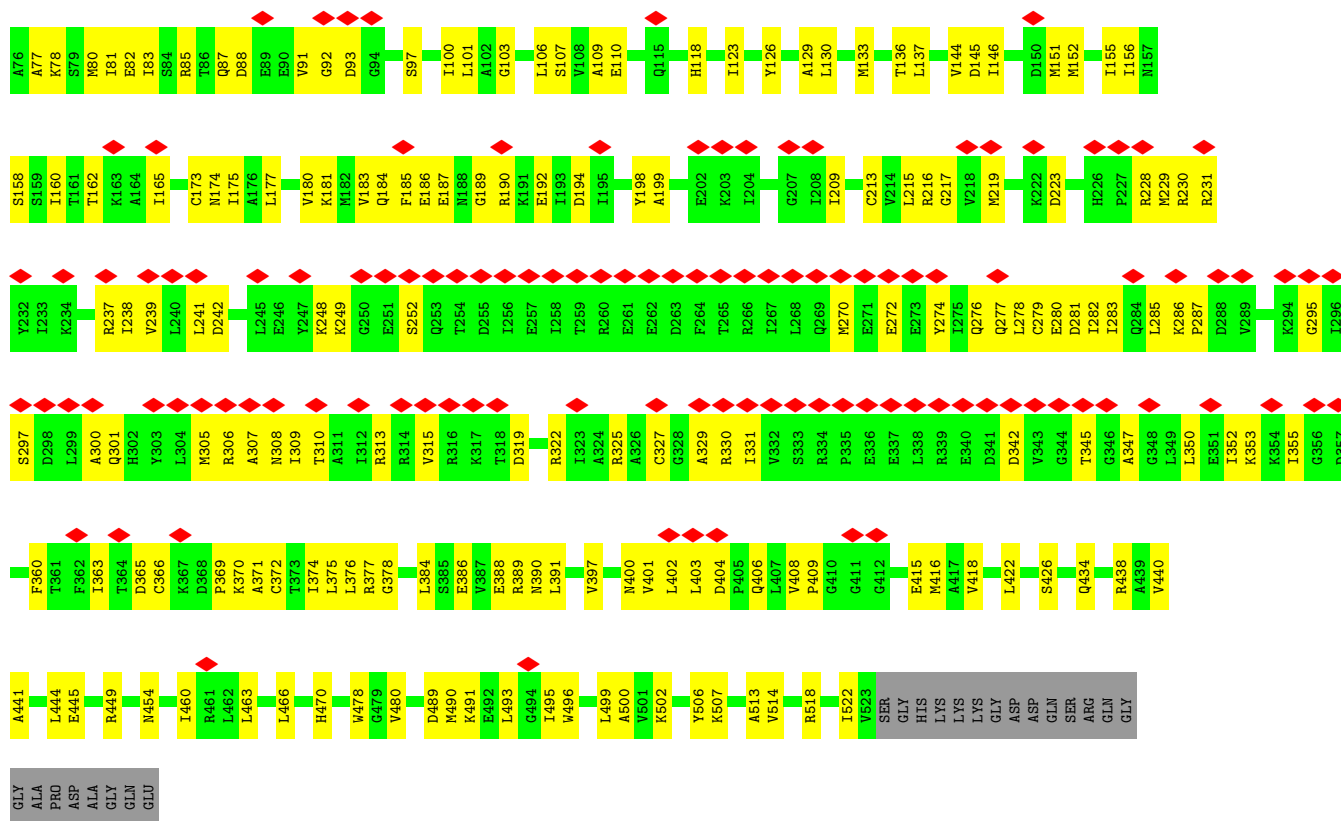


• Molecule 9: T-complex protein 1 subunit gamma

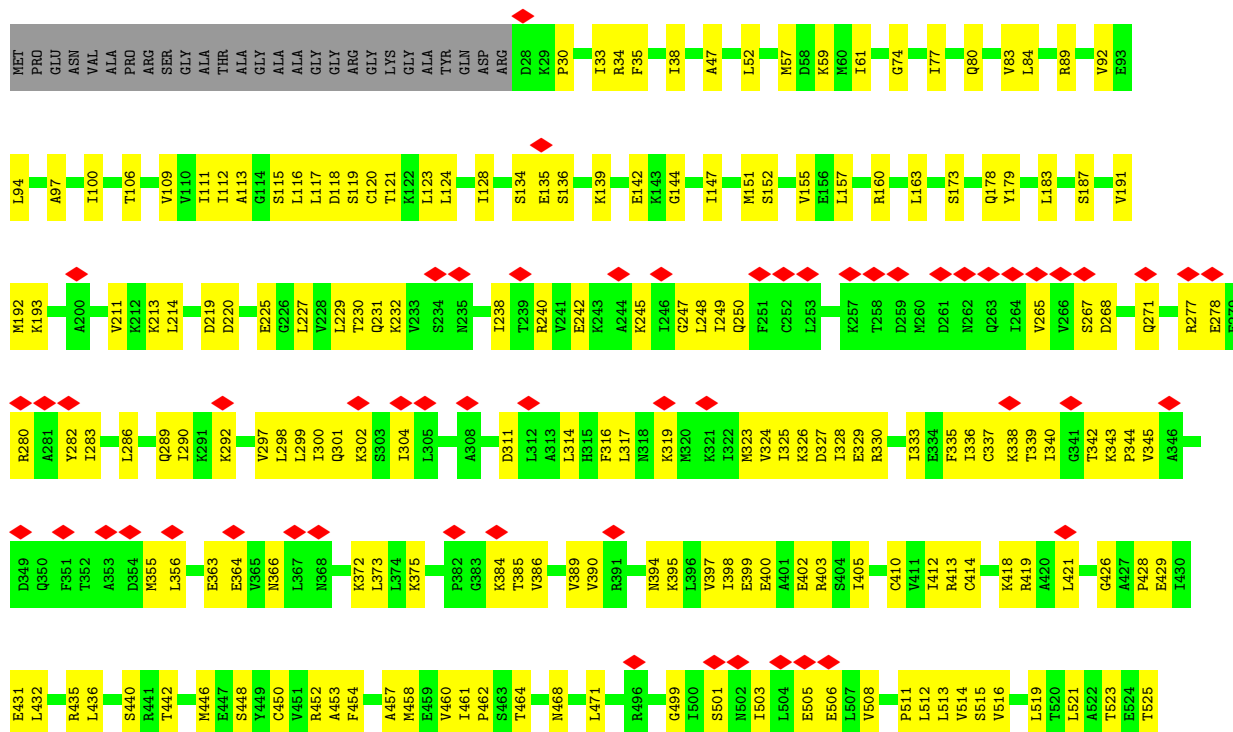


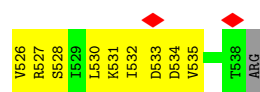
• Molecule 9: T-complex protein 1 subunit gamma



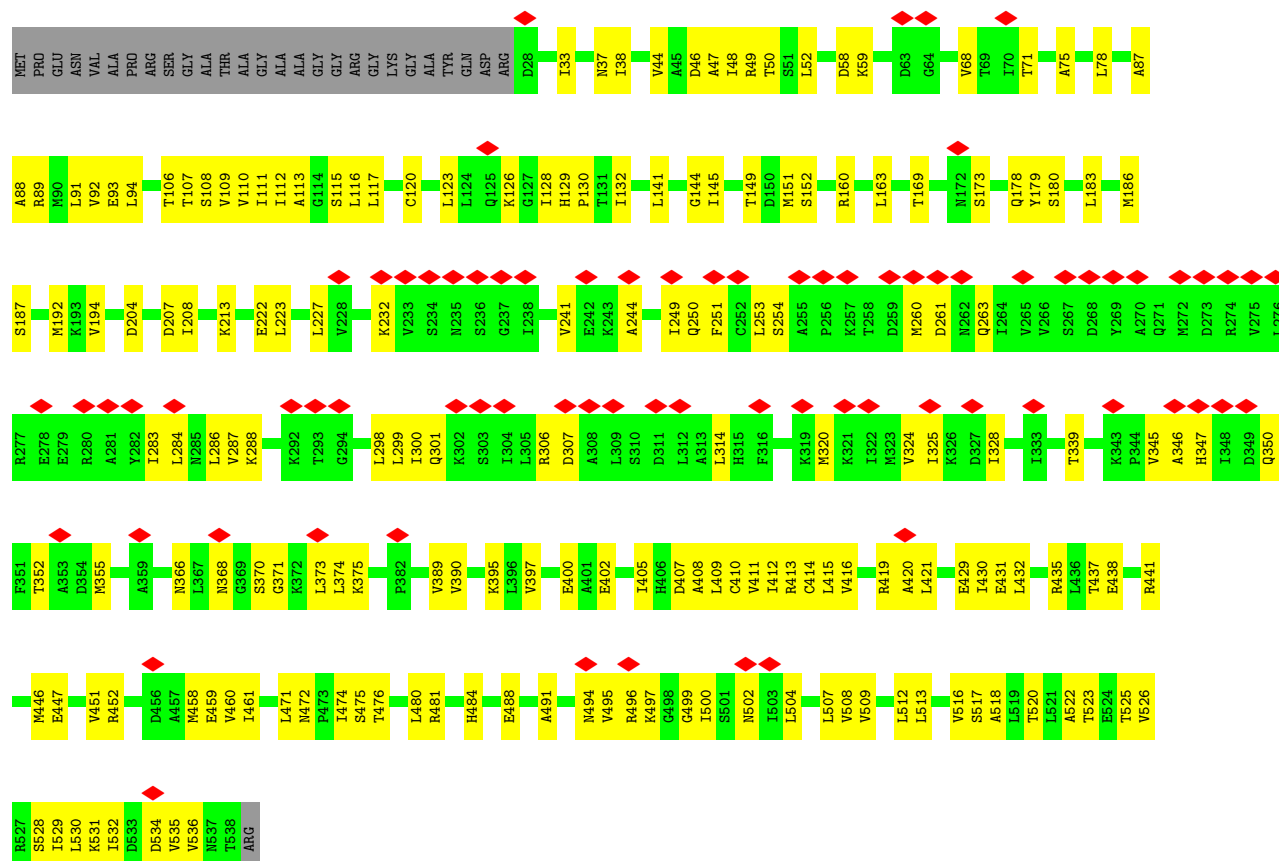


• Molecule 10: T-complex protein 1 subunit delta

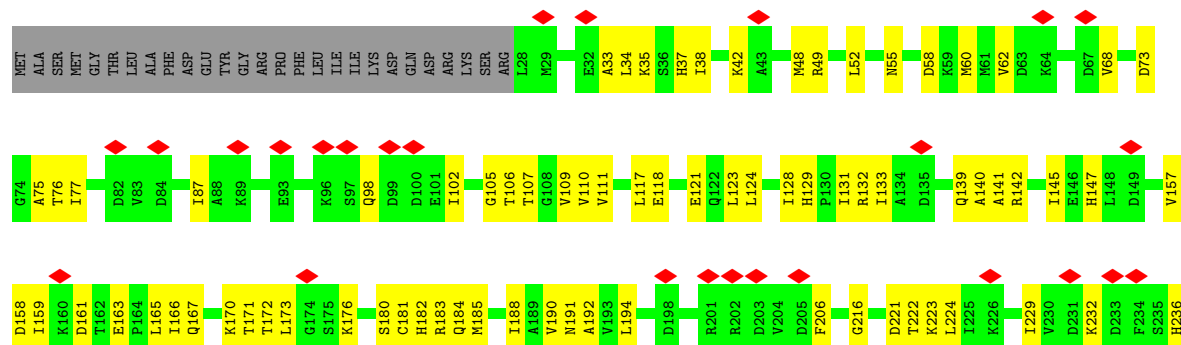


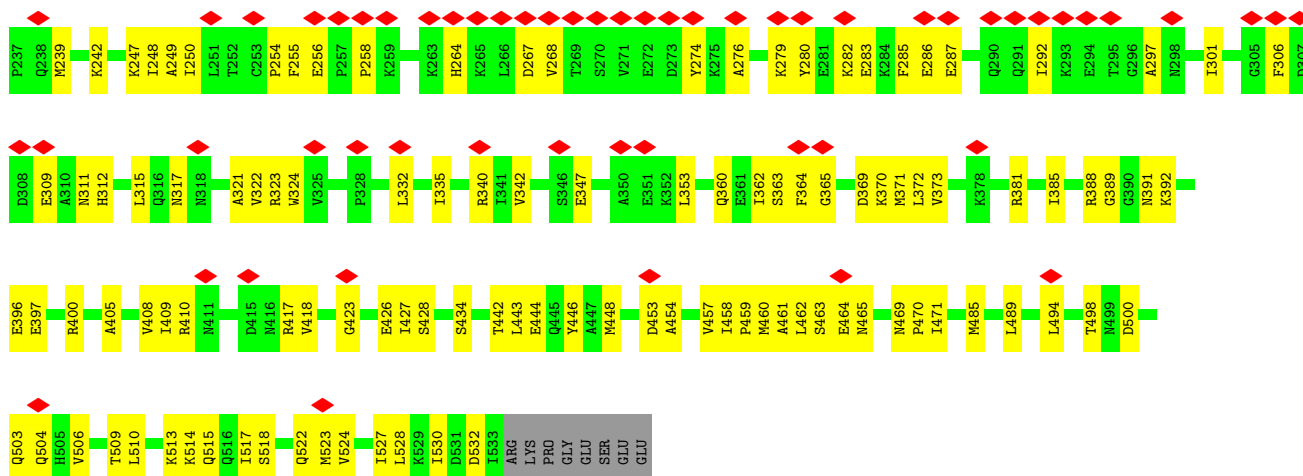


• Molecule 10: T-complex protein 1 subunit delta

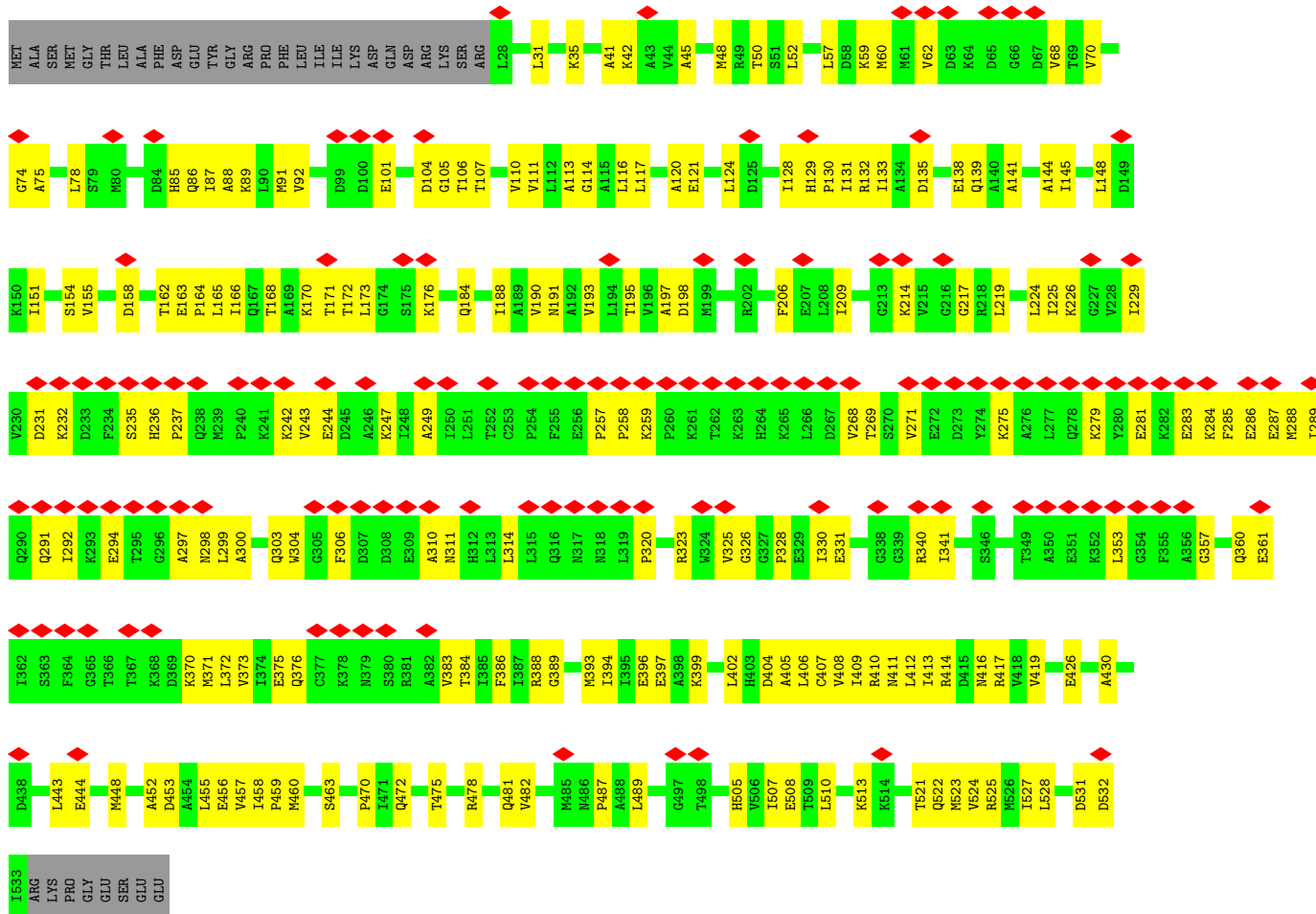


• Molecule 11: T-complex protein 1 subunit epsilon



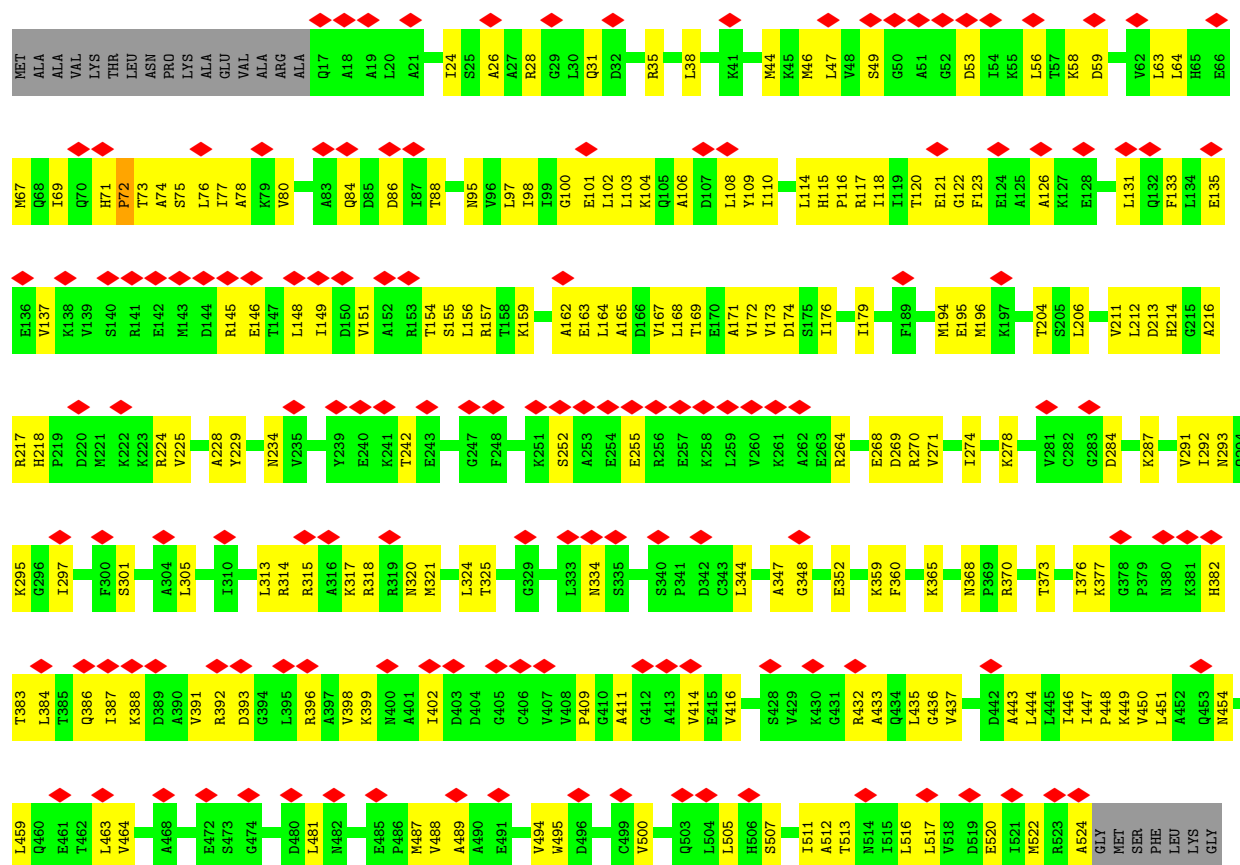


• Molecule 11: T-complex protein 1 subunit epsilon

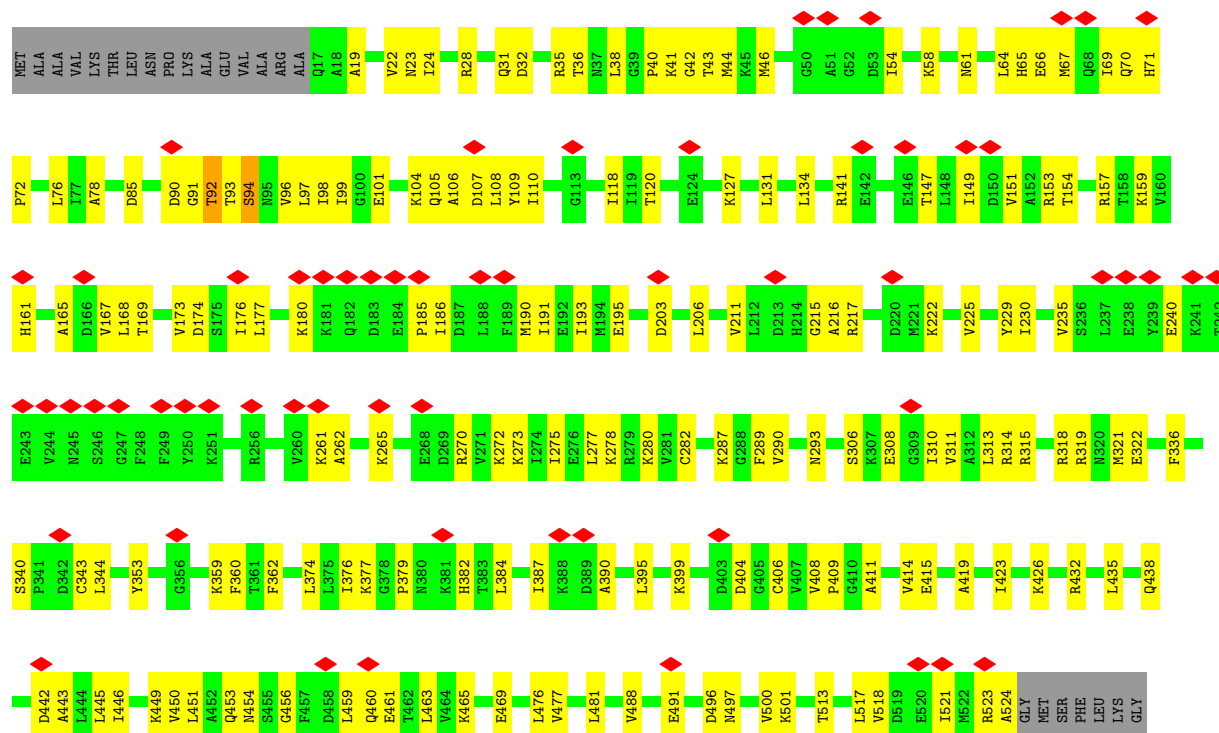


• Molecule 12: T-complex protein 1 subunit zeta

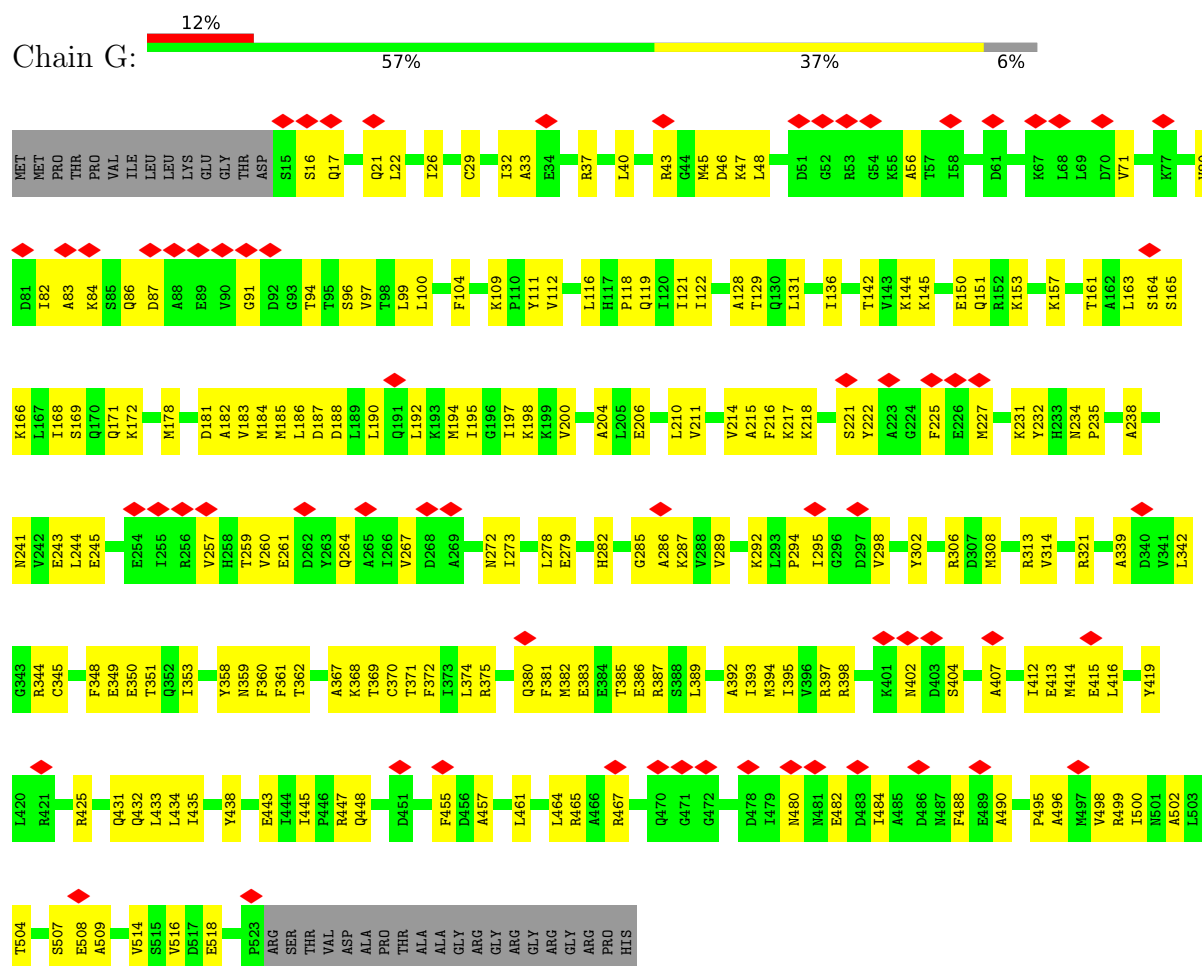




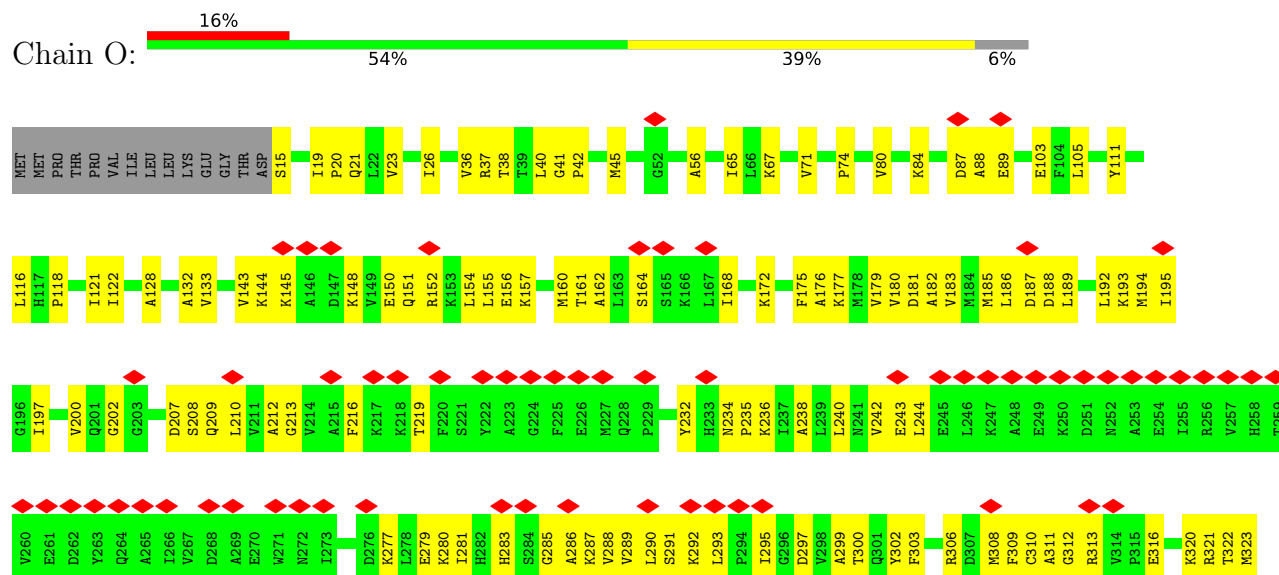
• Molecule 12: T-complex protein 1 subunit zeta

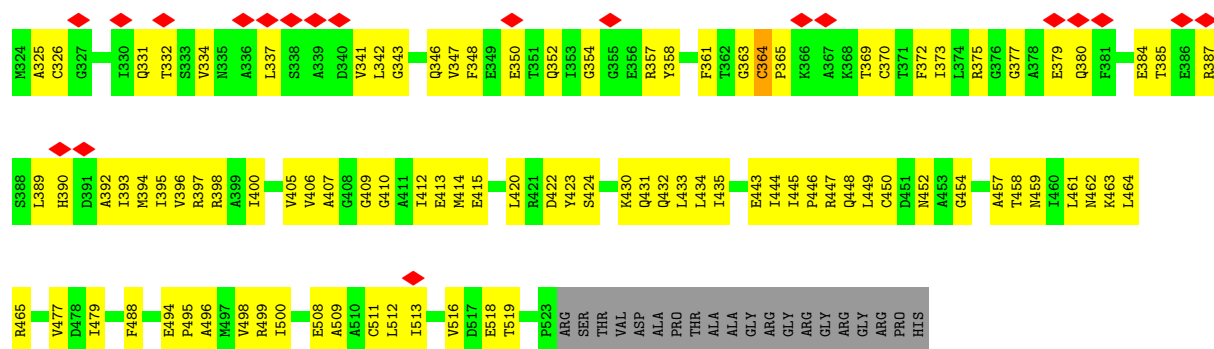


- Molecule 13: T-complex protein 1 subunit eta

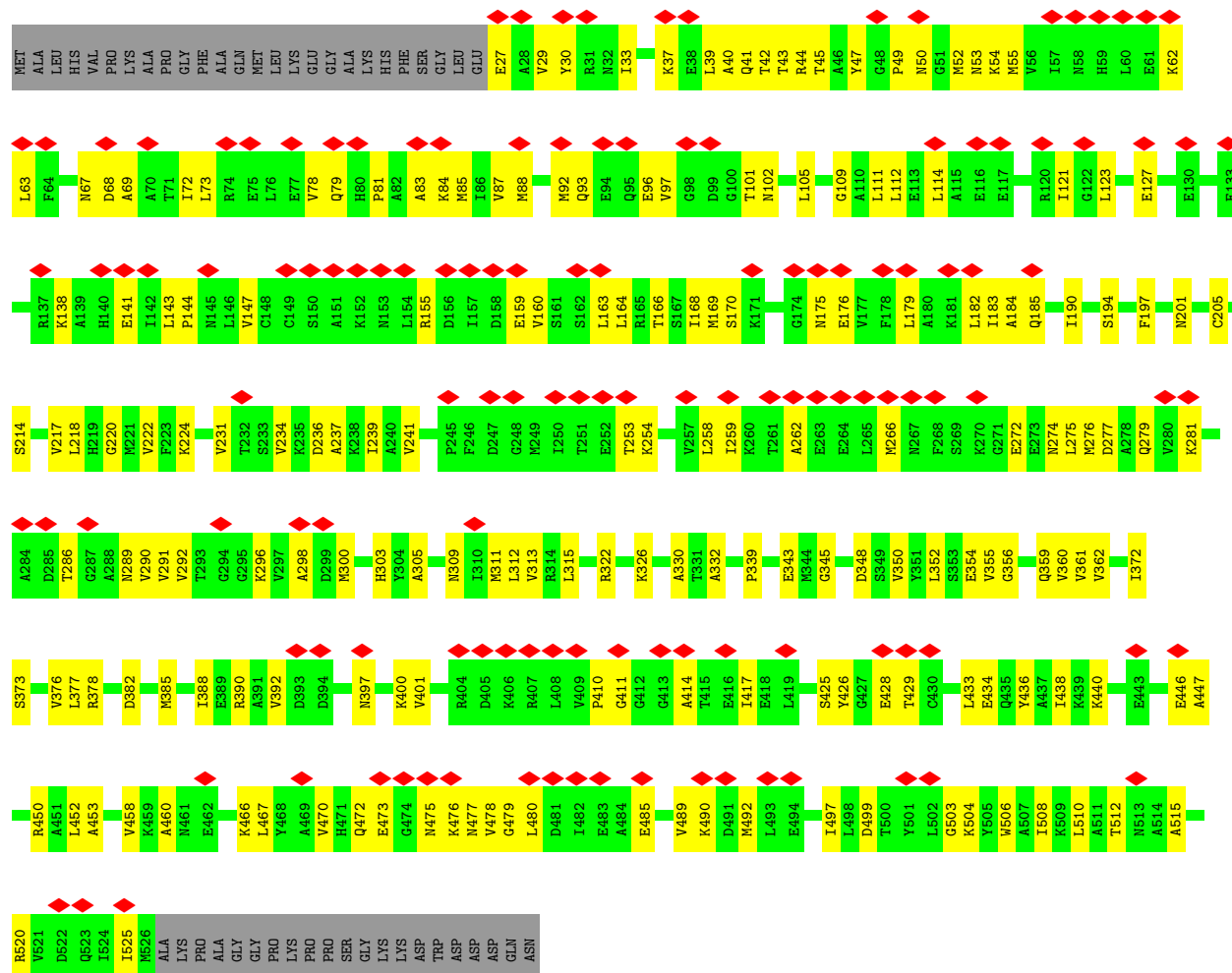


- Molecule 13: T-complex protein 1 subunit eta



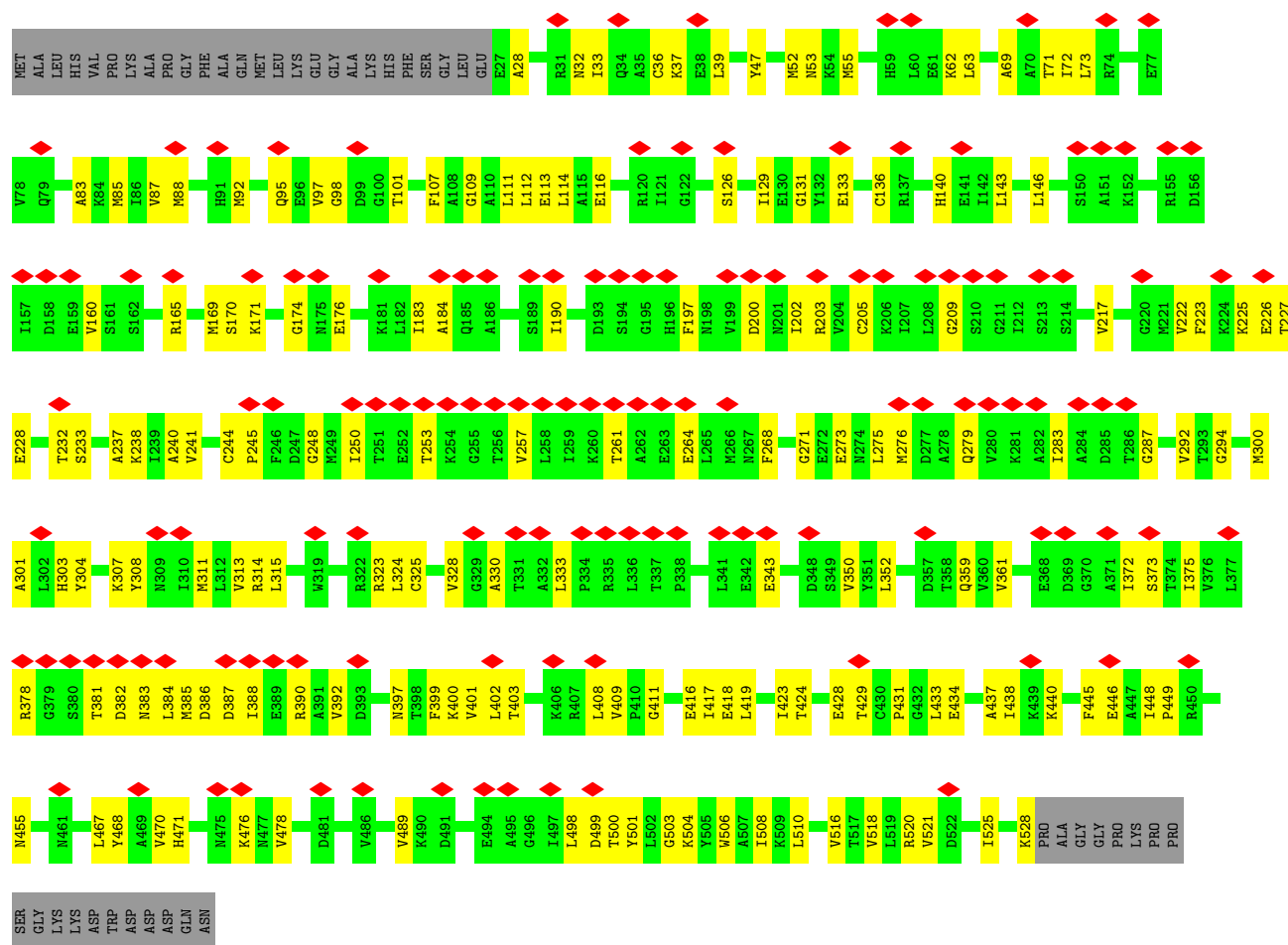


• Molecule 14: T-complex protein 1 subunit theta



• Molecule 14: T-complex protein 1 subunit theta





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	194013	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE; CTF correction was performed for every micrographs	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	11.117	Depositor
Minimum map value	-7.622	Depositor
Average map value	0.019	Depositor
Map value standard deviation	0.246	Depositor
Recommended contour level	0.943	Depositor
Map size (Å)	326.4, 326.4, 326.4	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.02, 1.02, 1.02	Depositor

5 Model quality

5.1 Standard geometry

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

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	1	0.23	0/879	0.58	0/1173
2	2	0.15	0/670	0.41	0/897
3	3	0.18	0/969	0.53	0/1300
4	4	0.18	0/715	0.51	0/959
5	5	0.21	0/1031	0.59	0/1385
6	6	0.16	0/829	0.47	0/1109
7	A	0.15	0/3955	0.40	0/5340
7	I	0.15	0/3939	0.44	1/5318 (0.0%)
8	B	0.14	0/3776	0.39	0/5090
8	J	0.15	0/3776	0.40	0/5090
9	C	0.15	0/3968	0.42	0/5355
9	K	0.17	0/3968	0.46	0/5355
10	D	0.16	0/3878	0.41	0/5237
10	L	0.15	0/3878	0.40	0/5237
11	E	0.15	0/3928	0.40	0/5295
11	M	0.15	0/3928	0.44	0/5295
12	F	0.14	0/3949	0.40	0/5324
12	N	0.18	0/3949	0.46	1/5324 (0.0%)
13	G	0.15	0/3965	0.43	0/5351
13	O	0.17	0/3965	0.46	0/5351
14	H	0.14	0/3867	0.39	0/5229
14	P	0.14	0/3881	0.39	0/5247
All	All	0.16	0/67663	0.43	2/91261 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	N	92	THR	N-CA-C	10.94	123.21	111.28
7	I	39	VAL	N-CA-C	-5.08	107.51	112.29

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	1	873	0	902	47	0
2	2	667	0	693	27	0
3	3	956	0	970	39	0
4	4	711	0	699	36	0
5	5	1017	0	1042	76	0
6	6	825	0	850	50	0
7	A	3919	0	4084	134	0
7	I	3903	0	4062	129	0
8	B	3736	0	3846	123	0
8	J	3736	0	3846	139	0
9	C	3924	0	4050	188	0
9	K	3924	0	4050	169	0
10	D	3847	0	4056	150	0
10	L	3847	0	4051	139	0
11	E	3883	0	3994	158	0
11	M	3883	0	3994	153	0
12	F	3903	0	4030	169	0
12	N	3903	0	4030	142	0
13	G	3910	0	4005	160	0
13	O	3910	0	4005	179	0
14	H	3816	0	3879	142	0
14	P	3830	0	3897	125	0
15	F	27	0	11	1	0
15	H	27	0	11	4	0
15	N	27	0	11	1	0
15	P	27	0	11	2	0
All	All	67031	0	69079	2506	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 18.

