



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 07:36 PM UTC

PDB ID : 6WLZ / pdb_00006wlz
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:

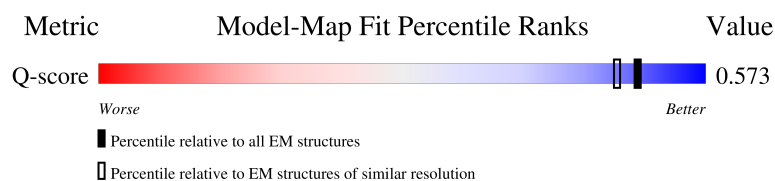
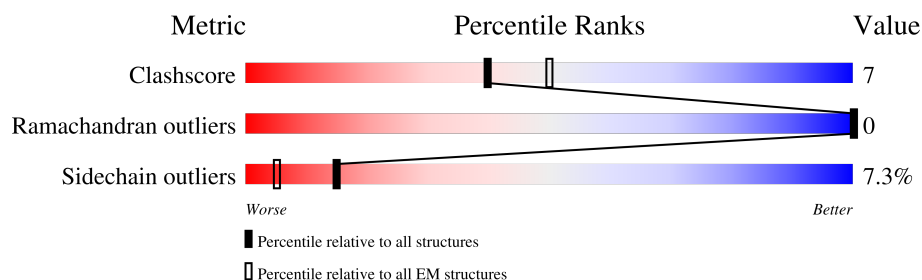
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13054 (2.40 - 3.40)

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	

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Mol	Chain	Length	Quality of chain
2	E	511	
2	F	511	
3	X	573	
3	Y	573	
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		

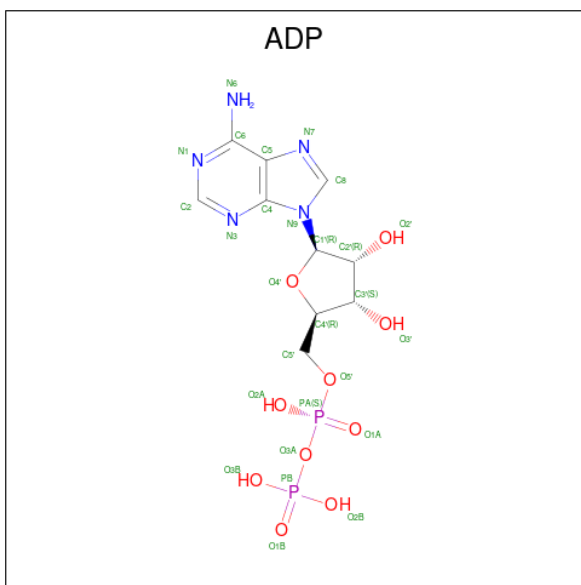
- Molecule 6 is a protein called V-type proton ATPase subunit D.

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 (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).

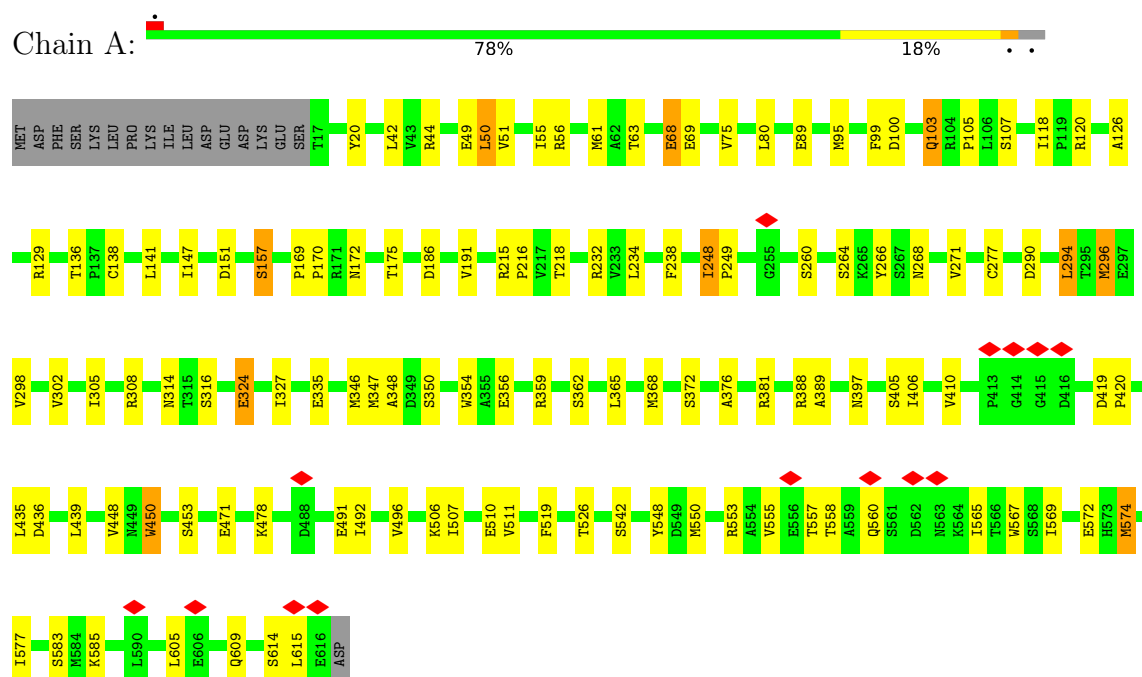


Mol	Chain	Residues	Atoms					AltConf
8	C	1	Total	C	N	O	P	0
			27	10	5	10	2	

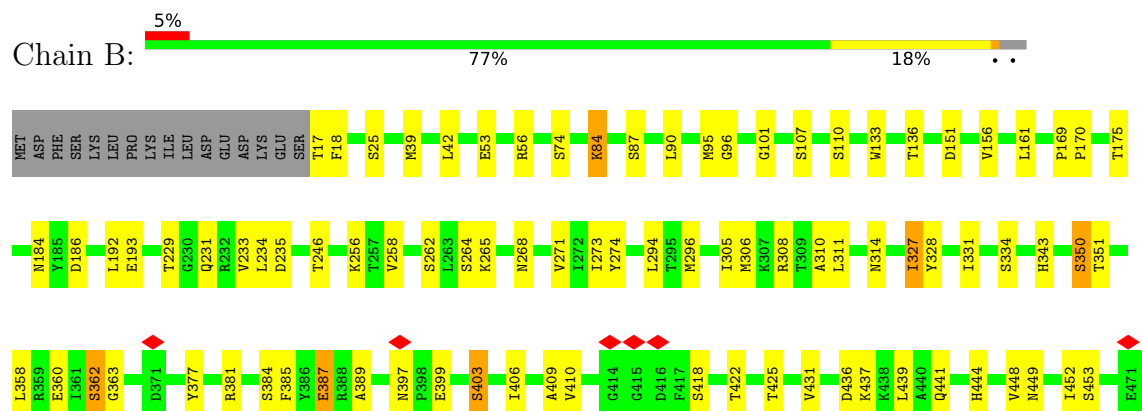
3 Residue-property plots [i](#)

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.

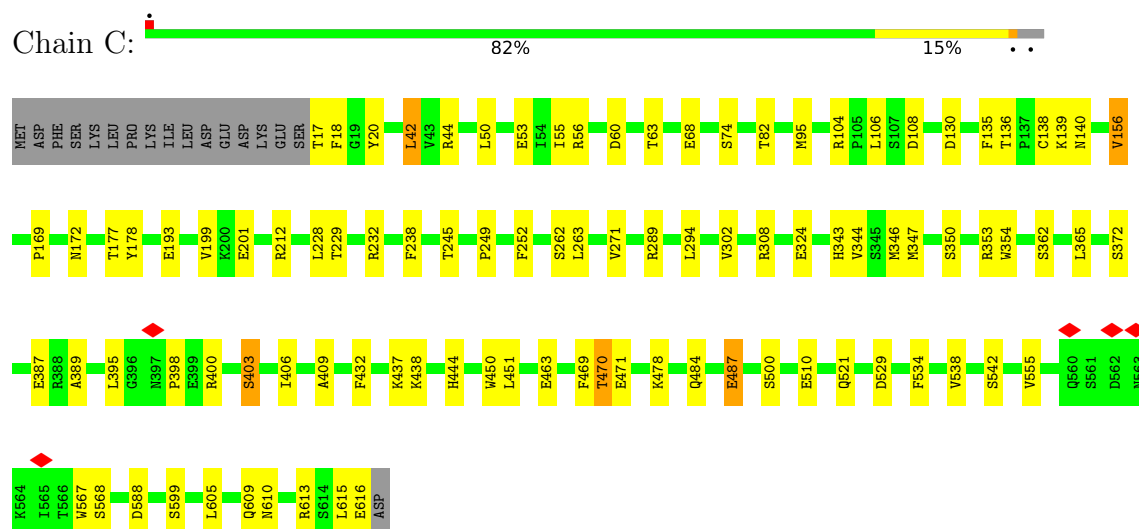
- Molecule 1: V-type proton ATPase catalytic subunit A



