



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 03:32 AM UTC

PDB ID : 6KS8 / pdb_00006ks8
EMDB ID : EMD-0760
Title : TRiC at 0.1 mM ADP-AlFx, Conformation 4, 0.1-C4
Authors : Jin, M.; Cong, Y.
Deposited on : 2019-08-23
Resolution : 4.69 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.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

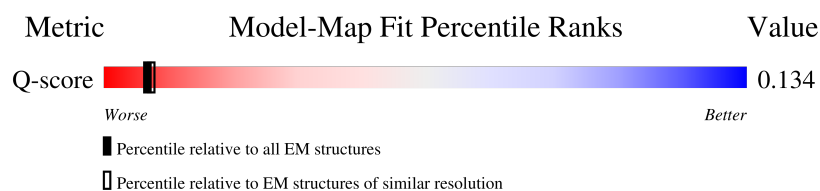
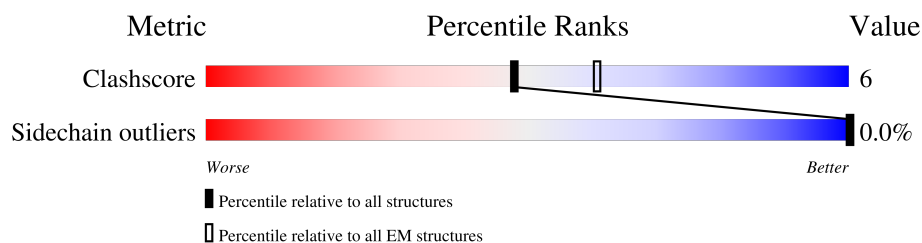
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.69 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	1970 (4.19 - 5.19)

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

Mol	Chain	Length	Quality of chain
1	A	559	
1	a	559	
2	B	527	
2	b	527	
3	D	528	

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Mol	Chain	Length	Quality of chain
3	d	528	
4	E	562	
4	e	562	
5	G	594	
5	g	594	
6	H	550	
6	h	550	
7	Q	568	
7	q	568	
8	Z	546	
8	z	546	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 61943 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 T-complex protein 1 subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	a	519	Total	C	N	O	S	0	0
			3908	2447	682	759	20		
1	A	512	Total	C	N	O	S	0	0
			3859	2417	673	750	19		

- Molecule 2 is a protein called T-complex protein 1 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	b	502	Total	C	N	O	S	0	0
			3811	2385	658	754	14		
2	B	489	Total	C	N	O	S	0	0
			3708	2316	642	736	14		

- Molecule 3 is a protein called T-complex protein 1 subunit delta.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	d	499	Total	C	N	O	S	0	0
			3816	2384	675	740	17		
3	D	480	Total	C	N	O	S	0	0
			3655	2284	647	708	16		

- Molecule 4 is a protein called T-complex protein 1 subunit epsilon.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	e	518	Total	C	N	O	S	0	0
			3982	2500	678	783	21		
4	E	502	Total	C	N	O	S	0	0
			3848	2416	656	755	21		

- Molecule 5 is a protein called fusion protein of T-complex protein 1 subunit gamma, rep-His-CBP and T-complex protein 1 subunit gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	g	493	Total	C	N	O	S	0	0
			3775	2374	661	715	25		
5	G	485	Total	C	N	O	S	0	0
			3709	2332	648	704	25		

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
g	375	LEU	-	see sequence details	UNP P39077
g	376	GLU	-	see sequence details	UNP P39077
g	377	GLY	-	see sequence details	UNP P39077
g	378	SER	-	see sequence details	UNP P39077
g	379	GLY	-	see sequence details	UNP P39077
g	380	SER	-	see sequence details	UNP P39077
g	381	GLY	-	see sequence details	UNP P39077
g	382	TRP	-	see sequence details	UNP P39077
g	383	SER	-	see sequence details	UNP P39077
g	384	HIS	-	see sequence details	UNP P39077
g	385	PRO	-	see sequence details	UNP P39077
g	386	GLN	-	see sequence details	UNP P39077
g	387	PHE	-	see sequence details	UNP P39077
g	388	GLU	-	see sequence details	UNP P39077
g	389	LYS	-	see sequence details	UNP P39077
g	390	GLY	-	see sequence details	UNP P39077
g	391	SER	-	see sequence details	UNP P39077
g	392	GLY	-	see sequence details	UNP P39077
g	393	LYS	-	see sequence details	UNP P39077
g	394	ARG	-	see sequence details	UNP P39077
g	395	ARG	-	see sequence details	UNP P39077
g	396	TRP	-	see sequence details	UNP P39077
g	397	LYS	-	see sequence details	UNP P39077
g	398	LYS	-	see sequence details	UNP P39077
g	399	ASN	-	see sequence details	UNP P39077
g	400	PHE	-	see sequence details	UNP P39077
g	401	ILE	-	see sequence details	UNP P39077
g	402	ALA	-	see sequence details	UNP P39077
g	403	VAL	-	see sequence details	UNP P39077
g	404	SER	-	see sequence details	UNP P39077
g	405	ALA	-	see sequence details	UNP P39077
g	406	ALA	-	see sequence details	UNP P39077
g	407	ASN	-	see sequence details	UNP P39077
g	408	ARG	-	see sequence details	UNP P39077
g	409	PHE	-	see sequence details	UNP P39077

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Chain	Residue	Modelled	Actual	Comment	Reference
g	410	LYS	-	see sequence details	UNP P39077
g	411	LYS	-	see sequence details	UNP P39077
g	412	ILE	-	see sequence details	UNP P39077
g	413	SER	-	see sequence details	UNP P39077
g	414	SER	-	see sequence details	UNP P39077
g	415	SER	-	see sequence details	UNP P39077
g	416	GLY	-	see sequence details	UNP P39077
g	417	ALA	-	see sequence details	UNP P39077
g	418	LEU	-	see sequence details	UNP P39077
g	419	GLY	-	see sequence details	UNP P39077
g	420	SER	-	see sequence details	UNP P39077
g	421	GLY	-	see sequence details	UNP P39077
g	422	HIS	-	see sequence details	UNP P39077
g	423	HIS	-	see sequence details	UNP P39077
g	424	HIS	-	see sequence details	UNP P39077
g	425	HIS	-	see sequence details	UNP P39077
g	426	HIS	-	see sequence details	UNP P39077
g	427	HIS	-	see sequence details	UNP P39077
g	428	HIS	-	see sequence details	UNP P39077
g	429	HIS	-	see sequence details	UNP P39077
g	430	GLY	-	see sequence details	UNP P39077
g	431	SER	-	see sequence details	UNP P39077
g	432	GLY	-	see sequence details	UNP P39077
g	433	LEU	-	see sequence details	UNP P39077
g	434	GLN	-	see sequence details	UNP P39077
G	375	LEU	-	see sequence details	UNP P39077
G	376	GLU	-	see sequence details	UNP P39077
G	377	GLY	-	see sequence details	UNP P39077
G	378	SER	-	see sequence details	UNP P39077
G	379	GLY	-	see sequence details	UNP P39077
G	380	SER	-	see sequence details	UNP P39077
G	381	GLY	-	see sequence details	UNP P39077
G	382	TRP	-	see sequence details	UNP P39077
G	383	SER	-	see sequence details	UNP P39077
G	384	HIS	-	see sequence details	UNP P39077
G	385	PRO	-	see sequence details	UNP P39077
G	386	GLN	-	see sequence details	UNP P39077
G	387	PHE	-	see sequence details	UNP P39077
G	388	GLU	-	see sequence details	UNP P39077
G	389	LYS	-	see sequence details	UNP P39077
G	390	GLY	-	see sequence details	UNP P39077
G	391	SER	-	see sequence details	UNP P39077

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Chain	Residue	Modelled	Actual	Comment	Reference
G	392	GLY	-	see sequence details	UNP P39077
G	393	LYS	-	see sequence details	UNP P39077
G	394	ARG	-	see sequence details	UNP P39077
G	395	ARG	-	see sequence details	UNP P39077
G	396	TRP	-	see sequence details	UNP P39077
G	397	LYS	-	see sequence details	UNP P39077
G	398	LYS	-	see sequence details	UNP P39077
G	399	ASN	-	see sequence details	UNP P39077
G	400	PHE	-	see sequence details	UNP P39077
G	401	ILE	-	see sequence details	UNP P39077
G	402	ALA	-	see sequence details	UNP P39077
G	403	VAL	-	see sequence details	UNP P39077
G	404	SER	-	see sequence details	UNP P39077
G	405	ALA	-	see sequence details	UNP P39077
G	406	ALA	-	see sequence details	UNP P39077
G	407	ASN	-	see sequence details	UNP P39077
G	408	ARG	-	see sequence details	UNP P39077
G	409	PHE	-	see sequence details	UNP P39077
G	410	LYS	-	see sequence details	UNP P39077
G	411	LYS	-	see sequence details	UNP P39077
G	412	ILE	-	see sequence details	UNP P39077
G	413	SER	-	see sequence details	UNP P39077
G	414	SER	-	see sequence details	UNP P39077
G	415	SER	-	see sequence details	UNP P39077
G	416	GLY	-	see sequence details	UNP P39077
G	417	ALA	-	see sequence details	UNP P39077
G	418	LEU	-	see sequence details	UNP P39077
G	419	GLY	-	see sequence details	UNP P39077
G	420	SER	-	see sequence details	UNP P39077
G	421	GLY	-	see sequence details	UNP P39077
G	422	HIS	-	see sequence details	UNP P39077
G	423	HIS	-	see sequence details	UNP P39077
G	424	HIS	-	see sequence details	UNP P39077
G	425	HIS	-	see sequence details	UNP P39077
G	426	HIS	-	see sequence details	UNP P39077
G	427	HIS	-	see sequence details	UNP P39077
G	428	HIS	-	see sequence details	UNP P39077
G	429	HIS	-	see sequence details	UNP P39077
G	430	GLY	-	see sequence details	UNP P39077
G	431	SER	-	see sequence details	UNP P39077
G	432	GLY	-	see sequence details	UNP P39077
G	433	LEU	-	see sequence details	UNP P39077

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Chain	Residue	Modelled	Actual	Comment	Reference
G	434	GLN	-	see sequence details	UNP P39077

- Molecule 6 is a protein called T-complex protein 1 subunit eta.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	h	507	Total	C	N	O	S	0	0
			3882	2447	664	752	19		
6	H	507	Total	C	N	O	S	0	0
			3882	2447	664	752	19		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	q	523	Total	C	N	O	S	0	0
			3974	2506	676	766	26		
7	Q	524	Total	C	N	O	S	0	0
			3978	2508	677	767	26		

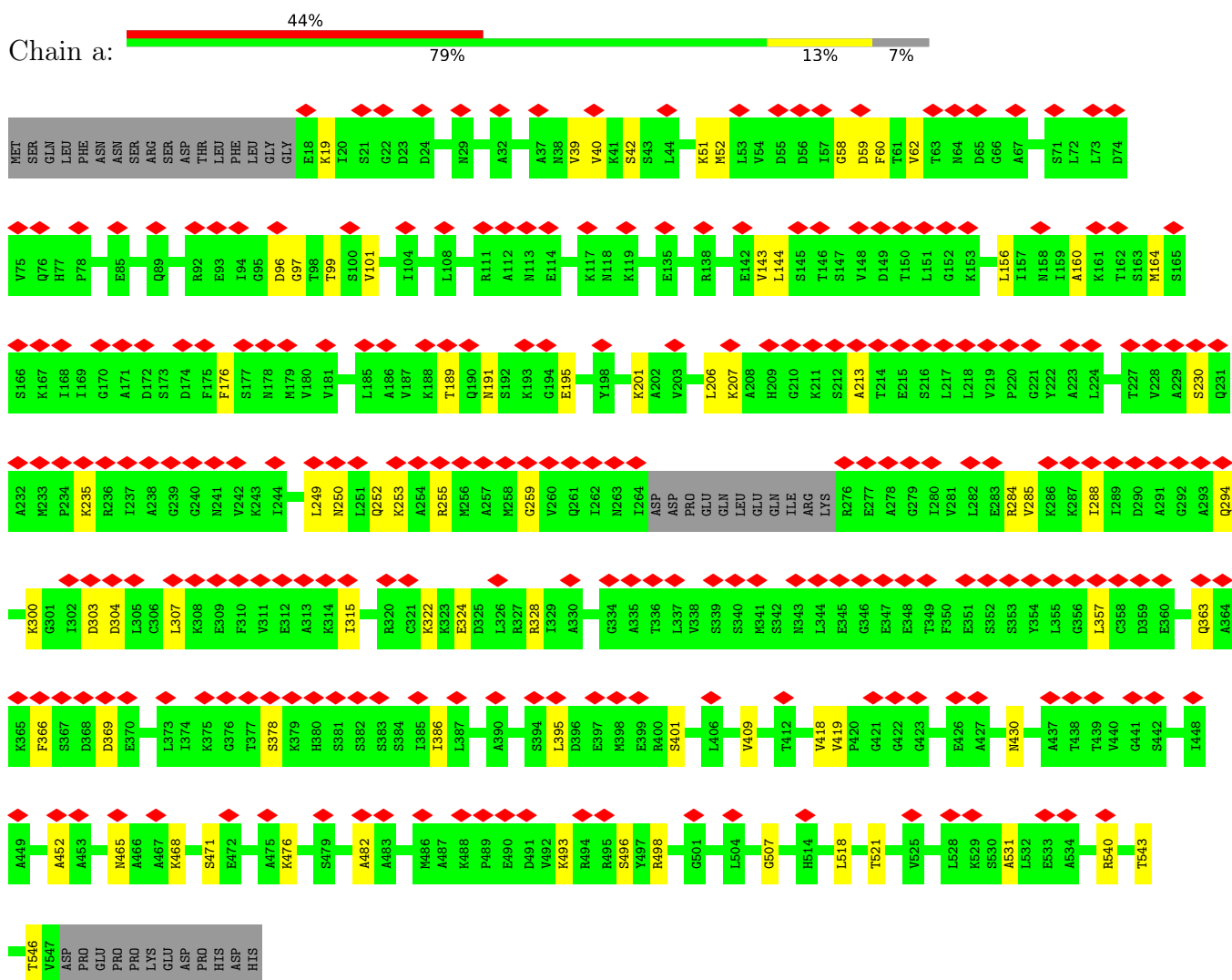
- Molecule 8 is a protein called T-complex protein 1 subunit zeta.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	z	531	Total	C	N	O	S	0	0
			4086	2566	708	795	17		
8	Z	529	Total	C	N	O	S	0	0
			4070	2555	705	793	17		

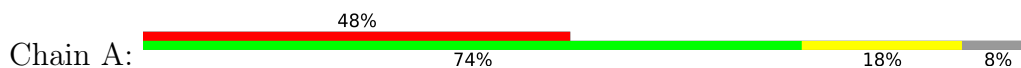
3 Residue-property plots

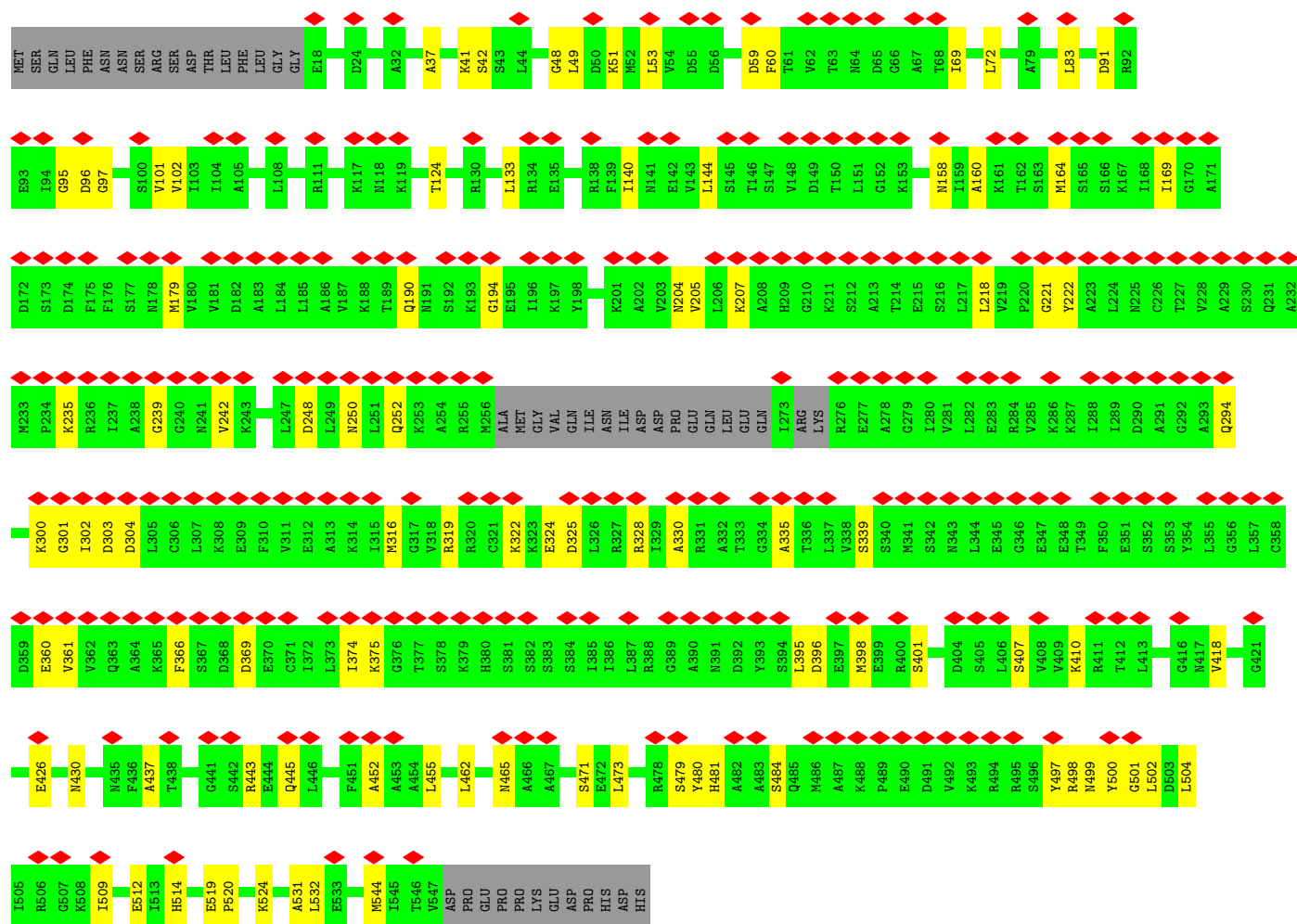
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: T-complex protein 1 subunit alpha

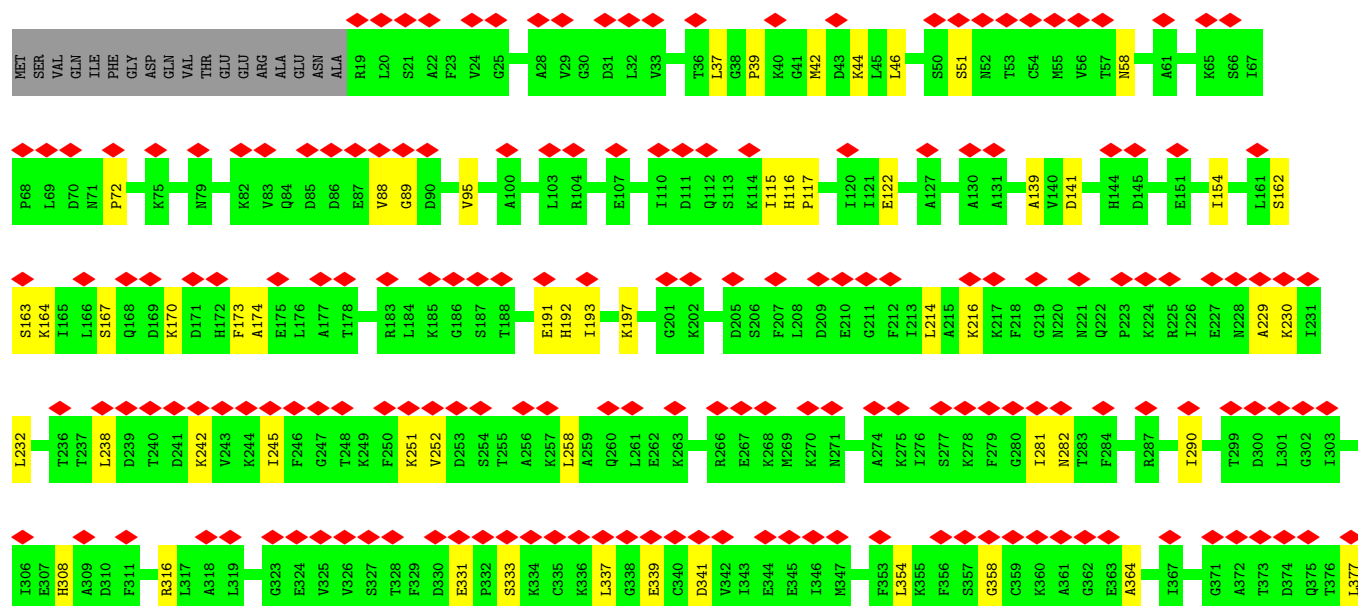
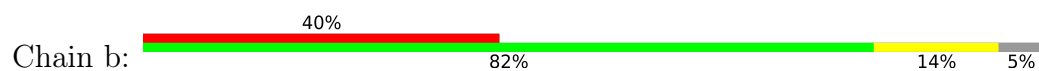


