



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 09:00 AM UTC

PDB ID : 6VQ8 / pdb_00006vq8
EMDB ID : EMD-21319
Title : Mammalian V-ATPase from rat brain - composite model of rotational state 3 bound to ADP and SidK (built from focused refinement models)
Authors : Abbas, Y.M.; Rubinstein, J.L.
Deposited on : 2020-02-04
Resolution : 3.90 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.

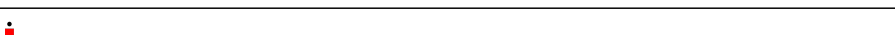
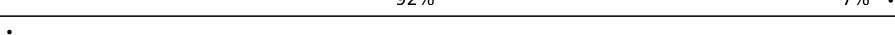
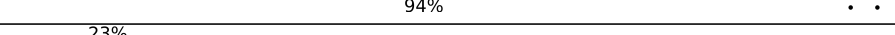
The types of validation reports are described at

<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

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Mol	Chain	Length	Quality of chain
2	E	511	
2	F	511	
3	G	382	
4	H	247	
5	I	226	
5	J	226	
5	K	226	
6	L	119	
7	M	118	
7	N	118	
7	O	118	
8	Q	301	
8	R	301	
8	S	301	
9	a	838	
10	b	205	
11	c	463	
12	d	351	
13	e	81	
14	f	98	
15	g	155	
15	h	155	
15	i	155	
15	j	155	
15	k	155	

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Mol	Chain	Length	Quality of chain
15	l	155	13% 85% 12%
15	m	155	13% 78% 16%
15	n	155	12% 82% 14%
15	o	155	10% 72% 24%
16	p	350	13% 85%

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 60714 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 ATPase H⁺-transporting V1 subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	600	Total	C	N	O	S	0	0
			4651	2949	786	889	27		
1	B	600	Total	C	N	O	S	0	0
			4651	2949	786	889	27		
1	C	600	Total	C	N	O	S	0	0
			4651	2949	786	889	27		

- Molecule 2 is a protein called V-type proton ATPase subunit B, brain isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	459	Total	C	N	O	S	0	0
			3595	2282	613	680	20		
2	E	459	Total	C	N	O	S	0	0
			3595	2282	613	680	20		
2	F	459	Total	C	N	O	S	0	0
			3595	2282	613	680	20		

- Molecule 3 is a protein called V-type proton ATPase subunit C 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	G	360	Total	C	N	O	0	0
			1790	1070	360	360		

- Molecule 4 is a protein called ATPase H⁺-transporting V1 subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	214	Total	C	N	O	S	0	0
			1726	1095	311	315	5		

- Molecule 5 is a protein called V-type proton ATPase subunit E 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	225	Total	C	N	O	S	0	0
			1607	1005	296	299	7		
5	J	224	Total	C	N	O	S	0	0
			1602	1002	295	298	7		
5	K	225	Total	C	N	O	S	0	0
			1607	1005	296	299	7		

- Molecule 6 is a protein called V-type proton ATPase subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	L	110	Total	C	N	O	S	0	0
			866	548	154	163	1		

- Molecule 7 is a protein called V-type proton ATPase subunit G.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	M	114	Total	C	N	O	S	0	0
			714	426	147	138	3		
7	N	114	Total	C	N	O	S	0	0
			714	426	147	138	3		
7	O	113	Total	C	N	O	S	0	0
			709	423	146	137	3		

- Molecule 8 is a protein called Effector protein SidK.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Q	232	Total	C	N	O	S	0	0
			1878	1197	316	354	11		
8	R	224	Total	C	N	O	S	0	0
			1824	1162	306	346	10		
8	S	212	Total	C	N	O	S	0	0
			1722	1096	292	325	9		

There are 69 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	0	GLY	-	expression tag	UNP Q5ZWW6
Q	279	ASP	-	expression tag	UNP Q5ZWW6
Q	280	TYR	-	expression tag	UNP Q5ZWW6
Q	281	LYS	-	expression tag	UNP Q5ZWW6
Q	282	ASP	-	expression tag	UNP Q5ZWW6
Q	283	HIS	-	expression tag	UNP Q5ZWW6
Q	284	ASP	-	expression tag	UNP Q5ZWW6

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	285	GLY	-	expression tag	UNP Q5ZWW6
Q	286	ASP	-	expression tag	UNP Q5ZWW6
Q	287	TYR	-	expression tag	UNP Q5ZWW6
Q	288	LYS	-	expression tag	UNP Q5ZWW6
Q	289	ASP	-	expression tag	UNP Q5ZWW6
Q	290	HIS	-	expression tag	UNP Q5ZWW6
Q	291	ASP	-	expression tag	UNP Q5ZWW6
Q	292	ILE	-	expression tag	UNP Q5ZWW6
Q	293	ASP	-	expression tag	UNP Q5ZWW6
Q	294	TYR	-	expression tag	UNP Q5ZWW6
Q	295	LYS	-	expression tag	UNP Q5ZWW6
Q	296	ASP	-	expression tag	UNP Q5ZWW6
Q	297	ASP	-	expression tag	UNP Q5ZWW6
Q	298	ASP	-	expression tag	UNP Q5ZWW6
Q	299	ASP	-	expression tag	UNP Q5ZWW6
Q	300	LYS	-	expression tag	UNP Q5ZWW6
R	0	GLY	-	expression tag	UNP Q5ZWW6
R	279	ASP	-	expression tag	UNP Q5ZWW6
R	280	TYR	-	expression tag	UNP Q5ZWW6
R	281	LYS	-	expression tag	UNP Q5ZWW6
R	282	ASP	-	expression tag	UNP Q5ZWW6
R	283	HIS	-	expression tag	UNP Q5ZWW6
R	284	ASP	-	expression tag	UNP Q5ZWW6
R	285	GLY	-	expression tag	UNP Q5ZWW6
R	286	ASP	-	expression tag	UNP Q5ZWW6
R	287	TYR	-	expression tag	UNP Q5ZWW6
R	288	LYS	-	expression tag	UNP Q5ZWW6
R	289	ASP	-	expression tag	UNP Q5ZWW6
R	290	HIS	-	expression tag	UNP Q5ZWW6
R	291	ASP	-	expression tag	UNP Q5ZWW6
R	292	ILE	-	expression tag	UNP Q5ZWW6
R	293	ASP	-	expression tag	UNP Q5ZWW6
R	294	TYR	-	expression tag	UNP Q5ZWW6
R	295	LYS	-	expression tag	UNP Q5ZWW6
R	296	ASP	-	expression tag	UNP Q5ZWW6
R	297	ASP	-	expression tag	UNP Q5ZWW6
R	298	ASP	-	expression tag	UNP Q5ZWW6
R	299	ASP	-	expression tag	UNP Q5ZWW6
R	300	LYS	-	expression tag	UNP Q5ZWW6
S	0	GLY	-	expression tag	UNP Q5ZWW6
S	279	ASP	-	expression tag	UNP Q5ZWW6
S	280	TYR	-	expression tag	UNP Q5ZWW6

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Chain	Residue	Modelled	Actual	Comment	Reference
S	281	LYS	-	expression tag	UNP Q5ZWW6
S	282	ASP	-	expression tag	UNP Q5ZWW6
S	283	HIS	-	expression tag	UNP Q5ZWW6
S	284	ASP	-	expression tag	UNP Q5ZWW6
S	285	GLY	-	expression tag	UNP Q5ZWW6
S	286	ASP	-	expression tag	UNP Q5ZWW6
S	287	TYR	-	expression tag	UNP Q5ZWW6
S	288	LYS	-	expression tag	UNP Q5ZWW6
S	289	ASP	-	expression tag	UNP Q5ZWW6
S	290	HIS	-	expression tag	UNP Q5ZWW6
S	291	ASP	-	expression tag	UNP Q5ZWW6
S	292	ILE	-	expression tag	UNP Q5ZWW6
S	293	ASP	-	expression tag	UNP Q5ZWW6
S	294	TYR	-	expression tag	UNP Q5ZWW6
S	295	LYS	-	expression tag	UNP Q5ZWW6
S	296	ASP	-	expression tag	UNP Q5ZWW6
S	297	ASP	-	expression tag	UNP Q5ZWW6
S	298	ASP	-	expression tag	UNP Q5ZWW6
S	299	ASP	-	expression tag	UNP Q5ZWW6
S	300	LYS	-	expression tag	UNP Q5ZWW6

- Molecule 9 is a protein called V-type proton ATPase 116 kDa subunit a isoform 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	a	749	Total	C	N	O	0	0
			3703	2205	749	749		

- Molecule 10 is a protein called ATPase, H⁺ transporting, V0 subunit B (Predicted), isoform CRA_a.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	b	203	Total	C	N	O	S	0	0
			1503	996	237	259	11		

- Molecule 11 is a protein called V-type proton ATPase subunit S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	c	41	Total	C	N	O	S	0	0
			337	228	51	54	4		

- Molecule 12 is a protein called V-type proton ATPase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	d	350	Total	C	N	O	S	0	0
			2833	1829	460	530	14		

- Molecule 13 is a protein called V-type proton ATPase subunit e 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	e	78	Total	C	N	O	0	0
			384	228	78	78		

- Molecule 14 is a protein called Ribonuclease K.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	f	84	Total	C	N	O	0	0
			412	244	84	84		

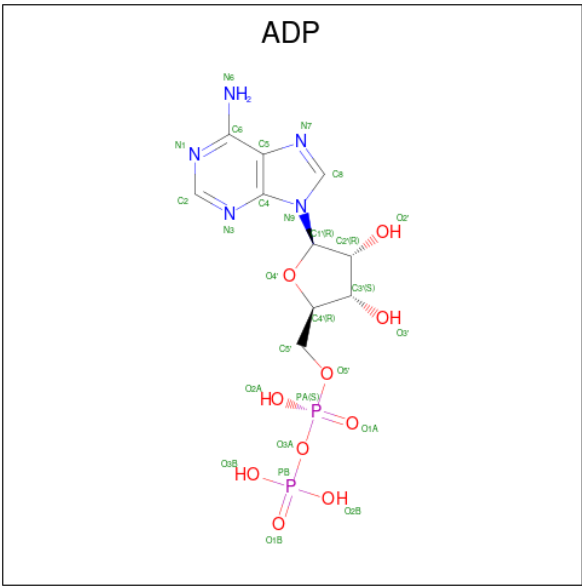
- Molecule 15 is a protein called V-type proton ATPase 16 kDa proteolipid subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	g	150	Total	C	N	O	S	0	0
			1068	699	171	190	8		
15	h	150	Total	C	N	O	S	0	0
			1068	699	171	190	8		
15	i	150	Total	C	N	O	S	0	0
			1068	699	171	190	8		
15	j	150	Total	C	N	O	S	0	0
			1068	699	171	190	8		
15	k	150	Total	C	N	O	S	0	0
			1068	699	171	190	8		
15	l	150	Total	C	N	O	S	0	0
			1068	699	171	190	8		
15	m	150	Total	C	N	O	S	0	0
			1068	699	171	190	8		
15	n	150	Total	C	N	O	S	0	0
			1068	699	171	190	8		
15	o	150	Total	C	N	O	S	0	0
			1068	699	171	190	8		

- Molecule 16 is a protein called Renin receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	p	52	Total	C	N	O	S	0	0
			406	269	61	73	3		

- Molecule 17 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).

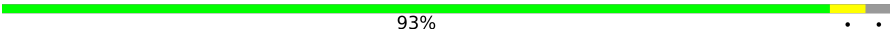


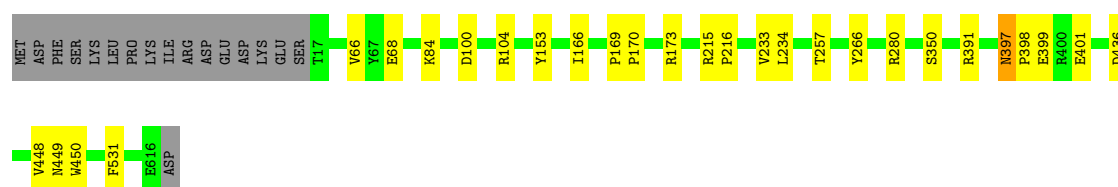
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
17	A	1	27	10	5	10	2	0

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.

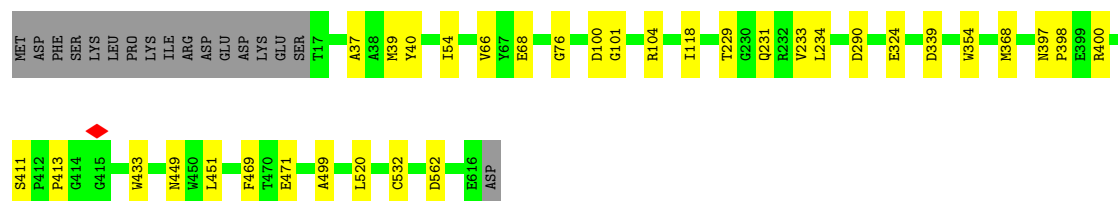
- Molecule 1: ATPase H⁺-transporting V1 subunit A

Chain A:  93%

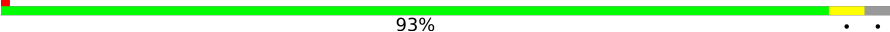


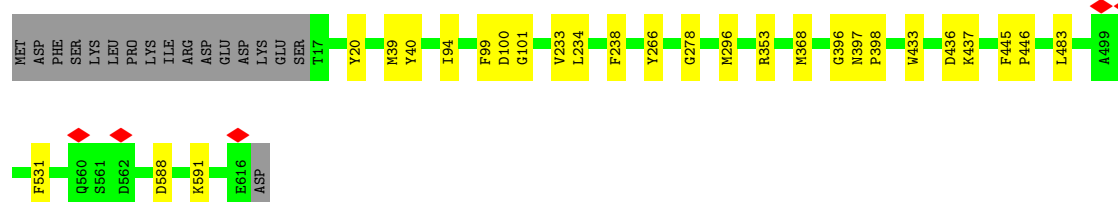
- Molecule 1: ATPase H⁺-transporting V1 subunit A

