



Full wwPDB EM Validation Report ⓘ

Mar 25, 2026 – 04:07 AM UTC

PDB ID : 8HKI / pdb_00008hki
EMDB ID : EMD-34852
Title : Human TRiC open state
Authors : Cong, Y.; Liu, C.X.
Deposited on : 2022-11-27
Resolution : 3.10 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:

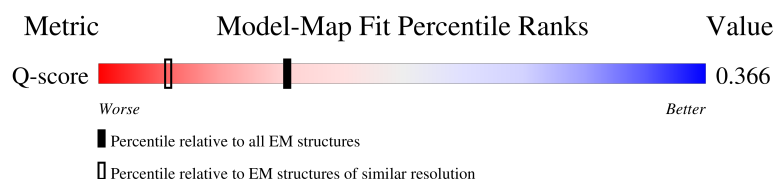
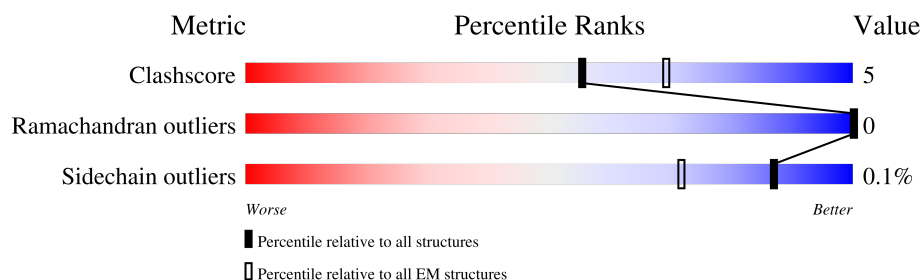
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.10 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14724 (2.60 - 3.60)

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	556	
1	a	556	
2	B	535	
2	b	535	

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Mol	Chain	Length	Quality of chain
3	D	539	
3	d	539	
4	E	539	
4	e	539	
5	G	545	
5	g	545	
6	H	543	
6	h	543	
7	Q	548	
7	q	548	
8	Z	531	
8	z	531	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
9	ADP	G	601	-	-	X	-
9	ADP	g	601	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 33926 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	291	Total	C	N	O	S	0	0
			2182	1369	377	429	7		
1	A	255	Total	C	N	O	S	0	0
			1918	1210	330	373	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	b	327	Total	C	N	O	S	0	0
			2407	1482	430	483	12		
2	B	250	Total	C	N	O	S	0	0
			1842	1141	326	365	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	250	Total	C	N	O	S	0	0
			1870	1164	328	369	9		
3	d	278	Total	C	N	O	S	0	0
			2086	1295	366	416	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	254	Total	C	N	O	S	0	0
			1916	1180	338	379	19		
4	e	321	Total	C	N	O	S	0	0
			2433	1494	436	481	22		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	g	239	Total	C	N	O	S	0	0
			1822	1137	320	350	15		
5	G	257	Total	C	N	O	S	0	0
			1946	1215	339	377	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	h	339	Total	C	N	O	S	0	0
			2585	1631	454	488	12		
6	H	255	Total	C	N	O	S	0	0
			1929	1216	337	370	6		

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

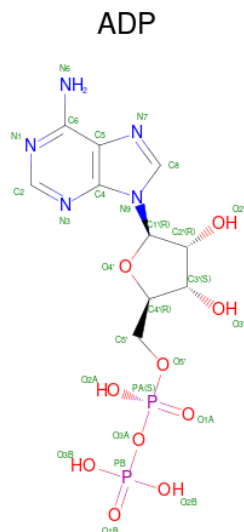
- Molecule 7 is a protein called T-complex protein 1 subunit theta.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	Q	262	Total	C	N	O	S	0	0
			1998	1272	336	379	11		
7	q	338	Total	C	N	O	S	0	0
			2574	1622	438	498	16		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Z	255	Total	C	N	O	S	0	0
			1887	1188	325	364	10		
8	z	316	Total	C	N	O	S	0	0
			2369	1480	420	458	11		

- Molecule 9 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).

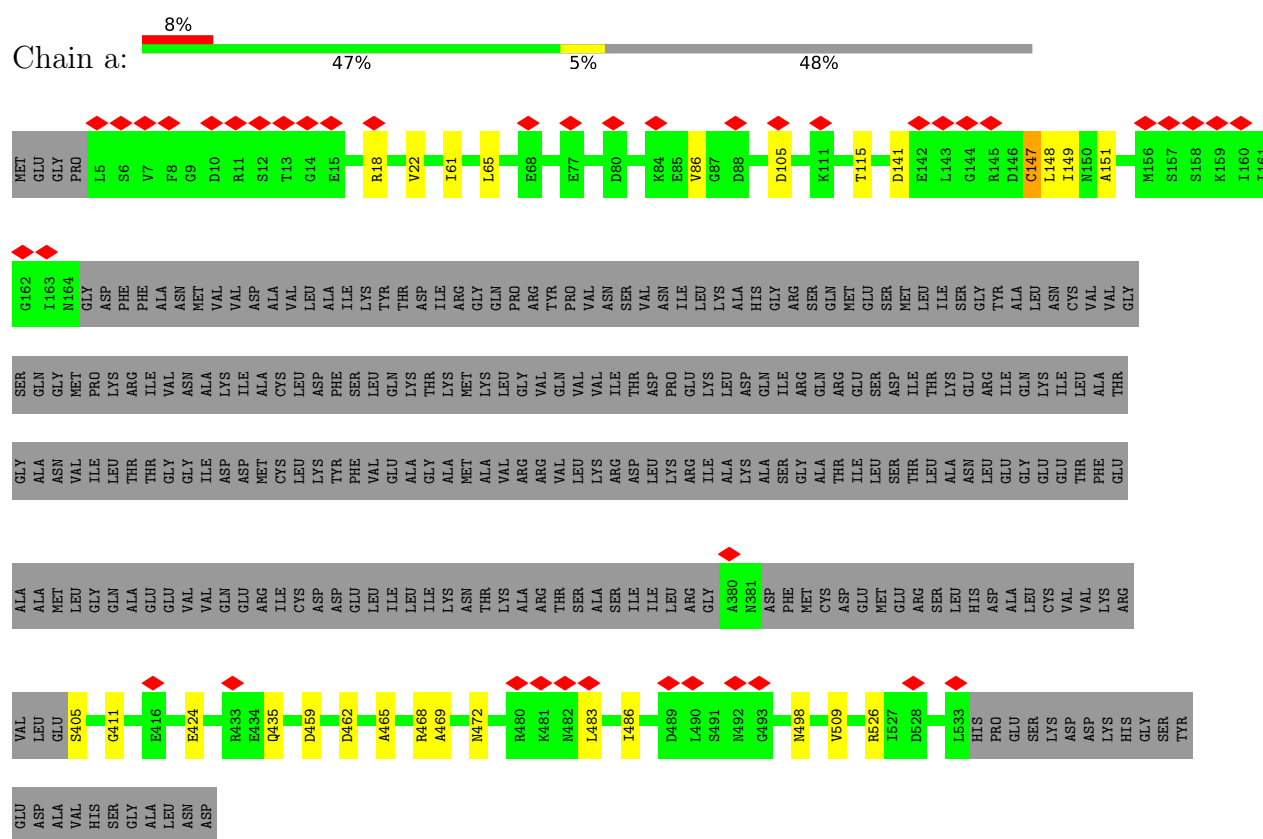


Mol	Chain	Residues	Atoms					AltConf
9	g	1	Total 27	C 10	N 5	O 10	P 2	0
9	G	1	Total 27	C 10	N 5	O 10	P 2	0
9	Q	1	Total 27	C 10	N 5	O 10	P 2	0
9	q	1	Total 27	C 10	N 5	O 10	P 2	0
9	Z	1	Total 27	C 10	N 5	O 10	P 2	0
9	z	1	Total 27	C 10	N 5	O 10	P 2	0

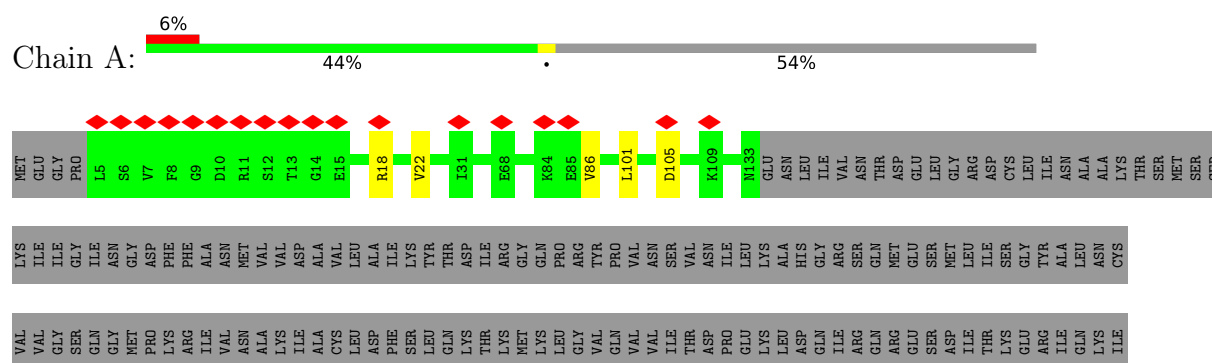
3 Residue-property plots

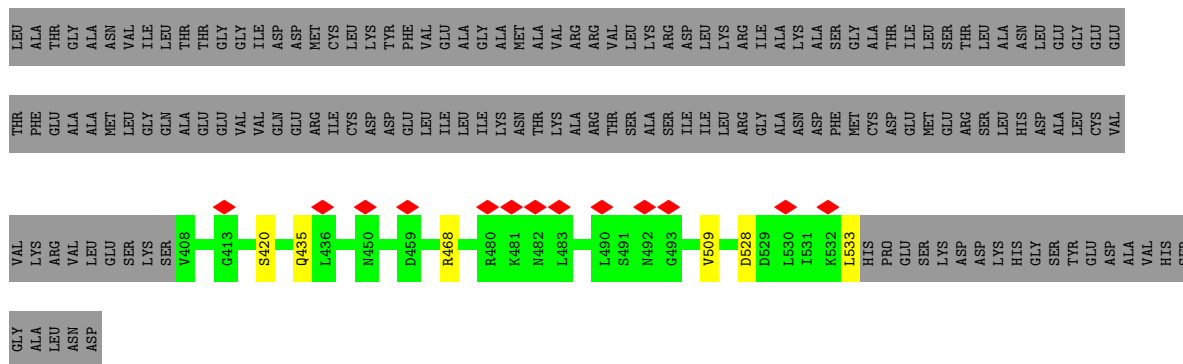
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: T-complex protein 1 subunit alpha

