



Full wwPDB EM Validation Report ⓘ

Sep 29, 2021 – 11:11 am BST

PDB ID : 7OLE
EMDB ID : EMD-12979
Title : Cryo-EM structure of the TELO2-TTI1-TTI2-RUVBL1-RUVBL2 complex
Authors : Pal, M.; Llorca, O.; Pearl, L.
Deposited on : 2021-05-19
Resolution : 3.41 Å (reported)
Based on initial model : 6FO1

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

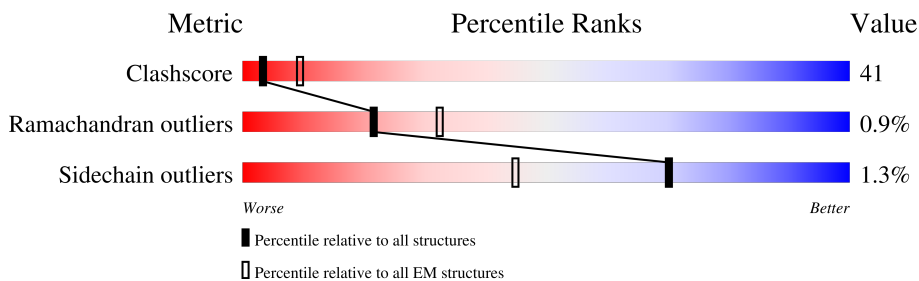
EMDB validation analysis : 0.0.0.dev97
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.41 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	A	456	
1	C	456	
1	E	456	
2	B	463	
2	D	463	
2	F	463	
3	H	1733	
4	J	964	

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Mol	Chain	Length	Quality of chain
5	K	491	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	ADP	B	501	-	-	X	-
6	ADP	D	501	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 26995 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 RuvB-like 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	433	Total	C	N	O	S	0	0
			3328	2095	568	651	14		
1	C	427	Total	C	N	O	S	0	0
			3281	2065	561	641	14		
1	E	413	Total	C	N	O	S	0	0
			3156	1988	538	618	12		

- Molecule 2 is a protein called RuvB-like 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	418	Total	C	N	O	S	0	0
			3209	2003	562	628	16		
2	D	419	Total	C	N	O	S	0	0
			3224	2013	564	631	16		
2	F	419	Total	C	N	O	S	0	0
			3232	2019	567	630	16		

- Molecule 3 is a protein called TELO2-interacting protein 1 homolog,TELO2-interacting protein 1 homolog,TTI1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	H	644	Total	C	N	O	0	0
			3208	1922	644	642		

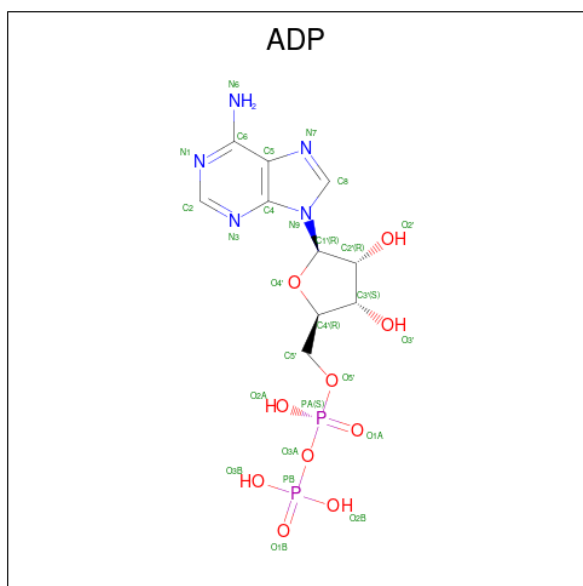
- Molecule 4 is a protein called TELO2-interacting protein 2,TELO2-interacting protein 2,TTI2.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	J	456	Total	C	N	O	0	0
			2273	1362	456	455		

- Molecule 5 is a protein called Telomere length regulation protein TEL2 homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	K	394	1949	1161	394	394	0	0

- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).

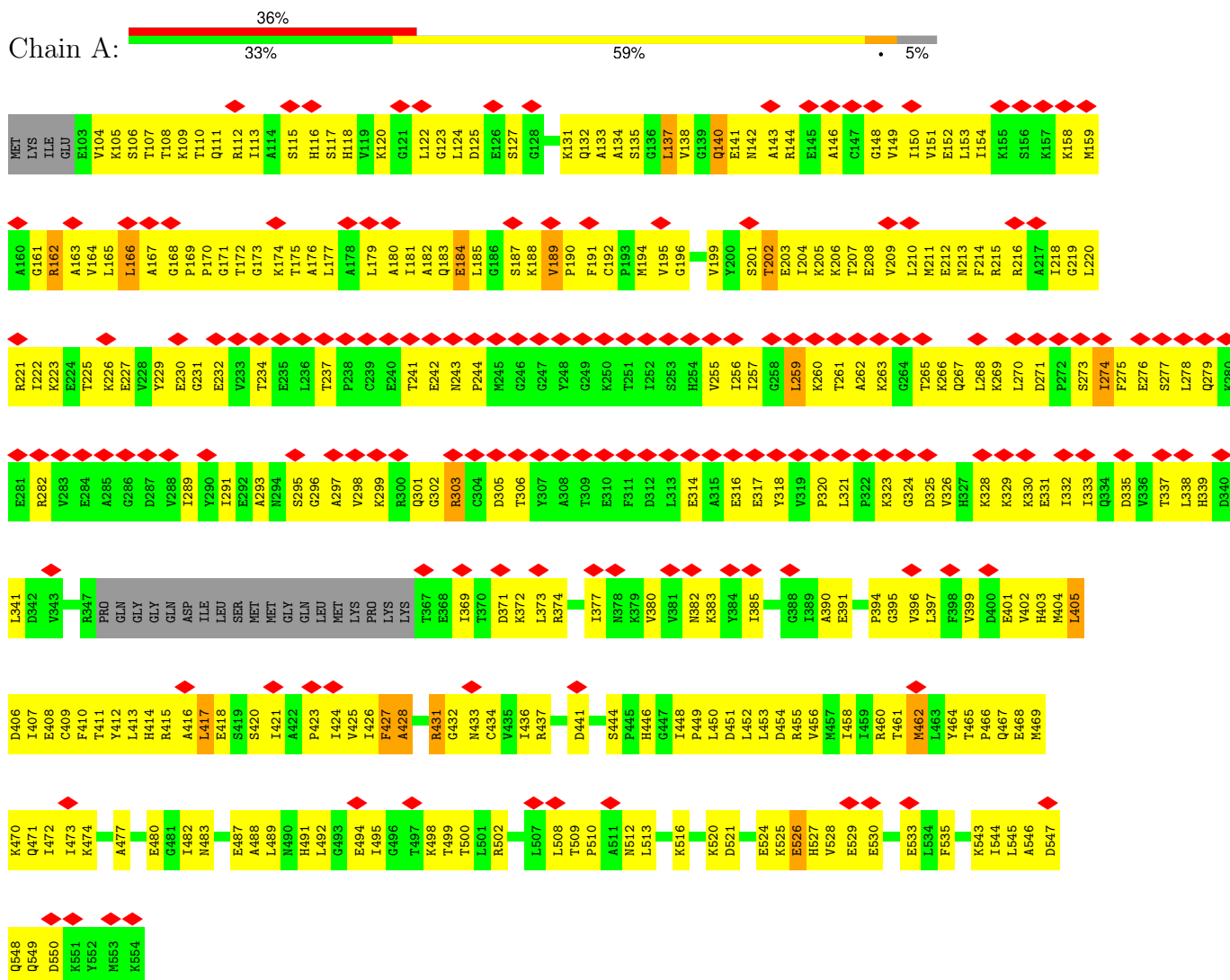


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
6	B	1	27	10	5	10	2	0
6	C	1	27	10	5	10	2	0
6	D	1	27	10	5	10	2	0
6	E	1	27	10	5	10	2	0
6	F	1	27	10	5	10	2	0

3 Residue-property plots

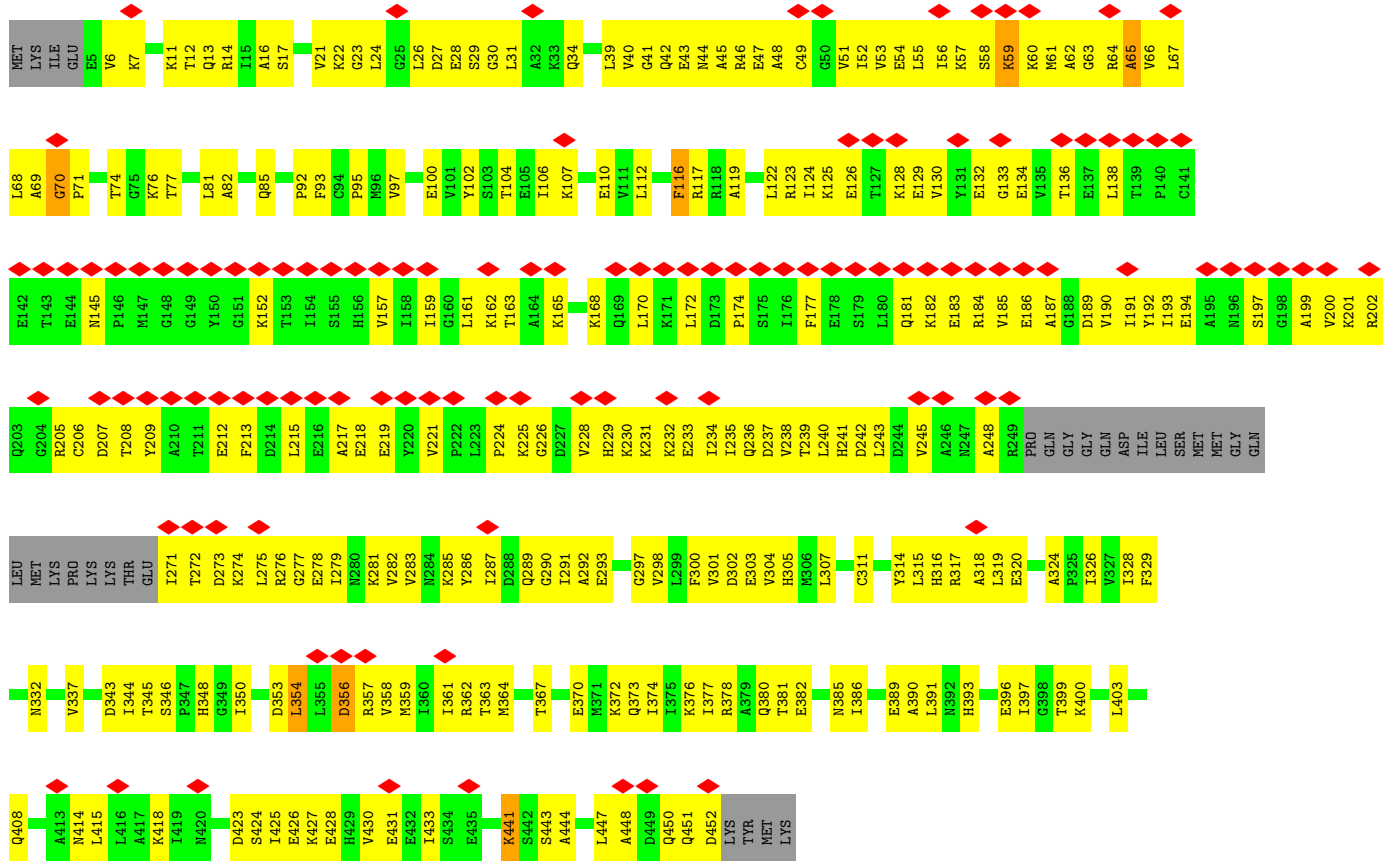
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: RuvB-like 1

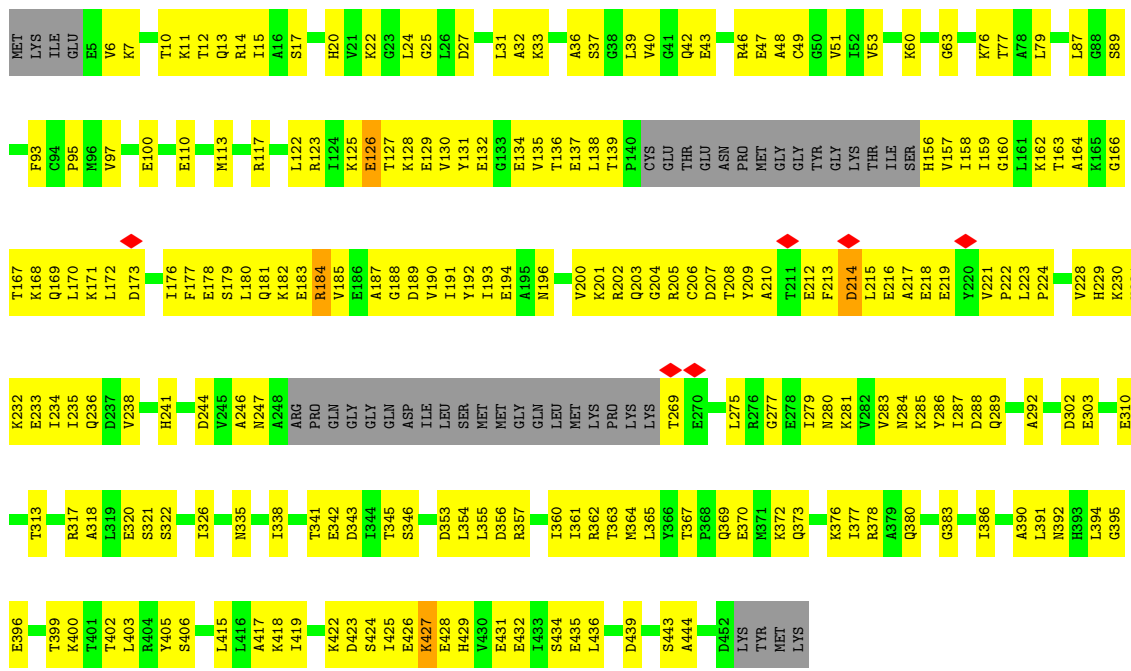


- Molecule 1: RuvB-like 1

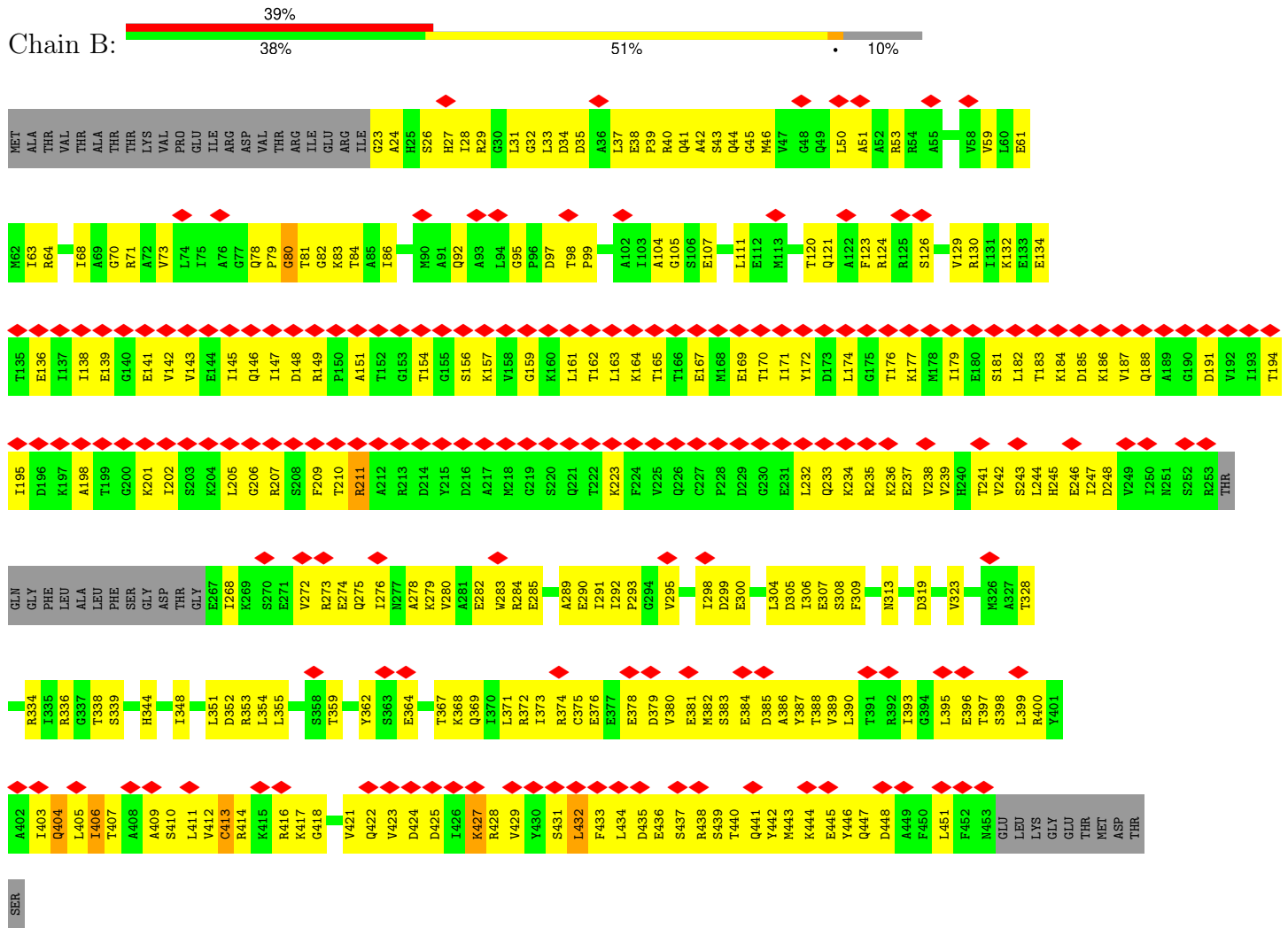




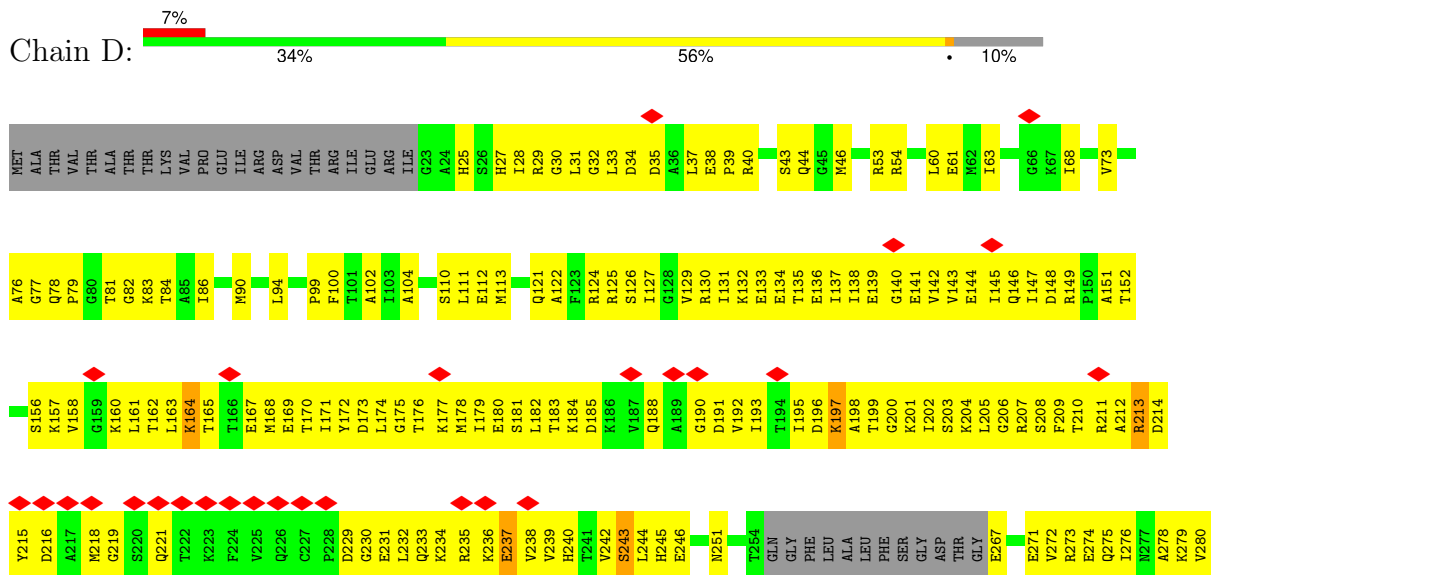
• Molecule 1: RuvB-like 1

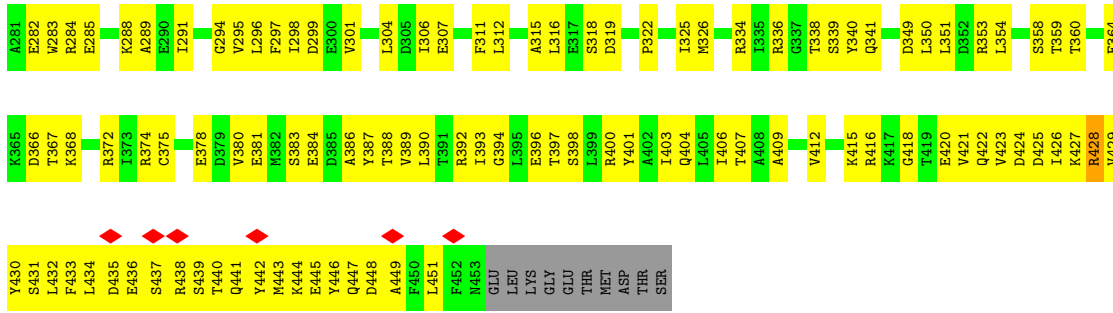


• Molecule 2: RuvB-like 2

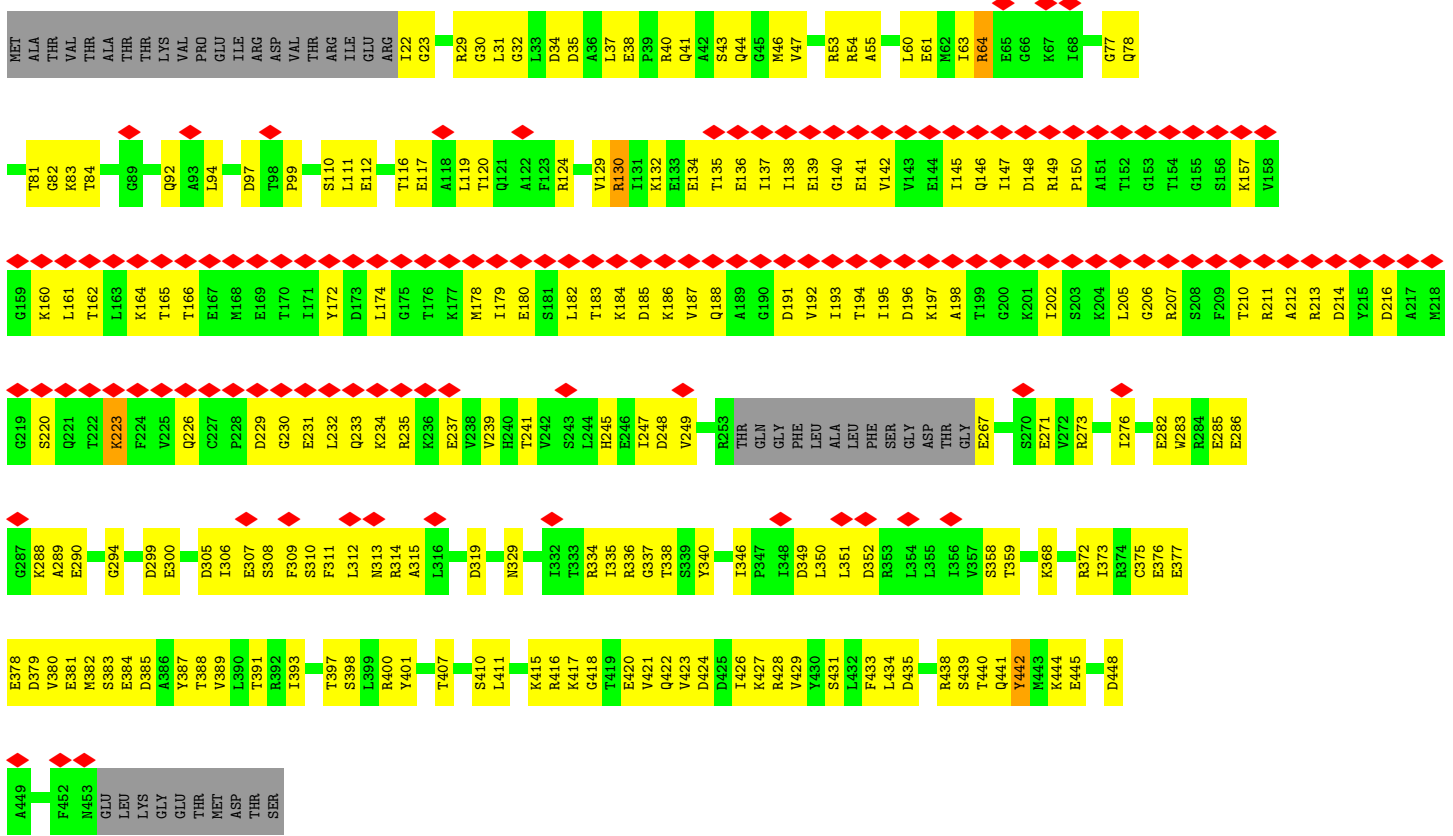


Molecule 2: RuvB-like 2

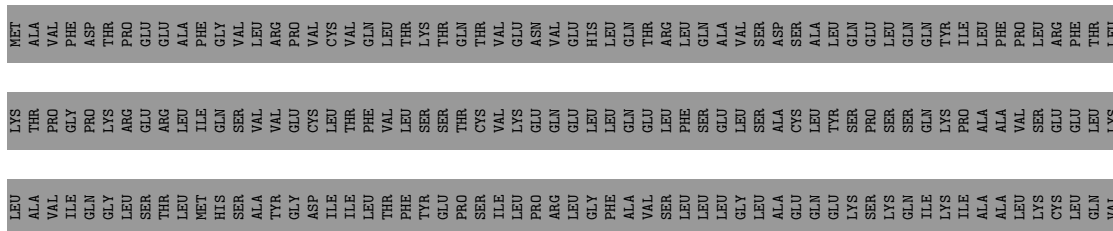


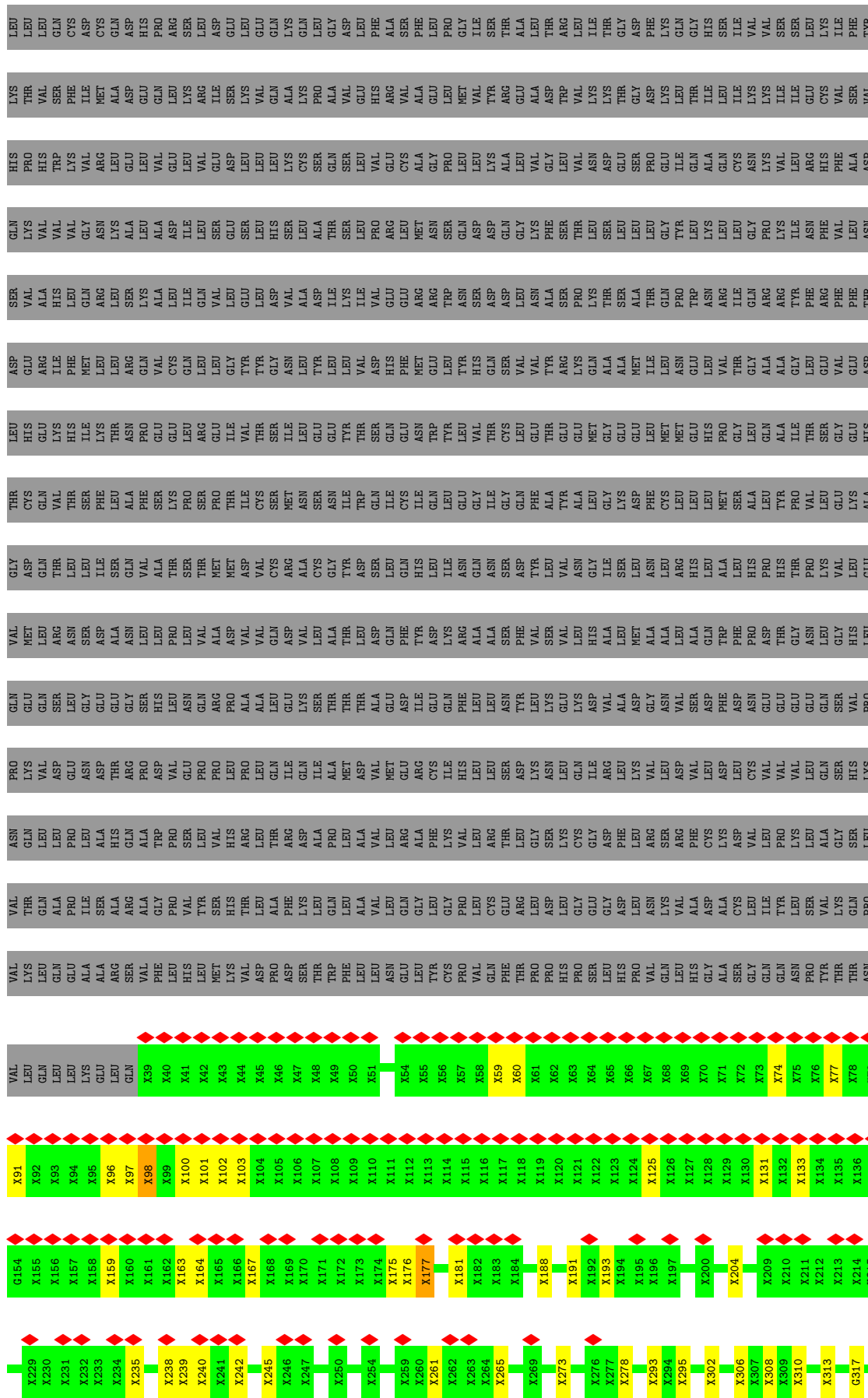


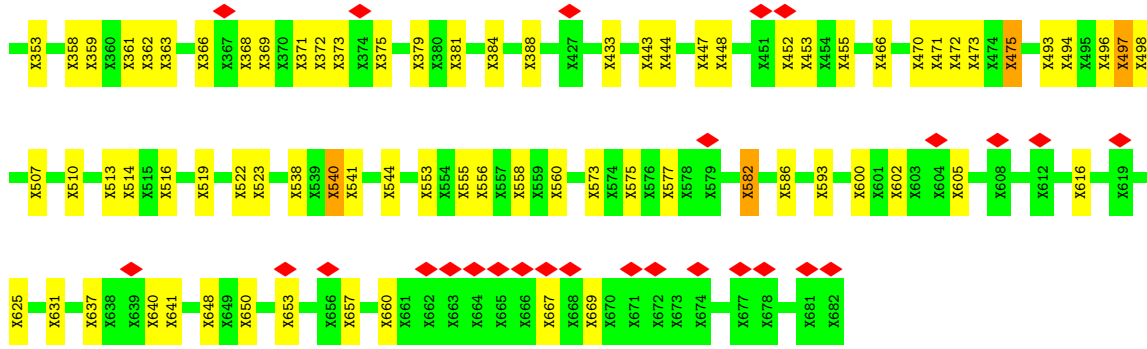
• Molecule 2: RuvB-like 2



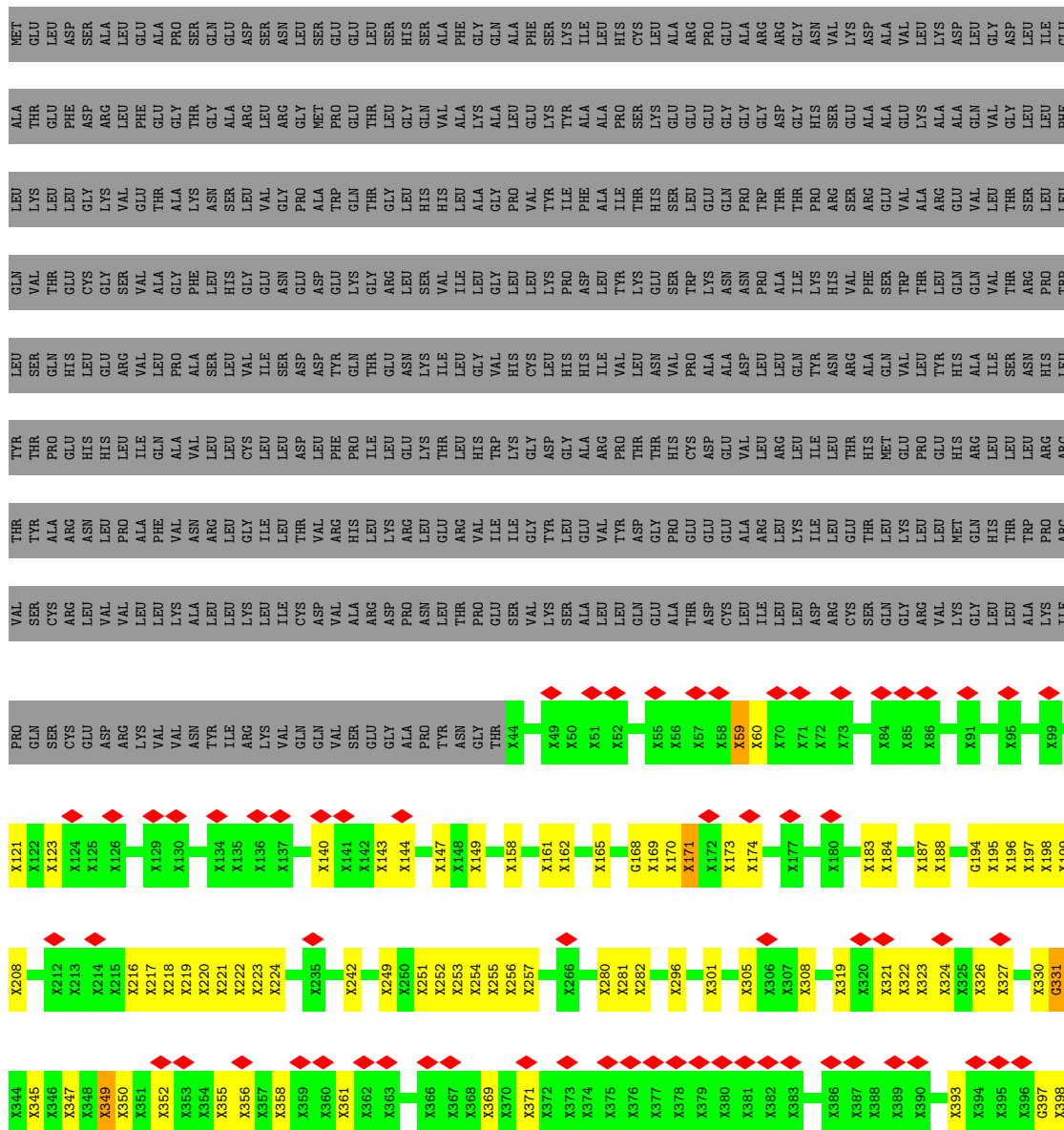
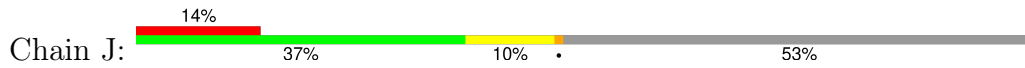
• Molecule 3: TELO2-interacting protein 1 homolog, TELO2-interacting protein 1 homolog, TTI1

