



Full wwPDB EM Validation Report ⓘ

Nov 13, 2022 – 08:15 PM EST

PDB ID : 6WLZ
EMDB ID : EMD-21845
Title : The V1 region of human V-ATPase in state 1 (focused refinement)
Authors : Wang, L.; Wu, H.; Fu, T.M.
Deposited on : 2020-04-20
Resolution : 2.90 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.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

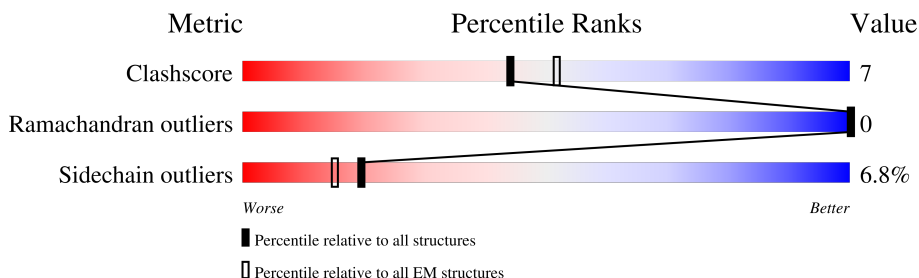
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	617	
1	B	617	
1	C	617	
2	D	511	
2	E	511	
2	F	511	
3	X	573	
3	Y	573	

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Mol	Chain	Length	Quality of chain
3	Z	573	
4	H	226	
4	I	226	
4	J	226	
5	K	118	
5	L	118	
5	M	118	
6	G	247	
7	N	119	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 40657 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 V-type proton ATPase catalytic subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	600	Total	C	N	O	S	0	0
			4652	2949	785	890	28		
1	B	600	Total	C	N	O	S	0	0
			4656	2952	786	890	28		
1	C	600	Total	C	N	O	S	0	0
			4656	2952	786	890	28		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	460	Total	C	N	O	S	0	0
			3600	2284	616	680	20		
2	E	460	Total	C	N	O	S	0	0
			3589	2278	616	676	19		
2	F	460	Total	C	N	O	S	0	0
			3596	2282	616	678	20		

- Molecule 3 is a protein called SidK.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	X	262	Total	C	N	O	S	0	0
			2110	1339	353	408	10		
3	Y	267	Total	C	N	O	S	0	0
			2136	1355	359	411	11		
3	Z	262	Total	C	N	O	S	0	0
			2105	1333	354	408	10		

- Molecule 4 is a protein called V-type proton ATPase subunit E 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	J	193	Total	C	N	O	S	0	0
			1570	988	280	294	8		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	I	193	Total	C	N	O	S	0	0
			1570	988	280	294	8		
4	H	193	Total	C	N	O	S	0	0
			1570	988	280	294	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	M	89	Total	C	N	O	S	0	0
			744	457	140	144	3		
5	L	89	Total	C	N	O	S	0	0
			744	457	140	144	3		
5	K	89	Total	C	N	O	S	0	0
			744	457	140	144	3		

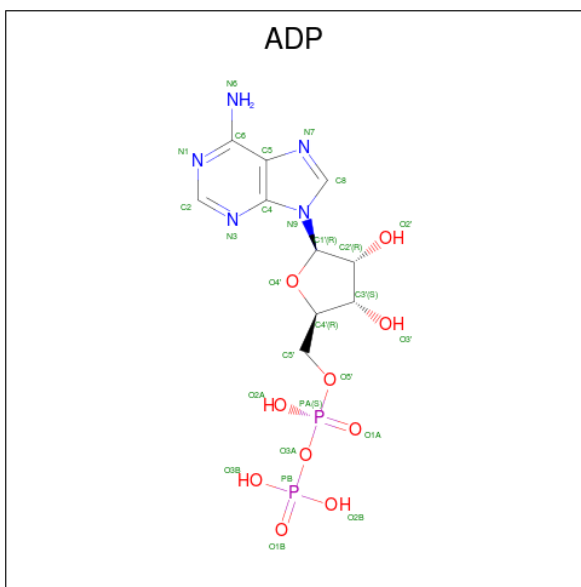
- Molecule 6 is a protein called V-type proton ATPase subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	213	Total	C	N	O	S	0	0
			1713	1087	309	312	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	N	110	Total	C	N	O	S	0	0
			875	552	157	164	2		

- Molecule 8 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

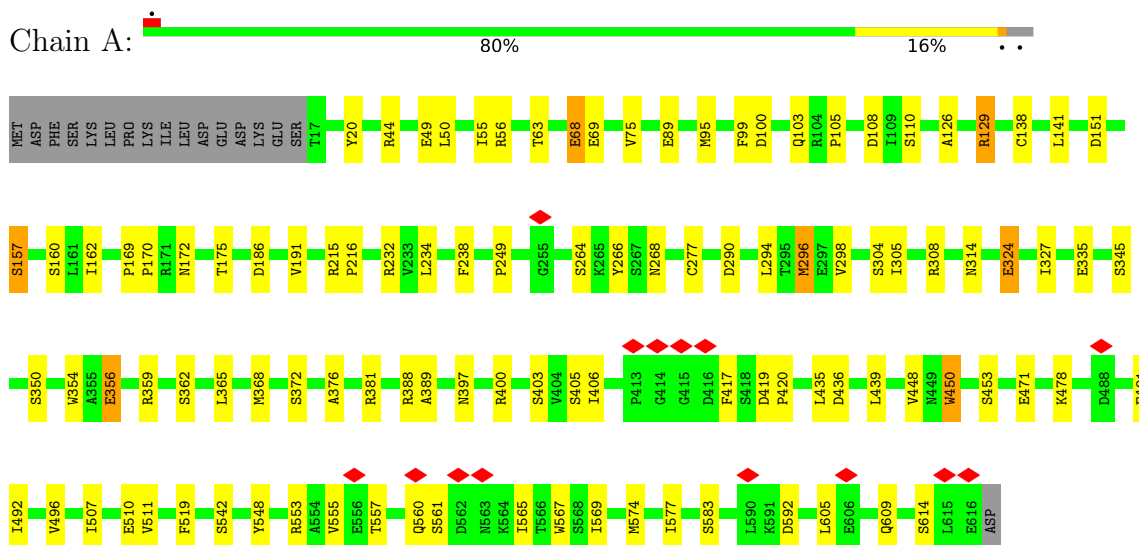


Mol	Chain	Residues	Atoms					AltConf
8	C	1	Total	C	N	O	P	0
			27	10	5	10	2	

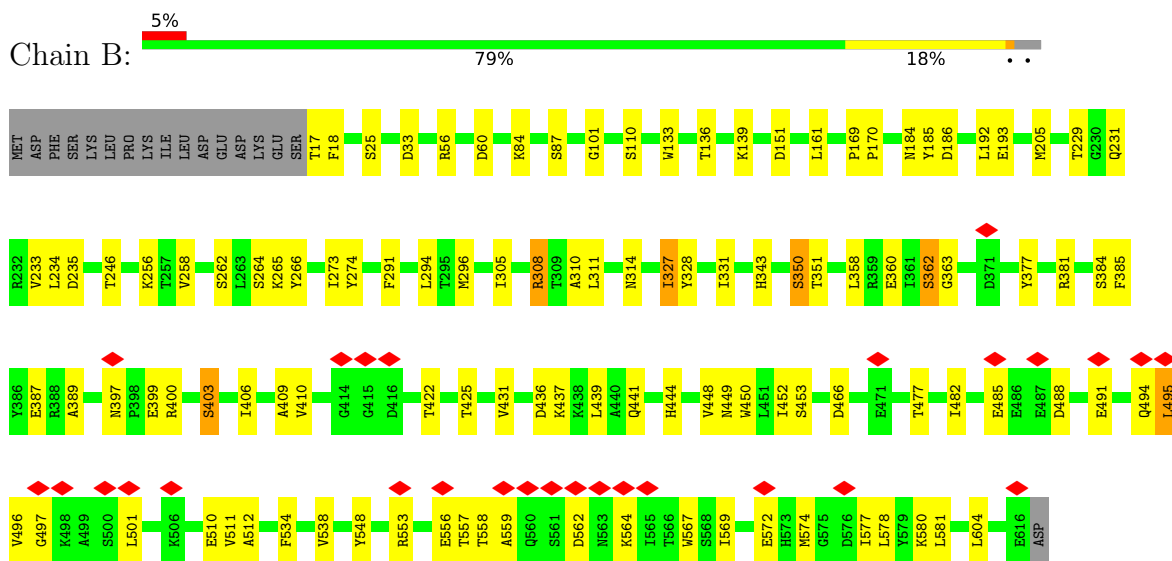
3 Residue-property plots [i](#)

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

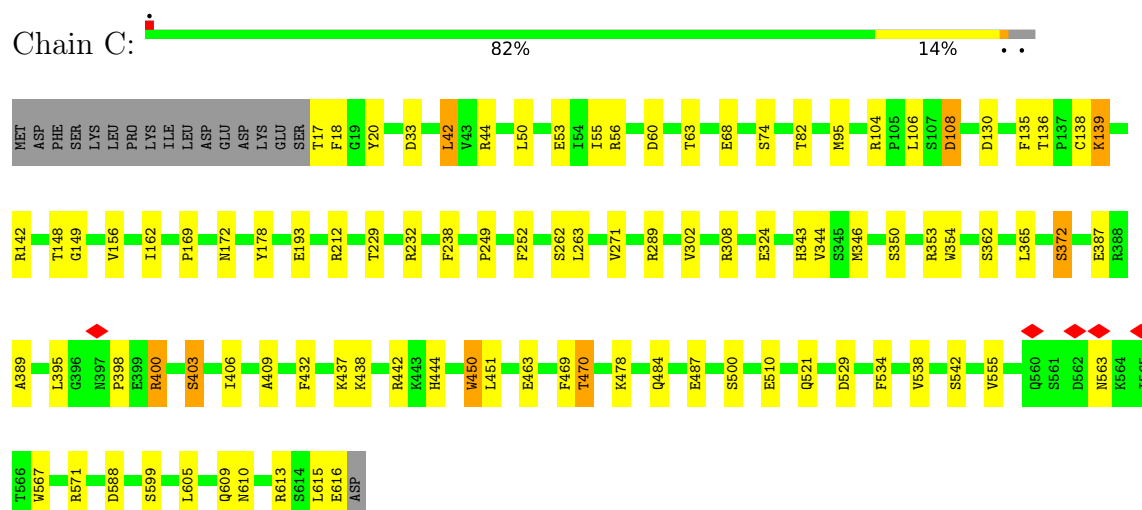
- Molecule 1: V-type proton ATPase catalytic subunit A



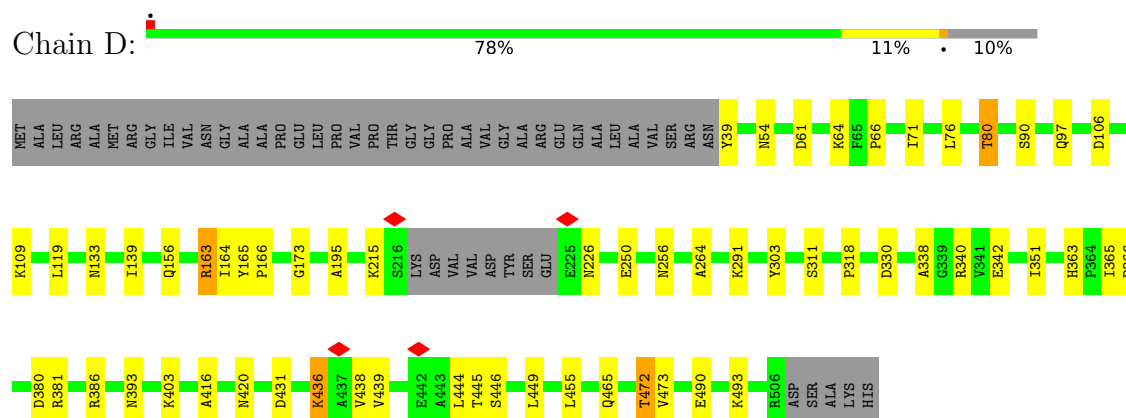
- Molecule 1: V-type proton ATPase catalytic subunit A



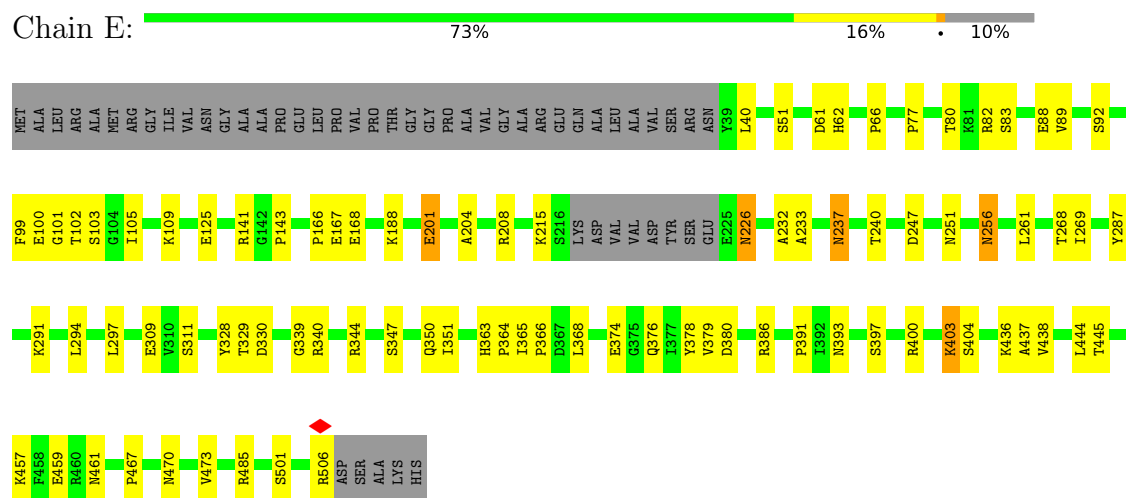
- Molecule 1: V-type proton ATPase catalytic subunit A



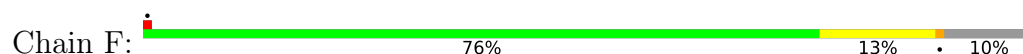
- Molecule 2: V-type proton ATPase subunit B, brain isoform

