



Full wwPDB EM Validation Report ⓘ

Nov 6, 2022 – 07:43 PM EST

PDB ID : 6NR8
EMDB ID : EMD-0490
Title : hTRiC-hPFD Class6
Authors : Gestaut, D.R.; Roh, S.H.; Ma, B.; Pintilie, G.; Joachimiak, L.A.; Leitner, A.; Walzthoeni, T.; Aebersold, R.; Chiu, W.; Frydman, J.
Deposited on : 2019-01-23
Resolution : 7.80 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

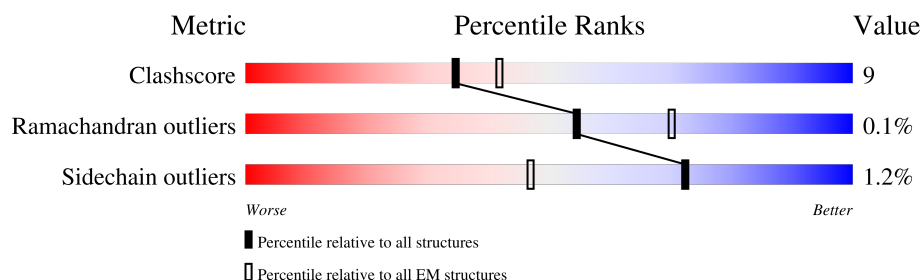
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 7.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	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	1	107	<div> <div>12%</div> <div>87%</div> <div>13%</div> </div>
2	2	103	<div> <div>58%</div> <div>83%</div> <div>17%</div> </div>
3	3	132	<div> <div>25%</div> <div>72%</div> <div>26%</div> </div>
4	4	104	<div> <div>14%</div> <div>81%</div> <div>18%</div> </div>
5	5	127	<div> <div>17%</div> <div>81%</div> <div>19%</div> </div>
6	6	102	<div> <div>14%</div> <div>80%</div> <div>20%</div> </div>
7	A	534	<div> <div>22%</div> <div>69%</div> <div>27%</div> </div>
7	I	534	<div> <div>32%</div> <div>81%</div> <div>19%</div> </div>

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Mol	Chain	Length	Quality of chain
8	B	509	
8	J	509	
9	C	513	
9	K	513	
10	D	514	
10	L	514	
11	E	517	
11	M	517	
12	F	515	
12	N	515	
13	G	514	
13	O	514	
14	H	514	
14	P	514	

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 68284 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Prefoldin subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	107	Total	C	N	O	S	0	0
			874	546	150	173	5		

- Molecule 2 is a protein called Prefoldin subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	103	Total	C	N	O	S	0	0
			830	513	151	163	3		

- Molecule 3 is a protein called Prefoldin subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	132	Total	C	N	O	S	0	0
			1087	690	179	210	8		

- Molecule 4 is a protein called Prefoldin subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	104	Total	C	N	O	S	0	0
			847	523	142	177	5		

- Molecule 5 is a protein called Prefoldin subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	5	127	Total	C	N	O	S	0	0
			1018	647	166	197	8		

- Molecule 6 is a protein called Prefoldin subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6	102	Total	C	N	O	S	0	0
			826	511	148	166	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A	521	Total	C	N	O	S	0	0
			3956	2479	691	763	23		
7	I	534	Total	C	N	O	S	0	0
			4056	2540	709	783	24		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	B	509	Total	C	N	O	S	0	0
			3829	2392	673	745	19		
8	J	508	Total	C	N	O	S	0	0
			3823	2389	672	743	19		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	C	509	Total	C	N	O	S	0	0
			3956	2465	697	764	30		
9	K	513	Total	C	N	O	S	0	0
			3985	2481	703	771	30		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	D	508	Total	C	N	O	S	0	0
			3832	2398	665	746	23		
10	L	513	Total	C	N	O	S	0	0
			3873	2422	674	754	23		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	E	517	Total	C	N	O	S	0	0
			3974	2483	692	769	30		
11	M	517	Total	C	N	O	S	0	0
			3974	2483	692	769	30		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	F	514	Total	C	N	O	S	0	0
			3945	2478	690	757	20		
12	N	513	Total	C	N	O	S	0	0
			3940	2476	689	755	20		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	G	512	Total	C	N	O	S	0	0
			3936	2485	682	746	23		
13	O	514	Total	C	N	O	S	0	0
			3947	2490	684	750	23		

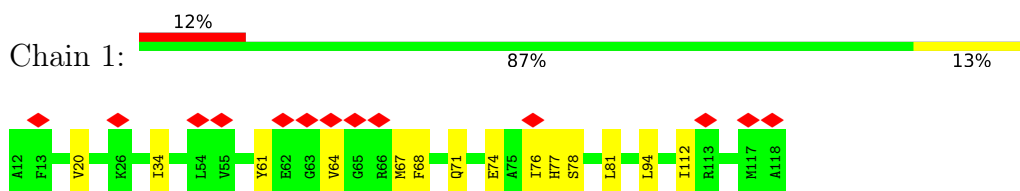
- Molecule 14 is a protein called T-complex protein 1 subunit theta.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	H	510	Total	C	N	O	S	0	0
			3892	2451	661	754	26		
14	P	509	Total	C	N	O	S	0	0
			3884	2447	659	752	26		

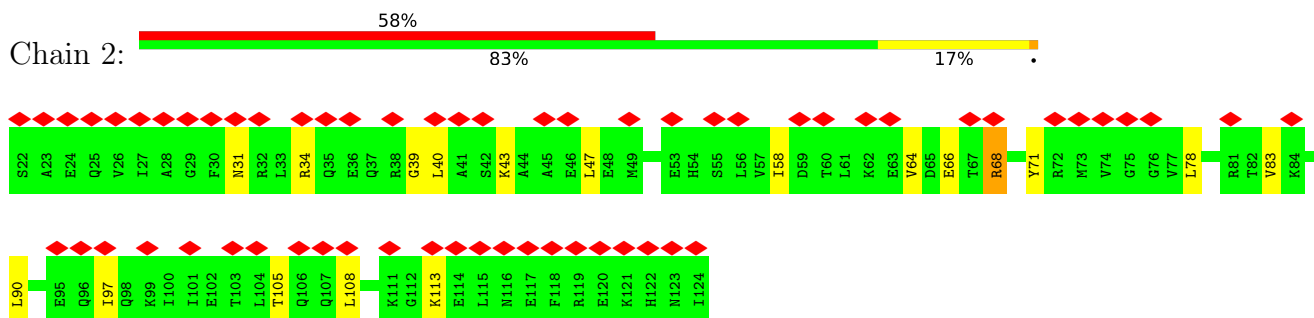
3 Residue-property plots

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.

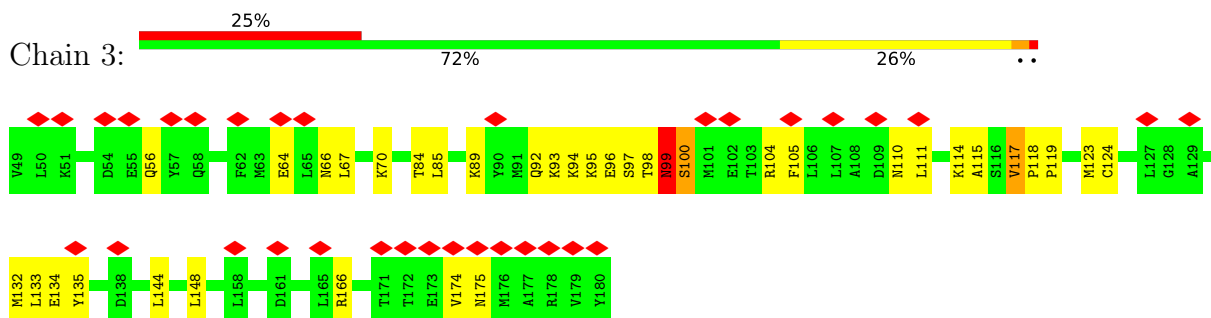
- Molecule 1: Prefoldin subunit 1



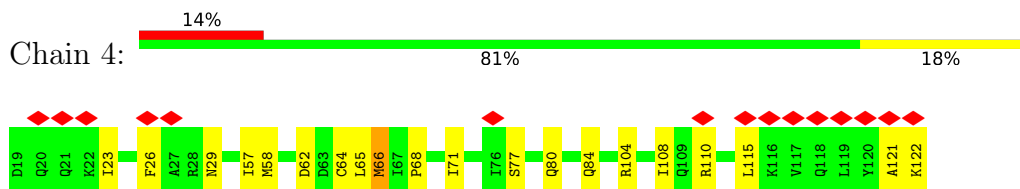
- Molecule 2: Prefoldin subunit 2



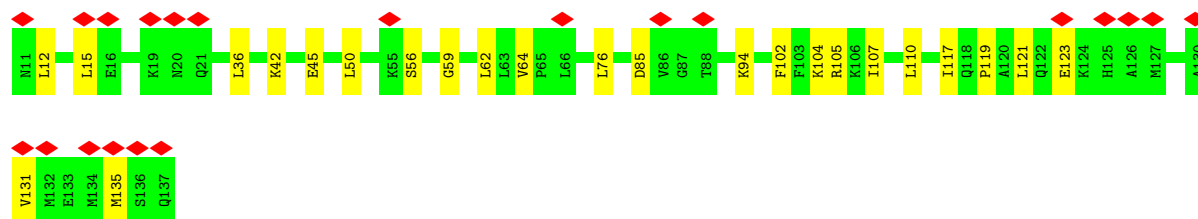
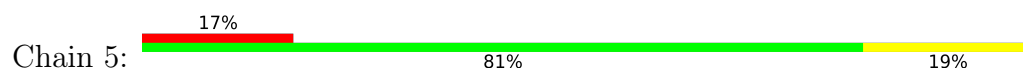
- Molecule 3: Prefoldin subunit 3



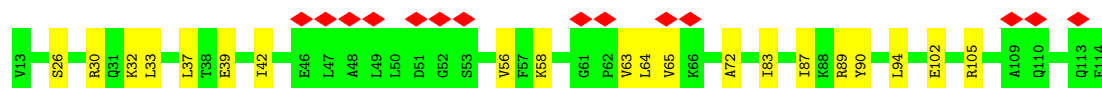
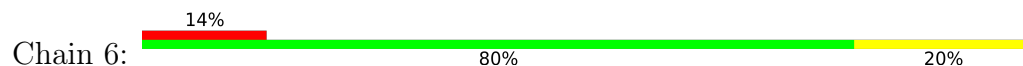
- Molecule 4: Prefoldin subunit 4



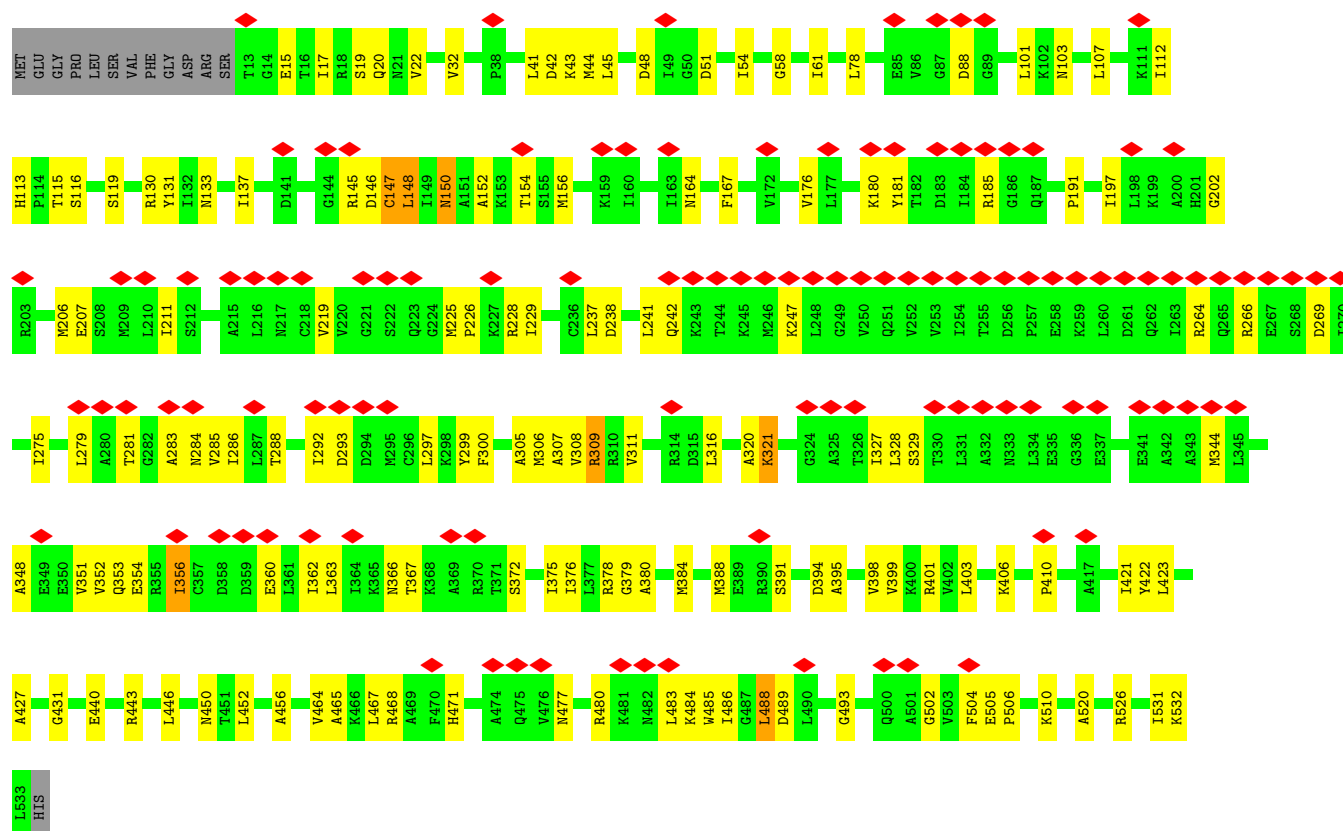
- Molecule 5: Prefoldin subunit 5



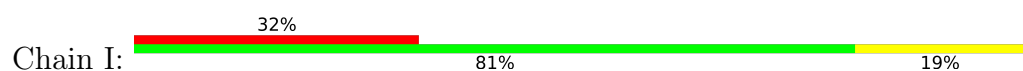
• Molecule 6: Prefoldin subunit 6

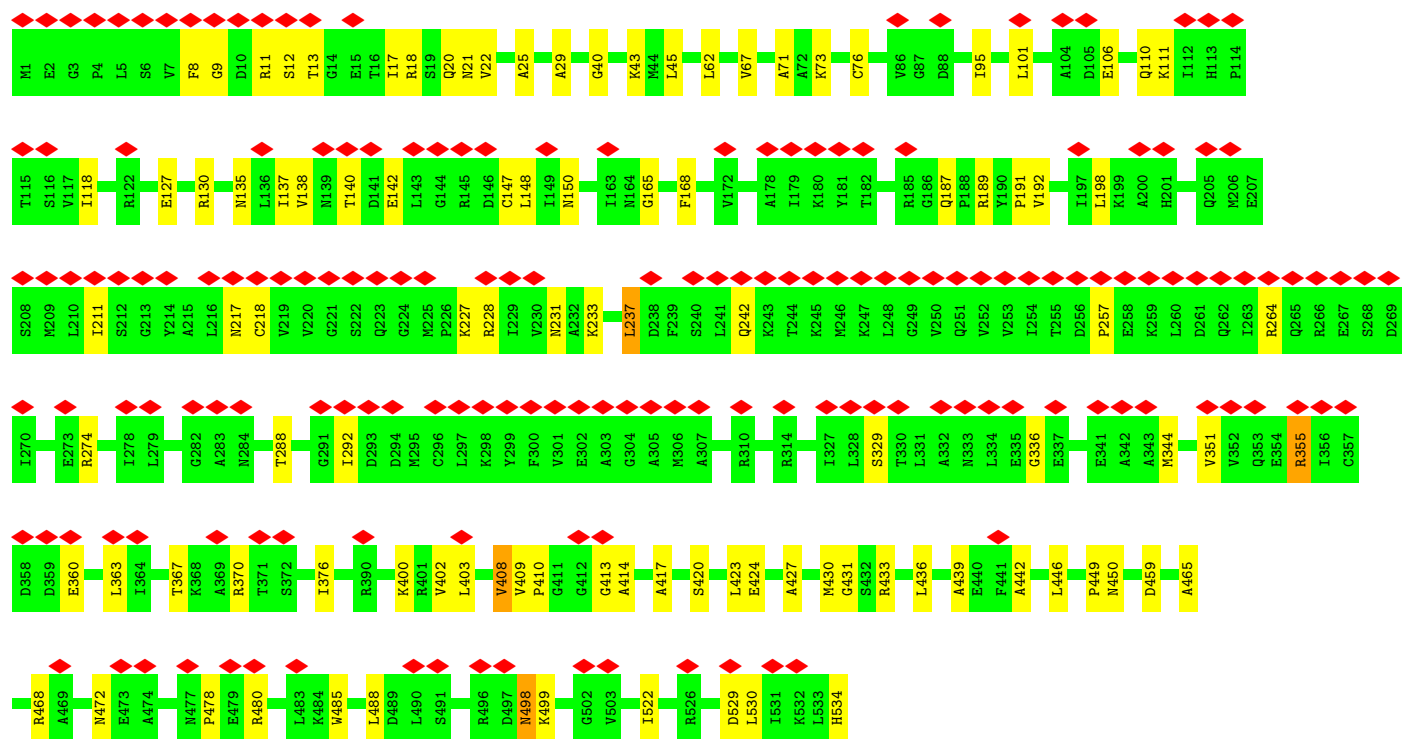


• Molecule 7: T-complex protein 1 subunit alpha

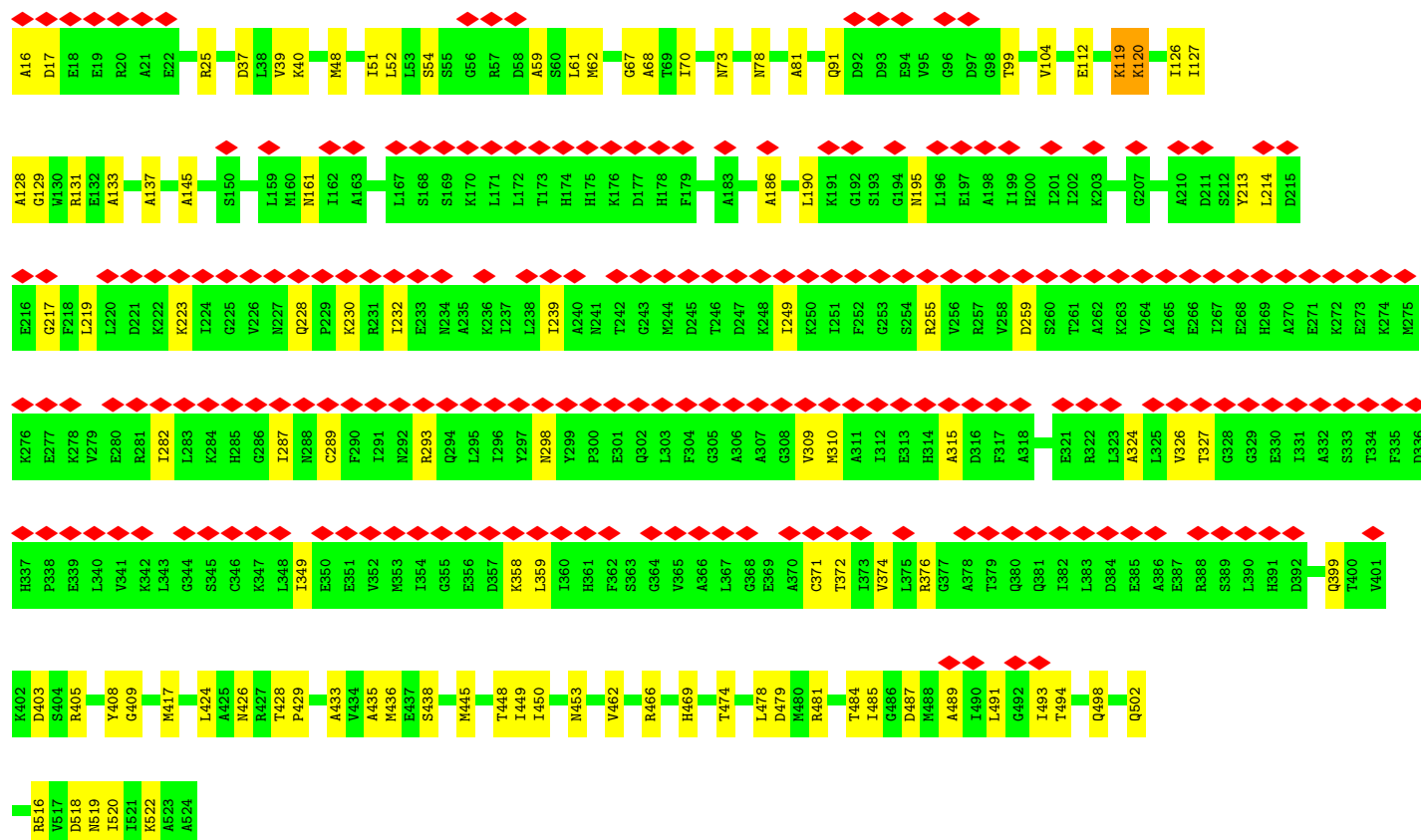
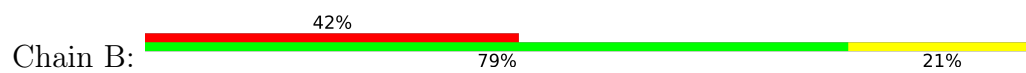


• Molecule 7: T-complex protein 1 subunit alpha

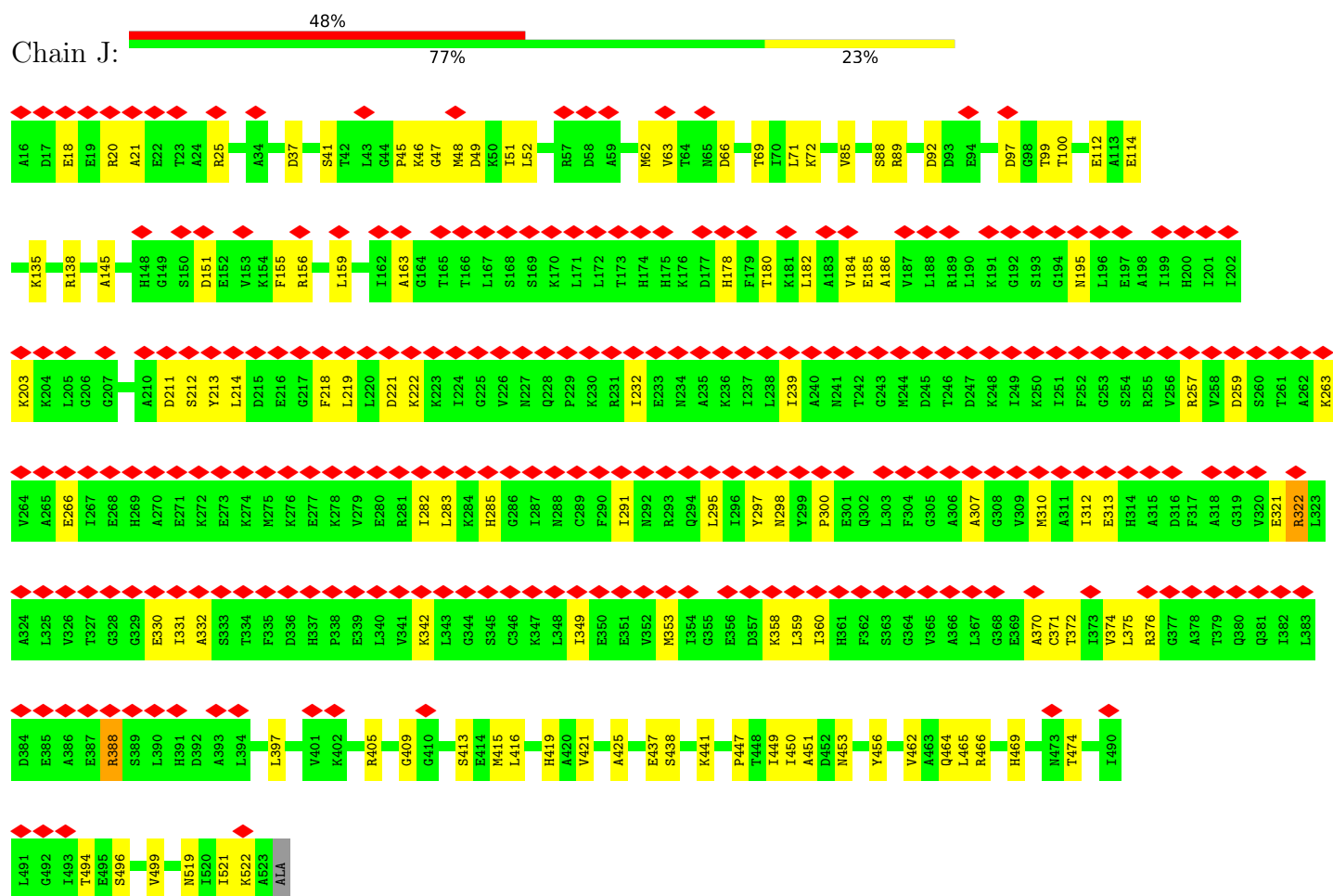




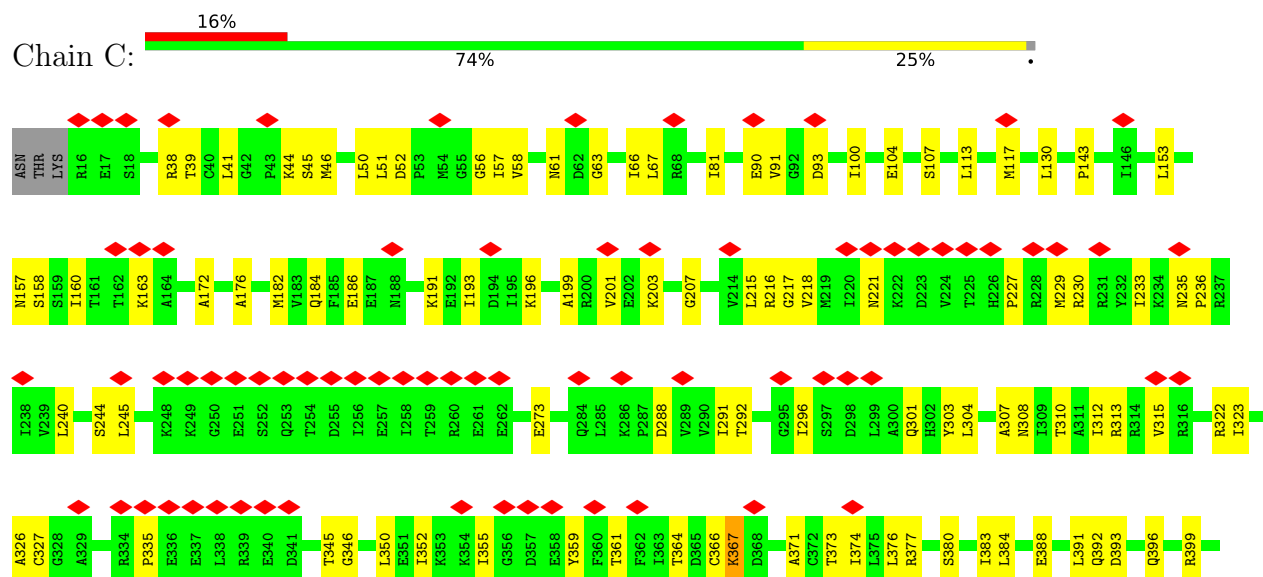
• Molecule 8: T-complex protein 1 subunit beta