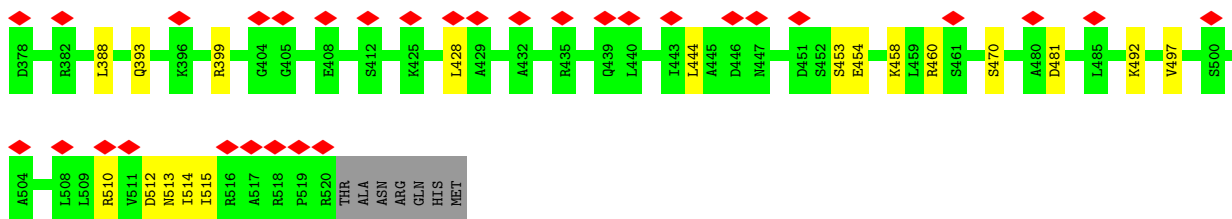
• Molecule 1: T-complex protein 1 subunit alpha



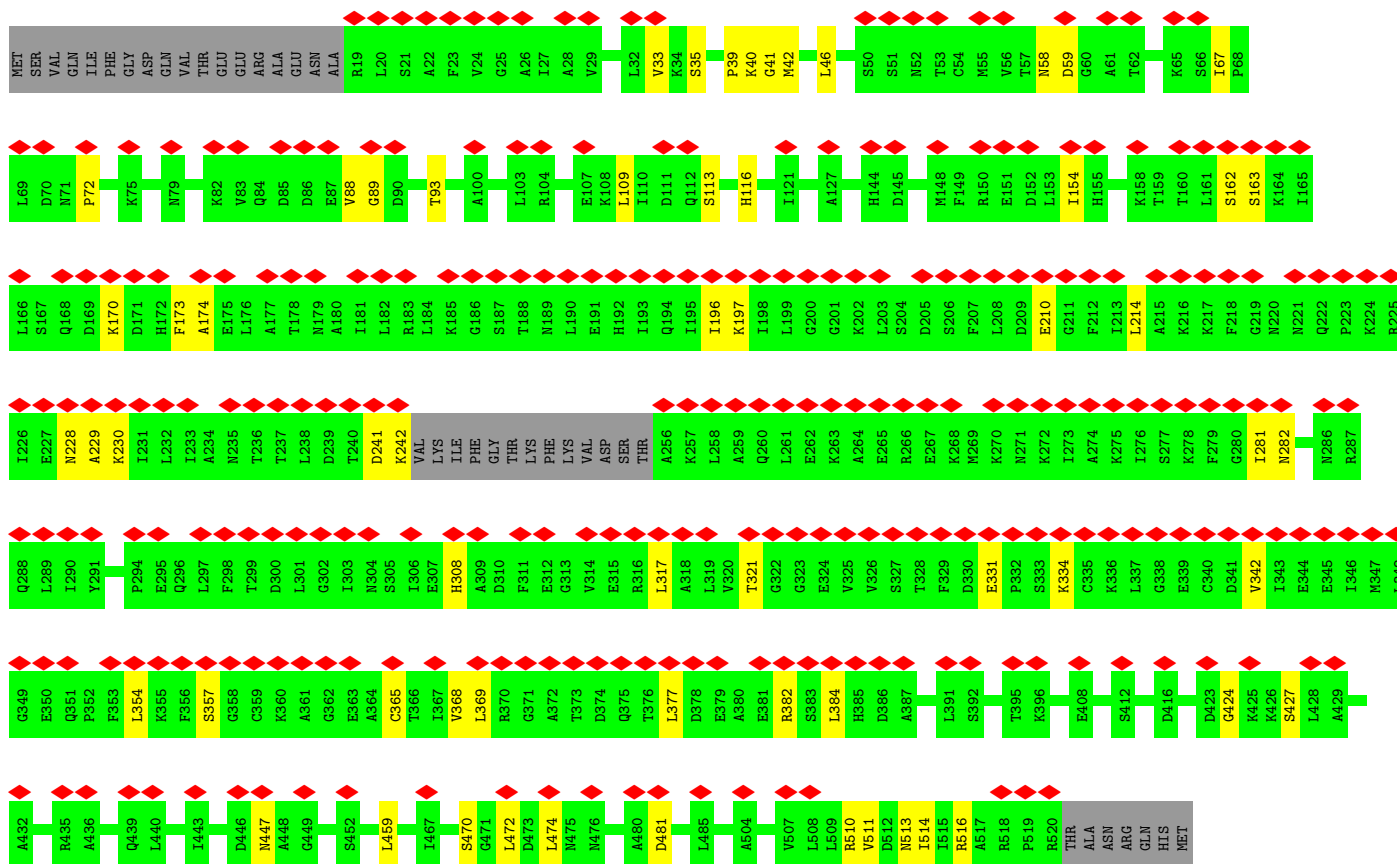
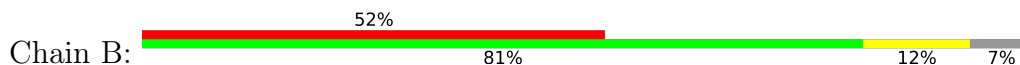


• Molecule 2: T-complex protein 1 subunit beta

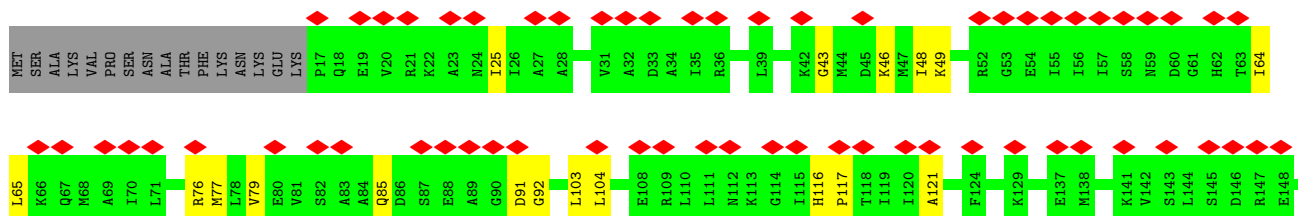


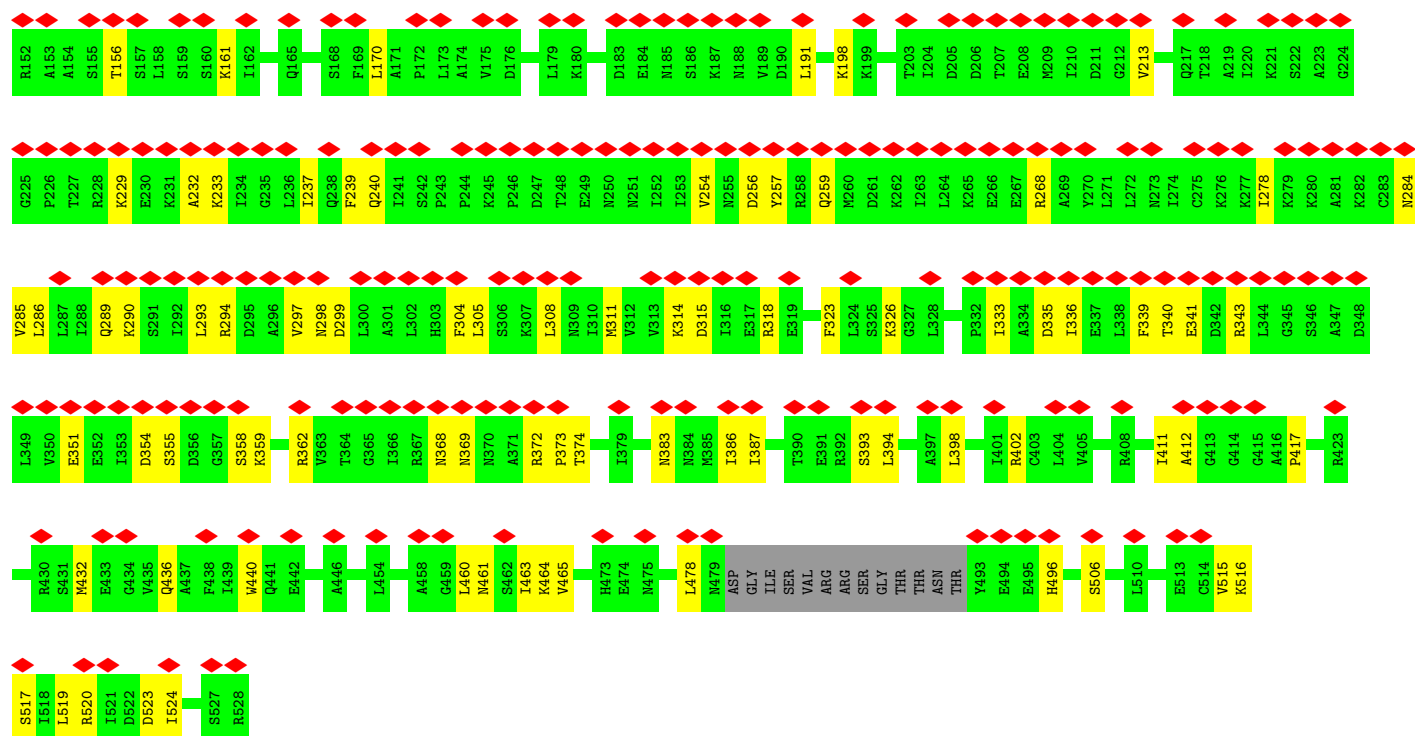


• Molecule 2: T-complex protein 1 subunit beta

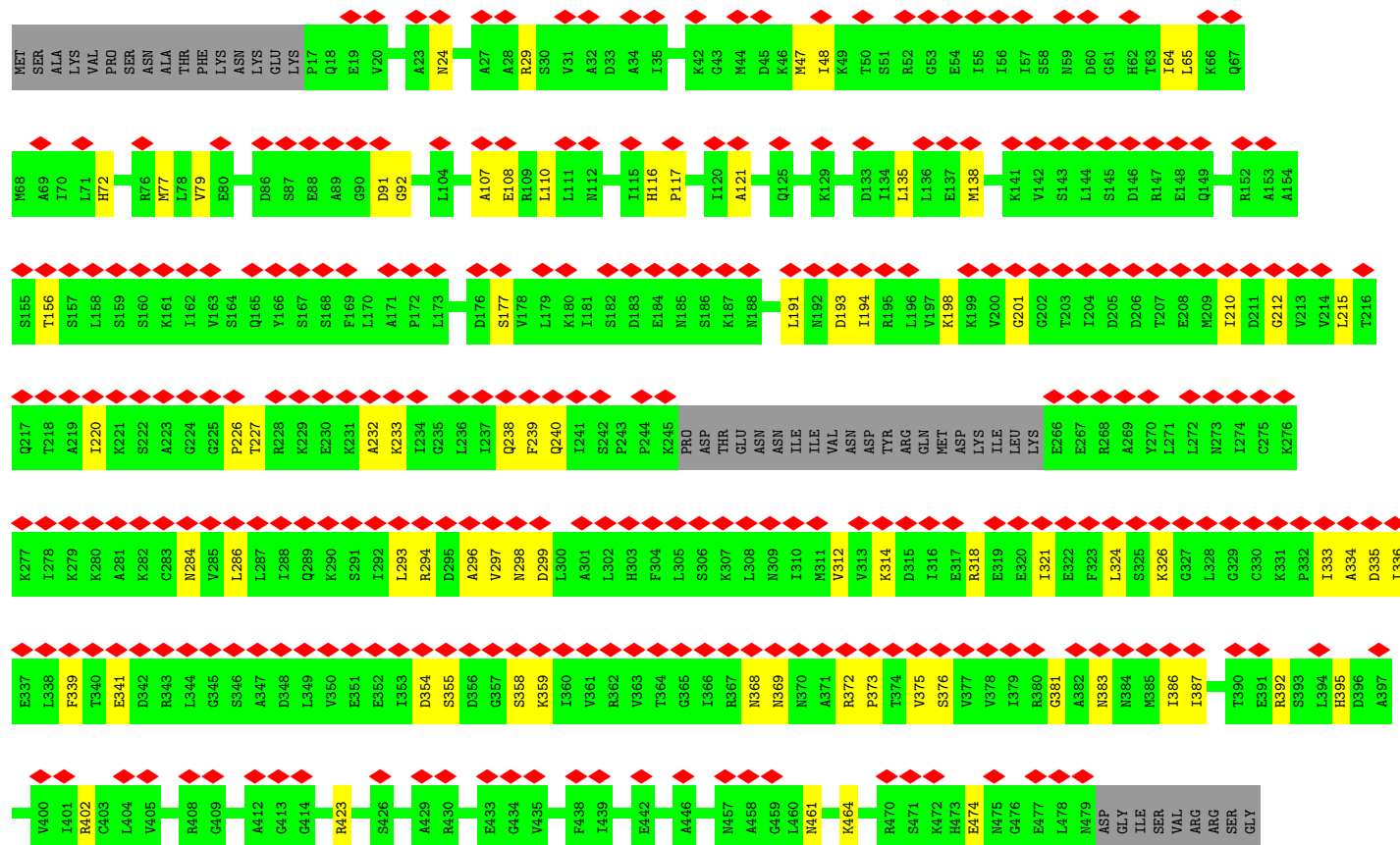
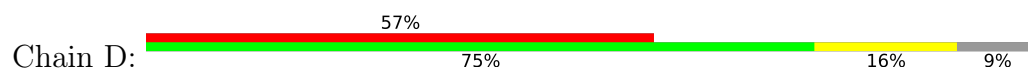


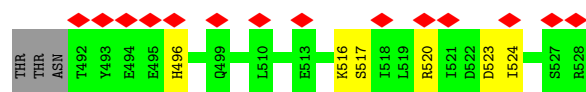
• Molecule 3: T-complex protein 1 subunit delta



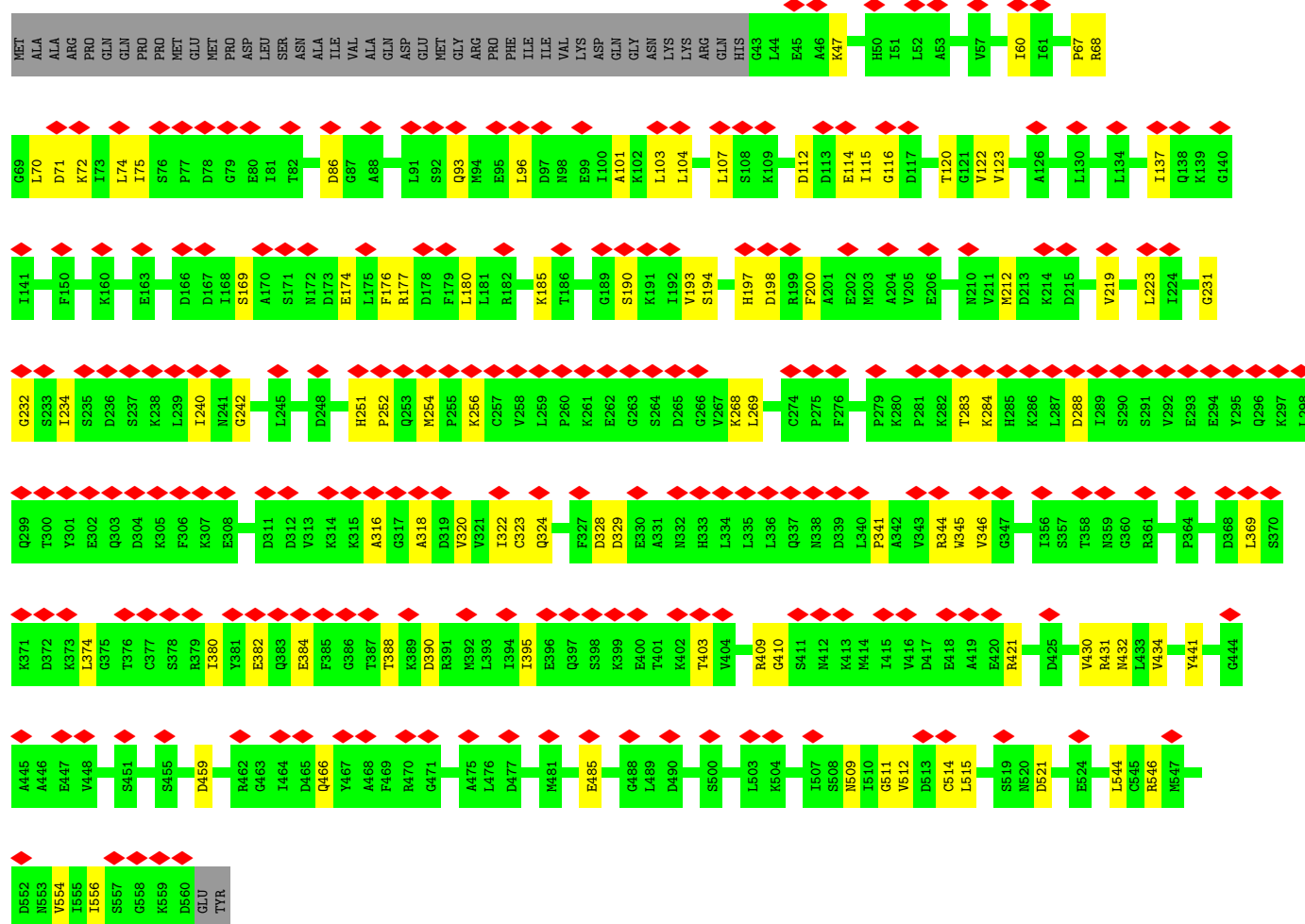
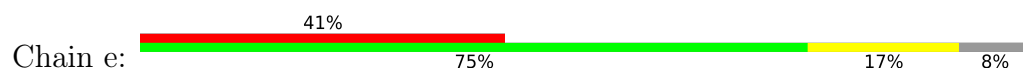