All (2506) 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)
12:F:71:HIS:ND1	12:F:72:PRO:HD2	1.39	1.31
9:K:152:MET:HE3	9:K:156:ILE:HD11	1.21	1.18
7:I:168:PHE:CZ	7:I:388:MET:HE1	1.80	1.15
13:O:186:LEU:HD12	13:O:186:LEU:O	1.42	1.15
7:I:168:PHE:HZ	7:I:388:MET:HE1	1.08	1.13
7:I:161:ILE:HD12	7:I:388:MET:SD	1.98	1.03
11:M:154:SER:HB3	11:M:417:ARG:HG2	1.40	1.01
9:K:152:MET:HE3	9:K:156:ILE:CD1	1.93	0.99
12:F:71:HIS:ND1	12:F:72:PRO:CD	2.29	0.94
9:C:156:ILE:HG21	9:C:173:CYS:HB3	1.53	0.90
7:I:168:PHE:HZ	7:I:388:MET:CE	1.86	0.89
13:G:287:LYS:HA	13:G:308:MET:HE2	1.56	0.88
9:K:165:ILE:HD11	9:K:386:GLU:HG2	1.55	0.88
9:C:182:MET:HE1	9:C:216:ARG:HH21	1.39	0.88
10:L:115:SER:OG	10:L:460:VAL:HG21	1.74	0.87
13:G:83:ALA:HB1	13:G:94:THR:HG23	1.57	0.86
7:A:458:GLN:HE21	7:A:493:GLY:HA3	1.41	0.86
12:F:71:HIS:CE1	12:F:72:PRO:HD2	2.12	0.85
9:K:400:ASN:HD22	9:K:500:ALA:H	1.21	0.85
9:C:219:MET:HE1	9:C:221:ASN:HB3	1.59	0.85
9:K:152:MET:CE	9:K:156:ILE:HD11	2.07	0.83
11:M:91:MET:HB2	11:M:523:MET:HE3	1.60	0.83
9:K:249:LYS:HB3	9:K:278:LEU:HD12	1.60	0.83
8:B:182:LEU:HB3	8:B:214:LEU:HD22	1.58	0.83
14:P:97:VAL:HG23	14:P:401:VAL:HG11	1.59	0.83
11:M:154:SER:CB	11:M:417:ARG:HG2	2.07	0.83
9:C:27:ILE:HG21	9:C:110:GLU:HB2	1.61	0.83
8:J:238:LEU:HB2	8:J:287:ILE:HG21	1.62	0.82
8:B:415:MET:HE1	8:B:444:ARG:HG2	1.61	0.82
12:N:91:GLY:N	12:N:500:VAL:HG21	1.93	0.82
7:I:22:VAL:HA	7:I:101:LEU:HD21	1.61	0.82
8:J:415:MET:HE1	8:J:444:ARG:HE	1.44	0.81
9:C:47:MET:H	12:F:517:LEU:HB3	1.46	0.81
9:C:236:PRO:HA	9:C:348:GLY:H	1.46	0.81
13:O:186:LEU:O	13:O:186:LEU:CD1	2.25	0.81
10:D:94:LEU:HD11	10:D:521:LEU:HB3	1.62	0.80
12:F:71:HIS:CG	12:F:72:PRO:HD2	2.16	0.80
10:D:231:GLN:HB2	10:D:372:LYS:HB2	1.61	0.80
10:L:298:LEU:HD23	10:L:324:VAL:HG12	1.62	0.79
10:D:83:VAL:HG21	10:D:92:VAL:HG11	1.64	0.79
7:A:242:GLN:HG3	7:A:244:THR:H	1.48	0.79
14:P:470:VAL:HG11	14:P:489:VAL:HG21	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:431:GLU:HB2	10:L:435:ARG:HH21	1.47	0.79
12:N:185:PRO:HB3	12:N:399:LYS:HE3	1.65	0.78
11:E:340:ARG:HB2	13:G:298:VAL:HG23	1.66	0.77
13:O:303:PHE:HD2	13:O:308:MET:HE3	1.49	0.77
8:B:348:LEU:HB3	8:B:363:SER:HB2	1.66	0.77
10:D:432:LEU:HD13	10:D:458:MET:HE1	1.64	0.77
9:K:31:LYS:HD3	9:K:107:SER:HB2	1.65	0.77
7:A:128:ALA:HB1	7:A:419:LEU:HD21	1.67	0.77
13:O:162:ALA:HB1	13:O:395:ILE:CD1	2.14	0.77
8:J:213:TYR:HB2	8:J:376:ARG:HH21	1.50	0.77
7:A:71:ALA:HB1	7:A:524:ILE:HD11	1.67	0.76
8:B:49:ASP:H	10:D:531:LYS:HG3	1.51	0.76
11:M:60:MET:HG2	11:M:70:VAL:HG12	1.67	0.76
11:E:131:ILE:HB	13:G:45:MET:HE1	1.65	0.76
12:N:272:LYS:HA	12:N:275:ILE:HG12	1.68	0.76
11:E:232:LYS:H	11:E:371:MET:HE1	1.50	0.76
11:E:247:LYS:HG3	11:E:297:ALA:HB2	1.66	0.75
13:G:186:LEU:HD11	13:G:367:ALA:HB3	1.67	0.75
13:G:171:GLN:HG3	13:G:206:GLU:HG3	1.68	0.75
7:I:103:ASN:HD22	7:I:444:SER:HB2	1.50	0.75
7:I:168:PHE:CZ	7:I:388:MET:CE	2.63	0.75
12:F:71:HIS:CG	12:F:72:PRO:CD	2.70	0.75
11:M:247:LYS:HB3	11:M:297:ALA:HA	1.68	0.74
14:P:411:GLY:H	14:P:498:LEU:HA	1.51	0.74
10:L:409:LEU:HD13	10:L:412:ILE:HD11	1.68	0.74
11:M:232:LYS:HB2	11:M:372:LEU:HG	1.67	0.74
5:5:50:LEU:HD21	5:5:107:ILE:HG13	1.69	0.74
11:E:206:PHE:HD2	11:E:410:ARG:HG3	1.53	0.74
7:I:506:PRO:HB2	7:I:509:VAL:HG12	1.70	0.74
11:M:155:VAL:O	11:M:416:ASN:ND2	2.21	0.74
13:O:414:MET:HE3	13:O:446:PRO:HG3	1.69	0.74
9:K:283:ILE:HG23	9:K:307:ALA:HB2	1.69	0.73
9:C:26:ASN:HD21	9:C:519:ILE:HB	1.50	0.73
10:L:109:VAL:HG12	10:L:518:ALA:HA	1.71	0.73
14:P:97:VAL:HG21	14:P:503:GLY:HA2	1.70	0.73
5:5:114:MET:HG2	5:5:118:GLN:HE22	1.52	0.73
14:P:197:PHE:O	14:P:400:LYS:NZ	2.21	0.73
9:K:183:VAL:O	9:K:186:GLU:HG3	1.89	0.73
13:O:195:ILE:HA	13:O:393:ILE:HD11	1.70	0.73
8:B:517:VAL:HG11	11:E:60:MET:HB2	1.70	0.73
1:1:15:GLU:OE1	1:1:19:LYS:NZ	2.21	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:N:195:GLU:HG3	12:N:384:LEU:HD21	1.71	0.73
4:4:65:LEU:HD23	4:4:66:MET:HG2	1.69	0.73
10:L:144:GLY:HA2	10:L:432:LEU:HD11	1.70	0.73
10:D:136:SER:HG	10:D:450:CYS:HG	1.31	0.72
13:G:286:ALA:HB2	13:G:342:LEU:HD13	1.71	0.72
9:K:190:ARG:HH11	9:K:192:GLU:HG3	1.54	0.72
9:K:199:ALA:HA	9:K:372:CYS:HB2	1.71	0.72
8:J:207:GLY:H	8:J:376:ARG:HB2	1.54	0.72
9:C:215:LEU:HB2	9:C:375:LEU:HD12	1.71	0.72
13:G:383:GLU:HB3	13:G:387:ARG:HH12	1.54	0.72
14:H:43:THR:HG21	14:H:105:LEU:HD13	1.71	0.72
10:D:265:VAL:HG12	10:D:267:SER:H	1.55	0.72
8:J:353:MET:SD	8:J:358:LYS:NZ	2.60	0.72
12:N:449:LYS:HG3	12:N:459:LEU:HD11	1.71	0.72
12:F:69:ILE:HD11	12:F:75:SER:HA	1.72	0.72
7:I:171:MET:HE3	7:I:375:ILE:HD12	1.72	0.72
7:A:440:GLU:OE1	7:A:443:ARG:NH2	2.23	0.72
14:P:417:ILE:HD11	14:P:449:PRO:HG2	1.72	0.72
12:F:171:ALA:HA	12:F:206:LEU:HD23	1.71	0.72
8:J:237:ILE:H	8:J:289:CYS:HB2	1.53	0.72
3:3:105:PHE:HB3	5:5:64:VAL:HG21	1.70	0.71
7:A:234:ILE:HG12	7:A:351:VAL:HG21	1.73	0.71
10:D:231:GLN:NE2	10:D:364:GLU:OE2	2.20	0.71
14:H:175:ASN:HB3	14:H:179:LEU:HD23	1.70	0.71
8:B:235:ALA:HA	8:B:289:CYS:HB3	1.71	0.71
12:F:376:ILE:HD12	12:F:387:ILE:HG23	1.72	0.71
12:N:277:LEU:HD21	12:N:344:LEU:HD21	1.73	0.71
7:A:294:ASP:OD1	7:A:298:LYS:NZ	2.23	0.71
8:J:298:ASN:ND2	10:L:346:ALA:O	2.23	0.71
11:M:42:LYS:NZ	11:M:121:GLU:OE1	2.22	0.71
11:M:419:VAL:HB	11:M:510:LEU:HA	1.71	0.71
8:B:235:ALA:HB2	8:B:349:ILE:HD11	1.72	0.70
11:E:460:MET:HE3	11:E:471:ILE:HD11	1.73	0.70
8:B:124:GLN:NE2	11:E:55:ASN:OD1	2.24	0.70
11:E:62:VAL:HG12	11:E:68:VAL:HG12	1.73	0.70
14:H:114:LEU:HB3	14:H:440:LYS:HB3	1.72	0.70
11:E:216:GLY:HA3	11:E:388:ARG:HH21	1.54	0.70
10:L:91:LEU:HD12	10:L:110:VAL:HG23	1.71	0.70
7:A:44:MET:HE2	9:C:519:ILE:HG21	1.74	0.70
13:G:467:ARG:HD3	13:G:484:ILE:HG21	1.74	0.70
11:E:188:ILE:HG13	11:E:224:LEU:HB2	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:130:LEU:HA	9:K:133:MET:HE3	1.73	0.70
8:B:441:LYS:HA	8:B:444:ARG:HD2	1.73	0.70
12:F:154:THR:HG21	12:F:495:TRP:H	1.56	0.70
11:M:396:GLU:HA	11:M:399:LYS:HZ3	1.55	0.70
9:C:231:ARG:HE	9:C:232:TYR:H	1.39	0.70
9:K:365:ASP:OD1	9:K:366:CYS:N	2.23	0.70
13:O:193:LYS:HE3	13:O:321:ARG:HE	1.54	0.70
7:A:112:ILE:HD11	7:A:436:LEU:HD23	1.74	0.69
11:E:129:HIS:HB2	13:G:455:PHE:HB2	1.72	0.69
13:G:183:VAL:HG11	13:G:393:ILE:HB	1.73	0.69
9:K:51:LEU:HB2	12:N:523:ARG:HA	1.73	0.69
9:C:22:VAL:HG21	9:C:520:ASP:HA	1.74	0.69
13:G:128:ALA:HB2	13:G:435:ILE:HD12	1.74	0.69
12:N:277:LEU:HA	12:N:280:LYS:HE2	1.74	0.69
10:L:38:ILE:HG12	10:L:117:LEU:HD12	1.74	0.69
11:M:172:THR:O	11:M:176:LYS:NZ	2.20	0.69
8:B:356:GLU:OE2	8:B:376:ARG:NH1	2.25	0.69
11:E:500:ASP:OD1	11:E:503:GLN:NE2	2.25	0.69
3:3:89:LYS:O	3:3:94:LYS:NZ	2.26	0.69
14:H:183:ILE:HD11	14:H:392:VAL:HG23	1.74	0.69
10:L:75:ALA:HB2	10:L:106:THR:HG21	1.73	0.69
12:F:487:MET:HE3	12:F:488:VAL:H	1.57	0.69
4:4:84:GLN:HA	4:4:87:LEU:HB2	1.74	0.69
14:H:492:MET:HE1	14:H:497:ILE:HB	1.73	0.69
7:I:300:PHE:HB3	7:I:305:ALA:HB2	1.73	0.69
9:K:365:ASP:HB3	9:K:370:LYS:HD2	1.75	0.69
9:K:400:ASN:HB3	9:K:500:ALA:HB2	1.75	0.69
12:N:94:SER:O	12:N:98:ILE:HG12	1.93	0.69
10:D:225:GLU:HG3	10:D:386:VAL:HG22	1.74	0.69
9:C:330:ARG:NH1	9:C:342:ASP:OD2	2.25	0.68
12:F:388:LYS:O	12:F:392:ARG:HG2	1.93	0.68
13:G:339:ALA:HA	13:G:342:LEU:HD12	1.75	0.68
13:O:495:PRO:HG2	13:O:498:VAL:HB	1.73	0.68
9:C:416:MET:HE1	9:C:445:GLU:HG2	1.74	0.68
12:N:174:ASP:HB3	12:N:206:LEU:HD21	1.75	0.68
12:N:40:PRO:HB3	12:N:157:ARG:HG2	1.75	0.68
8:B:215:ASP:OD2	8:B:361:HIS:NE2	2.27	0.68
12:N:445:LEU:HD23	12:N:463:LEU:HD21	1.76	0.68
13:O:519:THR:HG22	14:P:55:MET:HG3	1.76	0.68
2:2:51:LEU:HB2	2:2:97:ILE:HG21	1.76	0.68
8:J:322:ARG:HH21	8:J:371:CYS:HA	1.57	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:N:38:LEU:O	12:N:454:ASN:ND2	2.26	0.68
13:O:243:GLU:HB3	13:O:293:LEU:HD23	1.76	0.68
8:J:92:ASP:OD1	8:J:93:ASP:N	2.27	0.68
9:K:198:TYR:OH	9:K:325:ARG:NH1	2.27	0.68
9:K:230:ARG:HH12	9:K:352:ILE:HD11	1.58	0.68
14:H:53:ASN:ND2	14:H:67:ASN:OD1	2.26	0.68
14:H:231:VAL:HG23	14:H:352:LEU:HD13	1.76	0.68
9:K:144:VAL:CG2	9:K:152:MET:SD	2.82	0.68
14:P:200:ASP:O	14:P:203:ARG:NH1	2.27	0.68
11:M:154:SER:HB3	11:M:417:ARG:CG	2.20	0.68
1:I:70:LEU:HD22	5:5:61:GLU:HB3	1.76	0.68
3:3:87:ILE:HG12	4:4:72:GLY:HA3	1.76	0.68
7:I:196:ASN:OD1	7:I:318:ARG:NH2	2.27	0.68
8:J:275:MET:HE2	8:J:303:LEU:HB3	1.76	0.68
7:A:385:CYS:HA	7:A:388:MET:HE2	1.76	0.67
13:G:86:GLN:HG3	13:G:97:VAL:HG11	1.76	0.67
12:N:186:ILE:H	12:N:399:LYS:HG3	1.59	0.67
3:3:56:GLN:HA	3:3:59:LYS:HE2	1.76	0.67
9:C:313:ARG:HD3	9:C:314:ARG:HG2	1.76	0.67
8:J:211:ASP:HB2	8:J:376:ARG:HD2	1.77	0.67
8:J:230:LYS:NZ	8:J:351:GLU:OE2	2.26	0.67
13:O:162:ALA:CB	13:O:395:ILE:CD1	2.73	0.67
13:O:395:ILE:HG12	13:O:398:ARG:NH2	2.08	0.67
13:G:414:MET:HE1	13:G:443:GLU:HG3	1.75	0.67
9:C:477:THR:HG21	9:C:491:LYS:HB2	1.74	0.67
10:D:248:LEU:HA	10:D:299:LEU:HB3	1.77	0.67
11:E:182:HIS:HB3	11:E:184:GLN:HG3	1.77	0.67
7:A:275:ILE:HA	7:A:278:ILE:HG12	1.75	0.67
9:C:179:ALA:O	9:C:183:VAL:HG22	1.94	0.67
11:E:249:ALA:HA	11:E:353:LEU:HD13	1.77	0.67
11:E:396:GLU:HB2	11:E:400:ARG:HH21	1.60	0.67
9:K:280:GLU:HA	9:K:283:ILE:HD12	1.77	0.67
4:4:62:ASP:OD1	4:4:80:GLN:NE2	2.28	0.67
12:F:69:ILE:HD11	12:F:75:SER:CA	2.25	0.67
9:K:325:ARG:HH12	9:K:369:PRO:HB2	1.59	0.67
14:P:294:GLY:O	14:P:314:ARG:NH1	2.27	0.67
9:C:442:GLN:HA	9:C:445:GLU:HG3	1.76	0.66
9:K:37:ILE:HD13	9:K:67:LEU:HD21	1.76	0.66
14:P:209:GLY:HA3	14:P:378:ARG:HH21	1.61	0.66
3:3:131:VAL:O	3:3:132:MET:HE2	1.95	0.66
10:D:249:ILE:N	10:D:299:LEU:O	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:E:140:ALA:HB2	11:E:448:MET:HG2	1.76	0.66
8:J:236:LYS:HB2	8:J:287:ILE:HG23	1.75	0.66
5:5:105:ARG:HH22	6:6:50:LEU:HD22	1.61	0.66
12:F:446:ILE:HD12	12:F:449:LYS:HD3	1.77	0.66
7:I:161:ILE:CD1	7:I:388:MET:SD	2.81	0.66
12:N:46:MET:HE3	14:P:521:VAL:HG11	1.77	0.66
12:F:38:LEU:O	12:F:454:ASN:ND2	2.29	0.66
12:F:97:LEU:HD21	12:F:450:VAL:HG11	1.76	0.66
12:F:292:ILE:HD12	12:F:313:LEU:HB2	1.78	0.66
8:J:518:ASP:OD1	11:M:59:LYS:NZ	2.29	0.66
9:C:426:SER:OG	9:C:438:ARG:NH1	2.29	0.66
11:E:145:ILE:HD12	11:E:514:LYS:HG2	1.77	0.66
12:F:31:GLN:HG3	12:F:100:GLY:HA3	1.78	0.66
12:F:122:GLY:HA3	12:F:436:GLY:HA3	1.78	0.66
9:K:78:LYS:O	9:K:82:GLU:HG2	1.95	0.66
10:L:50:THR:HB	10:L:59:LYS:HE3	1.78	0.66
12:N:415:GLU:OE2	12:N:501:LYS:NZ	2.26	0.66
13:O:395:ILE:HA	13:O:398:ARG:NH2	2.11	0.66
5:5:36:LEU:HD11	5:5:118:GLN:HA	1.78	0.66
8:B:237:ILE:HG13	8:B:291:ILE:HG13	1.78	0.66
13:G:518:GLU:HB2	14:H:54:LYS:HE3	1.79	0.66
13:O:195:ILE:HD12	13:O:394:MET:HE3	1.77	0.66
14:P:225:LYS:NZ	14:P:226:GLU:O	2.27	0.66
5:5:36:LEU:HD21	5:5:118:GLN:HG3	1.76	0.65
11:E:132:ARG:HE	11:E:443:LEU:HD12	1.61	0.65
13:G:40:LEU:HD21	13:G:445:ILE:HG23	1.79	0.65
11:E:247:LYS:HD2	11:E:353:LEU:HB2	1.78	0.65
11:E:457:VAL:HA	11:E:460:MET:HB2	1.77	0.65
14:H:97:VAL:HG21	14:H:503:GLY:HA2	1.79	0.65
14:H:111:LEU:HD22	14:H:515:ALA:HB1	1.77	0.65
10:D:173:SER:HB2	10:D:508:VAL:HG13	1.79	0.65
9:K:123:ILE:HD12	9:K:514:VAL:HG23	1.78	0.65
13:O:280:LYS:HA	13:O:283:HIS:CE1	2.32	0.65
13:G:369:THR:OG1	13:G:371:THR:HG23	1.97	0.65
8:J:27:THR:N	8:J:518:ASP:O	2.30	0.65
13:O:235:PRO:HB3	13:O:287:LYS:HD2	1.79	0.65
7:A:201:HIS:NE2	7:A:382:ASP:OD1	2.29	0.65
14:H:127:GLU:HG3	14:H:433:LEU:HD23	1.79	0.65
9:K:306:ARG:H	9:K:306:ARG:HD2	1.62	0.65
10:L:145:ILE:HD12	10:L:516:VAL:HG13	1.79	0.65
9:K:144:VAL:HG21	9:K:152:MET:SD	2.37	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:C:407:LEU:HD23	9:C:499:LEU:HD12	1.79	0.65
11:E:128:ILE:HD11	10:L:474:ILE:HG21	1.78	0.65
13:O:148:LYS:HD3	13:O:150:GLU:HB2	1.79	0.65
8:J:33:ILE:HD13	8:J:111:ARG:HB2	1.79	0.65
5:5:115:GLU:HA	5:5:119:PRO:HD2	1.79	0.65
9:C:194:ASP:O	9:C:399:ARG:NH1	2.30	0.65
13:O:240:LEU:HB3	13:O:291:SER:HB3	1.79	0.65
12:N:230:ILE:HD13	12:N:290:VAL:HG23	1.78	0.64
12:F:114:LEU:HD11	12:N:460:GLN:HG2	1.79	0.64
13:O:182:ALA:HA	13:O:185:MET:HB3	1.78	0.64
9:C:350:LEU:HD21	9:C:361:THR:HG23	1.78	0.64
11:M:531:ASP:HB3	13:O:45:MET:HE2	1.77	0.64
10:D:429:GLU:HG3	10:D:461:ILE:HG23	1.77	0.64
11:E:110:VAL:HG22	11:E:523:MET:HE1	1.78	0.64
9:K:87:GLN:HE21	9:K:91:VAL:HB	1.63	0.64
10:L:173:SER:HB2	10:L:508:VAL:HG23	1.78	0.64
10:L:366:ASN:HB2	10:L:370:SER:HA	1.80	0.64
11:M:244:GLU:O	11:M:298:ASN:ND2	2.29	0.64
13:O:279:GLU:OE2	13:O:306:ARG:NH2	2.29	0.64
12:F:212:LEU:HG	12:F:214:HIS:H	1.63	0.64
9:K:376:LEU:HD13	9:K:384:LEU:HD22	1.80	0.64
10:D:38:ILE:HG22	10:D:117:LEU:HD12	1.79	0.64
13:O:385:THR:HG23	13:O:389:LEU:HD13	1.80	0.64
12:F:297:ILE:HG12	12:F:314:ARG:HB3	1.80	0.64
13:G:353:ILE:HD11	13:G:360:PHE:HZ	1.63	0.64
13:O:393:ILE:HA	13:O:396:VAL:HG22	1.79	0.64
12:F:148:LEU:HA	12:F:151:VAL:HG12	1.80	0.64
13:G:48:LEU:HD11	13:G:56:ALA:HB1	1.80	0.64
7:I:107:LEU:HD21	7:I:440:GLU:HG2	1.80	0.64
10:L:480:LEU:HD22	10:L:500:ILE:HD12	1.79	0.64
14:P:408:LEU:HB2	14:P:500:THR:HA	1.79	0.64
7:A:184:ILE:HG23	7:A:185:ARG:HG2	1.80	0.64
11:E:223:LYS:HE3	11:E:362:ILE:HG12	1.79	0.64
8:J:414:GLU:HG2	8:J:446:LEU:HD23	1.80	0.64
7:A:244:THR:HG21	7:A:246:MET:HE2	1.79	0.63
8:J:166:THR:HG21	8:J:396:VAL:HG21	1.80	0.63
8:J:295:LEU:HA	8:J:313:GLU:HB3	1.80	0.63
10:L:260:MET:HE3	10:L:261:ASP:H	1.62	0.63
11:M:198:ASP:OD1	11:M:198:ASP:O	2.15	0.63
5:5:26:VAL:HG11	5:5:132:MET:SD	2.38	0.63
9:K:45:SER:HA	9:K:454:ASN:HD21	1.61	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:422:ASP:OD1	13:O:423:TYR:N	2.32	0.63
8:B:219:LEU:HB3	8:B:359:LEU:HD21	1.79	0.63
13:G:382:MET:HA	13:G:385:THR:HB	1.80	0.63
14:P:381:THR:HG22	14:P:383:ASN:H	1.64	0.63
5:5:120:ALA:O	5:5:124:LYS:NZ	2.29	0.63
9:C:180:VAL:HG21	9:C:398:CYS:HB3	1.80	0.63
12:F:234:ASN:HD21	12:F:321:MET:HE1	1.63	0.63
14:P:73:LEU:HD13	14:P:87:VAL:HG22	1.80	0.63
9:C:50:LEU:HD21	9:C:66:ILE:HG13	1.79	0.63
13:G:214:VAL:HG21	13:G:321:ARG:HH11	1.63	0.63
7:I:101:LEU:HD12	7:I:524:ILE:HG21	1.79	0.63
9:K:180:VAL:HA	9:K:183:VAL:HB	1.81	0.63
12:N:106:ALA:O	12:N:110:ILE:HG12	1.98	0.63
2:2:91:GLU:HA	2:2:94:LYS:HE3	1.80	0.63
7:A:435:GLN:HE21	13:O:462:ASN:HD22	1.45	0.63
12:F:278:LYS:NZ	12:F:284:ASP:O	2.32	0.63
7:I:467:LEU:HD11	7:I:487:GLY:HA2	1.79	0.63
1:1:68:PHE:HB2	5:5:63:LEU:HB2	1.80	0.63
8:B:85:VAL:O	8:B:89:ARG:HG3	1.98	0.63
9:C:313:ARG:HH11	9:C:314:ARG:H	1.46	0.63
11:E:247:LYS:NZ	11:E:353:LEU:O	2.30	0.63
9:K:27:ILE:HG21	9:K:110:GLU:HB2	1.81	0.63
9:K:73:GLN:HE22	9:K:78:LYS:HD3	1.63	0.63
13:O:188:ASP:OD1	13:O:189:LEU:N	2.32	0.63
10:D:534:ASP:OD1	10:D:535:VAL:N	2.31	0.63
9:K:286:LYS:NZ	9:K:306:ARG:O	2.31	0.63
11:M:129:HIS:HD2	11:M:131:ILE:HG22	1.62	0.63
11:E:342:VAL:HG13	11:E:347:GLU:HB2	1.79	0.62
13:G:197:ILE:HD11	13:G:386:GLU:HA	1.81	0.62
2:2:92:ASN:ND2	2:2:95:GLU:OE2	2.31	0.62
11:E:161:ASP:HB3	11:E:165:LEU:HD13	1.81	0.62
9:K:177:LEU:O	9:K:181:LYS:HG2	2.00	0.62
10:L:504:LEU:HD23	10:L:507:LEU:HD23	1.82	0.62
8:B:167:LEU:HD21	8:B:393:ALA:HB2	1.80	0.62
9:C:168:TRP:NE1	9:C:209:ILE:O	2.32	0.62
10:D:325:ILE:HG22	10:D:328:ILE:HD11	1.80	0.62
10:L:123:LEU:HD13	10:L:128:ILE:HD11	1.81	0.62
12:N:235:VAL:O	12:N:270:ARG:NH1	2.32	0.62
14:H:114:LEU:HD12	14:H:440:LYS:HD2	1.81	0.62
10:L:52:LEU:HD12	10:L:111:ILE:HD12	1.81	0.62
2:2:60:THR:HA	2:2:64:VAL:HB	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:C:149:SER:HA	9:C:152:MET:HE2	1.80	0.62
12:F:67:MET:HG2	14:H:525:ILE:HG21	1.80	0.62
8:J:235:ALA:HB3	8:J:346:CYS:HB3	1.82	0.62
1:1:17:GLN:O	1:1:21:ILE:HG12	1.99	0.62
4:4:40:ILE:HG22	4:4:44:LYS:HZ2	1.63	0.62
14:H:254:LYS:HB3	14:H:259:ILE:HD12	1.82	0.62
7:I:32:VAL:HG23	7:I:61:ILE:HD11	1.81	0.62
5:5:89:GLY:O	6:6:59:LEU:N	2.33	0.62
12:F:520:GLU:HB3	12:F:522:MET:HE3	1.81	0.62
13:G:71:VAL:HG11	13:G:80:VAL:HG21	1.80	0.62
13:O:162:ALA:CB	13:O:395:ILE:HD13	2.30	0.62
13:O:240:LEU:N	13:O:290:LEU:O	2.32	0.62
7:A:208:SER:C	7:A:209:MET:HE2	2.25	0.62
8:B:83:VAL:O	8:B:87:MET:HG2	1.98	0.62
9:C:346:GLY:HA3	9:C:367:LYS:HG2	1.82	0.62
9:C:452:ILE:HD11	9:C:462:LEU:HB3	1.81	0.62
10:D:446:MET:HE2	11:M:472:GLN:HB2	1.80	0.62
14:H:218:LEU:HD11	14:H:355:VAL:HG21	1.81	0.62
7:I:203:ARG:N	7:I:379:GLY:O	2.28	0.62
5:5:82:VAL:O	5:5:94:LYS:N	2.30	0.61
9:C:200:ARG:HH22	9:C:318:THR:HG21	1.65	0.61
9:C:201:VAL:HG21	9:C:388:GLU:HG2	1.82	0.61
13:G:37:ARG:HA	13:G:99:LEU:HD21	1.81	0.61
13:O:200:VAL:HG22	13:O:358:TYR:HE2	1.64	0.61
7:I:146:ASP:OD1	7:I:150:ASN:ND2	2.33	0.61
7:I:103:ASN:ND2	7:I:440:GLU:HG3	2.15	0.61
14:H:179:LEU:HD13	14:H:182:LEU:HD21	1.82	0.61
7:I:298:LYS:NZ	9:K:342:ASP:OD1	2.28	0.61
14:P:160:VAL:HG13	14:P:184:ALA:HB1	1.81	0.61
10:D:458:MET:SD	10:D:519:LEU:HD11	2.41	0.61
13:G:278:LEU:O	13:G:282:HIS:ND1	2.24	0.61
7:I:234:ILE:HG13	7:I:346:GLY:HA3	1.82	0.61
13:O:38:THR:HA	13:O:452:ASN:HD21	1.66	0.61
5:5:44:VAL:HA	5:5:47:LYS:HD2	1.83	0.61
8:B:289:CYS:SG	8:B:290:PHE:N	2.74	0.61
11:E:458:ILE:O	11:E:462:LEU:HB2	2.00	0.61
14:H:190:ILE:HD11	14:H:373:SER:HB3	1.83	0.61
9:C:267:ILE:HA	9:C:270:MET:HG2	1.81	0.61
10:D:394:ASN:OD1	10:D:395:LYS:N	2.34	0.61
12:F:165:ALA:O	12:F:169:THR:HG23	2.00	0.61
13:G:188:ASP:O	13:G:397:ARG:NH2	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:237:ARG:HA	9:K:330:ARG:HB2	1.82	0.61
11:M:481:GLN:NE2	11:M:489:LEU:O	2.33	0.61
14:H:39:LEU:HG	14:H:105:LEU:HD21	1.83	0.61
11:M:299:LEU:HD22	11:M:320:PRO:HG2	1.82	0.61
14:P:129:ILE:HB	14:P:516:VAL:HG23	1.82	0.61
3:3:114:LYS:HE3	3:3:114:LYS:HA	1.83	0.61
5:5:40:GLN:NE2	5:5:118:GLN:OE1	2.31	0.61
6:6:33:LEU:O	6:6:36:GLN:NE2	2.32	0.61
8:B:236:LYS:HG3	8:B:343:LEU:HB2	1.82	0.61
14:P:434:GLU:O	14:P:438:ILE:HG12	2.01	0.61
6:6:78:LYS:HZ2	6:6:79:ARG:HH22	1.49	0.60
10:D:330:ARG:HA	10:D:333:ILE:HD12	1.83	0.60
12:F:464:VAL:HG11	12:N:432:ARG:HG3	1.82	0.60
9:K:229:MET:HE3	9:K:310:THR:HA	1.81	0.60
8:B:158:ASP:O	8:B:162:ILE:HG12	2.01	0.60
8:J:392:ASP:OD1	8:J:393:ALA:N	2.34	0.60
7:A:467:LEU:HD22	7:A:488:LEU:HD23	1.84	0.60
10:D:461:ILE:HA	10:D:464:THR:HG22	1.83	0.60
12:N:217:ARG:HB2	12:N:359:LYS:HD2	1.82	0.60
9:C:272:GLU:HA	9:C:299:LEU:HD12	1.82	0.60
10:D:38:ILE:HD12	10:D:121:THR:HB	1.82	0.60
12:F:159:LYS:NZ	15:F:601:ADP:O1B	2.34	0.60
13:G:264:GLN:HA	13:G:267:VAL:HG12	1.82	0.60
7:I:118:ILE:HG23	7:I:522:ILE:HG23	1.82	0.60
9:K:353:LYS:HD2	9:K:355:ILE:HD12	1.82	0.60
13:O:105:LEU:HD21	13:O:513:ILE:HG21	1.82	0.60
11:E:129:HIS:HD2	11:E:131:ILE:HG22	1.66	0.60
14:H:224:LYS:O	14:H:359:GLN:NE2	2.34	0.60
9:K:470:HIS:NE2	9:K:478:TRP:O	2.30	0.60
12:N:101:GLU:HB3	12:N:443:ALA:HA	1.84	0.60
12:N:379:PRO:HB3	14:P:92:MET:HE1	1.82	0.60
3:3:100:SER:O	3:3:101:MET:HE2	2.02	0.60
11:M:166:ILE:O	11:M:170:LYS:HG2	2.02	0.60
14:P:136:CYS:SG	14:P:140:HIS:NE2	2.75	0.60
14:P:386:ASP:O	14:P:390:ARG:NE	2.30	0.60
8:B:132:GLU:HG3	8:B:424:LEU:HD21	1.84	0.60
12:F:26:ALA:HB2	12:F:71:HIS:NE2	2.16	0.60
10:D:501:SER:OG	10:D:506:GLU:OE2	2.20	0.60
14:H:224:LYS:HA	14:H:360:VAL:HG12	1.84	0.60
14:H:272:GLU:HG2	14:H:276:MET:HE2	1.84	0.60
9:K:118:HIS:ND1	9:K:118:HIS:O	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:89:ARG:O	10:L:93:GLU:HG2	2.02	0.60
13:O:299:ALA:HA	13:O:302:TYR:HD2	1.65	0.60
7:A:341:GLU:HG3	7:A:343:ALA:H	1.66	0.60
8:B:154:LYS:NZ	8:B:158:ASP:OD1	2.35	0.60
13:G:389:LEU:O	13:G:393:ILE:HG12	2.00	0.60
7:I:135:ASN:O	7:I:484:LYS:NZ	2.32	0.60
12:N:91:GLY:N	12:N:500:VAL:CG2	2.62	0.60
5:5:114:MET:HG2	5:5:118:GLN:NE2	2.17	0.60
7:A:518:THR:O	7:A:522:ILE:HG13	2.02	0.60
9:C:454:ASN:O	12:F:115:HIS:NE2	2.35	0.60
12:N:105:GLN:NE2	12:N:442:ASP:OD2	2.35	0.60
12:N:159:LYS:HD2	12:N:390:ALA:HA	1.83	0.60
9:C:123:ILE:HD12	9:C:514:VAL:HG13	1.84	0.59
13:G:431:GLN:NE2	14:H:485:GLU:OE2	2.33	0.59
11:M:370:LYS:C	11:M:371:MET:HE2	2.27	0.59
13:O:207:ASP:HB2	13:O:375:ARG:HD3	1.83	0.59
8:B:48:MET:HA	10:D:531:LYS:HD2	1.84	0.59
7:I:154:THR:O	7:I:158:SER:OG	2.20	0.59
12:N:278:LYS:NZ	12:N:308:GLU:O	2.35	0.59
14:H:170:SER:OG	15:H:5000:ADP:O1A	2.20	0.59
8:J:49:ASP:N	10:L:531:LYS:O	2.34	0.59
9:K:327:CYS:HA	9:K:347:ALA:HB2	1.83	0.59
10:L:38:ILE:HG23	10:L:117:LEU:HB3	1.84	0.59
10:L:390:VAL:HG21	10:L:402:GLU:HG2	1.84	0.59
13:O:395:ILE:CG1	13:O:398:ARG:NH2	2.64	0.59
1:1:88:GLU:HG3	1:1:92:LYS:NZ	2.17	0.59
5:5:36:LEU:O	5:5:40:GLN:NE2	2.35	0.59
7:A:111:LYS:HA	7:A:111:LYS:HE3	1.84	0.59
14:H:27:GLU:HB3	14:H:30:TYR:HD2	1.68	0.59
10:L:169:THR:HB	10:L:509:VAL:HG21	1.85	0.59
13:O:387:ARG:O	13:O:390:HIS:HB3	2.02	0.59
7:A:133:ASN:HA	7:A:137:ILE:HD12	1.83	0.59
9:C:293:GLU:O	9:C:313:ARG:NH1	2.28	0.59
14:H:222:VAL:HG12	14:H:362:VAL:HG22	1.83	0.59
14:H:234:VAL:HG12	14:H:236:ASP:H	1.67	0.59
9:K:32:THR:O	9:K:36:ILE:HG12	2.01	0.59
9:K:144:VAL:HG22	9:K:152:MET:SD	2.43	0.59
11:M:173:LEU:HD21	11:M:408:VAL:HG11	1.82	0.59
13:O:413:GLU:HG3	13:O:445:ILE:HB	1.84	0.59
5:5:86:VAL:HG21	6:6:43:VAL:HG11	1.85	0.59
5:5:94:LYS:HZ1	5:5:103:PHE:HD1	1.49	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:D:134:SER:OG	10:D:527:ARG:NE	2.23	0.59
10:L:249:ILE:HG23	10:L:251:PHE:CE1	2.37	0.59
14:P:416:GLU:OE2	14:P:504:LYS:NZ	2.27	0.59
12:F:218:HIS:ND1	12:F:218:HIS:O	2.34	0.59
7:I:193:ASN:HB2	7:I:318:ARG:HD3	1.84	0.59
11:M:281:GLU:OE1	11:M:284:LYS:NZ	2.31	0.59
14:P:47:TYR:O	14:P:455:ASN:ND2	2.32	0.59
9:C:141:SER:HA	9:C:407:LEU:HA	1.85	0.59
11:E:434:SER:HB3	10:L:441:ARG:HH12	1.67	0.59
7:A:309:ARG:NH2	7:A:310:ARG:HD3	2.18	0.59
9:C:31:LYS:HD3	9:C:107:SER:HB2	1.84	0.59
9:C:195:ILE:HG23	9:C:197:LYS:H	1.67	0.59
7:I:370:ARG:NH1	7:I:371:THR:O	2.36	0.59
13:O:238:ALA:HB2	13:O:286:ALA:HB1	1.83	0.59
1:1:61:TYR:HD2	2:2:78:LEU:HD23	1.68	0.59
2:2:61:LEU:HD11	2:2:87:LEU:HD22	1.85	0.59
8:B:241:ASN:OD1	8:B:293:ARG:NH1	2.35	0.59
9:C:234:LYS:HG3	9:C:349:LEU:HA	1.85	0.59
9:C:314:ARG:HA	9:C:314:ARG:HE	1.67	0.59
10:D:191:VAL:HG21	10:D:412:ILE:HG21	1.84	0.59
10:D:238:ILE:HA	10:D:323:MET:HE2	1.84	0.59
8:J:203:LYS:NZ	8:J:384:ASP:OD1	2.34	0.59
9:K:422:LEU:HD23	9:K:441:ALA:HB2	1.85	0.59
10:D:286:LEU:O	10:D:290:ILE:HG12	2.03	0.58
12:F:31:GLN:HE21	12:F:97:LEU:HD12	1.68	0.58
10:L:115:SER:OG	10:L:460:VAL:CG2	2.50	0.58
1:1:61:TYR:HB2	2:2:78:LEU:HB3	1.85	0.58
11:E:75:ALA:HB2	11:E:106:THR:HG21	1.85	0.58
11:E:133:ILE:HG13	11:E:528:LEU:HD21	1.85	0.58
11:E:426:GLU:HG2	11:E:458:ILE:HG13	1.85	0.58
12:F:101:GLU:HG2	12:F:446:ILE:HB	1.85	0.58
8:J:198:ALA:HA	8:J:321:GLU:OE2	2.03	0.58
1:1:67:MET:HB2	5:5:62:LEU:HD12	1.85	0.58
7:I:100:LEU:HD23	7:I:444:SER:HB3	1.85	0.58
13:O:179:VAL:HG12	13:O:393:ILE:HG22	1.85	0.58
13:O:364:CYS:HB3	13:O:365:PRO:CD	2.33	0.58
10:D:414:CYS:HB2	10:D:513:LEU:HD23	1.84	0.58
11:E:147:HIS:NE2	11:E:428:SER:OG	2.36	0.58
8:J:148:HIS:ND1	8:J:158:ASP:OD2	2.37	0.58
7:A:125:CYS:HB2	7:A:518:THR:HG21	1.85	0.58
8:B:518:ASP:OD1	8:B:519:ASN:N	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:518:THR:O	7:I:522:ILE:HG13	2.04	0.58
14:P:33:ILE:HG21	14:P:116:GLU:HB2	1.86	0.58
14:P:303:HIS:O	14:P:307:LYS:HG3	2.03	0.58
10:D:363:GLU:HB3	10:D:375:LYS:HE3	1.86	0.58
11:E:363:SER:HA	11:E:370:LYS:HD3	1.85	0.58
13:O:15:SER:HA	13:O:20:PRO:HB2	1.84	0.58
5:5:35:GLN:O	5:5:39:VAL:HG13	2.03	0.58
9:C:218:VAL:HG13	9:C:363:ILE:HD13	1.86	0.58
12:N:101:GLU:HG3	12:N:446:ILE:HB	1.86	0.58
14:P:399:PHE:O	14:P:403:THR:HG23	2.04	0.58
3:3:168:GLN:HA	14:H:254:LYS:HB2	1.86	0.58
8:B:398:ALA:O	8:B:402:LYS:HG2	2.04	0.58
9:C:272:GLU:OE2	9:C:276:GLN:NE2	2.34	0.58
9:C:329:ALA:HB2	9:C:344:GLY:H	1.69	0.58
12:F:49:SER:OG	12:F:53:ASP:OD1	2.22	0.58
8:J:218:PHE:HD2	8:J:322:ARG:HH11	1.49	0.58
8:J:297:TYR:O	8:J:301:GLU:N	2.37	0.58
10:D:160:ARG:NH1	10:D:192:MET:SD	2.77	0.58
14:P:279:GLN:HG2	14:P:283:ILE:HD12	1.84	0.58
8:B:388:ARG:HH12	8:B:391:HIS:CG	2.22	0.58
8:J:238:LEU:O	8:J:291:ILE:HG12	2.03	0.58
9:K:57:ILE:HG21	12:N:76:LEU:HB2	1.84	0.58
10:L:314:LEU:HG	10:L:324:VAL:HG11	1.86	0.58
13:O:352:GLN:HB2	13:O:357:ARG:HH11	1.69	0.58
14:P:140:HIS:HE1	14:P:508:ILE:HG23	1.66	0.58
8:B:122:HIS:NE2	11:E:464:GLU:O	2.37	0.57
10:D:134:SER:HG	10:D:527:ARG:HE	1.46	0.57
12:N:193:ILE:HG22	12:N:374:LEU:HB2	1.84	0.57
12:N:451:LEU:HB3	12:N:481:LEU:HD21	1.85	0.57
8:B:37:ASP:OD1	8:B:40:LYS:NZ	2.36	0.57
8:J:72:LYS:HA	8:J:72:LYS:HE3	1.86	0.57
9:K:319:ASP:OD1	9:K:322:ARG:NH1	2.32	0.57
11:M:188:ILE:HG23	11:M:224:LEU:HB3	1.85	0.57
13:O:103:GLU:HG3	13:O:444:ILE:HG12	1.86	0.57
13:O:312:GLY:O	13:O:313:ARG:HD3	2.04	0.57
13:O:424:SER:O	13:O:432:GLN:HB2	2.05	0.57
5:5:35:GLN:HA	5:5:38:VAL:HG22	1.86	0.57
7:A:134:GLU:OE1	7:A:135:ASN:HB3	2.05	0.57
9:C:220:ILE:HD11	9:C:323:ILE:HD11	1.85	0.57
9:C:466:LEU:HD13	9:C:487:LEU:HD22	1.85	0.57
9:K:137:LEU:HD12	9:K:408:VAL:HG21	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:88:ALA:O	10:L:92:VAL:HG23	2.04	0.57
12:N:42:GLY:O	12:N:58:LYS:NZ	2.31	0.57
5:5:102:PHE:O	5:5:105:ARG:HG3	2.04	0.57
7:A:61:ILE:O	7:A:65:LEU:N	2.32	0.57
12:F:26:ALA:HB2	12:F:71:HIS:CE1	2.39	0.57
11:M:78:LEU:HD11	11:M:110:VAL:HG21	1.87	0.57
1:1:97:LYS:NZ	9:C:261:GLU:OE2	2.31	0.57
11:E:442:THR:HG23	11:E:444:GLU:H	1.68	0.57
10:L:495:VAL:HG23	10:L:496:ARG:HG2	1.86	0.57
11:M:113:ALA:HA	11:M:116:LEU:HD12	1.85	0.57
7:A:31:ILE:HG23	9:C:522:ILE:HG13	1.86	0.57
10:L:484:HIS:NE2	10:L:491:ALA:O	2.30	0.57
12:N:449:LYS:CG	12:N:459:LEU:HD11	2.34	0.57
1:1:35:GLU:HB3	1:1:39:ARG:CZ	2.33	0.57
5:5:114:MET:CG	5:5:118:GLN:HE22	2.18	0.57
8:B:425:ALA:HB2	8:B:436:MET:HG3	1.86	0.57
7:I:114:PRO:O	7:I:118:ILE:HG12	2.05	0.57
5:5:47:LYS:HA	5:5:50:LEU:HG	1.86	0.57
8:B:173:THR:HA	8:B:176:LYS:HD3	1.86	0.57
12:F:411:ALA:HB2	12:F:494:VAL:HG11	1.86	0.57
9:K:137:LEU:HD21	9:K:506:TYR:HE2	1.68	0.57
10:L:471:LEU:HD11	10:L:499:GLY:HA2	1.87	0.57
14:P:273:GLU:HB3	14:P:308:TYR:HD2	1.70	0.57
9:C:398:CYS:HA	9:C:401:VAL:HG22	1.87	0.57
14:H:478:VAL:HG22	14:H:489:VAL:HG12	1.86	0.57
9:K:279:CYS:HA	9:K:282:ILE:HD12	1.87	0.57
10:L:494:ASN:HB2	10:L:507:LEU:HD22	1.87	0.57
11:M:141:ALA:O	11:M:145:ILE:HG12	2.04	0.57
13:O:26:ILE:HG22	13:O:105:LEU:HD23	1.87	0.57
14:P:114:LEU:HB3	14:P:440:LYS:HB3	1.87	0.57
11:E:267:ASP:H	13:G:257:VAL:HG12	1.68	0.57
12:F:131:LEU:HD22	12:F:505:LEU:HD23	1.87	0.57
2:2:44:ALA:HB3	2:2:104:LEU:HD13	1.86	0.56
10:D:157:LEU:HG	10:D:419:ARG:HG2	1.87	0.56
11:E:364:PHE:O	11:E:388:ARG:NH1	2.38	0.56
14:H:322:ARG:HB3	14:H:326:LYS:NZ	2.20	0.56
9:K:60:THR:HG21	9:K:65:ALA:HB3	1.87	0.56
8:B:281:ARG:HH22	8:B:339:GLU:HB2	1.70	0.56
10:L:395:LYS:HA	10:L:395:LYS:HE3	1.86	0.56
13:O:36:VAL:HG23	13:O:65:ILE:HD11	1.86	0.56
3:3:152:THR:OG1	3:3:156:ASP:OD2	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:257:ARG:NH1	11:E:268:VAL:O	2.38	0.56
10:D:527:ARG:O	10:D:531:LYS:HB2	2.06	0.56
11:E:236:HIS:HE1	11:E:321:ALA:HB3	1.69	0.56
13:G:181:ASP:HA	13:G:184:MET:HG2	1.88	0.56
14:H:73:LEU:HD11	14:H:105:LEU:HD12	1.86	0.56
14:H:138:LYS:HE3	14:H:426:TYR:CG	2.41	0.56
8:J:232:ILE:HG12	8:J:310:MET:HE3	1.86	0.56
10:L:300:ILE:HD11	10:L:324:VAL:HB	1.88	0.56
11:M:197:ALA:HB1	11:M:413:ILE:HG12	1.87	0.56
12:N:149:ILE:HA	12:N:173:VAL:HG11	1.86	0.56
12:N:319:ARG:NH1	12:N:322:GLU:HB2	2.20	0.56
13:O:162:ALA:HB2	13:O:395:ILE:HD13	1.85	0.56
13:O:395:ILE:HG12	13:O:398:ARG:HH21	1.69	0.56
6:6:50:LEU:HD11	6:6:54:ASN:HB2	1.87	0.56
9:C:46:MET:HE2	12:F:115:HIS:HE1	1.69	0.56
9:C:352:ILE:HG12	9:C:361:THR:HA	1.87	0.56
12:F:284:ASP:OD2	12:F:287:LYS:NZ	2.30	0.56
14:P:240:ALA:O	14:P:292:VAL:N	2.33	0.56
11:E:52:LEU:O	11:E:465:ASN:ND2	2.37	0.56
7:I:274:ARG:NH2	7:I:338:GLU:O	2.37	0.56
8:J:219:LEU:HD21	8:J:359:LEU:HD22	1.87	0.56
9:K:228:ARG:HB3	9:K:305:MET:SD	2.46	0.56
10:L:33:ILE:HG21	10:L:534:ASP:H	1.68	0.56
8:B:222:LYS:HB2	8:B:312:ILE:HD11	1.86	0.56
9:C:280:GLU:OE1	9:C:303:TYR:OH	2.23	0.56
11:E:52:LEU:HD11	11:E:111:VAL:HG11	1.86	0.56
13:G:210:LEU:HG	13:G:372:PHE:HE1	1.71	0.56
14:H:123:LEU:HD22	9:K:460:ILE:HD13	1.86	0.56
11:M:405:ALA:O	11:M:409:ILE:HG12	2.06	0.56
10:D:336:ILE:O	10:D:340:ILE:HG12	2.04	0.56
11:E:276:ALA:HA	11:E:279:LYS:HG2	1.88	0.56
12:F:26:ALA:CB	12:F:71:HIS:CE1	2.88	0.56
7:I:202:GLY:N	7:I:379:GLY:O	2.36	0.56
11:M:48:MET:HA	11:M:48:MET:HE3	1.87	0.56
11:M:275:LYS:O	11:M:279:LYS:HG2	2.05	0.56
1:1:59:ASN:ND2	2:2:80:GLU:OE1	2.39	0.56
13:G:182:ALA:HA	13:G:185:MET:HE3	1.87	0.56
5:5:40:GLN:HE21	5:5:118:GLN:CD	2.13	0.56
8:B:232:ILE:HD12	8:B:310:MET:HB2	1.87	0.56
11:E:181:CYS:O	11:E:183:ARG:NH1	2.37	0.56
13:G:118:PRO:O	13:G:122:ILE:HG12	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:276:GLN:HG2	9:K:300:ALA:HB2	1.88	0.56
11:M:120:ALA:O	11:M:124:LEU:HG	2.06	0.56
13:O:210:LEU:HD23	13:O:372:PHE:HD1	1.70	0.56
12:F:204:THR:HG23	12:F:376:ILE:HA	1.88	0.56
14:H:377:LEU:HD21	14:H:388:ILE:HG23	1.88	0.56
9:K:81:ILE:O	9:K:85:ARG:HG2	2.06	0.56
13:O:195:ILE:HG13	13:O:393:ILE:HD11	1.87	0.56
13:O:414:MET:HG3	13:O:464:LEU:HB3	1.88	0.56
7:A:191:PRO:HG2	7:A:194:SER:HB3	1.86	0.55
9:C:101:LEU:O	9:C:105:MET:HG3	2.06	0.55
9:C:184:GLN:HB3	9:C:191:LYS:HB3	1.88	0.55
11:E:34:LEU:HD22	11:E:124:LEU:HD13	1.87	0.55
11:E:418:VAL:HG23	11:E:509:THR:HA	1.87	0.55
12:F:59:ASP:HA	12:F:159:LYS:HZ2	1.71	0.55
13:G:178:MET:HG2	13:G:210:LEU:HD21	1.88	0.55
9:K:64:ASN:HA	9:K:67:LEU:HD12	1.88	0.55
11:M:193:VAL:HG11	11:M:409:ILE:HD12	1.88	0.55
1:1:61:TYR:HB3	1:1:68:PHE:HB3	1.89	0.55
7:A:40:GLY:O	9:C:518:ARG:NH2	2.39	0.55
9:C:214:VAL:HG22	9:C:374:ILE:HA	1.88	0.55
10:D:345:VAL:HG22	10:D:355:MET:HE2	1.86	0.55
12:F:133:PHE:CZ	12:F:137:VAL:HG21	2.42	0.55
13:G:285:GLY:HA3	13:G:339:ALA:HB2	1.89	0.55
13:G:457:ALA:O	13:G:461:LEU:HB2	2.06	0.55
14:H:121:ILE:HG22	9:K:460:ILE:HD11	1.89	0.55
7:I:203:ARG:HD2	7:I:358:ASP:HB2	1.87	0.55
8:J:163:ALA:HB3	8:J:180:THR:HG23	1.88	0.55
9:K:404:ASP:C	9:K:406:GLN:H	2.14	0.55
9:K:449:ARG:HB2	9:K:463:LEU:HD11	1.88	0.55
12:F:156:LEU:HD13	12:F:168:LEU:HB2	1.87	0.55
12:F:293:ASN:N	12:F:313:LEU:O	2.39	0.55
8:J:212:SER:O	8:J:376:ARG:NH2	2.39	0.55
9:K:133:MET:O	9:K:137:LEU:HD23	2.06	0.55
9:K:493:LEU:HD22	9:K:495:ILE:HG12	1.88	0.55
1:1:37:LEU:HD13	1:1:90:LYS:HZ2	1.70	0.55
3:3:166:ARG:HA	3:3:169:PHE:HB3	1.89	0.55
9:C:230:ARG:NH2	9:C:309:ILE:O	2.39	0.55
10:D:30:PRO:HB3	10:D:533:ASP:HB3	1.89	0.55
10:D:426:GLY:HA2	10:D:429:GLU:OE2	2.06	0.55
10:D:513:LEU:HA	10:D:516:VAL:HG12	1.87	0.55
13:G:198:LYS:HD2	13:G:217:LYS:HZ2	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:80:GLU:O	3:3:84:THR:HG23	2.07	0.55
6:6:22:ASP:HA	6:6:25:LYS:HZ2	1.72	0.55
8:B:415:MET:HA	8:B:415:MET:HE3	1.88	0.55
9:C:183:VAL:HG12	9:C:371:ALA:H	1.72	0.55
9:C:215:LEU:HD23	9:C:219:MET:HB2	1.89	0.55
9:C:330:ARG:NH1	9:C:343:VAL:HG23	2.21	0.55
9:C:436:PRO:O	9:C:440:VAL:HG23	2.07	0.55
7:I:483:LEU:HD12	7:I:486:ILE:HD13	1.87	0.55
8:J:409:GLY:H	8:J:494:THR:HA	1.72	0.55
10:L:284:LEU:O	10:L:288:LYS:HD3	2.06	0.55
13:O:21:GLN:HG3	13:O:518:GLU:HA	1.88	0.55
2:2:50:GLU:O	2:2:54:HIS:ND1	2.31	0.55
3:3:111:LEU:HD21	5:5:103:PHE:CZ	2.41	0.55
8:B:222:LYS:HE3	8:B:314:HIS:HB2	1.87	0.55
11:E:279:LYS:HA	11:E:282:LYS:HD2	1.89	0.55
7:I:252:VAL:HG23	9:K:248:LYS:HA	1.89	0.55
11:M:135:ASP:O	11:M:139:GLN:HG2	2.06	0.55
11:M:399:LYS:HA	11:M:402:LEU:HG	1.88	0.55
13:O:67:LYS:HE2	13:O:84:LYS:HE2	1.88	0.55
14:P:417:ILE:HG23	14:P:468:TYR:HE1	1.72	0.55
1:1:105:VAL:O	1:1:109:GLU:HG2	2.07	0.55
8:B:48:MET:HG3	10:D:531:LYS:HD3	1.88	0.55
8:B:211:ASP:HB3	8:B:376:ARG:HB2	1.89	0.55
9:C:235:ASN:HB3	9:C:288:ASP:HB3	1.89	0.55
13:G:431:GLN:O	13:G:435:ILE:HG12	2.07	0.55
9:K:33:ILE:HD13	9:K:81:ILE:HD11	1.89	0.55
3:3:91:MET:HB2	4:4:71:ILE:HG21	1.89	0.55
4:4:92:LYS:HA	4:4:95:GLN:HG2	1.88	0.55
7:A:435:GLN:NE2	13:O:462:ASN:HD22	2.03	0.55
11:E:123:LEU:HD21	11:E:446:TYR:HB3	1.87	0.55
13:G:119:GLN:HG2	14:H:50:ASN:HB3	1.87	0.55
13:G:412:ILE:HD12	13:G:415:GLU:HB3	1.88	0.55
12:N:408:VAL:HG21	12:N:501:LYS:HG3	1.89	0.55
14:P:237:ALA:HB1	14:P:350:VAL:HG23	1.89	0.55
11:E:454:ALA:O	11:E:457:VAL:HG12	2.06	0.55
13:G:87:ASP:HA	13:G:91:GLY:HA2	1.89	0.55
13:G:232:TYR:HD1	13:G:348:PHE:CD1	2.25	0.55
10:L:144:GLY:CA	10:L:432:LEU:HD11	2.36	0.55
11:E:417:ARG:HB3	11:E:510:LEU:HD13	1.89	0.55
12:F:217:ARG:NH2	12:F:297:ILE:O	2.35	0.55
13:G:181:ASP:HA	13:G:184:MET:HE2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:G:375:ARG:HG2	13:G:375:ARG:HH11	1.72	0.55
9:K:66:ILE:O	9:K:70:ILE:HG22	2.06	0.55
13:G:22:LEU:HD11	13:G:514:VAL:HG23	1.87	0.54
14:H:220:GLY:H	14:H:373:SER:HA	1.72	0.54
14:P:409:VAL:O	14:P:499:ASP:N	2.40	0.54
7:A:225:MET:HE3	7:A:227:LYS:HD3	1.89	0.54
7:A:246:MET:HE1	9:C:334:ARG:H	1.72	0.54
9:C:406:GLN:HA	9:C:499:LEU:H	1.73	0.54
12:F:86:ASP:O	12:F:396:ARG:NH2	2.40	0.54
5:5:91:TYR:CZ	5:5:93:GLU:HB3	2.43	0.54
10:D:35:PHE:HA	10:D:38:ILE:HG12	1.90	0.54
12:F:122:GLY:HA2	12:F:433:ALA:HB1	1.90	0.54
7:I:351:VAL:HG13	7:I:364:ILE:HG13	1.90	0.54
8:J:302:GLN:OE1	10:L:347:HIS:HB2	2.08	0.54
11:M:521:THR:HA	11:M:524:VAL:HG12	1.89	0.54
7:A:43:LYS:HE3	9:C:520:ASP:HB3	1.90	0.54
10:D:33:ILE:HG21	10:D:534:ASP:HA	1.89	0.54
13:G:192:LEU:HG	13:G:195:ILE:HG23	1.88	0.54
14:H:85:MET:HA	14:H:88:MET:SD	2.47	0.54
8:J:155:PHE:O	8:J:159:LEU:HD23	2.07	0.54
8:J:170:LYS:O	8:J:176:LYS:HD3	2.07	0.54
8:J:415:MET:SD	8:J:444:ARG:HG3	2.47	0.54
10:L:298:LEU:HB3	10:L:324:VAL:HA	1.89	0.54
11:M:226:LYS:HA	11:M:383:VAL:HA	1.90	0.54
3:3:136:ASP:OD1	3:3:137:ILE:N	2.36	0.54
5:5:57:ASN:HD22	5:5:100:LYS:HD2	1.72	0.54
10:D:432:LEU:HD21	10:D:436:LEU:HD13	1.88	0.54
10:D:452:ARG:NH1	11:M:453:ASP:OD1	2.38	0.54
11:E:221:ASP:HB2	11:E:388:ARG:HB2	1.90	0.54
14:H:40:ALA:HB2	14:H:109:GLY:HA3	1.90	0.54
7:I:288:THR:H	7:I:308:VAL:HG22	1.72	0.54
8:J:517:VAL:HG21	11:M:60:MET:HG3	1.88	0.54
1:1:109:GLU:HA	1:1:112:ILE:HG22	1.87	0.54
5:5:30:SER:HA	5:5:33:ILE:HG12	1.90	0.54
9:C:78:LYS:O	9:C:82:GLU:HG2	2.07	0.54
12:F:24:ILE:HG12	12:F:103:LEU:HD22	1.90	0.54
14:H:289:ASN:ND2	14:H:309:ASN:O	2.41	0.54
8:J:203:LYS:HD2	8:J:383:LEU:HG	1.90	0.54
12:N:109:TYR:CD2	12:N:435:LEU:HD21	2.43	0.54
8:B:326:VAL:HA	8:B:367:LEU:HB2	1.89	0.54
8:B:388:ARG:HA	8:B:388:ARG:NH1	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:C:150:ASP:HA	9:C:153:LEU:HD13	1.88	0.54
10:D:152:SER:HB2	10:D:512:LEU:HD23	1.90	0.54
14:H:40:ALA:O	14:H:44:ARG:HB2	2.07	0.54
11:M:62:VAL:HG22	11:M:68:VAL:HG22	1.90	0.54
11:M:430:ALA:HB2	11:M:455:LEU:HB2	1.89	0.54
13:O:320:LYS:HA	13:O:323:MET:HG3	1.89	0.54
14:P:203:ARG:HE	14:P:323:ARG:HD2	1.72	0.54
8:B:51:ILE:HD11	10:D:532:ILE:HG13	1.90	0.54
9:C:215:LEU:HD22	9:C:362:PHE:HD1	1.72	0.54
10:D:248:LEU:HD22	10:D:337:CYS:SG	2.48	0.54
11:E:117:LEU:HD11	11:E:527:ILE:HD11	1.90	0.54
5:5:21:GLN:HA	5:5:24:GLN:HG3	1.90	0.54
7:A:485:TRP:NE1	7:A:499:LYS:HB2	2.23	0.54
8:B:475:THR:OG1	8:B:487:ASP:OD1	2.25	0.54
10:D:119:SER:HB3	10:D:453:ALA:HB1	1.89	0.54
10:D:123:LEU:HD12	10:D:128:ILE:HG13	1.90	0.54
14:H:159:GLU:O	14:H:163:LEU:HG	2.07	0.54
14:H:475:ASN:OD1	14:H:478:VAL:N	2.41	0.54
7:I:140:THR:OG1	7:I:406:LYS:O	2.21	0.54
11:M:135:ASP:O	11:M:138:GLU:HG3	2.08	0.54
12:N:446:ILE:HG13	12:N:450:VAL:HG23	1.89	0.54
8:B:177:ASP:O	8:B:181:LYS:HD3	2.09	0.54
11:M:74:GLY:HA3	11:M:107:THR:HB	1.91	0.54
12:N:35:ARG:NH2	12:N:453:GLN:OE1	2.33	0.54
12:N:270:ARG:HA	12:N:273:LYS:HD2	1.89	0.54
12:N:469:GLU:HG3	12:N:477:VAL:HG11	1.88	0.54
7:A:401:ARG:HA	7:A:404:GLU:HG2	1.90	0.53
9:C:168:TRP:O	9:C:172:ALA:N	2.37	0.53
11:E:418:VAL:HA	11:E:510:LEU:H	1.73	0.53
13:G:33:ALA:O	13:G:37:ARG:N	2.40	0.53
9:K:386:GLU:HG3	9:K:390:ASN:OD1	2.08	0.53
10:L:430:ILE:HG13	10:L:480:LEU:HB3	1.89	0.53
11:M:219:LEU:HD13	11:M:389:GLY:HA2	1.90	0.53
12:N:497:ASN:HB2	12:N:500:VAL:HG12	1.90	0.53
2:2:41:ALA:HA	2:2:104:LEU:HD11	1.90	0.53
3:3:110:ASN:ND2	5:5:42:LYS:HG2	2.23	0.53
7:A:418:ALA:HB2	7:A:471:HIS:CE1	2.43	0.53
8:B:298:ASN:O	8:B:301:GLU:HB3	2.07	0.53
13:G:22:LEU:O	13:G:26:ILE:HG12	2.08	0.53
13:G:245:GLU:OE1	13:G:245:GLU:N	2.41	0.53
14:H:426:TYR:HA	14:H:429:THR:HG22	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:132:ILE:HG21	10:L:446:MET:HG3	1.89	0.53
11:M:117:LEU:CD2	11:M:524:VAL:HG23	2.37	0.53
13:O:71:VAL:HG21	13:O:80:VAL:HG21	1.89	0.53
3:3:78:ILE:HD13	3:3:81:ILE:HD11	1.91	0.53
9:C:498:PRO:HG2	9:C:501:VAL:HG12	1.91	0.53
10:D:429:GLU:HG3	10:D:462:PRO:HD3	1.90	0.53
13:G:414:MET:HG3	13:G:464:LEU:CD2	2.39	0.53
14:H:300:MET:HA	14:H:303:HIS:CE1	2.43	0.53
11:M:129:HIS:CD2	11:M:131:ILE:HG22	2.43	0.53
8:B:480:MET:HA	8:B:480:MET:HE2	1.91	0.53
9:C:137:LEU:HD22	9:C:407:LEU:HD22	1.90	0.53
10:D:343:LYS:HG3	10:D:355:MET:HE1	1.90	0.53
10:D:399:GLU:O	10:D:402:GLU:HG3	2.08	0.53
7:I:267:GLU:HA	7:I:270:ILE:HG22	1.88	0.53
7:I:312:LEU:HG	7:I:315:ASP:H	1.73	0.53
8:J:172:LEU:O	8:J:176:LYS:HG2	2.08	0.53
13:O:449:LEU:HD22	13:O:477:VAL:HG21	1.90	0.53
13:G:195:ILE:HD13	13:G:370:CYS:H	1.74	0.53
7:I:209:MET:HA	7:I:209:MET:HE3	1.89	0.53
10:L:232:LYS:HA	10:L:325:ILE:HA	1.89	0.53
10:L:429:GLU:HG3	10:L:461:ILE:HB	1.90	0.53
11:M:419:VAL:HG21	11:M:513:LYS:HG2	1.91	0.53
8:B:203:LYS:HB3	8:B:383:LEU:HD21	1.90	0.53
8:B:481:ARG:NH1	8:B:482:GLU:OE1	2.42	0.53
14:H:205:CYS:SG	14:H:376:VAL:HA	2.48	0.53
9:K:184:GLN:HG3	9:K:185:PHE:CD2	2.43	0.53
13:O:303:PHE:HB3	13:O:308:MET:HG3	1.91	0.53
13:O:443:GLU:OE1	13:O:465:ARG:NH2	2.42	0.53
7:A:118:ILE:HG23	7:A:522:ILE:HG23	1.90	0.53
7:A:272:LYS:HA	7:A:275:ILE:HG12	1.89	0.53
7:A:286:ILE:O	7:A:307:ALA:HA	2.09	0.53
9:C:158:SER:HB3	9:C:495:ILE:HA	1.91	0.53
11:E:129:HIS:CD2	11:E:131:ILE:HG22	2.44	0.53
12:F:117:ARG:NH1	12:F:517:LEU:HD21	2.24	0.53
14:H:480:LEU:HA	14:H:489:VAL:HA	1.91	0.53
7:I:241:LEU:HD21	7:I:275:ILE:HG21	1.90	0.53
8:J:172:LEU:HB3	8:J:174:HIS:CE1	2.44	0.53
8:J:201:ILE:HG22	8:J:373:ILE:HB	1.89	0.53
1:1:17:GLN:HA	1:1:20:VAL:HG12	1.91	0.53
8:B:229:PRO:HG2	8:B:232:ILE:HD11	1.91	0.53
9:C:227:PRO:HD3	9:C:359:TYR:CD2	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:D:232:LYS:HD2	10:D:326:LYS:HB3	1.90	0.53
10:D:442:THR:HA	11:M:482:VAL:HG11	1.91	0.53
12:F:270:ARG:O	12:F:274:ILE:HG13	2.07	0.53
14:H:69:ALA:HA	14:H:72:ILE:HD12	1.89	0.53
14:H:78:VAL:HG21	14:H:87:VAL:HG21	1.90	0.53
14:H:79:GLN:O	14:H:84:LYS:NZ	2.42	0.53
7:I:427:ALA:HB2	7:I:438:ILE:HB	1.91	0.53
10:L:431:GLU:HB2	10:L:435:ARG:NH2	2.21	0.53
13:O:447:ARG:HB2	13:O:461:LEU:HD11	1.91	0.53
3:3:104:ARG:NH2	4:4:73:ASP:OD1	2.41	0.53
