Full wwPDB EM Validation Report ⓘ

Jun 26, 2025 – 06:11 PM JST

PDB ID	:	7WZ3 / pdb_00007wz3
EMDB ID	:	EMD-32903
Title	:	Cryo-EM structure of human TRiC-tubulin-S1 state
Authors	:	Cong, Y.; Liu, C.X.
Deposited on	:	2022-02-16
Resolution	:	4.10 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:

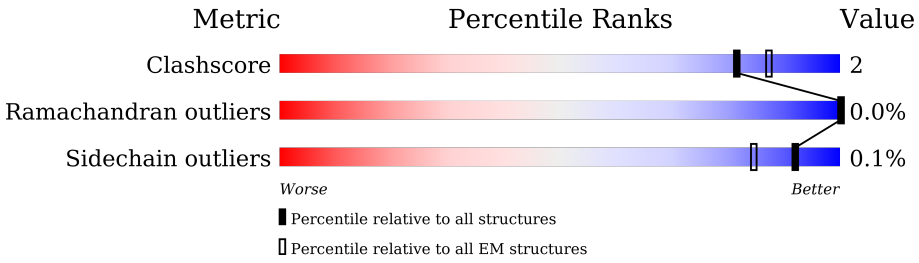
EMDB validation analysis	:	0.0.1.dev118
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0rc1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.44

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.10 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 <=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	556	34% 78% 8% 14%
1	a	556	23% 87% 6% • 6%
2	B	535	17% 58% • 39%
2	b	535	27% 84% 5% 11%
3	D	539	32% 76% 5% 19%
3	d	539	20% 91% 5% •
4	E	539	33% 88% 7% 5%
4	e	539	18% 88% 7% 5%

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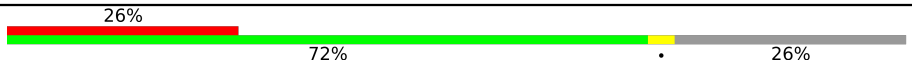
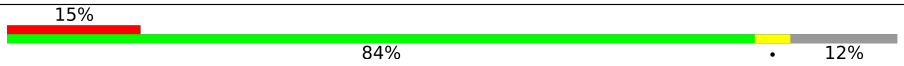
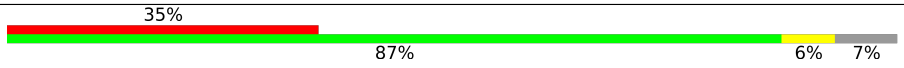
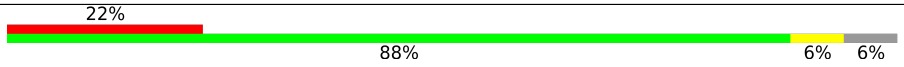
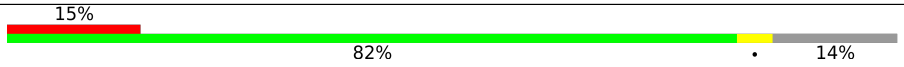
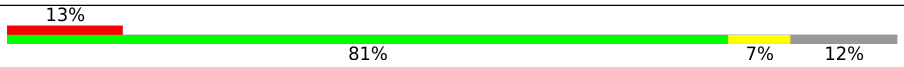
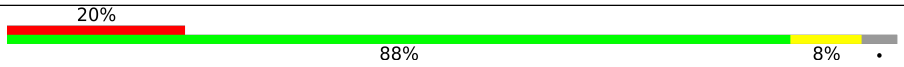
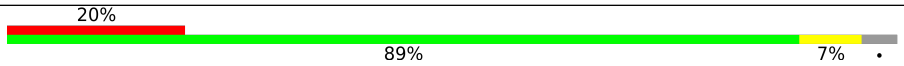
Mol	Chain	Length	Quality of chain
5	G	545	
5	g	545	
6	H	543	
6	h	543	
7	Q	548	
7	q	548	
8	Z	531	
8	z	531	

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 58551 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	520	Total	C	N	O	S	0	0
			3949	2475	690	761	23		
1	A	476	Total	C	N	O	S	0	0
			3590	2250	626	692	22		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	b	477	Total	C	N	O	S	0	0
			3580	2243	629	690	18		
2	B	327	Total	C	N	O	S	0	0
			2426	1503	432	479	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	435	Total	C	N	O	S	0	0
			3259	2044	563	633	19		
3	d	516	Total	C	N	O	S	0	0
			3902	2440	678	761	23		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	512	Total	C	N	O	S	0	0
			3936	2463	687	756	30		
4	e	510	Total	C	N	O	S	0	0
			3921	2454	684	753	30		

- Molecule 5 is a protein called T-complex protein 1 subunit gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	g	481	Total	C	N	O	S	0	0
			3724	2326	659	709	30		
5	G	406	Total	C	N	O	S	0	0
			3165	1986	557	599	23		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	h	511	Total	C	N	O	S	0	0
			3927	2478	681	745	23		
6	H	507	Total	C	N	O	S	0	0
			3898	2463	676	736	23		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
h	290	SER	LEU	engineered mutation	UNP Q99832
H	290	SER	LEU	engineered mutation	UNP Q99832

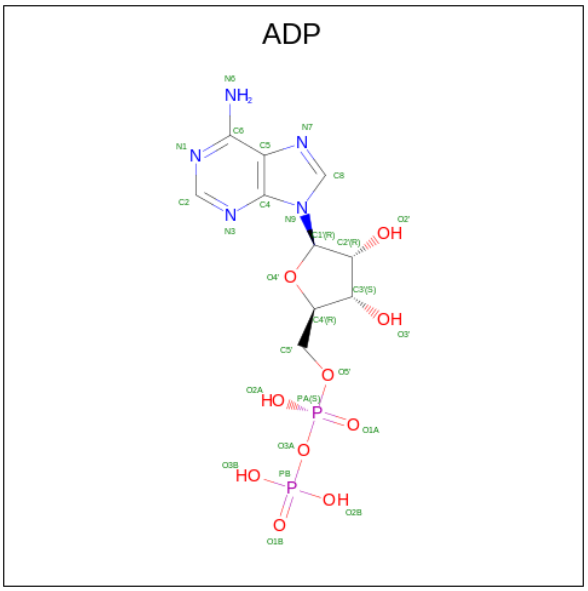
- Molecule 7 is a protein called T-complex protein 1 subunit theta.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	Q	472	Total	C	N	O	S	0	0
			3602	2271	616	692	23		
7	q	483	Total	C	N	O	S	0	0
			3688	2324	629	711	24		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Z	509	Total	C	N	O	S	0	0
			3907	2456	682	749	20		
8	z	510	Total	C	N	O	S	0	0
			3915	2461	683	750	21		

- Molecule 9 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).

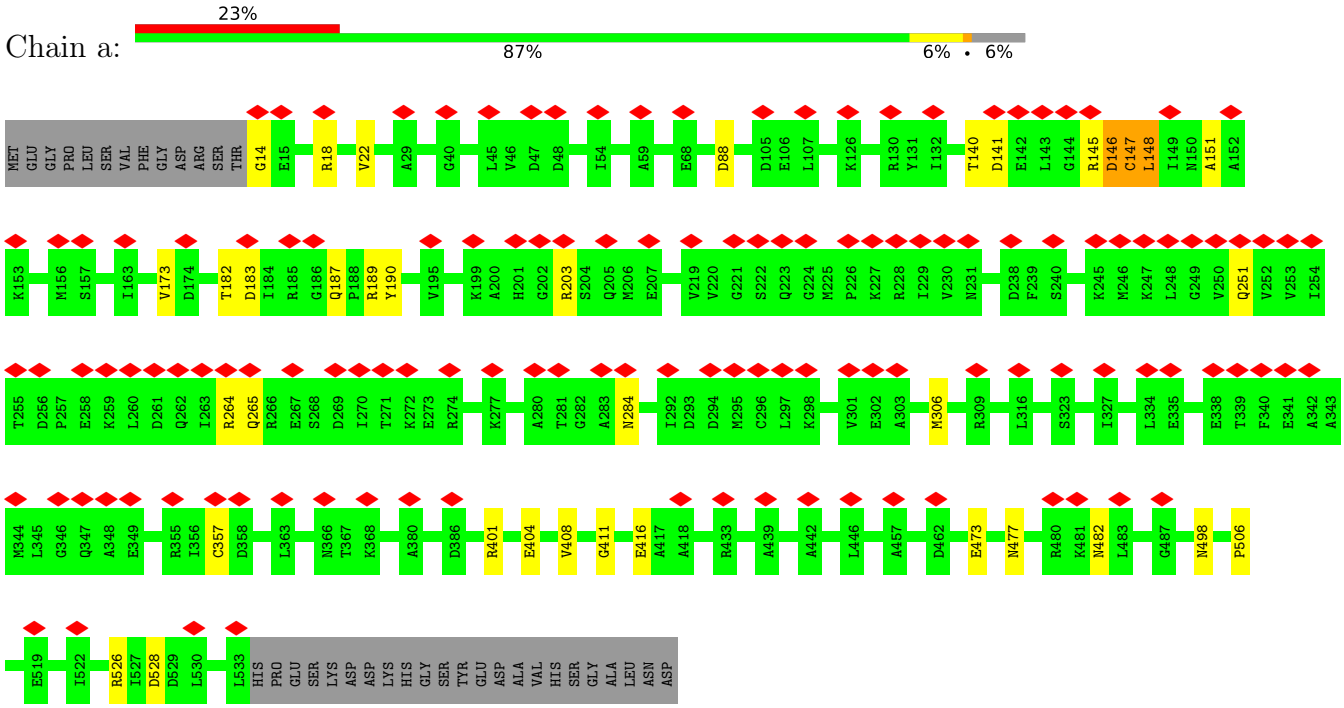


Mol	Chain	Residues	Atoms					AltConf
9	g	1	Total	C	N	O	P	0
			27	10	5	10	2	
9	G	1	Total	C	N	O	P	0
			27	10	5	10	2	
9	Q	1	Total	C	N	O	P	0
			27	10	5	10	2	
9	q	1	Total	C	N	O	P	0
			27	10	5	10	2	
9	Z	1	Total	C	N	O	P	0
			27	10	5	10	2	
9	z	1	Total	C	N	O	P	0
			27	10	5	10	2	

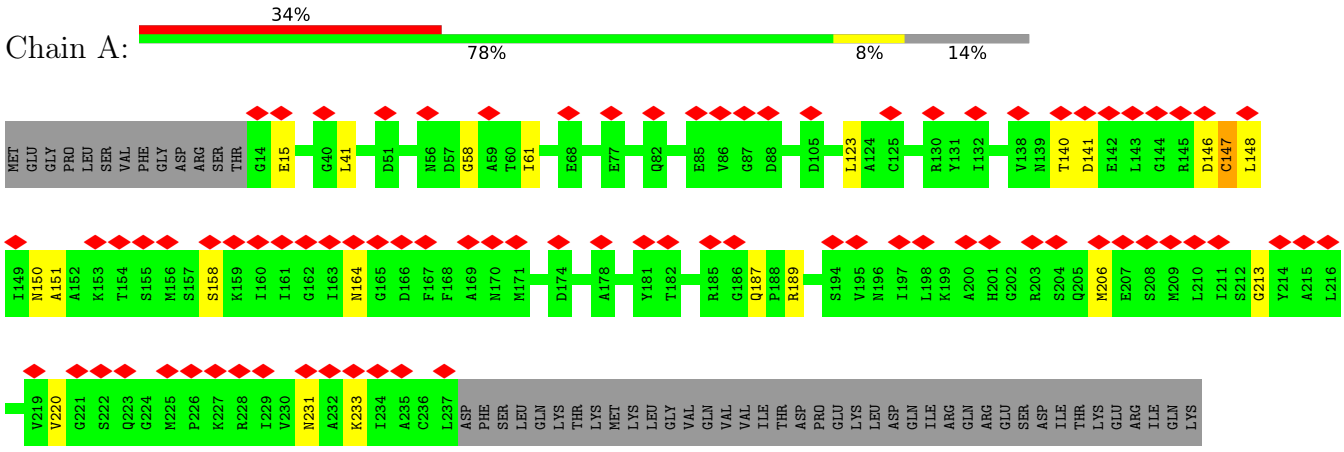
3 Residue-property plots (i)

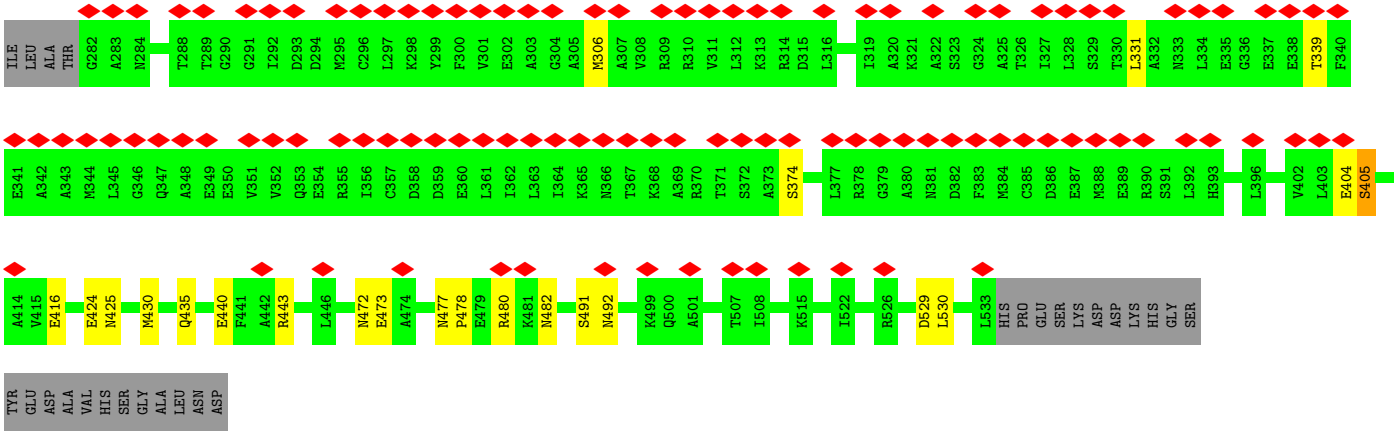
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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



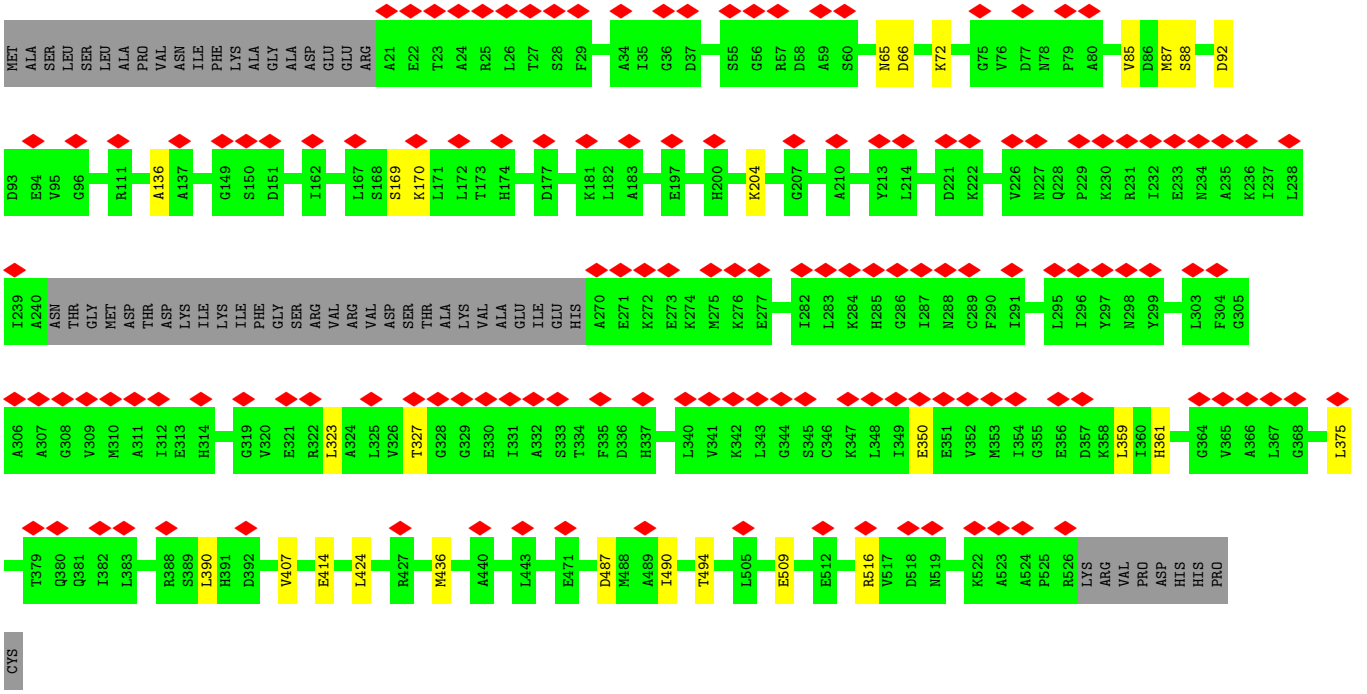
• Molecule 1: T-complex protein 1 subunit alpha





