



Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 03:07 PM JST

PDB ID : 7C4J
EMDB ID : EMD-30285
Title : Cryo-EM structure of the yeast Swi/Snf complex in a nucleosome free state
Authors : Wang, C.C.; Guo, Z.Y.; Zhan, X.C.; Zhang, X.F.
Deposited on : 2020-05-18
Resolution : 2.89 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
MolProbity : 4.02b-467
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) : 2.31.3

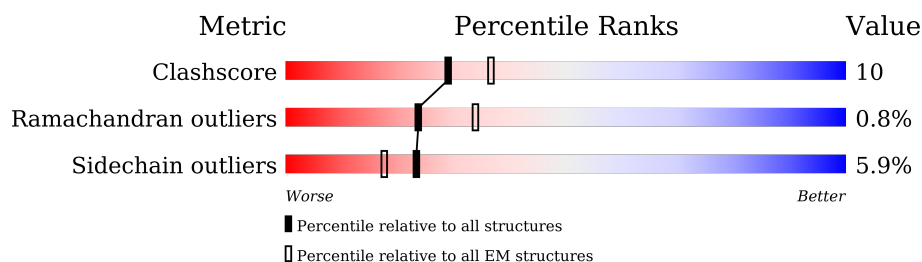
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.89 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	566	
2	B	825	
2	D	825	
3	C	332	
4	E	623	
5	F	905	
6	H	1703	
7	I	1314	

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Mol	Chain	Length	Quality of chain
8	G	82	<div><div><div></div><div></div><div></div></div><div>46%10%43%</div></div>
9	J	157	<div><div><div></div><div></div><div></div></div><div>34%20%13%66%</div></div>
10	K	477	<div><div><div></div><div></div><div></div></div><div>81%55%23%19%</div></div>
11	L	467	<div><div><div></div><div></div><div></div></div><div>84%61%21%16%</div></div>

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 29757 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 Transcription regulatory protein SNF12.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	374	Total	C	N	O	S	0	0
			3048	1928	529	581	10		

- Molecule 2 is a protein called SWI/SNF complex subunit SWI3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	395	Total	C	N	O	S	0	0
			3250	2082	560	597	11		
2	D	421	Total	C	N	O	S	0	0
			3445	2203	592	638	12		

- Molecule 3 is a protein called Transcription regulatory protein SNF6.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	154	Total	C	N	O	S	0	0
			1266	793	232	236	5		

- Molecule 4 is a protein called SWI/SNF global transcription activator complex subunit SWP82.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	288	Total	C	N	O	S	0	0
			2355	1529	412	411	3		

- Molecule 5 is a protein called SWI/SNF chromatin-remodeling complex subunit SNF5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	383	Total	C	N	O	S	0	0
			3134	1977	529	618	10		

- Molecule 6 is a protein called Transcription regulatory protein SNF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	242	Total	C	N	O	S	0	0
			1966	1233	354	373	6		

- Molecule 7 is a protein called SWI/SNF chromatin-remodeling complex subunit SWI1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	524	Total	C	N	O	S	0	0
			4242	2754	703	774	11		

- Molecule 8 is a protein called Unkown.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	G	47	Total	C	N	O	0	0
			271	166	56	49		

- Molecule 9 is a protein called Regulator of Ty1 transposition protein 102.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	J	53	Total	C	N	O	0	0
			482	308	83	91		

- Molecule 10 is a protein called Actin-related protein 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	387	Total	C	N	O	S	3	0
			3131	2020	516	591	4		

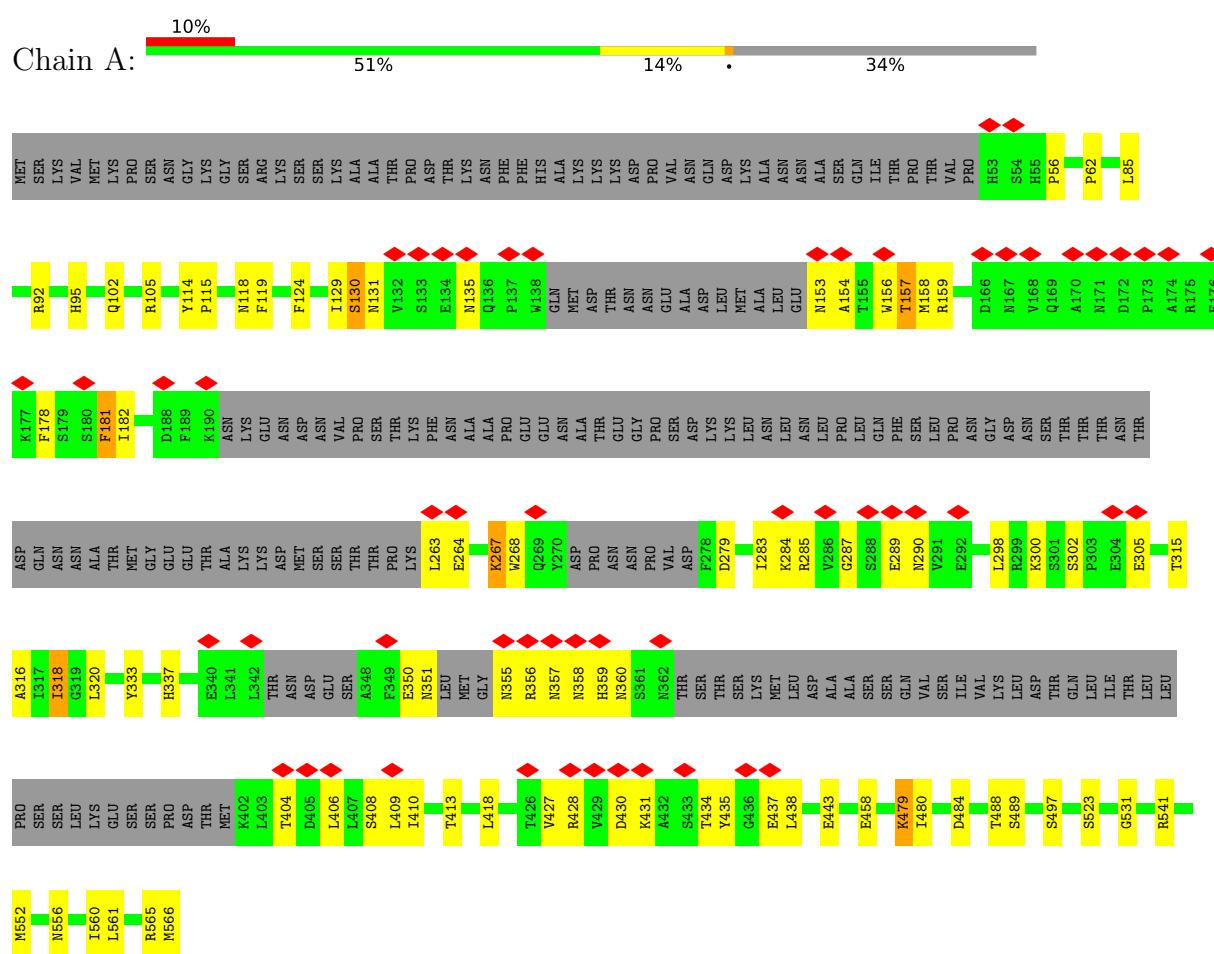
- Molecule 11 is a protein called Actin-like protein ARP9.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	392	Total	C	N	O	S	1	0
			3167	2033	519	611	4		

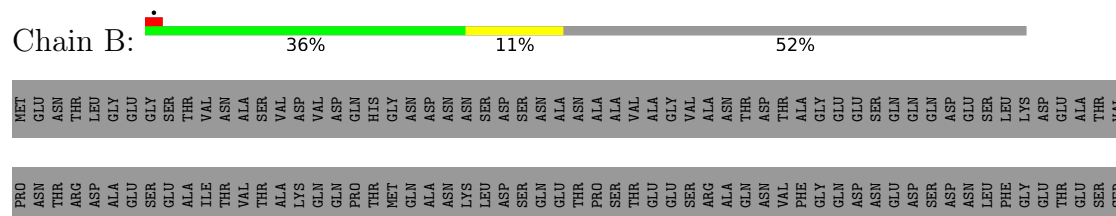
3 Residue-property plots

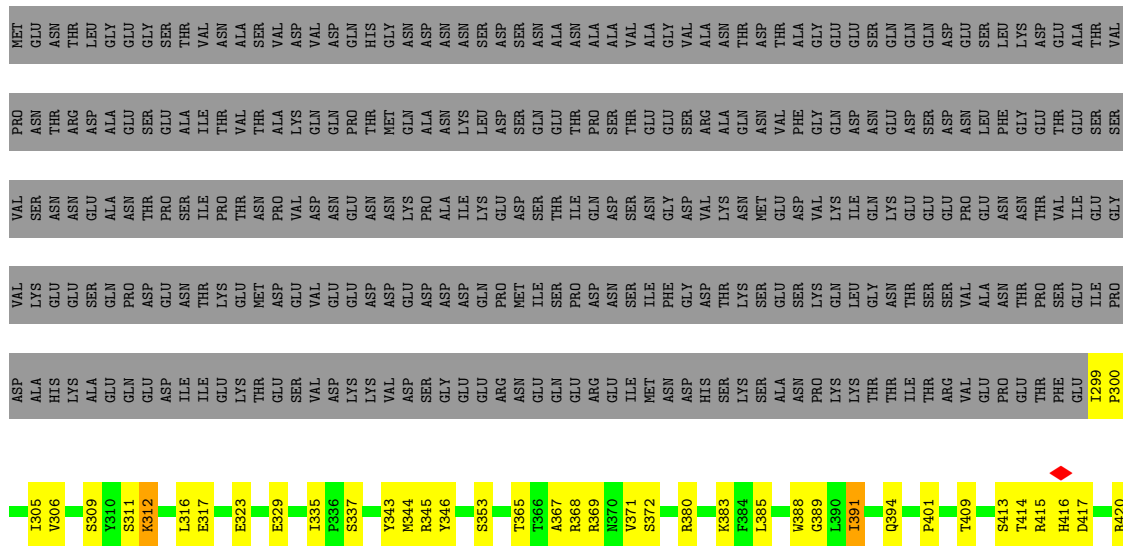
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

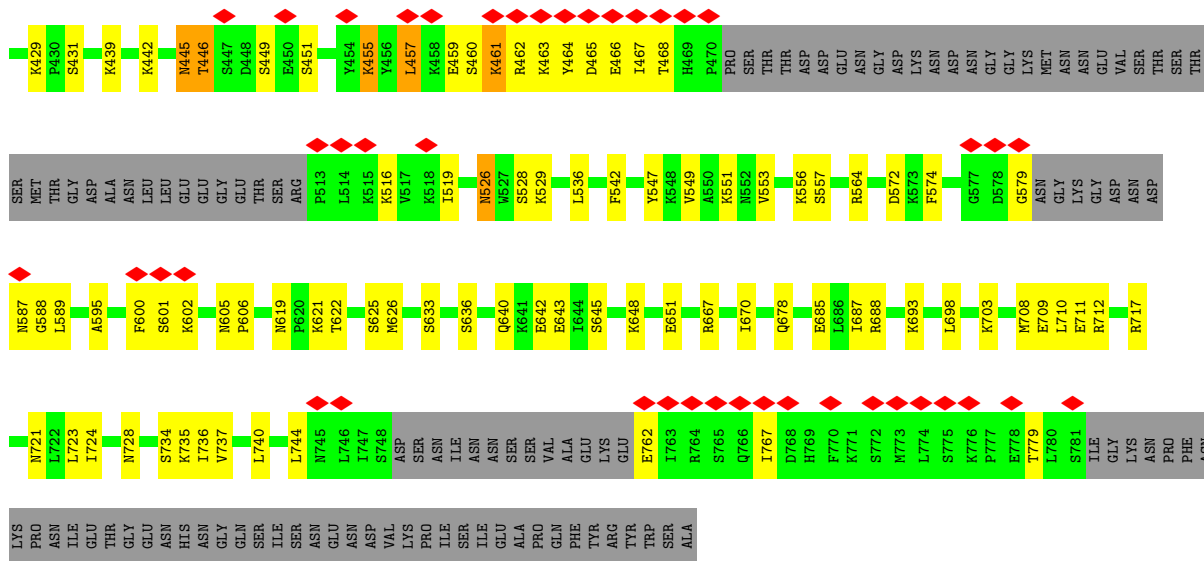
• Molecule 1: Transcription regulatory protein SNF12