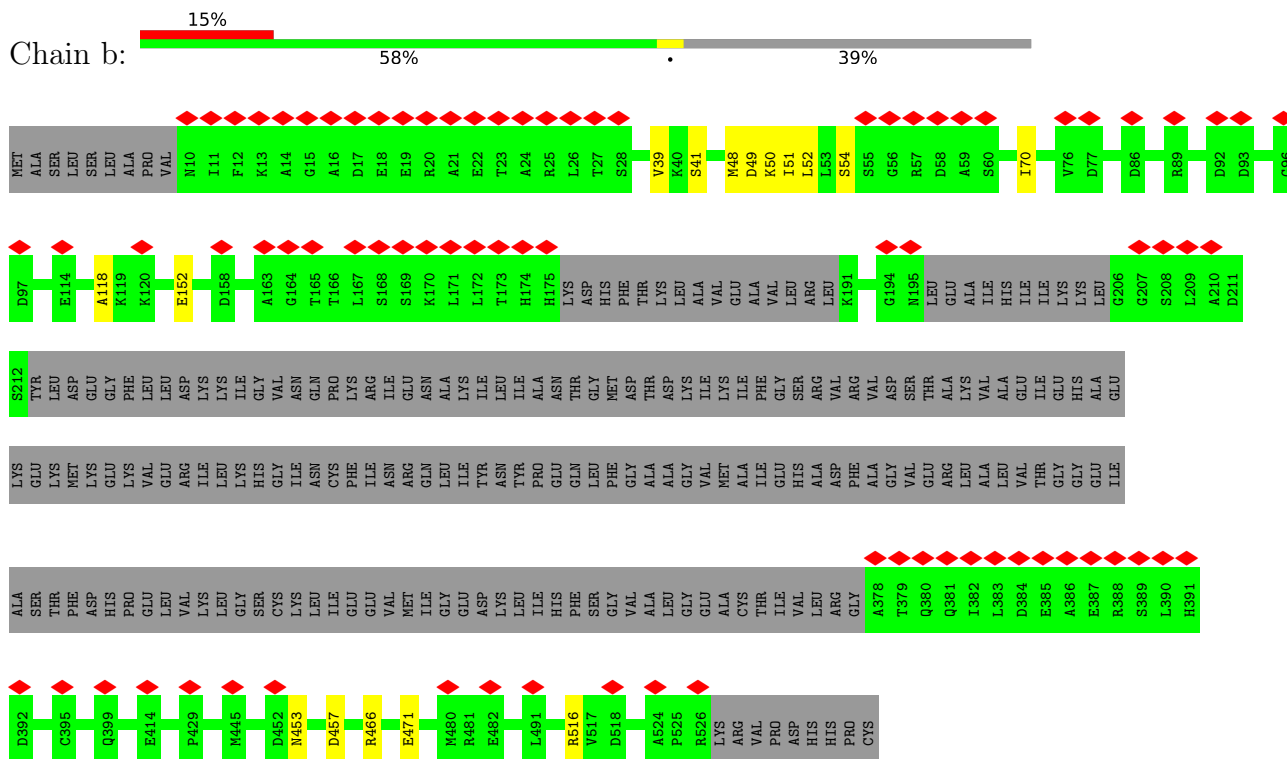


• Molecule 1: T-complex protein 1 subunit alpha

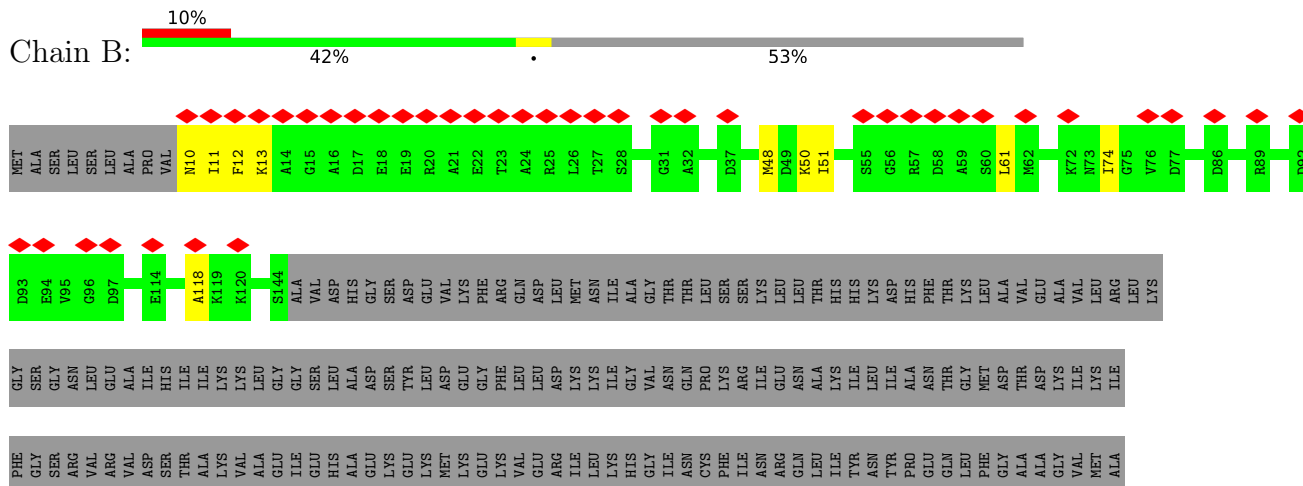


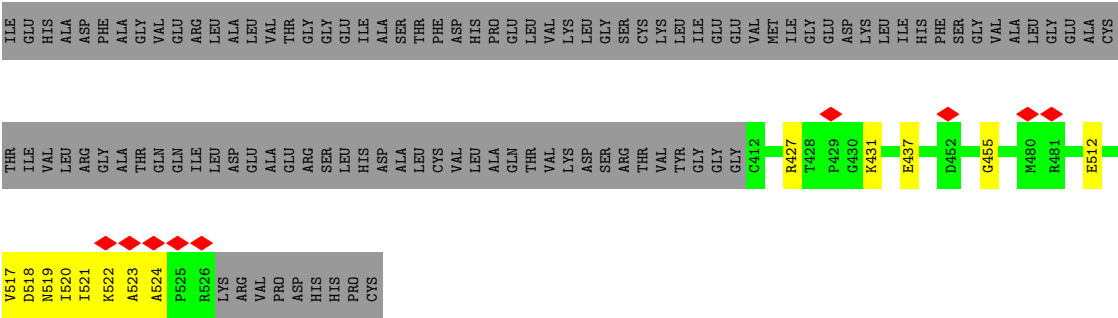


- Molecule 2: T-complex protein 1 subunit beta

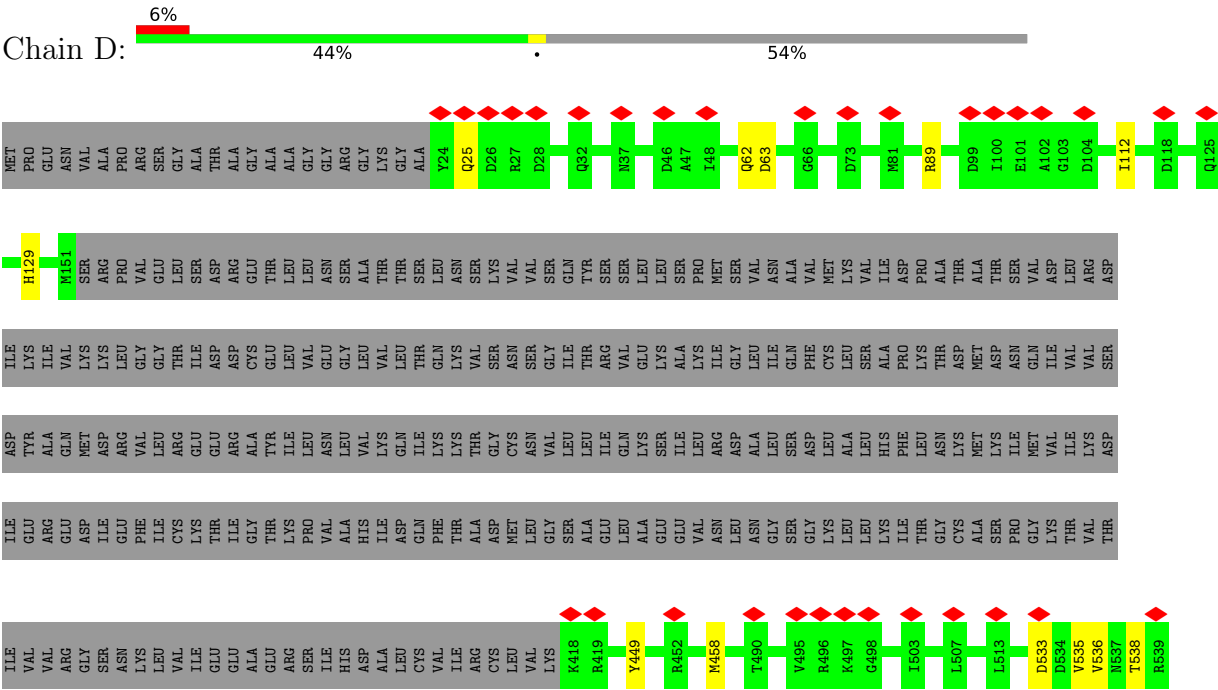


- Molecule 2: T-complex protein 1 subunit beta

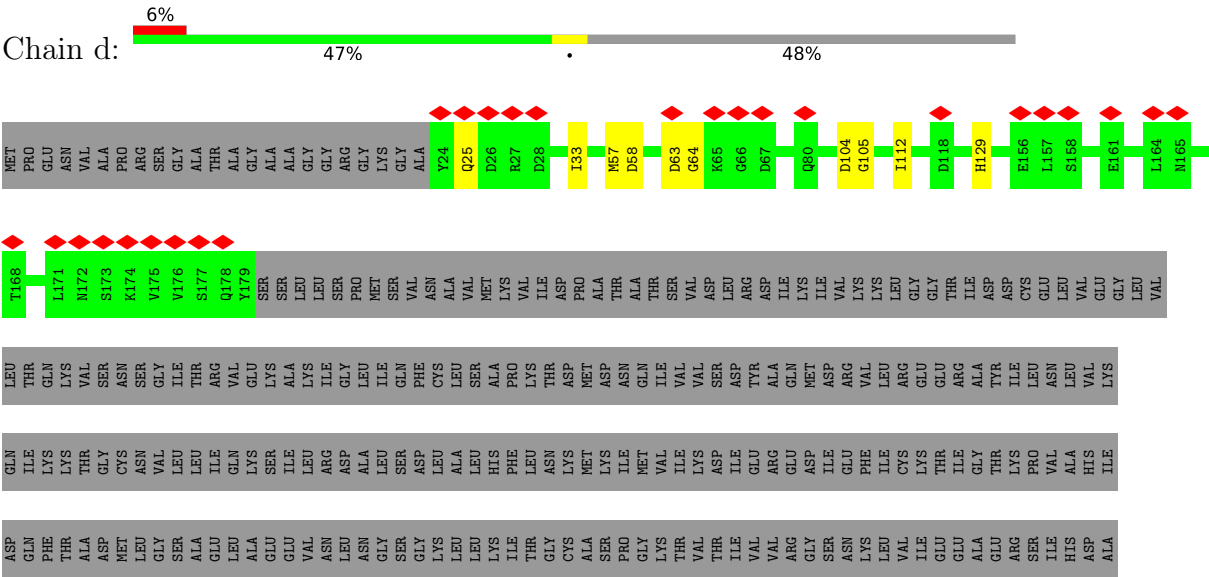


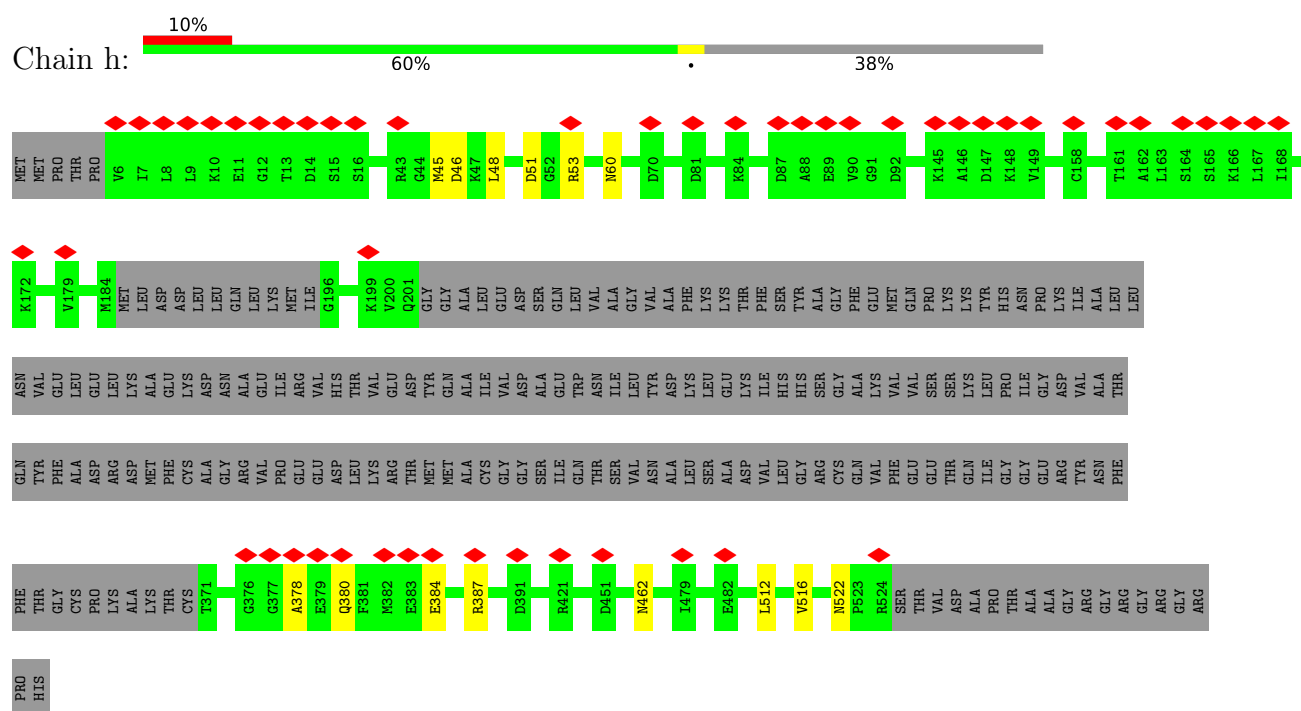


● Molecule 3: T-complex protein 1 subunit delta

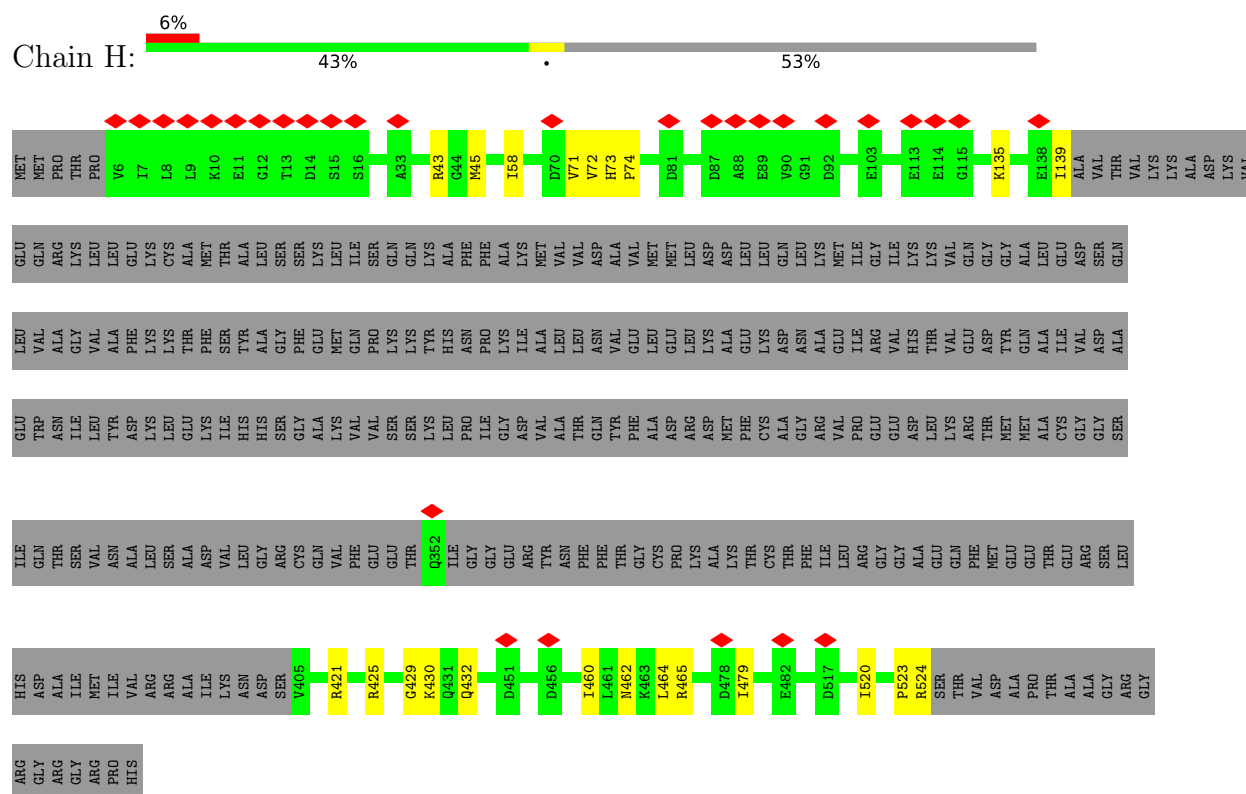


● Molecule 3: T-complex protein 1 subunit delta



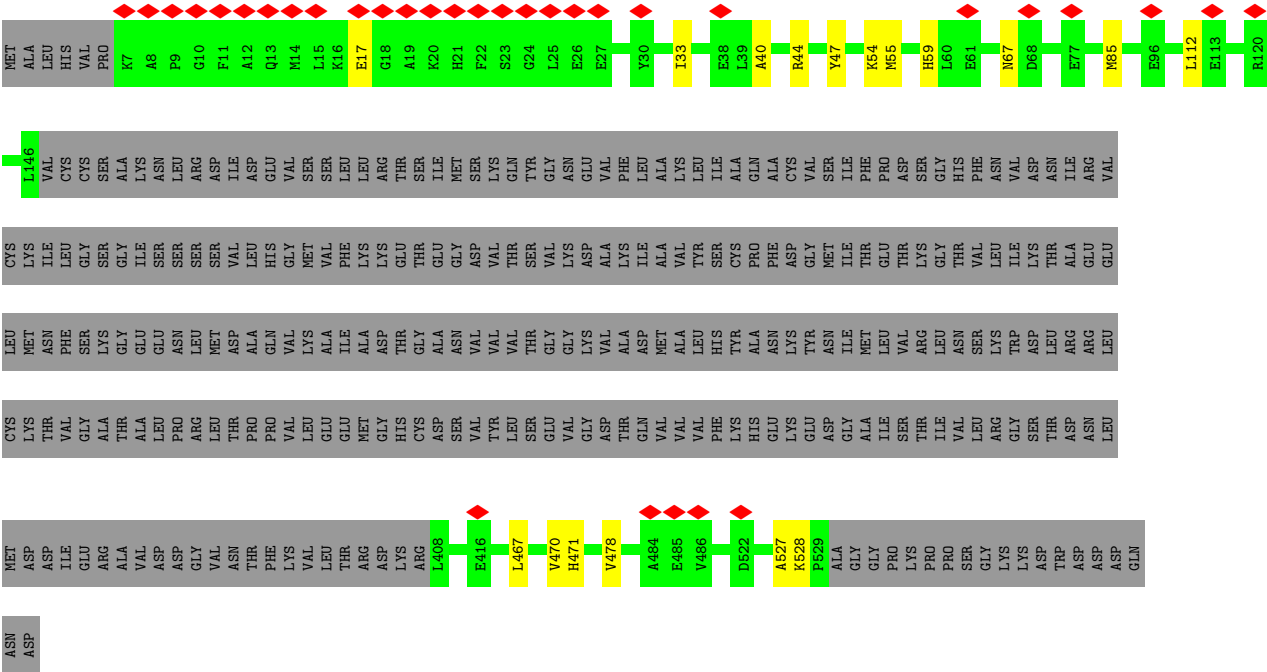


• Molecule 6: T-complex protein 1 subunit eta

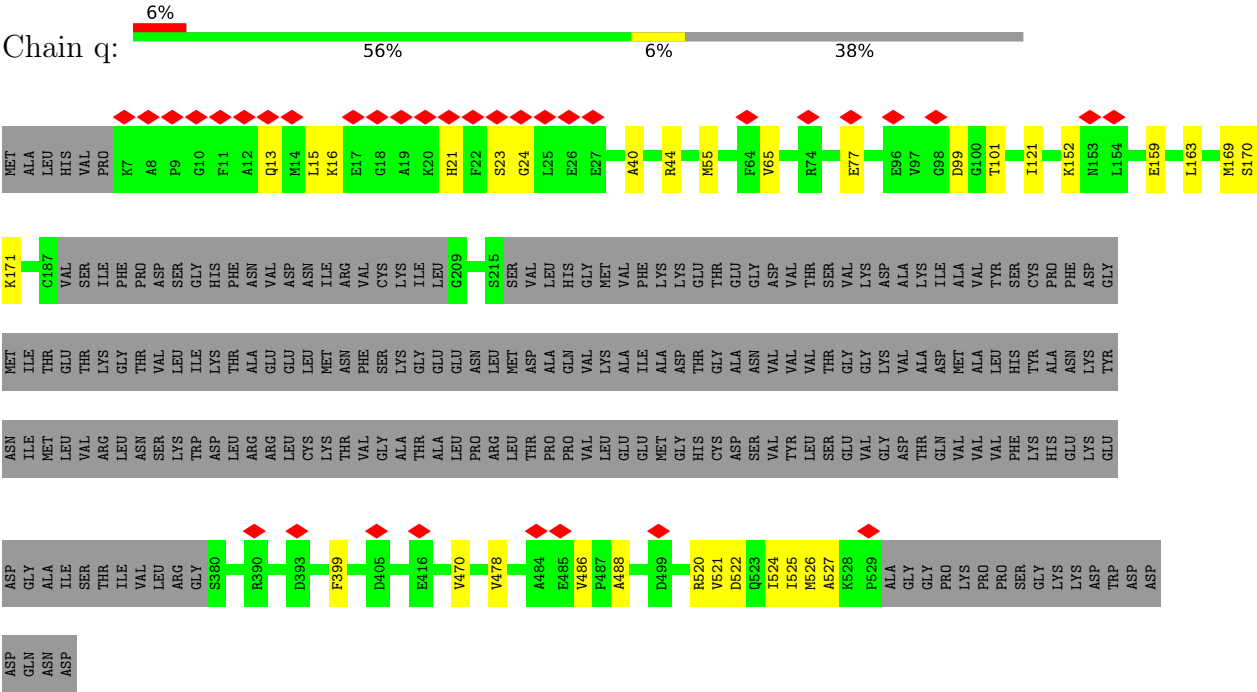


• Molecule 7: T-complex protein 1 subunit theta

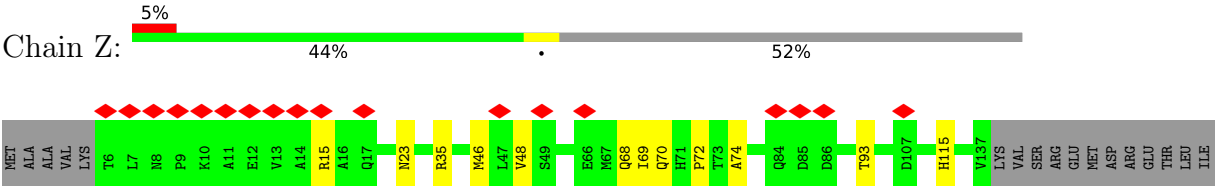




• Molecule 7: T-complex protein 1 subunit theta



• Molecule 8: T-complex protein 1 subunit zeta



ASP	ALA	VAL	VAL	ASP	THR	SER	LEU	ARG	LEU	ALA	THR	GLY	LEU	VAL	ASP	GLY
LEU	VAL	LEU	LEU	ASP	THR	GLY	ALA	ARG	ALA	ARG	THR	LEU	VAL	LEU	VAL	ASP
ARG	LYS	LYS	ILE	ASP	THR	ILE	GLU	LEU	ASP	LEU	THR	LEU	VAL	LEU	VAL	ASP
GLY	VAL	ALA	ALA	ASP	THR	ASP	PHE	LEU	ASP	LEU	THR	LEU	VAL	LEU	VAL	ASP