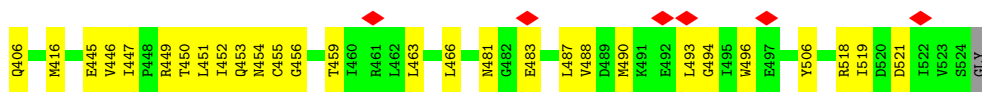


• Molecule 8: T-complex protein 1 subunit beta

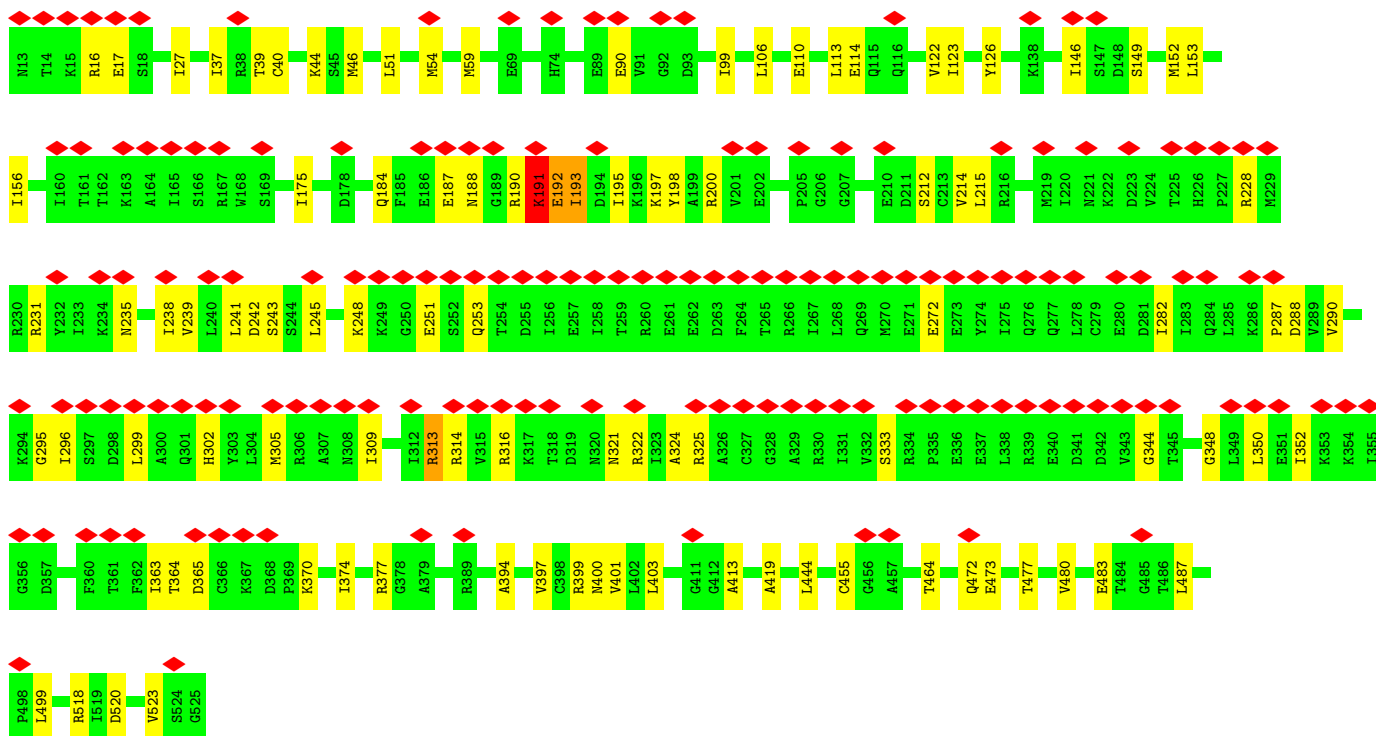
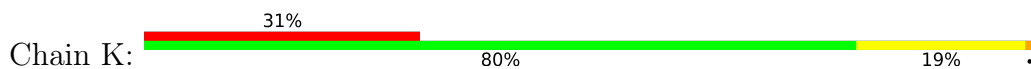


• Molecule 9: T-complex protein 1 subunit gamma

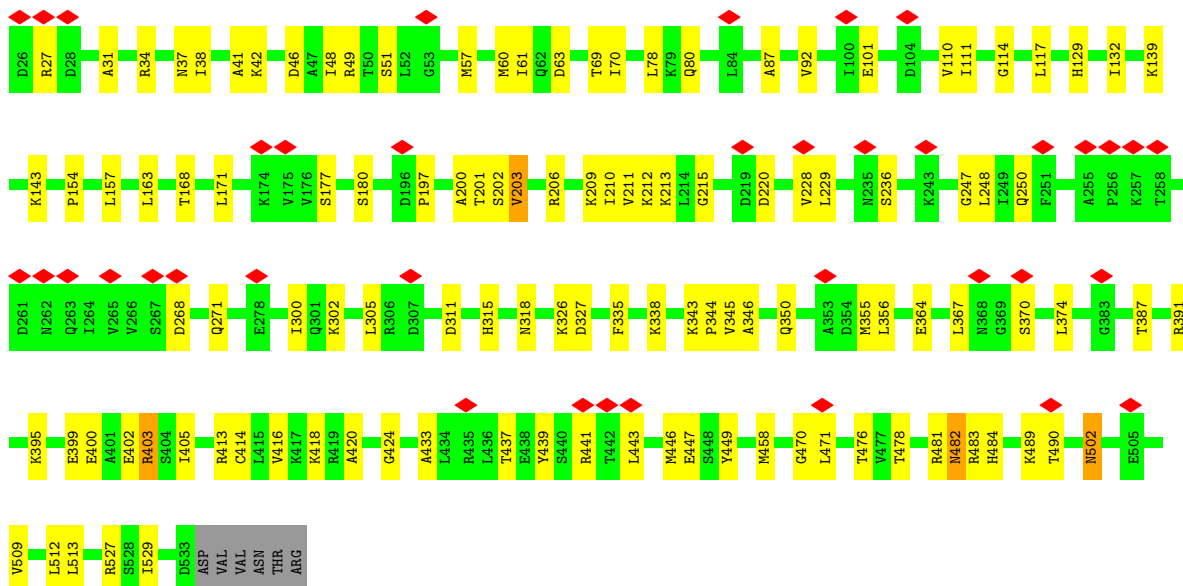
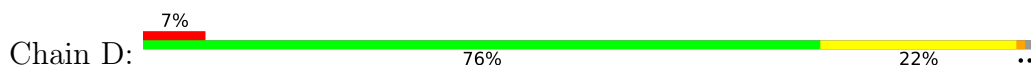




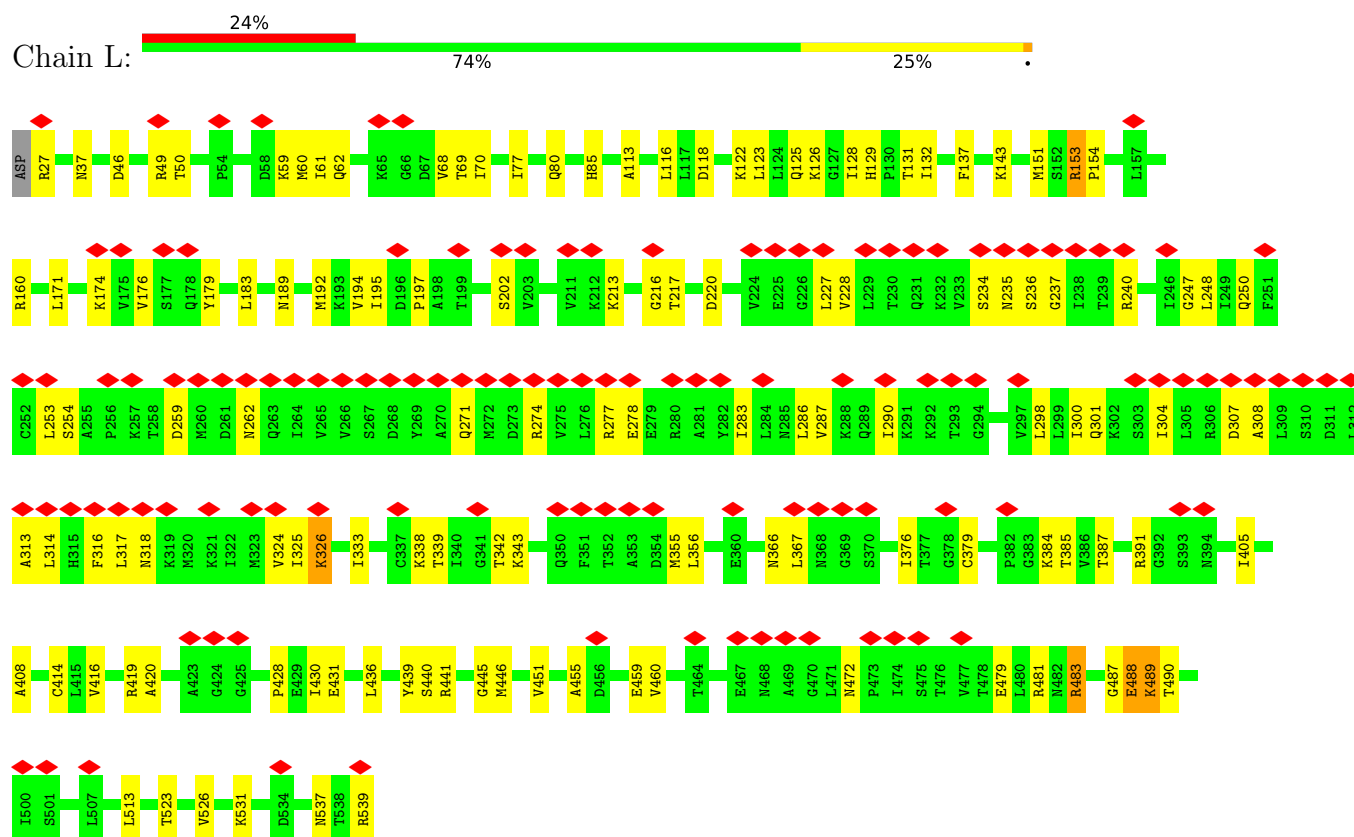
• Molecule 9: T-complex protein 1 subunit gamma



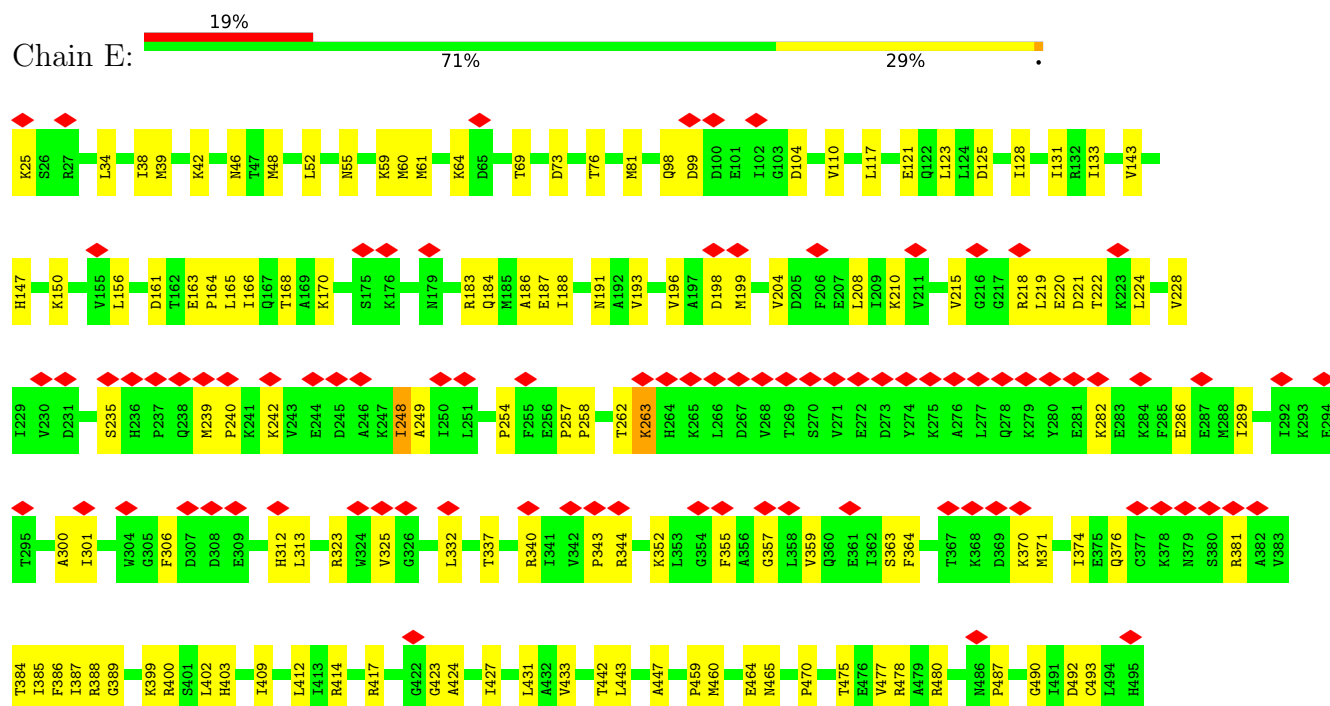
• Molecule 10: T-complex protein 1 subunit delta

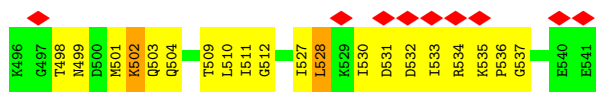


• Molecule 10: T-complex protein 1 subunit delta

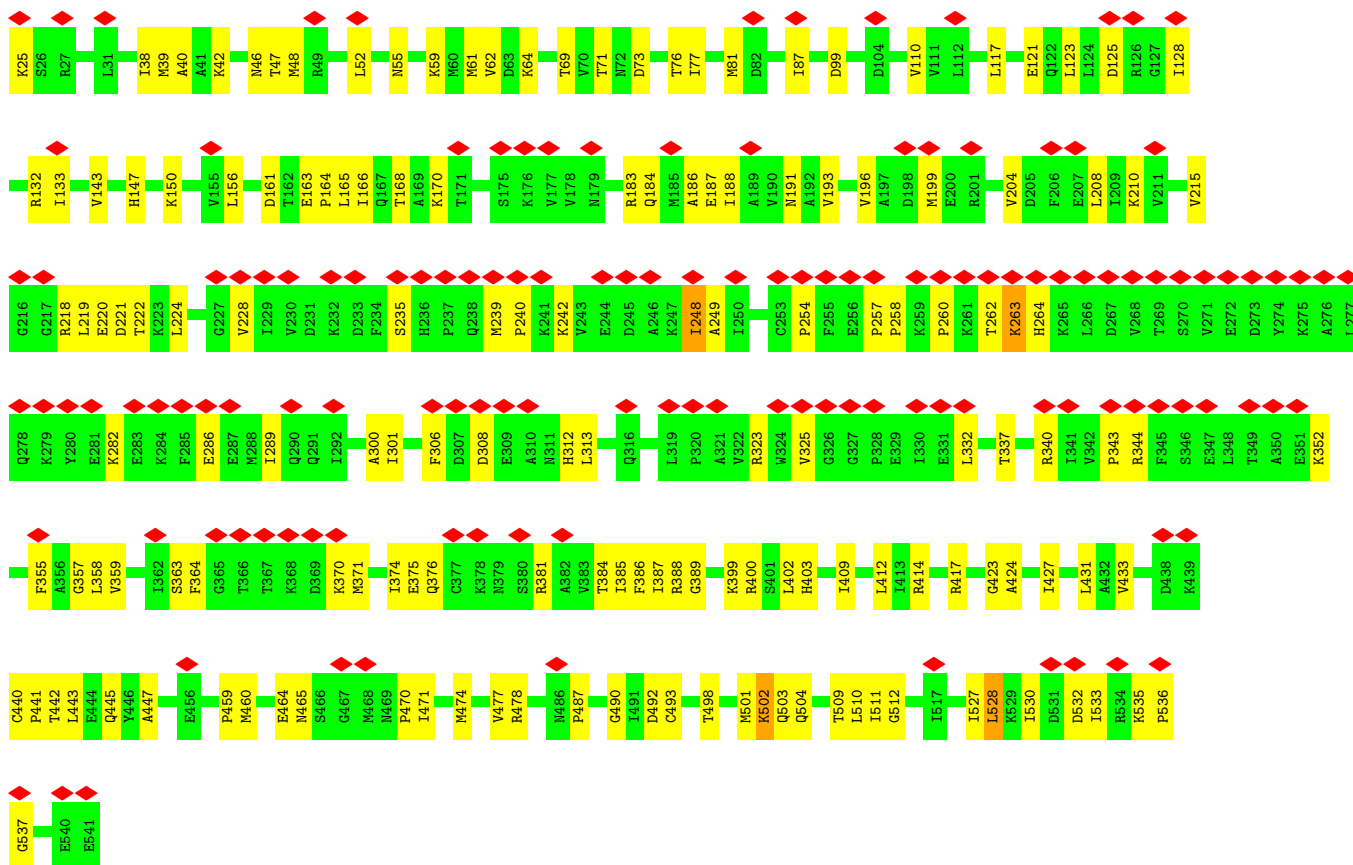


• Molecule 11: T-complex protein 1 subunit epsilon

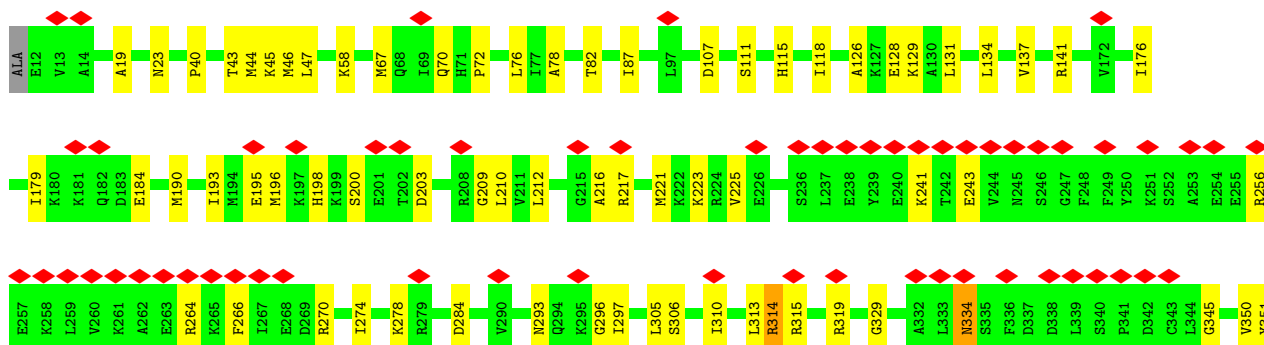
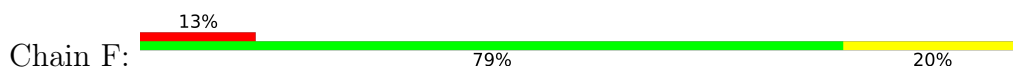


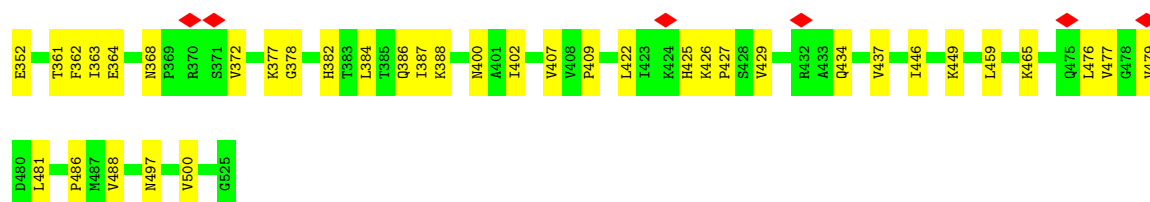


• Molecule 11: T-complex protein 1 subunit epsilon

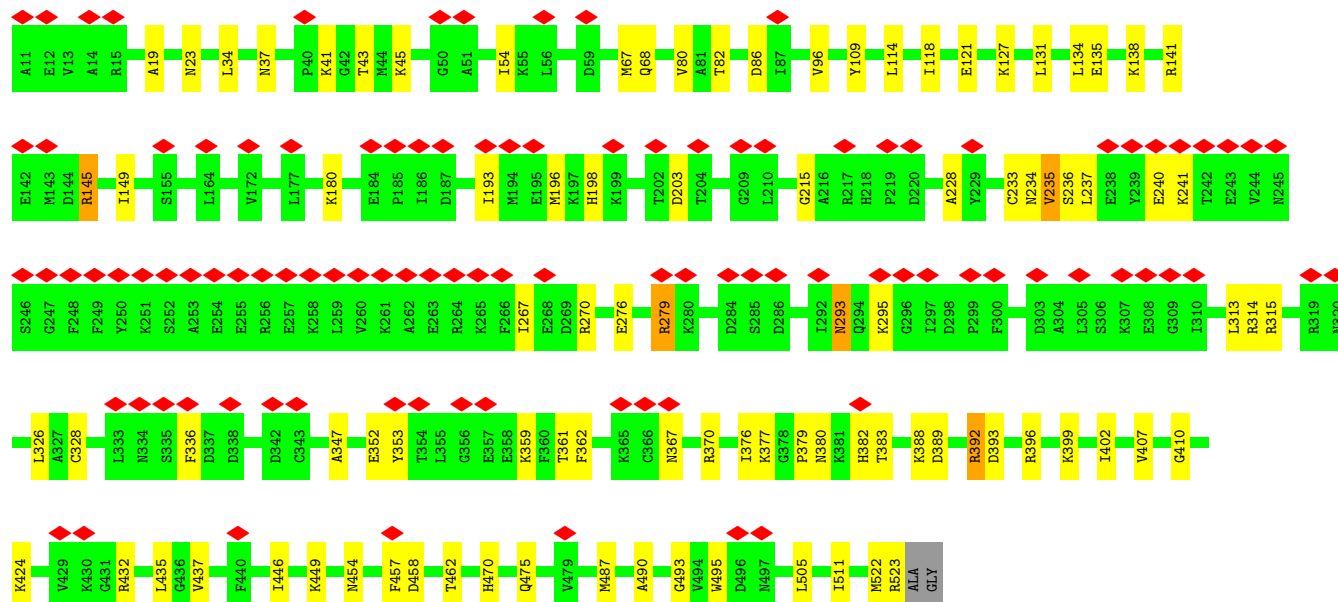
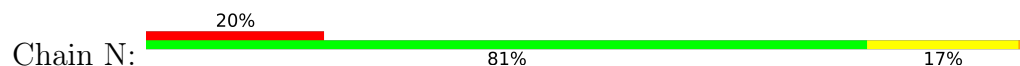


• Molecule 12: T-complex protein 1 subunit zeta

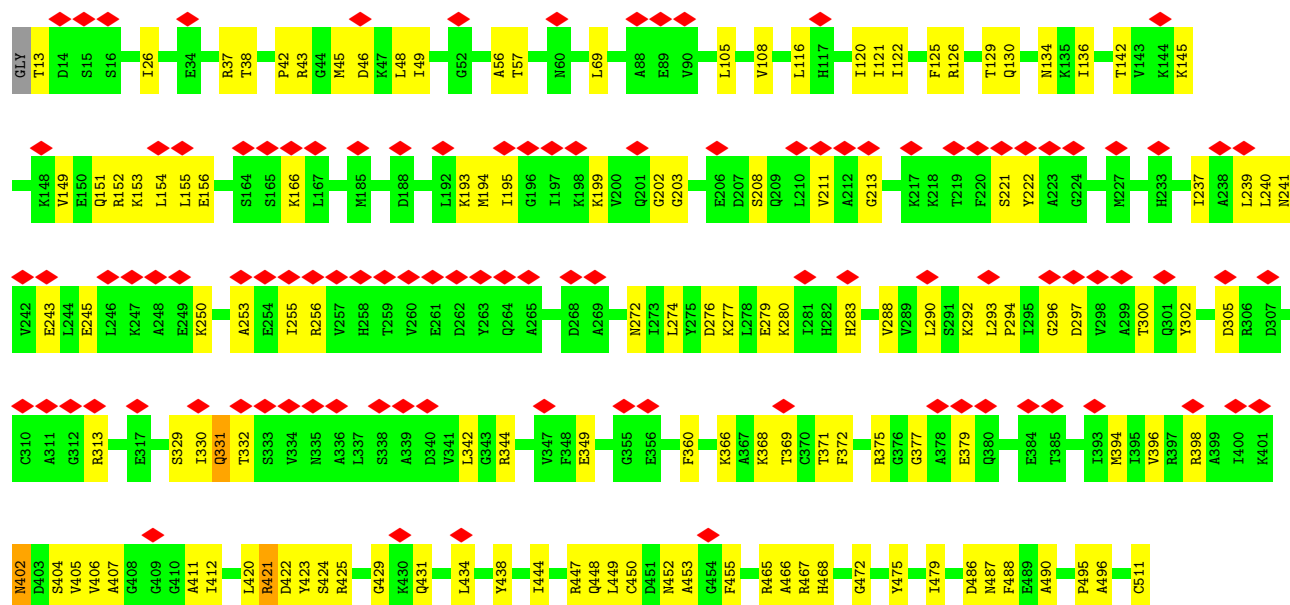
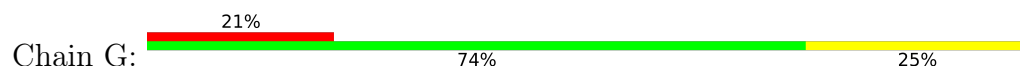