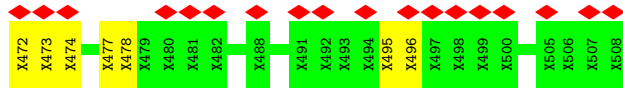
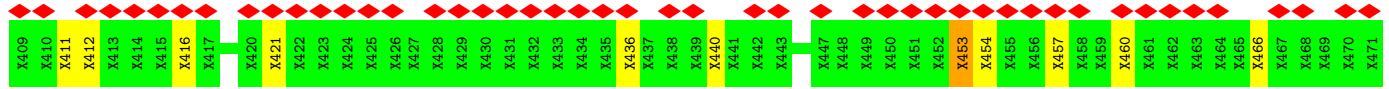




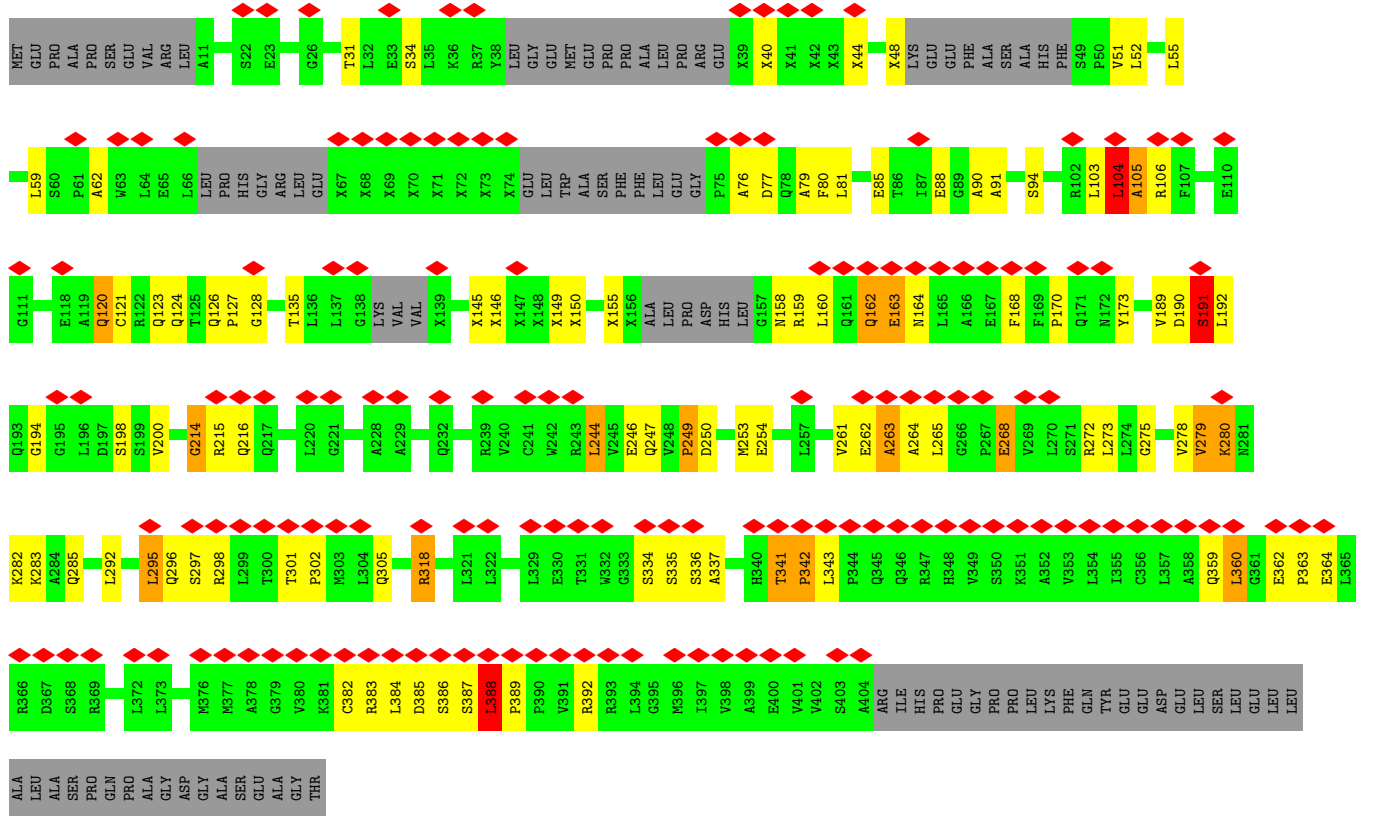


• Molecule 4: TELO2-interacting protein 2,TELO2-interacting protein 2,TTI2





• Molecule 5: Telomere length regulation protein TEL2 homolog



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	267149	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60.17	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.054	Depositor
Minimum map value	-0.019	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0106	Depositor
Map size (Å)	299.6, 299.6, 299.6	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: 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	A	0.44	0/3371	0.70	2/4548 (0.0%)
1	C	0.43	0/3323	0.60	0/4483
1	E	0.45	0/3195	0.53	0/4313
2	B	0.44	1/3244 (0.0%)	0.57	0/4370
2	D	0.43	0/3260	0.56	0/4391
2	F	0.44	0/3268	0.54	1/4401 (0.0%)
3	H	1.14	0/18	1.42	0/12
4	J	1.31	0/18	2.23	1/12 (8.3%)
5	K	1.17	3/1766 (0.2%)	1.35	18/2453 (0.7%)
All	All	0.54	4/21463 (0.0%)	0.69	22/28983 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	10
1	C	0	4
1	E	0	1
2	B	0	3
2	D	0	1
2	F	0	1
3	H	0	12
4	J	0	8
5	K	0	7
All	All	0	47

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	K	280	LYS	C-O	6.40	1.35	1.23
5	K	120	GLN	C-O	-5.84	1.12	1.23
2	B	359	THR	C-N	-5.66	1.21	1.34
5	K	268	GLU	C-O	-5.42	1.13	1.23

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	166	LEU	CA-CB-CG	10.99	140.58	115.30
5	K	191	SER	N-CA-C	-10.09	83.75	111.00
5	K	214	GLY	O-C-N	-8.22	109.55	122.70
5	K	318	ARG	C-N-CA	7.66	154.17	122.00
5	K	273	LEU	N-CA-C	-7.33	91.22	111.00
5	K	387	SER	O-C-N	7.25	134.29	122.70
4	J	331	GLY	N-CA-C	-7.07	95.43	113.10
5	K	249	PRO	N-CA-C	-6.91	94.15	112.10
5	K	278	VAL	N-CA-C	-6.85	92.49	111.00
5	K	279	VAL	N-CA-C	6.47	128.46	111.00
5	K	388	LEU	N-CA-C	-5.89	95.09	111.00
5	K	359	GLN	N-CA-C	5.75	126.51	111.00
5	K	121	CYS	N-CA-C	-5.61	95.85	111.00
5	K	282	LYS	N-CA-C	5.51	125.88	111.00
5	K	104	LEU	O-C-N	-5.27	114.27	122.70
5	K	384	LEU	O-C-N	5.24	131.08	122.70
5	K	295	LEU	C-N-CA	5.23	134.76	121.70
2	F	379	ASP	CB-CG-OD1	5.15	122.94	118.30
5	K	279	VAL	O-C-N	-5.13	114.50	122.70
5	K	162	GLN	O-C-N	5.10	130.85	122.70
1	A	137	LEU	CA-CB-CG	5.07	126.96	115.30
5	K	387	SER	CA-C-N	-5.04	106.11	117.20

There are no chirality outliers.

All (47) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	140	GLN	Peptide
1	A	184	GLU	Peptide
1	A	187	SER	Peptide
1	A	189	VAL	Peptide
1	A	202	THR	Peptide
1	A	259	LEU	Peptide
1	A	274	ILE	Peptide

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Mol	Chain	Res	Type	Group
1	A	417	LEU	Peptide
1	A	427	PHE	Peptide
1	A	462	MET	Peptide
2	B	404	GLN	Peptide
2	B	406	ILE	Peptide
2	B	432	LEU	Peptide
1	C	354	LEU	Peptide
1	C	356	ASP	Peptide
1	C	65	ALA	Peptide
1	C	70	GLY	Peptide
2	D	237	GLU	Peptide
1	E	214	ASP	Peptide
2	F	307	GLU	Peptide
3	H	103	UNK	Mainchain
3	H	177	UNK	Peptide
3	H	220	UNK	Mainchain
3	H	433	UNK	Mainchain
3	H	475	UNK	Mainchain
3	H	497	UNK	Mainchain
3	H	540	UNK	Mainchain
3	H	556	UNK	Peptide
3	H	582	UNK	Mainchain
3	H	600	UNK	Peptide
3	H	84	UNK	Mainchain
3	H	98	UNK	Mainchain
4	J	171	UNK	Peptide
4	J	242	UNK	Peptide
4	J	305	UNK	Mainchain
4	J	349	UNK	Peptide
4	J	421	UNK	Peptide
4	J	453	UNK	Peptide
4	J	473	UNK	Mainchain
4	J	59	UNK	Mainchain
5	K	104	LEU	Mainchain
5	K	168	PHE	Mainchain
5	K	214	GLY	Mainchain
5	K	247	GLN	Mainchain
5	K	263	ALA	Mainchain
5	K	279	VAL	Mainchain
5	K	360	LEU	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3328	0	3405	458	0
1	C	3281	0	3363	283	0
1	E	3156	0	3214	216	0
2	B	3209	0	3254	352	0
2	D	3224	0	3270	362	0
2	F	3232	0	3286	197	0
3	H	3208	0	680	117	0
4	J	2273	0	495	91	0
5	K	1949	0	857	87	0
6	B	27	0	12	13	0
6	C	27	0	12	0	0
6	D	27	0	11	20	0
6	E	27	0	12	5	0
6	F	27	0	12	6	0
All	All	26995	0	21883	1993	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 41.

All (1993) 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)
5:K:250:ASP:HA	5:K:253:MET:CB	1.27	1.57
5:K:124:GLN:HA	5:K:127:PRO:CB	1.32	1.56
4:J:416:UNK:HA	4:J:466:UNK:CB	1.36	1.54
5:K:302:PRO:CA	5:K:305:GLN:CB	1.86	1.53
3:H:593:UNK:CB	3:H:631:UNK:CB	1.85	1.51
4:J:416:UNK:CA	4:J:466:UNK:CB	1.95	1.45
5:K:91:ALA:O	5:K:94:SER:CB	1.70	1.40
4:J:416:UNK:CB	4:J:466:UNK:CB	1.97	1.38
5:K:302:PRO:HA	5:K:305:GLN:CB	0.90	1.38
5:K:124:GLN:CA	5:K:127:PRO:CB	2.02	1.36
1:A:123:GLY:N	2:B:410:SER:HA	1.38	1.36
3:H:91:UNK:CB	3:H:141:UNK:CB	2.04	1.35
2:B:362:TYR:OH	6:B:501:ADP:N7	1.57	1.33