9:C:153:LEU:HG	9:C:173:CYS:SG	2.48	0.53
9:C:193:ILE:HG23	9:C:399:ARG:NH1	2.24	0.53
12:F:348:GLY:HA3	12:F:365:LYS:HG3	1.90	0.53
14:H:73:LEU:HD22	14:H:87:VAL:HG22	1.89	0.53
9:K:440:VAL:O	9:K:444:LEU:HG	2.09	0.53
4:4:66:MET:HE3	4:4:77:SER:OG	2.09	0.53
8:B:71:LEU:HD12	8:B:85:VAL:HG22	1.90	0.53
10:D:109:VAL:HA	10:D:112:ILE:HG22	1.91	0.53
8:J:262:ALA:O	10:L:263:GLN:NE2	2.28	0.53
14:P:424:THR:O	14:P:428:GLU:HG2	2.09	0.53
7:A:67:VAL:HG23	7:A:73:LYS:HD3	1.92	0.52
12:F:317:LYS:HB3	12:F:320:ASN:OD1	2.08	0.52
8:J:247:ASP:HB3	8:J:274:LYS:HB3	1.91	0.52
9:K:109:ALA:HB2	9:K:126:TYR:OH	2.09	0.52
9:K:219:MET:HE1	9:K:360:PHE:HA	1.91	0.52
12:N:90:ASP:C	12:N:500:VAL:HG21	2.34	0.52
12:N:97:LEU:HD22	12:N:450:VAL:HG21	1.90	0.52
12:N:426:LYS:HD2	12:N:438:GLN:HB2	1.91	0.52
9:C:407:LEU:HD12	9:C:408:VAL:O	2.09	0.52
13:G:145:LYS:O	13:G:151:GLN:HG3	2.10	0.52
8:J:112:GLU:HB3	8:J:438:SER:OG	2.09	0.52
11:M:288:MET:HA	11:M:291:GLN:HB3	1.90	0.52
13:O:179:VAL:O	13:O:183:VAL:HG23	2.10	0.52
14:P:69:ALA:HB3	14:P:101:THR:HG23	1.91	0.52
4:4:70:GLN:HB2	4:4:75:PHE:CE1	2.44	0.52
6:6:68:GLU:CD	6:6:70:GLY:H	2.17	0.52
8:B:33:ILE:HG21	8:B:111:ARG:HE	1.74	0.52
9:C:216:ARG:HH11	9:C:216:ARG:HG3	1.73	0.52
9:C:235:ASN:ND2	9:C:287:PRO:O	2.43	0.52
9:C:346:GLY:HA3	9:C:367:LYS:CG	2.39	0.52
11:E:172:THR:HA	11:E:176:LYS:HZ3	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:G:395:ILE:HG22	13:G:398:ARG:HH21	1.73	0.52
13:G:504:THR:O	13:G:508:GLU:HG2	2.08	0.52
14:H:155:ARG:NH2	14:H:194:SER:OG	2.39	0.52
7:I:136:LEU:HD11	7:I:415:VAL:HG23	1.90	0.52
11:M:306:PHE:O	11:M:311:ASN:ND2	2.30	0.52
12:N:446:ILE:HD12	12:N:449:LYS:HD2	1.92	0.52
13:O:111:TYR:CE1	13:O:433:LEU:HD21	2.44	0.52
5:5:41:THR:HA	5:5:44:VAL:HG22	1.92	0.52
10:D:335:PHE:HA	10:D:338:LYS:HZ3	1.74	0.52
11:E:250:ILE:HG12	11:E:353:LEU:HA	1.91	0.52
13:G:279:GLU:OE1	13:G:306:ARG:NH1	2.37	0.52
14:H:397:ASN:O	14:H:401:VAL:HG23	2.09	0.52
9:K:502:LYS:HE3	9:K:506:TYR:CZ	2.44	0.52
10:L:232:LYS:HD3	10:L:374:LEU:HD21	1.91	0.52
11:M:135:ASP:HA	11:M:138:GLU:HG3	1.91	0.52
11:M:286:GLU:HA	11:M:289:ILE:HD12	1.91	0.52
13:O:213:GLY:N	13:O:370:CYS:HA	2.24	0.52
14:P:226:GLU:HB2	14:P:314:ARG:H	1.74	0.52
4:4:89:GLU:OE1	4:4:92:LYS:NZ	2.32	0.52
4:4:100:ALA:O	4:4:103:SER:OG	2.23	0.52
5:5:91:TYR:HD1	6:6:57:PHE:HB2	1.73	0.52
5:5:118:GLN:HB2	5:5:119:PRO:HD3	1.91	0.52
7:A:198:LEU:O	7:A:377:LEU:N	2.31	0.52
8:B:298:ASN:O	8:B:301:GLU:N	2.43	0.52
12:N:459:LEU:HD12	12:N:459:LEU:O	2.08	0.52
13:O:392:ALA:HA	13:O:395:ILE:HD12	1.92	0.52
13:O:431:GLN:O	13:O:435:ILE:HG12	2.10	0.52
14:P:470:VAL:HG13	14:P:478:VAL:HG21	1.91	0.52
1:1:102:GLU:HA	1:1:105:VAL:HG22	1.92	0.52
7:A:103:ASN:HD22	7:A:444:SER:HB2	1.75	0.52
8:B:51:ILE:HB	10:D:535:VAL:HG23	1.91	0.52
9:C:223:ASP:OD1	9:C:224:VAL:N	2.40	0.52
11:E:268:VAL:HG21	11:E:274:TYR:HD1	1.74	0.52
13:G:516:VAL:HG21	14:H:55:MET:HE3	1.91	0.52
14:H:83:ALA:O	14:H:87:VAL:HG23	2.09	0.52
14:H:417:ILE:HG13	14:H:467:LEU:HD22	1.91	0.52
13:O:450:CYS:SG	13:O:457:ALA:HA	2.49	0.52
1:1:16:LEU:HD13	9:C:314:ARG:HH12	1.74	0.52
6:6:89:ARG:O	6:6:93:GLN:HG2	2.09	0.52
12:F:320:ASN:O	12:F:324:LEU:HG	2.09	0.52
13:G:100:LEU:HD12	13:G:104:PHE:CZ	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:H:239:ILE:H	14:H:239:ILE:HD12	1.75	0.52
7:I:81:LEU:HD23	7:I:84:LYS:HE3	1.92	0.52
9:K:230:ARG:NH1	9:K:352:ILE:HD11	2.24	0.52
10:L:213:LYS:HE2	10:L:371:GLY:HA3	1.91	0.52
13:O:210:LEU:HD23	13:O:372:PHE:CD1	2.45	0.52
14:P:268:PHE:O	14:P:271:GLY:N	2.42	0.52
7:A:101:LEU:HD21	7:A:521:ALA:HA	1.92	0.52
8:B:227:ASN:OD1	8:B:228:GLN:N	2.39	0.52
10:D:106:THR:HA	10:D:109:VAL:HG12	1.91	0.52
11:E:165:LEU:HB3	11:E:190:VAL:HG11	1.92	0.52
13:G:111:TYR:HB3	13:G:116:LEU:HD21	1.92	0.52
14:H:434:GLU:O	14:H:438:ILE:HG12	2.09	0.52
13:O:197:ILE:HD12	13:O:372:PHE:HB3	1.91	0.52
1:I:82:GLU:O	1:I:86:ILE:HG12	2.10	0.52
7:I:45:LEU:HG	7:I:64:LEU:HD22	1.92	0.52
8:J:179:PHE:CD1	8:J:390:LEU:HD11	2.44	0.52
10:L:413:ARG:HA	10:L:416:VAL:HG12	1.91	0.52
14:P:165:ARG:NH2	14:P:176:GLU:HB3	2.25	0.52
14:P:325:CYS:O	14:P:330:ALA:N	2.43	0.52
9:C:404:ASP:OD1	9:C:405:PRO:HD2	2.09	0.52
11:E:256:GLU:OE2	11:E:306:PHE:N	2.33	0.52
7:I:99:GLU:HG2	7:I:447:VAL:HB	1.92	0.52
12:N:31:GLN:HG2	12:N:97:LEU:HD23	1.92	0.52
12:N:222:LYS:NZ	12:N:306:SER:O	2.36	0.52
12:N:225:VAL:HG21	12:N:311:VAL:HG21	1.91	0.52
14:P:382:ASP:HA	14:P:385:MET:HB2	1.92	0.52
7:A:231:ASN:OD1	7:A:232:ALA:N	2.43	0.51
9:C:240:LEU:HD11	9:C:324:ALA:HB2	1.93	0.51
10:D:34:ARG:NH2	10:D:533:ASP:OD1	2.44	0.51
10:D:119:SER:OG	10:D:457:ALA:HB2	2.09	0.51
11:E:280:TYR:HB3	13:G:260:VAL:HG22	1.92	0.51
8:J:350:GLU:HG2	8:J:363:SER:HB2	1.92	0.51
11:M:117:LEU:HD21	11:M:524:VAL:HG23	1.91	0.51
14:P:202:ILE:HA	14:P:373:SER:O	2.10	0.51
7:A:69:HIS:HD2	7:A:71:ALA:HB3	1.75	0.51
9:C:416:MET:HE3	9:C:448:PRO:HG3	1.92	0.51
14:H:446:GLU:HB3	14:H:450:ARG:HH21	1.76	0.51
8:J:51:ILE:HD11	10:L:535:VAL:HG12	1.93	0.51
9:K:297:SER:O	9:K:301:GLN:HG2	2.09	0.51
10:L:192:MET:HE2	10:L:192:MET:HA	1.92	0.51
10:L:414:CYS:HB2	10:L:513:LEU:HD22	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:M:50:THR:O	11:M:57:LEU:N	2.35	0.51
12:N:216:ALA:HB2	12:N:314:ARG:HG2	1.92	0.51
12:N:318:ARG:O	12:N:321:MET:N	2.43	0.51
14:P:304:TYR:HA	14:P:307:LYS:HD2	1.90	0.51
11:E:171:THR:HG22	11:E:506:VAL:HA	1.92	0.51
13:G:349:GLU:OE2	13:G:351:THR:OG1	2.25	0.51
14:H:305:ALA:O	14:H:309:ASN:N	2.44	0.51
13:O:496:ALA:O	13:O:500:ILE:HG12	2.11	0.51
5:5:22:LEU:O	5:5:26:VAL:HG23	2.10	0.51
7:A:480:ARG:HB3	7:A:483:LEU:HD23	1.93	0.51
10:D:52:LEU:HD21	10:D:461:ILE:HG13	1.92	0.51
11:E:76:THR:HG21	11:E:400:ARG:NH1	2.25	0.51
12:F:72:PRO:O	12:F:75:SER:N	2.44	0.51
11:M:191:ASN:O	11:M:195:THR:HG23	2.10	0.51
12:N:85:ASP:OD2	12:N:92:THR:HA	2.10	0.51
14:P:301:ALA:HA	14:P:304:TYR:HD2	1.75	0.51
7:I:241:LEU:HD21	7:I:275:ILE:HD13	1.92	0.51
7:I:379:GLY:HA3	7:I:385:CYS:SG	2.51	0.51
8:J:127:ILE:HD11	8:J:515:LEU:HD22	1.92	0.51
10:L:194:VAL:HG21	10:L:208:ILE:HD11	1.93	0.51
11:M:206:PHE:HA	11:M:209:ILE:HG22	1.92	0.51
13:O:168:ILE:HB	13:O:172:LYS:HB3	1.91	0.51
1:1:51:ILE:HD12	1:1:54:LEU:HD11	1.92	0.51
7:A:29:ALA:O	7:A:33:LYS:HB2	2.11	0.51
9:C:288:ASP:OD1	9:C:289:VAL:N	2.43	0.51
10:D:410:CYS:HA	10:D:413:ARG:HG2	1.92	0.51
13:G:241:ASN:HD22	13:G:292:LYS:HD3	1.76	0.51
9:K:158:SER:O	9:K:162:THR:HG23	2.10	0.51
11:M:31:LEU:O	11:M:35:LYS:HG2	2.11	0.51
13:O:118:PRO:HD2	14:P:52:MET:HE1	1.93	0.51
13:O:156:GLU:HG2	13:O:176:ALA:HB1	1.92	0.51
13:O:232:TYR:HB2	13:O:348:PHE:HB3	1.93	0.51
1:1:67:MET:HE1	5:5:49:CYS:SG	2.51	0.51
4:4:107:SER:HA	4:4:110:ARG:HG2	1.93	0.51
5:5:105:ARG:NH2	6:6:50:LEU:HD22	2.25	0.51
7:A:238:ASP:H	7:A:327:ILE:HG12	1.75	0.51
9:C:231:ARG:NE	9:C:232:TYR:H	2.08	0.51
10:D:335:PHE:HA	10:D:338:LYS:NZ	2.25	0.51
12:F:321:MET:O	12:F:325:THR:HG23	2.11	0.51
9:K:129:ALA:O	9:K:133:MET:HG3	2.10	0.51
9:K:434:GLN:HG2	9:K:438:ARG:HH12	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:46:ASP:HB2	10:L:49:ARG:NH2	2.26	0.51
7:A:242:GLN:HG3	7:A:244:THR:N	2.23	0.51
12:F:352:GLU:OE2	12:F:359:LYS:NZ	2.37	0.51
14:H:239:ILE:H	14:H:345:GLY:HA3	1.76	0.51
8:J:50:LYS:NZ	10:L:534:ASP:HB2	2.26	0.51
11:M:168:THR:HG23	11:M:507:ILE:HG21	1.93	0.51
11:M:225:ILE:O	11:M:384:THR:N	2.44	0.51
13:O:202:GLY:H	13:O:377:GLY:HA2	1.75	0.51
13:O:303:PHE:CD1	13:O:310:CYS:HB2	2.45	0.51
12:F:46:MET:HB3	12:F:56:LEU:HD13	1.92	0.51
13:G:86:GLN:HE21	13:G:502:ALA:HA	1.75	0.51
13:G:234:ASN:HB2	13:G:344:ARG:HH12	1.76	0.51
8:J:190:LEU:HG	8:J:192:GLY:H	1.76	0.51
8:J:413:SER:O	8:J:417:MET:HG3	2.11	0.51
13:O:162:ALA:HB1	13:O:395:ILE:HD12	1.91	0.51
13:O:213:GLY:HA3	13:O:361:PHE:O	2.11	0.51
14:P:506:TRP:HE3	14:P:510:LEU:HD11	1.76	0.51
1:1:109:GLU:O	1:1:113:ARG:HG2	2.11	0.51
4:4:56:ASP:O	4:4:60:ALA:N	2.39	0.51
4:4:94:LEU:O	4:4:98:ILE:HG12	2.11	0.51
8:B:51:ILE:HG21	8:B:61:LEU:HD12	1.93	0.51
8:B:228:GLN:HG2	8:B:311:ALA:H	1.74	0.51
8:B:322:ARG:O	8:B:326:VAL:HG22	2.11	0.51
11:E:132:ARG:NH1	13:G:482:GLU:HG3	2.25	0.51
12:F:109:TYR:CZ	12:F:435:LEU:HD22	2.46	0.51
13:G:398:ARG:HD2	13:G:495:PRO:HG2	1.92	0.51
8:J:43:LEU:HD12	8:J:104:VAL:HG21	1.93	0.51
10:L:488:GLU:OE2	10:L:502:ASN:ND2	2.36	0.51
12:N:376:ILE:O	12:N:376:ILE:HG13	2.11	0.51
3:3:126:TRP:HB2	3:3:132:MET:HE1	1.93	0.50
13:G:259:THR:HG23	13:G:261:GLU:H	1.75	0.50
8:J:205:LEU:HB3	8:J:378:ALA:HA	1.94	0.50
10:L:52:LEU:HA	10:L:107:THR:HG21	1.92	0.50
12:N:28:ARG:CZ	12:N:104:LYS:HE2	2.42	0.50
13:O:192:LEU:O	13:O:195:ILE:HG22	2.12	0.50
5:5:29:LEU:HD12	5:5:125:HIS:NE2	2.26	0.50
7:A:175:ALA:O	7:A:179:ILE:HG13	2.10	0.50
8:B:205:LEU:O	8:B:376:ARG:NH2	2.43	0.50
9:C:46:MET:HE2	12:F:115:HIS:CE1	2.46	0.50
9:C:204:ILE:HB	9:C:377:ARG:HA	1.94	0.50
10:D:74:GLY:HA2	10:D:77:ILE:HD12	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:E:139:GLN:HA	11:E:142:ARG:HD2	1.92	0.50
12:F:95:ASN:ND2	12:F:507:SER:OG	2.36	0.50
12:F:98:ILE:HD11	12:F:444:LEU:HD22	1.92	0.50
13:G:96:SER:O	13:G:100:LEU:HD23	2.11	0.50
9:K:386:GLU:OE2	9:K:390:ASN:ND2	2.44	0.50
10:L:58:ASP:OD2	10:L:71:THR:N	2.44	0.50
10:L:117:LEU:HD11	10:L:529:ILE:HG21	1.92	0.50
10:L:397:VAL:O	10:L:400:GLU:HG2	2.12	0.50
13:O:182:ALA:O	13:O:186:LEU:HG	2.10	0.50
14:P:387:ASP:OD1	14:P:390:ARG:NH2	2.45	0.50
7:A:196:ASN:ND2	7:A:215:ALA:O	2.44	0.50
7:A:227:LYS:NZ	7:A:360:GLU:OE2	2.34	0.50
11:E:185:MET:HA	11:E:188:ILE:HG22	1.92	0.50
14:H:473:GLU:OE1	14:H:473:GLU:N	2.45	0.50
7:I:462:ASP:OD2	7:I:466:LYS:NZ	2.44	0.50
8:J:417:MET:HB2	8:J:443:LEU:HD21	1.92	0.50
11:M:235:SER:HB3	11:M:311:ASN:ND2	2.26	0.50
12:N:153:ARG:HA	12:N:169:THR:HG21	1.92	0.50
4:4:39:GLU:HA	4:4:42:VAL:HG22	1.93	0.50
12:F:97:LEU:HD21	12:F:450:VAL:HG21	1.94	0.50
12:F:156:LEU:HD11	12:F:172:VAL:HG21	1.93	0.50
7:I:430:MET:SD	7:I:432:SER:OG	2.66	0.50
8:J:466:ARG:O	8:J:470:SER:HB2	2.12	0.50
11:M:214:LYS:HB3	11:M:388:ARG:HH21	1.76	0.50
14:P:112:LEU:HD11	14:P:518:VAL:HG11	1.94	0.50
14:P:228:GLU:OE1	14:P:359:GLN:NE2	2.33	0.50
9:C:165:ILE:HG13	9:C:390:ASN:HD22	1.76	0.50
14:H:49:PRO:HG3	15:H:5000:ADP:C5	2.47	0.50
14:H:277:ASP:O	14:H:281:LYS:HG2	2.10	0.50
7:I:156:MET:HE1	7:I:501:ALA:HB1	1.94	0.50
9:K:215:LEU:HB2	9:K:375:LEU:HB2	1.92	0.50
13:O:122:ILE:HG23	13:O:511:CYS:HB2	1.93	0.50
10:D:316:PHE:O	10:D:319:LYS:HG2	2.12	0.50
13:G:121:ILE:HG22	13:G:434:LEU:HD13	1.94	0.50
13:G:215:ALA:HB3	13:G:358:TYR:HE1	1.75	0.50
14:H:214:SER:OG	14:H:378:ARG:NE	2.31	0.50
7:I:183:ASP:HB3	7:I:189:ARG:HH21	1.76	0.50
9:K:198:TYR:HB3	9:K:370:LYS:O	2.12	0.50
9:K:466:LEU:HD22	9:K:480:VAL:HG13	1.94	0.50
3:3:91:MET:HE1	4:4:76:ILE:HD13	1.94	0.50
5:5:41:THR:O	5:5:44:VAL:HG22	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:6:15:LYS:HB2	6:6:104:GLN:HG2	1.92	0.50
11:E:530:ILE:HA	13:G:46:ASP:O	2.12	0.50
12:F:106:ALA:O	12:F:110:ILE:HG12	2.11	0.50
9:K:216:ARG:NH2	9:K:366:CYS:HA	2.27	0.50
14:P:261:THR:OG1	14:P:264:GLU:OE2	2.28	0.50
3:3:81:ILE:O	3:3:84:THR:OG1	2.24	0.50
9:C:456:GLY:O	12:F:432:ARG:NH2	2.44	0.50
13:G:190:LEU:N	13:G:397:ARG:HH22	2.10	0.50
7:I:35:SER:OG	7:I:56:ASN:O	2.29	0.50
14:P:408:LEU:HA	14:P:501:TYR:H	1.76	0.50
5:5:114:MET:O	5:5:118:GLN:NE2	2.45	0.50
6:6:78:LYS:HZ1	6:6:79:ARG:HH12	1.60	0.50
7:A:197:ILE:HD12	7:A:389:GLU:HG3	1.94	0.50
7:A:485:TRP:CD2	7:A:499:LYS:HD3	2.47	0.50
9:C:289:VAL:HG21	9:C:350:LEU:HD13	1.93	0.50
9:C:407:LEU:HD23	9:C:499:LEU:HA	1.93	0.50
11:E:35:LYS:HE3	11:E:121:GLU:HG2	1.94	0.50
11:E:37:HIS:CD2	11:E:87:ILE:HD12	2.46	0.50
11:E:247:LYS:HD3	11:E:248:ILE:H	1.77	0.50
11:E:434:SER:OG	10:L:441:ARG:NH2	2.43	0.50
8:J:421:VAL:HG11	8:J:439:TYR:HD1	1.76	0.50
9:K:34:ALA:O	9:K:38:ARG:HB2	2.12	0.50
9:K:194:ASP:OD2	9:K:198:TYR:HB2	2.11	0.50
9:K:217:GLY:HA2	9:K:370:LYS:HE3	1.94	0.50
11:M:217:GLY:HA3	11:M:388:ARG:HD3	1.94	0.50
8:B:112:GLU:HB3	8:B:438:SER:OG	2.11	0.49
8:B:151:ASP:OD1	8:B:155:PHE:HB2	2.12	0.49
8:B:232:ILE:HB	8:B:349:ILE:HD12	1.93	0.49
12:F:317:LYS:HG3	12:F:318:ARG:H	1.76	0.49
13:G:200:VAL:N	13:G:374:LEU:O	2.45	0.49
7:I:207:GLU:O	7:I:378:ARG:HB3	2.12	0.49
7:I:242:GLN:NE2	7:I:271:THR:OG1	2.41	0.49
8:J:236:LYS:HA	8:J:236:LYS:HE3	1.93	0.49
10:L:48:ILE:HG13	10:L:78:LEU:HD21	1.93	0.49
11:M:214:LYS:NZ	11:M:231:ASP:OD1	2.42	0.49
11:M:225:ILE:HG13	11:M:386:PHE:HB2	1.94	0.49
12:N:191:ILE:HG13	12:N:191:ILE:O	2.11	0.49
12:N:275:ILE:HA	12:N:278:LYS:HG2	1.93	0.49
12:N:409:PRO:HG3	12:N:476:LEU:HD13	1.93	0.49
13:O:209:GLN:O	13:O:373:ILE:HG22	2.12	0.49
5:5:83:LEU:CB	5:5:91:TYR:HE2	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:D:314:LEU:HA	10:D:317:LEU:HG	1.93	0.49
11:E:180:SER:HB3	11:E:182:HIS:CE1	2.47	0.49
11:E:322:VAL:HG11	11:E:372:LEU:HD11	1.92	0.49
12:F:176:ILE:HG13	12:F:398:VAL:CG1	2.42	0.49
12:F:234:ASN:ND2	12:F:334:ASN:OD1	2.45	0.49
13:G:395:ILE:HG22	13:G:398:ARG:NH2	2.27	0.49
14:H:163:LEU:O	14:H:166:THR:HG22	2.12	0.49
7:I:18:ARG:HH12	7:I:108:VAL:HG11	1.76	0.49
7:I:239:PHE:HB3	7:I:288:THR:HA	1.93	0.49
9:K:145:ASP:OD1	9:K:146:ILE:N	2.42	0.49
11:M:148:LEU:HG	11:M:510:LEU:HD11	1.93	0.49
12:N:28:ARG:HH11	12:N:28:ARG:HG3	1.76	0.49
14:P:183:ILE:HD11	14:P:392:VAL:HG22	1.92	0.49
7:A:209:MET:HB2	7:A:376:ILE:HD11	1.93	0.49
8:B:326:VAL:HG23	8:B:327:THR:HG23	1.94	0.49
10:D:297:VAL:HG12	10:D:323:MET:HB2	1.94	0.49
11:E:498:THR:OG1	11:E:500:ASP:OD2	2.29	0.49
12:F:196:MET:SD	12:F:377:LYS:HE3	2.52	0.49
13:G:394:MET:O	13:G:398:ARG:HG2	2.12	0.49
7:I:125:CYS:HB2	7:I:518:THR:HG21	1.94	0.49
8:J:222:LYS:NZ	8:J:228:GLN:OE1	2.41	0.49
8:J:244:MET:SD	8:J:304:PHE:HZ	2.35	0.49
8:J:491:LEU:HB3	8:J:493:ILE:HD12	1.94	0.49
11:M:279:LYS:O	11:M:283:GLU:HG2	2.11	0.49
12:N:229:TYR:HB2	12:N:289:PHE:HD2	1.77	0.49
14:P:250:ILE:HG22	14:P:253:THR:HG22	1.94	0.49
1:I:88:GLU:HG3	1:I:92:LYS:HZ1	1.76	0.49
7:A:180:LYS:HE3	7:A:188:PRO:HB2	1.93	0.49
7:A:520:ALA:O	7:A:524:ILE:HG22	2.12	0.49
11:E:76:THR:HG21	11:E:400:ARG:HH12	1.77	0.49
7:I:264:ARG:NH1	9:K:241:LEU:O	2.45	0.49
8:J:244:MET:HG2	8:J:248:LYS:HG2	1.94	0.49
9:K:88:ASP:HA	9:K:92:GLY:HA2	1.94	0.49
11:M:284:LYS:O	11:M:287:GLU:HG3	2.13	0.49
12:N:31:GLN:O	12:N:35:ARG:N	2.46	0.49
7:A:325:ALA:HA	7:A:344:MET:HA	1.94	0.49
8:B:130:TRP:O	8:B:134:THR:HG23	2.12	0.49
8:B:173:THR:O	8:B:176:LYS:NZ	2.34	0.49
12:F:164:LEU:O	12:F:168:LEU:HG	2.12	0.49
14:H:68:ASP:HB3	14:H:390:ARG:HD2	1.95	0.49
14:H:81:PRO:HA	14:H:84:LYS:HE2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:H:138:LYS:O	14:H:141:GLU:HG3	2.12	0.49
13:O:303:PHE:CD2	13:O:308:MET:HE3	2.39	0.49
14:P:98:GLY:HA3	14:P:397:ASN:HB3	1.94	0.49
1:1:37:LEU:HD12	1:1:40:THR:OG1	2.12	0.49
6:6:83:ILE:O	6:6:87:ILE:HG13	2.13	0.49
8:B:51:ILE:HG13	8:B:63:VAL:HG12	1.94	0.49
11:E:38:ILE:HG23	11:E:117:LEU:HB3	1.95	0.49
11:E:158:ASP:OD1	11:E:159:ILE:N	2.45	0.49
11:E:258:PRO:O	11:E:264:HIS:ND1	2.46	0.49
12:F:137:VAL:HG11	12:F:414:VAL:HG23	1.95	0.49
12:F:211:VAL:HG23	12:F:373:THR:HG21	1.94	0.49
13:G:235:PRO:HG2	13:G:345:CYS:HB2	1.94	0.49
8:J:239:ILE:HG22	8:J:291:ILE:HD11	1.95	0.49
9:K:34:ALA:HB2	9:K:103:GLY:HA3	1.94	0.49
10:L:437:THR:O	10:L:441:ARG:HG3	2.12	0.49
11:M:288:MET:O	11:M:292:ILE:N	2.38	0.49
7:A:418:ALA:HB2	7:A:471:HIS:ND1	2.28	0.49
9:C:64:ASN:O	9:C:68:ARG:HG2	2.13	0.49
9:C:214:VAL:HA	9:C:375:LEU:H	1.77	0.49
11:E:102:ILE:HD11	11:E:515:GLN:HB3	1.93	0.49
14:H:241:VAL:HG12	14:H:332:ALA:HB2	1.95	0.49
7:I:272:LYS:HA	7:I:275:ILE:HG12	1.94	0.49
7:I:418:ALA:HB2	7:I:471:HIS:CD2	2.48	0.49
8:J:296:ILE:HG22	8:J:300:PRO:HB2	1.95	0.49
10:L:227:LEU:HD11	10:L:339:THR:HG21	1.95	0.49
11:M:328:PRO:HA	11:M:331:GLU:OE2	2.13	0.49
7:A:132:ILE:HD11	7:A:419:LEU:HD22	1.95	0.49
8:B:40:LYS:HA	8:B:43:LEU:HD23	1.95	0.49
10:D:219:ASP:OD1	10:D:220:ASP:N	2.46	0.49
11:E:458:ILE:O	11:E:462:LEU:CB	2.61	0.49
12:F:451:LEU:HD12	12:F:481:LEU:HD12	1.94	0.49
13:O:394:MET:HE2	13:O:394:MET:HA	1.95	0.49
7:A:198:LEU:N	7:A:375:ILE:O	2.46	0.49
7:A:499:LYS:HA	7:A:504:PHE:CZ	2.48	0.49
8:B:162:ILE:HG22	8:B:494:THR:HG21	1.94	0.49
10:D:213:LYS:HD3	10:D:373:LEU:HD21	1.93	0.49
11:E:286:GLU:OE2	11:E:317:ASN:ND2	2.28	0.49
12:F:115:HIS:O	12:F:118:ILE:HG12	2.13	0.49
12:F:176:ILE:HA	12:F:179:ILE:HG22	1.95	0.49
13:O:152:ARG:HB2	13:O:180:VAL:HG21	1.94	0.49
13:O:392:ALA:O	13:O:395:ILE:HB	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:57:GLU:HB3	1:1:60:MET:HE3	1.95	0.49
2:2:66:GLU:HA	3:3:133:LEU:HD21	1.94	0.49
7:A:136:LEU:HD23	7:A:415:VAL:HG13	1.95	0.49
7:A:433:ARG:NH1	13:O:458:THR:OG1	2.46	0.49
10:D:120:CYS:HB3	10:D:530:LEU:HD21	1.94	0.49
11:E:170:LYS:HD2	11:E:173:LEU:HD12	1.93	0.49
12:F:109:TYR:HB3	12:F:114:LEU:HG	1.95	0.49
7:I:143:LEU:HD23	7:I:499:LYS:HD2	1.94	0.49
10:L:113:ALA:O	10:L:117:LEU:HD23	2.13	0.49
11:M:41:ALA:CB	11:M:117:LEU:HD12	2.43	0.49
11:M:340:ARG:HD2	11:M:341:ILE:O	2.13	0.49
11:M:444:GLU:OE1	11:M:444:GLU:N	2.41	0.49
12:N:314:ARG:HD3	12:N:315:ARG:NH1	2.28	0.49
13:O:395:ILE:HA	13:O:398:ARG:CZ	2.42	0.49
5:5:83:LEU:HB2	5:5:91:TYR:HE2	1.78	0.48
7:A:357:CYS:SG	7:A:378:ARG:NH2	2.86	0.48
10:D:345:VAL:HG22	10:D:355:MET:CE	2.43	0.48
11:E:141:ALA:O	11:E:145:ILE:HG12	2.12	0.48
13:G:183:VAL:O	13:G:187:ASP:HB2	2.13	0.48
7:I:218:CYS:SG	7:I:219:VAL:N	2.86	0.48
11:M:236:HIS:HD2	11:M:237:PRO:HD2	1.78	0.48
11:M:394:ILE:O	11:M:397:GLU:HG3	2.13	0.48
5:5:65:PRO:HA	5:5:70:MET:O	2.13	0.48
6:6:30:ARG:NH2	6:6:83:ILE:HD12	2.28	0.48
6:6:95:ARG:O	6:6:98:GLU:HG3	2.13	0.48
7:A:434:GLU:O	7:A:438:ILE:HG12	2.12	0.48
9:C:290:VAL:O	9:C:312:ILE:N	2.44	0.48
9:C:416:MET:HE3	9:C:448:PRO:CG	2.44	0.48
10:D:116:LEU:HD11	10:D:454:PHE:CD2	2.48	0.48
11:E:49:ARG:NE	11:E:464:GLU:OE1	2.43	0.48
12:F:109:TYR:O	12:F:114:LEU:HD23	2.14	0.48
13:G:166:LYS:NZ	13:G:381:PHE:HB3	2.28	0.48
13:G:188:ASP:O	13:G:368:LYS:NZ	2.46	0.48
7:I:168:PHE:O	7:I:172:VAL:HG23	2.13	0.48
7:I:402:VAL:O	7:I:405:SER:OG	2.26	0.48
9:K:409:PRO:HA	9:K:496:TRP:CE3	2.48	0.48
10:L:352:THR:O	10:L:355:MET:HG3	2.14	0.48
13:O:152:ARG:CB	13:O:180:VAL:HG21	2.43	0.48
14:P:238:LYS:HB3	14:P:287:GLY:C	2.38	0.48
7:A:143:LEU:HD11	7:A:504:PHE:CE2	2.47	0.48
10:D:418:LYS:HD2	10:D:512:LEU:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:E:323:ARG:HG3	11:E:324:TRP:CD1	2.47	0.48
13:G:136:ILE:HD11	13:G:416:LEU:HD11	1.95	0.48
13:G:294:PRO:HB3	13:G:313:ARG:HE	1.77	0.48
7:I:430:MET:HE1	7:I:434:GLU:HG2	1.95	0.48
8:J:136:ALA:HB2	8:J:424:LEU:HD13	1.95	0.48
9:K:223:ASP:O	9:K:229:MET:HG2	2.13	0.48
13:O:242:VAL:HB	13:O:334:VAL:HB	1.96	0.48
14:P:39:LEU:HD22	14:P:83:ALA:HB1	1.94	0.48
7:A:450:ASN:O	7:A:454:VAL:HG23	2.13	0.48
12:F:131:LEU:O	12:F:135:GLU:HG2	2.14	0.48
13:G:194:MET:HG3	13:G:368:LYS:HG3	1.96	0.48
9:K:272:GLU:HG2	9:K:297:SER:HB2	1.95	0.48
11:M:460:MET:HG3	11:M:470:PRO:HB2	1.95	0.48
12:N:36:THR:HA	12:N:454:ASN:OD1	2.14	0.48
12:N:165:ALA:O	12:N:169:THR:HG23	2.13	0.48
13:O:405:VAL:HA	13:O:495:PRO:HA	1.95	0.48
14:P:300:MET:HG3	14:P:304:TYR:CE2	2.48	0.48
4:4:57:ILE:HG21	6:6:63:VAL:HG21	1.94	0.48
5:5:91:TYR:CD1	6:6:57:PHE:HB2	2.49	0.48
5:5:93:GLU:HG3	6:6:55:VAL:H	1.78	0.48
14:H:62:LYS:HD2	14:H:63:LEU:H	1.78	0.48
14:H:169:MET:HG2	14:H:176:GLU:HG2	1.95	0.48
7:I:142:GLU:HB3	7:I:149:ILE:HD12	1.94	0.48
7:I:260:LEU:HG	9:K:248:LYS:NZ	2.29	0.48
12:N:23:ASN:HD22	12:N:518:VAL:HG21	1.79	0.48
12:N:319:ARG:HH12	12:N:322:GLU:HB2	1.78	0.48
14:P:467:LEU:O	14:P:471:HIS:HB2	2.13	0.48
5:5:21:GLN:O	5:5:25:GLU:HG2	2.13	0.48
10:D:250:GLN:HA	10:D:301:GLN:CD	2.38	0.48
10:D:400:GLU:O	10:D:403:ARG:HD3	2.14	0.48
11:E:34:LEU:O	11:E:38:ILE:HG12	2.13	0.48
11:E:365:GLY:N	11:E:369:ASP:OD1	2.46	0.48
8:J:396:VAL:HA	8:J:399:GLN:NE2	2.27	0.48
9:K:57:ILE:HG23	12:N:76:LEU:HD13	1.94	0.48
9:K:160:ILE:HG23	9:K:390:ASN:ND2	2.28	0.48
9:K:270:MET:HG3	9:K:274:TYR:HE2	1.79	0.48
10:L:149:THR:HA	10:L:512:LEU:HD11	1.95	0.48
10:L:415:LEU:O	10:L:419:ARG:N	2.37	0.48
11:M:249:ALA:HB3	11:M:300:ALA:HA	1.95	0.48
13:O:145:LYS:HD2	13:O:148:LYS:HE3	1.95	0.48
13:O:406:VAL:HG21	13:O:412:ILE:HD13	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:81:GLU:O	4:4:84:GLN:HG3	2.14	0.48
7:A:97:ALA:O	7:A:101:LEU:HG	2.14	0.48
7:A:421:ILE:HD11	7:A:468:ARG:CG	2.44	0.48
9:C:247:TYR:HD1	9:C:297:SER:HB2	1.78	0.48
12:F:399:LYS:HD2	12:F:402:ILE:HD11	1.96	0.48
14:H:45:THR:HB	14:H:52:MET:HB2	1.94	0.48
14:H:190:ILE:O	14:H:190:ILE:HG22	2.13	0.48
14:H:356:GLY:O	14:H:378:ARG:NH1	2.47	0.48
7:I:104:ALA:O	7:I:108:VAL:HG23	2.14	0.48
8:J:202:ILE:HG22	8:J:204:LYS:H	1.79	0.48
11:M:154:SER:HA	11:M:417:ARG:HA	1.95	0.48
11:M:523:MET:O	11:M:527:ILE:HG12	2.14	0.48
14:P:223:PHE:HZ	14:P:324:LEU:HB3	1.79	0.48
6:6:30:ARG:HE	6:6:87:ILE:HD11	1.78	0.48
7:A:322:ALA:HB2	7:A:370:ARG:NH2	2.29	0.48
9:C:401:VAL:HG23	9:C:402:LEU:HD22	1.96	0.48
9:C:407:LEU:HD21	9:C:502:LYS:HB3	1.96	0.48
12:F:435:LEU:HD11	12:N:460:GLN:NE2	2.29	0.48
14:H:450:ARG:HB2	14:H:460:ALA:HB1	1.96	0.48
11:M:463:SER:HB3	11:M:470:PRO:HA	1.95	0.48
12:N:93:THR:O	12:N:96:VAL:N	2.46	0.48
7:A:218:CYS:SG	7:A:362:ILE:HG12	2.54	0.48
8:J:223:LYS:HE2	8:J:226:VAL:HG21	1.95	0.48
9:K:65:ALA:HA	9:K:68:ARG:HH11	1.79	0.48
14:P:171:LYS:HE2	14:P:171:LYS:HA	1.95	0.48
14:P:419:LEU:O	14:P:423:ILE:HG12	2.14	0.48
5:5:105:ARG:HD2	5:5:105:ARG:C	2.39	0.48
9:C:178:ASP:O	9:C:182:MET:HE2	2.13	0.48
9:C:470:HIS:CE1	9:C:476:GLU:HA	2.49	0.48
11:E:494:LEU:HB2	11:E:504:GLN:HE22	1.79	0.48
12:F:512:ALA:O	12:F:516:LEU:HD23	2.13	0.48
13:G:17:GLN:HG2	13:G:518:GLU:CD	2.39	0.48
13:G:129:THR:HG22	13:G:438:TYR:OH	2.13	0.48
14:H:322:ARG:HB3	14:H:326:LYS:HZ3	1.79	0.48
14:H:447:ALA:HA	14:H:450:ARG:HE	1.79	0.48
7:I:446:LEU:HD11	7:I:468:ARG:NH1	2.29	0.48
9:K:330:ARG:HH22	9:K:345:THR:HG23	1.79	0.48
9:K:355:ILE:HD13	9:K:377:ARG:HH12	1.78	0.48
10:L:108:SER:O	10:L:112:ILE:HG12	2.13	0.48
4:4:67:ILE:O	4:4:77:SER:HA	2.14	0.47
10:D:461:ILE:HG23	10:D:462:PRO:HD3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:H:27:GLU:OE2	14:H:29:VAL:N	2.43	0.47
14:H:179:LEU:HA	14:H:182:LEU:HG	1.94	0.47
7:I:250:VAL:HB	7:I:260:LEU:HD21	1.95	0.47
9:K:38:ARG:HA	9:K:100:ILE:HG12	1.94	0.47
12:N:161:HIS:HE1	14:P:133:GLU:HG3	1.79	0.47
13:O:350:GLU:HG2	13:O:357:ARG:HE	1.79	0.47
13:O:414:MET:HE2	13:O:414:MET:HA	1.96	0.47
1:1:116:LEU:HD13	9:C:314:ARG:HH11	1.79	0.47
8:B:127:ILE:HD12	8:B:512:GLU:HG3	1.96	0.47
8:B:141:LEU:HD11	8:B:407:VAL:HG21	1.96	0.47
9:C:102:ALA:O	9:C:106:LEU:HD23	2.14	0.47
9:C:310:THR:HG22	9:C:311:ALA:N	2.28	0.47
9:C:497:GLU:HG2	9:C:498:PRO:HD2	1.96	0.47
10:D:300:ILE:HB	10:D:326:LYS:HA	1.96	0.47
11:E:216:GLY:N	11:E:389:GLY:O	2.44	0.47
7:I:330:THR:OG1	7:I:341:GLU:OE1	2.25	0.47
8:J:415:MET:HG2	8:J:465:LEU:HD23	1.95	0.47
9:K:209:ILE:HG22	9:K:378:GLY:HA2	1.95	0.47
11:M:128:ILE:HG23	11:M:443:LEU:HD11	1.96	0.47
13:O:292:LYS:HE2	13:O:316:GLU:OE2	2.13	0.47
9:C:168:TRP:HD1	9:C:171:LEU:HD21	1.79	0.47
13:G:80:VAL:O	13:G:84:LYS:HG2	2.14	0.47
7:I:198:LEU:HB2	7:I:375:ILE:O	2.13	0.47
8:J:236:LYS:HG3	8:J:287:ILE:HA	1.96	0.47
9:K:386:GLU:OE1	9:K:389:ARG:NE	2.48	0.47
10:L:346:ALA:H	10:L:350:GLN:NE2	2.11	0.47
11:M:158:ASP:OD2	11:M:165:LEU:HG	2.15	0.47
13:O:121:ILE:HA	13:O:434:LEU:HD13	1.95	0.47
13:O:161:THR:HA	13:O:164:SER:HB2	1.96	0.47
2:2:96:GLN:O	2:2:100:ILE:HG12	2.15	0.47
7:A:319:ILE:HG22	7:A:325:ALA:HB3	1.96	0.47
8:B:141:LEU:HG	8:B:497:PHE:HE1	1.78	0.47
9:C:419:ALA:HB1	9:C:441:ALA:HB1	1.96	0.47
10:D:214:LEU:HD13	10:D:395:LYS:HD2	1.96	0.47
12:F:163:GLU:O	12:F:167:VAL:HG23	2.14	0.47
12:F:295:LYS:O	12:F:314:ARG:HB2	2.15	0.47
8:J:167:LEU:HG	8:J:179:PHE:HB3	1.95	0.47
8:J:238:LEU:HG	8:J:341:VAL:HG21	1.95	0.47
9:K:73:GLN:O	9:K:78:LYS:HE2	2.15	0.47
10:L:410:CYS:O	10:L:413:ARG:HG2	2.13	0.47
13:O:385:THR:HG23	13:O:389:LEU:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:82:GLU:OE1	4:4:82:GLU:N	2.46	0.47
7:A:103:ASN:HB3	7:A:440:GLU:HG3	1.96	0.47
7:A:214:TYR:CE2	7:A:364:ILE:HD13	2.50	0.47
8:B:127:ILE:HD11	8:B:515:LEU:HD22	1.97	0.47
9:C:71:GLN:H	12:F:524:ALA:HB2	1.79	0.47
12:F:102:LEU:HD11	12:F:123:PHE:CE1	2.50	0.47
12:F:387:ILE:O	12:F:391:VAL:HG23	2.14	0.47
12:F:487:MET:HE3	12:F:488:VAL:N	2.28	0.47
8:J:30:ILE:H	8:J:30:ILE:HD12	1.79	0.47
9:K:426:SER:OG	9:K:438:ARG:NH2	2.47	0.47
10:L:91:LEU:HD13	10:L:94:LEU:HD13	1.97	0.47
10:L:115:SER:OG	10:L:460:VAL:HG11	2.14	0.47
12:N:120:THR:HB	12:N:513:THR:HG22	1.97	0.47
13:O:312:GLY:C	13:O:313:ARG:HD3	2.40	0.47
1:1:60:MET:SD	2:2:79:VAL:HA	2.54	0.47
7:A:35:SER:HB2	7:A:56:ASN:O	2.14	0.47
8:B:164:GLY:HA2	8:B:180:THR:HG21	1.96	0.47
8:B:189:ARG:HH12	8:B:216:GLU:HB2	1.79	0.47
11:E:170:LYS:HZ2	11:E:181:CYS:HB2	1.79	0.47
11:E:427:ILE:CG2	11:E:459:PRO:HG2	2.45	0.47
13:G:413:GLU:CD	13:G:499:ARG:HH12	2.23	0.47
14:H:144:PRO:HA	14:H:147:VAL:HG23	1.95	0.47
14:H:179:LEU:HG	14:H:388:ILE:HD11	1.97	0.47
8:J:102:VAL:HB	8:J:503:VAL:HG23	1.95	0.47
9:K:62:ASP:OD2	9:K:64:ASN:ND2	2.47	0.47
10:L:44:VAL:O	10:L:48:ILE:HG12	2.14	0.47
14:P:169:MET:SD	15:P:601:ADP:N6	2.88	0.47
1:1:65:GLY:O	5:5:71:TYR:OH	2.33	0.47
4:4:70:GLN:HB2	4:4:75:PHE:CD1	2.49	0.47
5:5:33:ILE:O	5:5:36:LEU:HB3	2.15	0.47
5:5:79:VAL:HA	5:5:82:VAL:HG23	1.96	0.47
9:C:326:ALA:HB2	9:C:371:ALA:HB3	1.96	0.47
10:D:118:ASP:O	10:D:121:THR:HG22	2.14	0.47
10:D:240:ARG:HH12	10:D:242:GLU:HB2	1.80	0.47
11:E:163:GLU:O	11:E:167:GLN:HG2	2.15	0.47
11:E:188:ILE:HG12	11:E:385:ILE:HD12	1.96	0.47
11:E:206:PHE:CD2	11:E:410:ARG:HG3	2.42	0.47
11:E:229:ILE:HA	11:E:373:VAL:HG13	1.97	0.47
11:E:463:SER:HB2	11:E:470:PRO:HA	1.97	0.47
12:F:155:SER:OG	12:F:393:ASP:OD2	2.30	0.47
12:F:195:GLU:HG3	12:F:376:ILE:HD11	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:F:234:ASN:HB2	12:F:334:ASN:HA	1.97	0.47
13:G:190:LEU:H	13:G:397:ARG:HH22	1.62	0.47
14:H:497:ILE:HG21	15:H:5000:ADP:C5	2.50	0.47
9:K:230:ARG:HG3	9:K:308:ASN:O	2.14	0.47
9:K:239:VAL:HG21	9:K:285:LEU:HD13	1.96	0.47
10:L:37:ASN:OD1	10:L:87:ALA:HB2	2.15	0.47
11:M:243:VAL:HG11	11:M:360:GLN:HA	1.97	0.47
12:N:38:LEU:N	12:N:454:ASN:HD21	2.13	0.47
12:N:261:LYS:HE3	12:N:265:LYS:HB2	1.96	0.47
12:N:353:TYR:N	12:N:360:PHE:O	2.47	0.47
12:N:488:VAL:HG23	12:N:491:GLU:HG3	1.97	0.47
13:O:40:LEU:HD23	13:O:41:GLY:N	2.30	0.47
13:O:394:MET:HE1	13:O:397:ARG:NH1	2.29	0.47
14:P:28:ALA:O	14:P:32:ASN:ND2	2.46	0.47
14:P:62:LYS:HB2	14:P:62:LYS:HE3	1.68	0.47
7:A:21:ASN:OD1	7:A:71:ALA:HB2	2.14	0.47
10:D:157:LEU:HB2	10:D:163:LEU:HD22	1.97	0.47
12:F:196:MET:HB3	12:F:360:PHE:CE2	2.50	0.47
13:G:40:LEU:HD13	13:G:99:LEU:HD12	1.97	0.47
14:H:411:GLY:HA3	14:H:499:ASP:HB2	1.96	0.47
10:L:94:LEU:HD12	10:L:525:THR:HG21	1.95	0.47
11:M:407:CYS:O	11:M:411:ASN:ND2	2.44	0.47
13:O:187:ASP:OD1	13:O:188:ASP:N	2.47	0.47
4:4:57:ILE:HD11	4:4:87:LEU:HD11	1.97	0.47
5:5:40:GLN:O	5:5:44:VAL:HG13	2.14	0.47
9:C:104:GLU:HG2	9:C:446:VAL:HB	1.97	0.47
9:C:200:ARG:HG2	9:C:200:ARG:HH11	1.80	0.47
11:E:42:LYS:NZ	11:E:118:GLU:OE1	2.43	0.47
12:F:157:ARG:HD3	12:F:162:ALA:HA	1.97	0.47
13:G:407:ALA:HB2	13:G:488:PHE:HB2	1.96	0.47
13:G:516:VAL:HA	14:H:53:ASN:O	2.15	0.47
14:H:479:GLY:O	14:H:490:LYS:N	2.41	0.47
14:H:508:ILE:O	14:H:512:THR:HG23	2.14	0.47
7:I:28:ILE:HA	7:I:31:ILE:HD12	1.97	0.47
9:K:415:GLU:OE2	9:K:502:LYS:NZ	2.37	0.47
10:L:528:SER:O	10:L:532:ILE:HG13	2.15	0.47
12:N:61:ASN:O	12:N:65:HIS:ND1	2.46	0.47
12:N:69:ILE:O	12:N:70:GLN:HG2	2.15	0.47
12:N:215:GLY:O	12:N:359:LYS:HE2	2.15	0.47
13:O:116:LEU:HD11	13:O:430:LYS:NZ	2.29	0.47
14:P:471:HIS:HE2	14:P:476:LYS:HA	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:80:GLU:HA	5:5:96:ALA:N	2.29	0.47
9:C:216:ARG:HG3	9:C:216:ARG:NH1	2.30	0.47
9:C:467:ARG:O	9:C:471:THR:HG23	2.15	0.47
7:I:234:ILE:HG12	7:I:348:ALA:H	1.80	0.47
8:J:447:PRO:HA	8:J:450:ILE:HD12	1.96	0.47
11:M:162:THR:O	11:M:166:ILE:HG12	2.14	0.47
11:M:242:LYS:N	11:M:361:GLU:OE2	2.48	0.47
13:O:212:ALA:HB3	13:O:363:GLY:H	1.79	0.47
1:1:98:LYS:HA	1:1:101:LEU:HG	1.95	0.46
7:A:515:LYS:O	7:A:519:GLU:HG2	2.15	0.46
8:B:499:VAL:O	8:B:503:VAL:HG23	2.14	0.46
12:F:409:PRO:HB2	12:F:489:ALA:HB3	1.97	0.46
14:H:290:VAL:HG12	14:H:311:MET:HB2	1.97	0.46
9:K:238:ILE:HD11	9:K:331:ILE:HG12	1.96	0.46
12:N:151:VAL:HA	12:N:154:THR:HG22	1.97	0.46
13:O:193:LYS:HE3	13:O:193:LYS:HB2	1.70	0.46
11:E:453:ASP:OD2	10:L:452:ARG:NH2	2.48	0.46
12:F:145:ARG:O	12:F:149:ILE:HG12	2.15	0.46
8:J:220:LEU:HB2	8:J:360:ILE:HG22	1.96	0.46
8:J:244:MET:HE3	8:J:247:ASP:HA	1.97	0.46
10:L:459:GLU:OE1	10:L:481:ARG:NH1	2.44	0.46
11:M:129:HIS:CD2	13:O:454:GLY:HA2	2.50	0.46
14:P:205:CYS:SG	14:P:222:VAL:HG23	2.55	0.46
8:B:70:ILE:O	8:B:74:ILE:HB	2.16	0.46
8:J:199:ILE:HD12	8:J:371:CYS:O	2.15	0.46
11:M:258:PRO:HA	11:M:304:TRP:CG	2.51	0.46
12:N:28:ARG:HG3	12:N:28:ARG:NH1	2.31	0.46
12:N:54:ILE:HG23	12:N:382:HIS:HB3	1.96	0.46
12:N:71:HIS:CG	12:N:72:PRO:HD2	2.50	0.46
13:O:132:ALA:HB2	13:O:420:LEU:HD11	1.97	0.46
13:O:154:LEU:HD12	13:O:155:LEU:HD22	1.97	0.46
13:O:414:MET:HE3	13:O:446:PRO:CG	2.43	0.46
14:P:227:THR:HG23	14:P:314:ARG:HB3	1.98	0.46
14:P:419:LEU:HB3	14:P:445:PHE:CE2	2.50	0.46
5:5:91:TYR:CE1	5:5:93:GLU:HB3	2.51	0.46
6:6:78:LYS:HZ1	6:6:79:ARG:NH1	2.13	0.46
6:6:84:THR:HB	6:6:88:LYS:NZ	2.30	0.46
7:A:107:LEU:HB3	7:A:112:ILE:HD12	1.97	0.46
8:B:37:ASP:HA	8:B:40:LYS:NZ	2.31	0.46
11:E:532:ASP:HB2	13:G:48:LEU:O	2.15	0.46
12:F:447:ILE:O	12:F:450:VAL:HG12	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:G:225:PHE:HE1	13:G:350:GLU:CD	2.24	0.46
8:J:184:VAL:HG12	8:J:188:LEU:HD23	1.96	0.46
8:J:291:ILE:HG22	8:J:312:ILE:HB	1.97	0.46
9:K:408:VAL:HG23	9:K:499:LEU:HD13	1.97	0.46
10:L:283:ILE:O	10:L:287:VAL:HG23	2.15	0.46
13:O:71:VAL:HG11	13:O:80:VAL:HG11	1.97	0.46
3:3:91:MET:HB2	4:4:71:ILE:CG2	2.46	0.46
3:3:103:THR:HG21	3:3:117:VAL:HG12	1.97	0.46
7:A:128:ALA:HA	7:A:419:LEU:HD11	1.97	0.46
9:C:193:ILE:C	9:C:399:ARG:HH12	2.23	0.46
10:D:440:SER:O	10:D:448:SER:OG	2.21	0.46
11:E:165:LEU:HG	11:E:409:ILE:HD11	1.97	0.46
12:F:44:MET:SD	12:F:58:LYS:HD3	2.55	0.46
13:G:198:LYS:HD2	13:G:217:LYS:NZ	2.30	0.46
13:G:465:ARG:NH1	7:I:435:GLN:OE1	2.49	0.46
14:H:62:LYS:HD2	14:H:63:LEU:N	2.30	0.46
7:I:58:GLY:O	7:I:62:LEU:HD23	2.16	0.46
7:I:171:MET:SD	7:I:172:VAL:N	2.89	0.46
8:J:399:GLN:O	8:J:403:ASP:N	2.33	0.46
9:K:175:ILE:HD12	9:K:374:ILE:HG12	1.98	0.46
11:M:249:ALA:HA	11:M:353:LEU:HD12	1.97	0.46
12:N:24:ILE:HD13	12:N:107:ASP:HB2	1.96	0.46
13:O:509:ALA:O	13:O:513:ILE:HG12	2.15	0.46
3:3:104:ARG:HD3	4:4:75:PHE:CD2	2.50	0.46
4:4:89:GLU:HA	4:4:92:LYS:NZ	2.30	0.46
6:6:30:ARG:HH12	6:6:34:GLU:HB2	1.79	0.46
7:A:278:ILE:HG22	7:A:340:PHE:CE1	2.50	0.46
7:A:480:ARG:HE	7:A:483:LEU:HD21	1.80	0.46
9:C:238:ILE:HD11	9:C:348:GLY:HA2	1.98	0.46
10:D:112:ILE:O	10:D:116:LEU:HD23	2.16	0.46
10:D:429:GLU:CG	10:D:462:PRO:HD3	2.45	0.46
12:F:28:ARG:HD3	12:F:104:LYS:HB2	1.97	0.46
12:F:271:VAL:HG21	12:F:301:SER:OG	2.16	0.46
13:G:121:ILE:HG22	13:G:434:LEU:HD22	1.98	0.46
13:G:131:LEU:HG	13:G:419:TYR:HE2	1.81	0.46
13:G:282:HIS:HB3	13:G:308:MET:SD	2.55	0.46
14:H:45:THR:OG1	14:H:54:LYS:NZ	2.49	0.46
7:I:446:LEU:HD11	7:I:468:ARG:HH11	1.79	0.46
10:L:494:ASN:ND2	10:L:497:LYS:HB2	2.31	0.46
10:L:522:ALA:O	10:L:526:VAL:HG23	2.15	0.46
12:N:36:THR:O	12:N:43:THR:HG22	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:P:131:GLY:HA3	14:P:437:ALA:HB3	1.96	0.46
7:A:355:ARG:CZ	7:A:360:GLU:HB2	2.46	0.46
8:B:228:GLN:HB3	8:B:310:MET:HA	1.96	0.46
10:D:277:ARG:NH1	10:D:278:GLU:OE2	2.49	0.46
12:F:168:LEU:HD21	12:F:387:ILE:HD11	1.98	0.46
12:F:435:LEU:HD11	12:N:460:GLN:CD	2.40	0.46
13:G:17:GLN:NE2	14:H:42:THR:HA	2.31	0.46
14:H:436:TYR:O	14:H:440:LYS:HG2	2.15	0.46
7:I:70:PRO:HB3	10:L:68:VAL:HG12	1.97	0.46
9:K:130:LEU:HD21	9:K:507:LYS:HD3	1.97	0.46
13:O:326:CYS:HB2	13:O:343:GLY:HA3	1.97	0.46
13:O:494:GLU:HA	13:O:494:GLU:OE2	2.15	0.46
5:5:98:ASP:HA	5:5:102:PHE:HB3	1.97	0.46
6:6:42:ILE:HG13	6:6:43:VAL:N	2.31	0.46
8:B:40:LYS:HB2	8:B:449:ILE:HG21	1.97	0.46
8:B:64:THR:HG21	8:B:69:THR:HB	1.98	0.46
9:C:386:GLU:HG3	9:C:389:ARG:NH1	2.31	0.46
10:D:94:LEU:HD13	10:D:525:THR:OG1	2.15	0.46
12:F:47:LEU:HG	14:H:525:ILE:HB	1.98	0.46
14:H:43:THR:HG21	14:H:105:LEU:CD1	2.44	0.46
14:H:354:GLU:HA	14:H:359:GLN:HA	1.97	0.46
7:I:235:ALA:HA	7:I:346:GLY:H	1.80	0.46
9:K:23:GLN:O	9:K:27:ILE:HG12	2.16	0.46
9:K:151:MET:O	9:K:155:ILE:HD12	2.16	0.46
9:K:287:PRO:HD2	9:K:309:ILE:HD13	1.98	0.46
10:L:407:ASP:OD1	10:L:408:ALA:N	2.48	0.46
11:M:453:ASP:O	11:M:457:VAL:HG23	2.16	0.46
13:O:219:THR:OG1	13:O:357:ARG:HB3	2.16	0.46
13:O:325:ALA:HB2	13:O:369:THR:HG21	1.97	0.46
9:C:48:LYS:HE2	9:C:48:LYS:HA	1.98	0.46
9:C:118:HIS:ND1	9:C:119:PRO:HD2	2.31	0.46
10:D:277:ARG:HG3	10:D:278:GLU:OE2	2.16	0.46
8:J:330:GLU:HG2	8:J:342:LYS:HD2	1.98	0.46
10:L:435:ARG:HA	10:L:438:GLU:HG3	1.98	0.46
11:M:326:GLY:O	11:M:330:ILE:HG13	2.16	0.46
13:O:364:CYS:HB3	13:O:365:PRO:HD2	1.98	0.46
2:2:33:LEU:O	2:2:37:GLN:HG2	2.15	0.46
7:A:143:LEU:HD23	7:A:144:GLY:N	2.31	0.46
9:C:418:VAL:HG13	9:C:444:LEU:HD13	1.98	0.46
10:D:61:ILE:HD11	10:D:77:ILE:HA	1.98	0.46
10:D:229:LEU:HD23	10:D:230:THR:N	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:E:332:LEU:HA	11:E:335:ILE:HG22	1.96	0.46
12:F:108:LEU:HD13	12:N:108:LEU:HD11	1.98	0.46
12:F:149:ILE:HD13	12:F:173:VAL:HG11	1.98	0.46
9:K:47:MET:SD	9:K:61:ASN:HB3	2.55	0.46
9:K:69:GLU:OE2	12:N:524:ALA:HB1	2.16	0.46
11:M:173:LEU:HG	11:M:405:ALA:HB2	1.98	0.46
12:N:32:ASP:HA	12:N:35:ARG:HD3	1.98	0.46
12:N:118:ILE:HD13	12:N:432:ARG:NH1	2.31	0.46
11:E:117:LEU:HD21	11:E:524:VAL:HG13	1.98	0.45
12:F:80:VAL:O	12:F:84:GLN:HG2	2.16	0.45
13:G:16:SER:O	13:G:21:GLN:HB2	2.16	0.45
14:H:253:THR:HG22	14:H:258:LEU:HD12	1.97	0.45
7:I:467:LEU:HD12	7:I:471:HIS:HE1	1.80	0.45
9:K:400:ASN:OD1	9:K:401:VAL:N	2.49	0.45
10:L:160:ARG:HA	10:L:163:LEU:HD12	1.97	0.45
10:L:409:LEU:HA	10:L:412:ILE:HG12	1.96	0.45
11:M:154:SER:CA	11:M:417:ARG:HG2	2.44	0.45
11:M:163:GLU:HB3	11:M:164:PRO:HD3	1.98	0.45
13:O:143:VAL:O	13:O:143:VAL:HG13	2.16	0.45
13:O:410:GLY:HA2	13:O:413:GLU:HG2	1.98	0.45
14:P:448:ILE:HB	14:P:449:PRO:HD3	1.98	0.45
7:A:405:SER:C	7:A:407:SER:H	2.24	0.45
10:D:61:ILE:HD13	10:D:80:GLN:HB2	1.97	0.45
10:D:326:LYS:HD3	10:D:327:ASP:HB2	1.98	0.45
12:F:145:ARG:HH12	12:F:174:ASP:HA	1.81	0.45
14:H:93:GLN:HG2	14:H:101:THR:HA	1.98	0.45
14:H:241:VAL:HG21	14:H:330:ALA:HB3	1.99	0.45
14:H:382:ASP:HA	14:H:385:MET:HB3	1.99	0.45
10:L:253:LEU:HD22	10:L:306:ARG:HH12	1.81	0.45
10:L:534:ASP:O	10:L:536:VAL:HG23	2.17	0.45
11:M:190:VAL:HA	11:M:193:VAL:HG12	1.98	0.45
11:M:426:GLU:OE2	11:M:513:LYS:NZ	2.38	0.45
12:N:134:LEU:HD11	12:N:408:VAL:HG11	1.99	0.45
14:P:37:LYS:NZ	14:P:113:GLU:HG2	2.31	0.45
14:P:190:ILE:HG23	14:P:197:PHE:HE1	1.80	0.45
3:3:156:ASP:O	3:3:160:GLU:HG2	2.16	0.45
5:5:41:THR:OG1	5:5:42:LYS:N	2.49	0.45
6:6:96:ASP:O	6:6:100:GLN:HG2	2.16	0.45
9:C:152:MET:HA	9:C:155:ILE:HG12	1.98	0.45
9:C:408:VAL:O	9:C:410:GLY:N	2.49	0.45
9:C:416:MET:HE1	9:C:445:GLU:CG	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:D:144:GLY:HA2	10:D:147:ILE:HG22	1.98	0.45
10:D:337:CYS:HB3	10:D:342:THR:O	2.17	0.45
14:H:237:ALA:N	14:H:348:ASP:O	2.49	0.45
7:I:149:ILE:O	7:I:153:LYS:N	2.45	0.45
7:I:234:ILE:HB	7:I:285:VAL:CG2	2.45	0.45
8:J:215:ASP:O	8:J:367:LEU:HD21	2.16	0.45
13:O:236:LYS:HB3	13:O:285:GLY:O	2.15	0.45
2:2:69:LYS:HE3	2:2:80:GLU:HG2	1.97	0.45
2:2:72:ARG:N	2:2:79:VAL:O	2.49	0.45
4:4:40:ILE:HG22	4:4:44:LYS:NZ	2.30	0.45
5:5:124:LYS:O	5:5:127:MET:HG3	2.17	0.45
8:B:37:ASP:HA	8:B:40:LYS:HZ1	1.80	0.45
9:C:44:LYS:NZ	9:C:483:GLU:O	2.47	0.45
9:C:375:LEU:HD23	9:C:375:LEU:O	2.16	0.45
10:D:249:ILE:HB	10:D:300:ILE:HA	1.98	0.45
12:F:126:ALA:HB2	12:F:437:VAL:HA	1.99	0.45
13:G:29:CYS:HA	13:G:32:ILE:HG22	1.99	0.45
13:G:37:ARG:HG3	13:G:448:GLN:OE1	2.16	0.45
14:H:279:GLN:HA	14:H:339:PRO:HD2	1.99	0.45
14:H:476:LYS:HG2	14:H:476:LYS:O	2.16	0.45
7:I:245:LYS:HB3	7:I:264:ARG:NH1	2.31	0.45
7:I:456:ALA:HB1	7:I:491:SER:HA	1.99	0.45
9:K:173:CYS:SG	9:K:174:ASN:N	2.90	0.45
13:O:297:ASP:O	13:O:300:THR:OG1	2.21	0.45
14:P:446:GLU:O	14:P:449:PRO:HD2	2.16	0.45
1:1:93:GLU:O	1:1:96:GLN:HG3	2.17	0.45
7:A:351:VAL:HG22	7:A:364:ILE:HG23	1.97	0.45
7:A:384:MET:O	7:A:388:MET:HG2	2.16	0.45
9:C:237:ARG:NH1	9:C:345:THR:HA	2.32	0.45
10:D:47:ALA:O	10:D:59:LYS:NZ	2.48	0.45
10:D:52:LEU:HD22	10:D:111:ILE:HG21	1.98	0.45
10:D:151:MET:HE3	10:D:428:PRO:HA	1.99	0.45
10:D:400:GLU:HA	10:D:403:ARG:CD	2.47	0.45
13:G:216:PHE:CD1	13:G:314:VAL:HG12	2.50	0.45
8:J:149:GLY:HA2	8:J:155:PHE:CZ	2.52	0.45
13:O:118:PRO:O	13:O:122:ILE:HG12	2.17	0.45
12:F:71:HIS:CE1	12:F:73:THR:HG22	2.52	0.45
13:G:43:ARG:NH2	13:G:480:ASN:OD1	2.49	0.45
14:H:292:VAL:HG23	14:H:313:VAL:HB	1.99	0.45
8:J:170:LYS:HB3	8:J:176:LYS:HD2	1.99	0.45
12:N:319:ARG:HA	12:N:319:ARG:HH11	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:508:GLU:HA	13:O:511:CYS:SG	2.57	0.45
7:A:262:GLN:HG3	7:A:265:GLN:CD	2.42	0.45
8:B:237:ILE:HD13	8:B:327:THR:HB	1.98	0.45
8:B:244:MET:HG3	8:B:297:TYR:H	1.80	0.45
9:C:297:SER:HB2	9:C:299:LEU:HD23	1.99	0.45
10:D:193:LYS:HD3	10:D:386:VAL:HG21	1.98	0.45
10:D:280:ARG:HA	10:D:283:ILE:HG12	1.99	0.45
12:F:97:LEU:CD2	12:F:450:VAL:HG11	2.46	0.45
13:G:150:GLU:HA	13:G:153:LYS:HZ2	1.82	0.45
13:G:204:ALA:HB1	13:G:206:GLU:OE1	2.16	0.45
9:K:402:LEU:HD12	9:K:403:LEU:HG	1.98	0.45
9:K:491:LYS:C	9:K:493:LEU:H	2.24	0.45
10:L:250:GLN:HB2	10:L:345:VAL:O	2.16	0.45
10:L:432:LEU:HD23	10:L:458:MET:HE2	1.98	0.45
11:M:285:PHE:CE2	11:M:289:ILE:HD11	2.52	0.45
12:N:518:VAL:HB	12:N:521:ILE:HD11	1.99	0.45
13:O:133:VAL:HG13	13:O:500:ILE:HD12	1.99	0.45
14:P:314:ARG:HD2	14:P:315:LEU:H	1.81	0.45
9:C:364:THR:O	9:C:366:CYS:N	2.50	0.45
9:C:404:ASP:CG	9:C:499:LEU:HD23	2.41	0.45
10:D:136:SER:HG	10:D:450:CYS:CB	2.30	0.45
12:F:64:LEU:HB3	12:F:78:ALA:HB1	1.99	0.45
13:G:86:GLN:NE2	13:G:502:ALA:HA	2.32	0.45
14:H:33:ILE:HG23	14:H:112:LEU:HB3	1.97	0.45
14:H:466:LYS:O	14:H:470:VAL:HG23	2.17	0.45
14:H:475:ASN:OD1	14:H:477:ASN:N	2.38	0.45
7:I:263:ILE:HG13	7:I:264:ARG:N	2.32	0.45
8:J:204:LYS:NZ	8:J:359:LEU:HD11	2.32	0.45
10:L:373:LEU:O	10:L:375:LYS:NZ	2.43	0.45