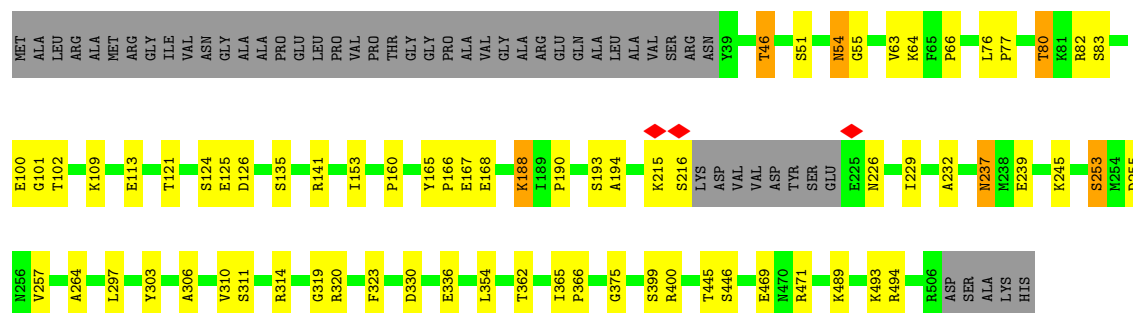


- Molecule 2: V-type proton ATPase subunit B, brain isoform

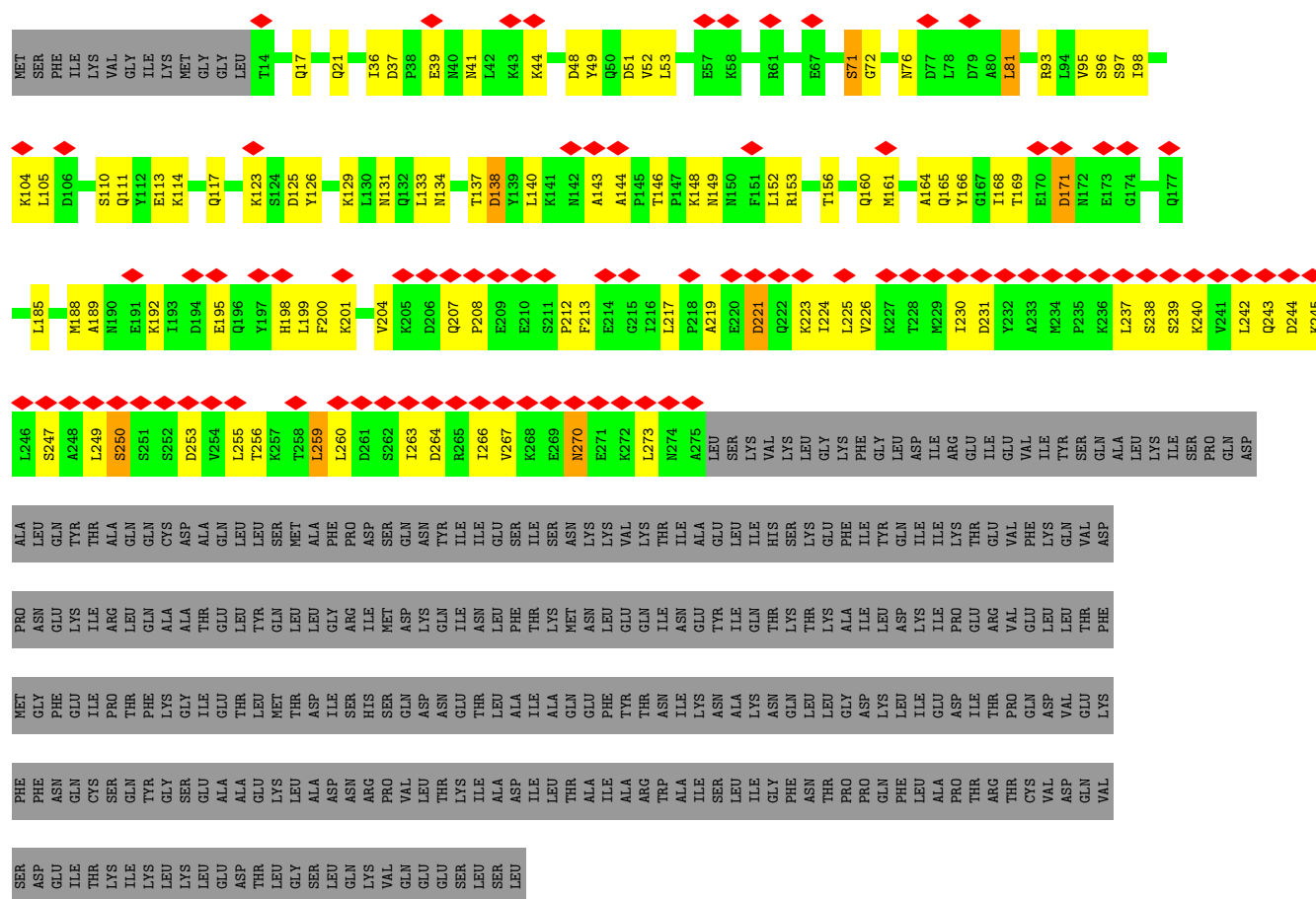
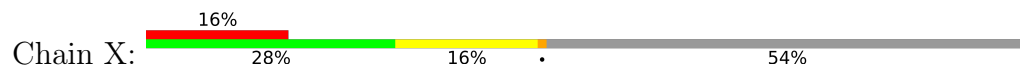


- Molecule 2: V-type proton ATPase subunit B, brain isoform

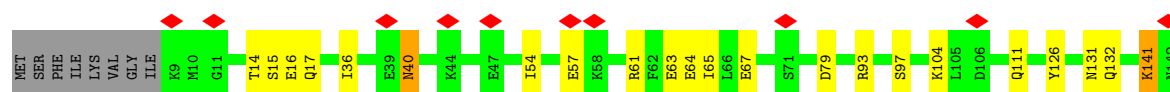
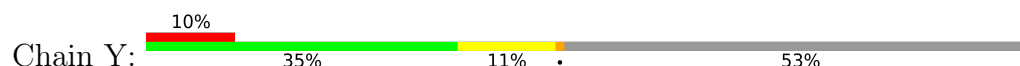


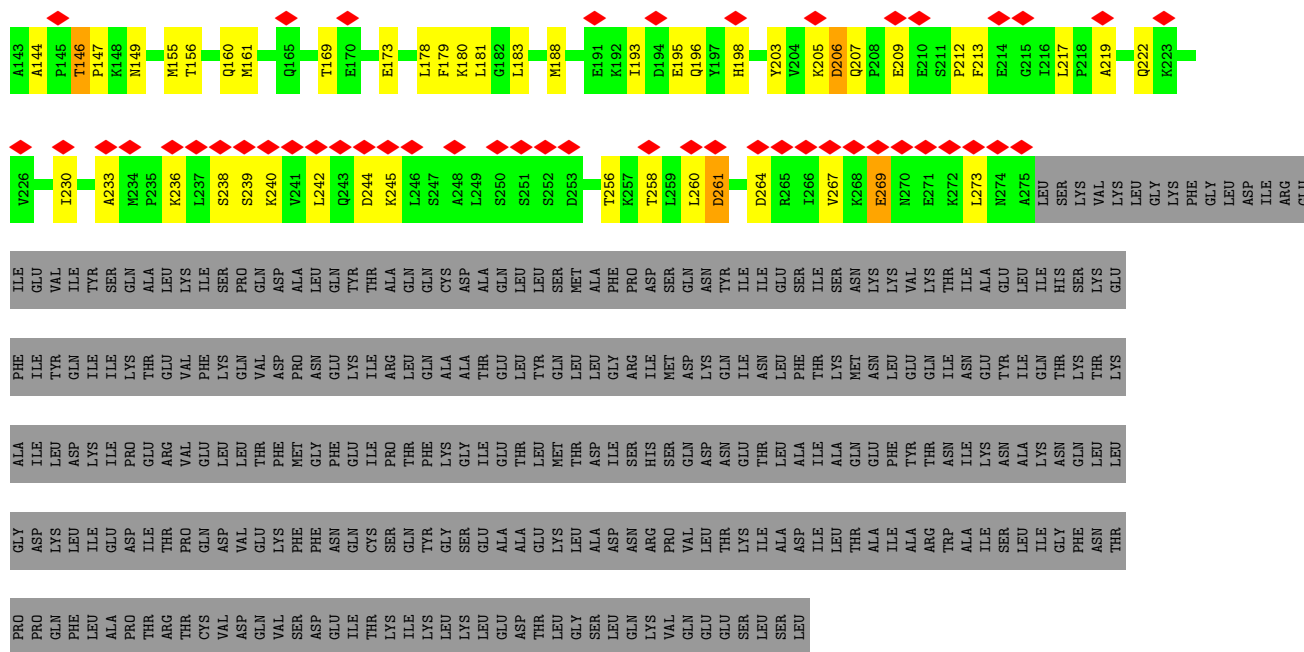


• Molecule 3: SidK

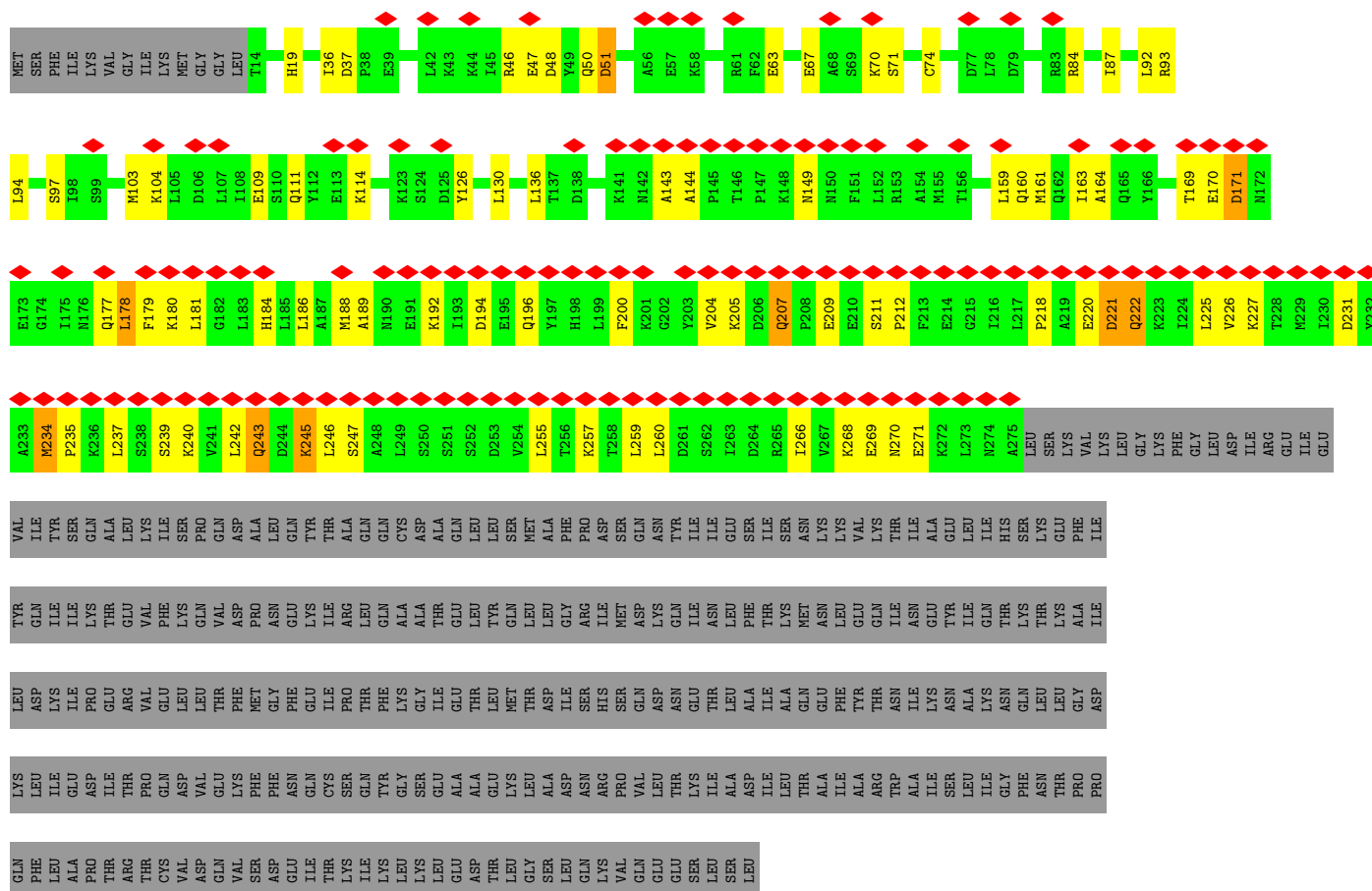
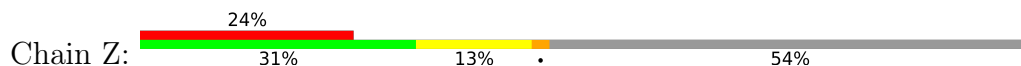


• Molecule 3: SidK

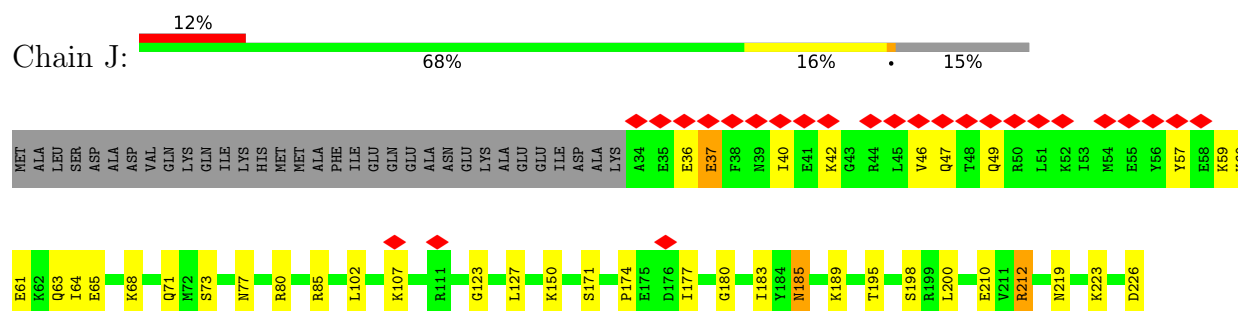




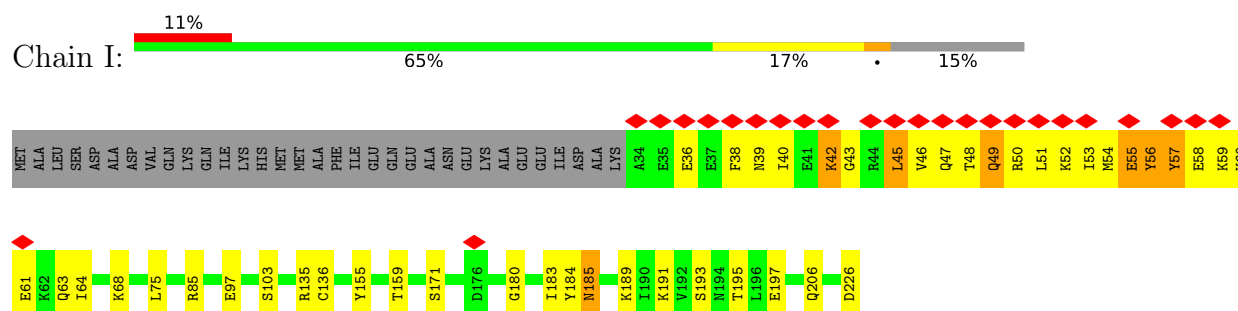
• Molecule 3: SidK



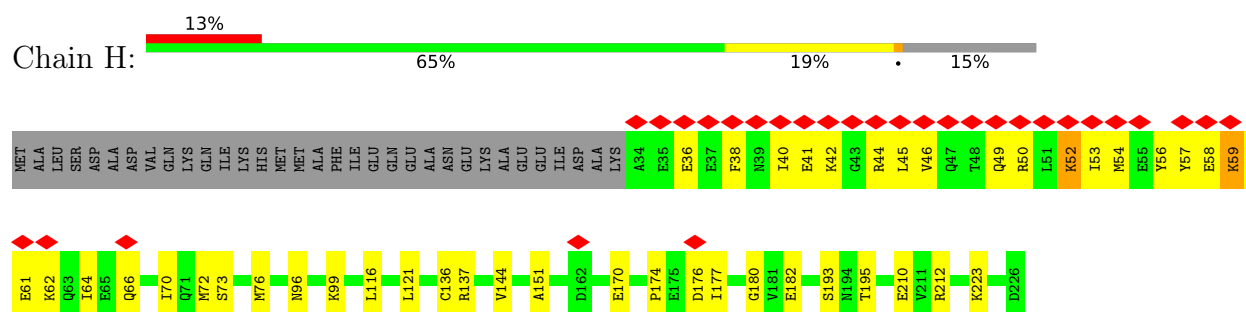
- Molecule 4: V-type proton ATPase subunit E 1