• Molecule 3: T-complex protein 1 subunit delta

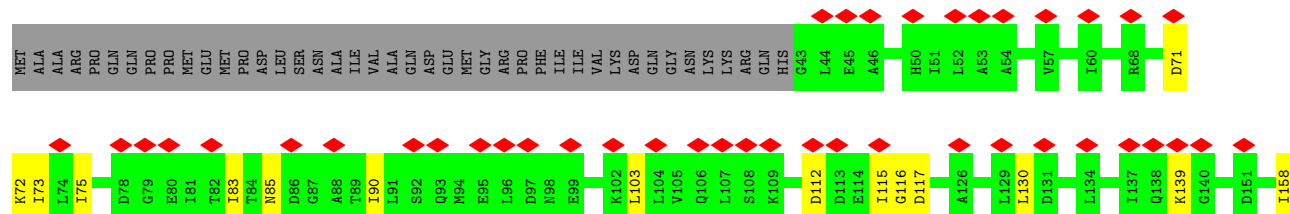


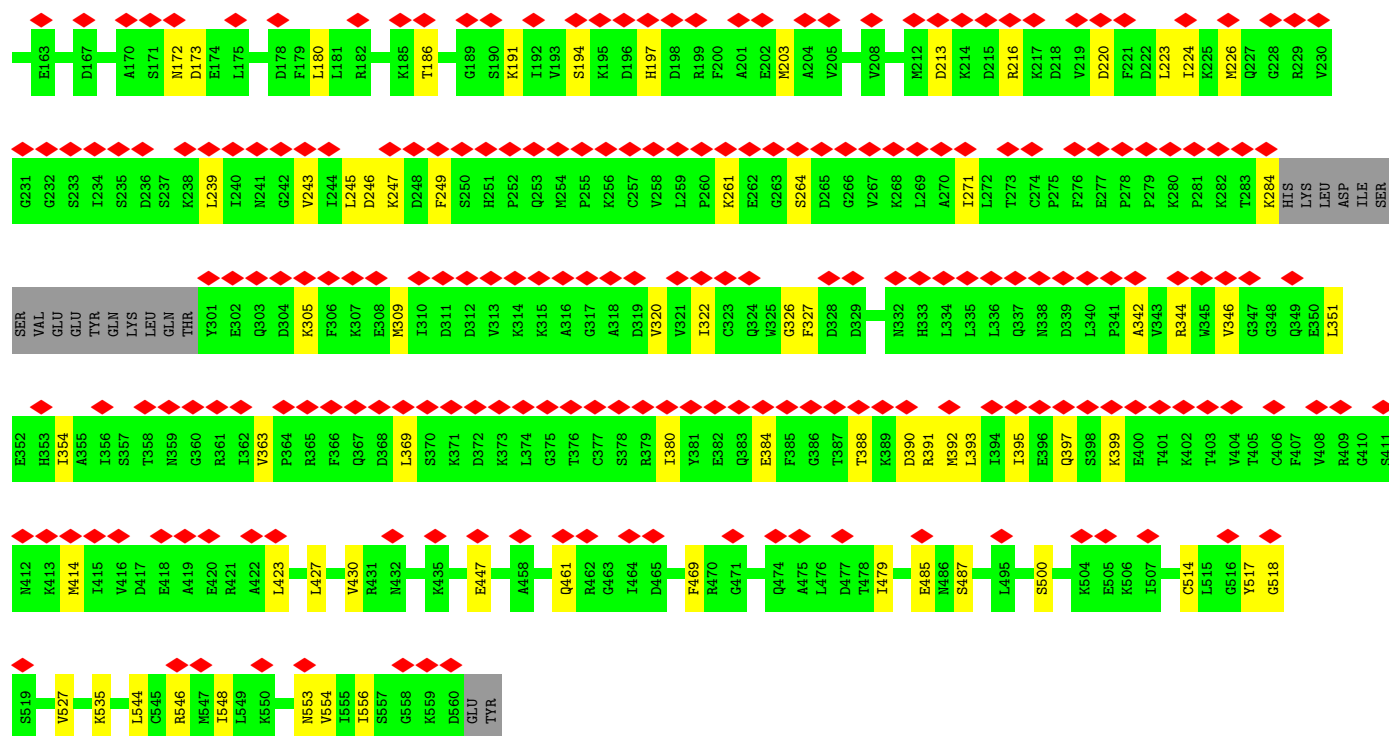


• Molecule 4: T-complex protein 1 subunit epsilon

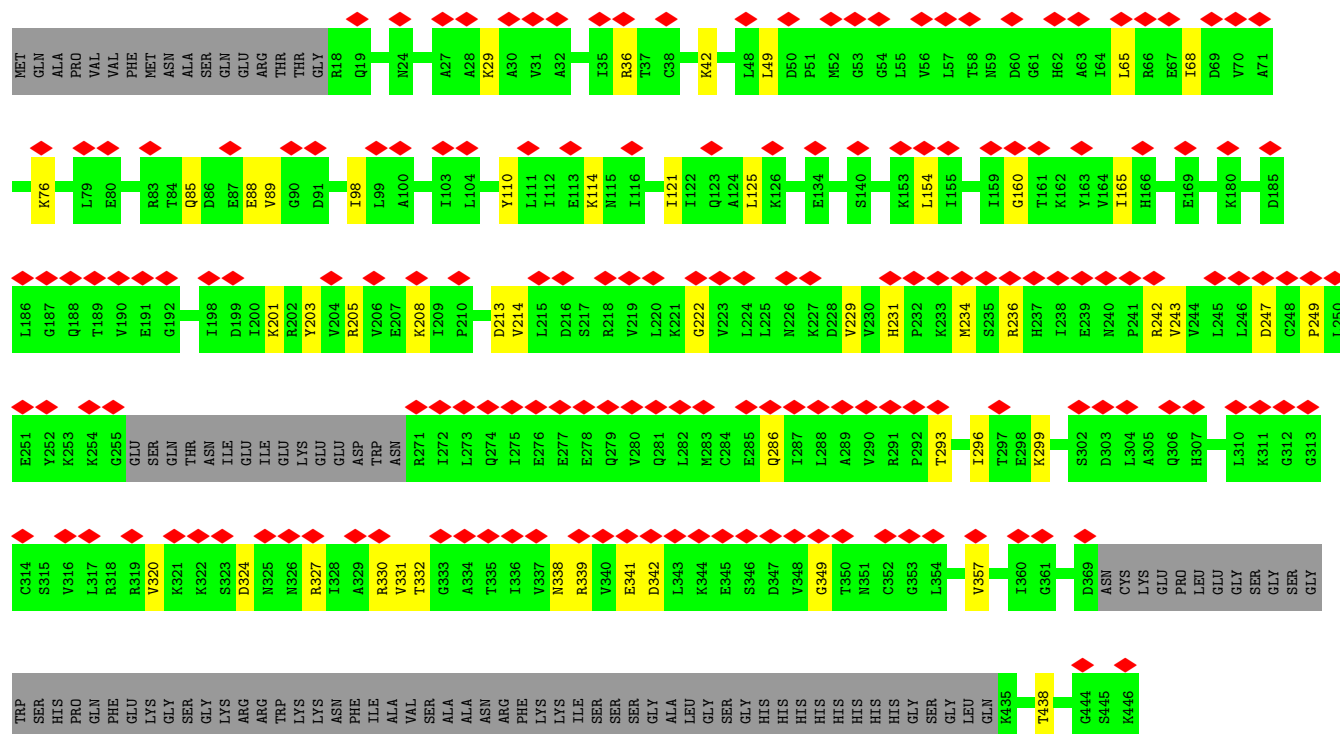


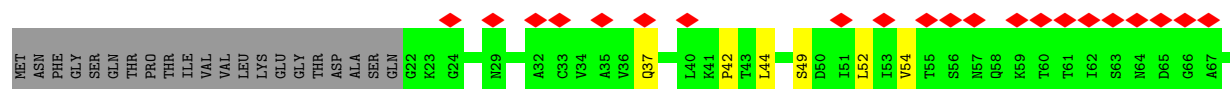
• Molecule 4: T-complex protein 1 subunit epsilon

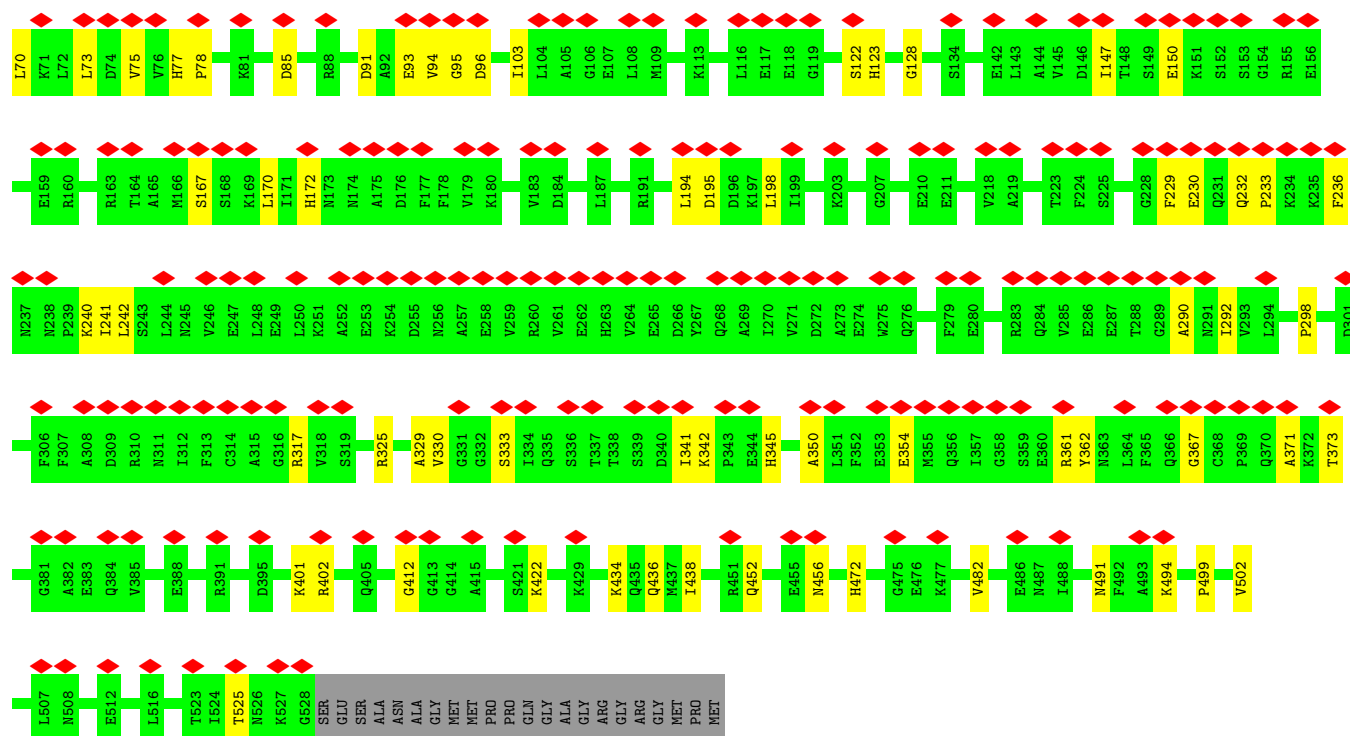




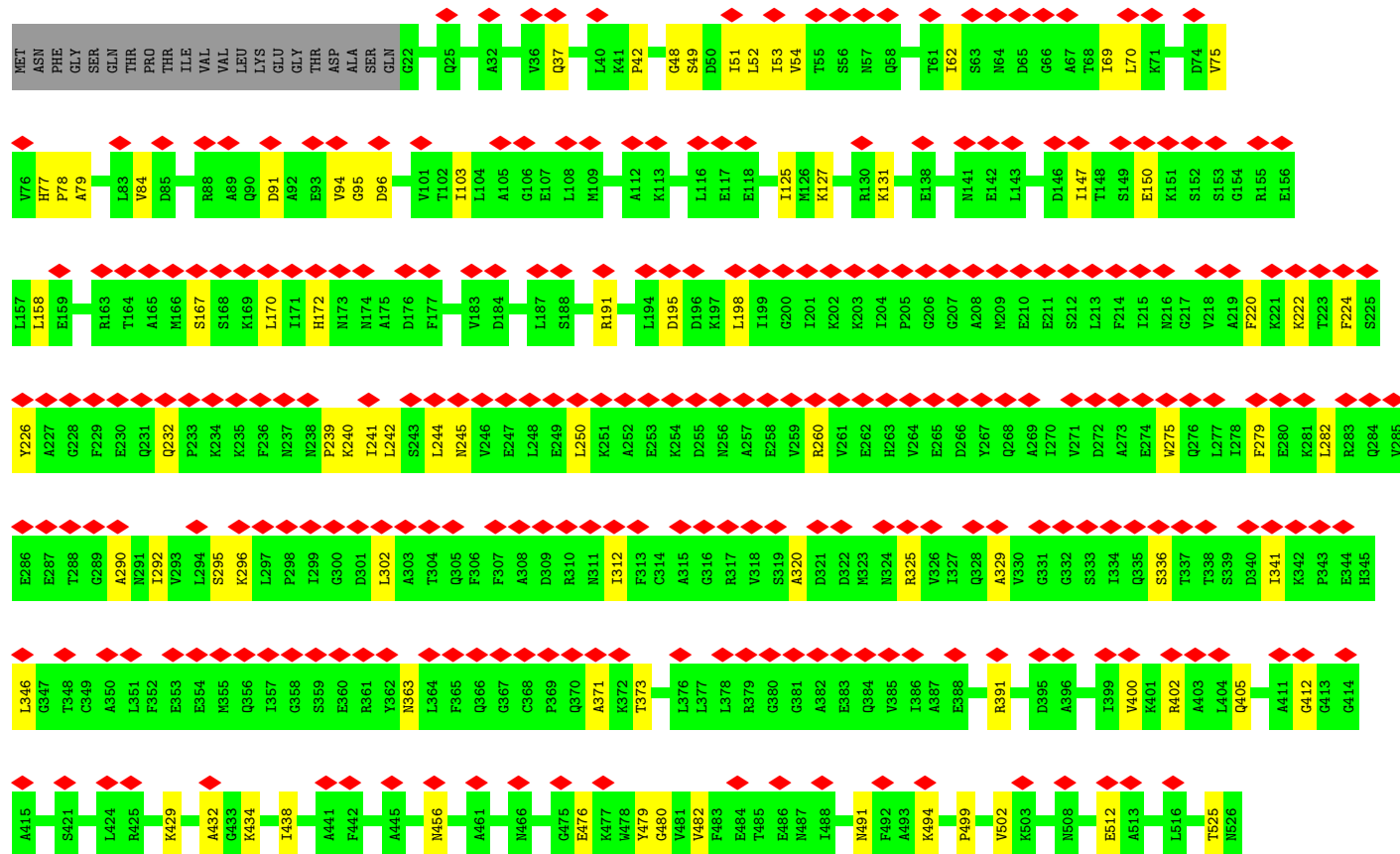
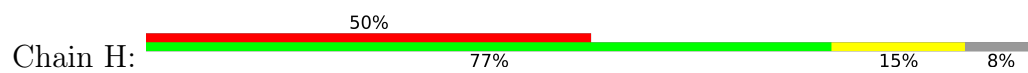
• Molecule 5: fusion protein of T-complex protein 1 subunit gamma, rep-His-CBP and T-complex protein 1 subunit gamma

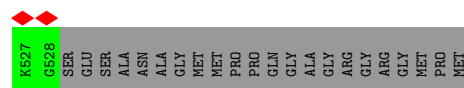




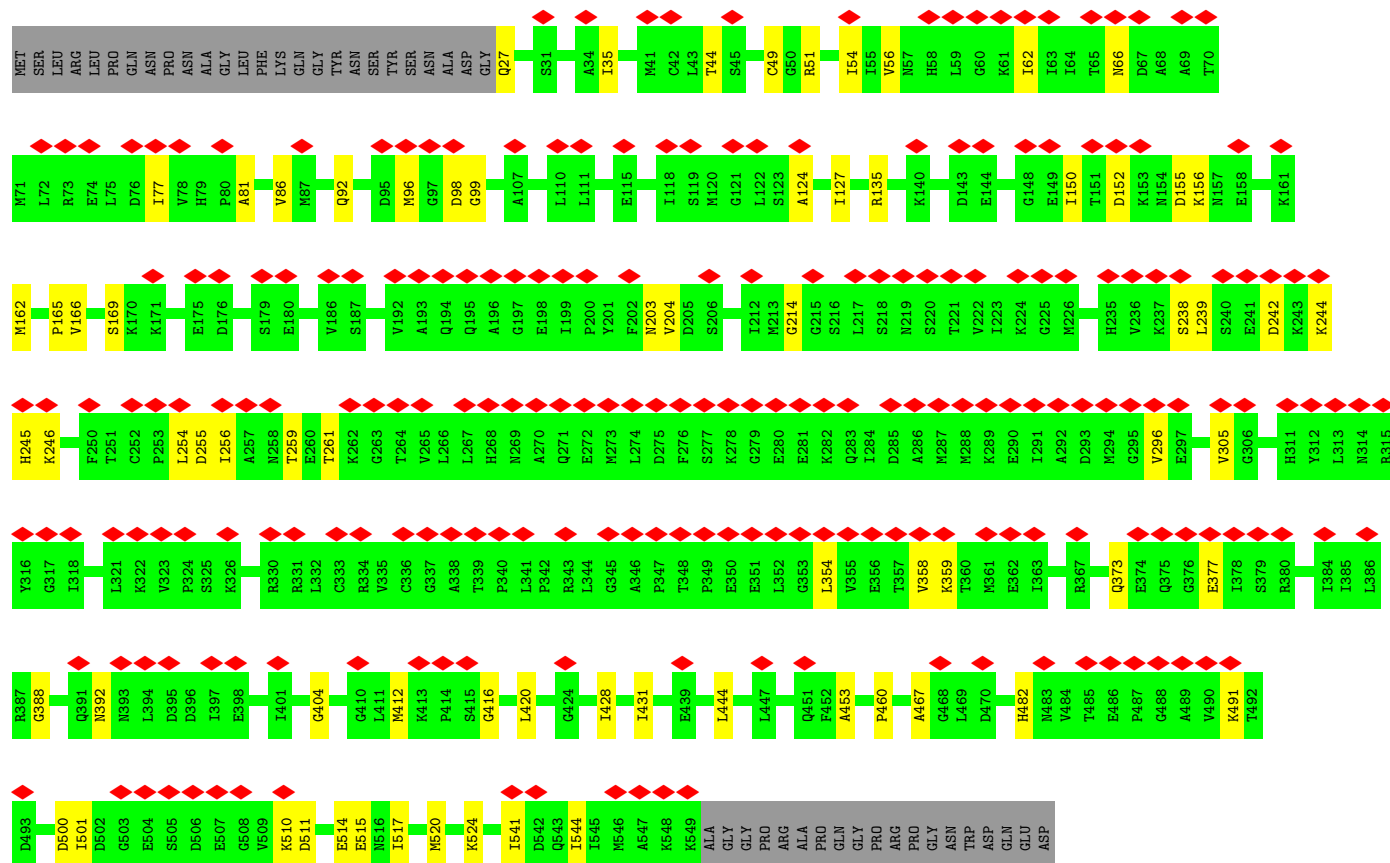
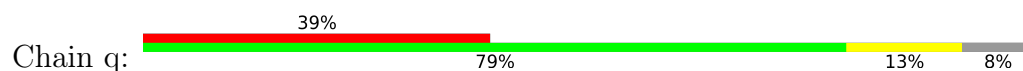


• Molecule 6: T-complex protein 1 subunit eta

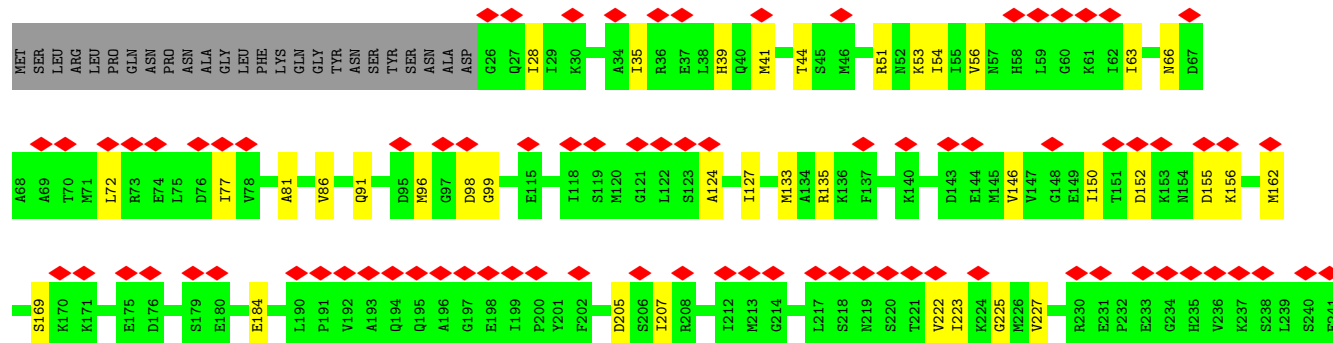
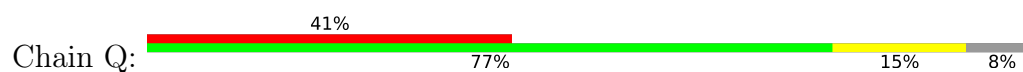