11:M:193:VAL:CG1	11:M:409:ILE:HD12	2.47	0.45
11:M:232:LYS:HB3	11:M:371:MET:HA	1.98	0.45
13:O:37:ARG:NE	13:O:448:GLN:OE1	2.47	0.45
13:O:384:GLU:HA	13:O:387:ARG:HH21	1.82	0.45
14:P:92:MET:HA	14:P:95:GLN:HG2	1.99	0.45
6:6:108:LEU:O	6:6:112:GLN:HG2	2.17	0.45
9:C:133:MET:SD	9:C:444:LEU:HD11	2.57	0.45
9:C:169:SER:HA	9:C:172:ALA:HB3	1.99	0.45
9:C:401:VAL:HG12	9:C:498:PRO:HB3	1.99	0.45
10:D:178:GLN:HG2	10:D:179:TYR:N	2.31	0.45
10:D:282:TYR:O	10:D:286:LEU:HG	2.17	0.45
11:E:232:LYS:HG3	11:E:322:VAL:HG12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:F:216:ALA:HB3	12:F:218:HIS:CD2	2.52	0.45
13:G:383:GLU:HB3	13:G:387:ARG:NH1	2.27	0.45
14:H:143:LEU:N	14:H:144:PRO:HD2	2.31	0.45
14:H:205:CYS:HG	14:H:376:VAL:HA	1.82	0.45
7:I:405:SER:C	7:I:407:SER:H	2.24	0.45
8:J:379:THR:HG22	8:J:382:ILE:H	1.81	0.45
13:O:157:LYS:HA	13:O:160:MET:HG3	1.99	0.45
13:O:434:LEU:HD23	13:O:434:LEU:HA	1.84	0.45
14:P:226:GLU:OE2	14:P:361:VAL:HB	2.17	0.45
10:D:183:LEU:HD13	10:D:405:ILE:HG22	1.98	0.45
11:E:518:SER:OG	13:G:380:GLN:NE2	2.50	0.45
12:F:44:MET:N	14:H:520:ARG:O	2.36	0.45
12:F:69:ILE:HD12	12:F:74:ALA:CB	2.47	0.45
14:H:179:LEU:O	14:H:183:ILE:HG12	2.17	0.45
11:M:52:LEU:HD13	11:M:111:VAL:HG11	1.99	0.45
11:M:104:ASP:OD1	11:M:105:GLY:N	2.50	0.45
12:N:168:LEU:HD11	12:N:387:ILE:HD12	1.98	0.45
14:P:325:CYS:HB2	14:P:330:ALA:C	2.42	0.45
2:2:44:ALA:HB3	2:2:104:LEU:HD22	1.98	0.44
4:4:70:GLN:HA	4:4:74:VAL:O	2.17	0.44
6:6:30:ARG:NH1	6:6:34:GLU:HB2	2.33	0.44
6:6:39:GLU:O	6:6:43:VAL:HG23	2.17	0.44
10:D:471:LEU:HD21	10:D:499:GLY:HA2	1.98	0.44
12:F:146:GLU:OE1	12:F:146:GLU:N	2.47	0.44
12:F:432:ARG:HD3	12:N:461:GLU:HB2	1.99	0.44
12:F:449:LYS:HB3	12:F:463:LEU:HD13	1.98	0.44
8:J:160:MET:SD	8:J:184:VAL:HG11	2.57	0.44
8:J:187:VAL:HG21	8:J:397:LEU:HB3	1.99	0.44
9:K:31:LYS:HA	9:K:31:LYS:HD2	1.78	0.44
9:K:66:ILE:H	9:K:66:ILE:HD12	1.82	0.44
9:K:130:LEU:HA	9:K:133:MET:CE	2.44	0.44
9:K:213:CYS:H	9:K:375:LEU:HD22	1.81	0.44
9:K:404:ASP:C	9:K:406:GLN:N	2.75	0.44
11:M:247:LYS:HZ1	11:M:297:ALA:HB2	1.82	0.44
14:P:69:ALA:HA	14:P:72:ILE:HG22	1.97	0.44
8:B:46:LYS:NZ	10:D:135:GLU:OE1	2.48	0.44
9:C:28:ASN:O	9:C:32:THR:HG23	2.17	0.44
10:D:112:ILE:HD11	10:D:458:MET:SD	2.57	0.44
11:E:185:MET:O	11:E:188:ILE:HG22	2.16	0.44
11:E:283:GLU:O	11:E:287:GLU:HB3	2.16	0.44
12:F:44:MET:HE1	12:F:386:GLN:HE21	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:463:LEU:O	7:I:467:LEU:HD23	2.18	0.44
11:M:475:THR:HG22	11:M:478:ARG:HH21	1.81	0.44
11:M:481:GLN:HG2	11:M:487:PRO:HA	1.99	0.44
12:N:67:MET:HB2	14:P:528:LYS:H	1.81	0.44
12:N:91:GLY:HA3	12:N:500:VAL:HG22	2.00	0.44
12:N:141:ARG:HD2	12:N:147:THR:HG21	1.98	0.44
13:O:23:VAL:HA	13:O:26:ILE:HG12	2.00	0.44
13:O:42:PRO:HG3	13:O:479:ILE:HD13	1.98	0.44
13:O:287:LYS:HB2	13:O:287:LYS:HE3	1.75	0.44
13:O:300:THR:HA	13:O:303:PHE:CD1	2.52	0.44
13:O:409:GLY:O	13:O:477:VAL:HG22	2.17	0.44
6:6:30:ARG:HD2	6:6:30:ARG:HA	1.73	0.44
6:6:102:GLU:O	6:6:106:GLU:HG2	2.18	0.44
6:6:103:GLN:O	6:6:107:THR:HG23	2.18	0.44
8:B:220:LEU:HB2	8:B:360:ILE:HB	2.00	0.44
9:C:354:LYS:HB3	9:C:359:TYR:CD1	2.51	0.44
11:E:311:ASN:O	11:E:315:LEU:HG	2.17	0.44
11:E:397:GLU:O	11:E:400:ARG:HG2	2.18	0.44
12:F:314:ARG:HG2	12:F:315:ARG:HG3	1.98	0.44
12:F:416:VAL:HG13	12:F:448:PRO:HG3	1.99	0.44
13:G:153:LYS:O	13:G:157:LYS:HE3	2.17	0.44
13:G:292:LYS:HA	13:G:314:VAL:HG22	1.99	0.44
14:H:497:ILE:HG22	14:H:497:ILE:O	2.17	0.44
8:J:95:VAL:HG21	8:J:499:VAL:HA	1.99	0.44
8:J:236:LYS:CB	8:J:287:ILE:HG23	2.43	0.44
8:J:250:LYS:HD2	8:J:281:ARG:HD3	2.00	0.44
9:K:295:GLY:HA2	9:K:313:ARG:HB2	1.98	0.44
10:L:517:SER:HA	10:L:520:THR:HG22	1.99	0.44
12:N:318:ARG:HA	12:N:321:MET:HE2	2.00	0.44
13:O:290:LEU:HD23	13:O:311:ALA:HB3	1.99	0.44
13:O:516:VAL:HA	14:P:53:ASN:O	2.17	0.44
14:P:402:LEU:HD12	14:P:402:LEU:HA	1.85	0.44
5:5:128:LYS:O	5:5:132:MET:HG2	2.18	0.44
8:B:137:ALA:HB1	8:B:417:MET:HB3	2.00	0.44
11:E:132:ARG:HH12	13:G:482:GLU:HG3	1.82	0.44
14:H:220:GLY:N	14:H:373:SER:HA	2.33	0.44
14:H:425:SER:O	14:H:428:GLU:HG3	2.17	0.44
14:H:504:LYS:O	14:H:508:ILE:HD12	2.17	0.44
8:J:251:ILE:H	8:J:251:ILE:HD12	1.82	0.44
9:K:75:PRO:HG2	9:K:77:ALA:HB3	1.99	0.44
9:K:322:ARG:HG3	9:K:371:ALA:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:M:78:LEU:HB3	11:M:92:VAL:HG23	1.99	0.44
11:M:303:GLN:O	11:M:323:ARG:NH1	2.46	0.44
11:M:357:GLY:H	11:M:376:GLN:HB3	1.83	0.44
12:N:408:VAL:HG23	12:N:496:ASP:HB3	1.99	0.44
2:2:72:ARG:HA	3:3:132:MET:HB2	2.00	0.44
3:3:71:LYS:HG2	3:3:75:LYS:NZ	2.32	0.44
4:4:39:GLU:O	4:4:43:LYS:HG2	2.17	0.44
5:5:40:GLN:HA	5:5:114:MET:HE2	1.99	0.44
8:B:219:LEU:HB2	8:B:372:THR:HG21	2.00	0.44
9:C:26:ASN:ND2	9:C:519:ILE:HB	2.26	0.44
9:C:45:SER:OG	9:C:61:ASN:OD1	2.35	0.44
9:C:237:ARG:HH11	9:C:345:THR:HA	1.81	0.44
9:C:469:LYS:HE2	9:C:469:LYS:HB2	1.90	0.44
10:D:120:CYS:O	10:D:124:LEU:HG	2.17	0.44
11:E:301:ILE:HD12	11:E:322:VAL:HG23	1.99	0.44
14:H:47:TYR:HD1	14:H:102:ASN:HD22	1.64	0.44
14:H:183:ILE:CD1	14:H:392:VAL:HG23	2.45	0.44
8:J:134:THR:HG22	8:J:439:TYR:OH	2.18	0.44
8:J:178:HIS:ND1	8:J:210:ALA:O	2.46	0.44
8:J:396:VAL:HA	8:J:399:GLN:CD	2.43	0.44
9:K:239:VAL:HG12	9:K:287:PRO:HG3	1.99	0.44
9:K:388:GLU:HA	9:K:391:LEU:HG	1.99	0.44
10:L:187:SER:HB3	10:L:405:ILE:HD11	1.99	0.44
12:N:71:HIS:ND1	12:N:72:PRO:HD2	2.33	0.44
13:O:332:THR:O	13:O:332:THR:HG22	2.18	0.44
4:4:102:GLU:HA	4:4:105:VAL:HG12	1.98	0.44
6:6:13:VAL:HG23	6:6:104:GLN:HG3	1.99	0.44
9:C:459:THR:HG23	9:C:460:ILE:HG13	2.00	0.44
10:D:113:ALA:O	10:D:117:LEU:HD23	2.17	0.44
10:D:193:LYS:O	10:D:384:LYS:HE3	2.17	0.44
8:J:159:LEU:HA	8:J:162:ILE:HG22	1.98	0.44
11:M:291:GLN:O	11:M:294:GLU:HG2	2.17	0.44
12:N:66:GLU:OE1	14:P:525:ILE:HG21	2.17	0.44
7:A:29:ALA:HB2	7:A:98:ALA:HB3	1.99	0.44
8:B:333:SER:O	8:B:333:SER:OG	2.34	0.44
13:G:241:ASN:HB3	13:G:292:LYS:HE2	2.00	0.44
8:J:238:LEU:HB2	8:J:287:ILE:HD13	2.00	0.44
8:J:299:TYR:O	8:J:303:LEU:HG	2.18	0.44
8:J:473:ASN:ND2	8:J:476:ALA:HB2	2.32	0.44
9:K:146:ILE:HB	9:K:401:VAL:HG12	2.00	0.44
11:M:232:LYS:HZ3	11:M:361:GLU:CD	2.25	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:208:SER:HB3	13:O:372:PHE:CZ	2.52	0.44
13:O:277:LYS:O	13:O:281:ILE:HG12	2.18	0.44
1:1:31:ASP:OD1	1:1:32:ILE:N	2.51	0.44
1:1:51:ILE:O	1:1:55:VAL:HG13	2.17	0.44
7:A:322:ALA:HA	7:A:370:ARG:HB3	2.00	0.44
8:B:48:MET:HG2	10:D:531:LYS:O	2.17	0.44
8:B:388:ARG:HA	8:B:388:ARG:CZ	2.48	0.44
11:E:167:GLN:O	11:E:170:LYS:HB2	2.18	0.44
11:E:396:GLU:HB2	11:E:400:ARG:NH2	2.31	0.44
12:F:69:ILE:HD11	12:F:75:SER:N	2.32	0.44
14:H:164:LEU:O	14:H:168:ILE:HG12	2.17	0.44
7:I:244:THR:HA	7:I:264:ARG:NH2	2.32	0.44
9:K:160:ILE:HG23	9:K:390:ASN:HD22	1.83	0.44
9:K:277:GLN:NE2	9:K:281:ASP:OD2	2.51	0.44
13:O:183:VAL:HG13	13:O:400:ILE:HG13	2.00	0.44
13:O:396:VAL:O	13:O:400:ILE:HG12	2.18	0.44
3:3:126:TRP:NE1	5:5:69:SER:HA	2.33	0.44
5:5:26:VAL:HG13	5:5:128:LYS:CG	2.47	0.44
6:6:42:ILE:O	6:6:43:VAL:C	2.61	0.44
8:B:252:PHE:CE1	8:B:277:GLU:HG3	2.53	0.44
9:C:313:ARG:HD3	9:C:314:ARG:N	2.32	0.44
11:E:133:ILE:HD11	11:E:528:LEU:HD11	1.99	0.44
12:F:120:THR:HG21	12:F:513:THR:HG23	2.00	0.44
12:F:269:ASP:OD1	12:F:270:ARG:NH2	2.50	0.44
12:F:382:HIS:CE1	12:F:383:THR:HG23	2.53	0.44
13:G:82:ILE:HG21	13:G:509:ALA:HB2	1.99	0.44
13:G:150:GLU:HA	13:G:153:LYS:NZ	2.33	0.44
14:H:452:LEU:HD22	14:H:480:LEU:HD21	2.00	0.44
7:I:100:LEU:HD22	7:I:441:PHE:CD2	2.53	0.44
7:I:467:LEU:HD21	7:I:488:LEU:HD22	2.00	0.44
8:J:156:ARG:HB3	8:J:160:MET:HE1	2.00	0.44
9:K:70:ILE:HG23	9:K:70:ILE:O	2.17	0.44
12:N:19:ALA:O	12:N:22:VAL:HG12	2.18	0.44
13:O:111:TYR:CZ	13:O:433:LEU:HD21	2.53	0.44
14:P:143:LEU:HD12	14:P:419:LEU:HD11	1.99	0.44
9:C:44:LYS:HD2	12:F:117:ARG:NH2	2.32	0.43
9:C:214:VAL:HG13	9:C:374:ILE:HA	2.00	0.43
10:D:394:ASN:O	10:D:398:ILE:HG12	2.19	0.43
11:E:247:LYS:HZ2	11:E:353:LEU:C	2.22	0.43
12:F:71:HIS:CG	12:F:72:PRO:HD3	2.53	0.43
12:F:118:ILE:HA	12:F:121:GLU:HG2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:42:ASP:OD1	9:K:518:ARG:NE	2.51	0.43
7:I:145:ARG:HA	7:I:145:ARG:HE	1.82	0.43
9:K:378:GLY:HA3	9:K:384:LEU:HD21	1.98	0.43
10:L:94:LEU:HD21	10:L:109:VAL:HB	1.99	0.43
11:M:144:ALA:O	11:M:148:LEU:HB2	2.18	0.43
11:M:303:GLN:NE2	11:M:325:VAL:O	2.34	0.43
14:P:170:SER:HB2	15:P:601:ADP:C8	2.53	0.43
14:P:241:VAL:HA	14:P:292:VAL:HB	1.99	0.43
8:B:52:LEU:HD21	8:B:70:ILE:HD13	2.00	0.43
11:E:123:LEU:HD23	11:E:123:LEU:HA	1.79	0.43
11:E:335:ILE:HD11	13:G:222:TYR:HA	2.00	0.43
13:G:432:GLN:NE2	13:G:433:LEU:HG	2.32	0.43
14:H:453:ALA:HB1	14:H:458:VAL:HG13	2.00	0.43
8:J:263:LYS:HA	10:L:263:GLN:NE2	2.33	0.43
8:J:375:LEU:HD23	8:J:383:LEU:HD13	1.99	0.43
9:K:97:SER:HA	9:K:100:ILE:HD13	1.99	0.43
10:L:408:ALA:O	10:L:412:ILE:HG12	2.18	0.43
10:L:432:LEU:HB3	10:L:458:MET:HE1	2.00	0.43
11:M:184:GLN:O	11:M:188:ILE:HG12	2.18	0.43
3:3:105:PHE:HE2	5:5:74:GLY:HA3	1.83	0.43
8:B:251:ILE:HG21	8:B:270:ALA:O	2.18	0.43
9:C:194:ASP:CG	9:C:195:ILE:H	2.26	0.43
10:D:397:VAL:O	10:D:400:GLU:HG3	2.18	0.43
10:D:528:SER:O	10:D:532:ILE:HG12	2.18	0.43
12:F:443:ALA:O	12:F:446:ILE:HG22	2.18	0.43
13:G:425:ARG:HD2	7:I:421:ILE:CD1	2.48	0.43
7:I:118:ILE:HD12	7:I:522:ILE:HG23	2.00	0.43
7:I:389:GLU:CD	7:I:389:GLU:C	2.86	0.43
8:J:47:GLY:HA2	8:J:453:ASN:HB3	2.00	0.43
9:K:77:ALA:O	9:K:81:ILE:HG12	2.18	0.43
11:M:88:ALA:HA	11:M:91:MET:HG2	1.99	0.43
11:M:257:PRO:HG2	11:M:306:PHE:CD1	2.53	0.43
12:N:293:ASN:HB3	12:N:313:LEU:O	2.18	0.43
13:O:288:VAL:HG12	13:O:309:PHE:HB3	1.99	0.43
14:P:232:THR:HG22	14:P:311:MET:SD	2.58	0.43
5:5:98:ASP:HA	5:5:102:PHE:CB	2.49	0.43
6:6:27:MET:HB2	6:6:90:TYR:CE2	2.53	0.43
6:6:50:LEU:CD1	6:6:54:ASN:HB2	2.48	0.43
7:A:69:HIS:CD2	7:A:71:ALA:HB3	2.54	0.43
11:E:249:ALA:HB2	11:E:292:ILE:HG21	1.99	0.43
11:E:471:ILE:HB	10:L:446:MET:HE1	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:F:133:PHE:CE2	12:F:137:VAL:HG21	2.53	0.43
13:G:392:ALA:HA	13:G:395:ILE:HG12	2.00	0.43
14:H:182:LEU:HA	14:H:185:GLN:HG2	2.00	0.43
7:I:151:ALA:HA	7:I:169:ALA:HB2	2.01	0.43
7:I:226:PRO:C	7:I:231:ASN:HD21	2.26	0.43
10:L:130:PRO:HB3	10:L:530:LEU:HD12	1.99	0.43
11:M:75:ALA:HB2	11:M:106:THR:HG21	2.00	0.43
11:M:531:ASP:OD1	11:M:532:ASP:N	2.51	0.43
12:N:195:GLU:HB2	12:N:384:LEU:HD11	1.99	0.43
5:5:94:LYS:HG3	5:5:98:ASP:CG	2.44	0.43
5:5:123:GLU:OE2	5:5:124:LYS:NZ	2.39	0.43
7:A:149:ILE:HG12	7:A:173:VAL:HG11	2.00	0.43
7:A:255:THR:HG23	9:C:270:MET:HB3	2.00	0.43
7:A:300:PHE:HB3	7:A:305:ALA:O	2.19	0.43
9:C:230:ARG:HH12	9:C:305:MET:HA	1.83	0.43
11:E:242:LYS:HE3	11:E:360:GLN:HG2	2.01	0.43
11:E:255:PHE:HB3	11:E:285:PHE:HE1	1.83	0.43
11:E:258:PRO:HG2	11:E:264:HIS:CE1	2.54	0.43
12:F:63:LEU:HG	12:F:67:MET:SD	2.58	0.43
12:F:229:TYR:HB3	12:F:344:LEU:HD11	2.01	0.43
13:G:243:GLU:OE1	13:G:243:GLU:N	2.52	0.43
13:G:350:GLU:HG2	13:G:359:ASN:HA	2.00	0.43
13:G:496:ALA:O	13:G:500:ILE:HG12	2.19	0.43
8:J:36:GLY:HA3	8:J:107:ALA:CB	2.48	0.43
10:L:180:SER:HA	10:L:183:LEU:HG	2.01	0.43
11:M:101:GLU:CD	11:M:414:ARG:HH22	2.25	0.43
11:M:138:GLU:HB3	11:M:525:ARG:HE	1.82	0.43
13:O:193:LYS:HG3	13:O:194:MET:N	2.33	0.43
2:2:46:GLU:O	2:2:50:GLU:HG3	2.19	0.43
8:B:251:ILE:HG22	8:B:252:PHE:N	2.33	0.43
9:C:476:GLU:OE1	9:C:476:GLU:N	2.51	0.43
11:E:423:GLY:O	11:E:427:ILE:HG12	2.19	0.43
12:F:71:HIS:ND1	12:F:73:THR:HG22	2.33	0.43
12:F:228:ALA:O	12:F:347:ALA:N	2.42	0.43
13:G:129:THR:HG21	13:G:507:SER:CB	2.48	0.43
14:H:217:VAL:C	14:H:218:LEU:HD12	2.44	0.43
8:J:67:GLY:HA2	8:J:70:ILE:HD13	1.99	0.43
10:L:52:LEU:HD12	10:L:111:ILE:CD1	2.47	0.43
11:M:129:HIS:ND1	11:M:130:PRO:HD2	2.33	0.43
12:N:270:ARG:HB3	12:N:336:PHE:CZ	2.53	0.43
13:O:152:ARG:HH11	13:O:177:LYS:HE2	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:238:ALA:HA	13:O:342:LEU:HD13	1.99	0.43
13:O:346:GLN:NE2	13:O:364:CYS:O	2.51	0.43
5:5:41:THR:O	5:5:42:LYS:C	2.62	0.43
9:C:236:PRO:HA	9:C:348:GLY:N	2.23	0.43
10:D:245:LYS:HB3	10:D:356:LEU:HD13	1.99	0.43
13:G:192:LEU:HD11	13:G:393:ILE:HG13	2.01	0.43
13:G:244:LEU:H	13:G:295:ILE:HD12	1.82	0.43
14:H:102:ASN:HB3	15:H:5000:ADP:O2A	2.18	0.43
8:J:238:LEU:HD12	8:J:287:ILE:HD12	1.99	0.43
9:K:46:MET:HE3	12:N:517:LEU:O	2.19	0.43
10:L:120:CYS:SG	10:L:530:LEU:HD11	2.59	0.43
11:M:310:ALA:O	11:M:314:LEU:HG	2.18	0.43
11:M:419:VAL:HG12	11:M:508:GLU:O	2.19	0.43
12:N:44:MET:HE3	14:P:520:ARG:HD2	2.01	0.43
13:O:74:PRO:HB3	14:P:63:LEU:HD11	1.99	0.43
2:2:112:GLY:HA3	12:F:242:THR:HA	1.99	0.43
6:6:78:LYS:HZ2	6:6:79:ARG:NH2	2.14	0.43
7:A:427:ALA:O	7:A:435:GLN:HB2	2.19	0.43
9:C:106:LEU:HD21	9:C:513:ALA:HA	1.99	0.43
9:C:156:ILE:CG2	9:C:173:CYS:HB3	2.36	0.43
10:D:311:ASP:N	10:D:311:ASP:OD1	2.50	0.43
11:E:157:VAL:H	11:E:161:ASP:CG	2.27	0.43
7:I:181:TYR:HB2	7:I:189:ARG:O	2.18	0.43
8:J:201:ILE:HD12	8:J:387:GLU:HA	2.00	0.43
9:K:63:GLY:O	9:K:67:LEU:HG	2.19	0.43
9:K:409:PRO:HA	9:K:496:TRP:HE3	1.83	0.43
10:L:438:GLU:O	10:L:441:ARG:HB2	2.19	0.43
11:M:525:ARG:HH12	13:O:380:GLN:NE2	2.17	0.43
14:P:238:LYS:HD2	14:P:287:GLY:HA2	2.01	0.43
7:A:170:ASN:HA	7:A:173:VAL:HG12	2.00	0.43
8:B:251:ILE:HG22	8:B:252:PHE:H	1.84	0.43
11:E:52:LEU:HD12	11:E:461:ALA:HB3	2.01	0.43
11:E:381:ARG:NH1	13:G:221:SER:O	2.52	0.43
11:E:485:MET:O	11:E:485:MET:HE3	2.18	0.43
12:F:368:ASN:O	12:F:370:ARG:HD3	2.18	0.43
13:G:211:VAL:HG12	13:G:362:THR:HG21	2.01	0.43
7:I:156:MET:HE1	7:I:502:GLY:H	1.83	0.43
10:L:33:ILE:HD11	10:L:535:VAL:HG22	2.00	0.43
11:M:373:VAL:HG22	11:M:375:GLU:OE1	2.19	0.43
11:M:410:ARG:HA	11:M:413:ILE:HG22	1.99	0.43
11:M:478:ARG:O	11:M:482:VAL:HG23	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:21:ILE:HG21	5:5:133:GLU:OE1	2.19	0.43
1:1:37:LEU:CD2	1:1:94:LEU:HD13	2.48	0.43
6:6:30:ARG:NH1	6:6:30:ARG:O	2.50	0.43
7:A:115:THR:HA	7:A:118:ILE:HG12	2.01	0.43
8:B:176:LYS:O	8:B:180:THR:HG23	2.19	0.43
9:C:247:TYR:HE1	9:C:298:ASP:H	1.66	0.43
11:E:170:LYS:HD2	11:E:170:LYS:HA	1.82	0.43
11:E:405:ALA:HA	11:E:408:VAL:HG22	2.01	0.43
13:G:129:THR:HG21	13:G:507:SER:HB2	2.01	0.43
13:G:215:ALA:HB2	13:G:361:PHE:H	1.84	0.43
13:G:402:ASN:OD1	13:G:498:VAL:HG23	2.19	0.43
14:H:197:PHE:O	14:H:400:LYS:HE2	2.19	0.43
7:I:279:LEU:HD21	7:I:306:MET:HG3	2.01	0.43
8:J:41:SER:HB2	8:J:48:MET:HG3	2.01	0.43
8:J:227:ASN:HD21	8:J:305:GLY:HA3	1.84	0.43
8:J:248:LYS:HA	8:J:248:LYS:HD2	1.72	0.43
10:L:46:ASP:HB2	10:L:49:ARG:HH22	1.83	0.43
10:L:58:ASP:C	10:L:59:LYS:HD3	2.43	0.43
10:L:241:VAL:HG13	10:L:244:ALA:HB2	2.01	0.43
11:M:85:HIS:CE1	11:M:87:ILE:HG22	2.53	0.43
11:M:89:LYS:HA	11:M:92:VAL:HG12	2.00	0.43
11:M:383:VAL:O	11:M:383:VAL:HG23	2.19	0.43
11:M:444:GLU:O	11:M:448:MET:HG2	2.19	0.43
12:N:377:LYS:HE3	12:N:377:LYS:HB3	1.92	0.43
12:N:411:ALA:N	15:N:601:ADP:O2'	2.47	0.43
14:P:83:ALA:O	14:P:87:VAL:HG23	2.19	0.43
14:P:223:PHE:HD2	14:P:313:VAL:HG21	1.84	0.43
1:1:109:GLU:OE1	1:1:113:ARG:HD3	2.19	0.42
7:A:181:TYR:HD1	7:A:370:ARG:HG3	1.83	0.42
7:A:213:GLY:O	7:A:374:SER:OG	2.33	0.42
7:A:467:LEU:HD11	7:A:487:GLY:HA2	2.01	0.42
7:A:526:ARG:O	10:D:57:MET:HB3	2.19	0.42
9:C:33:ILE:O	9:C:37:ILE:HG12	2.19	0.42
9:C:302:HIS:O	9:C:305:MET:HG2	2.19	0.42
11:E:489:LEU:HD13	11:E:500:ASP:HA	2.01	0.42
12:F:194:MET:HE1	12:F:213:ASP:HB3	2.01	0.42
12:F:225:VAL:HG12	12:F:228:ALA:HB2	2.01	0.42
13:G:238:ALA:HB3	13:G:289:VAL:HG23	2.01	0.42
13:G:443:GLU:OE1	13:G:447:ARG:NH2	2.42	0.42
7:I:48:ASP:OD1	7:I:49:ILE:N	2.51	0.42
7:I:245:LYS:HE2	7:I:264:ARG:NH1	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:92:ASP:CG	8:J:99:THR:HG22	2.44	0.42
9:K:101:LEU:HD23	9:K:101:LEU:HA	1.85	0.42
9:K:152:MET:HB3	9:K:156:ILE:HD13	2.01	0.42
12:N:177:LEU:HD12	12:N:180:LYS:HG3	2.01	0.42
14:P:85:MET:O	14:P:88:MET:HG3	2.19	0.42
1:1:116:LEU:HD13	9:C:314:ARG:NH1	2.33	0.42
7:A:421:ILE:HD11	7:A:468:ARG:HG3	2.01	0.42
10:D:339:THR:HG21	10:D:385:THR:HG21	2.00	0.42
11:E:184:GLN:OE1	11:E:222:THR:OG1	2.29	0.42
13:G:166:LYS:HZ2	13:G:381:PHE:HB3	1.84	0.42
13:G:227:MET:N	13:G:227:MET:SD	2.92	0.42
14:H:92:MET:HG2	14:H:510:LEU:HD21	2.01	0.42
7:I:235:ALA:HB2	7:I:283:ALA:HB3	2.00	0.42
8:J:448:THR:OG1	8:J:462:VAL:HG11	2.19	0.42
9:K:93:ASP:OD1	9:K:93:ASP:N	2.48	0.42
9:K:350:LEU:HA	9:K:363:ILE:HA	2.00	0.42
10:L:141:LEU:HD22	10:L:523:THR:OG1	2.19	0.42
10:L:222:GLU:O	10:L:389:VAL:HG12	2.19	0.42
11:M:133:ILE:HG13	11:M:528:LEU:HD13	2.00	0.42
14:P:146:LEU:HD11	14:P:418:GLU:HB3	2.01	0.42
14:P:271:GLY:O	14:P:275:LEU:HG	2.18	0.42
1:1:57:GLU:CD	2:2:81:ARG:HE	2.27	0.42
5:5:96:ALA:HB1	5:5:100:LYS:NZ	2.35	0.42
7:A:236:CYS:SG	7:A:325:ALA:HB1	2.59	0.42
7:A:278:ILE:HG22	7:A:340:PHE:CZ	2.54	0.42
7:A:467:LEU:HD22	7:A:488:LEU:CD2	2.47	0.42
10:D:84:LEU:HA	10:D:89:ARG:HH21	1.84	0.42
10:D:418:LYS:HB2	10:D:418:LYS:HE3	1.80	0.42
7:I:264:ARG:NH2	9:K:242:ASP:OD1	2.53	0.42
7:I:512:LYS:HG2	7:I:516:PHE:CE2	2.54	0.42
9:K:216:ARG:HG3	9:K:216:ARG:O	2.19	0.42
9:K:365:ASP:HB3	9:K:370:LYS:CD	2.48	0.42
10:L:299:LEU:HD12	10:L:328:ILE:HG12	2.02	0.42
10:L:472:ASN:HB2	10:L:475:SER:OG	2.18	0.42
12:N:211:VAL:HG23	12:N:362:PHE:CD1	2.55	0.42
13:O:38:THR:O	13:O:452:ASN:ND2	2.51	0.42
14:P:409:VAL:N	14:P:499:ASP:O	2.51	0.42
1:1:73:LYS:HA	1:1:76:ILE:HD12	2.02	0.42
1:1:88:GLU:O	1:1:91:ILE:HG22	2.20	0.42
2:2:104:LEU:O	2:2:108:LEU:HG	2.19	0.42
3:3:165:LEU:O	3:3:169:PHE:N	2.41	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:6:68:GLU:OE1	6:6:70:GLY:N	2.44	0.42
7:A:27:SER:O	7:A:31:ILE:HG12	2.19	0.42
8:B:152:GLU:O	8:B:156:ARG:HG2	2.19	0.42
9:C:368:ASP:O	9:C:370:LYS:N	2.52	0.42
11:E:229:ILE:HG13	11:E:373:VAL:HG22	2.00	0.42
12:F:77:ILE:HG12	12:F:511:ILE:HD11	2.01	0.42
13:G:168:ILE:HG22	13:G:169:SER:N	2.35	0.42
13:G:353:ILE:HD11	13:G:360:PHE:CZ	2.50	0.42
13:G:394:MET:O	13:G:397:ARG:HG2	2.20	0.42
8:J:245:ASP:OD1	8:J:294:GLN:HG2	2.19	0.42
9:K:238:ILE:HG23	9:K:329:ALA:HB1	2.01	0.42
10:L:204:ASP:HB3	10:L:207:ASP:HB2	2.01	0.42
12:N:127:LYS:O	12:N:131:LEU:HD23	2.20	0.42
5:5:41:THR:O	5:5:44:VAL:N	2.53	0.42
6:6:78:LYS:HB3	6:6:78:LYS:HE3	1.79	0.42
9:C:488:VAL:HG11	9:C:493:LEU:HD11	2.02	0.42
10:D:97:ALA:HA	10:D:100:ILE:HG22	2.02	0.42
11:E:52:LEU:HD23	11:E:107:THR:HB	2.01	0.42
12:F:271:VAL:HG13	12:F:305:LEU:HD21	2.01	0.42
7:I:99:GLU:HG3	7:I:444:SER:OG	2.19	0.42
8:J:466:ARG:O	8:J:470:SER:CB	2.68	0.42
9:K:230:ARG:HG2	9:K:231:ARG:N	2.34	0.42
10:L:368:ASN:C	10:L:368:ASN:HD22	2.27	0.42
12:N:173:VAL:HA	12:N:176:ILE:HG22	2.01	0.42
13:O:413:GLU:CD	13:O:499:ARG:HH21	2.27	0.42
1:1:91:ILE:O	1:1:95:GLU:OE1	2.38	0.42
2:2:92:ASN:HA	2:2:95:GLU:HG2	2.00	0.42
4:4:56:ASP:HA	4:4:59:LEU:HD23	2.00	0.42
7:A:100:LEU:HD21	7:A:441:PHE:HE2	1.85	0.42
8:B:36:GLY:HA3	8:B:107:ALA:HB2	2.00	0.42
8:B:81:ALA:O	8:B:85:VAL:HG23	2.19	0.42
8:B:214:LEU:HG	8:B:215:ASP:N	2.35	0.42
9:C:151:MET:O	9:C:155:ILE:HG12	2.20	0.42
9:C:461:ARG:NH2	12:N:456:GLY:O	2.53	0.42
10:D:147:ILE:O	10:D:151:MET:N	2.53	0.42
10:D:211:VAL:O	10:D:390:VAL:HG12	2.19	0.42
10:D:366:ASN:HB3	10:D:372:LYS:NZ	2.35	0.42
7:I:107:LEU:CD2	7:I:440:GLU:HG2	2.48	0.42
7:I:199:LYS:HE3	7:I:385:CYS:HB2	2.00	0.42
7:I:252:VAL:O	9:K:252:SER:HA	2.20	0.42
7:I:490:LEU:O	7:I:492:ASN:ND2	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:N:61:ASN:CG	12:N:92:THR:HG21	2.45	0.42
13:O:181:ASP:HB2	13:O:210:LEU:HD11	2.01	0.42
13:O:244:LEU:HB2	13:O:295:ILE:HG23	2.01	0.42
14:P:107:PHE:O	14:P:111:LEU:HD23	2.19	0.42
14:P:248:GLY:HA3	14:P:276:MET:HE1	2.01	0.42
1:1:64:VAL:O	1:1:64:VAL:HG12	2.19	0.42
3:3:82:LYS:O	3:3:86:GLU:OE1	2.37	0.42
3:3:112:TYR:HB2	5:5:83:LEU:O	2.18	0.42
4:4:54:CYS:SG	4:4:87:LEU:HD13	2.60	0.42
7:A:218:CYS:SG	7:A:362:ILE:N	2.85	0.42
7:A:435:GLN:HE22	13:O:465:ARG:HD2	1.84	0.42
8:B:244:MET:HE2	8:B:300:PRO:HG2	2.01	0.42
8:B:393:ALA:O	8:B:397:LEU:HD13	2.20	0.42
9:C:72:VAL:HG23	9:C:72:VAL:O	2.19	0.42
9:C:119:PRO:O	9:C:123:ILE:HG12	2.20	0.42
9:C:389:ARG:HA	9:C:392:GLN:HG3	2.00	0.42
10:D:302:LYS:NZ	10:D:304:ILE:HG12	2.35	0.42
12:F:384:LEU:HA	12:F:387:ILE:HG22	2.02	0.42
7:I:216:LEU:O	7:I:362:ILE:HG22	2.19	0.42
7:I:384:MET:O	7:I:388:MET:HG2	2.20	0.42
8:J:218:PHE:CD2	8:J:322:ARG:HD3	2.54	0.42
9:K:229:MET:HE1	9:K:301:GLN:OE1	2.19	0.42
10:L:46:ASP:OD1	10:L:47:ALA:N	2.53	0.42
10:L:160:ARG:NE	10:L:192:MET:HG3	2.35	0.42
11:M:35:LYS:HE3	11:M:124:LEU:HB2	2.02	0.42
11:M:107:THR:O	11:M:111:VAL:HG12	2.20	0.42
12:N:340:SER:HB3	12:N:343:CYS:HB2	2.02	0.42
13:O:395:ILE:CA	13:O:398:ARG:NH2	2.82	0.42
4:4:95:GLN:HA	4:4:98:ILE:HG12	2.02	0.42
7:A:296:CYS:HA	7:A:299:TYR:HD2	1.84	0.42
7:A:499:LYS:HG2	7:A:504:PHE:HE2	1.85	0.42
8:B:395:CYS:SG	8:B:399:GLN:NE2	2.76	0.42
8:B:517:VAL:HG11	11:E:60:MET:HE2	2.00	0.42
9:C:41:LEU:HB3	9:C:450:THR:HG21	2.02	0.42
9:C:108:VAL:HG21	9:C:443:ALA:HB2	2.02	0.42
9:C:168:TRP:CD1	9:C:171:LEU:HD21	2.54	0.42
9:C:253:GLN:NE2	9:C:255:ASP:OD1	2.49	0.42
11:E:170:LYS:NZ	11:E:181:CYS:HB2	2.35	0.42
14:H:262:ALA:O	14:H:266:MET:HG3	2.20	0.42
14:H:298:ALA:HB3	14:H:300:MET:HG2	2.00	0.42
8:J:234:ASN:O	8:J:236:LYS:HD2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:278:LYS:O	8:J:282:ILE:HG12	2.19	0.42
9:K:80:MET:O	9:K:83:ILE:HG22	2.20	0.42
9:K:136:THR:HG21	9:K:418:VAL:HG13	2.02	0.42
9:K:145:ASP:O	9:K:152:MET:HG2	2.20	0.42
9:K:187:GLU:HB2	9:K:192:GLU:O	2.20	0.42
11:M:229:ILE:HG21	11:M:386:PHE:CE1	2.54	0.42
11:M:259:LYS:H	11:M:304:TRP:CD1	2.38	0.42
12:N:41:LYS:HD2	14:P:126:SER:OG	2.20	0.42
6:6:80:LEU:O	6:6:84:THR:HG23	2.20	0.42
7:A:46:VAL:HG12	7:A:52:VAL:HA	2.02	0.42
8:B:520:ILE:HG22	11:E:60:MET:HB3	2.00	0.42
9:C:229:MET:C	9:C:230:ARG:HD3	2.44	0.42
10:D:155:VAL:HG11	10:D:421:LEU:HG	2.01	0.42
10:D:248:LEU:HD23	10:D:344:PRO:HA	2.01	0.42
12:F:44:MET:HE1	12:F:386:GLN:NE2	2.35	0.42
12:F:69:ILE:O	12:F:69:ILE:HG13	2.20	0.42
12:F:228:ALA:HB3	12:F:347:ALA:HB3	2.02	0.42
12:F:447:ILE:O	12:F:451:LEU:HD23	2.19	0.42
13:G:163:LEU:O	13:G:165:SER:N	2.52	0.42
7:I:25:ALA:HA	7:I:28:ILE:HG22	2.01	0.42
10:L:152:SER:OG	10:L:421:LEU:O	2.36	0.42
10:L:283:ILE:HG13	10:L:284:LEU:N	2.35	0.42
11:M:209:ILE:HG13	11:M:383:VAL:O	2.20	0.42
11:M:271:VAL:HG12	11:M:275:LYS:NZ	2.35	0.42
11:M:285:PHE:CE1	11:M:314:LEU:HD22	2.55	0.42
12:N:308:GLU:O	12:N:310:ILE:N	2.50	0.42
13:O:289:VAL:HG12	13:O:309:PHE:O	2.20	0.42
13:O:331:GLN:HG2	13:O:337:LEU:HD22	2.02	0.42
1:1:112:ILE:HD12	9:C:314:ARG:HD2	2.01	0.42
5:5:43:TYR:OH	6:6:39:GLU:OE2	2.38	0.42
6:6:58:LYS:HG3	6:6:60:LEU:HD22	2.01	0.42
8:B:30:ILE:HA	8:B:33:ILE:HD13	2.01	0.42
8:B:236:LYS:HE2	8:B:238:LEU:HD21	2.02	0.42
9:C:95:THR:HA	9:C:98:VAL:HG12	2.01	0.42
9:C:223:ASP:OD1	9:C:224:VAL:HG23	2.19	0.42
9:C:399:ARG:HG2	9:C:399:ARG:HH11	1.84	0.42
10:D:139:LYS:O	10:D:142:GLU:HG2	2.19	0.42
11:E:192:ALA:HB2	11:E:385:ILE:HD11	2.00	0.42
14:H:96:GLU:HG2	14:H:506:TRP:CD2	2.55	0.42
14:H:286:THR:HG21	14:H:339:PRO:HB3	2.02	0.42
8:J:445:MET:O	8:J:449:ILE:HG12	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:489:ASP:OD1	9:K:490:MET:N	2.52	0.42
13:O:87:ASP:O	13:O:89:GLU:N	2.53	0.42
13:O:162:ALA:CB	13:O:395:ILE:HD12	2.48	0.42
14:P:165:ARG:HH22	14:P:176:GLU:HB3	1.84	0.42
14:P:233:SER:H	14:P:311:MET:HE1	1.85	0.42
4:4:100:ALA:O	4:4:104:ARG:HG2	2.20	0.41
7:A:430:MET:HG3	7:A:435:GLN:HB3	2.02	0.41
8:B:238:LEU:HD12	8:B:332:ALA:HB2	2.02	0.41
10:D:157:LEU:HD12	10:D:157:LEU:O	2.20	0.41
10:D:227:LEU:HB2	10:D:336:ILE:HD13	2.02	0.41
11:E:105:GLY:O	11:E:109:VAL:HG12	2.19	0.41
11:E:391:ASN:OD1	11:E:392:LYS:N	2.53	0.41
12:F:47:LEU:HD11	12:F:63:LEU:HD12	2.01	0.41
7:I:429:SER:O	7:I:429:SER:OG	2.28	0.41
8:J:167:LEU:HD13	8:J:389:SER:OG	2.20	0.41
9:K:146:ILE:HB	9:K:401:VAL:CG1	2.50	0.41
9:K:156:ILE:HD11	9:K:397:VAL:HG11	2.01	0.41
13:O:208:SER:HB3	13:O:372:PHE:HZ	1.85	0.41
13:O:341:VAL:HG13	13:O:342:LEU:HG	2.02	0.41
14:P:36:CYS:HB2	14:P:112:LEU:HD12	2.01	0.41
14:P:416:GLU:HG2	14:P:448:ILE:HG13	2.00	0.41
6:6:42:ILE:O	6:6:46:GLU:OE1	2.38	0.41
6:6:44:LYS:HD3	6:6:44:LYS:HA	1.80	0.41
10:D:329:GLU:O	10:D:333:ILE:HG13	2.20	0.41
11:E:309:GLU:HA	11:E:312:HIS:ND1	2.34	0.41
12:F:449:LYS:O	12:F:459:LEU:HB2	2.20	0.41
14:H:160:VAL:HG13	14:H:184:ALA:HB1	2.01	0.41
14:H:291:VAL:O	14:H:312:LEU:HA	2.20	0.41
9:K:106:LEU:HD11	9:K:513:ALA:HA	2.01	0.41
9:K:416:MET:HE1	9:K:445:GLU:CD	2.45	0.41
10:L:151:MET:HE3	10:L:151:MET:O	2.19	0.41
10:L:476:THR:O	10:L:480:LEU:HD23	2.19	0.41
12:N:240:GLU:HB2	12:N:262:ALA:HB2	2.01	0.41
12:N:318:ARG:HA	12:N:321:MET:CE	2.50	0.41
13:O:26:ILE:HA	13:O:105:LEU:HD23	2.01	0.41
13:O:512:LEU:O	13:O:516:VAL:HG13	2.21	0.41
1:1:35:GLU:HB3	1:1:39:ARG:NH2	2.35	0.41
1:1:37:LEU:HD22	1:1:94:LEU:HD13	2.00	0.41
5:5:111:THR:O	5:5:115:GLU:HG2	2.19	0.41
6:6:37:LEU:HD11	6:6:41:ASN:HD21	1.84	0.41
8:B:40:LYS:HD3	8:B:449:ILE:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:182:LEU:HD13	8:B:214:LEU:HB2	2.02	0.41
10:D:115:SER:OG	10:D:460:VAL:HG11	2.20	0.41
10:D:440:SER:HB2	10:D:448:SER:O	2.20	0.41
11:E:311:ASN:HD21	11:E:323:ARG:NH2	2.19	0.41
12:F:88:THR:OG1	12:F:500:VAL:HA	2.20	0.41
13:G:157:LYS:O	13:G:161:THR:HG23	2.20	0.41
13:G:348:PHE:HD2	13:G:361:PHE:HB3	1.84	0.41
7:I:234:ILE:O	7:I:346:GLY:N	2.53	0.41
7:I:241:LEU:HD23	7:I:271:THR:HG22	2.02	0.41
7:I:260:LEU:HG	9:K:248:LYS:HZ3	1.85	0.41
7:I:448:ILE:HB	7:I:449:PRO:HD3	2.02	0.41
10:L:411:VAL:HA	10:L:414:CYS:SG	2.61	0.41
11:M:132:ARG:CG	13:O:454:GLY:HA3	2.50	0.41
11:M:148:LEU:HD12	11:M:151:ILE:HG21	2.01	0.41
11:M:268:VAL:HG22	11:M:269:THR:H	1.85	0.41
12:N:167:VAL:HG21	12:N:203:ASP:HA	2.01	0.41
12:N:186:ILE:HD12	12:N:395:LEU:HB3	2.02	0.41
13:O:407:ALA:HB2	13:O:488:PHE:HB2	2.02	0.41
13:O:415:GLU:OE1	13:O:415:GLU:HA	2.20	0.41
14:P:314:ARG:HG3	14:P:315:LEU:HG	2.01	0.41
3:3:106:LEU:HG	4:4:73:ASP:OD2	2.20	0.41
8:B:156:ARG:O	8:B:160:MET:HG2	2.20	0.41
8:B:516:ARG:O	11:E:58:ASP:N	2.53	0.41
9:C:118:HIS:HD2	9:C:120:THR:HB	1.85	0.41
9:C:152:MET:HA	9:C:155:ILE:CG1	2.51	0.41
10:D:187:SER:O	10:D:191:VAL:HG22	2.19	0.41
8:J:205:LEU:HD13	8:J:378:ALA:C	2.46	0.41
10:L:112:ILE:O	10:L:116:LEU:HG	2.20	0.41
10:L:254:SER:N	10:L:307:ASP:OD2	2.52	0.41
12:N:96:VAL:O	12:N:99:ILE:HG12	2.21	0.41
12:N:419:ALA:O	12:N:423:ILE:HG12	2.20	0.41
14:P:223:PHE:HB2	14:P:361:VAL:HG12	2.03	0.41
4:4:35:GLU:O	4:4:38:GLU:HG3	2.21	0.41
6:6:91:GLU:HG3	6:6:95:ARG:HH11	1.85	0.41
7:A:91:THR:O	7:A:95:ILE:HD12	2.20	0.41
7:A:314:ARG:O	7:A:317:LYS:HG2	2.20	0.41
7:A:395:ALA:O	7:A:398:VAL:HG12	2.21	0.41
9:C:39:THR:HB	9:C:46:MET:HG3	2.03	0.41
10:D:247:GLY:O	10:D:299:LEU:N	2.45	0.41
11:E:98:GLN:OE1	11:E:98:GLN:N	2.54	0.41
11:E:132:ARG:HH21	11:E:443:LEU:HG	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:F:252:SER:OG	12:F:255:GLU:OE1	2.39	0.41
12:F:318:ARG:NH2	12:F:321:MET:SD	2.91	0.41
7:I:125:CYS:SG	7:I:515:LYS:HG2	2.60	0.41
8:J:204:LYS:NZ	8:J:354:ILE:O	2.54	0.41
8:J:405:ARG:HG3	8:J:405:ARG:HH11	1.86	0.41
11:M:45:ALA:HB2	11:M:114:GLY:HA3	2.03	0.41
12:N:64:LEU:HB3	12:N:78:ALA:HB1	2.03	0.41
12:N:195:GLU:HB3	12:N:376:ILE:HG13	2.01	0.41
12:N:270:ARG:HB3	12:N:336:PHE:CE1	2.55	0.41
13:O:186:LEU:HD12	13:O:186:LEU:C	2.33	0.41
13:O:354:GLY:CA	13:O:375:ARG:HH12	2.32	0.41
14:P:71:THR:HG21	14:P:390:ARG:HH11	1.84	0.41
14:P:109:GLY:O	14:P:113:GLU:HG3	2.20	0.41
1:I:93:GLU:HA	1:I:96:GLN:HG3	2.03	0.41
7:A:435:GLN:HE21	13:O:462:ASN:ND2	2.14	0.41
7:A:530:LEU:H	7:A:530:LEU:HD23	1.85	0.41
9:C:130:LEU:HA	9:C:133:MET:HE3	2.01	0.41
9:C:218:VAL:HG11	9:C:323:ILE:HG13	2.01	0.41
9:C:504:GLN:HE21	9:C:504:GLN:HB3	1.74	0.41
10:D:298:LEU:HB2	10:D:324:VAL:HG12	2.02	0.41
11:E:129:HIS:NE2	13:G:45:MET:HE3	2.36	0.41
11:E:254:PRO:HD2	13:G:264:GLN:OE1	2.21	0.41
11:E:267:ASP:H	13:G:257:VAL:CG1	2.34	0.41
12:F:31:GLN:HE22	12:F:35:ARG:NH2	2.19	0.41
12:F:116:PRO:HB3	12:F:516:LEU:HB3	2.02	0.41
8:J:349:ILE:HG23	8:J:362:PHE:HA	2.01	0.41
9:K:190:ARG:NH1	9:K:192:GLU:HG3	2.29	0.41
13:O:459:ASN:O	13:O:463:LYS:HG2	2.20	0.41
14:P:174:GLY:N	14:P:176:GLU:OE1	2.52	0.41
3:3:110:ASN:HD22	5:5:42:LYS:HG2	1.85	0.41
5:5:33:ILE:O	5:5:37:LYS:HD3	2.20	0.41
7:A:284:ASN:O	7:A:305:ALA:HA	2.21	0.41
9:C:29:ALA:HB1	9:C:77:ALA:HB2	2.03	0.41
9:C:37:ILE:HG13	9:C:99:ILE:HG21	2.02	0.41
9:C:218:VAL:O	9:C:363:ILE:HB	2.21	0.41
9:C:237:ARG:HG2	9:C:285:LEU:HD22	2.02	0.41
10:D:503:ILE:H	10:D:503:ILE:HD12	1.86	0.41
11:E:73:ASP:O	11:E:77:ILE:HG12	2.20	0.41
11:E:87:ILE:HG23	11:E:527:ILE:HG21	2.02	0.41
12:F:44:MET:HG3	14:H:520:ARG:HB3	2.02	0.41
12:F:133:PHE:O	12:F:137:VAL:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:G:190:LEU:HD23	13:G:190:LEU:HA	1.94	0.41
14:H:37:LYS:O	14:H:41:GLN:HG2	2.21	0.41
14:H:330:ALA:HB1	14:H:343:GLU:HA	2.02	0.41
10:L:126:LYS:O	10:L:126:LYS:HG2	2.21	0.41
10:L:249:ILE:HG23	10:L:251:PHE:CD1	2.55	0.41
10:L:405:ILE:O	10:L:409:LEU:HD23	2.20	0.41
10:L:420:ALA:O	10:L:512:LEU:HB2	2.20	0.41
11:M:458:ILE:HB	11:M:459:PRO:HD3	2.03	0.41
12:N:127:LYS:HG2	12:N:131:LEU:HD23	2.02	0.41
12:N:195:GLU:OE1	12:N:195:GLU:N	2.53	0.41
12:N:404:ASP:C	12:N:406:CYS:H	2.29	0.41
14:P:372:ILE:O	14:P:372:ILE:HG13	2.20	0.41
2:2:59:ASP:OD1	2:2:60:THR:N	2.53	0.41
7:A:103:ASN:HD22	7:A:444:SER:CB	2.33	0.41
7:A:103:ASN:HB3	7:A:440:GLU:CG	2.51	0.41
8:B:347:LYS:HG2	8:B:364:GLY:HA3	2.02	0.41
10:D:289:GLN:HA	10:D:292:LYS:HG2	2.01	0.41
11:E:513:LYS:O	11:E:517:ILE:HG12	2.21	0.41
11:E:522:GLN:HB2	13:G:380:GLN:HB3	2.02	0.41
12:F:73:THR:O	12:F:76:LEU:HG	2.21	0.41
12:F:224:ARG:HH11	12:F:224:ARG:HG3	1.85	0.41
12:F:376:ILE:HG21	12:F:391:VAL:HG21	2.02	0.41
13:G:161:THR:HG21	13:G:490:ALA:O	2.20	0.41
13:G:282:HIS:O	13:G:308:MET:HE1	2.21	0.41
14:H:290:VAL:HG21	14:H:350:VAL:HG11	2.01	0.41
7:I:44:MET:HB2	9:K:522:ILE:HA	2.02	0.41
7:I:405:SER:HB2	7:I:506:PRO:HB3	2.03	0.41
8:J:37:ASP:HA	8:J:40:LYS:HD3	2.01	0.41
8:J:255:ARG:HH11	8:J:255:ARG:HG3	1.85	0.41
11:M:171:THR:HG21	11:M:505:HIS:HB3	2.03	0.41
11:M:452:ALA:O	11:M:456:GLU:HG2	2.21	0.41
12:N:31:GLN:CG	12:N:97:LEU:HD23	2.51	0.41
12:N:190:MET:N	12:N:190:MET:SD	2.93	0.41
13:O:128:ALA:HB2	13:O:435:ILE:HD12	2.03	0.41
13:O:175:PHE:O	13:O:179:VAL:HG13	2.21	0.41
14:P:397:ASN:O	14:P:400:LYS:HB2	2.21	0.41
1:1:36:GLN:O	1:1:40:THR:HG23	2.21	0.41
1:1:88:GLU:HA	1:1:91:ILE:HG22	2.02	0.41
3:3:138:ASP:HA	3:3:141:GLN:NE2	2.36	0.41
6:6:33:LEU:HA	6:6:36:GLN:HG3	2.03	0.41
6:6:57:PHE:CD2	6:6:66:LYS:HA	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:101:LEU:HD11	7:A:524:ILE:HG21	2.02	0.41
7:A:115:THR:HG21	10:D:468:ASN:O	2.21	0.41
7:A:133:ASN:HA	7:A:137:ILE:CD1	2.49	0.41
7:A:157:SER:HA	7:A:160:ILE:HG12	2.02	0.41
7:A:415:VAL:HG21	7:A:510:LYS:HE2	2.02	0.41
7:A:432:SER:OG	7:A:434:GLU:OE1	2.34	0.41
8:B:133:ALA:HB2	8:B:436:MET:HB2	2.02	0.41
8:B:170:LYS:HG3	8:B:389:SER:HB3	2.03	0.41
8:B:220:LEU:O	8:B:360:ILE:N	2.47	0.41
9:C:46:MET:HA	12:F:517:LEU:HD23	2.02	0.41
10:D:240:ARG:HH22	10:D:242:GLU:HB2	1.85	0.41
10:D:330:ARG:O	10:D:333:ILE:HB	2.21	0.41
10:D:511:PRO:O	10:D:514:VAL:HG12	2.21	0.41
11:E:33:ALA:O	11:E:37:HIS:ND1	2.53	0.41
11:E:163:GLU:OE1	11:E:166:ILE:HD11	2.21	0.41
12:F:149:ILE:CD1	12:F:173:VAL:HG11	2.51	0.41
12:F:291:VAL:HG12	12:F:292:ILE:N	2.36	0.41
13:G:46:ASP:OD1	13:G:47:LYS:N	2.54	0.41
13:G:231:LYS:HA	13:G:231:LYS:HD2	1.79	0.41
13:G:272:ASN:OD1	13:G:273:ILE:N	2.54	0.41
13:G:298:VAL:HG22	13:G:302:TYR:HE2	1.85	0.41
13:G:414:MET:HG3	13:G:464:LEU:HD22	2.03	0.41
14:H:55:MET:HE2	14:H:55:MET:HB3	1.90	0.41
14:H:218:LEU:HD13	14:H:376:VAL:CG2	2.51	0.41
14:H:410:PRO:O	14:H:414:ALA:HB3	2.21	0.41
7:I:27:SER:O	7:I:31:ILE:HG13	2.21	0.41
7:I:237:LEU:HD13	7:I:278:ILE:HG23	2.02	0.41
7:I:486:ILE:HG13	7:I:497:ASP:HA	2.03	0.41
8:J:40:LYS:HE3	8:J:449:ILE:HD12	2.02	0.41
8:J:199:ILE:HG12	8:J:394:LEU:HD22	2.03	0.41
8:J:211:ASP:O	8:J:376:ARG:HG2	2.21	0.41
9:K:65:ALA:HA	9:K:68:ARG:NH1	2.36	0.41
9:K:184:GLN:HG3	9:K:185:PHE:CE2	2.56	0.41
9:K:287:PRO:HD2	9:K:309:ILE:CD1	2.51	0.41
10:L:250:GLN:NE2	10:L:301:GLN:OE1	2.31	0.41
10:L:287:VAL:HG11	10:L:320:MET:SD	2.61	0.41
11:M:86:GLN:NE2	13:O:56:ALA:HB2	2.35	0.41
11:M:393:MET:N	11:M:393:MET:SD	2.94	0.41
12:N:445:LEU:HG	12:N:463:LEU:HD11	2.01	0.41
13:O:144:LYS:HD2	13:O:151:GLN:HE21	1.86	0.41
13:O:234:ASN:N	13:O:346:GLN:O	2.43	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:P:257:VAL:HG23	14:P:268:PHE:HB2	2.02	0.41
14:P:324:LEU:O	14:P:328:VAL:HG22	2.20	0.41
14:P:352:LEU:HD21	14:P:359:GLN:HG3	2.02	0.41
2:2:70:CYS:HA	3:3:134:GLU:OE2	2.21	0.41
2:2:90:LEU:HD12	2:2:93:ASN:HD21	1.85	0.41
3:3:78:ILE:CG2	3:3:82:LYS:HE3	2.51	0.41
7:A:233:LYS:HB2	7:A:283:ALA:HA	2.03	0.41
8:B:95:VAL:HG11	8:B:499:VAL:HG23	2.03	0.41
9:C:134:ILE:O	9:C:138:LYS:HG2	2.21	0.41
9:C:165:ILE:HG21	9:C:390:ASN:ND2	2.36	0.41
9:C:515:LEU:O	9:C:519:ILE:HG12	2.21	0.41
9:C:521:ASP:O	9:C:522:ILE:HD13	2.21	0.41
10:D:268:ASP:HB3	10:D:271:GLN:HB2	2.01	0.41
11:E:48:MET:HE3	11:E:48:MET:HB3	1.74	0.41
11:E:191:ASN:HA	11:E:194:LEU:HG	2.03	0.41
11:E:239:MET:HE3	11:E:315:LEU:HA	2.02	0.41
12:F:28:ARG:CZ	12:F:104:LYS:HD2	2.51	0.41
12:F:174:ASP:HB3	12:F:206:LEU:CD2	2.51	0.41
12:F:176:ILE:HG13	12:F:398:VAL:HG13	2.03	0.41
12:F:214:HIS:HB3	12:F:314:ARG:NH1	2.36	0.41
13:G:109:LYS:HA	13:G:112:VAL:HG12	2.03	0.41
13:G:218:LYS:O	13:G:218:LYS:HD2	2.21	0.41
7:I:292:ILE:HB	7:I:310:ARG:HD2	2.03	0.41
8:J:71:LEU:O	8:J:74:ILE:HG22	2.21	0.41
8:J:415:MET:HE1	8:J:444:ARG:NE	2.24	0.41
9:K:278:LEU:HD23	9:K:278:LEU:HA	1.79	0.41
10:L:178:GLN:HG2	10:L:179:TYR:N	2.36	0.41
11:M:165:LEU:HD12	11:M:412:LEU:HD13	2.02	0.41
12:N:461:GLU:OE2	12:N:465:LYS:HD3	2.21	0.41
6:6:42:ILE:O	6:6:45:GLU:HG2	2.21	0.40
8:B:180:THR:O	8:B:184:VAL:HG12	2.21	0.40
10:D:249:ILE:HD11	10:D:298:LEU:HD12	2.03	0.40
13:G:131:LEU:HG	13:G:419:TYR:CE2	2.56	0.40
13:G:443:GLU:CD	13:G:465:ARG:HH21	2.29	0.40
7:I:349:GLU:HG2	7:I:350:GLU:HG2	2.03	0.40
8:J:99:THR:HA	8:J:102:VAL:HG12	2.03	0.40
9:K:87:GLN:NE2	9:K:91:VAL:HB	2.34	0.40
10:L:186:MET:CE	10:L:223:LEU:H	2.34	0.40
11:M:206:PHE:CE1	11:M:406:LEU:HG	2.56	0.40
11:M:284:LYS:HA	11:M:287:GLU:HG3	2.03	0.40
11:M:388:ARG:NE	11:M:388:ARG:HA	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:M:522:GLN:HE22	13:O:379:GLU:HG3	1.85	0.40
12:N:318:ARG:HG3	12:N:321:MET:CE	2.50	0.40
14:P:384:LEU:O	14:P:388:ILE:HG12	2.21	0.40
7:A:171:MET:HE3	7:A:375:ILE:HG23	2.04	0.40
7:A:214:TYR:CE2	7:A:319:ILE:HG12	2.56	0.40
8:B:112:GLU:HB3	8:B:438:SER:HG	1.86	0.40
8:B:354:ILE:O	8:B:354:ILE:HG13	2.21	0.40
9:C:313:ARG:HH11	9:C:314:ARG:N	2.17	0.40
9:C:374:ILE:HG22	9:C:376:LEU:H	1.86	0.40
10:D:211:VAL:HG23	10:D:389:VAL:HA	2.03	0.40
12:F:73:THR:HA	12:F:76:LEU:HG	2.03	0.40
12:F:176:ILE:HG13	12:F:398:VAL:HG11	2.03	0.40
8:J:173:THR:O	8:J:176:LYS:HB2	2.21	0.40
9:K:280:GLU:HA	9:K:283:ILE:CD1	2.48	0.40
9:K:315:VAL:HB	9:K:319:ASP:HB2	2.03	0.40
10:L:283:ILE:O	10:L:286:LEU:HG	2.21	0.40
11:M:226:LYS:O	11:M:375:GLU:HB2	2.21	0.40
12:N:24:ILE:O	12:N:28:ARG:HG2	2.21	0.40
13:O:238:ALA:HB3	13:O:289:VAL:HA	2.03	0.40
14:P:408:LEU:HA	14:P:501:TYR:N	2.36	0.40
14:P:418:GLU:CD	14:P:476:LYS:HG3	2.47	0.40
7:A:69:HIS:ND1	7:A:70:PRO:HD2	2.35	0.40
7:A:100:LEU:HD12	7:A:444:SER:OG	2.22	0.40
7:A:448:ILE:HB	7:A:449:PRO:HD3	2.02	0.40
8:B:88:SER:HG	8:B:99:THR:HG1	1.61	0.40
8:B:408:TYR:CE2	8:B:475:THR:HG22	2.56	0.40
10:D:461:ILE:N	10:D:462:PRO:HD2	2.35	0.40
11:E:427:ILE:HG21	11:E:459:PRO:HG2	2.04	0.40
12:F:264:ARG:NH2	12:F:268:GLU:OE2	2.48	0.40
13:G:166:LYS:HD3	13:G:385:THR:OG1	2.21	0.40
14:H:274:ASN:OD1	14:H:275:LEU:N	2.54	0.40
8:J:114:GLU:HA	8:J:117:ILE:HG22	2.03	0.40
8:J:187:VAL:HG11	8:J:397:LEU:HD13	2.03	0.40
10:L:414:CYS:HB2	10:L:513:LEU:HB3	2.02	0.40
12:N:282:CYS:HB3	12:N:287:LYS:HG3	2.03	0.40
13:O:19:ILE:H	13:O:19:ILE:HD12	1.86	0.40
13:O:232:TYR:O	13:O:347:VAL:HA	2.21	0.40
14:P:217:VAL:HG12	14:P:375:ILE:HG22	2.04	0.40
14:P:433:LEU:O	14:P:434:GLU:HB2	2.21	0.40
7:A:378:ARG:O	7:A:388:MET:HE1	2.21	0.40
8:B:161:ASN:OD1	8:B:162:ILE:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:D:431:GLU:OE2	10:D:435:ARG:HG3	2.21	0.40
10:D:523:THR:HA	10:D:526:VAL:HG12	2.03	0.40
11:E:364:PHE:HB2	11:E:371:MET:HG2	2.04	0.40
11:E:469:ASN:HA	11:E:470:PRO:HD3	1.98	0.40
12:F:104:LYS:O	12:F:108:LEU:HG	2.21	0.40
13:G:142:THR:HG22	13:G:404:SER:HA	2.03	0.40
13:G:164:SER:HA	13:G:172:LYS:CE	2.52	0.40
14:H:201:ASN:O	14:H:372:ILE:HG13	2.21	0.40
14:H:296:LYS:HZ1	14:H:315:LEU:HG	1.86	0.40
14:H:472:GLN:OE1	14:H:472:GLN:HA	2.21	0.40
7:I:417:ALA:HB3	7:I:471:HIS:CE1	2.56	0.40
8:J:50:LYS:HZ2	10:L:534:ASP:HB2	1.85	0.40
8:J:200:HIS:HB3	8:J:372:THR:HG22	2.02	0.40
11:M:404:ASP:HA	11:M:407:CYS:SG	2.62	0.40
12:N:282:CYS:HA	12:N:287:LYS:HE2	2.04	0.40
14:P:244:CYS:HB2	14:P:245:PRO:HD2	2.03	0.40
14:P:333:LEU:HD11	14:P:343:GLU:CD	2.46	0.40
14:P:402:LEU:HD11	14:P:408:LEU:HD13	2.03	0.40
14:P:429:THR:O	14:P:431:PRO:HD3	2.22	0.40
3:3:63:MET:HB3	3:3:166:ARG:HD3	2.03	0.40
3:3:131:VAL:C	3:3:132:MET:HE2	2.46	0.40
5:5:15:LEU:HG	5:5:19:LYS:HE3	2.04	0.40
5:5:113:GLN:HG3	6:6:39:GLU:HG2	2.03	0.40
7:A:144:GLY:HA2	7:A:148:LEU:HG	2.03	0.40
8:B:230:LYS:HE2	8:B:358:LYS:NZ	2.36	0.40
8:B:250:LYS:O	8:B:251:ILE:HD13	2.21	0.40
9:C:142:ILE:HG23	9:C:144:VAL:HG23	2.02	0.40
9:C:144:VAL:HB	9:C:406:GLN:NE2	2.36	0.40
9:C:399:ARG:NH1	9:C:399:ARG:HG2	2.36	0.40
9:C:410:GLY:HA2	9:C:414:SER:HB3	2.04	0.40
10:D:248:LEU:HB3	10:D:345:VAL:HG23	2.03	0.40
10:D:515:SER:O	10:D:519:LEU:HD23	2.21	0.40
12:F:446:ILE:HD12	12:F:446:ILE:HA	1.97	0.40
13:G:298:VAL:HG22	13:G:302:TYR:CE2	2.57	0.40
14:H:222:VAL:HA	14:H:361:VAL:O	2.22	0.40
14:H:253:THR:HG22	14:H:258:LEU:HA	2.03	0.40
8:J:455:GLY:HA2	10:L:129:HIS:CG	2.56	0.40
10:L:78:LEU:HD12	10:L:92:VAL:HG22	2.03	0.40
10:L:438:GLU:HA	10:L:441:ARG:HD2	2.03	0.40
10:L:447:GLU:O	10:L:451:VAL:HG23	2.21	0.40
12:N:58:LYS:HD3	12:N:159:LYS:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:N:414:VAL:HG11	12:N:501:LYS:HE3	2.04	0.40
13:O:216:PHE:HZ	13:O:322:THR:HG21	1.86	0.40
13:O:288:VAL:HG21	13:O:361:PHE:CE1	2.56	0.40
14:P:146:LEU:HA	14:P:476:LYS:NZ	2.35	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 PDB entries followed by that with respect to all EM entries.