Chain B:  92% 6%



- Molecule 1: ATPase H⁺-transporting V1 subunit A

Chain C:  93%



- Molecule 2: V-type proton ATPase subunit B, brain isoform

Chain D:  85% 5% 10%

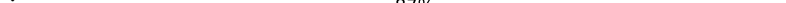


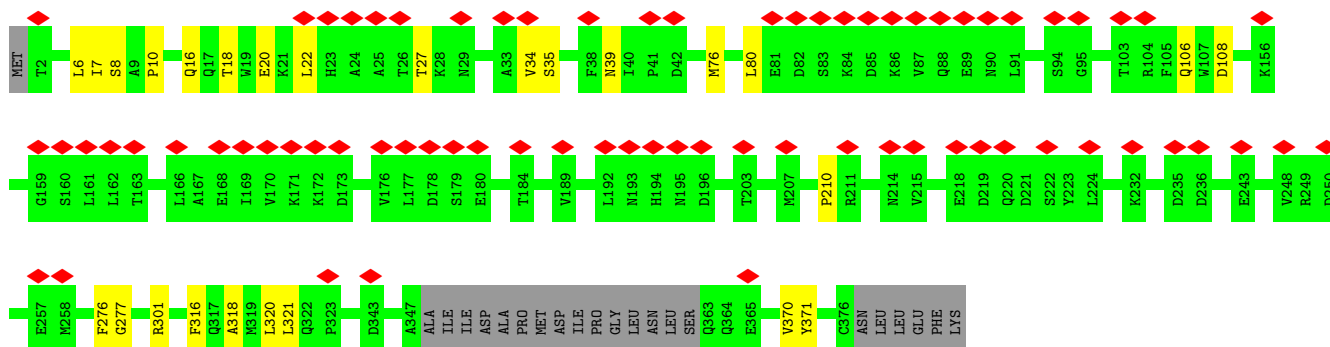
- Chain E:  85% 5% 10%

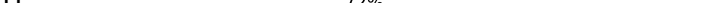


- Chain F: 85% . . 10%

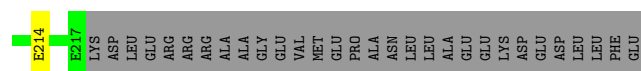


- Chain G:  19% 87% 7% 6%

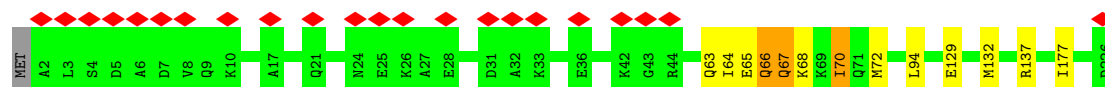


- Chain H:  72% 12% 3% 13%





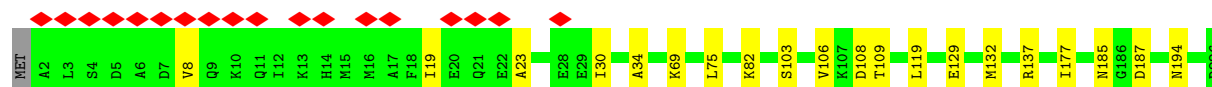
- Molecule 5: V-type proton ATPase subunit E 1



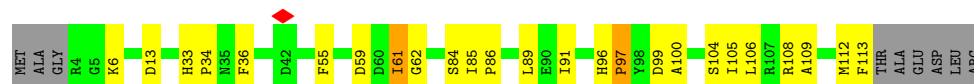
- Molecule 5: V-type proton ATPase subunit E 1



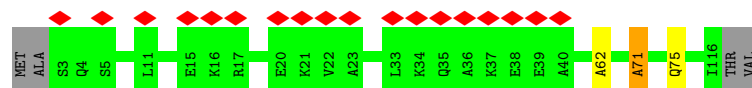
- Molecule 5: V-type proton ATPase subunit E 1



- Molecule 6: V-type proton ATPase subunit F



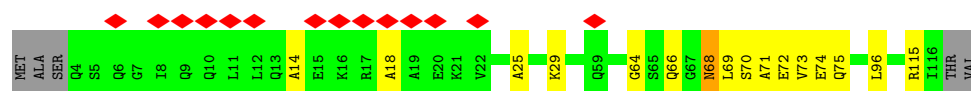
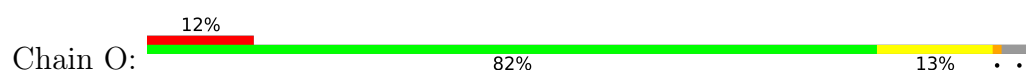
- Molecule 7: V-type proton ATPase subunit G



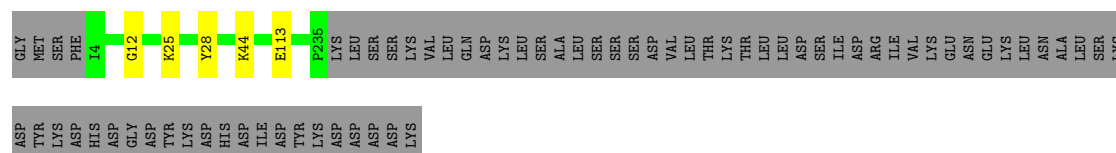
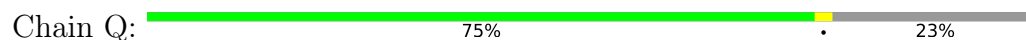
- Molecule 7: V-type proton ATPase subunit G



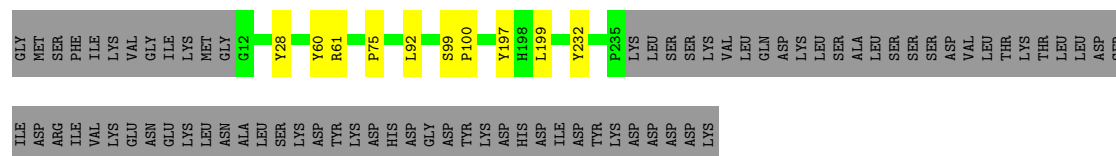
- Molecule 7: V-type proton ATPase subunit G



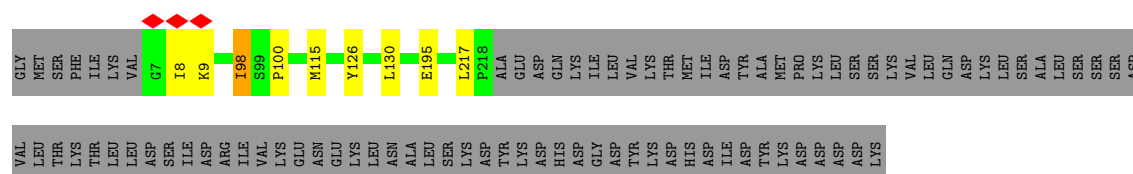
• Molecule 8: Effector protein SidK



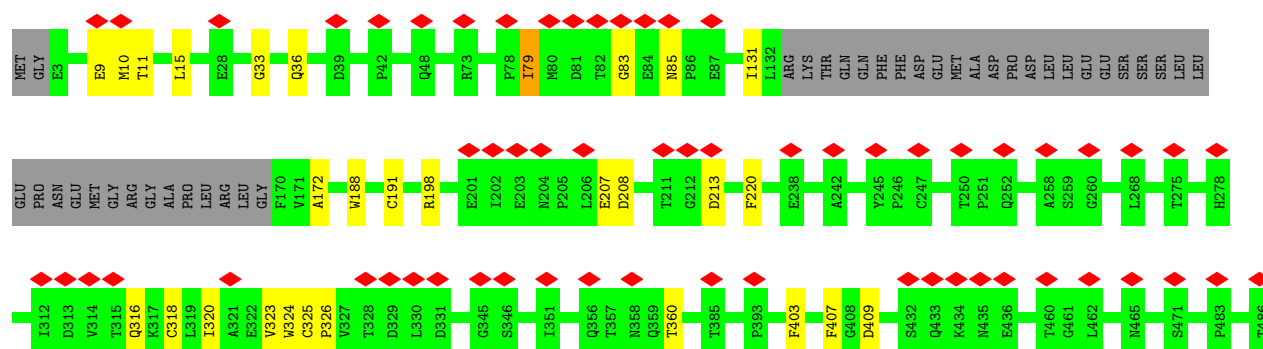
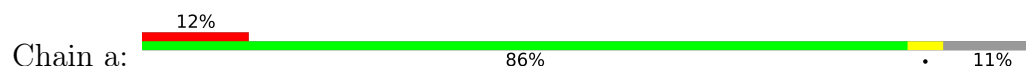
• Molecule 8: Effector protein SidK

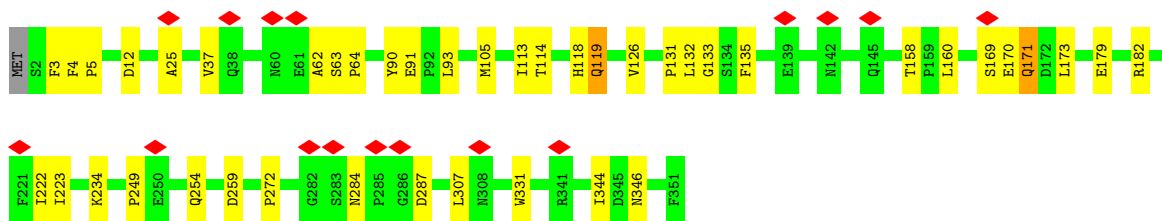


• Molecule 8: Effector protein SidK

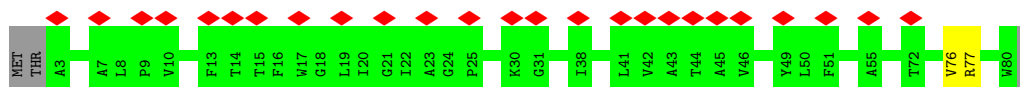
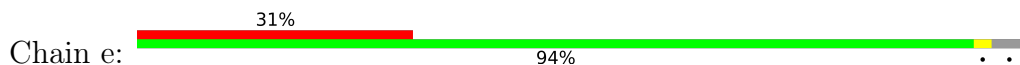


• Molecule 9: V-type proton ATPase 116 kDa subunit a isoform 1

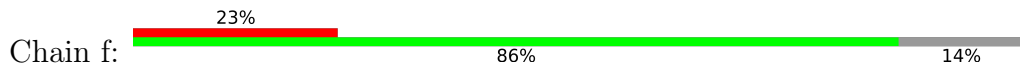




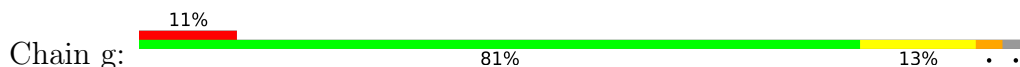
- Molecule 13: V-type proton ATPase subunit e 2



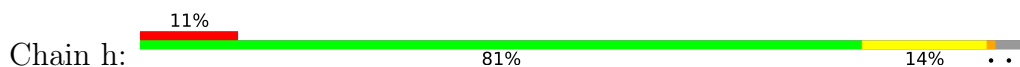
- Molecule 14: Ribonuclease K



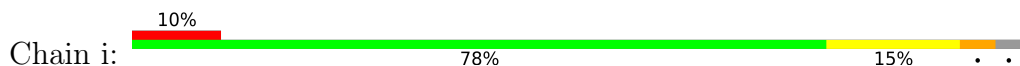
- Molecule 15: V-type proton ATPase 16 kDa proteolipid subunit

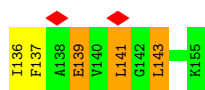


- Molecule 15: V-type proton ATPase 16 kDa proteolipid subunit

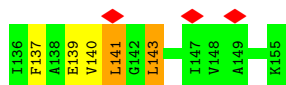
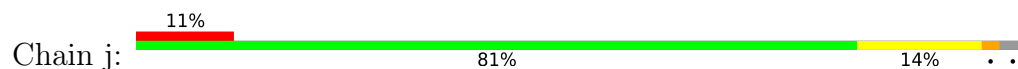


- Molecule 15: V-type proton ATPase 16 kDa proteolipid subunit

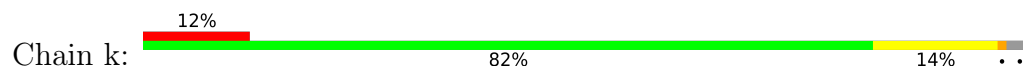




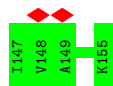
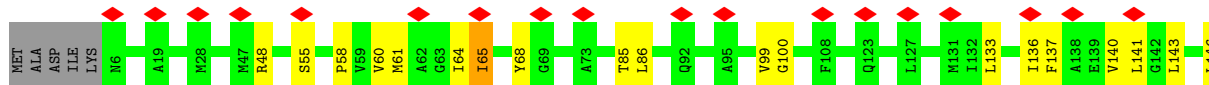
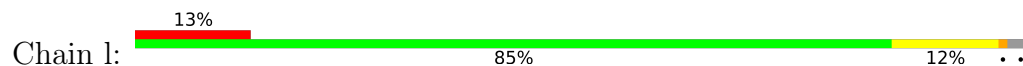
- Molecule 15: V-type proton ATPase 16 kDa proteolipid subunit



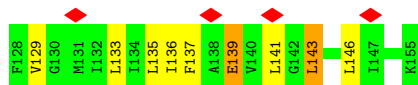
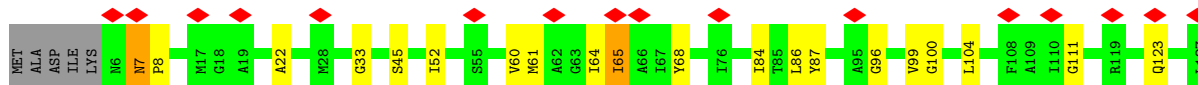
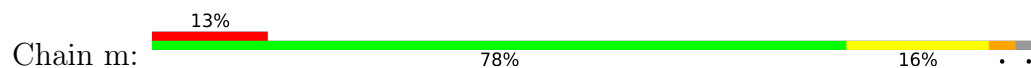
- Molecule 15: V-type proton ATPase 16 kDa proteolipid subunit



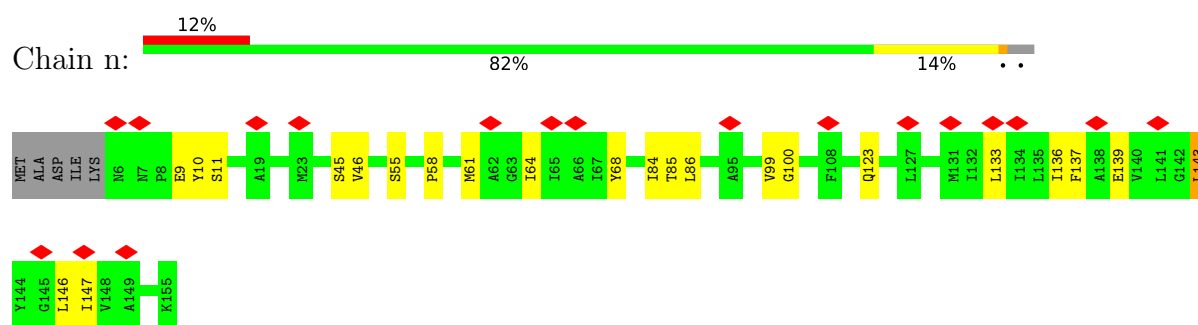
- Molecule 15: V-type proton ATPase 16 kDa proteolipid subunit



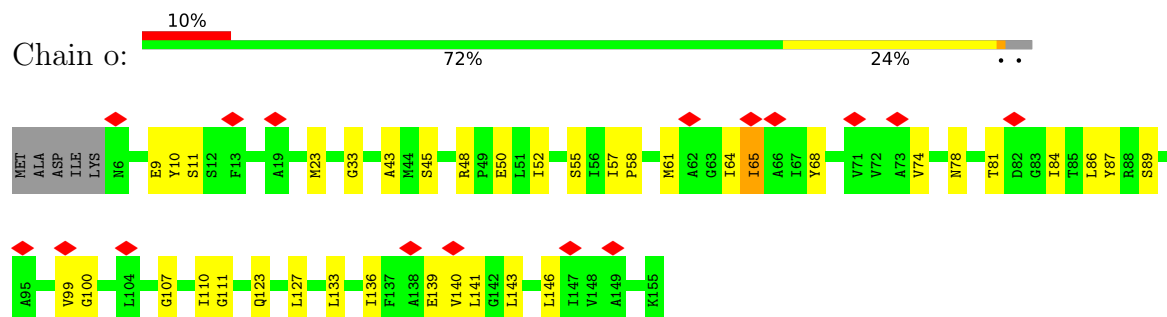
- Molecule 15: V-type proton ATPase 16 kDa proteolipid subunit