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:201:LYS:HE3	4:J:281:UNK:O	1.27	1.32
4:J:350:UNK:O	4:J:355:UNK:CB	1.80	1.30
3:H:273:UNK:CB	3:H:302:UNK:CB	2.12	1.28
5:K:250:ASP:CA	5:K:253:MET:CB	2.18	1.21
5:K:261:VAL:O	5:K:264:ALA:HB3	1.39	1.20
5:K:123:GLN:O	5:K:127:PRO:N	1.79	1.16
1:A:138:VAL:HG23	2:B:433:PHE:HD2	0.97	1.14
1:A:138:VAL:HG23	2:B:433:PHE:CD2	1.80	1.14
1:A:134:ALA:HB1	2:B:412:VAL:HG12	1.32	1.11
2:D:37:LEU:HD11	1:E:419:ILE:HG13	1.32	1.11
4:J:393:UNK:HA	4:J:400:GLY:CA	1.78	1.10
1:C:314:TYR:HB2	2:D:111:LEU:HD13	1.21	1.10
4:J:350:UNK:O	4:J:355:UNK:CA	2.00	1.10
5:K:200:VAL:CB	5:K:244:LEU:CB	2.31	1.08
3:H:125:UNK:CB	3:H:163:UNK:CA	2.30	1.08
3:H:125:UNK:CB	3:H:163:UNK:HA	1.83	1.07
3:H:125:UNK:CB	3:H:163:UNK:CB	2.32	1.07
1:A:144:ARG:HD2	2:B:407:THR:HG22	1.33	1.06
3:H:369:UNK:O	3:H:373:UNK:N	1.89	1.06
1:A:131:LYS:HE3	2:B:413:CYS:HB3	1.35	1.06
2:D:201:LYS:CE	4:J:281:UNK:O	2.03	1.05
3:H:204:UNK:CB	5:K:336:SER:CB	2.34	1.05
1:A:132:GLN:HB3	2:B:425:ASP:HB3	1.36	1.05
1:A:138:VAL:HB	2:B:433:PHE:H	0.87	1.04
2:D:81:THR:HB	6:D:501:ADP:H4'	1.36	1.04
1:A:138:VAL:HB	2:B:433:PHE:N	1.73	1.03
1:A:134:ALA:HB1	2:B:412:VAL:CG1	1.87	1.03
2:B:46:MET:SD	2:B:53:ARG:NH2	2.32	1.03
4:J:301:UNK:CB	4:J:308:UNK:CB	2.36	1.03
1:A:182:ALA:HA	1:A:185:LEU:HB2	1.40	1.01
4:J:350:UNK:C	4:J:355:UNK:CB	2.39	0.99
1:A:124:LEU:O	2:B:410:SER:OG	1.78	0.99
4:J:319:UNK:O	4:J:323:UNK:CB	2.10	0.99
4:J:280:UNK:O	4:J:282:UNK:N	1.96	0.98
4:J:352:UNK:O	4:J:356:UNK:N	1.97	0.98
4:J:319:UNK:O	4:J:323:UNK:N	1.97	0.97
1:A:138:VAL:CG2	2:B:433:PHE:HD2	1.77	0.97
3:H:593:UNK:CA	3:H:631:UNK:CB	2.43	0.96
2:B:362:TYR:OH	6:B:501:ADP:C5	2.18	0.96
1:A:109:LYS:N	1:A:427:PHE:O	1.99	0.95
1:A:133:ALA:HB3	2:B:427:LYS:H	1.31	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:THR:HA	1:A:427:PHE:HB2	1.48	0.94
1:A:123:GLY:H	2:B:410:SER:HA	0.88	0.94
1:A:133:ALA:HB1	2:B:429:VAL:H	1.33	0.94
1:A:170:PRO:HA	1:A:446:HIS:HD2	1.33	0.94
1:A:123:GLY:HA2	2:B:411:LEU:N	1.82	0.94
3:H:616:UNK:HA	3:H:625:UNK:CB	1.98	0.93
2:D:430:TYR:HA	2:D:433:PHE:HB2	1.50	0.93
2:B:78:GLN:NE2	1:C:450:GLN:OE1	2.01	0.93
1:A:133:ALA:O	2:B:427:LYS:HE3	1.70	0.92
1:C:314:TYR:HB2	2:D:111:LEU:CD1	2.00	0.92
4:J:220:UNK:O	4:J:224:UNK:N	2.02	0.92
1:C:65:ALA:H	1:C:354:LEU:H	1.02	0.92
1:A:131:LYS:HE3	2:B:413:CYS:CB	1.98	0.91
1:A:123:GLY:CA	2:B:410:SER:HA	2.00	0.91
1:A:275:PHE:H	1:A:296:GLY:H	1.14	0.91
4:J:208:UNK:CB	4:J:216:UNK:CB	2.47	0.91
5:K:334:SER:HA	5:K:337:ALA:HB3	1.53	0.91
1:E:386:ILE:HD11	1:E:391:LEU:HG	1.51	0.90
1:C:42:GLN:NE2	1:C:362:ARG:O	2.03	0.90
1:A:104:VAL:HB	1:A:188:LYS:HB2	1.51	0.90
1:A:204:ILE:N	2:F:308:SER:O	2.03	0.90
2:D:81:THR:CB	6:D:501:ADP:H4'	2.02	0.90
5:K:189:VAL:O	5:K:191:SER:N	2.04	0.90
1:A:124:LEU:N	2:B:410:SER:OG	2.05	0.89
4:J:408:UNK:O	4:J:412:UNK:N	2.05	0.89
2:D:434:LEU:HB2	2:D:438:ARG:HD2	1.54	0.89
1:A:470:LYS:HA	1:A:474:LYS:HB2	1.52	0.89
4:J:393:UNK:HA	4:J:400:GLY:HA3	1.54	0.89
1:A:123:GLY:N	2:B:410:SER:CA	2.32	0.89
1:A:116:HIS:O	1:A:462:MET:N	2.06	0.89
1:A:162:ARG:HH22	1:A:418:GLU:HB3	1.36	0.88
2:D:81:THR:O	6:D:501:ADP:O2'	1.89	0.88
2:D:81:THR:HB	6:D:501:ADP:C4'	2.03	0.88
5:K:40:UNK:CB	5:K:44:UNK:CB	2.52	0.88
3:H:125:UNK:CA	3:H:163:UNK:CB	2.52	0.88
1:C:74:THR:O	1:C:362:ARG:NE	2.07	0.87
1:A:133:ALA:CB	2:B:428:ARG:H	1.87	0.87
5:K:76:ALA:O	5:K:80:PHE:N	2.08	0.87
2:D:400:ARG:HH22	6:D:501:ADP:H2	1.22	0.87
1:A:202:THR:HG22	2:F:306:ILE:HG22	1.58	0.86
1:A:222:ILE:HG13	1:A:390:ALA:HB2	1.57	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:519:UNK:O	3:H:523:UNK:CB	2.23	0.86
2:B:362:TYR:CZ	6:B:501:ADP:N7	2.43	0.86
5:K:123:GLN:HA	5:K:126:GLN:CB	2.06	0.85
5:K:77:ASP:O	5:K:81:LEU:N	2.09	0.85
1:A:399:VAL:H	1:A:425:VAL:HG21	1.41	0.85
4:J:168:GLY:O	4:J:171:UNK:N	2.09	0.85
3:H:238:UNK:O	3:H:240:UNK:N	2.10	0.85
1:C:65:ALA:N	1:C:354:LEU:H	1.73	0.85
2:B:413:CYS:SG	2:B:414:ARG:NH1	2.50	0.85
3:H:125:UNK:HA	3:H:163:UNK:CB	2.07	0.85
5:K:302:PRO:HA	5:K:305:GLN:CA	2.05	0.85
1:A:259:LEU:O	1:A:266:LYS:HB3	1.76	0.84
2:D:137:ILE:N	2:D:206:GLY:O	2.08	0.84
4:J:218:UNK:O	4:J:222:UNK:N	2.10	0.84
1:A:144:ARG:CD	2:B:407:THR:HG22	2.07	0.84
1:A:123:GLY:H	2:B:410:SER:CA	1.82	0.84
5:K:301:THR:O	5:K:305:GLN:N	2.08	0.84
1:E:40:VAL:H	6:E:501:ADP:HN62	1.22	0.84
2:D:435:ASP:O	2:D:439:SER:N	2.11	0.83
2:F:420:GLU:O	2:F:422:GLN:NE2	2.10	0.83
2:B:374:ARG:NE	2:B:374:ARG:O	2.11	0.82
1:A:396:VAL:HA	1:A:424:ILE:HB	1.60	0.82
5:K:124:GLN:C	5:K:127:PRO:CB	2.47	0.82
2:D:37:LEU:O	2:D:54:ARG:NH1	2.13	0.82
3:H:261:UNK:HA	3:H:265:UNK:CB	2.10	0.82
2:D:436:GLU:O	2:D:440:THR:N	2.12	0.82
2:D:359:THR:H	6:D:501:ADP:PB	2.03	0.82
5:K:262:GLU:O	5:K:265:LEU:N	2.14	0.81
1:A:123:GLY:CA	2:B:411:LEU:N	2.44	0.81
1:A:229:TYR:HB3	1:A:266:LYS:HG2	1.62	0.81
2:B:148:ASP:HB2	2:B:182:LEU:HD13	1.63	0.81
1:C:165:LYS:HD3	1:C:225:LYS:HB3	1.62	0.81
2:D:437:SER:O	2:D:442:TYR:N	2.13	0.81
2:D:445:GLU:HA	2:D:448:ASP:HB2	1.63	0.81
1:A:166:LEU:HD22	1:A:456:VAL:HB	1.63	0.81
1:C:161:LEU:HD22	1:C:191:ILE:HD11	1.59	0.81
1:A:133:ALA:HB1	2:B:429:VAL:N	1.95	0.81
1:E:134:GLU:HB2	1:E:187:ALA:HA	1.63	0.81
1:C:65:ALA:HB1	1:C:350:ILE:HG22	1.62	0.80
1:A:125:ASP:OD1	2:B:414:ARG:NH2	2.14	0.80
1:A:122:LEU:HB3	2:B:409:ALA:O	1.81	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:GLY:O	1:A:424:ILE:N	2.14	0.80
2:D:139:GLU:OE1	2:D:234:LYS:NZ	2.14	0.80
1:A:203:GLU:HG3	2:F:311:PHE:H	1.46	0.80
5:K:170:PRO:HA	5:K:173:TYR:CB	2.12	0.80
1:A:138:VAL:CB	2:B:433:PHE:H	1.83	0.80
1:A:158:LYS:HG2	1:A:159:MET:HG3	1.62	0.80
2:B:441:GLN:HA	2:B:444:LYS:HB2	1.62	0.80
3:H:494:UNK:C	3:H:496:UNK:N	2.43	0.80
2:B:375:CYS:HB2	2:B:380:VAL:H	1.46	0.79
2:D:441:GLN:O	2:D:445:GLU:N	2.14	0.79
3:H:637:UNK:N	3:H:640:UNK:CB	2.45	0.79
1:C:389:GLU:O	1:C:427:LYS:NZ	2.14	0.79
2:B:375:CYS:O	2:B:379:ASP:N	2.13	0.79
2:B:400:ARG:NH2	6:B:501:ADP:O3A	2.15	0.79
1:C:69:ALA:HA	1:C:348:HIS:NE2	1.98	0.79
5:K:261:VAL:O	5:K:264:ALA:CB	2.27	0.79
2:F:286:GLU:HG3	2:F:288:LYS:H	1.47	0.79
3:H:261:UNK:O	3:H:265:UNK:CB	2.31	0.78
2:F:138:ILE:HG21	2:F:198:ALA:HB2	1.64	0.78
5:K:123:GLN:O	5:K:127:PRO:CA	2.31	0.78
1:C:125:LYS:HE2	1:C:235:ILE:HB	1.63	0.78
1:A:105:LYS:HG3	1:A:107:THR:HG23	1.64	0.78
1:C:190:VAL:HG23	1:C:206:CYS:HA	1.64	0.78
2:D:359:THR:OG1	6:D:501:ADP:O3B	2.00	0.78
1:C:373:GLN:HA	1:C:376:LYS:HB3	1.64	0.78
3:H:593:UNK:CB	3:H:631:UNK:CA	2.61	0.78
3:H:657:UNK:O	3:H:660:UNK:CB	2.31	0.78
4:J:350:UNK:O	4:J:355:UNK:N	2.16	0.78
2:B:78:GLN:HB2	2:B:79:PRO:HD3	1.63	0.78
2:D:37:LEU:CD1	1:E:419:ILE:HG13	2.12	0.78
1:A:142:ASN:HB3	2:B:400:ARG:HB3	1.63	0.77
1:A:212:GLU:O	1:A:216:ARG:N	2.17	0.77
1:E:134:GLU:OE1	1:E:188:GLY:N	2.17	0.77
3:H:368:UNK:O	3:H:372:UNK:N	2.17	0.77
2:D:37:LEU:HG	1:E:419:ILE:HG21	1.66	0.77
1:A:170:PRO:HA	1:A:446:HIS:CD2	2.17	0.77
5:K:250:ASP:O	5:K:254:GLU:N	2.15	0.77
2:D:129:VAL:H	2:D:242:VAL:HG13	1.49	0.77
3:H:519:UNK:HA	3:H:522:UNK:CB	2.13	0.77
4:J:161:UNK:O	4:J:165:UNK:N	2.17	0.77
1:E:426:GLU:OE1	1:E:428:GLU:N	2.17	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:VAL:H	2:B:433:PHE:HB2	1.50	0.77
2:D:165:THR:HG23	2:D:167:GLU:H	1.48	0.77
4:J:350:UNK:CB	4:J:355:UNK:CB	2.63	0.77
3:H:159:UNK:O	3:H:164:UNK:CB	2.33	0.77
2:B:80:GLY:HA2	2:B:83:LYS:HE2	1.68	0.77
4:J:319:UNK:O	4:J:323:UNK:CA	2.33	0.76
1:E:201:LYS:HD2	1:E:203:GLN:HB2	1.67	0.76
2:D:197:LYS:HD2	2:D:199:THR:H	1.50	0.76
2:B:23:GLY:HA2	2:B:404:GLN:HE22	1.48	0.76
1:C:48:ALA:HB1	1:C:358:VAL:H	1.50	0.76
2:B:437:SER:O	2:B:440:THR:OG1	2.01	0.76
2:F:29:ARG:HA	2:F:92:GLN:HE21	1.51	0.76
2:F:306:ILE:HG21	2:F:335:ILE:HG22	1.67	0.76
1:A:116:HIS:O	1:A:461:THR:OG1	2.02	0.76
1:A:219:GLY:N	1:A:421:ILE:O	2.16	0.75
1:A:138:VAL:HG11	2:B:432:LEU:H	1.49	0.75
2:B:78:GLN:OE1	2:B:78:GLN:N	2.18	0.75
2:D:132:LYS:HB3	2:D:237:GLU:HG2	1.68	0.75
2:D:170:THR:HA	2:D:200:GLY:HA2	1.68	0.75
1:E:136:THR:OG1	1:E:137:GLU:OE1	2.03	0.75
1:C:117:ARG:HB2	1:C:240:LEU:HB2	1.69	0.75
1:E:193:ILE:HB	1:E:200:VAL:HB	1.68	0.75
5:K:189:VAL:O	5:K:191:SER:O	2.04	0.75
4:J:168:GLY:O	4:J:169:UNK:C	2.35	0.74
1:A:131:LYS:HG2	2:B:418:GLY:O	1.86	0.74
1:A:397:LEU:HD23	1:A:423:PRO:HG3	1.67	0.74
1:C:132:GLU:O	1:C:168:LYS:NZ	2.18	0.74
1:C:76:LYS:HG2	1:C:362:ARG:HG3	1.69	0.74
4:J:143:UNK:O	4:J:147:UNK:N	2.19	0.74
2:B:372:ARG:NH1	2:B:381:GLU:OE2	2.20	0.74
2:D:434:LEU:HD12	2:D:438:ARG:HB3	1.69	0.74
2:F:60:LEU:HA	2:F:63:ILE:HD12	1.68	0.74
1:A:131:LYS:CG	2:B:418:GLY:O	2.36	0.74
1:C:205:ARG:H	1:C:218:GLU:HG2	1.53	0.74
1:E:125:LYS:NZ	1:E:127:THR:OG1	2.20	0.74
4:J:183:UNK:O	4:J:187:UNK:N	2.21	0.74
1:A:303:ARG:NH1	1:A:318:TYR:OH	2.20	0.74
1:A:273:SER:HA	1:A:297:ALA:HB3	1.69	0.74
2:B:146:GLN:NE2	2:B:185:ASP:O	2.20	0.74
1:E:183:GLU:OE2	1:E:205:ARG:NH1	2.21	0.74
2:F:400:ARG:NH1	6:F:501:ADP:O3A	2.21	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:162:LYS:HA	1:E:166:GLY:O	1.88	0.73
1:A:177:LEU:HD21	1:A:194:MET:HB2	1.69	0.73
2:D:160:LYS:HG3	2:D:171:ILE:HB	1.70	0.73
3:H:191:UNK:O	3:H:193:UNK:N	2.20	0.73
1:A:123:GLY:HA2	2:B:410:SER:C	2.08	0.73
2:F:38:GLU:OE2	2:F:54:ARG:NH1	2.21	0.73
2:F:112:GLU:OE2	2:F:267:GLU:N	2.20	0.73
3:H:541:UNK:O	3:H:544:UNK:CB	2.35	0.73
1:A:144:ARG:HH11	2:B:407:THR:N	1.84	0.73
3:H:349:UNK:CB	3:H:384:UNK:CB	2.66	0.73
1:A:203:GLU:HG2	2:F:308:SER:O	1.89	0.73
1:A:274:ILE:HB	1:A:295:SER:HA	1.69	0.73
1:A:417:LEU:O	1:A:455:ARG:NH1	2.21	0.73
2:F:82:GLY:N	6:F:501:ADP:O2B	2.22	0.73
1:C:34:GLN:OE1	1:C:46:ARG:NH2	2.19	0.73
1:C:354:LEU:HD12	1:C:357:ARG:HE	1.54	0.73
1:A:144:ARG:HD2	2:B:407:THR:CG2	2.16	0.73
1:C:63:GLY:N	1:C:315:LEU:O	2.21	0.73
3:H:273:UNK:CB	3:H:302:UNK:C	2.66	0.73
1:E:130:VAL:O	1:E:229:HIS:HA	1.89	0.72
2:D:440:THR:OG1	2:D:441:GLN:OE1	2.07	0.72
1:E:213:PHE:HE1	1:E:216:GLU:HG2	1.54	0.72
4:J:173:UNK:O	4:J:174:UNK:CB	2.37	0.72
1:A:405:LEU:HD13	1:A:409:CYS:HB2	1.72	0.72
1:C:343:ASP:OD2	2:D:334:ARG:NH1	2.22	0.72
1:A:183:GLN:NE2	1:A:184:GLU:OE2	2.23	0.72
2:B:440:THR:OG1	2:B:441:GLN:NE2	2.22	0.72
4:J:184:UNK:O	4:J:188:UNK:CB	2.37	0.72
2:D:400:ARG:NH2	6:D:501:ADP:H2	1.87	0.72
1:E:285:LYS:O	1:E:289:GLN:NE2	2.22	0.72
1:C:51:VAL:O	1:C:55:LEU:HG	1.89	0.72
2:D:139:GLU:OE2	2:D:208:SER:OG	2.08	0.72
4:J:217:UNK:O	4:J:220:UNK:CB	2.37	0.72
2:F:195:ILE:HD12	2:F:211:ARG:HG3	1.72	0.72
1:A:165:LEU:HD11	1:A:410:PHE:HB3	1.72	0.72
2:B:34:ASP:OD1	2:B:38:GLU:N	2.19	0.72
1:C:74:THR:OG1	1:C:362:ARG:NH2	2.23	0.72
2:D:445:GLU:O	2:D:449:ALA:N	2.22	0.72
2:F:311:PHE:O	2:F:315:ALA:N	2.19	0.72
4:J:393:UNK:HA	4:J:400:GLY:HA2	1.72	0.72
1:A:452:LEU:HG	1:A:454:ASP:HB2	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:61:GLU:OE2	2:F:64:ARG:NH2	2.22	0.71
1:A:205:LYS:NZ	1:A:208:GLU:OE1	2.15	0.71
5:K:91:ALA:O	5:K:94:SER:CA	2.36	0.71
5:K:124:GLN:O	5:K:127:PRO:CB	2.38	0.71
1:A:231:GLY:H	1:A:260:LYS:HA	1.55	0.71
1:A:451:ASP:OD1	1:A:452:LEU:N	2.23	0.71
1:C:302:ASP:OD1	1:C:303:GLU:N	2.23	0.71
4:J:217:UNK:O	4:J:221:UNK:N	2.24	0.71
2:D:129:VAL:O	2:D:130:ARG:NE	2.23	0.71
2:D:165:THR:HB	2:D:198:ALA:HB3	1.72	0.71
3:H:191:UNK:C	3:H:193:UNK:N	2.53	0.71
1:A:133:ALA:HB1	2:B:428:ARG:H	1.54	0.71
1:A:204:ILE:N	2:F:308:SER:HB2	2.04	0.71
2:D:78:GLN:O	2:D:81:THR:OG1	2.09	0.71
2:D:139:GLU:OE2	2:D:210:THR:OG1	2.07	0.71
1:A:111:GLN:OE1	1:A:502:ARG:NE	2.24	0.71
1:A:138:VAL:HG11	2:B:432:LEU:N	2.05	0.71
1:C:303:GLU:OE2	1:C:305:HIS:NE2	2.23	0.71
1:E:203:GLN:O	1:E:205:ARG:NH1	2.24	0.71
1:E:277:GLY:O	1:E:281:LYS:NZ	2.24	0.71
1:A:140:GLN:O	1:A:142:ASN:N	2.23	0.71
1:A:277:SER:HB3	1:A:298:VAL:HA	1.73	0.71
2:B:416:ARG:CZ	2:B:418:GLY:HA3	2.21	0.71
2:D:426:ILE:O	2:D:430:TYR:N	2.24	0.71
2:B:141:GLU:HG2	2:B:165:THR:HG23	1.72	0.71
2:B:132:LYS:HG2	2:B:237:GLU:HB3	1.73	0.70
1:E:163:THR:HG22	1:E:164:ALA:H	1.56	0.70
3:H:91:UNK:CA	3:H:141:UNK:CB	2.70	0.70
1:A:123:GLY:CA	2:B:410:SER:CA	2.68	0.70
1:A:162:ARG:C	1:A:414:HIS:HA	2.11	0.70
1:A:201:SER:HB2	2:F:309:PHE:HB2	1.72	0.70
3:H:637:UNK:O	3:H:641:UNK:N	2.24	0.70
1:A:170:PRO:HG3	1:A:433:ASN:HB2	1.74	0.70
2:D:443:MET:HA	2:D:446:TYR:HB2	1.74	0.70
1:E:110:GLU:OE1	1:E:110:GLU:N	2.20	0.70
1:C:193:ILE:HG22	1:C:201:LYS:H	1.57	0.70
2:D:271:GLU:OE1	2:D:271:GLU:N	2.23	0.70
1:A:465:THR:HG22	1:A:468:GLU:HB2	1.72	0.70
2:B:384:GLU:OE1	2:B:384:GLU:N	2.25	0.70
1:C:367:THR:N	1:C:370:GLU:OE2	2.22	0.70
2:D:131:ILE:H	2:D:239:VAL:HG12	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:368:LYS:HG3	2:F:372:ARG:HH12	1.57	0.70
1:E:156:HIS:HD2	1:E:173:ASP:HA	1.55	0.70
1:A:123:GLY:HA2	2:B:410:SER:CA	2.22	0.69
2:D:138:ILE:HG12	2:D:205:LEU:HA	1.72	0.69
2:D:364:GLU:O	2:D:367:THR:OG1	2.10	0.69
1:A:204:ILE:HG12	2:F:311:PHE:HB2	1.74	0.69
1:A:301:GLN:NE2	1:A:305:ASP:OD2	2.21	0.69
2:B:43:SER:O	2:B:46:MET:N	2.24	0.69
2:D:206:GLY:HA2	2:D:235:ARG:HD3	1.75	0.69
1:A:210:LEU:O	1:A:214:PHE:N	2.22	0.69
2:B:31:LEU:HB3	2:B:33:LEU:HD23	1.73	0.69
1:C:65:ALA:H	1:C:354:LEU:N	1.85	0.69
4:J:407:UNK:O	4:J:411:UNK:N	2.25	0.69
2:D:366:ASP:N	2:D:366:ASP:OD1	2.22	0.69
3:H:273:UNK:CB	3:H:302:UNK:CA	2.71	0.69
1:A:468:GLU:HG2	1:A:472:ILE:HG22	1.72	0.69
2:B:307:GLU:HA	1:C:102:TYR:O	1.92	0.69
2:D:60:LEU:HA	2:D:63:ILE:HD12	1.73	0.69
1:A:144:ARG:HD2	2:B:407:THR:H	1.58	0.69
1:A:263:LYS:HD3	1:A:324:GLY:H	1.58	0.69
2:F:283:TRP:HB3	2:F:289:ALA:HB3	1.74	0.69
2:F:197:LYS:HG3	2:F:205:LEU:HD22	1.73	0.69
3:H:494:UNK:O	3:H:496:UNK:N	2.26	0.69
1:A:141:GLU:OE2	1:A:144:ARG:NE	2.25	0.69
4:J:347:UNK:HA	4:J:454:UNK:O	1.93	0.69
1:C:304:VAL:HG11	1:C:329:PHE:HB3	1.76	0.68
1:E:184:ARG:HG2	1:E:212:GLU:HB3	1.75	0.68
4:J:252:UNK:O	4:J:255:UNK:N	2.26	0.68
1:A:369:ILE:HG13	1:A:373:LEU:HD12	1.75	0.68
2:F:338:THR:HG23	2:F:340:TYR:H	1.56	0.68
1:E:376:LYS:HD2	1:E:380:GLN:HE22	1.58	0.68
2:D:177:LYS:HE2	2:D:205:LEU:HD22	1.74	0.68
2:F:186:LYS:O	2:F:213:ARG:NH2	2.26	0.68
5:K:382:CYS:O	5:K:385:ASP:CB	2.41	0.68
1:A:133:ALA:HB3	2:B:428:ARG:H	1.58	0.68
1:E:126:GLU:OE1	1:E:128:LYS:NZ	2.26	0.68
1:E:367:THR:N	1:E:370:GLU:OE1	2.22	0.68
1:C:71:PRO:HB3	1:C:362:ARG:HB3	1.75	0.68
1:C:124:ILE:HA	1:C:292:ALA:HA	1.76	0.68
1:C:286:TYR:HB3	1:C:291:ILE:HG12	1.76	0.68
1:C:315:LEU:HB3	1:C:319:LEU:HD11	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:204:LYS:HD3	2:D:205:LEU:H	1.59	0.68
2:F:149:ARG:NH2	2:F:180:GLU:OE2	2.27	0.68
2:F:220:SER:OG	2:F:223:LYS:O	2.11	0.68
2:F:137:ILE:HG13	2:F:206:GLY:HA2	1.74	0.68
3:H:242:UNK:O	3:H:245:UNK:CB	2.42	0.68
3:H:444:UNK:O	3:H:448:UNK:N	2.26	0.68
1:C:34:GLN:NE2	1:C:39:LEU:O	2.26	0.68
2:D:174:LEU:HD12	2:D:203:SER:HB3	1.76	0.68
2:D:430:TYR:CZ	2:D:434:LEU:HA	2.29	0.68
3:H:353:UNK:HA	3:H:388:UNK:HA	1.75	0.68
1:C:194:GLU:HB3	1:C:197:SER:HB2	1.74	0.67
2:D:316:LEU:HD11	2:D:353:ARG:HH12	1.57	0.67
2:D:416:ARG:NH2	2:D:424:ASP:OD2	2.27	0.67
2:D:160:LYS:HA	2:D:171:ILE:HA	1.75	0.67
2:D:438:ARG:HA	2:D:442:TYR:HB3	1.74	0.67
1:C:190:VAL:HG11	1:C:224:PRO:HB2	1.75	0.67
1:A:135:SER:H	2:B:412:VAL:HB	1.58	0.67
1:A:372:LYS:H	1:A:372:LYS:HD2	1.58	0.67
1:C:13:GLN:OE1	1:C:13:GLN:N	2.26	0.67
1:A:132:GLN:HG2	2:B:425:ASP:N	2.09	0.67
2:F:194:THR:N	2:F:212:ALA:O	2.27	0.67
1:A:123:GLY:HA3	2:B:412:VAL:H	1.58	0.67
5:K:91:ALA:O	5:K:94:SER:N	2.26	0.67
2:D:77:GLY:HA2	6:D:501:ADP:O1B	1.95	0.67
2:F:37:LEU:O	2:F:54:ARG:NH1	2.27	0.67
1:A:397:LEU:HB3	1:A:423:PRO:HB2	1.77	0.67
1:C:283:VAL:HA	1:C:286:TYR:HB2	1.75	0.67
1:E:63:GLY:O	1:E:357:ARG:NH2	2.27	0.67
1:E:89:SER:O	1:E:123:ARG:NH2	2.28	0.67
1:C:61:MET:HG3	1:C:319:LEU:HD12	1.77	0.67
5:K:189:VAL:O	5:K:191:SER:C	2.33	0.67
1:A:221:ARG:HH22	1:A:391:GLU:HB3	1.60	0.66
1:A:549:GLN:OE1	2:F:78:GLN:NE2	2.25	0.66
2:F:149:ARG:HH12	2:F:179:ILE:HG23	1.59	0.66
1:A:204:ILE:HD13	2:F:311:PHE:HD1	1.59	0.66
1:A:205:LYS:HG2	1:A:206:LYS:H	1.60	0.66
2:B:27:HIS:O	2:B:29:ARG:NH1	2.28	0.66
2:B:29:ARG:HA	2:B:92:GLN:HG3	1.78	0.66
2:B:383:SER:O	2:B:386:ALA:N	2.24	0.66
2:D:396:GLU:OE1	2:D:397:THR:OG1	2.13	0.66
2:F:34:ASP:OD1	2:F:40:ARG:NH2	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:146:GLN:HE22	2:D:163:LEU:HG	1.59	0.66
1:E:122:LEU:HB3	1:E:238:VAL:O	1.95	0.66
2:F:192:VAL:HB	2:F:214:ASP:HB3	1.77	0.66
1:A:144:ARG:HG2	2:B:405:LEU:HA	1.77	0.66
3:H:444:UNK:O	3:H:447:UNK:CB	2.43	0.66
5:K:383:ARG:O	5:K:386:SER:CB	2.43	0.66
1:A:134:ALA:HB1	2:B:412:VAL:HG11	1.75	0.66
1:E:135:VAL:HA	1:E:159:ILE:HG23	1.78	0.66
4:J:219:UNK:O	4:J:223:UNK:N	2.28	0.66
1:A:289:ILE:HB	1:A:301:GLN:HG2	1.78	0.66
2:B:375:CYS:O	2:B:378:GLU:N	2.27	0.66
1:C:346:SER:OG	1:C:350:ILE:O	2.13	0.66
1:A:431:ARG:NH1	1:A:432:GLY:O	2.29	0.66
2:F:179:ILE:HA	2:F:182:LEU:HD12	1.77	0.66
5:K:386:SER:O	5:K:389:PRO:CA	2.44	0.66
1:A:201:SER:O	2:F:308:SER:N	2.27	0.65
1:A:225:THR:HA	1:A:331:GLU:HA	1.76	0.65
1:E:369:GLN:OE1	1:E:369:GLN:N	2.23	0.65
1:A:138:VAL:N	2:B:433:PHE:HB2	2.11	0.65
2:D:381:GLU:HB2	2:D:420:GLU:HA	1.77	0.65
5:K:383:ARG:O	5:K:386:SER:N	2.29	0.65
1:A:123:GLY:CA	2:B:411:LEU:H	2.08	0.65
1:A:141:GLU:OE2	1:A:144:ARG:NH2	2.30	0.65
2:D:176:THR:HB	2:D:177:LYS:HD3	1.76	0.65
1:E:97:VAL:N	1:E:100:GLU:OE2	2.23	0.65
1:E:177:PHE:O	1:E:202:ARG:NH1	2.29	0.65
1:E:210:ALA:HA	1:E:213:PHE:HB3	1.79	0.65
1:E:321:SER:OG	1:E:322:SER:N	2.28	0.65
3:H:369:UNK:O	3:H:373:UNK:CB	2.44	0.65
1:A:132:GLN:HG3	2:B:425:ASP:O	1.97	0.65
1:A:203:GLU:HG3	2:F:311:PHE:N	2.11	0.65
1:C:65:ALA:O	1:C:354:LEU:N	2.29	0.65
1:E:390:ALA:O	1:E:394:LEU:N	2.23	0.65
1:A:123:GLY:HA3	2:B:412:VAL:N	2.12	0.65
1:A:135:SER:H	2:B:412:VAL:CB	2.09	0.65
1:A:524:GLU:H	1:A:527:HIS:CE1	2.15	0.65
1:A:546:ALA:O	1:A:550:ASP:N	2.23	0.65
1:A:204:ILE:HB	2:F:116:THR:HG22	1.77	0.65
2:B:24:ALA:HB3	6:B:501:ADP:O2'	1.97	0.65
2:D:76:ALA:HB3	2:D:358:SER:HB2	1.79	0.65
2:F:136:GLU:HB2	2:F:235:ARG:HE	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:91:ALA:C	5:K:94:SER:CB	2.59	0.65
1:E:130:VAL:HG22	1:E:232:LYS:HD3	1.78	0.65
1:A:117:SER:HA	1:A:462:MET:HB2	1.79	0.65
1:E:373:GLN:OE1	1:E:373:GLN:N	2.22	0.65
3:H:573:UNK:O	3:H:575:UNK:N	2.29	0.65
1:C:396:GLU:OE1	1:C:396:GLU:N	2.29	0.64
2:D:34:ASP:OD1	2:D:38:GLU:N	2.26	0.64
4:J:199:UNK:O	4:J:202:UNK:CB	2.44	0.64
4:J:327:UNK:HA	4:J:331:GLY:H	1.62	0.64
2:B:61:GLU:OE2	2:B:64:ARG:NH1	2.30	0.64
2:B:164:LYS:HA	2:B:169:GLU:HG2	1.80	0.64
2:B:280:VAL:HA	2:B:283:TRP:HD1	1.61	0.64
2:D:73:VAL:HG13	2:D:325:ILE:HG22	1.79	0.64
2:D:130:ARG:HH21	2:D:242:VAL:HG21	1.61	0.64
2:F:32:GLY:HA3	2:F:43:SER:OG	1.98	0.64
1:A:227:GLU:OE1	1:A:229:TYR:OH	2.15	0.64
2:D:442:TYR:O	2:D:446:TYR:N	2.30	0.64
1:E:194:GLU:OE1	1:E:194:GLU:N	2.29	0.64
4:J:301:UNK:CA	4:J:308:UNK:CB	2.75	0.64
2:B:362:TYR:CE2	6:B:501:ADP:N7	2.66	0.64
2:B:428:ARG:HD2	2:B:431:SER:OG	1.98	0.64
2:D:25:HIS:NE2	2:D:84:THR:OG1	2.29	0.64
1:E:33:LYS:O	1:E:46:ARG:NH1	2.30	0.64
1:A:399:VAL:HB	1:A:425:VAL:HG11	1.77	0.64
1:E:192:TYR:O	1:E:232:LYS:NZ	2.31	0.64
2:F:188:GLN:HG3	2:F:191:ASP:HB2	1.77	0.64
2:D:129:VAL:HG12	2:D:291:ILE:HG22	1.78	0.64
5:K:59:LEU:HA	5:K:62:ALA:HB3	1.78	0.64
2:D:157:LYS:HE3	2:D:174:LEU:HD23	1.80	0.64
1:A:110:THR:OG1	1:A:502:ARG:NH2	2.30	0.64
1:A:134:ALA:CB	2:B:412:VAL:CG1	2.70	0.64
1:A:433:ASN:OD1	1:A:434:CYS:N	2.30	0.64
1:E:424:SER:OG	1:E:425:ILE:N	2.30	0.64
1:A:374:ARG:HH12	1:A:415:ARG:HH12	1.46	0.64
1:C:44:ASN:HB3	1:C:68:LEU:HD11	1.78	0.64
3:H:261:UNK:CA	3:H:265:UNK:CB	2.75	0.64
1:A:165:LEU:N	1:A:451:ASP:OD1	2.30	0.64
1:C:67:LEU:CD2	2:D:440:THR:HG21	2.27	0.64
5:K:123:GLN:O	5:K:127:PRO:CB	2.46	0.64
2:B:351:LEU:HA	2:B:354:LEU:HD12	1.80	0.63
2:B:435:ASP:O	2:B:439:SER:N	2.24	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:23:GLY:HA2	1:C:82:ALA:HB1	1.81	0.63
2:F:193:ILE:HD12	2:F:213:ARG:HH11	1.63	0.63
3:H:593:UNK:N	3:H:631:UNK:CB	2.61	0.63
2:B:285:GLU:N	2:B:285:GLU:OE1	2.28	0.63
1:C:128:LYS:HB2	1:C:232:LYS:HG2	1.80	0.63
3:H:471:UNK:C	3:H:473:UNK:N	2.59	0.63
1:E:426:GLU:HG3	1:E:429:HIS:CE1	2.32	0.63
2:F:110:SER:OG	2:F:111:LEU:N	2.31	0.63
2:F:381:GLU:N	2:F:381:GLU:OE1	2.32	0.63
4:J:398:UNK:HA	4:J:453:UNK:CB	2.28	0.63
1:C:356:ASP:H	1:C:357:ARG:HD3	1.64	0.63
1:C:358:VAL:HG12	1:C:359:MET:H	1.61	0.63
1:A:487:GLU:O	1:A:525:LYS:NZ	2.28	0.63
2:B:82:GLY:O	2:B:86:ILE:N	2.23	0.63
1:C:130:VAL:HG21	1:C:232:LYS:HB3	1.79	0.63
2:B:448:ASP:HA	2:B:451:LEU:HB2	1.80	0.63
3:H:308:UNK:CB	3:H:358:UNK:CB	2.77	0.63
5:K:383:ARG:CB	5:K:392:ARG:CB	2.77	0.63
1:A:138:VAL:H	2:B:433:PHE:CB	2.12	0.63
1:A:544:ILE:O	1:A:548:GLN:NE2	2.32	0.63
2:F:382:MET:HG2	2:F:421:VAL:HB	1.81	0.63
1:A:487:GLU:OE1	1:A:487:GLU:N	2.25	0.62
2:D:359:THR:N	6:D:501:ADP:O3B	2.32	0.62
5:K:261:VAL:O	5:K:268:GLU:CB	2.46	0.62
1:A:138:VAL:O	2:B:433:PHE:HB2	1.99	0.62
1:A:151:VAL:HA	1:A:154:ILE:HG12	1.80	0.62
1:E:42:GLN:HE22	1:E:364:MET:H	1.47	0.62
2:F:299:ASP:OD1	2:F:300:GLU:N	2.31	0.62
1:A:110:THR:O	1:A:502:ARG:NH2	2.31	0.62
2:B:438:ARG:NH1	2:B:441:GLN:HB2	2.15	0.62
2:D:239:VAL:HG23	2:D:240:HIS:H	1.64	0.62
2:F:441:GLN:NE2	2:F:445:GLU:OE2	2.32	0.62
3:H:637:UNK:O	3:H:640:UNK:N	2.32	0.62
1:A:382:ASN:HA	1:A:385:ILE:HD12	1.82	0.62
1:C:194:GLU:HB2	1:C:199:ALA:HB3	1.81	0.62
3:H:471:UNK:O	3:H:473:UNK:N	2.33	0.62
5:K:135:THR:HA	5:K:198:SER:CB	2.29	0.62
1:C:183:GLU:OE1	1:C:202:ARG:N	2.25	0.62
2:D:77:GLY:HA3	2:D:83:LYS:HD2	1.82	0.62
1:A:464:TYR:CD2	1:A:472:ILE:HG21	2.35	0.62
3:H:637:UNK:C	3:H:640:UNK:N	2.62	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:393:ILE:HA	2:B:396:GLU:HB2	1.82	0.62
1:C:27:ASP:N	1:C:31:LEU:O	2.32	0.62
2:D:428:ARG:HH11	2:D:429:VAL:HA	1.63	0.62
1:E:205:ARG:HE	1:E:218:GLU:HA	1.63	0.62
1:A:132:GLN:CB	2:B:425:ASP:HB3	2.20	0.62
1:A:275:PHE:O	1:A:279:GLN:N	2.30	0.62
1:A:495:ILE:HG13	1:A:498:LYS:HD2	1.81	0.62
2:B:97:ASP:N	2:B:97:ASP:OD1	2.31	0.62
1:E:192:TYR:HB3	1:E:203:GLN:HB3	1.82	0.62
1:A:403:HIS:CD2	1:A:404:MET:HB2	2.35	0.61
1:A:527:HIS:HA	1:A:530:GLU:OE1	1.99	0.61
2:B:174:LEU:HD22	2:B:179:ILE:HD13	1.80	0.61
1:C:110:GLU:OE1	1:C:110:GLU:N	2.22	0.61
1:A:134:ALA:CA	2:B:412:VAL:HG11	2.30	0.61
2:B:23:GLY:HA2	2:B:404:GLN:NE2	2.13	0.61
2:D:134:GLU:HA	2:D:207:ARG:HD3	1.81	0.61
2:D:197:LYS:CD	2:D:199:THR:H	2.13	0.61
2:F:142:VAL:HG13	2:F:161:LEU:HD21	1.82	0.61
1:C:71:PRO:HB3	1:C:362:ARG:CB	2.31	0.61
2:D:177:LYS:HB2	2:D:205:LEU:HD21	1.83	0.61
2:D:282:GLU:HA	2:D:285:GLU:HG2	1.81	0.61
1:E:128:LYS:HZ1	1:E:234:ILE:HB	1.65	0.61
2:F:149:ARG:HG3	2:F:183:THR:HG21	1.81	0.61
1:A:141:GLU:HG2	1:A:144:ARG:HB2	1.83	0.61
1:A:203:GLU:CG	2:F:311:PHE:H	2.11	0.61
1:A:397:LEU:O	1:A:425:VAL:HB	2.00	0.61
2:D:400:ARG:NH1	6:D:501:ADP:N3	2.49	0.61
4:J:280:UNK:C	4:J:282:UNK:N	2.63	0.61
2:D:144:GLU:OE2	2:D:188:GLN:N	2.27	0.61
2:D:170:THR:OG1	2:D:197:LYS:NZ	2.33	0.61
5:K:302:PRO:N	5:K:305:GLN:CB	2.61	0.61
1:E:207:ASP:HB3	1:E:223:LEU:HD22	1.81	0.61
1:A:132:GLN:HG2	2:B:425:ASP:C	2.21	0.61
1:E:40:VAL:O	6:E:501:ADP:N6	2.34	0.61
1:C:168:LYS:HB3	1:C:170:LEU:HD13	1.81	0.61
2:D:138:ILE:CG1	2:D:205:LEU:HA	2.31	0.61
1:E:213:PHE:CE1	1:E:216:GLU:HG2	2.36	0.61
2:F:31:LEU:O	2:F:53:ARG:NH2	2.31	0.61
1:A:132:GLN:HE21	2:B:423:VAL:C	2.05	0.60
1:A:176:ALA:HB2	1:A:456:VAL:HA	1.81	0.60
1:A:234:THR:OG1	1:A:256:ILE:O	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:ASP:HB3	1:A:328:LYS:HB3	1.82	0.60
2:B:376:GLU:N	2:B:376:GLU:OE1	2.33	0.60
1:C:316:HIS:O	1:C:320:GLU:N	2.25	0.60
2:D:400:ARG:NH2	6:D:501:ADP:C2	2.68	0.60
1:E:162:LYS:HG2	1:E:167:THR:HA	1.83	0.60
1:A:138:VAL:CA	2:B:433:PHE:HB2	2.31	0.60
2:D:284:ARG:NH1	2:D:285:GLU:OE2	2.33	0.60
1:A:122:LEU:HD11	1:A:144:ARG:CZ	2.32	0.60
2:F:196:ASP:HA	2:F:205:LEU:HD13	1.83	0.60
3:H:493:UNK:O	3:H:496:UNK:N	2.34	0.60
4:J:251:UNK:O	4:J:254:UNK:CB	2.49	0.60
1:A:138:VAL:C	2:B:433:PHE:HB2	2.21	0.60
2:D:201:LYS:NZ	4:J:281:UNK:O	2.34	0.60
1:E:17:SER:O	1:E:378:ARG:NH1	2.34	0.60
2:D:149:ARG:HD3	2:D:182:LEU:HB3	1.83	0.60
1:A:533:GLU:OE1	1:A:533:GLU:N	2.33	0.60
2:B:121:GLN:OE1	2:B:245:HIS:NE2	2.34	0.60
1:C:162:LYS:O	1:C:208:THR:OG1	2.16	0.60
1:A:146:ALA:HB3	1:A:454:ASP:HA	1.84	0.60
2:D:374:ARG:NH2	2:D:378:GLU:OE2	2.35	0.60
1:A:183:GLN:HG3	1:A:184:GLU:HG2	1.82	0.60
1:E:126:GLU:OE2	1:E:236:GLN:N	2.34	0.60
4:J:393:UNK:CB	4:J:404:UNK:CB	2.80	0.60
1:A:132:GLN:CG	2:B:425:ASP:C	2.70	0.60
1:E:138:LEU:HA	1:E:157:VAL:HG13	1.84	0.60
1:E:193:ILE:HG22	1:E:202:ARG:HA	1.83	0.60
1:E:281:LYS:HA	1:E:284:ASN:HB2	1.83	0.60
1:A:113:ILE:HG22	1:A:460:ARG:HB2	1.82	0.60
1:A:116:HIS:H	1:A:461:THR:HA	1.67	0.60
1:A:231:GLY:N	1:A:261:THR:H	2.00	0.60
1:C:362:ARG:HD3	1:C:363:THR:O	2.02	0.60
2:D:76:ALA:O	2:D:358:SER:OG	2.12	0.60
3:H:261:UNK:C	3:H:265:UNK:CB	2.79	0.60
1:A:134:ALA:CB	2:B:412:VAL:HG11	2.31	0.59
2:B:305:ASP:O	2:B:308:SER:OG	2.15	0.59
1:C:64:ARG:HH22	1:C:357:ARG:HH21	1.48	0.59
2:D:84:THR:HG22	2:D:297:PHE:HE2	1.66	0.59
3:H:637:UNK:O	3:H:640:UNK:CB	2.50	0.59
1:A:181:ILE:HG12	1:A:455:ARG:HD3	1.83	0.59
2:B:378:GLU:HG2	2:B:380:VAL:HG23	1.84	0.59
2:D:146:GLN:NE2	2:D:196:ASP:HB2	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:LEU:HB3	1:A:214:PHE:CZ	2.37	0.59
2:B:280:VAL:HA	2:B:283:TRP:CD1	2.36	0.59
1:C:6:VAL:HG11	1:C:242:ASP:HB3	1.83	0.59
2:D:138:ILE:HD12	2:D:178:MET:SD	2.42	0.59
2:F:388:THR:O	2:F:391:THR:OG1	2.17	0.59
1:A:209:VAL:O	1:A:213:ASN:ND2	2.34	0.59
1:C:319:LEU:HA	1:C:324:ALA:HB2	1.84	0.59
2:D:384:GLU:HA	2:D:387:TYR:HB2	1.84	0.59
1:E:283:VAL:HG12	1:E:287:ILE:HD11	1.83	0.59
1:A:135:SER:H	2:B:412:VAL:CG1	2.16	0.59
4:J:350:UNK:O	4:J:355:UNK:HA	1.99	0.59
2:F:174:LEU:HD22	2:F:182:LEU:HD13	1.85	0.59
2:F:352:ASP:N	2:F:352:ASP:OD1	2.33	0.59
3:H:514:UNK:C	3:H:516:UNK:N	2.65	0.59
3:H:514:UNK:O	3:H:516:UNK:N	2.36	0.59
4:J:330:UNK:C	4:J:332:UNK:N	2.62	0.59
2:B:70:GLY:O	2:B:353:ARG:NH1	2.36	0.59
1:C:279:ILE:HA	1:C:282:VAL:HG12	1.84	0.59
1:A:399:VAL:H	1:A:425:VAL:CG2	2.13	0.59
1:A:480:GLU:OE1	1:A:480:GLU:N	2.35	0.59
1:C:48:ALA:HB1	1:C:358:VAL:N	2.18	0.59
2:D:374:ARG:O	2:D:378:GLU:HG2	2.03	0.59
1:E:341:THR:O	1:E:342:GLU:HG2	2.03	0.59
3:H:573:UNK:C	3:H:575:UNK:N	2.62	0.59
5:K:250:ASP:C	5:K:253:MET:CB	2.69	0.59
1:A:132:GLN:NE2	2:B:423:VAL:O	2.36	0.59
2:B:195:ILE:HG13	2:B:210:THR:H	1.68	0.59
2:B:364:GLU:HB2	2:B:395:LEU:HD21	1.85	0.59
2:F:401:TYR:OH	2:F:433:PHE:O	2.16	0.59
1:A:231:GLY:H	1:A:261:THR:H	1.49	0.59
1:A:494:GLU:HG3	1:A:498:LYS:NZ	2.17	0.59
1:C:301:VAL:HG12	1:C:304:VAL:HG12	1.85	0.59
2:D:132:LYS:HB3	2:D:237:GLU:CG	2.33	0.59
4:J:147:UNK:C	4:J:149:UNK:N	2.65	0.59
2:B:194:THR:HG23	2:B:195:ILE:HG12	1.84	0.58
2:B:233:GLN:NE2	2:B:234:LYS:O	2.36	0.58
1:C:273:ASP:O	1:C:277:GLY:N	2.35	0.58
2:D:206:GLY:HA3	2:D:235:ARG:HB2	1.85	0.58
1:E:25:GLY:O	1:E:46:ARG:NH2	2.36	0.58
1:A:204:ILE:O	2:F:308:SER:HA	2.03	0.58
2:B:149:ARG:NH1	2:B:183:THR:O	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:92:PRO:HD2	1:C:297:GLY:HA3	1.85	0.58
2:D:279:LYS:HG2	2:D:283:TRP:HE1	1.67	0.58
2:D:397:THR:HG23	2:D:436:GLU:HB2	1.85	0.58
2:F:407:THR:O	2:F:410:SER:OG	2.16	0.58
5:K:302:PRO:C	5:K:305:GLN:CB	2.69	0.58
1:A:306:THR:HG22	1:A:321:LEU:H	1.68	0.58
2:D:124:ARG:O	2:D:245:HIS:N	2.36	0.58
1:A:441:ASP:N	1:A:441:ASP:OD1	2.35	0.58
1:E:353:ASP:OD1	1:E:354:LEU:N	2.35	0.58
2:F:81:THR:N	6:F:501:ADP:O2B	2.35	0.58
3:H:444:UNK:HA	3:H:447:UNK:CB	2.33	0.58
1:A:109:LYS:HG2	1:A:427:PHE:O	2.03	0.58
1:A:111:GLN:O	1:A:112:ARG:HG3	2.03	0.58
1:C:43:GLU:O	1:C:47:GLU:HG2	2.03	0.58
1:C:61:MET:N	1:C:320:GLU:OE1	2.37	0.58
2:D:134:GLU:HG3	2:D:207:ARG:CZ	2.34	0.58
1:E:42:GLN:HE22	1:E:364:MET:N	2.02	0.58
2:F:148:ASP:HB3	2:F:157:LYS:HB2	1.85	0.58
4:J:345:UNK:O	4:J:349:UNK:N	2.36	0.58
1:A:163:ALA:HB2	1:A:414:HIS:N	2.18	0.58
2:B:142:VAL:N	2:B:191:ASP:O	2.31	0.58
1:C:314:TYR:CB	2:D:111:LEU:HD13	2.14	0.58
1:E:20:HIS:O	1:E:22:LYS:NZ	2.34	0.58
2:F:135:THR:HA	2:F:207:ARG:HB2	1.84	0.58
2:F:426:ILE:HA	2:F:429:VAL:HG12	1.84	0.58
1:A:138:VAL:N	2:B:433:PHE:CD2	2.71	0.58
1:A:190:PRO:HD3	1:A:394:PRO:HG3	1.86	0.58
1:C:81:LEU:HG	1:C:85:GLN:HE22	1.69	0.58
1:C:27:ASP:H	1:C:31:LEU:N	2.01	0.58
1:C:51:VAL:HG21	2:D:404:GLN:HE21	1.67	0.58
1:C:63:GLY:HA2	1:C:315:LEU:HB2	1.86	0.58
4:J:393:UNK:CA	4:J:400:GLY:CA	2.66	0.58
1:A:124:LEU:HD23	1:A:135:SER:OG	2.02	0.58
1:A:225:THR:HG22	1:A:329:LYS:HE3	1.86	0.58
2:B:195:ILE:HG21	2:B:209:PHE:HA	1.85	0.58
2:B:403:ILE:HG12	2:B:404:GLN:OE1	2.04	0.58
1:C:123:ARG:HB3	1:C:293:GLU:HB3	1.86	0.58
1:A:444:SER:OG	1:A:448:ILE:O	2.14	0.57
1:E:373:GLN:HA	1:E:376:LYS:HB3	1.86	0.57
2:F:47:VAL:H	6:F:501:ADP:HN62	1.52	0.57
3:H:175:UNK:C	3:H:177:UNK:H	2.16	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:PHE:HD2	1:A:425:VAL:H	1.52	0.57
2:B:130:ARG:HG3	2:B:241:THR:HG22	1.85	0.57
2:D:334:ARG:HB2	2:D:341:GLN:HE22	1.69	0.57
3:H:91:UNK:HA	3:H:141:UNK:CB	2.34	0.57
2:B:352:ASP:O	1:C:408:GLN:NE2	2.36	0.57
2:D:351:LEU:HA	2:D:354:LEU:HD12	1.85	0.57
1:A:259:LEU:O	1:A:266:LYS:CB	2.51	0.57
1:A:265:THR:HG22	1:A:267:GLN:HG2	1.86	0.57
1:A:276:GLU:HG2	1:A:297:ALA:HA	1.86	0.57