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	1	105/122 (86%)	103 (98%)	2 (2%)	0	100	100
2	2	81/154 (53%)	80 (99%)	1 (1%)	0	100	100
3	3	114/197 (58%)	108 (95%)	6 (5%)	0	100	100
4	4	86/140 (61%)	82 (95%)	4 (5%)	0	100	100
5	5	125/140 (89%)	118 (94%)	7 (6%)	0	100	100
6	6	100/129 (78%)	97 (97%)	3 (3%)	0	100	100
7	A	514/556 (92%)	495 (96%)	19 (4%)	0	100	100
7	I	512/556 (92%)	474 (93%)	38 (7%)	0	100	100
8	B	495/535 (92%)	472 (95%)	23 (5%)	0	100	100
8	J	495/535 (92%)	470 (95%)	25 (5%)	0	100	100
9	C	503/545 (92%)	477 (95%)	25 (5%)	1 (0%)	43	74
9	K	503/545 (92%)	466 (93%)	36 (7%)	1 (0%)	43	74
10	D	509/539 (94%)	486 (96%)	22 (4%)	1 (0%)	43	74
10	L	509/539 (94%)	479 (94%)	30 (6%)	0	100	100
11	E	504/541 (93%)	472 (94%)	32 (6%)	0	100	100
11	M	504/541 (93%)	478 (95%)	26 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	F	506/531 (95%)	484 (96%)	21 (4%)	1 (0%)	43	74
12	N	506/531 (95%)	471 (93%)	34 (7%)	1 (0%)	43	74
13	G	507/543 (93%)	477 (94%)	29 (6%)	1 (0%)	43	74
13	O	507/543 (93%)	472 (93%)	33 (6%)	2 (0%)	30	64
14	H	498/547 (91%)	482 (97%)	16 (3%)	0	100	100
14	P	500/547 (91%)	476 (95%)	24 (5%)	0	100	100
All	All	8683/9556 (91%)	8219 (95%)	456 (5%)	8 (0%)	49	80