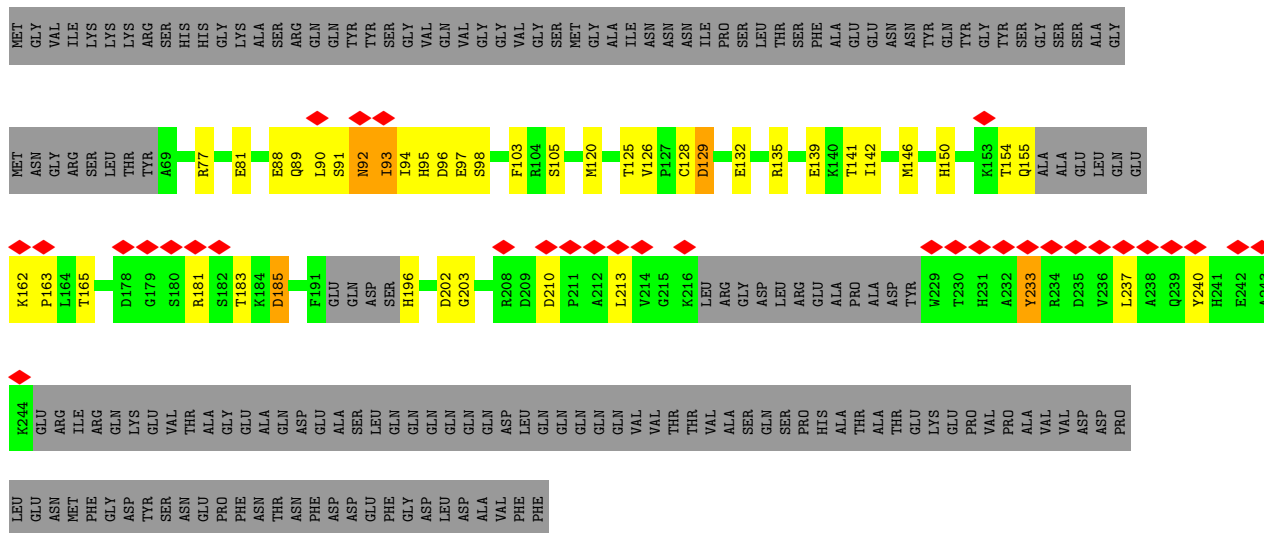
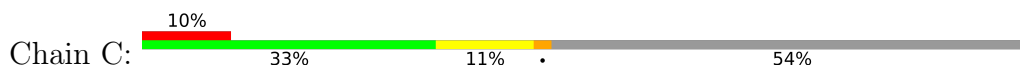
• Molecule 2: SWI/SNF complex subunit SWI3



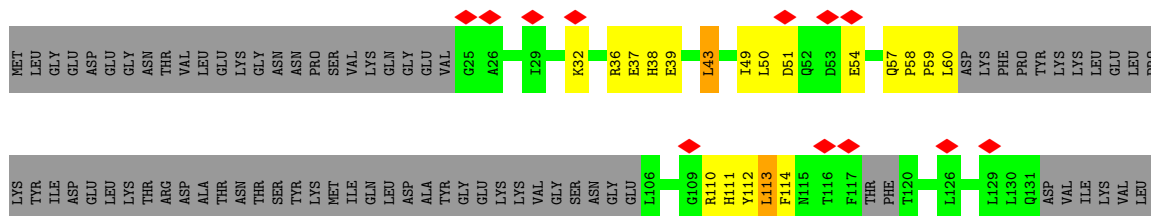
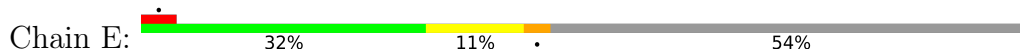


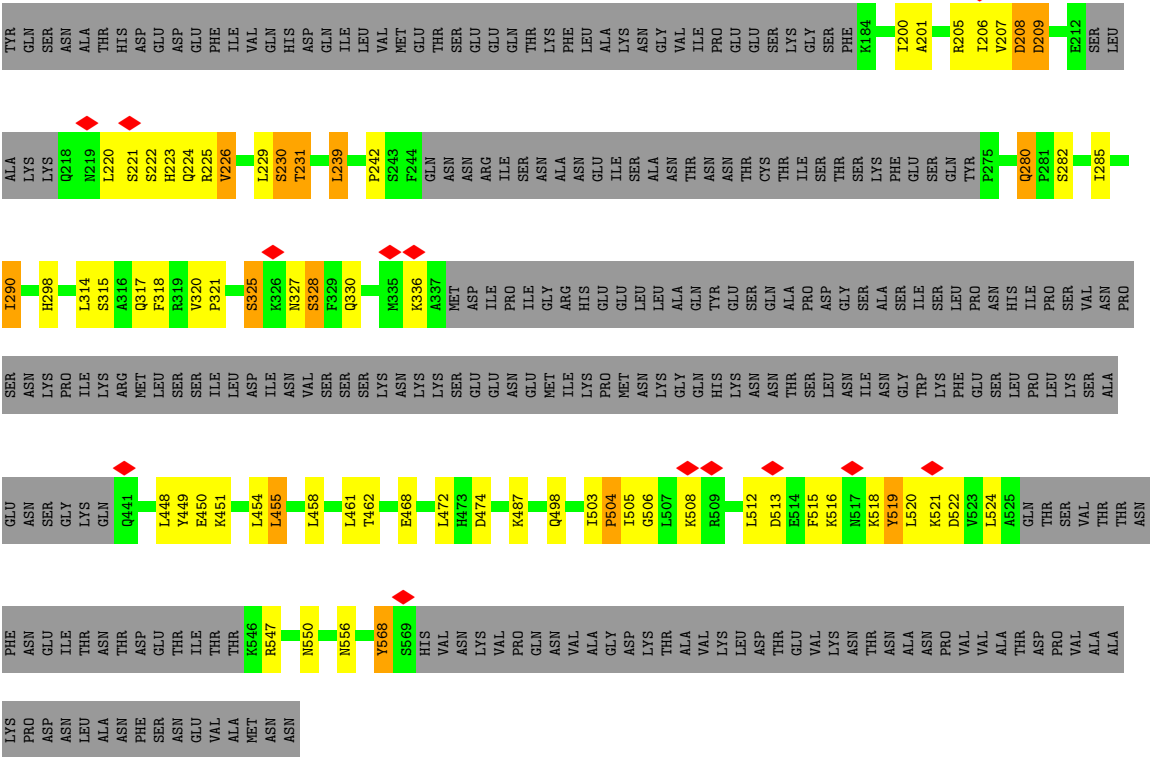


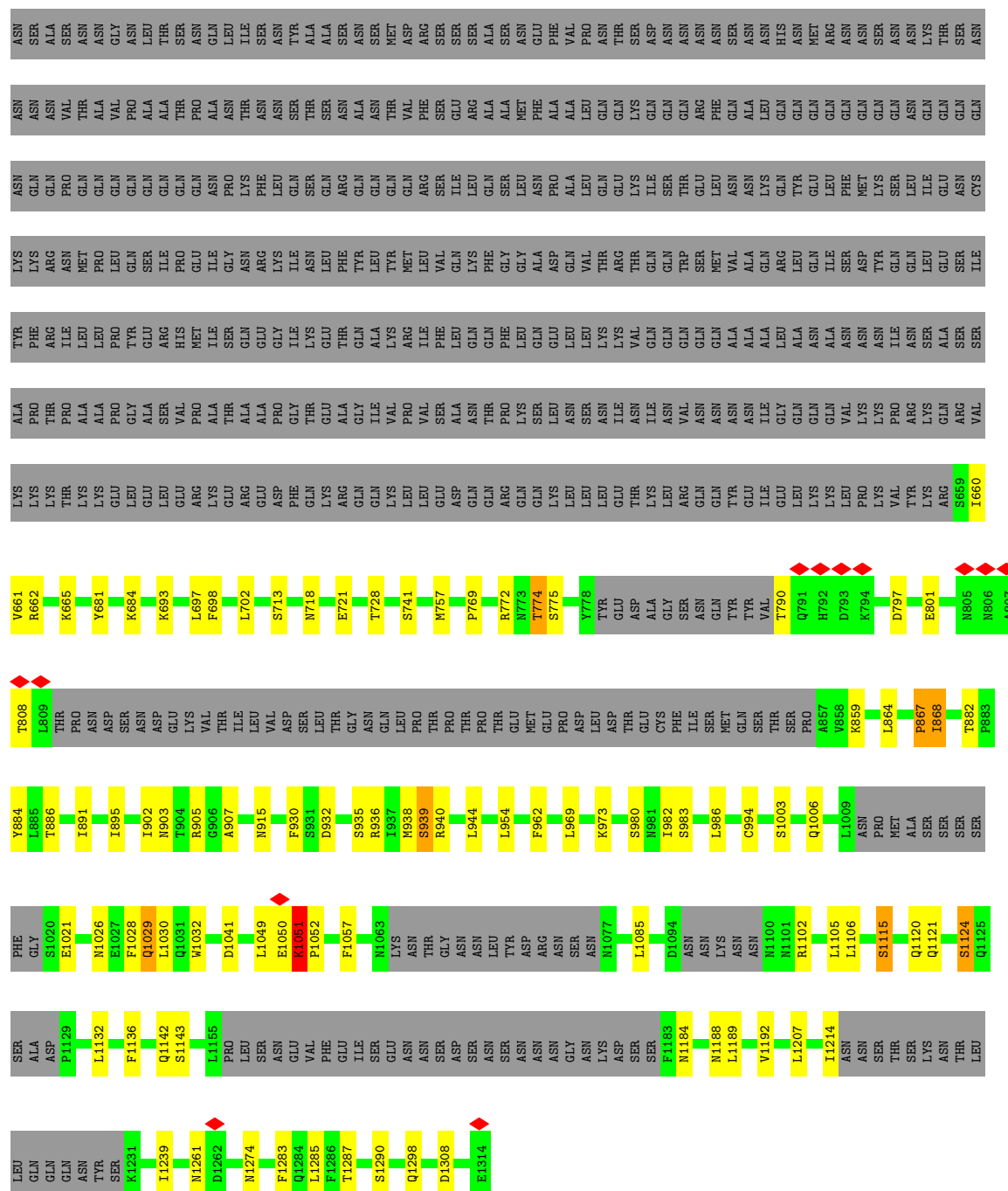
- Molecule 3: Transcription regulatory protein SNF6