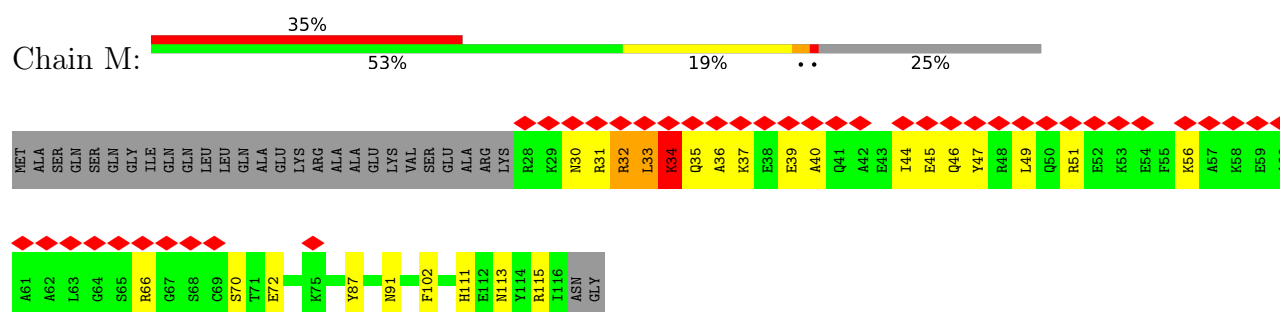
- Molecule 4: V-type proton ATPase subunit E 1



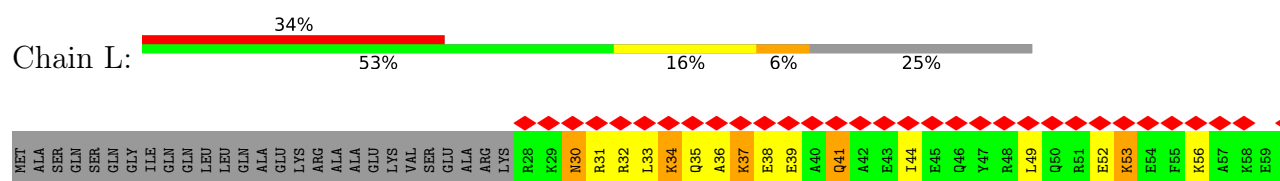
- Molecule 4: V-type proton ATPase subunit E 1



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



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

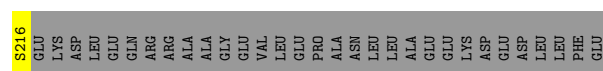




• Molecule 5: V-type proton ATPase subunit G 1



• Molecule 6: V-type proton ATPase subunit D



• Molecule 7: V-type proton ATPase subunit F



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1000000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50.1	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	4.183	Depositor
Minimum map value	-2.507	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.095	Depositor
Recommended contour level	0.6	Depositor
Map size (\AA)	388.80002, 388.80002, 388.80002	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.08, 1.08, 1.08	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.37	0/4748	0.46	0/6431
1	B	0.36	0/4752	0.48	0/6435
1	C	0.39	0/4752	0.47	0/6435
2	D	0.40	0/3671	0.47	0/4973
2	E	0.39	0/3660	0.47	0/4960
2	F	0.38	0/3667	0.47	0/4968
3	X	0.27	0/2143	0.47	0/2888
3	Y	0.27	0/2170	0.42	0/2926
3	Z	0.26	0/2138	0.44	0/2884
4	H	0.31	0/1585	0.44	0/2123
4	I	0.31	0/1585	0.47	1/2123 (0.0%)
4	J	0.31	0/1585	0.42	0/2123
5	K	0.30	0/751	0.44	0/1001
5	L	0.30	0/751	0.50	0/1001
5	M	0.31	0/751	0.48	1/1001 (0.1%)
6	G	0.30	0/1731	0.47	0/2316
7	N	0.26	0/889	0.49	0/1200
All	All	0.35	0/41329	0.46	2/55788 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
5	L	0	1
5	M	0	1
All	All	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	45	LEU	CA-CB-CG	5.32	127.53	115.30
5	M	33	LEU	CA-CB-CG	5.16	127.16	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	L	30	ASN	Peptide
5	M	34	LYS	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4652	0	4631	47	0
1	B	4656	0	4642	61	0
1	C	4656	0	4642	45	0
2	D	3600	0	3605	27	0
2	E	3589	0	3590	46	0
2	F	3596	0	3601	37	0
3	X	2110	0	2132	57	0
3	Y	2136	0	2158	37	0
3	Z	2105	0	2127	44	0
4	H	1570	0	1640	37	0
4	I	1570	0	1640	31	0
4	J	1570	0	1640	27	0
5	K	744	0	744	17	0
5	L	744	0	744	16	0
5	M	744	0	744	15	0
6	G	1713	0	1818	31	0
7	N	875	0	878	30	0
8	C	27	0	12	1	0
All	All	40657	0	40988	561	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 7.