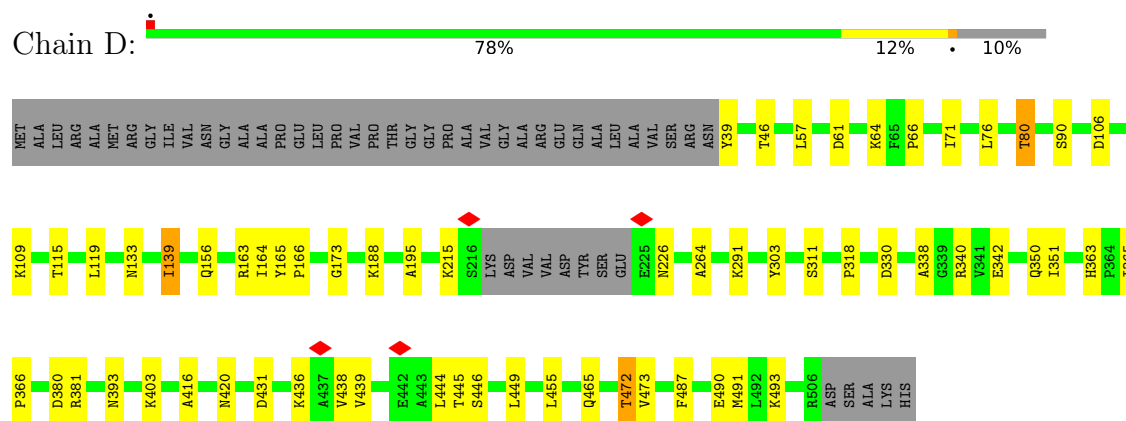
- Molecule 1: V-type proton ATPase catalytic subunit A



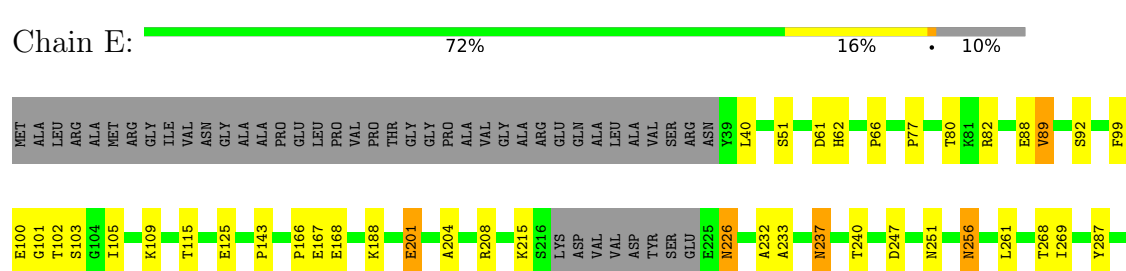
- Molecule 1: V-type proton ATPase catalytic subunit A

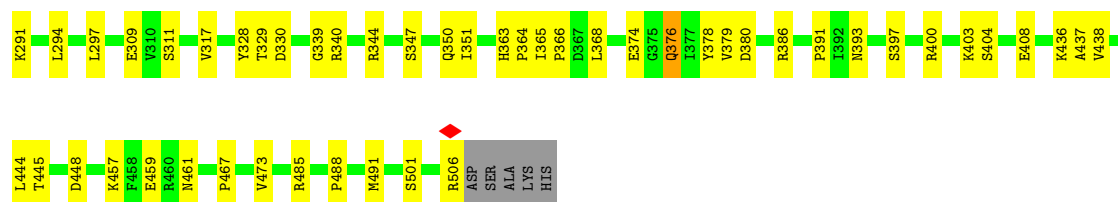


- Molecule 2: V-type proton ATPase subunit B, brain isoform



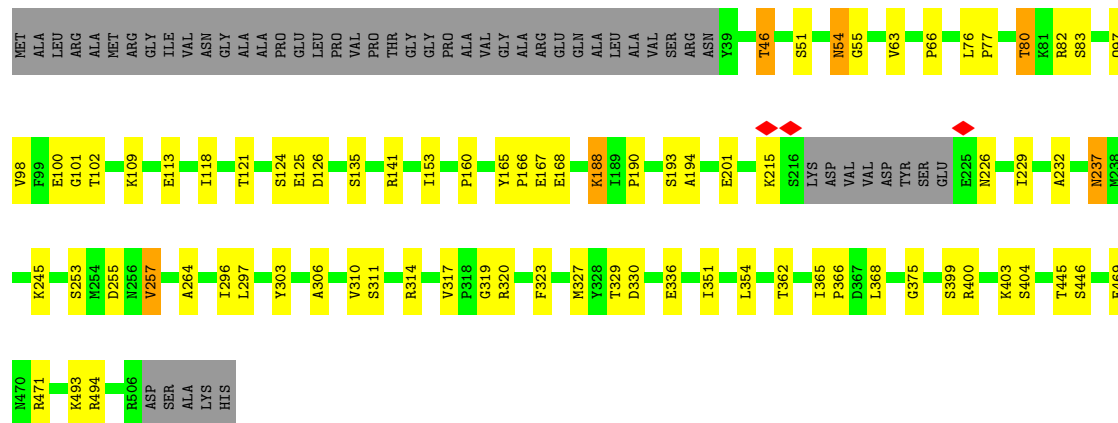
- Molecule 2: V-type proton ATPase subunit B, brain isoform





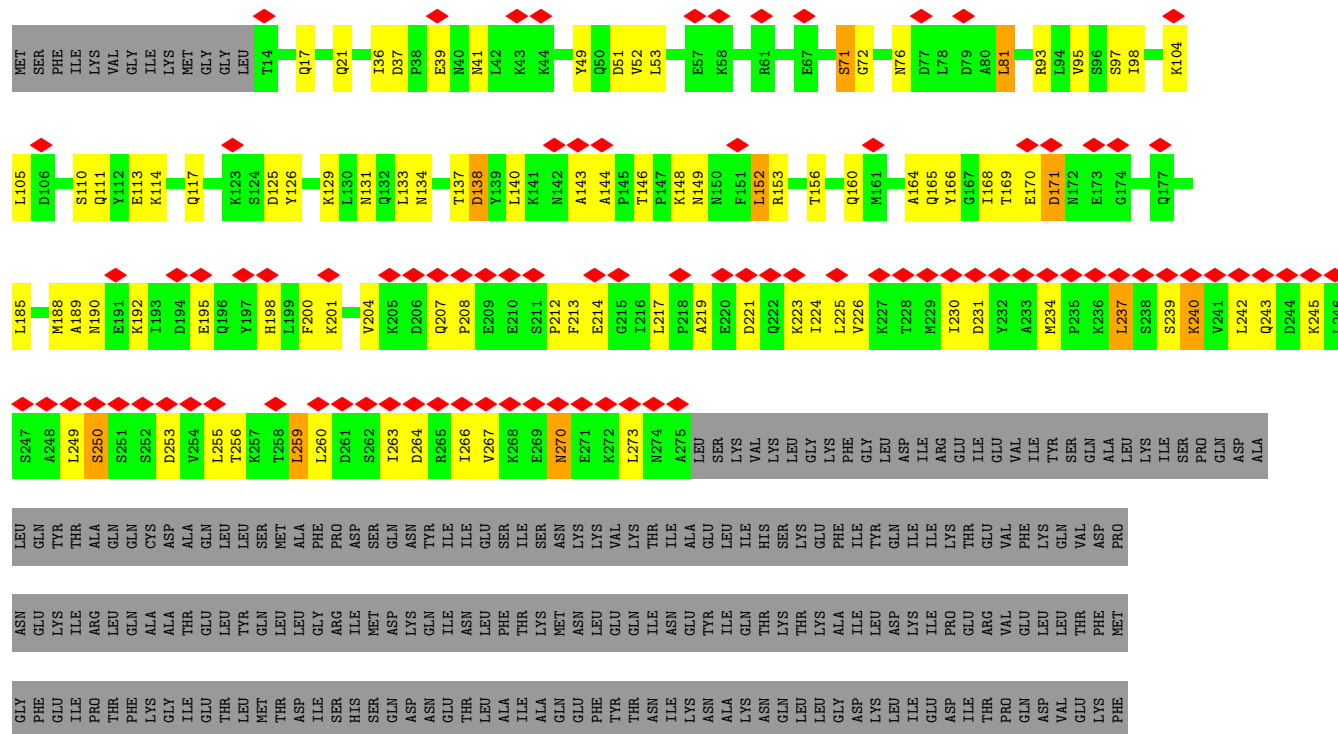
• Molecule 2: V-type proton ATPase subunit B, brain isoform

Chain F: 75% 14% 10%

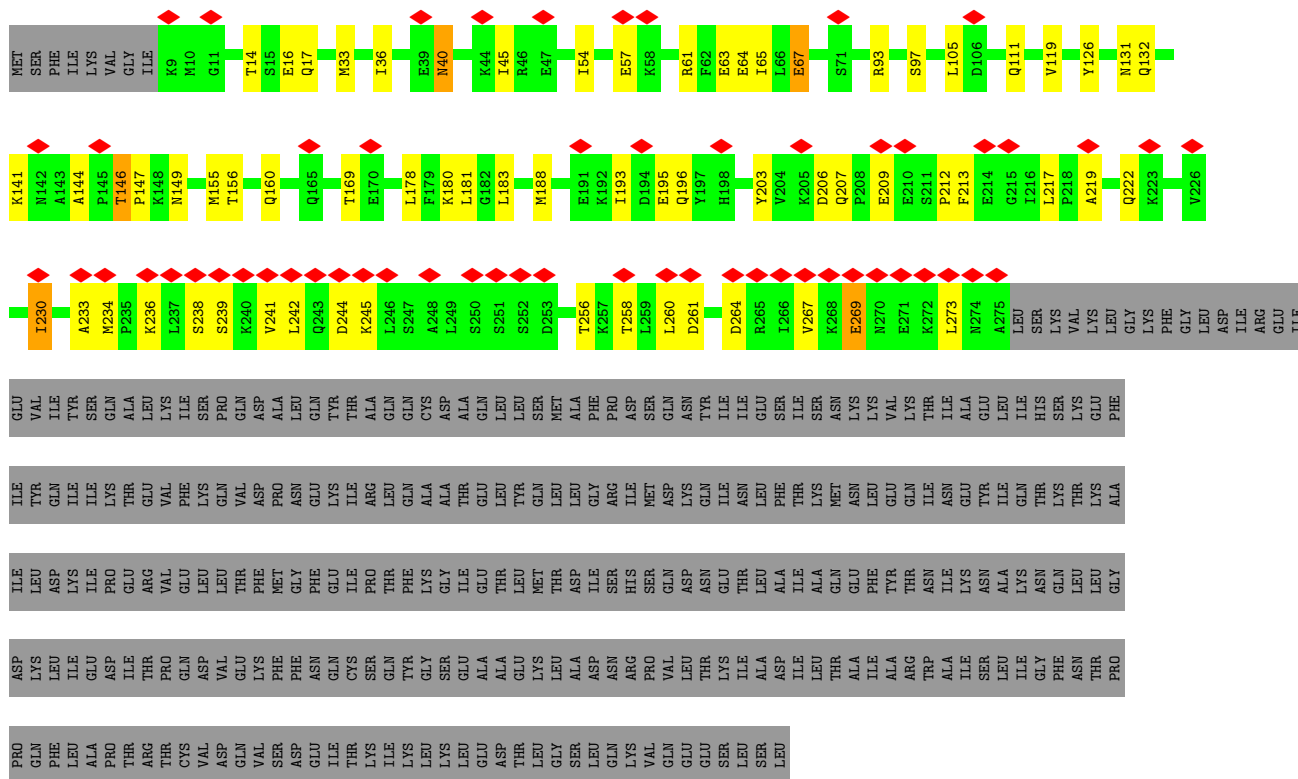
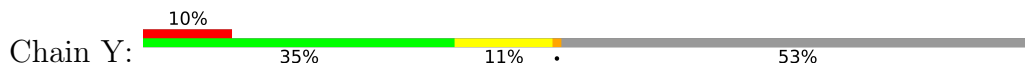