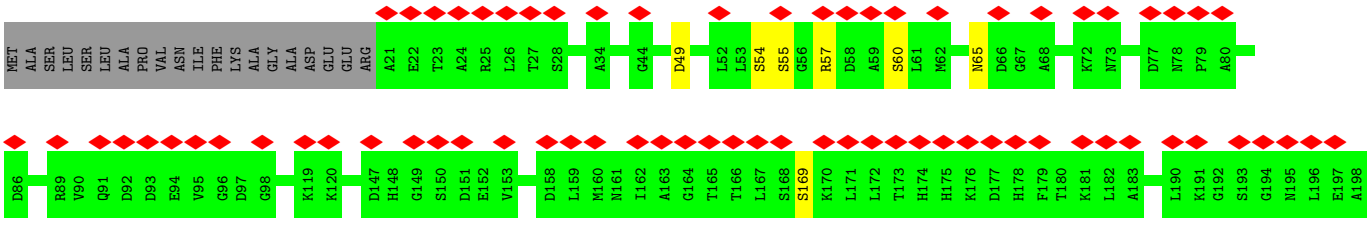
• Molecule 2: T-complex protein 1 subunit beta

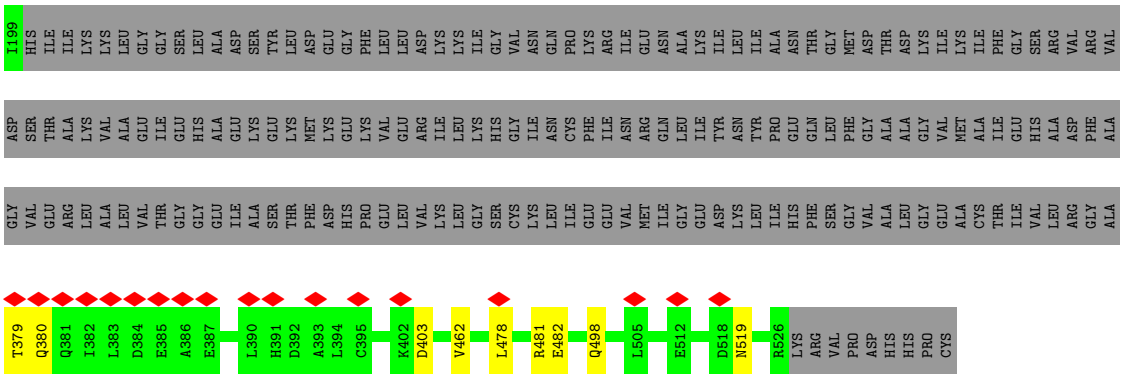
Chain b:



• Molecule 2: T-complex protein 1 subunit beta

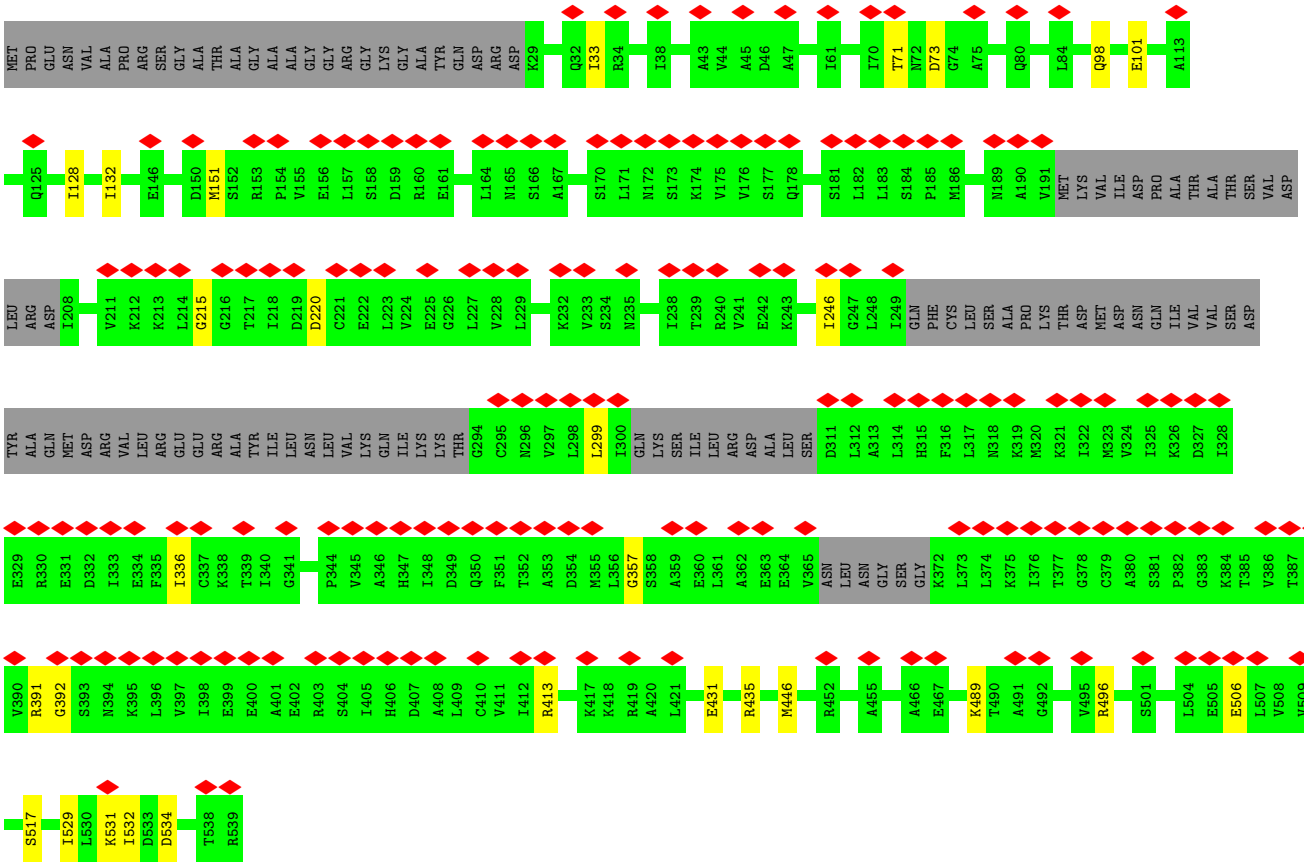
Chain B:





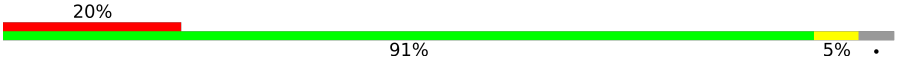
• Molecule 3: T-complex protein 1 subunit delta

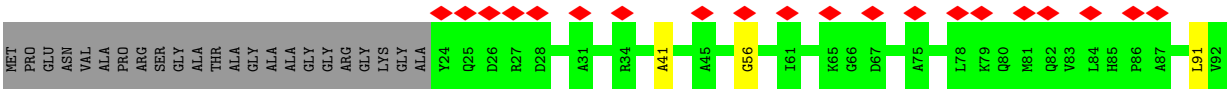
Chain D:

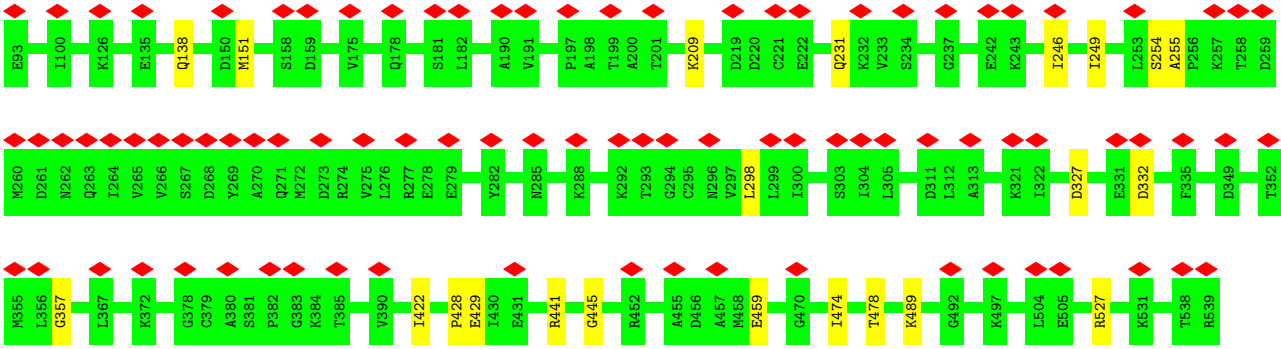


• Molecule 3: T-complex protein 1 subunit delta

Chain d:

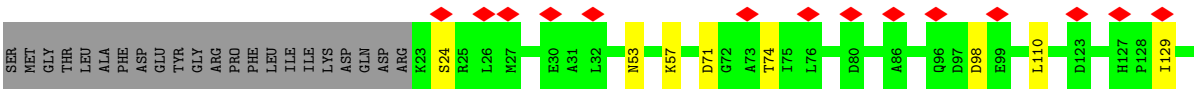






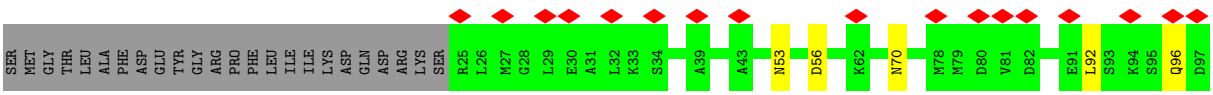
• Molecule 4: T-complex protein 1 subunit epsilon

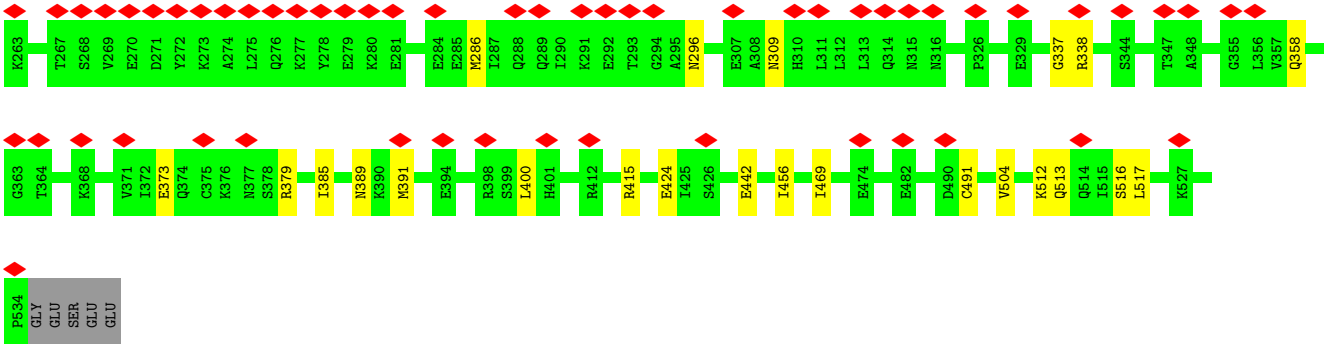
Chain E:



• Molecule 4: T-complex protein 1 subunit epsilon

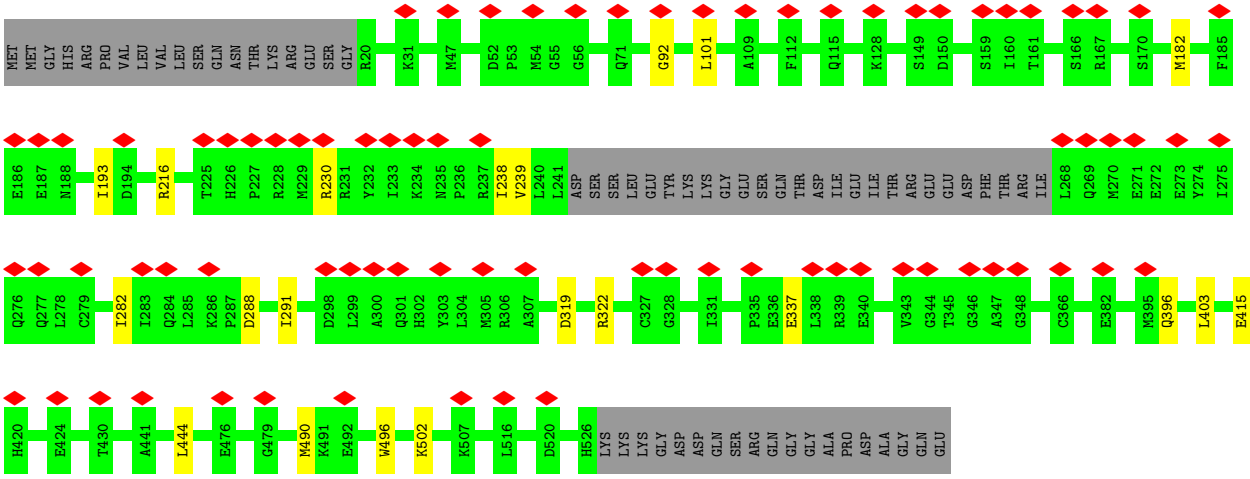
Chain e:





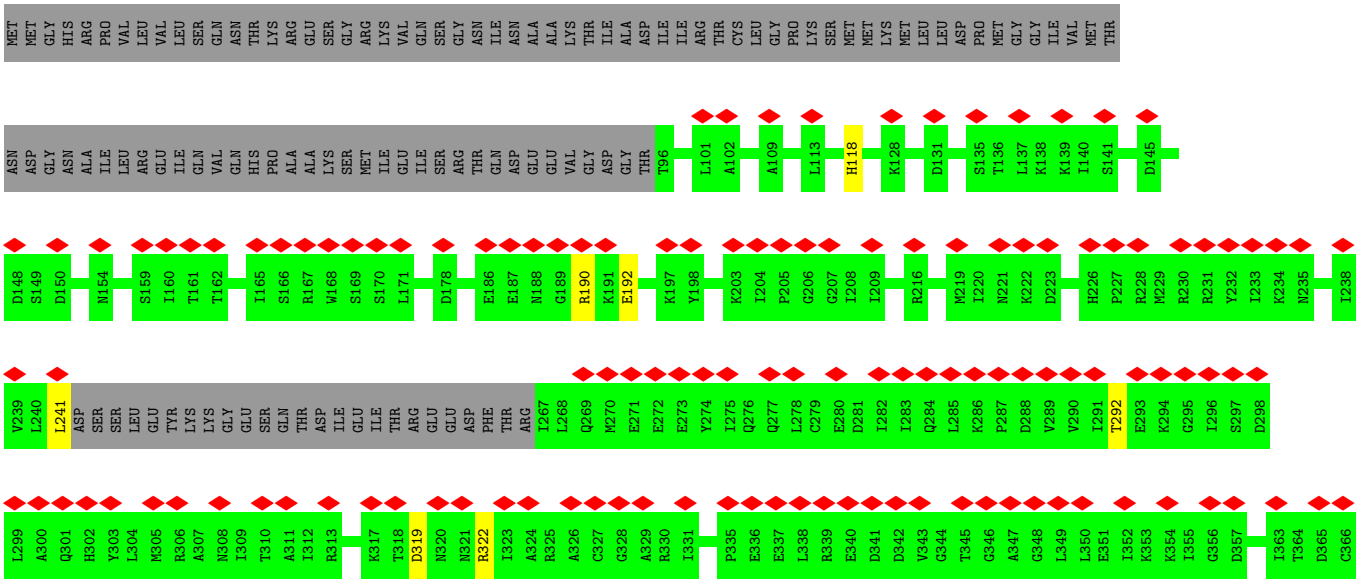
• Molecule 5: T-complex protein 1 subunit gamma