All (561) 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)
7:N:8:ILE:HB	7:N:25:ILE:HG12	1.48	0.92
7:N:14:GLU:HG2	7:N:38:VAL:HG11	1.54	0.86
4:H:42:LYS:HD2	5:K:40:ALA:HB2	1.58	0.85
6:G:91:GLN:HE22	7:N:24:GLY:HA3	1.43	0.83
7:N:65:LEU:HB3	7:N:91:ILE:HD11	1.62	0.81
2:E:208:ARG:NH2	2:E:467:PRO:O	2.13	0.80
7:N:16:THR:HG21	7:N:67:ASN:HD21	1.52	0.73
1:C:289:ARG:NH1	2:F:167:GLU:OE2	2.22	0.72
1:B:410:VAL:HG11	1:B:425:THR:HG21	1.72	0.72
2:E:403:LYS:H	2:E:403:LYS:HD2	1.55	0.71
3:X:242:LEU:HD12	3:X:266:ILE:HG23	1.71	0.71
4:H:180:GLY:HA3	4:H:195:THR:HA	1.72	0.71
3:Z:47:GLU:HA	3:Z:50:GLN:HG2	1.74	0.70
6:G:27:GLN:O	6:G:31:ASN:ND2	2.26	0.68
1:B:17:THR:OG1	1:B:18:PHE:N	2.25	0.68
4:H:46:VAL:HA	5:K:44:ILE:HD11	1.74	0.68
3:Y:146:THR:HG22	3:Y:147:PRO:HD2	1.76	0.68
1:A:50:LEU:HB3	1:A:68:GLU:HG3	1.77	0.67
3:X:201:LYS:HA	3:X:204:VAL:HG12	1.76	0.67
1:B:151:ASP:OD2	1:B:397:ASN:ND2	2.28	0.67
1:B:491:GLU:HB2	1:B:495:LEU:HD23	1.77	0.67
1:B:101:GLY:H	1:B:314:ASN:HD21	1.43	0.67
2:F:141:ARG:O	4:J:85:ARG:NH1	2.27	0.67
3:Y:144:ALA:O	3:Y:149:ASN:ND2	2.28	0.67
4:H:49:GLN:HB2	5:K:44:ILE:HD12	1.77	0.67
3:X:230:ILE:HG21	3:X:250:SER:HB3	1.78	0.66
5:M:111:HIS:HD2	5:M:113:ASN:H	1.44	0.66
7:N:28:LEU:HB3	7:N:32:ARG:HE	1.60	0.65
6:G:149:ALA:HB2	7:N:89:LEU:HD11	1.77	0.65
6:G:121:LEU:HD13	6:G:123:GLY:H	1.61	0.65
1:A:565:ILE:HA	1:A:569:ILE:HD11	1.77	0.65
4:I:47:GLN:HA	4:I:50:ARG:HB2	1.78	0.65
3:Y:54:ILE:HA	3:Y:57:GLU:HG2	1.77	0.64
2:F:445:THR:HG22	2:F:446:SER:H	1.61	0.64
1:B:580:LYS:HE3	1:B:604:LEU:HD13	1.80	0.64
3:Z:51:ASP:OD2	3:Z:84:ARG:NH1	2.29	0.64
2:D:438:VAL:HG12	2:D:439:VAL:HG23	1.78	0.64
3:Y:111:GLN:NE2	3:Y:169:THR:OG1	2.31	0.64
5:M:36:ALA:HA	5:M:39:GLU:HB2	1.79	0.64
3:Z:111:GLN:NE2	3:Z:169:THR:OG1	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:180:GLY:HA3	4:I:195:THR:HA	1.79	0.63
6:G:134:LEU:HD23	7:N:22:LEU:HG	1.80	0.63
2:E:393:ASN:O	2:E:397:SER:OG	2.16	0.63
5:K:30:ASN:O	5:K:34:LYS:HD2	1.99	0.63
1:A:151:ASP:OD2	1:A:397:ASN:ND2	2.32	0.63
1:C:232:ARG:NH2	1:C:529:ASP:OD1	2.32	0.63
2:E:436:LYS:HG3	2:E:444:LEU:HD11	1.80	0.63
3:Z:37:ASP:HB3	3:Z:46:ARG:HH21	1.64	0.62
2:D:445:THR:HG22	2:D:446:SER:H	1.65	0.62
2:D:173:GLY:O	2:D:465:GLN:NE2	2.25	0.62
3:X:148:LYS:NZ	3:X:188:MET:O	2.32	0.62
5:L:32:ARG:HA	5:L:35:GLN:HG2	1.81	0.62
4:H:58:GLU:HA	4:H:61:GLU:HB2	1.82	0.62
2:D:39:TYR:OH	4:H:210:GLU:OE1	2.16	0.62
1:A:138:CYS:HB2	1:A:141:LEU:HD12	1.81	0.61
2:F:82:ARG:NH1	2:F:101:GLY:O	2.33	0.61
3:Y:207:GLN:HE21	3:Y:209:GLU:HB2	1.65	0.61
3:Y:93:ARG:NH2	3:Y:131:ASN:OD1	2.33	0.61
5:L:41:GLN:HE21	5:L:44:ILE:HD12	1.64	0.61
3:X:242:LEU:HD23	3:X:242:LEU:H	1.65	0.61
2:D:163:ARG:NH2	2:D:338:ALA:O	2.33	0.61
7:N:29:ASN:HB3	7:N:33:HIS:H	1.66	0.61
1:A:296:MET:HG2	1:A:305:ILE:HG22	1.82	0.61
2:D:195:ALA:O	2:D:381:ARG:NH2	2.31	0.61
4:H:53:ILE:HD12	4:H:54:MET:N	2.16	0.61
2:E:256:ASN:H	2:E:256:ASN:HD22	1.49	0.60
3:X:223:LYS:HG2	3:X:253:ASP:HA	1.83	0.60
4:J:61:GLU:O	4:J:65:GLU:HG2	2.02	0.60
5:K:36:ALA:HA	5:K:39:GLU:HB3	1.82	0.60
7:N:85:ILE:HG13	7:N:86:PRO:HD3	1.83	0.60
1:A:264:SER:O	1:A:308:ARG:NH2	2.35	0.60
1:B:511:VAL:HG11	1:B:548:TYR:HD1	1.67	0.59
3:X:242:LEU:HA	3:X:245:LYS:HG2	1.84	0.59
6:G:92:VAL:HG23	7:N:25:ILE:HD13	1.85	0.59
3:X:105:LEU:HD22	3:X:105:LEU:H	1.68	0.59
3:X:226:VAL:HG12	3:X:255:LEU:HD23	1.84	0.59
4:H:38:PHE:HA	4:H:41:GLU:HB2	1.85	0.59
3:Y:233:ALA:HA	3:Y:236:LYS:HE2	1.83	0.59
3:Z:136:LEU:HD23	3:Z:186:LEU:HD22	1.85	0.59
7:N:29:ASN:OD1	7:N:30:LYS:N	2.36	0.59
3:X:171:ASP:OD1	3:X:171:ASP:N	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:ARG:HD3	2:F:54:ASN:HD22	1.67	0.59
1:C:463:GLU:N	1:C:463:GLU:OE1	2.35	0.59
7:N:8:ILE:HG23	7:N:63:ILE:HB	1.84	0.58
1:C:178:TYR:HB3	1:C:193:GLU:HB3	1.86	0.58
4:I:185:ASN:HD21	4:I:189:LYS:H	1.51	0.58
5:M:33:LEU:HD12	5:M:34:LYS:HG2	1.86	0.58
4:J:71:GLN:OE1	5:M:66:ARG:NE	2.29	0.58
2:D:490:GLU:O	2:D:493:LYS:NZ	2.34	0.58
2:D:133:ASN:HB3	2:D:139:ILE:HD12	1.86	0.57
2:D:436:LYS:HG3	2:D:444:LEU:HD11	1.85	0.57
3:Y:213:PHE:HB3	3:Y:217:LEU:HB2	1.86	0.57
1:C:372:SER:OG	1:C:372:SER:O	2.21	0.57
5:K:78:GLN:O	5:K:82:THR:HG23	2.04	0.57
3:Y:213:PHE:O	3:Y:222:GLN:NE2	2.35	0.57
2:D:106:ASP:OD2	2:D:109:LYS:NZ	2.35	0.57
2:F:55:GLY:O	2:F:102:THR:OG1	2.20	0.57
2:F:320:ARG:NH2	2:F:362:THR:O	2.34	0.57
3:Y:181:LEU:HD23	3:Y:203:TYR:HB2	1.87	0.57
4:I:52:LYS:O	4:I:55:GLU:HB3	2.04	0.57
6:G:95:ARG:NH1	6:G:110:GLU:OE2	2.37	0.57
1:A:89:GLU:OE1	1:A:129:ARG:NH2	2.36	0.57
2:F:82:ARG:HD3	2:F:100:GLU:HB2	1.88	0.56
3:Z:234:MET:HG3	3:Z:235:PRO:HD3	1.86	0.56
2:E:247:ASP:O	2:E:251:ASN:ND2	2.34	0.56
2:F:124:SER:OG	2:F:125:GLU:N	2.38	0.56
3:X:93:ARG:NH2	3:X:131:ASN:OD1	2.29	0.56
3:X:213:PHE:HB3	3:X:217:LEU:HD22	1.88	0.56
1:B:246:THR:HG23	1:B:431:VAL:HB	1.86	0.56
4:H:182:GLU:HG2	4:H:193:SER:HA	1.87	0.56
3:X:260:LEU:O	3:X:263:ILE:HG13	2.06	0.56
1:B:233:VAL:HG13	1:B:234:LEU:HG	1.86	0.56
1:C:387:GLU:HG3	2:D:264:ALA:HB3	1.88	0.56
4:I:57:TYR:CE2	4:I:58:GLU:HG3	2.41	0.56
3:Z:240:LYS:HA	3:Z:243:GLN:HB2	1.87	0.56
1:B:511:VAL:HG11	1:B:548:TYR:CD1	2.41	0.56
3:Y:242:LEU:HD23	3:Y:245:LYS:HD3	1.88	0.56
1:C:95:MET:HE3	1:C:162:ILE:HG13	1.87	0.55
1:B:296:MET:HG3	1:B:305:ILE:HG22	1.88	0.55
3:Z:143:ALA:HB1	3:Z:149:ASN:ND2	2.20	0.55
7:N:9:ALA:HB1	7:N:55:PHE:HE1	1.71	0.55
1:B:496:VAL:HG12	1:B:497:GLY:H	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:469:GLU:OE2	2:F:471:ARG:NH1	2.39	0.55
6:G:179:ARG:O	6:G:183:THR:HG22	2.07	0.55
4:I:50:ARG:CZ	4:I:53:ILE:HG13	2.37	0.55
2:E:61:ASP:OD1	2:E:62:HIS:N	2.38	0.55
3:X:260:LEU:H	3:X:260:LEU:HD23	1.71	0.55
3:Y:193:ILE:HA	3:Y:196:GLN:HG2	1.88	0.55
1:A:507:ILE:HD11	1:A:555:VAL:HG21	1.87	0.55
1:B:273:ILE:HD13	1:B:310:ALA:HB3	1.89	0.55
3:Y:93:ARG:O	3:Y:97:SER:OG	2.23	0.54
4:H:46:VAL:O	4:H:50:ARG:HB2	2.07	0.54
1:C:42:LEU:O	1:C:82:THR:OG1	2.26	0.54
3:Z:268:LYS:HA	3:Z:271:GLU:HB3	1.90	0.54
2:F:253:SER:OG	2:F:255:ASP:OD1	2.19	0.54
3:Y:264:ASP:HA	3:Y:267:VAL:HG12	1.89	0.54
7:N:10:VAL:O	7:N:36:PHE:HA	2.08	0.54
2:D:303:TYR:OH	2:D:330:ASP:OD2	2.23	0.54
3:Z:207:GLN:HE22	3:Z:212:PRO:HG3	1.73	0.54
3:Y:63:GLU:N	3:Y:63:GLU:OE2	2.37	0.54
2:F:229:ILE:HB	2:F:257:VAL:HG13	1.89	0.53
4:I:39:ASN:HA	4:I:42:LYS:HG2	1.89	0.53
4:I:185:ASN:H	4:I:185:ASN:HD22	1.55	0.53
5:K:67:GLY:O	5:K:71:THR:HG23	2.08	0.53
2:E:457:LYS:O	2:E:461:ASN:HB2	2.09	0.53
5:L:53:LYS:HA	5:L:56:LYS:HG2	1.89	0.53
4:H:42:LYS:HE3	5:K:36:ALA:HB1	1.91	0.53
1:B:553:ARG:O	1:B:557:THR:HG23	2.10	0.52
1:B:581:LEU:HD23	1:B:604:LEU:HD21	1.91	0.52
3:X:250:SER:O	3:X:250:SER:OG	2.26	0.52
3:Z:171:ASP:OD1	3:Z:171:ASP:N	2.41	0.52
1:A:100:ASP:N	1:A:100:ASP:OD1	2.40	0.52
1:A:169:PRO:HB2	1:A:172:ASN:HD22	1.74	0.52
1:C:53:GLU:OE2	1:C:212:ARG:NH2	2.41	0.52
7:N:66:ILE:O	7:N:90:GLU:HA	2.10	0.52
2:D:318:PRO:HG3	6:G:201:ARG:HD2	1.91	0.52
2:F:188:LYS:NZ	2:F:336:GLU:OE2	2.37	0.52
3:X:129:LYS:HB3	3:X:168:ILE:HD11	1.92	0.52
3:Z:143:ALA:HB1	3:Z:149:ASN:HD22	1.75	0.52
5:K:69:CYS:O	5:K:73:VAL:HG23	2.10	0.52
1:A:335:GLU:OE1	1:A:388:ARG:NH1	2.42	0.52
3:X:207:GLN:HG2	3:X:208:PRO:HD2	1.92	0.52
2:F:77:PRO:HB3	2:F:109:LYS:HE2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:365:ILE:HB	2:F:366:PRO:HD3	1.91	0.52
1:A:75:VAL:HB	2:D:66:PRO:HD2	1.93	0.51
3:X:113:GLU:O	3:X:117:GLN:HG2	2.09	0.51
1:B:327:ILE:HG23	1:B:385:PHE:CE1	2.46	0.51
6:G:68:SER:OG	6:G:133:LYS:NZ	2.44	0.51
5:M:33:LEU:CD1	5:M:34:LYS:HG2	2.41	0.51
2:E:82:ARG:HD3	2:E:100:GLU:HB2	1.92	0.51
2:E:386:ARG:NH2	2:E:459:GLU:OE1	2.43	0.51
1:A:553:ARG:O	1:A:557:THR:HG23	2.11	0.51
1:A:389:ALA:HB2	1:A:406:ILE:HG13	1.93	0.51
1:B:534:PHE:O	1:B:538:VAL:HG22	2.11	0.51
2:D:365:ILE:HB	2:D:366:PRO:HD3	1.93	0.51
3:X:219:ALA:O	3:X:223:LYS:HG3	2.11	0.51
1:A:232:ARG:NH1	1:A:519:PHE:O	2.44	0.50
6:G:131:LEU:O	6:G:135:LYS:HG2	2.11	0.50
3:X:200:PHE:HZ	3:X:225:LEU:HD21	1.76	0.50
2:E:376:GLN:HG3	2:E:378:TYR:CE2	2.46	0.50
3:X:240:LYS:HA	3:X:243:GLN:HG3	1.92	0.50
3:Z:245:LYS:HG3	3:Z:266:ILE:HD12	1.93	0.50
3:X:152:LEU:HG	3:X:185:LEU:HD23	1.94	0.50
3:Y:256:THR:HG22	3:Y:258:THR:H	1.77	0.50
1:C:106:LEU:HD13	2:F:160:PRO:HD2	1.94	0.50
1:C:229:THR:HG22	1:C:263:LEU:HG	1.94	0.50
1:C:324:GLU:HG3	1:C:354:TRP:HE1	1.75	0.50
2:F:63:VAL:HB	2:F:66:PRO:HG3	1.93	0.50
4:J:123:GLY:HA3	4:J:183:ILE:HD12	1.94	0.50
1:A:496:VAL:HG21	2:E:438:VAL:HG12	1.93	0.49
4:I:55:GLU:O	4:I:59:LYS:HB2	2.11	0.49
1:C:252:PHE:O	1:C:437:LYS:NZ	2.42	0.49
6:G:212:LEU:HD23	6:G:213:LYS:HD2	1.93	0.49
1:B:377:TYR:O	1:B:381:ARG:HG2	2.13	0.49
1:C:484:GLN:O	1:C:484:GLN:NE2	2.42	0.49
1:C:615:LEU:HD12	1:C:616:GLU:HG3	1.94	0.49
2:D:416:ALA:O	2:D:420:ASN:ND2	2.33	0.49
6:G:4:LYS:HG2	6:G:5:ASP:H	1.78	0.49
1:A:56:ARG:HB3	1:A:63:THR:HB	1.94	0.49
1:A:605:LEU:O	1:A:609:GLN:HG3	2.13	0.49
2:D:436:LYS:HB2	2:D:444:LEU:HD21	1.95	0.49
2:E:66:PRO:HB2	2:E:89:VAL:HG22	1.95	0.49
3:X:72:GLY:HA2	3:X:76:ASN:HD21	1.77	0.49
4:I:155:TYR:O	4:I:159:THR:OG1	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:34:LYS:HA	5:L:37:LYS:HG3	1.95	0.49
1:B:258:VAL:O	1:B:262:SER:OG	2.20	0.49
4:I:42:LYS:HG3	4:I:43:GLY:N	2.27	0.49
3:X:49:TYR:O	3:X:53:LEU:HB2	2.13	0.49
1:B:25:SER:HB2	2:E:88:GLU:HG3	1.93	0.49
2:F:303:TYR:OH	2:F:330:ASP:OD2	2.28	0.49
1:C:169:PRO:HB2	1:C:172:ASN:HD22	1.78	0.48
3:X:195:GLU:HA	3:X:198:HIS:HB3	1.95	0.48
4:H:121:LEU:HD13	4:H:151:ALA:HB1	1.95	0.48
1:C:610:ASN:OD1	1:C:613:ARG:NH1	2.46	0.48
3:X:98:ILE:HD12	3:X:164:ALA:HB2	1.94	0.48
4:I:45:LEU:O	4:I:48:THR:HG22	2.13	0.48
4:J:185:ASN:HD21	4:J:189:LYS:H	1.62	0.48
2:E:99:PHE:HA	2:E:269:ILE:HD13	1.96	0.48
4:J:210:GLU:OE1	4:J:210:GLU:N	2.46	0.48
2:D:445:THR:HG22	2:D:446:SER:N	2.28	0.48
1:B:360:GLU:OE2	2:E:329:THR:OG1	2.16	0.48
2:E:125:GLU:OE2	2:E:291:LYS:NZ	2.45	0.48
3:Y:155:MET:HB3	3:Y:178:LEU:HD11	1.95	0.48
3:Z:222:GLN:HE22	3:Z:255:LEU:H	1.62	0.48
1:C:350:SER:H	1:C:409:ALA:HB3	1.79	0.48
4:I:43:GLY:HA2	4:I:46:VAL:HB	1.95	0.48
1:B:186:ASP:OD1	1:B:186:ASP:N	2.36	0.48
3:X:140:LEU:HD21	3:X:152:LEU:HB3	1.96	0.48
3:Z:218:PRO:HG2	3:Z:221:ASP:HB2	1.96	0.48
6:G:95:ARG:HH21	7:N:4:ARG:HB2	1.78	0.48
2:F:76:LEU:HB2	2:F:80:THR:HG23	1.95	0.48
3:Z:114:LYS:HD3	3:Z:169:THR:HB	1.95	0.48
4:H:53:ILE:HD12	4:H:54:MET:H	1.79	0.48
1:B:491:GLU:HA	1:B:494:GLN:CG	2.44	0.47
1:B:510:GLU:HG2	1:B:567:TRP:CZ2	2.48	0.47
2:E:379:VAL:HG13	2:E:391:PRO:HG2	1.96	0.47
3:Z:205:LYS:HA	3:Z:257:LYS:HE2	1.96	0.47
4:J:180:GLY:HA3	4:J:195:THR:HA	1.95	0.47
6:G:57:LEU:O	6:G:60:GLU:HG3	2.13	0.47
3:X:134:ASN:O	3:X:138:ASP:HB2	2.15	0.47
3:Y:195:GLU:OE1	3:Y:195:GLU:N	2.47	0.47
3:Z:225:LEU:HD12	3:Z:226:VAL:HG23	1.96	0.47
1:A:372:SER:O	1:A:372:SER:OG	2.30	0.47
2:E:287:TYR:OH	2:E:339:GLY:O	2.30	0.47
3:Z:94:LEU:HB2	3:Z:130:LEU:HD21	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Z:180:LYS:HB3	3:Z:180:LYS:HE3	1.62	0.47
1:B:449:ASN:HD22	1:B:452:ILE:HG12	1.77	0.47
2:E:77:PRO:HB3	2:E:109:LYS:HE2	1.96	0.47
2:E:365:ILE:HB	2:E:366:PRO:HD3	1.97	0.47
2:F:121:THR:HG22	2:F:153:ILE:HG22	1.96	0.47
3:X:72:GLY:HA2	3:X:76:ASN:ND2	2.29	0.47
4:I:36:GLU:O	4:I:40:ILE:HD13	2.15	0.47
3:Z:19:HIS:CG	3:Z:70:LYS:HG3	2.49	0.47
4:I:54:MET:HA	4:I:57:TYR:HD2	1.80	0.47
1:A:290:ASP:O	1:A:294:LEU:HD13	2.14	0.47
3:X:36:ILE:HG13	3:X:95:VAL:HG21	1.96	0.47
3:X:97:SER:O	3:X:160:GLN:NE2	2.48	0.47
3:Y:61:ARG:NH1	3:Y:64:GLU:OE2	2.48	0.47
3:Y:213:PHE:CD1	3:Y:217:LEU:HD12	2.50	0.47
4:I:97:GLU:HG2	5:L:92:ARG:NH2	2.29	0.47
4:J:185:ASN:H	4:J:185:ASN:HD22	1.61	0.47
3:X:110:SER:O	3:X:114:LYS:HG2	2.15	0.47
3:X:189:ALA:HB3	3:X:192:LYS:HD2	1.97	0.47
5:L:74:GLU:O	5:L:74:GLU:HG2	2.15	0.47
4:I:51:LEU:HA	4:I:54:MET:HB2	1.97	0.47
2:F:237:ASN:H	2:F:237:ASN:ND2	2.13	0.46
3:Z:200:PHE:O	3:Z:204:VAL:HG23	2.15	0.46
1:B:362:SER:OG	1:B:363:GLY:N	2.48	0.46
1:B:485:GLU:HA	1:B:488:ASP:OD2	2.15	0.46
3:X:165:GLN:HG3	3:X:166:TYR:HD2	1.80	0.46
6:G:130:GLN:O	6:G:133:LYS:HG3	2.16	0.46
6:G:91:GLN:NE2	7:N:24:GLY:HA3	2.23	0.46
1:A:277:CYS:O	1:A:314:ASN:ND2	2.33	0.46
2:E:374:GLU:HA	2:E:400:ARG:HD2	1.97	0.46
2:F:193:SER:OG	2:F:194:ALA:N	2.48	0.46
4:I:46:VAL:O	4:I:49:GLN:HG3	2.14	0.46
4:H:50:ARG:CZ	5:K:47:TYR:HB3	2.46	0.46
4:H:136:CYS:SG	4:H:144:VAL:HG21	2.55	0.46
1:C:350:SER:HB3	1:C:353:ARG:HG2	1.97	0.46
1:C:510:GLU:HG3	1:C:567:TRP:CE2	2.51	0.46
4:H:54:MET:HA	4:H:57:TYR:HB3	1.97	0.46
1:A:186:ASP:OD1	1:A:186:ASP:N	2.45	0.46
2:D:380:ASP:HB2	2:D:393:ASN:HB2	1.96	0.46
2:E:485:ARG:NH2	2:E:506:ARG:HB2	2.31	0.46
1:C:398:PRO:O	1:C:400:ARG:HD3	2.16	0.46
3:X:264:ASP:HA	3:X:267:VAL:HG22	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Z:160:GLN:O	3:Z:163:ILE:HG12	2.16	0.46
3:Z:169:THR:OG1	3:Z:170:GLU:OE2	2.26	0.46
6:G:215:LYS:NZ	6:G:216:SER:OG	2.42	0.46
1:B:439:LEU:HD23	1:B:444:HIS:CD2	2.51	0.46
6:G:53:GLU:O	6:G:57:LEU:HG	2.16	0.46
1:A:356:GLU:OE2	1:A:359:ARG:NH2	2.46	0.45
3:Y:207:GLN:NE2	3:Y:212:PRO:HB3	2.31	0.45
3:Z:239:SER:O	3:Z:243:GLN:N	2.49	0.45
4:J:36:GLU:O	4:J:40:ILE:HD12	2.16	0.45
5:K:49:LEU:HD12	5:K:49:LEU:HA	1.75	0.45
1:A:510:GLU:HG3	1:A:567:TRP:NE1	2.30	0.45
1:B:265:LYS:HD2	1:B:294:LEU:HG	1.98	0.45
1:B:562:ASP:H	1:B:564:LYS:NZ	2.14	0.45
1:C:389:ALA:HB2	1:C:406:ILE:HG13	1.98	0.45