• Molecule 3: SidK

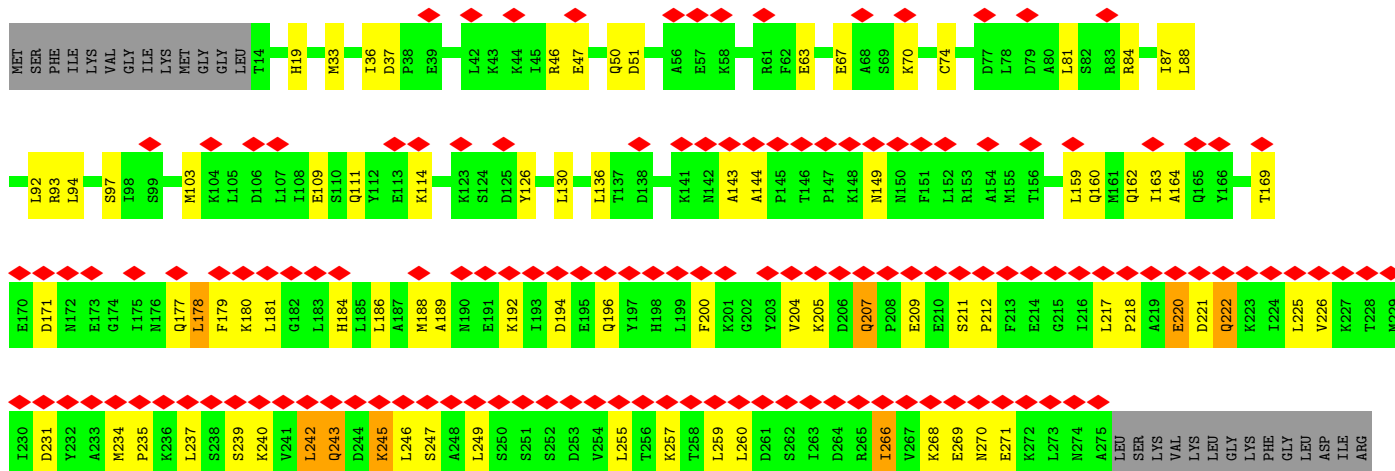
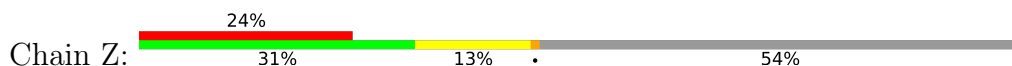
Chain X: 16% 29% 15% 54%



- Molecule 3: SidK

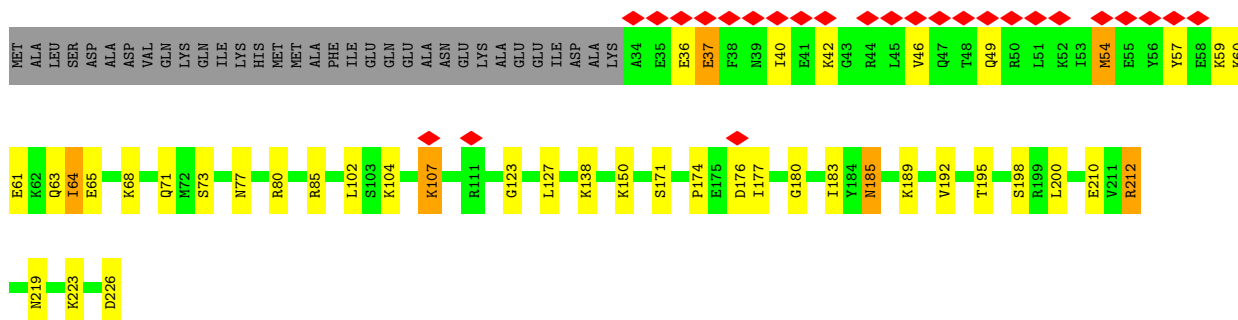


- Molecule 3: SidK

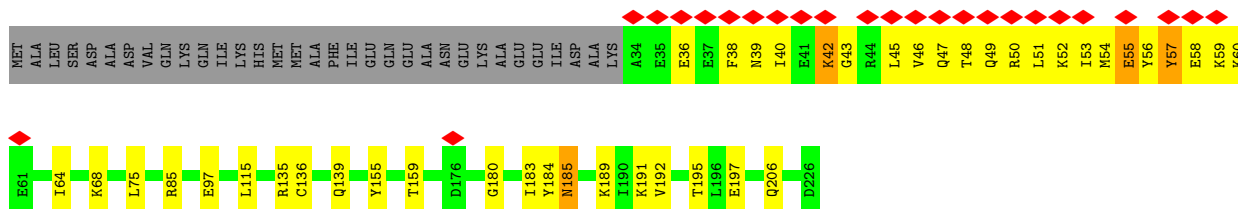




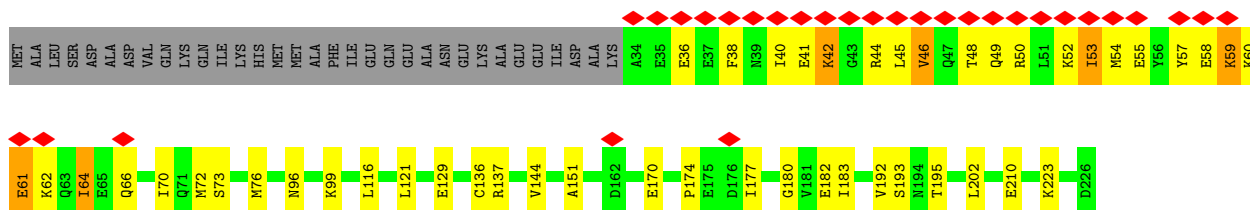
- Molecule 4: V-type proton ATPase subunit E 1



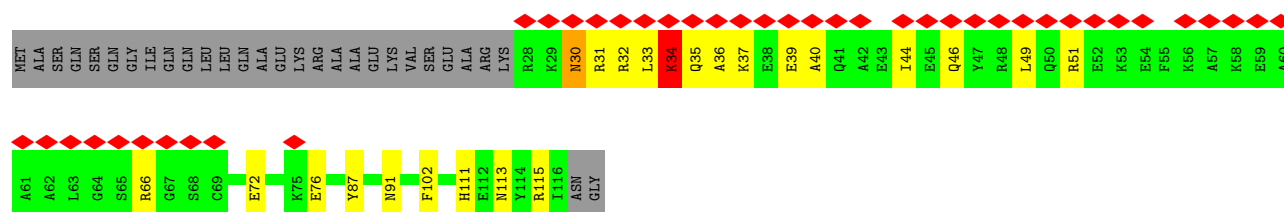
- Molecule 4: V-type proton ATPase subunit E 1



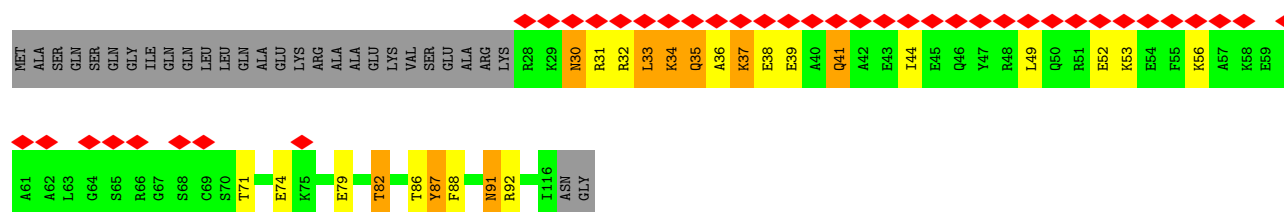
- Molecule 4: V-type proton ATPase subunit E 1



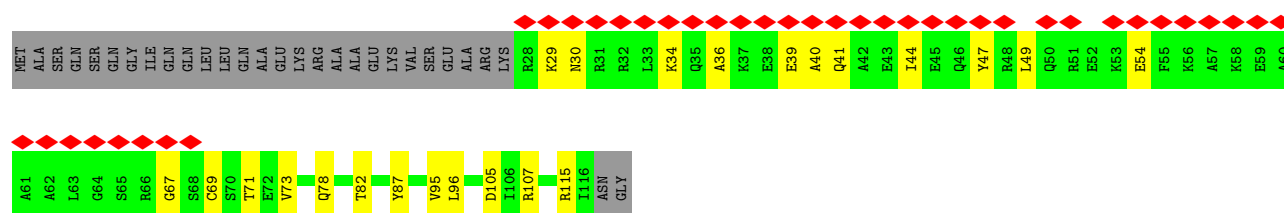
- Molecule 5: V-type proton ATPase subunit G 1