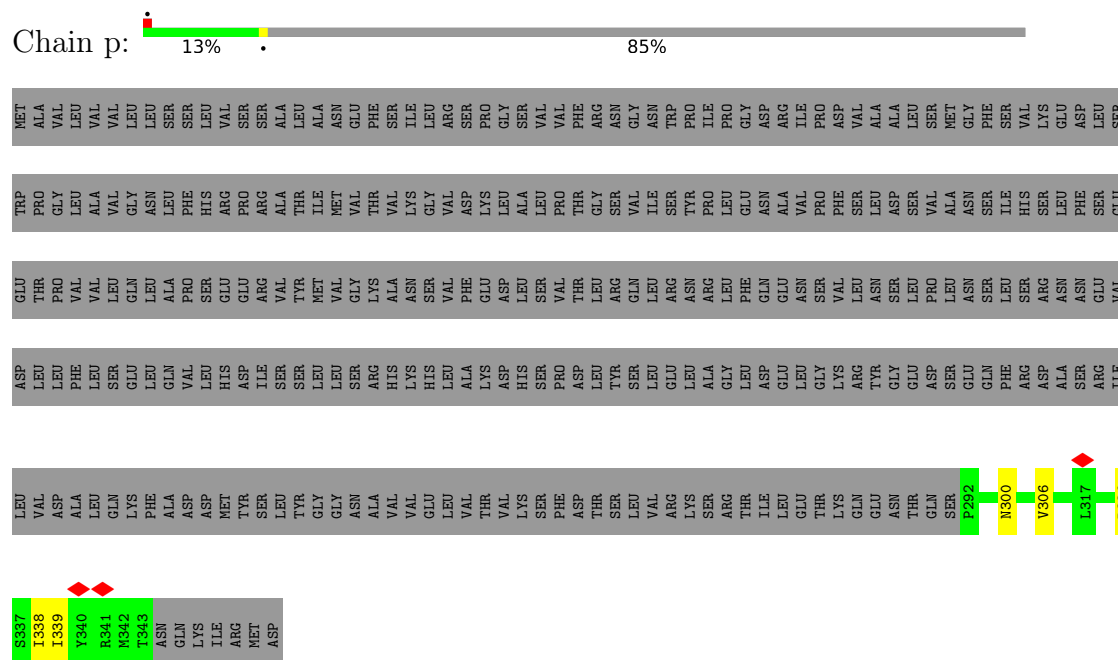
- Molecule 15: V-type proton ATPase 16 kDa proteolipid subunit



- Molecule 15: V-type proton ATPase 16 kDa proteolipid subunit



- Molecule 16: Renin receptor



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	79654	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 ($e^-/\text{\AA}^2$)	43	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	1.467	Depositor
Minimum map value	-0.788	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.070	Depositor
Recommended contour level	0.25	Depositor
Map size (Å)	360.4, 360.4, 360.4	wwPDB
Map dimensions	340, 340, 340	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	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	0.60	5/4746 (0.1%)	0.69	10/6425 (0.2%)
1	B	0.66	5/4746 (0.1%)	0.78	13/6425 (0.2%)
1	C	0.60	0/4746	0.71	4/6425 (0.1%)
2	D	0.59	2/3666 (0.1%)	0.68	4/4967 (0.1%)
2	E	0.57	2/3666 (0.1%)	0.63	3/4967 (0.1%)
2	F	0.60	3/3666 (0.1%)	0.68	8/4967 (0.2%)
3	G	0.39	0/1788	0.96	2/2494 (0.1%)
4	H	0.73	1/1744 (0.1%)	0.93	5/2332 (0.2%)
5	I	0.52	0/1619	0.69	0/2192
5	J	0.57	0/1614	0.74	0/2185
5	K	0.51	0/1619	0.63	0/2192
6	L	0.85	0/880	1.33	13/1189 (1.1%)
7	M	0.51	0/717	0.78	2/980 (0.2%)
7	N	0.58	0/717	0.91	2/980 (0.2%)
7	O	0.52	0/712	0.83	1/973 (0.1%)
8	Q	0.56	0/1912	0.60	0/2575
8	R	0.55	0/1858	0.58	0/2505
8	S	0.53	0/1754	0.58	1/2362 (0.0%)
9	a	0.42	0/3700	0.90	4/5150 (0.1%)
10	b	0.45	0/1537	0.68	1/2088 (0.0%)
11	c	0.57	1/347 (0.3%)	0.91	3/466 (0.6%)
12	d	0.59	0/2899	0.70	3/3927 (0.1%)
13	e	0.29	0/383	0.60	0/531
14	f	0.43	0/410	0.81	0/566
15	g	0.53	0/1083	0.82	5/1466 (0.3%)
15	h	0.50	0/1083	0.75	1/1466 (0.1%)
15	i	0.52	0/1083	0.77	4/1466 (0.3%)
15	j	0.47	0/1083	0.68	0/1466
15	k	0.51	0/1083	0.79	3/1466 (0.2%)
15	l	0.49	0/1083	0.75	2/1466 (0.1%)
15	m	0.56	0/1083	0.93	3/1466 (0.2%)
15	n	0.46	0/1083	0.69	0/1466

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
15	o	0.51	0/1083	0.73	0/1466
16	p	0.48	0/416	0.68	1/571 (0.2%)
All	All	0.56	19/61609 (0.0%)	0.75	98/83628 (0.1%)

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	290	ASP	C-N	-9.36	1.22	1.33
2	F	391	PRO	N-CA	8.46	1.53	1.47
2	E	504	TYR	C-N	6.62	1.41	1.34
2	E	352	PRO	N-CA	5.74	1.54	1.47
1	A	397	ASN	C-N	5.65	1.40	1.34
2	F	396	PRO	N-CA	5.64	1.54	1.47
2	D	487	PHE	C-N	5.59	1.40	1.33
1	A	216	PRO	N-CA	5.58	1.53	1.47
4	H	107	PRO	C-O	-5.58	1.17	1.23
1	B	104	ARG	C-N	5.52	1.39	1.33
1	A	104	ARG	C-N	5.42	1.40	1.33
1	A	170	PRO	N-CA	5.29	1.53	1.47
1	B	368	MET	C-N	5.25	1.39	1.33
2	D	165	TYR	C-N	5.19	1.39	1.33
1	B	532	CYS	C-N	5.14	1.40	1.33
1	B	118	ILE	C-N	5.06	1.40	1.33
2	F	190	PRO	N-CA	5.04	1.53	1.47
11	c	417	PRO	N-CD	5.03	1.54	1.47
1	A	84	LYS	C-N	5.01	1.39	1.33

All (98) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	189	ILE	CA-C-N	9.41	129.35	119.85
2	F	189	ILE	C-N-CA	9.41	129.35	119.85
1	A	215	ARG	CA-C-N	9.31	129.34	119.76
1	A	215	ARG	C-N-CA	9.31	129.34	119.76
1	B	411	SER	CA-C-N	8.43	129.06	120.38
1	B	411	SER	C-N-CA	8.43	129.06	120.38
6	L	91	ILE	CA-C-N	8.01	127.77	119.76
6	L	91	ILE	C-N-CA	8.01	127.77	119.76
2	F	395	LEU	CA-C-N	7.83	128.50	120.04
2	F	395	LEU	C-N-CA	7.83	128.50	120.04
1	A	397	ASN	CA-C-N	7.67	127.34	119.82
1	A	397	ASN	C-N-CA	7.67	127.34	119.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	108	ARG	CA-C-N	-7.66	112.33	123.05
6	L	108	ARG	C-N-CA	-7.66	112.33	123.05
2	D	487	PHE	CA-C-N	7.62	127.58	120.03
2	D	487	PHE	C-N-CA	7.62	127.58	120.03
6	L	104	SER	N-CA-C	-7.55	103.06	111.82
2	E	351	ILE	CA-C-N	7.40	127.40	119.78
2	E	351	ILE	C-N-CA	7.40	127.40	119.78
15	m	7	ASN	CA-C-N	7.33	127.31	119.76
15	m	7	ASN	C-N-CA	7.33	127.31	119.76
1	C	368	MET	CA-C-N	7.31	127.23	119.85
1	C	368	MET	C-N-CA	7.31	127.23	119.85
12	d	171	GLN	N-CA-C	-7.27	102.53	111.33
11	c	416	SER	CA-C-N	7.18	126.71	119.24
11	c	416	SER	C-N-CA	7.18	126.71	119.24
1	A	169	PRO	CA-C-N	7.17	127.17	119.78
1	A	169	PRO	C-N-CA	7.17	127.17	119.78
9	a	360	THR	CA-C-N	7.08	127.67	120.38
9	a	360	THR	C-N-CA	7.08	127.67	120.38
2	F	165	TYR	CA-C-N	7.02	126.99	119.76
2	F	165	TYR	C-N-CA	7.02	126.99	119.76
1	C	238	PHE	CA-C-N	6.95	126.94	119.78
1	C	238	PHE	C-N-CA	6.95	126.94	119.78
6	L	55	PHE	N-CA-C	-6.88	103.86	111.36
7	N	107	ARG	CA-C-N	6.85	126.77	119.85
7	N	107	ARG	C-N-CA	6.85	126.77	119.85
1	A	84	LYS	CA-C-N	6.75	127.21	120.52
1	A	84	LYS	C-N-CA	6.75	127.21	120.52
11	c	417	PRO	N-CA-C	-6.71	102.91	113.78
12	d	3	PHE	N-CA-C	-6.69	104.69	112.92
15	l	48	ARG	CA-C-N	6.49	126.72	119.32
15	l	48	ARG	C-N-CA	6.49	126.72	119.32
1	B	368	MET	CA-C-N	6.44	126.90	120.52
1	B	368	MET	C-N-CA	6.44	126.90	120.52
15	k	7	ASN	CA-C-N	6.33	126.28	119.76
15	k	7	ASN	C-N-CA	6.33	126.28	119.76
6	L	91	ILE	O-C-N	6.30	128.28	121.10
6	L	97	PRO	N-CA-C	6.28	120.83	111.41
15	g	10	TYR	N-CA-C	-6.13	104.19	113.51
4	H	172	ILE	N-CA-C	-6.12	104.78	110.53
8	S	98	ILE	N-CA-C	-6.03	105.49	111.88
2	E	300	MET	N-CA-C	-5.91	106.07	113.28
2	D	165	TYR	CA-C-N	5.89	126.19	119.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	165	TYR	C-N-CA	5.89	126.19	119.83
15	m	129	VAL	N-CA-C	-5.84	104.82	110.72
15	k	9	GLU	CA-C-O	-5.82	115.38	121.55
7	O	68	ASN	N-CA-C	-5.80	104.96	111.28
1	B	104	ARG	CA-C-N	5.79	126.69	119.98
1	B	104	ARG	C-N-CA	5.79	126.69	119.98
1	B	532	CYS	CA-C-N	5.73	125.66	119.76
1	B	532	CYS	C-N-CA	5.73	125.66	119.76
1	A	104	ARG	CA-C-N	5.68	125.96	119.83
1	A	104	ARG	C-N-CA	5.68	125.96	119.83
10	b	94	ILE	N-CA-C	-5.63	105.03	110.72
15	i	9	GLU	CA-C-O	-5.60	115.37	121.87
1	B	413	PRO	N-CA-C	-5.60	106.56	113.84
15	i	7	ASN	CA-C-N	5.57	125.85	119.83
15	i	7	ASN	C-N-CA	5.57	125.85	119.83
1	B	118	ILE	CA-C-N	5.49	125.43	119.78
1	B	118	ILE	C-N-CA	5.49	125.43	119.78
15	g	9	GLU	CA-C-O	-5.48	115.52	121.87
2	F	390	PRO	CA-C-N	5.48	129.30	121.91
2	F	390	PRO	C-N-CA	5.48	129.30	121.91
9	a	529	LYS	N-CA-C	-5.44	105.45	111.71
3	G	301	ARG	N-CA-C	-5.41	105.28	111.07
16	p	306	VAL	N-CA-C	-5.36	105.30	110.72
15	g	8	PRO	N-CA-C	-5.36	102.52	111.26
6	L	33	HIS	CA-C-N	5.36	126.54	119.84
6	L	33	HIS	C-N-CA	5.36	126.54	119.84
15	h	58	PRO	N-CA-C	-5.35	105.12	113.78
4	H	106	LEU	CA-C-N	5.27	125.43	119.90
4	H	106	LEU	C-N-CA	5.27	125.43	119.90
6	L	105	ILE	N-CA-C	-5.19	105.35	111.00
9	a	79	ILE	N-CA-C	5.17	120.09	109.34
3	G	108	ASP	N-CA-C	5.15	116.70	108.41
6	L	105	ILE	CA-C-N	-5.11	112.92	120.28
6	L	105	ILE	C-N-CA	-5.11	112.92	120.28
7	M	71	ALA	CA-C-N	5.09	127.56	120.63
7	M	71	ALA	C-N-CA	5.09	127.56	120.63
15	g	7	ASN	CA-C-N	5.08	125.37	119.93
15	g	7	ASN	C-N-CA	5.08	125.37	119.93
15	i	10	TYR	N-CA-C	-5.06	105.34	113.28
4	H	113	HIS	CA-C-N	5.06	127.31	120.38
4	H	113	HIS	C-N-CA	5.06	127.31	120.38
12	d	126	VAL	CB-CA-C	-5.04	109.01	114.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	76	GLY	CA-C-N	-5.04	112.89	120.60
1	B	76	GLY	C-N-CA	-5.04	112.89	120.60

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	4651	0	4644	14	0
1	B	4651	0	4644	26	0
1	C	4651	0	4644	15	0
2	D	3595	0	3602	14	0
2	E	3595	0	3602	13	0
2	F	3595	0	3602	13	0
3	G	1790	0	794	14	0
4	H	1726	0	1835	60	0
5	I	1607	0	1516	11	0
5	J	1602	0	1511	12	0
5	K	1607	0	1516	22	0
6	L	866	0	865	17	0
7	M	714	0	551	3	0
7	N	714	0	551	4	0
7	O	709	0	549	22	0
8	Q	1878	0	1898	3	0
8	R	1824	0	1835	6	0
8	S	1722	0	1733	7	0
9	a	3703	0	1623	19	0
10	b	1503	0	1551	15	0
11	c	337	0	338	1	0
12	d	2833	0	2770	32	0
13	e	384	0	176	1	0
14	f	412	0	186	0	0
15	g	1068	0	1136	13	0
15	h	1068	0	1136	18	0
15	i	1068	0	1136	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	j	1068	0	1136	20	0
15	k	1068	0	1136	19	0
15	l	1068	0	1136	9	0
15	m	1068	0	1136	23	0
15	n	1068	0	1136	15	0
15	o	1068	0	1136	28	0
16	p	406	0	384	3	0
17	A	27	0	12	1	0
All	All	60714	0	57156	438	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 4.