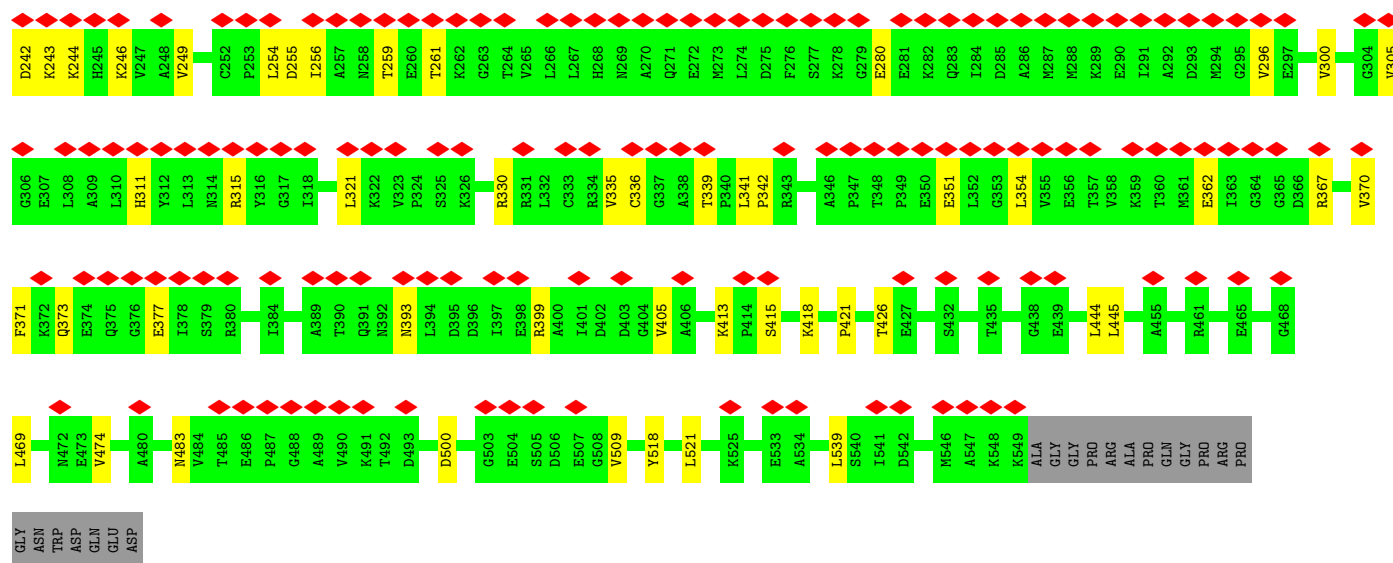


• Molecule 7: T-complex protein 1 subunit theta

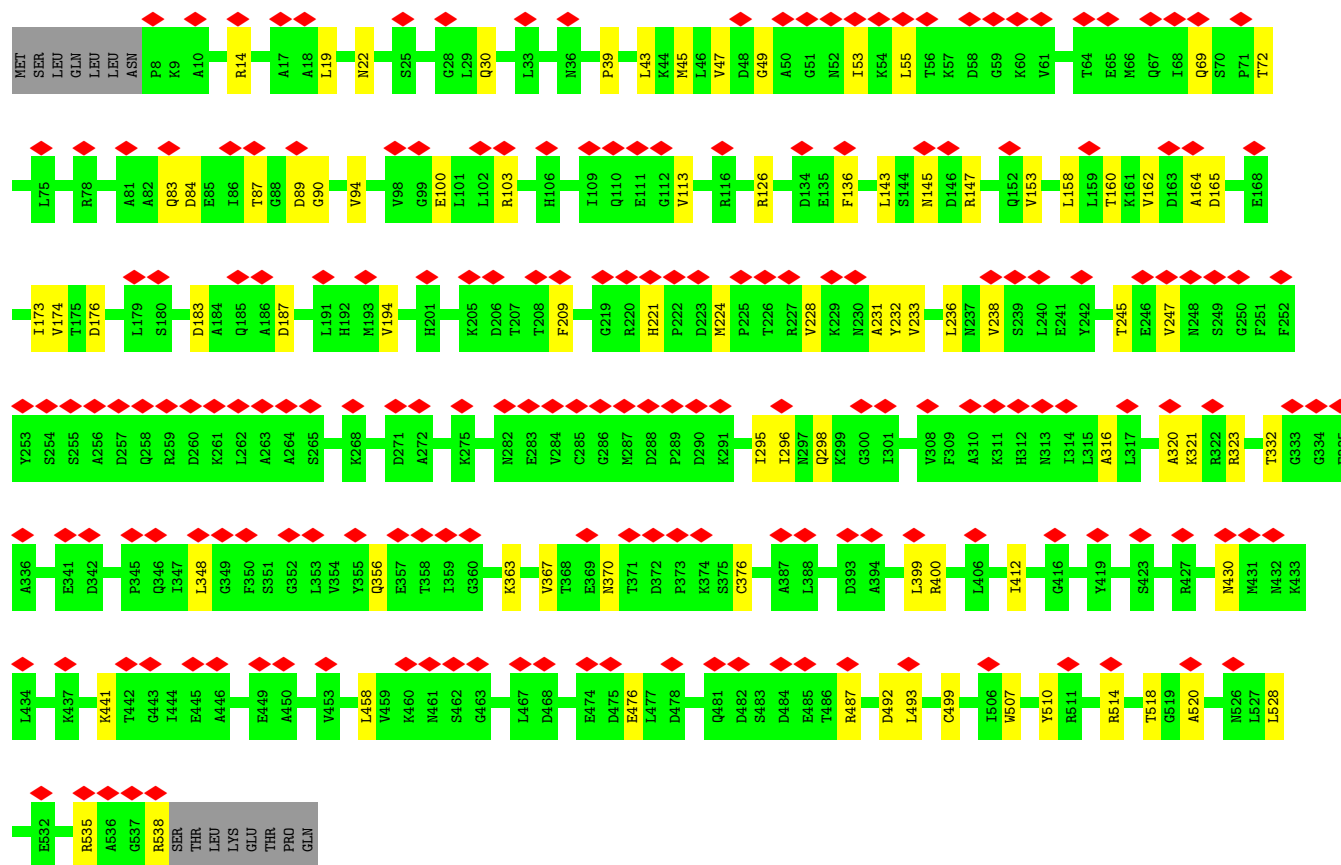
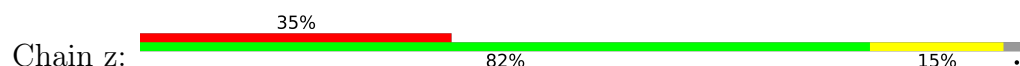


• Molecule 7: T-complex protein 1 subunit theta

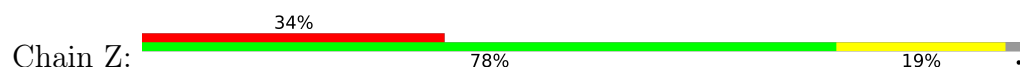


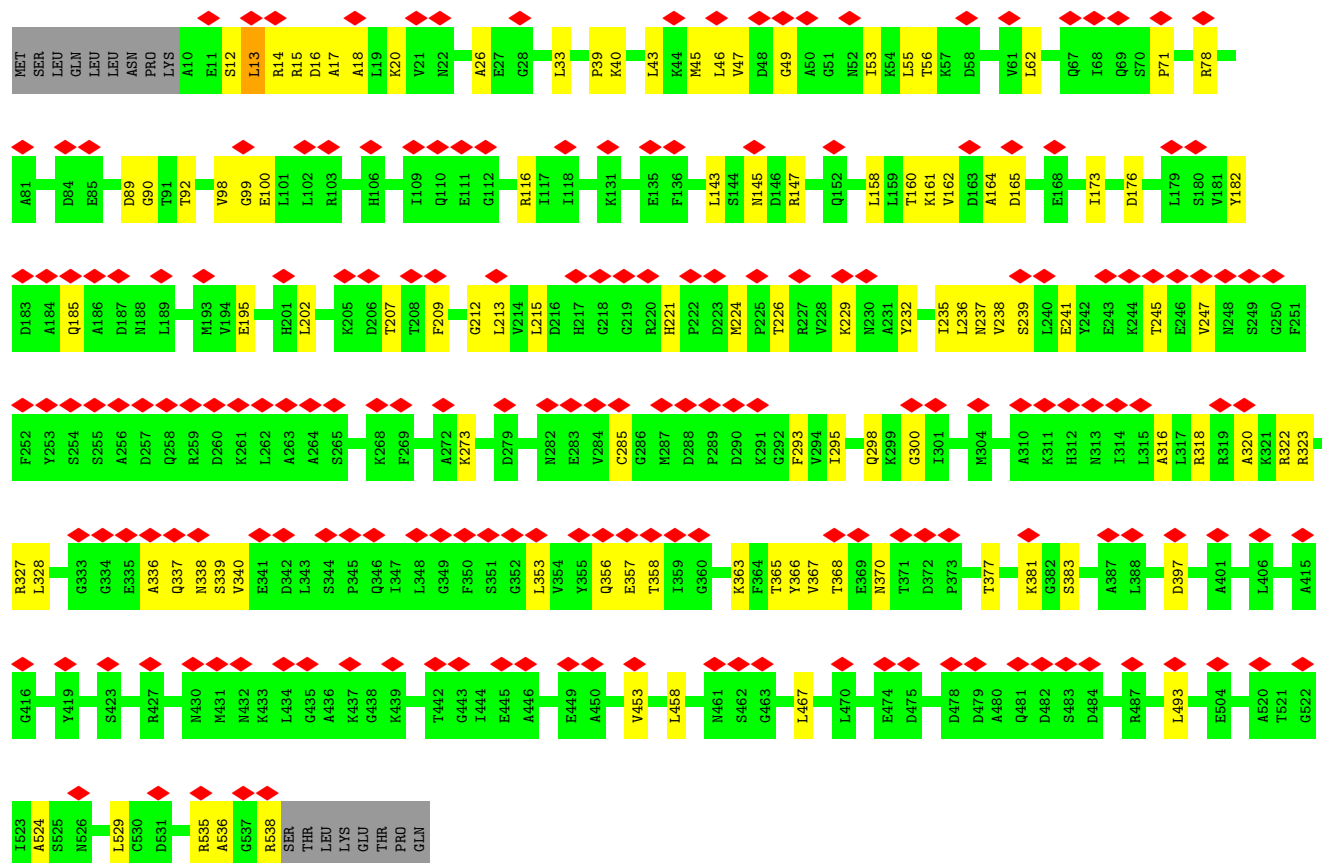


• Molecule 8: T-complex protein 1 subunit zeta



• Molecule 8: T-complex protein 1 subunit zeta





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	53539	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	38	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	3.268	Depositor
Minimum map value	-1.235	Depositor
Average map value	0.021	Depositor
Map value standard deviation	0.143	Depositor
Recommended contour level	0.85	Depositor
Map size ($\text{\AA}$)	337.408, 337.408, 337.408	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.318, 1.318, 1.318	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	A	0.08	0/3891	0.24	0/5247
1	a	0.07	0/3941	0.24	0/5316
2	B	0.07	0/3743	0.22	0/5043
2	b	0.07	0/3849	0.23	0/5186
3	D	0.07	0/3687	0.23	0/4967
3	d	0.07	0/3851	0.23	0/5190
4	E	0.07	0/3893	0.23	0/5240
4	e	0.07	0/4030	0.22	0/5426
5	G	0.07	0/3751	0.24	0/5065
5	g	0.08	0/3817	0.23	0/5152
6	H	0.06	0/3931	0.21	0/5304
6	h	0.06	0/3931	0.21	0/5304
7	Q	0.07	0/4024	0.22	0/5431
7	q	0.12	0/4020	0.22	0/5426
8	Z	0.09	0/4121	0.30	1/5568 (0.0%)
8	z	0.08	0/4138	0.26	1/5590 (0.0%)
All	All	0.08	0/62618	0.23	2/84455 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	Z	13	LEU	CB-CA-C	-5.94	109.15	117.23
8	z	14	ARG	N-CA-C	-5.90	106.04	113.18

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3859	0	4033	60	0
1	a	3908	0	4085	46	0
2	B	3708	0	3815	40	0
2	b	3811	0	3928	50	0
3	D	3655	0	3824	46	0
3	d	3816	0	3986	61	0
4	E	3848	0	3941	52	0
4	e	3982	0	4075	61	0
5	G	3709	0	3861	48	0
5	g	3775	0	3937	45	0
6	H	3882	0	3964	54	0
6	h	3882	0	3964	47	0
7	Q	3978	0	4132	52	0
7	q	3974	0	4129	44	0
8	Z	4070	0	4156	61	0
8	z	4086	0	4177	47	0
All	All	61943	0	64007	744	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 6.