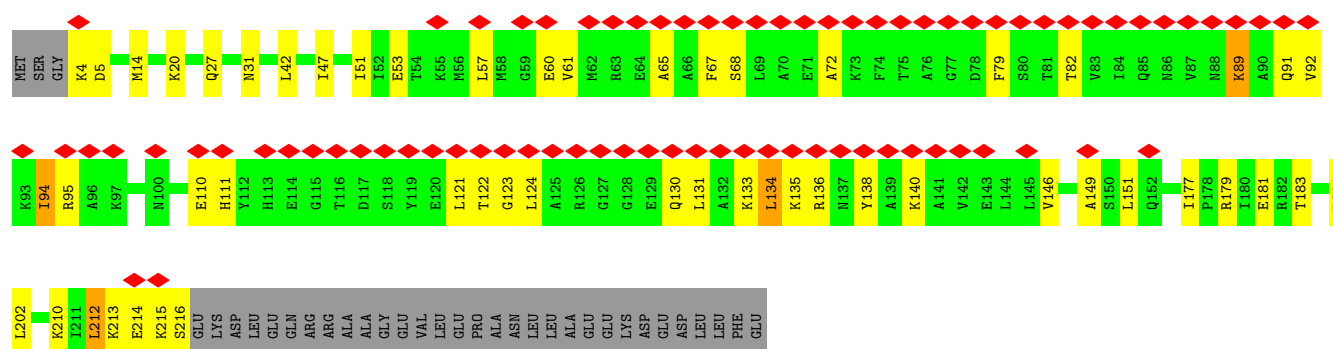
• Molecule 5: V-type proton ATPase subunit G 1



• 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 ($\text{\AA}$)	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 ($\text{\AA}$)	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	0.27	0/4748	0.36	0/6431
1	B	0.27	0/4752	0.40	0/6435
1	C	0.29	0/4752	0.38	0/6435
2	D	0.31	0/3671	0.39	0/4973
2	E	0.30	0/3660	0.38	0/4960
2	F	0.30	0/3667	0.38	0/4968
3	X	0.17	0/2143	0.38	0/2888
3	Y	0.18	0/2170	0.35	0/2926
3	Z	0.16	0/2138	0.38	0/2884
4	H	0.23	0/1585	0.36	0/2123
4	I	0.24	0/1585	0.43	0/2123
4	J	0.22	0/1585	0.36	0/2123
5	K	0.20	0/751	0.38	0/1001
5	L	0.22	0/751	0.53	0/1001
5	M	0.23	0/751	0.47	0/1001
6	G	0.21	0/1731	0.42	0/2316
7	N	0.16	0/889	0.44	0/1200
All	All	0.26	0/41329	0.39	0/55788

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.

There are no bond angle outliers.

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 ⓘ

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	51	0
1	B	4656	0	4642	65	0
1	C	4656	0	4642	46	0
2	D	3600	0	3605	29	0
2	E	3589	0	3590	49	0
2	F	3596	0	3601	38	0
3	X	2110	0	2132	59	0
3	Y	2136	0	2158	39	0
3	Z	2105	0	2127	44	0
4	H	1570	0	1640	39	0
4	I	1570	0	1640	31	0
4	J	1570	0	1640	29	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	582	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 (582) 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
1:C:95:MET:HE1	1:C:271:VAL:HG13	1.73	0.70
3:Z:47:GLU:HA	3:Z:50:GLN:HG2	1.74	0.70
1:A:95:MET:HE1	1:A:271:VAL:HG13	1.74	0.69
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
1:A:550:MET:HE1	1:A:609:GLN:HG2	1.78	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Z:111:GLN:NE2	3:Z:169:THR:OG1	2.29	0.63
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:D:39:TYR:OH	4:H:210:GLU:OE1	2.16	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
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:95:MET:HE3	1:A:308:ARG:HA	1.84	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:N:29:ASN:OD1	7:N:30:LYS:N	2.36	0.59
1:A:346:MET:HE2	1:A:348:ALA:HB2	1.84	0.59
3:X:171:ASP:OD1	3:X:171:ASP:N	2.32	0.59
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
2:F:188:LYS:NZ	2:F:336:GLU:OE2	2.37	0.57
1:C:372:SER:O	1:C:372:SER:OG	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
1:C:95:MET:HE3	1:C:308:ARG:HA	1.87	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:C:263:LEU:HD22	1:C:347:MET:HE1	1.87	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
3:Z:188:MET:HE3	3:Z:196:GLN:HG2	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:252:PHE:O	1:C:437:LYS:NZ	2.42	0.52
1:C:53:GLU:OE2	1:C:212:ARG:NH2	2.41	0.52
2:D:487:PHE:HD2	2:D:491:MET:HE3	1.73	0.52
1:B:95:MET:HE1	1:B:271:VAL:HG13	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
4:H:44:ARG:O	4:H:48:THR:OG1	2.25	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:96:GLY:HA2	1:B:306:MET:HE3	1.95	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
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
2:E:488:PRO:HD2	2:E:491:MET:HE3	1.94	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:33:MET:HE1	3:Y:45:ILE:HG22	1.95	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:B:583:SER:O	1:B:583:SER:OG	2.30	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:Y:238:SER:O	3:Y:238:SER:OG	2.29	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
2:F:327:MET:HE2	2:F:368:LEU:HD12	1.96	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
3:Z:220:GLU:CD	3:Z:220:GLU:H	2.22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:368:MET:HE2	2:E:317:VAL:HA	1.98	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
3:Z:160:GLN:O	3:Z:163:ILE:HG12	2.16	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
1:A:248:ILE:HD11	1:A:347:MET:HE1	1.99	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
2:D:226:ASN:OD1	2:D:226:ASN:N	2.50	0.45
2:E:237:ASN:C	2:E:237:ASN:HD22	2.25	0.45
1:C:108:ASP:OD1	1:C:108:ASP:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:562:ASP:H	1:B:564:LYS:HZ3	1.65	0.44
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
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:OD1	3:Y:40:ASN:N	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:39:MET:HE3	1:B:39:MET:HB3	1.92	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
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
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:J:54:MET:HE2	4:J:54:MET:HB3	1.73	0.42
4:H:62:LYS:HE3	4:H:62:LYS:HA	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:F:226:ASN:OD1	2:F:226:ASN:N	2.51	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
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
3:X:234:MET:HE3	3:X:234:MET:HB3	1.83	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:33:MET:HE2	3:Z:88:LEU:HD21	2.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:521:GLN:HE22	2:F:494:ARG:NH2	2.18	0.41
4:J:104:LYS:C	4:J:104:LYS:HD3	2.46	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
2:D:64:LYS:NZ	4:H:129:GLU:OE2	2.42	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
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
3:X:170:GLU:CD	3:X:170:GLU:H	2.28	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:155:MET:HE1	3:Y:181:LEU:HB3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:61:MET:HE3	1:A:61:MET:HB3	1.85	0.40
1:B:296:MET:HE3	1:B:296:MET:HB2	1.71	0.40
1:C:55:ILE:HD12	1:C:365:LEU:HD11	2.03	0.40
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: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
1:A:368:MET:HE1	6:G:202:LEU:HB3	2.03	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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 [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%)	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	458 (90%)	49 (10%)	8	25
1	B	508/525 (97%)	475 (94%)	33 (6%)	15	44
1	C	508/525 (97%)	476 (94%)	32 (6%)	16	45
2	D	393/430 (91%)	374 (95%)	19 (5%)	23	55
2	E	390/430 (91%)	368 (94%)	22 (6%)	19	50
2	F	392/430 (91%)	367 (94%)	25 (6%)	16	44
3	X	237/519 (46%)	219 (92%)	18 (8%)	12	36
3	Y	239/519 (46%)	223 (93%)	16 (7%)	15	43
3	Z	237/519 (46%)	213 (90%)	24 (10%)	7	24
4	H	172/199 (86%)	160 (93%)	12 (7%)	14	40
4	I	172/199 (86%)	160 (93%)	12 (7%)	14	40
4	J	172/199 (86%)	159 (92%)	13 (8%)	12	36
5	K	79/101 (78%)	77 (98%)	2 (2%)	42	74
5	L	79/101 (78%)	67 (85%)	12 (15%)	3	9
5	M	79/101 (78%)	72 (91%)	7 (9%)	9	28
6	G	183/212 (86%)	167 (91%)	16 (9%)	9	30
7	N	94/100 (94%)	84 (89%)	10 (11%)	6	22
All	All	4441/5634 (79%)	4119 (93%)	322 (7%)	15	38

All (322) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	LEU
1	A	50	LEU
1	A	51	VAL
1	A	68	GLU
1	A	69	GLU
1	A	80	LEU
1	A	103	GLN
1	A	107	SER
1	A	118	ILE
1	A	120	ARG
1	A	136	THR
1	A	147	ILE
1	A	157	SER
1	A	175	THR
1	A	191	VAL
1	A	218	THR
1	A	248	ILE
1	A	260	SER
1	A	266	TYR
1	A	268	ASN
1	A	294	LEU
1	A	296	MET
1	A	298	VAL
1	A	302	VAL
1	A	316	SER
1	A	324	GLU
1	A	327	ILE
1	A	350	SER
1	A	362	SER
1	A	381	ARG
1	A	405	SER
1	A	410	VAL
1	A	450	TRP
1	A	453	SER
1	A	471	GLU
1	A	478	LYS
1	A	491	GLU
1	A	506	LYS
1	A	526	THR
1	A	542	SER
1	A	558	THR
1	A	560	GLN