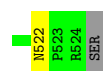


• Molecule 12: T-complex protein 1 subunit zeta

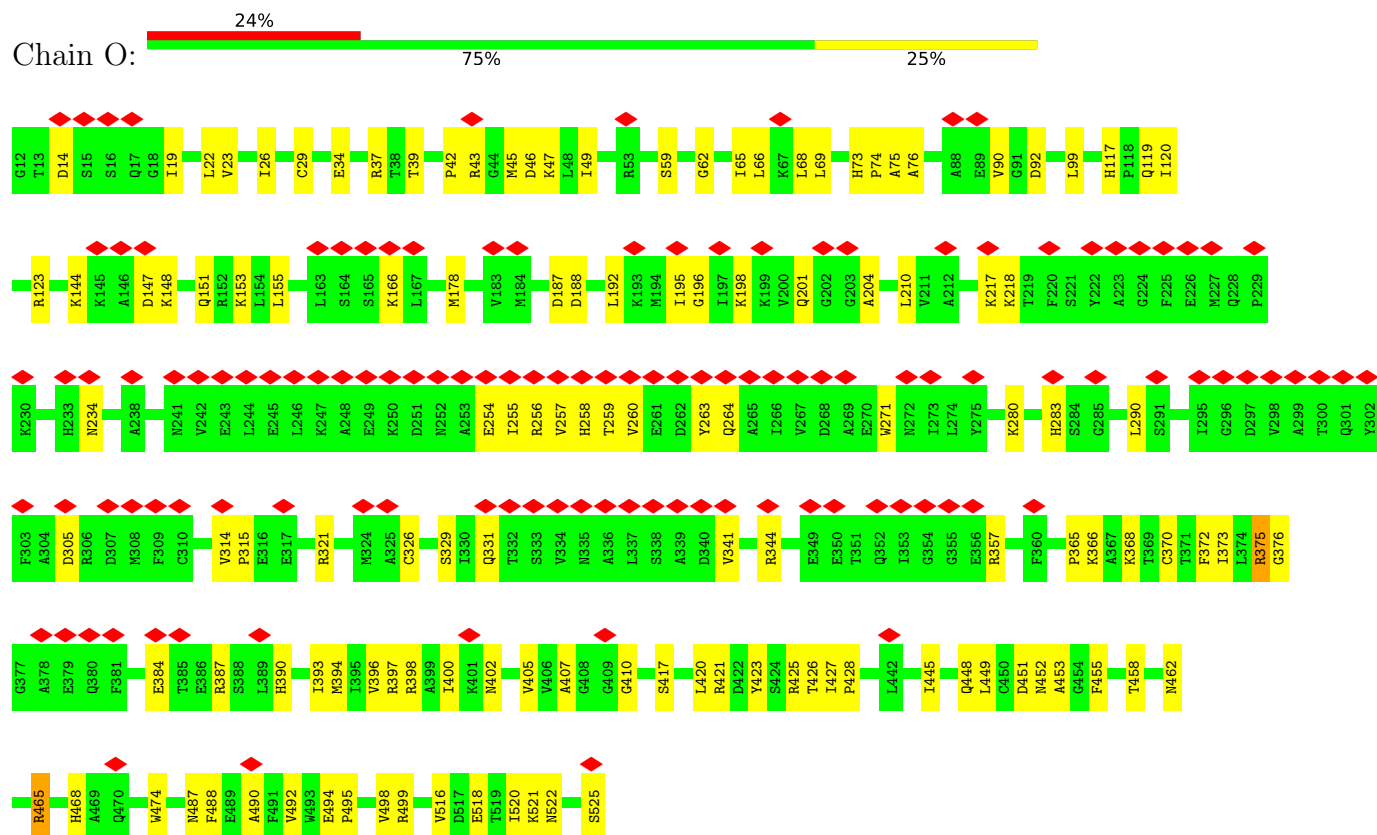


• Molecule 13: T-complex protein 1 subunit eta

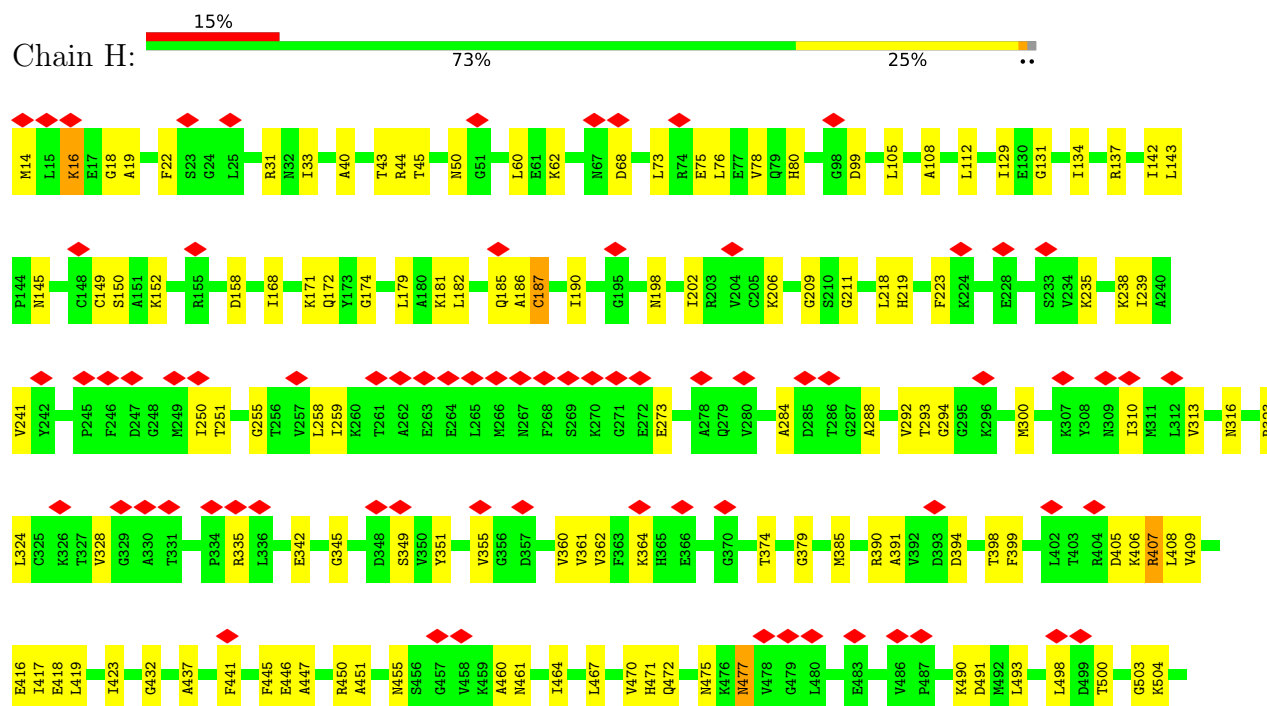


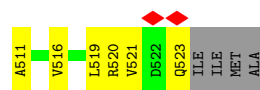


• Molecule 13: T-complex protein 1 subunit eta

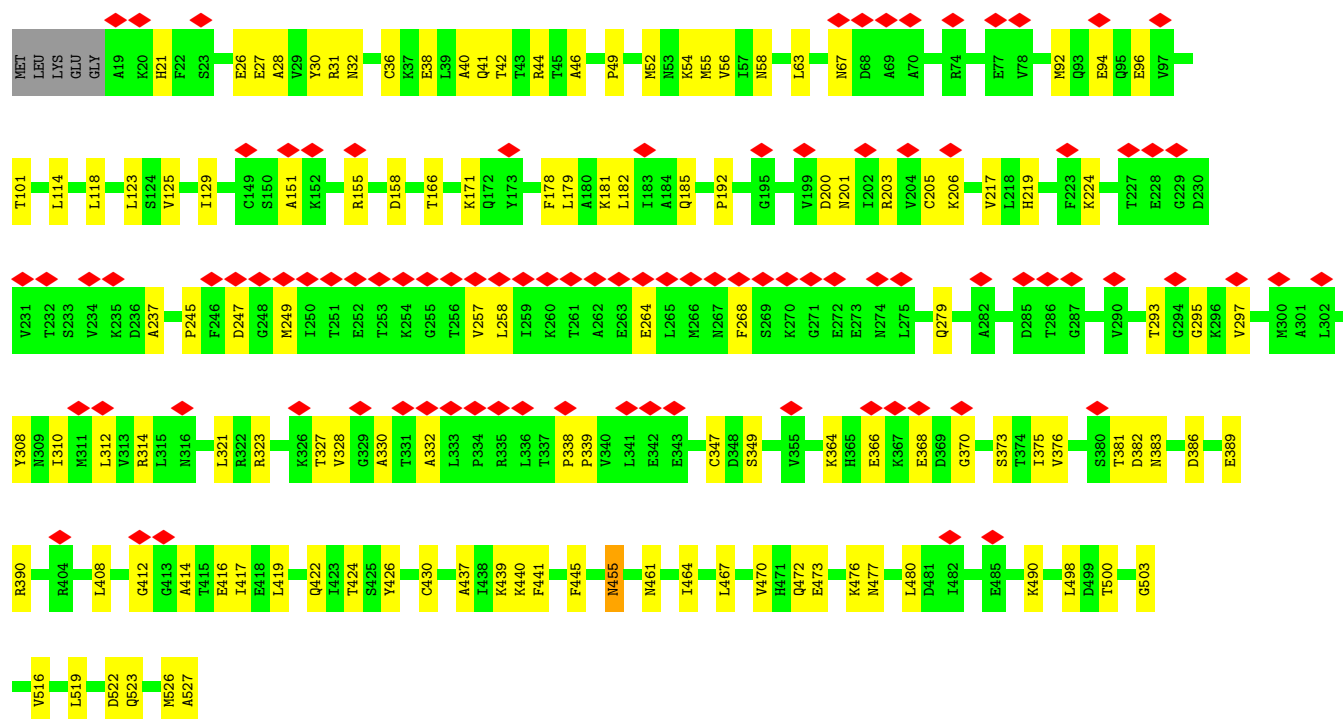
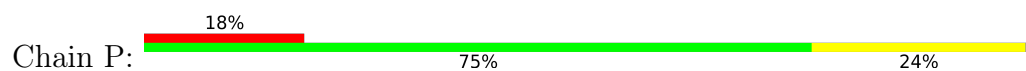


• Molecule 14: T-complex protein 1 subunit theta





• Molecule 14: T-complex protein 1 subunit theta



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	38032	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL 3200FSC	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	48	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.758	Depositor
Minimum map value	-0.616	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.117	Depositor
Recommended contour level	0.55	Depositor
Map size (Å)	408.0, 408.0, 408.0	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.7, 1.7, 1.7	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	1	0.25	0/880	0.46	0/1173
2	2	0.27	0/835	0.50	0/1116
3	3	0.28	0/1101	0.56	0/1476
4	4	0.27	0/852	0.46	0/1140
5	5	0.28	0/1032	0.49	0/1385
6	6	0.27	0/830	0.48	0/1109
7	A	0.30	0/3992	0.56	2/5389 (0.0%)
7	I	0.28	0/4095	0.55	1/5526 (0.0%)
8	B	0.28	0/3869	0.51	0/5214
8	J	0.27	0/3863	0.52	0/5207
9	C	0.28	0/4000	0.53	0/5397
9	K	0.28	0/4029	0.55	1/5434 (0.0%)
10	D	0.29	0/3863	0.54	0/5214
10	L	0.28	0/3904	0.54	0/5269
11	E	0.27	0/4020	0.55	1/5414 (0.0%)
11	M	0.28	0/4020	0.55	1/5414 (0.0%)
12	F	0.28	0/3991	0.51	0/5379
12	N	0.29	0/3986	0.52	0/5374
13	G	0.30	0/3991	0.53	0/5386
13	O	0.31	0/4002	0.56	2/5399 (0.0%)
14	H	0.28	0/3945	0.53	0/5331
14	P	0.29	0/3937	0.51	0/5321
All	All	0.28	0/69037	0.53	8/93067 (0.0%)

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
3	3	0	5
7	A	0	2
7	I	0	4

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Mol	Chain	#Chirality outliers	#Planarity outliers
8	B	0	3
9	C	0	1
9	K	0	3
10	D	0	2
10	L	0	4
12	N	0	2
13	G	0	2
13	O	0	5
14	H	0	4
14	P	0	2
All	All	0	39

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	K	191	LYS	C-N-CA	8.42	142.74	121.70
13	O	188	ASP	CB-CG-OD1	8.11	125.60	118.30
7	A	148	LEU	CA-CB-CG	5.92	128.92	115.30
7	I	237	LEU	CA-CB-CG	5.34	127.59	115.30
13	O	187	ASP	C-N-CA	5.33	135.03	121.70
11	E	492	ASP	CB-CG-OD1	5.12	122.90	118.30
7	A	488	LEU	CA-CB-CG	5.11	127.05	115.30
11	M	492	ASP	CB-CG-OD1	5.09	122.88	118.30

There are no chirality outliers.

All (39) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	3	117	VAL	Peptide
3	3	92	GLN	Peptide
3	3	97	SER	Peptide
3	3	98	THR	Peptide
3	3	99	ASN	Peptide
7	A	147	CYS	Peptide
7	A	242	GLN	Peptide
8	B	120	LYS	Peptide
8	B	428	THR	Peptide
8	B	489	ALA	Peptide
9	C	367	LYS	Peptide
10	D	201	THR	Peptide

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Mol	Chain	Res	Type	Group
10	D	202	SER	Peptide
13	G	166	LYS	Peptide
13	G	331	GLN	Peptide
14	H	187	CYS	Peptide
14	H	211	GLY	Peptide
14	H	255	GLY	Peptide
14	H	470	VAL	Peptide
7	I	111	LYS	Peptide
7	I	459	ASP	Peptide
7	I	478	PRO	Peptide
7	I	480	ARG	Peptide
9	K	191	LYS	Peptide
9	K	192	GLU	Peptide
9	K	477	THR	Peptide
10	L	197	PRO	Peptide
10	L	307	ASP	Peptide
10	L	487	GLY	Peptide
10	L	488	GLU	Peptide
12	N	235	VAL	Peptide
12	N	458	ASP	Peptide
13	O	147	ASP	Peptide
13	O	255	ILE	Peptide
13	O	258	HIS	Peptide
13	O	427	ILE	Peptide
13	O	46	ASP	Peptide
14	P	430	CYS	Peptide
14	P	472	GLN	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	874	0	902	9	0
2	2	830	0	852	13	0
3	3	1087	0	1114	27	0
4	4	847	0	845	12	0
5	5	1018	0	1042	15	0
6	6	826	0	850	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	3956	0	4124	91	0
7	I	4056	0	4218	58	0
8	B	3829	0	3932	61	0
8	J	3823	0	3927	80	0
9	C	3956	0	4079	84	0
9	K	3985	0	4108	61	0
10	D	3832	0	4042	75	0
10	L	3873	0	4086	84	0
11	E	3974	0	4084	94	0
11	M	3974	0	4084	102	0
12	F	3945	0	4071	67	0
12	N	3940	0	4068	58	0
13	G	3936	0	4029	87	0
13	O	3947	0	4037	83	0
14	H	3892	0	3949	83	0
14	P	3884	0	3943	75	0
All	All	68284	0	70386	1226	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 9.