ALA	VAL	VAL	ASP	GLY	LEU	ARG	ALA	VAL	VAL	LYS	ASN	ALA	ASP	ASP	D404	E415	S428	V429	K430	D442	Q453	D458	E472	S473	G474	G478	M487	E491	I521	M522	G525	M526	SER	LEU	LYS	GLY
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• Molecule 8: T-complex protein 1 subunit zeta



MET	ALA	ALA	VAL	LYS	T6	L7	N8	P9	K10	A11	E12	V13	A14	R15	A16	Q17	R28	T36	T43	M44	K45	M46	L47	V48	S49	D53	L56	L63	E66	M67	Q68	I69	Q70	L76	A81	Q84	D85	D107	E112	M143	D144	R153	T154	R157																		
	H161			L164	ALA	ASP	VAL	VAL	THR	GLU	ALA	VAL	VAL	ASP	SER	ILE	LEU	ALA	ILE	LYS	LYS	GLN	ASP	GLU	PRO	ILE	ASP	PHE	MET	ILE	GLU	ILE	MET	GLU	MET	K197	H198	E201	T202	D203	T204	SER	LEU	ILE	ARG	GLY	LEU	VAL	LYS	LEU	ASP	HIS	GLY	ALA	ARG	HIS	PRO	LYS	ASP	MET		
LYS	LYS	ARG	VAL	GLU	ASP	ALA	ALA	THR	LEU	THR	CYS	ASN	VAL	VAL	ASP	SER	GLU	TYR	GLU	LYS	THR	GLU	VAL	ASN	SER	GLY	PHE	PHE	TYR	LYS	ALA	SER	ALA	GLU	GLU	GLU	LYS	VAL	LYS	ALA	GLU	ARG	GLU	GLY	LEU	VAL	LYS	LYS	ILE	ILE	GLU	LEU	LYS	ARG	LYS	VAL						
CYS	GLY	ASP	SER	ASP	LYS	GLY	PHE	VAL	VAL	ILE	ASN	GLN	GLY	GLY	ILE	ASP	PRO	PHE	SER	LYS	LEU	ASP	ALA	LEU	SER	LYS	GLY	GLY	ILE	VAL	ALA	LEU	ARG	ALA	ALA	LYS	ARG	ARG	ASN	MET	GLU	ARG	GLU	LEU	THR	LYS	LEU	ALA	CYS	GLY	GLY	VAL	ALA	LEU	ASN	SER	PHE	ASP	ASP	LEU	SER	PRO
ASP	CYS	GLY	GLY	HIS	ALA	GLY	LEU	VAL	VAL	TYR	GLU	THR	GLU	GLY	GLY	GLU	GLU	PHE	THR	PHE	THR	ILE	GLU	GLU	LYS	CYS	ASN	ASN	PRO	ARG	THR	THR	LEU	ILE	LYS	GLY	G378	K381	D389	D393	V398	L402	A411	E415	V416	S428	V429	K430	D442	D458												
	T466	Q467	H470	S471	E472	S473	G474		R523	A524	G525	M526	SER	SER	LEU	LYS	GLY	ASP	CYS	ASN	ASN	PRO	ARG	THR	THR	LEU	LEU	LEU	LYS	G378	K381	D389	D393	V398	L402	A411	E415	V416	S428	V429	K430	D442	D458																			

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	185216	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	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	2.892	Depositor
Minimum map value	-1.544	Depositor
Average map value	0.014	Depositor
Map value standard deviation	0.124	Depositor
Recommended contour level	0.663	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	0.14	0/1938	0.26	0/2626
1	a	0.14	0/2201	0.28	0/2978
2	B	0.13	0/1856	0.24	0/2507
2	b	0.13	0/2425	0.25	0/3271
3	D	0.13	0/1885	0.25	0/2544
3	d	0.14	0/2103	0.26	0/2841
4	E	0.13	0/1930	0.27	0/2592
4	e	0.14	0/2450	0.29	0/3293
5	G	0.13	0/1970	0.28	0/2665
5	g	0.13	0/1843	0.27	0/2489
6	H	0.14	0/1952	0.26	0/2645
6	h	0.13	0/2613	0.26	0/3525
7	Q	0.12	0/2028	0.26	0/2741
7	q	0.13	0/2606	0.28	0/3516
8	Z	0.12	0/1907	0.27	0/2582
8	z	0.13	0/2392	0.28	0/3232
All	All	0.13	0/34099	0.27	0/46047

There are no bond length outliers.

There are no bond angle outliers.

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	1918	0	1992	9	0
1	a	2182	0	2264	36	0
2	B	1842	0	1896	54	0
2	b	2407	0	2445	41	0
3	D	1870	0	1948	25	0
3	d	2086	0	2166	46	0
4	E	1916	0	1956	53	0
4	e	2433	0	2492	17	0
5	G	1946	0	2002	48	0
5	g	1822	0	1880	18	0
6	H	1929	0	1983	38	0
6	h	2585	0	2690	14	0
7	Q	1998	0	2033	18	0
7	q	2574	0	2613	39	0
8	Z	1887	0	1951	38	0
8	z	2369	0	2450	53	0
9	G	27	0	12	14	0
9	Q	27	0	12	1	0
9	Z	27	0	12	1	0
9	g	27	0	12	11	0
9	q	27	0	10	5	0
9	z	27	0	12	6	0
All	All	33926	0	34831	343	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 5.