1:C:21:VAL:HG23	1:C:85:GLN:HG2	1.86	0.57
1:C:55:LEU:HD11	1:C:354:LEU:HD11	1.87	0.57
1:C:191:ILE:HG22	1:C:202:ARG:HD3	1.84	0.57
2:D:439:SER:OG	2:D:440:THR:N	2.37	0.57
2:F:187:VAL:HG22	2:F:213:ARG:HH12	1.69	0.57
4:J:217:UNK:O	4:J:220:UNK:N	2.37	0.57
1:A:229:TYR:HD2	1:A:259:LEU:HD22	1.68	0.57
1:A:477:ALA:HB1	1:A:508:LEU:HD11	1.87	0.57
1:C:27:ASP:OD1	1:C:28:GLU:N	2.38	0.57
2:D:82:GLY:O	6:D:501:ADP:O2'	2.22	0.57
2:D:297:PHE:HD1	2:D:325:ILE:HG13	1.70	0.57
2:F:142:VAL:HG21	2:F:193:ILE:HG22	1.86	0.57
2:D:137:ILE:HG12	2:D:211:ARG:HH11	1.70	0.57
1:E:166:GLY:HA2	1:E:228:VAL:HG22	1.87	0.57
1:E:338:ILE:HD11	1:E:346:SER:HB3	1.85	0.57
3:H:648:UNK:C	3:H:650:UNK:N	2.64	0.57
5:K:77:ASP:HA	5:K:80:PHE:CB	2.34	0.57
1:A:134:ALA:HA	2:B:412:VAL:HG11	1.85	0.57
2:D:436:GLU:HA	2:D:439:SER:OG	2.05	0.57
1:E:396:GLU:O	1:E:400:LYS:N	2.36	0.57
3:H:125:UNK:CA	3:H:163:UNK:HA	2.34	0.57
3:H:493:UNK:O	3:H:496:UNK:CA	2.53	0.57
4:J:198:UNK:O	4:J:201:UNK:CB	2.52	0.57
1:A:131:LYS:CE	2:B:413:CYS:CB	2.77	0.57
1:A:431:ARG:NH1	1:A:434:CYS:SG	2.77	0.57
2:B:104:ALA:N	2:B:107:GLU:OE2	2.30	0.57
2:D:132:LYS:HA	2:D:238:VAL:O	2.05	0.57
1:A:412:TYR:HB2	2:B:111:LEU:HD23	1.87	0.57
1:A:470:LYS:HG2	1:A:489:LEU:HD11	1.86	0.57
1:C:311:CYS:HA	2:D:111:LEU:HD11	1.87	0.57
1:C:428:GLU:OE1	1:C:428:GLU:N	2.29	0.57
2:D:146:GLN:HB3	2:D:149:ARG:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:180:GLU:O	2:D:184:LYS:N	2.37	0.57
5:K:386:SER:O	5:K:389:PRO:N	2.38	0.57
2:D:403:ILE:O	2:D:406:ILE:HG22	2.04	0.56
1:E:439:ASP:N	1:E:439:ASP:OD1	2.36	0.56
2:F:99:PRO:HG2	2:F:294:GLY:HA3	1.86	0.56
3:H:472:UNK:O	3:H:475:UNK:N	2.38	0.56
2:B:362:TYR:OH	6:B:501:ADP:N6	2.38	0.56
1:C:168:LYS:HD2	1:C:228:VAL:HA	1.86	0.56
1:C:414:ASN:HA	1:C:425:ILE:HD11	1.87	0.56
2:D:156:SER:HA	2:D:174:LEU:H	1.70	0.56
1:A:141:GLU:O	1:A:144:ARG:N	2.27	0.56
1:A:203:GLU:CD	2:F:312:LEU:H	2.09	0.56
1:C:129:GLU:HG2	1:C:231:LYS:HE3	1.87	0.56
1:C:426:GLU:HB2	1:C:428:GLU:OE2	2.05	0.56
2:D:142:VAL:HG23	2:D:164:LYS:HB3	1.88	0.56
2:D:274:GLU:O	2:D:278:ALA:N	2.37	0.56
2:D:383:SER:HG	2:D:386:ALA:H	1.53	0.56
2:F:185:ASP:OD2	2:F:213:ARG:NH1	2.38	0.56
2:F:358:SER:OG	2:F:359:THR:N	2.37	0.56
3:H:593:UNK:CB	3:H:631:UNK:HA	2.33	0.56
4:J:121:UNK:C	4:J:123:UNK:H	2.18	0.56
2:B:383:SER:HB3	2:B:423:VAL:HA	1.87	0.56
1:C:396:GLU:HA	1:C:399:THR:HB	1.87	0.56
1:A:116:HIS:HE1	1:A:118:HIS:O	1.88	0.56
1:A:162:ARG:N	1:A:414:HIS:O	2.38	0.56
1:C:14:ARG:NH1	1:C:95:PRO:O	2.37	0.56
1:C:62:ALA:HB1	1:C:316:HIS:CE1	2.40	0.56
2:D:422:GLN:HB2	2:D:424:ASP:H	1.71	0.56
2:F:385:ASP:N	2:F:385:ASP:OD1	2.36	0.56
4:J:168:GLY:O	4:J:170:UNK:N	2.38	0.56
1:A:107:THR:O	1:A:427:PHE:N	2.38	0.56
2:B:146:GLN:HE22	2:B:187:VAL:H	1.53	0.56
1:C:307:LEU:HB3	1:C:311:CYS:SG	2.44	0.56
2:D:428:ARG:NH1	2:D:429:VAL:HA	2.21	0.56
2:D:190:GLY:HA3	2:D:215:TYR:HA	1.88	0.56
2:D:218:MET:HG2	2:D:219:GLY:H	1.71	0.56
2:D:318:SER:OG	2:D:319:ASP:N	2.38	0.56
1:A:133:ALA:HB1	2:B:428:ARG:N	2.21	0.56
1:A:306:THR:HA	1:A:320:PRO:HA	1.88	0.56
2:D:442:TYR:HA	2:D:445:GLU:HB2	1.87	0.56
4:J:158:UNK:CB	4:J:197:UNK:CB	2.84	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:GLY:H	1:A:402:VAL:N	2.04	0.56
1:A:302:GLY:HA3	1:A:316:GLU:CD	2.26	0.56
2:B:422:GLN:HB3	2:B:425:ASP:HB2	1.88	0.56
1:C:44:ASN:OD1	2:D:439:SER:HA	2.05	0.56
1:C:381:THR:OG1	1:C:382:GLU:OE1	2.18	0.56
2:D:251:ASN:HD22	2:D:276:ILE:HD11	1.70	0.56
4:J:59:UNK:O	4:J:60:UNK:C	2.51	0.56
1:A:229:TYR:CE2	1:A:293:ALA:HA	2.40	0.56
1:A:396:VAL:CA	1:A:424:ILE:HB	2.35	0.56
2:B:352:ASP:OD1	2:B:352:ASP:N	2.38	0.56
2:B:438:ARG:HA	2:B:441:GLN:HG2	1.88	0.56
1:C:205:ARG:NE	1:C:215:LEU:O	2.38	0.56
2:D:429:VAL:HB	2:D:433:PHE:CE2	2.41	0.56
2:F:83:LYS:NZ	6:F:501:ADP:O1B	2.28	0.56
2:F:319:ASP:N	2:F:319:ASP:OD1	2.36	0.56
3:H:359:UNK:C	3:H:361:UNK:N	2.66	0.56
1:C:28:GLU:OE2	1:C:57:LYS:NZ	2.26	0.55
1:C:116:PHE:O	1:C:119:ALA:N	2.37	0.55
1:C:189:ASP:HB3	1:C:205:ARG:HA	1.87	0.55
2:D:312:LEU:O	2:D:315:ALA:N	2.38	0.55
1:E:190:VAL:HG11	1:E:224:PRO:HG2	1.88	0.55
1:E:219:GLU:O	1:E:221:VAL:N	2.36	0.55
1:E:402:THR:HG22	1:E:405:TYR:H	1.71	0.55
2:B:374:ARG:HH22	2:B:406:ILE:HB	1.71	0.55
1:C:125:LYS:HD2	1:C:233:GLU:HB3	1.88	0.55
2:D:146:GLN:HG3	2:D:148:ASP:H	1.71	0.55
1:E:156:HIS:HB2	1:E:171:LYS:HB3	1.88	0.55
5:K:123:GLN:C	5:K:127:PRO:N	2.54	0.55
1:A:237:THR:HG22	1:A:257:ILE:HG22	1.88	0.55
1:A:414:HIS:CG	1:A:415:ARG:N	2.75	0.55
2:B:130:ARG:HA	2:B:241:THR:HG22	1.88	0.55
1:C:24:LEU:HD21	1:C:34:GLN:HA	1.88	0.55
1:A:397:LEU:O	1:A:399:VAL:HG23	2.07	0.55
1:C:193:ILE:HB	1:C:200:VAL:HA	1.88	0.55
2:D:372:ARG:HG2	2:D:387:TYR:CE1	2.42	0.55
2:D:389:VAL:HG13	2:D:426:ILE:HD11	1.88	0.55
2:F:193:ILE:HG12	2:F:195:ILE:HG22	1.88	0.55
2:B:299:ASP:OD1	2:B:300:GLU:N	2.37	0.55
1:C:134:GLU:HG2	1:C:162:LYS:H	1.71	0.55
1:C:374:ILE:HA	1:C:377:ILE:HD12	1.88	0.55
1:C:393:HIS:N	1:C:427:LYS:HZ1	2.04	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:381:GLU:O	2:D:421:VAL:N	2.34	0.55
2:F:35:ASP:N	2:F:35:ASP:OD1	2.37	0.55
1:A:278:LEU:HD13	1:A:301:GLN:HB3	1.88	0.55
2:B:170:THR:HB	2:B:198:ALA:HA	1.88	0.55
1:C:51:VAL:CG2	2:D:404:GLN:HE21	2.19	0.55
1:C:248:ALA:HA	1:C:275:LEU:HD11	1.87	0.55
1:E:36:ALA:O	1:E:39:LEU:N	2.37	0.55
2:B:79:PRO:O	2:B:81:THR:N	2.39	0.55
2:D:141:GLU:HG2	2:D:191:ASP:O	2.07	0.55
2:D:448:ASP:HA	2:D:451:LEU:HG	1.87	0.55
1:A:227:GLU:HB2	1:A:293:ALA:HB2	1.88	0.55
1:A:278:LEU:HD21	1:A:289:ILE:HD12	1.87	0.55
1:A:149:VAL:HA	1:A:152:GLU:CD	2.28	0.55
2:B:309:PHE:O	2:B:313:ASN:ND2	2.39	0.55
1:C:452:ASP:N	1:C:452:ASP:OD1	2.38	0.55
2:D:283:TRP:O	2:D:288:LYS:HG2	2.06	0.55
1:E:49:CYS:O	1:E:53:VAL:HG23	2.07	0.55
1:E:373:GLN:O	1:E:377:ILE:N	2.35	0.55
1:A:111:GLN:HE22	1:A:502:ARG:HG3	1.72	0.55
2:F:306:ILE:HG23	2:F:336:ARG:O	2.07	0.55
5:K:292:LEU:HA	5:K:295:LEU:O	2.07	0.55
1:A:199:VAL:HA	1:A:206:LYS:HD2	1.89	0.54
2:D:284:ARG:HG3	2:D:285:GLU:OE2	2.07	0.54
1:A:237:THR:HG21	1:A:256:ILE:HD12	1.89	0.54
2:D:28:ILE:O	2:D:29:ARG:NE	2.40	0.54
3:H:602:UNK:O	3:H:605:UNK:CB	2.55	0.54
1:C:337:VAL:HA	1:C:345:THR:HA	1.90	0.54
2:D:182:LEU:HA	2:D:185:ASP:HB2	1.89	0.54
2:D:394:GLY:O	2:D:397:THR:N	2.38	0.54
3:H:278:UNK:CB	3:H:310:UNK:O	2.55	0.54
5:K:280:LYS:O	5:K:285:GLN:CB	2.55	0.54
1:A:203:GLU:HG3	2:F:311:PHE:CB	2.37	0.54
2:D:161:LEU:O	2:D:170:THR:HG23	2.08	0.54
5:K:170:PRO:O	5:K:173:TYR:CB	2.55	0.54
1:C:418:LYS:HA	1:C:418:LYS:HE2	1.90	0.54
2:D:386:ALA:HB2	2:D:422:GLN:C	2.27	0.54
1:A:232:GLU:OE2	1:A:260:LYS:NZ	2.41	0.54
1:C:52:ILE:HG13	1:C:358:VAL:HA	1.90	0.54
1:E:135:VAL:HG13	1:E:159:ILE:HG12	1.89	0.54
3:H:96:UNK:O	3:H:100:UNK:CB	2.55	0.54
3:H:496:UNK:O	3:H:498:UNK:N	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:416:ALA:O	1:A:417:LEU:HD22	2.07	0.54
1:C:157:VAL:HB	1:C:174:PRO:HG3	1.90	0.54
1:C:328:ILE:HG12	1:C:359:MET:SD	2.47	0.54
2:D:199:THR:OG1	2:D:233:GLN:NE2	2.41	0.54
2:F:194:THR:HB	2:F:212:ALA:HB3	1.89	0.54
3:H:273:UNK:O	3:H:306:UNK:CB	2.55	0.54
5:K:302:PRO:C	5:K:305:GLN:N	2.61	0.54
1:A:218:ILE:N	1:A:423:PRO:HD3	2.23	0.54
1:A:316:GLU:OE1	1:A:318:TYR:OH	2.13	0.54
1:C:161:LEU:HD11	1:C:170:LEU:HD22	1.89	0.54
2:D:140:GLY:HA2	2:D:231:GLU:O	2.07	0.54
2:D:172:TYR:HB3	2:D:197:LYS:HZ1	1.73	0.54
1:E:32:ALA:N	1:E:47:GLU:OE2	2.40	0.54
2:F:117:GLU:O	2:F:120:THR:OG1	2.25	0.54
5:K:77:ASP:O	5:K:80:PHE:N	2.41	0.54
1:A:124:LEU:HD12	1:A:125:ASP:O	2.07	0.54
2:B:157:LYS:HZ3	2:B:174:LEU:HB3	1.73	0.54
2:D:438:ARG:HA	2:D:442:TYR:CB	2.37	0.54
2:D:438:ARG:O	2:D:443:MET:HG2	2.08	0.54
1:A:171:GLY:HA2	1:A:431:ARG:H	1.72	0.54
1:C:52:ILE:HG13	1:C:357:ARG:O	2.08	0.54
1:C:77:THR:HG22	1:C:300:PHE:HE2	1.73	0.54
2:D:146:GLN:H	2:D:149:ARG:HH21	1.55	0.54
2:D:441:GLN:HA	2:D:444:LYS:HB2	1.90	0.54
1:E:77:THR:N	6:E:501:ADP:O1A	2.41	0.54
1:E:427:LYS:HG3	1:E:428:GLU:OE1	2.08	0.54
3:H:667:UNK:C	3:H:669:UNK:N	2.69	0.54
1:A:144:ARG:HG2	2:B:406:ILE:H	1.73	0.53
1:A:221:ARG:NH2	1:A:391:GLU:HB3	2.23	0.53
1:A:399:VAL:HG21	1:A:423:PRO:HG2	1.90	0.53
2:B:298:ILE:HG22	2:B:299:ASP:H	1.73	0.53
2:F:166:THR:HG23	2:F:229:ASP:HA	1.88	0.53
1:C:51:VAL:HB	1:C:357:ARG:HB3	1.89	0.53
2:D:61:GLU:HB3	1:E:415:LEU:HD23	1.90	0.53
2:D:139:GLU:HB2	2:D:234:LYS:HB2	1.91	0.53
3:H:452:UNK:O	3:H:455:UNK:N	2.42	0.53
1:A:124:LEU:HD21	1:A:144:ARG:HH12	1.72	0.53
1:A:164:VAL:HG21	1:A:454:ASP:HB3	1.90	0.53
1:E:232:LYS:HD2	1:E:234:ILE:HD11	1.89	0.53
2:F:124:ARG:HB3	2:F:245:HIS:HB2	1.89	0.53
2:F:145:ILE:HG22	2:F:147:ILE:HG23	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:416:ARG:NH1	2:F:418:GLY:HA3	2.23	0.53
2:F:439:SER:OG	2:F:440:THR:N	2.39	0.53
3:H:293:UNK:C	3:H:295:UNK:N	2.71	0.53
4:J:330:UNK:O	4:J:332:UNK:N	2.42	0.53
1:A:116:HIS:CE1	1:A:118:HIS:H	2.26	0.53
1:A:260:LYS:H	1:A:291:ILE:HD11	1.72	0.53
2:B:364:GLU:HA	2:B:395:LEU:HD11	1.90	0.53
2:B:413:CYS:HB2	2:B:418:GLY:O	2.08	0.53
1:A:231:GLY:O	1:A:260:LYS:HA	2.08	0.53
2:B:384:GLU:O	2:B:388:THR:HG23	2.09	0.53
1:C:129:GLU:HB3	1:C:229:HIS:NE2	2.24	0.53
2:D:319:ASP:N	2:D:319:ASP:OD1	2.40	0.53
1:E:207:ASP:OD1	1:E:207:ASP:N	2.41	0.53
2:F:124:ARG:NH1	2:F:273:ARG:HD2	2.22	0.53
1:A:166:LEU:HD13	1:A:456:VAL:HG23	1.90	0.53
2:B:275:GLN:O	2:B:279:LYS:N	2.38	0.53
1:C:159:ILE:HG21	1:C:172:LEU:HD22	1.91	0.53
1:C:348:HIS:HB2	1:C:350:ILE:HG13	1.90	0.53
2:D:182:LEU:HD11	2:D:195:ILE:HA	1.91	0.53
2:D:372:ARG:HG2	2:D:387:TYR:CZ	2.42	0.53
3:H:131:UNK:C	3:H:133:UNK:N	2.71	0.53
5:K:90:ALA:O	5:K:94:SER:N	2.41	0.53
1:A:166:LEU:HG	1:A:174:LYS:HD3	1.90	0.53
1:A:377:ILE:HA	1:A:380:VAL:HG22	1.91	0.53
2:D:279:LYS:O	2:D:283:TRP:HD1	1.90	0.53
2:D:389:VAL:HG23	2:D:392:ARG:HE	1.73	0.53
2:D:437:SER:HA	2:D:441:GLN:OE1	2.08	0.53
1:E:443:SER:OG	1:E:444:ALA:N	2.42	0.53
3:H:361:UNK:O	3:H:363:UNK:N	2.41	0.53
3:H:493:UNK:O	3:H:496:UNK:HA	2.09	0.53
1:A:189:VAL:HB	1:A:394:PRO:HG2	1.91	0.53
2:B:369:GLN:HA	2:B:372:ARG:CG	2.39	0.53
1:C:106:ILE:C	1:C:107:LYS:HE2	2.28	0.53
1:C:145:ASN:HD21	1:C:152:LYS:HB3	1.74	0.53
1:C:272:THR:OG1	1:C:274:LYS:NZ	2.35	0.53
2:D:151:ALA:N	2:D:179:ILE:HB	2.24	0.53
2:D:427:LYS:HA	2:D:430:TYR:HB2	1.91	0.53
2:F:146:GLN:HB3	2:F:183:THR:HG23	1.91	0.53
2:D:441:GLN:O	2:D:445:GLU:HG3	2.09	0.53
2:F:134:GLU:O	2:F:207:ARG:NH1	2.42	0.53
1:C:189:ASP:HB2	1:C:202:ARG:HD2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:205:ARG:HE	1:C:217:ALA:H	1.55	0.53
1:C:430:VAL:HA	1:C:433:ILE:HG22	1.90	0.53
1:E:188:GLY:HA3	1:E:208:THR:OG1	2.09	0.53
1:E:286:TYR:HB3	1:E:292:ALA:HB2	1.90	0.53
1:E:343:ASP:OD2	2:F:334:ARG:NH2	2.34	0.53
2:F:141:GLU:HA	2:F:192:VAL:HG22	1.91	0.53
4:J:199:UNK:O	4:J:202:UNK:N	2.42	0.53
1:A:111:GLN:HG3	1:A:428:ALA:O	2.09	0.52
1:A:204:ILE:HD13	2:F:311:PHE:CD1	2.43	0.52
1:C:61:MET:HB3	1:C:319:LEU:O	2.10	0.52
2:D:138:ILE:HG13	2:D:205:LEU:HG	1.91	0.52
1:E:356:ASP:OD1	1:E:357:ARG:N	2.42	0.52
2:F:29:ARG:H	2:F:44:GLN:HB3	1.75	0.52
2:F:384:GLU:O	2:F:388:THR:HG23	2.10	0.52
3:H:368:UNK:O	3:H:372:UNK:CB	2.57	0.52
1:A:122:LEU:HB3	2:B:409:ALA:C	2.30	0.52
1:A:131:LYS:HE3	2:B:413:CYS:HB2	1.89	0.52
1:A:168:GLY:O	1:A:446:HIS:HB2	2.08	0.52
1:A:190:PRO:CD	1:A:394:PRO:HG3	2.39	0.52
2:B:142:VAL:HA	2:B:163:LEU:HD13	1.90	0.52
1:C:343:ASP:OD1	1:C:344:ILE:HD12	2.09	0.52
3:H:453:UNK:C	3:H:455:UNK:N	2.71	0.52
1:A:195:VAL:HB	1:A:401:GLU:HA	1.92	0.52
2:B:397:THR:HG23	2:B:398:SER:H	1.73	0.52
2:D:216:ASP:HB3	2:D:229:ASP:OD1	2.10	0.52
2:D:272:VAL:O	2:D:275:GLN:HG3	2.09	0.52
2:D:440:THR:HG1	2:D:441:GLN:CD	2.11	0.52
1:E:139:THR:O	1:E:158:ILE:HG22	2.09	0.52
1:E:317:ARG:HH22	2:F:112:GLU:HB3	1.74	0.52
2:F:178:MET:HG3	2:F:211:ARG:HH21	1.75	0.52
1:A:231:GLY:H	1:A:260:LYS:CA	2.22	0.52
2:D:161:LEU:HB3	2:D:172:TYR:CE1	2.44	0.52
2:F:245:HIS:O	2:F:249:VAL:HG23	2.09	0.52
1:A:140:GLN:OE1	2:B:436:GLU:N	2.43	0.52
1:A:180:ALA:HB3	1:A:455:ARG:HG2	1.92	0.52
1:A:314:GLU:HB3	1:A:318:TYR:HE2	1.74	0.52
2:B:143:VAL:O	2:B:164:LYS:NZ	2.40	0.52
2:D:301:VAL:HG11	2:D:326:MET:HB3	1.92	0.52
1:A:144:ARG:NH1	2:B:406:ILE:C	2.63	0.52
1:A:179:LEU:HD21	1:A:183:GLN:HA	1.91	0.52
1:A:215:ARG:HH22	1:A:371:ASP:HA	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:370:GLU:O	1:C:374:ILE:HG12	2.10	0.52
2:D:148:ASP:HB3	2:D:178:MET:HG2	1.91	0.52
2:D:430:TYR:OH	2:D:438:ARG:NE	2.42	0.52
1:E:130:VAL:HB	1:E:230:LYS:HG2	1.92	0.52
2:F:148:ASP:HB2	2:F:179:ILE:HG12	1.90	0.52
4:J:162:UNK:O	4:J:165:UNK:CB	2.57	0.52
1:C:376:LYS:NZ	1:C:380:GLN:OE1	2.40	0.52
2:D:130:ARG:O	2:D:289:ALA:HA	2.09	0.52
2:D:145:ILE:HA	2:D:149:ARG:HH21	1.74	0.52
2:D:147:ILE:HG13	2:D:161:LEU:HD11	1.91	0.52
2:D:197:LYS:HD2	2:D:198:ALA:N	2.25	0.52
1:E:428:GLU:N	1:E:428:GLU:OE1	2.43	0.52
1:E:386:ILE:HG22	1:E:425:ILE:HB	1.92	0.52
1:C:396:GLU:O	1:C:400:LYS:N	2.32	0.52
1:E:129:GLU:HG2	1:E:194:GLU:HA	1.91	0.52
1:C:133:GLY:O	1:C:190:VAL:HA	2.09	0.52
1:C:138:LEU:HA	1:C:157:VAL:HG21	1.91	0.52
2:D:141:GLU:OE2	2:D:164:LYS:NZ	2.43	0.52
2:D:141:GLU:HB2	2:D:230:GLY:HA3	1.92	0.52
2:D:209:PHE:HA	2:D:211:ARG:CZ	2.40	0.52
2:D:437:SER:O	2:D:441:GLN:N	2.43	0.52
1:E:279:ILE:O	1:E:283:VAL:HG23	2.10	0.52
3:H:582:UNK:O	3:H:586:UNK:N	2.43	0.52
1:A:431:ARG:HD3	1:A:432:GLY:N	2.25	0.51
2:D:206:GLY:CA	2:D:235:ARG:HD3	2.40	0.51
2:D:280:VAL:O	2:D:284:ARG:HG2	2.10	0.51
2:D:383:SER:N	2:D:420:GLU:OE2	2.44	0.51
1:E:163:THR:HG22	1:E:164:ALA:N	2.25	0.51
3:H:470:UNK:O	3:H:473:UNK:CB	2.58	0.51
1:A:201:SER:HB2	2:F:309:PHE:CG	2.45	0.51
2:B:61:GLU:HB3	1:C:415:LEU:HD13	1.93	0.51
2:B:439:SER:HA	2:B:442:TYR:HB2	1.92	0.51
2:B:441:GLN:O	2:B:445:GLU:HG3	2.11	0.51
3:H:373:UNK:C	3:H:375:UNK:N	2.69	0.51
2:B:434:LEU:HD13	2:B:439:SER:HB3	1.92	0.51
2:D:179:ILE:O	2:D:183:THR:HG23	2.11	0.51
2:D:182:LEU:HD21	2:D:195:ILE:HG12	1.92	0.51
1:E:178:GLU:O	1:E:182:LYS:NZ	2.27	0.51
1:E:188:GLY:O	1:E:206:CYS:HB3	2.09	0.51
1:E:234:ILE:HG22	1:E:235:ILE:H	1.75	0.51
1:A:135:SER:O	1:A:144:ARG:NH2	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:LEU:N	1:A:452:LEU:O	2.44	0.51
2:B:388:THR:OG1	2:B:389:VAL:N	2.43	0.51
1:C:11:LYS:HE2	1:C:14:ARG:HD2	1.92	0.51
1:E:128:LYS:NZ	1:E:234:ILE:HB	2.26	0.51
1:E:185:VAL:HG12	1:E:189:ASP:OD1	2.10	0.51
2:F:195:ILE:HG12	2:F:205:LEU:HD12	1.92	0.51
3:H:538:UNK:C	3:H:540:UNK:N	2.66	0.51
4:J:195:UNK:O	4:J:198:UNK:CB	2.59	0.51
1:A:127:SER:O	1:A:127:SER:OG	2.24	0.51
1:A:203:GLU:OE2	2:F:312:LEU:N	2.43	0.51
2:B:362:TYR:OH	6:B:501:ADP:C6	2.61	0.51
1:C:17:SER:HA	1:C:378:ARG:HH22	1.74	0.51
2:F:166:THR:HG22	2:F:226:GLN:HE22	1.75	0.51
1:C:378:ARG:HA	1:C:381:THR:OG1	2.11	0.51
2:D:429:VAL:O	2:D:433:PHE:N	2.44	0.51
1:A:132:GLN:HG2	2:B:425:ASP:CA	2.40	0.51
2:B:129:VAL:HA	2:B:291:ILE:HA	1.92	0.51
2:B:382:MET:HG3	2:B:383:SER:H	1.76	0.51
2:D:182:LEU:HD21	2:D:195:ILE:HA	1.93	0.51
4:J:369:UNK:C	4:J:371:UNK:N	2.69	0.51
1:A:123:GLY:N	2:B:411:LEU:H	2.08	0.51
2:B:43:SER:H	2:B:46:MET:HG2	1.76	0.51
1:C:427:LYS:HB3	1:C:431:GLU:OE1	2.10	0.51
2:D:63:ILE:HG12	2:D:68:ILE:HD13	1.93	0.51
2:D:181:SER:O	2:D:185:ASP:N	2.44	0.51
2:D:439:SER:O	2:D:443:MET:HB2	2.10	0.51
1:E:27:ASP:OD1	1:E:31:LEU:N	2.44	0.51
1:E:302:ASP:OD1	1:E:303:GLU:N	2.43	0.51
2:F:385:ASP:O	2:F:388:THR:OG1	2.18	0.51
5:K:249:PRO:O	5:K:253:MET:N	2.44	0.51
1:A:232:GLU:HA	1:A:260:LYS:HD3	1.92	0.51
1:A:520:LYS:NZ	1:A:526:GLU:OE2	2.43	0.51
2:B:400:ARG:HD3	6:B:501:ADP:O1B	2.11	0.51
2:B:123:PHE:O	2:B:126:SER:OG	2.21	0.51
2:B:369:GLN:HA	2:B:372:ARG:HG2	1.92	0.51
2:B:380:VAL:HG12	2:B:381:GLU:H	1.75	0.51
2:D:172:TYR:HE2	2:D:174:LEU:HD13	1.76	0.51
2:F:282:GLU:HA	2:F:285:GLU:HB3	1.92	0.51
3:H:235:UNK:O	3:H:239:UNK:N	2.44	0.51
1:A:221:ARG:HD2	1:A:222:ILE:N	2.25	0.50
1:A:492:LEU:HD13	1:A:528:VAL:HG21	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:42:GLN:O	1:C:45:ALA:HB3	2.10	0.50
1:C:49:CYS:HB2	1:C:359:MET:HG3	1.93	0.50
1:E:10:THR:OG1	1:E:11:LYS:N	2.43	0.50
1:E:190:VAL:O	1:E:204:GLY:HA3	2.11	0.50
1:E:247:ASN:O	1:E:269:THR:N	2.44	0.50
1:E:341:THR:HA	2:F:336:ARG:HH21	1.76	0.50
2:F:286:GLU:OE2	2:F:288:LYS:HE3	2.11	0.50
2:B:132:LYS:HG3	2:B:239:VAL:HG12	1.92	0.50
2:B:236:LYS:NZ	2:B:238:VAL:HA	2.26	0.50
2:B:319:ASP:OD1	2:B:319:ASP:N	2.45	0.50
2:B:348:ILE:O	2:B:351:LEU:N	2.44	0.50
1:C:185:VAL:HG21	1:C:202:ARG:HE	1.77	0.50
1:E:93:PHE:CD2	1:E:95:PRO:HD3	2.46	0.50
1:E:129:GLU:OE2	1:E:196:ASN:N	2.44	0.50
1:E:423:ASP:OD1	1:E:423:ASP:N	2.41	0.50
1:E:426:GLU:HG3	1:E:429:HIS:ND1	2.27	0.50
1:A:170:PRO:HG2	2:B:443:MET:HB3	1.94	0.50
1:A:499:THR:OG1	1:A:500:THR:N	2.44	0.50
2:B:50:LEU:O	2:B:53:ARG:N	2.44	0.50
2:B:243:SER:OG	2:B:246:GLU:N	2.31	0.50
3:H:85:UNK:O	3:H:90:UNK:N	2.44	0.50
5:K:301:THR:O	5:K:305:GLN:CB	2.59	0.50
1:A:201:SER:HB2	2:F:309:PHE:CB	2.39	0.50
1:A:203:GLU:H	2:F:308:SER:C	2.15	0.50
2:B:151:ALA:HA	2:B:179:ILE:HG13	1.94	0.50
1:C:56:ILE:HG12	1:C:324:ALA:HB3	1.92	0.50
2:D:81:THR:O	2:D:400:ARG:NH1	2.45	0.50
2:F:231:GLU:CD	2:F:232:LEU:H	2.15	0.50
2:F:424:ASP:OD1	2:F:424:ASP:N	2.43	0.50
4:J:217:UNK:HA	4:J:220:UNK:CB	2.41	0.50
1:A:162:ARG:O	1:A:417:LEU:HD23	2.11	0.50
1:A:487:GLU:HG2	1:A:525:LYS:HB2	1.93	0.50
2:B:381:GLU:HG3	2:B:382:MET:H	1.76	0.50
1:C:52:ILE:O	1:C:55:LEU:HB2	2.12	0.50
1:C:61:MET:HB3	1:C:320:GLU:HA	1.94	0.50
2:D:397:THR:CG2	2:D:436:GLU:H	2.24	0.50
3:H:59:UNK:O	3:H:60:UNK:CB	2.60	0.50
3:H:125:UNK:CB	3:H:163:UNK:N	2.75	0.50
5:K:120:GLN:HA	5:K:123:GLN:CB	2.42	0.50
5:K:249:PRO:O	5:K:253:MET:CB	2.60	0.50
1:A:166:LEU:CD2	1:A:456:VAL:HB	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:145:ILE:HG23	2:B:147:ILE:HG23	1.93	0.50
2:B:161:LEU:HB3	2:B:172:TYR:CZ	2.47	0.50
1:C:192:TYR:OH	1:C:230:LYS:HD2	2.12	0.50
1:C:285:LYS:HG2	1:C:289:GLN:NE2	2.27	0.50
1:E:280:ASN:O	1:E:284:ASN:N	2.32	0.50
2:B:32:GLY:HA3	2:B:46:MET:SD	2.52	0.50
1:C:46:ARG:O	1:C:49:CYS:HB3	2.12	0.50
2:D:112:GLU:N	2:D:112:GLU:OE2	2.45	0.50
2:D:393:ILE:HG23	2:D:435:ASP:CG	2.32	0.50
1:A:161:GLY:O	1:A:414:HIS:HB2	2.12	0.49
1:C:126:GLU:HB2	1:C:128:LYS:HZ2	1.75	0.49
2:D:192:VAL:N	2:D:216:ASP:OD1	2.45	0.49
2:D:280:VAL:HA	2:D:283:TRP:HB2	1.92	0.49
2:F:282:GLU:O	2:F:286:GLU:N	2.28	0.49
1:A:132:GLN:CG	2:B:425:ASP:O	2.60	0.49
1:A:190:PRO:HG3	1:A:394:PRO:HG3	1.94	0.49
1:A:472:ILE:HG23	1:A:473:ILE:HD12	1.94	0.49
1:C:133:GLY:HA3	1:C:161:LEU:HB3	1.94	0.49
1:C:389:GLU:OE1	1:C:427:LYS:HG3	2.11	0.49
2:D:146:GLN:HE21	2:D:195:ILE:HG22	1.76	0.49
2:D:170:THR:HG21	2:D:198:ALA:HA	1.94	0.49
1:E:418:LYS:HE2	1:E:418:LYS:HA	1.94	0.49
2:F:428:ARG:O	2:F:431:SER:OG	2.13	0.49
3:H:466:UNK:CB	3:H:507:UNK:HA	2.42	0.49
2:B:378:GLU:N	2:B:378:GLU:OE2	2.45	0.49
1:C:390:ALA:HB2	1:C:426:GLU:HA	1.94	0.49
2:D:149:ARG:HA	2:D:182:LEU:HB2	1.95	0.49
2:D:389:VAL:HG11	2:D:423:VAL:HG13	1.94	0.49
3:H:650:UNK:HA	3:H:653:UNK:CB	2.42	0.49
1:A:148:GLY:O	1:A:151:VAL:HG22	2.12	0.49
1:A:231:GLY:H	1:A:261:THR:N	2.10	0.49
1:A:397:LEU:HB3	1:A:423:PRO:CB	2.40	0.49
2:B:290:GLU:OE1	2:B:290:GLU:N	2.46	0.49
2:B:304:LEU:O	2:B:336:ARG:HB2	2.11	0.49
2:D:199:THR:HG1	2:D:233:GLN:HE22	1.60	0.49
2:D:447:GLN:HB3	2:D:451:LEU:HD23	1.93	0.49
2:F:207:ARG:HE	2:F:235:ARG:HH21	1.59	0.49
2:B:380:VAL:HG12	2:B:381:GLU:N	2.27	0.49
1:C:67:LEU:HD23	2:D:440:THR:CG2	2.41	0.49
1:C:386:ILE:HD11	1:C:391:LEU:HB2	1.93	0.49
1:C:390:ALA:HA	1:C:427:LYS:HG2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:310:GLU:HB3	2:F:111:LEU:HD21	1.93	0.49
2:F:41:GLN:NE2	2:F:41:GLN:O	2.45	0.49
2:F:84:THR:N	6:F:501:ADP:O2A	2.45	0.49
2:B:186:LYS:NZ	2:B:188:GLN:OE1	2.31	0.49
1:C:26:LEU:HA	1:C:31:LEU:C	2.33	0.49
1:C:271:ILE:HG12	1:C:275:LEU:HD13	1.95	0.49
1:E:177:PHE:O	1:E:181:GLN:HB2	2.13	0.49
5:K:124:GLN:O	5:K:128:GLY:N	2.37	0.49
5:K:159:ARG:O	5:K:163:GLU:N	2.42	0.49
5:K:341:THR:CB	5:K:342:PRO:CD	2.90	0.49
1:A:115:SER:OG	1:A:460:ARG:HG3	2.12	0.49
1:A:183:GLN:NE2	1:A:183:GLN:O	2.46	0.49
1:A:207:THR:O	1:A:210:LEU:HB2	2.12	0.49
1:A:210:LEU:HD22	1:A:214:PHE:CE1	2.47	0.49
1:A:232:GLU:CD	1:A:260:LYS:HZ3	2.16	0.49
1:A:314:GLU:HB3	1:A:318:TYR:CE2	2.48	0.49
1:A:412:TYR:C	1:A:414:HIS:H	2.16	0.49
1:C:367:THR:O	1:C:370:GLU:HG2	2.13	0.49
1:C:443:SER:OG	1:C:444:ALA:N	2.46	0.49
2:D:236:LYS:HE3	2:D:238:VAL:HA	1.94	0.49
1:A:115:SER:HB2	1:A:460:ARG:O	2.13	0.49
1:A:216:ARG:NH2	1:A:397:LEU:HD21	2.28	0.49
2:B:27:HIS:CD2	2:B:45:GLY:HA3	2.48	0.49
2:B:59:VAL:O	2:B:63:ILE:HG12	2.12	0.49
1:C:317:ARG:HH11	1:C:318:ALA:HB2	1.78	0.49
1:C:361:ILE:O	1:C:361:ILE:HG13	2.13	0.49
2:D:73:VAL:CG1	2:D:325:ILE:HG22	2.42	0.49
1:A:111:GLN:HG2	1:A:428:ALA:HB3	1.94	0.49
1:A:150:ILE:O	1:A:154:ILE:HG12	2.13	0.49
1:A:203:GLU:C	2:F:308:SER:HB2	2.32	0.49
1:A:208:GLU:OE1	1:A:208:GLU:N	2.28	0.49
1:A:399:VAL:O	1:A:425:VAL:HG21	2.13	0.49
1:A:525:LYS:O	1:A:529:GLU:HG2	2.11	0.49
1:C:219:GLU:O	1:C:221:VAL:N	2.39	0.49
1:C:363:THR:HG23	1:C:364:MET:O	2.13	0.49
2:F:271:GLU:H	2:F:271:GLU:CD	2.16	0.49
1:A:122:LEU:O	1:A:135:SER:HA	2.13	0.49
1:C:122:LEU:HA	1:C:293:GLU:O	2.13	0.49
1:C:426:GLU:OE1	1:C:426:GLU:N	2.45	0.49
2:D:110:SER:OG	2:D:113:MET:N	2.46	0.49
2:F:43:SER:O	2:F:46:MET:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:149:ARG:HB2	2:F:150:PRO:HD3	1.95	0.49
2:F:283:TRP:HA	2:F:286:GLU:OE2	2.13	0.49
3:H:510:UNK:O	3:H:513:UNK:CB	2.60	0.49
1:A:218:ILE:HB	1:A:338:LEU:HB3	1.94	0.48
1:C:27:ASP:HB3	1:C:30:GLY:H	1.78	0.48
1:C:187:ALA:O	1:C:212:GLU:HB2	2.13	0.48
1:A:142:ASN:H	1:A:142:ASN:ND2	2.10	0.48
1:A:256:ILE:HG13	1:A:268:LEU:O	2.13	0.48
1:C:134:GLU:OE1	1:C:209:TYR:HB2	2.12	0.48
2:D:130:ARG:NH2	2:D:242:VAL:HG21	2.26	0.48
2:D:311:PHE:HD2	2:D:312:LEU:HD23	1.78	0.48
1:A:166:LEU:O	1:A:450:LEU:HA	2.13	0.48
1:A:226:LYS:HE3	1:A:293:ALA:HB3	1.95	0.48
2:B:105:GLY:N	2:B:300:GLU:OE2	2.46	0.48
1:C:70:GLY:O	2:D:447:GLN:OE1	2.31	0.48
1:C:128:LYS:O	1:C:231:LYS:HA	2.13	0.48
1:C:134:GLU:OE1	1:C:208:THR:OG1	2.30	0.48
2:D:316:LEU:HD21	2:D:353:ARG:HH22	1.78	0.48
1:E:127:THR:OG1	1:E:233:GLU:OE1	2.30	0.48
1:E:406:SER:O	1:E:406:SER:OG	2.31	0.48
4:J:140:UNK:O	4:J:144:UNK:N	2.46	0.48
1:A:135:SER:H	2:B:412:VAL:HG11	1.77	0.48
2:B:39:PRO:HG2	2:B:50:LEU:HD23	1.95	0.48
1:C:124:ILE:O	1:C:235:ILE:HG13	2.14	0.48
2:D:102:ALA:HA	2:D:297:PHE:O	2.13	0.48
1:E:24:LEU:O	1:E:46:ARG:NH2	2.35	0.48
1:E:181:GLN:NE2	1:E:185:VAL:O	2.47	0.48
5:K:77:ASP:C	5:K:80:PHE:H	2.16	0.48
1:A:465:THR:HG23	1:A:468:GLU:H	1.77	0.48
1:A:546:ALA:HA	1:A:549:GLN:HB3	1.95	0.48
2:B:124:ARG:HH21	2:B:244:LEU:HB3	1.79	0.48
2:B:195:ILE:HD12	2:B:206:GLY:HA2	1.95	0.48
2:B:427:LYS:O	2:B:431:SER:HB3	2.13	0.48
1:C:69:ALA:HA	1:C:348:HIS:CE1	2.49	0.48
3:H:97:UNK:O	3:H:101:UNK:N	2.47	0.48
4:J:217:UNK:O	4:J:220:UNK:CA	2.61	0.48
1:A:133:ALA:C	2:B:428:ARG:HB3	2.33	0.48
1:A:218:ILE:H	1:A:423:PRO:HD3	1.77	0.48
2:B:35:ASP:OD2	2:B:35:ASP:N	2.46	0.48
2:B:43:SER:O	2:B:46:MET:HG2	2.14	0.48
2:B:181:SER:OG	2:B:211:ARG:NE	2.37	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:416:ARG:HH12	2:B:422:GLN:HE21	1.61	0.48
1:C:40:VAL:HG12	1:C:41:GLY:N	2.28	0.48
2:D:61:GLU:OE1	1:E:415:LEU:HD23	2.13	0.48
2:D:390:LEU:HD13	2:D:426:ILE:HD12	1.96	0.48
2:D:440:THR:O	2:D:444:LYS:HG2	2.13	0.48
1:E:137:GLU:OE1	1:E:137:GLU:N	2.46	0.48
3:H:88:UNK:HA	3:H:91:UNK:CB	2.44	0.48
3:H:176:UNK:CB	3:H:226:UNK:O	2.61	0.48
1:A:153:LEU:HB3	1:A:159:MET:SD	2.53	0.48
2:B:24:ALA:N	2:B:403:ILE:HG21	2.28	0.48
2:B:417:LYS:HD2	2:B:417:LYS:HA	1.70	0.48
1:C:66:VAL:HG22	1:C:67:LEU:N	2.28	0.48
1:C:123:ARG:CB	1:C:293:GLU:HB3	2.42	0.48
3:H:637:UNK:O	3:H:640:UNK:CA	2.62	0.48
1:A:207:THR:O	1:A:211:MET:HG2	2.14	0.48
2:B:134:GLU:O	2:B:207:ARG:NH1	2.47	0.48
2:B:185:ASP:OD2	2:B:187:VAL:HB	2.13	0.48
1:C:189:ASP:OD1	1:C:205:ARG:HG3	2.13	0.48
2:D:81:THR:CB	6:D:501:ADP:HO3'	2.27	0.48
2:D:218:MET:HG2	2:D:219:GLY:N	2.29	0.48
1:E:132:GLU:HG2	1:E:190:VAL:HG23	1.95	0.48
5:K:31:THR:O	5:K:34:SER:CB	2.62	0.48
2:B:159:GLY:HA3	2:B:174:LEU:HB2	1.95	0.48
2:B:161:LEU:HD12	2:B:174:LEU:HD11	1.94	0.48
1:E:431:GLU:O	1:E:435:GLU:HG2	2.14	0.48
3:H:444:UNK:O	3:H:447:UNK:N	2.47	0.48
1:A:133:ALA:CB	2:B:429:VAL:H	2.17	0.48
1:A:144:ARG:HH11	2:B:406:ILE:C	2.16	0.48
1:A:203:GLU:N	2:F:308:SER:OG	2.47	0.48
1:A:211:MET:HA	1:A:214:PHE:CD2	2.49	0.48
1:A:491:HIS:O	1:A:494:GLU:HG2	2.13	0.48
2:B:272:VAL:O	2:B:276:ILE:HG13	2.14	0.48
2:B:339:SER:O	2:B:339:SER:OG	2.25	0.48
5:K:103:LEU:O	5:K:105:ALA:N	2.47	0.48
2:D:126:SER:O	2:D:126:SER:OG	2.21	0.47
2:D:351:LEU:HD23	2:D:354:LEU:HD12	1.96	0.47
2:D:390:LEU:O	2:D:393:ILE:HB	2.13	0.47
1:E:283:VAL:O	1:E:287:ILE:HD12	2.14	0.47
1:A:169:PRO:HD2	1:A:458:ILE:HD12	1.96	0.47
1:A:191:PHE:CE2	1:A:424:ILE:HG23	2.49	0.47
1:A:205:LYS:HG2	1:A:206:LYS:N	2.26	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:372:ARG:HD2	2:B:381:GLU:OE1	2.14	0.47
2:B:400:ARG:CZ	6:B:501:ADP:O3A	2.61	0.47
1:C:122:LEU:O	1:C:237:ASP:HA	2.14	0.47
1:A:196:GLY:N	1:A:403:HIS:H	2.12	0.47
2:B:138:ILE:HD11	2:B:205:LEU:HD22	1.96	0.47
2:B:142:VAL:HG22	2:B:163:LEU:HD13	1.95	0.47
2:B:149:ARG:HH21	2:B:186:LYS:HD3	1.79	0.47
2:B:201:LYS:HG3	2:B:202:ILE:H	1.80	0.47
1:C:64:ARG:NH2	1:C:357:ARG:HH21	2.11	0.47
2:D:124:ARG:NH2	2:D:273:ARG:HD2	2.29	0.47
2:D:152:THR:H	2:D:157:LYS:HD2	1.80	0.47
2:D:172:TYR:HA	2:D:201:LYS:O	2.15	0.47
1:E:40:VAL:N	6:E:501:ADP:HN62	2.03	0.47
1:E:184:ARG:NH2	1:E:217:ALA:O	2.46	0.47
2:F:34:ASP:OD2	2:F:38:GLU:HB2	2.14	0.47
4:J:217:UNK:C	4:J:220:UNK:N	2.77	0.47
5:K:77:ASP:O	5:K:80:PHE:CA	2.63	0.47
1:A:142:ASN:OD1	2:B:400:ARG:N	2.46	0.47
1:A:204:ILE:HG23	2:F:119:LEU:HD12	1.96	0.47
1:A:266:LYS:HD3	1:A:326:VAL:HG22	1.97	0.47
1:A:275:PHE:N	1:A:296:GLY:H	1.97	0.47
2:B:146:GLN:NE2	2:B:187:VAL:H	2.12	0.47
2:B:400:ARG:NH2	6:B:501:ADP:PA	2.87	0.47
2:D:138:ILE:HG22	2:D:139:GLU:N	2.29	0.47
2:F:202:ILE:HG13	2:F:202:ILE:O	2.15	0.47
1:A:133:ALA:HA	2:B:429:VAL:HG23	1.95	0.47
1:A:170:PRO:HB3	1:A:432:GLY:C	2.35	0.47
1:A:170:PRO:HB3	1:A:433:ASN:N	2.29	0.47
1:A:196:GLY:HA2	1:A:403:HIS:HB3	1.97	0.47
1:A:203:GLU:HB3	2:F:312:LEU:HG	1.95	0.47
2:B:161:LEU:HB2	2:B:174:LEU:HG	1.96	0.47
2:B:373:ILE:HG23	2:B:379:ASP:CG	2.34	0.47
2:B:383:SER:CB	2:B:423:VAL:HA	2.44	0.47
2:B:397:THR:HG23	2:B:398:SER:N	2.29	0.47
2:D:77:GLY:HA2	6:D:501:ADP:PB	2.54	0.47
1:E:135:VAL:HG22	1:E:159:ILE:HD13	1.95	0.47
1:E:285:LYS:HA	1:E:288:ASP:OD2	2.14	0.47
2:F:138:ILE:HD12	2:F:233:GLN:HA	1.96	0.47
3:H:362:UNK:O	3:H:366:UNK:N	2.47	0.47
4:J:319:UNK:HA	4:J:322:UNK:CB	2.45	0.47
2:B:136:GLU:OE1	2:B:235:ARG:NH1	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:393:ILE:O	2:B:397:THR:HG22	2.15	0.47
1:C:112:LEU:HD23	1:C:112:LEU:HA	1.67	0.47
2:D:139:GLU:HB3	2:D:231:GLU:OE1	2.14	0.47
2:D:170:THR:CG2	2:D:198:ALA:HA	2.45	0.47
2:D:380:VAL:HG21	2:D:406:ILE:HD11	1.97	0.47
1:A:120:LYS:O	1:A:183:GLN:HG2	2.15	0.47
1:A:282:ARG:NH2	1:A:303:ARG:HB3	2.29	0.47
2:B:141:GLU:O	2:B:165:THR:OG1	2.18	0.47
2:B:383:SER:OG	2:B:421:VAL:HG13	2.15	0.47
1:C:26:LEU:HD21	1:C:46:ARG:CZ	2.44	0.47
2:D:142:VAL:HG21	2:D:163:LEU:HD12	1.95	0.47
2:D:279:LYS:O	2:D:282:GLU:HG3	2.14	0.47
2:D:368:LYS:NZ	2:D:388:THR:HA	2.30	0.47
2:D:428:ARG:NH1	2:D:431:SER:OG	2.48	0.47
1:E:14:ARG:NH1	1:E:95:PRO:O	2.48	0.47
3:H:369:UNK:O	3:H:373:UNK:CA	2.61	0.47
4:J:196:UNK:O	4:J:199:UNK:CB	2.63	0.47
4:J:218:UNK:O	4:J:221:UNK:N	2.48	0.47
5:K:76:ALA:O	5:K:79:ALA:HB3	2.15	0.47
5:K:192:LEU:C	5:K:194:GLY:H	2.18	0.47
1:A:116:HIS:CG	1:A:117:SER:N	2.83	0.47
1:A:144:ARG:HD2	2:B:407:THR:N	2.28	0.47
1:A:256:ILE:HD11	1:A:269:LYS:HB3	1.97	0.47
1:A:408:GLU:O	1:A:411:THR:OG1	2.33	0.47
1:A:453:LEU:HB3	1:A:456:VAL:HG21	1.96	0.47
1:A:470:LYS:HA	1:A:474:LYS:CB	2.35	0.47
1:A:543:LYS:O	1:A:547:ASP:N	2.33	0.47
1:C:26:LEU:HG	1:C:31:LEU:HA	1.96	0.47
1:C:77:THR:HG22	1:C:300:PHE:CE2	2.49	0.47
2:D:384:GLU:HA	2:D:387:TYR:HD2	1.80	0.47
1:E:417:ALA:HB1	1:E:422:LYS:HB2	1.97	0.47
2:F:130:ARG:HE	2:F:290:GLU:HB3	1.80	0.47
4:J:457:UNK:O	4:J:460:UNK:CB	2.62	0.47
5:K:77:ASP:O	5:K:80:PHE:C	2.52	0.47
1:A:138:VAL:HG21	2:B:432:LEU:H	1.79	0.47
1:A:144:ARG:CD	2:B:407:THR:H	2.26	0.47
2:B:120:THR:O	2:B:124:ARG:HG2	2.15	0.47
2:B:136:GLU:HG3	2:B:233:GLN:NE2	2.30	0.47
2:B:382:MET:HE3	2:B:421:VAL:HG13	1.97	0.47
1:C:130:VAL:HA	1:C:193:ILE:O	2.15	0.47
1:C:185:VAL:HG12	1:C:205:ARG:NH1	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:240:LEU:O	1:C:243:LEU:HG	2.15	0.47
1:E:157:VAL:HG12	1:E:159:ILE:HG13	1.97	0.47
1:E:180:LEU:HD12	1:E:202:ARG:H	1.80	0.47
2:F:383:SER:N	2:F:420:GLU:OE2	2.48	0.47
4:J:352:UNK:O	4:J:355:UNK:N	2.47	0.47
2:B:157:LYS:NZ	2:B:174:LEU:HB3	2.29	0.47
2:B:443:MET:O	2:B:447:GLN:N	2.46	0.47
1:C:236:GLN:NE2	1:C:237:ASP:O	2.48	0.47
1:C:236:GLN:OE1	1:C:238:VAL:HG13	2.14	0.47
1:C:403:LEU:HD12	1:C:403:LEU:HA	1.74	0.47
2:D:207:ARG:HG3	2:D:235:ARG:HD2	1.96	0.47
2:D:383:SER:OG	2:D:422:GLN:HA	2.15	0.47
2:F:310:SER:O	2:F:314:ARG:NE	2.40	0.47
1:A:124:LEU:HD23	1:A:135:SER:CB	2.45	0.46
2:B:334:ARG:NH1	2:B:338:THR:O	2.47	0.46
1:C:55:LEU:HD11	1:C:354:LEU:CD1	2.45	0.46