1:C:534:PHE:O	1:C:538:VAL:HG23	2.16	0.45
1:B:264:SER:O	1:B:308:ARG:NH2	2.50	0.45
6:G:95:ARG:HE	7:N:4:ARG:HB3	1.82	0.45
1:B:229:THR:OG1	1:B:235:ASP:OD1	2.33	0.45
1:B:328:TYR:HA	1:B:331:ILE:HG22	1.98	0.45
1:C:444:HIS:ND1	1:C:521:GLN:OE1	2.48	0.45
3:X:221:ASP:OD2	3:X:221:ASP:N	2.36	0.45
3:Y:61:ARG:O	3:Y:65:ILE:HG22	2.17	0.45
1:B:558:THR:O	1:B:558:THR:OG1	2.35	0.45
2:D:226:ASN:OD1	2:D:226:ASN:N	2.50	0.45
1:C:108:ASP:OD1	1:C:108:ASP:N	2.49	0.45
1:A:215:ARG:HE	1:A:215:ARG:HB3	1.55	0.45
1:A:324:GLU:HA	1:A:354:TRP:CD1	2.52	0.45
3:Y:64:GLU:O	3:Y:67:GLU:HG3	2.17	0.45
3:Z:93:ARG:O	3:Z:97:SER:OG	2.30	0.45
1:C:249:PRO:HG2	1:C:432:PHE:HE1	1.82	0.44
2:E:256:ASN:HD22	2:E:256:ASN:N	2.15	0.44
2:F:215:LYS:HE2	2:F:215:LYS:HB2	1.86	0.44
3:Y:269:GLU:H	3:Y:269:GLU:HG2	1.42	0.44
5:M:30:ASN:OD1	5:M:34:LYS:HE3	2.17	0.44
4:I:46:VAL:O	4:I:50:ARG:HG2	2.16	0.44
1:B:84:LYS:HE2	1:B:84:LYS:HB2	1.62	0.44
1:B:578:LEU:HD23	1:B:578:LEU:HA	1.78	0.44
1:C:139:LYS:HB2	1:C:139:LYS:HE2	1.78	0.44
2:E:40:LEU:H	4:I:206:GLN:HE22	1.65	0.44
2:F:126:ASP:OD2	4:J:212:ARG:NH2	2.50	0.44
3:Y:219:ALA:HA	3:Y:222:GLN:HG3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:174:PRO:O	4:H:177:ILE:HG12	2.17	0.44
7:N:39:VAL:HG21	7:N:48:ILE:HD11	1.99	0.44
1:B:387:GLU:HG3	2:F:264:ALA:HB3	1.98	0.44
1:C:238:PHE:CZ	1:C:450:TRP:HA	2.52	0.44
1:C:343:HIS:ND1	1:C:403:SER:HB3	2.32	0.44
3:Y:40:ASN:N	3:Y:40:ASN:OD1	2.51	0.44
3:Y:239:SER:HB2	3:Y:273:LEU:HG	1.99	0.44
4:H:41:GLU:OE1	4:H:44:ARG:NH1	2.50	0.44
7:N:21:LEU:HD13	7:N:25:ILE:O	2.18	0.44
1:B:482:ILE:HG22	1:B:512:ALA:HB2	2.00	0.44
6:G:94:ILE:HG12	7:N:63:ILE:HD11	2.00	0.44
1:A:238:PHE:CZ	1:A:450:TRP:HA	2.52	0.44
2:E:143:PRO:HD3	4:I:85:ARG:HG2	2.00	0.44
1:A:157:SER:O	1:A:157:SER:OG	2.30	0.44
1:B:350:SER:H	1:B:409:ALA:HB3	1.83	0.44
1:B:397:ASN:O	1:B:399:GLU:N	2.50	0.44
4:J:150:LYS:HB2	4:J:150:LYS:HE3	1.86	0.44
3:X:36:ILE:HG23	3:X:37:ASP:OD1	2.18	0.44
3:Z:194:ASP:OD2	3:Z:194:ASP:N	2.51	0.44
6:G:94:ILE:HD12	6:G:111:HIS:HA	1.99	0.44
1:B:574:MET:HB3	1:B:577:ILE:HB	2.00	0.44
2:E:232:ALA:HB3	2:E:297:LEU:HD23	1.99	0.44
3:Z:240:LYS:O	3:Z:240:LYS:HD3	2.18	0.44
7:N:45:ILE:H	7:N:45:ILE:HG13	1.59	0.44
1:B:491:GLU:HA	1:B:494:GLN:HG2	1.98	0.44
2:E:350:GLN:HE21	2:E:350:GLN:HB3	1.52	0.44
2:D:291:LYS:HE2	2:D:291:LYS:HB3	1.75	0.43
2:E:201:GLU:H	2:E:201:GLU:HG2	1.45	0.43
4:J:42:LYS:HZ1	5:M:40:ALA:N	2.16	0.43
4:I:53:ILE:HA	4:I:56:TYR:HB2	1.99	0.43
5:L:88:PHE:O	5:L:92:ARG:HB2	2.17	0.43
7:N:16:THR:HG21	7:N:67:ASN:ND2	2.28	0.43
1:B:256:LYS:HB3	1:B:256:LYS:HE2	1.72	0.43
1:C:238:PHE:HZ	1:C:450:TRP:HA	1.83	0.43
3:X:237:LEU:HD22	3:X:270:ASN:HB2	2.00	0.43
3:X:249:LEU:HD13	3:X:263:ILE:HG22	1.99	0.43
3:Z:189:ALA:HB3	3:Z:192:LYS:HG3	2.00	0.43
4:I:56:TYR:O	4:I:60:LYS:HG2	2.18	0.43
1:A:105:PRO:HG3	1:A:126:ALA:HA	1.99	0.43
1:C:271:VAL:HB	1:C:344:VAL:HG22	2.00	0.43
2:D:472:THR:HG22	2:D:473:VAL:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:226:ASN:N	2:F:226:ASN:OD1	2.51	0.43
1:B:496:VAL:HG12	1:B:497:GLY:N	2.33	0.43
2:D:363:HIS:HB3	2:D:366:PRO:HD2	2.00	0.43
3:X:134:ASN:HA	3:X:137:THR:HG22	2.00	0.43
3:Y:213:PHE:CG	3:Y:217:LEU:HD12	2.54	0.43
3:Z:222:GLN:O	3:Z:226:VAL:HG23	2.17	0.43
1:B:437:LYS:O	1:B:441:GLN:HG3	2.19	0.43
1:C:44:ARG:HA	1:C:50:LEU:O	2.19	0.43
1:C:451:LEU:HD11	1:C:487:GLU:HG3	2.01	0.43
3:X:17:GLN:O	3:X:21:GLN:HG2	2.18	0.43
3:X:256:THR:OG1	3:X:259:LEU:HD23	2.19	0.43
3:Z:63:GLU:OE2	3:Z:63:GLU:N	2.47	0.43
6:G:177:ILE:O	6:G:181:GLU:HG3	2.18	0.43
5:L:82:THR:O	5:L:86:THR:HG22	2.19	0.43
4:H:96:ASN:HA	4:H:99:LYS:HD2	2.00	0.43
3:Y:260:LEU:HD12	3:Y:260:LEU:HA	1.86	0.43
4:H:42:LYS:HD3	4:H:42:LYS:HA	1.37	0.43
4:H:53:ILE:H	4:H:53:ILE:HG13	1.66	0.43
1:B:274:TYR:HB3	1:B:311:LEU:HD23	2.00	0.43
1:B:569:ILE:O	1:B:572:GLU:HG3	2.19	0.43
2:E:166:PRO:HA	2:E:340:ARG:HD3	2.00	0.43
6:G:65:ALA:HB1	6:G:138:TYR:CZ	2.54	0.43
6:G:72:ALA:HB1	6:G:131:LEU:HD23	2.01	0.43
4:H:59:LYS:HG3	4:H:60:LYS:N	2.34	0.43
1:A:55:ILE:HD12	1:A:365:LEU:HD11	2.00	0.43
2:F:493:LYS:HB2	2:F:493:LYS:HE3	1.82	0.43
3:X:143:ALA:HB1	3:X:149:ASN:ND2	2.34	0.43
3:Y:238:SER:O	3:Y:238:SER:OG	2.29	0.43
1:B:343:HIS:ND1	1:B:403:SER:HB3	2.34	0.43
1:C:20:TYR:CZ	5:M:115:ARG:HD3	2.53	0.43
2:E:204:ALA:O	2:E:208:ARG:HG2	2.19	0.43
2:E:287:TYR:O	2:E:344:ARG:NH1	2.52	0.43
3:X:144:ALA:H	3:X:149:ASN:ND2	2.17	0.43
3:Y:261:ASP:HA	3:Y:264:ASP:OD2	2.19	0.43
3:Z:159:LEU:HB2	3:Z:178:LEU:HD22	2.00	0.43
6:G:89:LYS:HA	6:G:89:LYS:HD3	1.75	0.43
1:A:95:MET:HE2	1:A:162:ILE:HG13	2.00	0.43
1:B:231:GLN:O	1:B:235:ASP:HB2	2.19	0.43
1:C:469:PHE:O	1:C:470:THR:HG22	2.18	0.43
2:E:167:GLU:HG3	2:E:168:GLU:HG2	2.01	0.43
2:E:294:LEU:HD11	2:E:351:ILE:HG13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:38:PHE:CD1	5:L:33:LEU:HD23	2.54	0.43
2:E:226:ASN:HD22	2:E:226:ASN:HA	1.64	0.42
4:H:46:VAL:O	4:H:50:ARG:CB	2.67	0.42
1:B:559:ALA:O	1:B:564:LYS:HE3	2.19	0.42
8:C:701:ADP:O1B	2:F:400:ARG:NH2	2.51	0.42
2:E:82:ARG:NH1	2:E:101:GLY:O	2.52	0.42
2:F:46:THR:HG23	2:F:113:GLU:HB2	2.00	0.42
4:J:37:GLU:OE2	5:M:33:LEU:HB3	2.19	0.42
2:F:237:ASN:H	2:F:237:ASN:HD22	1.66	0.42
5:M:32:ARG:HD2	5:M:35:GLN:NE2	2.35	0.42
5:L:36:ALA:O	5:L:39:GLU:HB3	2.18	0.42
7:N:51:THR:HA	7:N:54:GLN:NE2	2.34	0.42
1:A:44:ARG:HD2	1:A:49:GLU:HB3	2.01	0.42
1:A:419:ASP:OD1	1:A:420:PRO:HD2	2.20	0.42
3:Z:205:LYS:HE2	3:Z:260:LEU:HB3	2.00	0.42
4:J:174:PRO:O	4:J:177:ILE:HG12	2.20	0.42
7:N:40:GLU:HB2	7:N:42:ASP:OD2	2.18	0.42
1:A:574:MET:HE2	1:A:577:ILE:HG21	2.01	0.42
2:D:76:LEU:HB2	2:D:80:THR:HG23	2.01	0.42
3:X:200:PHE:CZ	3:X:225:LEU:HD21	2.54	0.42
3:Z:103:MET:HG2	3:Z:164:ALA:HA	2.02	0.42
4:H:62:LYS:HE3	4:H:62:LYS:HA	2.01	0.42
1:A:368:MET:HE3	6:G:202:LEU:HD13	2.01	0.42
1:C:500:SER:O	1:C:500:SER:OG	2.38	0.42
2:F:306:ALA:O	2:F:310:VAL:HG23	2.19	0.42
6:G:210:LYS:O	6:G:214:GLU:HG2	2.20	0.42
1:A:249:PRO:HG2	1:A:435:LEU:HB2	2.02	0.42
1:A:511:VAL:HG11	1:A:548:TYR:HB2	2.02	0.42
2:E:269:ILE:HD12	2:E:269:ILE:H	1.85	0.42
3:Z:220:GLU:CD	3:Z:220:GLU:H	2.22	0.42
5:L:49:LEU:HD23	5:L:49:LEU:HA	1.88	0.42
4:J:60:LYS:O	4:J:64:ILE:HG23	2.19	0.42
1:A:376:ALA:HB1	2:E:309:GLU:HA	2.02	0.42
1:B:389:ALA:HB2	1:B:406:ILE:HG13	2.02	0.42
2:D:165:TYR:HA	2:D:166:PRO:HD3	1.92	0.42
3:X:133:LEU:O	3:X:137:THR:HG22	2.19	0.42
3:Y:132:GLN:HB3	3:Y:183:LEU:HD11	2.01	0.42
7:N:21:LEU:HD13	7:N:21:LEU:HA	1.92	0.42
1:A:436:ASP:HB3	1:A:439:LEU:HB2	2.01	0.42
1:A:574:MET:H	1:A:574:MET:HG2	1.72	0.42
2:D:71:ILE:HD11	2:D:119:LEU:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:319:GLY:N	2:F:323:PHE:O	2.42	0.42
3:X:71:SER:O	3:X:71:SER:OG	2.32	0.42
4:J:59:LYS:O	4:J:63:GLN:HG3	2.20	0.42
4:J:102:LEU:HD12	4:J:200:LEU:HD22	2.01	0.42
1:B:494:GLN:HG3	1:B:495:LEU:N	2.35	0.41
3:X:207:GLN:NE2	3:X:212:PRO:HB3	2.35	0.41
1:C:289:ARG:HE	1:C:289:ARG:HB3	1.69	0.41
3:X:156:THR:O	3:X:160:GLN:HG3	2.20	0.41
3:Z:242:LEU:HB2	3:Z:270:ASN:ND2	2.35	0.41
4:H:38:PHE:CZ	5:K:29:LYS:HG2	2.55	0.41
1:A:169:PRO:HA	1:A:170:PRO:HD3	1.91	0.41
1:B:422:THR:HA	1:B:425:THR:HG22	2.02	0.41
2:E:102:THR:HA	2:E:105:ILE:HD12	2.02	0.41
2:E:363:HIS:CD2	2:E:364:PRO:HD2	2.55	0.41
3:X:239:SER:HB2	3:X:273:LEU:HD22	2.02	0.41
3:Z:188:MET:HE3	3:Z:196:GLN:HG2	2.03	0.41
3:Z:209:GLU:HG2	3:Z:211:SER:H	1.84	0.41
5:K:41:GLN:HA	5:K:44:ILE:HB	2.02	0.41
1:C:56:ARG:HB3	1:C:63:THR:HB	2.02	0.41
1:C:135:PHE:HD1	1:C:156:VAL:HG23	1.86	0.41
2:E:237:ASN:ND2	2:E:240:THR:H	2.18	0.41
3:Y:141:LYS:HE2	3:Y:141:LYS:HB2	1.85	0.41
4:J:223:LYS:HE2	4:J:223:LYS:HB3	1.80	0.41
1:B:192:LEU:HG	1:B:193:GLU:N	2.35	0.41
3:X:111:GLN:HG2	3:X:169:THR:HG23	2.01	0.41
4:I:42:LYS:HE3	5:L:37:LYS:HG2	2.01	0.41
4:I:64:ILE:HD13	4:I:64:ILE:HA	1.90	0.41
5:K:96:LEU:HD23	5:K:96:LEU:HA	1.87	0.41
1:A:20:TYR:CZ	5:K:115:ARG:HD3	2.56	0.41
1:A:108:ASP:N	1:A:108:ASP:OD2	2.54	0.41
1:C:148:THR:OG1	1:C:149:GLY:N	2.53	0.41
1:C:521:GLN:HE22	2:F:494:ARG:NH2	2.18	0.41
6:G:47:ILE:HD13	6:G:47:ILE:HA	1.94	0.41
4:I:59:LYS:HE3	4:I:59:LYS:HB3	1.69	0.41
3:Y:156:THR:O	3:Y:160:GLN:HG3	2.21	0.41
4:J:219:ASN:HD22	4:J:219:ASN:HA	1.74	0.41
6:G:136:ARG:HE	6:G:136:ARG:HB3	1.76	0.41
6:G:140:LYS:HB3	6:G:140:LYS:HE3	1.68	0.41
4:I:38:PHE:CD1	4:I:39:ASN:N	2.88	0.41
4:H:45:LEU:HD23	4:H:45:LEU:HA	1.77	0.41
4:H:50:ARG:HD2	4:H:53:ILE:HG12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:60:LYS:HA	4:H:60:LYS:HD3	1.74	0.41
4:H:223:LYS:HA	4:H:223:LYS:HD3	1.90	0.41
1:B:133:TRP:O	1:B:184:ASN:HA	2.21	0.41
1:B:501:LEU:HD23	1:B:501:LEU:HA	1.91	0.41
3:X:52:VAL:HG11	3:X:81:LEU:HD11	2.02	0.41
4:J:127:LEU:HA	4:J:127:LEU:HD23	1.86	0.41
5:L:30:ASN:HD22	5:L:33:LEU:HB2	1.86	0.41
1:A:215:ARG:HA	1:A:216:PRO:HD3	1.93	0.41
1:B:491:GLU:H	1:B:491:GLU:HG2	1.61	0.41
1:C:605:LEU:O	1:C:609:GLN:HG3	2.21	0.41
3:X:93:ARG:O	3:X:97:SER:OG	2.29	0.41
3:X:140:LEU:HD13	3:X:153:ARG:HA	2.03	0.41
3:Y:180:LYS:HE2	3:Y:180:LYS:HB2	1.80	0.41
3:Z:144:ALA:O	3:Z:149:ASN:ND2	2.53	0.41
3:Z:207:GLN:NE2	3:Z:209:GLU:O	2.54	0.41
4:J:59:LYS:HA	4:J:59:LYS:HD3	1.84	0.41
4:J:107:LYS:HA	4:J:107:LYS:HD3	1.59	0.41
5:M:37:LYS:HD2	5:M:37:LYS:HA	1.81	0.41
5:L:87:TYR:O	5:L:91:ASN:ND2	2.54	0.41
4:H:36:GLU:O	4:H:40:ILE:HG12	2.21	0.41
4:H:57:TYR:HE2	5:K:54:GLU:HB2	1.85	0.41
4:H:72:MET:O	4:H:76:MET:HG2	2.20	0.41
4:H:116:LEU:HD13	4:H:144:VAL:HG12	2.03	0.41
7:N:39:VAL:HG21	7:N:48:ILE:CD1	2.51	0.41
1:B:169:PRO:HA	1:B:170:PRO:HD3	1.93	0.41
2:E:380:ASP:HB2	2:E:393:ASN:HB2	2.01	0.41
2:F:190:PRO:HD2	2:F:375:GLY:O	2.21	0.41
3:X:125:ASP:OD1	3:X:125:ASP:N	2.53	0.41
3:X:223:LYS:O	3:X:226:VAL:HG22	2.21	0.41
3:Z:177:GLN:HE21	3:Z:181:LEU:HG	1.86	0.41
3:Z:222:GLN:HA	3:Z:225:LEU:HG	2.02	0.41
4:J:42:LYS:O	4:J:46:VAL:HB	2.21	0.41
3:Y:206:ASP:OD1	3:Y:206:ASP:N	2.54	0.40
3:Y:230:ILE:HD12	3:Y:230:ILE:HA	1.90	0.40
4:J:57:TYR:CD2	5:M:51:ARG:HD2	2.57	0.40
4:J:77:ASN:ND2	4:J:80:ARG:HH12	2.18	0.40
5:M:31:ARG:H	5:M:31:ARG:HG2	1.60	0.40
4:I:135:ARG:HE	4:I:135:ARG:HB3	1.72	0.40
4:H:66:GLN:O	4:H:70:ILE:HG13	2.21	0.40
7:N:106:LEU:HD23	7:N:106:LEU:HA	1.85	0.40
1:C:55:ILE:HD12	1:C:365:LEU:HD11	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:245:LYS:HE3	2:F:245:LYS:HB3	1.76	0.40
5:M:46:GLN:O	5:M:49:LEU:HG	2.21	0.40
4:I:60:LYS:HD2	4:I:60:LYS:N	2.36	0.40
5:K:105:ASP:OD2	5:K:107:ARG:NH1	2.54	0.40
1:A:99:PHE:HB3	1:A:103:GLN:HA	2.03	0.40
1:A:234:LEU:HD21	1:A:448:VAL:HG21	2.03	0.40
1:B:185:TYR:HB2	1:B:205:MET:HE3	2.04	0.40
1:B:234:LEU:HD21	1:B:448:VAL:HG21	2.03	0.40
1:C:50:LEU:HB3	1:C:68:GLU:HG3	2.03	0.40
1:C:438:LYS:HD3	1:C:438:LYS:HA	1.80	0.40
2:E:233:ALA:HB3	2:E:261:LEU:HD23	2.02	0.40
2:F:232:ALA:HB3	2:F:297:LEU:HD23	2.04	0.40
3:X:39:GLU:O	3:X:41:ASN:ND2	2.55	0.40
5:L:41:GLN:HA	5:L:44:ILE:HB	2.03	0.40
4:H:52:LYS:H	4:H:52:LYS:HG3	1.67	0.40
2:E:328:TYR:HD2	2:E:368:LEU:HD22	1.85	0.40
3:Z:36:ILE:HB	3:Z:92:LEU:HD13	2.03	0.40
3:Z:237:LEU:HD23	3:Z:270:ASN:HD22	1.86	0.40
4:J:65:GLU:HA	4:J:68:LYS:HG2	2.03	0.40
4:I:184:TYR:CE2	4:I:191:LYS:HD2	2.57	0.40
5:L:31:ARG:HG3	5:L:35:GLN:HE22	1.86	0.40
4:H:60:LYS:O	4:H:64:ILE:HG23	2.22	0.40
1:A:492:ILE:HG21	2:E:437:ALA:HB1	2.03	0.40
2:D:164:ILE:HD11	2:D:342:GLU:HA	2.03	0.40
2:E:188:LYS:HB2	2:E:188:LYS:HE2	1.80	0.40
2:F:165:TYR:HA	2:F:166:PRO:HD3	1.94	0.40
4:J:49:GLN:HG3	5:M:44:ILE:HD13	2.03	0.40
4:H:137:ARG:HD3	4:H:177:ILE:HG13	2.04	0.40
7:N:69:TYR:HA	7:N:72:GLU:HG2	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	575 (96%)	23 (4%)	0	100	100
1	B	598/617 (97%)	557 (93%)	41 (7%)	0	100	100
1	C	598/617 (97%)	574 (96%)	24 (4%)	0	100	100
2	D	456/511 (89%)	433 (95%)	23 (5%)	0	100	100
2	E	456/511 (89%)	438 (96%)	18 (4%)	0	100	100
2	F	456/511 (89%)	440 (96%)	16 (4%)	0	100	100
3	X	258/573 (45%)	243 (94%)	15 (6%)	0	100	100
3	Y	265/573 (46%)	252 (95%)	13 (5%)	0	100	100
3	Z	260/573 (45%)	238 (92%)	22 (8%)	0	100	100
4	H	191/226 (84%)	191 (100%)	0	0	100	100
4	I	191/226 (84%)	187 (98%)	4 (2%)	0	100	100
4	J	191/226 (84%)	188 (98%)	3 (2%)	0	100	100
5	K	87/118 (74%)	85 (98%)	2 (2%)	0	100	100
5	L	87/118 (74%)	85 (98%)	2 (2%)	0	100	100
5	M	87/118 (74%)	82 (94%)	5 (6%)	0	100	100
6	G	211/247 (85%)	199 (94%)	12 (6%)	0	100	100
7	N	108/119 (91%)	97 (90%)	11 (10%)	0	100	100
All	All	5098/6501 (78%)	4864 (95%)	234 (5%)	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	507/525 (97%)	472 (93%)	35 (7%)	15	41
1	B	508/525 (97%)	483 (95%)	25 (5%)	25	57
1	C	508/525 (97%)	476 (94%)	32 (6%)	18	46
2	D	393/430 (91%)	372 (95%)	21 (5%)	22	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	E	390/430 (91%)	369 (95%)	21 (5%)	22	54
2	F	392/430 (91%)	374 (95%)	18 (5%)	27	60
3	X	237/519 (46%)	214 (90%)	23 (10%)	8	25
3	Y	239/519 (46%)	217 (91%)	22 (9%)	9	27
3	Z	237/519 (46%)	211 (89%)	26 (11%)	6	19
4	H	172/199 (86%)	165 (96%)	7 (4%)	30	64
4	I	172/199 (86%)	155 (90%)	17 (10%)	8	24
4	J	172/199 (86%)	164 (95%)	8 (5%)	26	59
5	K	79/101 (78%)	73 (92%)	6 (8%)	13	36
5	L	79/101 (78%)	68 (86%)	11 (14%)	3	10
5	M	79/101 (78%)	69 (87%)	10 (13%)	4	13
6	G	183/212 (86%)	171 (93%)	12 (7%)	16	44
7	N	94/100 (94%)	86 (92%)	8 (8%)	10	31
All	All	4441/5634 (79%)	4139 (93%)	302 (7%)	19	42