All (343) 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)
8:z:154:THR:HG23	8:z:157:ARG:NH2	1.45	1.28
4:e:527:LYS:NZ	6:h:384:GLU:OE2	1.68	1.25
8:z:154:THR:CG2	8:z:157:ARG:HH22	1.61	1.13
5:G:93:ASP:OD1	9:G:601:ADP:O3A	1.67	1.11
5:G:93:ASP:OD2	9:G:601:ADP:O1A	1.68	1.11
5:g:93:ASP:OD1	9:g:601:ADP:O3A	1.69	1.11
8:z:154:THR:CG2	8:z:157:ARG:NH2	2.13	1.08
5:G:57:ILE:HD11	8:Z:72:PRO:HB2	1.36	1.06
7:q:171:LYS:NZ	9:q:601:ADP:O2B	1.87	1.05
8:z:157:ARG:NE	9:z:601:ADP:HN61	1.55	1.05
8:z:154:THR:HG23	8:z:157:ARG:HH22	0.95	1.04
1:a:141:ASP:HB2	1:a:147:CYS:HB2	1.39	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:129:ILE:HD11	6:H:45:MET:HG2	1.38	1.02
2:B:524:ALA:O	4:E:62:LYS:HB3	1.61	1.01
2:b:118:ALA:HB1	3:D:25:GLN:CG	1.91	1.01
5:g:93:ASP:OD1	9:g:601:ADP:PA	2.18	1.01
8:z:154:THR:HA	8:z:157:ARG:CZ	1.90	1.01
1:a:462:ASP:OD1	6:H:430:LYS:NZ	1.94	1.00
2:B:524:ALA:N	4:E:62:LYS:HG2	1.77	0.99
2:B:523:ALA:HB1	4:E:62:LYS:HG3	1.41	0.99
8:z:153:ARG:O	8:z:157:ARG:HG2	1.61	0.97
8:z:154:THR:HG23	8:z:157:ARG:CZ	1.93	0.97
7:q:16:LYS:NZ	8:z:63:LEU:O	1.97	0.97
5:G:50:LEU:HA	8:Z:522:MET:O	1.64	0.95
5:G:93:ASP:OD1	9:G:601:ADP:PB	2.26	0.94
2:B:51:ILE:HB	3:D:535:VAL:HG23	1.47	0.93
5:g:93:ASP:OD1	9:g:601:ADP:O1A	1.86	0.93
2:B:48:MET:HE2	3:D:533:ASP:OD1	1.67	0.93
8:z:154:THR:CB	8:z:157:ARG:NH2	2.32	0.93
1:a:141:ASP:CB	1:a:147:CYS:HB2	1.99	0.92
2:B:523:ALA:HB1	4:E:62:LYS:CG	2.00	0.91
2:B:48:MET:CE	3:D:533:ASP:OD1	2.20	0.88
5:G:57:ILE:HD11	8:Z:72:PRO:CB	2.04	0.87
2:B:10:ASN:O	4:E:82:ASP:HB2	1.75	0.86
2:b:50:LYS:NZ	3:d:534:ASP:OD1	2.09	0.85
2:B:524:ALA:H	4:E:62:LYS:HG2	1.39	0.85
5:g:57:ILE:HG21	8:z:76:LEU:HD11	1.58	0.85
2:b:52:LEU:HD23	3:d:536:VAL:HB	1.59	0.85
2:B:520:ILE:HA	4:E:58:MET:O	1.77	0.84
5:G:53:PRO:HA	8:Z:526:MET:HG3	1.58	0.84
2:B:524:ALA:O	4:E:62:LYS:CB	2.26	0.84
5:G:70:ILE:HD13	8:Z:522:MET:SD	2.17	0.83
5:G:70:ILE:CD1	8:Z:522:MET:SD	2.67	0.83
5:G:49:MET:HB3	8:Z:521:ILE:HG12	1.61	0.82
2:B:523:ALA:HB3	4:E:62:LYS:N	1.94	0.82
1:a:435:GLN:NE2	6:H:465:ARG:HH11	1.77	0.81
1:a:141:ASP:HB2	1:a:147:CYS:CB	2.11	0.80
8:z:154:THR:OG1	8:z:157:ARG:NH2	2.15	0.80
7:q:527:ALA:N	8:z:48:VAL:O	2.14	0.80
2:b:50:LYS:HG3	3:d:534:ASP:OD1	1.82	0.79
5:g:93:ASP:CG	9:g:601:ADP:O1A	2.26	0.79
2:b:48:MET:CB	3:d:533:ASP:HB2	2.12	0.79
2:b:118:ALA:HB1	3:D:25:GLN:CD	2.08	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:52:LEU:CD2	3:d:536:VAL:HB	2.15	0.77
5:G:57:ILE:CD1	8:Z:72:PRO:HB2	2.15	0.76
1:a:472:ASN:OD1	6:H:425:ARG:HD3	1.86	0.75
2:b:51:ILE:CB	3:d:535:VAL:HG23	2.16	0.75
8:z:154:THR:HG23	8:z:157:ARG:NH1	2.02	0.75
7:q:525:ILE:O	8:z:48:VAL:N	2.13	0.74
2:B:50:LYS:HD3	3:D:536:VAL:CG2	2.18	0.74
8:z:154:THR:HA	8:z:157:ARG:NE	2.02	0.74
7:q:525:ILE:HB	8:z:46:MET:O	1.88	0.73
2:b:51:ILE:HB	3:d:535:VAL:HG23	1.71	0.73
2:b:52:LEU:HA	3:d:536:VAL:O	1.89	0.73
7:q:99:ASP:OD1	9:q:601:ADP:O3A	2.06	0.72
2:b:453:ASN:O	3:d:129:HIS:CE1	2.42	0.72
5:G:32:THR:HG23	8:Z:15:ARG:HH21	1.54	0.72
1:a:141:ASP:OD2	1:a:147:CYS:SG	2.46	0.71
1:a:424:GLU:CD	6:H:421:ARG:HH21	1.98	0.71
2:b:48:MET:HB3	3:d:533:ASP:HB2	1.71	0.71
6:h:60:ASN:OD1	6:h:387:ARG:NH1	2.23	0.71
2:b:51:ILE:HG22	3:d:535:VAL:HG23	1.73	0.71
8:z:154:THR:CA	8:z:157:ARG:CZ	2.67	0.71
1:a:424:GLU:OE2	6:H:421:ARG:NH2	2.25	0.70
2:b:51:ILE:CG2	3:d:535:VAL:HG23	2.22	0.70
2:B:50:LYS:HD3	3:D:536:VAL:HG23	1.74	0.70
2:B:118:ALA:HB1	3:d:25:GLN:HB2	1.74	0.70
5:G:32:THR:HG23	8:Z:15:ARG:NH2	2.07	0.69
5:g:57:ILE:CG2	8:z:76:LEU:HD11	2.22	0.69
7:q:527:ALA:CB	8:z:47:LEU:HD21	2.23	0.69
5:g:94:GLY:N	9:g:601:ADP:O3B	2.27	0.68
3:d:475:SER:OG	4:E:441:LEU:HD21	1.93	0.68
5:G:49:MET:HE1	8:Z:23:ASN:OD1	1.94	0.68
2:b:51:ILE:HB	3:d:535:VAL:CG2	2.24	0.68
2:B:48:MET:HG3	3:D:533:ASP:OD2	1.94	0.68
2:B:523:ALA:HB3	4:E:61:ASP:C	2.18	0.68
1:A:420:SER:OG	1:A:468:ARG:NH1	2.27	0.67
1:a:462:ASP:CG	6:H:430:LYS:HZ2	1.99	0.67
5:G:93:ASP:OD1	9:G:601:ADP:O2B	2.13	0.66
7:q:524:ILE:HA	8:z:46:MET:HB3	1.76	0.66
4:e:531:ILE:HG23	6:h:48:LEU:HD22	1.78	0.66
2:b:118:ALA:HB1	3:D:25:GLN:HG3	1.78	0.65
5:G:57:ILE:CD1	8:Z:72:PRO:CB	2.73	0.65
2:b:118:ALA:HB1	3:D:25:GLN:HG2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:415:GLU:OE2	5:G:502:LYS:NZ	2.30	0.64
6:h:512:LEU:HD11	7:q:65:VAL:HG11	1.80	0.64
2:B:517:VAL:HG21	4:E:58:MET:HE3	1.79	0.64
2:b:54:SER:HA	3:d:538:THR:O	1.97	0.64
2:B:10:ASN:O	4:E:82:ASP:C	2.41	0.64
7:q:99:ASP:OD2	9:q:601:ADP:O1A	2.16	0.63
8:z:157:ARG:NE	9:z:601:ADP:N6	2.38	0.63
2:B:61:LEU:HD22	3:D:89:ARG:CZ	2.28	0.62
1:a:472:ASN:OD1	6:H:425:ARG:CD	2.47	0.62
2:B:48:MET:HG3	3:D:533:ASP:CG	2.23	0.62
2:B:48:MET:HE3	3:D:533:ASP:OD1	1.99	0.62
7:q:527:ALA:CB	8:z:47:LEU:CD2	2.77	0.62
7:Q:528:LYS:HB3	8:Z:68:GLN:HG3	1.81	0.62
1:a:411:GLY:O	1:a:498:ASN:ND2	2.32	0.62
5:G:460:ILE:HD11	7:q:121:ILE:O	1.98	0.62
5:G:94:GLY:N	9:G:601:ADP:O3B	2.33	0.62
2:b:51:ILE:HB	3:d:535:VAL:CB	2.31	0.61
7:q:171:LYS:HE2	9:q:601:ADP:O2A	2.00	0.61
2:B:521:ILE:O	4:E:60:VAL:N	2.23	0.61
5:g:93:ASP:OD2	9:g:601:ADP:O1A	2.19	0.61
1:a:472:ASN:CG	6:H:425:ARG:HB3	2.25	0.61
5:g:95:THR:N	9:g:601:ADP:O3B	2.34	0.60
7:Q:47:TYR:CZ	9:Q:601:ADP:H4'	2.36	0.60
2:B:10:ASN:O	4:E:82:ASP:CB	2.49	0.60
5:G:50:LEU:HD23	8:Z:522:MET:HB3	1.83	0.60
5:G:93:ASP:OD1	9:G:601:ADP:PA	2.60	0.60
7:q:152:LYS:N	7:q:159:GLU:OE2	2.34	0.59
2:b:50:LYS:HA	3:d:534:ASP:O	2.02	0.59
5:G:497:GLU:OE2	9:G:601:ADP:H3'	2.01	0.59
6:h:516:VAL:HG21	7:q:55:MET:HE3	1.83	0.59
2:b:51:ILE:HB	3:d:535:VAL:HB	1.84	0.59
2:B:518:ASP:OD1	4:E:56:ASP:O	2.20	0.59
4:E:18:LYS:N	6:H:72:VAL:CG1	2.66	0.59
4:e:147:ASP:OD1	4:e:415:ARG:NH1	2.35	0.59
8:z:157:ARG:CZ	9:z:601:ADP:HN61	2.16	0.59
2:B:74:ILE:CG1	3:D:538:THR:HG22	2.33	0.58
1:a:469:ALA:HA	6:H:425:ARG:O	2.03	0.58
2:B:523:ALA:HB1	4:E:62:LYS:HG2	1.84	0.58
1:a:424:GLU:OE2	6:H:421:ARG:NE	2.37	0.58
2:b:49:ASP:N	3:d:531:LYS:O	2.35	0.58
2:b:51:ILE:O	3:d:536:VAL:N	2.23	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:q:526:MET:HA	8:z:48:VAL:O	2.04	0.58
4:E:129:ILE:CD1	6:H:45:MET:HG2	2.23	0.58
6:H:523:PRO:O	6:H:524:ARG:NH1	2.35	0.58
1:A:18:ARG:NH1	1:A:528:ASP:OD2	2.36	0.58
4:e:529:ASP:OD1	6:h:46:ASP:O	2.22	0.58
2:B:74:ILE:HG12	3:D:538:THR:HG22	1.86	0.57
2:B:512:GLU:OE2	2:B:516:ARG:NH2	2.37	0.57
5:g:94:GLY:H	9:g:601:ADP:PB	2.27	0.57
2:b:50:LYS:HZ3	3:d:534:ASP:CG	2.07	0.57
7:q:527:ALA:O	8:z:49:SER:HA	2.05	0.57
8:z:154:THR:HA	8:z:157:ARG:NH2	2.20	0.57
5:G:94:GLY:CA	9:G:601:ADP:O3B	2.52	0.57
5:G:495:ILE:HD12	9:G:601:ADP:N6	2.19	0.57
7:q:525:ILE:HG21	8:z:67:MET:SD	2.45	0.56
7:q:470:VAL:HG21	7:q:478:VAL:HG11	1.88	0.56
8:Z:35:ARG:NH1	8:Z:453:GLN:OE1	2.38	0.56
5:G:454:ASN:O	8:Z:115:HIS:CE1	2.58	0.56
2:B:50:LYS:HD3	3:D:536:VAL:HG21	1.88	0.56
2:B:517:VAL:HG11	4:E:58:MET:HB2	1.87	0.56
5:G:53:PRO:CA	8:Z:526:MET:HA	2.36	0.56
2:b:457:ASP:OD2	2:B:431:LYS:NZ	2.39	0.56
1:a:526:ARG:NE	3:d:58:ASP:OD2	2.35	0.55
2:B:10:ASN:C	4:E:82:ASP:HB2	2.30	0.55
4:E:22:ARG:NH1	4:E:536:GLU:O	2.40	0.55
8:z:154:THR:CA	8:z:157:ARG:NH2	2.69	0.55
2:b:118:ALA:HB1	3:D:25:GLN:NE2	2.22	0.55
5:G:49:MET:HE1	8:Z:23:ASN:CG	2.32	0.55
4:E:524:MET:HE2	6:H:58:ILE:HD13	1.89	0.55
2:b:41:SER:OG	3:d:533:ASP:OD1	2.20	0.54
5:G:49:MET:O	8:Z:522:MET:N	2.41	0.54
5:G:49:MET:O	8:Z:521:ILE:HA	2.08	0.54
1:a:435:GLN:OE1	6:H:462:ASN:HA	2.08	0.54
2:B:521:ILE:HD12	4:E:59:MET:HG2	1.90	0.54
2:B:12:PHE:HA	4:E:82:ASP:OD1	2.08	0.53
5:G:93:ASP:CG	9:G:601:ADP:O1A	2.50	0.53
3:D:449:TYR:OH	4:e:476:ARG:NH2	2.41	0.53
1:a:472:ASN:CB	6:H:425:ARG:HB3	2.39	0.53
2:B:455:GLY:HA2	3:D:129:HIS:CG	2.44	0.53
2:b:48:MET:HB2	3:d:533:ASP:HB2	1.88	0.53
7:Q:40:ALA:O	7:Q:44:ARG:N	2.41	0.52
2:b:49:ASP:HB2	3:d:532:ILE:HD13	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:148:LEU:O	1:a:151:ALA:N	2.40	0.52
5:g:94:GLY:CA	9:g:601:ADP:O3B	2.57	0.52
1:a:465:ALA:CB	6:H:429:GLY:O	2.58	0.52
3:d:33:ILE:HD13	3:d:534:ASP:HA	1.92	0.52
8:z:157:ARG:CD	9:z:601:ADP:HN61	2.21	0.52
1:A:435:GLN:NE2	6:h:462:ASN:O	2.43	0.52
1:a:141:ASP:HB3	1:a:147:CYS:HB2	1.86	0.51
7:Q:467:LEU:O	7:Q:471:HIS:ND1	2.43	0.51
1:a:115:THR:OG1	3:d:57:MET:HE3	2.09	0.51
6:h:522:ASN:ND2	7:q:77:GLU:OE2	2.38	0.51
4:E:120:GLN:O	4:E:120:GLN:NE2	2.43	0.51
7:q:163:LEU:HD12	7:q:399:PHE:CZ	2.45	0.51
8:z:154:THR:CG2	8:z:157:ARG:CZ	2.72	0.51
8:z:157:ARG:CZ	9:z:601:ADP:N6	2.74	0.51
7:q:13:GLN:O	7:q:21:HIS:ND1	2.41	0.51
8:z:523:ARG:NH1	8:z:526:MET:SD	2.83	0.51
2:B:523:ALA:CB	4:E:62:LYS:HG3	2.28	0.51
2:B:523:ALA:CB	4:E:62:LYS:N	2.72	0.51
7:q:40:ALA:O	7:q:44:ARG:N	2.43	0.50
7:q:525:ILE:HD13	8:z:67:MET:SD	2.52	0.50
2:b:51:ILE:C	3:d:535:VAL:HG23	2.36	0.50
1:a:459:ASP:OD2	6:H:430:LYS:NZ	2.45	0.50
7:Q:470:VAL:HG21	7:Q:478:VAL:HG11	1.94	0.50
7:q:524:ILE:HG12	8:z:46:MET:SD	2.51	0.50
1:a:472:ASN:CG	6:H:425:ARG:CB	2.85	0.50
2:b:453:ASN:O	3:d:129:HIS:HE1	1.92	0.50
7:q:163:LEU:HD12	7:q:399:PHE:HZ	1.75	0.50
5:G:49:MET:CB	8:Z:521:ILE:HG12	2.37	0.50
6:H:520:ILE:HD12	7:Q:54:LYS:HB3	1.93	0.50
4:e:416:VAL:HG12	4:e:507:THR:HA	1.93	0.49
4:E:442:GLU:N	4:E:442:GLU:OE1	2.45	0.49
7:q:527:ALA:HB3	8:z:47:LEU:CD2	2.42	0.49
5:G:49:MET:HB3	8:Z:521:ILE:CG1	2.40	0.49
5:G:415:GLU:OE1	5:G:415:GLU:N	2.45	0.49
2:b:50:LYS:HD3	3:d:536:VAL:CG2	2.42	0.49
2:B:12:PHE:CA	4:E:82:ASP:OD1	2.59	0.49
7:q:23:SER:OG	7:q:24:GLY:N	2.44	0.49
3:d:429:GLU:N	3:d:429:GLU:OE1	2.46	0.49
5:G:36:ILE:HD11	8:Z:522:MET:HE1	1.93	0.49
5:G:70:ILE:HD11	8:Z:522:MET:SD	2.52	0.49
2:b:51:ILE:CG2	3:d:535:VAL:CG2	2.89	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:416:VAL:HG12	4:E:507:THR:HA	1.94	0.49
8:z:415:GLU:OE1	8:z:415:GLU:N	2.46	0.49
4:e:529:ASP:HB3	6:h:45:MET:CE	2.43	0.49
2:b:516:ARG:O	4:e:56:ASP:N	2.46	0.48
5:G:36:ILE:CD1	8:Z:522:MET:HE1	2.43	0.48
3:d:449:TYR:CE2	4:E:469:ILE:HG23	2.49	0.48
3:d:478:THR:OG1	4:E:444:TYR:HE1	1.96	0.48
8:Z:93:THR:HB	9:Z:601:ADP:O3B	2.13	0.48
6:H:43:ARG:NH1	6:H:479:ILE:O	2.46	0.48
2:b:51:ILE:HG22	3:d:535:VAL:CG2	2.42	0.48
4:E:424:GLU:N	4:E:424:GLU:OE1	2.47	0.48
7:Q:85:MET:CE	8:Z:46:MET:HE2	2.43	0.48
4:e:424:GLU:N	4:e:424:GLU:OE1	2.47	0.48
7:q:520:ARG:CD	8:z:161:HIS:ND1	2.77	0.48
2:B:522:LYS:HA	4:E:60:VAL:HB	1.96	0.47
2:B:519:ASN:O	4:E:58:MET:N	2.45	0.47
2:B:523:ALA:CB	4:E:62:LYS:CG	2.84	0.47
1:a:18:ARG:O	1:a:22:VAL:HG23	2.15	0.47
6:H:524:ARG:NE	7:Q:59:HIS:HB2	2.30	0.47
1:a:435:GLN:CD	6:H:465:ARG:HH11	2.23	0.47
1:A:18:ARG:O	1:A:22:VAL:HG23	2.15	0.47
6:h:51:ASP:OD2	6:h:53:ARG:NE	2.45	0.47
2:B:11:ILE:O	4:E:81:VAL:HA	2.15	0.47
3:D:112:ILE:HG23	3:D:458:MET:HE1	1.96	0.47
3:d:478:THR:OG1	4:E:444:TYR:CE1	2.68	0.47
5:g:490:MET:O	5:g:496:TRP:NE1	2.48	0.47
5:g:520:ASP:OD1	5:g:520:ASP:N	2.47	0.47
1:a:468:ARG:NH1	6:H:432:GLN:OE1	2.41	0.46
1:A:533:LEU:HD22	3:D:63:ASP:HA	1.97	0.46
2:B:11:ILE:O	4:E:82:ASP:N	2.32	0.46
7:Q:528:LYS:O	8:Z:68:GLN:NE2	2.49	0.46
1:a:462:ASP:OD1	6:H:430:LYS:CE	2.64	0.46
5:G:497:GLU:OE2	9:G:601:ADP:H2'	2.15	0.46
8:z:416:VAL:HG21	8:z:466:ILE:HD12	1.98	0.46
2:b:152:GLU:N	2:b:152:GLU:OE1	2.48	0.46
4:e:45:THR:O	4:e:57:LYS:NZ	2.44	0.46
5:G:113:LEU:O	5:G:116:GLN:NE2	2.48	0.46
7:q:522:ASP:OD1	8:z:44:MET:O	2.32	0.46
1:A:86:VAL:HG11	1:A:509:VAL:HG22	1.96	0.46
7:q:169:MET:O	7:q:170:SER:OG	2.28	0.46
3:d:475:SER:OG	4:E:441:LEU:CD2	2.63	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:74:PRO:CB	7:Q:55:MET:SD	3.04	0.45
7:q:524:ILE:HG23	8:z:46:MET:SD	2.56	0.45
7:q:527:ALA:HB3	8:z:47:LEU:HD23	1.98	0.45
8:Z:478:GLY:N	8:Z:487:MET:O	2.46	0.45
2:B:13:LYS:N	4:E:82:ASP:OD1	2.49	0.45
4:e:478:ARG:NH1	4:e:482:GLU:OE1	2.49	0.45
5:G:50:LEU:CD2	8:Z:522:MET:HB3	2.45	0.45
5:G:112:PHE:HE1	5:G:122:VAL:HG21	1.81	0.45
8:Z:415:GLU:OE1	8:Z:415:GLU:N	2.49	0.45
8:z:467:GLN:O	8:z:470:HIS:NE2	2.50	0.45
1:a:22:VAL:HG21	1:a:105:ASP:HB2	1.98	0.45
4:e:524:MET:SD	6:h:380:GLN:CD	2.99	0.45
2:B:10:ASN:O	4:E:83:HIS:N	2.49	0.44
5:G:495:ILE:HD12	9:G:601:ADP:C6	2.52	0.44
3:d:104:ASP:OD1	3:d:105:GLY:N	2.50	0.44
5:G:497:GLU:OE2	9:G:601:ADP:C3'	2.66	0.44
6:H:460:ILE:O	6:H:464:LEU:N	2.49	0.44
7:Q:17:GLU:H	8:Z:70:GLN:HB2	1.82	0.44
7:q:101:THR:N	9:q:601:ADP:O1B	2.50	0.44
7:q:521:VAL:HG22	8:z:56:LEU:HD22	1.98	0.44
2:B:51:ILE:CB	3:D:535:VAL:HG23	2.32	0.44
7:q:486:VAL:HG12	7:q:488:ALA:H	1.83	0.44
7:Q:527:ALA:HB3	8:Z:48:VAL:O	2.17	0.44
7:q:526:MET:HA	8:z:48:VAL:HB	2.00	0.44
4:e:520:GLN:HE22	6:h:378:ALA:CB	2.31	0.44
5:G:42:GLY:O	5:G:45:SER:OG	2.35	0.44
2:B:524:ALA:O	4:E:62:LYS:CA	2.65	0.44
4:E:524:MET:CE	6:H:58:ILE:HD13	2.48	0.44
7:q:15:LEU:O	8:z:70:GLN:N	2.39	0.44
5:g:415:GLU:OE1	5:g:415:GLU:N	2.50	0.43
5:g:415:GLU:OE2	5:g:502:LYS:NZ	2.50	0.43
2:B:74:ILE:HG13	3:D:538:THR:HG22	2.00	0.43
8:z:398:VAL:HG12	8:z:402:ILE:HD12	2.00	0.43
2:B:517:VAL:CG1	4:E:58:MET:HB2	2.47	0.43
4:E:45:THR:O	4:E:57:LYS:NZ	2.29	0.43
1:A:22:VAL:HG22	1:A:101:LEU:HB3	2.01	0.43
1:a:86:VAL:HG11	1:a:509:VAL:HG22	2.01	0.43
2:b:50:LYS:CG	3:d:534:ASP:O	2.67	0.43
2:b:466:ARG:NH1	2:B:437:GLU:OE2	2.52	0.43
8:z:144:ASP:OD1	8:z:144:ASP:N	2.52	0.43
1:a:483:LEU:HD13	1:a:486:ILE:HD11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:61:LEU:HD22	3:D:89:ARG:NH1	2.34	0.43
4:e:159:ASP:OD1	4:e:160:THR:N	2.50	0.43
8:z:154:THR:O	8:z:157:ARG:NH1	2.52	0.42
4:E:18:LYS:N	6:H:72:VAL:HG13	2.34	0.42
6:H:71:VAL:HG12	6:H:73:HIS:H	1.85	0.42
7:q:527:ALA:HB2	8:z:47:LEU:CD2	2.50	0.42
4:e:529:ASP:OD2	6:h:45:MET:CB	2.67	0.42
6:H:74:PRO:HB2	7:Q:55:MET:SD	2.60	0.42
2:b:471:GLU:OE2	2:B:427:ARG:NE	2.53	0.42
1:a:424:GLU:CD	6:H:421:ARG:NH2	2.74	0.42
1:a:424:GLU:OE2	6:H:421:ARG:CZ	2.67	0.42
3:d:474:ILE:HG21	4:E:126:ILE:HD11	2.02	0.42
1:a:435:GLN:CD	6:H:465:ARG:NH1	2.78	0.42
4:e:529:ASP:HB3	6:h:45:MET:HE2	2.00	0.42
7:Q:33:ILE:HG23	7:Q:112:LEU:HB3	2.02	0.42
5:G:136:THR:HG21	5:G:418:VAL:HA	2.02	0.42
7:Q:528:LYS:CB	8:Z:68:GLN:HG3	2.48	0.42
8:z:411:ALA:HB2	9:z:601:ADP:C2	2.54	0.42
1:a:61:ILE:O	1:a:65:LEU:N	2.50	0.42
1:A:533:LEU:HD13	3:D:62:GLN:O	2.20	0.42
2:b:39:VAL:HG12	2:b:70:ILE:HG21	2.02	0.41
8:z:36:THR:O	8:z:43:THR:N	2.48	0.41
6:H:74:PRO:HB3	7:Q:55:MET:SD	2.61	0.41
1:A:22:VAL:HG21	1:A:105:ASP:HB2	2.01	0.41
5:g:94:GLY:C	9:g:601:ADP:O3B	2.63	0.41
5:G:53:PRO:HA	8:Z:526:MET:HA	2.01	0.41
7:Q:67:ASN:OD1	7:Q:67:ASN:N	2.53	0.41
1:a:148:LEU:O	1:a:149:ILE:C	2.64	0.41
3:d:478:THR:HG1	4:E:444:TYR:HE1	1.61	0.41
5:g:497:GLU:OE2	9:g:601:ADP:H3'	2.21	0.41
2:b:50:LYS:NZ	3:d:534:ASP:CG	2.74	0.41
2:B:521:ILE:N	4:E:58:MET:O	2.50	0.41
3:d:112:ILE:HG23	3:d:458:MET:HE1	2.03	0.41
4:e:154:LEU:HD21	4:e:162:PRO:HG2	2.02	0.41
5:G:94:GLY:H	9:G:601:ADP:PB	2.43	0.41
6:H:135:LYS:O	6:H:139:ILE:HG22	2.20	0.41
5:G:53:PRO:HB3	8:Z:526:MET:HA	2.03	0.41
3:d:449:TYR:HE2	4:E:469:ILE:HG12	1.86	0.40
5:g:136:THR:HG21	5:g:418:VAL:HA	2.02	0.40
5:G:53:PRO:CB	8:Z:526:MET:HA	2.51	0.40
8:z:154:THR:CG2	8:z:157:ARG:NH1	2.80	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:d:63:ASP:OD2	3:d:64:GLY:N	2.53	0.40
6:H:524:ARG:HE	7:Q:59:HIS:HB2	1.85	0.40
8:Z:69:ILE:HG21	8:Z:74:ALA:HB3	2.04	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	251/556 (45%)	250 (100%)	1 (0%)	0	100	100
1	a	285/556 (51%)	273 (96%)	12 (4%)	0	100	100
2	B	246/535 (46%)	239 (97%)	7 (3%)	0	100	100
2	b	319/535 (60%)	311 (98%)	8 (2%)	0	100	100
3	D	246/539 (46%)	245 (100%)	1 (0%)	0	100	100
3	d	274/539 (51%)	270 (98%)	4 (2%)	0	100	100
4	E	249/539 (46%)	243 (98%)	6 (2%)	0	100	100
4	e	315/539 (58%)	305 (97%)	10 (3%)	0	100	100
5	G	253/545 (46%)	244 (96%)	9 (4%)	0	100	100
5	g	235/545 (43%)	228 (97%)	7 (3%)	0	100	100
6	H	250/543 (46%)	245 (98%)	5 (2%)	0	100	100
6	h	333/543 (61%)	326 (98%)	7 (2%)	0	100	100
7	Q	258/548 (47%)	248 (96%)	10 (4%)	0	100	100
7	q	332/548 (61%)	320 (96%)	12 (4%)	0	100	100
8	Z	251/531 (47%)	248 (99%)	3 (1%)	0	100	100
8	z	310/531 (58%)	305 (98%)	5 (2%)	0	100	100
All	All	4407/8672 (51%)	4300 (98%)	107 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	209/463 (45%)	209 (100%)	0	100	100
1	a	240/463 (52%)	238 (99%)	2 (1%)	73	81
2	B	192/427 (45%)	192 (100%)	0	100	100
2	b	253/427 (59%)	253 (100%)	0	100	100
3	D	205/452 (45%)	205 (100%)	0	100	100
3	d	232/452 (51%)	232 (100%)	0	100	100
4	E	208/455 (46%)	208 (100%)	0	100	100
4	e	268/455 (59%)	268 (100%)	0	100	100
5	G	215/469 (46%)	215 (100%)	0	100	100
5	g	200/469 (43%)	200 (100%)	0	100	100
6	H	205/443 (46%)	205 (100%)	0	100	100
6	h	276/443 (62%)	276 (100%)	0	100	100
7	Q	207/452 (46%)	207 (100%)	0	100	100
7	q	274/452 (61%)	274 (100%)	0	100	100
8	Z	201/442 (46%)	201 (100%)	0	100	100
8	z	255/442 (58%)	255 (100%)	0	100	100
All	All	3640/7206 (50%)	3638 (100%)	2 (0%)	87	90