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Mol	Chain	Res	Type
1	A	572	GLU
1	A	574	MET
1	A	577	ILE
1	A	583	SER
1	A	585	LYS
1	A	614	SER
1	A	615	LEU
1	B	42	LEU
1	B	53	GLU
1	B	74	SER
1	B	84	LYS
1	B	87	SER
1	B	90	LEU
1	B	107	SER
1	B	110	SER
1	B	136	THR
1	B	156	VAL
1	B	161	LEU
1	B	175	THR
1	B	268	ASN
1	B	327	ILE
1	B	334	SER
1	B	350	SER
1	B	351	THR
1	B	358	LEU
1	B	362	SER
1	B	384	SER
1	B	387	GLU
1	B	403	SER
1	B	418	SER
1	B	436	ASP
1	B	453	SER
1	B	475	LEU
1	B	477	THR
1	B	478	LYS
1	B	491	GLU
1	B	495	LEU
1	B	556	GLU
1	B	558	THR
1	B	581	LEU
1	C	17	THR
1	C	18	PHE

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Mol	Chain	Res	Type
1	C	42	LEU
1	C	60	ASP
1	C	74	SER
1	C	104	ARG
1	C	130	ASP
1	C	136	THR
1	C	138	CYS
1	C	140	ASN
1	C	156	VAL
1	C	177	THR
1	C	199	VAL
1	C	201	GLU
1	C	228	LEU
1	C	245	THR
1	C	262	SER
1	C	294	LEU
1	C	302	VAL
1	C	346	MET
1	C	362	SER
1	C	395	LEU
1	C	403	SER
1	C	470	THR
1	C	471	GLU
1	C	478	LYS
1	C	487	GLU
1	C	542	SER
1	C	555	VAL
1	C	568	SER
1	C	588	ASP
1	C	599	SER
2	D	46	THR
2	D	57	LEU
2	D	61	ASP
2	D	80	THR
2	D	90	SER
2	D	115	THR
2	D	139	ILE
2	D	156	GLN
2	D	188	LYS
2	D	215	LYS
2	D	311	SER
2	D	340	ARG

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Mol	Chain	Res	Type
2	D	350	GLN
2	D	351	ILE
2	D	403	LYS
2	D	431	ASP
2	D	449	LEU
2	D	455	LEU
2	D	472	THR
2	E	51	SER
2	E	80	THR
2	E	89	VAL
2	E	92	SER
2	E	103	SER
2	E	115	THR
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	376	GLN
2	E	404	SER
2	E	408	GLU
2	E	445	THR
2	E	448	ASP
2	E	473	VAL
2	E	501	SER
2	F	46	THR
2	F	51	SER
2	F	54	ASN
2	F	80	THR
2	F	83	SER
2	F	97	GLN
2	F	98	VAL
2	F	118	ILE
2	F	135	SER
2	F	168	GLU
2	F	188	LYS
2	F	201	GLU
2	F	237	ASN

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Mol	Chain	Res	Type
2	F	239	GLU
2	F	257	VAL
2	F	296	ILE
2	F	311	SER
2	F	314	ARG
2	F	317	VAL
2	F	329	THR
2	F	351	ILE
2	F	354	LEU
2	F	399	SER
2	F	403	LYS
2	F	404	SER
3	X	51	ASP
3	X	71	SER
3	X	81	LEU
3	X	104	LYS
3	X	126	TYR
3	X	138	ASP
3	X	146	THR
3	X	152	LEU
3	X	171	ASP
3	X	190	ASN
3	X	214	GLU
3	X	224	ILE
3	X	231	ASP
3	X	237	LEU
3	X	240	LYS
3	X	250	SER
3	X	259	LEU
3	X	270	ASN
3	Y	14	THR
3	Y	16	GLU
3	Y	17	GLN
3	Y	36	ILE
3	Y	40	ASN
3	Y	67	GLU
3	Y	105	LEU
3	Y	119	VAL
3	Y	126	TYR
3	Y	146	THR
3	Y	188	MET
3	Y	230	ILE

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Mol	Chain	Res	Type
3	Y	234	MET
3	Y	241	VAL
3	Y	244	ASP
3	Y	269	GLU
3	Z	67	GLU
3	Z	74	CYS
3	Z	81	LEU
3	Z	87	ILE
3	Z	109	GLU
3	Z	126	TYR
3	Z	162	GLN
3	Z	178	LEU
3	Z	179	PHE
3	Z	184	HIS
3	Z	207	GLN
3	Z	217	LEU
3	Z	220	GLU
3	Z	222	GLN
3	Z	231	ASP
3	Z	242	LEU
3	Z	243	GLN
3	Z	245	LYS
3	Z	246	LEU
3	Z	247	SER
3	Z	249	LEU
3	Z	259	LEU
3	Z	266	ILE
3	Z	269	GLU
4	J	37	GLU
4	J	54	MET
4	J	64	ILE
4	J	73	SER
4	J	107	LYS
4	J	138	LYS
4	J	171	SER
4	J	176	ASP
4	J	185	ASN
4	J	192	VAL
4	J	198	SER
4	J	212	ARG
4	J	226	ASP
5	M	30	ASN

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Mol	Chain	Res	Type
5	M	34	LYS
5	M	72	GLU
5	M	76	GLU
5	M	87	TYR
5	M	91	ASN
5	M	102	PHE
6	G	14	MET
6	G	20	LYS
6	G	42	LEU
6	G	51	ILE
6	G	61	VAL
6	G	67	PHE
6	G	79	PHE
6	G	82	THR
6	G	89	LYS
6	G	94	ILE
6	G	122	THR
6	G	124	LEU
6	G	134	LEU
6	G	146	VAL
6	G	151	LEU
6	G	212	LEU
4	I	42	LYS
4	I	55	GLU
4	I	57	TYR
4	I	68	LYS
4	I	75	LEU
4	I	115	LEU
4	I	136	CYS
4	I	139	GLN
4	I	183	ILE
4	I	185	ASN
4	I	192	VAL
4	I	197	GLU
5	L	33	LEU
5	L	34	LYS
5	L	35	GLN
5	L	37	LYS
5	L	38	GLU
5	L	41	GLN
5	L	52	GLU
5	L	71	THR

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Mol	Chain	Res	Type
5	L	79	GLU
5	L	82	THR
5	L	87	TYR
5	L	91	ASN
4	H	42	LYS
4	H	46	VAL
4	H	53	ILE
4	H	55	GLU
4	H	59	LYS
4	H	61	GLU
4	H	64	ILE
4	H	73	SER
4	H	170	GLU
4	H	183	ILE
4	H	192	VAL
4	H	202	LEU
5	K	87	TYR
5	K	95	VAL
7	N	8	ILE
7	N	16	THR
7	N	25	ILE
7	N	37	LEU
7	N	45	ILE
7	N	46	ASN
7	N	66	ILE
7	N	74	VAL
7	N	102	LYS
7	N	105	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (94) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	172	ASN
1	A	213	GLN
1	A	261	GLN
1	A	430	GLN
1	A	441	GLN
1	A	444	HIS
1	A	603	GLN
1	B	65	GLN
1	B	172	ASN
1	B	231	GLN

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Mol	Chain	Res	Type
1	B	261	GLN
1	B	314	ASN
1	B	430	GLN
1	B	444	HIS
1	B	560	GLN
1	C	140	ASN
1	C	164	HIS
1	C	172	ASN
1	C	231	GLN
1	C	261	GLN
1	C	441	GLN
1	C	563	ASN
2	D	42	GLN
2	D	54	ASN
2	D	97	GLN
2	D	156	GLN
2	D	171	GLN
2	D	350	GLN
2	E	54	ASN
2	E	156	GLN
2	E	205	GLN
2	E	209	GLN
2	E	226	ASN
2	E	237	ASN
2	E	256	ASN
2	E	265	ASN
2	E	350	GLN
2	E	363	HIS
2	E	382	GLN
2	E	470	ASN
2	F	54	ASN
2	F	73	HIS
2	F	85	GLN
2	F	97	GLN
2	F	237	ASN
2	F	288	GLN
2	F	350	GLN
3	X	40	ASN
3	X	149	ASN
3	X	150	ASN
3	X	222	GLN
3	Y	196	GLN

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Mol	Chain	Res	Type
3	Y	207	GLN
3	Y	270	ASN
3	Z	177	GLN
3	Z	207	GLN
3	Z	222	GLN
4	J	47	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	206	GLN
4	I	39	ASN
4	I	71	GLN
4	I	77	ASN
4	I	126	GLN
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	39	ASN
4	H	100	GLN
4	H	126	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	76	HIS
7	N	82	GLN
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 oligosaccharides 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	-	28,29,29	1.38	5 (17%)	43,45,45	1.80	9 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	ADP	C	701	-	-	3/16/32/32	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	701	ADP	C5-C4	4.30	1.46	1.39
8	C	701	ADP	C5-N7	-2.54	1.34	1.39
8	C	701	ADP	C5-C6	2.48	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	701	ADP	C8-N7	2.18	1.35	1.31
8	C	701	ADP	C4-N9	-2.12	1.33	1.37

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	701	ADP	C5-C4-N3	-5.81	118.72	126.72
8	C	701	ADP	N3-C4-N9	4.47	134.76	127.17
8	C	701	ADP	C2-N3-C4	3.65	120.74	111.83
8	C	701	ADP	C4-C5-N7	-3.39	106.70	110.58
8	C	701	ADP	N3-C2-N1	-3.10	123.89	128.58
8	C	701	ADP	C4-N9-C8	2.40	108.25	105.74
8	C	701	ADP	C5-N7-C8	2.36	107.16	103.45
8	C	701	ADP	C3'-C2'-C1'	2.33	105.87	101.46
8	C	701	ADP	C6-C5-N7	2.01	135.97	132.09

There are no chirality outliers.