All (744) 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)
4:E:247:LYS:HG3	4:E:249:PHE:H	1.51	0.76
4:E:380:ILE:HG12	4:E:395:ILE:HG12	1.69	0.73
7:q:428:ILE:HD11	7:q:460:PRO:HG3	1.70	0.73
4:e:194:SER:O	4:e:197:HIS:ND1	2.23	0.72
8:Z:212:GLY:H	8:Z:368:THR:HG22	1.55	0.72
2:B:331:GLU:HB3	2:B:334:LYS:HE3	1.71	0.71
6:h:42:PRO:HB2	6:h:49:SER:HB2	1.73	0.70
4:e:380:ILE:HG12	4:e:395:ILE:HG12	1.75	0.69
2:b:39:PRO:HB3	2:b:162:SER:HB2	1.73	0.69
1:A:207:LYS:HB2	1:A:395:LEU:HD13	1.75	0.68
7:q:482:HIS:O	7:q:491:LYS:NZ	2.26	0.67
4:E:203:MET:HA	4:E:239:LEU:HD22	1.76	0.67
8:Z:15:ARG:HH21	8:Z:20:LYS:HE3	1.60	0.66
4:E:245:LEU:HD21	4:E:354:ILE:HD11	1.77	0.65
4:E:194:SER:O	4:E:197:HIS:ND1	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:214:LEU:HD23	2:b:354:LEU:HD12	1.79	0.65
5:G:155:ILE:HD11	5:G:463:ALA:HB2	1.79	0.64
2:B:58:ASN:ND2	2:B:163:SER:O	2.30	0.64
4:e:67:PRO:HG3	4:e:515:LEU:HD23	1.78	0.64
1:a:476:LYS:HG2	6:H:432:ALA:HB1	1.80	0.64
6:H:62:ILE:O	6:H:391:ARG:NH1	2.31	0.64
1:A:140:ILE:HG22	1:A:144:LEU:HD23	1.80	0.64
2:b:139:ALA:HB1	2:b:399:ARG:HB3	1.80	0.64
7:Q:91:GLN:NE2	8:Z:383:SER:OG	2.31	0.63
4:e:388:THR:HG22	4:e:390:ASP:H	1.63	0.63
5:G:526:ARG:HA	7:q:444:LEU:HD21	1.80	0.63
4:E:220:ASP:HB3	4:E:223:LEU:HD13	1.81	0.62
6:H:244:LEU:HB3	6:H:295:SER:HB2	1.80	0.62
5:G:198:ILE:O	5:G:464:ARG:NH2	2.33	0.62
3:D:210:ILE:HG22	3:D:212:GLY:H	1.65	0.62
1:a:430:ASN:HA	1:a:452:ALA:HB1	1.82	0.62
4:e:180:LEU:HD11	4:e:430:VAL:HG12	1.79	0.62
4:E:388:THR:HG22	4:E:390:ASP:H	1.64	0.62
4:e:103:LEU:HB3	4:e:544:LEU:HD11	1.82	0.62
5:G:110:TYR:HB3	5:G:116:ILE:HD12	1.81	0.62
6:H:91:ASP:HA	6:H:95:GLY:HA2	1.81	0.62
8:z:69:GLN:HE21	8:z:538:ARG:HH12	1.47	0.61
7:q:246:LYS:HB2	7:q:296:VAL:HA	1.83	0.61
4:E:203:MET:HG2	4:E:239:LEU:HB2	1.82	0.61
5:g:526:ARG:HA	7:Q:444:LEU:HD21	1.82	0.61
3:d:233:LYS:NZ	3:d:341:GLU:OE2	2.33	0.61
7:q:431:ILE:HG23	7:q:453:ALA:HB1	1.83	0.61
5:G:37:THR:HB	5:G:44:MET:HB2	1.83	0.61
5:G:54:GLY:HA2	8:Z:78:ARG:HH22	1.66	0.61
5:G:249:PRO:HB3	5:G:299:LYS:HB2	1.81	0.61
5:G:69:ASP:H	8:Z:536:ALA:HB1	1.66	0.61
4:E:326:GLY:HA2	4:E:344:ARG:HB2	1.84	0.60
6:h:412:GLY:O	6:h:491:ASN:ND2	2.35	0.60
8:Z:207:THR:HA	8:Z:381:LYS:HD2	1.82	0.60
5:g:88:GLU:O	5:g:464:ARG:NH2	2.34	0.60
5:g:456:LEU:HG	5:g:460:MET:HE2	1.83	0.60
1:a:40:VAL:HB	1:a:99:THR:HG23	1.82	0.60
3:d:354:ASP:HA	3:d:359:LYS:H	1.67	0.60
4:E:284:LYS:HE3	6:H:260:ARG:HD2	1.82	0.60
8:z:356:GLN:HE21	8:z:363:LYS:HB3	1.67	0.60
2:b:58:ASN:ND2	2:b:163:SER:O	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:q:244:LYS:HB3	7:q:354:LEU:HD22	1.84	0.60
3:d:289:GLN:HE21	3:d:318:ARG:HG2	1.66	0.60
6:H:512:GLU:OE2	7:Q:393:ASN:ND2	2.34	0.60
8:Z:33:LEU:HB3	8:Z:92:THR:HG23	1.84	0.60
1:a:58:GLY:O	5:g:76:LYS:NZ	2.34	0.59
1:A:53:LEU:HD21	1:A:69:ILE:HG23	1.84	0.59
4:e:232:GLY:HA3	4:e:409:ARG:HH21	1.67	0.59
7:q:254:LEU:HD12	7:q:305:VAL:HG13	1.85	0.59
2:b:512:ASP:OD1	4:e:72:LYS:NZ	2.34	0.59
1:A:158:ASN:ND2	1:A:514:HIS:O	2.34	0.59
3:d:25:ILE:HG23	3:d:104:LEU:HB3	1.84	0.59
5:G:242:ARG:NH1	5:G:243:VAL:O	2.36	0.59
6:H:127:LYS:HE3	6:H:131:LYS:HE3	1.85	0.59
8:z:100:GLU:OE1	8:z:103:ARG:NH1	2.36	0.59
1:A:53:LEU:HD11	1:A:69:ILE:HA	1.85	0.59
3:D:392:ARG:HA	3:D:395:HIS:HD2	1.67	0.59
1:a:322:LYS:HE2	1:a:324:GLU:HB2	1.85	0.59
4:E:83:ILE:H	4:E:414:MET:HE2	1.68	0.59
2:b:232:LEU:HD13	2:b:337:LEU:HG	1.84	0.59
3:D:193:ASP:OD1	3:D:372:ARG:NH1	2.36	0.59
4:E:546:ARG:HH12	6:H:170:LEU:HD21	1.68	0.59
2:B:39:PRO:HB3	2:B:162:SER:HB2	1.85	0.58
1:a:259:GLY:O	5:g:286:GLN:NE2	2.36	0.58
2:b:154:ILE:HG23	2:b:174:ALA:HB1	1.83	0.58
5:G:456:LEU:HG	5:G:460:MET:HE2	1.83	0.58
2:b:460:ARG:NH2	2:B:427:SER:OG	2.37	0.58
3:d:278:ILE:HG21	3:d:286:LEU:HD11	1.84	0.58
6:H:525:THR:HA	7:Q:56:VAL:HB	1.85	0.58
8:Z:337:GLN:NE2	8:Z:339:SER:O	2.36	0.58
2:B:229:ALA:HA	2:B:282:ASN:HB2	1.84	0.58
3:D:65:LEU:HB3	3:D:79:VAL:HG22	1.84	0.58
5:G:208:LYS:HD2	5:G:449:LEU:HB3	1.85	0.58
1:a:191:ASN:HB2	1:a:195:GLU:HB2	1.85	0.58
2:b:252:VAL:HG21	2:b:258:LEU:HB2	1.85	0.58
5:G:140:SER:HB3	5:G:471:SER:HB2	1.84	0.58
1:A:124:THR:HG21	1:A:443:ARG:HD2	1.86	0.58
5:g:160:GLY:HA2	5:g:165:ILE:HD13	1.85	0.58
1:a:546:THR:HG23	3:d:49:LYS:HD3	1.84	0.58
6:h:525:THR:HA	7:q:56:VAL:HB	1.86	0.58
6:H:158:LEU:HD22	6:H:400:VAL:HG13	1.86	0.58
6:H:240:LYS:HB2	6:H:290:ALA:HA	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:540:ARG:NH2	3:d:43:GLY:O	2.37	0.58
8:z:232:TYR:HB3	8:z:348:LEU:HD23	1.85	0.58
7:Q:66:ASN:ND2	7:Q:169:SER:O	2.37	0.57
4:e:546:ARG:HH12	6:h:170:LEU:HD21	1.68	0.57
4:E:85:ASN:OD1	4:E:191:LYS:NZ	2.34	0.57
7:Q:300:VAL:HG22	7:Q:321:LEU:HD23	1.86	0.57
1:a:201:LYS:HE2	1:a:328:ARG:HD3	1.86	0.57
2:B:154:ILE:HG23	2:B:174:ALA:HB1	1.85	0.57
3:d:156:THR:HG21	3:d:496:HIS:HB3	1.86	0.57
3:d:232:ALA:HA	3:d:284:ASN:HD22	1.69	0.57
7:Q:44:THR:HB	7:Q:51:ARG:HB2	1.85	0.57
8:Z:161:LYS:NZ	8:Z:397:ASP:OD2	2.38	0.57
4:e:174:GLU:OE1	4:e:177:ARG:NH2	2.37	0.57
4:e:185:LYS:HE2	4:e:198:ASP:HA	1.86	0.57
7:Q:249:VAL:HA	7:Q:300:VAL:HB	1.86	0.57
4:E:115:ILE:HG22	4:E:117:ASP:H	1.70	0.57
7:q:259:THR:HG22	7:q:261:THR:H	1.69	0.57
7:q:412:MET:H	7:q:416:GLY:HA3	1.69	0.57
6:H:191:ARG:O	6:H:405:GLN:NE2	2.38	0.57
6:H:329:ALA:HA	6:H:371:ALA:HA	1.87	0.57
7:q:56:VAL:HG22	7:q:62:ILE:HG12	1.86	0.57
7:q:511:ASP:HB2	7:q:514:GLU:HG3	1.86	0.57
7:Q:63:ILE:HG23	7:Q:399:ARG:HH12	1.69	0.57
6:h:241:ILE:HA	6:h:292:ILE:HB	1.87	0.57
7:Q:150:ILE:HG12	7:Q:152:ASP:H	1.69	0.57
8:Z:232:TYR:OH	8:Z:285:CYS:SG	2.61	0.57
2:b:197:LYS:HD2	2:b:377:LEU:HB3	1.86	0.56
6:h:233:PRO:HG2	6:h:236:PHE:HE1	1.70	0.56
8:z:221:HIS:HB3	8:z:224:MET:HG2	1.87	0.56
4:e:74:LEU:HB3	4:e:93:GLN:HG2	1.86	0.56
7:q:44:THR:O	7:q:51:ARG:N	2.33	0.56
1:a:468:LYS:HE3	1:a:507:GLY:HA3	1.86	0.56
2:b:116:HIS:NE2	4:e:485:GLU:O	2.37	0.56
4:E:245:LEU:HB2	4:E:393:LEU:HD21	1.86	0.56
5:g:539:ASN:ND2	5:g:541:THR:OG1	2.39	0.56
3:D:238:GLN:HB2	3:D:334:ALA:HA	1.88	0.56
5:g:324:ASP:OD1	5:g:327:ARG:NH2	2.37	0.56
2:b:515:ILE:HD11	4:e:60:ILE:HD13	1.88	0.56
3:d:161:LYS:HE3	3:d:393:SER:HA	1.88	0.56
4:e:251:HIS:HB3	4:e:254:MET:HG3	1.88	0.56
5:g:491:ALA:HA	5:g:494:LEU:HD12	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:q:66:ASN:ND2	7:q:169:SER:O	2.39	0.56
3:D:121:ALA:HB1	3:D:516:LYS:HG3	1.88	0.56
7:q:27:GLN:HE22	7:q:544:ILE:HG12	1.71	0.56
1:A:462:LEU:HG	1:A:504:LEU:HD11	1.86	0.56
5:G:354:LEU:HD13	5:G:356:LYS:HB2	1.88	0.56
8:z:510:TYR:OH	8:z:514:ARG:NH1	2.38	0.56
3:d:355:SER:H	3:d:358:SER:HB2	1.71	0.55
8:Z:46:LEU:HD11	8:Z:62:LEU:HD23	1.88	0.55
2:b:393:GLN:HB3	2:b:492:LYS:HD3	1.87	0.55
6:H:78:PRO:HB2	7:Q:54:ILE:HD13	1.87	0.55
6:H:275:TRP:HE1	6:H:302:LEU:HD11	1.72	0.55
4:e:104:LEU:HD22	4:e:123:VAL:HG13	1.87	0.55
5:G:49:LEU:HB2	8:Z:535:ARG:HA	1.89	0.55
8:Z:147:ARG:NH1	8:Z:176:ASP:OD1	2.40	0.55
8:z:295:ILE:HB	8:z:316:ALA:HA	1.89	0.55
3:d:121:ALA:HB1	3:d:516:LYS:HG3	1.87	0.55
4:E:180:LEU:HD11	4:E:430:VAL:HG22	1.87	0.55
8:z:236:LEU:HG	8:z:238:VAL:H	1.72	0.55
4:E:553:ASN:HB3	6:H:51:ILE:HG13	1.89	0.55
5:g:484:SER:HB3	5:g:509:MET:HB2	1.88	0.55
6:H:224:PHE:CZ	6:H:226:TYR:HB2	2.42	0.55
7:Q:96:MET:HG3	7:Q:98:ASP:H	1.72	0.55
8:Z:458:LEU:HG	8:Z:493:LEU:HD21	1.89	0.55
2:b:242:LYS:HB3	2:b:245:ILE:HB	1.89	0.55
2:B:40:LYS:NZ	2:B:474:LEU:O	2.38	0.55
5:g:331:VAL:HG23	5:g:332:THR:HG23	1.89	0.55
5:G:53:GLY:O	8:Z:78:ARG:NH2	2.40	0.55
7:Q:500:ASP:HB2	7:Q:509:VAL:HG12	1.88	0.55
8:Z:15:ARG:HG3	8:Z:17:ALA:H	1.72	0.55
3:d:298:ASN:OD1	3:d:299:ASP:N	2.40	0.54
6:H:94:VAL:O	6:H:402:ARG:NH2	2.40	0.54
3:D:354:ASP:HA	3:D:359:LYS:H	1.72	0.54
4:e:268:LYS:HB2	4:e:318:ALA:HA	1.89	0.54
6:H:48:GLY:HA2	6:H:456:ASN:HB3	1.89	0.54
6:H:240:LYS:HD3	6:H:346:LEU:HD13	1.90	0.54
6:H:245:ASN:HD22	6:H:336:SER:HA	1.72	0.54
2:b:214:LEU:HG	2:b:216:LYS:H	1.72	0.54
3:d:412:ALA:HB3	3:d:478:LEU:HG	1.88	0.54
3:D:298:ASN:OD1	3:D:299:ASP:N	2.41	0.54
3:d:432:MET:O	4:E:500:SER:OG	2.24	0.54
7:q:373:GLN:NE2	7:q:377:GLU:O	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:z:19:LEU:HD11	8:z:528:LEU:HD23	1.89	0.54
1:a:207:LYS:HB2	1:a:395:LEU:HD13	1.89	0.54
5:G:225:LEU:HB2	5:G:366:SER:HB2	1.88	0.54
8:Z:367:VAL:O	8:Z:370:ASN:ND2	2.40	0.54
1:A:207:LYS:NZ	1:A:396:ASP:OD1	2.39	0.54
7:Q:341:LEU:HD12	7:Q:342:PRO:HD2	1.90	0.54
1:A:407:SER:HA	1:A:410:LYS:HE2	1.89	0.54
2:b:341:ASP:HB2	2:b:358:GLY:HA3	1.89	0.54
2:b:470:SER:HA	2:b:481:ASP:HA	1.89	0.54
2:B:41:GLY:HA2	2:B:447:ASN:HB3	1.89	0.54
2:B:197:LYS:HD2	2:B:377:LEU:HB3	1.88	0.54
5:g:242:ARG:HA	5:g:349:GLY:HA3	1.90	0.54
6:h:229:PHE:HZ	6:h:361:ARG:HD2	1.72	0.54
3:D:29:ARG:NH1	3:D:108:GLU:OE1	2.41	0.54
4:E:461:GLN:HG3	4:E:469:PHE:HE2	1.73	0.54
1:A:250:ASN:HB3	1:A:300:LYS:HB2	1.89	0.53
4:E:103:LEU:HB3	4:E:544:LEU:HD11	1.91	0.53
2:B:511:VAL:HG11	4:E:73:ILE:HG13	1.89	0.53
3:D:135:LEU:HA	3:D:138:MET:HE3	1.89	0.53
5:G:21:GLN:NE2	5:G:584:ASP:OD1	2.41	0.53
3:d:372:ARG:HB2	3:d:373:PRO:HD2	1.90	0.53
4:e:96:LEU:HD11	4:e:101:ALA:HB3	1.90	0.53
4:E:72:LYS:HD2	4:E:90:ILE:HD13	1.89	0.53
6:H:125:ILE:HA	6:H:438:ILE:HD13	1.89	0.53
4:e:316:ALA:HB2	4:e:369:LEU:HD13	1.89	0.53
5:g:121:ILE:HG12	5:g:501:PRO:HB3	1.90	0.53
5:G:181:THR:HG21	5:G:437:CYS:HB3	1.90	0.53
7:q:150:ILE:HG22	7:q:152:ASP:H	1.73	0.53
7:q:541:ILE:HG12	8:z:45:MET:HB2	1.90	0.53
8:Z:221:HIS:HB3	8:Z:224:MET:HG3	1.91	0.53
1:A:430:ASN:HA	1:A:452:ALA:HB1	1.91	0.53
4:E:363:VAL:HG11	4:E:369:LEU:HD23	1.89	0.53
8:Z:245:THR:HG22	8:Z:247:VAL:H	1.74	0.53
6:h:85:ASP:OD2	7:q:392:ASN:ND2	2.40	0.53
8:Z:298:GLN:HG3	8:Z:320:ALA:HB3	1.90	0.53
2:B:317:LEU:O	2:B:321:THR:OG1	2.24	0.53
2:B:342:VAL:HB	2:B:357:SER:HB3	1.91	0.53
6:H:412:GLY:O	6:H:491:ASN:ND2	2.35	0.53
7:q:96:MET:HG3	7:q:98:ASP:H	1.73	0.53
8:Z:16:ASP:O	8:Z:18:ALA:N	2.41	0.53
1:a:176:PHE:HZ	1:a:213:ALA:HB1	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:251:LYS:HB2	4:e:288:ASP:HB3	1.90	0.53
6:H:325:ARG:NH1	6:H:373:THR:OG1	2.42	0.53
6:H:70:LEU:HB3	6:H:84:VAL:HG22	1.91	0.53
8:z:84:ASP:O	8:z:400:ARG:NH1	2.40	0.53
5:g:85:GLN:HE21	5:g:89:VAL:HG22	1.73	0.52
2:b:513:ASN:OD1	2:b:514:ILE:N	2.42	0.52
2:B:59:ASP:OD2	2:B:382:ARG:NE	2.42	0.52
2:B:197:LYS:HB3	2:B:377:LEU:HD22	1.91	0.52
3:D:355:SER:H	3:D:358:SER:HB2	1.74	0.52
4:e:114:GLU:O	4:e:431:ARG:NH2	2.39	0.52
6:H:94:VAL:HG12	6:H:96:ASP:H	1.73	0.52
8:z:113:VAL:HG22	8:Z:467:LEU:HD22	1.90	0.52
1:A:418:VAL:HA	1:A:520:PRO:HA	1.91	0.52
3:D:326:LYS:HB3	3:D:372:ARG:HE	1.73	0.52
5:g:229:VAL:HG12	5:g:231:HIS:H	1.74	0.52
2:B:510:ARG:HG2	4:E:71:ASP:H	1.74	0.52
5:g:495:GLU:OE2	7:Q:483:ASN:ND2	2.43	0.52
8:Z:26:ALA:HB1	8:Z:99:GLY:HA2	1.92	0.52
1:a:493:LYS:HD2	1:a:496:SER:HB3	1.90	0.52
1:A:242:VAL:HG23	1:A:294:GLN:HB2	1.92	0.52
2:B:196:ILE:HB	2:B:368:VAL:HG22	1.91	0.52
4:E:226:MET:HE1	4:E:423:LEU:HD23	1.90	0.52
7:Q:336:CYS:HB2	7:Q:354:LEU:H	1.74	0.52
6:h:482:VAL:HG13	6:h:494:LYS:HE2	1.91	0.52
4:e:283:THR:HG23	4:e:284:LYS:H	1.73	0.52
8:Z:358:THR:HG23	8:Z:363:LYS:HG2	1.91	0.52
2:b:72:PRO:HG3	2:b:514:ILE:HG21	1.92	0.52
3:d:117:PRO:HB2	3:d:519:LEU:HB3	1.91	0.52
3:d:523:ASP:OD1	3:d:524:ILE:N	2.43	0.52
4:E:305:LYS:HG3	4:E:309:MET:HE2	1.92	0.52
6:H:279:PHE:HA	6:H:282:LEU:HB3	1.92	0.52
4:e:234:ILE:HG22	4:e:410:GLY:HA2	1.92	0.52
6:h:242:LEU:HD11	6:h:341:ILE:HD13	1.92	0.52
7:Q:256:ILE:HB	7:Q:280:GLU:HG2	1.92	0.52
8:Z:229:LYS:HA	8:Z:353:LEU:HA	1.92	0.52
6:h:94:VAL:HG12	6:h:96:ASP:H	1.75	0.52
8:z:30:GLN:HE22	8:z:100:GLU:HB2	1.74	0.52
4:e:269:LEU:HD21	4:e:322:ILE:HD12	1.92	0.51
4:E:243:VAL:HG21	4:E:354:ILE:HG12	1.93	0.51
7:Q:223:ILE:HG22	7:Q:225:GLY:H	1.74	0.51
5:g:296:ILE:HG23	5:g:320:VAL:HG21	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Q:227:VAL:HG13	7:Q:370:VAL:HG12	1.90	0.51
3:D:383:ASN:H	3:D:386:ILE:HD12	1.75	0.51
4:E:186:THR:HG21	4:E:527:VAL:HG13	1.91	0.51
6:h:329:ALA:HA	6:h:371:ALA:HA	1.93	0.51
7:Q:373:GLN:NE2	7:Q:377:GLU:O	2.39	0.51
4:e:223:LEU:O	4:e:403:THR:OG1	2.28	0.51
4:e:344:ARG:HH21	4:e:345:TRP:HE1	1.59	0.51
4:E:247:LYS:HB3	4:E:393:LEU:HD23	1.93	0.51
7:q:255:ASP:OD1	7:q:256:ILE:N	2.44	0.51
8:z:194:VAL:HG22	8:z:376:CYS:HB2	1.92	0.51
3:d:463:ILE:HD11	4:E:139:LYS:HB3	1.93	0.51
5:g:203:TYR:OH	5:g:330:ARG:NH1	2.39	0.51
5:G:339:ARG:HG2	5:G:341:GLU:H	1.76	0.51
3:d:48:ILE:HD11	3:d:64:ILE:HG23	1.93	0.51
3:D:523:ASP:OD1	3:D:524:ILE:N	2.44	0.51
4:e:86:ASP:OD1	4:e:120:THR:OG1	2.28	0.51
4:e:107:LEU:HD21	4:e:122:VAL:HG22	1.93	0.51
4:E:384:GLU:HG2	4:E:391:ARG:HG2	1.92	0.51
5:G:242:ARG:HB3	5:G:292:PRO:HA	1.93	0.51
6:H:37:GLN:HE21	6:H:103:ILE:HG23	1.76	0.51
2:b:510:ARG:O	4:e:71:ASP:N	2.43	0.51
5:g:481:MET:HG2	5:g:531:LEU:HG	1.93	0.51
5:G:180:LYS:HG2	5:G:183:ARG:HE	1.75	0.51
6:h:499:PRO:HG2	6:h:502:VAL:HG23	1.93	0.51
4:e:240:ILE:HG22	4:e:242:GLY:H	1.75	0.51
5:g:339:ARG:NH2	5:g:342:ASP:OD1	2.43	0.51
1:A:221:GLY:HA3	1:A:375:LYS:HG2	1.93	0.51
2:B:470:SER:HA	2:B:481:ASP:HA	1.93	0.51
6:H:242:LEU:HD11	6:H:341:ILE:HD13	1.93	0.51
2:b:229:ALA:HA	2:b:282:ASN:HB2	1.93	0.50
7:Q:135:ARG:NH2	8:Z:165:ASP:OD2	2.43	0.50
7:Q:155:ASP:OD1	7:Q:156:LYS:N	2.43	0.50
2:b:230:LYS:HA	2:b:339:GLU:HA	1.93	0.50
8:z:173:ILE:HG12	8:z:209:PHE:HB2	1.92	0.50
1:A:164:MET:HG2	1:A:401:SER:HB2	1.93	0.50
3:D:293:LEU:HG	3:D:294:ARG:HG2	1.93	0.50
5:g:236:ARG:HA	5:g:357:VAL:HG22	1.92	0.50
8:Z:202:LEU:HD23	8:Z:381:LYS:HD3	1.93	0.50
3:d:340:THR:OG1	3:d:343:ARG:NH1	2.44	0.50
5:g:229:VAL:HG11	5:g:234:MET:HG3	1.93	0.50
7:Q:207:ILE:HD12	7:Q:405:VAL:HG13	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Q:339:THR:HB	7:Q:351:GLU:HG2	1.93	0.50
8:Z:235:ILE:HB	8:Z:336:ALA:HA	1.94	0.50
5:G:211:GLY:O	5:G:442:ARG:NE	2.34	0.50
1:A:190:GLN:HE21	1:A:194:GLY:H	1.60	0.50
1:A:252:GLN:HA	1:A:303:ASP:HB2	1.93	0.50
1:A:302:ILE:H	1:A:319:ARG:HG2	1.77	0.50
2:b:51:SER:O	3:d:76:ARG:NH1	2.44	0.50
6:H:239:PRO:HB2	6:H:292:ILE:HG12	1.94	0.50
2:b:192:HIS:HB3	2:b:364:ALA:HA	1.93	0.50
1:a:51:LYS:HA	5:g:583:VAL:HG13	1.93	0.49
1:A:322:LYS:HE2	1:A:324:GLU:HB2	1.92	0.49
6:H:241:ILE:HA	6:H:292:ILE:HB	1.93	0.49
7:q:92:GLN:NE2	7:q:98:ASP:O	2.45	0.49
6:H:42:PRO:HB2	6:H:49:SER:HB2	1.94	0.49
6:H:220:PHE:HD1	6:H:222:LYS:H	1.60	0.49
6:H:232:GLN:NE2	6:H:312:ILE:O	2.46	0.49
6:H:482:VAL:HG13	6:H:494:LYS:HE2	1.92	0.49
8:Z:215:LEU:HD11	8:Z:365:THR:HB	1.95	0.49
2:B:214:LEU:HD23	2:B:354:LEU:HD12	1.94	0.49
4:e:441:TYR:HD2	4:e:509:ASN:HB2	1.77	0.49
6:h:75:VAL:HG12	6:h:77:HIS:H	1.77	0.49
6:h:123:HIS:NE2	7:q:49:CYS:SG	2.80	0.49
8:Z:323:ARG:HE	8:Z:327:ARG:HH21	1.60	0.49
3:D:333:ILE:HD13	3:D:339:PHE:HA	1.93	0.49
7:Q:162:MET:SD	7:Q:518:TYR:OH	2.65	0.49
2:B:88:VAL:HG23	2:B:89:GLY:H	1.77	0.49
3:d:436:GLN:HA	3:d:440:TRP:CE3	2.47	0.49
5:G:51:PRO:HB3	8:Z:538:ARG:HB2	1.92	0.49
8:z:43:LEU:HD21	8:z:55:LEU:HB3	1.95	0.49
8:Z:12:SER:HB3	8:Z:13:LEU:HD13	1.94	0.49
6:h:325:ARG:NH1	6:h:373:THR:OG1	2.46	0.49
7:q:77:ILE:HG13	7:q:86:VAL:HG21	1.95	0.49
8:Z:295:ILE:HB	8:Z:316:ALA:HA	1.94	0.49
2:B:228:ASN:O	2:B:282:ASN:ND2	2.43	0.49
4:e:193:VAL:HG13	4:e:200:PHE:HD2	1.77	0.49
7:q:242:ASP:O	7:q:245:HIS:NE2	2.45	0.49
7:q:98:ASP:OD1	7:q:99:GLY:N	2.46	0.49
7:q:162:MET:HE1	7:q:520:MET:HB3	1.95	0.49
4:e:67:PRO:HA	4:e:190:SER:HB3	1.94	0.49
4:e:511:GLY:H	4:e:521:ASP:H	1.60	0.49
5:g:125:LEU:HB3	5:g:574:ILE:HG23	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:q:135:ARG:NH2	8:z:165:ASP:OD2	2.45	0.49
7:q:203:ASN:OD1	7:q:204:VAL:N	2.45	0.49
1:A:426:GLU:HB3	1:A:455:LEU:HB3	1.95	0.48
2:B:35:SER:O	2:B:42:MET:N	2.36	0.48
2:B:230:LYS:HB2	2:B:281:ILE:HA	1.95	0.48
3:D:215:LEU:HD21	3:D:324:LEU:HD11	1.93	0.48
4:E:172:ASN:OD1	4:E:173:ASP:N	2.46	0.48
5:g:242:ARG:HB2	5:g:293:THR:H	1.78	0.48
7:q:155:ASP:OD1	7:q:156:LYS:N	2.46	0.48
1:a:189:THR:HG23	1:a:191:ASN:H	1.78	0.48
1:a:303:ASP:OD1	1:a:304:ASP:N	2.41	0.48
1:A:96:ASP:OD1	1:A:97:GLY:N	2.46	0.48
5:G:563:GLU:HG2	5:G:567:GLN:HG3	1.95	0.48
6:h:70:LEU:HA	6:h:73:LEU:HD13	1.95	0.48
6:h:342:LYS:H	6:h:345:HIS:HD2	1.62	0.48
1:A:51:LYS:HD3	5:G:585:ASP:HB3	1.96	0.48
3:d:284:ASN:O	3:d:311:MET:N	2.41	0.48
5:G:178:ALA:HB2	5:G:439:ILE:HD11	1.95	0.48
3:d:91:ASP:OD1	3:d:92:GLY:N	2.45	0.48
2:B:511:VAL:HG13	4:E:72:LYS:HA	1.95	0.48
4:e:115:ILE:HG23	4:e:432:ASN:HD21	1.79	0.48
4:E:158:ILE:HD13	4:E:535:LYS:HE3	1.94	0.48
4:E:320:VAL:HG21	4:E:380:ILE:HD12	1.95	0.48
4:E:556:ILE:HA	6:H:54:VAL:HB	1.95	0.48
7:Q:184:GLU:HB3	7:Q:222:VAL:HG21	1.96	0.48
1:A:303:ASP:OD1	1:A:304:ASP:N	2.41	0.48
3:d:412:ALA:H	3:d:478:LEU:HD21	1.79	0.48
4:e:459:ASP:OD1	4:e:466:GLN:NE2	2.46	0.48
5:G:160:GLY:O	5:G:161:THR:OG1	2.30	0.48