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	C	365	ASP
12	F	72	PRO
12	N	94	SER
13	O	364	CYS
13	G	144	LYS
9	K	189	GLY
13	O	88	ALA
10	D	505	GLU

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 PDB entries followed by that with respect to all EM entries.

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	1	97/109 (89%)	97 (100%)	0	100	100
2	2	74/122 (61%)	74 (100%)	0	100	100
3	3	107/175 (61%)	107 (100%)	0	100	100
4	4	81/125 (65%)	81 (100%)	0	100	100
5	5	116/128 (91%)	116 (100%)	0	100	100
6	6	91/108 (84%)	91 (100%)	0	100	100
7	A	430/463 (93%)	430 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	I	428/463 (92%)	427 (100%)	1 (0%)	87	87
8	B	397/427 (93%)	397 (100%)	0	100	100
8	J	397/427 (93%)	397 (100%)	0	100	100
9	C	437/469 (93%)	437 (100%)	0	100	100
9	K	437/469 (93%)	437 (100%)	0	100	100
10	D	435/452 (96%)	435 (100%)	0	100	100
10	L	435/452 (96%)	435 (100%)	0	100	100
11	E	426/456 (93%)	426 (100%)	0	100	100
11	M	426/456 (93%)	426 (100%)	0	100	100
12	F	426/442 (96%)	426 (100%)	0	100	100
12	N	426/442 (96%)	426 (100%)	0	100	100
13	G	417/443 (94%)	417 (100%)	0	100	100
13	O	417/443 (94%)	417 (100%)	0	100	100
14	H	416/451 (92%)	416 (100%)	0	100	100
14	P	417/451 (92%)	417 (100%)	0	100	100
All	All	7333/7973 (92%)	7332 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	I	389	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
6	6	54	ASN
7	A	103	ASN
7	A	284	ASN
7	A	393	HIS
7	A	435	GLN
7	A	458	GLN
7	A	472	ASN
8	B	157	GLN
8	B	174	HIS
8	B	175	HIS
8	B	269	HIS