All (438) 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)
3:G:7:ILE:HA	3:G:370:VAL:O	1.45	1.14
1:B:499:ALA:HB1	4:H:103:GLY:CA	1.80	1.11
1:B:499:ALA:CB	4:H:103:GLY:HA2	1.85	1.07
5:K:23:ALA:CB	7:O:18:ALA:HA	1.84	1.07
1:B:499:ALA:CB	4:H:103:GLY:CA	2.33	1.06
1:B:499:ALA:HB1	4:H:103:GLY:HA2	1.32	1.04
4:H:106:LEU:HG	4:H:157:THR:OG1	1.62	0.98
4:H:107:PRO:HD2	4:H:157:THR:HG21	1.44	0.96
4:H:47:ILE:HD11	4:H:154:SER:HB2	1.47	0.96
4:H:155:PHE:HZ	6:L:109:ALA:HB2	1.32	0.95
4:H:101:VAL:CG2	4:H:106:LEU:HD13	1.97	0.94
4:H:47:ILE:CD1	4:H:154:SER:HB2	1.97	0.93
9:a:33:GLY:HA2	9:a:826:PHE:O	1.68	0.92
15:o:133:LEU:HA	15:o:136:ILE:HD12	1.55	0.89
5:K:30:ILE:CB	7:O:25:ALA:HB1	2.02	0.87
4:H:101:VAL:HG21	4:H:106:LEU:HD13	1.56	0.87
3:G:6:LEU:O	3:G:371:TYR:HA	1.75	0.86
4:H:106:LEU:HD21	4:H:158:LEU:CD2	2.05	0.86
4:H:153:THR:HG23	6:L:84:SER:HB2	1.58	0.85
1:B:499:ALA:HB1	4:H:103:GLY:O	1.78	0.83
1:B:499:ALA:HB1	4:H:103:GLY:C	2.04	0.82
15:g:61:MET:HA	15:g:64:ILE:HD12	1.59	0.82
5:K:23:ALA:HB2	7:O:18:ALA:HA	1.62	0.81
5:K:23:ALA:HB1	7:O:18:ALA:HA	1.61	0.81
1:B:499:ALA:HB3	4:H:103:GLY:CA	2.10	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:106:LEU:HD21	4:H:158:LEU:HD21	1.64	0.78
15:k:133:LEU:HA	15:k:136:ILE:HD12	1.69	0.74
15:n:133:LEU:HA	15:n:136:ILE:HD12	1.67	0.74
15:n:61:MET:HA	15:n:64:ILE:HD12	1.68	0.74
3:G:35:SER:HA	3:G:320:LEU:O	1.88	0.73
4:H:155:PHE:CZ	6:L:109:ALA:HB2	2.21	0.73
5:K:34:ALA:HB1	7:O:29:LYS:HA	1.71	0.72
4:H:101:VAL:HG21	4:H:106:LEU:CD1	2.21	0.71
10:b:59:SER:HB2	15:g:101:LEU:HD23	1.73	0.71
15:i:61:MET:HE2	15:i:139:GLU:HG2	1.74	0.70
1:B:499:ALA:HB3	4:H:103:GLY:HA3	1.72	0.69
9:a:208:ASP:N	9:a:213:ASP:O	2.22	0.69
15:j:30:ALA:HB3	15:k:141:LEU:HD21	1.73	0.69
9:a:11:THR:H	9:a:325:CYS:H	1.40	0.68
4:H:101:VAL:HG22	4:H:106:LEU:HD13	1.75	0.68
4:H:48:LEU:HD12	4:H:48:LEU:C	2.19	0.67
15:h:30:ALA:HB3	15:i:141:LEU:HD21	1.75	0.67
15:i:143:LEU:HD12	15:i:143:LEU:O	1.93	0.67
1:B:499:ALA:CB	4:H:103:GLY:HA3	2.24	0.67
15:j:143:LEU:HD12	15:j:143:LEU:O	1.95	0.67
9:a:198:ARG:O	9:a:220:PHE:HA	1.95	0.66
5:K:34:ALA:CB	7:O:29:LYS:HA	2.25	0.66
5:K:30:ILE:CB	7:O:25:ALA:CB	2.75	0.65
4:H:51:ILE:HG12	4:H:151:LEU:HB3	1.79	0.65
2:D:266:ASP:OD1	8:S:9:LYS:NZ	2.30	0.64
15:j:60:VAL:HG22	15:k:137:PHE:CZ	2.33	0.64
5:K:23:ALA:HB2	7:O:18:ALA:CB	2.28	0.64
4:H:43:ARG:HA	4:H:46:GLN:HB2	1.80	0.64
15:m:68:TYR:HD1	15:m:146:LEU:HD22	1.63	0.64
15:o:61:MET:N	15:o:61:MET:HE2	2.12	0.64
15:l:61:MET:HA	15:l:64:ILE:HD12	1.78	0.63
2:F:251:ASN:HA	5:K:69:LYS:HE2	1.79	0.63
5:K:23:ALA:HB2	7:O:18:ALA:CA	2.28	0.62
15:m:143:LEU:O	15:m:143:LEU:HD12	1.99	0.62
5:J:66:GLN:HA	5:J:69:LYS:HD2	1.82	0.62
15:o:61:MET:HA	15:o:64:ILE:HD12	1.81	0.62
6:L:62:GLY:O	6:L:86:PRO:HA	1.99	0.62
10:b:168:GLN:HG2	12:d:25:ALA:HB2	1.80	0.61
2:D:374:GLU:HA	2:D:400:ARG:HD2	1.82	0.61
12:d:12:ASP:OD1	15:g:36:LYS:NZ	2.34	0.61
2:E:189:ILE:HG23	2:E:189:ILE:O	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:a:11:THR:O	9:a:324:TRP:HA	2.01	0.61
10:b:132:HIS:CE1	15:o:81:THR:O	2.54	0.61
1:B:499:ALA:HB3	4:H:103:GLY:HA2	1.74	0.60
2:D:298:THR:O	2:D:299:ASP:C	2.44	0.60
15:i:8:PRO:HB2	15:i:11:SER:OG	2.01	0.60
15:h:62:ALA:HA	15:h:65:ILE:HD12	1.83	0.60
15:o:68:TYR:HD1	15:o:146:LEU:HD22	1.67	0.59
6:L:85:ILE:N	6:L:86:PRO:HD2	2.17	0.59
9:a:33:GLY:CA	9:a:826:PHE:O	2.47	0.59
2:F:89:VAL:O	2:F:89:VAL:HG23	2.03	0.59
15:n:143:LEU:HD12	15:n:147:ILE:HG13	1.85	0.59
1:A:397:ASN:N	1:A:398:PRO:CD	2.66	0.59
1:B:66:VAL:HG12	1:B:68:GLU:H	1.68	0.59
6:L:85:ILE:N	6:L:86:PRO:CD	2.66	0.59
2:F:360:ASP:OD2	4:H:20:LYS:NZ	2.36	0.58
12:d:249:PRO:O	15:m:123:GLN:NE2	2.36	0.58
15:g:33:GLY:HA2	15:g:111:GLY:HA3	1.85	0.58
5:J:135:ARG:NE	5:J:171:ALA:O	2.36	0.58
5:J:66:GLN:HA	5:J:66:GLN:OE1	2.04	0.58
4:H:107:PRO:CD	4:H:157:THR:HG21	2.28	0.58
15:h:143:LEU:O	15:h:143:LEU:HD12	2.03	0.58
15:m:61:MET:HE2	15:m:139:GLU:HG2	1.85	0.57
1:C:397:ASN:N	1:C:398:PRO:CD	2.66	0.57
4:H:42:LEU:O	4:H:46:GLN:N	2.32	0.57
4:H:106:LEU:HD21	4:H:158:LEU:CG	2.32	0.57
15:g:143:LEU:HD12	15:g:143:LEU:O	2.03	0.57
15:l:60:VAL:HG22	15:m:137:PHE:CZ	2.39	0.57
15:k:84:ILE:HG12	15:k:89:SER:HB2	1.85	0.57
1:A:436:ASP:OD2	4:H:4:LYS:NZ	2.38	0.56
4:H:101:VAL:CG2	4:H:106:LEU:CD1	2.78	0.56
3:G:7:ILE:CA	3:G:370:VAL:O	2.38	0.56
4:H:106:LEU:HD21	4:H:158:LEU:HG	1.87	0.56
5:I:65:GLU:HA	5:I:68:LYS:HD2	1.87	0.56
15:m:68:TYR:CD1	15:m:146:LEU:HD22	2.39	0.56
5:I:67:GLN:O	5:I:70:ILE:HG22	2.05	0.56
12:d:4:PHE:N	12:d:5:PRO:CD	2.67	0.56
9:a:10:MET:CB	9:a:324:TRP:CB	2.84	0.56
12:d:37:VAL:HG13	12:d:344:ILE:HG12	1.88	0.56
7:O:69:LEU:HA	7:O:72:GLU:HB2	1.88	0.56
1:A:391:ARG:NH1	1:A:401:GLU:OE2	2.39	0.56
15:n:143:LEU:HD12	15:n:143:LEU:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:b:58:ILE:CD1	10:b:105:ILE:HG12	2.36	0.55
15:i:65:ILE:HA	15:i:68:TYR:CD2	2.42	0.55
12:d:284:ASN:HB2	12:d:287:ASP:HB2	1.89	0.55
10:b:58:ILE:HD11	10:b:105:ILE:HG12	1.89	0.55
5:K:119:LEU:O	5:K:194:ASN:ND2	2.40	0.55
15:i:60:VAL:HG22	15:j:137:PHE:CZ	2.41	0.55
4:H:44:PHE:HA	4:H:47:ILE:HG22	1.89	0.54
9:a:11:THR:H	9:a:325:CYS:N	2.04	0.54
15:o:68:TYR:CD1	15:o:146:LEU:HD22	2.42	0.54
12:d:169:SER:C	12:d:171:GLN:H	2.15	0.54
5:J:75:LEU:CD2	7:N:70:SER:HB2	2.38	0.54
15:l:133:LEU:HA	15:l:136:ILE:HD12	1.88	0.54
15:k:61:MET:N	15:k:61:MET:HE2	2.23	0.54
4:H:45:ARG:HA	4:H:48:LEU:CD2	2.37	0.53
4:H:101:VAL:HG11	4:H:106:LEU:HD22	1.89	0.53
4:H:43:ARG:O	4:H:47:ILE:N	2.22	0.53
9:a:15:LEU:O	9:a:320:ILE:HA	2.08	0.53
15:i:61:MET:HA	15:i:64:ILE:HD12	1.90	0.53
15:m:60:VAL:HG22	15:n:137:PHE:CZ	2.43	0.53
1:A:280:ARG:NH1	2:D:372:ILE:O	2.42	0.53
15:m:45:SER:HB2	15:m:52:ILE:HD11	1.90	0.53
4:H:106:LEU:HG	4:H:157:THR:HG1	1.68	0.52
15:i:46:VAL:HA	15:j:124:GLN:HB2	1.92	0.52
15:o:33:GLY:HA2	15:o:111:GLY:CA	2.40	0.52
15:o:57:ILE:HG23	15:o:61:MET:HE3	1.91	0.52
9:a:83:GLY:C	9:a:85:ASN:H	2.17	0.52
5:J:67:GLN:OE1	5:J:67:GLN:HA	2.08	0.52
10:b:70:TYR:C	10:b:70:TYR:CD1	2.88	0.52
15:n:84:ILE:HG22	15:n:86:LEU:H	1.75	0.52
3:G:10:PRO:O	3:G:316:PHE:HA	2.10	0.52
5:I:72:MET:HA	5:I:72:MET:HE3	1.92	0.52
15:h:60:VAL:HG22	15:i:137:PHE:HZ	1.74	0.52
8:R:60:TYR:O	8:R:61:ARG:HB2	2.09	0.51
7:O:69:LEU:O	7:O:73:VAL:N	2.34	0.51
15:o:9:GLU:O	15:o:11:SER:N	2.44	0.51
1:A:449:ASN:O	1:A:450:TRP:CG	2.63	0.51
2:E:173:GLY:O	2:E:465:GLN:NE2	2.38	0.51
5:I:63:GLN:HA	5:I:66:GLN:HB3	1.91	0.51
8:R:99:SER:N	8:R:100:PRO:HD2	2.26	0.51
12:d:131:PRO:O	12:d:132:LEU:HB2	2.11	0.51
15:j:33:GLY:HA2	15:j:111:GLY:HA3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:49:LYS:HB2	4:H:49:LYS:NZ	2.25	0.51
12:d:307:LEU:HA	15:o:43:ALA:HB1	1.92	0.51
15:n:61:MET:HE2	15:n:61:MET:N	2.25	0.51
2:F:505:PRO:O	2:F:506:ARG:HB2	2.11	0.51
6:L:96:HIS:CG	6:L:97:PRO:HD2	2.46	0.51
3:G:34:VAL:O	3:G:321:LEU:HA	2.11	0.50
9:a:33:GLY:HA2	9:a:827:SER:HA	1.92	0.50
1:B:234:LEU:HD22	1:B:433:TRP:CD2	2.45	0.50
15:g:41:ILE:HG12	15:g:55:SER:HB2	1.93	0.50
9:a:316:GLN:O	9:a:318:CYS:N	2.43	0.50
15:g:33:GLY:HA2	15:g:111:GLY:CA	2.40	0.50
15:m:65:ILE:HA	15:m:68:TYR:CD2	2.46	0.50
1:C:436:ASP:OD1	1:C:437:LYS:N	2.45	0.50
4:H:55:LYS:NZ	6:L:99:ASP:OD2	2.34	0.50
12:d:169:SER:O	12:d:171:GLN:N	2.43	0.50
15:h:65:ILE:HD11	15:h:110:ILE:HG13	1.94	0.50
15:m:65:ILE:HA	15:m:68:TYR:HD2	1.76	0.50
1:B:39:MET:HG2	1:B:40:TYR:CD1	2.47	0.50
5:J:137:ARG:NH1	5:J:177:ILE:O	2.45	0.50
5:K:19:ILE:CB	7:O:14:ALA:HB1	2.41	0.50
5:K:129:GLU:H	5:K:132:MET:CE	2.25	0.50
15:j:33:GLY:HA2	15:j:111:GLY:CA	2.41	0.50
2:F:395:LEU:N	2:F:396:PRO:HD2	2.26	0.49
12:d:4:PHE:N	12:d:5:PRO:HD2	2.26	0.49
4:H:106:LEU:CD2	4:H:158:LEU:HD21	2.40	0.49
15:m:61:MET:HA	15:m:64:ILE:HD12	1.94	0.49
1:C:100:ASP:OD1	1:C:101:GLY:N	2.45	0.49
10:b:72:THR:HG23	10:b:156:GLY:HA2	1.95	0.49
12:d:62:ALA:HB1	12:d:64:PRO:HD2	1.94	0.49
6:L:112:MET:O	6:L:113:PHE:C	2.55	0.49
15:n:46:VAL:HG11	15:o:123:GLN:OE1	2.12	0.49
15:n:85:THR:O	15:n:86:LEU:HB3	2.13	0.49
4:H:49:LYS:NZ	4:H:49:LYS:CB	2.76	0.49
4:H:47:ILE:HG21	4:H:158:LEU:HD12	1.95	0.49
15:i:60:VAL:HG22	15:j:137:PHE:HZ	1.78	0.49
2:E:255:ASP:OD1	5:J:80:ARG:NH1	2.44	0.48
4:H:154:SER:O	4:H:158:LEU:HG	2.13	0.48
12:d:169:SER:O	12:d:170:GLU:HB2	2.13	0.48
2:E:118:ILE:O	2:E:120:ARG:N	2.46	0.48
15:k:33:GLY:HA2	15:k:111:GLY:HA3	1.95	0.48
15:o:9:GLU:C	15:o:11:SER:H	2.22	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:o:86:LEU:O	15:o:89:SER:N	2.47	0.48
1:B:499:ALA:CB	4:H:103:GLY:O	2.56	0.48
10:b:34:ARG:HH21	11:c:413:GLY:HA2	1.78	0.48
15:n:9:GLU:O	15:n:11:SER:N	2.46	0.48
15:o:45:SER:HB2	15:o:52:ILE:HD11	1.96	0.48
15:o:86:LEU:O	15:o:87:TYR:C	2.55	0.48
2:E:84:GLY:CA	2:E:97:GLN:O	2.62	0.48
3:G:20:GLU:O	3:G:27:THR:HA	2.14	0.48
2:E:106:ASP:OD1	2:E:106:ASP:C	2.57	0.47
6:L:62:GLY:HA2	6:L:85:ILE:HG22	1.96	0.47
8:R:199:LEU:HD23	8:R:199:LEU:C	2.40	0.47
5:I:68:LYS:HE2	7:M:62:ALA:HB1	1.95	0.47
7:M:71:ALA:O	7:M:75:GLN:HG3	2.14	0.47
8:S:115:MET:SD	8:S:126:TYR:CE2	3.08	0.47
15:h:60:VAL:HG22	15:i:137:PHE:CZ	2.49	0.47
15:o:65:ILE:HA	15:o:68:TYR:HD2	1.78	0.47
1:A:399:GLU:OE2	8:Q:25:LYS:NZ	2.45	0.47
5:K:185:ASN:ND2	5:K:187:ASP:OD1	2.47	0.47
10:b:196:LEU:HD22	15:o:78:ASN:OD1	2.15	0.47
4:H:45:ARG:HA	4:H:48:LEU:HD23	1.96	0.47
2:F:273:ILE:O	2:F:274:THR:C	2.58	0.47
4:H:47:ILE:CD1	4:H:154:SER:CB	2.84	0.47
8:S:217:LEU:HD12	8:S:217:LEU:C	2.40	0.47
5:I:94:LEU:HD23	5:I:94:LEU:C	2.39	0.46
1:A:100:ASP:C	1:A:100:ASP:OD1	2.58	0.46
2:E:273:ILE:O	2:E:274:THR:C	2.58	0.46
15:i:8:PRO:HG2	15:i:86:LEU:HD22	1.96	0.46
15:i:61:MET:HA	15:i:64:ILE:CD1	2.46	0.46
10:b:196:LEU:CD1	15:o:74:VAL:HG13	2.46	0.46
12:d:105:MET:HG2	12:d:133:GLY:HA2	1.96	0.46
15:h:60:VAL:HA	15:i:137:PHE:CE2	2.50	0.46
15:j:60:VAL:HG22	15:k:137:PHE:HZ	1.77	0.46
2:D:365:ILE:HB	2:D:366:PRO:CD	2.46	0.46
2:F:194:ALA:H	2:F:197:LEU:HD12	1.81	0.46
12:d:331:TRP:CE2	12:d:346:ASN:HB2	2.51	0.46
12:d:158:THR:HG22	12:d:160:LEU:H	1.80	0.46
15:i:33:GLY:HA2	15:i:111:GLY:HA3	1.97	0.46
15:m:133:LEU:HA	15:m:136:ILE:HD12	1.98	0.46
4:H:49:LYS:HB2	4:H:49:LYS:HZ1	1.81	0.46
2:E:187:GLN:CG	2:E:188:LYS:H	2.29	0.46
2:F:186:GLY:N	2:F:349:THR:HG22	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:64:GLY:O	7:O:68:ASN:N	2.44	0.46
7:O:71:ALA:O	7:O:75:GLN:N	2.47	0.46
15:l:68:TYR:CD1	15:l:146:LEU:HD22	2.51	0.46
15:m:133:LEU:O	15:m:136:ILE:HB	2.16	0.46
2:F:190:PRO:HA	2:F:352:PRO:O	2.16	0.46
3:G:39:ASN:O	3:G:106:GLN:HA	2.16	0.46
9:a:9:GLU:O	9:a:326:PRO:N	2.48	0.46
12:d:63:SER:N	12:d:64:PRO:HD2	2.31	0.46
1:A:448:VAL:O	1:A:450:TRP:CE3	2.69	0.46
1:C:588:ASP:OD2	1:C:591:LYS:NZ	2.45	0.45
10:b:168:GLN:HG2	12:d:25:ALA:CB	2.45	0.45
15:g:107:GLY:HA2	15:g:110:ILE:HD12	1.97	0.45
15:i:46:VAL:HG21	16:p:338:ILE:HG21	1.98	0.45
15:k:33:GLY:HA2	15:k:111:GLY:CA	2.46	0.45
15:m:84:ILE:HG22	15:m:86:LEU:H	1.81	0.45
15:g:84:ILE:HG22	15:g:86:LEU:H	1.82	0.45
1:C:353:ARG:NH2	2:F:371:TYR:O	2.47	0.45
1:B:499:ALA:CB	4:H:103:GLY:C	2.81	0.45
9:a:403:PHE:O	9:a:407:PHE:N	2.49	0.45
15:j:52:ILE:CD1	15:k:127:LEU:HA	2.46	0.45
4:H:52:ILE:O	4:H:56:MET:HG2	2.17	0.45
8:S:8:ILE:O	8:S:9:LYS:C	2.60	0.45
15:j:58:PRO:HG3	15:j:135:LEU:HD11	1.99	0.45
1:C:397:ASN:N	1:C:398:PRO:HD3	2.31	0.45
2:D:154:MET:O	2:D:337:ARG:NH2	2.49	0.45
2:F:106:ASP:OD1	2:F:106:ASP:C	2.60	0.45
5:J:152:ILE:HG22	5:J:153:PRO:HD3	1.98	0.45
15:i:30:ALA:HB3	15:j:141:LEU:HD21	1.99	0.45
5:J:152:ILE:N	5:J:153:PRO:HD2	2.32	0.45
8:R:92:LEU:HD23	8:R:92:LEU:C	2.41	0.45
9:a:188:TRP:HA	9:a:191:CYS:O	2.17	0.45
12:d:118:HIS:O	12:d:119:GLN:C	2.60	0.45
12:d:331:TRP:CZ2	12:d:346:ASN:HB2	2.52	0.45
15:m:65:ILE:O	15:m:68:TYR:HB2	2.16	0.45
15:o:133:LEU:O	15:o:136:ILE:HB	2.17	0.45
1:B:37:ALA:HB1	1:B:54:ILE:CD1	2.48	0.44
15:n:68:TYR:CD1	15:n:146:LEU:HD22	2.52	0.44
1:A:257:THR:HB	17:A:701:ADP:O2A	2.18	0.44
3:G:18:THR:O	3:G:22:LEU:N	2.33	0.44
5:I:64:ILE:O	5:I:68:LYS:HG3	2.16	0.44
5:J:185:ASN:ND2	5:J:187:ASP:OD1	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:b:190:GLY:HA2	15:o:23:MET:HG2	1.99	0.44
2:D:188:LYS:HD3	2:D:335:TYR:O	2.18	0.44
2:D:389:TYR:C	2:D:389:TYR:CD2	2.95	0.44
2:E:194:ALA:H	2:E:197:LEU:HD12	1.81	0.44
7:O:96:LEU:C	7:O:96:LEU:HD23	2.42	0.44
8:Q:44:LYS:NZ	8:Q:113:GLU:OE2	2.50	0.44
12:d:234:LYS:HE2	12:d:259:ASP:OD1	2.18	0.44
15:h:55:SER:O	15:h:58:PRO:HD2	2.18	0.44
15:k:61:MET:HE2	15:k:61:MET:CA	2.47	0.44
15:m:33:GLY:HA2	15:m:111:GLY:HA3	1.99	0.44
15:m:99:VAL:HG13	15:m:100:GLY:N	2.33	0.44
1:A:66:VAL:HG12	1:A:68:GLU:H	1.82	0.44
15:j:62:ALA:HA	15:j:110:ILE:HD12	2.00	0.44
15:h:9:GLU:O	15:h:11:SER:N	2.51	0.44
1:C:94:ILE:HD12	1:C:99:PHE:CZ	2.53	0.44
10:b:59:SER:O	10:b:63:VAL:HG23	2.17	0.44
15:k:99:VAL:HG13	15:k:100:GLY:N	2.33	0.44
15:m:22:ALA:HB2	15:m:96:GLY:HA2	1.99	0.44
1:B:100:ASP:OD1	1:B:101:GLY:N	2.49	0.44
1:C:483:LEU:C	1:C:483:LEU:HD23	2.43	0.44
2:D:380:ASP:C	2:D:380:ASP:OD1	2.60	0.44
3:G:16:GLN:O	3:G:20:GLU:N	2.47	0.44
15:h:9:GLU:HG3	15:h:10:TYR:N	2.33	0.44
4:H:52:ILE:HD11	6:L:106:LEU:HD21	2.00	0.44
15:j:80:LEU:C	15:k:87:TYR:OH	2.61	0.44
15:o:65:ILE:N	15:o:65:ILE:CD1	2.81	0.44
15:o:107:GLY:HA2	15:o:110:ILE:HD12	1.99	0.44
15:o:65:ILE:HA	15:o:68:TYR:CD2	2.52	0.43
15:o:84:ILE:HG22	15:o:86:LEU:H	1.82	0.43
2:E:187:GLN:CG	2:E:188:LYS:N	2.80	0.43
1:B:449:ASN:OD1	1:B:451:LEU:HB2	2.18	0.43
1:B:469:PHE:C	1:B:471:GLU:H	2.26	0.43
2:E:365:ILE:HB	2:E:366:PRO:CD	2.49	0.43
6:L:34:PRO:HB2	6:L:36:PHE:CE2	2.53	0.43
15:m:104:LEU:C	15:m:104:LEU:HD23	2.44	0.43
12:d:169:SER:C	12:d:171:GLN:N	2.76	0.43
4:H:148:LEU:HG	6:L:89:LEU:HD22	1.99	0.43
12:d:113:ILE:O	12:d:114:THR:HB	2.19	0.43
15:g:65:ILE:O	15:g:68:TYR:HB2	2.19	0.43
15:i:143:LEU:HD12	15:i:143:LEU:C	2.39	0.43
15:i:104:LEU:HD23	15:i:104:LEU:C	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:39:MET:HE2	1:C:40:TYR:CZ	2.53	0.43
2:D:201:GLU:OE1	2:D:201:GLU:N	2.49	0.43
5:I:66:GLN:HG2	5:I:67:GLN:N	2.34	0.43
5:I:68:LYS:HE2	7:M:62:ALA:CB	2.49	0.43
15:i:61:MET:SD	15:i:135:LEU:HB3	2.59	0.43
5:K:108:ASP:OD1	5:K:109:THR:N	2.48	0.43
6:L:6:LYS:NZ	6:L:59:ASP:O	2.48	0.43
10:b:58:ILE:HG23	10:b:59:SER:N	2.34	0.43
15:g:82:ASP:OD1	15:g:83:GLY:N	2.52	0.43
15:h:61:MET:HA	15:h:64:ILE:CD1	2.49	0.43
15:m:61:MET:SD	15:m:135:LEU:HB3	2.59	0.43
2:D:504:TYR:HB3	2:D:505:PRO:HD3	2.00	0.43
5:K:23:ALA:CB	7:O:18:ALA:CA	2.73	0.43
6:L:61:ILE:HG22	6:L:62:GLY:N	2.33	0.43
15:n:99:VAL:HG13	15:n:100:GLY:N	2.34	0.43
1:C:445:PHE:HA	1:C:446:PRO:C	2.43	0.42
15:j:80:LEU:C	15:k:87:TYR:HH	2.27	0.42
15:k:60:VAL:HG22	15:l:137:PHE:CZ	2.54	0.42
1:A:233:VAL:O	1:A:234:LEU:HB2	2.19	0.42
1:C:234:LEU:HD22	1:C:433:TRP:CG	2.54	0.42
7:O:66:GLN:HA	7:O:69:LEU:CB	2.49	0.42
1:B:233:VAL:CG1	1:B:520:LEU:O	2.67	0.42
8:S:195:GLU:OE1	8:S:195:GLU:N	2.50	0.42
15:j:85:THR:O	15:j:86:LEU:HB3	2.19	0.42
4:H:50:LYS:HE2	4:H:151:LEU:HD21	2.01	0.42
10:b:67:TRP:HA	10:b:70:TYR:CE2	2.54	0.42
15:i:65:ILE:O	15:i:68:TYR:HB2	2.19	0.42
7:N:70:SER:O	7:N:73:VAL:HB	2.19	0.42
15:h:61:MET:HA	15:h:64:ILE:HD12	2.01	0.42
15:o:48:ARG:HB2	15:o:50:GLU:CD	2.45	0.42
1:C:20:TYR:CE2	7:O:115:ARG:HG3	2.55	0.42
1:B:339:ASP:O	1:B:400:ARG:NE	2.45	0.42
1:B:397:ASN:HB3	8:R:28:TYR:CG	2.55	0.42
5:I:129:GLU:H	5:I:132:MET:CE	2.32	0.42
5:I:137:ARG:NH1	5:I:177:ILE:O	2.53	0.42
5:J:75:LEU:HD22	7:N:70:SER:HB2	2.00	0.42
5:K:137:ARG:NH1	5:K:177:ILE:O	2.52	0.42
9:a:36:GLN:O	9:a:323:VAL:HA	2.19	0.42
9:a:407:PHE:O	9:a:409:ASP:N	2.53	0.42
15:j:9:GLU:C	15:j:10:TYR:CD2	2.98	0.42
1:B:562:ASP:OD1	1:B:562:ASP:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:389:TYR:C	2:E:389:TYR:CD2	2.97	0.42
3:G:76:MET:O	3:G:80:LEU:N	2.48	0.42
5:K:75:LEU:HD13	7:O:70:SER:CB	2.49	0.42
15:j:82:ASP:OD1	15:j:83:GLY:N	2.53	0.42
15:j:119:ARG:HH11	16:p:339:ILE:HD12	1.85	0.42
15:k:55:SER:O	15:k:58:PRO:HD2	2.19	0.42
16:p:336:ASP:C	16:p:336:ASP:OD1	2.62	0.42
3:G:8:SER:HA	3:G:318:ALA:HA	2.00	0.42
4:H:177:ILE:O	4:H:178:PRO:C	2.63	0.42
15:i:8:PRO:O	15:i:11:SER:OG	2.36	0.42
15:l:99:VAL:HG13	15:l:100:GLY:N	2.34	0.42
15:m:7:ASN:HA	15:m:8:PRO:HD3	1.94	0.42
1:A:397:ASN:HB3	8:Q:28:TYR:CG	2.55	0.42
8:S:126:TYR:CZ	8:S:130:LEU:HD11	2.55	0.42
15:h:33:GLY:HA2	15:h:111:GLY:CA	2.50	0.42
15:o:55:SER:O	15:o:58:PRO:HD2	2.20	0.42
4:H:46:GLN:O	4:H:50:LYS:HG3	2.20	0.41
5:K:103:SER:O	5:K:106:VAL:HG22	2.19	0.41
12:d:133:GLY:O	12:d:135:PHE:N	2.53	0.41
15:h:30:ALA:CB	15:i:141:LEU:HD21	2.46	0.41
15:h:85:THR:O	15:h:86:LEU:HB3	2.19	0.41
5:K:129:GLU:H	5:K:132:MET:HE2	1.85	0.41
15:g:9:GLU:O	15:g:10:TYR:HB2	2.19	0.41
15:j:55:SER:O	15:j:58:PRO:HD2	2.20	0.41
15:k:7:ASN:HB3	15:k:8:PRO:HD2	2.01	0.41
15:m:86:LEU:O	15:m:87:TYR:C	2.62	0.41
15:n:55:SER:O	15:n:58:PRO:HD2	2.20	0.41
2:F:395:LEU:HB2	2:F:396:PRO:HD3	2.02	0.41
7:O:69:LEU:HA	7:O:72:GLU:CD	2.45	0.41
9:a:131:ILE:HA	9:a:172:ALA:O	2.20	0.41
15:i:99:VAL:HG13	15:i:100:GLY:N	2.35	0.41
1:A:153:TYR:CZ	1:A:166:ILE:HG22	2.55	0.41
1:C:233:VAL:O	1:C:234:LEU:HB2	2.20	0.41
4:H:44:PHE:CD2	4:H:44:PHE:C	2.99	0.41
15:n:45:SER:HB2	15:o:127:LEU:HD21	2.03	0.41
6:L:13:ASP:OD1	6:L:13:ASP:C	2.64	0.41
15:l:85:THR:O	15:l:86:LEU:HB3	2.20	0.41
15:o:99:VAL:HG13	15:o:100:GLY:N	2.35	0.41
1:B:397:ASN:N	1:B:398:PRO:CD	2.83	0.41
7:N:110:VAL:O	7:N:111:HIS:C	2.64	0.41
4:H:88:ASN:OD1	4:H:89:LYS:N	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:108:ASP:CG	5:J:109:THR:N	2.78	0.41
12:d:254:GLN:OE1	12:d:254:GLN:N	2.49	0.41
15:i:133:LEU:HA	15:i:136:ILE:HD12	2.02	0.41
9:a:207:GLU:HA	9:a:213:ASP:C	2.46	0.41
12:d:170:GLU:O	12:d:173:LEU:N	2.53	0.41
13:e:76:VAL:O	13:e:77:ARG:C	2.63	0.41
2:D:269:ILE:O	2:D:272:ILE:HG12	2.21	0.41
2:E:133:ASN:OD1	2:E:133:ASN:C	2.64	0.41
3:G:276:PHE:O	3:G:277:GLY:C	2.64	0.41
7:O:69:LEU:O	7:O:73:VAL:HG23	2.21	0.41
8:S:98:ILE:C	8:S:100:PRO:HD2	2.45	0.41
12:d:179:GLU:O	12:d:182:ARG:HG2	2.21	0.41
12:d:272:PRO:HD2	15:n:123:GLN:HG2	2.03	0.41
15:i:109:ALA:O	15:i:113:VAL:HG22	2.21	0.41
15:k:133:LEU:O	15:k:136:ILE:HB	2.21	0.41
1:A:266:TYR:HB3	1:A:531:PHE:CD1	2.56	0.41
4:H:69:LEU:C	4:H:69:LEU:HD23	2.46	0.41
5:K:82:LYS:NZ	7:O:74:GLU:OE2	2.52	0.41
6:L:85:ILE:HB	6:L:86:PRO:HD3	2.03	0.41
12:d:90:TYR:O	12:d:91:GLU:C	2.62	0.41
12:d:93:LEU:C	12:d:93:LEU:HD23	2.45	0.41
15:k:68:TYR:CD1	15:k:146:LEU:HD22	2.57	0.41
15:l:55:SER:O	15:l:58:PRO:HD2	2.21	0.41
15:m:61:MET:HA	15:m:64:ILE:CD1	2.51	0.41
2:D:299:ASP:OD1	2:D:301:SER:HB2	2.21	0.40
12:d:131:PRO:O	12:d:132:LEU:CB	2.69	0.40
12:d:222:ILE:HG23	12:d:223:ILE:N	2.36	0.40
15:h:82:ASP:OD1	15:h:83:GLY:N	2.51	0.40
15:h:99:VAL:HG13	15:h:100:GLY:N	2.35	0.40
1:B:324:GLU:HG3	1:B:354:TRP:HE1	1.87	0.40
2:D:504:TYR:N	2:D:505:PRO:CD	2.85	0.40
3:G:210:PRO:CB	5:K:8:VAL:CB	3.00	0.40
15:k:61:MET:HE2	15:k:61:MET:HA	2.04	0.40
1:C:266:TYR:HB3	1:C:531:PHE:CD1	2.56	0.40
2:F:99:PHE:CD1	2:F:269:ILE:HG21	2.56	0.40
4:H:122:THR:O	4:H:126:ARG:HA	2.22	0.40
4:H:210:LYS:NZ	4:H:214:GLU:OE2	2.54	0.40
15:g:22:ALA:HB2	15:g:96:GLY:HA2	2.02	0.40
15:h:81:THR:H	15:h:84:ILE:HD11	1.87	0.40
15:i:85:THR:O	15:i:86:LEU:HB3	2.21	0.40
1:B:229:THR:HG23	1:B:231:GLN:H	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:396:GLY:C	1:C:398:PRO:HD2	2.46	0.40
15:l:65:ILE:HA	15:l:68:TYR:CD2	2.57	0.40
8:R:197:TYR:CZ	8:R:232:TYR:HB2	2.57	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	598/617 (97%)	573 (96%)	24 (4%)	1 (0%)	43	74
1	B	598/617 (97%)	580 (97%)	18 (3%)	0	100	100
1	C	598/617 (97%)	575 (96%)	22 (4%)	1 (0%)	43	74
2	D	455/511 (89%)	443 (97%)	9 (2%)	3 (1%)	18	53
2	E	455/511 (89%)	442 (97%)	11 (2%)	2 (0%)	30	64
2	F	455/511 (89%)	442 (97%)	13 (3%)	0	100	100
3	G	356/382 (93%)	353 (99%)	3 (1%)	0	100	100
4	H	212/247 (86%)	205 (97%)	7 (3%)	0	100	100
5	I	223/226 (99%)	223 (100%)	0	0	100	100
5	J	222/226 (98%)	222 (100%)	0	0	100	100
5	K	223/226 (99%)	222 (100%)	1 (0%)	0	100	100
6	L	108/119 (91%)	101 (94%)	5 (5%)	2 (2%)	6	33
7	M	112/118 (95%)	111 (99%)	1 (1%)	0	100	100
7	N	112/118 (95%)	111 (99%)	1 (1%)	0	100	100
7	O	111/118 (94%)	109 (98%)	2 (2%)	0	100	100
8	Q	230/301 (76%)	223 (97%)	6 (3%)	1 (0%)	30	64
8	R	222/301 (74%)	214 (96%)	7 (3%)	1 (0%)	24	59