All (1226) 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)
13:O:39:THR:HA	13:O:45:MET:HB2	1.73	0.71
7:A:480:ARG:HE	7:A:483:LEU:HB3	1.56	0.71
13:O:148:LYS:HE2	13:O:153:LYS:HB2	1.73	0.71
7:A:22:VAL:HG22	7:A:101:LEU:HB3	1.73	0.70
10:D:250:GLN:HB2	10:D:346:ALA:HA	1.73	0.70
7:A:181:TYR:HB3	7:A:191:PRO:HG3	1.72	0.69
7:I:9:GLY:HA2	10:L:62:GLN:H	1.56	0.69
11:E:131:ILE:HD12	13:G:43:ARG:HB3	1.75	0.69
10:L:60:MET:HG2	10:L:70:ILE:HG12	1.74	0.69
14:P:470:VAL:HG21	14:P:476:LYS:HG3	1.73	0.69
9:C:230:ARG:HE	9:C:288:ASP:HB3	1.56	0.68
14:P:49:PRO:HD2	14:P:480:LEU:HD23	1.75	0.68
7:A:238:ASP:HB2	7:A:329:SER:HA	1.75	0.68
10:L:217:THR:H	10:L:220:ASP:HB2	1.60	0.67
11:M:530:ILE:HA	13:O:45:MET:HB3	1.76	0.67
8:B:133:ALA:HB2	8:B:436:MET:HG2	1.77	0.67
12:F:70:GLN:H	14:H:18:GLY:HA2	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:F:129:LYS:HD2	12:F:427:PRO:HB3	1.77	0.67
14:H:241:VAL:HA	14:H:292:VAL:HB	1.78	0.66
14:H:33:ILE:HD12	14:H:112:LEU:HB3	1.78	0.66
10:D:78:LEU:HB3	10:D:92:VAL:HG12	1.78	0.66
12:N:109:TYR:HB3	12:N:114:LEU:HD12	1.77	0.66
10:D:441:ARG:HB3	11:M:478:ARG:HH21	1.61	0.65
14:H:45:THR:HG22	14:H:50:ASN:HD22	1.62	0.65
11:M:340:ARG:HB2	11:M:352:LYS:HA	1.78	0.65
11:E:235:SER:HB2	11:E:312:HIS:HB3	1.78	0.65
11:M:235:SER:HB2	11:M:312:HIS:HB3	1.78	0.65
11:E:239:MET:HG3	11:E:312:HIS:HB2	1.78	0.65
11:M:239:MET:HG3	11:M:312:HIS:HB2	1.77	0.65
10:L:317:LEU:HD13	10:L:324:VAL:HG11	1.79	0.65
10:D:46:ASP:HA	10:D:49:ARG:HD3	1.79	0.65
3:3:117:VAL:HG22	3:3:119:PRO:HD3	1.79	0.64
8:J:41:SER:HB2	8:J:48:MET:HG3	1.80	0.64
8:J:409:GLY:H	8:J:494:THR:HA	1.63	0.64
11:E:340:ARG:HB2	11:E:352:LYS:HA	1.78	0.64
13:G:13:THR:HG21	14:H:76:LEU:HA	1.80	0.64
7:A:150:ASN:HD21	7:A:154:THR:HG23	1.62	0.64
10:L:254:SER:HA	10:L:259:ASP:HB2	1.79	0.64
12:N:424:LYS:HE3	12:N:437:VAL:HG23	1.80	0.64
13:O:14:ASP:HB2	13:O:521:LYS:HB3	1.78	0.63
7:I:12:SER:HB2	7:I:17:ILE:HB	1.80	0.63
14:H:223:PHE:HB2	14:H:361:VAL:HB	1.81	0.63
9:C:296:ILE:HD11	9:C:301:GLN:HB3	1.81	0.63
10:D:197:PRO:HG2	10:D:200:ALA:H	1.62	0.63
9:K:350:LEU:HD23	9:K:363:ILE:HD12	1.81	0.62
13:O:204:ALA:HB3	13:O:375:ARG:HH21	1.63	0.62
7:A:526:ARG:HD3	10:D:57:MET:HA	1.79	0.62
8:J:469:HIS:HB2	8:J:474:THR:HA	1.81	0.62
7:I:147:CYS:SG	7:I:148:LEU:N	2.73	0.62
11:M:156:LEU:HB3	11:M:161:ASP:HB3	1.82	0.62
8:J:447:PRO:HB2	8:J:462:VAL:HG12	1.82	0.62
9:K:228:ARG:NH2	9:K:305:MET:SD	2.72	0.62
9:C:346:GLY:HA3	9:C:367:LYS:HG3	1.82	0.62
8:J:321:GLU:HB2	8:J:331:ILE:HD12	1.81	0.62
9:K:239:VAL:HG21	9:K:287:PRO:HB3	1.82	0.62
12:N:141:ARG:NH1	12:N:407:VAL:O	2.32	0.62
13:G:294:PRO:HG3	13:G:313:ARG:HE	1.65	0.61
3:3:85:LEU:HD12	3:3:89:LYS:HE3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:N:410:GLY:H	12:N:495:TRP:HA	1.64	0.61
14:P:424:THR:O	14:P:439:LYS:NZ	2.32	0.61
10:L:171:LEU:HD23	10:L:174:LYS:HD2	1.82	0.61
13:G:240:LEU:HD22	13:G:332:THR:HG23	1.83	0.61
10:L:202:SER:HB3	10:L:384:LYS:HD3	1.83	0.61
8:B:127:ILE:HD13	8:B:516:ARG:HE	1.66	0.61
9:C:50:LEU:HB2	9:C:58:VAL:HB	1.81	0.61
4:4:62:ASP:HA	4:4:80:GLN:HE21	1.66	0.60
10:D:229:LEU:HB2	10:D:374:LEU:HB3	1.83	0.60
14:P:118:LEU:HB3	14:P:123:LEU:HD12	1.83	0.60
9:C:229:MET:O	9:C:310:THR:OG1	2.19	0.60
9:K:44:LYS:NZ	12:N:121:GLU:OE2	2.34	0.60
9:K:175:ILE:HA	9:K:214:VAL:HG13	1.83	0.60
6:6:30:ARG:HH21	6:6:87:ILE:HG23	1.66	0.60
7:A:228:ARG:HE	7:A:352:VAL:HG22	1.65	0.60
7:A:237:LEU:HG	7:A:328:LEU:HD23	1.83	0.60
12:F:477:VAL:HA	12:F:488:VAL:HA	1.82	0.60
14:H:99:ASP:OD1	14:H:171:LYS:NZ	2.33	0.60
7:I:106:GLU:OE2	10:L:472:ASN:ND2	2.35	0.60
8:B:145:ALA:HB1	8:B:405:ARG:HD2	1.84	0.60
11:E:156:LEU:HB3	11:E:161:ASP:HB3	1.82	0.60
14:P:200:ASP:OD2	14:P:203:ARG:NH1	2.35	0.60
10:D:203:VAL:HB	10:D:413:ARG:HG3	1.82	0.60
11:M:260:PRO:HD2	13:O:257:VAL:HG21	1.82	0.60
8:J:52:LEU:HB3	8:J:62:MET:HB2	1.83	0.60
8:J:145:ALA:HB1	8:J:405:ARG:HB3	1.84	0.60
10:L:298:LEU:HB2	10:L:324:VAL:HG12	1.83	0.60
14:P:46:ALA:HA	14:P:52:MET:H	1.67	0.60
8:B:408:TYR:HA	8:B:494:THR:HG23	1.83	0.59
10:D:482:ASN:HA	11:M:441:PRO:HB2	1.83	0.59
11:M:340:ARG:NH1	13:O:305:ASP:OD1	2.35	0.59
8:B:403:ASP:O	8:B:498:GLN:NE2	2.35	0.59
13:G:398:ARG:HE	13:G:495:PRO:HD2	1.67	0.59
12:N:45:LYS:HG3	14:P:522:ASP:HB2	1.83	0.59
2:2:66:GLU:HB3	2:2:83:VAL:HG21	1.84	0.59
14:H:78:VAL:HG22	14:H:80:HIS:H	1.67	0.59
3:3:93:LYS:HB3	3:3:96:GLU:H	1.68	0.59
7:A:354:GLU:HB2	7:A:363:LEU:HD13	1.84	0.59
10:D:61:ILE:HB	10:D:69:THR:HB	1.85	0.59
7:A:103:ASN:HB3	7:A:440:GLU:HB3	1.85	0.59
11:M:240:PRO:HB2	11:M:242:LYS:HZ2	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:462:ASN:OD1	13:O:465:ARG:NH2	2.36	0.59
7:A:237:LEU:HB2	7:A:288:THR:HA	1.84	0.59
13:G:241:ASN:HD21	13:G:330:ILE:HB	1.68	0.59
8:J:322:ARG:HG2	8:J:370:ALA:HB1	1.84	0.59
13:O:522:ASN:ND2	14:P:58:ASN:OD1	2.36	0.59
4:4:66:MET:HB2	4:4:77:SER:HB3	1.84	0.59
12:F:278:LYS:NZ	12:F:284:ASP:O	2.36	0.59
8:J:71:LEU:HD22	8:J:85:VAL:HG22	1.83	0.59
10:L:253:LEU:HB3	10:L:286:LEU:HD13	1.85	0.59
14:P:166:THR:HG21	14:P:498:LEU:H	1.67	0.59
11:E:364:PHE:HB2	11:E:371:MET:HG3	1.85	0.58
7:A:348:ALA:HA	7:A:367:THR:HA	1.84	0.58
11:M:61:MET:HB3	11:M:69:THR:HB	1.85	0.58
6:6:26:SER:HB3	6:6:89:ARG:HH12	1.68	0.58
9:C:233:ILE:HG23	9:C:236:PRO:HD2	1.85	0.58
10:L:129:HIS:HB2	10:L:132:ILE:HG12	1.86	0.58
10:L:160:ARG:NH1	10:L:189:ASN:OD1	2.36	0.58
11:M:460:MET:HG3	11:M:470:PRO:HB2	1.86	0.58
12:N:328:CYS:O	12:N:367:ASN:ND2	2.36	0.58
7:A:197:ILE:HG12	7:A:375:ILE:H	1.68	0.58
11:M:364:PHE:HB2	11:M:371:MET:HG3	1.85	0.58
7:I:40:GLY:O	9:K:518:ARG:NH2	2.37	0.58
13:O:373:ILE:O	13:O:375:ARG:NH1	2.37	0.58
7:A:115:THR:HG22	7:A:526:ARG:HH22	1.69	0.58
7:A:264:ARG:NH1	9:C:273:GLU:O	2.36	0.58
12:F:19:ALA:O	12:F:23:ASN:ND2	2.37	0.58
11:E:431:LEU:HB2	11:E:478:ARG:HH12	1.69	0.58
10:L:220:ASP:O	10:L:391:ARG:NH1	2.37	0.58
12:N:141:ARG:HD2	12:N:407:VAL:HB	1.86	0.58
10:L:61:ILE:HB	10:L:69:THR:HB	1.86	0.57
12:N:393:ASP:OD1	12:N:396:ARG:NH2	2.36	0.57
14:P:28:ALA:O	14:P:32:ASN:ND2	2.37	0.57
10:D:213:LYS:HB3	10:D:391:ARG:HG2	1.86	0.57
7:I:231:ASN:ND2	7:I:233:LYS:O	2.38	0.57
14:P:21:HIS:ND1	14:P:526:MET:SD	2.77	0.57
8:B:409:GLY:H	8:B:494:THR:HA	1.69	0.57
11:E:460:MET:HG3	11:E:470:PRO:HB2	1.86	0.57
13:G:422:ASP:HA	13:G:425:ARG:HE	1.69	0.57
14:H:149:CYS:SG	14:H:152:LYS:NZ	2.77	0.57
14:H:158:ASP:OD1	14:H:181:LYS:NZ	2.38	0.57
8:J:218:PHE:HB3	8:J:322:ARG:HD2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:M:431:LEU:HB2	11:M:478:ARG:HH12	1.69	0.57
14:P:185:GLN:HE22	14:P:219:HIS:HE1	1.51	0.57
11:E:61:MET:HB3	11:E:69:THR:HB	1.85	0.57
11:E:240:PRO:HB2	11:E:242:LYS:HZ2	1.68	0.57
3:3:94:LYS:HE2	3:3:100:SER:HA	1.85	0.57
7:I:62:LEU:HD23	7:I:76:CYS:HA	1.86	0.57
14:P:389:GLU:OE1	14:P:390:ARG:NH1	2.37	0.57
7:A:107:LEU:HD11	7:A:440:GLU:HG3	1.85	0.57
14:P:205:CYS:HB2	14:P:376:VAL:HA	1.87	0.57
1:1:20:VAL:HG21	1:1:112:ILE:HG13	1.87	0.57
8:B:491:LEU:HB3	8:B:493:ILE:HG22	1.87	0.57
9:C:91:VAL:O	9:C:396:GLN:NE2	2.37	0.57
8:J:20:ARG:HE	8:J:21:ALA:H	1.52	0.57
8:J:332:ALA:HB3	8:J:342:LYS:H	1.70	0.57
11:M:249:ALA:HB3	11:M:300:ALA:HA	1.87	0.57
11:M:530:ILE:HD12	11:M:532:ASP:HB2	1.87	0.57
9:C:449:ARG:HG2	9:C:463:LEU:HD11	1.87	0.57
11:E:530:ILE:HD12	11:E:532:ASP:HB2	1.87	0.57
12:F:190:MET:HA	12:F:372:VAL:H	1.68	0.57
14:P:158:ASP:OD1	14:P:181:LYS:NZ	2.37	0.57
8:B:223:LYS:HG2	8:B:358:LYS:HB2	1.86	0.57
8:J:371:CYS:SG	8:J:372:THR:N	2.77	0.57
13:O:117:HIS:NE2	13:O:119:GLN:OE1	2.38	0.57
7:A:181:TYR:HA	7:A:372:SER:HA	1.87	0.57
9:C:130:LEU:HA	9:C:506:TYR:HE2	1.70	0.57
13:O:405:VAL:HA	13:O:495:PRO:HA	1.86	0.57
11:E:218:ARG:HG2	11:E:220:GLU:H	1.70	0.56
11:E:337:THR:HB	11:E:355:PHE:H	1.70	0.56
14:H:323:ARG:NH2	14:H:374:THR:OG1	2.37	0.56
8:B:259:ASP:OD2	13:G:256:ARG:NH1	2.38	0.56
8:J:182:LEU:HD11	8:J:214:LEU:HB3	1.85	0.56
13:O:254:GLU:HB3	13:O:256:ARG:HH21	1.69	0.56
8:B:519:ASN:HB2	11:E:59:LYS:HA	1.85	0.56
8:J:186:ALA:O	8:J:195:ASN:ND2	2.38	0.56
10:L:430:ILE:HG12	10:L:459:GLU:HA	1.86	0.56
11:M:282:LYS:HZ1	11:M:313:LEU:HD22	1.69	0.56
13:O:326:CYS:HA	13:O:365:PRO:HD2	1.87	0.56
14:P:412:GLY:O	14:P:477:ASN:ND2	2.37	0.56
2:2:39:GLY:O	2:2:43:LYS:NZ	2.37	0.56
10:D:215:GLY:HA3	10:D:370:SER:H	1.70	0.56
12:F:129:LYS:HD3	12:F:422:LEU:HD23	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:198:LEU:HB2	7:I:376:ILE:HG12	1.87	0.56
11:M:337:THR:HA	11:M:376:GLN:HG2	1.88	0.56
11:E:282:LYS:HZ1	11:E:313:LEU:HD22	1.69	0.56
13:G:237:ILE:HA	13:G:288:VAL:HB	1.88	0.56
8:J:159:LEU:HD22	8:J:397:LEU:HG	1.86	0.56
9:C:191:LYS:HG2	9:C:193:ILE:HD11	1.88	0.56
10:D:399:GLU:O	10:D:403:ARG:NE	2.38	0.56
11:E:381:ARG:HH21	13:G:221:SER:HB3	1.70	0.56
10:L:300:ILE:HB	10:L:326:LYS:HA	1.88	0.56
8:B:51:ILE:HD11	8:B:61:LEU:HB2	1.87	0.56
9:C:186:GLU:HB3	9:C:193:ILE:HA	1.88	0.56
11:E:337:THR:HA	11:E:376:GLN:HG2	1.88	0.56
7:I:135:ASN:HD22	7:I:409:VAL:HG12	1.71	0.56
10:L:446:MET:SD	10:L:446:MET:N	2.78	0.56
1:I:71:GLN:HB2	1:I:76:ILE:HD11	1.86	0.56
13:G:394:MET:HG3	13:G:398:ARG:HH12	1.71	0.56
13:G:466:ALA:HB2	7:I:431:GLY:HA2	1.87	0.56
8:J:519:ASN:ND2	11:M:47:THR:OG1	2.39	0.56
11:M:218:ARG:HG2	11:M:220:GLU:H	1.70	0.56
11:M:187:GLU:O	11:M:191:ASN:ND2	2.39	0.56
7:A:152:ALA:O	7:A:156:MET:N	2.34	0.55
9:C:41:LEU:HD11	9:C:100:ILE:HG13	1.88	0.55
11:E:221:ASP:HB2	11:E:388:ARG:HB2	1.88	0.55
12:F:47:LEU:HD11	12:F:67:MET:HG2	1.89	0.55
12:F:479:VAL:HA	12:F:486:PRO:HA	1.87	0.55
7:I:138:VAL:HB	7:I:410:PRO:HG3	1.88	0.55
9:K:455:CYS:O	12:N:432:ARG:NH1	2.39	0.55
3:3:93:LYS:HE3	3:3:123:MET:HG3	1.89	0.55
7:A:211:ILE:HG12	7:A:376:ILE:HG13	1.88	0.55
11:E:249:ALA:HB3	11:E:300:ALA:HA	1.87	0.55
14:H:405:ASP:O	14:H:407:ARG:NH1	2.39	0.55
9:K:187:GLU:OE1	9:K:190:ARG:NH1	2.39	0.55
11:M:337:THR:HB	11:M:355:PHE:H	1.69	0.55
11:E:170:LYS:HD2	11:E:183:ARG:HH12	1.72	0.55
13:G:467:ARG:NH2	13:G:475:TYR:OH	2.40	0.55
9:K:251:GLU:HG2	9:K:253:GLN:H	1.71	0.55
10:L:62:GLN:HE22	10:L:68:VAL:HG22	1.71	0.55
11:M:170:LYS:HD2	11:M:183:ARG:HH12	1.72	0.55
12:N:198:HIS:H	12:N:379:PRO:HD3	1.70	0.55
12:N:237:LEU:HB3	12:N:267:ILE:HA	1.88	0.55
13:O:42:PRO:HB3	13:O:166:LYS:HD2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:E:187:GLU:O	11:E:191:ASN:ND2	2.39	0.55
11:E:490:GLY:H	11:E:501:MET:HG2	1.72	0.55
12:F:198:HIS:ND1	12:F:200:SER:O	2.40	0.55
11:M:490:GLY:H	11:M:501:MET:HG2	1.72	0.55
9:C:466:LEU:HD13	9:C:487:LEU:HD22	1.87	0.55
9:K:90:GLU:O	9:K:399:ARG:NH1	2.40	0.55
9:K:272:GLU:HG2	9:K:299:LEU:HD23	1.89	0.55
8:J:145:ALA:O	8:J:405:ARG:NH1	2.40	0.55
7:I:20:GLN:NE2	7:I:21:ASN:OD1	2.40	0.55
7:A:320:ALA:HB1	7:A:327:ILE:HG21	1.89	0.55
12:F:209:GLY:HA3	12:F:364:GLU:HA	1.88	0.55
8:J:413:SER:HA	8:J:416:LEU:HD12	1.87	0.55
9:K:193:ILE:HD12	9:K:399:ARG:HH21	1.71	0.55
13:O:259:THR:OG1	13:O:260:VAL:N	2.34	0.55
8:B:91:GLN:HE22	8:B:502:GLN:HB3	1.72	0.55
9:C:91:VAL:HG12	9:C:93:ASP:H	1.71	0.55
8:J:88:SER:HB2	8:J:99:THR:HA	1.89	0.55
10:L:428:PRO:HA	10:L:431:GLU:HB3	1.89	0.55
13:G:522:ASN:ND2	14:H:75:GLU:OE1	2.39	0.54
7:I:118:ILE:HD12	7:I:522:ILE:HG12	1.89	0.54
11:M:221:ASP:HB2	11:M:388:ARG:HB2	1.88	0.54
5:5:59:GLY:N	5:5:76:LEU:O	2.38	0.54
6:6:33:LEU:HD22	6:6:83:ILE:HG12	1.88	0.54
11:E:442:THR:OG1	11:E:443:LEU:N	2.40	0.54
14:H:294:GLY:HA2	14:H:316:ASN:HB2	1.88	0.54
7:I:11:ARG:NH1	7:I:13:THR:OG1	2.39	0.54
8:J:37:ASP:OD2	10:L:27:ARG:NH2	2.40	0.54
8:J:283:LEU:HD13	8:J:307:ALA:HB1	1.88	0.54
12:F:141:ARG:NH1	12:F:407:VAL:O	2.40	0.54
13:G:136:ILE:HD12	13:G:412:ILE:HD12	1.90	0.54
8:J:25:ARG:NH1	8:J:114:GLU:OE1	2.40	0.54
8:J:298:ASN:HD22	10:L:250:GLN:HB3	1.72	0.54
12:N:470:HIS:ND1	12:N:475:GLN:O	2.40	0.54
9:C:451:LEU:HA	9:C:454:ASN:HB2	1.89	0.54
11:E:417:ARG:HE	11:E:510:LEU:HD12	1.72	0.54
14:H:68:ASP:OD2	14:H:390:ARG:NH2	2.41	0.54
8:J:298:ASN:ND2	10:L:250:GLN:O	2.40	0.54
9:K:413:ALA:HB2	9:K:480:VAL:HG12	1.89	0.54
14:P:201:ASN:O	14:P:373:SER:N	2.40	0.54
2:2:47:LEU:HB3	2:2:97:ILE:HG23	1.90	0.54
8:B:282:ILE:HG23	8:B:287:ILE:HD11	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:C:199:ALA:HA	9:C:373:THR:HG22	1.90	0.54
11:E:248:ILE:HD13	11:E:374:ILE:HG12	1.90	0.54
12:F:43:THR:O	12:F:58:LYS:NZ	2.39	0.54
12:F:352:GLU:HA	12:F:361:THR:HA	1.90	0.54
9:K:16:ARG:NH1	9:K:17:GLU:O	2.41	0.54
11:M:363:SER:HA	11:M:370:LYS:HA	1.89	0.54
1:I:61:TYR:HB2	2:2:78:LEU:HB3	1.89	0.54
7:A:145:ARG:HB3	7:A:398:VAL:HG13	1.89	0.54
9:C:233:ILE:HB	9:C:350:LEU:HB3	1.88	0.54
7:I:264:ARG:HG3	9:K:242:ASP:HB3	1.89	0.54
11:M:248:ILE:HD13	11:M:374:ILE:HG12	1.90	0.54
14:H:198:ASN:HB2	14:H:202:ILE:HG23	1.90	0.54
8:J:92:ASP:OD1	8:J:388:ARG:NH2	2.41	0.54
8:J:203:LYS:HG2	8:J:375:LEU:HD22	1.90	0.54
13:O:522:ASN:HD22	14:P:58:ASN:HA	1.71	0.54
3:3:67:LEU:HD11	3:3:166:ARG:HB2	1.90	0.54
11:E:39:MET:SD	11:E:42:LYS:NZ	2.81	0.54
12:F:141:ARG:HH12	12:F:409:PRO:HD3	1.71	0.54
14:H:149:CYS:SG	14:H:150:SER:N	2.81	0.54
7:I:257:PRO:HG3	9:K:248:LYS:HD3	1.90	0.54
8:B:68:ALA:HB2	8:B:99:THR:HG21	1.90	0.54
10:D:60:MET:SD	10:D:60:MET:N	2.80	0.54
13:G:153:LYS:HA	13:G:156:GLU:HB2	1.90	0.54
9:K:197:LYS:O	9:K:200:ARG:NH1	2.41	0.54
10:L:342:THR:HG23	10:L:356:LEU:HA	1.90	0.54
10:L:343:LYS:HB2	10:L:355:MET:HB3	1.90	0.54
10:L:430:ILE:HG23	10:L:459:GLU:HG2	1.90	0.54
11:M:306:PHE:HB2	11:M:323:ARG:HH21	1.73	0.54
13:O:384:GLU:OE2	13:O:387:ARG:NH2	2.41	0.54
7:A:293:ASP:O	7:A:297:LEU:N	2.39	0.53
8:B:54:SER:HB2	8:B:59:ALA:HA	1.90	0.53
13:O:155:LEU:HD22	13:O:396:VAL:HG13	1.90	0.53
7:A:247:LYS:HD2	7:A:264:ARG:HD2	1.90	0.53
10:D:236:SER:H	10:D:318:ASN:HB3	1.72	0.53
10:D:335:PHE:HA	10:D:338:LYS:HE3	1.90	0.53
10:D:478:THR:HG21	11:M:443:LEU:HD23	1.89	0.53
10:L:488:GLU:HB3	10:L:489:LYS:HD3	1.88	0.53
14:P:94:GLU:HG2	14:P:101:THR:HG21	1.90	0.53
9:C:490:MET:O	9:C:496:TRP:NE1	2.42	0.53
10:D:220:ASP:O	10:D:391:ARG:NH1	2.41	0.53
8:J:48:MET:HA	10:L:531:LYS:HE2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:522:LYS:HA	11:M:62:VAL:HB	1.89	0.53
7:A:421:ILE:HD11	7:A:468:ARG:HE	1.73	0.53
11:M:258:PRO:O	13:O:263:TYR:OH	2.20	0.53
14:P:382:ASP:O	14:P:386:ASP:N	2.42	0.53
7:A:281:THR:HG21	7:A:344:MET:H	1.74	0.53
9:C:207:GLY:HA3	9:C:377:ARG:HD2	1.89	0.53
10:L:143:LYS:NZ	10:L:439:TYR:O	2.40	0.53
4:4:122:LYS:HE3	13:G:280:LYS:HD2	1.89	0.53
7:A:164:ASN:HD21	7:A:206:MET:HG3	1.74	0.53
11:E:121:GLU:O	11:E:125:ASP:N	2.38	0.53
11:E:306:PHE:HB2	11:E:323:ARG:HH21	1.73	0.53
12:F:195:GLU:HB3	12:F:384:LEU:HD21	1.90	0.53
13:G:279:GLU:OE1	13:G:283:HIS:NE2	2.42	0.53
11:M:39:MET:SD	11:M:42:LYS:NZ	2.81	0.53
11:M:343:PRO:HB2	11:M:344:ARG:HD3	1.90	0.53
13:O:19:ILE:HA	13:O:22:LEU:HB3	1.91	0.53
13:O:43:ARG:NH2	13:O:453:ALA:O	2.42	0.53
13:O:487:ASN:HA	13:O:490:ALA:HB3	1.89	0.53
14:P:249:MET:O	14:P:279:GLN:NE2	2.42	0.53
8:B:37:ASP:HA	8:B:40:LYS:HE3	1.91	0.53
8:B:112:GLU:HB3	8:B:438:SER:HB3	1.91	0.53
9:C:176:ALA:HB2	9:C:391:LEU:HG	1.89	0.53
10:D:31:ALA:HA	10:D:34:ARG:HE	1.73	0.53
11:E:343:PRO:HB2	11:E:344:ARG:HD3	1.90	0.53
7:I:142:GLU:HG2	7:I:403:LEU:HD23	1.90	0.53
14:P:416:GLU:HB3	14:P:445:PHE:HB3	1.91	0.53
1:1:64:VAL:HG12	5:5:45:GLU:HG3	1.91	0.53
9:C:45:SER:OG	9:C:61:ASN:ND2	2.42	0.53
10:D:60:MET:HG3	10:D:70:ILE:HG13	1.89	0.53
13:G:122:ILE:HA	13:G:125:PHE:HD2	1.73	0.53
14:H:22:PHE:O	14:H:31:ARG:NH2	2.42	0.53
12:N:135:GLU:HA	12:N:138:LYS:HE3	1.90	0.53
5:5:12:LEU:HD22	5:5:135:MET:HG2	1.91	0.53
8:B:161:ASN:HD21	8:B:494:THR:HB	1.74	0.53
10:D:210:ILE:HD12	10:D:405:ILE:HD11	1.92	0.53
10:D:414:CYS:HB3	10:D:513:LEU:HB3	1.89	0.53
13:G:108:VAL:HG13	13:G:116:LEU:HD23	1.89	0.53
8:J:353:MET:HG3	8:J:358:LYS:HG2	1.90	0.53
8:J:449:ILE:O	8:J:453:ASN:ND2	2.42	0.53
14:P:381:THR:HG22	14:P:383:ASN:H	1.73	0.53
3:3:104:ARG:HH21	6:6:64:LEU:HD23	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:G:202:GLY:H	13:G:377:GLY:HA2	1.74	0.52
10:L:46:ASP:HA	10:L:49:ARG:HH21	1.74	0.52
13:O:394:MET:SD	13:O:397:ARG:NH2	2.82	0.52
7:A:489:ASP:HB3	7:A:493:GLY:H	1.74	0.52
9:C:447:ILE:HA	9:C:450:THR:HG22	1.90	0.52
11:E:357:GLY:H	11:E:376:GLN:HA	1.74	0.52
13:G:420:LEU:O	13:G:424:SER:N	2.42	0.52
13:G:487:ASN:HA	13:G:490:ALA:HB3	1.91	0.52
10:L:338:LYS:NZ	10:L:385:THR:OG1	2.42	0.52
11:M:52:LEU:O	11:M:465:ASN:ND2	2.40	0.52
2:2:71:TYR:HB2	3:3:132:MET:HB3	1.91	0.52
9:C:352:ILE:HG12	9:C:361:THR:HA	1.90	0.52
11:E:530:ILE:HG13	13:G:46:ASP:HA	1.92	0.52
11:M:417:ARG:HE	11:M:510:LEU:HD12	1.72	0.52
14:P:349:SER:H	14:P:364:LYS:HB3	1.74	0.52
3:3:105:PHE:HB3	5:5:64:VAL:HG11	1.91	0.52
9:C:57:ILE:HG21	12:F:76:LEU:HD11	1.91	0.52
11:E:363:SER:HA	11:E:370:LYS:HA	1.90	0.52
14:H:293:THR:OG1	14:H:313:VAL:O	2.23	0.52
7:A:15:GLU:O	7:A:19:SER:N	2.39	0.52
11:E:534:ARG:HH12	13:G:69:LEU:HB2	1.74	0.52
9:K:212:SER:HB2	9:K:377:ARG:HB2	1.92	0.52
10:L:228:VAL:H	10:L:387:THR:HG21	1.73	0.52
13:O:516:VAL:HG21	14:P:55:MET:HG2	1.92	0.52
7:A:477:ASN:HD21	7:A:484:LYS:HE2	1.74	0.52
12:F:384:LEU:HD12	12:F:387:ILE:HD11	1.91	0.52
14:H:149:CYS:O	14:H:408:LEU:N	2.42	0.52
7:A:44:MET:HG3	9:C:519:ILE:HD12	1.91	0.52
9:C:52:ASP:HB2	9:C:56:GLY:H	1.75	0.52
10:D:400:GLU:HA	10:D:403:ARG:HH21	1.74	0.52
12:F:217:ARG:HG3	12:F:314:ARG:HE	1.74	0.52
9:C:201:VAL:HA	9:C:374:ILE:HB	1.90	0.52
7:I:413:GLY:HA3	7:I:449:PRO:HD3	1.91	0.52
8:J:257:ARG:NH2	8:J:266:GLU:OE1	2.43	0.52
11:M:357:GLY:H	11:M:376:GLN:HA	1.74	0.52
8:B:52:LEU:HD12	8:B:62:MET:HB2	1.92	0.52
10:D:206:ARG:O	10:D:338:LYS:NZ	2.42	0.52
9:K:228:ARG:HE	9:K:305:MET:HB3	1.75	0.52
12:F:270:ARG:NE	12:F:334:ASN:O	2.42	0.51
7:I:211:ILE:HG21	7:I:363:LEU:HD22	1.92	0.51
14:P:203:ARG:HB3	14:P:323:ARG:HD2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:356:ILE:HG12	7:A:376:ILE:HG21	1.92	0.51
11:E:222:THR:HG23	11:E:387:ILE:HG22	1.92	0.51
14:H:239:ILE:HB	14:H:328:VAL:HG11	1.92	0.51
7:I:29:ALA:HB1	7:I:95:ILE:HA	1.92	0.51
7:A:443:ARG:HH21	7:A:446:LEU:HD11	1.75	0.51
8:B:520:ILE:HA	11:E:60:MET:HB3	1.93	0.51
12:F:176:ILE:HB	12:F:402:ILE:HD11	1.93	0.51
9:K:215:LEU:HD23	9:K:374:ILE:HA	1.93	0.51
11:M:210:LYS:HB3	11:M:384:THR:HG22	1.92	0.51
11:M:498:THR:O	11:M:504:GLN:NE2	2.42	0.51
13:G:297:ASP:OD1	13:G:297:ASP:N	2.44	0.51
14:H:447:ALA:HA	14:H:450:ARG:HE	1.75	0.51
10:L:304:ILE:HA	10:L:308:ALA:HB2	1.92	0.51
13:O:47:LYS:HB2	13:O:59:SER:H	1.75	0.51
13:O:494:GLU:OE2	13:O:499:ARG:NE	2.44	0.51
11:E:61:MET:N	11:E:69:THR:O	2.43	0.51
13:O:90:VAL:HG12	13:O:92:ASP:H	1.75	0.51
10:D:213:LYS:NZ	10:D:367:LEU:O	2.41	0.51
11:E:52:LEU:O	11:E:465:ASN:ND2	2.40	0.51
11:E:210:LYS:HB3	11:E:384:THR:HG22	1.92	0.51
11:E:257:PRO:O	11:E:323:ARG:NH2	2.44	0.51
7:I:446:LEU:HG	7:I:450:ASN:HD21	1.75	0.51
12:N:236:SER:OG	12:N:237:LEU:N	2.43	0.51
9:C:218:VAL:HG13	9:C:373:THR:HG21	1.92	0.51
13:G:130:GLN:O	13:G:134:ASN:ND2	2.43	0.51
7:A:116:SER:O	7:A:119:SER:OG	2.29	0.51
8:B:48:MET:SD	10:D:27:ARG:NH1	2.84	0.51
12:N:114:LEU:HB3	12:N:118:ILE:HD11	1.93	0.51
12:N:490:ALA:HA	12:N:495:TRP:HE1	1.74	0.51
7:A:48:ASP:HB2	7:A:51:ASP:HB2	1.92	0.51
8:B:426:ASN:OD1	8:J:466:ARG:NH2	2.43	0.51
9:C:240:LEU:HD21	9:C:323:ILE:HG22	1.93	0.51
12:F:293:ASN:HD22	12:F:297:ILE:HG12	1.76	0.51
13:G:48:LEU:HD11	13:G:56:ALA:HB1	1.93	0.51
9:K:243:SER:HB2	9:K:333:SER:HB3	1.93	0.51
11:M:344:ARG:HD2	13:O:271:TRP:HB3	1.93	0.51
12:N:457:PHE:HB3	12:N:462:THR:HG21	1.92	0.51
7:A:403:LEU:O	7:A:406:LYS:NZ	2.43	0.51
13:G:329:SER:O	13:G:331:GLN:NE2	2.43	0.51
14:H:467:LEU:HD21	14:H:477:ASN:HA	1.92	0.51
8:J:47:GLY:H	8:J:453:ASN:HB3	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:40:CYS:HA	9:K:46:MET:H	1.76	0.51
9:K:231:ARG:HH22	9:K:352:ILE:HG21	1.75	0.51
11:M:257:PRO:O	11:M:323:ARG:NH2	2.44	0.51
7:A:137:ILE:HG22	7:A:410:PRO:HD3	1.93	0.50
8:B:219:LEU:HD21	8:B:359:LEU:HD12	1.93	0.50
12:F:274:ILE:HD13	12:F:305:LEU:HD21	1.94	0.50
13:G:194:MET:HB3	13:G:369:THR:HA	1.92	0.50
14:H:108:ALA:HB2	14:H:511:ALA:HB1	1.93	0.50
11:M:423:GLY:HA2	11:M:459:PRO:HB3	1.94	0.50
9:C:230:ARG:NH2	9:C:308:ASN:O	2.43	0.50
9:K:37:ILE:HG21	9:K:99:ILE:HD11	1.92	0.50
12:N:145:ARG:HE	12:N:149:ILE:HD11	1.77	0.50
12:N:233:CYS:HB3	12:N:336:PHE:HE1	1.75	0.50
14:P:151:ALA:H	14:P:408:LEU:HD13	1.76	0.50
14:H:73:LEU:HD23	14:H:76:LEU:HD12	1.93	0.50
9:K:193:ILE:HG23	9:K:403:LEU:HB2	1.94	0.50
13:O:449:LEU:HD23	13:O:452:ASN:HD21	1.76	0.50
3:3:104:ARG:HH22	4:4:68:PRO:HB2	1.77	0.50
8:B:219:LEU:HB3	8:B:372:THR:HG21	1.92	0.50
8:B:479:ASP:N	8:B:484:THR:O	2.44	0.50
12:F:78:ALA:O	12:F:82:THR:OG1	2.27	0.50
13:G:149:VAL:HG11	13:G:154:LEU:HB2	1.93	0.50
8:J:156:ARG:HH11	8:J:184:VAL:HG12	1.75	0.50
9:K:146:ILE:HG22	9:K:401:VAL:HG22	1.92	0.50
12:N:215:GLY:N	12:N:359:LYS:O	2.43	0.50
8:B:445:MET:O	8:B:448:THR:OG1	2.26	0.50
9:C:143:PRO:HA	9:C:406:GLN:HA	1.94	0.50
9:C:455:CYS:SG	9:C:456:GLY:N	2.85	0.50
11:E:99:ASP:OD2	11:E:400:ARG:NH2	2.43	0.50
14:H:206:LYS:HG2	14:H:385:MET:HG2	1.94	0.50
14:H:241:VAL:HG21	14:H:324:LEU:HB3	1.94	0.50
10:L:247:GLY:HA2	10:L:356:LEU:HD22	1.92	0.50
11:M:222:THR:HG23	11:M:387:ILE:HG22	1.92	0.50
12:N:134:LEU:HD11	12:N:505:LEU:HD13	1.94	0.50
12:F:409:PRO:HD2	12:F:476:LEU:HD22	1.94	0.50
7:I:137:ILE:HD11	7:I:485:TRP:HA	1.93	0.50
9:K:110:GLU:HG2	9:K:114:GLU:HG3	1.94	0.50
13:G:449:LEU:HD23	13:G:452:ASN:HD22	1.75	0.50
10:L:194:VAL:HA	10:L:384:LYS:HA	1.93	0.50
11:M:228:VAL:HG11	11:M:332:LEU:HB3	1.93	0.50
13:O:62:GLY:O	13:O:66:LEU:N	2.37	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:329:SER:HB3	13:O:341:VAL:HG13	1.93	0.50
13:O:398:ARG:HG3	13:O:495:PRO:HG2	1.93	0.50
11:E:423:GLY:HA2	11:E:459:PRO:HB3	1.94	0.50
11:E:478:ARG:HH21	10:L:441:ARG:HD3	1.77	0.50
14:H:238:LYS:HA	14:H:345:GLY:HA3	1.94	0.50
8:J:282:ILE:HA	8:J:285:HIS:HD2	1.77	0.50
10:L:154:PRO:HA	10:L:420:ALA:HA	1.94	0.50
4:4:104:ARG:HH12	4:4:108:ILE:HD13	1.77	0.49
7:I:446:LEU:O	7:I:450:ASN:ND2	2.45	0.49
11:M:264:HIS:HB2	13:O:259:THR:H	1.77	0.49
14:P:114:LEU:HB3	14:P:440:LYS:HD2	1.92	0.49
1:1:61:TYR:HB3	1:1:68:PHE:HB3	1.93	0.49
8:B:128:ALA:HA	8:B:131:ARG:HE	1.76	0.49
10:D:41:ALA:HB2	10:D:87:ALA:HB1	1.92	0.49
10:D:210:ILE:HD11	10:D:402:GLU:HG2	1.95	0.49
12:F:107:ASP:O	12:F:111:SER:N	2.40	0.49
11:M:99:ASP:OD2	11:M:400:ARG:NH2	2.42	0.49
12:N:67:MET:HB3	14:P:526:MET:HA	1.94	0.49
14:P:500:THR:HG23	14:P:503:GLY:H	1.77	0.49
7:A:286:ILE:HB	7:A:307:ALA:HA	1.93	0.49
9:C:203:LYS:H	9:C:221:ASN:HD22	1.60	0.49
10:D:37:ASN:HB3	10:D:529:ILE:HD11	1.94	0.49
12:F:179:ILE:HG12	12:F:184:GLU:HB2	1.93	0.49
13:G:136:ILE:HG22	13:G:496:ALA:HB1	1.94	0.49
7:I:192:VAL:HG13	7:I:400:LYS:HD3	1.94	0.49
12:N:235:VAL:HA	12:N:295:LYS:HD3	1.94	0.49
13:O:407:ALA:HB2	13:O:474:TRP:HD1	1.77	0.49
14:P:328:VAL:HG23	14:P:330:ALA:H	1.76	0.49
7:A:145:ARG:HH21	7:A:398:VAL:HA	1.77	0.49
9:C:67:LEU:HB3	9:C:81:ILE:HG12	1.94	0.49
12:N:19:ALA:O	12:N:23:ASN:ND2	2.45	0.49
12:N:389:ASP:OD1	12:N:392:ARG:NH2	2.45	0.49
6:6:58:LYS:HB3	6:6:65:VAL:HG23	1.95	0.49
8:B:129:GLY:HA3	8:B:435:ALA:HB3	1.94	0.49
10:D:481:ARG:HA	10:D:484:HIS:HB2	1.94	0.49
11:E:228:VAL:HG11	11:E:332:LEU:HB3	1.93	0.49
8:J:163:ALA:HB3	8:J:180:THR:HG23	1.93	0.49
9:K:235:ASN:ND2	9:K:344:GLY:O	2.46	0.49
12:N:276:GLU:HA	12:N:279:ARG:HE	1.76	0.49
14:P:217:VAL:HG22	14:P:375:ILE:HG12	1.93	0.49
8:B:478:LEU:HA	8:B:485:ILE:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:D:101:GLU:O	10:D:413:ARG:NH1	2.45	0.49
12:F:241:LYS:HE2	12:F:264:ARG:HH11	1.77	0.49
13:O:34:GLU:HG2	13:O:37:ARG:HH12	1.77	0.49
7:A:423:LEU:O	7:A:427:ALA:N	2.42	0.49
10:D:157:LEU:HA	10:D:163:LEU:HD21	1.93	0.49
12:F:426:LYS:HE3	12:F:434:GLN:HG2	1.94	0.49
11:M:399:LYS:O	11:M:403:HIS:N	2.46	0.49
14:P:321:LEU:HD11	14:P:332:ALA:HB2	1.94	0.49
14:P:416:GLU:HA	14:P:419:LEU:HD12	1.95	0.49
3:3:66:ASN:O	3:3:70:LYS:NZ	2.43	0.49
9:C:327:CYS:O	9:C:345:THR:OG1	2.31	0.49
10:D:302:LYS:H	10:D:305:LEU:HD12	1.78	0.49
12:F:40:PRO:HD2	12:F:481:LEU:HD22	1.95	0.49
7:I:414:ALA:HB2	7:I:488:LEU:HB3	1.93	0.49
10:D:154:PRO:HA	10:D:420:ALA:HA	1.95	0.49
10:D:268:ASP:HB3	10:D:271:GLN:HG2	1.95	0.49
11:E:531:ASP:HA	13:G:45:MET:H	1.78	0.49
8:J:18:GLU:HG3	8:J:521:ILE:HG12	1.95	0.49
8:J:112:GLU:OE1	8:J:441:LYS:NZ	2.44	0.49
8:J:437:GLU:HG2	8:J:441:LYS:HE3	1.94	0.49
10:L:436:LEU:O	10:L:440:SER:N	2.46	0.49
14:P:237:ALA:HB3	14:P:347:CYS:HB2	1.95	0.49
4:4:110:ARG:HG2	13:G:253:ALA:HB1	1.94	0.49
8:B:239:ILE:HG21	8:B:324:ALA:HB2	1.95	0.49
9:C:230:ARG:HG3	9:C:233:ILE:HD11	1.95	0.49
9:C:376:LEU:HD11	9:C:391:LEU:HD13	1.94	0.49
10:D:229:LEU:HD12	10:D:374:LEU:HD22	1.94	0.49
11:E:427:ILE:HD13	11:E:477:VAL:HG13	1.95	0.49
12:N:54:ILE:HG13	12:N:382:HIS:HB3	1.95	0.49
1:1:34:ILE:HB	1:1:94:LEU:HD12	1.95	0.48
8:B:25:ARG:HH12	8:B:518:ASP:HB3	1.78	0.48
10:D:129:HIS:HB2	10:D:132:ILE:HG12	1.94	0.48
13:G:42:PRO:HG2	13:G:43:ARG:HG2	1.94	0.48
13:G:122:ILE:HG13	13:G:511:CYS:HB2	1.95	0.48
13:G:222:TYR:HB3	13:G:300:THR:HG21	1.95	0.48
10:L:137:PHE:HB3	10:L:523:THR:HG23	1.94	0.48
12:N:234:ASN:O	12:N:293:ASN:ND2	2.40	0.48
13:O:410:GLY:H	13:O:499:ARG:HH22	1.60	0.48
7:A:300:PHE:HB3	7:A:305:ALA:HB3	1.94	0.48
12:F:128:GLU:HA	12:F:131:LEU:HB2	1.94	0.48
14:H:349:SER:HB2	14:H:364:LYS:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:H:399:PHE:O	14:H:406:LYS:NZ	2.34	0.48
10:L:537:ASN:O	10:L:539:ARG:NH1	2.45	0.48
11:M:502:LYS:HD2	11:M:503:GLN:HG2	1.95	0.48
6:6:90:TYR:O	6:6:94:LEU:N	2.45	0.48
7:A:41:LEU:HD12	9:C:518:ARG:HG2	1.96	0.48
7:A:275:ILE:HG13	7:A:299:TYR:HB3	1.95	0.48
14:H:477:ASN:O	14:H:490:LYS:N	2.45	0.48
12:N:352:GLU:HA	12:N:361:THR:HA	1.94	0.48
14:P:26:GLU:O	14:P:31:ARG:N	2.40	0.48
14:H:235:LYS:HB3	14:H:349:SER:HA	1.95	0.48
7:A:88:ASP:OD2	7:A:401:ARG:NE	2.46	0.48
14:H:131:GLY:HA3	14:H:437:ALA:HB3	1.94	0.48
14:H:238:LYS:HB2	14:H:288:ALA:HA	1.95	0.48
8:J:71:LEU:HB3	8:J:85:VAL:HG13	1.95	0.48
11:M:427:ILE:HD13	11:M:477:VAL:HG13	1.95	0.48
12:N:203:ASP:HB3	12:N:377:LYS:HG3	1.95	0.48
14:P:417:ILE:HG21	14:P:467:LEU:HB3	1.96	0.48
8:B:462:VAL:O	8:B:466:ARG:N	2.39	0.48
10:D:343:LYS:HB2	10:D:355:MET:HA	1.96	0.48
13:G:155:LEU:HG	13:G:396:VAL:HB	1.95	0.48
11:M:254:PRO:HB2	13:O:264:GLN:HE22	1.78	0.48
9:C:104:GLU:HA	9:C:107:SER:HB2	1.95	0.48
10:D:247:GLY:HA2	10:D:356:LEU:HD22	1.94	0.48
10:D:424:GLY:H	10:D:509:VAL:HA	1.77	0.48
12:F:46:MET:HG3	14:H:521:VAL:HG11	1.96	0.48
7:I:43:LYS:NZ	9:K:520:ASP:OD1	2.36	0.48
10:L:274:ARG:HG2	10:L:277:ARG:HH21	1.78	0.48
4:4:57:ILE:HD13	6:6:63:VAL:HG21	1.95	0.48
9:C:229:MET:HA	9:C:312:ILE:HD11	1.95	0.48
14:H:168:ILE:HG23	14:H:391:ALA:HB1	1.96	0.48
14:P:247:ASP:HB3	14:P:257:VAL:HG23	1.95	0.48
9:C:456:GLY:HA3	12:F:118:ILE:HB	1.96	0.48
11:E:359:VAL:HG22	11:E:374:ILE:HG23	1.96	0.48
13:G:450:CYS:HB3	13:G:455:PHE:HB2	1.96	0.48
11:M:359:VAL:HG22	11:M:374:ILE:HG23	1.96	0.48
12:N:237:LEU:HD13	12:N:267:ILE:HG23	1.96	0.48
7:A:532:LYS:NZ	10:D:63:ASP:O	2.38	0.48
11:E:147:HIS:HD2	11:E:150:LYS:HE2	1.79	0.48
12:F:87:ILE:HG22	12:F:400:ASN:HD21	1.78	0.48
12:F:351:TYR:O	12:F:362:PHE:N	2.42	0.48
14:H:450:ARG:HG2	14:H:460:ALA:HB1	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:271:GLN:HG2	10:L:274:ARG:HH21	1.78	0.48
11:M:163:GLU:HA	11:M:166:ILE:HB	1.96	0.48
12:F:43:THR:HB	14:H:520:ARG:HB3	1.95	0.47
7:I:329:SER:OG	7:I:344:MET:SD	2.66	0.47
10:L:451:VAL:O	10:L:455:ALA:N	2.42	0.47
11:M:121:GLU:O	11:M:125:ASP:N	2.37	0.47
11:M:442:THR:OG1	11:M:443:LEU:N	2.40	0.47
12:N:193:ILE:HG23	12:N:376:ILE:HG13	1.95	0.47
6:6:33:LEU:O	6:6:37:LEU:N	2.46	0.47
11:E:163:GLU:HA	11:E:166:ILE:HB	1.96	0.47
12:F:126:ALA:HB2	12:F:437:VAL:HG22	1.96	0.47
12:F:378:GLY:HA3	12:F:384:LEU:HD13	1.96	0.47
13:G:402:ASN:HB3	13:G:495:PRO:HB3	1.96	0.47
14:H:182:LEU:HA	14:H:185:GLN:HB2	1.95	0.47
11:M:143:VAL:HG23	11:M:433:VAL:HG22	1.96	0.47
11:M:254:PRO:HB3	11:M:258:PRO:HD3	1.96	0.47
12:N:353:TYR:HB3	12:N:362:PHE:HE2	1.78	0.47
4:4:64:CYS:SG	4:4:65:LEU:N	2.87	0.47
10:D:38:ILE:HG23	10:D:117:LEU:HB3	1.96	0.47
11:E:502:LYS:HD2	11:E:503:GLN:HG2	1.95	0.47
12:F:44:MET:HA	12:F:58:LYS:HD2	1.96	0.47
11:M:42:LYS:O	11:M:46:ASN:ND2	2.47	0.47
7:A:202:GLY:N	7:A:379:GLY:O	2.40	0.47
8:B:16:ALA:HB3	11:E:81:MET:HG2	1.96	0.47
10:D:446:MET:HB2	11:M:471:ILE:HG22	1.95	0.47
11:E:530:ILE:O	13:G:45:MET:N	2.47	0.47
7:I:18:ARG:HH12	7:I:530:LEU:HD21	1.79	0.47
10:L:489:LYS:HG2	10:L:490:THR:HG23	1.96	0.47
13:O:178:MET:HB3	13:O:372:PHE:HE1	1.79	0.47
14:P:26:GLU:HA	14:P:30:TYR:HB2	1.96	0.47
3:3:104:ARG:HD2	3:3:114:LYS:HE2	1.96	0.47
9:C:227:PRO:HD3	9:C:359:TYR:HB2	1.95	0.47
11:E:399:LYS:O	11:E:403:HIS:N	2.46	0.47
13:G:152:ARG:NH1	13:G:156:GLU:OE2	2.48	0.47
9:K:44:LYS:HE3	9:K:483:GLU:HA	1.96	0.47