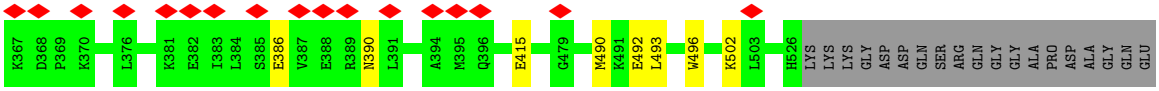
Chain g:



• Molecule 5: T-complex protein 1 subunit gamma

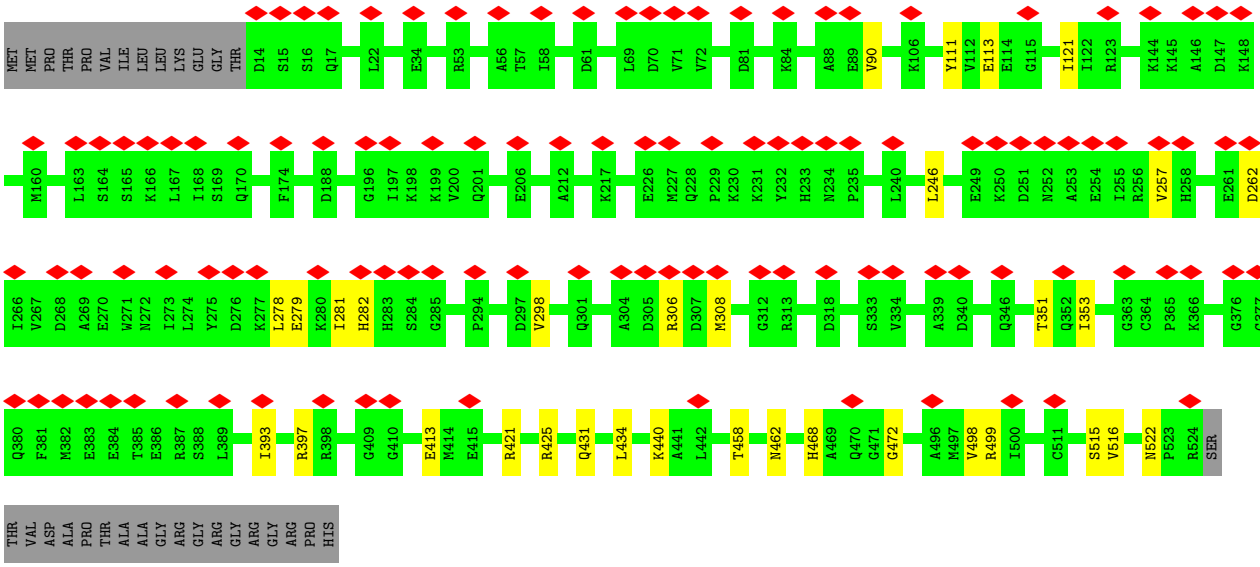
Chain G:





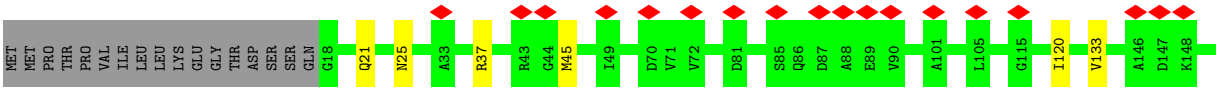
• Molecule 6: T-complex protein 1 subunit eta

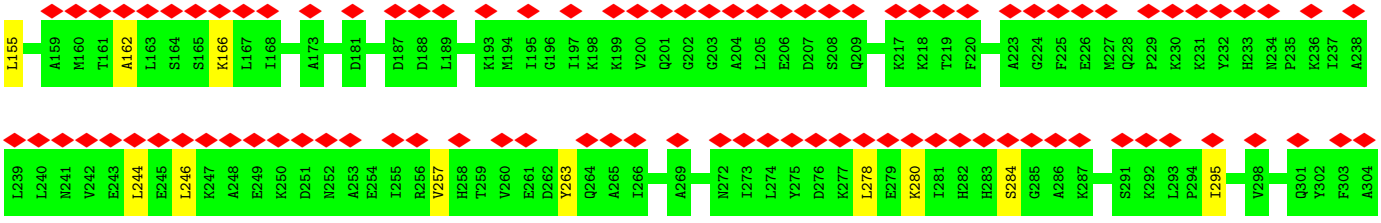
Chain h:



• Molecule 6: T-complex protein 1 subunit eta

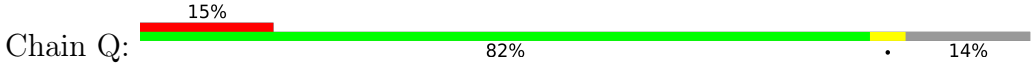
Chain H:

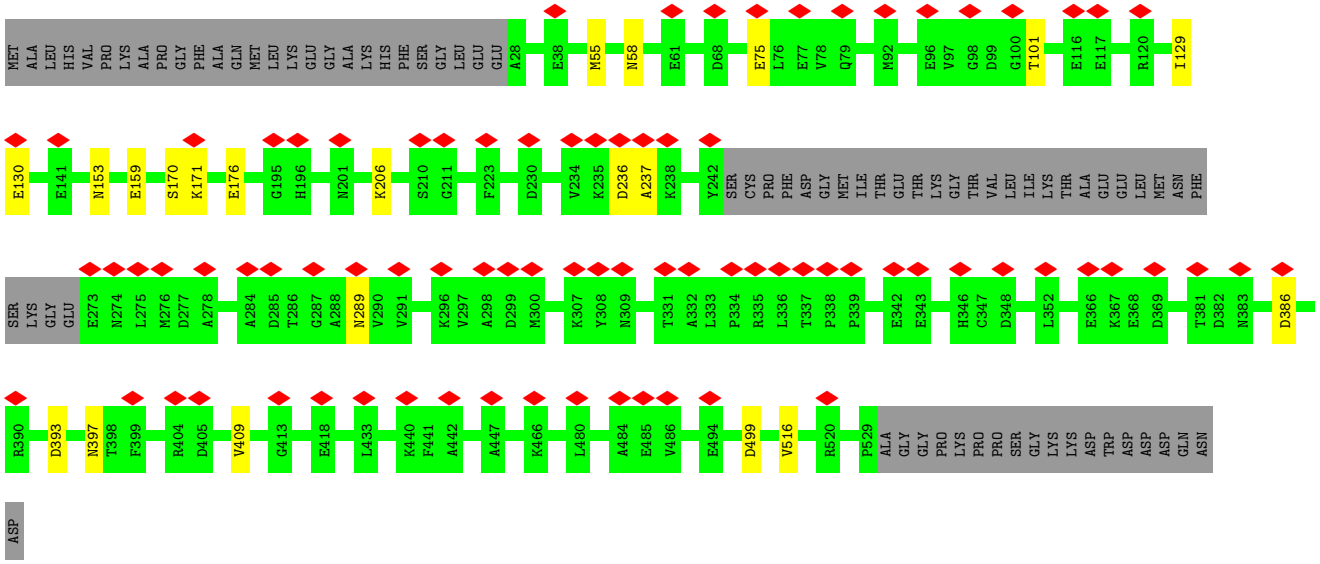




• Molecule 7: T-complex protein 1 subunit theta

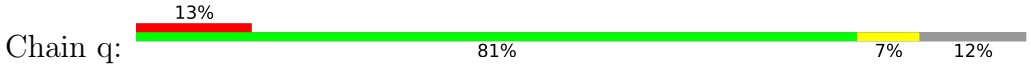
Chain Q:

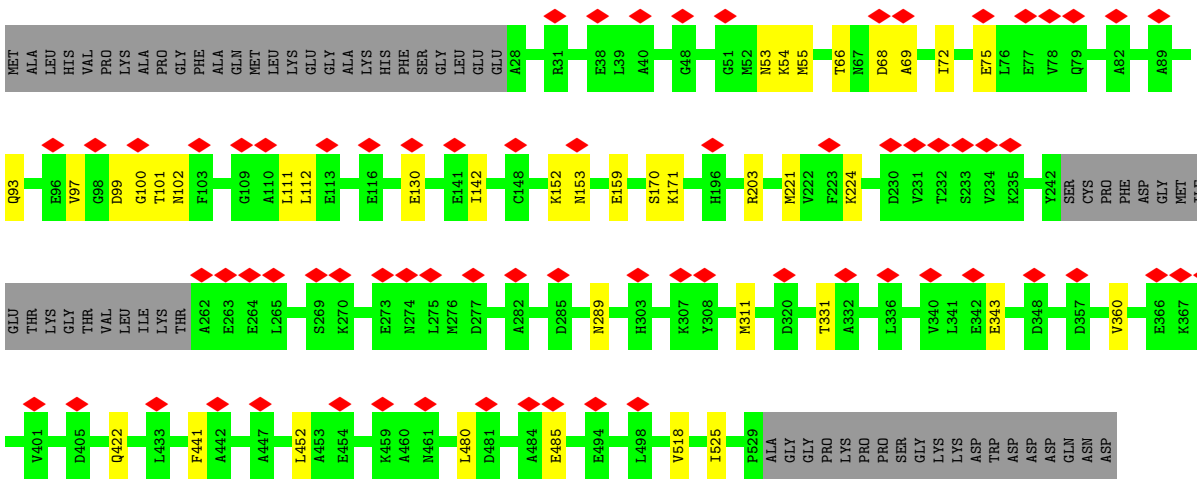




• Molecule 7: T-complex protein 1 subunit theta

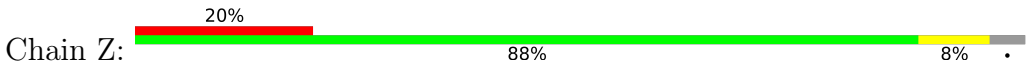
Chain q:

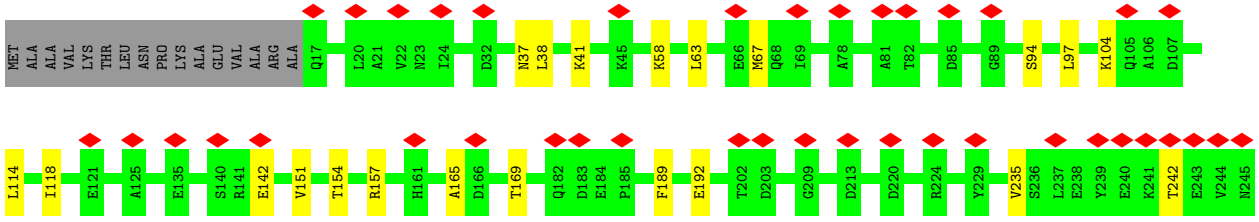


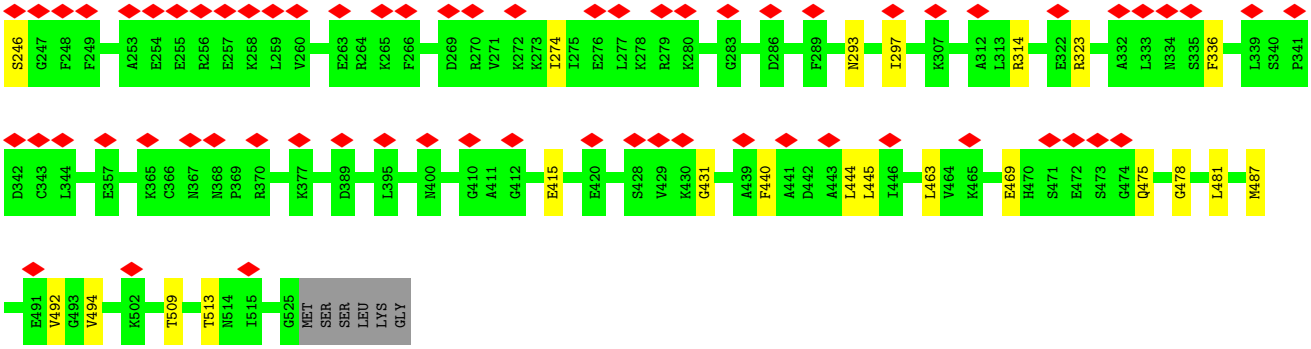


• Molecule 8: T-complex protein 1 subunit zeta

Chain Z:

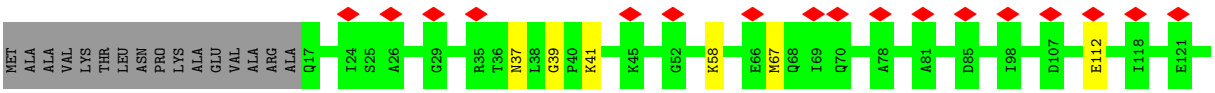


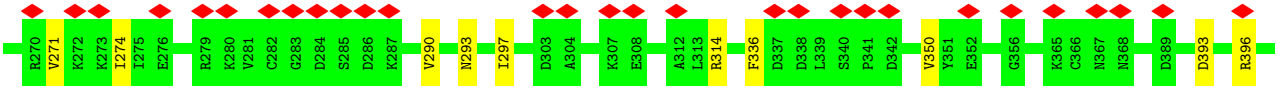


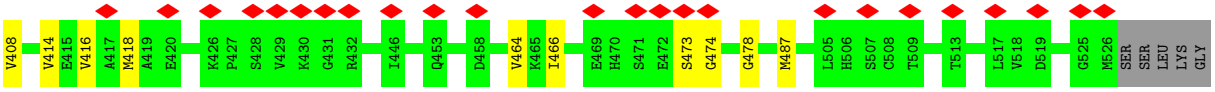


• Molecule 8: T-complex protein 1 subunit zeta

Chain z:







4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	115666	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	38	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	3.520	Depositor
Minimum map value	-2.264	Depositor
Average map value	0.019	Depositor
Map value standard deviation	0.164	Depositor
Recommended contour level	0.7	Depositor
Map size (Å)	337.408, 337.408, 337.408	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.318, 1.318, 1.318	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.16	0/3623	0.36	0/4893
1	a	0.16	0/3985	0.34	0/5379
2	B	0.14	0/2447	0.30	0/3306
2	b	0.14	0/3618	0.30	0/4878
3	D	0.15	0/3281	0.34	0/4423
3	d	0.14	0/3934	0.32	0/5310
4	E	0.15	0/3982	0.31	0/5365
4	e	0.15	0/3967	0.32	0/5346
5	G	0.16	0/3203	0.32	0/4327
5	g	0.16	0/3766	0.33	0/5083
6	H	0.14	0/3953	0.31	0/5334
6	h	0.14	0/3982	0.32	0/5373
7	Q	0.14	0/3650	0.31	0/4937
7	q	0.13	0/3737	0.31	0/5052
8	Z	0.14	0/3953	0.31	0/5329
8	z	0.14	0/3961	0.32	0/5339
All	All	0.15	0/59042	0.32	0/79674

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	a	0	2
All	All	0	4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	146	ASP	Peptide
1	A	187	GLN	Peptide
1	a	146	ASP	Peptide
1	a	187	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	A	3590	0	3728	37	0
1	a	3949	0	4117	33	0
2	B	2426	0	2491	9	0
2	b	3580	0	3690	17	0
3	D	3259	0	3450	15	0
3	d	3902	0	4107	15	0
4	E	3936	0	4058	23	0
4	e	3921	0	4040	23	0
5	G	3165	0	3280	8	0
5	g	3724	0	3858	11	0
6	H	3898	0	3994	19	0
6	h	3927	0	4016	23	0
7	Q	3602	0	3670	13	0
7	q	3688	0	3749	25	0
8	Z	3907	0	4031	26	0
8	z	3915	0	4039	21	0
9	G	27	0	12	0	0
9	Q	27	0	11	1	0
9	Z	27	0	12	3	0
9	g	27	0	12	0	0
9	q	27	0	12	4	0
9	z	27	0	10	0	0
All	All	58551	0	60387	290	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 2.