All (302) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	GLU
1	A	69	GLU
1	A	110	SER
1	A	129	ARG
1	A	157	SER
1	A	160	SER
1	A	175	THR
1	A	191	VAL
1	A	266	TYR
1	A	268	ASN
1	A	296	MET
1	A	298	VAL
1	A	304	SER
1	A	324	GLU
1	A	327	ILE
1	A	345	SER
1	A	350	SER
1	A	356	GLU
1	A	362	SER

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Mol	Chain	Res	Type
1	A	381	ARG
1	A	400	ARG
1	A	403	SER
1	A	405	SER
1	A	417	PHE
1	A	450	TRP
1	A	453	SER
1	A	471	GLU
1	A	478	LYS
1	A	491	GLU
1	A	542	SER
1	A	560	GLN
1	A	561	SER
1	A	583	SER
1	A	592	ASP
1	A	614	SER
1	B	33	ASP
1	B	60	ASP
1	B	87	SER
1	B	110	SER
1	B	136	THR
1	B	139	LYS
1	B	161	LEU
1	B	266	TYR
1	B	291	PHE
1	B	308	ARG
1	B	327	ILE
1	B	350	SER
1	B	351	THR
1	B	358	LEU
1	B	362	SER
1	B	384	SER
1	B	400	ARG
1	B	403	SER
1	B	436	ASP
1	B	450	TRP
1	B	453	SER
1	B	466	ASP
1	B	477	THR
1	B	495	LEU
1	B	556	GLU
1	C	17	THR

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Mol	Chain	Res	Type
1	C	18	PHE
1	C	33	ASP
1	C	42	LEU
1	C	60	ASP
1	C	74	SER
1	C	104	ARG
1	C	108	ASP
1	C	130	ASP
1	C	136	THR
1	C	138	CYS
1	C	139	LYS
1	C	142	ARG
1	C	262	SER
1	C	302	VAL
1	C	308	ARG
1	C	346	MET
1	C	362	SER
1	C	372	SER
1	C	395	LEU
1	C	400	ARG
1	C	403	SER
1	C	442	ARG
1	C	450	TRP
1	C	470	THR
1	C	478	LYS
1	C	542	SER
1	C	555	VAL
1	C	563	ASN
1	C	571	ARG
1	C	588	ASP
1	C	599	SER
2	D	54	ASN
2	D	61	ASP
2	D	64	LYS
2	D	80	THR
2	D	90	SER
2	D	97	GLN
2	D	156	GLN
2	D	163	ARG
2	D	215	LYS
2	D	250	GLU
2	D	256	ASN

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Mol	Chain	Res	Type
2	D	311	SER
2	D	340	ARG
2	D	351	ILE
2	D	386	ARG
2	D	403	LYS
2	D	431	ASP
2	D	436	LYS
2	D	449	LEU
2	D	455	LEU
2	D	472	THR
2	E	51	SER
2	E	80	THR
2	E	83	SER
2	E	92	SER
2	E	103	SER
2	E	141	ARG
2	E	201	GLU
2	E	215	LYS
2	E	226	ASN
2	E	237	ASN
2	E	256	ASN
2	E	268	THR
2	E	311	SER
2	E	330	ASP
2	E	347	SER
2	E	403	LYS
2	E	404	SER
2	E	445	THR
2	E	470	ASN
2	E	473	VAL
2	E	501	SER
2	F	46	THR
2	F	51	SER
2	F	54	ASN
2	F	64	LYS
2	F	80	THR
2	F	83	SER
2	F	135	SER
2	F	168	GLU
2	F	188	LYS
2	F	216	SER
2	F	237	ASN

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Mol	Chain	Res	Type
2	F	239	GLU
2	F	253	SER
2	F	311	SER
2	F	314	ARG
2	F	354	LEU
2	F	399	SER
2	F	489	LYS
3	X	44	LYS
3	X	48	ASP
3	X	51	ASP
3	X	71	SER
3	X	81	LEU
3	X	96	SER
3	X	104	LYS
3	X	123	LYS
3	X	126	TYR
3	X	138	ASP
3	X	146	THR
3	X	161	MET
3	X	171	ASP
3	X	199	LEU
3	X	221	ASP
3	X	224	ILE
3	X	231	ASP
3	X	238	SER
3	X	244	ASP
3	X	247	SER
3	X	250	SER
3	X	259	LEU
3	X	270	ASN
3	Y	14	THR
3	Y	15	SER
3	Y	16	GLU
3	Y	17	GLN
3	Y	36	ILE
3	Y	40	ASN
3	Y	79	ASP
3	Y	104	LYS
3	Y	126	TYR
3	Y	141	LYS
3	Y	146	THR
3	Y	161	MET

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Mol	Chain	Res	Type
3	Y	173	GLU
3	Y	179	PHE
3	Y	188	MET
3	Y	198	HIS
3	Y	205	LYS
3	Y	206	ASP
3	Y	240	LYS
3	Y	244	ASP
3	Y	261	ASP
3	Y	269	GLU
3	Z	48	ASP
3	Z	51	ASP
3	Z	67	GLU
3	Z	71	SER
3	Z	74	CYS
3	Z	87	ILE
3	Z	104	LYS
3	Z	109	GLU
3	Z	126	TYR
3	Z	161	MET
3	Z	171	ASP
3	Z	178	LEU
3	Z	179	PHE
3	Z	184	HIS
3	Z	207	GLN
3	Z	221	ASP
3	Z	222	GLN
3	Z	227	LYS
3	Z	231	ASP
3	Z	234	MET
3	Z	243	GLN
3	Z	245	LYS
3	Z	246	LEU
3	Z	247	SER
3	Z	259	LEU
3	Z	269	GLU
4	J	37	GLU
4	J	47	GLN
4	J	73	SER
4	J	171	SER
4	J	185	ASN
4	J	198	SER

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Mol	Chain	Res	Type
4	J	212	ARG
4	J	226	ASP
5	M	32	ARG
5	M	34	LYS
5	M	45	GLU
5	M	47	TYR
5	M	56	LYS
5	M	70	SER
5	M	72	GLU
5	M	87	TYR
5	M	91	ASN
5	M	102	PHE
6	G	5	ASP
6	G	42	LEU
6	G	58	MET
6	G	67	PHE
6	G	78	ASP
6	G	79	PHE
6	G	122	THR
6	G	126	ARG
6	G	133	LYS
6	G	136	ARG
6	G	140	LYS
6	G	215	LYS
4	I	42	LYS
4	I	49	GLN
4	I	55	GLU
4	I	56	TYR
4	I	57	TYR
4	I	61	GLU
4	I	63	GLN
4	I	68	LYS
4	I	75	LEU
4	I	103	SER
4	I	136	CYS
4	I	171	SER
4	I	183	ILE
4	I	185	ASN
4	I	193	SER
4	I	197	GLU
4	I	226	ASP
5	L	34	LYS

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Mol	Chain	Res	Type
5	L	37	LYS
5	L	38	GLU
5	L	41	GLN
5	L	52	GLU
5	L	53	LYS
5	L	68	SER
5	L	79	GLU
5	L	87	TYR
5	L	91	ASN
5	L	98	ASN
4	H	52	LYS
4	H	56	TYR
4	H	59	LYS
4	H	73	SER
4	H	170	GLU
4	H	176	ASP
4	H	212	ARG
5	K	28	ARG
5	K	41	GLN
5	K	46	GLN
5	K	48	ARG
5	K	65	SER
5	K	87	TYR
7	N	6	LYS
7	N	15	ASP
7	N	30	LYS
7	N	41	LYS
7	N	66	ILE
7	N	68	GLN
7	N	74	VAL
7	N	110	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (83) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	146	HIS
1	A	172	ASN
1	A	213	GLN
1	A	261	GLN
1	A	430	GLN
1	A	441	GLN
1	A	444	HIS

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Mol	Chain	Res	Type
1	A	603	GLN
1	B	47	HIS
1	B	172	ASN
1	B	231	GLN
1	B	261	GLN
1	B	314	ASN
1	B	521	GLN
1	B	560	GLN
1	C	140	ASN
1	C	146	HIS
1	C	172	ASN
1	C	261	GLN
1	C	441	GLN
1	C	563	ASN
2	D	54	ASN
2	D	85	GLN
2	D	97	GLN
2	D	156	GLN
2	D	350	GLN
2	E	226	ASN
2	E	237	ASN
2	E	256	ASN
2	E	350	GLN
2	E	363	HIS
2	E	382	GLN
2	E	470	ASN
2	F	54	ASN
2	F	85	GLN
2	F	97	GLN
2	F	237	ASN
2	F	350	GLN
3	X	40	ASN
3	X	134	ASN
3	X	149	ASN
3	X	150	ASN
3	X	222	GLN
3	Y	184	HIS
3	Y	190	ASN
3	Y	196	GLN
3	Y	207	GLN
3	Y	270	ASN
3	Z	149	ASN

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Mol	Chain	Res	Type
3	Z	177	GLN
3	Z	222	GLN
4	J	49	GLN
4	J	77	ASN
4	J	185	ASN
4	J	219	ASN
5	M	35	GLN
5	M	111	HIS
6	G	31	ASN
6	G	152	GLN
6	G	206	GLN
4	I	71	GLN
4	I	77	ASN
4	I	149	GLN
4	I	185	ASN
4	I	206	GLN
4	I	219	ASN
5	L	30	ASN
5	L	35	GLN
5	L	41	GLN
5	L	78	GLN
5	L	91	ASN
5	L	98	ASN
4	H	100	GLN
4	H	139	GLN
4	H	219	ASN
5	K	35	GLN
5	K	46	GLN
5	K	78	GLN
7	N	31	ASN
7	N	33	HIS
7	N	67	ASN
7	N	81	HIS
7	N	83	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry

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	$\# Z > 2$
8	ADP	C	701	-	24,29,29	0.95	1 (4%)	29,45,45	1.42	4 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	ADP	C	701	-	-	3/12/32/32	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	701	ADP	C5-C4	2.20	1.46	1.40

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	701	ADP	C3'-C2'-C1'	3.25	105.87	100.98
8	C	701	ADP	N3-C2-N1	-3.06	123.89	128.68
8	C	701	ADP	PA-O3A-PB	-2.87	122.97	132.83
8	C	701	ADP	C4-C5-N7	-2.59	106.70	109.40

There are no chirality outliers.