- Molecule 4: SWI/SNF global transcription activator complex subunit SWP82





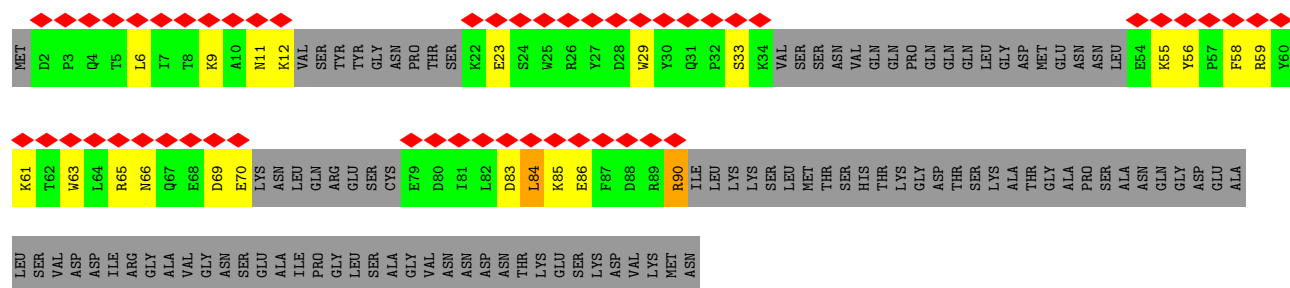


• Molecule 8: Unknown

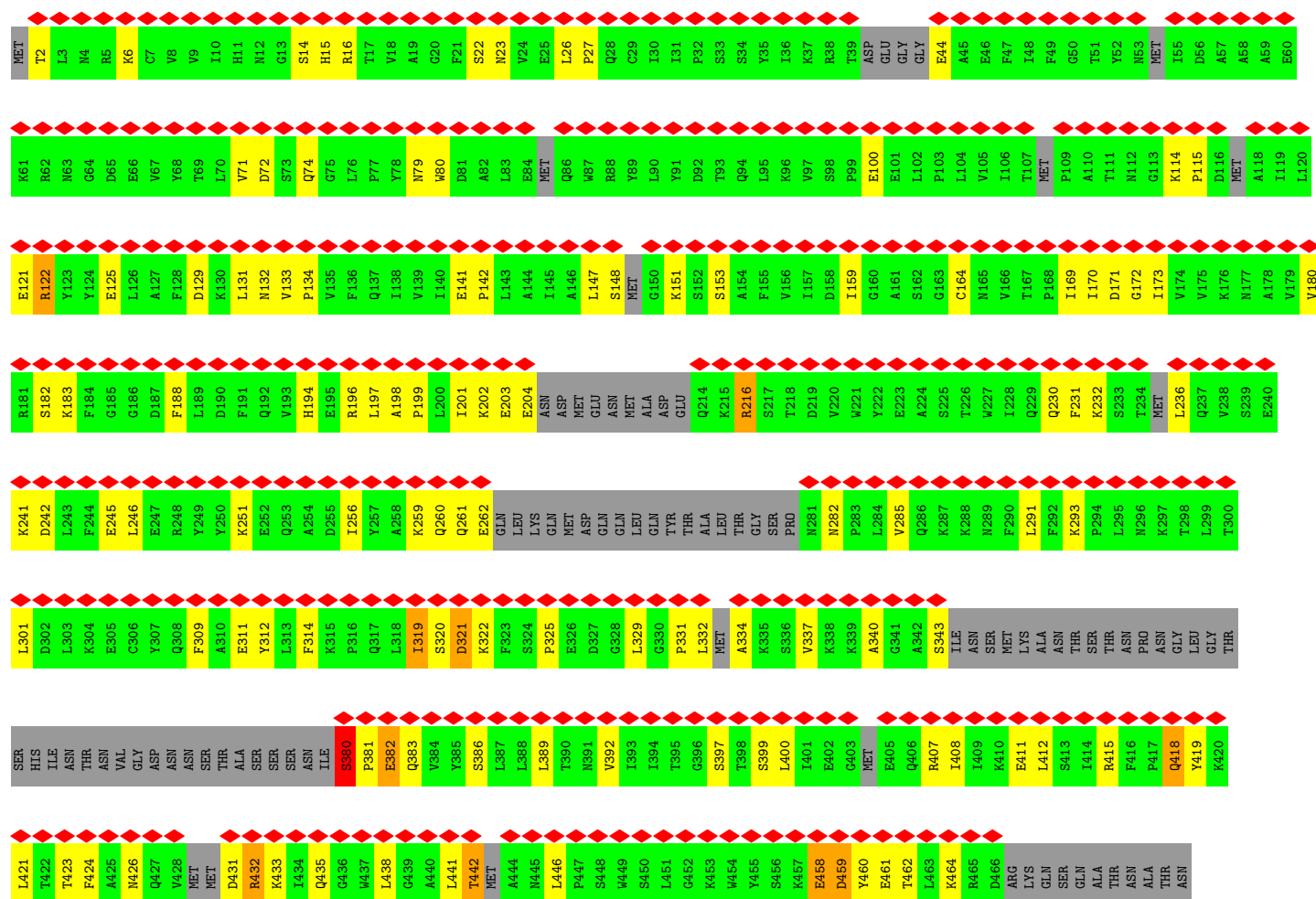
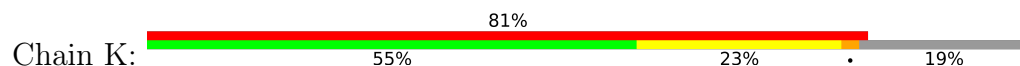


• Molecule 9: Regulator of Ty1 transposition protein 102

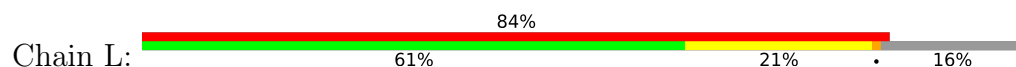




• Molecule 10: Actin-related protein 7



• Molecule 11: Actin-like protein ARP9



K421	S422	G423	Y424	S425	E426	I427	L428	F429	L430	G431	A432	Q433	L434	V435	S436	K437	Q438	I439	F440	T441	H442	P443	K444	D445	T446	F447	Y448	I449	T450	R451	E452	K453	Y454	N455	MET	K457	G458	P459	A460	A461	L462	W463	D464	V465	Q466	F467													
E361	P362	E363	E364	E365	K366	S367	K368	R369	E370	E371	E372	A373	K374	S375	VAL	LEU	PRO	ALA	ALA	THR	LYS	LYS	SER	LYS	PHE	MET	THR	ASN	SER	THR	ALA	F394	V395	P396	T397	I398	E399	Y400	Y401	Q402	C403	P404	T405	Y406	I407	K408	L409	A410	K411	Y412	F413	D414	Y415	F416	F417	E418	W419	K420	
G301	C302	N303	N304	L305	I306	K307	N308	I309	S310	N311	R312	V313	G314	L315	T316	L317	D318	N319	I320	D321	D322	I323	N324	K325	A326	K327	A328	V329	W330	E331	N332	I333	I334	I335	V336	G337	G338	T339	T340	S341	I342	S343	G344	F345	K346	E347	A348	L349	L350	G351	Q352	L353	Y354	K355	D356	H357	L358	I359	T360
GLU	ASP	GLU	GLY	THR	LEU	ASN	VAL	ALA	GLU	ILE	ILE	THR	SER	GLY	ARG	ASP	THR	ARG	GLU	VAL	LEU	GLU	GLY	VAL	LYS	ASN	VAL	K275	N276	S277	D278	L279	E280	F281	N282	T283	F284	W285	D286	E287	K288	G289	N290	E291	I292	K293	V294	G295	K296	Q297	R298	F299	Q300						
D181	H182	L183	V184	S185	S186	I187	P188	MET	G190	G191	Q192	S193	I194	N195	D196	S197	L198	K199	K200	L201	L202	P203	Q204	W205	D206	D207	D208	Q209	I210	E211	S212	L213	K214	K215	S216	P217	I218	F219	E220	V221	L222	S223	ASP	ASP	ALA	LYS	LYS	LEU	SER	K296	Q297	R298	F299	Q300					
Q121	S122	D123	L124	E125	I126	I127	T128	Q129	Y130	V131	F132	E133	S134	L135	E136	I137	N138	N139	L140	I141	Q142	L143	P144	A145	S146	L147	A148	S89	Q209	I210	E211	S212	L213	K214	K215	S216	P217	I218	F219	E220	V221	L222	D163	V164	G165	T166	H167	H168	T169	PHE	ASP	PHE	GLY	ASN	GLU	ASN	GLU	ASP	
K61	A62	E63	L64	I65	K66	P67	I68	Q69	N70	G71	E72	I73	I74	D75	I76	S77	A78	F79	T80	Q81	F82	L83	R84	L85	I86	F87	V88	S89	I90	L91	S92	D93	R94	A95	N96	K97	N98	Q99	D100	A101	F102	E103	A104	E105	L106	S107	N108	I109	P110	L111	L112	L113	I114	T115	H116	H117	S118	W119	S120

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	386469	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	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	0.094	Depositor
Minimum map value	-0.042	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.02	Depositor
Map size (\AA)	347.84, 347.84, 347.84	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.087, 1.087, 1.087	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.33	0/3104	0.44	0/4188
2	B	0.37	0/3318	0.47	0/4465
2	D	0.39	0/3517	0.47	0/4735
3	C	0.34	0/1287	0.46	0/1729
4	E	0.37	0/2404	0.50	1/3237 (0.0%)
5	F	0.39	0/3201	0.51	0/4336
6	H	0.39	0/2000	0.52	0/2706
7	I	0.38	0/4316	0.48	0/5843
8	G	0.38	0/101	0.59	0/123
9	J	0.41	0/493	0.58	0/659
10	K	0.44	0/3197	0.61	1/4313 (0.0%)
11	L	0.45	0/3234	0.59	0/4382
All	All	0.39	0/30172	0.51	2/40716 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	K	380	SER	C-N-CD	5.92	140.84	128.40
4	E	461	LEU	C-N-CA	5.82	136.25	121.70

There are no chirality outliers.

There are no planarity outliers.

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	3048	0	3012	56	0
2	B	3250	0	3302	74	0
2	D	3445	0	3505	86	0
3	C	1266	0	1264	36	0
4	E	2355	0	2416	67	0
5	F	3134	0	3045	54	0
6	H	1966	0	1991	61	0
7	I	4242	0	4401	72	0
8	G	271	0	129	10	0
9	J	482	0	455	19	0
10	K	3131	0	3132	108	0
11	L	3167	0	3149	87	0
All	All	29757	0	29801	613	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 10.