All (3) torsion outliers are listed below:

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

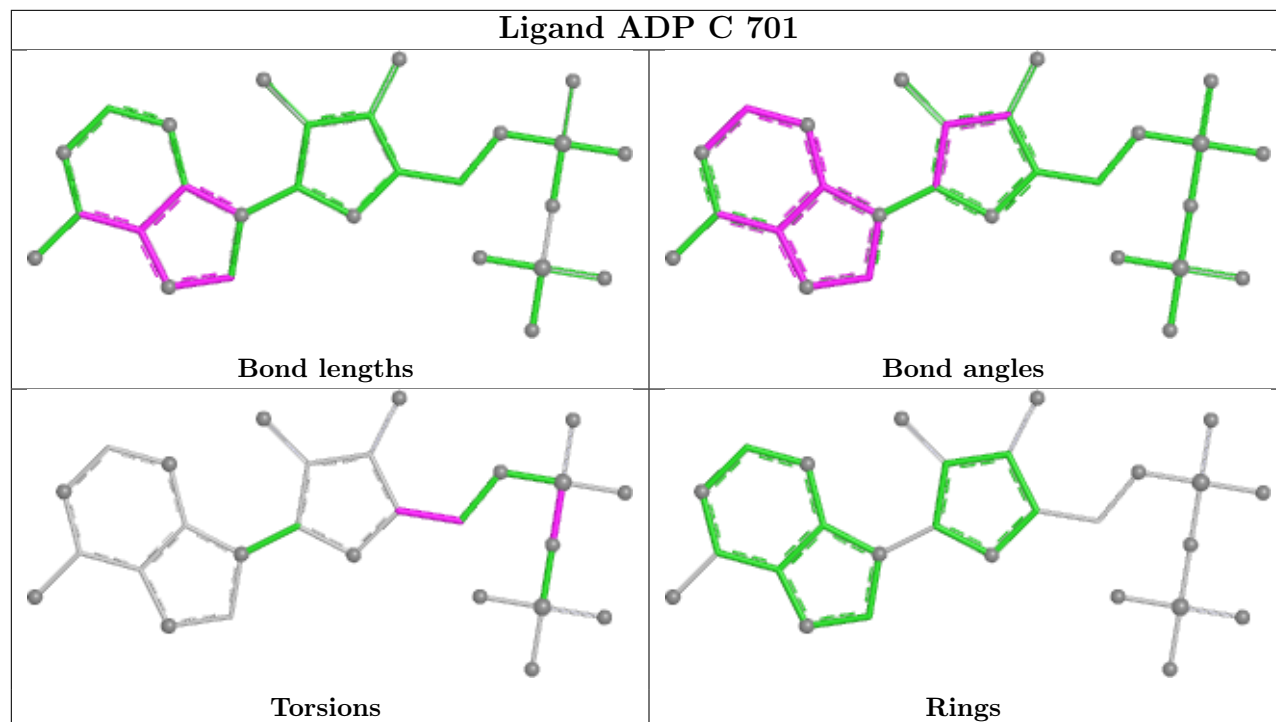
There are no ring outliers.

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.

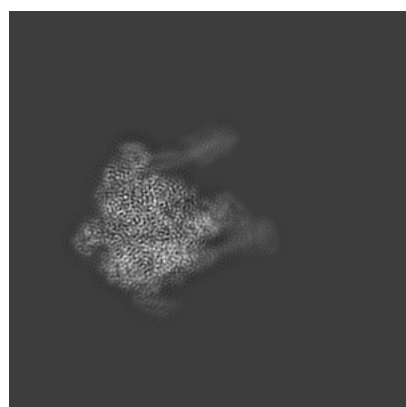
6 Map visualisation [i](#)

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.

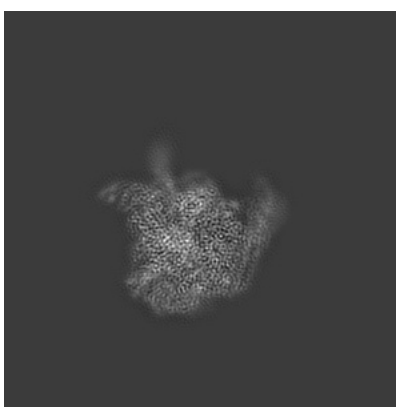
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X



Y

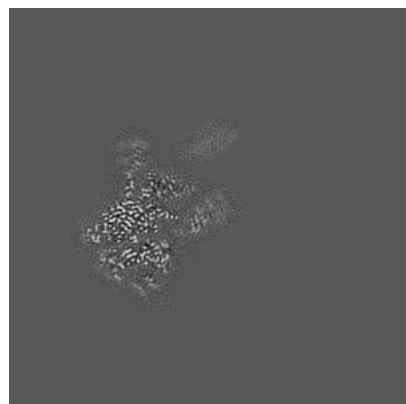


Z

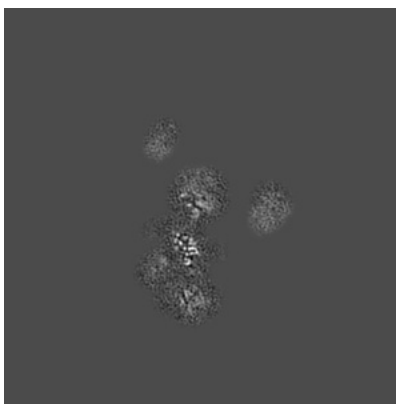
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

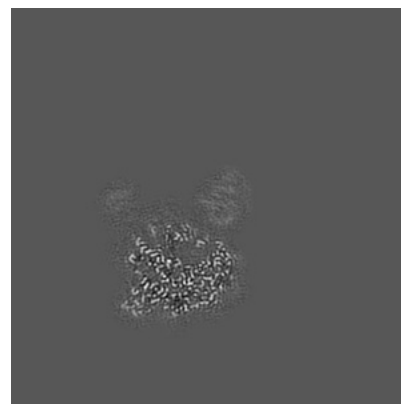
6.2.1 Primary map



X Index: 180



Y Index: 180

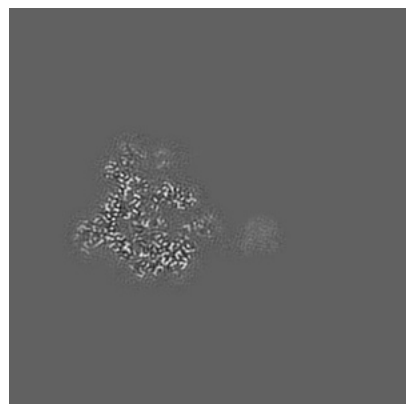


Z Index: 180

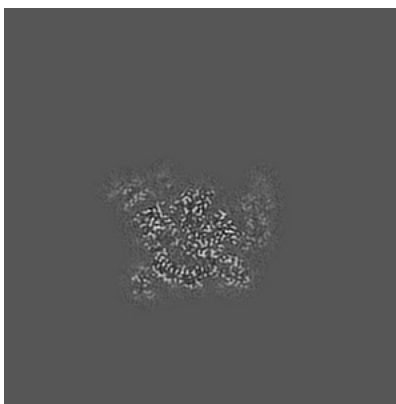
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

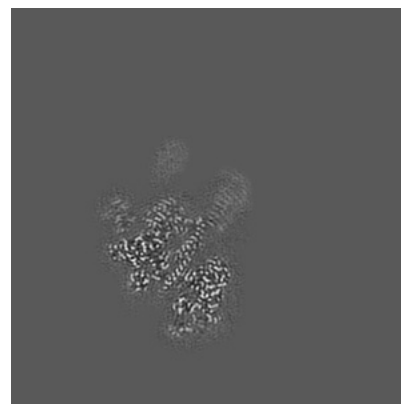
6.3.1 Primary map



X Index: 149



Y Index: 114

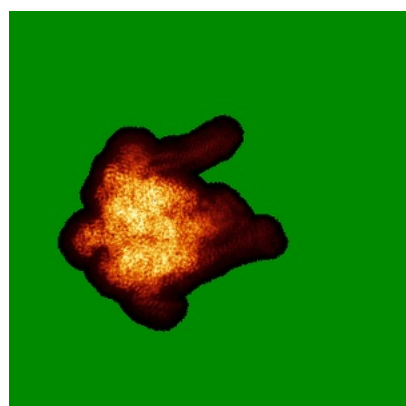


Z Index: 164

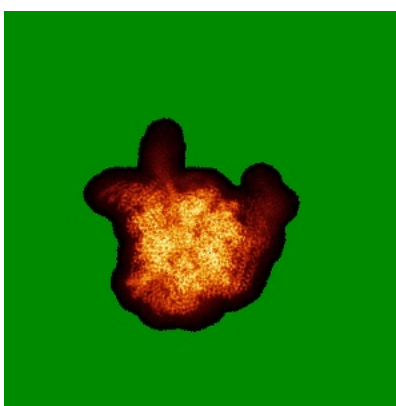
The images above show the largest variance slices of the map in three orthogonal directions.