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Mol	Chain	Res	Type
8	B	314	HIS
9	C	118	HIS
9	C	470	HIS
10	D	406	HIS
10	D	510	GLN
11	E	318	ASN
12	F	31	GLN
12	F	320	ASN
12	F	400	ASN
13	G	487	ASN
14	H	422	GLN
7	I	69	HIS
7	I	103	ASN
8	J	65	ASN
8	J	227	ASN
9	K	321	ASN
9	K	392	GLN
9	K	434	GLN
9	K	454	ASN
10	L	98	GLN
10	L	263	GLN
10	L	350	GLN
10	L	406	HIS
10	L	472	ASN
10	L	482	ASN
11	M	46	ASN
11	M	55	ASN
11	M	85	HIS
11	M	129	HIS
11	M	139	GLN
11	M	316	GLN
11	M	376	GLN
11	M	411	ASN
11	M	522	GLN
12	N	23	ASN
12	N	470	HIS
13	O	380	GLN
13	O	452	ASN
13	O	487	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 ⓘ

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
15	ADP	P	601	-	28,29,29	3.05	11 (39%)	43,45,45	1.81	8 (18%)
15	ADP	N	601	-	28,29,29	3.09	12 (42%)	43,45,45	1.82	8 (18%)
15	ADP	F	601	-	28,29,29	3.05	11 (39%)	43,45,45	1.88	9 (20%)
15	ADP	H	5000	-	28,29,29	3.06	11 (39%)	43,45,45	1.85	9 (20%)

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
15	ADP	P	601	-	-	6/16/32/32	0/3/3/3
15	ADP	N	601	-	-	1/16/32/32	0/3/3/3
15	ADP	F	601	-	-	5/16/32/32	0/3/3/3
15	ADP	H	5000	-	-	6/16/32/32	0/3/3/3

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	N	601	ADP	O4'-C4'	7.79	1.62	1.45
15	P	601	ADP	O4'-C4'	7.61	1.61	1.45
15	F	601	ADP	O4'-C4'	7.57	1.61	1.45
15	H	5000	ADP	O4'-C4'	7.45	1.61	1.45
15	P	601	ADP	C3'-C4'	-7.37	1.34	1.53
15	H	5000	ADP	C3'-C4'	-7.37	1.34	1.53
15	N	601	ADP	C3'-C4'	-7.29	1.34	1.53
15	F	601	ADP	C3'-C4'	-7.23	1.34	1.53
15	N	601	ADP	C6-N6	6.26	1.50	1.34
15	H	5000	ADP	C6-N6	6.25	1.50	1.34
15	F	601	ADP	C6-N6	6.23	1.50	1.34
15	P	601	ADP	C6-N6	6.19	1.50	1.34
15	H	5000	ADP	O4'-C1'	-5.98	1.28	1.42
15	F	601	ADP	O4'-C1'	-5.95	1.28	1.42
15	P	601	ADP	O4'-C1'	-5.78	1.28	1.42
15	N	601	ADP	O4'-C1'	-5.71	1.28	1.42
15	N	601	ADP	PA-O3A	4.78	1.64	1.59
15	H	5000	ADP	PA-O3A	4.64	1.64	1.59
15	F	601	ADP	PA-O3A	4.49	1.64	1.59
15	P	601	ADP	PA-O3A	4.49	1.64	1.59
15	P	601	ADP	C5-N7	-3.22	1.33	1.39
15	F	601	ADP	C5-N7	-3.22	1.33	1.39
15	H	5000	ADP	C5-N7	-3.20	1.33	1.39
15	N	601	ADP	C5-N7	-3.18	1.33	1.39
15	N	601	ADP	PB-O1B	2.93	1.59	1.50
15	H	5000	ADP	O3'-C3'	2.82	1.50	1.43
15	F	601	ADP	O3'-C3'	2.82	1.49	1.43
15	N	601	ADP	O3'-C3'	2.81	1.49	1.43
15	P	601	ADP	O3'-C3'	2.80	1.49	1.43
15	N	601	ADP	O2'-C2'	-2.78	1.36	1.43
15	F	601	ADP	O2'-C2'	-2.70	1.36	1.43
15	H	5000	ADP	O2'-C2'	-2.65	1.36	1.43
15	P	601	ADP	C8-N9	-2.65	1.33	1.37
15	N	601	ADP	C8-N9	-2.63	1.33	1.37
15	P	601	ADP	O2'-C2'	-2.62	1.36	1.43
15	F	601	ADP	C8-N9	-2.61	1.33	1.37
15	H	5000	ADP	C8-N9	-2.59	1.33	1.37
15	P	601	ADP	C4-N9	-2.39	1.32	1.37
15	H	5000	ADP	C4-N9	-2.35	1.32	1.37
15	F	601	ADP	C4-N9	-2.30	1.32	1.37
15	N	601	ADP	C4-N9	-2.24	1.33	1.37
15	H	5000	ADP	PB-O1B	2.03	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	F	601	ADP	PB-O1B	2.02	1.56	1.50
15	P	601	ADP	PB-O1B	2.01	1.56	1.50
15	N	601	ADP	PA-O5'	2.01	1.67	1.59

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	N	601	ADP	C5-C4-N3	-5.53	119.10	126.72
15	P	601	ADP	C5-C4-N3	-5.46	119.20	126.72
15	F	601	ADP	C5-C4-N3	-5.41	119.27	126.72
15	H	5000	ADP	C5-C4-N3	-5.37	119.32	126.72
15	N	601	ADP	N3-C2-N1	-4.60	121.62	128.58
15	H	5000	ADP	N3-C2-N1	-4.53	121.72	128.58
15	F	601	ADP	N3-C2-N1	-4.50	121.77	128.58
15	P	601	ADP	N3-C2-N1	-4.41	121.90	128.58
15	N	601	ADP	N3-C4-N9	3.94	133.86	127.17
15	P	601	ADP	N3-C4-N9	3.91	133.81	127.17
15	F	601	ADP	N3-C4-N9	3.86	133.73	127.17
15	H	5000	ADP	N3-C4-N9	3.86	133.73	127.17
15	N	601	ADP	C2-N3-C4	3.61	120.64	111.83
15	H	5000	ADP	C2-N3-C4	3.53	120.46	111.83
15	F	601	ADP	C2-N3-C4	3.53	120.44	111.83
15	P	601	ADP	C2-N3-C4	3.47	120.31	111.83
15	H	5000	ADP	N9-C8-N7	-3.30	109.25	113.94
15	N	601	ADP	C4-C5-N7	-3.29	106.82	110.58
15	N	601	ADP	N9-C8-N7	-3.28	109.28	113.94
15	P	601	ADP	N9-C8-N7	-3.22	109.37	113.94
15	N	601	ADP	C5-N7-C8	3.22	108.51	103.45
15	F	601	ADP	C4-C5-N7	-3.21	106.92	110.58
15	H	5000	ADP	C4-C5-N7	-3.20	106.92	110.58
15	F	601	ADP	N9-C8-N7	-3.20	109.40	113.94
15	P	601	ADP	C4-C5-N7	-3.18	106.94	110.58
15	H	5000	ADP	C5-N7-C8	3.17	108.43	103.45
15	F	601	ADP	C5-N7-C8	3.13	108.37	103.45
15	P	601	ADP	C5-N7-C8	3.11	108.34	103.45
15	H	5000	ADP	C4-N9-C8	2.57	108.44	105.74
15	P	601	ADP	C4-N9-C8	2.51	108.37	105.74
15	N	601	ADP	C4-N9-C8	2.49	108.35	105.74
15	F	601	ADP	C4-N9-C8	2.45	108.31	105.74
15	H	5000	ADP	C3'-C2'-C1'	2.20	105.63	101.46
15	F	601	ADP	C4'-O4'-C1'	-2.18	104.66	109.47

There are no chirality outliers.

All (18) torsion outliers are listed below:

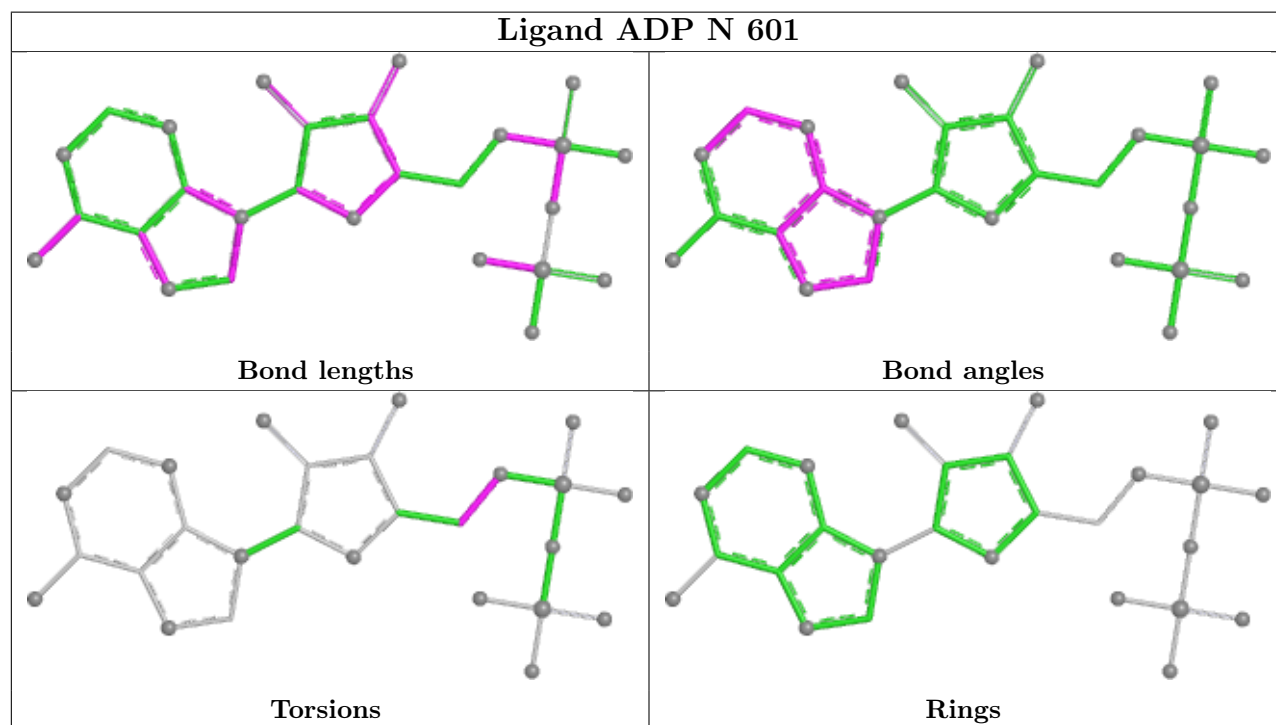
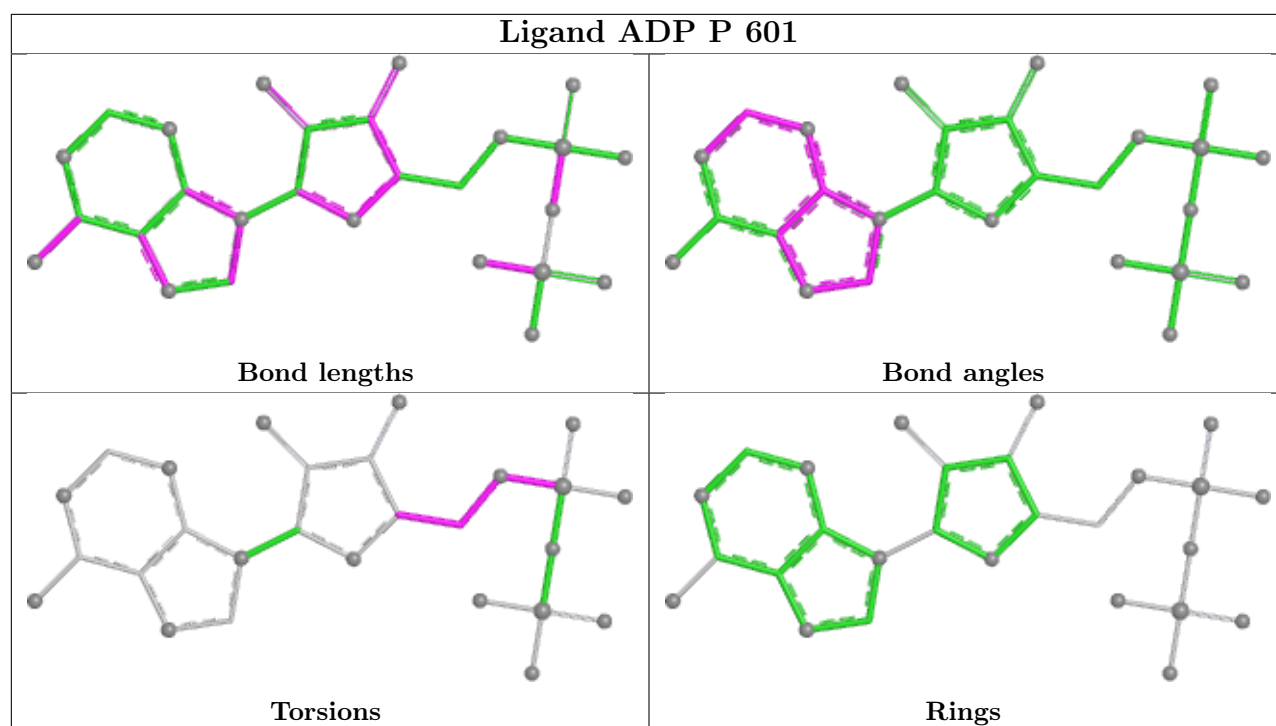
Mol	Chain	Res	Type	Atoms
15	F	601	ADP	C5'-O5'-PA-O1A
15	F	601	ADP	C5'-O5'-PA-O2A
15	F	601	ADP	C5'-O5'-PA-O3A
15	F	601	ADP	O4'-C4'-C5'-O5'
15	H	5000	ADP	PA-O3A-PB-O2B
15	H	5000	ADP	PA-O3A-PB-O3B
15	H	5000	ADP	C5'-O5'-PA-O1A
15	H	5000	ADP	C5'-O5'-PA-O2A
15	H	5000	ADP	C5'-O5'-PA-O3A
15	P	601	ADP	C5'-O5'-PA-O1A
15	P	601	ADP	C5'-O5'-PA-O3A
15	F	601	ADP	C3'-C4'-C5'-O5'
15	P	601	ADP	O4'-C4'-C5'-O5'
15	P	601	ADP	C3'-C4'-C5'-O5'
15	P	601	ADP	C4'-C5'-O5'-PA
15	P	601	ADP	C5'-O5'-PA-O2A
15	N	601	ADP	C4'-C5'-O5'-PA
15	H	5000	ADP	O4'-C4'-C5'-O5'

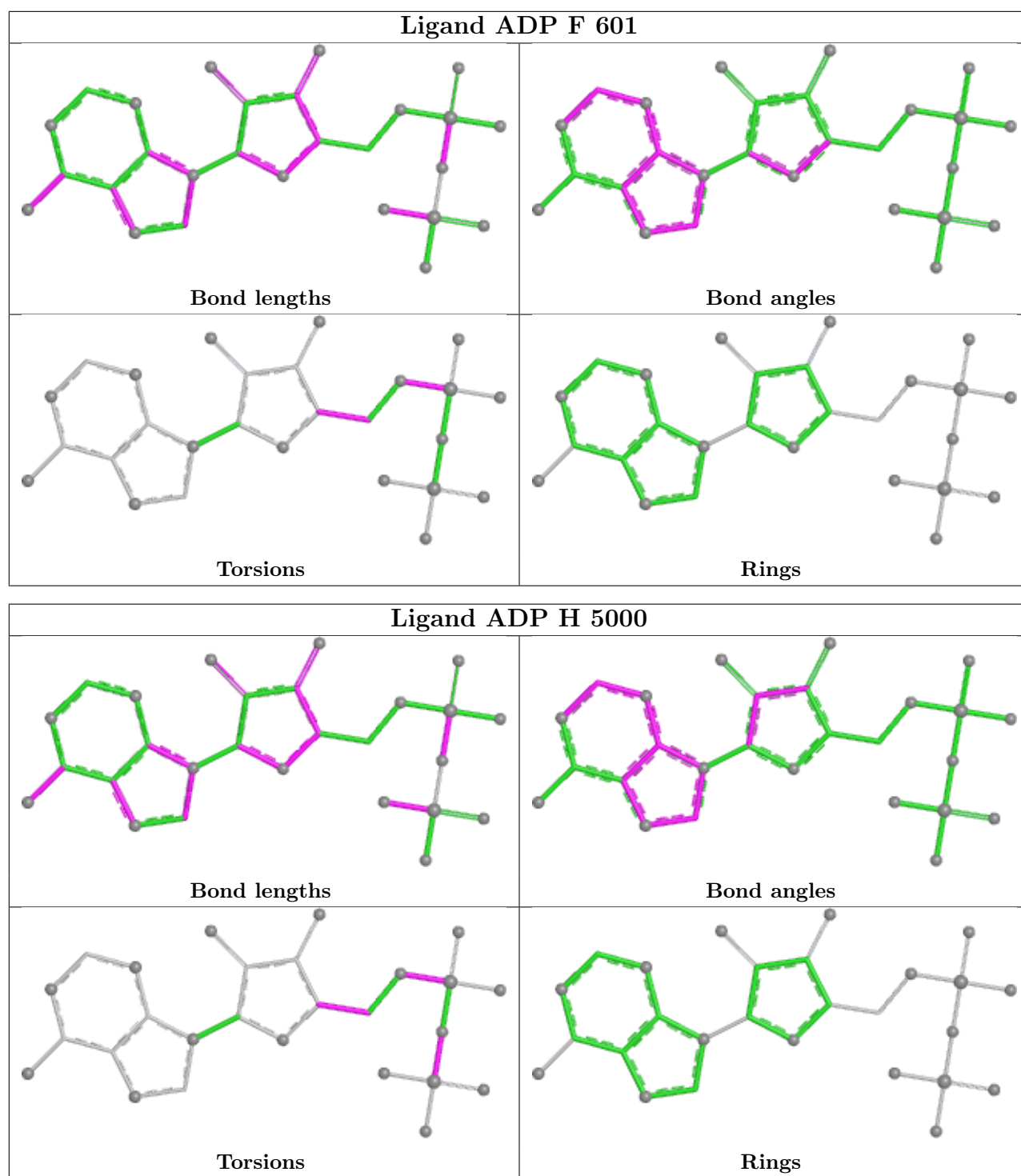
There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	P	601	ADP	2	0
15	N	601	ADP	1	0
15	F	601	ADP	1	0
15	H	5000	ADP	4	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

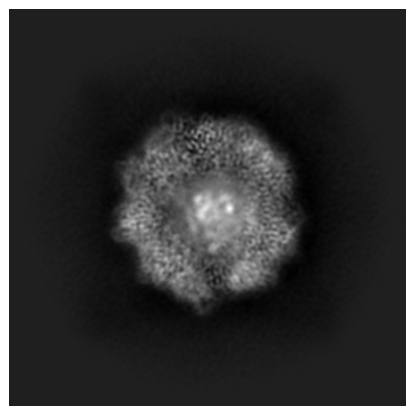
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32823. These allow visual inspection of the internal detail of the map and identification of artifacts.