All (613) 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:I:1051:LYS:HB3	7:I:1052:PRO:CD	1.70	1.19
11:L:403:CYS:SG	11:L:404:PRO:HD3	1.89	1.11
7:I:1051:LYS:HE2	7:I:1051:LYS:HA	1.17	1.08
10:K:216:ARG:HG2	10:K:216:ARG:HH11	1.17	1.07
11:L:359:ILE:HD11	11:L:404:PRO:HG2	1.34	1.07
11:L:359:ILE:HG12	11:L:404:PRO:O	1.55	1.06
10:K:114:LYS:HG3	10:K:115:PRO:HD3	1.37	1.06
4:E:58:PRO:HG2	4:E:59:PRO:HD3	1.37	1.05
4:E:206:ILE:HD11	4:E:221:SER:HA	1.40	1.03
1:A:56:PRO:HB3	7:I:1032:TRP:CD1	1.94	1.02
10:K:122:ARG:HH11	10:K:122:ARG:HG2	1.25	1.01
7:I:1051:LYS:CB	7:I:1052:PRO:HD2	1.94	0.97
7:I:1051:LYS:CB	7:I:1052:PRO:CD	2.42	0.97
7:I:1051:LYS:HB3	7:I:1052:PRO:HD3	1.46	0.97
7:I:1051:LYS:HB3	7:I:1052:PRO:HD2	1.50	0.92
7:I:1051:LYS:HA	7:I:1051:LYS:CE	2.00	0.92
2:D:429:LYS:HE2	5:F:360:TYR:CE2	2.06	0.91
6:H:619:ARG:HH21	10:K:441:LEU:HD23	1.37	0.90
7:I:1006:GLN:HE22	7:I:1032:TRP:HZ3	1.20	0.89
11:L:327:LYS:HE3	11:L:403:CYS:HA	1.52	0.88
4:E:57:GLN:HB2	4:E:225:ARG:HE	1.39	0.88
11:L:359:ILE:HG12	11:L:404:PRO:C	1.96	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:605:LEU:HD21	10:K:172:GLY:HA3	1.60	0.83
11:L:323:ILE:HG12	11:L:403:CYS:HB3	1.60	0.82
6:H:596:ARG:HH11	6:H:596:ARG:HA	1.45	0.80
7:I:1051:LYS:HE2	7:I:1051:LYS:CA	2.08	0.80
11:L:303:ASN:HD21	11:L:307:LYS:HZ1	1.29	0.80
4:E:290:ILE:HG13	5:F:745:VAL:HG21	1.64	0.80
10:K:216:ARG:HG2	10:K:216:ARG:NH1	1.94	0.80
4:E:58:PRO:CG	4:E:59:PRO:HD3	2.13	0.79
9:J:63:TRP:CD2	11:L:459:PRO:HG2	2.18	0.78
11:L:403:CYS:HG	11:L:404:PRO:HD3	1.45	0.78
6:H:596:ARG:HA	6:H:596:ARG:NH1	1.97	0.78
7:I:1006:GLN:NE2	7:I:1032:TRP:HZ3	1.82	0.77
7:I:868:ILE:HD11	7:I:954:LEU:HD13	1.66	0.77
10:K:159:ILE:HD11	10:K:408:ILE:HD11	1.65	0.77
10:K:122:ARG:HH11	10:K:122:ARG:CG	1.99	0.76
10:K:114:LYS:HG3	10:K:115:PRO:CD	2.14	0.75
2:B:301:GLN:HE22	4:E:449:TYR:HA	1.52	0.74
2:B:380:ARG:NH2	5:F:570:ASN:OD1	2.21	0.74
10:K:100:GLU:HG2	10:K:132:ASN:HB3	1.68	0.74
2:D:461:LYS:NZ	2:D:465:ASP:OD2	2.20	0.74
4:E:205:ARG:HG3	4:E:224:GLN:HB2	1.68	0.74
4:E:200:ILE:HD11	4:E:208:ASP:HB3	1.70	0.74
4:E:327:ASN:HB3	4:E:330:GLN:HE21	1.52	0.73
6:H:572:ARG:HG2	7:I:930:PHE:HE1	1.54	0.73
11:L:303:ASN:HD21	11:L:307:LYS:NZ	1.85	0.73
11:L:327:LYS:HG3	11:L:403:CYS:HB2	1.70	0.73
11:L:403:CYS:SG	11:L:404:PRO:CD	2.75	0.73
11:L:359:ILE:N	11:L:359:ILE:HD13	2.04	0.73
11:L:14:PRO:O	11:L:116[B]:HIS:HE1	1.72	0.73
2:B:437:MET:HE3	6:H:502:ALA:HB1	1.70	0.72
9:J:84:LEU:O	9:J:85:LYS:HB2	1.89	0.72
2:B:437:MET:CE	6:H:502:ALA:HB1	2.19	0.72
7:I:1051:LYS:HB2	7:I:1052:PRO:HD2	1.70	0.71
11:L:359:ILE:CG1	11:L:404:PRO:O	2.37	0.71
2:D:300:PRO:HD2	4:E:503:ILE:HG12	1.72	0.70
10:K:183:LYS:O	10:K:183:LYS:HG2	1.91	0.70
10:K:14:SER:HA	10:K:71:VAL:HB	1.74	0.70
6:H:619:ARG:NH2	10:K:441:LEU:HD23	2.07	0.69
6:H:595:GLU:OE2	6:H:595:GLU:HA	1.93	0.68
6:H:605:LEU:CD2	10:K:172:GLY:HA3	2.23	0.68
10:K:392:VAL:HB	10:K:423:THR:HG22	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:98:ASN:O	11:L:99:GLN:HG2	1.93	0.68
1:A:418:LEU:C	1:A:418:LEU:HD23	2.13	0.68
2:B:337:SER:HB3	5:F:633:ILE:HG22	1.74	0.68
2:B:541:GLU:HG2	4:E:242:PRO:HB2	1.75	0.68
2:D:439:LYS:NZ	2:D:595:ALA:O	2.27	0.68
9:J:11:ASN:HA	11:L:107:SER:O	1.95	0.67
10:K:458:GLU:HG2	10:K:459:ASP:N	2.10	0.67
3:C:237:LEU:C	3:C:237:LEU:HD13	2.14	0.67
11:L:275:LYS:HB3	11:L:278:ASP:OD2	1.94	0.67
11:L:303:ASN:ND2	11:L:307:LYS:NZ	2.43	0.67
2:B:736:ILE:HD11	2:D:740:LEU:HD13	1.75	0.67
1:A:356:ARG:HA	1:A:359:HIS:CE1	2.30	0.66
2:D:365:THR:HG22	2:D:368:ARG:HH22	1.60	0.66
10:K:311:GLU:OE2	10:K:407:ARG:NH2	2.28	0.66
3:C:233:TYR:H	3:C:233:TYR:HD2	1.44	0.66
7:I:868:ILE:CD1	7:I:954:LEU:HD13	2.26	0.66
10:K:180:VAL:HG11	10:K:332:LEU:HG	1.78	0.66
2:D:442:LYS:NZ	2:D:579:GLY:O	2.28	0.66
3:C:126:VAL:O	2:D:667:ARG:NH1	2.29	0.66
1:A:409:LEU:O	1:A:413:THR:HG23	1.96	0.65
7:I:1006:GLN:NE2	7:I:1032:TRP:CZ3	2.64	0.65
2:D:640:GLN:HA	2:D:643:GLU:HG2	1.77	0.65
2:B:685:GLU:OE1	2:B:688:ARG:NH1	2.30	0.64
4:E:225:ARG:O	4:E:225:ARG:HG3	1.97	0.64
1:A:130:SER:HB2	1:A:435:TYR:HA	1.79	0.64
10:K:121:GLU:O	10:K:125:GLU:HG3	1.98	0.64
5:F:469:ASP:OD2	5:F:469:ASP:N	2.31	0.63
5:F:536:ARG:NH2	5:F:540:ASP:OD1	2.31	0.63
2:D:464:TYR:O	2:D:468:THR:HG23	1.99	0.63
6:H:593:LYS:HD2	6:H:593:LYS:C	2.20	0.63
10:K:148:SER:HB2	10:K:442:THR:HG21	1.79	0.62
1:A:102:GLN:OE1	1:A:105:ARG:NH1	2.33	0.62
10:K:153:SER:HA	10:K:169:ILE:O	1.99	0.62
7:I:938:MET:HG2	7:I:944:LEU:HD22	1.81	0.62
1:A:458:GLU:OE2	2:D:717:ARG:NH1	2.32	0.62
2:B:712:ARG:NH2	2:D:711:GLU:OE1	2.33	0.62
4:E:512:LEU:O	4:E:515:PHE:HB3	2.00	0.61
11:L:47:GLN:O	11:L:48:ASP:HB3	1.99	0.61
3:C:141:THR:HG22	2:D:688:ARG:HD3	1.82	0.61
4:E:321:PRO:HD2	4:E:474:ASP:OD1	1.99	0.61
5:F:419:ILE:HG22	5:F:420:THR:O	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:778:GLU:OE1	2:D:735:LYS:NZ	2.34	0.61
10:K:203:GLU:O	10:K:204:GLU:HB2	2.00	0.61
10:K:382:GLU:CD	10:K:382:GLU:H	2.03	0.61
2:B:592:LEU:HG	6:H:494:THR:HG22	1.81	0.61
7:I:1029:GLN:C	7:I:1121:GLN:HE22	2.03	0.61
4:E:550:ASN:O	4:E:556:ASN:ND2	2.32	0.61
4:E:57:GLN:HB2	4:E:225:ARG:NE	2.14	0.61
7:I:718:ASN:HD22	7:I:721:GLU:HG2	1.66	0.60
2:B:429:LYS:HD2	4:E:568:TYR:CZ	2.36	0.60
5:F:336:THR:O	5:F:340:GLU:HG2	2.02	0.60
1:A:351:ASN:O	1:A:358:ASN:ND2	2.34	0.60
6:H:593:LYS:HD2	6:H:593:LYS:O	2.01	0.60
10:K:256:ILE:O	10:K:260:GLN:HB2	2.00	0.60
11:L:44:THR:OG1	11:L:62:ALA:HB2	2.02	0.60
7:I:932:ASP:OD1	7:I:932:ASP:N	2.30	0.60
5:F:574:GLU:OE2	7:I:790:THR:OG1	2.20	0.60
10:K:122:ARG:HG2	10:K:122:ARG:NH1	2.06	0.60
5:F:318:GLU:OE1	5:F:320:LYS:N	2.35	0.60
10:K:400:LEU:HD12	10:K:433:LYS:HE2	1.84	0.60
2:B:407:PRO:HG3	2:D:299:ILE:HD12	1.83	0.59
2:B:429:LYS:HD2	4:E:568:TYR:CE2	2.37	0.59
6:H:430:LEU:HD21	7:I:661:VAL:HG11	1.83	0.59
1:A:56:PRO:CB	7:I:1032:TRP:CD1	2.81	0.59
11:L:53:TYR:CD1	11:L:81:GLN:HG3	2.37	0.59
2:B:345:ARG:HD2	5:F:638:VAL:HG11	1.83	0.59
6:H:611:SER:O	6:H:615:GLN:HG3	2.03	0.59
7:I:1026:ASN:O	7:I:1115:SER:HB2	2.01	0.59
11:L:141:ILE:HG12	11:L:448:TYR:HB3	1.85	0.59
6:H:619:ARG:NH2	10:K:438:LEU:HD22	2.18	0.59
9:J:29:TRP:CD2	9:J:61:LYS:HD3	2.38	0.59
10:K:380:SER:O	10:K:383:GLN:HB2	2.03	0.58
1:A:131:ASN:HD22	1:A:427:VAL:HG13	1.68	0.58
2:B:533:GLN:NE2	6:H:527:GLU:OE2	2.37	0.58
4:E:57:GLN:OE1	4:E:57:GLN:N	2.36	0.58
6:H:519:ASP:HA	6:H:526:ARG:HH22	1.67	0.58
10:K:159:ILE:HG23	10:K:164:CYS:SG	2.44	0.58
10:K:389:LEU:HB3	10:K:421:LEU:HD23	1.84	0.58
11:L:14:PRO:O	11:L:116[B]:HIS:CE1	2.53	0.58
9:J:84:LEU:HD13	11:L:35:LEU:HD11	1.84	0.58
5:F:559:ASP:OD1	5:F:560:GLN:N	2.37	0.58
6:H:518:ASN:O	6:H:526:ARG:NH2	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:ALA:O	2:B:730:ASN:ND2	2.36	0.58
6:H:519:ASP:OD1	6:H:519:ASP:N	2.36	0.58
6:H:605:LEU:HD11	10:K:171:ASP:O	2.04	0.58
11:L:199:LYS:HD2	11:L:210:ILE:HD13	1.85	0.58
10:K:241:LYS:NZ	10:K:245:GLU:HB3	2.19	0.58
10:K:381:PRO:HG2	10:K:382:GLU:OE2	2.04	0.58
2:B:737:VAL:HG21	2:B:770:PHE:CE2	2.38	0.57
2:B:770:PHE:HE1	2:D:736:ILE:HG23	1.69	0.57
1:A:351:ASN:OD1	1:A:351:ASN:N	2.34	0.57
4:E:522:ASP:O	4:E:547:ARG:NH1	2.36	0.57
6:H:588:ASN:O	6:H:592:LEU:HD13	2.04	0.57
4:E:328:SER:OG	8:G:58:ARG:NH1	2.37	0.57
10:K:334:ALA:HB2	10:K:415:ARG:HD3	1.85	0.57
10:K:418:GLN:O	10:K:418:GLN:HG3	2.03	0.57
2:D:547:TYR:O	2:D:551:LYS:HG2	2.04	0.57
5:F:316:PRO:O	7:I:662:ARG:NH1	2.30	0.57
11:L:327:LYS:HE3	11:L:403:CYS:CA	2.28	0.57
11:L:327:LYS:HG2	11:L:403:CYS:O	2.05	0.57
2:B:314:PHE:HE1	2:B:347:ARG:HD2	1.69	0.57
6:H:521:CYS:HB2	6:H:526:ARG:HH21	1.70	0.57
5:F:420:THR:HG22	5:F:421:ASN:H	1.70	0.57
10:K:216:ARG:HA	10:K:216:ARG:NE	2.20	0.56
3:C:89:GLN:HG2	3:C:90:LEU:HG	1.86	0.56
4:E:498:GLN:OE1	4:E:506:GLY:N	2.38	0.56
2:D:316:LEU:O	2:D:317:GLU:HG2	2.05	0.56
2:D:429:LYS:HE2	5:F:360:TYR:HE2	1.65	0.56
10:K:44:GLU:O	10:K:44:GLU:HG2	2.04	0.56
10:K:72:ASP:OD1	10:K:74:GLN:HB2	2.05	0.56
11:L:359:ILE:CD1	11:L:404:PRO:HG2	2.23	0.56
3:C:88:GLU:HB3	3:C:93:ILE:HG22	1.88	0.56
1:A:285:ARG:HG2	1:A:285:ARG:HH11	1.71	0.56
5:F:423:THR:O	5:F:424:THR:OG1	2.21	0.56
2:D:305:ILE:HA	2:D:394:GLN:HE22	1.71	0.56
5:F:620:ILE:HG21	5:F:626:ARG:HG3	1.88	0.56
1:A:129:ILE:HB	1:A:438:LEU:HD23	1.88	0.56
7:I:1120:GLN:O	7:I:1124:SER:HB3	2.05	0.56
10:K:194:HIS:NE2	10:K:203:GLU:OE1	2.39	0.56
3:C:210:ASP:HB3	3:C:213:LEU:HB2	1.88	0.55
4:E:448:LEU:HD23	8:G:64:PRO:HB2	1.87	0.55
5:F:361:ASP:N	5:F:362:PRO:HD2	2.22	0.55
5:F:439:LEU:O	8:G:118:ARG:NH2	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:426:ASN:HB3	10:K:432:ARG:HG2	1.88	0.55
3:C:233:TYR:N	3:C:233:TYR:CD2	2.73	0.55
9:J:69:ASP:O	9:J:70:GLU:HG3	2.06	0.55
11:L:43:ARG:HG3	11:L:53:TYR:CE2	2.42	0.55
2:B:695:ASP:OD1	2:B:696:ALA:N	2.40	0.55
3:C:202:ASP:OD2	3:C:203:GLY:N	2.40	0.55
1:A:181:PHE:O	1:A:182:ILE:HG12	2.07	0.54
2:D:409:THR:O	2:D:409:THR:OG1	2.23	0.54
4:E:207:VAL:O	4:E:209:ASP:N	2.40	0.54
10:K:196:ARG:NH2	10:K:312:TYR:OH	2.39	0.54
10:K:26:LEU:HB3	10:K:27:PRO:HD2	1.88	0.54
11:L:327:LYS:CE	11:L:403:CYS:HA	2.29	0.54
1:A:56:PRO:HB3	7:I:1032:TRP:NE1	2.23	0.54
1:A:131:ASN:ND2	1:A:427:VAL:HG13	2.22	0.54
2:D:685:GLU:OE2	2:D:688:ARG:NH2	2.40	0.54
2:D:602:LYS:HE2	5:F:324:PRO:HG2	1.89	0.54
1:A:115:PRO:HG3	2:D:721:ASN:HA	1.89	0.54
7:I:1188:ASN:O	7:I:1192:VAL:HG13	2.08	0.54
10:K:438:LEU:O	10:K:442:THR:HG23	2.08	0.54