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

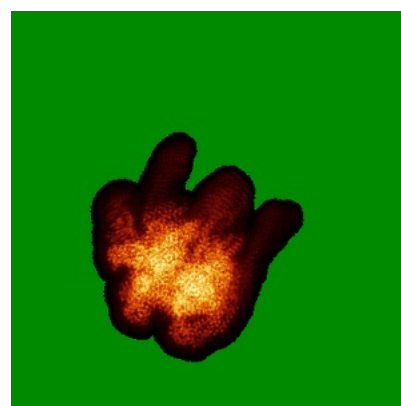
6.4.1 Primary map



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 0.6. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

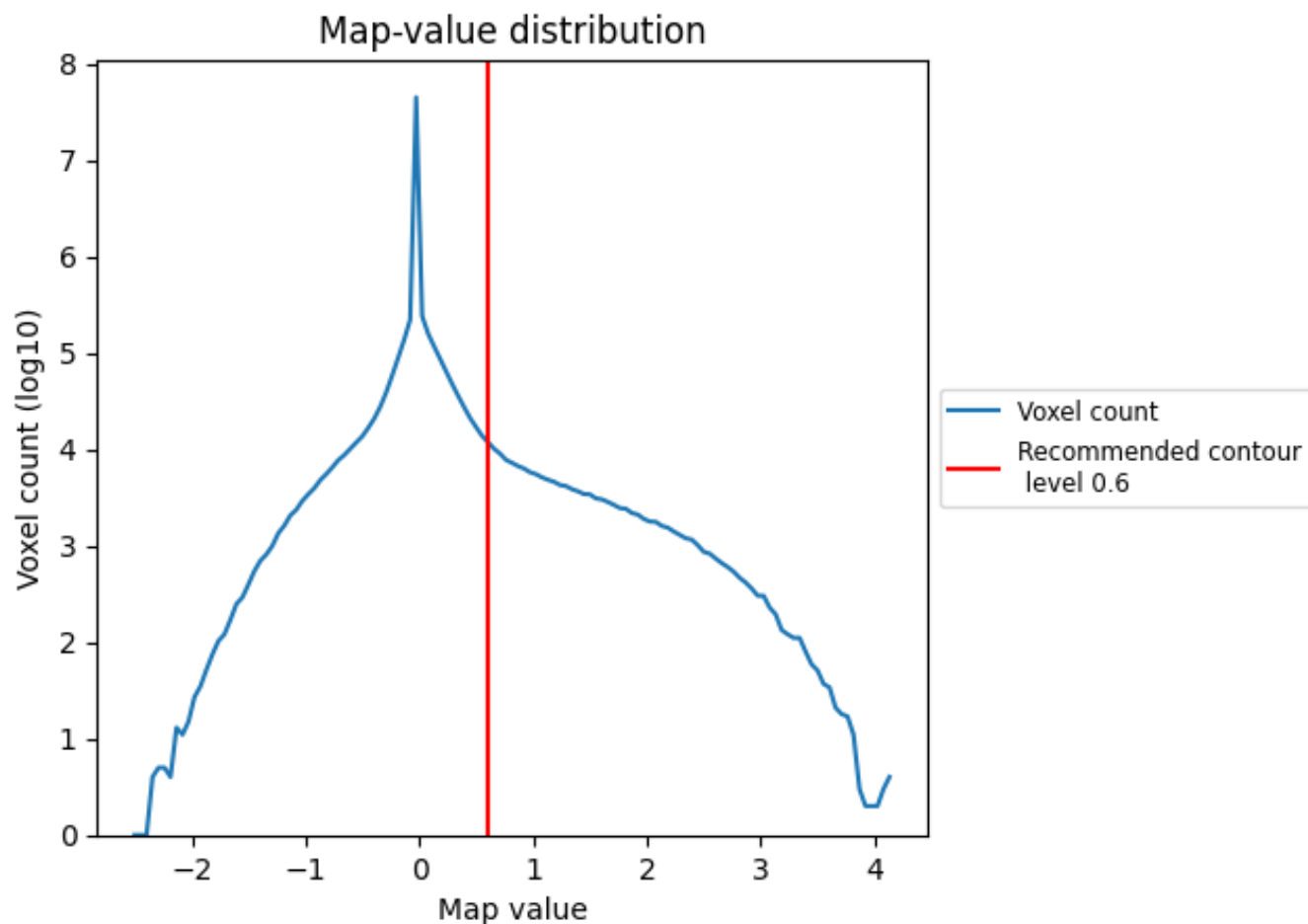
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

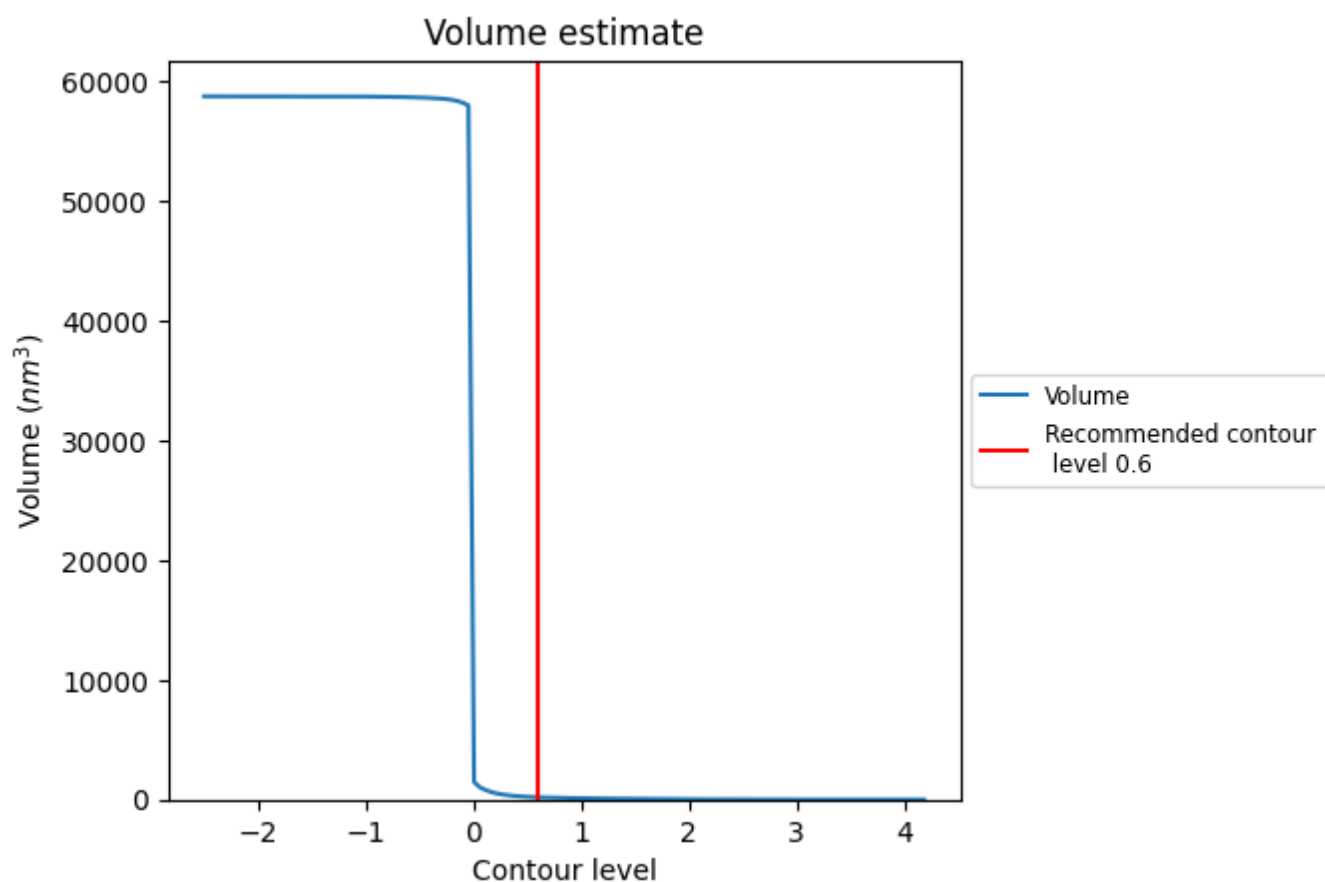
This section contains the results of statistical analysis of the map.

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.

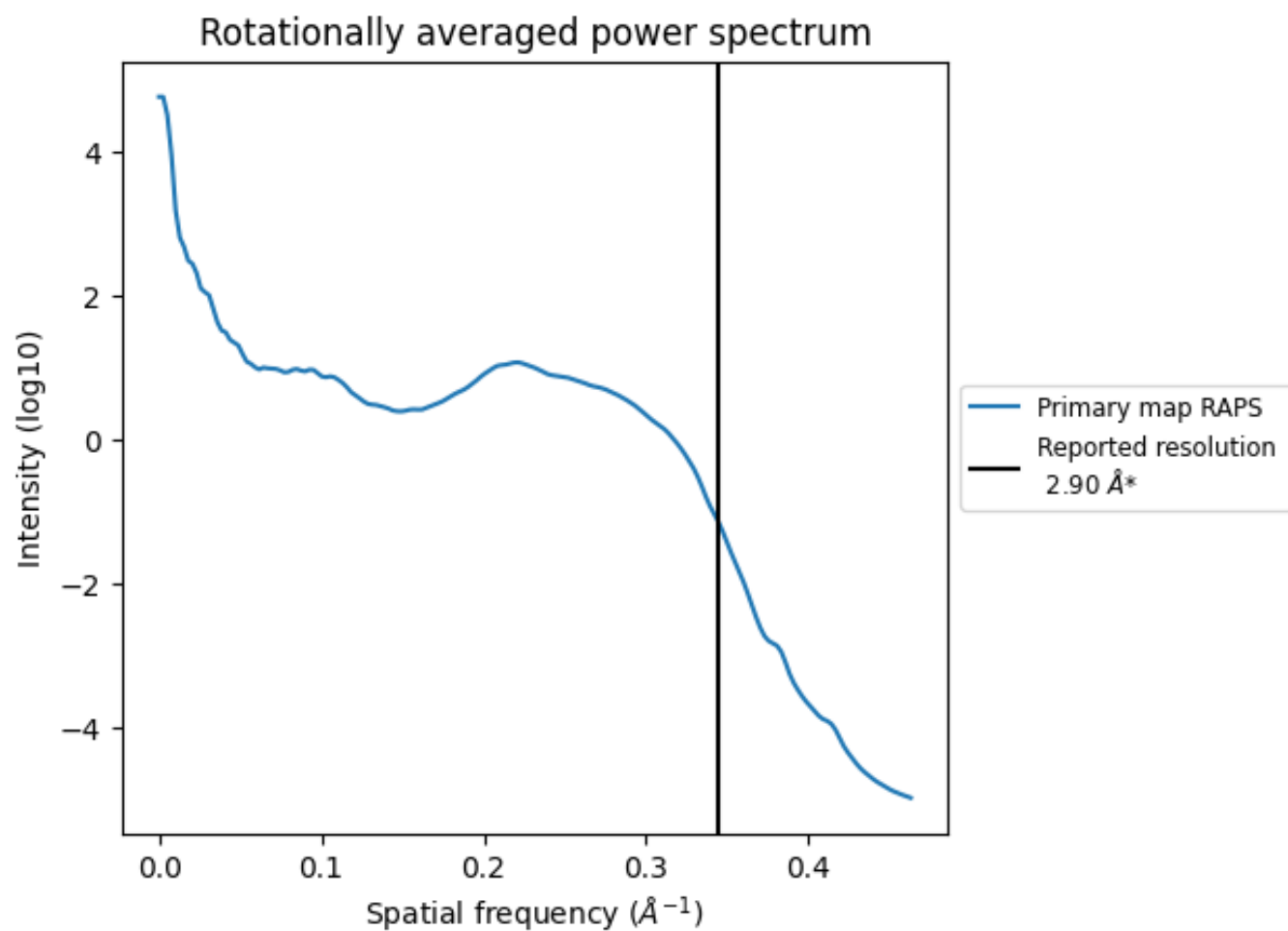
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 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.