All (290) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:189:ARG:HA	1:a:404:GLU:HG3	1.26	1.15
1:A:147:CYS:SG	1:A:150:ASN:ND2	2.26	1.07
1:A:189:ARG:HA	1:A:404:GLU:HG3	1.43	1.00
1:A:189:ARG:HB3	1:A:404:GLU:CD	1.86	1.00
1:A:189:ARG:HB3	1:A:404:GLU:CG	1.96	0.96
1:a:189:ARG:HE	1:a:404:GLU:HG2	1.30	0.94
1:a:189:ARG:NE	1:a:404:GLU:HG2	1.85	0.90
1:A:189:ARG:HE	1:A:404:GLU:HG2	1.43	0.83
1:a:148:LEU:HD12	1:a:173:VAL:HG13	1.59	0.83
1:A:189:ARG:CA	1:A:404:GLU:HG3	2.08	0.82
1:a:189:ARG:CD	1:a:404:GLU:HG2	2.13	0.78
1:a:190:TYR:N	1:a:404:GLU:OE2	2.12	0.78
7:q:170:SER:OG	9:q:601:ADP:O2A	2.02	0.75
1:a:189:ARG:HE	1:a:404:GLU:CG	1.99	0.73
1:a:189:ARG:HD2	1:a:404:GLU:HG2	1.72	0.71
1:a:477:ASN:O	1:a:482:ASN:ND2	2.24	0.70
6:H:37:ARG:NH1	6:H:448:GLN:OE1	2.25	0.70
4:e:147:ASP:OD1	4:e:415:ARG:NH1	2.25	0.70
1:A:213:GLY:O	1:A:374:SER:OG	2.09	0.70
6:H:413:GLU:OE2	6:H:499:ARG:NH1	2.25	0.70
3:d:138:GLN:OE1	3:d:527:ARG:NH1	2.25	0.69
5:G:415:GLU:OE2	5:G:502:LYS:NZ	2.24	0.69
1:a:189:ARG:CA	1:a:404:GLU:HG3	2.14	0.69
1:a:203:ARG:NH1	1:a:357:CYS:SG	2.65	0.69
1:A:189:ARG:NE	1:A:404:GLU:HG2	2.07	0.69
1:a:147:CYS:O	1:a:151:ALA:HB2	1.93	0.68
3:D:220:ASP:OD2	3:D:391:ARG:NH1	2.26	0.68
7:Q:206:LYS:NZ	7:Q:386:ASP:OD1	2.26	0.68
1:A:231:ASN:ND2	1:A:233:LYS:O	2.26	0.68
1:a:189:ARG:HA	1:a:404:GLU:CG	2.15	0.68
6:H:162:ALA:O	6:H:166:LYS:NZ	2.27	0.67
3:D:496:ARG:NH2	3:D:506:GLU:OE1	2.27	0.67
5:g:415:GLU:OE2	5:g:502:LYS:NZ	2.27	0.67
3:d:246:ILE:O	3:d:357:GLY:N	2.27	0.67
4:E:161:GLU:OE2	4:E:165:GLN:NE2	2.27	0.67
3:D:151:MET:O	3:D:489:LYS:NZ	2.26	0.67
7:Q:393:ASP:O	7:Q:397:ASN:ND2	2.27	0.67
3:d:151:MET:O	3:d:489:LYS:NZ	2.28	0.67
8:Z:37:ASN:ND2	8:Z:58:LYS:O	2.29	0.66
8:z:37:ASN:ND2	8:z:58:LYS:O	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:145:ARG:NH1	1:a:146:ASP:O	2.29	0.65
8:z:414:VAL:HG12	8:z:418:MET:HE2	1.78	0.65
1:A:147:CYS:O	1:A:150:ASN:N	2.29	0.65
8:z:297:ILE:O	8:z:314:ARG:NH1	2.30	0.65
4:e:358:GLN:NE2	4:e:373:GLU:OE2	2.29	0.65
5:g:92:GLY:N	5:g:396:GLN:OE1	2.29	0.65
4:E:98:ASP:O	4:E:408:ARG:NH1	2.30	0.65
1:A:473:GLU:O	1:A:482:ASN:ND2	2.31	0.64
4:e:243:ASP:OD2	4:e:296:ASN:ND2	2.30	0.64
1:A:440:GLU:OE2	6:h:440:LYS:NZ	2.30	0.64
1:a:14:GLY:N	1:a:528:ASP:OD2	2.31	0.63
7:q:130:GLU:OE2	8:z:41:LYS:NZ	2.32	0.63
7:Q:236:ASP:OD2	7:Q:289:ASN:N	2.32	0.63
8:z:39:GLY:O	8:z:58:LYS:NZ	2.28	0.63
2:B:481:ARG:NH1	2:B:482:GLU:OE2	2.32	0.63
2:b:407:VAL:O	2:b:494:THR:OG1	2.13	0.63
4:E:136:GLU:OE2	4:E:140:ARG:NH2	2.31	0.63
6:H:458:THR:O	6:H:462:ASN:ND2	2.32	0.63
5:g:230:ARG:NH1	5:g:288:ASP:OD1	2.32	0.63
3:d:459:GLU:OE2	4:E:447:ARG:NH1	2.32	0.62
5:g:238:ILE:HG23	5:g:291:ILE:HD12	1.80	0.62
4:e:130:ARG:NH1	4:e:442:GLU:OE2	2.33	0.62
5:G:386:GLU:O	5:G:390:ASN:ND2	2.32	0.62
6:H:133:VAL:HG22	6:H:500:ILE:HG23	1.81	0.62
1:A:424:GLU:OE2	6:h:421:ARG:NE	2.33	0.61
1:A:189:ARG:HB3	1:A:404:GLU:HG3	1.81	0.61
1:A:189:ARG:CB	1:A:404:GLU:CG	2.75	0.61
7:q:102:ASN:ND2	9:q:601:ADP:O3B	2.33	0.61
1:A:478:PRO:O	1:A:480:ARG:NH2	2.32	0.61
3:D:101:GLU:O	3:D:413:ARG:NH1	2.32	0.61
1:A:472:ASN:ND2	6:h:425:ARG:O	2.34	0.61
2:b:66:ASP:OD1	2:b:170:LYS:NZ	2.34	0.61
8:Z:165:ALA:O	8:Z:169:THR:OG1	2.08	0.61
1:A:443:ARG:NH2	6:h:111:TYR:OH	2.34	0.60
8:Z:469:GLU:OE2	8:Z:475:GLN:NE2	2.35	0.60
2:b:136:ALA:HB2	2:b:424:LEU:HD22	1.84	0.60
7:Q:130:GLU:OE2	8:Z:41:LYS:NZ	2.28	0.60
1:A:189:ARG:CB	1:A:404:GLU:HG3	2.32	0.59
1:a:526:ARG:NH2	3:d:56:GLY:O	2.36	0.58
2:b:424:LEU:HD23	2:b:436:MET:SD	2.43	0.58
1:A:491:SER:OG	1:A:492:ASN:ND2	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:53:ASN:ND2	4:E:491:CYS:O	2.36	0.58
4:E:336:GLY:O	4:E:338:ARG:NH1	2.36	0.58
1:A:220:VAL:HG12	1:A:306:MET:HE3	1.84	0.58
3:d:231:GLN:NE2	3:d:327:ASP:O	2.37	0.58
8:Z:63:LEU:O	8:Z:67:MET:HE3	2.04	0.58
4:e:512:LYS:O	4:e:516:SER:OG	2.11	0.58
8:Z:192:GLU:OE1	8:Z:323:ARG:NE	2.36	0.57
8:z:393:ASP:OD1	8:z:396:ARG:NH2	2.37	0.57
3:d:441:ARG:NH2	4:E:432:SER:OG	2.38	0.57
8:Z:157:ARG:NE	9:Z:601:ADP:N7	2.49	0.57
2:b:323:LEU:O	2:b:327:THR:OG1	2.21	0.57
3:D:246:ILE:O	3:D:357:GLY:N	2.37	0.57
4:e:233:SER:O	4:e:309:ASN:ND2	2.37	0.57
8:Z:274:ILE:HD11	8:Z:336:PHE:CZ	2.39	0.57
4:E:340:VAL:HG11	4:E:346:LEU:HD23	1.87	0.57
1:A:58:GLY:HA2	1:A:61:ILE:HD12	1.87	0.56
4:e:169:THR:HG21	4:e:504:VAL:HA	1.87	0.56
5:G:190:ARG:NH2	5:G:192:GLU:OE1	2.38	0.56
6:h:468:HIS:ND1	6:h:472:GLY:O	2.38	0.56
8:Z:445:LEU:HD22	8:Z:463:LEU:HD11	1.87	0.56
3:D:215:GLY:N	3:D:392:GLY:O	2.39	0.56
4:E:246:ILE:HG12	4:E:297:LEU:HD23	1.87	0.56
2:B:462:VAL:HG22	2:B:478:LEU:HD11	1.88	0.56
6:H:257:VAL:O	6:H:263:TYR:OH	2.13	0.56
7:Q:170:SER:OG	7:Q:171:LYS:NZ	2.39	0.55
2:B:65:ASN:ND2	2:B:169:SER:O	2.38	0.55
1:A:141:ASP:O	1:A:148:LEU:HD12	2.07	0.55
3:d:422:ILE:HD12	3:d:428:PRO:HG2	1.89	0.55
1:A:147:CYS:O	1:A:151:ALA:N	2.33	0.55
3:d:41:ALA:HB1	3:d:91:LEU:HD11	1.87	0.55
5:g:490:MET:O	5:g:496:TRP:NE1	2.40	0.55
1:a:189:ARG:HB3	1:a:404:GLU:CD	2.32	0.55
1:a:189:ARG:HB3	1:a:404:GLU:OE2	2.07	0.54
4:e:53:ASN:ND2	4:e:491:CYS:O	2.40	0.54
6:h:279:GLU:OE2	6:h:306:ARG:NH2	2.41	0.54
6:h:516:VAL:HG11	7:q:55:MET:HE3	1.89	0.54
7:Q:153:ASN:N	7:Q:159:GLU:OE2	2.41	0.54
2:B:403:ASP:OD2	2:B:498:GLN:NE2	2.40	0.54
4:e:96:GLN:HG2	4:e:100:ILE:HD12	1.90	0.54
8:Z:297:ILE:O	8:Z:314:ARG:NH1	2.41	0.53
3:d:445:GLY:O	4:E:473:THR:OG1	2.19	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:h:246:LEU:HD22	6:h:298:VAL:HG21	1.91	0.53
8:Z:492:VAL:HG23	8:Z:494:VAL:HG23	1.90	0.53
2:b:516:ARG:O	4:e:56:ASP:N	2.41	0.53
7:q:101:THR:N	9:q:601:ADP:O1B	2.41	0.53
1:a:473:GLU:O	1:a:482:ASN:ND2	2.42	0.52
5:G:490:MET:O	5:G:496:TRP:NE1	2.42	0.52
8:z:144:ASP:OD1	8:z:147:THR:OG1	2.15	0.52
5:g:319:ASP:OD1	5:g:322:ARG:NH2	2.42	0.52
1:A:435:GLN:NE2	6:h:462:ASN:O	2.43	0.52
7:q:525:ILE:HD12	8:z:67:MET:SD	2.50	0.52
4:E:341:PRO:HB3	6:H:246:LEU:HD21	1.91	0.52
7:q:99:ASP:OD1	7:q:100:GLY:N	2.43	0.52
8:z:473:SER:OG	8:z:474:GLY:N	2.43	0.52
1:A:141:ASP:O	1:A:148:LEU:CD1	2.58	0.52
1:A:331:LEU:HD22	1:A:339:THR:HA	1.91	0.52
3:D:128:ILE:HD11	4:e:469:ILE:HD13	1.92	0.52
4:e:110:LEU:HB2	4:e:456:ILE:HD11	1.92	0.52
5:G:319:ASP:OD1	5:G:322:ARG:NH2	2.42	0.52
8:z:478:GLY:N	8:z:487:MET:O	2.43	0.51
1:A:164:ASN:ND2	1:A:206:MET:SD	2.84	0.51
7:Q:129:ILE:HG23	7:Q:516:VAL:HG13	1.92	0.51
3:d:209:LYS:NZ	3:d:332:ASP:OD2	2.43	0.51
4:E:24:SER:OG	4:E:531:ILE:O	2.29	0.51
2:b:72:LYS:NZ	2:b:92:ASP:OD2	2.31	0.51
4:e:206:LEU:HD22	4:e:379:ARG:O	2.10	0.50
7:q:66:THR:OG1	7:q:68:ASP:OD2	2.30	0.50
7:q:69:ALA:HA	7:q:72:ILE:HD12	1.93	0.50
6:h:113:GLU:N	6:h:113:GLU:OE2	2.45	0.50
4:E:200:ARG:NH1	4:E:411:ILE:O	2.44	0.50
8:z:200:SER:OG	8:z:203:ASP:OD2	2.29	0.49
3:D:132:ILE:HD13	3:D:446:MET:SD	2.51	0.49
4:E:490:ASP:OD1	4:E:494:LYS:N	2.45	0.49
5:g:193:ILE:HD12	5:g:403:LEU:HG	1.95	0.49
1:a:408:VAL:HG12	1:a:506:PRO:HA	1.94	0.49
1:a:411:GLY:O	1:a:498:ASN:ND2	2.43	0.49
2:B:57:ARG:O	2:B:60:SER:OG	2.30	0.49
7:Q:58:ASN:ND2	7:Q:75:GLU:OE2	2.45	0.49
7:q:153:ASN:N	7:q:159:GLU:OE2	2.44	0.49
2:B:49:ASP:N	3:D:531:LYS:O	2.45	0.49
4:e:100:ILE:HD11	4:e:513:GLN:CB	2.42	0.49
7:q:289:ASN:O	7:q:311:MET:N	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:120:ILE:HD13	6:H:430:LYS:CD	2.43	0.49
1:a:189:ARG:HE	1:a:404:GLU:CD	2.21	0.48
4:e:253:PHE:HA	4:e:286:MET:HE2	1.94	0.48
6:H:244:LEU:HD13	6:H:278:LEU:HD21	1.94	0.48
3:d:249:ILE:HD12	3:d:298:LEU:HD22	1.95	0.48
8:Z:440:PHE:CE2	8:Z:444:LEU:HD11	2.48	0.48
4:e:173:SER:O	4:e:173:SER:OG	2.31	0.48
6:H:516:VAL:HG11	7:Q:55:MET:HE3	1.94	0.48
8:z:271:VAL:HA	8:z:274:ILE:HD12	1.96	0.48
1:A:425:ASN:OD1	6:h:425:ARG:NH1	2.46	0.48
7:q:142:ILE:HD13	7:q:422:GLN:HB2	1.95	0.48
1:A:416:GLU:OE1	1:A:416:GLU:N	2.47	0.48
2:B:54:SER:OG	2:B:55:SER:N	2.47	0.48
8:z:290:VAL:HG21	8:z:350:VAL:HG11	1.96	0.48
8:Z:415:GLU:N	8:Z:415:GLU:OE1	2.47	0.47
7:q:224:LYS:HA	7:q:360:VAL:HG12	1.96	0.47
2:b:65:ASN:ND2	2:b:169:SER:O	2.47	0.47
8:Z:189:PHE:O	8:Z:323:ARG:NH2	2.46	0.47
8:z:274:ILE:HD11	8:z:336:PHE:CZ	2.49	0.47
5:g:101:LEU:HD22	5:g:444:LEU:HD23	1.96	0.47
8:Z:142:GLU:OE2	8:Z:142:GLU:N	2.47	0.47
4:e:92:LEU:HD11	4:e:517:LEU:HB3	1.97	0.47
2:b:350:GLU:N	2:b:361:HIS:O	2.48	0.47
1:A:15:GLU:OE2	1:A:15:GLU:N	2.48	0.47
7:q:112:LEU:HD11	7:q:518:VAL:HG11	1.97	0.47
1:A:158:SER:O	1:A:158:SER:OG	2.28	0.46
6:H:280:LYS:O	6:H:284:SER:OG	2.19	0.46
1:A:477:ASN:OD1	1:A:482:ASN:ND2	2.45	0.46
3:d:254:SER:OG	3:d:255:ALA:N	2.47	0.46
5:g:182:MET:HE1	5:g:216:ARG:HA	1.98	0.46
2:b:375:LEU:HD21	2:b:390:LEU:HD22	1.98	0.46
6:h:458:THR:O	6:h:462:ASN:ND2	2.49	0.46
8:Z:104:LYS:NZ	8:z:112:GLU:OE1	2.49	0.46
1:a:416:GLU:OE1	1:a:416:GLU:N	2.49	0.46
6:h:515:SER:OG	7:q:53:ASN:ND2	2.49	0.46
7:Q:176:GLU:OE1	7:Q:176:GLU:N	2.46	0.45
8:Z:151:VAL:O	8:Z:154:THR:OG1	2.28	0.45
4:e:389:ASN:OD1	4:e:391:MET:N	2.49	0.45
6:h:413:GLU:OE2	6:h:499:ARG:NH1	2.50	0.45
7:q:452:LEU:HD23	7:q:480:LEU:HD23	1.99	0.45
8:z:214:HIS:ND1	8:z:314:ARG:O	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:87:MET:HE2	2:b:509:GLU:OE2	2.16	0.45
4:e:100:ILE:HD11	4:e:513:GLN:HB3	1.98	0.45
7:q:171:LYS:NZ	9:q:601:ADP:O2A	2.50	0.45
3:D:529:ILE:HA	3:D:532:ILE:HD12	1.98	0.45
4:e:424:GLU:N	4:e:424:GLU:OE1	2.50	0.45
8:Z:94:SER:HA	8:Z:97:LEU:HD12	1.97	0.45
1:a:148:LEU:HD22	1:a:148:LEU:HA	1.86	0.45
3:D:431:GLU:OE2	3:D:435:ARG:NE	2.50	0.45
6:h:522:ASN:ND2	7:q:75:GLU:O	2.50	0.45
6:H:408:GLY:O	6:H:487:ASN:ND2	2.50	0.45
3:d:474:ILE:O	3:d:478:THR:OG1	2.18	0.44
8:Z:478:GLY:N	8:Z:487:MET:O	2.48	0.44
4:E:383:ILE:HG21	4:E:400:LEU:HD21	2.00	0.44
3:D:71:THR:HG22	3:D:73:ASP:H	1.82	0.44
3:D:299:LEU:CD2	3:D:336:ILE:HD13	2.47	0.44
1:A:529:ASP:OD1	1:A:530:LEU:N	2.50	0.44
5:G:241:LEU:HD11	5:G:292:THR:HG22	1.99	0.44
1:a:189:ARG:HD2	1:a:404:GLU:CG	2.45	0.44
1:A:123:LEU:HD13	1:A:430:MET:HE2	2.00	0.44
4:E:71:ASP:OD2	4:E:74:THR:N	2.49	0.43
4:E:110:LEU:HB2	4:E:456:ILE:HD11	2.00	0.43
1:a:182:THR:OG1	1:a:183:ASP:N	2.51	0.43
3:D:98:GLN:NE2	3:D:517:SER:OG	2.48	0.43
4:E:163:LEU:HD23	4:E:188:VAL:HG13	1.98	0.43
4:E:129:ILE:HD11	6:H:45:MET:HG2	2.00	0.43
6:h:278:LEU:HD23	6:h:281:ILE:HD12	2.00	0.43
1:A:140:THR:OG1	1:A:141:ASP:N	2.51	0.43
4:e:70:ASN:OD1	4:e:70:ASN:N	2.52	0.43
1:a:251:GLN:NE2	5:g:337:GLU:OE2	2.50	0.43
2:b:204:LYS:HE3	2:b:359:LEU:HD21	2.01	0.43
6:H:460:ILE:O	6:H:464:LEU:N	2.50	0.43
1:a:189:ARG:NE	1:a:404:GLU:CG	2.65	0.43
6:H:120:ILE:HD13	6:H:430:LYS:HD3	1.99	0.43
1:a:264:ARG:NH2	1:a:265:GLN:OE1	2.52	0.43
8:Z:114:LEU:HD11	8:Z:118:ILE:HB	2.01	0.43
8:Z:242:THR:HG21	8:Z:246:SER:HB3	2.00	0.43
3:d:429:GLU:N	3:d:429:GLU:OE1	2.52	0.42
4:e:337:GLY:O	4:e:338:ARG:NH1	2.50	0.42
8:Z:38:LEU:HD12	9:Z:601:ADP:O3B	2.19	0.42
8:Z:431:GLY:CA	8:z:464:VAL:HG11	2.48	0.42
1:a:284:ASN:O	1:a:306:MET:N	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:254:GLU:OE1	4:E:305:ASP:N	2.48	0.42
6:h:121:ILE:HG13	6:h:434:LEU:HD22	2.02	0.42
2:b:350:GLU:N	2:b:350:GLU:OE2	2.51	0.42
6:h:351:THR:HG21	6:h:353:ILE:HD12	2.01	0.42
6:h:431:GLN:NE2	7:q:485:GLU:OE2	2.53	0.42
2:B:519:ASN:OD1	4:E:57:LYS:NZ	2.51	0.42
7:q:54:LYS:N	7:q:66:THR:O	2.50	0.42
8:z:235:VAL:O	8:z:293:ASN:ND2	2.49	0.42
2:b:414:GLU:N	2:b:414:GLU:OE1	2.53	0.42
5:g:239:VAL:HG11	5:g:282:ILE:HG23	2.01	0.42
6:h:282:HIS:HA	6:h:308:MET:HE1	2.02	0.42
5:G:492:GLU:C	5:G:493:LEU:HD12	2.44	0.42
7:q:111:LEU:HD21	7:q:441:PHE:CD1	2.54	0.42
6:H:21:GLN:O	6:H:25:ASN:ND2	2.53	0.41
6:H:155:LEU:HD11	6:H:400:ILE:HD11	2.03	0.41
7:q:331:THR:OG1	7:q:343:GLU:OE1	2.31	0.41
6:h:393:ILE:O	6:h:397:ARG:N	2.50	0.41
7:Q:101:THR:N	9:Q:601:ADP:O1B	2.47	0.41
8:Z:481:LEU:HD22	9:Z:601:ADP:N6	2.35	0.41
6:h:257:VAL:HG21	6:h:262:ASP:HB2	2.03	0.41
6:H:244:LEU:HB2	6:H:295:ILE:HG23	2.02	0.41
4:E:409:ASN:O	4:E:413:ASP:N	2.48	0.41
8:Z:235:VAL:O	8:Z:293:ASN:ND2	2.49	0.41
8:z:416:VAL:HG21	8:z:466:ILE:HD12	2.03	0.41
2:B:379:THR:OG1	2:B:380:GLN:N	2.53	0.41
7:q:152:LYS:N	7:q:159:GLU:OE2	2.54	0.41
1:a:88:ASP:OD2	1:a:401:ARG:NH1	2.53	0.41
4:e:385:ILE:HD11	4:e:400:LEU:HD12	2.01	0.41
8:Z:509:THR:O	8:Z:513:THR:OG1	2.25	0.41
8:z:261:LYS:O	8:z:265:LYS:N	2.54	0.41
2:b:65:ASN:OD1	2:b:65:ASN:N	2.54	0.40
7:q:93:GLN:O	7:q:97:VAL:HG13	2.21	0.40
7:q:203:ARG:HH11	7:q:221:MET:HE3	1.86	0.40
1:A:41:LEU:HD21	5:G:118:HIS:CE1	2.56	0.40
3:D:33:ILE:HG21	3:D:534:ASP:HA	2.03	0.40
6:h:90:VAL:HG13	6:h:498:VAL:HG22	2.02	0.40
1:a:18:ARG:O	1:a:22:VAL:HG23	2.22	0.40
2:b:487:ASP:HB3	2:b:490:ILE:HD12	2.03	0.40
1:a:140:THR:HG23	1:a:141:ASP:OD2	2.21	0.40
2:b:85:VAL:O	2:b:88:SER:OG	2.26	0.40
7:Q:409:VAL:O	7:Q:499:ASP:N	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:z:138:LYS:HA	8:z:408:VAL:HG12	2.03	0.40
4:E:145:HIS:NE2	4:E:426:SER:OG	2.49	0.40
6:H:351:THR:OG1	6:H:352:GLN:N	2.55	0.40
7:Q:236:ASP:OD1	7:Q:237:ALA:N	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	472/556 (85%)	454 (96%)	17 (4%)	1 (0%)	44 77
1	a	518/556 (93%)	501 (97%)	17 (3%)	0	100 100
2	B	323/535 (60%)	316 (98%)	7 (2%)	0	100 100
2	b	473/535 (88%)	459 (97%)	14 (3%)	0	100 100
3	D	425/539 (79%)	415 (98%)	10 (2%)	0	100 100
3	d	514/539 (95%)	504 (98%)	10 (2%)	0	100 100
4	E	510/539 (95%)	493 (97%)	17 (3%)	0	100 100
4	e	508/539 (94%)	490 (96%)	18 (4%)	0	100 100
5	G	402/545 (74%)	388 (96%)	14 (4%)	0	100 100
5	g	477/545 (88%)	463 (97%)	14 (3%)	0	100 100
6	H	505/543 (93%)	491 (97%)	14 (3%)	0	100 100
6	h	509/543 (94%)	495 (97%)	14 (3%)	0	100 100
7	Q	468/548 (85%)	462 (99%)	6 (1%)	0	100 100
7	q	479/548 (87%)	470 (98%)	9 (2%)	0	100 100
8	Z	507/531 (96%)	491 (97%)	16 (3%)	0	100 100
8	z	508/531 (96%)	494 (97%)	14 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	7598/8672 (88%)	7386 (97%)	211 (3%)	1 (0%)	100 100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	405	SER