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	147	CYS
1	a	405	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	a	133	ASN
1	a	435	GLN
2	b	380	GLN
3	d	129	HIS
3	d	537	ASN
4	E	493	HIS
4	e	443	GLN
4	e	520	GLN
6	h	380	GLN
6	H	17	GLN
6	H	25	ASN
7	q	477	ASN
7	q	523	GLN
8	z	23	ASN
8	z	482	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	Z	601	-	28,29,29	1.43	4 (14%)	43,45,45	1.83	10 (23%)
9	ADP	g	601	-	28,29,29	1.43	5 (17%)	43,45,45	1.82	9 (20%)
9	ADP	Q	601	-	28,29,29	1.44	5 (17%)	43,45,45	1.83	9 (20%)
9	ADP	q	601	-	28,29,29	1.43	5 (17%)	43,45,45	1.83	9 (20%)
9	ADP	z	601	-	28,29,29	1.43	4 (14%)	43,45,45	1.84	10 (23%)
9	ADP	G	601	-	28,29,29	1.43	5 (17%)	43,45,45	1.83	9 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	ADP	Z	601	-	-	2/16/32/32	0/3/3/3
9	ADP	g	601	-	-	2/16/32/32	0/3/3/3
9	ADP	Q	601	-	-	2/16/32/32	0/3/3/3
9	ADP	q	601	-	-	2/16/32/32	0/3/3/3
9	ADP	z	601	-	-	2/16/32/32	0/3/3/3
9	ADP	G	601	-	-	2/16/32/32	0/3/3/3

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	Q	601	ADP	C5-C4	4.79	1.47	1.39
9	G	601	ADP	C5-C4	4.78	1.47	1.39
9	q	601	ADP	C5-C4	4.75	1.47	1.39
9	g	601	ADP	C5-C4	4.75	1.47	1.39
9	z	601	ADP	C5-C4	4.75	1.47	1.39
9	Z	601	ADP	C5-C4	4.73	1.47	1.39
9	Z	601	ADP	C5-C6	2.77	1.48	1.41
9	g	601	ADP	C5-C6	2.76	1.48	1.41
9	Q	601	ADP	C5-C6	2.73	1.48	1.41
9	q	601	ADP	C5-C6	2.73	1.48	1.41
9	z	601	ADP	C5-C6	2.73	1.48	1.41
9	G	601	ADP	C5-C6	2.71	1.48	1.41
9	Z	601	ADP	C8-N7	2.43	1.36	1.31
9	Q	601	ADP	C8-N7	2.42	1.36	1.31
9	g	601	ADP	C8-N7	2.40	1.36	1.31
9	z	601	ADP	C8-N7	2.38	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	q	601	ADP	C8-N7	2.36	1.36	1.31
9	G	601	ADP	C8-N7	2.32	1.36	1.31
9	Z	601	ADP	C5-N7	-2.26	1.35	1.39
9	Q	601	ADP	C5-N7	-2.24	1.35	1.39
9	q	601	ADP	C5-N7	-2.22	1.35	1.39
9	g	601	ADP	C5-N7	-2.21	1.35	1.39
9	z	601	ADP	C5-N7	-2.21	1.35	1.39
9	G	601	ADP	C5-N7	-2.20	1.35	1.39
9	Q	601	ADP	PA-O3A	2.08	1.61	1.59
9	g	601	ADP	PA-O3A	2.03	1.61	1.59
9	q	601	ADP	PA-O3A	2.01	1.61	1.59
9	G	601	ADP	PA-O3A	2.00	1.61	1.59

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	G	601	ADP	C5-C4-N3	-5.88	118.62	126.72
9	z	601	ADP	C5-C4-N3	-5.87	118.64	126.72
9	q	601	ADP	C5-C4-N3	-5.86	118.65	126.72
9	g	601	ADP	C5-C4-N3	-5.86	118.65	126.72
9	Z	601	ADP	C5-C4-N3	-5.82	118.71	126.72
9	Q	601	ADP	C5-C4-N3	-5.81	118.72	126.72
9	G	601	ADP	N3-C4-N9	4.64	135.05	127.17
9	z	601	ADP	N3-C4-N9	4.61	135.01	127.17
9	Z	601	ADP	N3-C4-N9	4.60	134.98	127.17
9	Q	601	ADP	N3-C4-N9	4.59	134.97	127.17
9	g	601	ADP	N3-C4-N9	4.57	134.94	127.17
9	q	601	ADP	N3-C4-N9	4.57	134.94	127.17
9	z	601	ADP	C2-N3-C4	3.74	120.96	111.83
9	G	601	ADP	C2-N3-C4	3.73	120.94	111.83
9	g	601	ADP	C2-N3-C4	3.72	120.91	111.83
9	Q	601	ADP	C2-N3-C4	3.70	120.87	111.83
9	q	601	ADP	C2-N3-C4	3.70	120.86	111.83
9	Z	601	ADP	C2-N3-C4	3.69	120.84	111.83
9	q	601	ADP	C4-C5-N7	-3.57	106.50	110.58
9	G	601	ADP	C4-C5-N7	-3.56	106.51	110.58
9	z	601	ADP	C4-C5-N7	-3.56	106.52	110.58
9	Q	601	ADP	C4-C5-N7	-3.52	106.56	110.58
9	g	601	ADP	C4-C5-N7	-3.52	106.56	110.58
9	Z	601	ADP	C4-C5-N7	-3.49	106.59	110.58
9	z	601	ADP	N3-C2-N1	-3.29	123.60	128.58
9	g	601	ADP	N3-C2-N1	-3.27	123.63	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	Q	601	ADP	N3-C2-N1	-3.26	123.64	128.58
9	Z	601	ADP	N3-C2-N1	-3.25	123.66	128.58
9	G	601	ADP	N3-C2-N1	-3.23	123.69	128.58
9	q	601	ADP	N3-C2-N1	-3.21	123.73	128.58
9	Z	601	ADP	C4-N9-C8	2.68	108.55	105.74
9	z	601	ADP	C4-N9-C8	2.64	108.52	105.74
9	Q	601	ADP	C4-N9-C8	2.64	108.51	105.74
9	G	601	ADP	C4-N9-C8	2.61	108.48	105.74
9	q	601	ADP	C5-N7-C8	2.60	107.53	103.45
9	z	601	ADP	C5-N7-C8	2.59	107.53	103.45
9	Z	601	ADP	C5-N7-C8	2.59	107.52	103.45
9	G	601	ADP	C5-N7-C8	2.59	107.52	103.45
9	q	601	ADP	C4-N9-C8	2.58	108.45	105.74
9	g	601	ADP	C4-N9-C8	2.57	108.44	105.74
9	Q	601	ADP	C5-N7-C8	2.57	107.49	103.45
9	g	601	ADP	C5-N7-C8	2.56	107.47	103.45
9	Q	601	ADP	C3'-C2'-C1'	2.25	105.73	101.46
9	Z	601	ADP	C3'-C2'-C1'	2.24	105.71	101.46
9	g	601	ADP	C3'-C2'-C1'	2.24	105.70	101.46
9	G	601	ADP	C3'-C2'-C1'	2.23	105.68	101.46
9	q	601	ADP	C3'-C2'-C1'	2.21	105.64	101.46
9	z	601	ADP	C3'-C2'-C1'	2.18	105.59	101.46
9	z	601	ADP	C6-C5-N7	2.14	136.22	132.09
9	Q	601	ADP	C6-C5-N7	2.13	136.20	132.09
9	G	601	ADP	C6-C5-N7	2.13	136.19	132.09
9	q	601	ADP	C6-C5-N7	2.11	136.15	132.09
9	Z	601	ADP	C6-C5-N7	2.10	136.14	132.09
9	g	601	ADP	C6-C5-N7	2.09	136.12	132.09
9	Z	601	ADP	N9-C8-N7	-2.05	111.03	113.94
9	z	601	ADP	N9-C8-N7	-2.01	111.09	113.94

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	g	601	ADP	PB-O3A-PA-O1A
9	g	601	ADP	PB-O3A-PA-O2A
9	G	601	ADP	PB-O3A-PA-O1A
9	G	601	ADP	PB-O3A-PA-O2A
9	Q	601	ADP	PB-O3A-PA-O1A
9	Q	601	ADP	PB-O3A-PA-O2A
9	q	601	ADP	PB-O3A-PA-O1A

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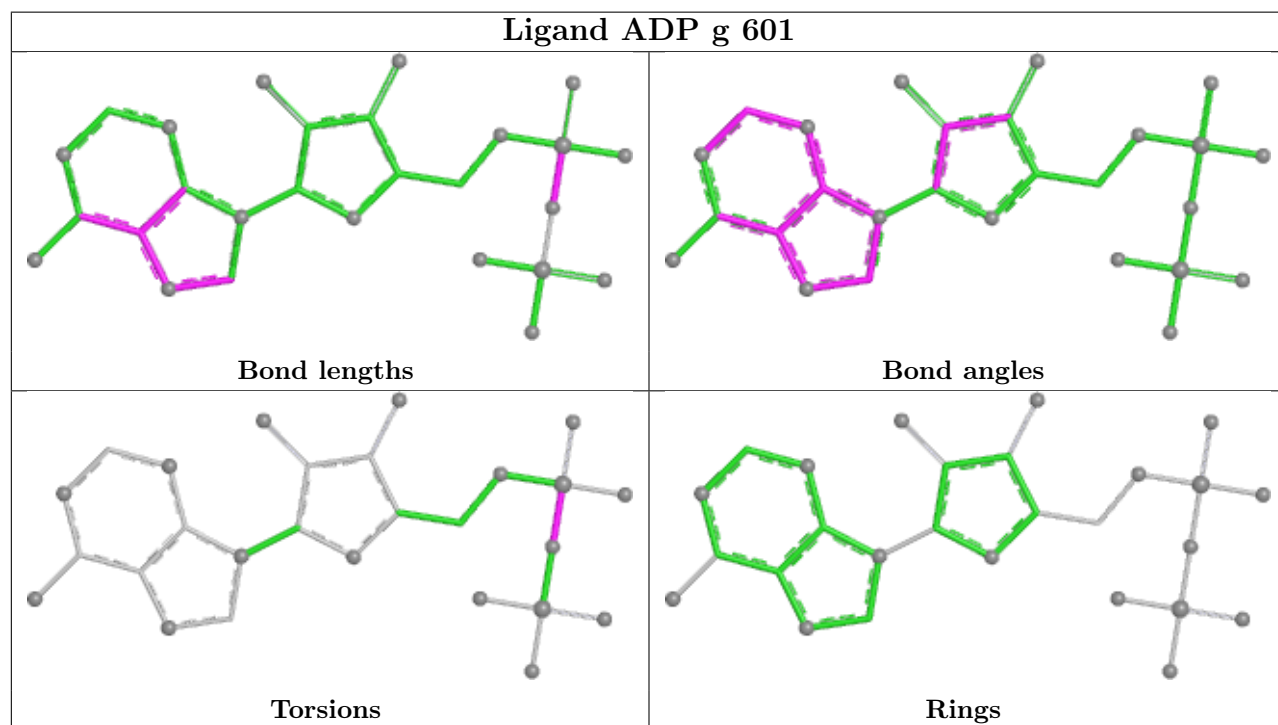
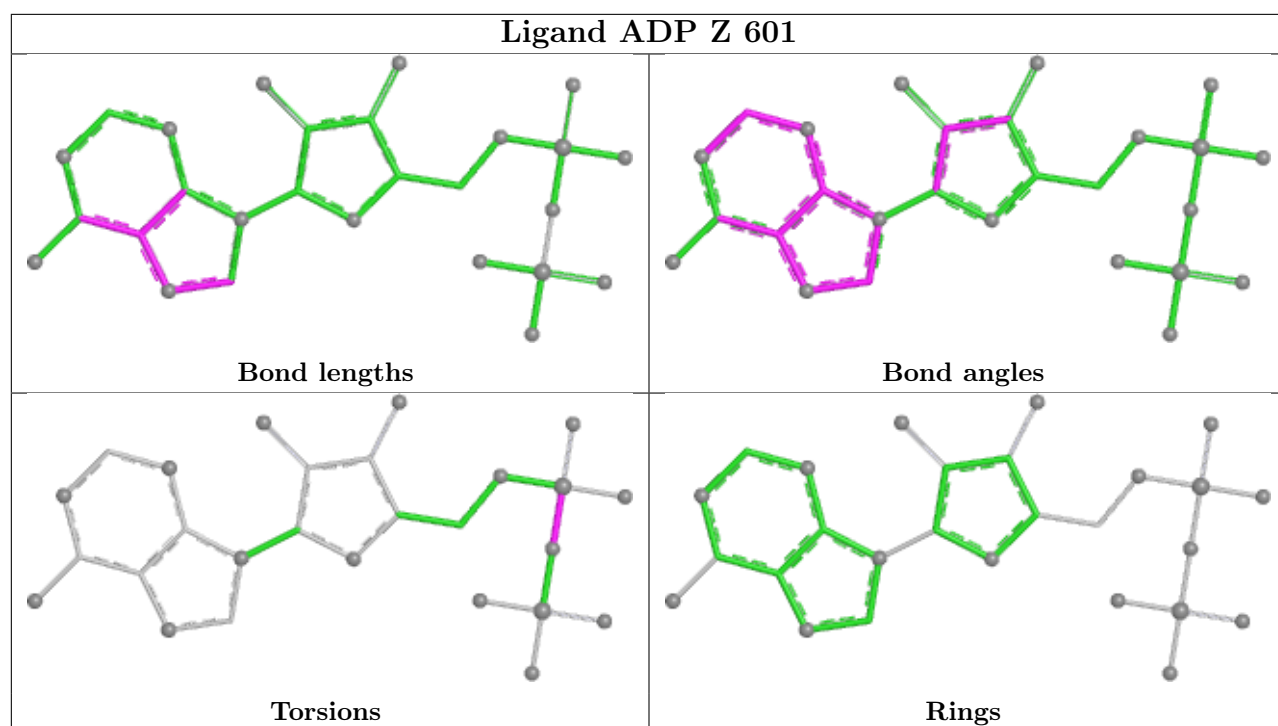
Mol	Chain	Res	Type	Atoms
9	q	601	ADP	PB-O3A-PA-O2A
9	Z	601	ADP	PB-O3A-PA-O1A
9	Z	601	ADP	PB-O3A-PA-O2A
9	z	601	ADP	PB-O3A-PA-O1A
9	z	601	ADP	PB-O3A-PA-O2A