1:C:138:LEU:HD12	1:C:174:PRO:HA	1.97	0.46
2:D:434:LEU:CD1	2:D:438:ARG:HB3	2.42	0.46
1:E:205:ARG:HB3	1:E:212:GLU:OE2	2.15	0.46
2:F:389:VAL:HG11	2:F:423:VAL:HG23	1.97	0.46
2:F:424:ASP:HA	2:F:427:LYS:HB2	1.97	0.46
2:F:134:GLU:HG3	2:F:237:GLU:HA	1.97	0.46
4:J:196:UNK:O	4:J:199:UNK:N	2.49	0.46
1:A:109:LYS:HZ2	1:A:428:ALA:H	1.62	0.46
1:A:402:VAL:O	1:A:402:VAL:HG12	2.15	0.46
2:B:154:THR:HA	2:B:176:THR:HG23	1.97	0.46
2:B:374:ARG:HH12	2:B:405:LEU:N	2.14	0.46
1:C:17:SER:C	1:C:378:ARG:HH12	2.16	0.46
1:C:190:VAL:O	1:C:202:ARG:HG3	2.15	0.46
2:D:158:VAL:HG21	2:D:172:TYR:CE2	2.50	0.46
2:D:440:THR:O	2:D:444:LYS:N	2.28	0.46
1:E:132:GLU:O	1:E:166:GLY:HA3	2.15	0.46
3:H:216:UNK:C	3:H:218:UNK:N	2.76	0.46
4:J:327:UNK:HA	4:J:331:GLY:N	2.30	0.46
1:A:133:ALA:CB	2:B:427:LYS:H	2.14	0.46
1:A:191:PHE:CD2	1:A:424:ILE:HG23	2.50	0.46
1:A:414:HIS:CG	1:A:415:ARG:H	2.32	0.46
1:A:466:PRO:HB2	1:A:467:GLN:NE2	2.31	0.46
1:C:177:PHE:O	1:C:181:GLN:HB3	2.14	0.46
2:D:84:THR:HG22	2:D:297:PHE:CE2	2.48	0.46
2:D:188:GLN:HE22	2:D:213:ARG:C	2.19	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:299:ASP:OD1	2:D:299:ASP:N	2.45	0.46
1:E:214:ASP:OD1	1:E:215:LEU:N	2.46	0.46
3:H:125:UNK:HA	3:H:163:UNK:CA	2.46	0.46
3:H:602:UNK:HA	3:H:605:UNK:CB	2.46	0.46
4:J:323:UNK:HA	4:J:326:UNK:CB	2.44	0.46
2:B:80:GLY:O	2:B:82:GLY:N	2.49	0.46
2:B:84:THR:OG1	6:B:501:ADP:O1A	2.28	0.46
2:B:142:VAL:HG13	2:B:163:LEU:HB2	1.96	0.46
2:B:432:LEU:HD23	2:B:433:PHE:CE2	2.50	0.46
2:B:443:MET:HA	2:B:446:TYR:HB3	1.97	0.46
1:C:6:VAL:HG12	1:C:7:LYS:H	1.81	0.46
1:C:45:ALA:HA	1:C:68:LEU:HD21	1.97	0.46
2:D:168:MET:HG3	2:D:169:GLU:O	2.16	0.46
1:E:128:LYS:O	1:E:231:LYS:HA	2.16	0.46
2:F:140:GLY:O	2:F:142:VAL:HG23	2.15	0.46
2:F:329:ASN:OD1	2:F:329:ASN:N	2.46	0.46
1:A:165:LEU:O	1:A:453:LEU:HD23	2.16	0.46
1:A:466:PRO:HB2	1:A:467:GLN:HE22	1.79	0.46
2:B:374:ARG:NH1	2:B:405:LEU:H	2.13	0.46
1:C:205:ARG:NE	1:C:217:ALA:H	2.14	0.46
2:F:373:ILE:O	2:F:377:GLU:N	2.37	0.46
4:J:472:UNK:C	4:J:474:UNK:N	2.76	0.46
5:K:170:PRO:CA	5:K:173:TYR:CB	2.91	0.46
1:A:132:GLN:HB2	2:B:422:GLN:O	2.16	0.46
1:A:141:GLU:OE2	1:A:144:ARG:CZ	2.63	0.46
1:A:149:VAL:O	1:A:153:LEU:HG	2.15	0.46
1:A:418:GLU:O	1:A:420:SER:N	2.45	0.46
2:B:247:ILE:HD12	2:B:247:ILE:HA	1.83	0.46
2:F:349:ASP:OD1	2:F:349:ASP:N	2.46	0.46
5:K:85:GLU:O	5:K:88:GLU:CB	2.63	0.46
1:A:150:ILE:HG12	1:A:455:ARG:HH21	1.81	0.46
1:A:341:LEU:HB3	1:A:377:ILE:HD13	1.98	0.46
1:A:466:PRO:HA	1:A:469:MET:SD	2.56	0.46
2:D:397:THR:OG1	2:D:435:ASP:HB3	2.16	0.46
2:F:411:LEU:O	2:F:415:LYS:N	2.43	0.46
1:A:109:LYS:HZ2	1:A:428:ALA:N	2.13	0.46
1:A:275:PHE:H	1:A:296:GLY:N	1.97	0.46
1:A:417:LEU:HD13	1:A:417:LEU:HA	1.81	0.46
2:B:31:LEU:O	2:B:53:ARG:NH2	2.42	0.46
2:B:146:GLN:OE1	2:B:187:VAL:N	2.49	0.46
1:C:51:VAL:HG21	2:D:404:GLN:HG2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:377:ILE:HA	1:C:380:GLN:NE2	2.31	0.46
2:D:146:GLN:H	2:D:149:ARG:NH2	2.14	0.46
2:F:139:GLU:H	2:F:234:LYS:NZ	2.13	0.46
2:F:388:THR:OG1	2:F:389:VAL:N	2.49	0.46
3:H:97:UNK:O	3:H:101:UNK:CB	2.64	0.46
3:H:443:UNK:O	3:H:447:UNK:N	2.48	0.46
1:A:162:ARG:NH2	1:A:418:GLU:HB3	2.17	0.46
1:A:191:PHE:CG	1:A:427:PHE:HZ	2.33	0.46
1:A:201:SER:CB	2:F:309:PHE:HB2	2.43	0.46
1:A:380:VAL:HA	1:A:383:LYS:HD3	1.97	0.46
1:A:425:VAL:HG22	1:A:426:ILE:N	2.31	0.46
2:B:373:ILE:HB	2:B:403:ILE:HG13	1.98	0.46
2:B:400:ARG:HG3	2:B:400:ARG:O	2.16	0.46
1:C:58:SER:C	1:C:59:LYS:HG3	2.37	0.46
1:C:117:ARG:HH12	1:C:276:ARG:CB	2.29	0.46
2:D:122:ALA:HB1	2:D:296:LEU:HD11	1.98	0.46
2:D:244:LEU:HD23	2:D:244:LEU:HA	1.68	0.46
1:E:190:VAL:N	1:E:206:CYS:HB2	2.31	0.46
1:E:378:ARG:HD2	1:E:378:ARG:HA	1.64	0.46
4:J:251:UNK:O	4:J:254:UNK:N	2.49	0.46
1:A:105:LYS:C	1:A:188:LYS:HD2	2.37	0.45
1:A:144:ARG:CD	2:B:407:THR:CG2	2.87	0.45
1:A:270:LEU:HG	1:A:271:ASP:H	1.80	0.45
2:B:268:ILE:HD11	2:B:273:ARG:HE	1.81	0.45
2:B:425:ASP:OD1	2:B:427:LYS:HG2	2.16	0.45
1:C:69:ALA:HB2	2:D:444:LYS:HD3	1.97	0.45
2:D:161:LEU:HD12	2:D:162:THR:H	1.81	0.45
2:D:213:ARG:HD3	2:D:213:ARG:H	1.81	0.45
4:J:252:UNK:O	4:J:256:UNK:N	2.49	0.45
1:A:179:LEU:HD12	1:A:182:ALA:HB3	1.99	0.45
2:B:282:GLU:HA	2:B:285:GLU:HB2	1.98	0.45
2:B:436:GLU:HA	2:B:439:SER:OG	2.17	0.45
1:C:30:GLY:C	1:C:31:LEU:HD22	2.37	0.45
1:C:314:TYR:O	1:C:316:HIS:N	2.45	0.45
2:D:349:ASP:OD1	2:D:350:LEU:N	2.48	0.45
1:E:117:ARG:NH2	1:E:244:ASP:OD2	2.49	0.45
1:E:123:ARG:HD3	1:E:235:ILE:HG21	1.97	0.45
1:E:185:VAL:HG13	1:E:205:ARG:HG3	1.99	0.45
2:F:141:GLU:HB3	2:F:164:LYS:HB2	1.97	0.45
2:F:180:GLU:O	2:F:184:LYS:HG2	2.16	0.45
1:A:171:GLY:HA2	1:A:431:ARG:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:162:THR:HG22	2:B:171:ILE:HG13	1.97	0.45
2:B:368:LYS:O	2:B:372:ARG:HG2	2.16	0.45
1:C:12:THR:O	1:C:16:ALA:N	2.50	0.45
1:C:380:GLN:HG2	1:C:381:THR:N	2.31	0.45
2:D:359:THR:O	6:D:501:ADP:O2B	2.34	0.45
2:F:94:LEU:HD23	2:F:94:LEU:HA	1.63	0.45
2:F:132:LYS:HZ2	2:F:239:VAL:HB	1.80	0.45
1:A:208:GLU:HG2	1:A:209:VAL:H	1.82	0.45
1:A:221:ARG:HG2	1:A:335:ASP:HA	1.97	0.45
1:A:374:ARG:HH12	1:A:415:ARG:NH1	2.13	0.45
2:B:32:GLY:HA2	2:B:44:GLN:NE2	2.31	0.45
2:B:374:ARG:NH1	2:B:405:LEU:N	2.65	0.45
1:C:326:ILE:HD11	1:C:359:MET:HE1	1.99	0.45
2:D:99:PRO:HG2	2:D:294:GLY:HA3	1.97	0.45
2:D:207:ARG:HG2	2:D:235:ARG:NH1	2.31	0.45
2:D:444:LYS:O	2:D:447:GLN:HB2	2.17	0.45
2:F:393:ILE:HD12	2:F:393:ILE:H	1.80	0.45
3:H:366:UNK:HA	3:H:369:UNK:CB	2.47	0.45
3:H:496:UNK:C	3:H:498:UNK:N	2.79	0.45
1:C:183:GLU:O	1:C:185:VAL:HG13	2.17	0.45
1:C:393:HIS:O	1:C:397:ILE:HG12	2.17	0.45
2:D:35:ASP:N	2:D:35:ASP:OD1	2.47	0.45
2:D:443:MET:O	2:D:447:GLN:N	2.42	0.45
1:E:51:VAL:HG13	2:F:411:LEU:HD23	1.99	0.45
1:E:187:ALA:N	1:E:209:TYR:OH	2.41	0.45
2:F:129:VAL:O	2:F:241:THR:HA	2.16	0.45
3:H:74:UNK:HA	3:H:77:UNK:CB	2.46	0.45
3:H:188:UNK:O	3:H:193:UNK:HA	2.16	0.45
3:H:558:UNK:C	3:H:560:UNK:N	2.78	0.45
1:A:301:GLN:HE22	1:A:317:GLU:CG	2.30	0.45
2:B:42:ALA:C	2:B:46:MET:HE2	2.36	0.45
1:C:185:VAL:HG11	1:C:202:ARG:HG2	1.98	0.45
1:C:354:LEU:CD1	1:C:357:ARG:HB2	2.46	0.45
2:D:188:GLN:HE22	2:D:214:ASP:N	2.14	0.45
2:D:231:GLU:HG2	2:D:234:LYS:NZ	2.32	0.45
2:F:306:ILE:HG12	2:F:337:GLY:HA3	1.97	0.45
4:J:321:UNK:O	4:J:324:UNK:N	2.50	0.45
1:A:133:ALA:CB	2:B:428:ARG:N	2.69	0.45
1:A:207:THR:HA	1:A:210:LEU:HB2	1.99	0.45
2:B:156:SER:OG	2:B:157:LYS:N	2.48	0.45
2:B:313:ASN:ND2	2:B:313:ASN:H	2.14	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:368:LYS:HG3	2:B:387:TYR:HB3	1.98	0.45
2:B:399:LEU:HG	2:B:399:LEU:O	2.17	0.45
1:C:51:VAL:HG11	1:C:357:ARG:HG2	1.97	0.45
1:C:71:PRO:O	1:C:332:ASN:HA	2.17	0.45
1:C:343:ASP:OD1	1:C:343:ASP:N	2.47	0.45
2:D:142:VAL:O	2:D:195:ILE:HD12	2.17	0.45
4:J:393:UNK:CA	4:J:400:GLY:HA3	2.37	0.45
5:K:155:UNK:HA	5:K:158:ASN:CB	2.47	0.45
2:B:23:GLY:O	2:B:26:SER:N	2.41	0.45
2:B:43:SER:O	2:B:45:GLY:N	2.50	0.45
2:B:209:PHE:O	2:B:211:ARG:NH1	2.49	0.45
1:C:27:ASP:OD1	1:C:29:SER:N	2.37	0.45
2:D:104:ALA:HA	2:D:299:ASP:OD1	2.17	0.45
2:D:232:LEU:HD23	2:D:232:LEU:HA	1.82	0.45
2:D:437:SER:HA	2:D:441:GLN:HB2	1.99	0.45
2:F:124:ARG:HD3	2:F:124:ARG:HA	1.70	0.45
2:F:132:LYS:NZ	2:F:239:VAL:HB	2.32	0.45
2:F:350:LEU:HD12	2:F:350:LEU:HA	1.75	0.45
1:A:132:GLN:HG3	2:B:425:ASP:C	2.37	0.45
1:A:167:ALA:HB2	1:A:450:LEU:HB3	1.99	0.45
1:A:216:ARG:HH21	1:A:397:LEU:HD21	1.82	0.45
1:C:134:GLU:H	1:C:161:LEU:HA	1.82	0.45
1:C:165:LYS:HG3	1:C:226:GLY:O	2.17	0.45
1:C:328:ILE:HG23	1:C:359:MET:HG2	1.99	0.45
1:C:393:HIS:H	1:C:427:LYS:HZ1	1.65	0.45
2:D:134:GLU:HG3	2:D:207:ARG:NH2	2.31	0.45
2:D:156:SER:O	2:D:157:LYS:HG2	2.17	0.45
2:D:204:LYS:HD3	2:D:205:LEU:N	2.28	0.45
2:D:428:ARG:HD3	2:D:429:VAL:HG22	1.99	0.45
2:F:305:ASP:O	2:F:308:SER:OG	2.35	0.45
1:A:223:LYS:HG2	1:A:333:ILE:HG23	1.99	0.45
2:B:33:LEU:O	2:B:40:ARG:NH2	2.50	0.45
2:B:143:VAL:O	2:B:164:LYS:HG2	2.17	0.45
2:B:383:SER:O	2:B:385:ASP:N	2.50	0.45
1:C:207:ASP:N	1:C:207:ASP:OD1	2.49	0.45
1:C:362:ARG:HG2	1:C:363:THR:H	1.82	0.45
2:D:33:LEU:HG	2:D:39:PRO:HA	1.98	0.45
2:D:243:SER:OG	2:D:246:GLU:N	2.44	0.45
2:F:306:ILE:O	2:F:306:ILE:HG13	2.16	0.45
2:F:444:LYS:O	2:F:448:ASP:N	2.33	0.45
1:A:162:ARG:H	1:A:162:ARG:HD3	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:THR:HA	2:F:305:ASP:O	2.17	0.44
1:C:104:THR:O	1:C:107:LYS:NZ	2.34	0.44
1:C:117:ARG:HH12	1:C:276:ARG:HB3	1.81	0.44
1:C:136:THR:HA	1:C:209:TYR:CE1	2.52	0.44
2:D:81:THR:CB	6:D:501:ADP:O3'	2.65	0.44
2:D:146:GLN:HG3	2:D:148:ASP:N	2.33	0.44
2:D:311:PHE:O	2:D:315:ALA:N	2.46	0.44
1:E:130:VAL:HG13	1:E:192:TYR:HA	1.98	0.44
2:D:28:ILE:HD13	2:D:28:ILE:HA	1.81	0.44
2:D:197:LYS:HD3	2:D:199:THR:OG1	2.18	0.44
2:D:236:LYS:HD2	2:D:237:GLU:N	2.33	0.44
2:D:318:SER:OG	2:D:319:ASP:OD1	2.35	0.44
1:E:13:GLN:OE1	1:E:13:GLN:N	2.25	0.44
1:E:60:LYS:HE2	1:E:60:LYS:HA	2.00	0.44
3:H:175:UNK:HA	3:H:181:UNK:CB	2.47	0.44
2:B:177:LYS:NZ	2:B:209:PHE:O	2.50	0.44
1:C:177:PHE:HE1	1:C:202:ARG:HH22	1.64	0.44
1:C:311:CYS:O	1:C:314:TYR:HB3	2.17	0.44
1:C:393:HIS:HB2	1:C:427:LYS:HD3	2.00	0.44
2:D:81:THR:C	2:D:400:ARG:HE	2.21	0.44
2:D:82:GLY:O	2:D:400:ARG:NH1	2.48	0.44
1:E:134:GLU:HG3	1:E:136:THR:HG23	1.99	0.44
1:E:183:GLU:HG2	1:E:205:ARG:HD2	1.99	0.44
2:F:124:ARG:HG2	2:F:248:ASP:OD2	2.17	0.44
4:J:457:UNK:O	4:J:460:UNK:N	2.49	0.44
1:A:482:ILE:HD12	1:A:512:ASN:HD22	1.81	0.44
2:B:165:THR:HG22	2:B:167:GLU:H	1.81	0.44
2:B:400:ARG:CZ	6:B:501:ADP:PB	3.05	0.44
1:C:125:LYS:NZ	1:C:233:GLU:HB3	2.32	0.44
2:D:306:ILE:HG13	2:D:307:GLU:N	2.32	0.44
1:E:43:GLU:O	1:E:46:ARG:N	2.50	0.44
1:E:386:ILE:HA	1:E:425:ILE:H	1.82	0.44
5:K:48:UNK:HA	5:K:51:VAL:CB	2.48	0.44
1:A:122:LEU:HD21	1:A:144:ARG:NH1	2.33	0.44
1:A:468:GLU:HG3	1:A:471:GLN:HB3	1.99	0.44
1:E:376:LYS:HD2	1:E:380:GLN:NE2	2.29	0.44
2:F:178:MET:SD	2:F:195:ILE:HD11	2.57	0.44
4:J:257:UNK:CB	4:J:296:UNK:CB	2.96	0.44
2:B:68:ILE:HD12	2:B:71:ARG:HB2	2.00	0.44
2:B:295:VAL:HG12	2:B:323:VAL:CG1	2.48	0.44
1:C:64:ARG:HA	1:C:353:ASP:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:46:MET:HG2	2:D:53:ARG:CZ	2.48	0.44
2:D:275:GLN:HA	2:D:278:ALA:HB3	1.99	0.44
2:D:443:MET:O	2:D:447:GLN:HG2	2.18	0.44
1:E:113:MET:O	1:E:117:ARG:HG2	2.18	0.44
1:E:360:ILE:HG13	2:F:434:LEU:HB2	1.99	0.44
5:K:263:ALA:O	5:K:265:LEU:N	2.51	0.44
1:A:110:THR:HB	1:A:473:ILE:HG12	2.00	0.44
1:A:166:LEU:HD13	1:A:456:VAL:CG2	2.48	0.44
1:A:406:ASP:OD1	1:A:437:ARG:NE	2.50	0.44
1:A:465:THR:OG1	1:A:466:PRO:HD2	2.18	0.44
2:B:328:THR:HG21	2:B:344:HIS:HB3	2.00	0.44
1:C:52:ILE:HD11	1:C:358:VAL:HG13	2.00	0.44
1:C:53:VAL:HA	1:C:56:ILE:HG22	2.00	0.44
1:C:66:VAL:HG22	1:C:67:LEU:H	1.82	0.44
1:C:239:THR:O	1:C:242:ASP:HB2	2.17	0.44
1:E:159:ILE:HD12	1:E:172:LEU:HB2	2.00	0.44
1:A:218:ILE:HD12	1:A:339:HIS:HB2	2.00	0.44
1:A:260:LYS:NZ	1:A:262:ALA:HA	2.33	0.44
2:B:284:ARG:HA	2:B:289:ALA:O	2.17	0.44
2:B:436:GLU:O	2:B:440:THR:HG23	2.18	0.44
2:B:439:SER:HA	2:B:442:TYR:CD2	2.53	0.44
1:C:281:LYS:HD3	1:C:281:LYS:HA	1.65	0.44
2:D:86:ILE:H	2:D:86:ILE:HD12	1.82	0.44
2:D:297:PHE:CD1	2:D:325:ILE:HG13	2.51	0.44
1:E:12:THR:O	1:E:15:ILE:N	2.45	0.44
1:E:131:TYR:HA	1:E:228:VAL:O	2.17	0.44
1:E:283:VAL:O	1:E:286:TYR:N	2.51	0.44
5:K:160:LEU:O	5:K:163:GLU:CB	2.66	0.44
1:A:131:LYS:CE	2:B:413:CYS:HB2	2.48	0.44
1:A:545:LEU:HA	1:A:548:GLN:OE1	2.17	0.44
1:C:22:LYS:HB2	1:C:22:LYS:HE3	1.82	0.44
2:D:82:GLY:HA3	2:D:400:ARG:HE	1.83	0.44
2:D:397:THR:HG21	2:D:436:GLU:H	1.83	0.44
1:E:76:LYS:HG2	1:E:363:THR:HG21	1.99	0.44
1:E:212:GLU:OE2	1:E:218:GLU:HB3	2.18	0.44
1:E:426:GLU:OE2	1:E:429:HIS:N	2.42	0.44
1:A:140:GLN:C	1:A:142:ASN:H	2.17	0.43
2:B:34:ASP:OD1	2:B:37:LEU:N	2.51	0.43
2:B:73:VAL:HG23	2:B:355:LEU:O	2.18	0.43
2:B:78:GLN:HB2	2:B:79:PRO:CD	2.41	0.43
2:B:385:ASP:O	2:B:388:THR:OG1	2.35	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:29:ARG:HB2	2:D:44:GLN:HA	2.00	0.43
2:D:174:LEU:HG	2:D:175:GLY:H	1.82	0.43
1:E:87:LEU:HD12	1:E:87:LEU:HA	1.78	0.43
1:E:380:GLN:O	1:E:383:GLY:N	2.49	0.43
3:H:496:UNK:O	3:H:497:UNK:C	2.66	0.43
4:J:121:UNK:C	4:J:123:UNK:N	2.79	0.43
4:J:321:UNK:O	4:J:324:UNK:CB	2.66	0.43
1:A:220:LEU:H	1:A:337:THR:HA	1.82	0.43
1:A:492:LEU:O	1:A:495:ILE:HG22	2.18	0.43
2:B:130:ARG:HB3	2:B:290:GLU:OE1	2.18	0.43
2:B:146:GLN:HE21	2:B:149:ARG:HG3	1.82	0.43
2:B:236:LYS:HZ3	2:B:238:VAL:HA	1.81	0.43
2:B:268:ILE:HD11	2:B:273:ARG:NE	2.32	0.43
2:B:292:ILE:HD12	2:B:293:PRO:HD2	2.00	0.43
2:B:367:THR:O	2:B:371:LEU:HD12	2.17	0.43
1:C:48:ALA:HB1	1:C:356:ASP:O	2.18	0.43
1:C:317:ARG:NH1	1:C:318:ALA:HB2	2.33	0.43
2:D:29:ARG:HB2	2:D:44:GLN:HB3	1.99	0.43
2:D:338:THR:OG1	2:D:339:SER:N	2.51	0.43
2:D:359:THR:OG1	6:D:501:ADP:O1A	2.36	0.43
2:D:428:ARG:HD3	2:D:429:VAL:CG2	2.48	0.43
1:E:131:TYR:CZ	1:E:229:HIS:CD2	3.06	0.43
1:E:395:GLY:O	1:E:399:THR:HG23	2.18	0.43
2:F:247:ILE:HG22	2:F:276:ILE:HD13	2.00	0.43
2:F:310:SER:O	2:F:310:SER:OG	2.37	0.43
5:K:192:LEU:C	5:K:194:GLY:N	2.71	0.43
1:A:150:ILE:O	1:A:154:ILE:N	2.49	0.43
1:A:231:GLY:HA3	1:A:265:THR:CA	2.48	0.43
1:A:263:LYS:HA	1:A:323:LYS:HD2	2.00	0.43
1:A:524:GLU:H	1:A:527:HIS:HD1	1.62	0.43
1:C:97:VAL:O	1:C:100:GLU:HG2	2.18	0.43
1:C:286:TYR:O	1:C:290:GLY:N	2.51	0.43
1:C:372:LYS:HB3	1:C:391:LEU:HD21	1.99	0.43
2:D:164:LYS:HB3	2:D:164:LYS:HE3	1.76	0.43
2:F:77:GLY:HA3	2:F:359:THR:CG2	2.48	0.43
2:F:165:THR:HG22	2:F:230:GLY:HA3	2.01	0.43
2:F:166:THR:CG2	2:F:229:ASP:HA	2.47	0.43
2:F:375:CYS:SG	2:F:376:GLU:N	2.91	0.43
2:F:378:GLU:O	2:F:380:VAL:HG23	2.18	0.43
1:A:131:LYS:CE	2:B:413:CYS:HB3	2.26	0.43
1:A:165:LEU:HD13	1:A:449:PRO:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:ARG:HH22	1:A:303:ARG:HB3	1.83	0.43
1:A:487:GLU:HG2	1:A:488:ALA:N	2.33	0.43
2:B:41:GLN:O	2:B:41:GLN:NE2	2.50	0.43
2:B:422:GLN:O	2:B:424:ASP:N	2.50	0.43
1:C:126:GLU:O	1:C:233:GLU:HA	2.18	0.43
1:C:354:LEU:O	1:C:356:ASP:N	2.52	0.43
1:C:418:LYS:NZ	1:C:423:ASP:HA	2.34	0.43
2:D:86:ILE:O	2:D:90:MET:HG3	2.18	0.43
2:D:112:GLU:HG2	2:D:113:MET:H	1.83	0.43
2:D:137:ILE:HG21	2:D:211:ARG:NH1	2.33	0.43
1:E:372:LYS:NZ	1:E:395:GLY:HA3	2.34	0.43
2:F:130:ARG:HH21	2:F:290:GLU:HB3	1.82	0.43
2:F:161:LEU:HD13	2:F:174:LEU:HD21	2.01	0.43
3:H:238:UNK:C	3:H:240:UNK:N	2.81	0.43
1:A:138:VAL:CG1	2:B:432:LEU:H	2.24	0.43
1:A:158:LYS:HE2	1:A:158:LYS:HB3	1.74	0.43
1:A:190:PRO:N	1:A:394:PRO:HB3	2.34	0.43
1:A:206:LYS:O	1:A:208:GLU:N	2.52	0.43
2:B:95:GLY:HA3	2:B:98:THR:HG23	2.00	0.43
1:C:27:ASP:OD1	1:C:28:GLU:HG2	2.19	0.43
1:C:64:ARG:HH22	1:C:357:ARG:NH2	2.16	0.43
1:C:427:LYS:O	1:C:430:VAL:N	2.51	0.43
2:D:29:ARG:C	2:D:44:GLN:HB3	2.39	0.43
2:D:31:LEU:HA	2:D:31:LEU:HD23	1.83	0.43
1:E:6:VAL:HB	1:E:236:GLN:HE21	1.83	0.43
5:K:76:ALA:HA	5:K:79:ALA:HB3	2.00	0.43
5:K:162:GLN:O	5:K:164:ASN:N	2.52	0.43
1:A:150:ILE:HG12	1:A:455:ARG:NH2	2.33	0.43
1:A:172:THR:HG1	1:A:174:LYS:HZ2	1.64	0.43
1:A:174:LYS:HE3	1:A:174:LYS:HB3	1.88	0.43
2:B:27:HIS:CE1	2:B:403:ILE:HD12	2.54	0.43
1:C:132:GLU:OE1	1:C:163:THR:HG21	2.18	0.43
1:E:191:ILE:HB	1:E:193:ILE:HG23	1.99	0.43
1:E:213:PHE:CZ	1:E:222:PRO:HA	2.53	0.43
3:H:510:UNK:O	3:H:513:UNK:N	2.52	0.43
4:J:477:UNK:HA	4:J:478:UNK:HA	1.53	0.43
1:A:133:ALA:O	2:B:428:ARG:CB	2.67	0.43
1:A:140:GLN:CD	2:B:434:LEU:HD12	2.39	0.43
1:A:163:ALA:HB2	1:A:413:LEU:C	2.39	0.43
2:B:306:ILE:HD12	1:C:102:TYR:CD1	2.54	0.43
1:C:185:VAL:HB	1:C:189:ASP:OD2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:113:MET:SD	2:D:267:GLU:N	2.92	0.43
2:D:275:GLN:O	2:D:279:LYS:N	2.37	0.43
2:D:375:CYS:O	2:D:380:VAL:HG22	2.18	0.43
1:E:79:LEU:HA	1:E:79:LEU:HD23	1.78	0.43
2:F:161:LEU:HD23	2:F:162:THR:N	2.33	0.43
4:J:397:GLY:C	4:J:453:UNK:CB	2.87	0.43
5:K:386:SER:O	5:K:389:PRO:CB	2.67	0.43
1:A:170:PRO:HB2	1:A:432:GLY:HA2	2.01	0.43
1:A:241:THR:HG22	1:A:242:GLU:N	2.33	0.43
1:C:129:GLU:HB3	1:C:229:HIS:CE1	2.54	0.43
1:C:359:MET:HE2	1:C:359:MET:HB2	1.60	0.43
1:C:389:GLU:OE2	1:C:427:LYS:HE2	2.19	0.43
2:D:409:ALA:O	2:D:412:VAL:HG22	2.19	0.43
1:E:126:GLU:HB2	1:E:128:LYS:HZ2	1.84	0.43
1:E:170:LEU:HD12	1:E:170:LEU:HA	1.84	0.43
1:A:232:GLU:N	1:A:265:THR:HA	2.34	0.43
2:B:28:ILE:HA	2:B:28:ILE:HD13	1.83	0.43
2:B:157:LYS:HD3	2:B:174:LEU:O	2.19	0.43
2:B:306:ILE:HG13	2:B:307:GLU:OE2	2.19	0.43
1:C:385:ASN:O	1:C:424:SER:HA	2.19	0.43
2:D:138:ILE:HG12	2:D:204:LYS:O	2.19	0.43
2:D:201:LYS:HE3	4:J:281:UNK:C	2.29	0.43
1:E:432:GLU:O	1:E:436:LEU:HG	2.19	0.43
2:F:130:ARG:HB3	2:F:239:VAL:HG21	2.01	0.43
2:F:160:LYS:HD3	2:F:172:TYR:O	2.19	0.43
4:J:495:UNK:HA	4:J:496:UNK:HA	1.47	0.43
5:K:301:THR:C	5:K:305:GLN:CB	2.87	0.43
1:E:97:VAL:HG22	1:E:100:GLU:OE2	2.19	0.43
1:E:234:ILE:HG22	1:E:235:ILE:N	2.33	0.43
3:H:369:UNK:C	3:H:371:UNK:N	2.67	0.43
1:A:172:THR:OG1	1:A:174:LYS:N	2.52	0.42
1:A:302:GLY:HA3	1:A:316:GLU:OE1	2.19	0.42
2:B:390:LEU:HA	2:B:390:LEU:HD23	1.73	0.42
1:C:181:GLN:HG3	1:C:182:LYS:HD3	2.00	0.42
1:C:315:LEU:C	1:C:319:LEU:HD21	2.40	0.42
2:D:94:LEU:HD23	2:D:94:LEU:HA	1.68	0.42
2:D:121:GLN:HB3	2:D:125:ARG:HH21	1.83	0.42
2:D:133:GLU:OE1	2:D:134:GLU:N	2.52	0.42
2:D:137:ILE:HA	2:D:205:LEU:HD23	2.01	0.42
3:H:164:UNK:HA	3:H:167:UNK:CB	2.49	0.42
1:A:436:ILE:HD11	1:A:449:PRO:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:64:ARG:HB3	1:C:354:LEU:N	2.34	0.42
2:D:132:LYS:HD3	2:D:237:GLU:HG2	1.99	0.42
2:D:430:TYR:HA	2:D:433:PHE:CB	2.33	0.42
1:E:37:SER:O	1:E:37:SER:OG	2.36	0.42
1:E:279:ILE:HD12	1:E:279:ILE:H	1.84	0.42
1:E:362:ARG:HD3	2:F:442:TYR:CD2	2.54	0.42
2:F:423:VAL:HG22	2:F:427:LYS:HG2	2.02	0.42
1:A:544:ILE:CG2	1:A:548:GLN:HE22	2.33	0.42
2:B:38:GLU:HA	2:B:39:PRO:HD3	1.94	0.42
2:B:86:ILE:HD13	2:B:86:ILE:HA	1.81	0.42
2:B:145:ILE:HD12	2:B:145:ILE:HA	1.91	0.42
1:C:93:PHE:HD1	1:C:298:VAL:HG11	1.84	0.42
1:C:122:LEU:HB2	1:C:238:VAL:HG23	2.00	0.42
1:C:185:VAL:HG21	1:C:202:ARG:HB3	2.01	0.42
2:D:32:GLY:CA	2:D:43:SER:HB2	2.49	0.42
2:D:393:ILE:HG23	2:D:435:ASP:OD2	2.18	0.42
2:D:444:LYS:O	2:D:448:ASP:N	2.33	0.42
1:E:32:ALA:HB1	1:E:46:ARG:CZ	2.49	0.42
1:E:160:GLY:HA3	1:E:162:LYS:NZ	2.34	0.42
1:E:168:LYS:NZ	1:E:169:GLN:O	2.52	0.42
2:F:195:ILE:HG23	2:F:196:ASP:OD1	2.19	0.42
3:H:553:UNK:C	3:H:555:UNK:N	2.80	0.42
1:A:494:GLU:HG3	1:A:498:LYS:HZ1	1.80	0.42
2:D:145:ILE:O	2:D:145:ILE:HG13	2.19	0.42
2:D:206:GLY:HA2	2:D:235:ARG:HH11	1.85	0.42
2:D:436:GLU:O	2:D:440:THR:OG1	2.37	0.42
1:E:234:ILE:O	1:E:235:ILE:HD13	2.20	0.42
2:F:309:PHE:CE2	2:F:313:ASN:HB2	2.54	0.42
1:A:170:PRO:CB	1:A:432:GLY:HA2	2.48	0.42
1:A:332:ILE:H	1:A:332:ILE:HG13	1.70	0.42
2:B:382:MET:HB3	2:B:387:TYR:CE1	2.54	0.42
1:C:54:GLU:O	1:C:58:SER:N	2.53	0.42
1:C:370:GLU:HA	1:C:373:GLN:NE2	2.35	0.42
3:H:558:UNK:O	3:H:560:UNK:N	2.53	0.42
5:K:52:LEU:HA	5:K:55:LEU:CB	2.49	0.42
5:K:91:ALA:CA	5:K:94:SER:CB	2.97	0.42
1:A:237:THR:HB	1:A:255:VAL:O	2.20	0.42
1:A:256:ILE:HG23	1:A:267:GLN:OE1	2.19	0.42
1:C:447:LEU:O	1:C:451:GLN:HG2	2.19	0.42
2:D:78:GLN:HG3	2:D:79:PRO:HD2	2.00	0.42
1:E:212:GLU:OE1	1:E:218:GLU:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:22:ILE:HG12	2:F:23:GLY:H	1.85	0.42
4:J:249:UNK:O	4:J:253:UNK:N	2.53	0.42
1:A:123:GLY:N	2:B:411:LEU:N	2.65	0.42
2:B:23:GLY:O	2:B:26:SER:OG	2.25	0.42
2:B:99:PRO:HG2	2:B:126:SER:O	2.20	0.42
1:C:186:GLU:OE1	1:C:213:PHE:HA	2.19	0.42
2:D:334:ARG:HA	2:D:340:TYR:O	2.20	0.42
1:E:126:GLU:HB2	1:E:128:LYS:NZ	2.34	0.42
1:E:365:LEU:HD23	1:E:365:LEU:HA	1.83	0.42
1:E:372:LYS:HE3	1:E:392:ASN:HA	2.01	0.42
1:E:403:LEU:HA	1:E:403:LEU:HD12	1.74	0.42
2:F:435:ASP:H	2:F:438:ARG:HH21	1.67	0.42
3:H:575:UNK:O	3:H:577:UNK:N	2.52	0.42
1:A:222:ILE:HA	1:A:390:ALA:HB1	2.01	0.42
1:A:277:SER:OG	1:A:299:LYS:N	2.53	0.42
2:B:284:ARG:HD2	2:B:291:ILE:HG23	2.02	0.42
2:B:382:MET:CG	2:B:383:SER:H	2.32	0.42
2:D:143:VAL:HG23	2:D:145:ILE:HG12	2.02	0.42
2:D:251:ASN:HD22	2:D:276:ILE:CD1	2.32	0.42
1:E:125:LYS:CE	1:E:233:GLU:HB3	2.50	0.42
1:E:313:THR:HG21	2:F:110:SER:HB2	2.01	0.42
1:E:317:ARG:HG3	1:E:318:ALA:N	2.35	0.42
1:E:326:ILE:HD12	1:E:326:ILE:HA	1.91	0.42
1:E:335:ASN:OD1	1:E:345:THR:HG22	2.20	0.42
2:F:97:ASP:OD1	2:F:97:ASP:N	2.52	0.42
2:F:119:LEU:HB3	2:F:311:PHE:CE2	2.55	0.42
2:F:416:ARG:C	2:F:417:LYS:HG2	2.40	0.42
5:K:261:VAL:C	5:K:264:ALA:HB3	2.28	0.42
5:K:383:ARG:C	5:K:385:ASP:N	2.70	0.42
1:A:118:HIS:HA	1:A:461:THR:OG1	2.20	0.42
1:A:303:ARG:HG2	1:A:318:TYR:OH	2.20	0.42
1:A:407:ILE:HD12	1:A:407:ILE:H	1.84	0.42
1:C:81:LEU:HD12	1:C:81:LEU:HA	1.88	0.42
1:C:241:HIS:O	1:C:245:VAL:HG12	2.20	0.42
1:C:319:LEU:N	1:C:319:LEU:HD23	2.35	0.42
1:A:175:THR:O	1:A:175:THR:OG1	2.28	0.42
1:A:189:VAL:HB	1:A:394:PRO:CG	2.48	0.42
1:A:535:PHE:HE1	2:F:55:ALA:HB1	1.84	0.42
2:B:372:ARG:HA	2:B:387:TYR:CZ	2.55	0.42
1:C:49:CYS:N	1:C:358:VAL:O	2.53	0.42
1:C:95:PRO:HA	1:C:300:PHE:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:142:VAL:HG21	2:D:163:LEU:HB3	2.01	0.42
2:D:193:ILE:HG22	2:D:212:ALA:O	2.20	0.42
1:E:12:THR:HA	1:E:15:ILE:HG12	2.02	0.42
1:E:48:ALA:HB1	1:E:361:ILE:HD13	2.00	0.42
2:F:30:GLY:O	2:F:31:LEU:HD23	2.20	0.42
2:F:346:ILE:HG22	2:F:351:LEU:HG	2.02	0.42
4:J:219:UNK:O	4:J:223:UNK:CB	2.68	0.42
1:A:106:SER:O	1:A:106:SER:OG	2.38	0.41
1:A:467:GLN:CD	1:A:467:GLN:N	2.73	0.41
2:B:43:SER:N	2:B:46:MET:HE2	2.35	0.41
2:B:434:LEU:HD13	2:B:439:SER:CB	2.50	0.41
2:D:296:LEU:HD21	2:D:298:ILE:HD11	2.01	0.41
2:D:372:ARG:HA	2:D:387:TYR:OH	2.20	0.41
1:E:209:TYR:HB3	1:E:212:GLU:HG3	2.01	0.41
1:E:431:GLU:O	1:E:434:SER:OG	2.23	0.41
1:A:149:VAL:HG23	1:A:152:GLU:OE1	2.19	0.41
1:C:185:VAL:HA	1:C:205:ARG:HH12	1.84	0.41
1:C:354:LEU:HD12	1:C:357:ARG:NE	2.29	0.41
2:D:81:THR:HB	6:D:501:ADP:O3'	2.19	0.41
2:D:209:PHE:HA	2:D:211:ARG:NE	2.35	0.41
2:D:375:CYS:HA	2:D:406:ILE:HD11	2.02	0.41
1:A:124:LEU:HB3	1:A:135:SER:CB	2.50	0.41
1:A:164:VAL:HG22	1:A:417:LEU:HG	2.01	0.41
1:A:177:LEU:HB3	1:A:192:CYS:O	2.21	0.41
2:B:139:GLU:O	2:B:232:LEU:HD13	2.20	0.41
2:B:248:ASP:HA	2:B:276:ILE:HD12	2.02	0.41
2:B:431:SER:H	2:B:431:SER:HG	1.63	0.41
1:C:69:ALA:HB2	2:D:444:LYS:CD	2.50	0.41
1:C:128:LYS:HZ1	1:C:234:ILE:H	1.68	0.41
1:C:293:GLU:HG3	2:D:221:GLN:OE1	2.20	0.41
2:D:100:PHE:HD1	2:D:295:VAL:HG13	1.85	0.41
1:E:43:GLU:OE1	1:E:43:GLU:N	2.47	0.41
1:E:241:HIS:HA	1:E:244:ASP:OD2	2.21	0.41
2:F:433:PHE:N	2:F:433:PHE:CD2	2.88	0.41
1:A:190:PRO:CG	1:A:394:PRO:HG3	2.51	0.41
1:A:191:PHE:HB2	1:A:425:VAL:H	1.85	0.41
2:B:24:ALA:HA	2:B:27:HIS:CE1	2.56	0.41
2:B:24:ALA:O	2:B:27:HIS:N	2.53	0.41
2:B:244:LEU:O	2:B:247:ILE:HG22	2.20	0.41
2:B:274:GLU:O	2:B:278:ALA:N	2.51	0.41
2:B:385:ASP:HA	2:B:388:THR:OG1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:141:GLU:CB	2:D:230:GLY:HA3	2.51	0.41
2:D:435:ASP:N	2:D:438:ARG:HB2	2.35	0.41
1:E:178:GLU:HA	1:E:181:GLN:HB2	2.02	0.41
5:K:272:ARG:HA	5:K:275:GLY:H	1.86	0.41
1:A:408:GLU:HB3	2:B:111:LEU:CD2	2.51	0.41
1:A:492:LEU:HD12	1:A:492:LEU:HA	1.73	0.41
2:B:161:LEU:HD13	2:B:174:LEU:HD21	2.02	0.41
1:C:441:LYS:HE3	1:C:441:LYS:HB2	1.82	0.41
2:D:113:MET:N	2:D:113:MET:SD	2.93	0.41
1:E:182:LYS:HB2	1:E:182:LYS:HE2	1.87	0.41
1:A:172:THR:HG1	1:A:173:GLY:N	2.18	0.41
1:A:418:GLU:OE1	1:A:420:SER:OG	2.26	0.41
2:B:438:ARG:HH22	2:B:445:GLU:HG2	1.85	0.41
2:D:412:VAL:HA	2:D:415:LYS:HB3	2.01	0.41
1:E:20:HIS:HE1	6:E:501:ADP:O2'	2.03	0.41
1:E:176:ILE:HA	1:E:179:SER:OG	2.21	0.41
1:E:212:GLU:O	1:E:217:ALA:HB3	2.21	0.41
2:F:384:GLU:O	2:F:387:TYR:HB2	2.21	0.41
3:H:497:UNK:O	3:H:498:UNK:C	2.69	0.41
1:A:231:GLY:N	1:A:260:LYS:HA	2.27	0.41
1:A:483:ASN:HD22	1:A:521:ASP:CG	2.21	0.41
1:A:509:THR:N	1:A:510:PRO:HD2	2.36	0.41
2:B:424:ASP:N	2:B:424:ASP:OD2	2.46	0.41
1:C:448:ALA:HA	1:C:451:GLN:HB2	2.03	0.41
2:D:156:SER:OG	2:D:173:ASP:HA	2.20	0.41
2:D:177:LYS:HB2	2:D:205:LEU:CD2	2.50	0.41
2:D:304:LEU:O	2:D:336:ARG:HB2	2.21	0.41
2:D:421:VAL:HA	2:D:425:ASP:OD2	2.21	0.41
2:F:60:LEU:HD12	2:F:63:ILE:HD12	2.03	0.41
2:F:134:GLU:HG2	2:F:207:ARG:HH22	1.85	0.41
2:F:309:PHE:HZ	2:F:350:LEU:HB2	1.85	0.41
4:J:252:UNK:O	4:J:255:UNK:CA	2.69	0.41
5:K:386:SER:CB	5:K:388:LEU:O	2.69	0.41
1:A:106:SER:HB2	1:A:191:PHE:CZ	2.56	0.41
1:A:230:GLU:HG3	1:A:261:THR:HB	2.03	0.41
1:A:495:ILE:HA	1:A:498:LYS:HD2	2.03	0.41
2:B:284:ARG:HG2	2:B:290:GLU:HA	2.02	0.41
1:C:34:GLN:OE1	1:C:46:ARG:NH1	2.54	0.41
1:C:54:GLU:HA	1:C:57:LYS:CB	2.50	0.41
1:C:354:LEU:O	1:C:357:ARG:N	2.48	0.41
2:D:60:LEU:HA	2:D:60:LEU:HD23	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:77:GLY:HA3	2:D:83:LYS:CD	2.50	0.41
2:D:81:THR:HB	6:D:501:ADP:C3'	2.49	0.41
2:D:137:ILE:CG2	2:D:209:PHE:H	2.33	0.41
2:D:359:THR:HB	2:D:360:THR:H	1.71	0.41
2:D:406:ILE:HG23	2:D:407:THR:N	2.36	0.41
3:H:379:UNK:C	3:H:381:UNK:N	2.83	0.41
1:A:134:ALA:HB2	2:B:416:ARG:HH21	1.85	0.41
2:B:50:LEU:O	2:B:51:ALA:C	2.59	0.41
2:B:132:LYS:CG	2:B:237:GLU:HB3	2.46	0.41
2:B:242:VAL:HG13	2:B:246:GLU:OE1	2.21	0.41
2:B:279:LYS:O	2:B:282:GLU:HG3	2.20	0.41
2:B:384:GLU:O	2:B:387:TYR:HB2	2.21	0.41
2:D:27:HIS:O	2:D:29:ARG:HG2	2.21	0.41
2:D:30:GLY:N	2:D:44:GLN:HB3	2.36	0.41
2:D:134:GLU:HA	2:D:207:ARG:CD	2.49	0.41
2:D:401:TYR:O	2:D:404:GLN:HB3	2.20	0.41
1:E:7:LYS:HD3	1:E:246:ALA:HB2	2.03	0.41
1:E:160:GLY:O	1:E:162:LYS:N	2.54	0.41
1:E:180:LEU:HD23	1:E:180:LEU:HA	1.90	0.41
2:F:164:LYS:HB3	2:F:164:LYS:HE2	1.77	0.41
2:F:442:TYR:HD1	2:F:442:TYR:HA	1.79	0.41
3:H:86:UNK:O	3:H:88:UNK:N	2.54	0.41
3:H:98:UNK:O	3:H:102:UNK:N	2.53	0.41
3:H:293:UNK:O	3:H:295:UNK:N	2.54	0.41
1:A:143:ALA:HB1	1:A:456:VAL:O	2.21	0.41
1:A:194:MET:HA	1:A:402:VAL:HB	2.03	0.41
1:A:513:LEU:O	1:A:516:LYS:HB3	2.21	0.41
2:B:368:LYS:NZ	2:B:372:ARG:HH12	2.19	0.41
1:C:55:LEU:HD13	1:C:60:LYS:O	2.21	0.41
1:C:232:LYS:HG3	1:C:234:ILE:HG12	2.03	0.41
2:D:172:TYR:HB2	2:D:202:ILE:HA	2.02	0.41
2:D:394:GLY:O	2:D:398:SER:N	2.54	0.41
1:E:183:GLU:OE2	1:E:203:GLN:HA	2.21	0.41
1:E:275:LEU:O	1:E:279:ILE:HD12	2.21	0.41
1:E:355:LEU:HD12	1:E:355:LEU:HA	1.84	0.41
4:J:343:UNK:O	4:J:347:UNK:N	2.54	0.41
1:A:179:LEU:HD13	1:A:189:VAL:HG22	2.03	0.40
1:A:243:ASN:HA	1:A:244:PRO:HD3	1.94	0.40
1:A:328:LYS:NZ	1:A:330:LYS:HB2	2.37	0.40
2:B:37:LEU:HD13	2:B:37:LEU:HA	1.90	0.40
2:D:135:THR:OG1	2:D:136:GLU:N	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:208:SER:O	2:D:210:THR:HG23	2.21	0.40
2:D:318:SER:HG	2:D:319:ASP:H	1.67	0.40
1:E:11:LYS:HE3	1:E:11:LYS:HB3	1.95	0.40
1:E:138:LEU:HA	1:E:157:VAL:CG1	2.49	0.40
1:E:317:ARG:O	1:E:320:GLU:HG2	2.21	0.40
1:E:343:ASP:OD1	1:E:343:ASP:N	2.52	0.40
1:E:376:LYS:O	1:E:380:GLN:NE2	2.54	0.40
2:F:139:GLU:H	2:F:234:LYS:HZ1	1.67	0.40
2:F:283:TRP:HA	2:F:286:GLU:HG2	2.04	0.40
1:A:162:ARG:HG2	1:A:417:LEU:HB2	2.03	0.40
1:A:241:THR:HG22	1:A:242:GLU:H	1.84	0.40
1:C:278:GLU:HG3	1:C:279:ILE:H	1.86	0.40
1:C:287:ILE:HA	1:C:287:ILE:HD12	1.77	0.40
2:D:46:MET:O	2:D:53:ARG:NH2	2.54	0.40
2:D:127:ILE:HD11	2:D:322:PRO:HD3	2.02	0.40
2:D:196:ASP:CG	2:D:197:LYS:H	2.25	0.40
2:D:416:ARG:CZ	2:D:418:GLY:HA3	2.52	0.40
1:E:128:LYS:HE2	1:E:128:LYS:HB2	1.92	0.40
1:E:394:LEU:HD12	1:E:394:LEU:HA	1.76	0.40
2:F:188:GLN:NE2	2:F:216:ASP:OD1	2.54	0.40
3:H:313:UNK:O	3:H:317:GLY:N	2.51	0.40
5:K:145:UNK:O	5:K:149:UNK:N	2.55	0.40
5:K:246:GLU:O	5:K:250:ASP:CB	2.69	0.40
1:A:138:VAL:CB	2:B:433:PHE:HD2	2.33	0.40
1:A:189:VAL:HB	1:A:190:PRO:HD3	2.04	0.40
2:B:24:ALA:H	2:B:403:ILE:HG21	1.85	0.40
2:D:425:ASP:O	2:D:429:VAL:N	2.42	0.40
1:E:218:GLU:HG3	1:E:219:GLU:O	2.21	0.40
1:E:232:LYS:CD	1:E:234:ILE:HD11	2.51	0.40
4:J:358:UNK:HA	4:J:361:UNK:CB	2.51	0.40
5:K:146:UNK:O	5:K:150:UNK:N	2.54	0.40
1:A:373:LEU:O	1:A:377:ILE:HG13	2.21	0.40
1:A:412:TYR:O	1:A:412:TYR:CG	2.75	0.40
2:D:129:VAL:H	2:D:242:VAL:CG1	2.25	0.40
2:D:135:THR:H	2:D:207:ARG:HH11	1.68	0.40
2:D:148:ASP:CG	2:D:174:LEU:HD22	2.42	0.40
2:D:429:VAL:O	2:D:432:LEU:N	2.55	0.40
2:F:161:LEU:HB3	2:F:172:TYR:CE1	2.56	0.40
3:H:175:UNK:C	3:H:177:UNK:N	2.83	0.40
1:A:202:THR:HA	2:F:306:ILE:HA	2.02	0.40
2:B:111:LEU:HD13	2:B:111:LEU:HA	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:189:ASP:C	1:C:206:CYS:HB2	2.42	0.40
1:C:353:ASP:OD1	1:C:353:ASP:N	2.54	0.40
2:D:134:GLU:HA	2:D:207:ARG:CZ	2.50	0.40
2:D:167:GLU:OE1	2:D:168:MET:HG2	2.21	0.40
2:D:179:ILE:HG23	2:D:180:GLU:H	1.86	0.40
2:D:425:ASP:O	2:D:429:VAL:HG23	2.21	0.40
1:E:184:ARG:HH12	1:E:217:ALA:HB1	1.87	0.40
2:F:77:GLY:HA3	2:F:359:THR:HG22	2.02	0.40
2:F:137:ILE:HG12	2:F:210:THR:OG1	2.22	0.40
2:F:397:THR:OG1	2:F:398:SER:N	2.54	0.40
4:J:436:UNK:O	4:J:440:UNK:N	2.55	0.40
5:K:362:GLU:O	5:K:364:GLU:N	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	A	429/456 (94%)	316 (74%)	111 (26%)	2 (0%)	29	65
1	C	423/456 (93%)	353 (84%)	70 (16%)	0	100	100
1	E	407/456 (89%)	347 (85%)	60 (15%)	0	100	100
2	B	414/463 (89%)	340 (82%)	73 (18%)	1 (0%)	47	80
2	D	415/463 (90%)	337 (81%)	78 (19%)	0	100	100
2	F	415/463 (90%)	373 (90%)	42 (10%)	0	100	100
3	H	6/1733 (0%)	6 (100%)	0	0	100	100
4	J	6/964 (1%)	5 (83%)	0	1 (17%)	0	1
5	K	356/491 (72%)	276 (78%)	59 (17%)	21 (6%)	1	14
All	All	2871/5945 (48%)	2353 (82%)	493 (17%)	25 (1%)	21	53