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	391/463 (84%)	389 (100%)	2 (0%)	86 90
1	a	433/463 (94%)	431 (100%)	2 (0%)	86 90
2	B	257/427 (60%)	257 (100%)	0	100 100
2	b	378/427 (88%)	378 (100%)	0	100 100
3	D	368/452 (81%)	368 (100%)	0	100 100
3	d	441/452 (98%)	441 (100%)	0	100 100
4	E	432/455 (95%)	432 (100%)	0	100 100
4	e	430/455 (94%)	430 (100%)	0	100 100
5	G	352/469 (75%)	352 (100%)	0	100 100
5	g	414/469 (88%)	414 (100%)	0	100 100
6	H	415/443 (94%)	415 (100%)	0	100 100
6	h	419/443 (95%)	419 (100%)	0	100 100
7	Q	391/452 (86%)	391 (100%)	0	100 100
7	q	400/452 (88%)	400 (100%)	0	100 100
8	Z	426/442 (96%)	426 (100%)	0	100 100
8	z	427/442 (97%)	427 (100%)	0	100 100
All	All	6374/7206 (88%)	6370 (100%)	4 (0%)	92 95

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	147	CYS
1	a	148	LEU
1	A	147	CYS
1	A	405	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	a	133	ASN
1	a	193	ASN
1	a	482	ASN
1	A	150	ASN
1	A	170	ASN
1	A	217	ASN
1	A	471	HIS
1	A	492	ASN
2	b	298	ASN
2	b	519	ASN
2	B	419	HIS
2	B	502	GLN
4	E	301	GLN
4	E	374	GLN
4	E	401	HIS
4	e	443	GLN
5	g	277	GLN
5	G	390	ASN
6	h	282	HIS
6	H	25	ASN
6	H	234	ASN
6	H	258	HIS
7	Q	201	ASN
7	Q	397	ASN
7	Q	477	ASN
7	q	53	ASN
7	q	289	ASN
7	q	306	ASN
8	Z	245	ASN
8	Z	380	ASN
8	Z	434	GLN
8	z	23	ASN
8	z	61	ASN
8	z	482	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)

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
9	ADP	Q	601	-	24,29,29	1.33	2 (8%)	29,45,45	1.83	7 (24%)
9	ADP	g	601	-	24,29,29	0.94	1 (4%)	29,45,45	1.48	4 (13%)
9	ADP	z	601	8	24,29,29	1.01	1 (4%)	29,45,45	1.56	5 (17%)
9	ADP	Z	601	-	24,29,29	1.08	2 (8%)	29,45,45	1.46	4 (13%)
9	ADP	q	601	-	24,29,29	0.97	1 (4%)	29,45,45	1.57	5 (17%)
9	ADP	G	601	-	24,29,29	0.95	1 (4%)	29,45,45	1.46	4 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	ADP	Q	601	-	-	2/12/32/32	0/3/3/3
9	ADP	g	601	-	-	3/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	ADP	z	601	8	-	2/12/32/32	0/3/3/3
9	ADP	Z	601	-	-	5/12/32/32	0/3/3/3
9	ADP	q	601	-	-	4/12/32/32	0/3/3/3
9	ADP	G	601	-	-	2/12/32/32	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	Q	601	ADP	O4'-C1'	4.60	1.47	1.41
9	q	601	ADP	C5-C4	2.48	1.47	1.40
9	Z	601	ADP	C5-C4	2.44	1.47	1.40
9	z	601	ADP	C5-C4	2.39	1.47	1.40
9	G	601	ADP	C5-C4	2.39	1.47	1.40
9	g	601	ADP	C5-C4	2.38	1.47	1.40
9	Q	601	ADP	C5-C4	2.35	1.47	1.40
9	Z	601	ADP	C2-N1	2.24	1.38	1.33

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	Q	601	ADP	C3'-C2'-C1'	4.76	108.14	100.98
9	q	601	ADP	PA-O3A-PB	-3.93	119.35	132.83
9	G	601	ADP	N3-C2-N1	-3.70	122.89	128.68
9	z	601	ADP	N3-C2-N1	-3.66	122.96	128.68
9	Q	601	ADP	N3-C2-N1	-3.64	122.99	128.68
9	g	601	ADP	N3-C2-N1	-3.63	123.01	128.68
9	Z	601	ADP	PA-O3A-PB	-3.63	120.38	132.83
9	q	601	ADP	N3-C2-N1	-3.61	123.03	128.68
9	q	601	ADP	C3'-C2'-C1'	3.57	106.36	100.98
9	Q	601	ADP	C5'-C4'-C3'	-3.48	102.13	115.18
9	g	601	ADP	PA-O3A-PB	-3.47	120.92	132.83
9	Z	601	ADP	C4-C5-N7	-3.41	105.85	109.40
9	z	601	ADP	C3'-C2'-C1'	3.35	106.02	100.98
9	z	601	ADP	PA-O3A-PB	-3.32	121.42	132.83
9	G	601	ADP	PA-O3A-PB	-3.32	121.43	132.83
9	Z	601	ADP	N3-C2-N1	-3.28	123.56	128.68
9	g	601	ADP	C3'-C2'-C1'	3.26	105.88	100.98
9	Z	601	ADP	C3'-C2'-C1'	3.10	105.64	100.98
9	G	601	ADP	C3'-C2'-C1'	3.05	105.56	100.98
9	Q	601	ADP	PA-O3A-PB	-2.98	122.60	132.83
9	q	601	ADP	C4-C5-N7	-2.97	106.30	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	Q	601	ADP	C4-C5-N7	-2.95	106.32	109.40
9	z	601	ADP	C4-C5-N7	-2.95	106.33	109.40
9	Q	601	ADP	O4'-C4'-C5'	-2.76	100.30	109.37
9	g	601	ADP	C4-C5-N7	-2.74	106.55	109.40
9	G	601	ADP	C4-C5-N7	-2.73	106.55	109.40
9	z	601	ADP	C2-N1-C6	2.52	123.06	118.75
9	q	601	ADP	C2-N1-C6	2.15	122.43	118.75
9	Q	601	ADP	O3B-PB-O2B	2.02	115.37	107.64

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	q	601	ADP	C5'-O5'-PA-O3A
9	Z	601	ADP	C5'-O5'-PA-O3A
9	G	601	ADP	PB-O3A-PA-O1A
9	Q	601	ADP	PB-O3A-PA-O1A
9	z	601	ADP	PB-O3A-PA-O1A
9	g	601	ADP	C5'-O5'-PA-O3A
9	g	601	ADP	PB-O3A-PA-O1A
9	q	601	ADP	PB-O3A-PA-O1A
9	Z	601	ADP	C5'-O5'-PA-O1A
9	Z	601	ADP	C5'-O5'-PA-O2A
9	g	601	ADP	PB-O3A-PA-O2A
9	G	601	ADP	PB-O3A-PA-O2A
9	q	601	ADP	PB-O3A-PA-O2A
9	Z	601	ADP	PB-O3A-PA-O1A
9	Z	601	ADP	PB-O3A-PA-O2A
9	z	601	ADP	PB-O3A-PA-O2A
9	Q	601	ADP	PB-O3A-PA-O2A
9	q	601	ADP	C5'-O5'-PA-O1A

There are no ring outliers.