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	S	210/301 (70%)	204 (97%)	6 (3%)	0	100	100
9	a	743/838 (89%)	720 (97%)	22 (3%)	1 (0%)	48	80
10	b	201/205 (98%)	198 (98%)	3 (2%)	0	100	100
11	c	39/463 (8%)	39 (100%)	0	0	100	100
12	d	348/351 (99%)	329 (94%)	18 (5%)	1 (0%)	36	69
13	e	76/81 (94%)	75 (99%)	1 (1%)	0	100	100
14	f	80/98 (82%)	77 (96%)	3 (4%)	0	100	100
15	g	148/155 (96%)	146 (99%)	2 (1%)	0	100	100
15	h	148/155 (96%)	145 (98%)	3 (2%)	0	100	100
15	i	148/155 (96%)	145 (98%)	3 (2%)	0	100	100
15	j	148/155 (96%)	146 (99%)	2 (1%)	0	100	100
15	k	148/155 (96%)	145 (98%)	3 (2%)	0	100	100
15	l	148/155 (96%)	145 (98%)	3 (2%)	0	100	100
15	m	148/155 (96%)	145 (98%)	3 (2%)	0	100	100
15	n	148/155 (96%)	145 (98%)	2 (1%)	1 (1%)	18	53
15	o	148/155 (96%)	143 (97%)	4 (3%)	1 (1%)	18	53
16	p	50/350 (14%)	46 (92%)	3 (6%)	1 (2%)	6	32
All	All	8369/9848 (85%)	8142 (97%)	211 (2%)	16 (0%)	44	74