6:h:78:PRO:HB2	7:q:54:ILE:HD13	1.95	0.48
7:Q:415:SER:HB3	7:Q:521:LEU:HD23	1.96	0.48
8:Z:43:LEU:HD21	8:Z:55:LEU:HB3	1.96	0.48
8:z:89:ASP:OD1	8:z:90:GLY:N	2.45	0.48
1:a:252:GLN:HA	1:a:303:ASP:HB2	1.96	0.48
5:g:154:LEU:HD13	5:g:466:VAL:HG21	1.96	0.48
5:G:494:LEU:HD11	5:G:498:GLN:HE21	1.79	0.48
8:z:183:ASP:HB2	8:z:187:ASP:HB2	1.96	0.48
1:A:325:ASP:OD1	1:A:328:ARG:NH2	2.43	0.48
2:B:516:ARG:HA	4:E:75:ILE:HB	1.95	0.48
3:d:368:ASN:OD1	3:d:369:ASN:N	2.47	0.48
3:D:423:ARG:NH2	3:D:474:GLU:OE1	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:g:485:VAL:HG21	5:g:535:HIS:HB2	1.96	0.48
2:B:210:GLU:HA	2:B:365:CYS:HA	1.97	0.47
7:Q:35:ILE:HD11	7:Q:81:ALA:HB1	1.96	0.47
7:Q:77:ILE:HG13	7:Q:86:VAL:HG21	1.96	0.47
8:z:245:THR:HG22	8:z:247:VAL:H	1.78	0.47
2:B:459:LEU:HD22	2:B:472:LEU:HG	1.95	0.47
4:e:268:LYS:HB3	4:e:374:LEU:HD13	1.95	0.47
4:E:447:GLU:HG2	4:E:479:ILE:HB	1.96	0.47
6:h:198:LEU:O	6:h:373:THR:OG1	2.25	0.47
6:h:241:ILE:HD12	6:h:330:VAL:HG11	1.97	0.47
3:d:383:ASN:H	3:d:386:ILE:HD12	1.79	0.47
5:G:231:HIS:ND1	5:G:232:PRO:HD2	2.29	0.47
7:Q:44:THR:O	7:Q:51:ARG:N	2.35	0.47
7:Q:124:ALA:HA	7:Q:127:ILE:HD12	1.95	0.47
8:z:367:VAL:O	8:z:370:ASN:ND2	2.44	0.47
1:A:519:GLU:HG2	1:A:524:LYS:HE2	1.95	0.47
2:b:141:ASP:HB3	2:b:399:ARG:HA	1.96	0.47
2:B:513:ASN:OD1	2:B:514:ILE:N	2.48	0.47
3:D:48:ILE:HD11	3:D:64:ILE:HG23	1.97	0.47
4:e:219:VAL:HB	4:e:431:ARG:HG3	1.96	0.47
5:g:208:LYS:HD2	5:g:449:LEU:HB3	1.95	0.47
8:z:147:ARG:NH1	8:z:176:ASP:OD1	2.47	0.47
3:D:156:THR:HG21	3:D:496:HIS:HB3	1.97	0.47
5:g:222:GLY:O	5:g:438:THR:OG1	2.27	0.47
6:h:240:LYS:HB2	6:h:290:ALA:HA	1.97	0.47
6:H:53:ILE:HD11	6:H:69:ILE:HG23	1.96	0.47
3:d:461:ASN:HB3	3:d:464:LYS:HB3	1.97	0.47
3:D:286:LEU:HB2	3:D:312:VAL:HG22	1.96	0.47
5:G:183:ARG:NH1	5:G:185:ASP:OD2	2.47	0.47
1:A:42:SER:HB2	1:A:51:LYS:HE3	1.97	0.47
2:B:470:SER:OG	2:B:481:ASP:OD1	2.29	0.47
3:d:326:LYS:HB3	3:d:372:ARG:HE	1.80	0.47
3:d:335:ASP:OD1	3:d:336:ILE:N	2.47	0.47
4:e:112:ASP:HA	4:e:116:GLY:HA2	1.96	0.47
6:H:220:PHE:HZ	6:H:363:ASN:HD22	1.62	0.47
1:A:484:SER:OG	1:A:497:TYR:O	2.30	0.47
5:g:65:LEU:HD23	5:g:68:ILE:HD12	1.97	0.47
5:G:236:ARG:HB3	5:G:356:LYS:HG2	1.97	0.47
8:Z:45:MET:HG3	8:Z:53:ILE:HG23	1.96	0.47
8:Z:300:GLY:HA2	8:Z:318:ARG:HB2	1.97	0.47
2:b:191:GLU:O	2:b:316:ARG:NH1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:z:430:ASN:HD21	8:z:441:LYS:HG2	1.80	0.47
1:A:480:TYR:HB3	1:A:500:TYR:HD2	1.80	0.47
1:A:498:ARG:HG3	1:A:499:ASN:HD22	1.80	0.47
2:b:72:PRO:HB3	4:e:75:ILE:HD11	1.97	0.47
2:b:88:VAL:HG23	2:b:89:GLY:H	1.81	0.47
3:D:461:ASN:HB3	3:D:464:LYS:HB3	1.97	0.47
4:e:322:ILE:HG23	4:e:346:VAL:HG21	1.96	0.47
6:h:325:ARG:HB3	6:h:373:THR:HG21	1.97	0.47
6:h:452:GLN:NE2	6:h:456:ASN:OD1	2.42	0.47
3:d:213:VAL:HG23	3:d:323:PHE:HE2	1.81	0.46
8:z:143:LEU:HG	8:z:145:ASN:H	1.79	0.46
8:Z:89:ASP:OD1	8:Z:90:GLY:N	2.48	0.46
1:A:160:ALA:HB1	1:A:164:MET:HE2	1.96	0.46
2:b:122:GLU:OE2	4:e:68:ARG:NH1	2.48	0.46
8:z:476:GLU:OE2	8:z:487:ARG:NH1	2.43	0.46
2:B:72:PRO:HD3	2:B:516:ARG:HH21	1.80	0.46
3:D:198:LYS:HB2	3:D:387:ILE:HB	1.97	0.46
1:a:235:LYS:HB3	1:a:363:GLN:HB3	1.96	0.46
5:G:49:LEU:HD21	8:Z:71:PRO:HG3	1.97	0.46
3:d:297:VAL:HB	3:d:314:LYS:HD3	1.97	0.46
4:e:556:ILE:HA	6:h:54:VAL:HB	1.98	0.46
6:h:37:GLN:HE21	6:h:103:ILE:HG23	1.79	0.46
6:h:195:ASP:HB3	6:h:198:LEU:HG	1.97	0.46
1:A:437:ALA:HB1	1:A:445:GLN:HG3	1.97	0.46
4:e:251:HIS:ND1	4:e:252:PRO:HD2	2.30	0.46
8:z:153:VAL:HG22	8:z:507:TRP:HB2	1.98	0.46
1:a:252:GLN:HG2	1:a:303:ASP:HB2	1.97	0.46
1:A:91:ASP:HA	1:A:95:GLY:HA2	1.96	0.46
1:A:301:GLY:HA2	1:A:319:ARG:HA	1.98	0.46
3:D:77:MET:SD	3:D:517:SER:OG	2.71	0.46
3:D:91:ASP:OD1	3:D:92:GLY:N	2.49	0.46
5:g:110:TYR:HA	5:g:114:LYS:HB2	1.98	0.46
7:Q:243:LYS:HG2	7:Q:244:LYS:HG3	1.97	0.46
7:Q:246:LYS:HB2	7:Q:296:VAL:HA	1.96	0.46
1:a:52:MET:HG2	1:a:62:VAL:HB	1.97	0.46
1:A:204:ASN:OD1	1:A:205:VAL:N	2.49	0.46
2:b:331:GLU:HG2	2:b:333:SER:H	1.80	0.46
3:d:285:VAL:HG22	3:d:311:MET:HB3	1.97	0.46
3:D:335:ASP:OD1	3:D:336:ILE:N	2.42	0.46
1:a:418:VAL:HG21	1:a:518:LEU:HD13	1.98	0.46
3:d:103:LEU:HB2	3:d:515:VAL:HG21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:d:256:ASP:OD1	3:d:257:TYR:N	2.49	0.46
7:q:420:LEU:HD11	7:q:524:LYS:HG3	1.97	0.46
8:Z:158:LEU:O	8:Z:162:VAL:HG22	2.16	0.46
1:a:164:MET:HG2	1:a:401:SER:HB2	1.98	0.46
2:b:37:LEU:HG	2:b:444:LEU:HD21	1.98	0.46
8:Z:100:GLU:HG2	8:Z:453:VAL:HB	1.96	0.46
1:A:544:MET:HA	3:D:47:MET:HB2	1.97	0.45
2:b:232:LEU:HD23	2:b:281:ILE:HD13	1.97	0.45
3:d:460:LEU:HB3	3:d:465:VAL:HG21	1.98	0.45
3:D:177:SER:HB2	3:D:375:VAL:HG11	1.97	0.45
3:D:220:ILE:HD11	3:D:312:VAL:HB	1.97	0.45
3:D:372:ARG:HB2	3:D:373:PRO:HD2	1.98	0.45
7:Q:41:MET:HB3	7:Q:53:LYS:HE3	1.97	0.45
1:a:101:VAL:HG13	1:a:531:ALA:HB2	1.99	0.45
6:H:75:VAL:HG12	6:H:77:HIS:H	1.81	0.45
1:A:59:ASP:OD1	1:A:60:PHE:N	2.42	0.45
7:Q:28:ILE:HD11	7:Q:539:LEU:HA	1.98	0.45
1:a:206:LEU:HD12	1:a:386:ILE:HG12	1.97	0.45
1:A:366:PHE:HB2	1:A:369:ASP:O	2.16	0.45
3:D:201:GLY:N	3:D:381:GLY:O	2.49	0.45
4:E:322:ILE:HG23	4:E:346:VAL:HG21	1.97	0.45
5:G:45:LEU:HD23	5:G:59:ASN:HB3	1.98	0.45
7:Q:335:VAL:HG11	7:Q:371:PHE:HE2	1.81	0.45
8:Z:40:LYS:HG2	8:Z:493:LEU:HD13	1.98	0.45
1:a:59:ASP:OD1	1:a:60:PHE:N	2.42	0.45
1:a:366:PHE:HB2	1:a:369:ASP:O	2.17	0.45
1:A:133:LEU:HD22	1:A:532:LEU:HD13	1.98	0.45
2:B:170:LYS:HA	2:B:173:PHE:HB2	1.98	0.45
4:e:47:LYS:HD3	4:e:137:ILE:HD13	1.98	0.45
4:E:271:ILE:HG23	4:E:351:LEU:HD22	1.99	0.45
5:G:213:ASP:OD1	5:G:214:VAL:N	2.49	0.45
6:h:422:LYS:HD3	6:h:472:HIS:CD2	2.51	0.45
7:q:124:ALA:HA	7:q:127:ILE:HD12	1.97	0.45
8:Z:236:LEU:HD11	8:Z:238:VAL:HG12	1.99	0.45
7:Q:242:ASP:OD1	7:Q:243:LYS:N	2.50	0.45
1:a:230:SER:HB2	1:a:307:LEU:HD21	1.99	0.45
4:e:512:VAL:HG12	4:e:514:CYS:H	1.81	0.45
8:z:94:VAL:HG13	8:z:520:ALA:HB2	1.99	0.45
3:d:411:ILE:HB	3:d:478:LEU:HD21	1.98	0.45
5:G:325:ASN:HB3	5:G:336:ILE:HD11	1.99	0.45
8:z:39:PRO:HA	8:z:160:THR:HA	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Z:232:TYR:HB2	8:Z:293:PHE:HD1	1.82	0.45
1:a:253:LYS:HB3	1:a:255:ARG:HH12	1.80	0.45
1:A:242:VAL:HG11	1:A:361:VAL:HG23	1.99	0.45
2:B:33:VAL:HB	2:B:93:THR:HG23	1.99	0.45
3:d:65:LEU:HB3	3:d:79:VAL:HG22	1.97	0.45
3:d:411:ILE:HD12	3:d:417:PRO:HG3	1.98	0.45
1:A:169:ILE:HB	1:A:398:MET:HG2	1.98	0.45
1:A:235:LYS:HA	1:A:316:MET:HE1	1.99	0.45
3:D:233:LYS:NZ	3:D:341:GLU:OE2	2.50	0.45
4:E:261:LYS:O	4:E:264:SER:OG	2.31	0.45
6:H:77:HIS:CE1	6:H:79:ALA:HB3	2.52	0.45
7:q:35:ILE:HD11	7:q:81:ALA:HB1	1.99	0.45
1:A:471:SER:HB2	6:h:434:LYS:HE2	1.98	0.44
5:G:296:ILE:HG12	5:G:317:LEU:HD12	1.99	0.44
7:Q:146:VAL:HG21	7:Q:418:LYS:HD3	2.00	0.44
8:z:136:PHE:HE2	8:z:412:ILE:HG23	1.82	0.44
3:D:194:ILE:HG12	3:D:375:VAL:HB	1.97	0.44
4:e:323:CYS:SG	4:e:324:GLN:N	2.90	0.44
6:h:91:ASP:HA	6:h:95:GLY:HA2	1.99	0.44
7:Q:98:ASP:OD1	7:Q:99:GLY:N	2.50	0.44
1:A:42:SER:O	1:A:465:ASN:ND2	2.50	0.44
6:H:42:PRO:O	6:H:49:SER:N	2.50	0.44
8:Z:273:LYS:HB3	8:Z:340:VAL:HG21	1.98	0.44
4:e:86:ASP:OD2	4:e:421:ARG:NH2	2.44	0.44
4:E:213:ASP:HB2	4:E:216:ARG:HB2	1.99	0.44
7:q:238:SER:HB2	7:q:359:LYS:HG2	1.98	0.44
8:z:47:VAL:HG12	8:z:49:GLY:H	1.83	0.44
1:A:101:VAL:HG13	1:A:531:ALA:HB2	2.00	0.44
4:E:112:ASP:HA	4:E:116:GLY:HA2	2.00	0.44
1:A:252:GLN:HG2	1:A:303:ASP:HB2	1.98	0.44
3:d:372:ARG:HG3	3:d:374:THR:HG23	1.99	0.44
4:e:231:GLY:N	4:e:410:GLY:O	2.51	0.44
4:E:246:ASP:HA	4:E:392:MET:HG2	1.98	0.44
5:g:249:PRO:HB3	5:g:299:LYS:HB2	1.99	0.44
8:Z:239:SER:OG	8:Z:241:GLU:HG2	2.18	0.44
1:A:83:LEU:HD23	1:A:102:VAL:HG13	2.00	0.44
4:e:256:LYS:NZ	4:e:384:GLU:OE2	2.51	0.44
5:g:89:VAL:HG12	5:g:465:ASN:HD21	1.82	0.44
5:g:247:ASP:HB3	5:g:338:ASN:HA	1.99	0.44
8:Z:47:VAL:HG12	8:Z:49:GLY:H	1.83	0.44
8:z:126:ARG:HD2	8:z:518:THR:HG23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Z:213:LEU:HD12	8:Z:328:LEU:HD23	2.00	0.44
1:a:96:ASP:OD1	1:a:97:GLY:N	2.51	0.44
1:a:471:SER:HB3	6:H:434:LYS:HG2	1.99	0.44
1:A:481:HIS:NE2	1:A:500:TYR:O	2.49	0.44
3:d:198:LYS:HB2	3:d:387:ILE:HB	1.99	0.44
3:d:254:VAL:HG13	3:d:259:GLN:HB3	1.99	0.44
8:z:298:GLN:HG3	8:z:320:ALA:HB3	1.99	0.44
8:Z:357:GLU:OE1	8:Z:366:TYR:OH	2.34	0.44
1:a:42:SER:O	1:a:465:ASN:ND2	2.51	0.43
3:D:368:ASN:OD1	3:D:369:ASN:N	2.50	0.43
4:e:344:ARG:HE	4:e:345:TRP:CD1	2.36	0.43
8:Z:39:PRO:HA	8:Z:160:THR:HA	2.00	0.43
1:A:49:LEU:HD22	5:G:582:ARG:HG2	2.00	0.43
1:A:222:TYR:HB2	1:A:374:ILE:HB	1.99	0.43
1:A:480:TYR:HE2	1:A:509:ILE:HG13	1.82	0.43
3:d:293:LEU:HG	3:d:294:ARG:HG2	1.98	0.43
5:g:563:GLU:HG2	5:g:567:GLN:HG3	2.00	0.43
6:h:298:PRO:HB3	6:h:317:ARG:HE	1.83	0.43
8:Z:143:LEU:HG	8:Z:145:ASN:H	1.82	0.43
1:a:156:LEU:HD13	1:a:409:VAL:HG13	2.00	0.43
1:a:543:THR:HB	3:d:46:LYS:HG3	2.00	0.43
1:a:419:VAL:HB	1:a:521:THR:HG22	2.00	0.43
1:A:501:GLY:HA3	1:A:512:GLU:HG2	2.00	0.43
2:b:170:LYS:HA	2:b:173:PHE:HB2	2.00	0.43
6:H:250:LEU:HB2	6:H:302:LEU:HD22	2.01	0.43
8:Z:195:GLU:HB2	8:Z:377:THR:HG23	2.00	0.43
3:d:305:LEU:HD23	3:d:308:LEU:HD12	2.00	0.43
3:D:232:ALA:HA	3:D:284:ASN:HD22	1.84	0.43
3:D:318:ARG:HA	3:D:321:ILE:HD12	2.01	0.43
4:e:320:VAL:HG22	4:e:341:PRO:HG2	2.00	0.43
8:Z:14:ARG:HG3	8:Z:15:ARG:N	2.34	0.43
8:Z:226:THR:HG23	8:Z:356:GLN:HB2	2.00	0.43
3:d:77:MET:SD	3:d:517:SER:OG	2.70	0.43
6:h:73:LEU:HB3	6:h:75:VAL:HG23	1.99	0.43
6:h:167:SER:HA	6:h:172:HIS:HD2	1.83	0.43
2:b:58:ASN:HD21	2:b:164:LYS:HD3	1.83	0.43
2:B:41:GLY:O	3:D:520:ARG:NH2	2.52	0.43
7:Q:255:ASP:OD1	7:Q:256:ILE:N	2.47	0.43
1:A:239:GLY:HA2	1:A:360:GLU:HG3	2.00	0.43
4:e:256:LYS:O	4:e:382:GLU:N	2.42	0.43
5:g:213:ASP:OD1	5:g:214:VAL:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:h:44:LEU:O	6:h:456:ASN:ND2	2.50	0.43
6:h:147:ILE:HG13	6:h:150:GLU:HB2	2.01	0.43
7:Q:254:LEU:HD12	7:Q:305:VAL:HG13	2.01	0.43
7:Q:259:THR:HG22	7:Q:261:THR:H	1.84	0.43
1:A:248:ASP:HB3	1:A:339:SER:HA	2.01	0.43
2:b:454:GLU:HG3	2:B:424:GLY:HA3	2.00	0.43
3:d:85:GLN:NE2	3:d:506:SER:OG	2.40	0.43
4:e:256:LYS:HB3	4:e:382:GLU:HB3	2.00	0.43
8:z:22:ASN:OD1	8:z:72:THR:OG1	2.37	0.43
2:b:454:GLU:HG2	2:b:458:LYS:HE3	2.00	0.43
6:h:128:GLY:HA3	6:h:438:ILE:HG21	1.99	0.43
8:z:158:LEU:O	8:z:162:VAL:HG22	2.18	0.43
2:b:193:ILE:HD13	2:b:388:LEU:HD13	2.01	0.42
3:D:239:PHE:CG	3:D:240:GLN:N	2.87	0.42
6:H:499:PRO:HG2	6:H:502:VAL:HG23	2.00	0.42
2:b:116:HIS:CG	2:b:117:PRO:HD2	2.54	0.42
2:b:453:SER:OG	2:B:113:SER:O	2.32	0.42
2:B:116:HIS:NE2	4:E:485:GLU:O	2.52	0.42
3:D:191:LEU:HG	3:D:402:ARG:HH11	1.83	0.42
6:h:350:ALA:HB3	6:h:367:GLY:HA3	1.99	0.42
2:B:241:ASP:CG	2:B:242:LYS:H	2.28	0.42
3:d:351:GLU:OE2	3:d:362:ARG:NH2	2.44	0.42
3:D:296:ALA:HB3	3:D:314:LYS:HD2	2.01	0.42
7:q:165:PRO:HB3	7:q:517:ILE:HG23	2.01	0.42
7:Q:133:MET:HG3	7:Q:445:LEU:HD13	2.00	0.42
7:Q:421:PRO:O	7:Q:426:THR:OG1	2.30	0.42
3:d:116:HIS:CG	3:d:117:PRO:HD2	2.54	0.42
3:d:229:LYS:HG2	3:d:284:ASN:HB3	2.01	0.42
4:e:328:ASP:OD1	4:e:329:ASP:N	2.42	0.42
6:H:147:ILE:HG13	6:H:150:GLU:HB2	2.01	0.42
7:q:510:LYS:NZ	7:q:515:GLU:OE1	2.38	0.42
1:a:143:VAL:O	1:a:498:ARG:NH2	2.53	0.42
1:A:473:LEU:HB3	1:A:502:LEU:HD22	2.02	0.42
2:b:167:SER:HA	2:b:170:LYS:HB2	2.00	0.42
3:D:210:ILE:HB	3:D:376:SER:HB3	2.01	0.42
4:e:169:SER:HA	4:e:176:PHE:HB2	2.01	0.42
5:g:339:ARG:HG2	5:g:341:GLU:H	1.84	0.42
5:G:296:ILE:HG23	5:G:320:VAL:HG21	2.00	0.42
5:G:331:VAL:HG23	5:G:332:THR:HG23	1.99	0.42
6:h:122:SER:OG	7:q:51:ARG:NH2	2.53	0.42
6:h:194:LEU:HD23	6:h:401:LYS:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:94:VAL:HG11	6:H:502:VAL:HG22	1.99	0.42
3:D:116:HIS:CG	3:D:117:PRO:HD2	2.54	0.42
5:G:44:MET:HB3	8:Z:529:LEU:O	2.19	0.42
6:h:93:GLU:O	6:h:402:ARG:NH2	2.52	0.42
6:H:476:GLU:HB2	6:H:479:TYR:CE2	2.55	0.42
2:b:44:LYS:HE3	2:b:46:LEU:HD21	2.02	0.42
4:e:554:VAL:HG22	6:h:52:LEU:HD23	2.01	0.42
5:g:29:LYS:HE3	5:g:36:ARG:HH22	1.85	0.42
8:z:162:VAL:HG23	8:z:164:ALA:H	1.85	0.42
8:z:458:LEU:HB3	8:z:493:LEU:HD21	2.02	0.42
1:A:48:GLY:HA2	1:A:465:ASN:HD22	1.84	0.42
4:E:397:GLN:HG3	4:E:399:LYS:HG2	2.01	0.42
5:G:531:LEU:HD22	5:G:544:ILE:HD11	2.02	0.42
2:b:95:VAL:HG22	2:b:497:VAL:HG13	2.01	0.42
5:g:201:LYS:O	5:g:205:ARG:HB2	2.19	0.42
1:a:482:ALA:HB1	6:H:429:LYS:HD3	2.00	0.42
8:z:174:VAL:HG13	8:z:399:LEU:HD23	2.02	0.42
2:b:115:ILE:HD11	2:b:428:LEU:HB2	2.01	0.41
2:b:510:ARG:HA	4:e:70:LEU:HD22	2.02	0.41
4:e:283:THR:HG23	4:e:284:LYS:N	2.34	0.41
6:h:37:GLN:NE2	6:h:103:ILE:O	2.53	0.41
6:H:325:ARG:HB3	6:H:373:THR:HG21	2.02	0.41
7:Q:35:ILE:O	7:Q:39:HIS:N	2.47	0.41
8:z:233:VAL:HG11	8:z:332:THR:HG21	2.01	0.41
1:a:19:LYS:HE2	1:a:543:THR:HG21	2.01	0.41
1:a:249:LEU:HD21	1:a:284:ARG:HH12	1.85	0.41
2:b:214:LEU:HB3	2:b:354:LEU:HB2	2.02	0.41
2:B:46:LEU:HD21	2:B:67:ILE:HD11	2.02	0.41
3:d:333:ILE:HG13	3:d:339:PHE:HD1	1.85	0.41
3:D:226:PRO:O	3:D:227:THR:OG1	2.30	0.41
5:g:243:VAL:HG13	5:g:296:ILE:HD12	2.03	0.41
5:G:475:GLY:H	5:G:559:ILE:HG23	1.85	0.41
8:z:45:MET:HG3	8:z:53:ILE:HG23	2.01	0.41
8:Z:98:VAL:HG13	8:Z:524:ALA:HB2	2.02	0.41
8:Z:173:ILE:HG12	8:Z:209:PHE:HB2	2.02	0.41
2:b:42:MET:HB3	3:d:520:ARG:O	2.20	0.41
2:B:109:LEU:C	2:B:113:SER:HB2	2.46	0.41
2:B:369:LEU:HD11	2:B:384:LEU:HD22	2.01	0.41
3:d:170:LEU:HD22	3:d:394:LEU:HD21	2.00	0.41
3:d:355:SER:O	3:d:358:SER:OG	2.27	0.41
5:g:243:VAL:HG11	5:g:332:THR:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Q:72:LEU:HD22	7:Q:86:VAL:HG22	2.02	0.41
2:B:308:HIS:O	2:B:308:HIS:ND1	2.53	0.41
5:G:585:ASP:OD1	5:G:586:ILE:N	2.53	0.41
7:q:166:VAL:HG11	7:q:404:GLY:HA2	2.01	0.41
7:Q:205:ASP:OD2	7:Q:330:ARG:NH2	2.38	0.41
7:Q:413:LYS:O	7:Q:415:SER:N	2.53	0.41
1:A:179:MET:HA	1:A:218:LEU:HD22	2.03	0.41
2:b:251:LYS:HD2	4:e:288:ASP:HB3	2.02	0.41
4:E:554:VAL:HG13	6:H:52:LEU:HD23	2.03	0.41
5:g:36:ARG:HA	5:g:98:ILE:HD11	2.02	0.41
7:q:214:GLY:N	7:q:388:GLY:O	2.45	0.41
7:q:239:LEU:HD12	7:q:358:VAL:HB	2.01	0.41
7:Q:311:HIS:HE1	7:Q:315:ARG:HH21	1.67	0.41
1:a:285:VAL:HA	1:a:288:ILE:HD12	2.01	0.41
1:A:37:ALA:O	1:A:41:LYS:HG3	2.21	0.41
1:A:53:LEU:HD13	1:A:72:LEU:HB2	2.02	0.41
1:A:330:ALA:O	1:A:335:ALA:N	2.51	0.41
3:d:239:PHE:CG	3:d:240:GLN:N	2.88	0.41
4:E:487:SER:HB3	4:E:514:CYS:SG	2.61	0.41
5:g:42:LYS:HE3	5:g:547:ASP:HA	2.03	0.41
5:g:562:PRO:HD2	5:g:565:ILE:HD12	2.02	0.41
5:G:221:LYS:O	5:G:369:ASP:HA	2.21	0.41
7:Q:362:GLU:HA	7:Q:367:ARG:HA	2.00	0.41
8:Z:162:VAL:HG23	8:Z:164:ALA:H	1.86	0.41
8:Z:237:ASN:HB3	8:Z:338:ASN:HA	2.03	0.41
3:d:290:LYS:HB2	3:d:315:ASP:HA	2.02	0.41
5:G:96:VAL:HG22	5:G:569:SER:HA	2.02	0.41
8:z:30:GLN:OE1	8:z:100:GLU:N	2.54	0.41
1:a:160:ALA:HB1	1:a:164:MET:HE2	2.03	0.41
6:h:232:GLN:OE1	6:h:233:PRO:HD2	2.20	0.41
8:z:321:LYS:HG2	8:z:323:ARG:H	1.85	0.41
1:a:39:VAL:HA	1:a:51:LYS:HZ1	1.86	0.41
1:A:479:SER:OG	6:h:436:GLN:OE1	2.38	0.41
3:D:24:ASN:OD1	3:D:72:HIS:NE2	2.50	0.41
4:e:212:MET:HE1	4:e:434:VAL:HG11	2.03	0.41
4:E:327:PHE:CE2	4:E:342:ALA:HB1	2.56	0.41
7:q:467:ALA:HB2	7:q:501:ILE:HD12	2.03	0.41
7:q:541:ILE:HG13	8:z:43:LEU:O	2.20	0.41
8:z:83:GLN:O	8:z:87:THR:OG1	2.38	0.41
4:E:517:TYR:CG	4:E:518:GLY:N	2.89	0.41
5:g:49:LEU:HD23	8:z:535:ARG:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:h:229:PHE:CG	6:h:230:GLU:N	2.89	0.41
6:H:167:SER:HA	6:H:172:HIS:HD2	1.86	0.41
8:z:296:ILE:HG22	8:z:296:ILE:O	2.21	0.41
1:a:143:VAL:HG23	1:a:144:LEU:H	1.86	0.40
1:a:294:GLN:HA	1:a:315:ILE:HG12	2.03	0.40
3:d:191:LEU:HD22	3:d:398:LEU:HB3	2.02	0.40
3:D:297:VAL:HB	3:D:314:LYS:HD3	2.03	0.40
6:h:333:SER:HB3	6:h:345:HIS:ND1	2.36	0.40
6:H:296:LYS:HE2	6:H:320:ALA:HA	2.03	0.40
7:Q:469:LEU:HD13	7:Q:474:VAL:HG21	2.03	0.40
2:b:308:HIS:O	2:b:308:HIS:ND1	2.54	0.40
3:d:191:LEU:HG	3:d:402:ARG:HD3	2.03	0.40
3:d:268:ARG:HE	3:d:304:PHE:HZ	1.70	0.40
7:q:500:ASP:OD1	7:q:501:ILE:N	2.54	0.40
8:z:492:ASP:HB2	8:z:499:CYS:HB3	2.02	0.40
3:d:237:ILE:HA	3:d:333:ILE:HB	2.02	0.40
3:D:107:ALA:HA	3:D:110:LEU:HD12	2.03	0.40
4:E:130:LEU:HD11	4:E:548:ILE:HD13	2.03	0.40
5:G:154:LEU:HD13	5:G:466:VAL:HG21	2.04	0.40
6:h:354:GLU:HG3	6:h:362:TYR:C	2.47	0.40
1:a:357:LEU:HB3	1:a:378:SER:HB3	2.04	0.40
4:E:224:ILE:HG21	4:E:427:LEU:HD13	2.04	0.40
6:H:195:ASP:HB3	6:H:198:LEU:HG	2.02	0.40
6:H:480:GLY:HA3	6:H:491:ASN:ND2	2.36	0.40
7:Q:243:LYS:HE2	7:Q:244:LYS:HE3	2.04	0.40
8:z:228:VAL:HG11	8:z:231:ALA:HB2	2.04	0.40
8:Z:182:TYR:OH	8:Z:185:GLN:O	2.23	0.40
1:a:250:ASN:HB3	1:a:300:LYS:HB2	2.03	0.40
2:b:238:LEU:HD13	2:b:290:ILE:HG13	2.04	0.40
5:G:65:LEU:HD23	5:G:68:ILE:HD12	2.03	0.40
5:G:520:ALA:O	8:Z:116:ARG:NH2	2.44	0.40
8:Z:298:GLN:HE22	8:Z:322:ARG:HG2	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