10:L:171:LEU:HD11	10:L:408:ALA:HB2	1.96	0.47
13:O:196:GLY:HA3	13:O:321:ARG:HH22	1.79	0.47
3:3:110:ASN:HD22	5:5:85:ASP:HB2	1.79	0.47
11:E:42:LYS:O	11:E:46:ASN:ND2	2.47	0.47
11:E:535:LYS:HG3	11:E:537:GLY:H	1.80	0.47
13:G:208:SER:HB3	13:G:372:PHE:HZ	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:H:417:ILE:HG12	14:H:467:LEU:HD23	1.96	0.47
7:I:242:GLN:HE21	7:I:292:ILE:HA	1.80	0.47
9:K:480:VAL:HA	9:K:487:LEU:HA	1.96	0.47
11:M:535:LYS:HG3	11:M:537:GLY:H	1.80	0.47
4:4:29:ASN:HD22	4:4:115:LEU:HD12	1.80	0.47
5:5:104:LYS:HA	5:5:107:ILE:HD12	1.96	0.47
7:A:147:CYS:SG	7:A:502:GLY:N	2.88	0.47
7:A:279:LEU:HA	7:A:283:ALA:HB3	1.96	0.47
7:A:388:MET:HA	7:A:391:SER:HB3	1.96	0.47
7:A:488:LEU:HG	7:A:493:GLY:HA2	1.97	0.47
9:C:217:GLY:HA2	9:C:366:CYS:HB2	1.95	0.47
9:C:291:ILE:HD11	9:C:315:VAL:HG21	1.95	0.47
9:C:374:ILE:HG12	9:C:391:LEU:HD21	1.96	0.47
10:D:433:ALA:HB2	10:D:458:MET:HB2	1.97	0.47
11:E:498:THR:O	11:E:504:GLN:NE2	2.42	0.47
14:H:129:ILE:HG23	14:H:516:VAL:HG13	1.97	0.47
7:I:122:VAL:HG12	7:I:101:LEU:HD12	1.97	0.47
8:J:310:MET:N	8:J:310:MET:SD	2.87	0.47
8:J:415:MET:HE2	8:J:462:VAL:HA	1.97	0.47
11:M:147:HIS:HD2	11:M:150:LYS:HE2	1.79	0.47
12:N:432:ARG:HA	12:N:435:LEU:HD12	1.95	0.47
13:O:42:PRO:HB3	13:O:166:LYS:HA	1.96	0.47
13:O:218:LYS:HB2	13:O:315:PRO:HD3	1.97	0.47
14:P:179:LEU:HD13	14:P:182:LEU:HD12	1.97	0.47
9:C:90:GLU:HG3	9:C:91:VAL:HG23	1.96	0.47
9:K:123:ILE:HA	9:K:126:TYR:HD2	1.79	0.47
9:K:419:ALA:HB2	9:K:444:LEU:HB2	1.97	0.47
10:L:116:LEU:HB3	10:L:526:VAL:HG11	1.97	0.47
11:M:184:GLN:NE2	11:M:220:GLU:O	2.48	0.47
14:P:461:ASN:HA	14:P:464:ILE:HB	1.96	0.47
8:B:126:ILE:HA	8:B:435:ALA:HB2	1.96	0.47
13:G:199:LYS:HD3	13:G:379:GLU:HA	1.97	0.47
10:L:250:GLN:O	10:L:301:GLN:NE2	2.48	0.47
12:N:80:VAL:HG11	12:N:511:ILE:HB	1.97	0.47
10:D:311:ASP:O	10:D:315:HIS:N	2.43	0.47
10:D:364:GLU:HA	10:D:374:LEU:HA	1.95	0.47
12:F:196:MET:HB3	12:F:377:LYS:HG2	1.97	0.47
12:F:278:LYS:HB2	12:F:310:ILE:HD11	1.96	0.47
8:J:438:SER:HA	8:J:441:LYS:HZ2	1.79	0.47
11:M:215:VAL:HA	11:M:389:GLY:H	1.80	0.47
8:B:213:TYR:HB3	8:B:374:VAL:HB	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:C:453:GLN:HG3	12:F:115:HIS:CE1	2.50	0.46
11:E:480:ARG:NH1	11:E:499:ASN:O	2.40	0.46
13:G:239:LEU:HB2	13:G:331:GLN:HE21	1.80	0.46
13:G:405:VAL:HA	13:G:495:PRO:HA	1.97	0.46
13:G:411:ALA:HB2	13:G:487:ASN:HD22	1.79	0.46
8:J:178:HIS:CE1	8:J:212:SER:H	2.33	0.46
13:O:201:GLN:OE1	13:O:376:GLY:N	2.43	0.46
7:A:308:VAL:HG21	7:A:362:ILE:HG13	1.97	0.46
8:B:223:LYS:HE2	8:B:358:LYS:H	1.80	0.46
11:E:254:PRO:HB3	11:E:258:PRO:HD3	1.96	0.46
12:F:329:GLY:HA3	12:F:345:GLY:HA3	1.97	0.46
13:G:120:ILE:HG12	13:G:431:GLN:HE21	1.80	0.46
8:J:453:ASN:HA	10:L:131:THR:HG21	1.97	0.46
9:K:288:ASP:HA	9:K:309:ILE:HD12	1.98	0.46
14:P:417:ILE:HD13	14:P:467:LEU:HD23	1.96	0.46
7:A:78:LEU:HD22	7:A:520:ALA:HB2	1.97	0.46
7:A:353:GLN:HE21	7:A:360:GLU:HB3	1.80	0.46
7:A:380:ALA:H	7:A:384:MET:HG3	1.80	0.46
8:B:429:PRO:HG2	8:J:464:GLN:HA	1.96	0.46
9:C:38:ARG:NH2	9:C:104:GLU:OE2	2.49	0.46
11:E:143:VAL:HG23	11:E:433:VAL:HG22	1.96	0.46
8:J:211:ASP:HB3	8:J:376:ARG:HH21	1.80	0.46
8:J:419:HIS:HA	8:J:466:ARG:HH11	1.79	0.46
7:A:42:ASP:HB3	7:A:54:ILE:HG22	1.98	0.46
9:C:158:SER:OG	9:C:494:GLY:O	2.33	0.46
10:D:437:THR:HB	10:D:441:ARG:HH12	1.79	0.46
7:I:402:VAL:HG13	7:I:408:VAL:HG11	1.97	0.46
8:J:156:ARG:HH12	8:J:185:GLU:HA	1.80	0.46
7:A:446:LEU:O	7:A:450:ASN:ND2	2.49	0.46
7:A:531:ILE:HD11	10:D:61:ILE:HD12	1.97	0.46
10:D:300:ILE:HB	10:D:326:LYS:HA	1.98	0.46
7:I:274:ARG:HD3	7:I:336:GLY:HA2	1.98	0.46
14:P:297:VAL:HG21	14:P:312:LEU:HD13	1.98	0.46
2:2:64:VAL:HG21	3:3:135:TYR:HE1	1.79	0.46
5:5:117:ILE:O	5:5:121:LEU:N	2.43	0.46
9:C:172:ALA:HB1	9:C:391:LEU:HD12	1.98	0.46
9:C:452:ILE:HG21	9:C:459:THR:HA	1.97	0.46
10:D:51:SER:HA	10:D:57:MET:H	1.79	0.46
13:G:453:ALA:HB2	13:G:479:ILE:HG13	1.97	0.46
11:M:164:PRO:O	11:M:168:THR:N	2.49	0.46
7:A:45:LEU:HD11	7:A:61:ILE:HB	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:H:14:MET:HG2	14:H:19:ALA:HB3	1.98	0.46
9:K:175:ILE:HG12	9:K:214:VAL:HA	1.98	0.46
12:N:446:ILE:HA	12:N:449:LYS:HB2	1.98	0.46
13:O:521:LYS:NZ	13:O:525:SER:OG	2.39	0.46
7:A:431:GLY:O	13:O:462:ASN:HB3	2.16	0.46
10:D:489:LYS:HG2	10:D:502:ASN:HD21	1.81	0.46
11:E:184:GLN:NE2	11:E:220:GLU:O	2.48	0.46
13:G:342:LEU:O	13:G:344:ARG:NH1	2.49	0.46
14:H:446:GLU:HG3	14:H:464:ILE:HG12	1.97	0.46
7:I:25:ALA:HB2	7:I:71:ALA:HB1	1.98	0.46
10:L:151:MET:O	10:L:153:ARG:NH1	2.48	0.46
13:O:47:LYS:N	13:O:59:SER:O	2.36	0.46
13:O:74:PRO:HB3	14:P:63:LEU:HD21	1.98	0.46
13:O:290:LEU:HD12	13:O:314:VAL:HG21	1.96	0.46
3:3:56:GLN:HE21	3:3:174:VAL:HG21	1.81	0.46
7:A:366:ASN:ND2	7:A:372:SER:O	2.49	0.46
13:G:434:LEU:O	13:G:438:TYR:N	2.44	0.46
14:H:142:ILE:HD12	14:H:145:ASN:HD22	1.81	0.46
9:K:296:ILE:O	9:K:314:ARG:NH1	2.48	0.46
12:N:389:ASP:HA	12:N:392:ARG:HH21	1.82	0.46
13:O:420:LEU:HA	13:O:423:TYR:HD2	1.80	0.46
14:P:125:VAL:HG13	14:P:519:LEU:HG	1.98	0.46
7:A:32:VAL:HG12	7:A:58:GLY:HA3	1.97	0.45
7:A:465:ALA:HB1	13:O:428:PRO:HB2	1.98	0.45
10:D:177:SER:HA	10:D:180:SER:HB2	1.97	0.45
12:F:210:LEU:N	12:F:363:ILE:O	2.42	0.45
7:I:127:GLU:OE1	7:I:130:ARG:NH2	2.47	0.45
11:M:193:VAL:HG21	11:M:409:ILE:HG21	1.98	0.45
11:M:286:GLU:HA	11:M:289:ILE:HD12	1.98	0.45
13:O:23:VAL:HA	13:O:26:ILE:HG12	1.98	0.45
8:B:429:PRO:HA	8:B:433:ALA:HB3	1.98	0.45
11:E:475:THR:HG23	10:L:445:GLY:HA2	1.98	0.45
12:F:449:LYS:HD2	12:F:459:LEU:HD12	1.98	0.45
13:G:203:GLY:HA3	13:G:375:ARG:HB3	1.98	0.45
14:H:418:GLU:OE2	14:H:472:GLN:NE2	2.49	0.45
7:I:420:SER:HA	7:I:442:ALA:HB1	1.98	0.45
8:J:222:LYS:HB3	8:J:360:ILE:HB	1.98	0.45
9:K:149:SER:O	9:K:153:LEU:N	2.49	0.45
9:K:156:ILE:HD11	9:K:394:ALA:HB1	1.98	0.45
10:L:227:LEU:HB2	10:L:339:THR:HG21	1.98	0.45
11:M:527:ILE:HG13	11:M:528:LEU:HD23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:P:36:CYS:O	14:P:40:ALA:N	2.47	0.45
2:2:113:LYS:HE2	12:F:266:PHE:HD1	1.80	0.45
3:3:105:PHE:HE2	3:3:115:ALA:HB3	1.82	0.45
11:E:188:ILE:HG23	11:E:224:LEU:HB2	1.99	0.45
11:E:215:VAL:HA	11:E:389:GLY:H	1.80	0.45
13:G:449:LEU:HD22	13:G:479:ILE:HD12	1.99	0.45
14:H:129:ILE:HD12	14:H:516:VAL:HG13	1.98	0.45
8:J:257:ARG:NH1	10:L:262:ASN:O	2.49	0.45
9:K:295:GLY:HA2	9:K:313:ARG:HB2	1.99	0.45
11:M:132:ARG:HB3	13:O:455:PHE:HE1	1.81	0.45
12:N:127:LYS:HG3	12:N:505:LEU:HD23	1.98	0.45
5:5:119:PRO:O	5:5:123:GLU:N	2.49	0.45
10:D:49:ARG:HD2	10:D:111:ILE:HD12	1.98	0.45
12:F:129:LYS:NZ	12:F:425:HIS:O	2.50	0.45
12:F:225:VAL:HB	12:F:350:VAL:HB	1.97	0.45
8:J:232:ILE:HB	8:J:349:ILE:HB	1.98	0.45
11:M:165:LEU:HD11	11:M:412:LEU:HD22	1.98	0.45
12:N:34:LEU:HD12	12:N:96:VAL:HG11	1.97	0.45
10:D:48:ILE:HG13	10:D:110:VAL:HG11	1.99	0.45
12:N:68:GLN:H	14:P:527:ALA:HB2	1.82	0.45
7:A:180:LYS:NZ	7:A:372:SER:O	2.49	0.45
7:A:219:VAL:HG12	7:A:309:ARG:HE	1.82	0.45
7:A:229:ILE:HG21	7:A:284:ASN:HB3	1.98	0.45
8:B:487:ASP:HB3	8:B:491:LEU:HD23	1.98	0.45
9:C:153:LEU:HG	9:C:157:ASN:HD21	1.81	0.45
10:D:248:LEU:HD23	10:D:345:VAL:H	1.81	0.45
11:E:424:ALA:HB1	11:E:487:PRO:HG2	1.99	0.45
10:L:248:LEU:HD21	10:L:333:ILE:HG23	1.98	0.45
11:E:193:VAL:HG21	11:E:409:ILE:HG21	1.98	0.45
11:E:286:GLU:HA	11:E:289:ILE:HD12	1.98	0.45
12:F:314:ARG:HD2	12:F:315:ARG:HG2	1.99	0.45
7:I:423:LEU:O	7:I:427:ALA:N	2.49	0.45
8:J:135:LYS:HG2	8:J:138:ARG:HH21	1.81	0.45
10:L:183:LEU:HD23	10:L:405:ILE:HB	1.98	0.45
10:L:236:SER:HB3	10:L:366:ASN:HD21	1.81	0.45
5:5:36:LEU:HB3	5:5:110:LEU:HD12	1.99	0.45
8:B:359:LEU:HD21	8:B:376:ARG:HH22	1.80	0.45
11:E:165:LEU:HD11	11:E:412:LEU:HD22	1.98	0.45
13:G:486:ASP:O	13:G:490:ALA:N	2.48	0.45
14:H:187:CYS:HB2	14:H:219:HIS:HE1	1.82	0.45
7:I:498:ASN:HD22	7:I:499:LYS:H	1.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:97:ASP:OD1	8:J:100:THR:OG1	2.29	0.45
13:O:474:TRP:CD1	13:O:488:PHE:HB2	2.52	0.45
14:P:258:LEU:HD12	14:P:268:PHE:HB2	1.99	0.45
10:D:483:ARG:HB3	10:D:490:THR:H	1.82	0.45
11:E:527:ILE:HG13	11:E:528:LEU:HD23	1.98	0.45
13:G:302:TYR:HA	13:G:305:ASP:HB2	1.99	0.45
14:H:149:CYS:HB3	14:H:408:LEU:HB2	1.98	0.45
14:H:355:VAL:HB	14:H:360:VAL:HG21	1.98	0.45
10:L:195:ILE:HD12	10:L:416:VAL:HG22	1.99	0.45
13:O:210:LEU:HD11	13:O:370:CYS:HB3	1.99	0.45
14:P:67:ASN:O	14:P:171:LYS:NZ	2.43	0.45
8:B:403:ASP:HB2	8:B:498:GLN:HE21	1.82	0.45
11:E:414:ARG:HH22	11:E:511:ILE:HG21	1.82	0.45
12:F:243:GLU:HB2	12:F:256:ARG:HB3	1.98	0.45
13:G:241:ASN:ND2	13:G:331:GLN:O	2.50	0.45
13:G:411:ALA:HB2	13:G:487:ASN:HB2	1.99	0.45
11:M:188:ILE:HG23	11:M:224:LEU:HB2	1.99	0.45
11:M:208:LEU:HD22	11:M:381:ARG:HA	1.99	0.45
12:N:241:LYS:H	12:N:270:ARG:NH1	2.14	0.45
13:O:198:LYS:HD2	13:O:217:LYS:HB2	1.97	0.45
13:O:280:LYS:HA	13:O:283:HIS:CE1	2.52	0.45
14:P:293:THR:HB	14:P:314:ARG:HA	1.99	0.45
7:A:266:ARG:NH1	7:A:269:ASP:OD2	2.50	0.44
8:B:228:GLN:NE2	8:B:309:VAL:O	2.50	0.44
10:D:157:LEU:HD22	10:D:416:VAL:HG12	1.99	0.44
13:G:398:ARG:HG2	13:G:495:PRO:HG2	1.98	0.44
9:K:282:ILE:HD13	9:K:290:VAL:HG11	2.00	0.44
13:O:144:LYS:HD2	13:O:151:GLN:HG3	1.99	0.44
14:P:366:GLU:O	14:P:370:GLY:N	2.44	0.44
7:A:464:VAL:HA	7:A:467:LEU:HD12	1.99	0.44
8:B:424:LEU:HD23	8:B:436:MET:HE1	2.00	0.44
9:C:244:SER:H	9:C:335:PRO:HG3	1.81	0.44
12:F:497:ASN:HB2	12:F:500:VAL:HG23	2.00	0.44
13:G:121:ILE:H	13:G:121:ILE:HG13	1.45	0.44
14:H:182:LEU:O	14:H:186:ALA:N	2.45	0.44
14:H:284:ALA:HB2	14:H:310:ILE:HD11	1.99	0.44
14:H:300:MET:SD	14:H:300:MET:N	2.90	0.44
14:H:351:TYR:HB2	14:H:362:VAL:HB	1.98	0.44
7:I:140:THR:HG22	7:I:499:LYS:HE2	1.98	0.44
9:K:156:ILE:HA	9:K:397:VAL:HG21	1.97	0.44
10:L:126:LYS:HD3	10:L:128:ILE:HD11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:D:211:VAL:HG21	10:D:228:VAL:HB	1.99	0.44
12:F:221:MET:HG2	12:F:306:SER:HB3	2.00	0.44
13:G:240:LEU:N	13:G:290:LEU:O	2.49	0.44
13:G:255:ILE:HD12	13:G:255:ILE:HA	1.83	0.44
13:G:467:ARG:O	13:G:472:GLY:N	2.49	0.44
14:H:129:ILE:HD11	14:H:519:LEU:HB3	2.00	0.44
14:H:209:GLY:N	14:H:379:GLY:O	2.49	0.44
7:I:21:ASN:HB3	7:I:71:ALA:HB2	1.98	0.44
6:6:58:LYS:N	6:6:65:VAL:O	2.43	0.44
10:D:168:THR:HA	10:D:171:LEU:HB2	1.99	0.44
9:K:59:MET:SD	9:K:59:MET:N	2.90	0.44
13:O:65:ILE:HG22	13:O:68:LEU:HD12	1.98	0.44
2:2:68:ARG:HG2	3:3:133:LEU:HD11	1.99	0.44
9:C:303:TYR:O	9:C:307:ALA:N	2.50	0.44
11:E:196:VAL:HB	11:E:204:VAL:HG23	2.00	0.44
14:H:172:GLN:HG3	14:H:174:GLY:H	1.82	0.44
8:J:450:ILE:HD12	8:J:453:ASN:HB2	1.98	0.44
8:J:450:ILE:HA	8:J:453:ASN:HD22	1.82	0.44
8:J:451:ALA:O	8:J:456:TYR:N	2.50	0.44
9:K:472:GLN:HG2	9:K:473:GLU:HG3	2.00	0.44
11:M:308:ASP:O	11:M:312:HIS:ND1	2.44	0.44
13:O:465:ARG:HA	13:O:468:HIS:HB2	1.98	0.44
14:P:293:THR:HG21	14:P:297:VAL:HG23	1.99	0.44
14:P:437:ALA:O	14:P:441:PHE:N	2.49	0.44
7:A:207:GLU:HB3	7:A:378:ARG:HH11	1.83	0.44
9:C:39:THR:O	9:C:46:MET:N	2.51	0.44
12:F:203:ASP:HB2	12:F:377:LYS:HD2	2.00	0.44
7:I:218:CYS:SG	7:I:227:LYS:NZ	2.76	0.44
12:N:399:LYS:HA	12:N:402:ILE:HG22	2.00	0.44
13:O:90:VAL:HG21	13:O:498:VAL:HG13	1.99	0.44
3:3:175:ASN:ND2	14:H:250:ILE:O	2.51	0.44
7:A:17:ILE:HD12	7:A:20:GLN:HB3	1.99	0.44
8:B:326:VAL:HG23	8:B:327:THR:HG23	2.00	0.44
9:C:196:LYS:HB3	9:C:399:ARG:HD3	1.99	0.44
9:C:322:ARG:O	9:C:326:ALA:N	2.50	0.44
11:E:262:THR:OG1	11:E:263:LYS:N	2.51	0.44
12:F:212:LEU:HD12	12:F:313:LEU:HD13	1.99	0.44
13:G:49:ILE:O	13:G:57:THR:OG1	2.28	0.44
13:G:126:ARG:HA	13:G:129:THR:HG22	1.98	0.44
8:J:259:ASP:H	8:J:263:LYS:HG3	1.82	0.44
11:M:133:ILE:HA	11:M:447:ALA:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:M:424:ALA:HB1	11:M:487:PRO:HG2	1.99	0.44
1:I:74:GLU:HA	1:I:77:HIS:HD2	1.82	0.44
8:B:293:ARG:HA	8:B:315:ALA:HB3	2.00	0.44
13:G:349:GLU:HB3	13:G:360:PHE:HB2	2.00	0.44
7:I:165:GLY:HA2	7:I:168:PHE:HB2	2.00	0.44
10:L:290:ILE:HD13	10:L:298:LEU:HD11	2.00	0.44
10:L:460:VAL:HA	10:L:481:ARG:HD3	1.99	0.44
11:M:73:ASP:O	11:M:76:THR:OG1	2.34	0.44
12:N:493:GLY:HA2	12:N:495:TRP:CE2	2.53	0.44
6:6:56:VAL:HG21	6:6:72:ALA:HB2	2.00	0.44
7:A:311:VAL:HG11	7:A:316:LEU:HD13	1.99	0.44
8:B:78:ASN:HB2	8:B:81:ALA:HB3	1.99	0.44
8:B:289:CYS:HA	8:B:310:MET:HB3	2.00	0.44
9:C:388:GLU:O	9:C:392:GLN:N	2.50	0.44
11:E:133:ILE:HA	11:E:447:ALA:HB2	1.99	0.44
13:G:272:ASN:O	13:G:276:ASP:N	2.51	0.44
14:H:432:GLY:H	9:K:464:THR:HG21	1.83	0.44
8:J:465:LEU:HG	8:J:469:HIS:HD2	1.83	0.44
14:P:92:MET:O	14:P:96:GLU:N	2.45	0.44
14:P:245:PRO:HG3	14:P:295:GLY:HA3	2.00	0.44
3:3:64:GLU:HG2	3:3:166:ARG:HH11	1.83	0.43
3:3:111:LEU:HD21	5:5:50:LEU:HD13	2.00	0.43
7:A:146:ASP:H	7:A:504:PHE:HD2	1.64	0.43
8:B:450:ILE:HA	8:B:453:ASN:HB2	2.00	0.43
9:C:113:LEU:O	9:C:117:MET:N	2.50	0.43
11:E:164:PRO:O	11:E:168:THR:N	2.48	0.43
8:J:49:ASP:H	10:L:531:LYS:HG3	1.83	0.43
10:L:479:GLU:O	10:L:483:ARG:NE	2.32	0.43
12:N:37:ASN:ND2	12:N:43:THR:O	2.51	0.43
12:N:131:LEU:HD23	12:N:134:LEU:HD12	1.99	0.43
13:O:195:ILE:HD13	13:O:393:ILE:HG21	2.00	0.43
14:P:455:ASN:HB3	14:P:480:LEU:HD21	1.99	0.43
7:A:113:HIS:CG	10:D:470:GLY:HA2	2.52	0.43
12:F:446:ILE:HA	12:F:449:LYS:HE3	1.99	0.43
14:H:258:LEU:HD23	14:H:258:LEU:HA	1.84	0.43
7:I:355:ARG:HA	7:I:360:GLU:HA	1.99	0.43
11:M:61:MET:N	11:M:69:THR:O	2.43	0.43
11:M:219:LEU:HA	11:M:389:GLY:HA2	2.00	0.43
13:O:144:LYS:HE2	13:O:400:ILE:HA	2.00	0.43
13:O:458:THR:O	13:O:462:ASN:ND2	2.48	0.43
13:O:487:ASN:O	13:O:492:VAL:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:520:ILE:HD12	14:P:56:VAL:HG22	1.99	0.43
14:P:417:ILE:HD12	14:P:473:GLU:HG3	1.99	0.43
2:2:58:ILE:HG22	2:2:90:LEU:HB3	2.00	0.43
10:D:302:LYS:HA	10:D:327:ASP:HA	2.00	0.43
14:H:187:CYS:HB3	14:H:190:ILE:HG23	2.01	0.43
14:H:409:VAL:HG21	14:H:504:LYS:HG3	2.00	0.43
8:J:295:LEU:HA	8:J:313:GLU:HB2	2.00	0.43
10:L:216:GLY:HA3	10:L:391:ARG:HD3	2.00	0.43
11:M:25:LYS:HG2	11:M:536:PRO:HA	2.00	0.43
1:1:67:MET:HB2	5:5:62:LEU:HD23	2.00	0.43
7:A:241:LEU:HD23	7:A:292:ILE:HG23	2.00	0.43
9:C:157:ASN:HA	9:C:160:ILE:HG12	1.99	0.43
12:F:449:LYS:HB2	12:F:459:LEU:HB2	1.99	0.43
13:G:145:LYS:HD2	13:G:151:GLN:HE22	1.83	0.43
13:G:468:HIS:CD2	13:G:472:GLY:HA2	2.54	0.43
14:H:40:ALA:O	14:H:44:ARG:NH1	2.51	0.43
14:H:416:GLU:HB3	14:H:445:PHE:HB3	2.00	0.43
11:M:196:VAL:HB	11:M:204:VAL:HG23	2.00	0.43
13:O:366:LYS:HB3	13:O:368:LYS:HG2	2.00	0.43
6:6:102:GLU:HA	6:6:105:ARG:HE	1.84	0.43
7:A:130:ARG:HA	7:A:133:ASN:HD22	1.84	0.43
8:B:119:LYS:HD3	8:B:120:LYS:HG2	2.00	0.43
11:E:61:MET:O	11:E:69:THR:N	2.49	0.43
11:E:460:MET:O	11:E:464:GLU:N	2.52	0.43
12:F:216:ALA:HB2	12:F:313:LEU:HD23	1.99	0.43
14:H:475:ASN:HA	14:H:493:LEU:HB3	2.01	0.43
10:L:283:ILE:HG21	10:L:313:ALA:HA	1.99	0.43
13:O:99:LEU:HD22	13:O:445:ILE:HG13	2.00	0.43
14:P:38:GLU:O	14:P:42:THR:OG1	2.36	0.43
14:P:308:TYR:HD2	14:P:310:ILE:HB	1.82	0.43
14:P:366:GLU:HB3	14:P:368:GLU:HG2	2.00	0.43
2:2:40:LEU:HD11	2:2:105:THR:HA	2.01	0.43
11:E:208:LEU:HD22	11:E:381:ARG:HA	1.99	0.43
11:E:219:LEU:HA	11:E:389:GLY:HA2	2.00	0.43
12:F:128:GLU:HG3	12:F:131:LEU:HD12	2.01	0.43
11:M:414:ARG:HH22	11:M:511:ILE:HG21	1.82	0.43
12:N:228:ALA:N	12:N:347:ALA:O	2.51	0.43
13:O:73:HIS:HB2	13:O:76:ALA:H	1.84	0.43
13:O:487:ASN:HB3	13:O:492:VAL:HB	1.99	0.43
5:5:15:LEU:HD22	5:5:131:VAL:HG13	2.01	0.43
7:A:176:VAL:HG12	7:A:399:VAL:HG11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:356:ILE:HA	7:A:378:ARG:HH21	1.82	0.43
9:C:63:GLY:HA2	9:C:66:ILE:HB	2.00	0.43
9:C:445:GLU:O	9:C:449:ARG:N	2.49	0.43
11:E:73:ASP:O	11:E:76:THR:OG1	2.34	0.43
13:G:406:VAL:HB	13:G:496:ALA:HB2	1.99	0.43
14:H:134:ILE:HG12	14:H:137:ARG:HH21	1.84	0.43
14:H:475:ASN:ND2	14:H:491:ASP:OD1	2.52	0.43
8:J:219:LEU:HD13	8:J:359:LEU:HD22	2.01	0.43
8:J:496:SER:HB3	8:J:499:VAL:HG12	2.01	0.43
9:K:238:ILE:HD11	9:K:324:ALA:HB2	1.99	0.43
11:M:417:ARG:HB3	11:M:510:LEU:HB3	2.01	0.43
13:O:37:ARG:HG3	13:O:99:LEU:HG	2.00	0.43
14:P:27:GLU:HG3	14:P:523:GLN:HA	2.01	0.43
2:2:71:TYR:HB3	2:2:78:LEU:HD11	2.00	0.43
3:3:94:LYS:HE3	3:3:118:PRO:HA	2.01	0.43
7:A:467:LEU:O	7:A:485:TRP:NE1	2.51	0.43
11:E:25:LYS:HG2	11:E:536:PRO:HA	2.00	0.43
14:H:218:LEU:HD21	14:H:362:VAL:HG22	2.00	0.43
9:K:195:ILE:HB	9:K:198:TYR:HD2	1.83	0.43
10:L:314:LEU:HD11	10:L:326:LYS:HD2	2.01	0.43
11:M:509:THR:HG23	11:M:512:GLY:H	1.84	0.43
5:5:94:LYS:HE2	5:5:102:PHE:HE2	1.84	0.43
12:F:382:HIS:O	12:F:386:GLN:N	2.50	0.43
14:H:408:LEU:HB3	14:H:498:LEU:HD12	2.00	0.43
8:J:52:LEU:N	8:J:62:MET:O	2.52	0.43
10:L:287:VAL:HG21	10:L:316:PHE:HB3	2.01	0.43
10:L:376:ILE:HG22	10:L:379:CYS:HB3	2.00	0.43
8:B:449:ILE:O	8:B:453:ASN:N	2.47	0.43
13:G:149:VAL:HG23	13:G:151:GLN:H	1.83	0.43
13:G:274:LEU:HD23	13:G:277:LYS:HD2	2.00	0.43
7:I:43:LYS:NZ	9:K:518:ARG:O	2.45	0.43
7:I:237:LEU:HB2	7:I:288:THR:HA	2.01	0.43
8:J:297:TYR:H	8:J:300:PRO:HD2	1.84	0.43
9:K:51:LEU:N	12:N:522:MET:O	2.47	0.43
9:K:322:ARG:HG2	9:K:325:ARG:HH21	1.83	0.43
11:M:262:THR:OG1	11:M:263:LYS:N	2.51	0.43
7:A:394:ASP:OD1	7:A:395:ALA:N	2.52	0.42
11:E:509:THR:HG23	11:E:512:GLY:H	1.84	0.42
10:L:213:LYS:HE3	10:L:367:LEU:HB2	2.01	0.42
11:M:59:LYS:N	11:M:71:THR:O	2.46	0.42
11:M:440:CYS:HA	11:M:441:PRO:HD3	1.79	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:164:ASN:HB3	7:A:167:PHE:HB3	2.01	0.42
8:B:469:HIS:HD2	8:B:474:THR:HG22	1.84	0.42
9:C:304:LEU:HA	9:C:307:ALA:HB3	2.00	0.42
10:D:49:ARG:HH22	10:D:114:GLY:HA3	1.83	0.42
11:E:98:GLN:NE2	11:E:104:ASP:O	2.42	0.42
13:G:37:ARG:HH11	13:G:444:ILE:HD11	1.83	0.42
8:J:72:LYS:HZ3	8:J:89:ARG:HD3	1.84	0.42
9:K:27:ILE:HG12	9:K:106:LEU:HG	2.01	0.42
9:K:152:MET:HG2	9:K:401:VAL:HG21	2.00	0.42
3:3:93:LYS:HG3	3:3:95:LYS:H	1.83	0.42
11:E:48:MET:HG3	11:E:110:VAL:HB	2.01	0.42
7:I:436:LEU:HA	7:I:439:ALA:HB3	2.00	0.42
8:J:219:LEU:HD21	8:J:374:VAL:HG11	2.00	0.42
9:K:299:LEU:HA	9:K:302:HIS:HD2	1.83	0.42
7:A:285:VAL:HG21	7:A:351:VAL:HG21	2.00	0.42
9:C:355:ILE:HG23	9:C:377:ARG:HH11	1.84	0.42
11:E:417:ARG:HB3	11:E:510:LEU:HB3	2.01	0.42
12:F:44:MET:HG2	12:F:58:LYS:HD2	2.01	0.42
12:F:45:LYS:HD2	14:H:523:GLN:HG3	2.01	0.42
14:H:16:LYS:HG2	14:H:18:GLY:H	1.84	0.42
14:H:218:LEU:HD22	14:H:355:VAL:HG21	2.01	0.42
7:I:529:ASP:H	10:L:50:THR:HB	1.84	0.42
8:J:45:PRO:HD2	8:J:450:ILE:HG12	2.02	0.42
9:K:184:GLN:NE2	9:K:188:ASN:OD1	2.53	0.42
10:L:283:ILE:HA	10:L:286:LEU:HD12	2.01	0.42
13:O:120:ILE:HG23	13:O:123:ARG:HD2	2.01	0.42
7:A:226:PRO:HG2	7:A:306:MET:HB2	2.01	0.42
9:C:245:LEU:HD22	9:C:292:THR:HG21	2.01	0.42
10:D:209:LYS:HB3	10:D:387:THR:HG23	2.02	0.42
10:D:484:HIS:HD2	10:D:489:LYS:HA	1.83	0.42
12:F:134:LEU:HA	12:F:137:VAL:HG12	2.02	0.42
12:F:426:LYS:HD2	12:F:429:VAL:HG13	2.01	0.42
14:H:60:LEU:HD12	14:H:62:LYS:HZ3	1.85	0.42
9:K:153:LEU:HA	9:K:156:ILE:HG22	2.01	0.42
12:N:127:LYS:HG3	12:N:505:LEU:HB3	2.00	0.42
7:A:486:ILE:HD12	7:A:486:ILE:HA	1.90	0.42
14:H:423:ILE:HG21	14:H:441:PHE:HD2	1.85	0.42
11:M:123:LEU:HD22	11:M:128:ILE:HD12	2.02	0.42
11:M:386:PHE:HE2	11:M:388:ARG:HE	1.68	0.42
5:5:105:ARG:HH22	6:6:42:ILE:HG23	1.84	0.42
9:C:51:LEU:HD13	12:F:72:PRO:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:D:69:THR:HG21	10:D:80:GLN:HE22	1.83	0.42
10:D:139:LYS:NZ	10:D:447:GLU:OE2	2.45	0.42
13:G:429:GLY:H	7:I:465:ALA:HA	1.85	0.42
9:K:348:GLY:N	9:K:364:THR:O	2.43	0.42
11:M:264:HIS:HA	13:O:256:ARG:HB2	2.00	0.42
11:M:460:MET:O	11:M:464:GLU:N	2.52	0.42
12:N:82:THR:O	12:N:86:ASP:N	2.49	0.42
12:N:240:GLU:HA	12:N:270:ARG:HD2	2.01	0.42
9:C:217:GLY:N	9:C:371:ALA:O	2.52	0.42
11:E:301:ILE:HG23	11:E:325:VAL:HG21	2.02	0.42
13:G:366:LYS:HB3	13:G:368:LYS:HG2	2.01	0.42
13:G:420:LEU:HA	13:G:423:TYR:HB3	2.02	0.42
7:A:145:ARG:HE	7:A:398:VAL:HA	1.85	0.42
7:A:452:LEU:O	7:A:456:ALA:N	2.46	0.42
11:E:254:PRO:HG3	11:E:258:PRO:HG3	2.02	0.42
13:G:142:THR:HA	13:G:404:SER:HA	2.02	0.42
8:J:421:VAL:O	8:J:425:ALA:N	2.53	0.42
11:M:61:MET:O	11:M:69:THR:N	2.49	0.42
11:M:478:ARG:HD2	11:M:478:ARG:HA	1.87	0.42
12:N:314:ARG:HG2	12:N:315:ARG:HG3	2.01	0.42
13:O:398:ARG:HE	13:O:498:VAL:HG22	1.85	0.42
3:3:56:GLN:NE2	14:H:251:THR:OG1	2.53	0.42
5:5:42:LYS:HA	5:5:45:GLU:HB3	2.00	0.42
9:C:163:LYS:NZ	9:C:393:ASP:OD2	2.46	0.42
9:C:227:PRO:HG3	9:C:359:TYR:HD2	1.85	0.42
14:H:143:LEU:HD13	14:H:419:LEU:HD11	2.02	0.42
7:I:367:THR:OG1	7:I:370:ARG:O	2.30	0.42
9:C:446:VAL:HA	9:C:449:ARG:HB2	2.02	0.41
11:E:386:PHE:HE2	11:E:388:ARG:HE	1.68	0.41
13:G:245:GLU:HA	13:G:296:GLY:HA3	2.01	0.41
13:G:407:ALA:HB2	13:G:488:PHE:HB2	2.02	0.41
14:H:446:GLU:HG2	14:H:450:ARG:NE	2.36	0.41
7:I:110:GLN:OE1	7:I:433:ARG:NH1	2.52	0.41
11:M:301:ILE:HG23	11:M:325:VAL:HG21	2.02	0.41
12:N:215:GLY:HA2	12:N:313:LEU:HD12	2.01	0.41
13:O:29:CYS:HB2	13:O:75:ALA:HB1	2.01	0.41
7:A:185:ARG:H	7:A:321:LYS:HB2	1.83	0.41
11:E:478:ARG:HA	11:E:478:ARG:HD2	1.87	0.41
13:G:38:THR:HB	13:G:448:GLN:HB3	2.02	0.41
14:H:43:THR:HG21	14:H:105:LEU:HD23	2.03	0.41
8:J:330:GLU:H	8:J:342:LYS:HG2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:192:LEU:HD22	13:O:390:HIS:HE1	1.84	0.41
7:A:131:TYR:HB2	7:A:422:TYR:CE2	2.55	0.41
7:I:187:GLN:OE1	7:I:189:ARG:NE	2.38	0.41
10:L:262:ASN:ND2	10:L:278:GLU:OE2	2.51	0.41
11:M:48:MET:HG3	11:M:110:VAL:HB	2.01	0.41
13:O:518:GLU:HG2	14:P:54:LYS:HD2	2.01	0.41
14:P:338:PRO:HA	14:P:339:PRO:HD3	1.86	0.41
14:P:422:GLN:O	14:P:426:TYR:N	2.52	0.41
2:2:31:ASN:HA	2:2:34:ARG:HE	1.85	0.41
4:4:58:MET:SD	4:4:84:GLN:NE2	2.93	0.41
13:G:421:ARG:HG2	13:G:465:ARG:HH22	1.85	0.41
7:I:8:PHE:HD2	7:I:534:HIS:HA	1.86	0.41
10:L:414:CYS:HA	10:L:513:LEU:HD23	2.02	0.41
11:M:254:PRO:HG3	11:M:258:PRO:HG3	2.02	0.41
12:N:326:LEU:HD21	12:N:370:ARG:HB3	2.02	0.41
14:P:41:GLN:H	14:P:44:ARG:HD2	1.86	0.41
14:P:327:THR:HG23	14:P:328:VAL:HG13	2.03	0.41
1:1:78:SER:HA	1:1:81:LEU:HD12	2.02	0.41
7:A:112:ILE:HD11	13:O:458:THR:HG21	2.03	0.41
9:C:229:MET:HB2	9:C:352:ILE:HD11	2.02	0.41
10:D:42:LYS:O	10:D:46:ASP:N	2.53	0.41
10:L:37:ASN:HA	10:L:85:HIS:CE1	2.55	0.41
11:M:77:ILE:O	11:M:81:MET:N	2.42	0.41
14:P:178:PHE:HD2	14:P:179:LEU:HD22	1.86	0.41
6:6:39:GLU:HG2	6:6:42:ILE:HD12	2.03	0.41
7:A:471:HIS:CE1	13:O:426:THR:HA	2.55	0.41
8:B:17:ASP:HB2	8:B:522:LYS:HB3	2.03	0.41
8:B:39:VAL:HG23	8:B:104:VAL:HB	2.02	0.41
9:C:184:GLN:HA	9:C:193:ILE:HG21	2.03	0.41
9:C:488:VAL:HG21	9:C:493:LEU:HD22	2.03	0.41
11:E:38:ILE:HD13	11:E:117:LEU:HD23	2.01	0.41
11:E:55:ASN:ND2	11:E:493:CYS:O	2.54	0.41
14:H:44:ARG:HB3	14:H:451:ALA:HB1	2.03	0.41
7:I:191:PRO:HA	7:I:400:LYS:HD2	2.03	0.41
7:I:424:GLU:HG2	7:I:439:ALA:HA	2.03	0.41
7:I:530:LEU:HA	10:L:59:LYS:HG3	2.03	0.41
2:2:40:LEU:HD12	2:2:108:LEU:HB2	2.02	0.41
7:A:505:GLU:HG2	7:A:510:LYS:HE2	2.02	0.41
8:B:217:GLY:H	8:B:371:CYS:HA	1.84	0.41
10:D:449:TYR:OH	11:M:474:MET:SD	2.65	0.41
13:G:243:GLU:HB2	13:G:293:LEU:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:118:ASP:O	10:L:122:LYS:NZ	2.53	0.41
10:L:122:LYS:HA	10:L:125:GLN:HB2	2.03	0.41
10:L:234:SER:OG	10:L:318:ASN:ND2	2.52	0.41
11:M:55:ASN:ND2	11:M:493:CYS:O	2.53	0.41
13:O:417:SER:HB3	13:O:421:ARG:HH12	1.86	0.41
13:O:522:ASN:HB2	14:P:58:ASN:HA	2.02	0.41
3:3:94:LYS:NZ	3:3:99:ASN:OD1	2.53	0.41
9:C:380:SER:H	9:C:383:ILE:HB	1.85	0.41
11:E:34:LEU:O	11:E:38:ILE:N	2.54	0.41
11:E:123:LEU:HD22	11:E:128:ILE:HD12	2.02	0.41
11:E:364:PHE:H	11:E:370:LYS:HA	1.85	0.41
12:F:296:GLY:HA2	12:F:314:ARG:HB2	2.02	0.41
13:G:239:LEU:H	13:G:331:GLN:HE21	1.69	0.41
8:J:213:TYR:H	8:J:376:ARG:HH12	1.67	0.41
10:L:176:VAL:HB	10:L:179:TYR:HB2	2.03	0.41
10:L:237:GLY:H	10:L:240:ARG:HH21	1.67	0.41
11:M:38:ILE:HD13	11:M:117:LEU:HD23	2.02	0.41
13:O:448:GLN:HA	13:O:451:ASP:HB2	2.03	0.41
14:P:155:ARG:NH2	14:P:192:PRO:O	2.54	0.41
14:P:206:LYS:NZ	14:P:386:ASP:OD1	2.34	0.41
14:P:414:ALA:HB2	14:P:477:ASN:HB2	2.02	0.41
3:3:84:THR:HB	3:3:144:LEU:HD13	2.02	0.41
8:B:67:GLY:HA2	8:B:70:ILE:HD12	2.02	0.41
8:B:137:ALA:HB1	8:B:417:MET:HB3	2.02	0.41
8:B:190:LEU:HD22	8:B:195:ASN:HB2	2.03	0.41
8:B:249:ILE:H	8:B:249:ILE:HG13	1.70	0.41
8:B:399:GLN:HB3	8:B:498:GLN:HG2	2.03	0.41
9:C:39:THR:HB	9:C:46:MET:HB2	2.02	0.41
9:C:44:LYS:HD2	9:C:483:GLU:HA	2.02	0.41
9:C:215:LEU:HD12	9:C:364:THR:HG21	2.02	0.41
9:C:296:ILE:HG12	9:C:313:ARG:HB3	2.01	0.41
10:D:248:LEU:HD23	10:D:344:PRO:HA	2.02	0.41
10:D:346:ALA:N	10:D:350:GLN:OE1	2.43	0.41
10:D:481:ARG:HD3	11:M:445:GLN:HE22	1.86	0.41
12:F:465:LYS:HB3	12:F:486:PRO:HG2	2.03	0.41
14:H:168:ILE:HD13	14:H:179:LEU:HB2	2.03	0.41
14:H:500:THR:HG23	14:H:503:GLY:H	1.86	0.41
7:I:45:LEU:HD22	9:K:523:VAL:HG22	2.02	0.41
7:I:67:VAL:HG11	7:I:73:LYS:HA	2.03	0.41
7:I:231:ASN:O	7:I:351:VAL:N	2.45	0.41
8:J:221:ASP:HA	8:J:359:LEU:HG	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:113:ALA:HA	10:L:116:LEU:HD12	2.03	0.41
10:L:160:ARG:NE	10:L:192:MET:HG3	2.36	0.41
10:L:325:ILE:HD12	10:L:325:ILE:HA	1.89	0.41
11:M:385:ILE:HD12	11:M:402:LEU:HD23	2.02	0.41
4:4:121:ALA:HB2	13:G:277:LYS:HG2	2.02	0.41
9:C:203:LYS:HA	9:C:384:LEU:HD11	2.02	0.41
9:C:416:MET:HG2	9:C:466:LEU:HG	2.03	0.41
10:D:471:LEU:O	10:D:476:THR:OG1	2.39	0.41
14:H:335:ARG:NH2	14:H:342:GLU:OE2	2.53	0.41
14:H:394:ASP:O	14:H:398:THR:OG1	2.31	0.41
9:K:113:LEU:HD13	9:K:122:VAL:HG22	2.03	0.41
10:L:123:LEU:HB3	10:L:128:ILE:HD12	2.03	0.41
11:M:183:ARG:HH21	11:M:186:ALA:HB3	1.86	0.41
7:A:401:ARG:HB3	7:A:506:PRO:HG3	2.03	0.40
10:D:143:LYS:HD2	10:D:439:TYR:CD2	2.55	0.40
13:G:195:ILE:HA	13:G:371:THR:HA	2.02	0.40
8:J:151:ASP:O	8:J:155:PHE:N	2.45	0.40
9:K:39:THR:O	9:K:46:MET:N	2.53	0.40
9:K:241:LEU:HA	9:K:245:LEU:HB2	2.02	0.40
10:L:77:ILE:HA	10:L:80:GLN:HG2	2.03	0.40
10:L:235:ASN:ND2	10:L:318:ASN:O	2.55	0.40
12:N:193:ILE:HG21	12:N:388:LYS:HG3	2.03	0.40
14:P:477:ASN:O	14:P:490:LYS:N	2.48	0.40
7:A:43:LYS:HD3	9:C:521:ASP:HB2	2.02	0.40
10:D:418:LYS:HB3	10:D:512:LEU:HD23	2.02	0.40
11:E:183:ARG:HH21	11:E:186:ALA:HB3	1.86	0.40
13:G:26:ILE:HG23	13:G:105:LEU:HB3	2.02	0.40
13:G:211:VAL:HG12	13:G:213:GLY:H	1.86	0.40
8:J:291:ILE:HG22	8:J:312:ILE:HB	2.03	0.40
12:N:41:LYS:HG3	12:N:454:ASN:HB3	2.03	0.40
12:N:196:MET:N	12:N:376:ILE:O	2.54	0.40
14:P:129:ILE:HG23	14:P:516:VAL:HB	2.04	0.40
3:3:85:LEU:HG	3:3:148:LEU:HD22	2.03	0.40
4:4:23:ILE:HA	4:4:26:PHE:HB3	2.03	0.40
8:B:186:ALA:HB2	8:B:214:LEU:HD11	2.04	0.40
8:J:51:ILE:HD12	8:J:63:VAL:HG22	2.02	0.40
8:J:239:ILE:HG12	8:J:291:ILE:HD11	2.03	0.40
11:M:358:LEU:O	11:M:375:GLU:N	2.52	0.40
11:M:364:PHE:H	11:M:370:LYS:HA	1.85	0.40
13:O:331:GLN:HE21	13:O:341:VAL:HG12	1.86	0.40
3:3:124:CYS:HA	3:3:134:GLU:HA	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:232:ILE:HB	8:B:349:ILE:HB	2.02	0.40
9:C:216:ARG:HB2	9:C:364:THR:HB	2.03	0.40
11:E:198:ASP:OD1	11:E:198:ASP:N	2.55	0.40
11:E:385:ILE:HD12	11:E:402:LEU:HD23	2.02	0.40
14:H:273:GLU:HG3	14:H:300:MET:HB3	2.04	0.40
7:I:417:ALA:HB1	7:I:468:ARG:HH22	1.86	0.40
8:J:66:ASP:O	8:J:69:THR:OG1	2.35	0.40
8:J:465:LEU:HG	8:J:469:HIS:CD2	2.57	0.40
9:K:365:ASP:HB2	9:K:370:LYS:HD3	2.03	0.40
14:P:258:LEU:HD13	14:P:264:GLU:HB3	2.03	0.40
7:A:107:LEU:HB3	7:A:112:ILE:HG13	2.04	0.40
9:C:38:ARG:HB3	9:C:100:ILE:HD12	2.03	0.40
10:D:212:LYS:HD2	10:D:395:LYS:HZ3	1.87	0.40
12:F:193:ILE:HG21	12:F:388:LYS:HG3	2.02	0.40
8:J:374:VAL:O	8:J:376:ARG:NH1	2.54	0.40
9:K:400:ASN:HD21	9:K:499:LEU:N	2.20	0.40
10:L:283:ILE:HD13	10:L:313:ALA:HB2	2.04	0.40
11:M:40:ALA:HB3	11:M:87:ILE:HB	2.03	0.40
12:N:380:ASN:O	12:N:383:THR:OG1	2.39	0.40
13:O:49:ILE:HG21	13:O:69:LEU:HD11	2.03	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	1	105/107 (98%)	103 (98%)	2 (2%)	0	100	100
2	2	101/103 (98%)	99 (98%)	2 (2%)	0	100	100
3	3	130/132 (98%)	118 (91%)	10 (8%)	2 (2%)	10	46
4	4	102/104 (98%)	95 (93%)	7 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	5	125/127 (98%)	119 (95%)	5 (4%)	1 (1%)	19	60
6	6	100/102 (98%)	100 (100%)	0	0	100	100
7	A	519/534 (97%)	473 (91%)	45 (9%)	1 (0%)	47	81
7	I	532/534 (100%)	494 (93%)	38 (7%)	0	100	100
8	B	507/509 (100%)	478 (94%)	28 (6%)	1 (0%)	47	81
8	J	506/509 (99%)	472 (93%)	34 (7%)	0	100	100
9	C	507/513 (99%)	478 (94%)	29 (6%)	0	100	100
9	K	511/513 (100%)	466 (91%)	42 (8%)	3 (1%)	25	66
10	D	506/514 (98%)	476 (94%)	28 (6%)	2 (0%)	34	72
10	L	511/514 (99%)	466 (91%)	45 (9%)	0	100	100
11	E	515/517 (100%)	489 (95%)	26 (5%)	0	100	100
11	M	515/517 (100%)	489 (95%)	26 (5%)	0	100	100
12	F	512/515 (99%)	480 (94%)	32 (6%)	0	100	100
12	N	511/515 (99%)	485 (95%)	26 (5%)	0	100	100
13	G	510/514 (99%)	481 (94%)	29 (6%)	0	100	100
13	O	512/514 (100%)	481 (94%)	31 (6%)	0	100	100
14	H	508/514 (99%)	480 (94%)	27 (5%)	1 (0%)	47	81
14	P	507/514 (99%)	484 (96%)	23 (4%)	0	100	100
All	All	8852/8935 (99%)	8306 (94%)	535 (6%)	11 (0%)	54	86