11:L:43:ARG:HD3	11:L:51:TYR:CD1	2.44	0.53
11:L:275:LYS:HE3	11:L:277:SER:H	1.73	0.53
1:A:560:ILE:HG22	1:A:566:MET:HB2	1.90	0.53
2:B:399:LEU:HD11	4:E:487:LYS:HE3	1.91	0.53
3:C:185:ASP:OD1	3:C:185:ASP:N	2.40	0.53
3:C:154:THR:OG1	3:C:155:GLN:OE1	2.22	0.53
2:D:417:ASP:OD1	2:D:417:ASP:N	2.32	0.53
10:K:381:PRO:C	10:K:383:GLN:H	2.11	0.53
6:H:619:ARG:HH21	10:K:441:LEU:CD2	2.17	0.53
7:I:1041:ASP:OD1	7:I:1142:GLN:NE2	2.42	0.53
11:L:359:ILE:N	11:L:359:ILE:CD1	2.72	0.53
1:A:182:ILE:O	1:A:300:LYS:NZ	2.40	0.52
5:F:345:ARG:NH1	6:H:484:LEU:O	2.42	0.52
5:F:622:ASP:OD1	5:F:623:ASP:N	2.40	0.52
10:K:399:SER:OG	10:K:432:ARG:NH1	2.42	0.52
10:K:80:TRP:NE1	10:K:122:ARG:HD3	2.25	0.52
2:B:429:LYS:HE3	2:D:416:HIS:CE1	2.43	0.52
2:B:450:GLU:HA	2:B:455:LYS:HE3	1.91	0.52
6:H:608:MET:HG3	10:K:446:LEU:CD1	2.39	0.52
2:D:306:VAL:H	2:D:394:GLN:NE2	2.08	0.52
10:K:133:VAL:HG13	10:K:134:PRO:HD2	1.91	0.52
10:K:197:LEU:HD11	10:K:231:PHE:CZ	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:606:PRO:HA	6:H:486:VAL:HG23	1.91	0.52
6:H:619:ARG:NH2	10:K:441:LEU:CD2	2.73	0.52
10:K:261:GLN:HB2	10:K:262:GLU:OE1	2.08	0.52
5:F:374:ILE:HD13	7:I:681:TYR:HD2	1.75	0.52
4:E:282:SER:OG	4:E:285:ILE:HD12	2.10	0.52
11:L:34:GLU:CD	11:L:34:GLU:H	2.13	0.52
2:B:301:GLN:NE2	4:E:450:GLU:OE2	2.43	0.52
3:C:91:SER:C	3:C:93:ILE:H	2.14	0.51
1:A:531:GLY:O	7:I:693:LYS:NZ	2.40	0.51
10:K:201:ILE:O	10:K:202:LYS:HB2	2.11	0.51
10:K:6:LYS:HE3	11:L:121:GLN:OE1	2.09	0.51
11:L:47:GLN:O	11:L:48:ASP:CB	2.59	0.51
11:L:335:ILE:HG22	11:L:340:THR:HG21	1.93	0.51
4:E:207:VAL:C	4:E:209:ASP:H	2.14	0.51
6:H:641:GLU:O	6:H:645:GLN:HG3	2.10	0.51
9:J:85:LYS:O	9:J:90:ARG:NH1	2.44	0.51
10:K:291:LEU:HB3	11:L:402:GLN:NE2	2.25	0.51
4:E:113:LEU:HG	4:E:201:ALA:HA	1.92	0.51
10:K:320:SER:OG	10:K:322:LYS:N	2.38	0.51
10:K:418:GLN:HG2	10:K:419:TYR:CE1	2.46	0.51
2:B:517:VAL:HG22	2:B:519:ILE:HG12	1.93	0.50
2:D:414:THR:O	2:D:415:ARG:NE	2.44	0.50
10:K:460:TYR:CZ	10:K:464:LYS:HE3	2.47	0.50
10:K:426:ASN:O	10:K:432:ARG:NE	2.35	0.50
1:A:131:ASN:HD21	1:A:428:ARG:H	1.59	0.50
4:E:516:LYS:O	4:E:519:TYR:HB2	2.11	0.50
9:J:6:LEU:CD2	11:L:102:PHE:HZ	2.25	0.50
3:C:103:PHE:CZ	7:I:902:ILE:HD11	2.47	0.50
4:E:221:SER:H	4:E:224:GLN:NE2	2.10	0.50
5:F:464:PHE:O	5:F:472:PHE:HA	2.12	0.50
11:L:32:VAL:HG23	11:L:33:PRO:HD2	1.92	0.50
11:L:359:ILE:HG21	11:L:402:GLN:HB2	1.93	0.50
3:C:120:MET:HB2	6:H:472:SER:HB2	1.93	0.50
2:D:317:GLU:HA	2:D:344:MET:HE1	1.93	0.50
7:I:935:SER:O	7:I:939:SER:OG	2.29	0.50
2:B:578:ASP:OD1	2:B:578:ASP:N	2.45	0.49
6:H:650:LYS:HE2	6:H:650:LYS:HA	1.94	0.49
10:K:141:GLU:HB3	10:K:142:PRO:HD3	1.94	0.49
11:L:171:ILE:HD13	11:L:312:ARG:CG	2.42	0.49
7:I:891:ILE:O	7:I:895:ILE:HG13	2.13	0.49
10:K:407:ARG:O	10:K:411:GLU:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:81:GLU:HB3	7:I:932:ASP:HB3	1.94	0.49
11:L:330:TRP:CD1	11:L:404:PRO:HB3	2.47	0.49
2:B:629:ARG:NH1	2:D:626:MET:O	2.45	0.49
2:D:311:SER:OG	2:D:388:TRP:O	2.21	0.49
2:D:642:GLU:O	2:D:645:SER:OG	2.21	0.49
3:C:77:ARG:HD2	8:G:128:TYR:CD1	2.47	0.49
2:D:744:LEU:HD11	2:D:767:ILE:HG23	1.94	0.49
7:I:938:MET:HB3	7:I:982:ILE:HD11	1.94	0.49
6:H:443:ILE:HD11	7:I:662:ARG:HG2	1.94	0.49
8:G:89:UNK:C	8:G:91:UNK:H	2.25	0.49
10:K:22:SER:HA	10:K:441:LEU:CD1	2.42	0.49
3:C:92:ASN:C	3:C:94:ILE:H	2.16	0.49
10:K:122:ARG:CG	10:K:122:ARG:NH1	2.66	0.49
1:A:552:MET:O	1:A:556:ASN:ND2	2.46	0.48
1:A:114:TYR:HB3	1:A:115:PRO:HD3	1.95	0.48
6:H:439:LYS:HB3	7:I:660:ILE:HG22	1.96	0.48
6:H:619:ARG:NH2	10:K:438:LEU:CD2	2.76	0.48
10:K:15:HIS:ND1	10:K:16[B]:ARG:HG2	2.28	0.48
11:L:120:SER:HB2	11:L:123:ASP:H	1.78	0.48
1:A:357:ASN:OD1	1:A:357:ASN:N	2.45	0.48
4:E:314:LEU:O	5:F:651:ASN:ND2	2.45	0.48
7:I:697:LEU:HD12	7:I:697:LEU:H	1.78	0.48
7:I:774:THR:HG22	7:I:775:SER:H	1.79	0.48
2:D:519:ILE:HG22	2:D:574:PHE:HB3	1.94	0.48
6:H:473:ASP:OD2	6:H:474:HIS:N	2.45	0.48
1:A:95:HIS:HD2	7:I:1274:ASN:HD21	1.60	0.48
1:A:178:PHE:HB3	1:A:279:ASP:HA	1.96	0.48
5:F:386:ASP:OD2	5:F:387:LEU:N	2.47	0.48
6:H:503:LEU:O	6:H:507:THR:HG23	2.14	0.48
10:K:389:LEU:O	10:K:421:LEU:HA	2.13	0.48
11:L:148:ALA:O	11:L:431:GLY:HA3	2.14	0.48
6:H:458:ILE:HD12	6:H:459:SER:N	2.28	0.48
11:L:286:ASP:HB3	11:L:290:ASN:H	1.79	0.48
4:E:60:LEU:HD22	4:E:229:LEU:HD12	1.95	0.48
6:H:557:ASN:HD22	7:I:907:ALA:HA	1.79	0.48
10:K:170:ILE:O	10:K:173:ILE:HG22	2.13	0.48
11:L:286:ASP:HB2	11:L:290:ASN:HB2	1.96	0.48
1:A:157:THR:HA	1:A:283:ILE:O	2.14	0.48
1:A:351:ASN:C	1:A:358:ASN:HD21	2.17	0.48
2:D:323:GLU:OE1	2:D:343:TYR:OH	2.24	0.48
2:D:385:LEU:HB3	2:D:391:ILE:HG21	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:39:GLU:HG3	6:H:517:LEU:HD23	1.95	0.48
7:I:1261:ASN:OD1	7:I:1261:ASN:N	2.47	0.48
10:K:259:LYS:HD2	10:K:259:LYS:O	2.14	0.48
1:A:434:THR:HG23	1:A:437:GLU:OE2	2.14	0.48
2:B:389:GLY:O	2:B:391:ILE:N	2.47	0.47
2:D:431:SER:O	2:D:431:SER:OG	2.30	0.47
2:D:648:LYS:HB2	2:D:651:GLU:HG2	1.96	0.47
6:H:464:ASP:OD1	6:H:464:ASP:N	2.38	0.47
7:I:1102:ARG:NH1	7:I:1184:ASN:O	2.47	0.47
11:L:327:LYS:HE2	11:L:403:CYS:O	2.14	0.47
2:B:688:ARG:NH1	2:B:688:ARG:HB3	2.28	0.47
2:D:678:GLN:HE22	6:H:466:GLN:HG2	1.78	0.47
4:E:550:ASN:HB2	5:F:751:SER:HB3	1.96	0.47
10:K:458:GLU:O	10:K:461:GLU:N	2.47	0.47
3:C:96:ASP:OD2	7:I:884:TYR:OH	2.28	0.47
3:C:129:ASP:OD2	3:C:129:ASP:N	2.46	0.47
2:D:459:GLU:O	2:D:463:LYS:HG2	2.14	0.47
4:E:315:SER:HB3	5:F:649:THR:HG21	1.96	0.47
5:F:624:ASP:O	5:F:627:SER:OG	2.33	0.47
6:H:596:ARG:NH1	6:H:596:ARG:CA	2.73	0.47
10:K:337:VAL:O	10:K:340:ALA:HB3	2.15	0.47
2:D:462:ARG:HD3	2:D:463:LYS:HD2	1.97	0.47
2:D:526:ASN:OD1	2:D:526:ASN:N	2.47	0.47
4:E:280:GLN:HE21	4:E:280:GLN:HB2	1.54	0.47
6:H:633:LEU:HD12	11:L:151:TYR:CD1	2.50	0.47
11:L:359:ILE:HB	11:L:405:THR:HG22	1.96	0.47
5:F:386:ASP:O	5:F:390:THR:HG23	2.14	0.47
11:L:303:ASN:ND2	11:L:307:LYS:HZ2	2.10	0.47
11:L:364:GLU:HG2	11:L:365:GLU:N	2.29	0.47
1:A:302:SER:HB2	1:A:305:GLU:HG3	1.96	0.47
2:B:437:MET:HE1	6:H:502:ALA:HB1	1.93	0.47
2:D:346:TYR:OH	2:D:372:SER:O	2.31	0.47
2:D:445:ASN:O	2:D:446:THR:HB	2.14	0.47
4:E:205:ARG:HD3	4:E:220:LEU:HD22	1.97	0.47
10:K:241:LYS:O	10:K:242:ASP:C	2.52	0.47
2:B:428:TYR:CG	2:D:420:ARG:HG2	2.50	0.47
2:D:306:VAL:H	2:D:394:GLN:HE22	1.62	0.47
6:H:608:MET:CG	10:K:446:LEU:HD11	2.44	0.47
11:L:30:PHE:HB3	11:L:433:GLN:OE1	2.14	0.47
1:A:484:ASP:O	1:A:488:THR:HG23	2.13	0.47
2:B:519:ILE:HG21	2:B:536:LEU:HD11	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:689:LEU:O	2:B:693:LYS:HG2	2.14	0.47
1:A:480:ILE:HG23	2:D:693:LYS:HE3	1.97	0.47
2:D:528:SER:OG	2:D:529:LYS:N	2.48	0.47
2:D:547:TYR:CZ	2:D:551:LYS:HD3	2.50	0.47
2:D:619:ASN:O	2:D:621:LYS:N	2.48	0.47
3:C:81:GLU:CB	7:I:932:ASP:HB3	2.45	0.46
2:D:413:SER:O	2:D:413:SER:OG	2.31	0.46
10:K:325:PRO:O	10:K:331:PRO:HG2	2.15	0.46
11:L:370:GLU:HG3	11:L:395:VAL:HG21	1.97	0.46
2:B:639:SER:OG	2:B:640:GLN:OE1	2.33	0.46
4:E:468:GLU:O	4:E:472:LEU:HG	2.15	0.46
10:K:188:PHE:HZ	10:K:319:ILE:HD13	1.80	0.46
2:D:329:GLU:OE1	2:D:380:ARG:NH1	2.48	0.46
2:D:572:ASP:HB2	2:D:605:ASN:HB3	1.98	0.46
4:E:230:SER:OG	4:E:231:THR:N	2.48	0.46
4:E:451:LYS:HE3	4:E:455:LEU:HD12	1.97	0.46
6:H:430:LEU:O	6:H:433:GLN:HG3	2.16	0.46
2:B:396:ASP:O	2:B:399:LEU:HB2	2.16	0.46
1:A:418:LEU:HD23	1:A:418:LEU:O	2.15	0.46
9:J:56:TYR:HB3	9:J:58:PHE:CE2	2.50	0.46
10:K:6:LYS:HD2	10:K:23:ASN:ND2	2.31	0.46
2:B:374:ASP:OD1	2:B:377:ALA:N	2.40	0.46
9:J:66:ASN:HB3	9:J:70:GLU:HB2	1.98	0.46
10:K:419:TYR:CD1	10:K:419:TYR:N	2.84	0.46
1:A:289:GLU:HG2	1:A:290:ASN:H	1.81	0.46
2:D:383:LYS:HA	2:D:383:LYS:HD3	1.70	0.46
9:J:83:ASP:C	9:J:84:LEU:O	2.52	0.46
10:K:236:LEU:HD22	10:K:309:PHE:CD2	2.51	0.46
11:L:359:ILE:CD1	11:L:404:PRO:O	2.64	0.46
11:L:359:ILE:CG2	11:L:402:GLN:HB2	2.46	0.46
2:B:780:LEU:HD12	2:D:728:ASN:OD1	2.16	0.46
6:H:611:SER:OG	10:K:446:LEU:HD23	2.16	0.46
7:I:684:LYS:HB3	7:I:684:LYS:HE2	1.55	0.46
9:J:23:GLU:OE2	9:J:65:ARG:HD3	2.16	0.46
11:L:26:ASN:O	11:L:27:GLU:HB2	2.15	0.46
1:A:131:ASN:HA	1:A:158:MET:HA	1.98	0.45
2:B:587:ASN:ND2	2:D:588:GLY:O	2.49	0.45
2:D:464:TYR:O	2:D:467:ILE:HG22	2.17	0.45
7:I:757:MET:HE1	7:I:864:LEU:HD13	1.97	0.45
11:L:143:LEU:HD12	11:L:144:PRO:HD2	1.98	0.45
1:A:428:ARG:HB3	1:A:431:LYS:HB3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:763:ILE:HD12	2:B:764:ARG:N	2.31	0.45
3:C:126:VAL:HG21	6:H:463:ILE:HD11	1.97	0.45
3:C:135:ARG:NH1	3:C:139:GLU:OE1	2.37	0.45
10:K:183:LYS:O	10:K:183:LYS:CG	2.61	0.45
10:K:282:ASN:O	10:K:285:VAL:HG22	2.16	0.45
10:K:334:ALA:CB	10:K:415:ARG:HD3	2.46	0.45
11:L:424:TYR:CD1	11:L:427:ILE:HD12	2.51	0.45
4:E:519:TYR:HD1	4:E:519:TYR:HA	1.60	0.45
7:I:769:PRO:HA	7:I:772:ARG:HE	1.81	0.45
1:A:404:THR:O	1:A:408:SER:OG	2.29	0.45
2:B:339:THR:HG22	2:B:341:GLU:H	1.82	0.45
5:F:659:GLU:OE1	5:F:659:GLU:N	2.48	0.45
10:K:164:CYS:HB2	10:K:182:SER:HB3	1.98	0.45
1:A:406:LEU:O	1:A:410:ILE:HG12	2.17	0.45
2:B:623:VAL:O	2:B:627:THR:HG22	2.16	0.45
11:L:286:ASP:CB	11:L:290:ASN:H	2.29	0.45
11:L:354:LEU:HD22	11:L:358:LEU:HD22	1.99	0.45
2:B:328:PRO:HB2	5:F:537:LEU:HD21	1.98	0.45
4:E:518:LYS:HA	4:E:521:LYS:HD2	1.99	0.45
9:J:9:LYS:HD2	9:J:12:LYS:HE2	1.97	0.45
10:K:241:LYS:HZ2	10:K:245:GLU:HB3	1.78	0.45
1:A:263:LEU:HB3	1:A:264:GLU:H	1.51	0.45
1:A:355:ASN:N	1:A:358:ASN:HD22	2.14	0.45