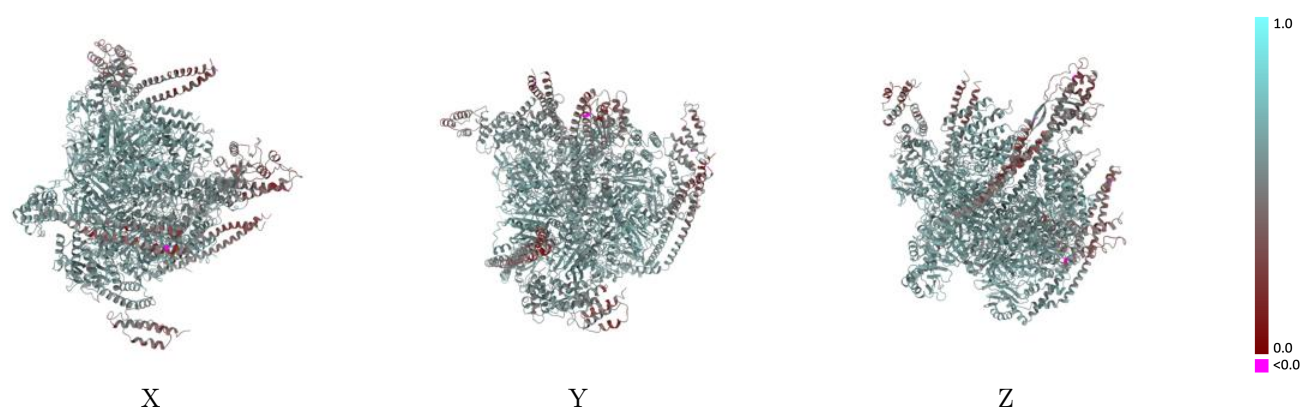
9 Map-model fit [i](#)

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](#)

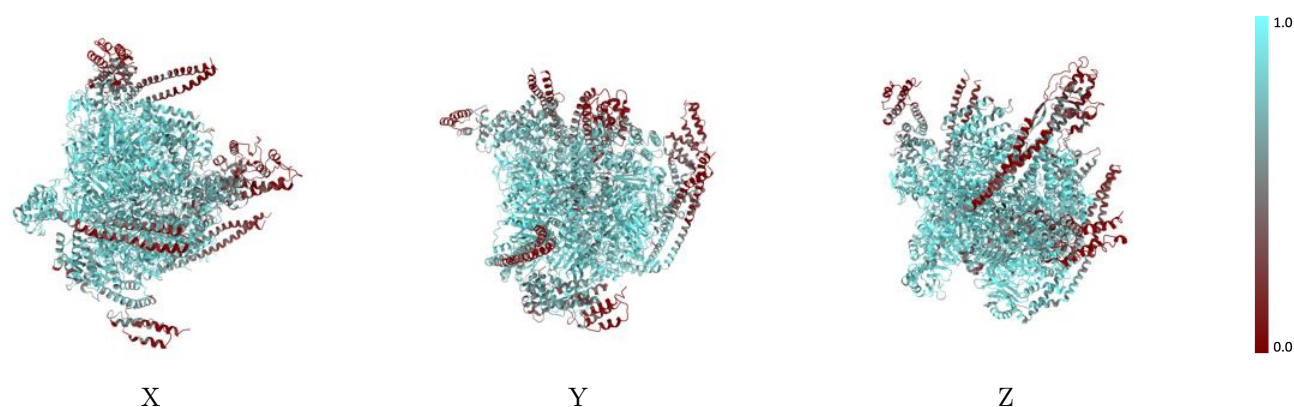
This section was not generated.

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



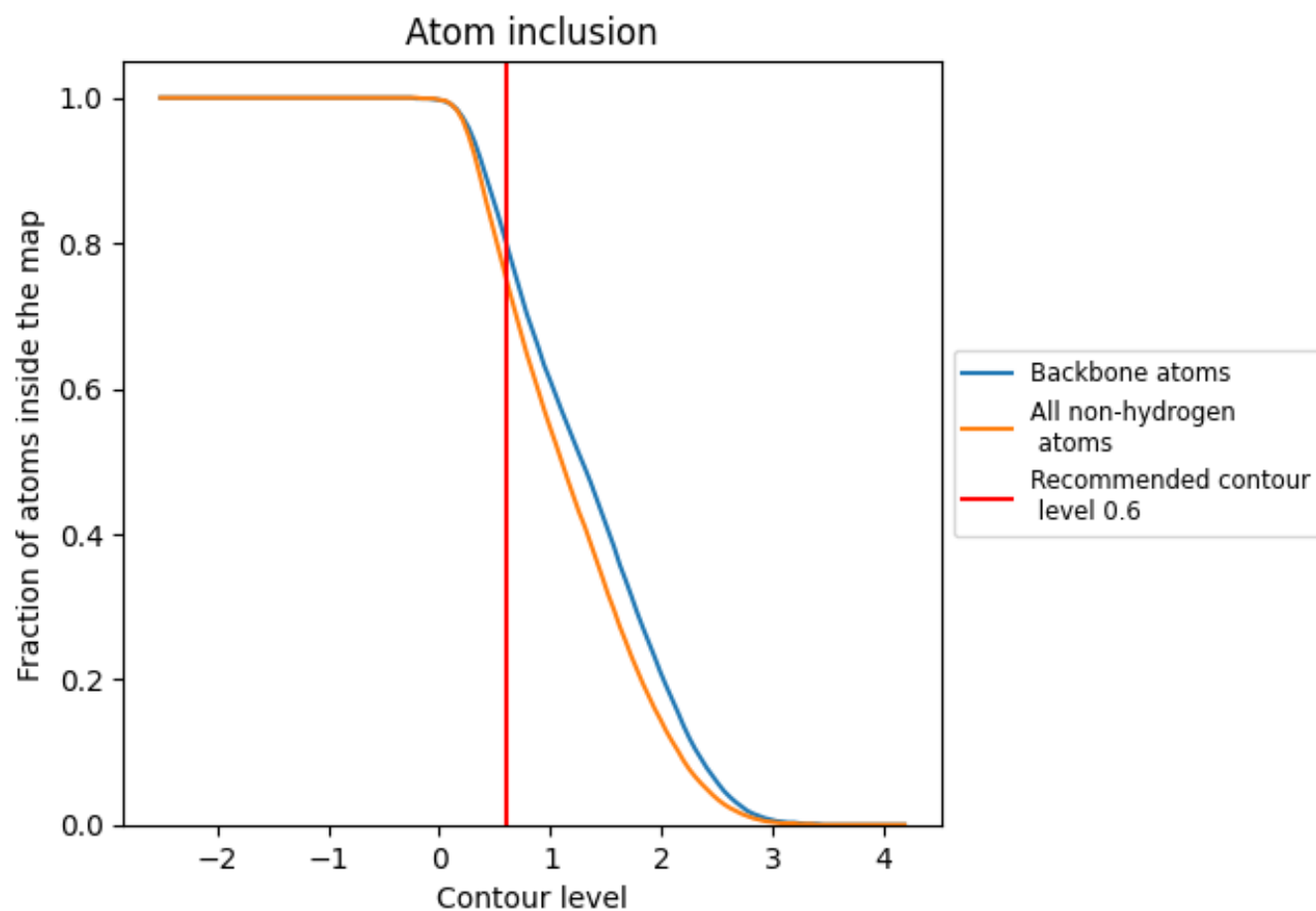
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	0.8560	0.6060
B	0.8370	0.5940
C	0.8950	0.6150
D	0.9060	0.6230
E	0.9150	0.6200
F	0.9100	0.6260
G	0.5420	0.5010
H	0.7090	0.5550
I	0.7090	0.5410
J	0.7210	0.5630
K	0.4850	0.4800
L	0.4590	0.4590
M	0.4610	0.4630
N	0.2400	0.4330
X	0.5030	0.5040
Y	0.5920	0.5280
Z	0.3880	0.4980

1.0

0.0

<0.0