All (3) torsion outliers are listed below:

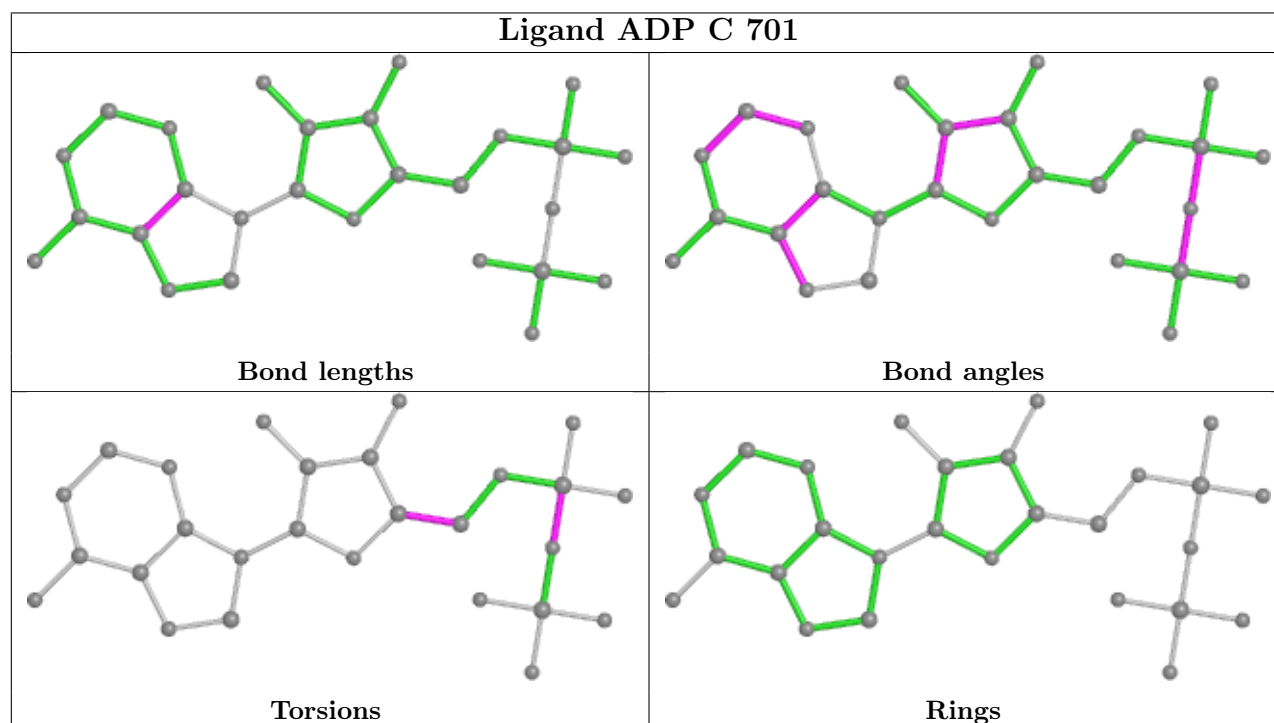
Mol	Chain	Res	Type	Atoms
8	C	701	ADP	O4'-C4'-C5'-O5'
8	C	701	ADP	PB-O3A-PA-O1A
8	C	701	ADP	PB-O3A-PA-O2A

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	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.

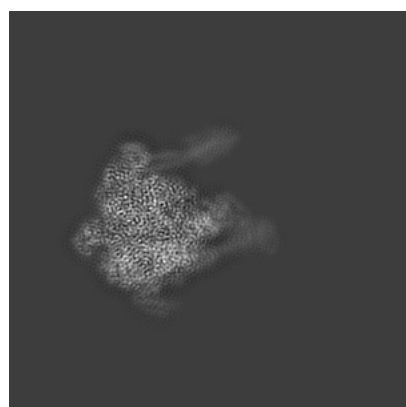
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21845. These allow visual inspection of the internal detail of the map and identification of artifacts.

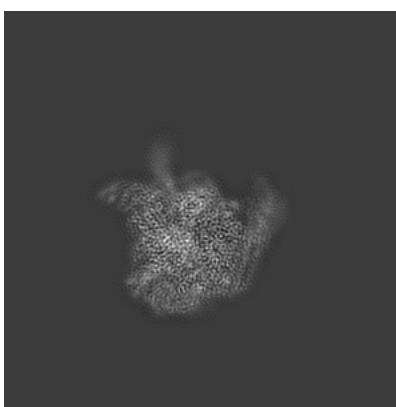
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X



Y

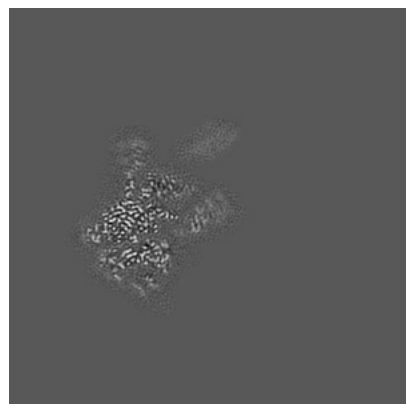


Z

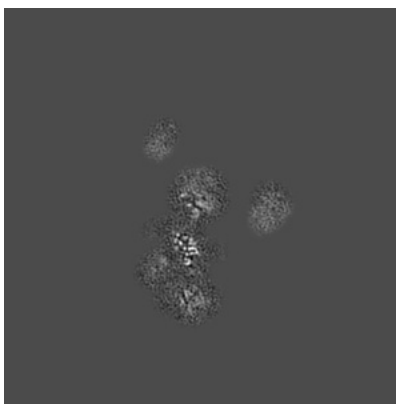
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

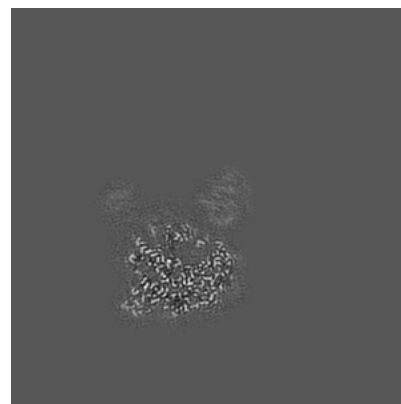
6.2.1 Primary map



X Index: 180



Y Index: 180

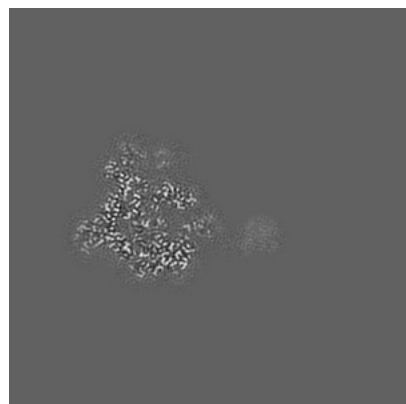


Z Index: 180

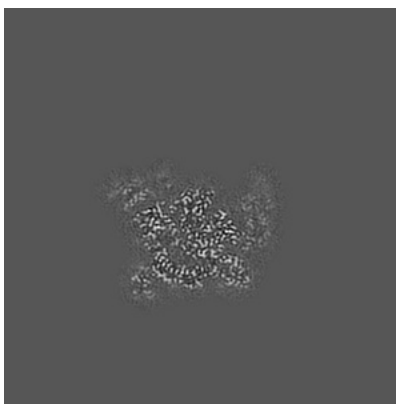
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

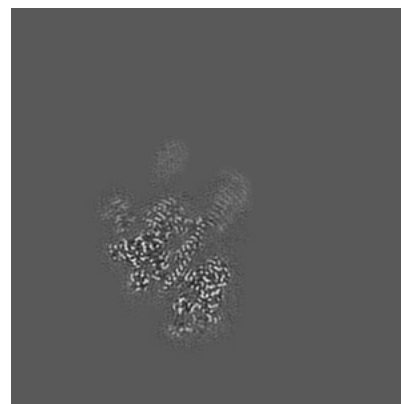
6.3.1 Primary map



X Index: 149



Y Index: 114



Z Index: 164

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.6. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

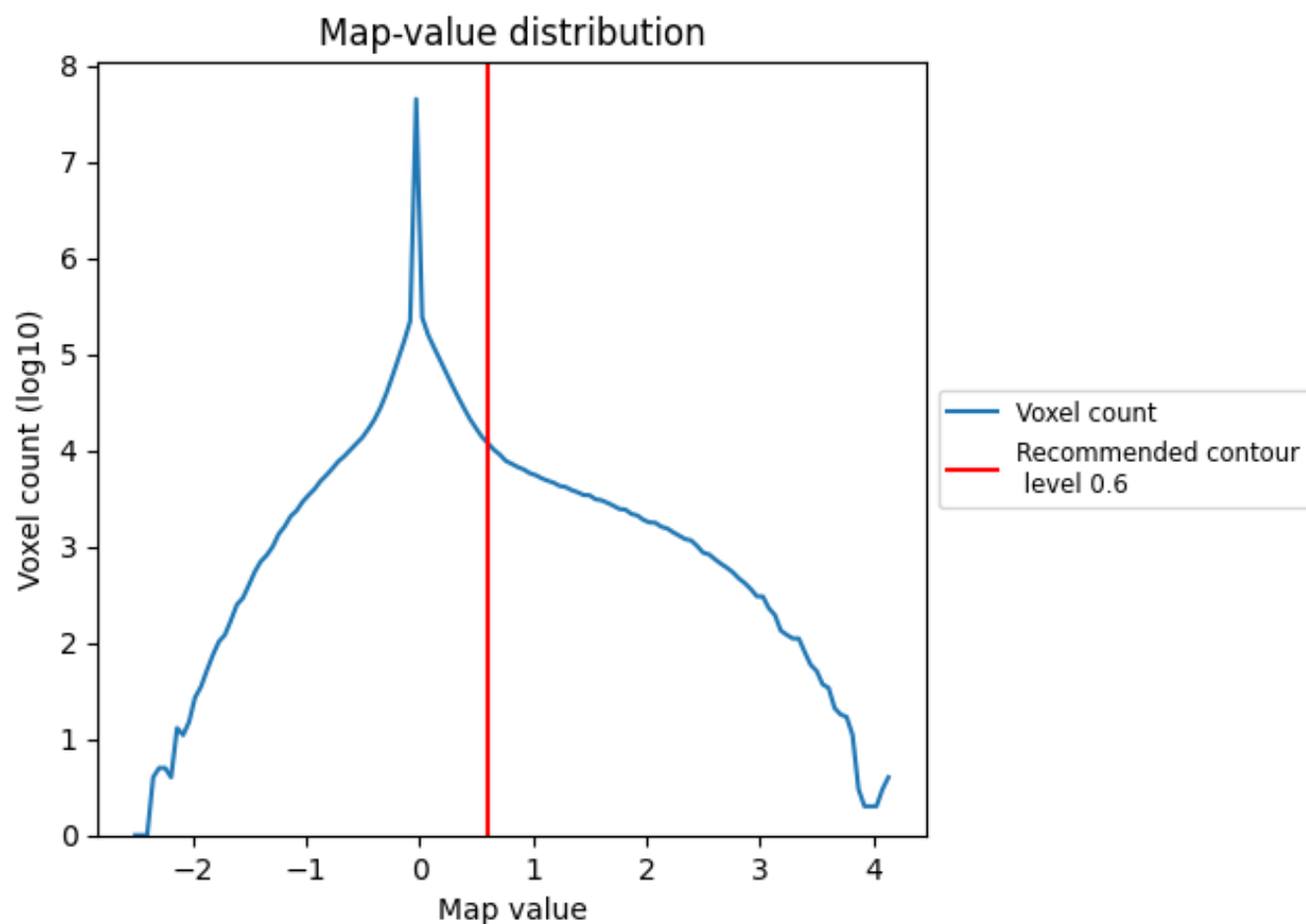
6.5 Mask visualisation

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

7 Map analysis [i](#)

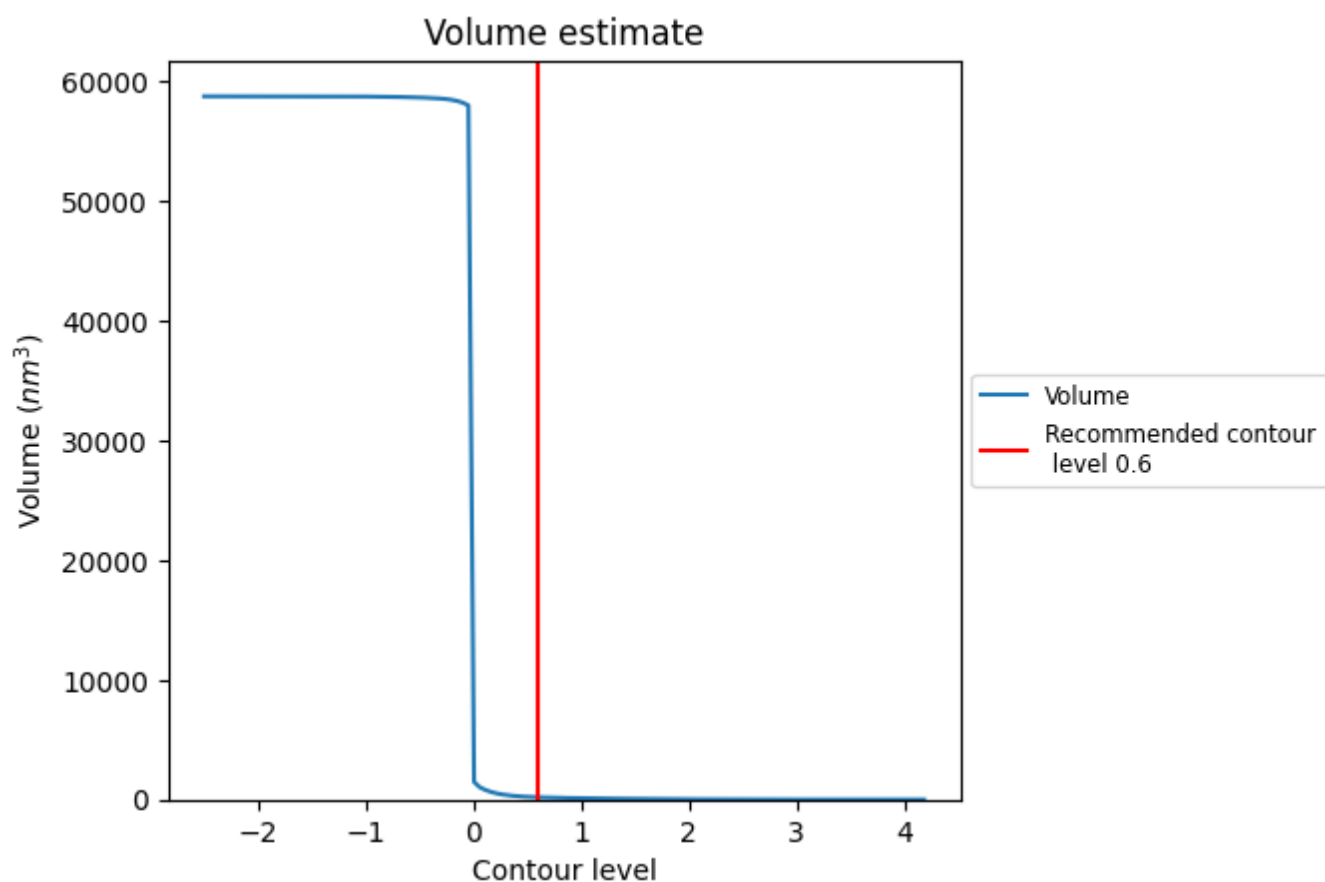
This section contains the results of statistical analysis of the map.