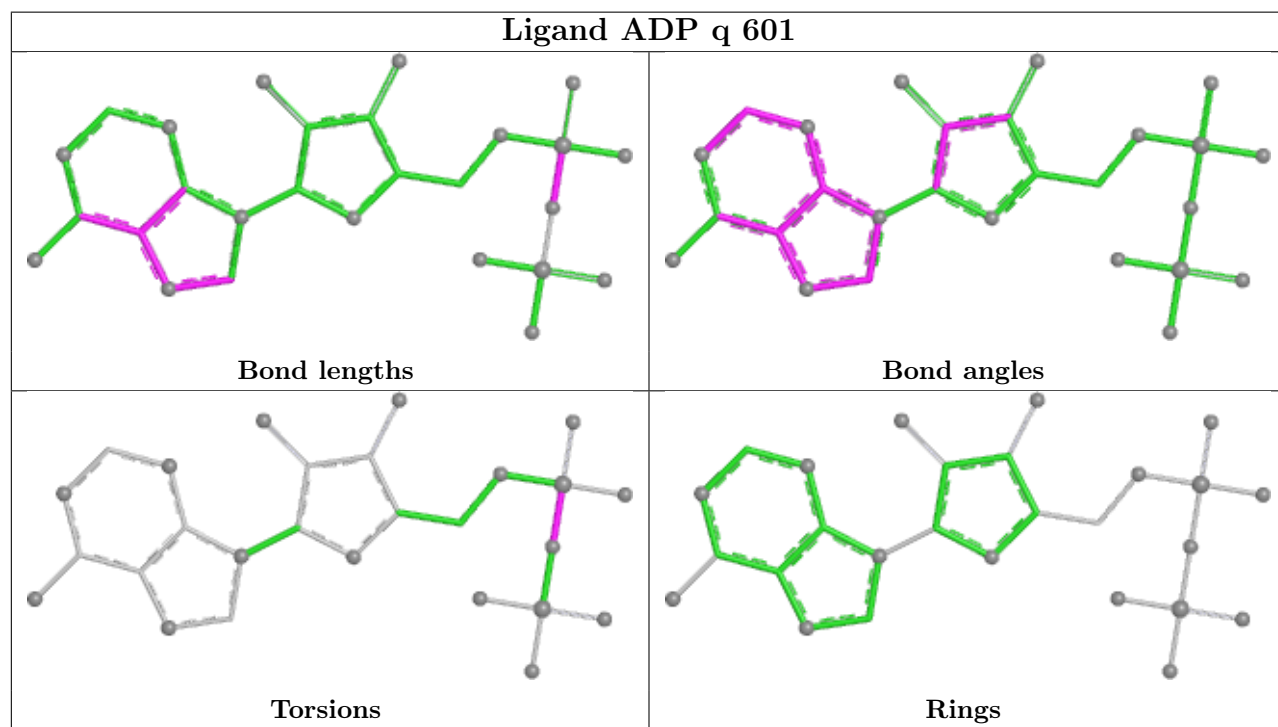
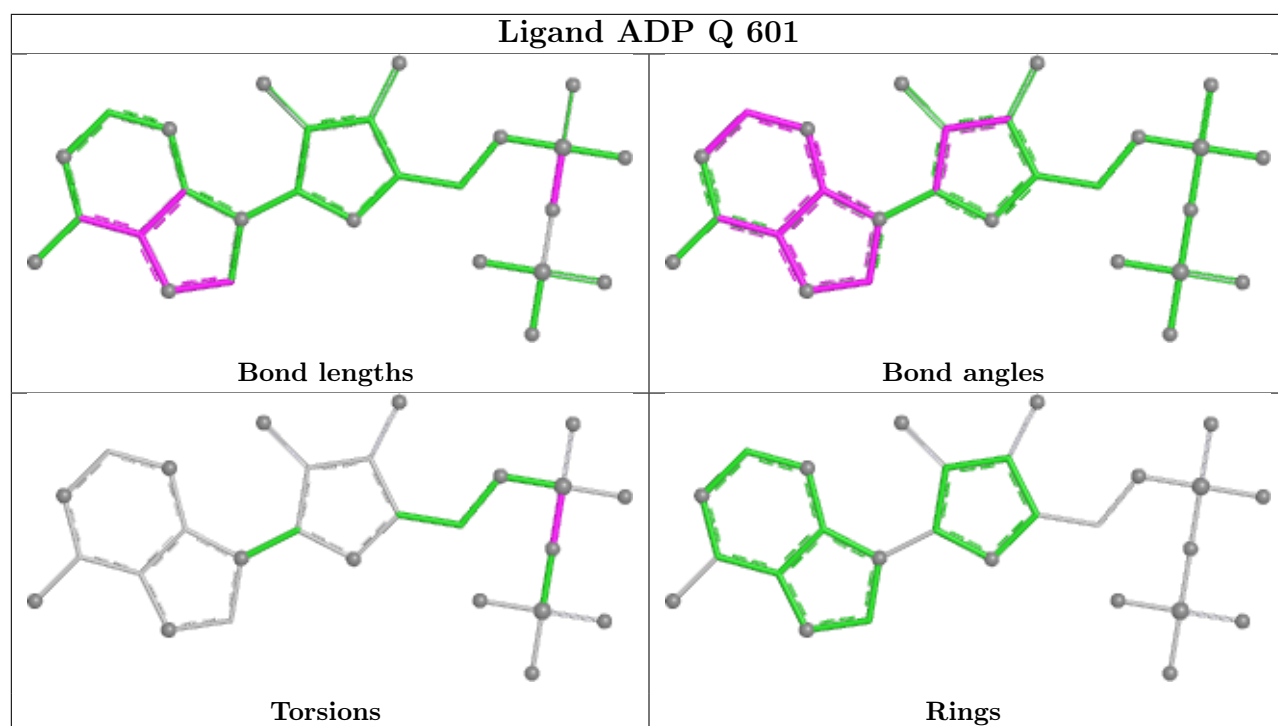
There are no ring outliers.

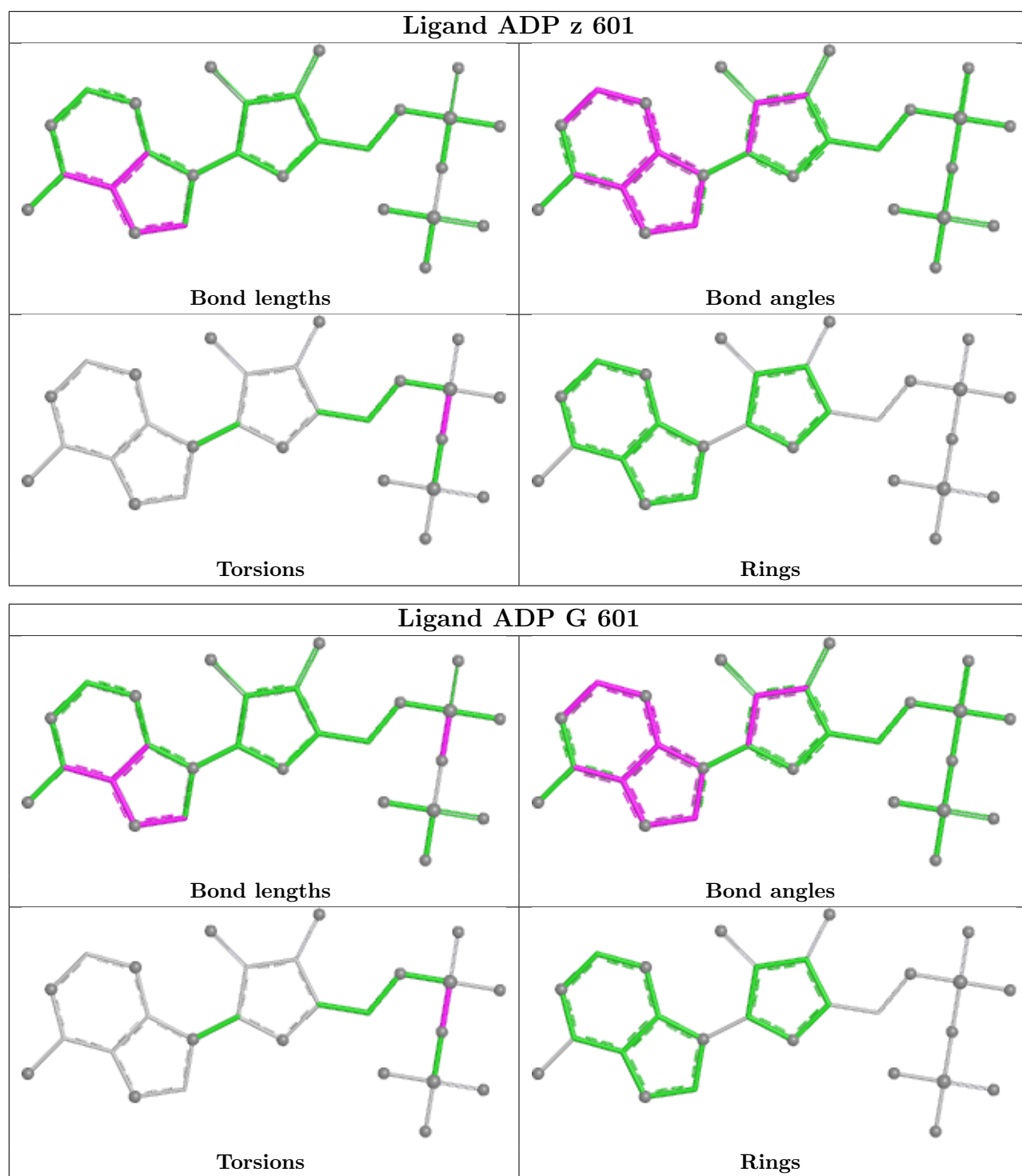
6 monomers are involved in 38 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	Z	601	ADP	1	0
9	g	601	ADP	11	0
9	Q	601	ADP	1	0
9	q	601	ADP	5	0
9	z	601	ADP	6	0
9	G	601	ADP	14	0

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







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

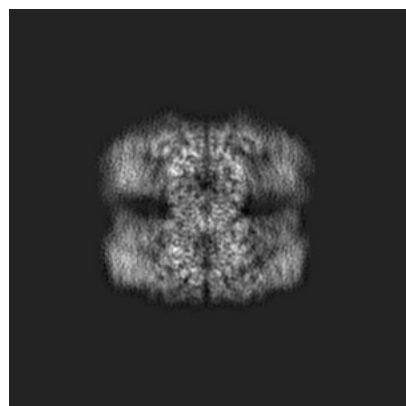
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-34852. These allow visual inspection of the internal detail of the map and identification of artifacts.

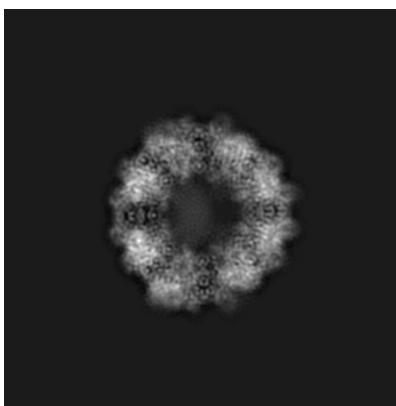
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

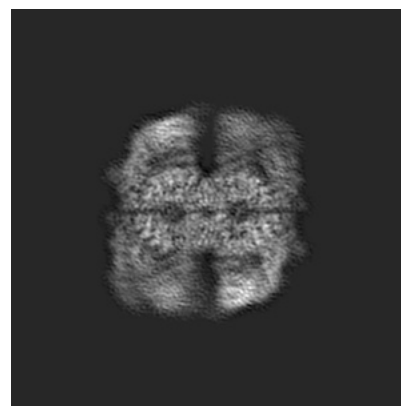
6.1.1 Primary map



X

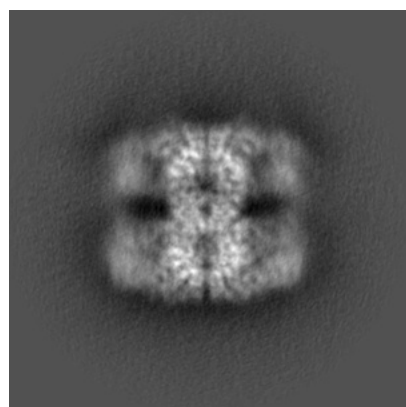


Y

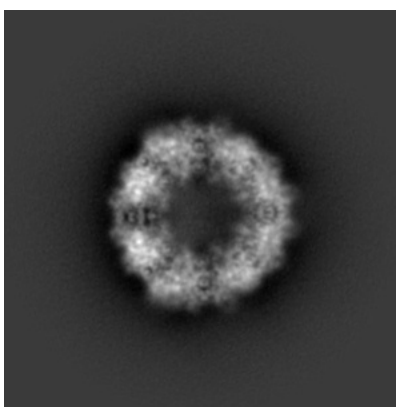


Z

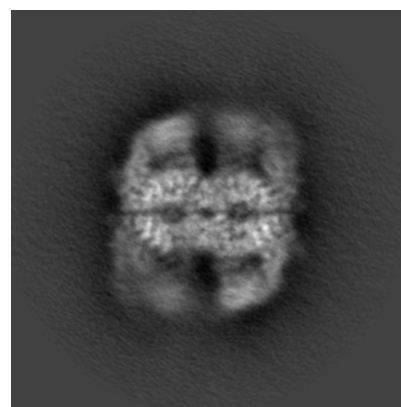
6.1.2 Raw map



X



Y

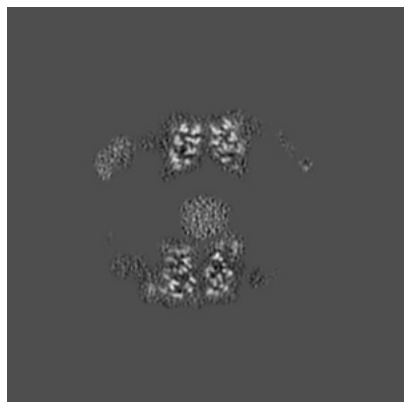


Z

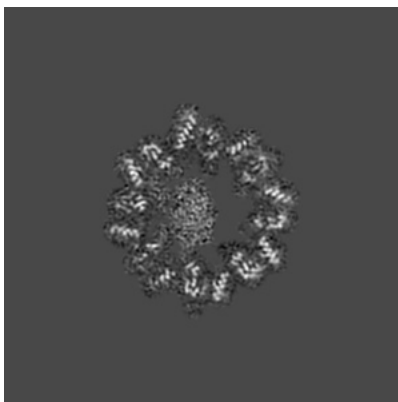
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

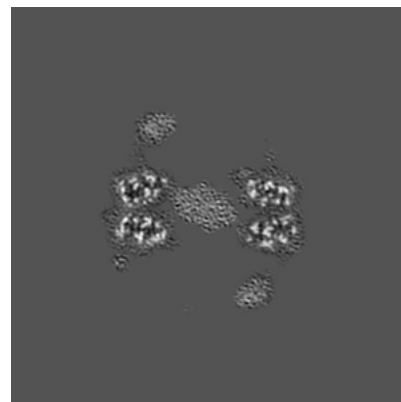
6.2.1 Primary map



X Index: 128

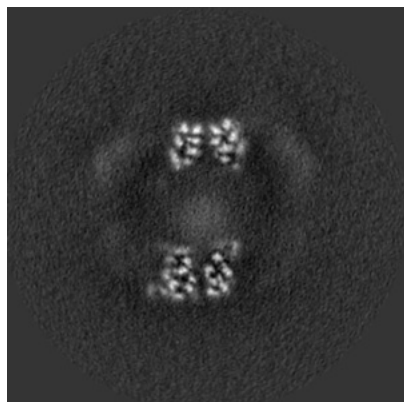


Y Index: 128

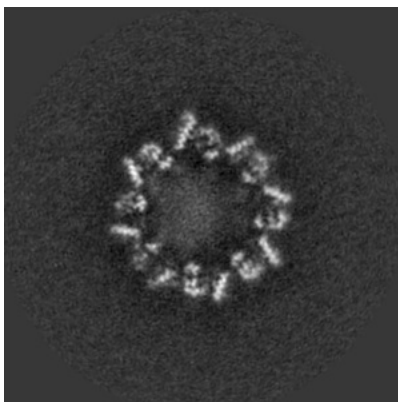


Z Index: 128

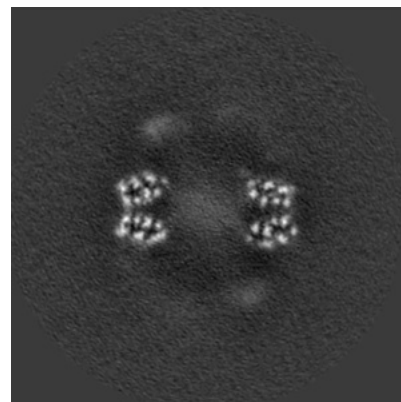
6.2.2 Raw map



X Index: 128



Y Index: 128



Z Index: 128

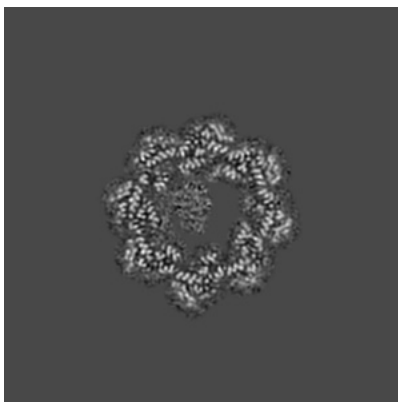
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