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	3	99	ASN
9	K	192	GLU
7	A	148	LEU
9	K	191	LYS
14	H	471	HIS
10	D	443	LEU
3	3	100	SER
5	5	56	SER
8	B	119	LYS
9	K	193	ILE
10	D	203	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	97/97 (100%)	97 (100%)	0	100	100
2	2	91/91 (100%)	90 (99%)	1 (1%)	73	84
3	3	122/122 (100%)	122 (100%)	0	100	100
4	4	96/96 (100%)	94 (98%)	2 (2%)	53	72
5	5	116/116 (100%)	116 (100%)	0	100	100
6	6	91/91 (100%)	90 (99%)	1 (1%)	73	84
7	A	434/445 (98%)	429 (99%)	5 (1%)	71	83
7	I	445/445 (100%)	437 (98%)	8 (2%)	59	77
8	B	405/405 (100%)	400 (99%)	5 (1%)	71	83
8	J	405/405 (100%)	402 (99%)	3 (1%)	84	90
9	C	441/444 (99%)	438 (99%)	3 (1%)	84	90
9	K	444/444 (100%)	440 (99%)	4 (1%)	78	87
10	D	433/439 (99%)	429 (99%)	4 (1%)	78	87
10	L	438/439 (100%)	433 (99%)	5 (1%)	73	84
11	E	436/436 (100%)	429 (98%)	7 (2%)	62	79
11	M	436/436 (100%)	429 (98%)	7 (2%)	62	79
12	F	429/429 (100%)	424 (99%)	5 (1%)	71	83
12	N	429/429 (100%)	422 (98%)	7 (2%)	62	79
13	G	420/421 (100%)	414 (99%)	6 (1%)	67	80
13	O	421/421 (100%)	414 (98%)	7 (2%)	60	78
14	H	423/426 (99%)	417 (99%)	6 (1%)	67	80
14	P	422/426 (99%)	420 (100%)	2 (0%)	88	93
All	All	7474/7503 (100%)	7386 (99%)	88 (1%)	72	83