There are no protein backbone outliers to report in this entry.

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	A	428/471 (91%)	428 (100%)	0	100	100
1	a	433/471 (92%)	433 (100%)	0	100	100
2	B	408/441 (92%)	408 (100%)	0	100	100
2	b	420/441 (95%)	420 (100%)	0	100	100
3	D	409/453 (90%)	409 (100%)	0	100	100
3	d	428/453 (94%)	428 (100%)	0	100	100
4	E	429/483 (89%)	429 (100%)	0	100	100
4	e	445/483 (92%)	445 (100%)	0	100	100
5	G	410/501 (82%)	410 (100%)	0	100	100
5	g	417/501 (83%)	417 (100%)	0	100	100
6	H	422/454 (93%)	422 (100%)	0	100	100
6	h	422/454 (93%)	422 (100%)	0	100	100
7	Q	439/473 (93%)	439 (100%)	0	100	100
7	q	439/473 (93%)	439 (100%)	0	100	100
8	Z	446/463 (96%)	445 (100%)	1 (0%)	87	86
8	z	448/463 (97%)	448 (100%)	0	100	100
All	All	6843/7478 (92%)	6842 (100%)	1 (0%)	100	100

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

Mol	Chain	Res	Type
8	Z	56	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (64) such sidechains are listed below:

Mol	Chain	Res	Type
1	a	90	GLN
1	a	113	ASN

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Mol	Chain	Res	Type
1	a	191	ASN
1	a	294	GLN
1	a	417	ASN
1	A	90	GLN
1	A	190	GLN
1	A	294	GLN
1	A	403	HIS
1	A	465	ASN
1	A	499	ASN
2	b	192	HIS
2	B	84	GLN
2	B	192	HIS
2	B	439	GLN
3	d	85	GLN
3	d	240	GLN
3	d	284	ASN
3	d	289	GLN
3	d	473	HIS
3	d	475	ASN
3	D	85	GLN
3	D	395	HIS
4	e	111	GLN
4	e	132	GLN
4	e	397	GLN
4	e	432	ASN
4	e	509	ASN
4	E	93	GLN
4	E	466	GLN
5	g	85	GLN
5	g	188	GLN
5	g	286	GLN
5	g	465	ASN
5	g	539	ASN
5	G	498	GLN
6	h	172	HIS
6	H	25	GLN
6	H	37	GLN
6	H	90	GLN
6	H	172	HIS
6	H	231	GLN
6	H	238	ASN
6	H	245	ASN

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Mol	Chain	Res	Type
6	H	345	HIS
6	H	363	ASN
6	H	515	ASN
7	q	52	ASN
7	q	66	ASN
7	q	92	GLN
7	q	451	GLN
7	Q	52	ASN
7	Q	66	ASN
7	Q	91	GLN
7	Q	92	GLN
7	Q	311	HIS
7	Q	446	GLN
8	z	69	GLN
8	z	192	HIS
8	z	230	ASN
8	z	356	GLN
8	z	430	ASN
8	Z	192	HIS
8	Z	430	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 oligosaccharides 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.

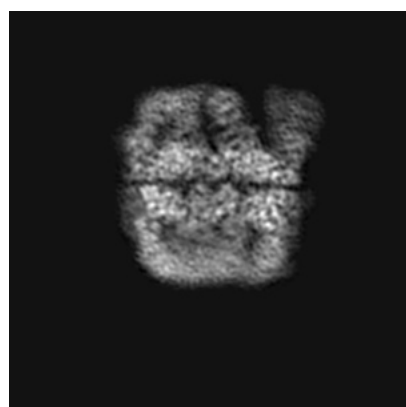
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0760. These allow visual inspection of the internal detail of the map and identification of artifacts.

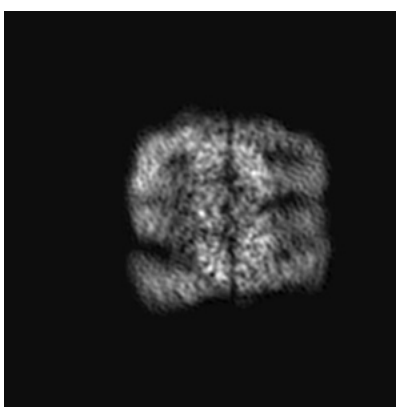
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

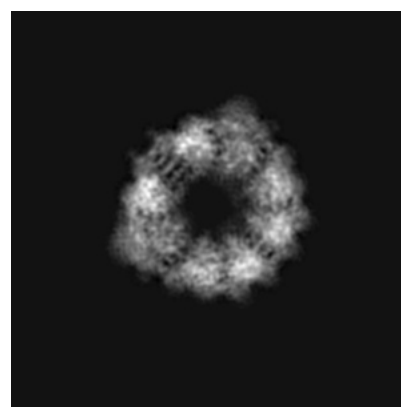
6.1.1 Primary map



X



Y



Z

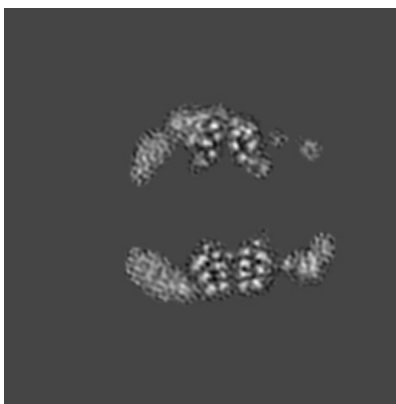
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

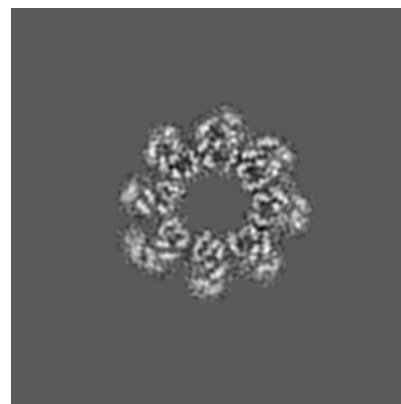
6.2.1 Primary map



X Index: 128



Y Index: 128



Z Index: 128

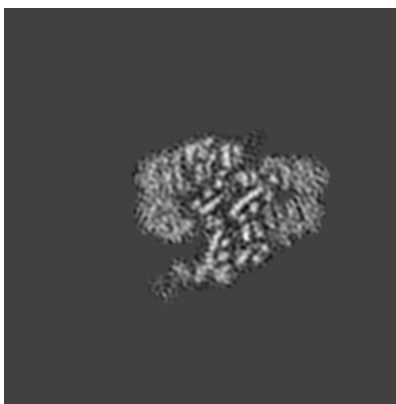
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 168



Y Index: 91

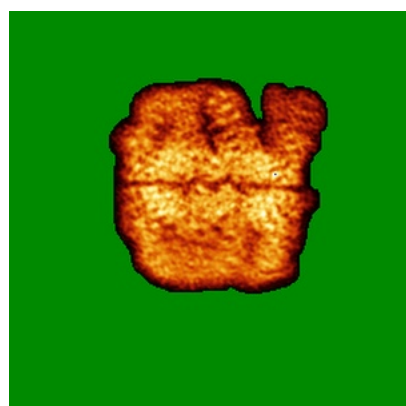


Z Index: 126

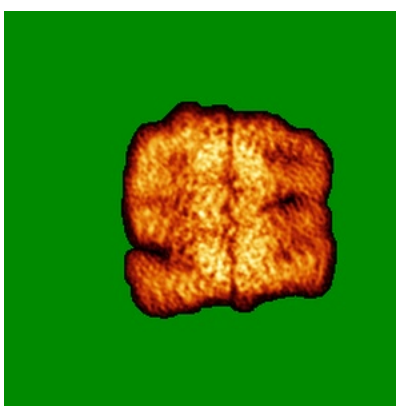
The images above show the largest variance slices of the map in three orthogonal directions.