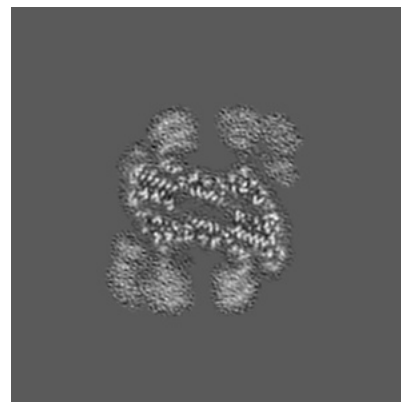
6.3.1 Primary map



X Index: 94

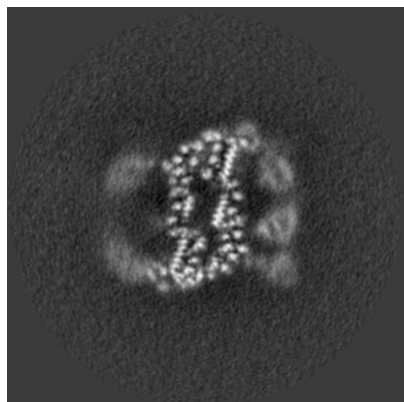


Y Index: 117

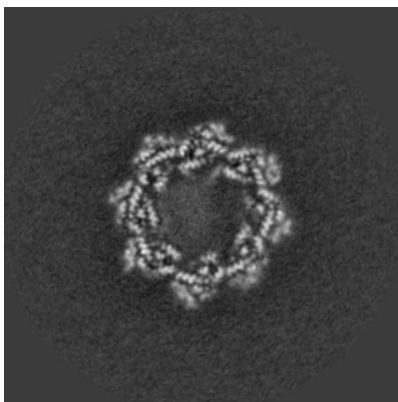


Z Index: 94

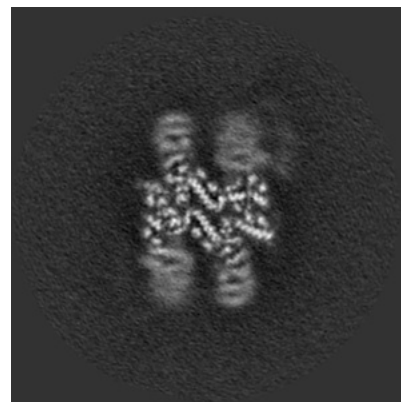
6.3.2 Raw map



X Index: 94



Y Index: 117

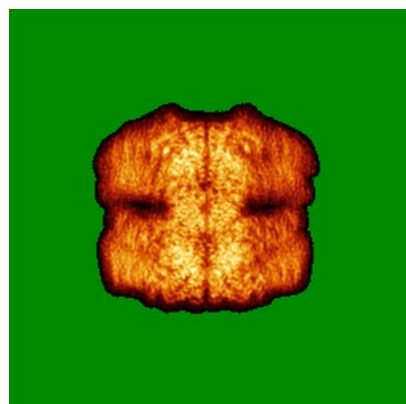


Z Index: 87

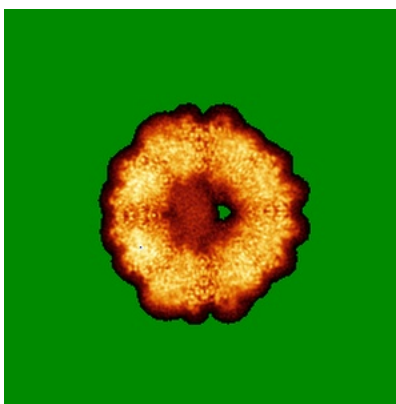
The images above show the largest variance slices of the map in three orthogonal directions.

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

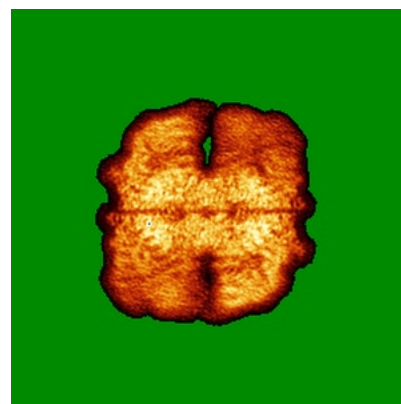
6.4.1 Primary map



X

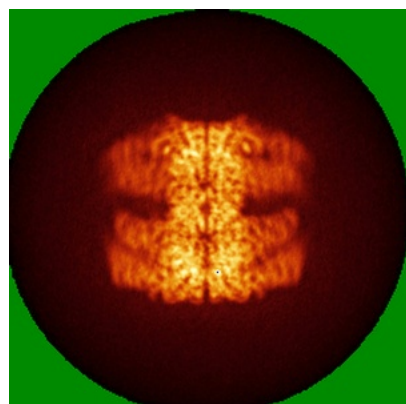


Y

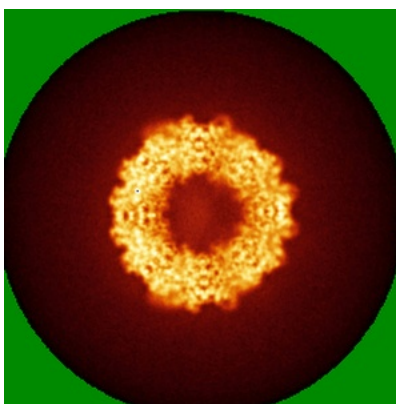


Z

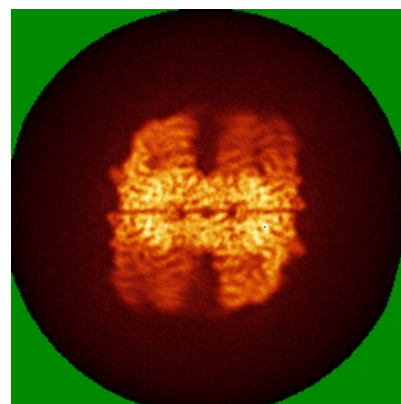
6.4.2 Raw map



X



Y

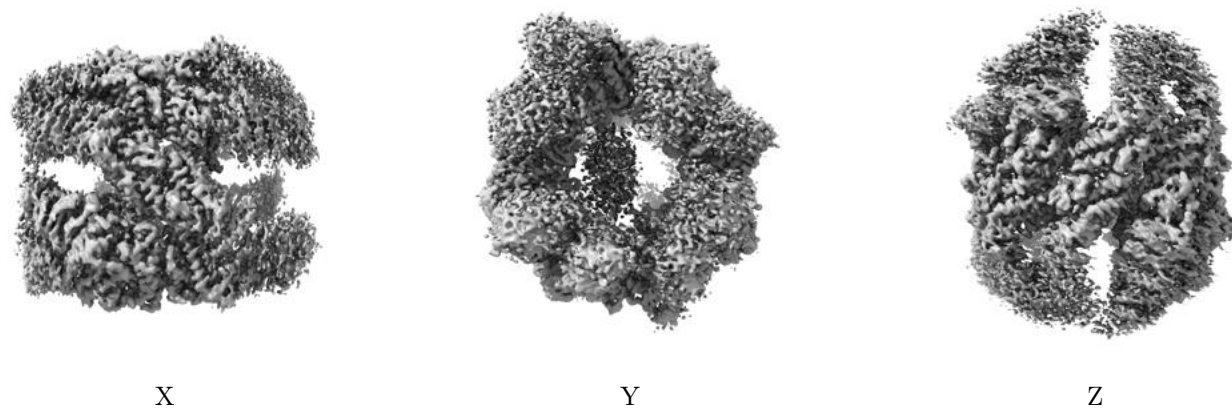


Z

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

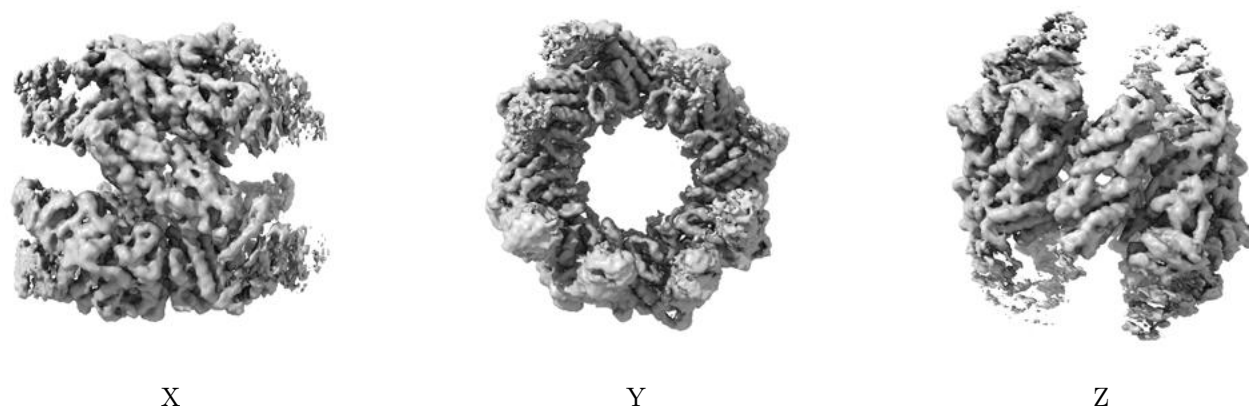
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.663. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

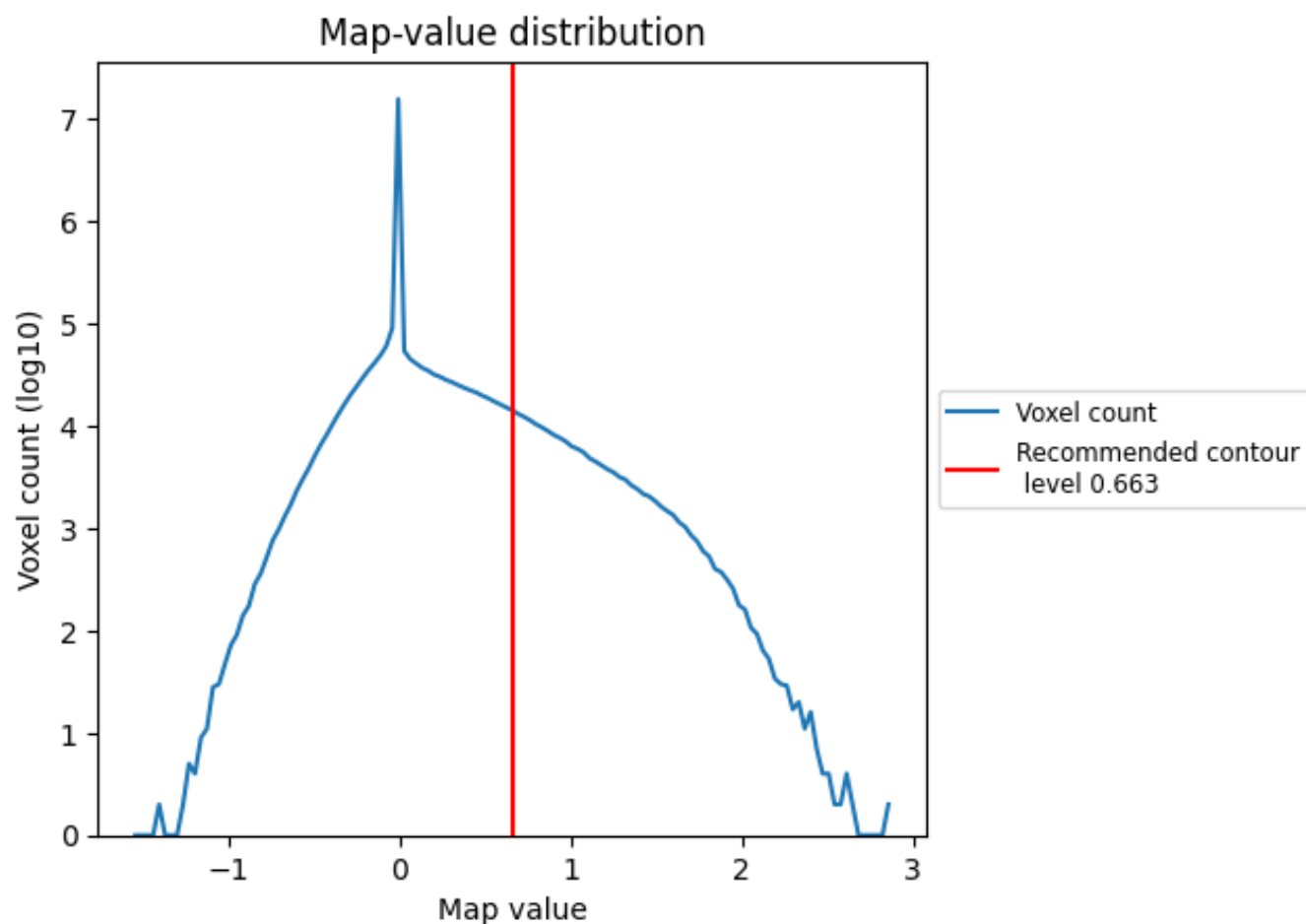
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

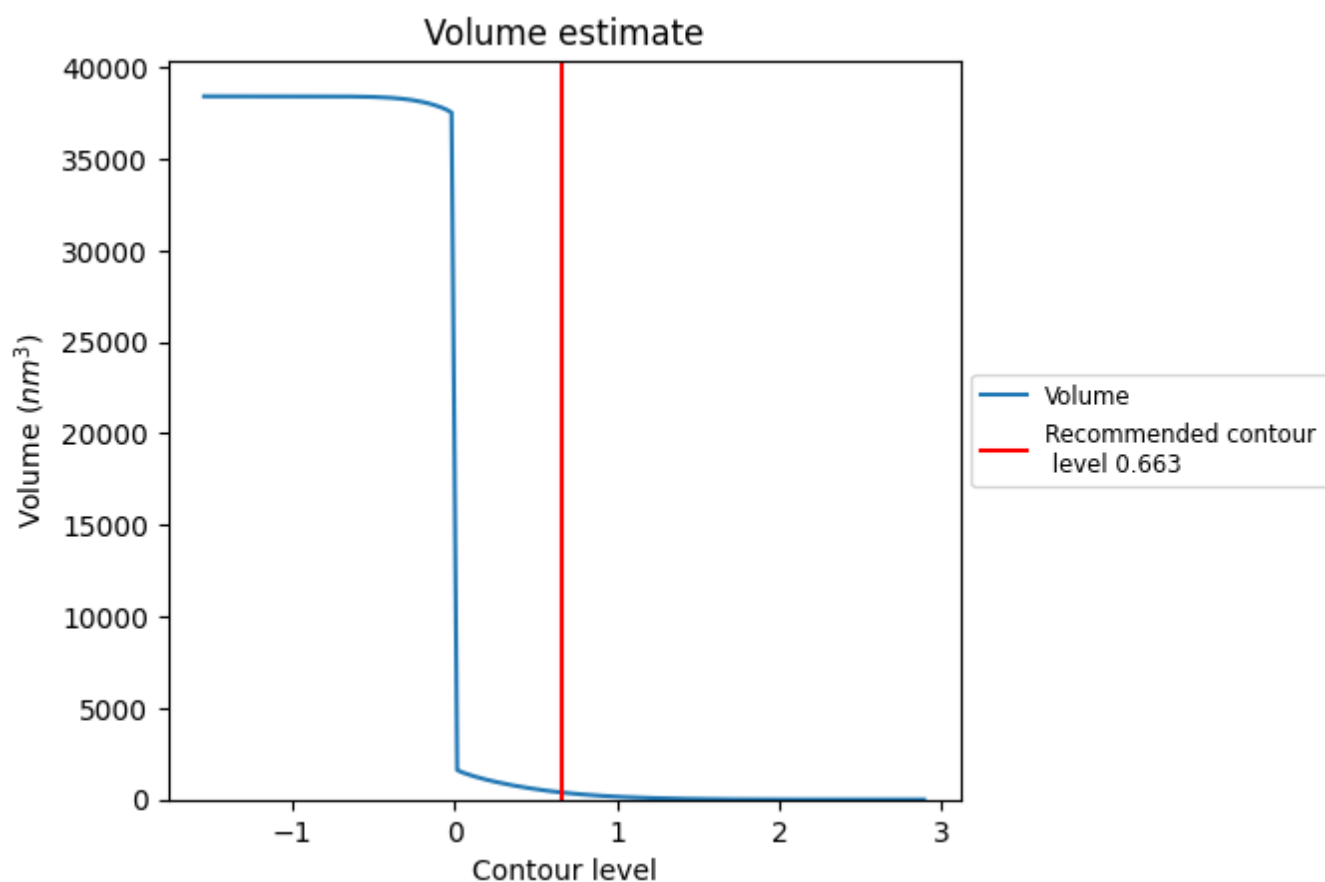
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