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	K	105	ALA
5	K	106	ARG
5	K	190	ASP
5	K	191	SER
5	K	283	LYS
5	K	296	GLN
5	K	318	ARG
5	K	342	PRO
5	K	388	LEU
2	B	80	GLY
4	J	194	GLY
5	K	104	LEU
5	K	163	GLU
5	K	343	LEU
5	K	216	GLN
5	K	244	LEU
5	K	297	SER
5	K	363	PRO
1	A	137	LEU
5	K	215	ARG
5	K	298	ARG
5	K	335	SER
5	K	360	LEU
1	A	428	ALA
5	K	341	THR

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	A	364/387 (94%)	359 (99%)	5 (1%)	67 85
1	C	360/387 (93%)	356 (99%)	4 (1%)	73 87
1	E	343/387 (89%)	340 (99%)	3 (1%)	78 90
2	B	343/390 (88%)	338 (98%)	5 (2%)	65 83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	346/390 (89%)	340 (98%)	6 (2%)	60	82
2	F	347/390 (89%)	343 (99%)	4 (1%)	71	87
5	K	1/383 (0%)	1 (100%)	0	100	100
All	All	2104/2714 (78%)	2077 (99%)	27 (1%)	70	86

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	162	ARG
1	A	303	ARG
1	A	405	LEU
1	A	431	ARG
1	A	526	GLU
2	B	184	LYS
2	B	211	ARG
2	B	223	LYS
2	B	413	CYS
2	B	427	LYS
1	C	59	LYS
1	C	116	PHE
1	C	184	ARG
1	C	441	LYS
2	D	40	ARG
2	D	164	LYS
2	D	197	LYS
2	D	213	ARG
2	D	243	SER
2	D	428	ARG
1	E	126	GLU
1	E	184	ARG
1	E	427	LYS
2	F	64	ARG
2	F	130	ARG
2	F	223	LYS
2	F	442	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	116	HIS