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.

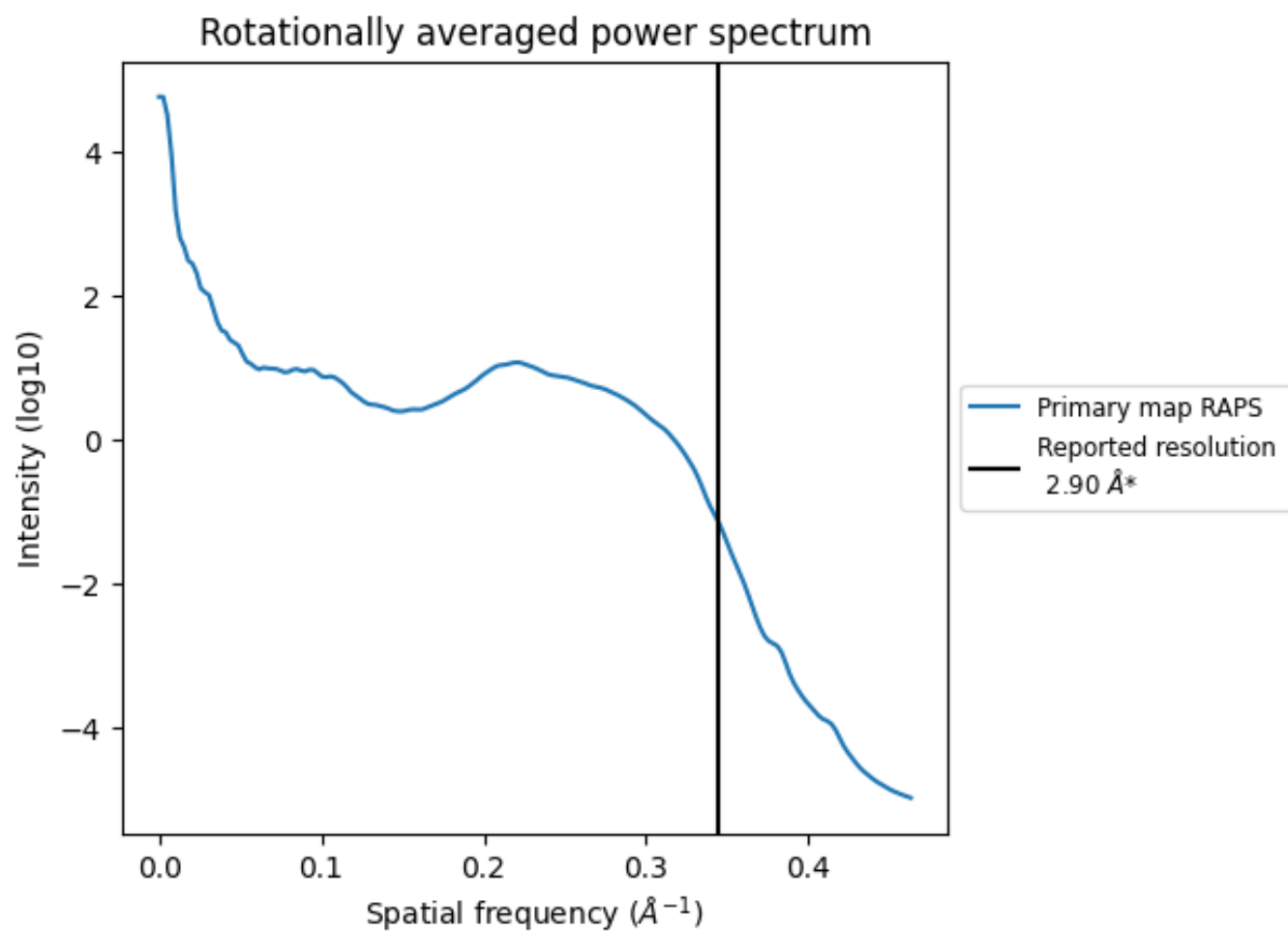
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 191 nm³; this corresponds to an approximate mass of 172 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 0.345 Å⁻¹

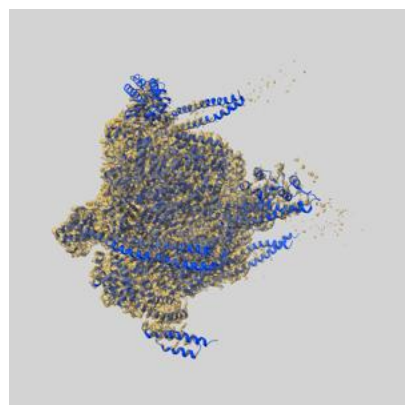
8 Fourier-Shell correlation ⓘ

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

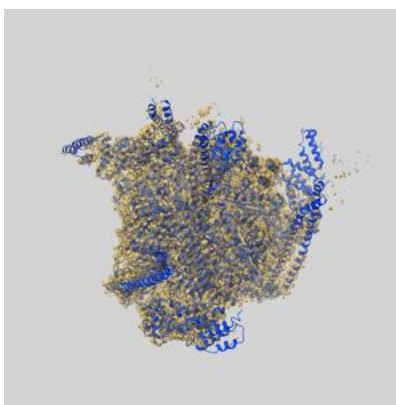
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-21845 and PDB model 6WLZ. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

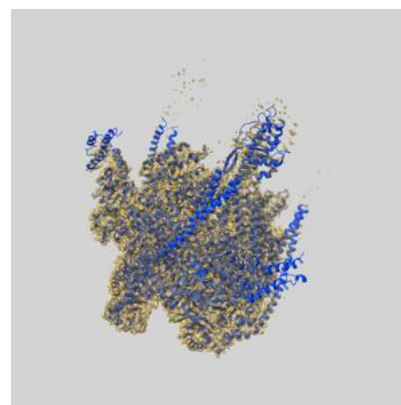
9.1 Map-model overlay [i](#)



X



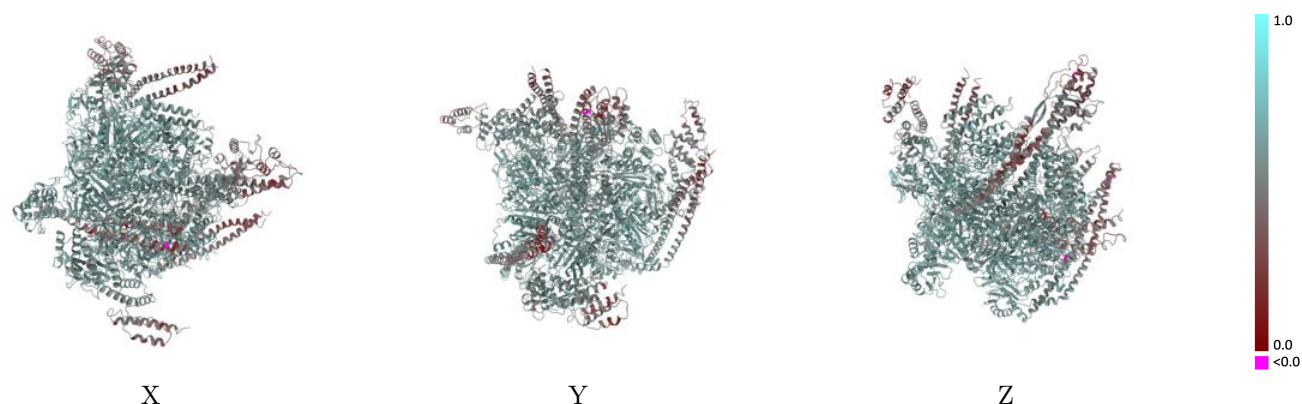
Y



Z

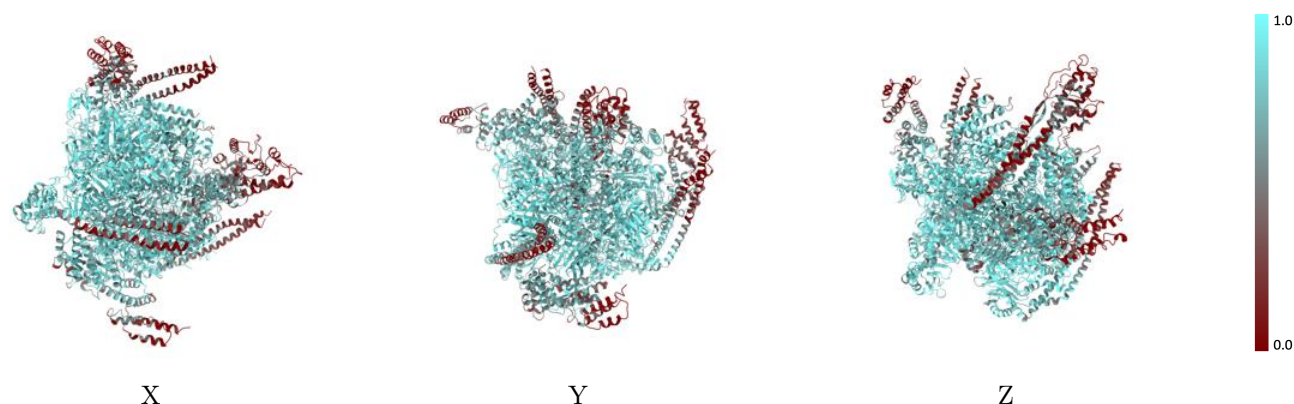
The images above show the 3D surface view of the map at the recommended contour level 0.6 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



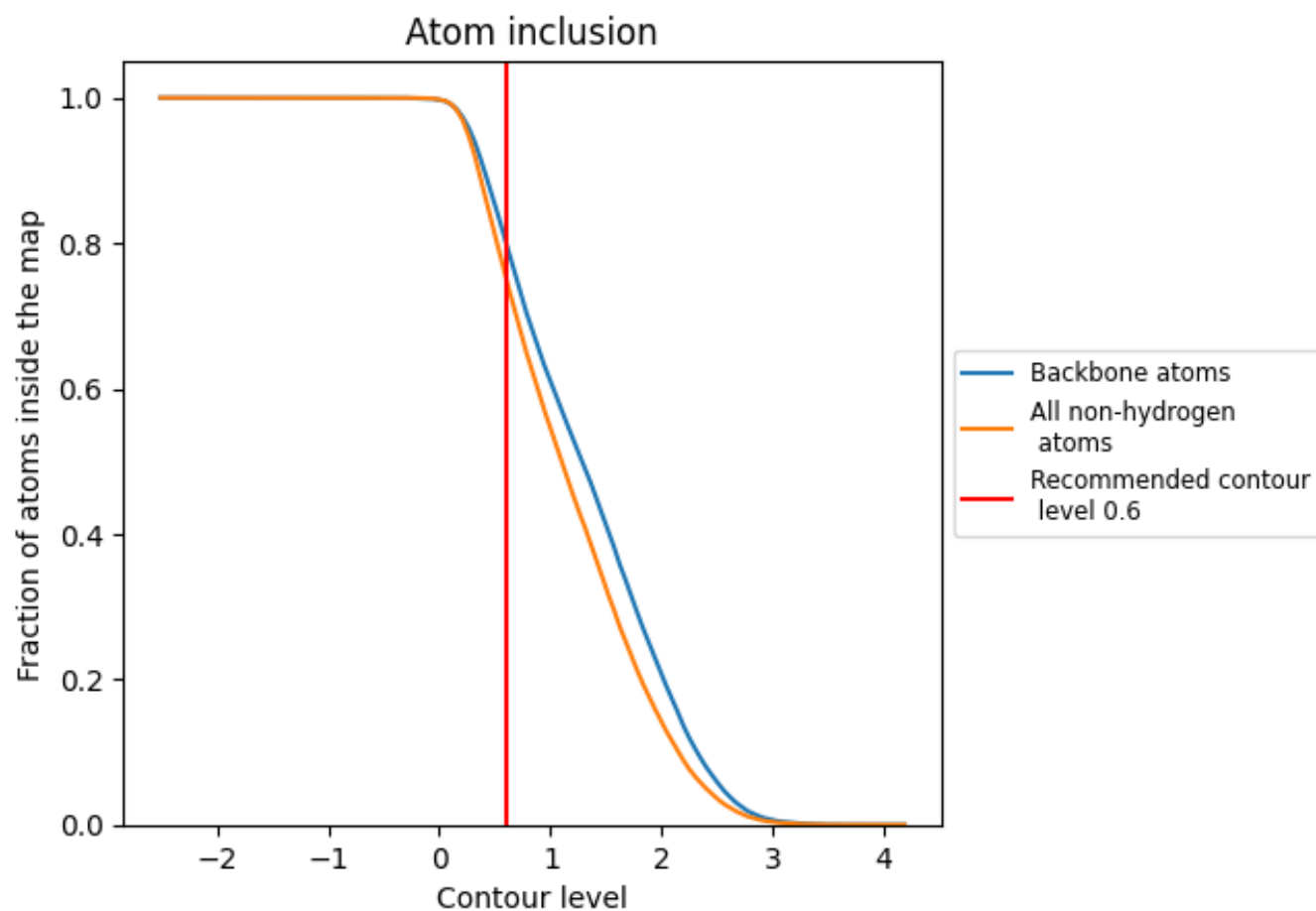
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.6).





































9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 75% 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 (0.6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7520	 0.5730
A	 0.8563	 0.6060
B	 0.8371	 0.5940
C	 0.8947	 0.6150
D	 0.9064	 0.6230
E	 0.9152	 0.6200
F	 0.9103	 0.6260
G	 0.5424	 0.5010
H	 0.7088	 0.5550
I	 0.7088	 0.5410
J	 0.7212	 0.5630
K	 0.4854	 0.4800
L	 0.4591	 0.4590
M	 0.4605	 0.4630
N	 0.2404	 0.4330
X	 0.5026	 0.5040
Y	 0.5923	 0.5280
Z	 0.3878	 0.4980