2:D:429:LYS:CE	5:F:360:TYR:CE2	2.92	0.45
2:D:455:LYS:O	2:D:459:GLU:HG2	2.17	0.45
9:J:33:SER:HB3	9:J:55:LYS:CD	2.46	0.45
7:I:1285:LEU:HD23	7:I:1285:LEU:HA	1.83	0.45
11:L:146:SER:HB2	11:L:174:ILE:HD11	1.99	0.45
1:A:356:ARG:HH12	2:B:735:LYS:HE2	1.82	0.45
2:D:312:LYS:HB3	2:D:312:LYS:HE3	1.51	0.45
9:J:6:LEU:HD23	11:L:102:PHE:HZ	1.82	0.45
2:B:613:PHE:HE2	6:H:490:THR:HG22	1.82	0.45
10:K:216:ARG:NH1	10:K:216:ARG:CG	2.69	0.45
11:L:212:SER:HB3	11:L:284:PHE:HE2	1.81	0.45
2:D:587:ASN:OD1	2:D:587:ASN:N	2.50	0.44
4:E:54:GLU:OE1	4:E:54:GLU:HA	2.17	0.44
4:E:325:SER:HB3	8:G:57:GLY:O	2.16	0.44
4:E:520:LEU:O	4:E:524:LEU:HG	2.17	0.44
7:I:1021:GLU:O	7:I:1192:VAL:HB	2.17	0.44
7:I:1189:LEU:O	7:I:1192:VAL:HG22	2.17	0.44
11:L:105:GLU:H	11:L:105:GLU:HG3	1.62	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:205:ARG:HB2	4:E:222:SER:HA	1.99	0.44
2:D:389:GLY:O	2:D:391:ILE:N	2.50	0.44
11:L:197:SER:HB3	11:L:301:GLY:HA2	2.00	0.44
11:L:359:ILE:HB	11:L:405:THR:HA	1.99	0.44
1:A:118:ASN:OD1	1:A:119:PHE:N	2.51	0.44
4:E:49:ILE:HD11	4:E:223:HIS:HB3	1.99	0.44
5:F:563:TRP:CZ2	5:F:570:ASN:HB3	2.53	0.44
11:L:121:GLN:HG2	11:L:463:TRP:CH2	2.52	0.44
1:A:267:LYS:HZ1	1:A:268:TRP:C	2.21	0.44
3:C:91:SER:O	3:C:93:ILE:N	2.50	0.44
3:C:103:PHE:CE1	7:I:902:ILE:HD11	2.52	0.44
2:D:698:LEU:HA	2:D:698:LEU:HD23	1.84	0.44
2:D:744:LEU:HD12	2:D:744:LEU:HA	1.81	0.44
6:H:526:ARG:HE	6:H:526:ARG:HB2	1.64	0.44
7:I:915:ASN:HD21	7:I:962:PHE:HA	1.82	0.44
7:I:969:LEU:HG	7:I:973:LYS:HE3	1.99	0.44
10:K:232:LYS:HA	10:K:236:LEU:HG	1.99	0.44
11:L:30:PHE:CD1	11:L:30:PHE:N	2.84	0.44
1:A:541:ARG:NH1	2:B:571:GLU:OE2	2.43	0.44
2:D:740:LEU:HD23	2:D:740:LEU:HA	1.78	0.44
7:I:882:THR:HG22	7:I:886:THR:OG1	2.17	0.44
10:K:320:SER:OG	10:K:321:ASP:N	2.49	0.44
1:A:298:LEU:HD21	1:A:418:LEU:HD22	1.99	0.44
2:D:703:LYS:HE2	2:D:703:LYS:H	1.82	0.44
4:E:504:PRO:HG3	4:E:518:LYS:HE3	2.00	0.44
6:H:608:MET:HG3	10:K:446:LEU:HD13	1.99	0.44
7:I:859:LYS:HB3	7:I:859:LYS:HE2	1.78	0.44
3:C:125:THR:O	6:H:460:HIS:NE2	2.51	0.44
7:I:1132:LEU:HD12	7:I:1132:LEU:HA	1.84	0.44
9:J:33:SER:HB3	9:J:55:LYS:HD3	1.98	0.44
11:L:286:ASP:HB2	11:L:290:ASN:O	2.18	0.44
3:C:142:ILE:O	3:C:146:MET:HG2	2.17	0.43
2:D:553:VAL:HG11	2:D:556:LYS:HD2	2.00	0.43
5:F:460:ILE:HD13	5:F:517:ILE:HG23	1.99	0.43
5:F:536:ARG:NH1	5:F:616:ASP:HA	2.32	0.43
7:I:1028:PHE:O	7:I:1028:PHE:CD1	2.70	0.43
3:C:77:ARG:HD2	8:G:128:TYR:CE1	2.53	0.43
4:E:206:ILE:HD11	4:E:221:SER:CA	2.29	0.43
5:F:620:ILE:HG12	5:F:626:ARG:HB2	2.00	0.43
7:I:1290:SER:O	7:I:1290:SER:OG	2.32	0.43
10:K:129:ASP:OD2	10:K:460:TYR:HE2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:337:SER:HB3	5:F:633:ILE:CG2	2.47	0.43
2:B:732:ASN:O	2:B:736:ILE:HG23	2.18	0.43
10:K:381:PRO:HG2	10:K:382:GLU:CD	2.39	0.43
1:A:92:ARG:NH2	2:D:708:MET:SD	2.91	0.43
10:K:151:LYS:HE3	10:K:424:PHE:CE1	2.53	0.43
10:K:381:PRO:C	10:K:383:GLN:N	2.72	0.43
11:L:354:LEU:HD23	11:L:354:LEU:HA	1.89	0.43
2:B:432:VAL:O	2:B:432:VAL:HG13	2.19	0.43
2:D:734:SER:O	2:D:737:VAL:HG12	2.19	0.43
10:K:458:GLU:O	10:K:459:ASP:C	2.56	0.43
11:L:361:GLU:HA	11:L:362:PRO:HD3	1.93	0.43
2:B:372:SER:O	5:F:633:ILE:HD11	2.19	0.43
2:B:387:LYS:HD3	2:B:387:LYS:HA	1.86	0.43
2:B:434:LEU:HD11	6:H:536:LEU:O	2.19	0.43
1:A:154:ALA:HB3	1:A:287:GLY:H	1.84	0.43
2:D:367:ALA:O	2:D:371:VAL:HG22	2.18	0.43
4:E:336:LYS:HD3	4:E:336:LYS:HA	1.91	0.43
5:F:613:TYR:CE2	5:F:615:PHE:HA	2.54	0.43
4:E:58:PRO:CG	4:E:59:PRO:CD	2.92	0.43
6:H:633:LEU:HA	6:H:633:LEU:HD23	1.82	0.43
2:B:698:LEU:HD23	2:B:698:LEU:HA	1.88	0.42
9:J:83:ASP:O	9:J:86:GLU:HG3	2.18	0.42
1:A:479:LYS:HD3	1:A:479:LYS:H	1.84	0.42
5:F:360:TYR:HB2	5:F:362:PRO:HD2	1.99	0.42
6:H:490:THR:O	6:H:494:THR:HG23	2.19	0.42
3:C:150:HIS:O	3:C:154:THR:HG23	2.20	0.42
5:F:357:THR:HG23	5:F:370:ASN:HB3	2.00	0.42
11:L:445:ASP:HA	11:L:448:TYR:CE1	2.55	0.42
2:D:369:ARG:NH2	5:F:499:TYR:OH	2.53	0.42
7:I:983:SER:HA	7:I:986:LEU:HB2	2.01	0.42
10:K:80:TRP:CE2	10:K:122:ARG:HD3	2.54	0.42
10:K:431:ASP:O	10:K:435:GLN:HB2	2.19	0.42
11:L:6:GLN:O	11:L:24:GLY:HA2	2.20	0.42
2:B:346:TYR:HE1	5:F:638:VAL:HG23	1.84	0.42
3:C:97:GLU:O	3:C:98:SER:HB3	2.20	0.42
2:D:457:LEU:HD11	4:E:111:HIS:NE2	2.35	0.42
6:H:608:MET:CE	10:K:147:LEU:HD13	2.49	0.42
7:I:1283:PHE:O	7:I:1287:THR:HG23	2.18	0.42
5:F:614:ASN:H	5:F:614:ASN:ND2	2.17	0.42
8:G:89:UNK:O	8:G:90:LEU:HB3	2.18	0.42
9:J:9:LYS:HD2	9:J:12:LYS:NZ	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:688:ARG:HB3	2:B:688:ARG:HH11	1.84	0.42
4:E:43:LEU:HD23	4:E:43:LEU:HA	1.77	0.42
4:E:110:ARG:HE	4:E:208:ASP:HA	1.85	0.42
4:E:239:LEU:HD23	4:E:239:LEU:HA	1.81	0.42
10:K:131:LEU:HD23	10:K:131:LEU:HA	1.90	0.42
10:K:412:LEU:HA	10:K:412:LEU:HD12	1.76	0.42
5:F:471:PHE:HD1	5:F:471:PHE:H	1.68	0.42
10:K:197:LEU:HD11	10:K:231:PHE:CE1	2.55	0.42
10:K:198:ALA:N	10:K:199:PRO:HD2	2.34	0.42
10:K:314:PHE:CZ	10:K:407:ARG:HG3	2.54	0.42
2:D:335:ILE:HG22	2:D:337:SER:H	1.83	0.42
4:E:58:PRO:N	4:E:59:PRO:CD	2.83	0.42
5:F:541:ASP:OD1	5:F:543:ARG:NH1	2.53	0.42
10:K:381:PRO:O	10:K:383:GLN:N	2.53	0.42
1:A:560:ILE:HG23	1:A:565:ARG:HB2	2.02	0.42
2:B:638:LYS:HD2	2:B:638:LYS:HA	1.54	0.42
2:D:547:TYR:CD1	6:H:458:ILE:HD13	2.55	0.42
4:E:298:HIS:HD2	5:F:466:GLN:OE1	2.03	0.42
4:E:49:ILE:O	4:E:51:ASP:N	2.53	0.41
1:A:124:PHE:CE1	1:A:443:GLU:HB3	2.54	0.41
1:A:318:ILE:O	1:A:320:LEU:N	2.50	0.41
2:B:320:HIS:CE1	2:B:322:ILE:HG13	2.55	0.41
2:B:437:MET:HE1	6:H:502:ALA:CB	2.49	0.41
3:C:132:GLU:HG3	6:H:462:ASN:HB3	2.03	0.41
11:L:66:LYS:HA	11:L:67:PRO:HD3	1.78	0.41
2:B:667:ARG:HD2	2:B:670:ILE:HD12	2.01	0.41
2:D:463:LYS:O	2:D:466:GLU:HG3	2.20	0.41
2:D:536:LEU:HD23	2:D:536:LEU:HA	1.92	0.41
11:L:112:LEU:HD12	11:L:141:ILE:HD12	2.02	0.41
1:A:115:PRO:HB3	2:D:724:ILE:HD12	2.02	0.41
4:E:205:ARG:HA	4:E:205:ARG:NE	2.36	0.41
6:H:468:LEU:HD23	6:H:468:LEU:HA	1.86	0.41
10:K:418:GLN:HG2	10:K:419:TYR:CD1	2.56	0.41
11:L:91:LEU:CD2	11:L:106:LEU:HD22	2.50	0.41
2:B:611:ILE:O	2:B:615:VAL:HG13	2.20	0.41
3:C:237:LEU:HD13	3:C:237:LEU:O	2.21	0.41
4:E:455:LEU:HD23	4:E:458:LEU:HD11	2.02	0.41
7:I:1049:LEU:C	7:I:1051:LYS:H	2.24	0.41
10:K:381:PRO:HG2	10:K:382:GLU:H	1.86	0.41
3:C:128:CYS:HB3	2:D:670:ILE:HD12	2.02	0.41
4:E:290:ILE:CG1	5:F:745:VAL:HG21	2.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:702:LEU:HD22	7:I:728:THR:HG23	2.02	0.41
7:I:994:CYS:HB3	7:I:1057:PHE:CE1	2.55	0.41
1:A:428:ARG:HA	1:A:428:ARG:HD3	1.77	0.41
2:B:740:LEU:HD12	2:B:740:LEU:HA	1.84	0.41
2:D:549:VAL:O	2:D:553:VAL:HG23	2.21	0.41
4:E:32:LYS:O	4:E:36:ARG:HG3	2.20	0.41
9:J:59:ARG:HE	9:J:59:ARG:HB2	1.63	0.41
11:L:156:LEU:HD23	11:L:156:LEU:HA	1.76	0.41
2:B:307:ILE:O	8:G:82:UNK:HA	2.21	0.41
2:B:307:ILE:HG22	2:B:311:SER:HB2	2.02	0.41
2:B:350:MET:HE2	2:B:385:LEU:HD12	2.02	0.41
2:B:385:LEU:HD23	2:B:385:LEU:HA	1.86	0.41
2:B:420:ARG:HG2	7:I:697:LEU:HD21	2.03	0.41
2:B:537:LYS:NZ	2:B:541:GLU:OE2	2.54	0.41
2:B:704:LEU:HD23	2:B:704:LEU:HA	1.76	0.41
2:D:516:LYS:O	2:D:519:ILE:HG12	2.21	0.41
7:I:665:LYS:HB2	7:I:665:LYS:HE2	1.72	0.41
7:I:1239:ILE:HG23	7:I:1298:GLN:HG3	2.03	0.41
10:K:180:VAL:CG1	10:K:332:LEU:HG	2.48	0.41
10:K:458:GLU:O	10:K:460:TYR:N	2.53	0.41
11:L:146:SER:O	11:L:149:ALA:HB3	2.21	0.41
11:L:166:THR:HG22	11:L:167:HIS:CE1	2.56	0.41
11:L:429:PHE:HE1	11:L:433:GLN:HE21	1.68	0.41
1:A:350:GLU:N	1:A:350:GLU:OE1	2.54	0.41
2:B:766:GLN:HE21	2:B:766:GLN:HB2	1.69	0.41
3:C:165:THR:HB	2:D:712:ARG:HH22	1.86	0.41
4:E:320:VAL:HG22	4:E:474:ASP:OD2	2.21	0.41
5:F:456:GLN:OE1	5:F:481:LYS:HD3	2.20	0.41
6:H:513:LEU:HD23	6:H:513:LEU:HA	1.91	0.41
5:F:360:TYR:HD2	5:F:362:PRO:HG2	1.87	0.40
5:F:466:GLN:C	5:F:468:ARG:H	2.24	0.40
10:K:314:PHE:CE1	10:K:329:LEU:HD23	2.57	0.40
11:L:403:CYS:N	11:L:404:PRO:CD	2.83	0.40
2:B:299:ILE:N	2:B:300:PRO:HD2	2.37	0.40
2:B:429:LYS:HB3	2:B:429:LYS:HE2	1.90	0.40
2:B:461:LYS:HE2	2:D:600:PHE:CE1	2.57	0.40
7:I:936:ARG:HD2	8:G:128:TYR:HB3	2.04	0.40
3:C:162:LYS:HA	3:C:163:PRO:HD3	1.87	0.40
3:C:237:LEU:C	3:C:237:LEU:CD1	2.85	0.40
4:E:207:VAL:C	4:E:209:ASP:N	2.74	0.40
7:I:797:ASP:O	7:I:801:GLU:HG2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:1030:LEU:HD13	7:I:1136:PHE:CZ	2.57	0.40
10:K:188:PHE:CZ	10:K:319:ILE:HD13	2.57	0.40
11:L:183:LEU:HD23	11:L:183:LEU:HA	1.81	0.40
2:B:687:ILE:HD11	2:D:687:ILE:HD13	2.03	0.40
2:B:715:LEU:HD23	2:B:715:LEU:HA	1.92	0.40
2:D:409:THR:HG22	5:F:407:ILE:HG22	2.03	0.40
4:E:38:HIS:CE1	4:E:113:LEU:HD11	2.56	0.40
4:E:205:ARG:HG2	4:E:226:VAL:CG1	2.52	0.40
5:F:448:GLN:OE1	5:F:485:LEU:HG	2.21	0.40
10:K:389:LEU:HD22	10:K:421:LEU:CD2	2.52	0.40
11:L:148:ALA:HB1	11:L:428:ILE:O	2.22	0.40
1:A:157:THR:HB	1:A:284:LYS:HG3	2.03	0.40
3:C:181:ARG:HB3	3:C:185:ASP:HB2	2.02	0.40
2:D:636:SER:HG	2:D:640:GLN:HG3	1.86	0.40
7:I:1050:GLU:O	7:I:1050:GLU:CG	2.70	0.40
11:L:26:ASN:HB3	11:L:29:THR:O	2.21	0.40
11:L:154:ILE:O	11:L:154:ILE:HG22	2.21	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	360/566 (64%)	344 (96%)	15 (4%)	1 (0%)	41	71
2	B	385/825 (47%)	361 (94%)	21 (6%)	3 (1%)	19	51
2	D	413/825 (50%)	383 (93%)	27 (6%)	3 (1%)	22	54
3	C	146/332 (44%)	134 (92%)	10 (7%)	2 (1%)	11	36
4	E	272/623 (44%)	245 (90%)	24 (9%)	3 (1%)	14	42
5	F	379/905 (42%)	333 (88%)	43 (11%)	3 (1%)	19	51
6	H	240/1703 (14%)	230 (96%)	9 (4%)	1 (0%)	34	66