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

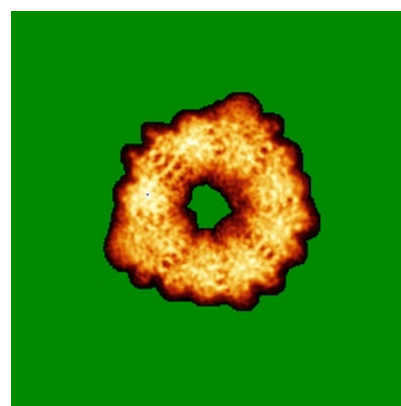
6.4.1 Primary map



X



Y

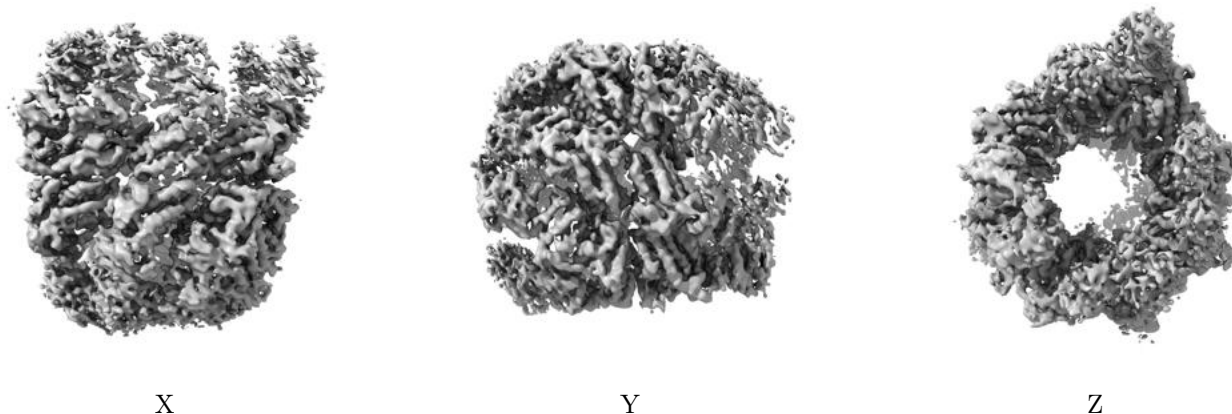


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.85. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

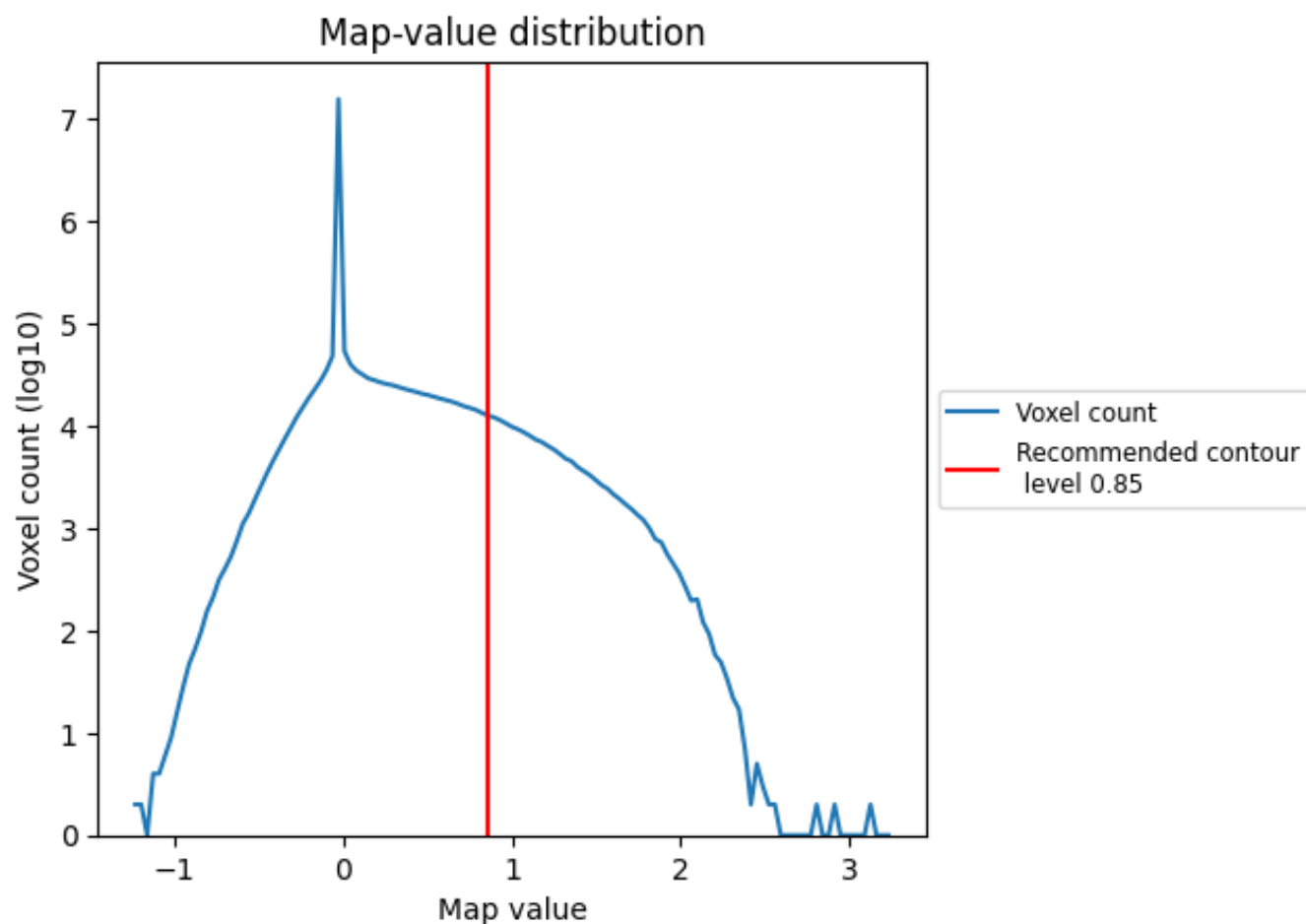
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

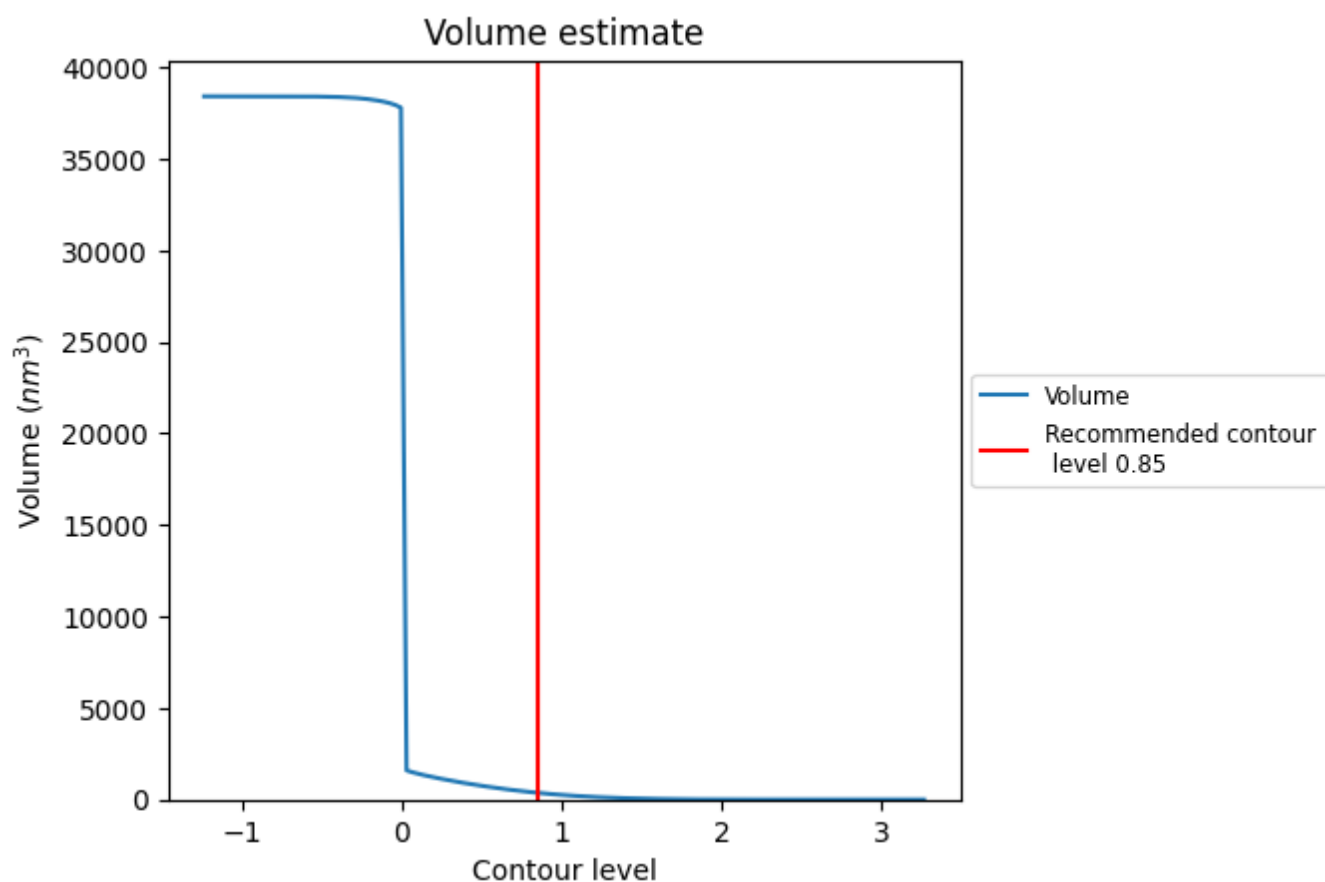
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

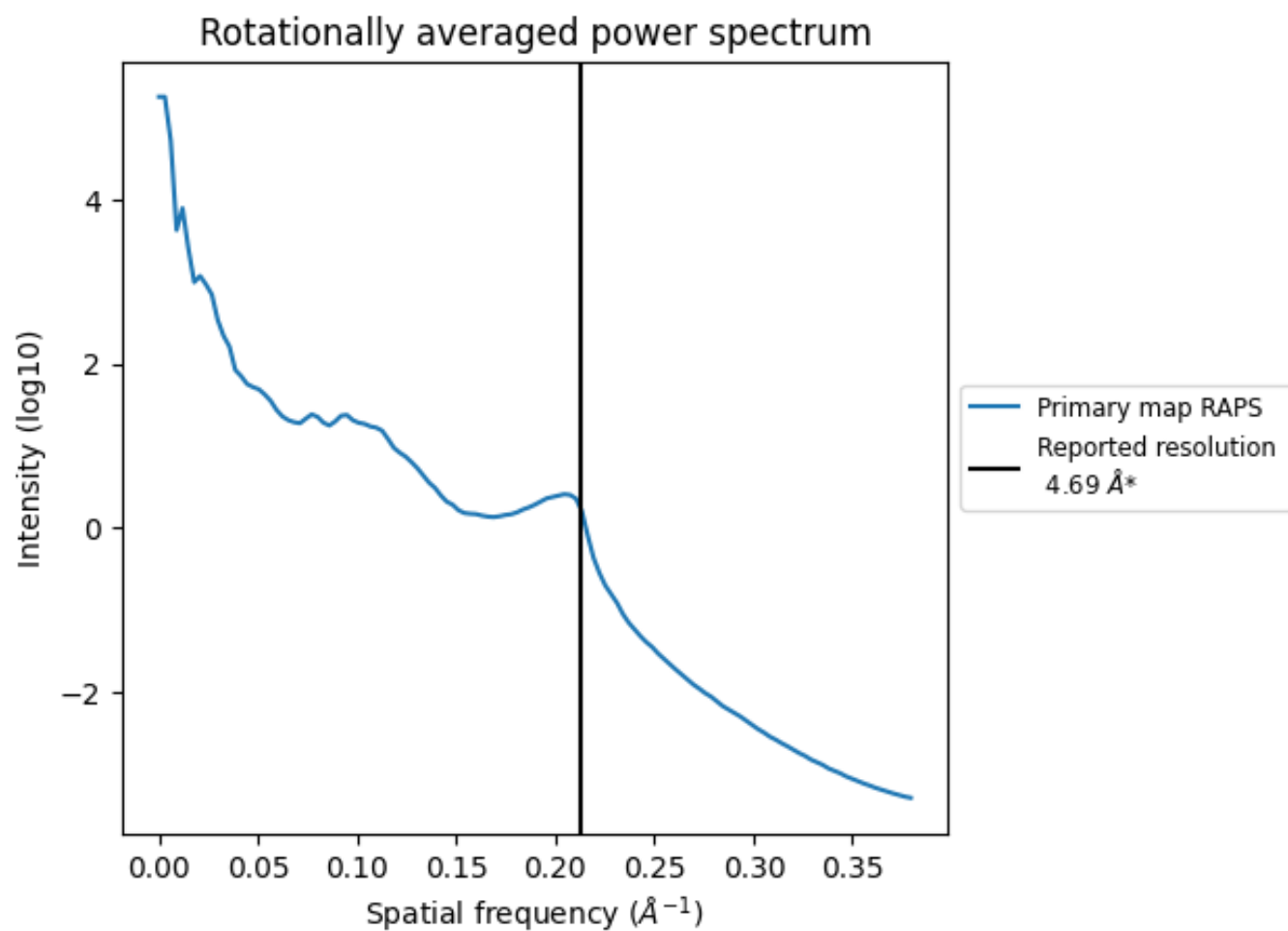
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 369 nm³; this corresponds to an approximate mass of 333 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 0.213 $\text{\AA}^{-1}$

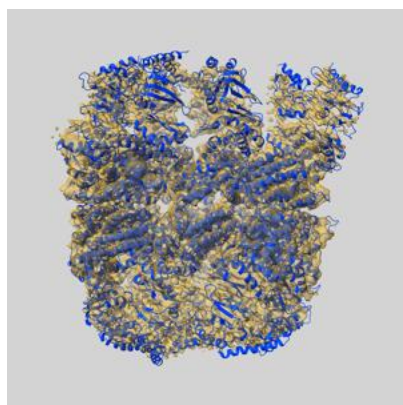
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

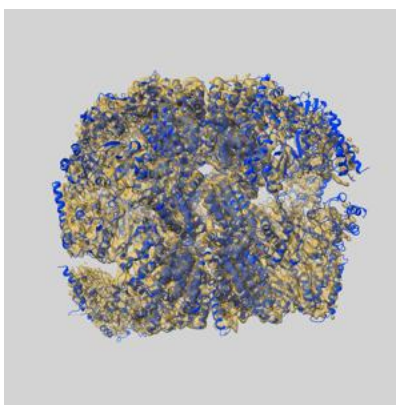
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-0760 and PDB model 6KS8. Per-residue inclusion information can be found in section [3](#) on page [9](#).

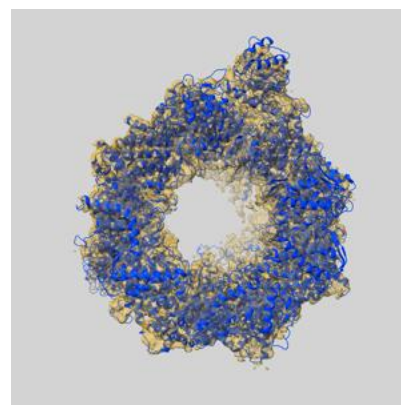
9.1 Map-model overlay [i](#)



X



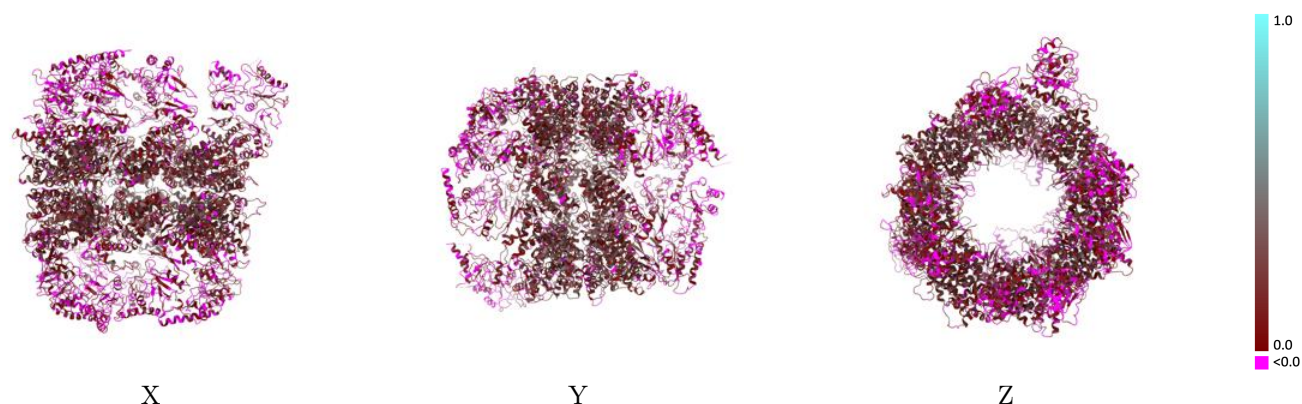
Y



Z

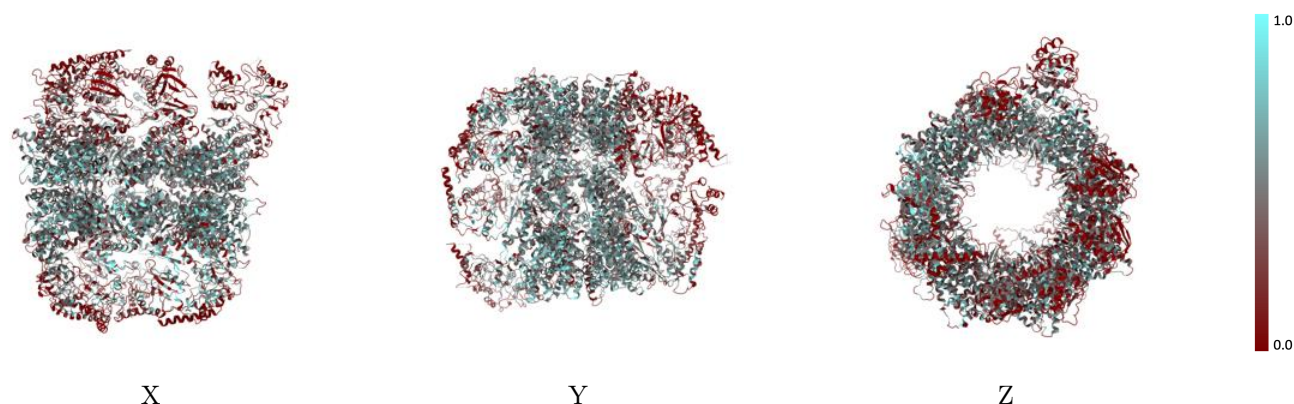
The images above show the 3D surface view of the map at the recommended contour level 0.85 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



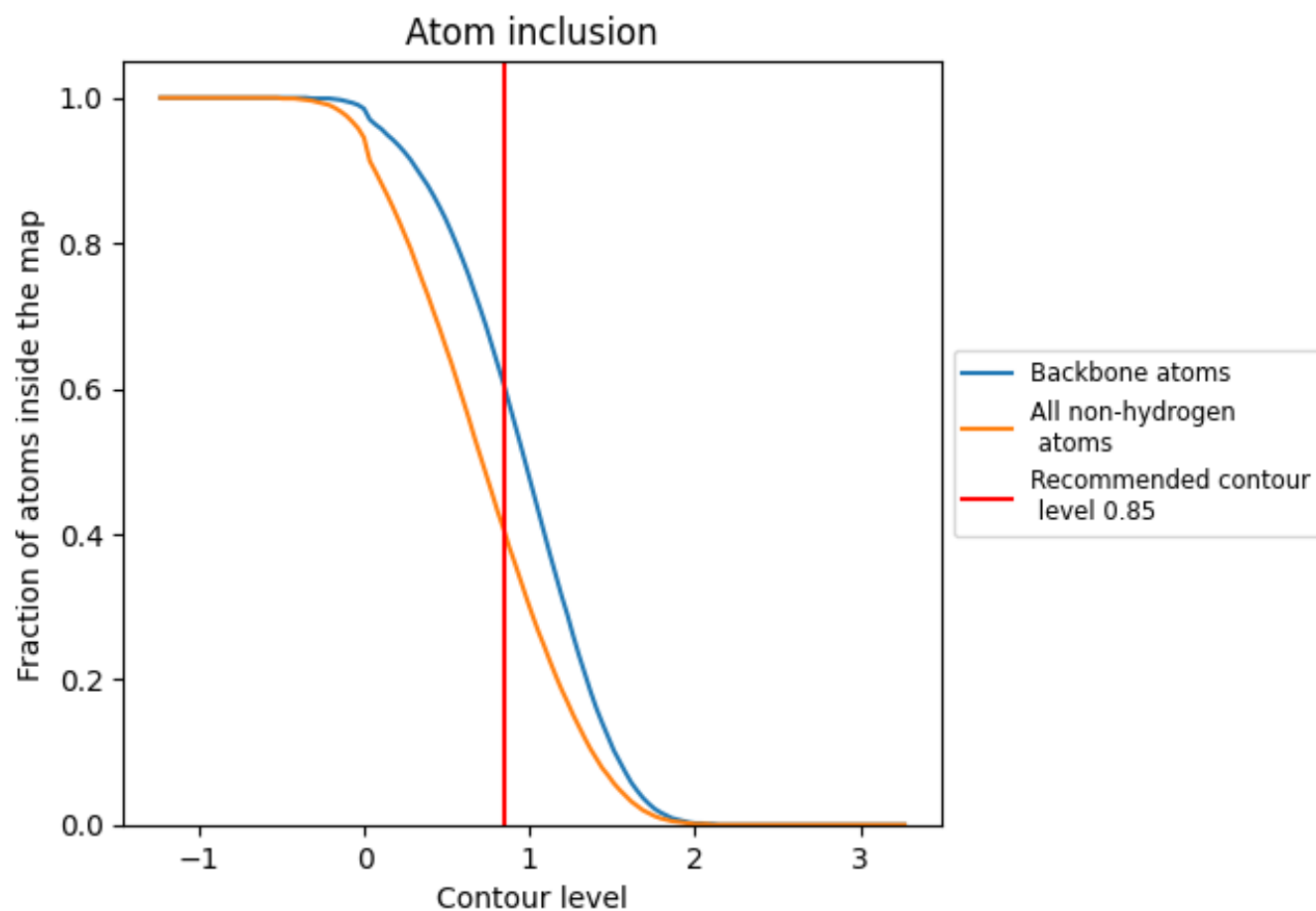
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.85).

9.4 Atom inclusion [i](#)



At the recommended contour level, 60% of all backbone atoms, 40% 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 (0.85) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4010	0.1340
A	0.3540	0.1310
B	0.3390	0.1300
D	0.2860	0.1030
E	0.3710	0.1140
G	0.3900	0.1390
H	0.3660	0.1270
Q	0.4040	0.1360
Z	0.4720	0.1730
a	0.4020	0.1280
b	0.4390	0.1390
d	0.3550	0.1160
e	0.4220	0.1170
g	0.4500	0.1440
h	0.4550	0.1360
q	0.4120	0.1340
z	0.4790	0.1750

1.0

0.0

<0.0