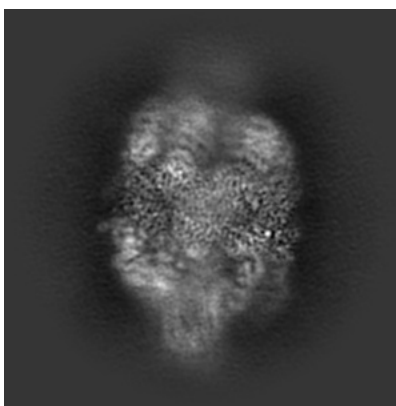
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

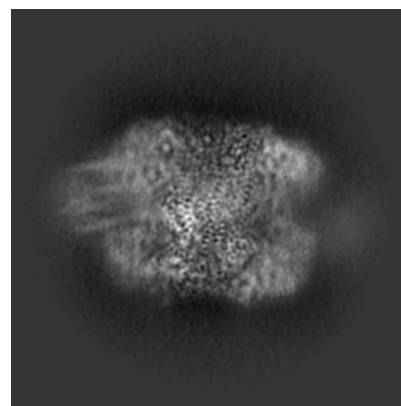
6.1.1 Primary map



X

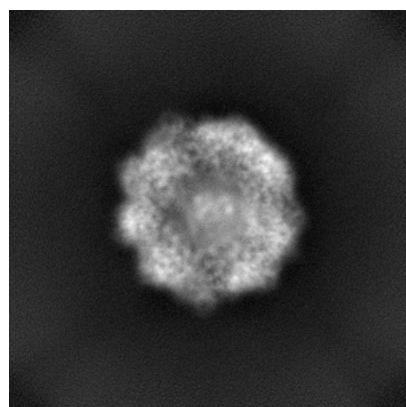


Y

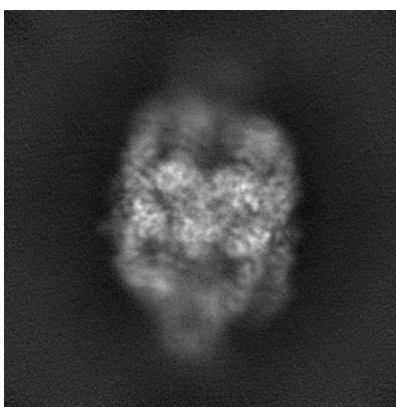


Z

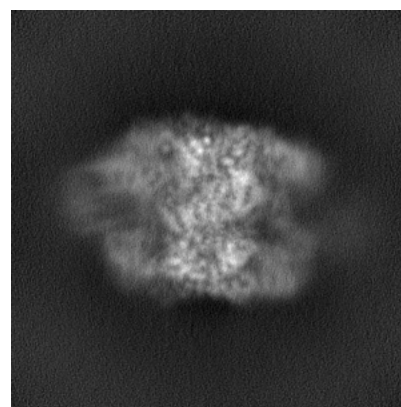
6.1.2 Raw map



X



Y

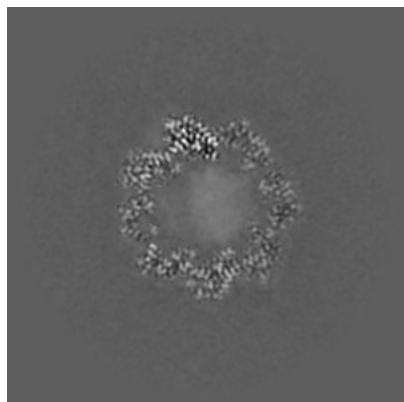


Z

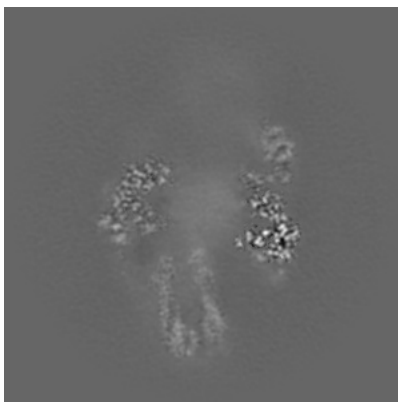
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

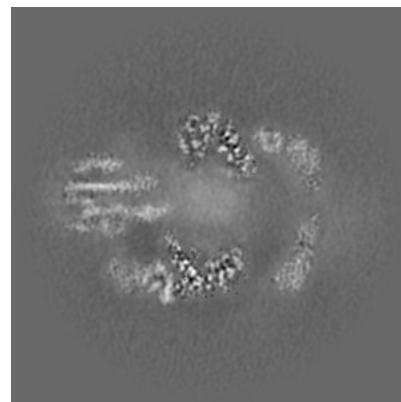
6.2.1 Primary map



X Index: 160

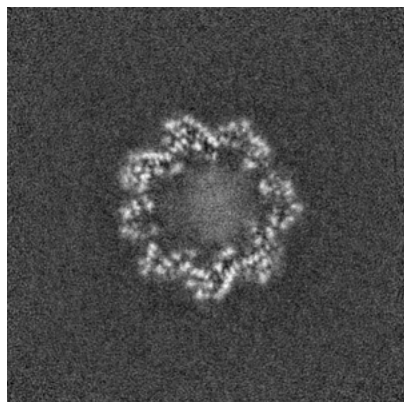


Y Index: 160

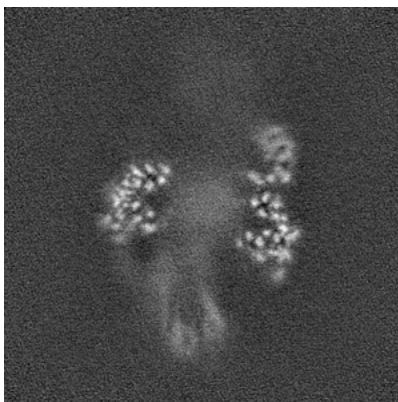


Z Index: 160

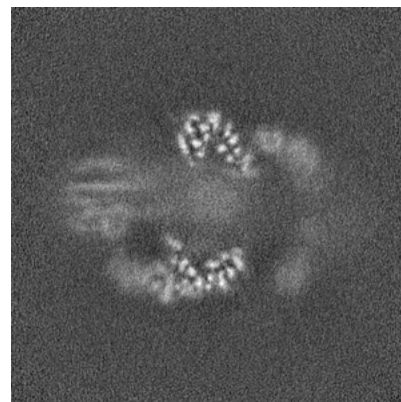
6.2.2 Raw map



X Index: 160



Y Index: 160

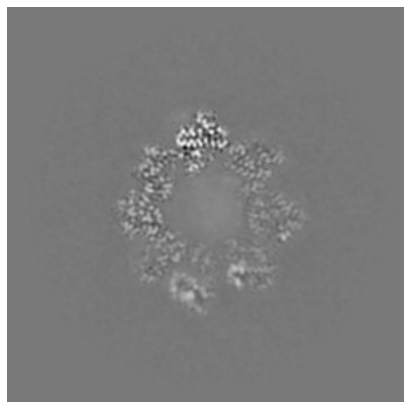


Z Index: 160

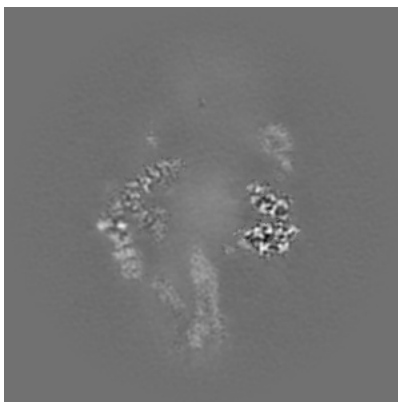
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

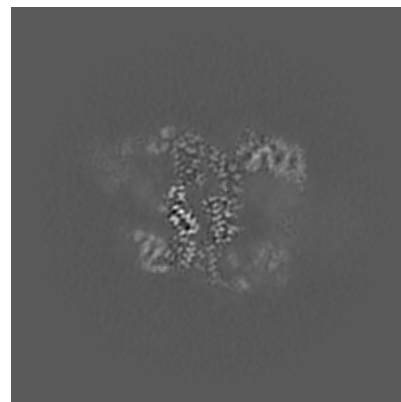
6.3.1 Primary map



X Index: 141

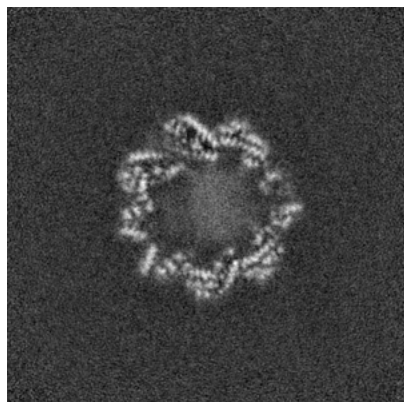


Y Index: 153

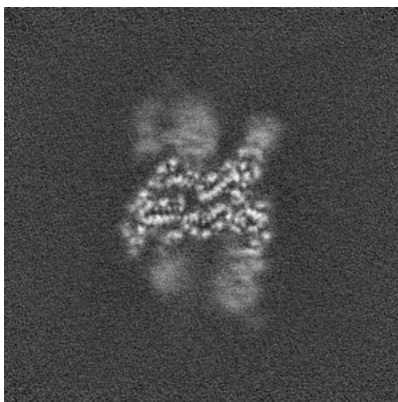


Z Index: 202

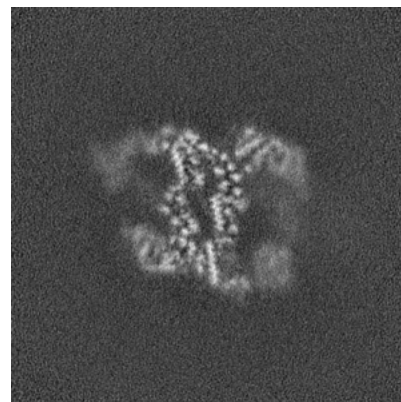
6.3.2 Raw map



X Index: 162



Y Index: 207

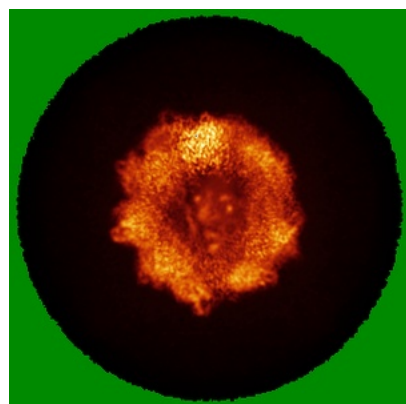


Z Index: 200

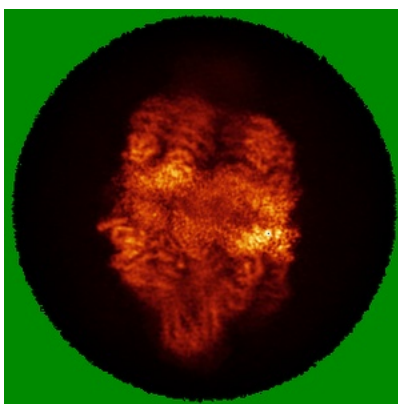
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

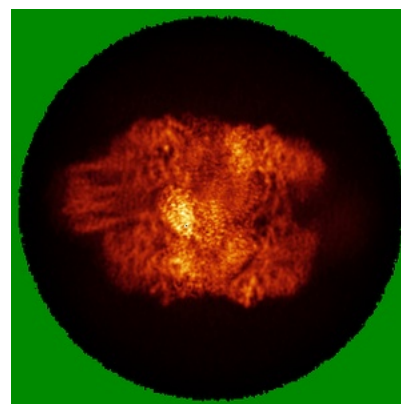
6.4.1 Primary map



X

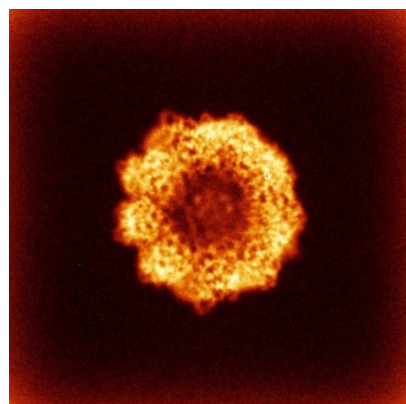


Y

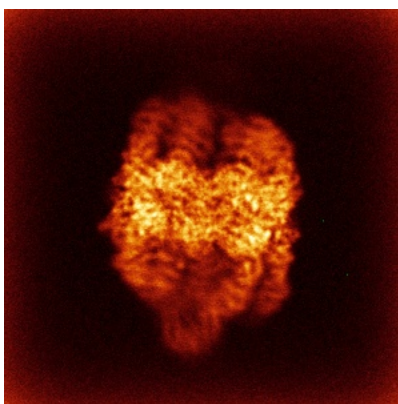


Z

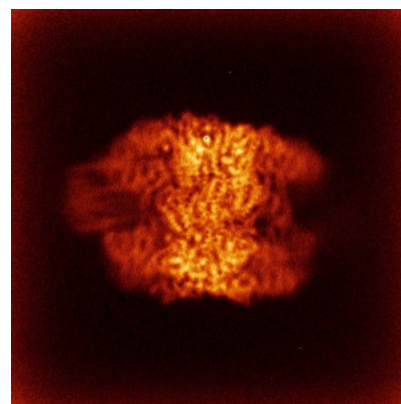
6.4.2 Raw map



X



Y

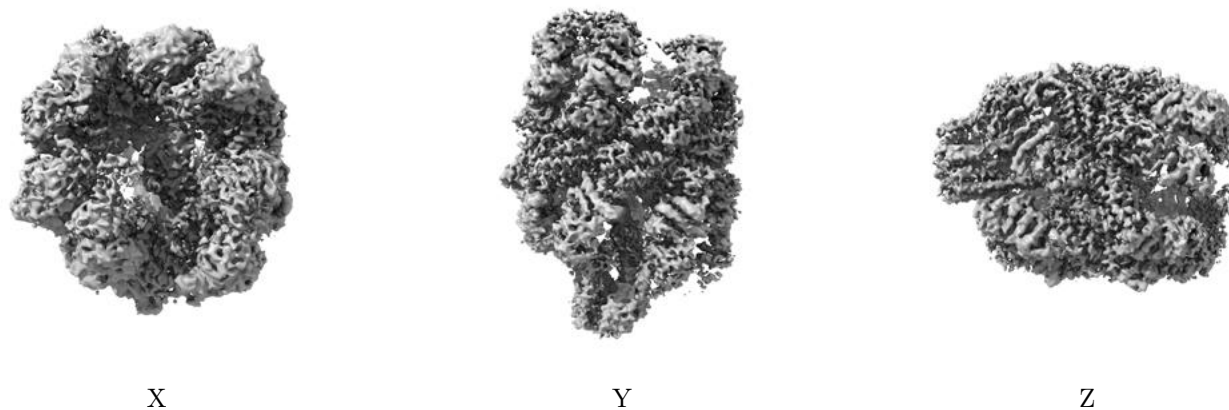


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

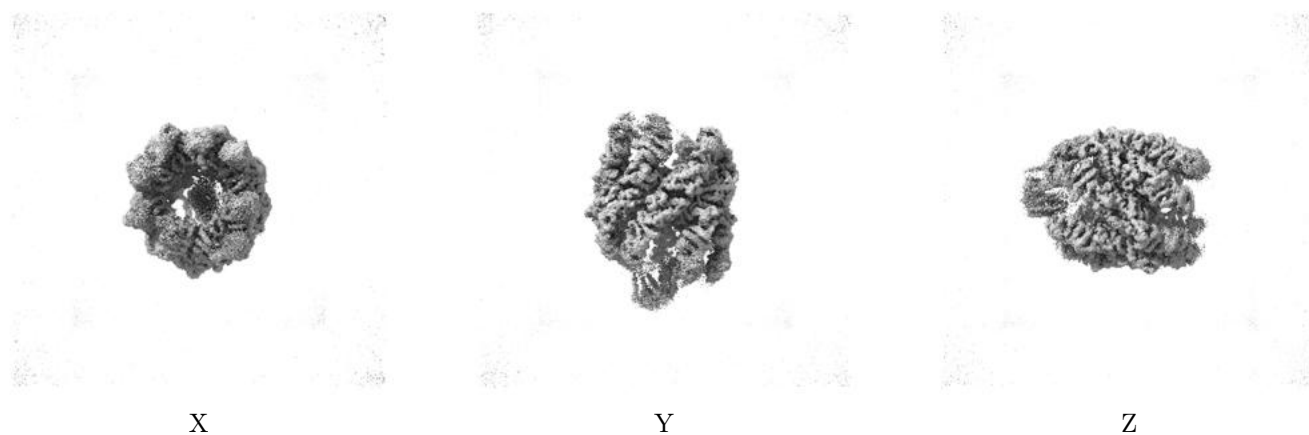
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.943. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

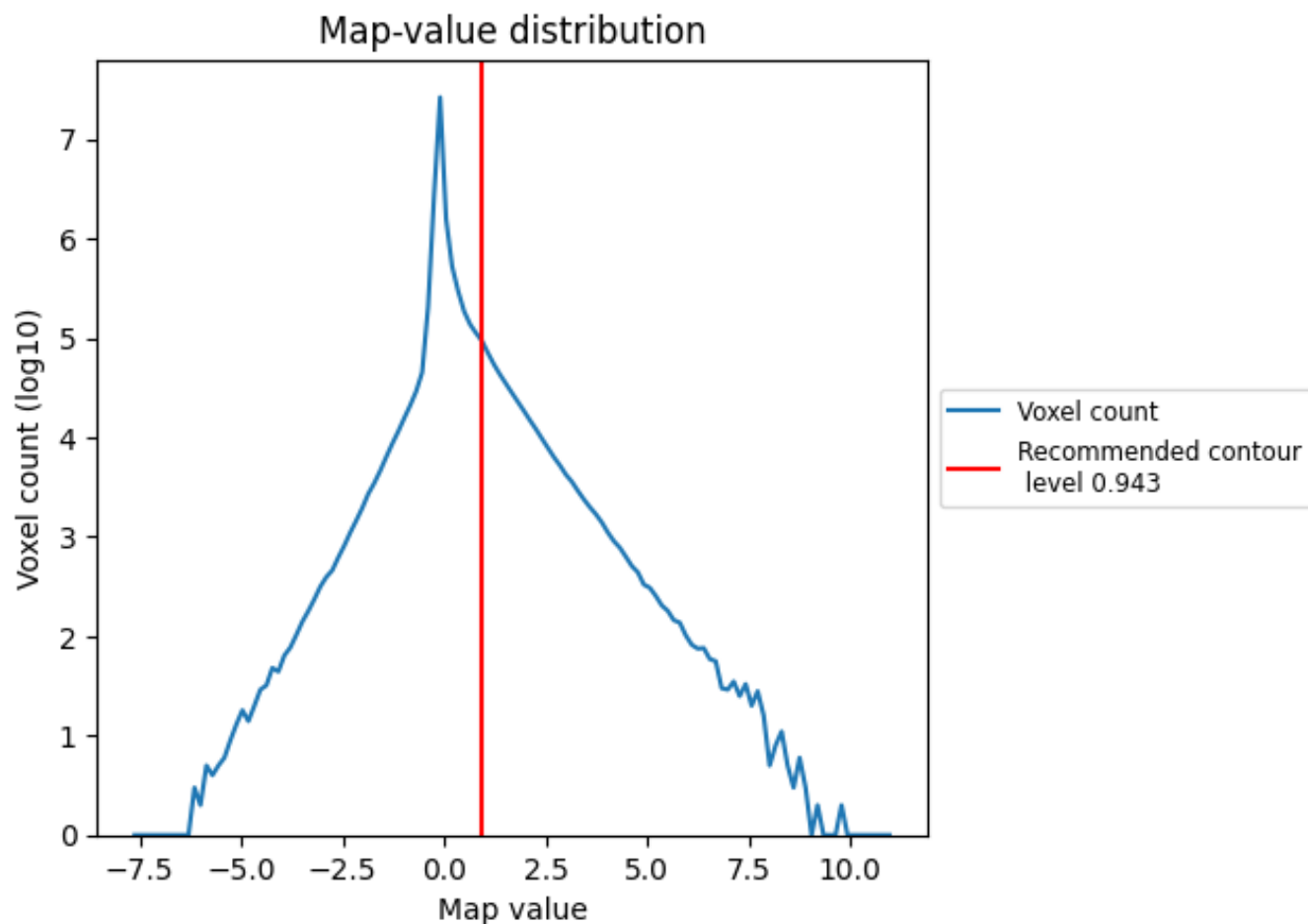
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

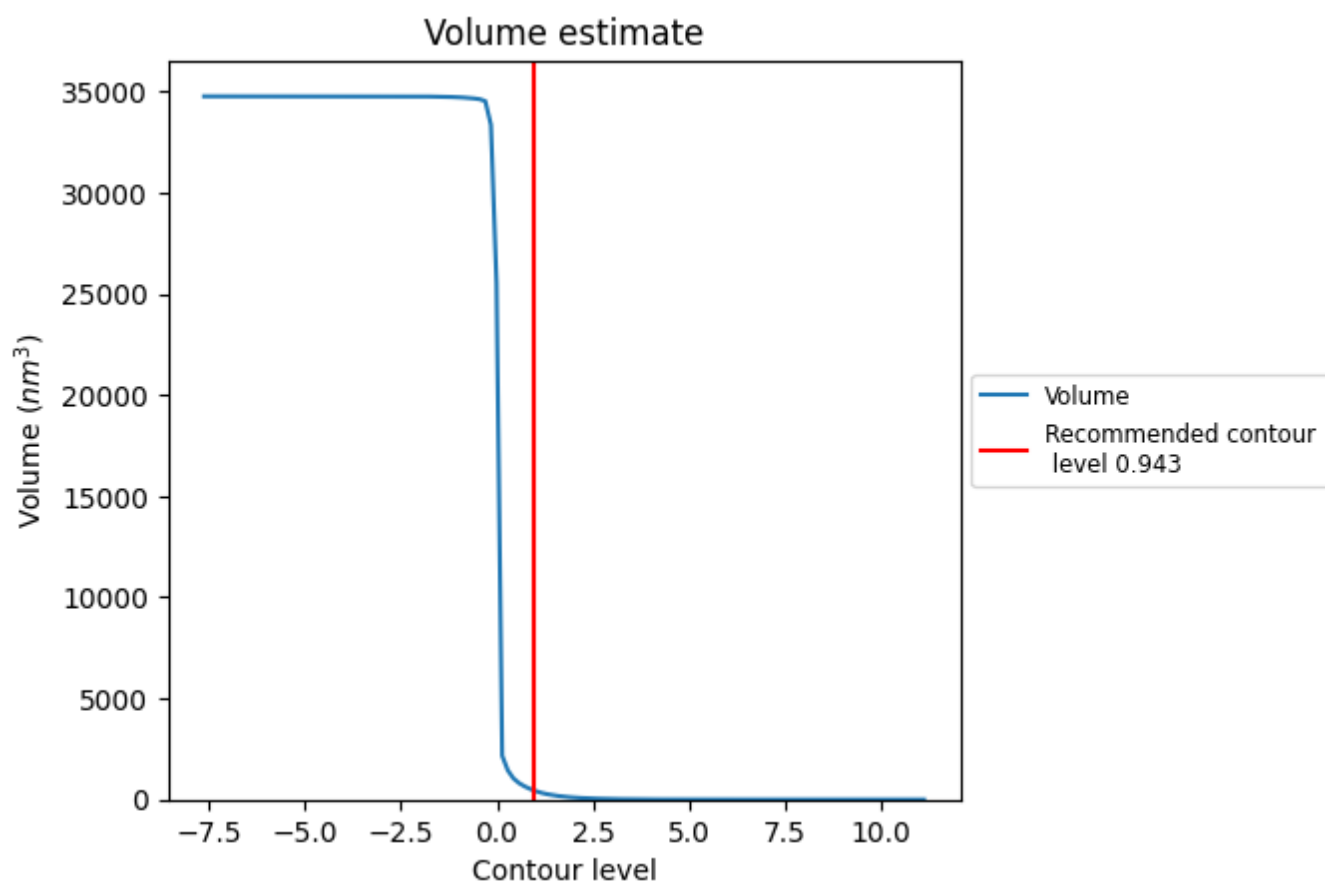
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

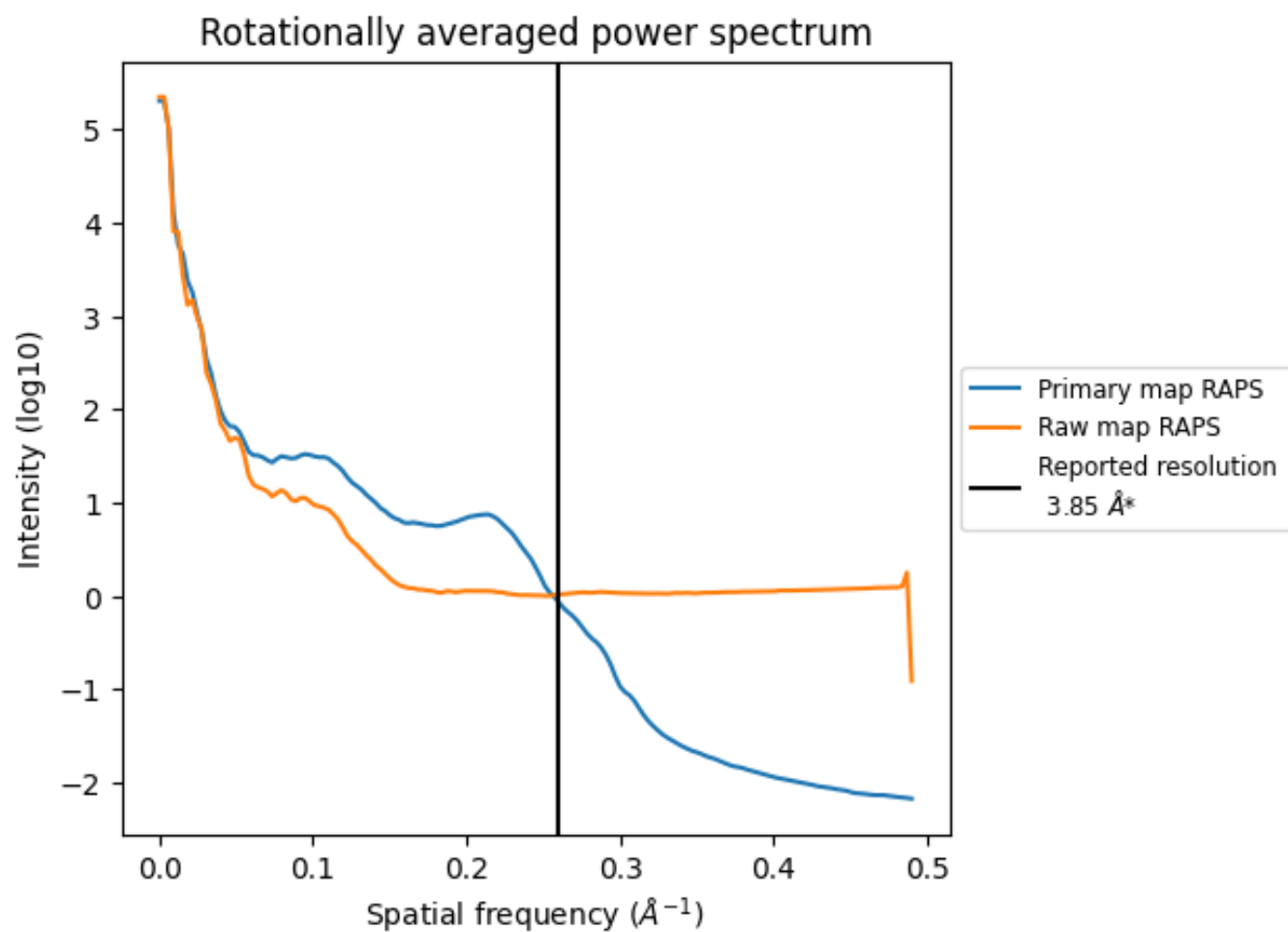
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 469 nm³; this corresponds to an approximate mass of 423 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

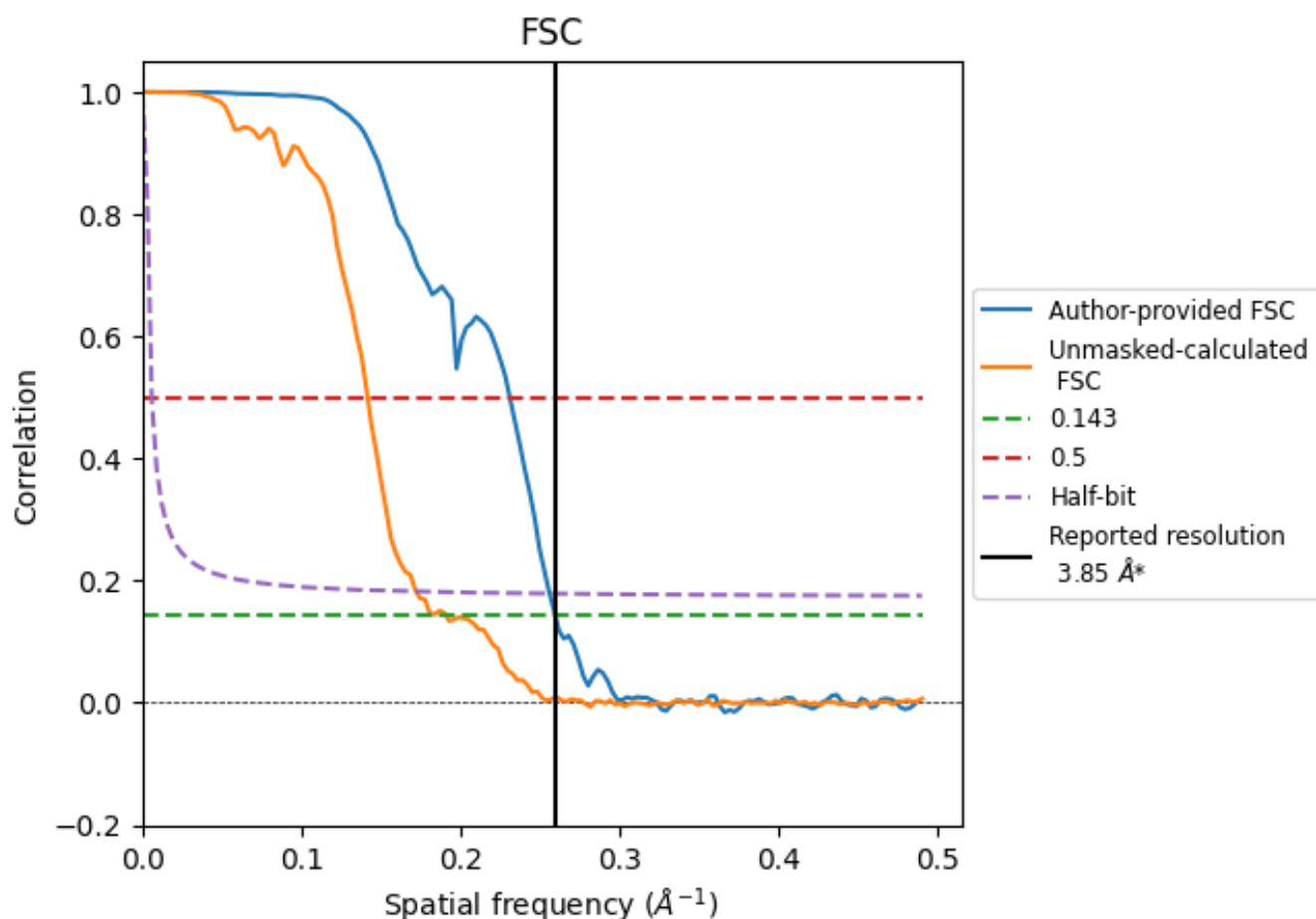


*Reported resolution corresponds to spatial frequency of 0.260 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.260 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

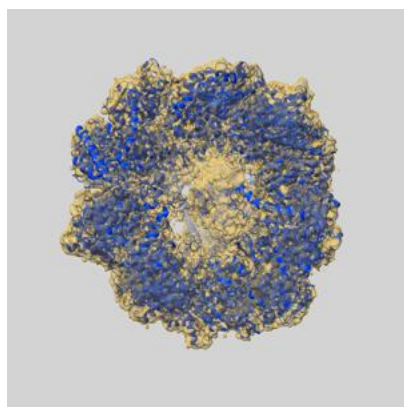
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.85	-	-
Author-provided FSC curve	3.85	4.33	3.90
Unmasked-calculated*	5.24	7.06	5.81

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 5.24 differs from the reported value 3.85 by more than 10 %

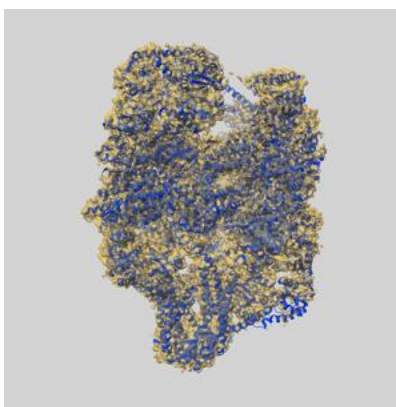
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-32823 and PDB model 7WU7. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

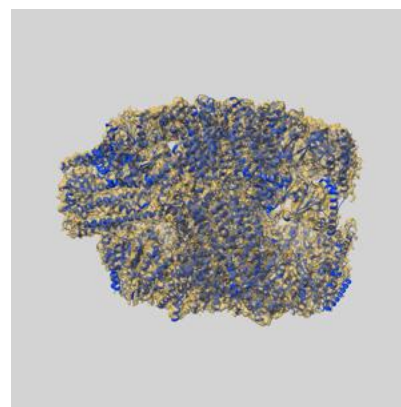
9.1 Map-model overlay [i](#)



X



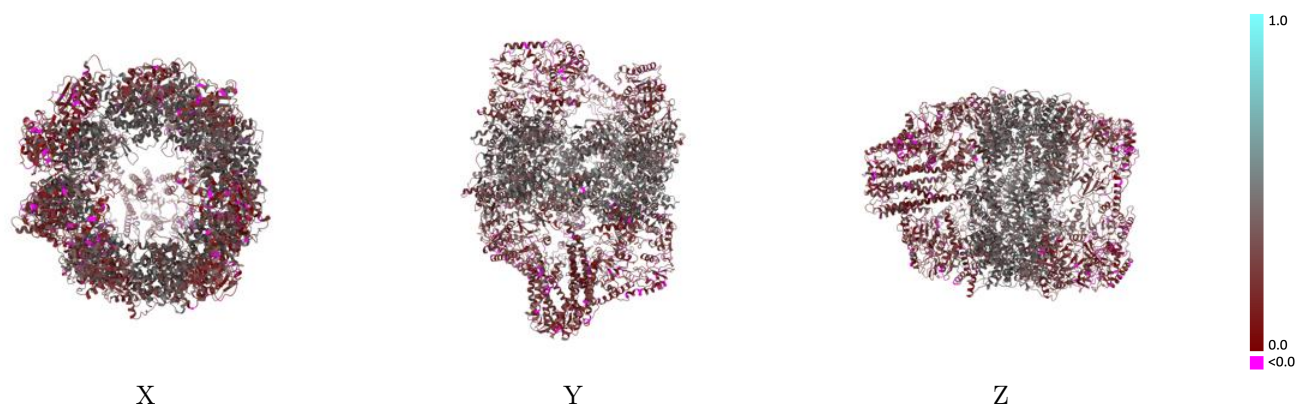
Y



Z

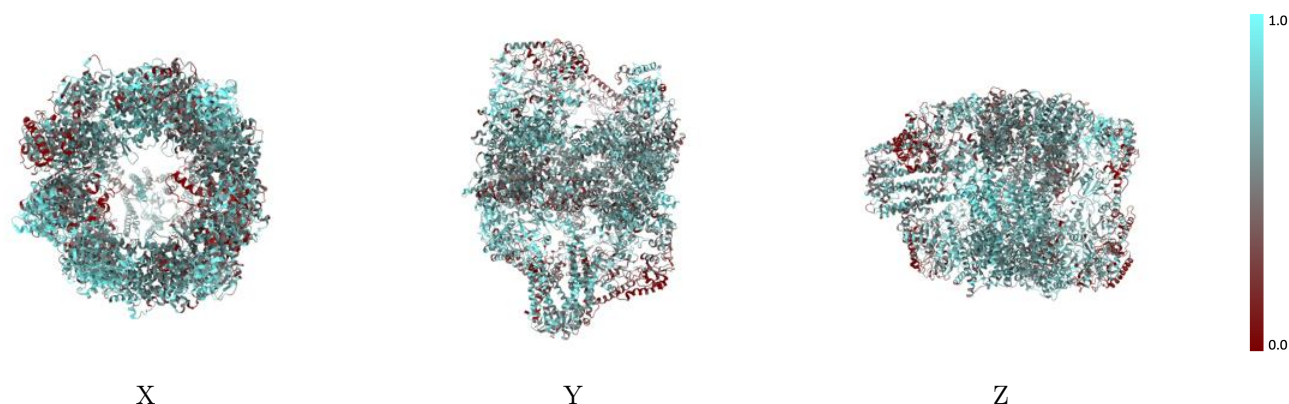
The images above show the 3D surface view of the map at the recommended contour level 0.943 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



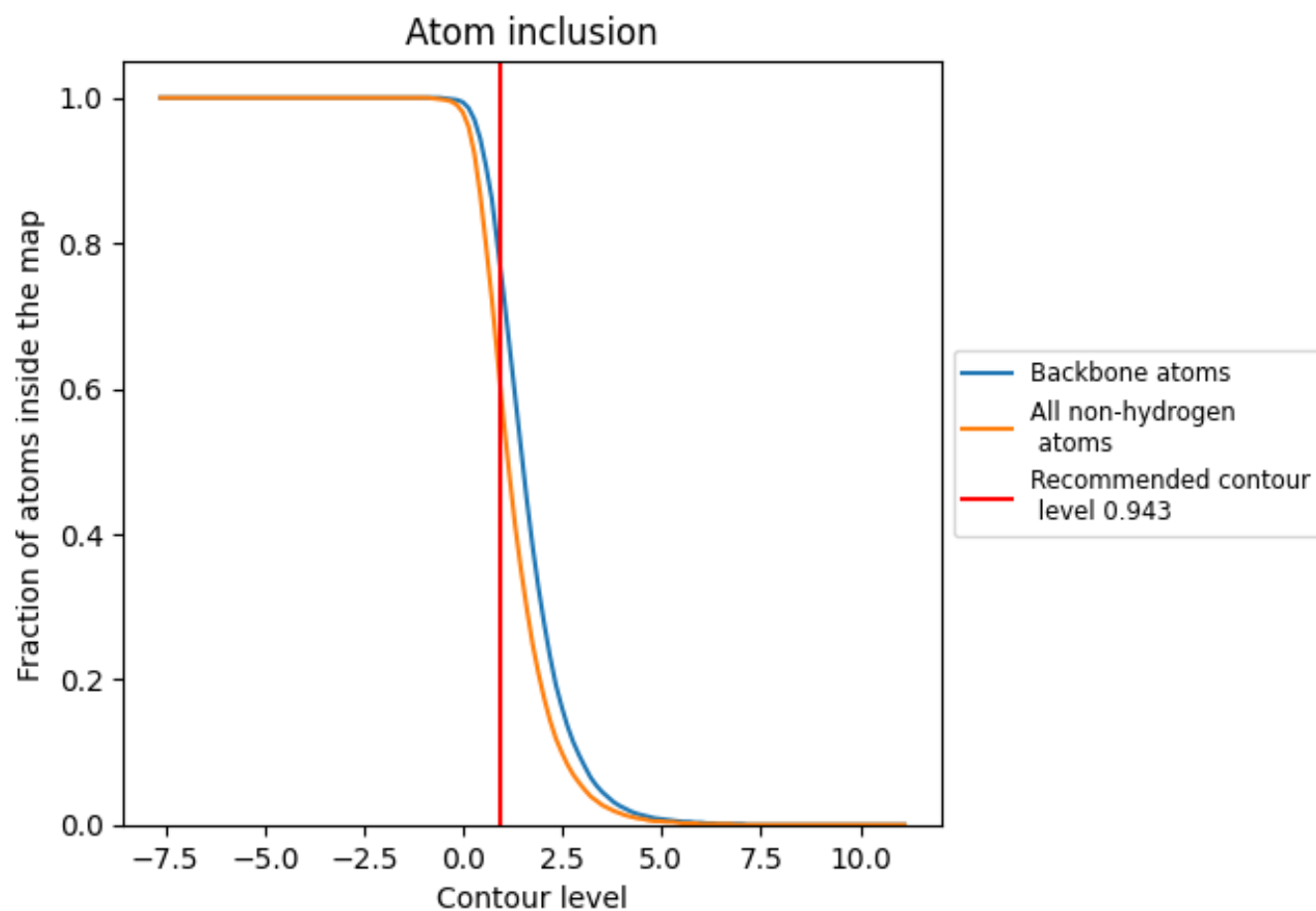
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.943).

9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 60% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.943) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5980	 0.3020
1	 0.6210	 0.2070
2	 0.5150	 0.2520
3	 0.7030	 0.2300
4	 0.6210	 0.2110
5	 0.5870	 0.2020
6	 0.6670	 0.1780
A	 0.5600	 0.3060
B	 0.5440	 0.2970
C	 0.5200	 0.2900
D	 0.6580	 0.3150
E	 0.6120	 0.2960
F	 0.5590	 0.3300
G	 0.6570	 0.3030
H	 0.5600	 0.3370
I	 0.6230	 0.3000
J	 0.6330	 0.2930
K	 0.5880	 0.2820
L	 0.6630	 0.3070
M	 0.5130	 0.2970
N	 0.6710	 0.3480
O	 0.6380	 0.3080
P	 0.5310	 0.3480