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	2	68	ARG
4	4	66	MET
4	4	71	ILE
6	6	32	LYS
7	A	150	ASN
7	A	225	MET
7	A	309	ARG
7	A	321	LYS
7	A	356	ILE
8	B	73	ASN
8	B	230	LYS
8	B	255	ARG
8	B	298	ASN
8	B	481	ARG
9	C	182	MET
9	C	235	ASN
9	C	481	ASN
10	D	403	ARG
10	D	482	ASN
10	D	502	ASN
10	D	527	ARG
11	E	64	LYS
11	E	199	MET
11	E	248	ILE
11	E	263	LYS
11	E	502	LYS
11	E	528	LEU
11	E	533	ILE
12	F	223	LYS
12	F	314	ARG
12	F	319	ARG
12	F	334	ASN
12	F	368	ASN
13	G	193	LYS
13	G	250	LYS
13	G	292	LYS
13	G	402	ASN
13	G	421	ARG
13	G	447	ARG
14	H	16	LYS
14	H	259	ILE
14	H	407	ARG
14	H	455	ASN

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Mol	Chain	Res	Type
14	H	461	ASN
14	H	477	ASN
7	I	150	ASN
7	I	217	ASN
7	I	228	ARG
7	I	355	ARG
7	I	408	VAL
7	I	430	MET
7	I	472	ASN
7	I	498	ASN
8	J	46	LYS
8	J	322	ARG
8	J	388	ARG
9	K	54	MET
9	K	313	ARG
9	K	316	ARG
9	K	321	ASN
10	L	153	ARG
10	L	326	LYS
10	L	419	ARG
10	L	483	ARG
10	L	489	LYS
11	M	64	LYS
11	M	199	MET
11	M	248	ILE
11	M	263	LYS
11	M	502	LYS
11	M	528	LEU
11	M	533	ILE
12	N	145	ARG
12	N	180	LYS
12	N	279	ARG
12	N	293	ASN
12	N	392	ARG
12	N	487	MET
12	N	523	ARG
13	O	234	ASN
13	O	344	ARG
13	O	357	ARG
13	O	375	ARG
13	O	402	ASN
13	O	425	ARG

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Mol	Chain	Res	Type
13	O	465	ARG
14	P	224	LYS
14	P	455	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (126) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	38	ASN
1	1	71	GLN
1	1	77	HIS
3	3	56	GLN
3	3	175	ASN
4	4	29	ASN
4	4	80	GLN
5	5	51	ASN
7	A	20	GLN
7	A	69	HIS
7	A	82	GLN
7	A	103	ASN
7	A	133	ASN
7	A	150	ASN
7	A	164	ASN
7	A	366	ASN
8	B	91	GLN
8	B	148	HIS
8	B	161	ASN
8	B	228	GLN
8	B	285	HIS
8	B	298	ASN
8	B	314	HIS
8	B	361	HIS
8	B	453	ASN
8	B	519	ASN
9	C	61	ASN
9	C	157	ASN
9	C	235	ASN
9	C	481	ASN
10	D	80	GLN
10	D	235	ASN
10	D	271	GLN
10	D	318	ASN
10	D	482	ASN

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Mol	Chain	Res	Type
10	D	484	HIS
10	D	502	ASN
11	E	85	HIS
11	E	86	GLN
11	E	191	ASN
11	E	236	HIS
11	E	317	ASN
12	F	23	ASN
12	F	115	HIS
12	F	334	ASN
12	F	368	ASN
12	F	460	GLN
13	G	21	GLN
13	G	134	ASN
13	G	151	GLN
13	G	241	ASN
13	G	331	GLN
13	G	431	GLN
13	G	448	GLN
13	G	452	ASN
13	G	487	ASN
14	H	50	ASN
14	H	80	HIS
14	H	145	ASN
14	H	219	HIS
14	H	267	ASN
14	H	316	ASN
14	H	346	HIS
14	H	422	GLN
14	H	461	ASN
14	H	472	GLN
14	H	477	ASN
7	I	20	GLN
7	I	135	ASN
7	I	217	ASN
7	I	242	GLN
7	I	450	ASN
7	I	458	GLN
7	I	498	ASN
8	J	241	ASN
8	J	285	HIS
8	J	399	GLN

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Mol	Chain	Res	Type
8	J	426	ASN
8	J	453	ASN
8	J	519	ASN
9	K	184	GLN
9	K	226	HIS
9	K	302	HIS
9	K	400	ASN
10	L	62	GLN
10	L	80	GLN
10	L	85	HIS
10	L	129	HIS
10	L	250	GLN
10	L	301	GLN
10	L	318	ASN
10	L	366	ASN
10	L	472	ASN
10	L	486	GLN
10	L	537	ASN
11	M	85	HIS
11	M	191	ASN
11	M	236	HIS
11	M	317	ASN
11	M	403	HIS
11	M	472	GLN
11	M	515	GLN
12	N	23	ASN
12	N	65	HIS
12	N	71	HIS
12	N	161	HIS
12	N	245	ASN
12	N	367	ASN
12	N	497	ASN
12	N	514	ASN
13	O	25	ASN
13	O	234	ASN
13	O	264	GLN
13	O	359	ASN
13	O	380	GLN
13	O	390	HIS
13	O	402	ASN
13	O	448	GLN
13	O	501	ASN

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Mol	Chain	Res	Type
13	O	522	ASN
14	P	67	ASN
14	P	198	ASN
14	P	219	HIS
14	P	303	HIS
14	P	455	ASN
14	P	461	ASN

5.3.3 RNA [i](#)

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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

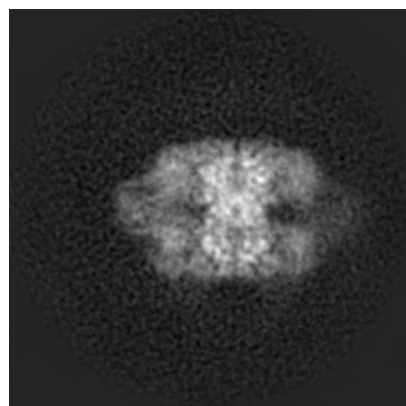
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0490. These allow visual inspection of the internal detail of the map and identification of artifacts.

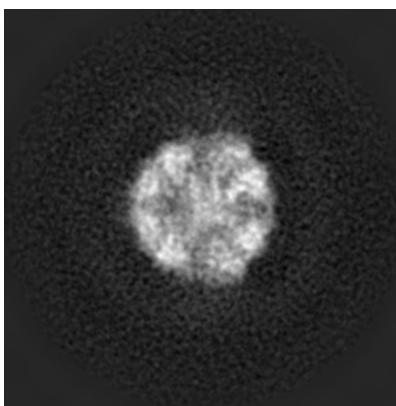
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

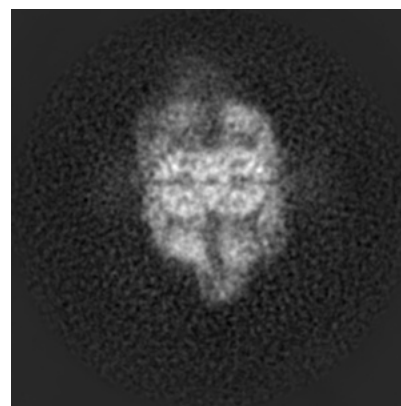
6.1.1 Primary map



X

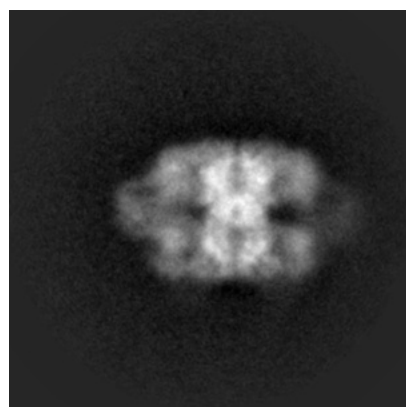


Y

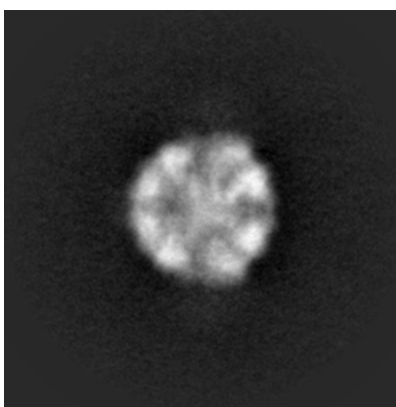


Z

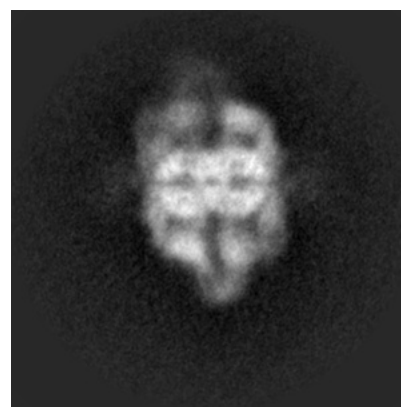
6.1.2 Raw map



X



Y

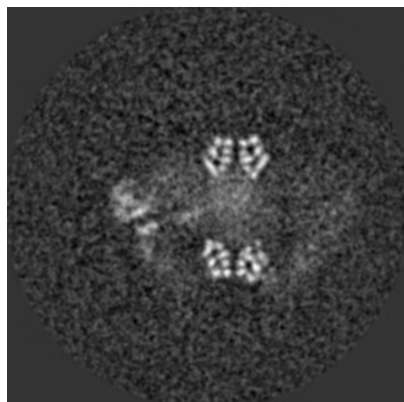


Z

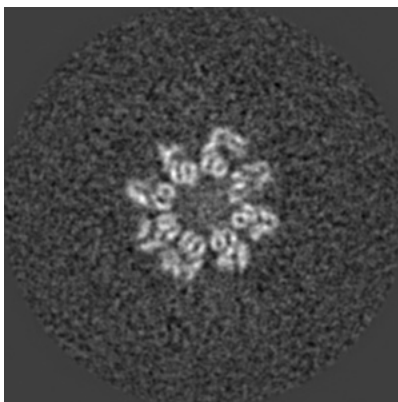
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

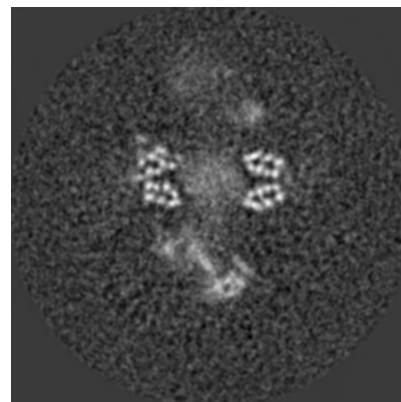
6.2.1 Primary map



X Index: 120

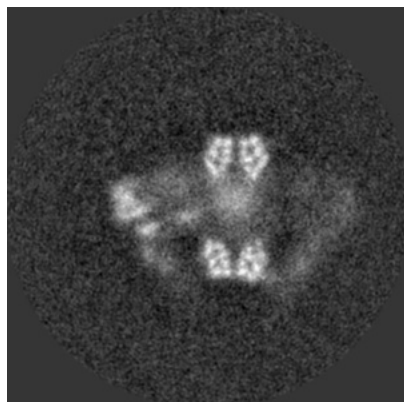


Y Index: 120

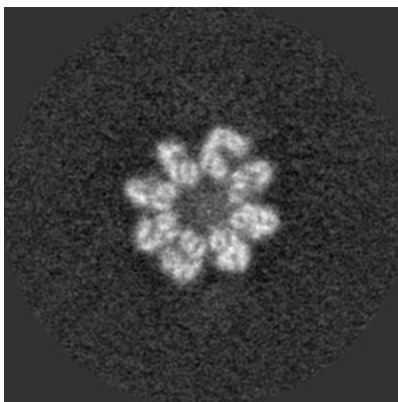


Z Index: 120

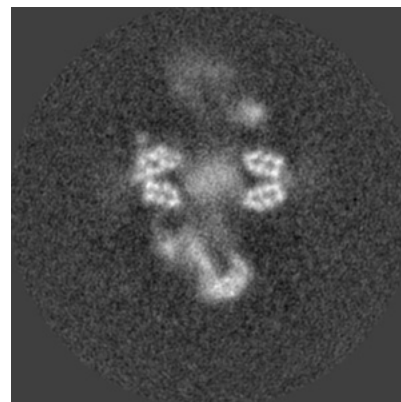
6.2.2 Raw map



X Index: 120



Y Index: 120

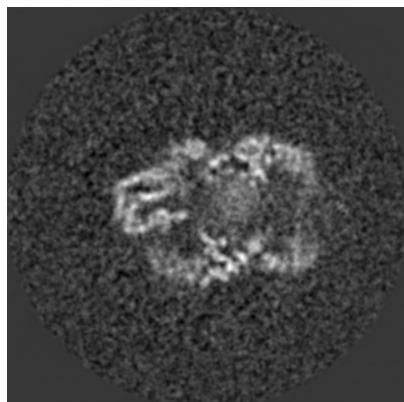


Z Index: 120

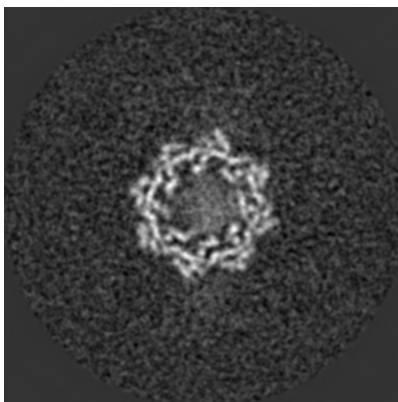
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

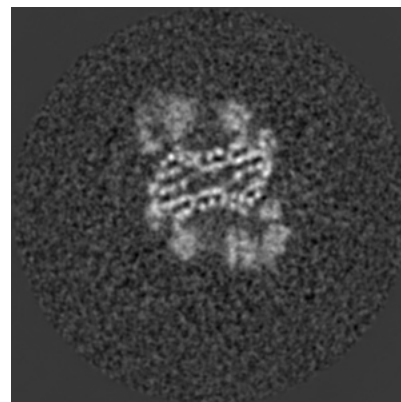
6.3.1 Primary map



X Index: 130

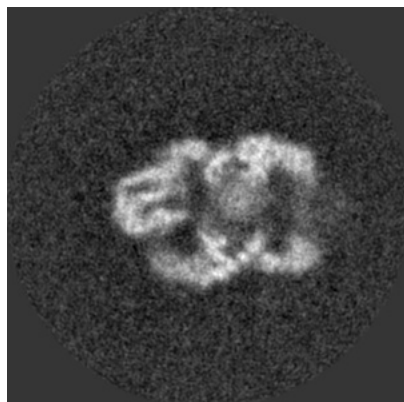


Y Index: 129

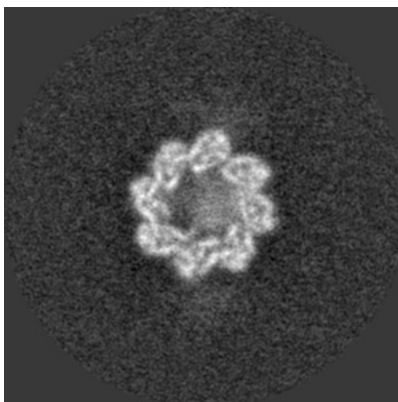


Z Index: 143

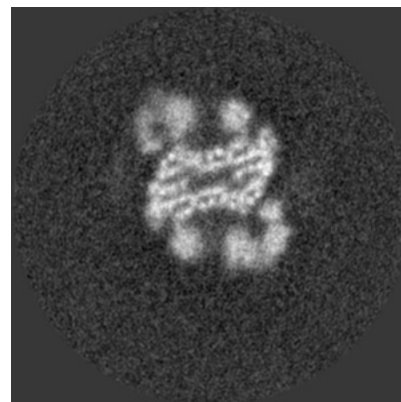
6.3.2 Raw map



X Index: 131



Y Index: 128

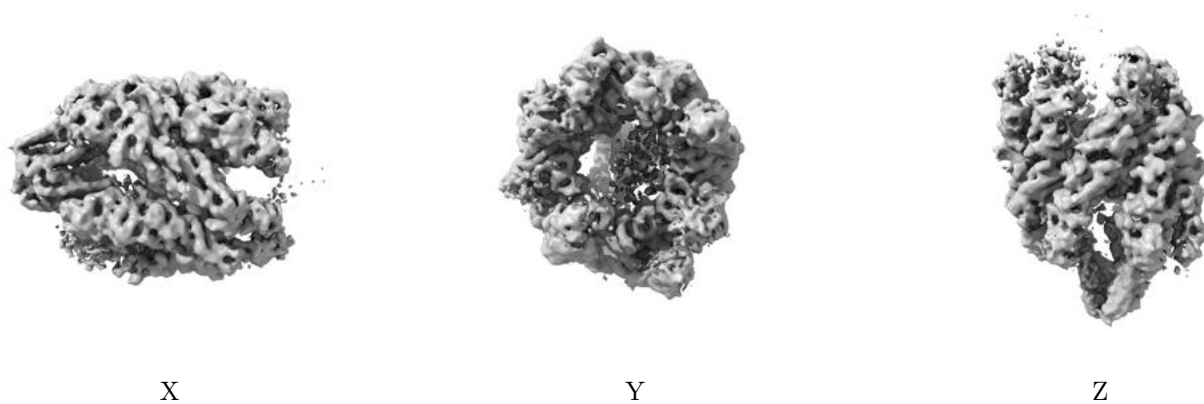


Z Index: 143

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

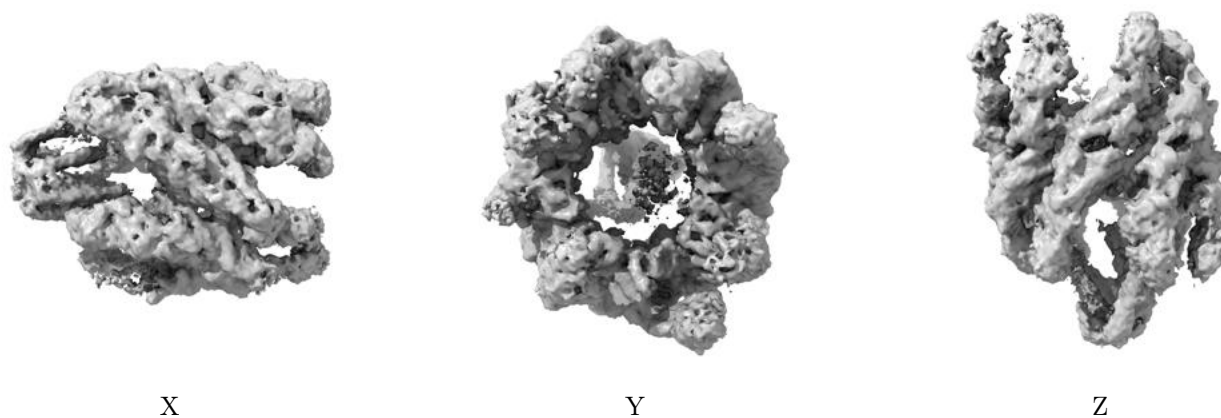
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.55. 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.