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	a	79	ILE
16	p	300	ASN
1	A	350	SER
2	D	299	ASP
2	E	119	LEU
15	n	10	TYR
15	o	10	TYR
2	D	119	LEU
6	L	100	ALA
8	Q	12	GLY
1	C	278	GLY
2	D	378	TYR
2	E	378	TYR
12	d	119	GLN

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Mol	Chain	Res	Type
6	L	61	ILE
8	R	75	PRO

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	507/524 (97%)	506 (100%)	1 (0%)	87	87
1	B	507/524 (97%)	507 (100%)	0	100	100
1	C	507/524 (97%)	506 (100%)	1 (0%)	87	87
2	D	393/431 (91%)	393 (100%)	0	100	100
2	E	393/431 (91%)	393 (100%)	0	100	100
2	F	393/431 (91%)	393 (100%)	0	100	100
4	H	185/212 (87%)	180 (97%)	5 (3%)	39	60
5	I	141/198 (71%)	138 (98%)	3 (2%)	47	65
5	J	141/198 (71%)	141 (100%)	0	100	100
5	K	141/198 (71%)	141 (100%)	0	100	100
6	L	92/100 (92%)	92 (100%)	0	100	100
7	M	43/100 (43%)	43 (100%)	0	100	100
7	N	43/100 (43%)	43 (100%)	0	100	100
7	O	43/100 (43%)	43 (100%)	0	100	100
8	Q	208/274 (76%)	208 (100%)	0	100	100
8	R	203/274 (74%)	203 (100%)	0	100	100
8	S	191/274 (70%)	191 (100%)	0	100	100
10	b	156/158 (99%)	156 (100%)	0	100	100
11	c	36/395 (9%)	36 (100%)	0	100	100
12	d	305/306 (100%)	305 (100%)	0	100	100
15	g	109/113 (96%)	106 (97%)	3 (3%)	38	59
15	h	109/113 (96%)	107 (98%)	2 (2%)	51	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	i	109/113 (96%)	102 (94%)	7 (6%)	16	42
15	j	109/113 (96%)	104 (95%)	5 (5%)	24	48
15	k	109/113 (96%)	106 (97%)	3 (3%)	38	59
15	l	109/113 (96%)	105 (96%)	4 (4%)	30	53
15	m	109/113 (96%)	105 (96%)	4 (4%)	30	53
15	n	109/113 (96%)	107 (98%)	2 (2%)	51	67
15	o	109/113 (96%)	104 (95%)	5 (5%)	24	48
16	p	41/313 (13%)	41 (100%)	0	100	100
All	All	5650/7082 (80%)	5605 (99%)	45 (1%)	70	77

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	173	ARG
1	C	296	MET
4	H	44	PHE
4	H	48	LEU
4	H	49	LYS
4	H	52	ILE
4	H	157	THR
5	I	66	GLN
5	I	67	GLN
5	I	70	ILE
15	g	61	MET
15	g	136	ILE
15	g	143	LEU
15	h	61	MET
15	h	139	GLU
15	i	61	MET
15	i	65	ILE
15	i	110	ILE
15	i	135	LEU
15	i	139	GLU
15	i	141	LEU
15	i	143	LEU
15	j	110	ILE
15	j	139	GLU
15	j	140	VAL
15	j	141	LEU

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Mol	Chain	Res	Type
15	j	143	LEU
15	k	139	GLU
15	k	141	LEU
15	k	143	LEU
15	l	65	ILE
15	l	140	VAL
15	l	141	LEU
15	l	143	LEU
15	m	65	ILE
15	m	139	GLU
15	m	141	LEU
15	m	143	LEU
15	n	139	GLU
15	n	143	LEU
15	o	65	ILE
15	o	139	GLU
15	o	140	VAL
15	o	141	LEU
15	o	143	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	HIS
1	B	103	GLN
1	B	146	HIS
1	B	268	ASN
1	B	441	GLN
1	C	213	GLN
1	C	231	GLN
2	D	85	GLN
2	D	181	ASN
2	E	73	HIS
2	E	358	ASN
2	F	181	ASN
2	F	384	HIS
4	H	85	GLN
4	H	137	ASN
5	I	67	GLN
5	J	206	GLN
8	Q	34	GLN
8	Q	184	HIS

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Mol	Chain	Res	Type
8	Q	222	GLN
8	R	177	GLN
8	R	184	HIS
8	R	207	GLN
8	S	160	GLN
12	d	30	GLN
12	d	88	HIS
15	m	124	GLN
16	p	308	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](#)

1 ligand is 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	$\# Z > 2$
17	ADP	A	701	-	28,29,29	0.47	0	43,45,45	0.43	0

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
17	ADP	A	701	-	-	5/16/32/32	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

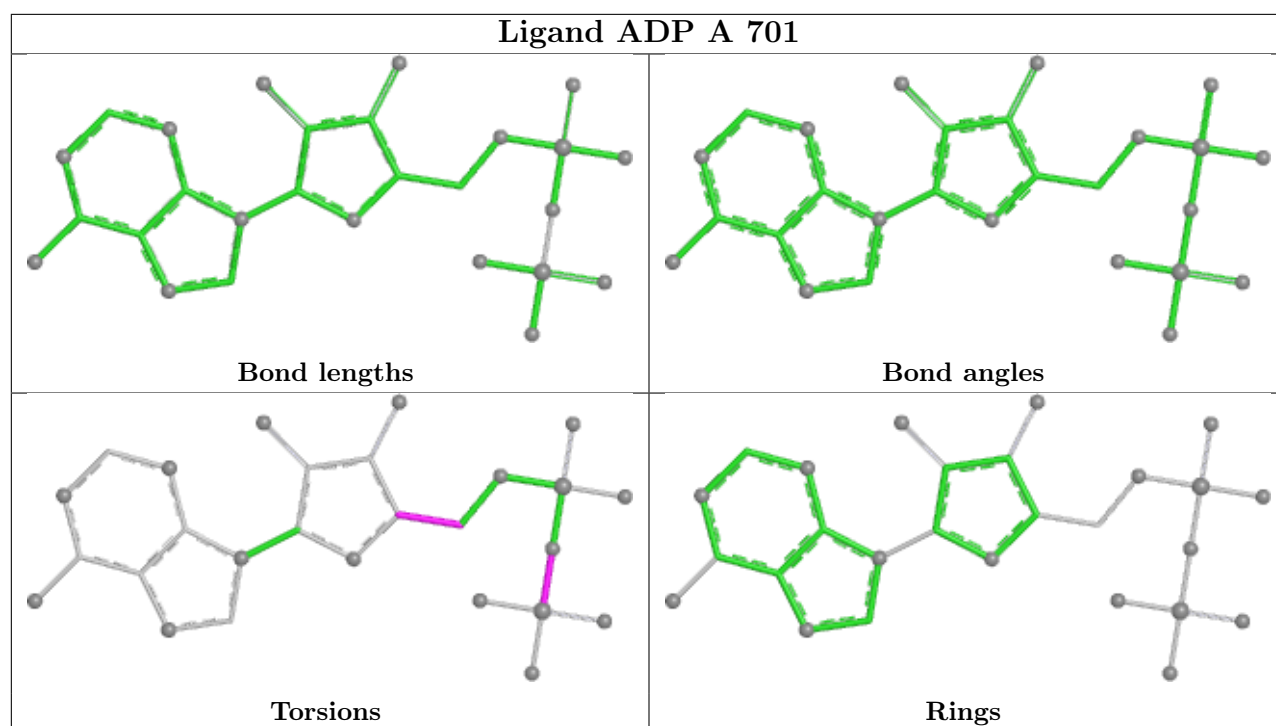
Mol	Chain	Res	Type	Atoms
17	A	701	ADP	O4'-C4'-C5'-O5'
17	A	701	ADP	C3'-C4'-C5'-O5'
17	A	701	ADP	PA-O3A-PB-O1B
17	A	701	ADP	PA-O3A-PB-O2B
17	A	701	ADP	PA-O3A-PB-O3B

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	A	701	ADP	1	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

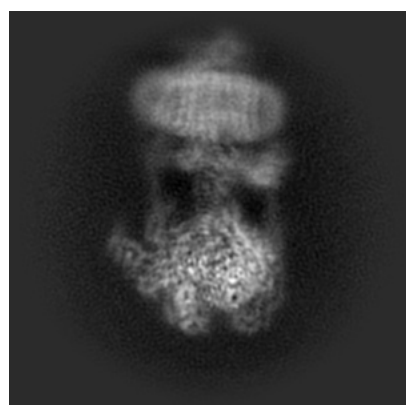
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21319. These allow visual inspection of the internal detail of the map and identification of artifacts.