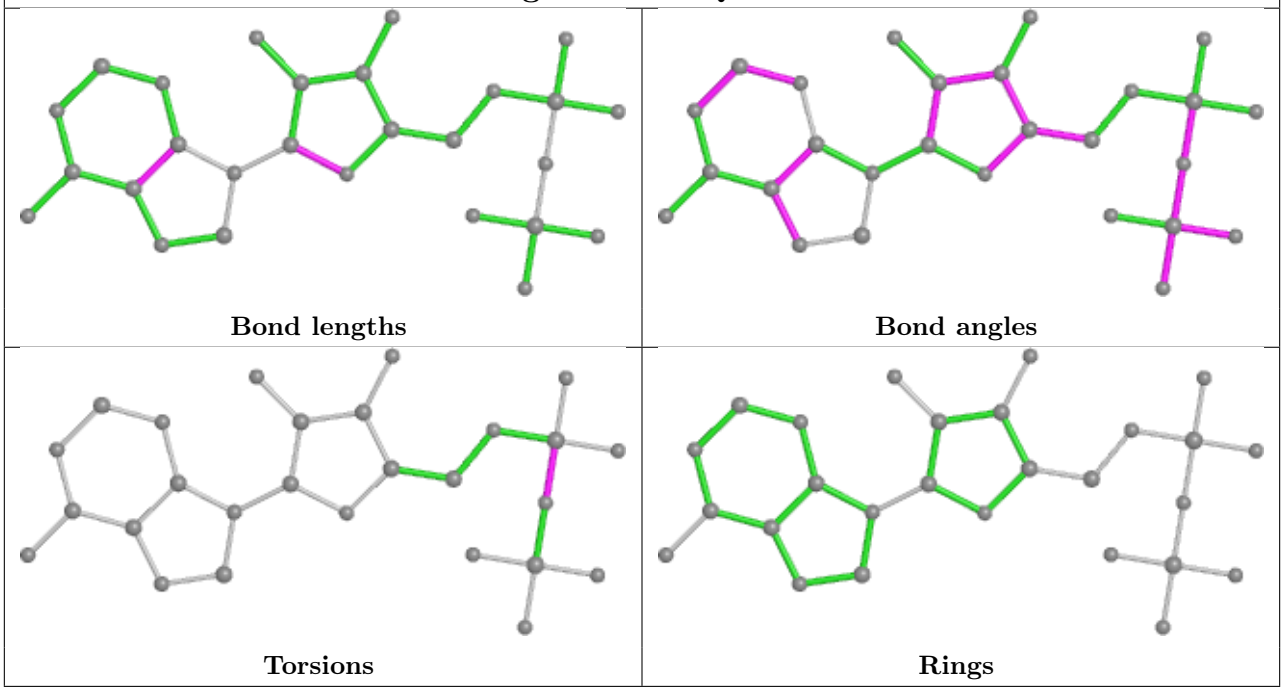
3 monomers are involved in 8 short contacts:

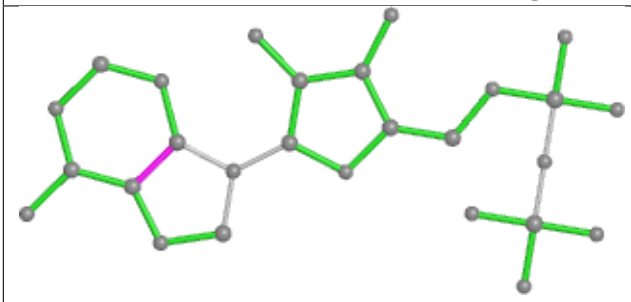
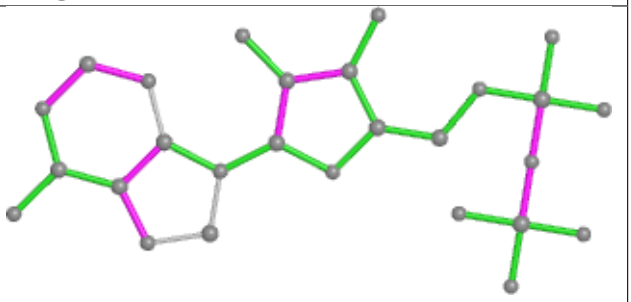
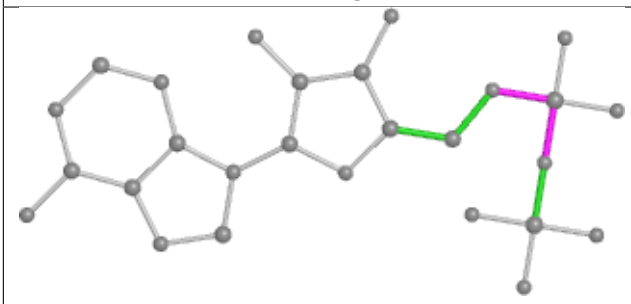
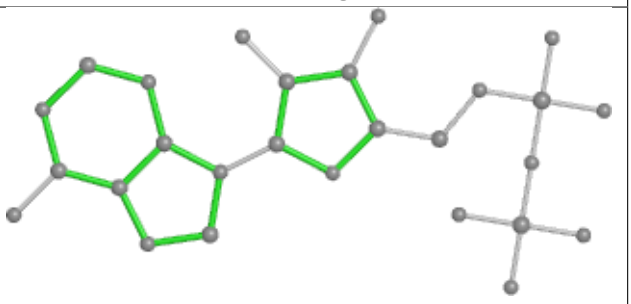
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	Q	601	ADP	1	0
9	Z	601	ADP	3	0
9	q	601	ADP	4	0

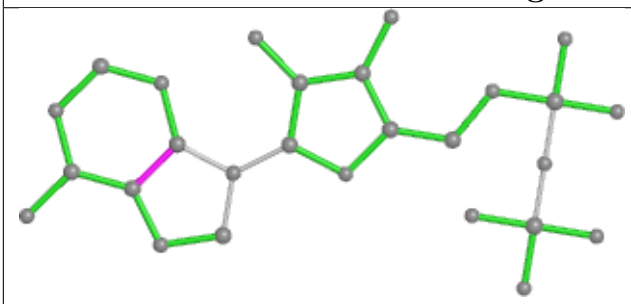
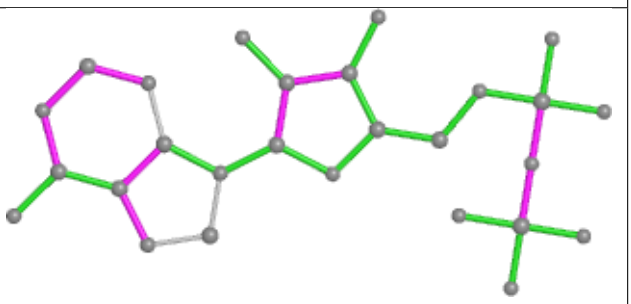
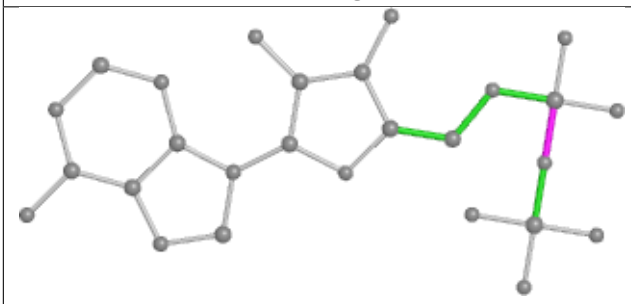
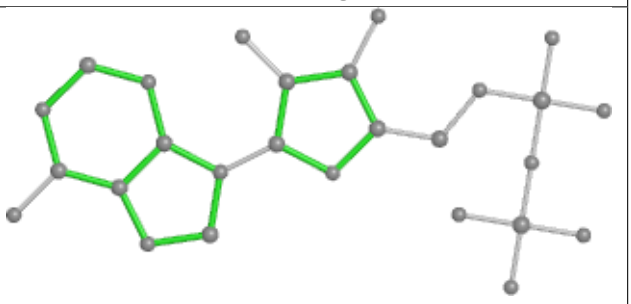
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

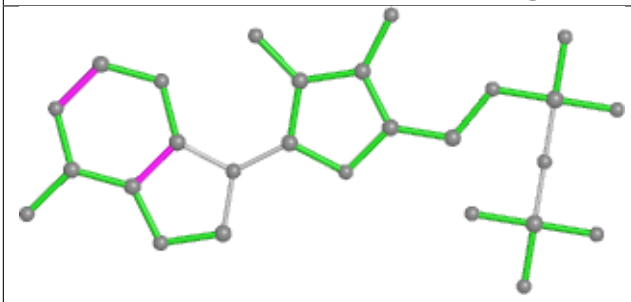
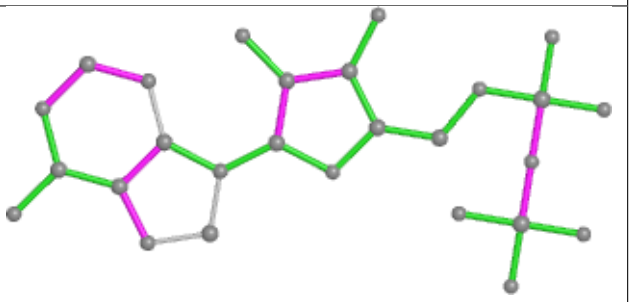
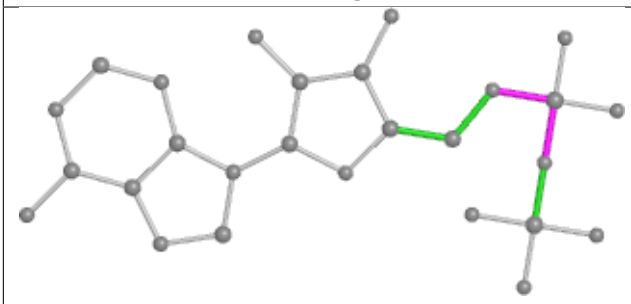
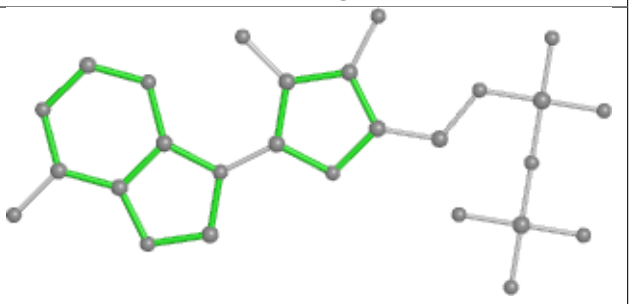
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within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

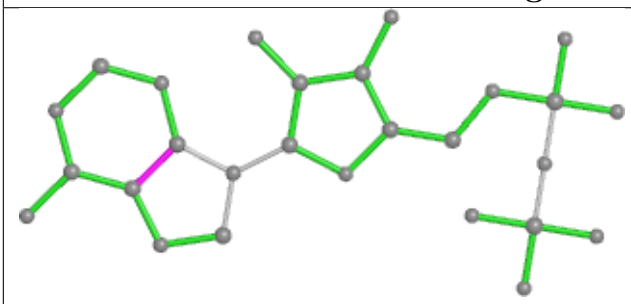
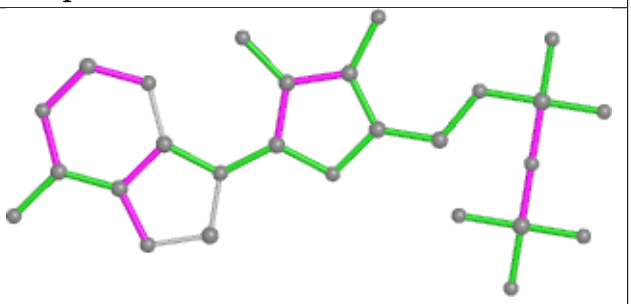
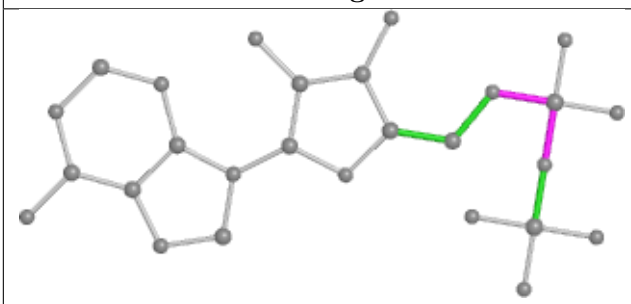
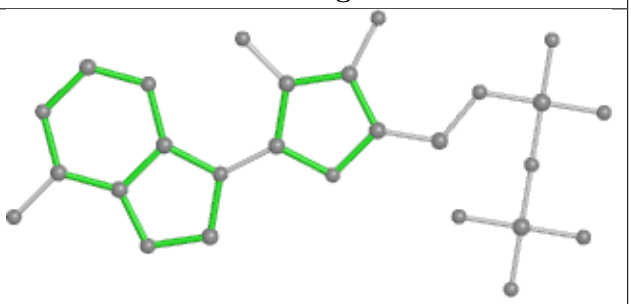
Ligand ADP Q 601



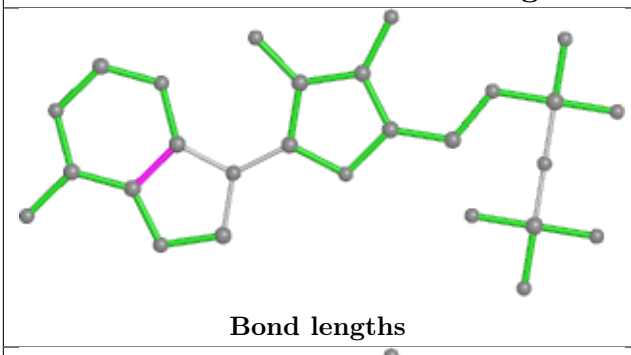
Ligand ADP g 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP z 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