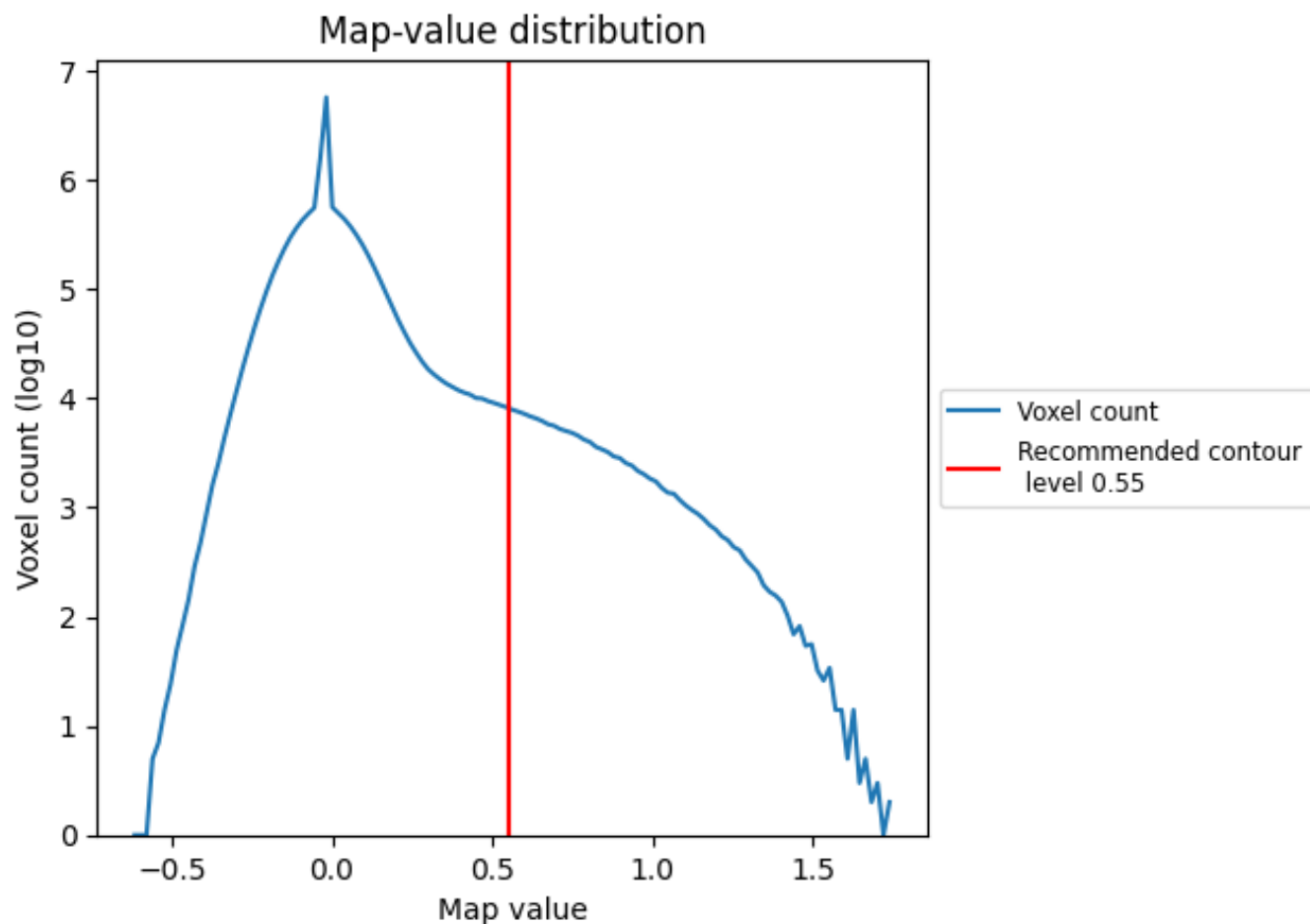
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

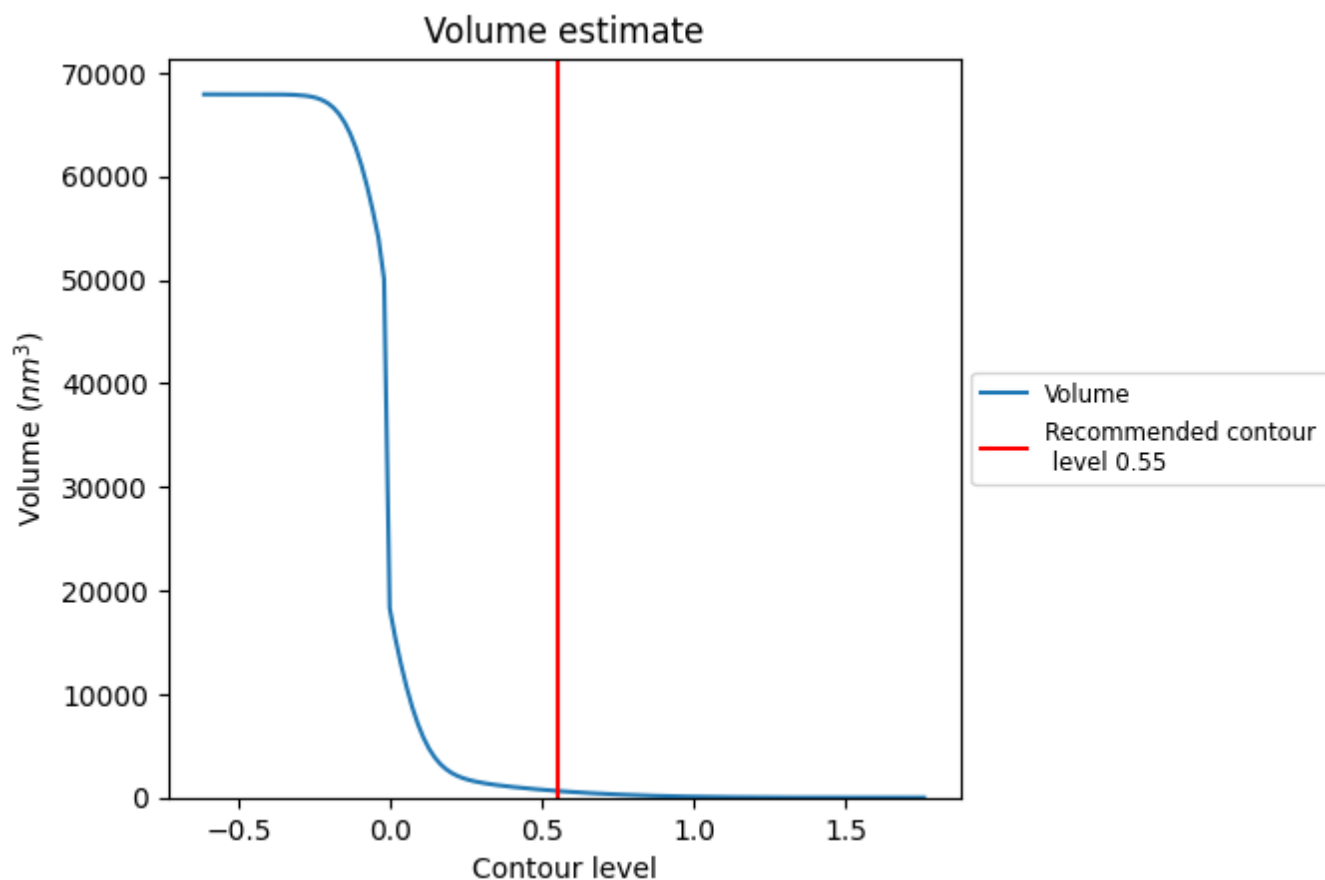
This section contains the results of statistical analysis of the map.

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.

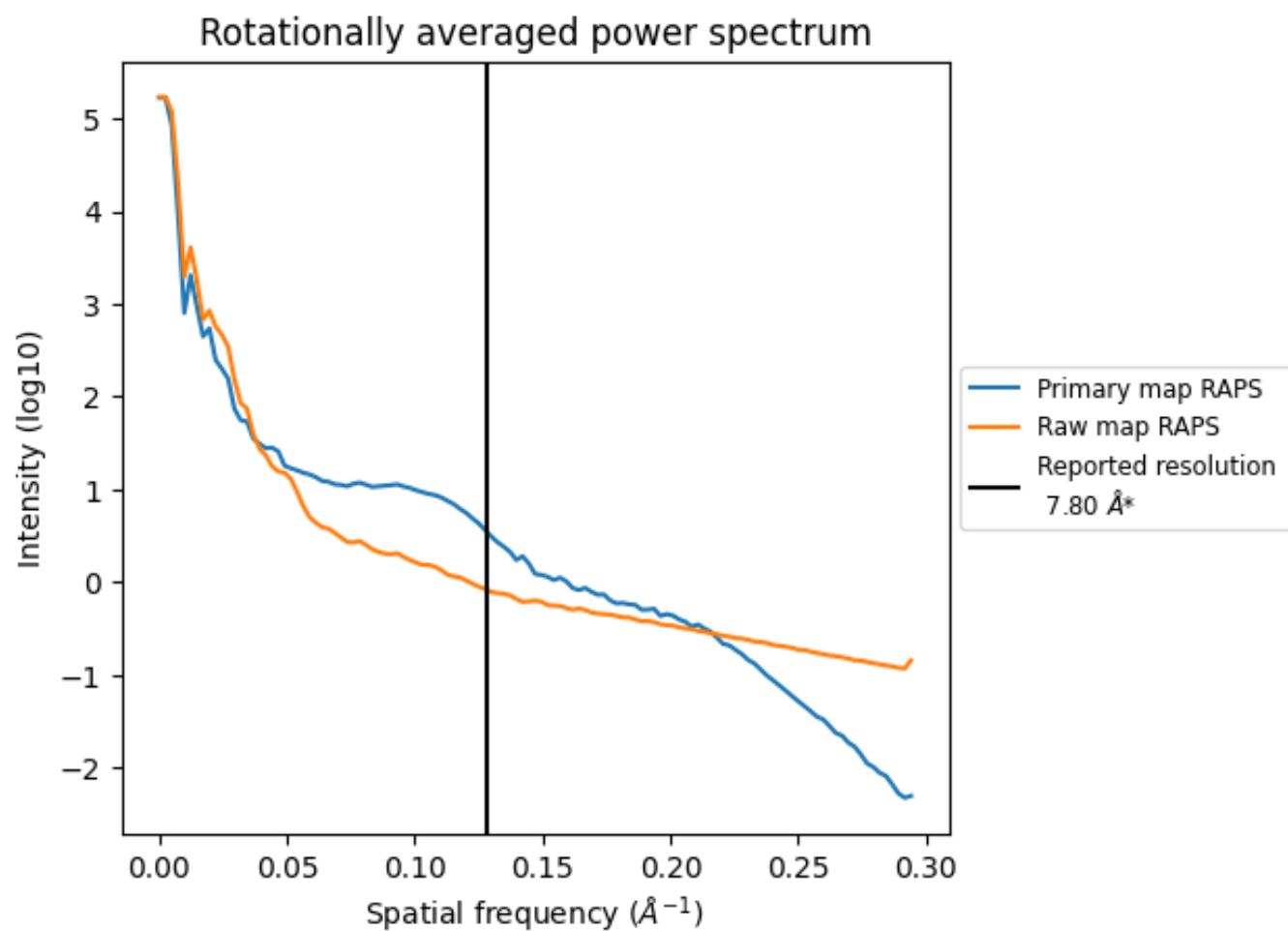
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 638 nm³; this corresponds to an approximate mass of 576 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

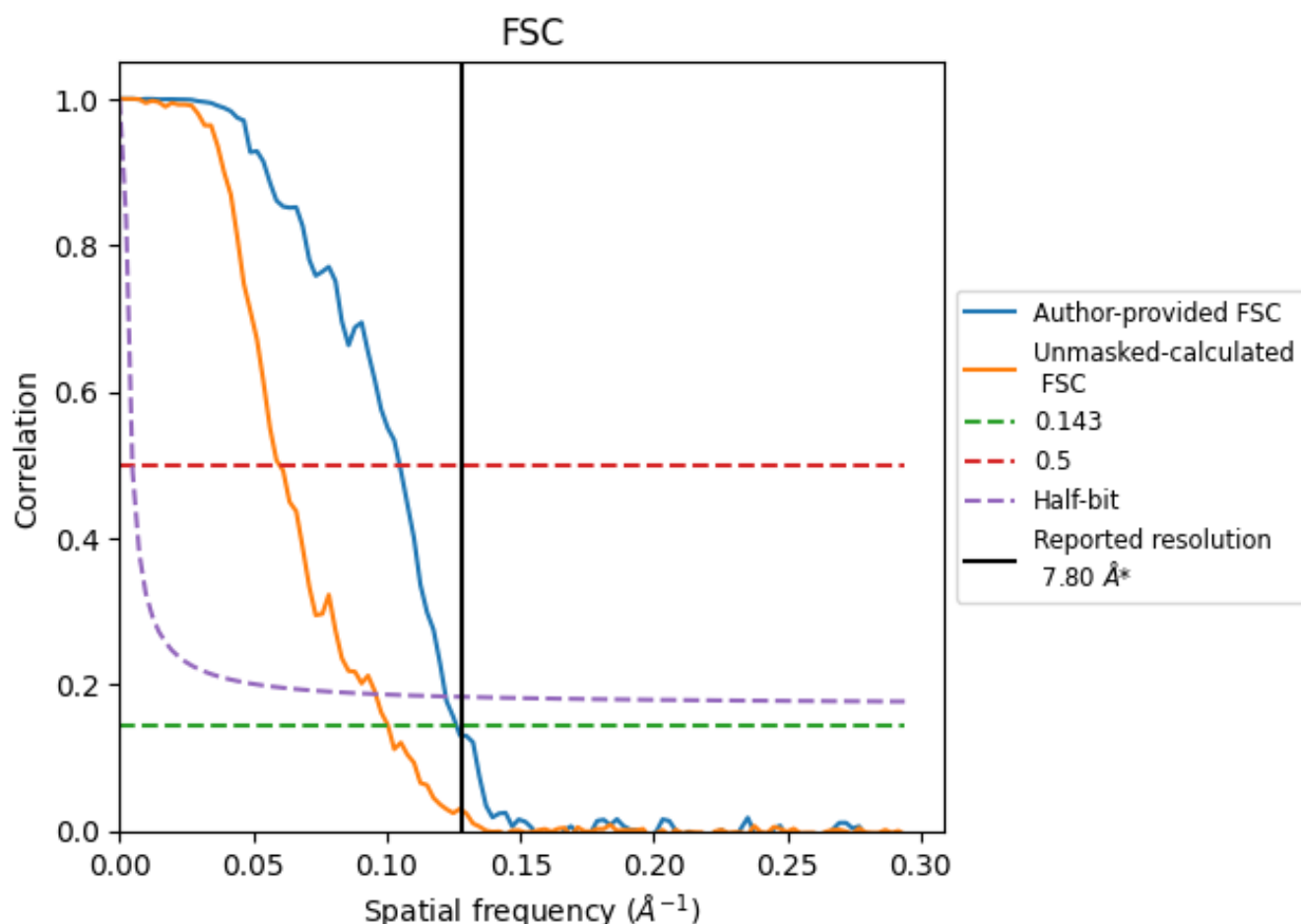


*Reported resolution corresponds to spatial frequency of 0.128 Å⁻¹

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 0.128 Å⁻¹

8.2 Resolution estimates [i](#)

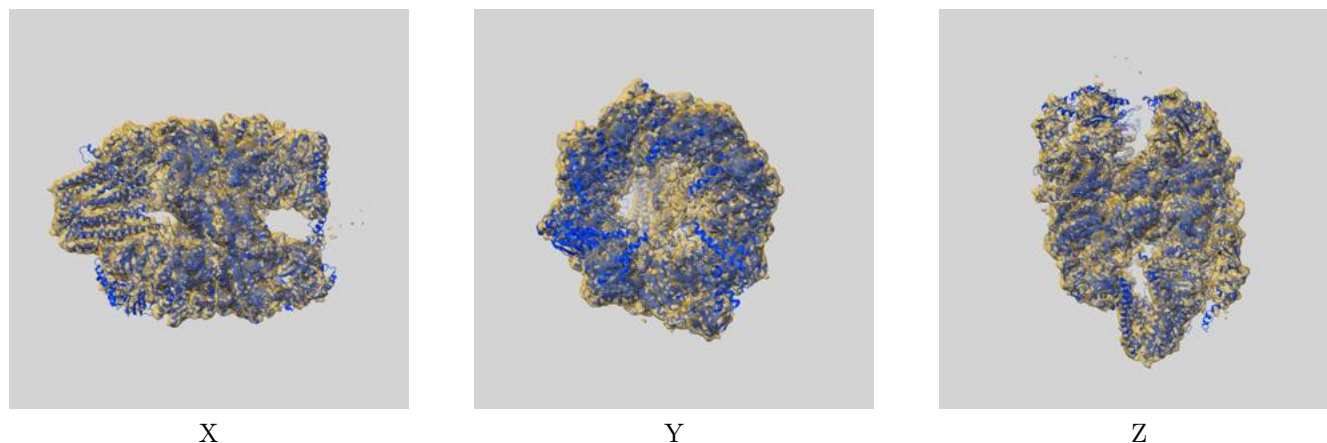
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	7.80	-	-
Author-provided FSC curve	7.92	9.53	8.18
Unmasked-calculated*	9.94	16.69	10.43

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 9.94 differs from the reported value 7.8 by more than 10 %

9 Map-model fit [i](#)

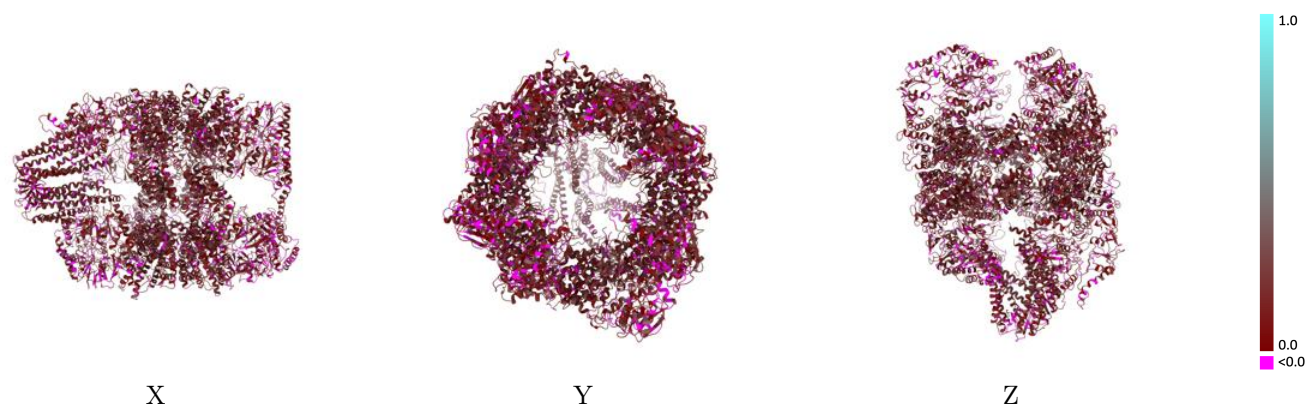
This section contains information regarding the fit between EMDB map EMD-0490 and PDB model 6NR8. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



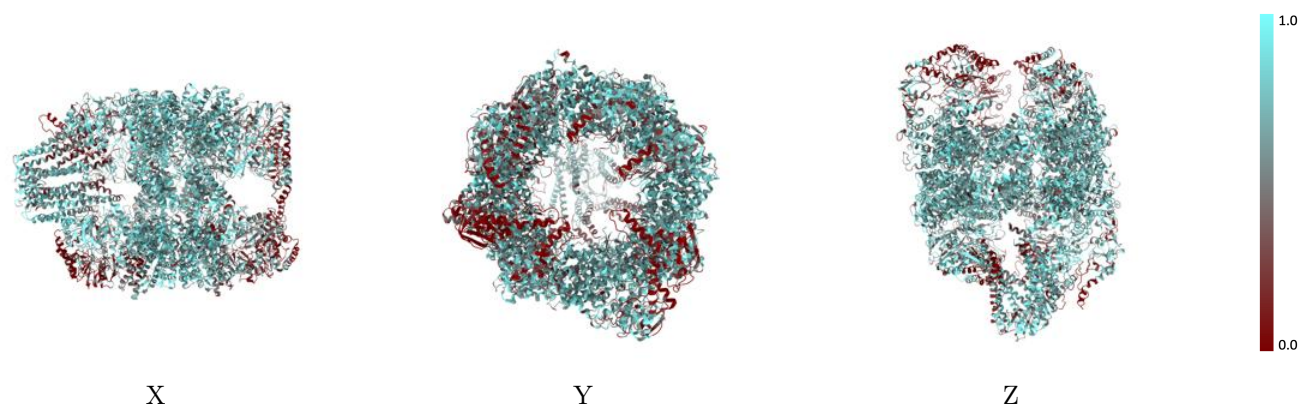
The images above show the 3D surface view of the map at the recommended contour level 0.55 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



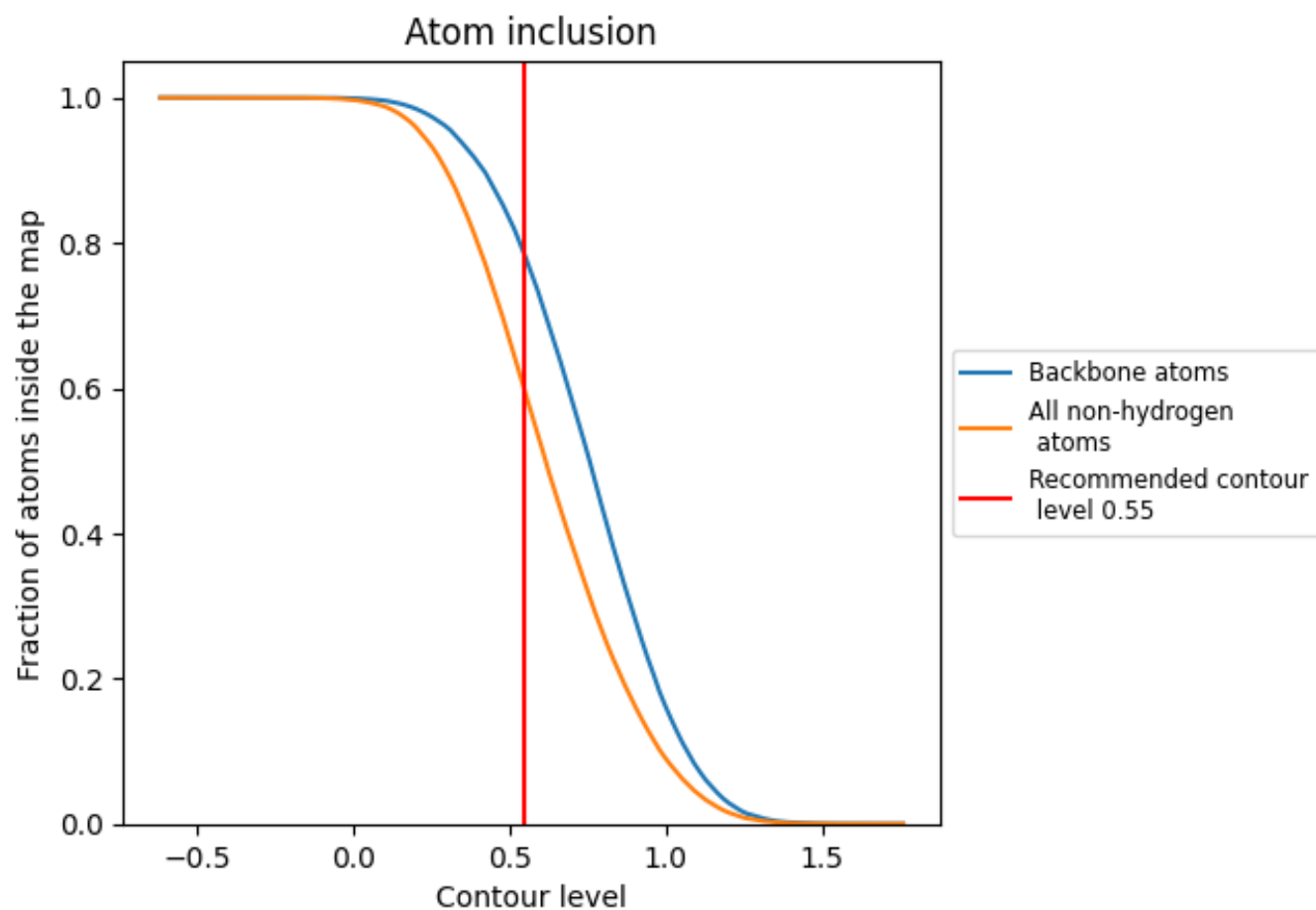
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.55).















































9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 60% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.55) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5953	 0.1370
1	 0.6829	 0.1560
2	 0.3644	 0.0990
3	 0.6047	 0.1150
4	 0.6607	 0.1380
5	 0.6453	 0.1470
6	 0.6489	 0.1560
A	 0.6270	 0.1450
B	 0.4486	 0.1370
C	 0.6523	 0.1350
D	 0.7319	 0.1610
E	 0.6220	 0.1340
F	 0.6668	 0.1410
G	 0.6166	 0.1340
H	 0.6704	 0.1430
I	 0.5450	 0.1270
J	 0.3981	 0.1220
K	 0.5246	 0.1330
L	 0.5930	 0.1420
M	 0.5774	 0.1190
N	 0.6244	 0.1440
O	 0.5740	 0.1400
P	 0.6371	 0.1440