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	I	506/1314 (38%)	486 (96%)	15 (3%)	5 (1%)	15	45
8	G	13/82 (16%)	12 (92%)	1 (8%)	0	100	100
9	J	45/157 (29%)	42 (93%)	2 (4%)	1 (2%)	6	24
10	K	360/477 (76%)	340 (94%)	17 (5%)	3 (1%)	19	51
11	L	381/467 (82%)	360 (94%)	19 (5%)	2 (0%)	29	61
All	All	3500/8276 (42%)	3270 (93%)	203 (6%)	27 (1%)	24	51

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	431	SER
2	B	432	VAL
4	E	208	ASP
5	F	358	ASN
7	I	867	PRO
7	I	868	ILE
7	I	1029	GLN
7	I	1051	LYS
11	L	48	ASP
1	A	62	PRO
3	C	92	ASN
5	F	369	SER
2	D	445	ASN
9	J	84	LEU
10	K	382	GLU
10	K	459	ASP
4	E	50	LEU
4	E	504	PRO
10	K	458	GLU
11	L	155	SER
2	D	401	PRO
2	D	446	THR
7	I	905	ARG
2	B	523	ILE
5	F	322	PRO
6	H	443	ILE
3	C	93	ILE

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	345/517 (67%)	325 (94%)	20 (6%)	20	50
2	B	368/751 (49%)	346 (94%)	22 (6%)	19	49
2	D	392/751 (52%)	367 (94%)	25 (6%)	17	45
3	C	141/288 (49%)	133 (94%)	8 (6%)	20	51
4	E	257/558 (46%)	233 (91%)	24 (9%)	9	27
5	F	351/823 (43%)	334 (95%)	17 (5%)	25	58
6	H	222/1520 (15%)	206 (93%)	16 (7%)	14	39
7	I	500/1218 (41%)	479 (96%)	21 (4%)	30	63
8	G	7/15 (47%)	6 (86%)	1 (14%)	3	10
9	J	52/140 (37%)	51 (98%)	1 (2%)	57	84
10	K	345/420 (82%)	326 (94%)	19 (6%)	21	53
11	L	359/423 (85%)	337 (94%)	22 (6%)	18	48
All	All	3339/7424 (45%)	3143 (94%)	196 (6%)	23	49