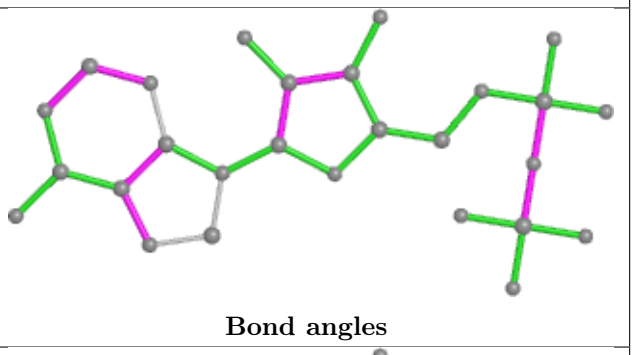
Ligand ADP Z 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP q 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

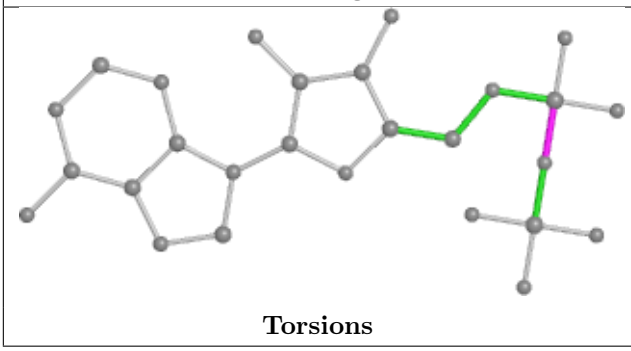
Ligand ADP G 601



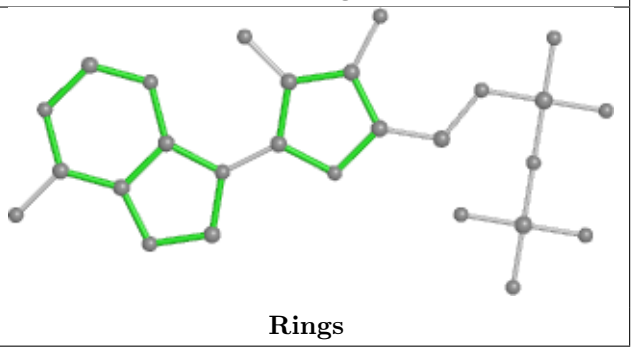
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

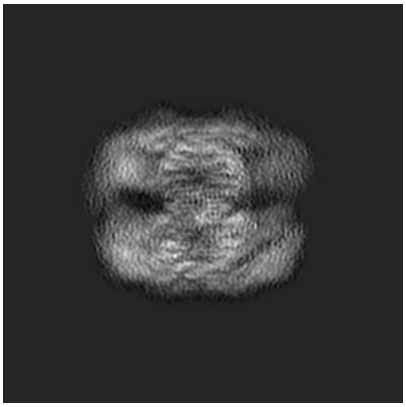
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-32903. These allow visual inspection of the internal detail of the map and identification of artifacts.

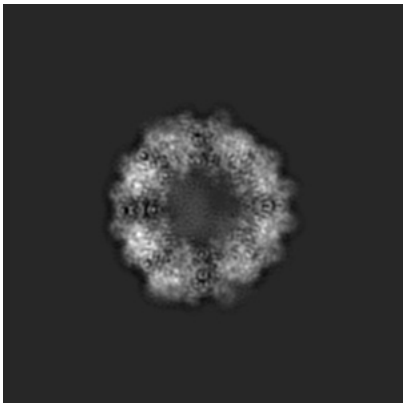
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

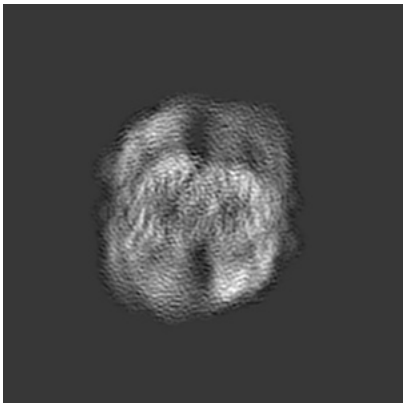
6.1.1 Primary map



X



Y

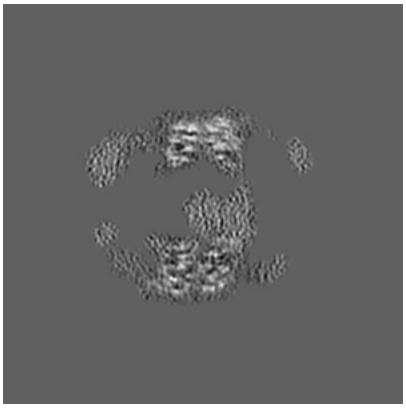


Z

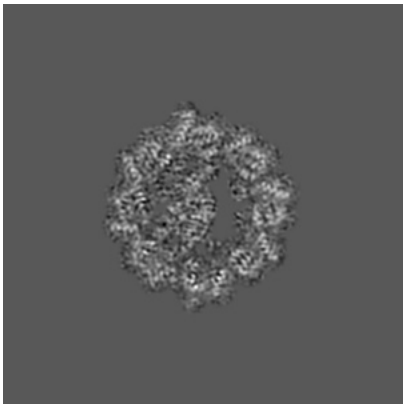
The images above show the map projected in three orthogonal directions.

6.2 Central slices

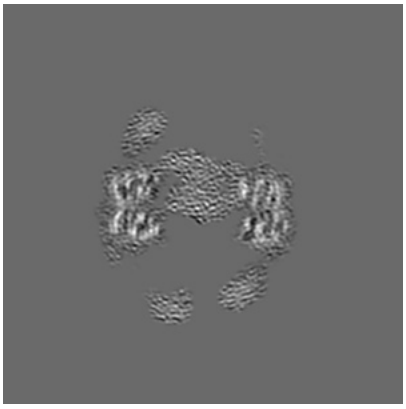
6.2.1 Primary map



X Index: 128



Y Index: 128

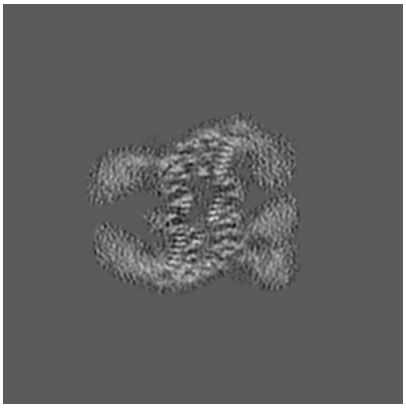


Z Index: 128

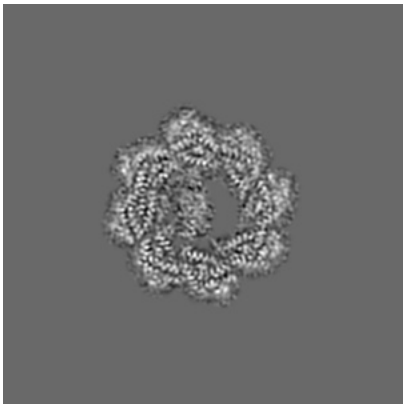
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

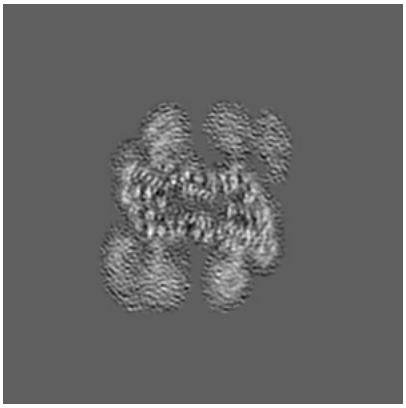
6.3.1 Primary map



X Index: 95



Y Index: 135

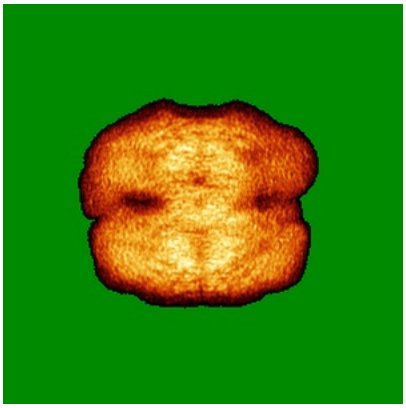


Z Index: 94

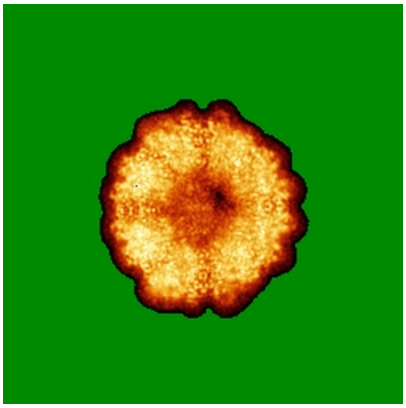
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

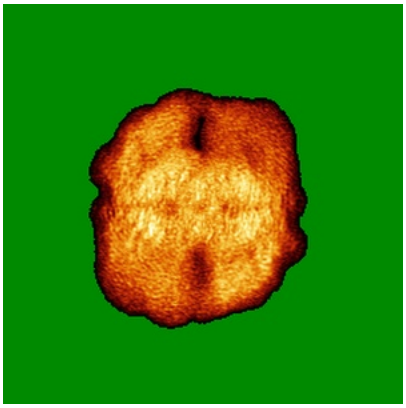
6.4.1 Primary map



X



Y

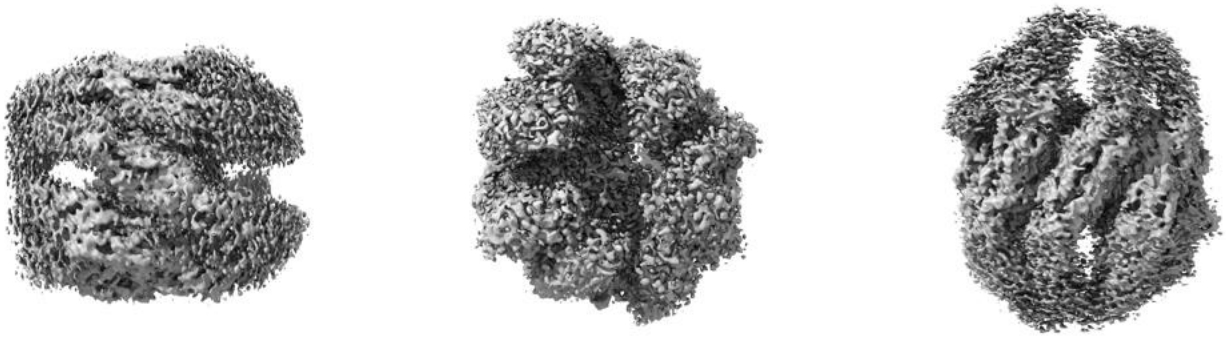


Z

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



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.7. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

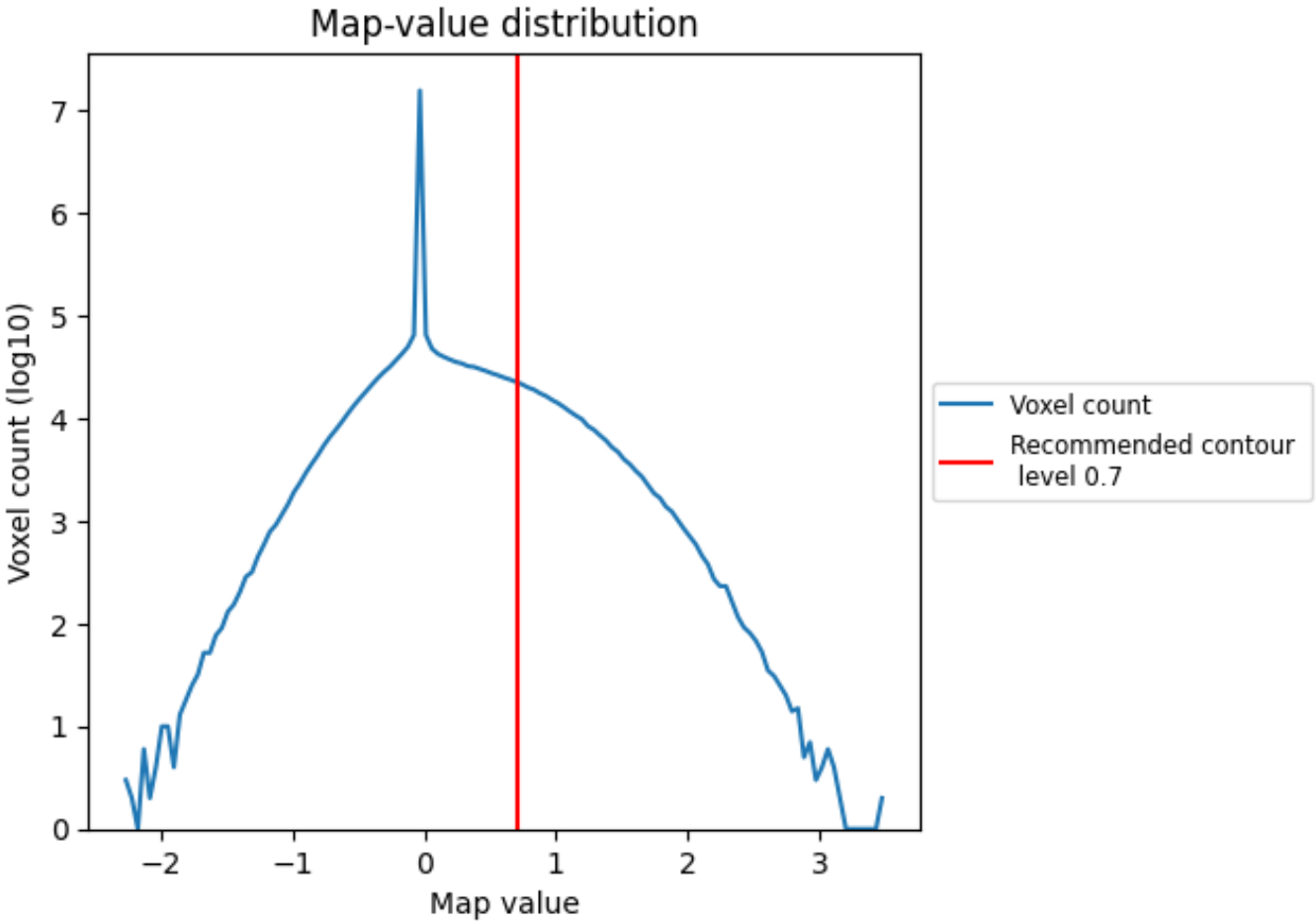
6.6 Mask visualisation (i)