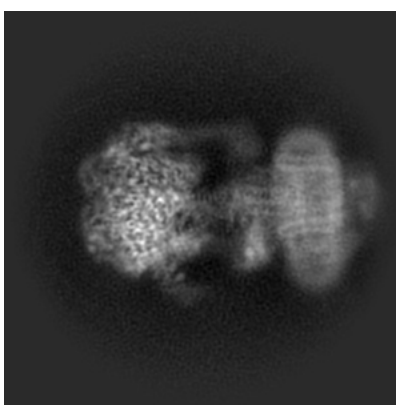
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

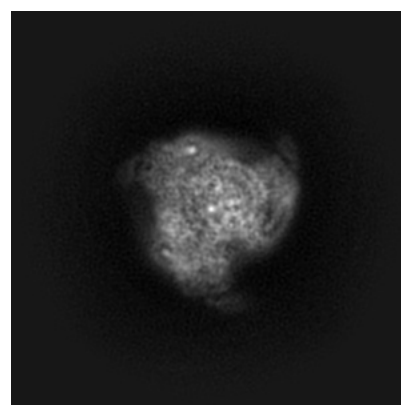
6.1.1 Primary map



X



Y

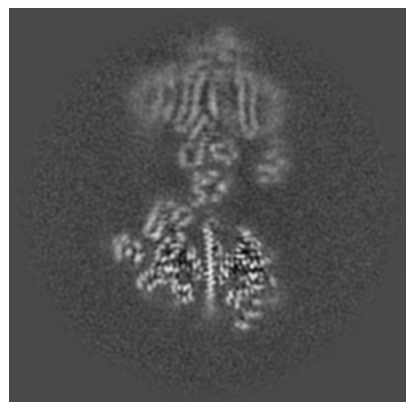


Z

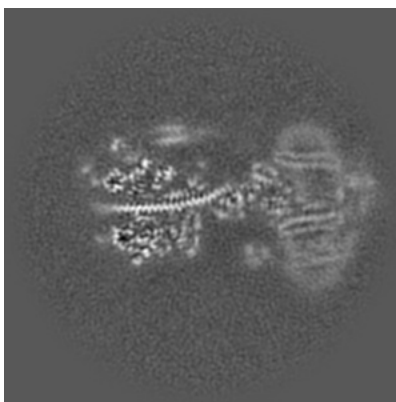
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

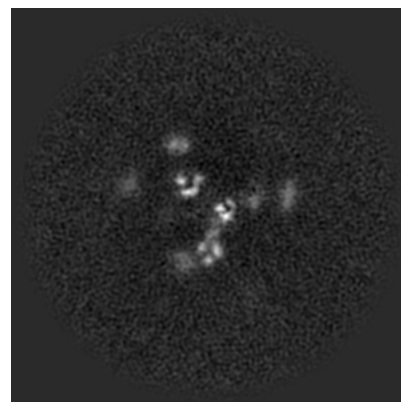
6.2.1 Primary map



X Index: 170



Y Index: 170

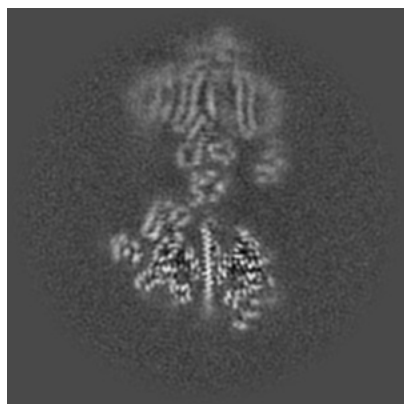


Z Index: 170

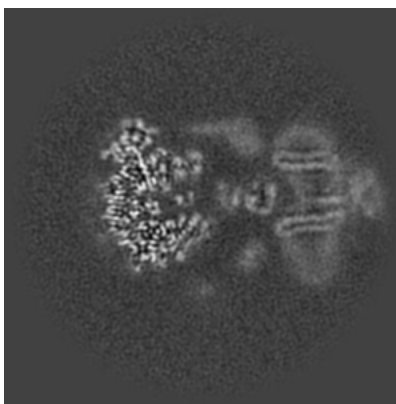
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

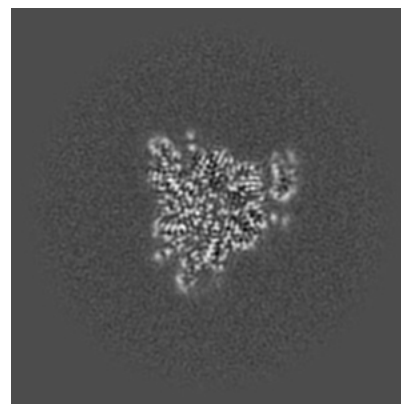
6.3.1 Primary map



X Index: 170



Y Index: 186

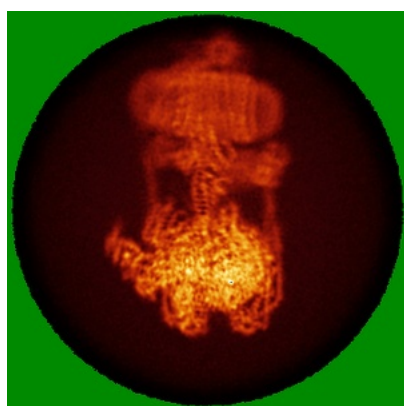


Z Index: 118

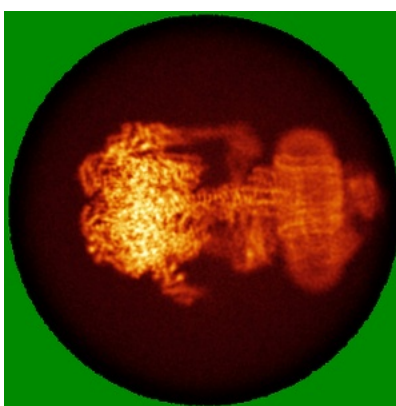
The images above show the largest variance slices of the map in three orthogonal directions.

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

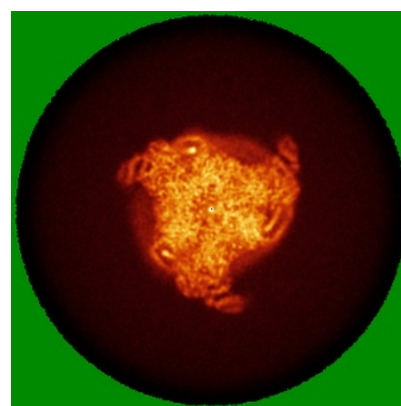
6.4.1 Primary map



X



Y

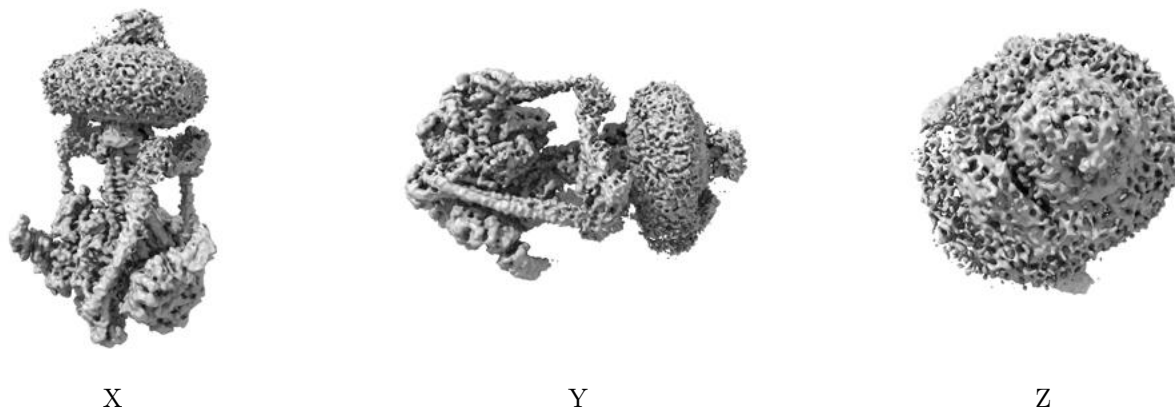


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.25. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

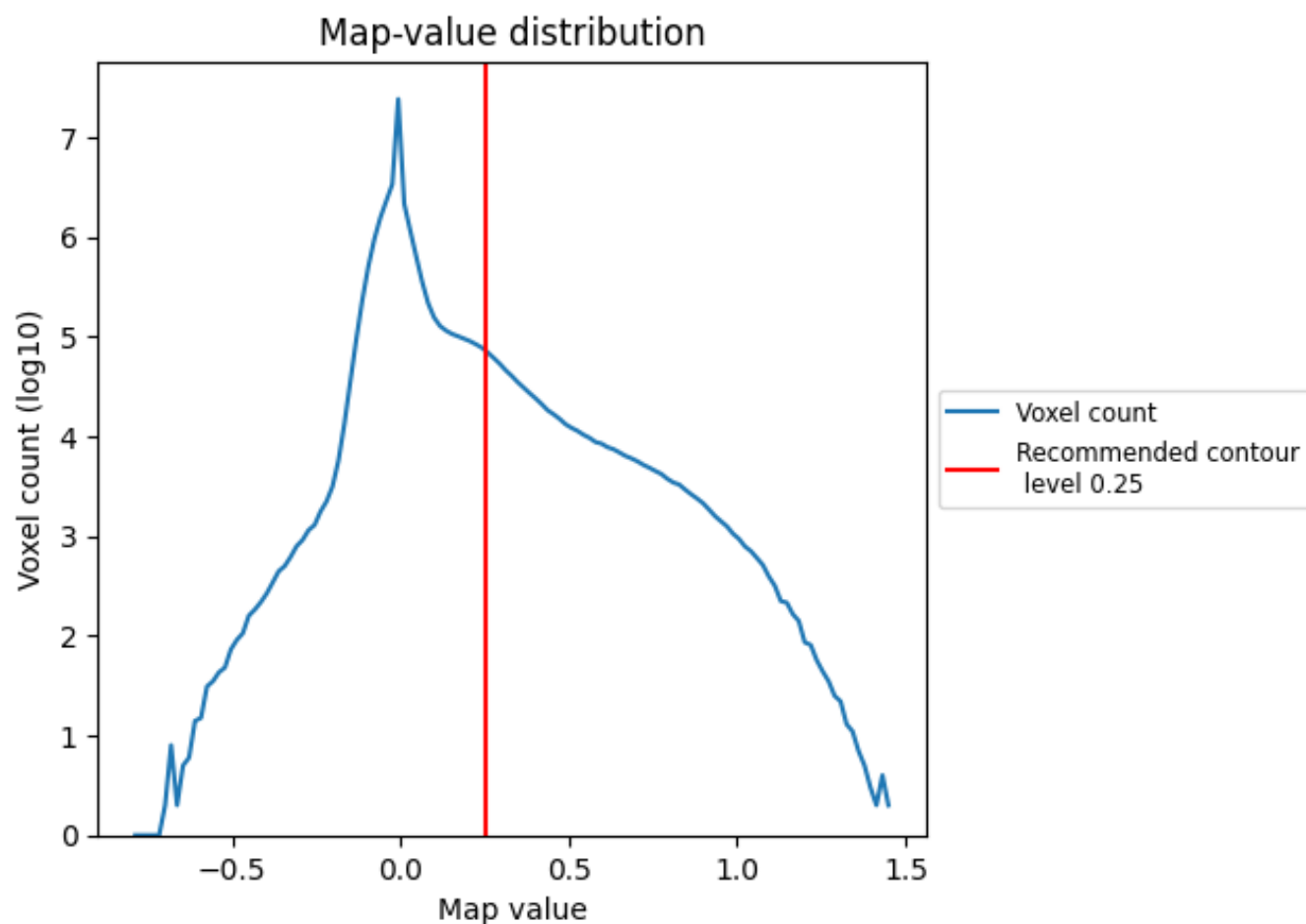
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

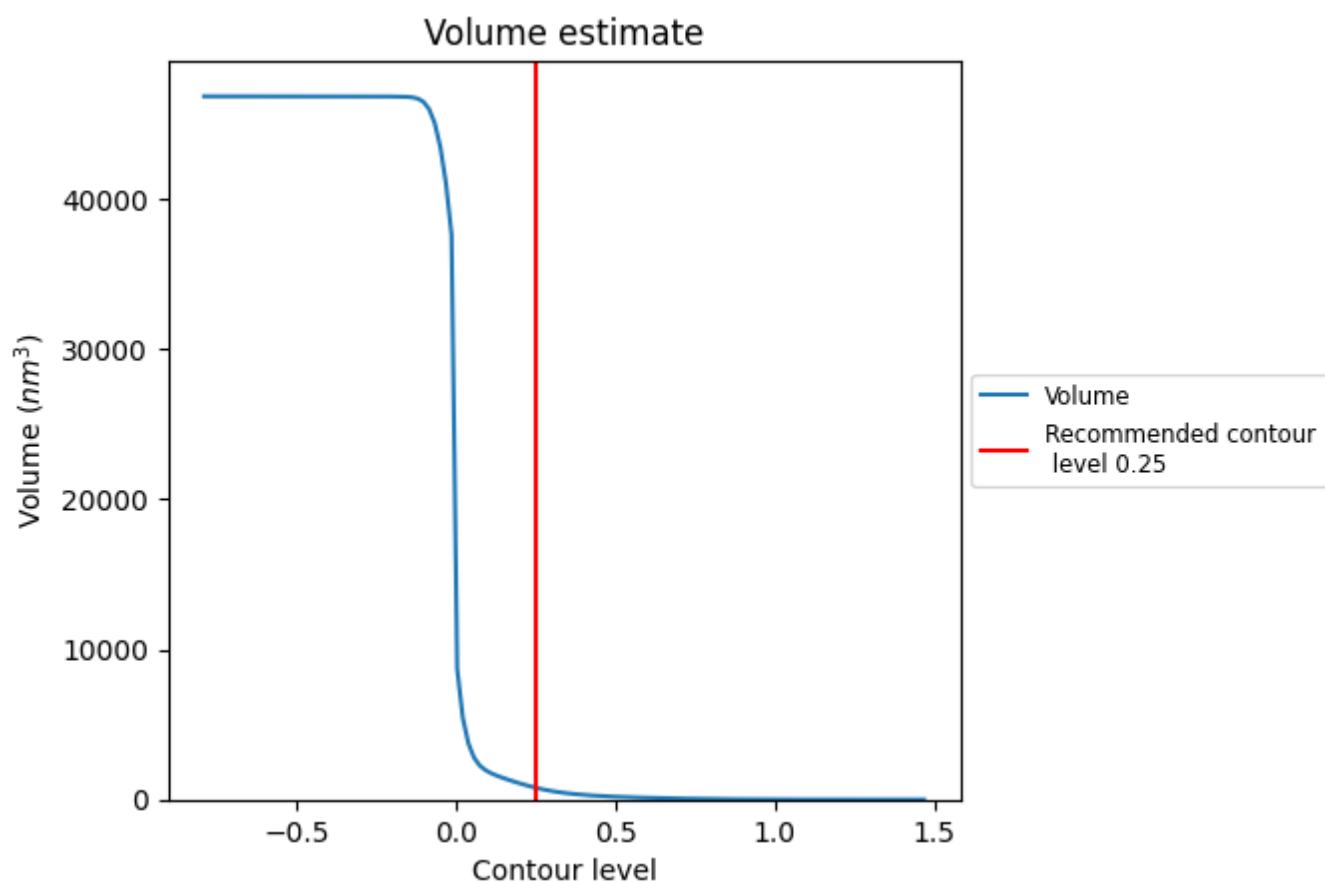
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