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Mol	Chain	Res	Type
1	A	132	GLN
1	A	213	ASN
1	A	382	ASN
1	A	506	GLN
1	A	512	ASN
1	A	548	GLN
2	B	27	HIS
2	B	41	GLN
2	B	233	GLN
2	B	275	GLN
2	B	313	ASN
2	B	422	GLN
2	B	441	GLN
1	C	18	HIS
1	C	115	ASN
1	C	181	GLN
1	C	284	ASN
1	C	316	HIS
2	D	146	GLN
2	D	188	GLN
2	D	233	GLN
2	D	251	ASN
2	D	302	HIS
2	D	341	GLN
2	D	404	GLN
2	D	453	ASN
1	E	34	GLN
1	E	42	GLN
1	E	156	HIS
1	E	169	GLN
1	E	229	HIS
1	E	289	GLN
2	F	92	GLN
2	F	226	GLN
2	F	233	GLN
2	F	447	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

5 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
6	ADP	C	501	1	24,29,29	0.97	1 (4%)	29,45,45	1.39	5 (17%)
6	ADP	E	501	1	24,29,29	0.98	2 (8%)	29,45,45	1.60	4 (13%)
6	ADP	D	501	2	24,29,29	0.89	1 (4%)	29,45,45	1.43	4 (13%)
6	ADP	F	501	2	24,29,29	0.98	1 (4%)	29,45,45	1.58	4 (13%)
6	ADP	B	501	-	24,29,29	1.08	2 (8%)	29,45,45	1.29	4 (13%)

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
6	ADP	C	501	1	-	3/12/32/32	0/3/3/3
6	ADP	E	501	1	-	3/12/32/32	0/3/3/3
6	ADP	D	501	2	-	4/12/32/32	0/3/3/3
6	ADP	F	501	2	-	7/12/32/32	0/3/3/3
6	ADP	B	501	-	-	3/12/32/32	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	501	ADP	C5-C4	2.42	1.47	1.40
6	B	501	ADP	C2'-C1'	-2.30	1.50	1.53
6	E	501	ADP	C2'-C1'	-2.15	1.50	1.53
6	D	501	ADP	C5-C4	2.10	1.46	1.40
6	B	501	ADP	C4-N3	-2.10	1.32	1.35
6	F	501	ADP	C5-C4	2.09	1.46	1.40
6	E	501	ADP	C5-C4	2.05	1.46	1.40

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	501	ADP	PA-O3A-PB	-5.00	115.66	132.83
6	F	501	ADP	PA-O3A-PB	-4.25	118.23	132.83
6	D	501	ADP	N3-C2-N1	-3.62	123.03	128.68
6	E	501	ADP	C3'-C2'-C1'	3.39	106.08	100.98
6	D	501	ADP	PA-O3A-PB	-3.31	121.46	132.83
6	C	501	ADP	N3-C2-N1	-3.26	123.58	128.68
6	F	501	ADP	N3-C2-N1	-2.98	124.02	128.68
6	F	501	ADP	C3'-C2'-C1'	2.91	105.36	100.98
6	B	501	ADP	C4-C5-N7	-2.91	106.37	109.40
6	D	501	ADP	C3'-C2'-C1'	2.81	105.22	100.98
6	E	501	ADP	N3-C2-N1	-2.74	124.39	128.68
6	B	501	ADP	C5'-C4'-C3'	-2.41	106.15	115.18
6	F	501	ADP	C4-C5-N7	-2.35	106.95	109.40
6	C	501	ADP	O4'-C1'-C2'	-2.20	103.72	106.93
6	C	501	ADP	O3B-PB-O2B	2.12	115.73	107.64
6	B	501	ADP	O3B-PB-O2B	2.10	115.65	107.64
6	C	501	ADP	PA-O3A-PB	-2.08	125.69	132.83
6	C	501	ADP	C4-C5-N7	-2.07	107.24	109.40
6	B	501	ADP	PA-O3A-PB	-2.06	125.77	132.83
6	E	501	ADP	C4-C5-N7	-2.06	107.26	109.40
6	D	501	ADP	C2-N1-C6	2.00	122.18	118.75

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	D	501	ADP	C5'-O5'-PA-O1A
6	D	501	ADP	C5'-O5'-PA-O2A
6	F	501	ADP	C5'-O5'-PA-O1A
6	F	501	ADP	C5'-O5'-PA-O3A
6	C	501	ADP	O4'-C4'-C5'-O5'

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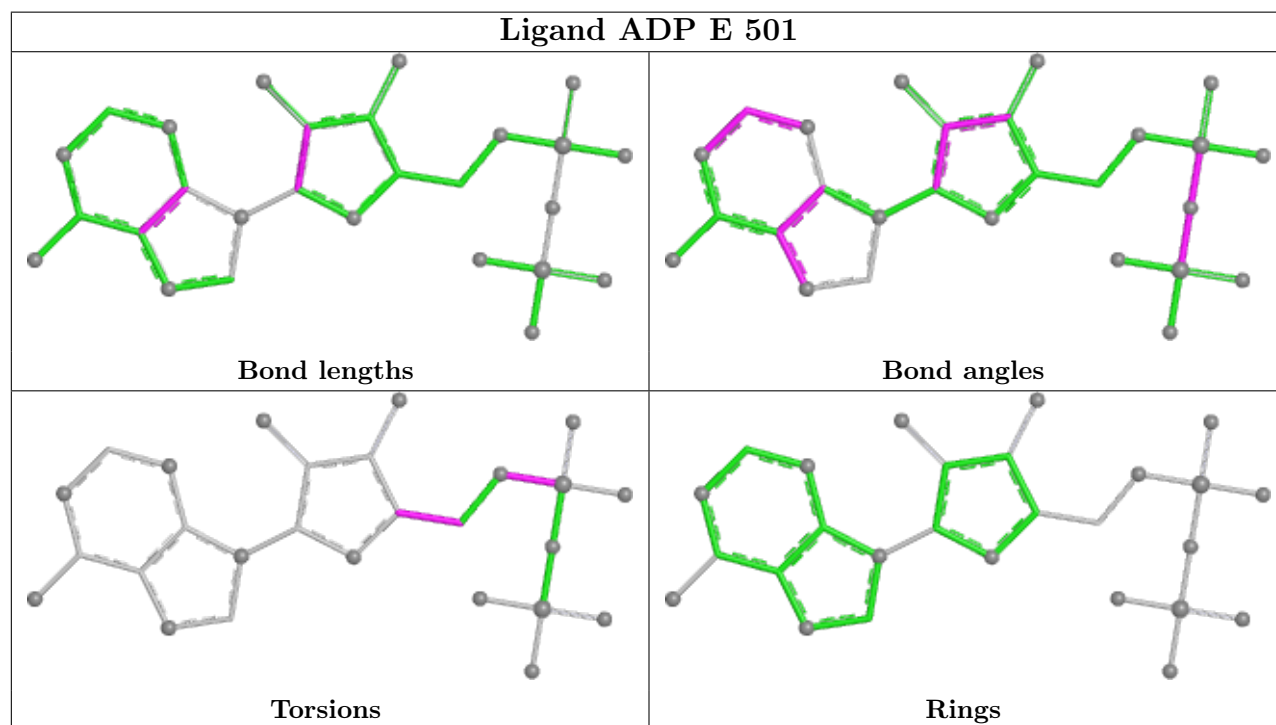
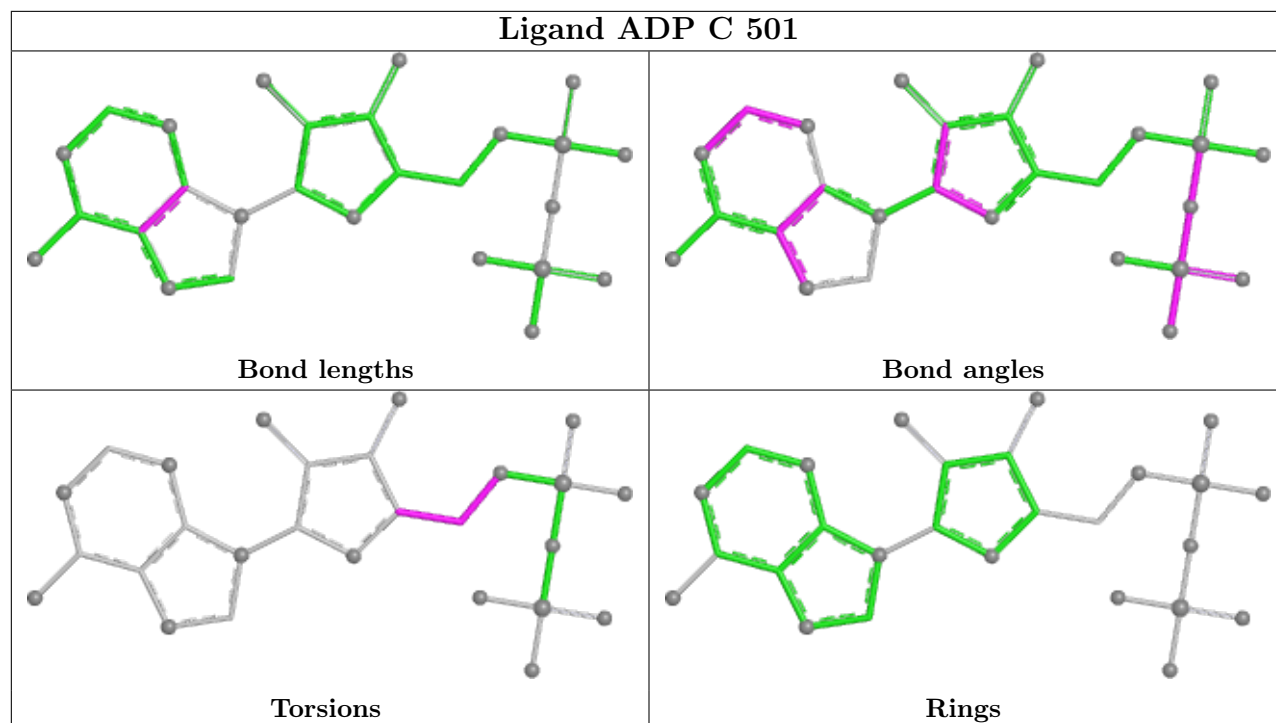
Mol	Chain	Res	Type	Atoms
6	C	501	ADP	C3'-C4'-C5'-O5'
6	B	501	ADP	O4'-C4'-C5'-O5'
6	B	501	ADP	C3'-C4'-C5'-O5'
6	E	501	ADP	O4'-C4'-C5'-O5'
6	D	501	ADP	O4'-C4'-C5'-O5'
6	E	501	ADP	C3'-C4'-C5'-O5'
6	F	501	ADP	O4'-C4'-C5'-O5'
6	F	501	ADP	PB-O3A-PA-O1A
6	F	501	ADP	C5'-O5'-PA-O2A
6	F	501	ADP	C3'-C4'-C5'-O5'
6	F	501	ADP	PB-O3A-PA-O2A
6	C	501	ADP	C4'-C5'-O5'-PA
6	D	501	ADP	C5'-O5'-PA-O3A
6	E	501	ADP	C5'-O5'-PA-O3A
6	B	501	ADP	C4'-C5'-O5'-PA

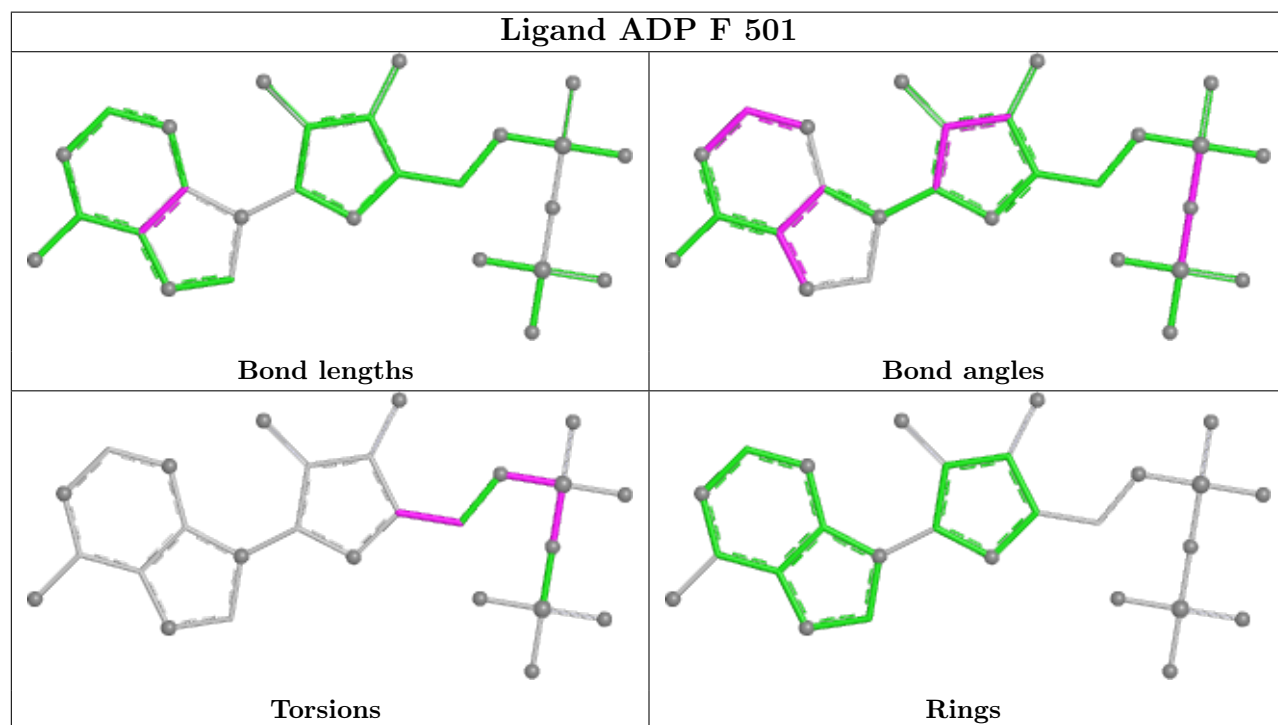
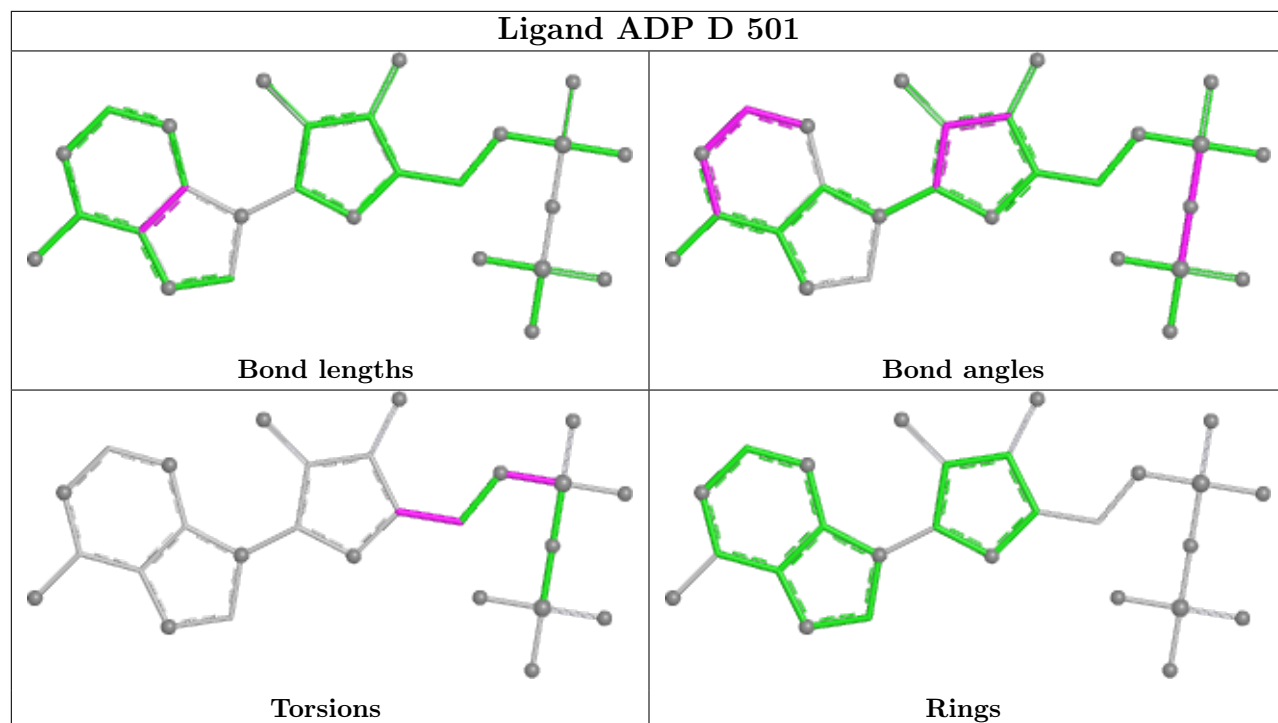
There are no ring outliers.

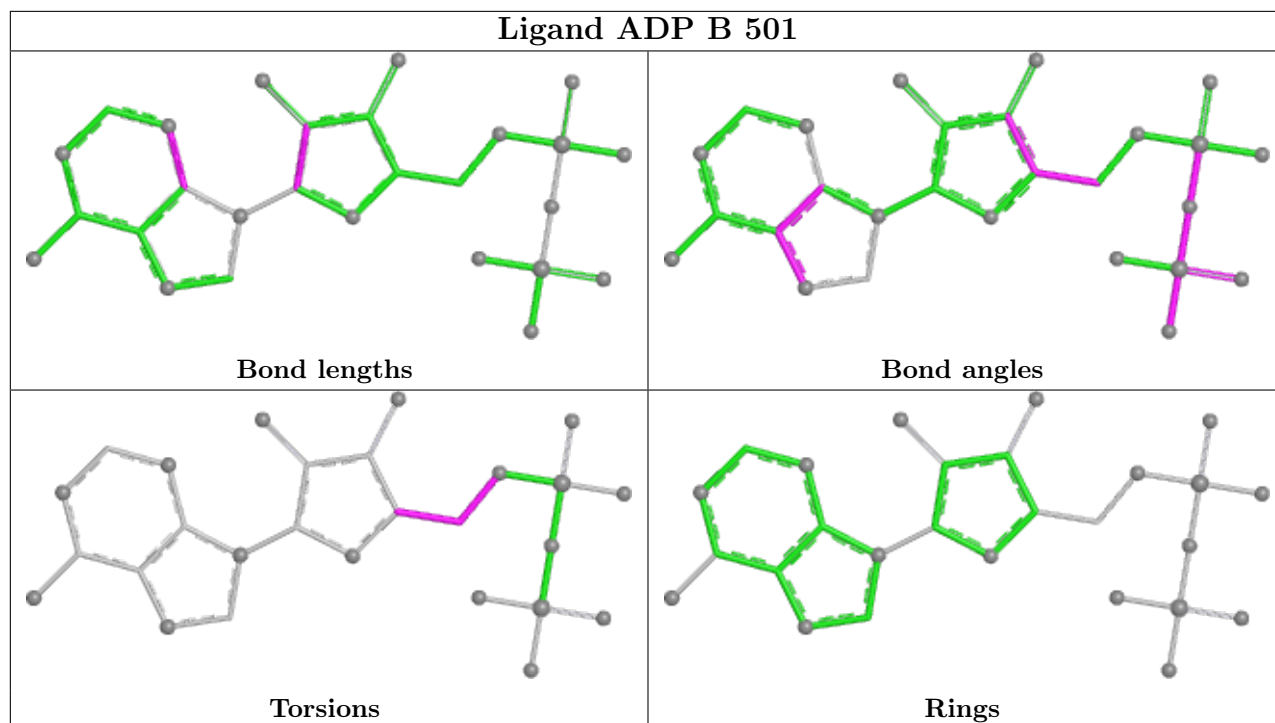
4 monomers are involved in 44 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	E	501	ADP	5	0
6	D	501	ADP	20	0
6	F	501	ADP	6	0
6	B	501	ADP	13	0

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







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	J	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	J	60:UNK	C	70:UNK	N	9.60

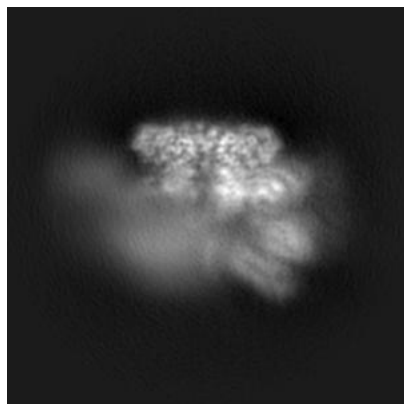
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12979. These allow visual inspection of the internal detail of the map and identification of artifacts.