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

7 Map analysis

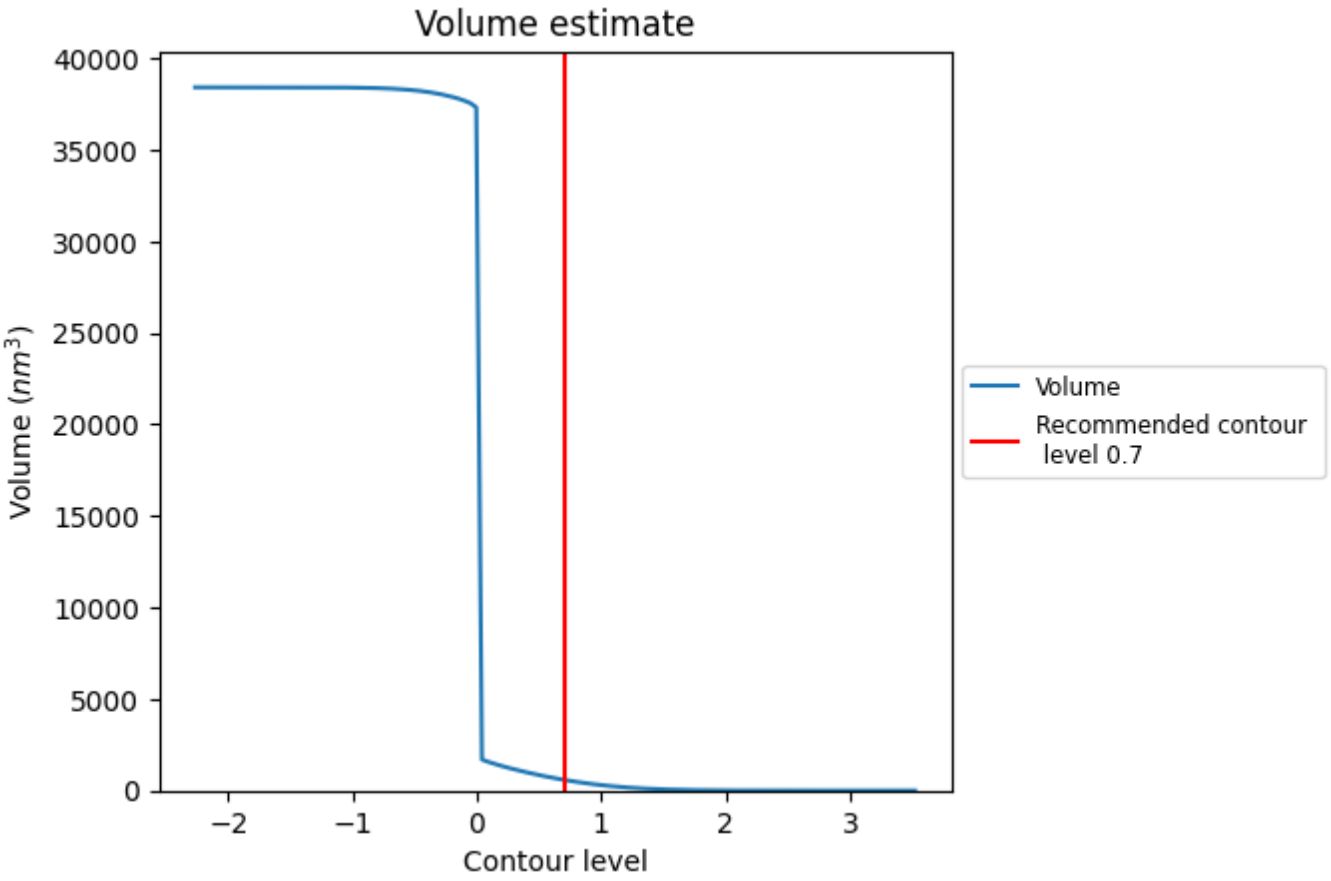
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

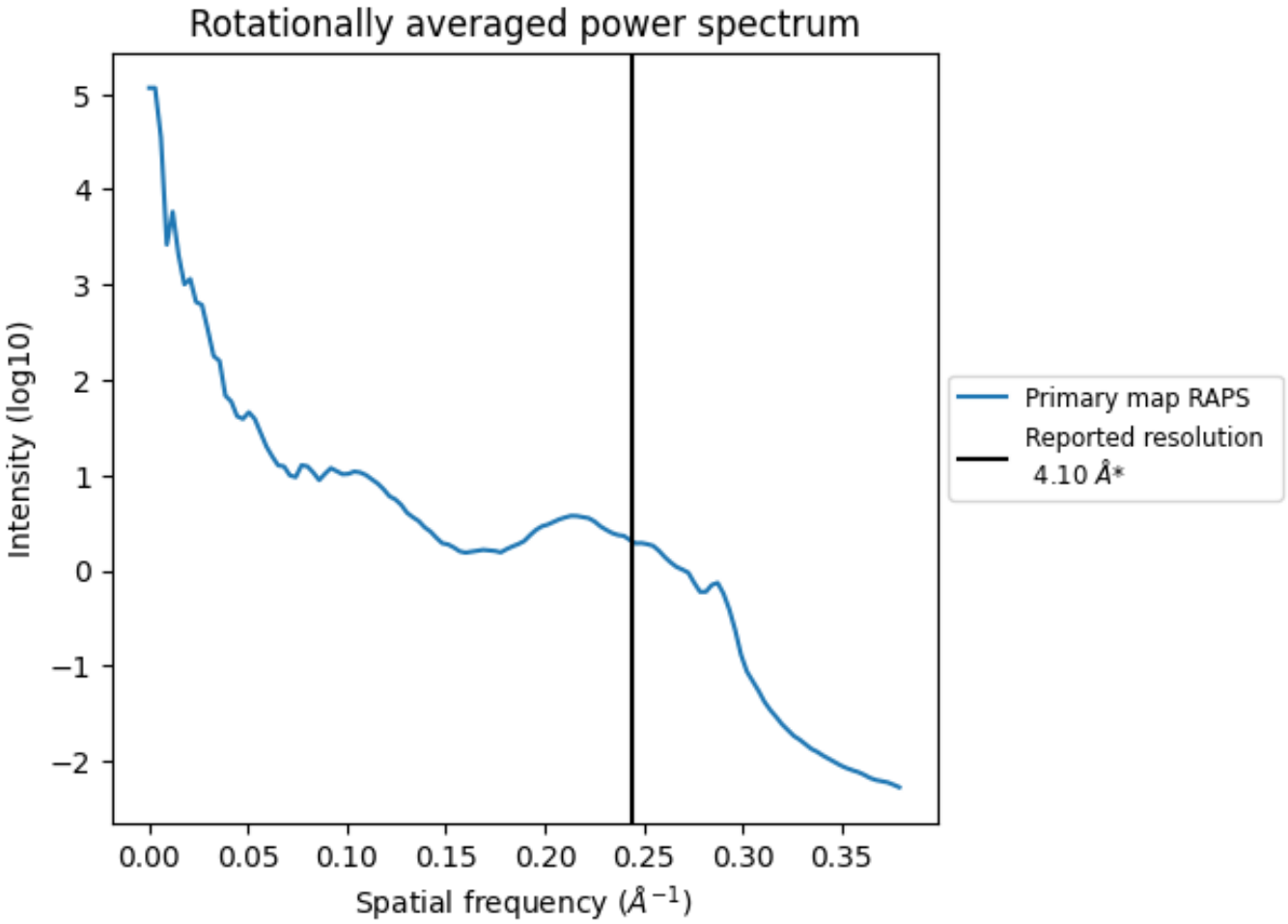
7.2 Volume estimate



The volume at the recommended contour level is 585 nm^3; this corresponds to an approximate mass of 529 kDa.

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

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.244 Å^{-1}

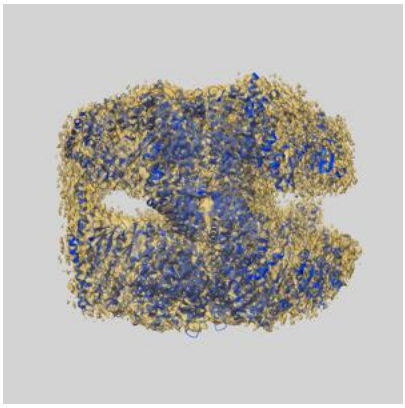
8 Fourier-Shell correlation (i)

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

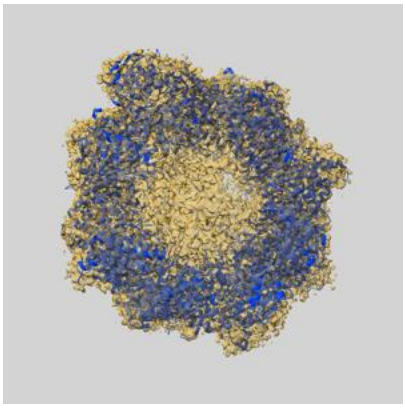
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-32903 and PDB model 7WZ3. Per-residue inclusion information can be found in section 3 on page 7.

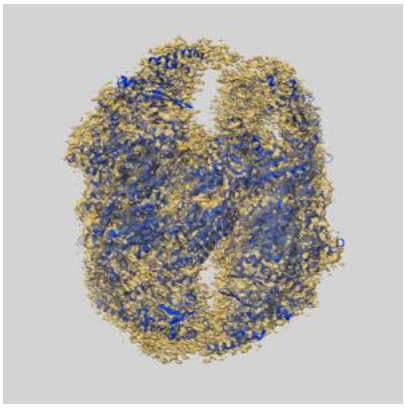
9.1 Map-model overlay



X



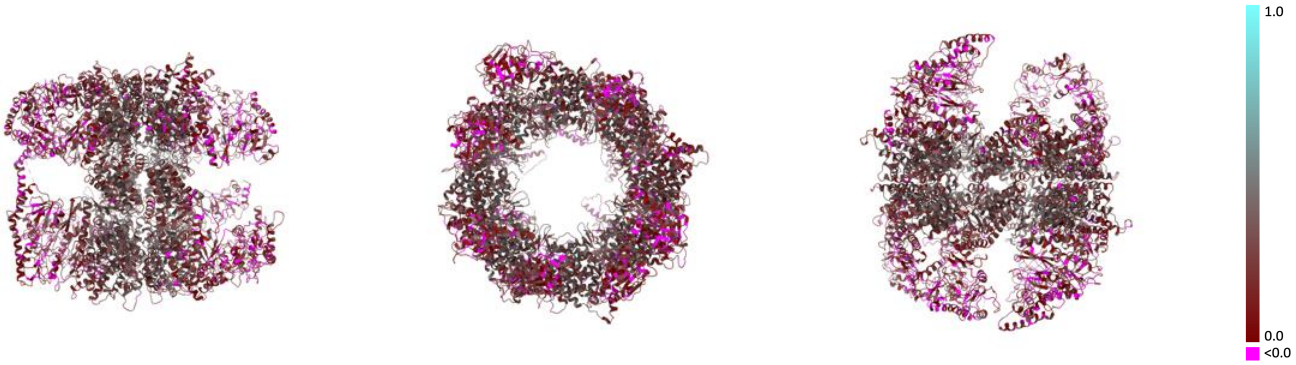
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.7 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.

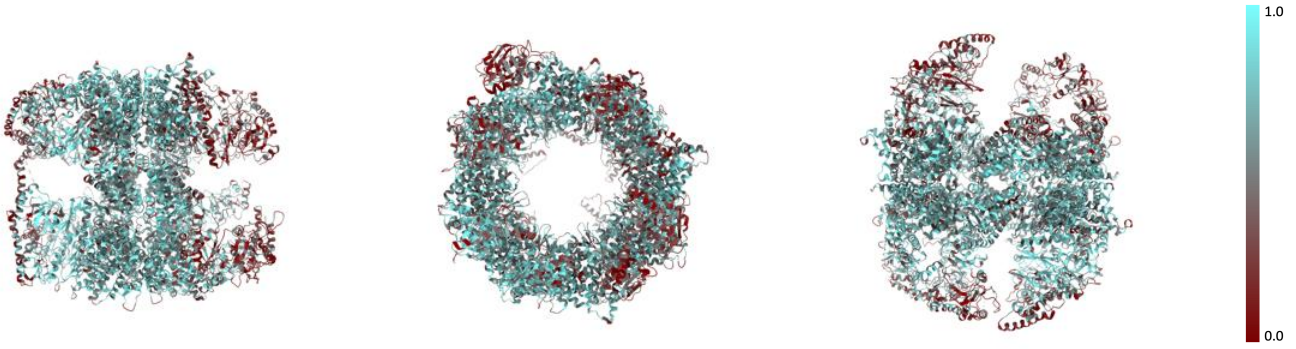
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

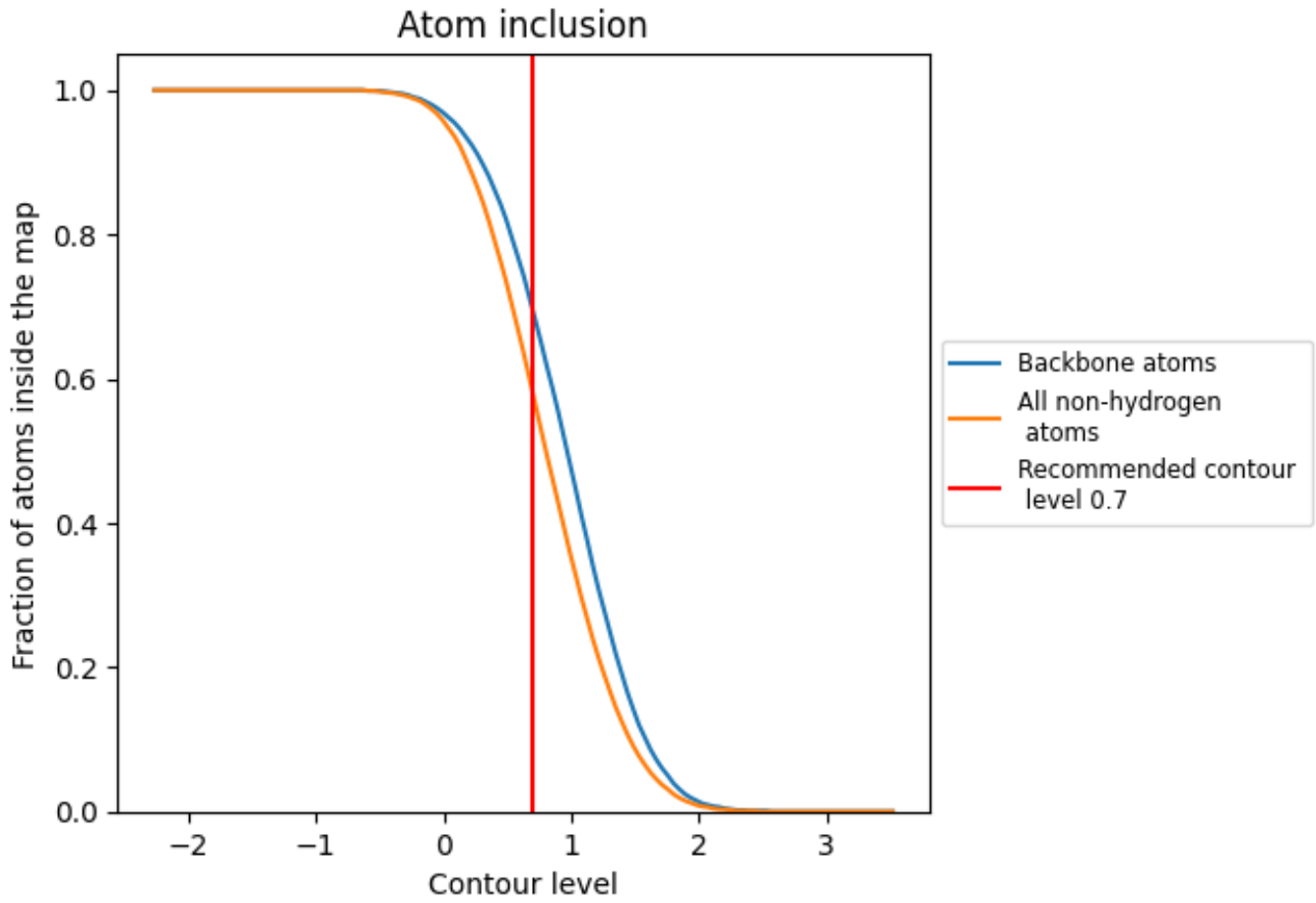
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.7).

9.4 Atom inclusion (i)



At the recommended contour level, 70% of all backbone atoms, 58% 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 (0.7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5800	0.2270
A	0.4820	0.2120
B	0.5690	0.2470
D	0.4770	0.2080
E	0.5230	0.2100
G	0.5350	0.2080
H	0.4930	0.2300
Q	0.6480	0.2550
Z	0.6050	0.2400
a	0.5910	0.2180
b	0.5520	0.2280
d	0.6090	0.2220
e	0.6400	0.2190
g	0.6370	0.2320
h	0.5950	0.2170
q	0.6610	0.2520
z	0.6320	0.2410