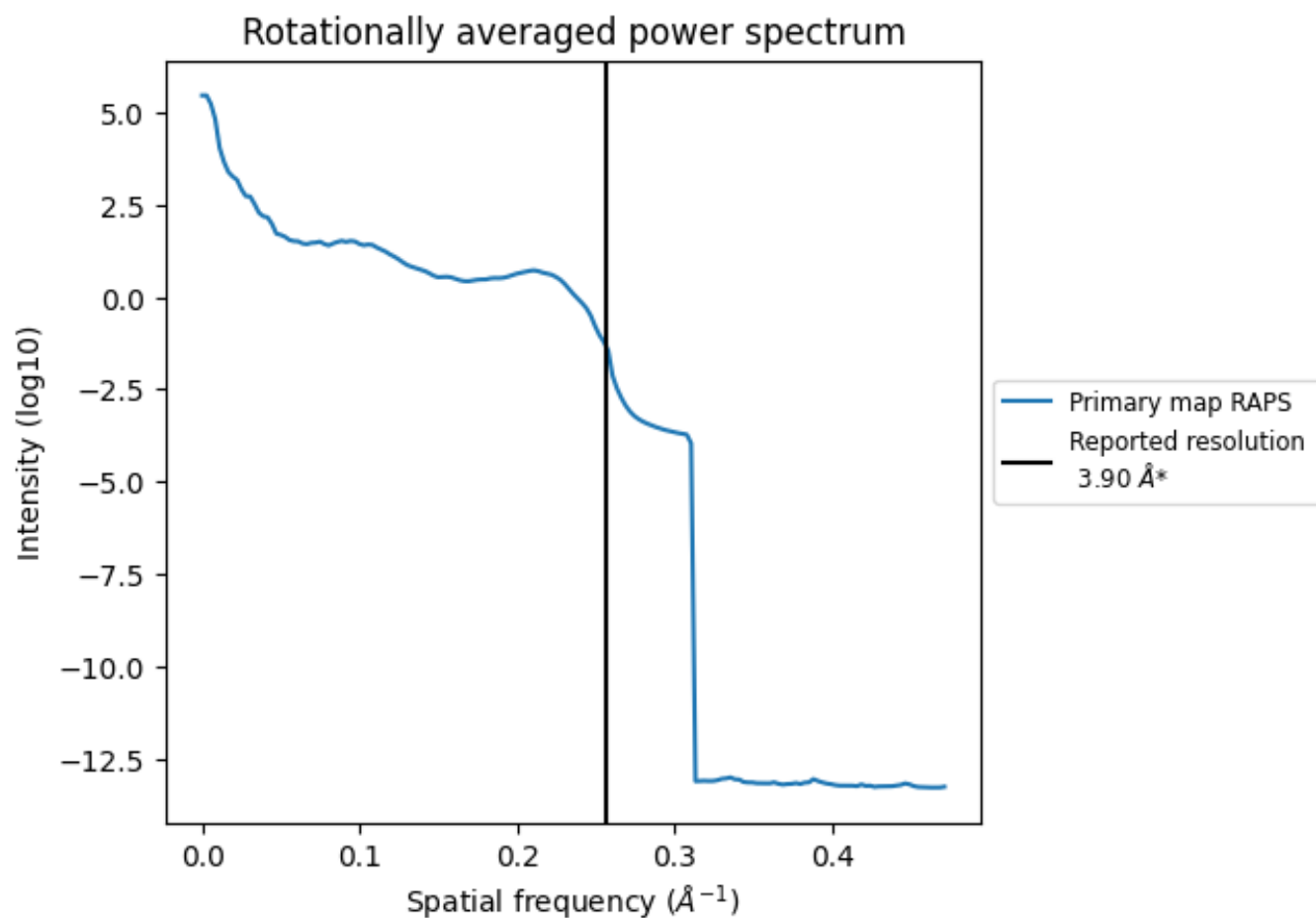
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 792 nm³; this corresponds to an approximate mass of 715 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 0.256 Å⁻¹

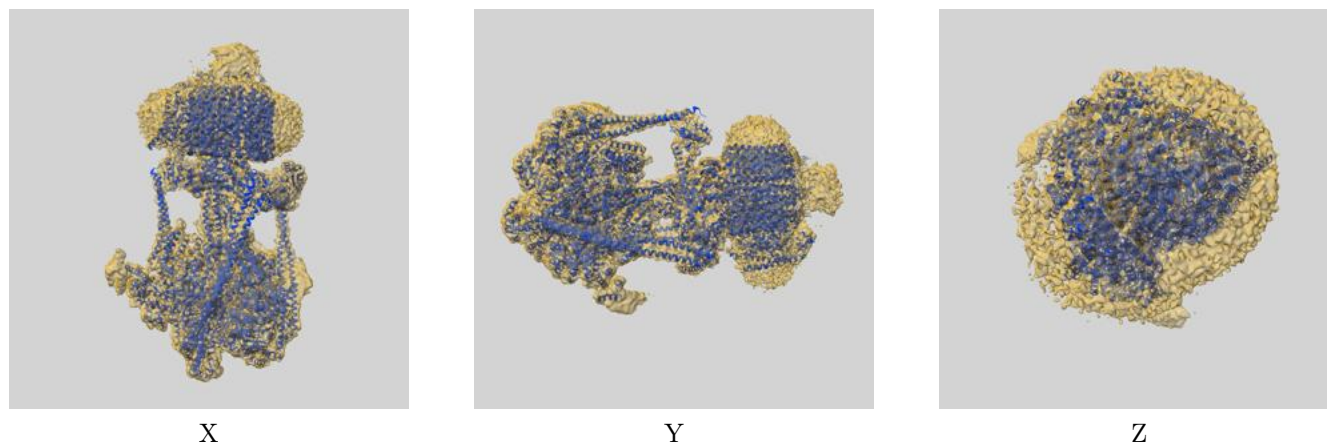
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

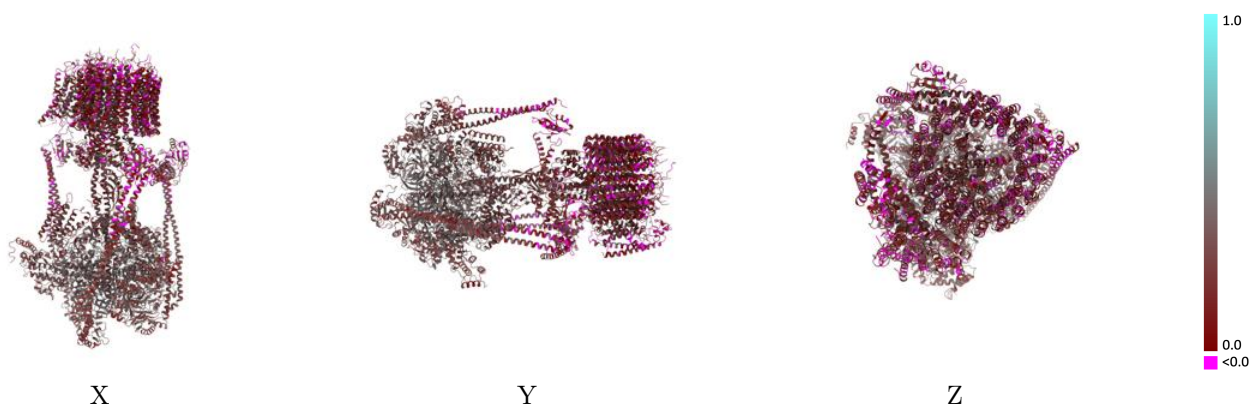
This section contains information regarding the fit between EMDB map EMD-21319 and PDB model 6VQ8. Per-residue inclusion information can be found in section [3](#) on page [11](#).

9.1 Map-model overlay [i](#)



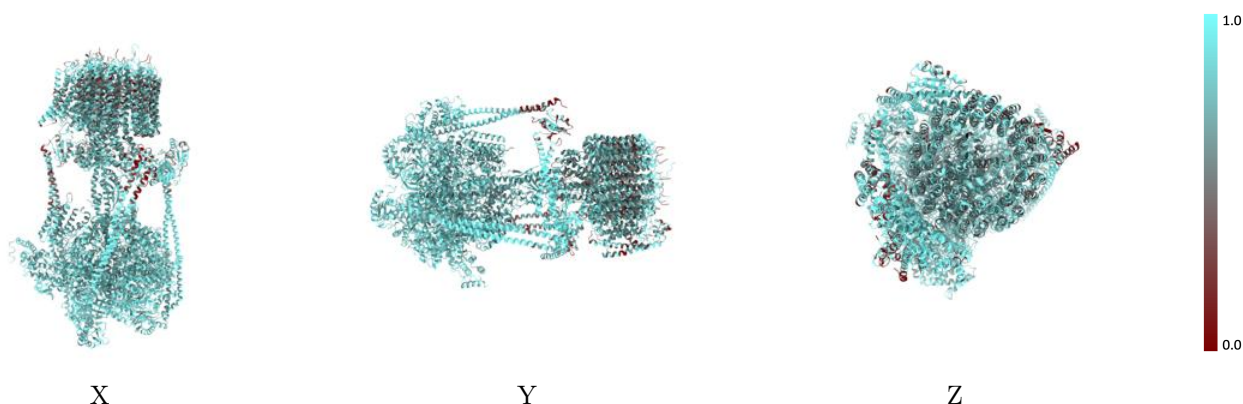
The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



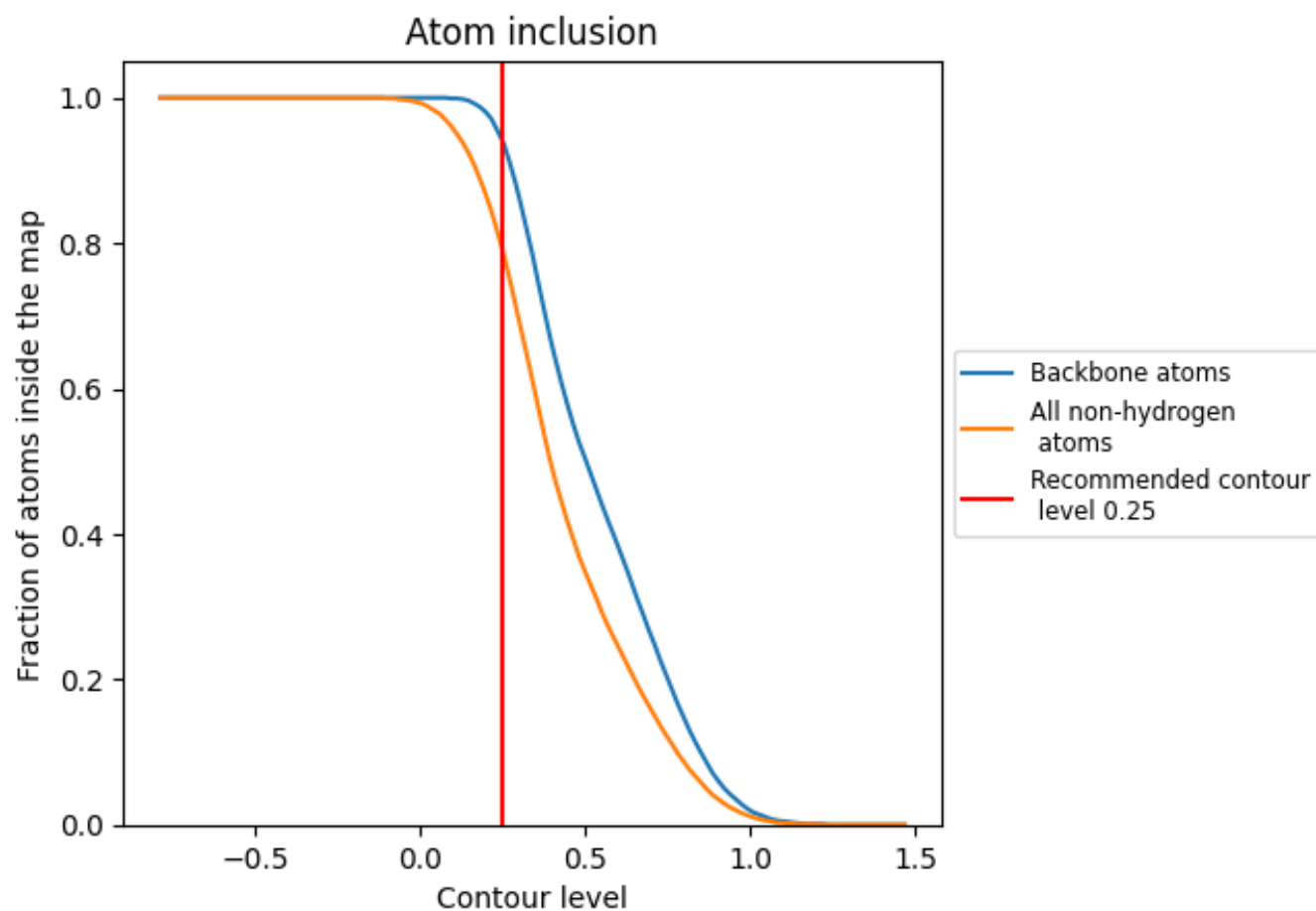
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.25).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 79% 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 (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7890	 0.2740
A	 0.8480	 0.3710
B	 0.8310	 0.3550
C	 0.8370	 0.3480
D	 0.8470	 0.3710
E	 0.8550	 0.3840
F	 0.8520	 0.3880
G	 0.7630	 0.1660
H	 0.7660	 0.2960
I	 0.7690	 0.2630
J	 0.8300	 0.2790
K	 0.7950	 0.2660
L	 0.7720	 0.2570
M	 0.7680	 0.2030
N	 0.8710	 0.2640
O	 0.7870	 0.2380
Q	 0.8230	 0.3000
R	 0.8210	 0.2750
S	 0.8230	 0.2720
a	 0.8140	 0.1880
b	 0.6750	 0.1580
c	 0.6100	 0.2040
d	 0.7080	 0.2200
e	 0.6330	 0.1350
f	 0.6750	 0.1350
g	 0.6890	 0.1680
h	 0.6740	 0.1610
i	 0.6940	 0.1590
j	 0.6840	 0.1350
k	 0.6740	 0.1140
l	 0.6890	 0.1370
m	 0.6750	 0.1210
n	 0.6780	 0.1320
o	 0.6810	 0.1500
p	 0.6930	 0.1900