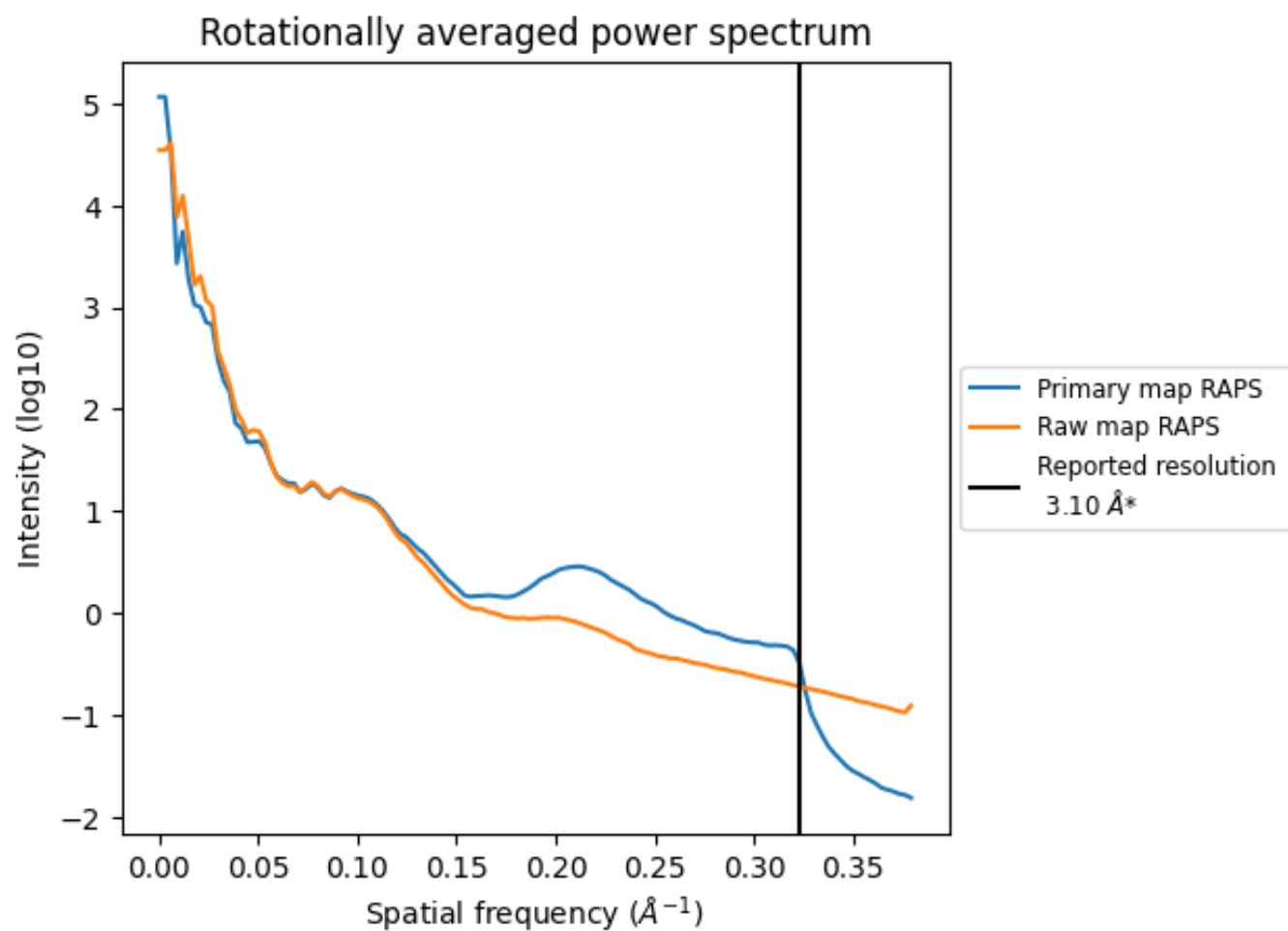
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 384 nm³; this corresponds to an approximate mass of 347 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 ⓘ

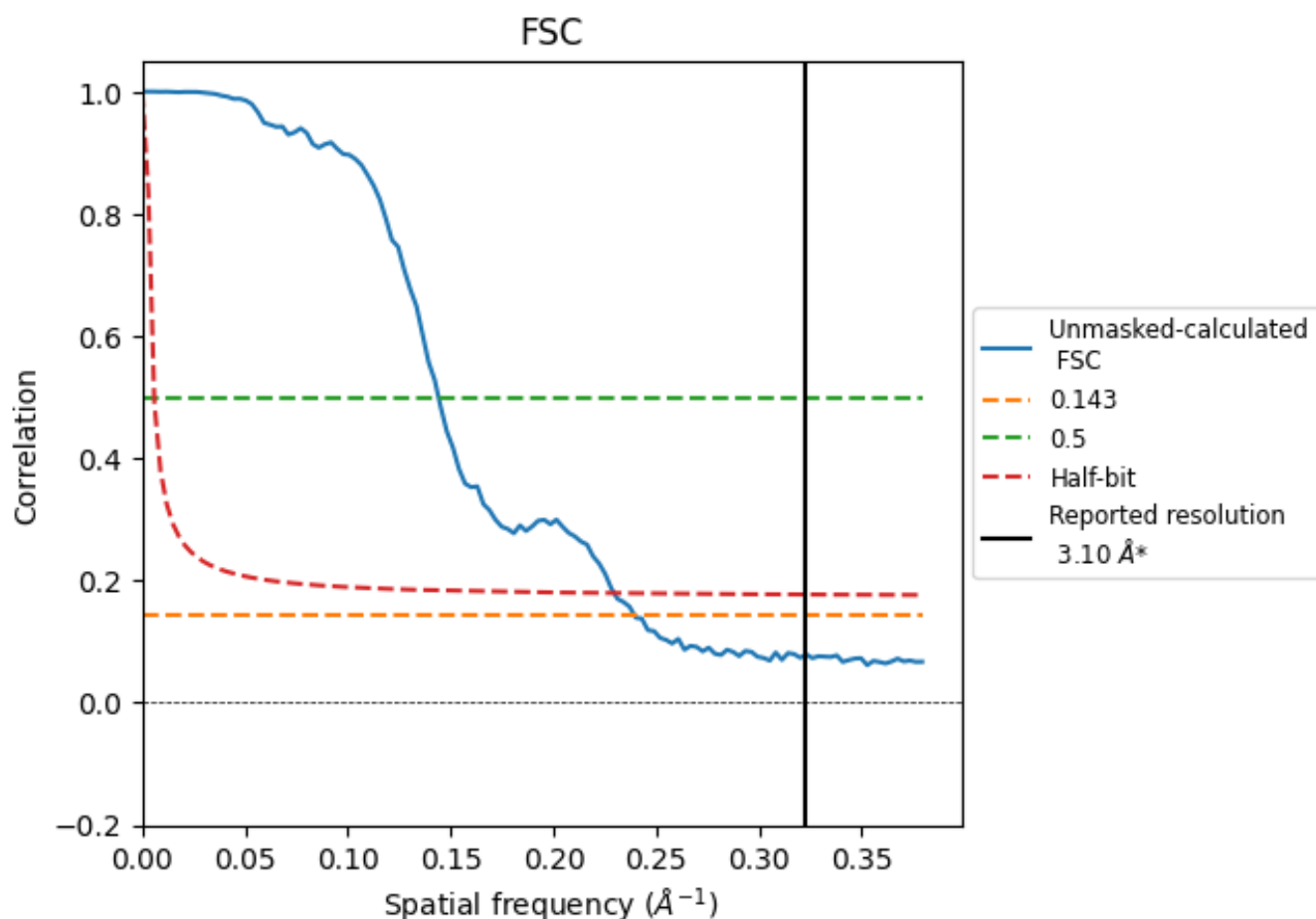


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.323 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

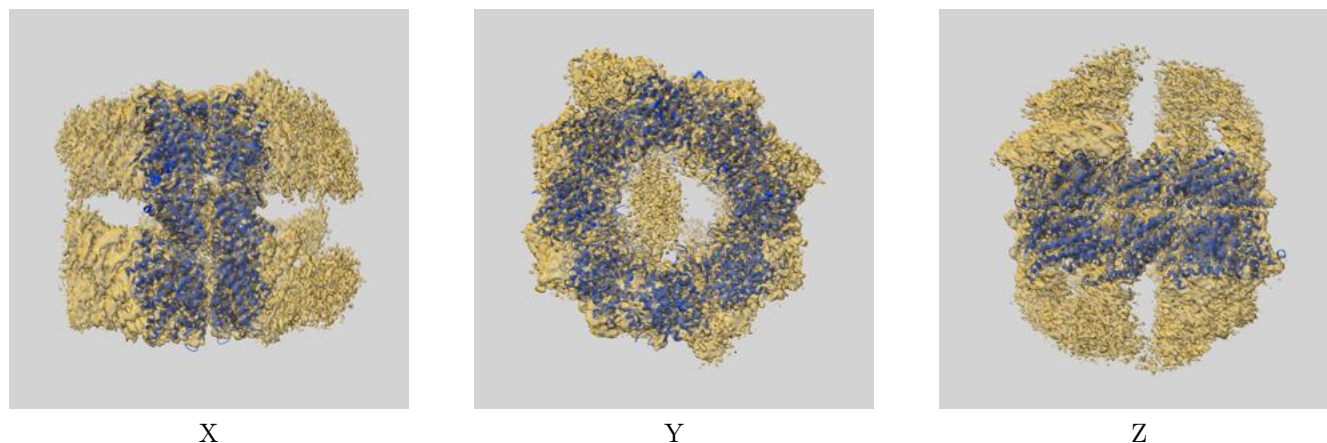
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.18	6.94	4.36

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.18 differs from the reported value 3.1 by more than 10 %

9 Map-model fit [i](#)

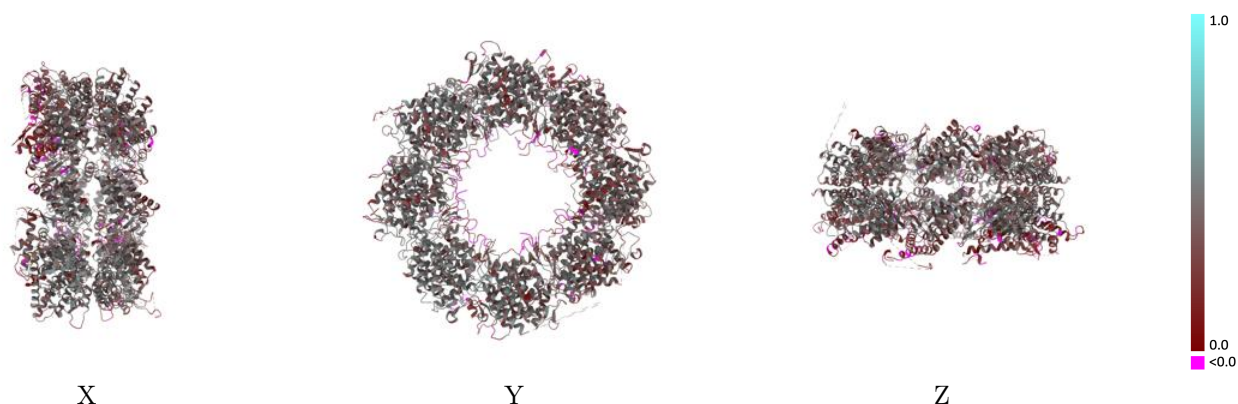
This section contains information regarding the fit between EMDB map EMD-34852 and PDB model 8HKI. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



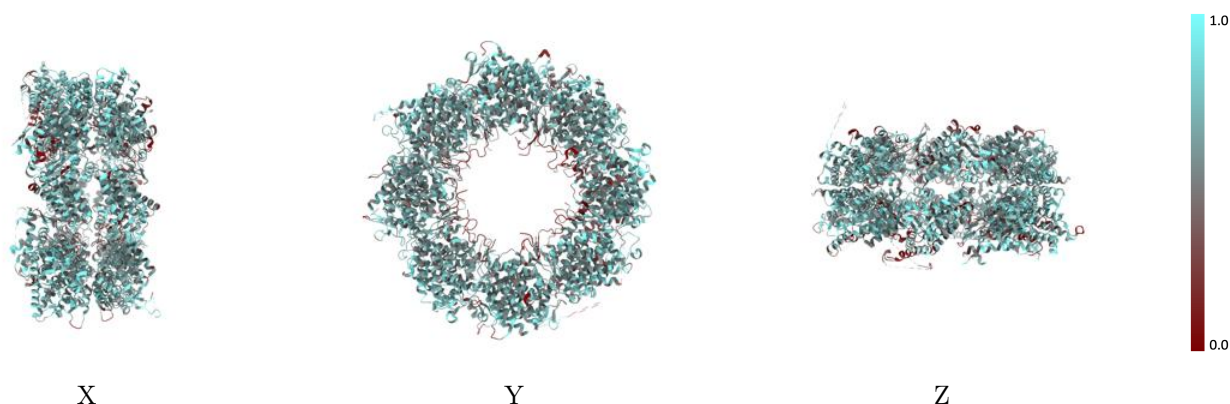
The images above show the 3D surface view of the map at the recommended contour level 0.663 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



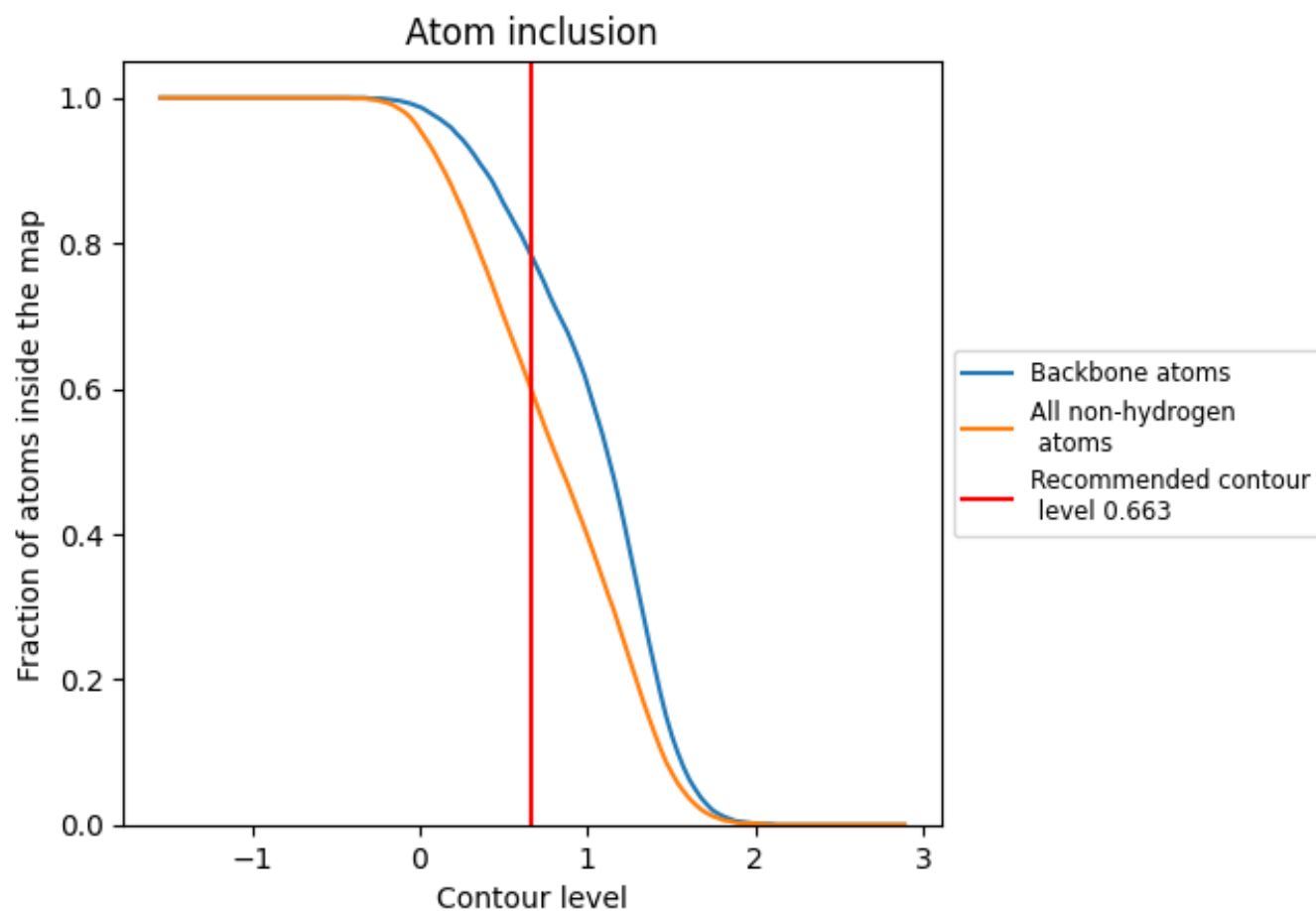
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.663).

9.4 Atom inclusion [i](#)



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

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.663) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6000	 0.3660
A	 0.6010	 0.3690
B	 0.5630	 0.3360
D	 0.5920	 0.3570
E	 0.6050	 0.3490
G	 0.6180	 0.3920
H	 0.6120	 0.3850
Q	 0.6000	 0.4040
Z	 0.5940	 0.3800
a	 0.5980	 0.3490
b	 0.5590	 0.3170
d	 0.6080	 0.3630
e	 0.6110	 0.3280
g	 0.6250	 0.4250
h	 0.5940	 0.3400
q	 0.6180	 0.3900
z	 0.6110	 0.3920