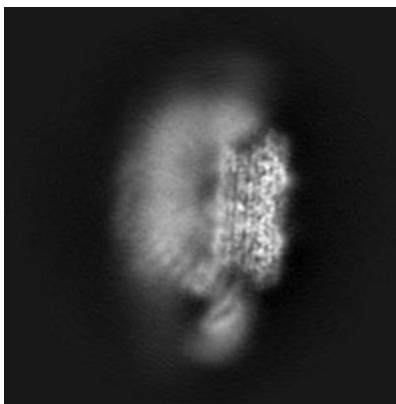
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

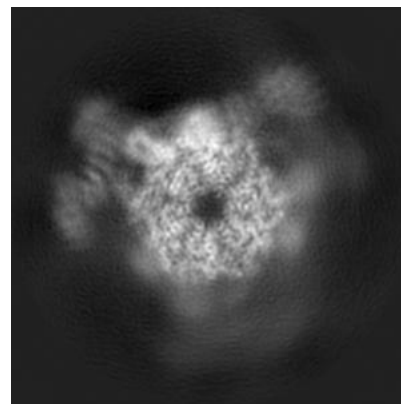
6.1.1 Primary map



X

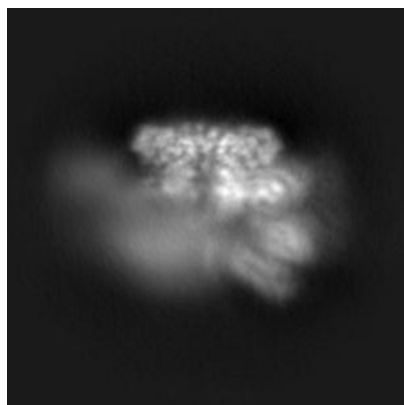


Y

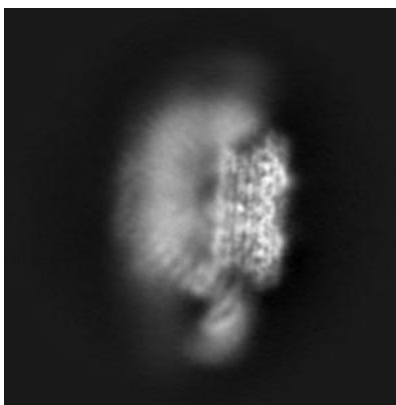


Z

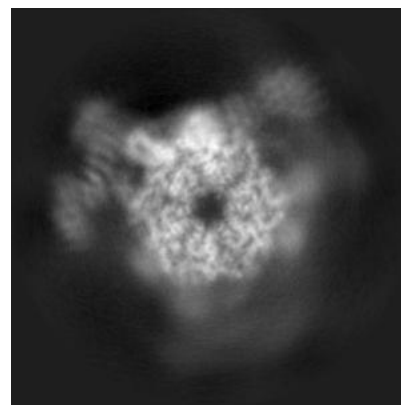
6.1.2 Raw map



X



Y

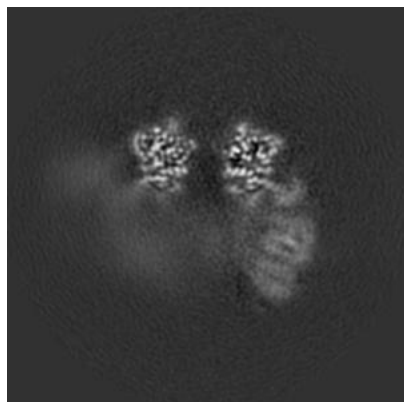


Z

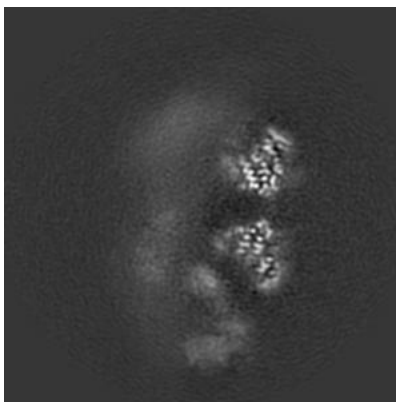
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

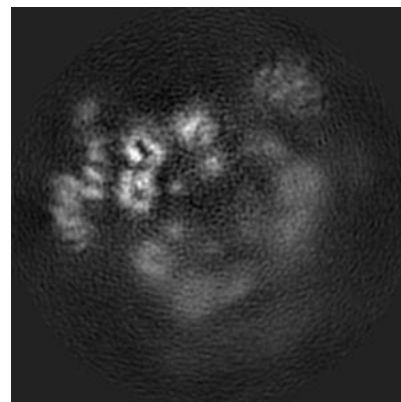
6.2.1 Primary map



X Index: 140

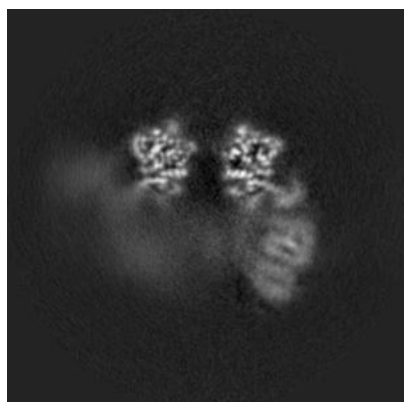


Y Index: 140

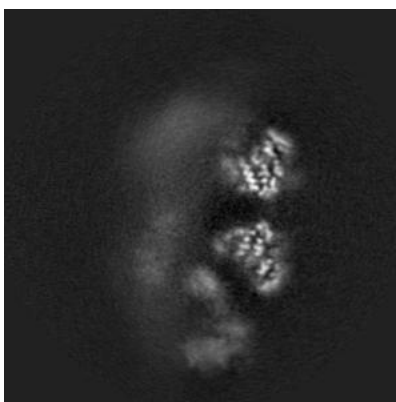


Z Index: 140

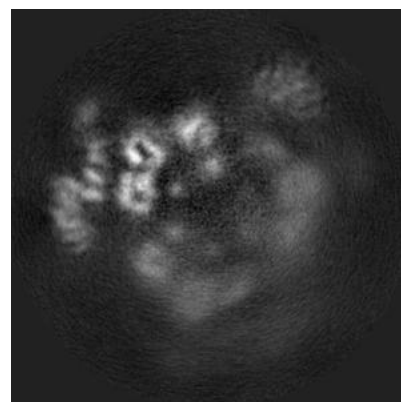
6.2.2 Raw map



X Index: 140



Y Index: 140

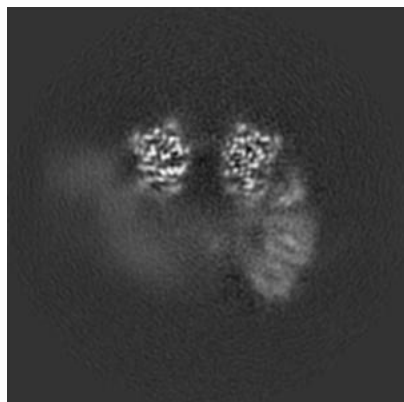


Z Index: 140

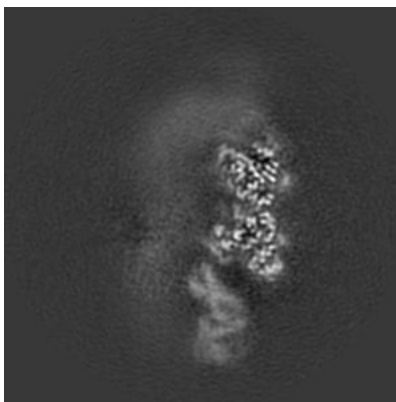
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

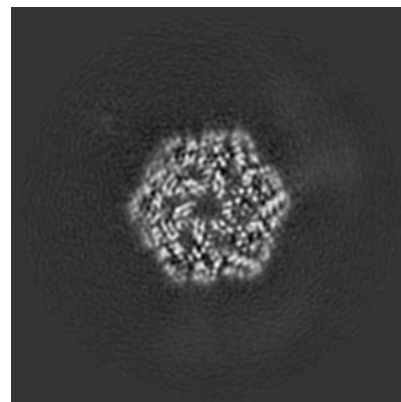
6.3.1 Primary map



X Index: 138

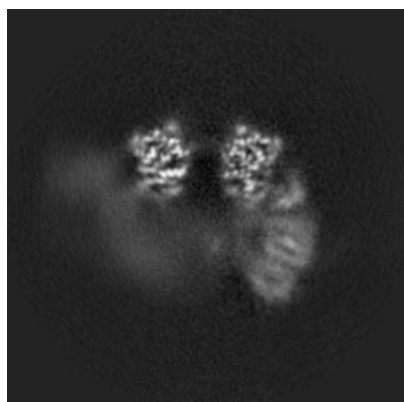


Y Index: 152

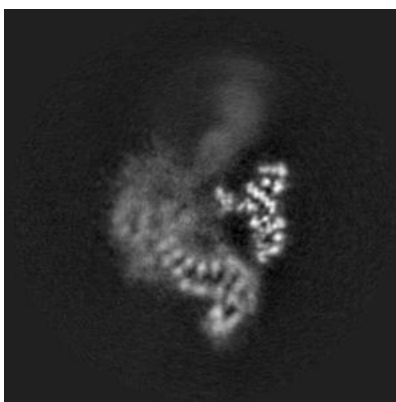


Z Index: 185

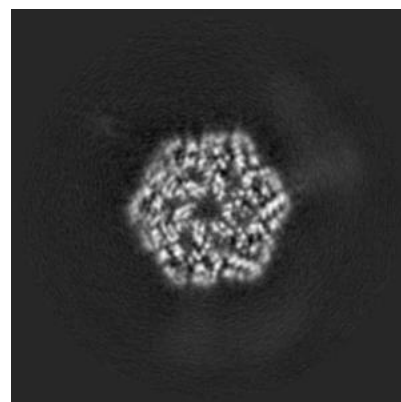
6.3.2 Raw map



X Index: 138



Y Index: 181

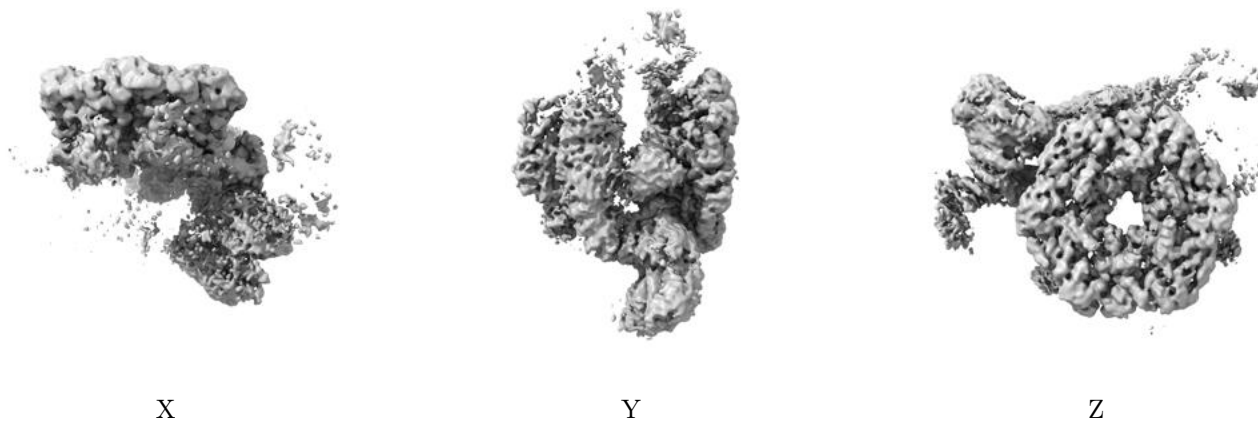


Z Index: 185

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

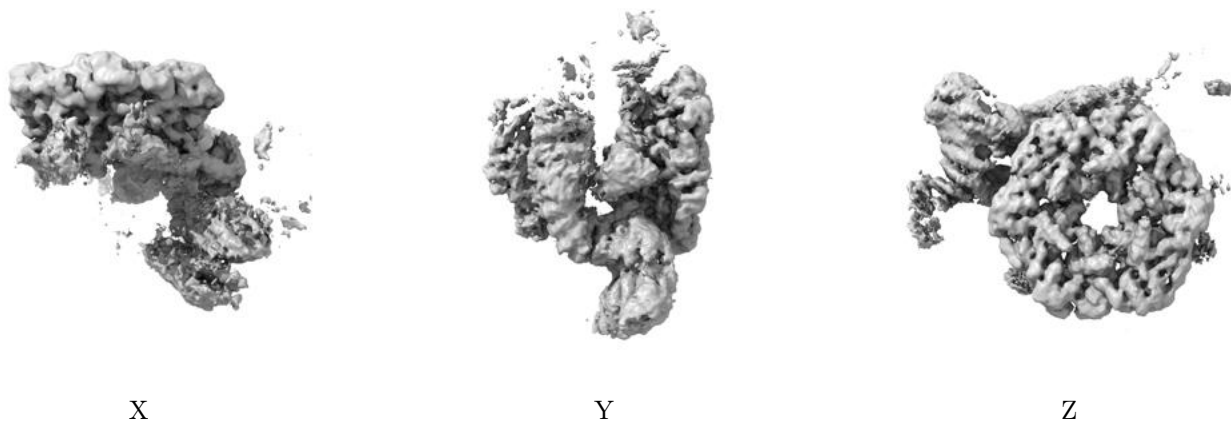
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0106. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

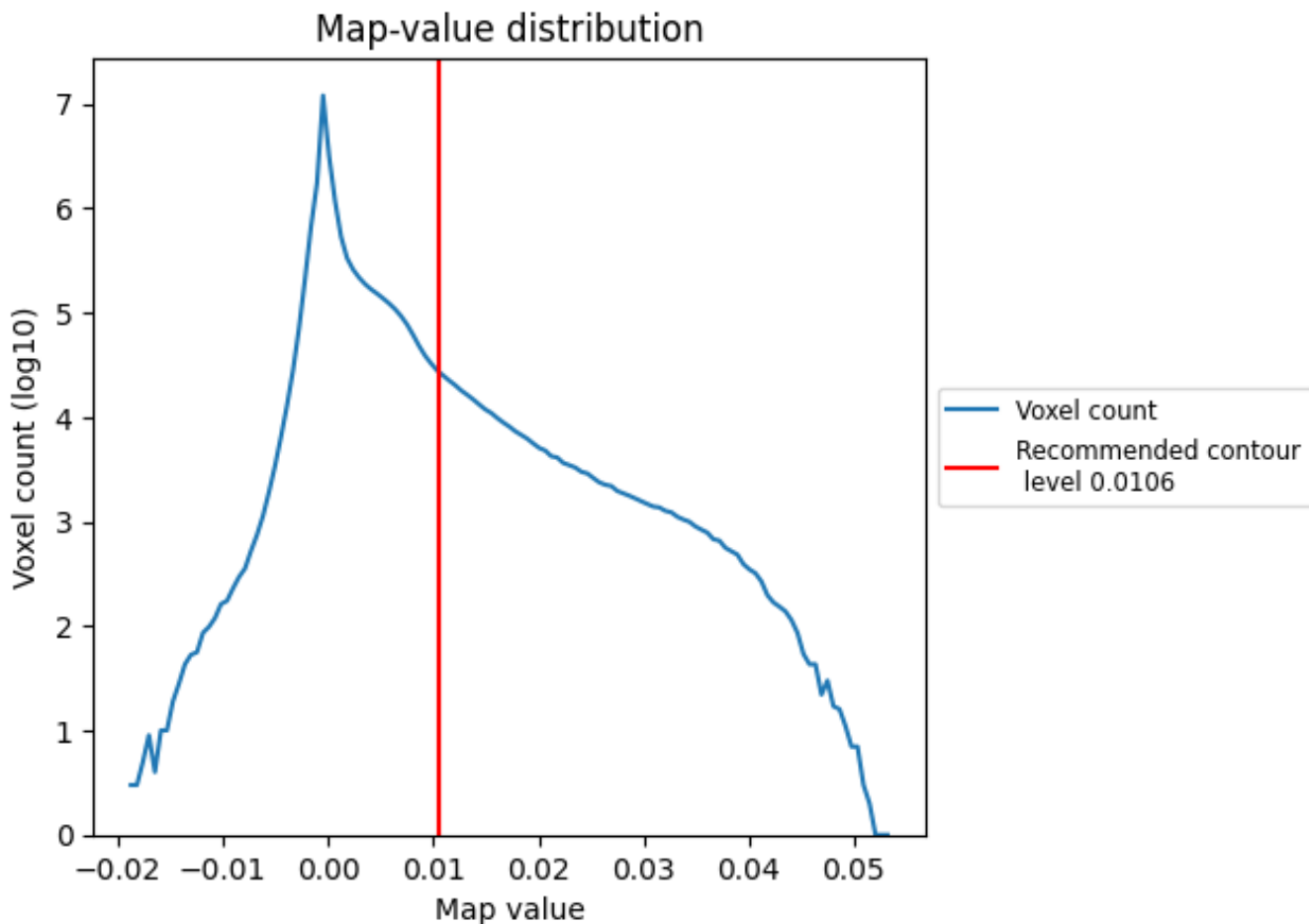
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

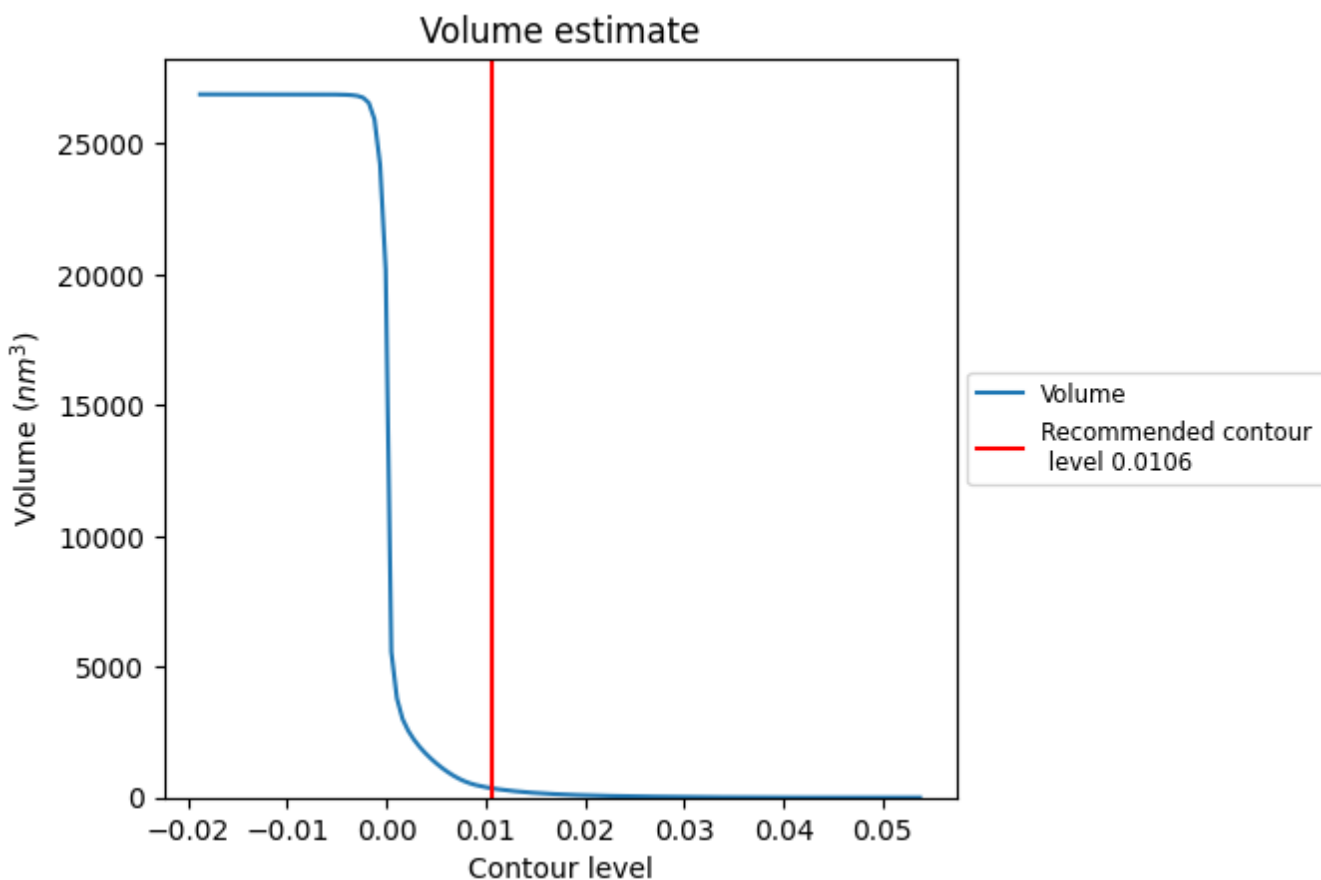
This section contains the results of statistical analysis of the map.

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.

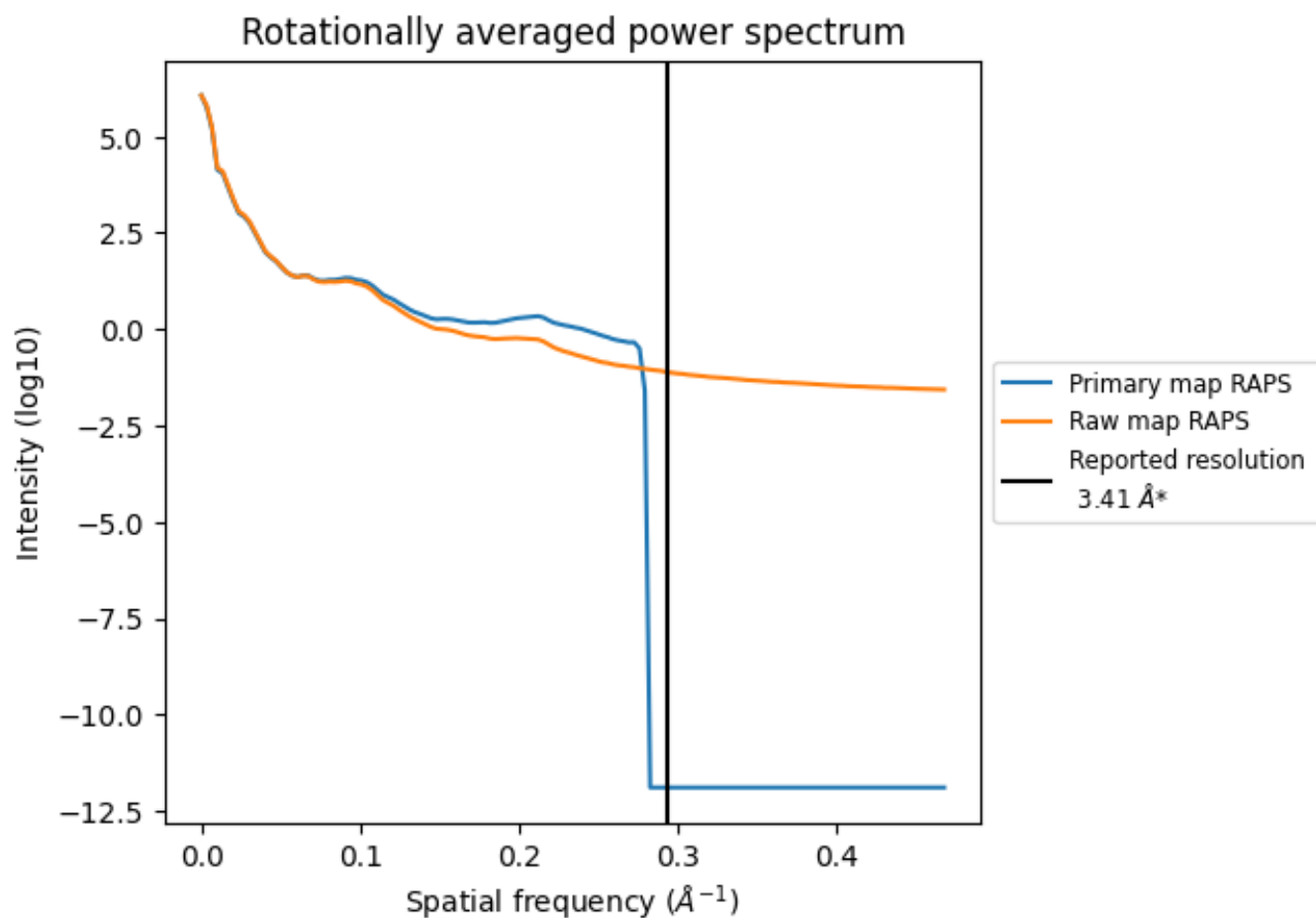
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 357 nm^3 ; this corresponds to an approximate mass of 323 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 [i](#)

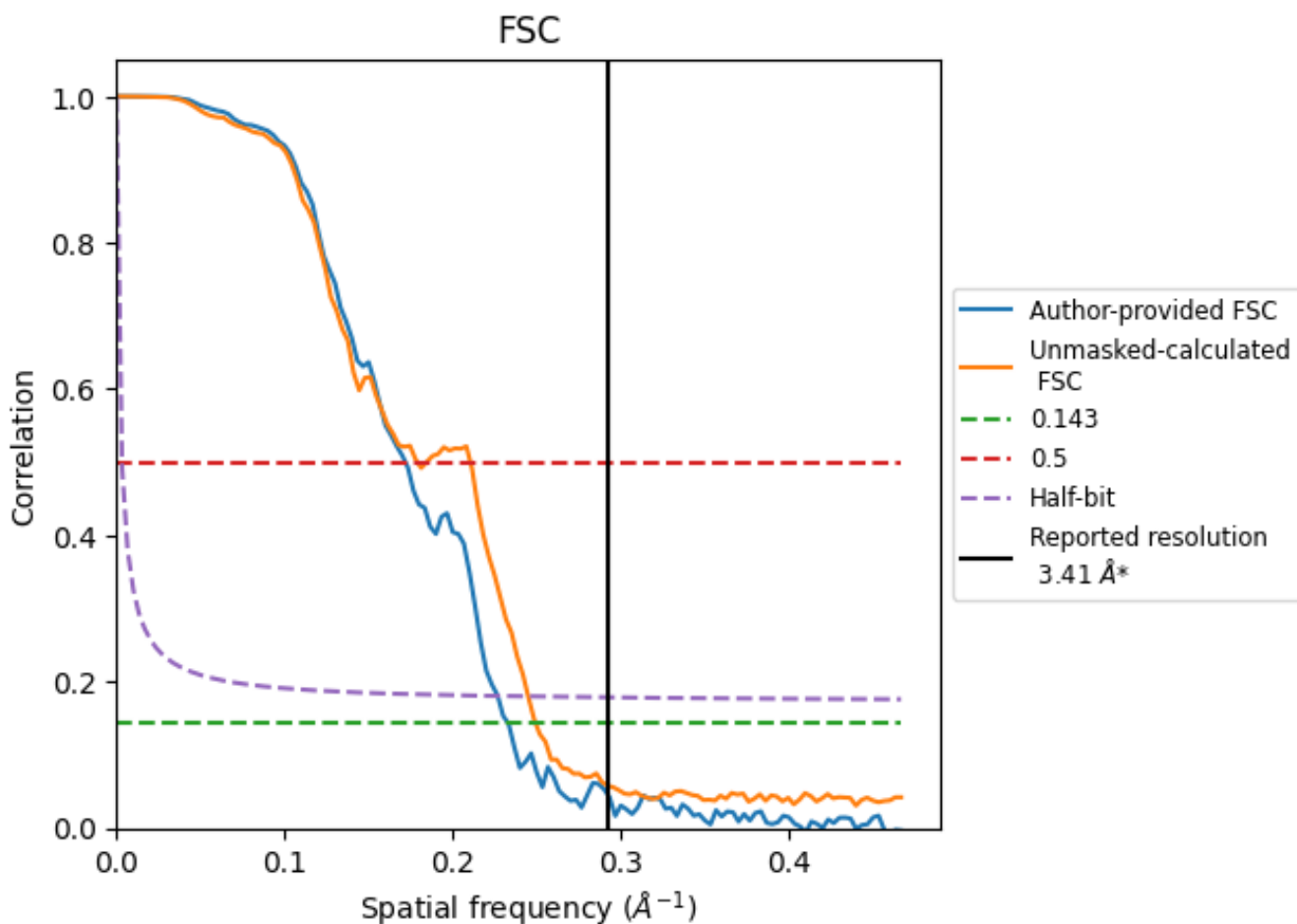


*Reported resolution corresponds to spatial frequency of 0.293 Å⁻¹

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 0.293\AA^{-1}

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.41	-	-
Author-provided FSC curve	4.28	5.81	4.40
Unmasked-calculated*	4.01	5.58	4.08

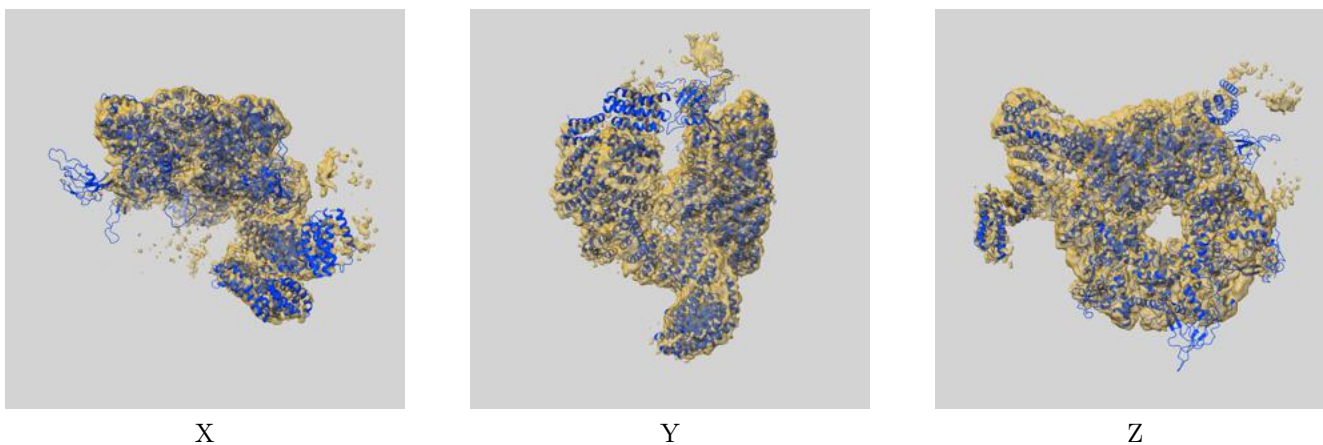
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 4.28 differs from the reported value 3.41 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.01 differs from the reported value 3.41 by more than 10 %

9 Map-model fit [i](#)

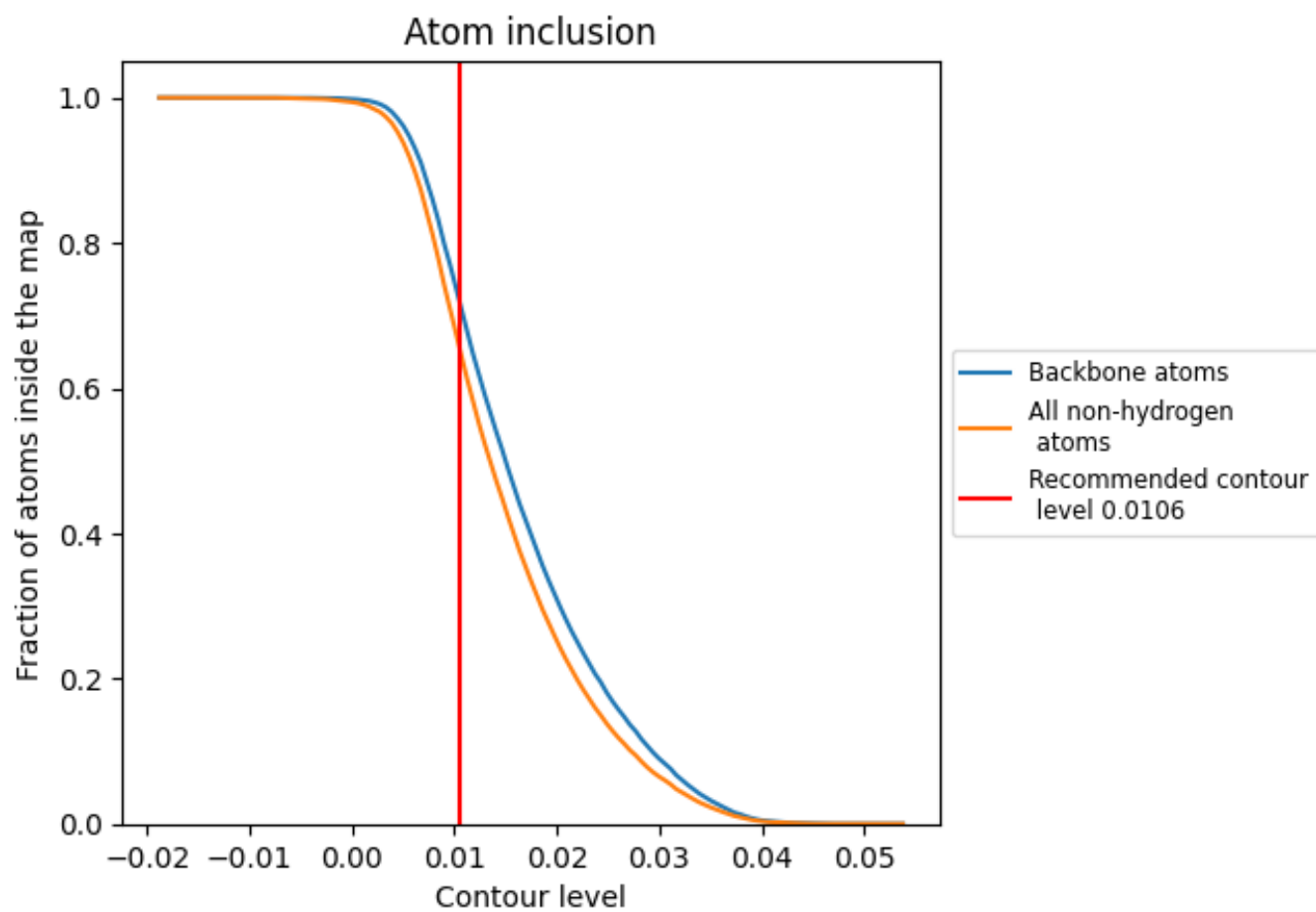
This section contains information regarding the fit between EMDB map EMD-12979 and PDB model 7OLE. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.0106 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 Atom inclusion [i](#)



At the recommended contour level, 71% of all backbone atoms, 65% of all non-hydrogen atoms, are inside the map.