All (196) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	85	LEU
1	A	130	SER
1	A	135	ASN
1	A	153	ASN
1	A	156	TRP
1	A	157	THR
1	A	159	ARG
1	A	181	PHE
1	A	267	LYS
1	A	315	THR
1	A	318	ILE
1	A	333	TYR
1	A	337	HIS
1	A	360	ASN

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Mol	Chain	Res	Type
1	A	430	ASP
1	A	479	LYS
1	A	489	SER
1	A	497	SER
1	A	523	SER
1	A	561	LEU
2	B	353	SER
2	B	387	LYS
2	B	391	ILE
2	B	432	VAL
2	B	452	THR
2	B	453	LEU
2	B	460	SER
2	B	462	ARG
2	B	465	ASP
2	B	535	LEU
2	B	542	PHE
2	B	555	ASN
2	B	563	LEU
2	B	578	ASP
2	B	635	GLU
2	B	711	GLU
2	B	734	SER
2	B	741	SER
2	B	773	MET
2	B	775	SER
2	B	780	LEU
2	B	787	PHE
3	C	95	HIS
3	C	105	SER
3	C	129	ASP
3	C	183	THR
3	C	185	ASP
3	C	196	HIS
3	C	233	TYR
3	C	240	TYR
2	D	309	SER
2	D	312	LYS
2	D	345	ARG
2	D	353	SER
2	D	391	ILE
2	D	449	SER

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Mol	Chain	Res	Type
2	D	451	SER
2	D	455	LYS
2	D	457	LEU
2	D	460	SER
2	D	461	LYS
2	D	526	ASN
2	D	542	PHE
2	D	557	SER
2	D	564	ARG
2	D	589	LEU
2	D	601	SER
2	D	622	THR
2	D	625	SER
2	D	633	SER
2	D	709	GLU
2	D	710	LEU
2	D	723	LEU
2	D	762	GLU
2	D	779	THR
4	E	37	GLU
4	E	43	LEU
4	E	112	TYR
4	E	113	LEU
4	E	114	PHE
4	E	209	ASP
4	E	226	VAL
4	E	230	SER
4	E	231	THR
4	E	239	LEU
4	E	280	GLN
4	E	290	ILE
4	E	317	GLN
4	E	318	PHE
4	E	325	SER
4	E	328	SER
4	E	454	LEU
4	E	455	LEU
4	E	462	THR
4	E	505	ILE
4	E	508	LYS
4	E	513	ASP
4	E	519	TYR

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Mol	Chain	Res	Type
4	E	568	TYR
5	F	321	LEU
5	F	328	SER
5	F	360	TYR
5	F	379	HIS
5	F	391	ARG
5	F	406	SER
5	F	425	ARG
5	F	467	ASP
5	F	554	GLN
5	F	578	SER
5	F	616	ASP
5	F	636	ASP
5	F	656	SER
5	F	728	ARG
5	F	730	PHE
5	F	736	SER
5	F	743	VAL
6	H	427	LEU
6	H	430	LEU
6	H	442	ASP
6	H	447	ASP
6	H	459	SER
6	H	480	GLU
6	H	511	ASP
6	H	522	THR
6	H	524	SER
6	H	558	SER
6	H	560	LEU
6	H	569	SER
6	H	596	ARG
6	H	650	LYS
6	H	651	LYS
6	H	659	LEU
7	I	698	PHE
7	I	713	SER
7	I	741	SER
7	I	774	THR
7	I	808	THR
7	I	867	PRO
7	I	903	ASN
7	I	939	SER

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Mol	Chain	Res	Type
7	I	940	ARG
7	I	980	SER
7	I	1003	SER
7	I	1051	LYS
7	I	1085	LEU
7	I	1105	LEU
7	I	1106	LEU
7	I	1115	SER
7	I	1124	SER
7	I	1143	SER
7	I	1207	LEU
7	I	1214	ILE
7	I	1308	ASP
8	G	118	ARG
9	J	90	ARG
10	K	2	THR
10	K	79	ASN
10	K	122	ARG
10	K	216	ARG
10	K	230	GLN
10	K	246	LEU
10	K	251	LYS
10	K	293	LYS
10	K	301	LEU
10	K	319	ILE
10	K	321	ASP
10	K	343	SER
10	K	380	SER
10	K	386	SER
10	K	397	SER
10	K	418	GLN
10	K	432	ARG
10	K	442	THR
10	K	462	THR
11	L	7	ASP
11	L	32	VAL
11	L	34	GLU
11	L	41	ILE
11	L	48	ASP
11	L	52	THR
11	L	54	HIS
11	L	56	THR

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Mol	Chain	Res	Type
11	L	69	GLN
11	L	94	ARG
11	L	100	ASP
11	L	105	GLU
11	L	122	SER
11	L	181	ASP
11	L	197	SER
11	L	291	GLU
11	L	321	ASP
11	L	323	ILE
11	L	347	GLU
11	L	359	ILE
11	L	422	SER
11	L	438	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	87	HIS
1	A	95	HIS
1	A	116	HIS
1	A	153	ASN
1	A	171	ASN
1	A	355	ASN
1	A	358	ASN
1	A	359	HIS
1	A	419	GLN
1	A	549	ASN
1	A	556	ASN
1	A	563	ASN
2	B	301	GLN
2	B	555	ASN
2	B	738	ASN
2	B	766	GLN
3	C	200	GLN
2	D	303	HIS
2	D	325	GLN
2	D	359	ASN
2	D	394	GLN
2	D	416	HIS
2	D	522	GLN
2	D	567	GLN

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Mol	Chain	Res	Type
2	D	587	ASN
2	D	640	GLN
2	D	678	GLN
2	D	680	ASN
2	D	690	GLN
4	E	280	GLN
4	E	298	HIS
4	E	317	GLN
4	E	330	GLN
4	E	452	ASN
4	E	473	HIS
5	F	434	ASN
5	F	534	GLN
5	F	556	GLN
5	F	614	ASN
6	H	462	ASN
6	H	537	GLN
6	H	564	HIS
6	H	589	HIS
7	I	675	ASN
7	I	718	ASN
7	I	805	ASN
7	I	915	ASN
7	I	970	ASN
7	I	981	ASN
7	I	1006	GLN
7	I	1029	GLN
7	I	1100	ASN
7	I	1120	GLN
7	I	1300	GLN
11	L	303	ASN
11	L	304	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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.

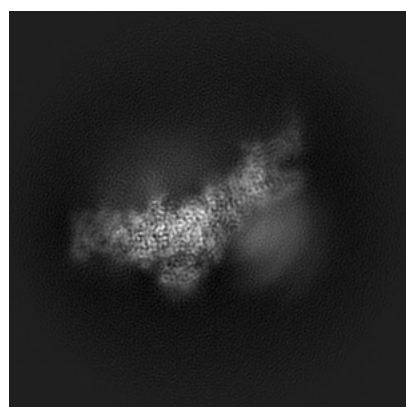
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30285. These allow visual inspection of the internal detail of the map and identification of artifacts.

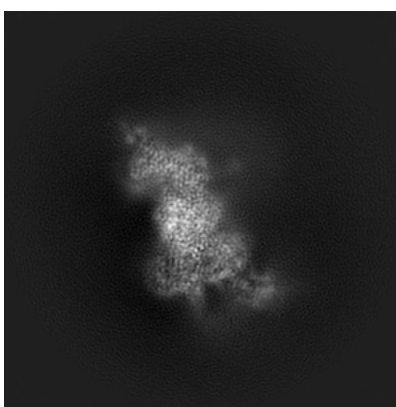
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

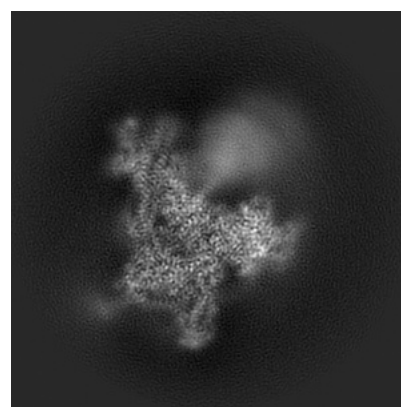
6.1.1 Primary map



X



Y

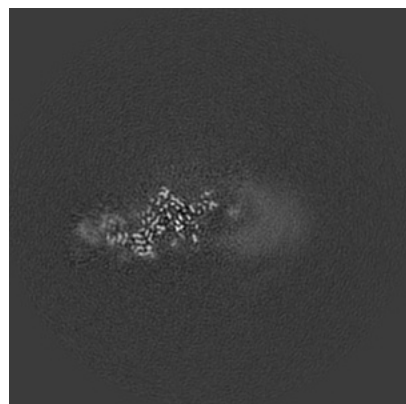


Z

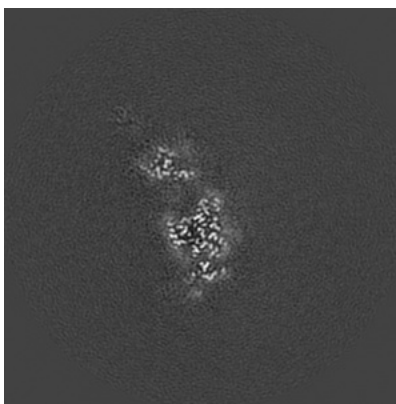
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

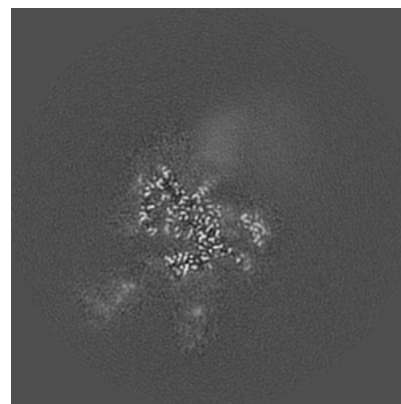
6.2.1 Primary map



X Index: 160



Y Index: 160

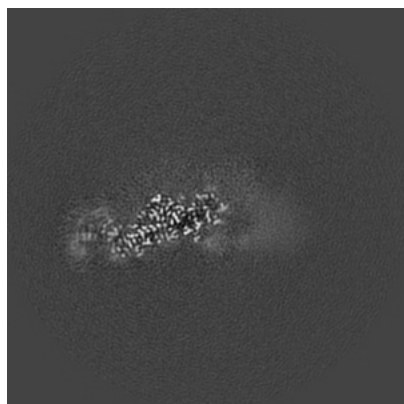


Z Index: 160

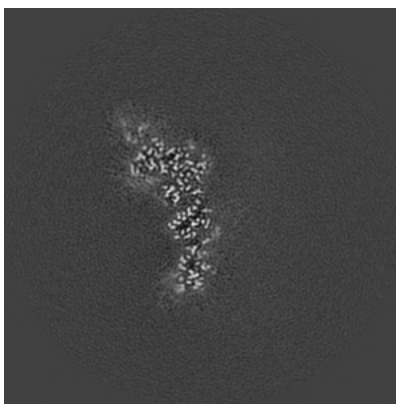
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

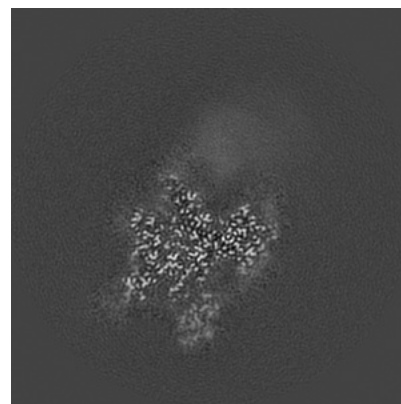
6.3.1 Primary map



X Index: 152



Y Index: 143

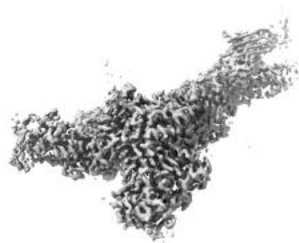


Z Index: 146

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

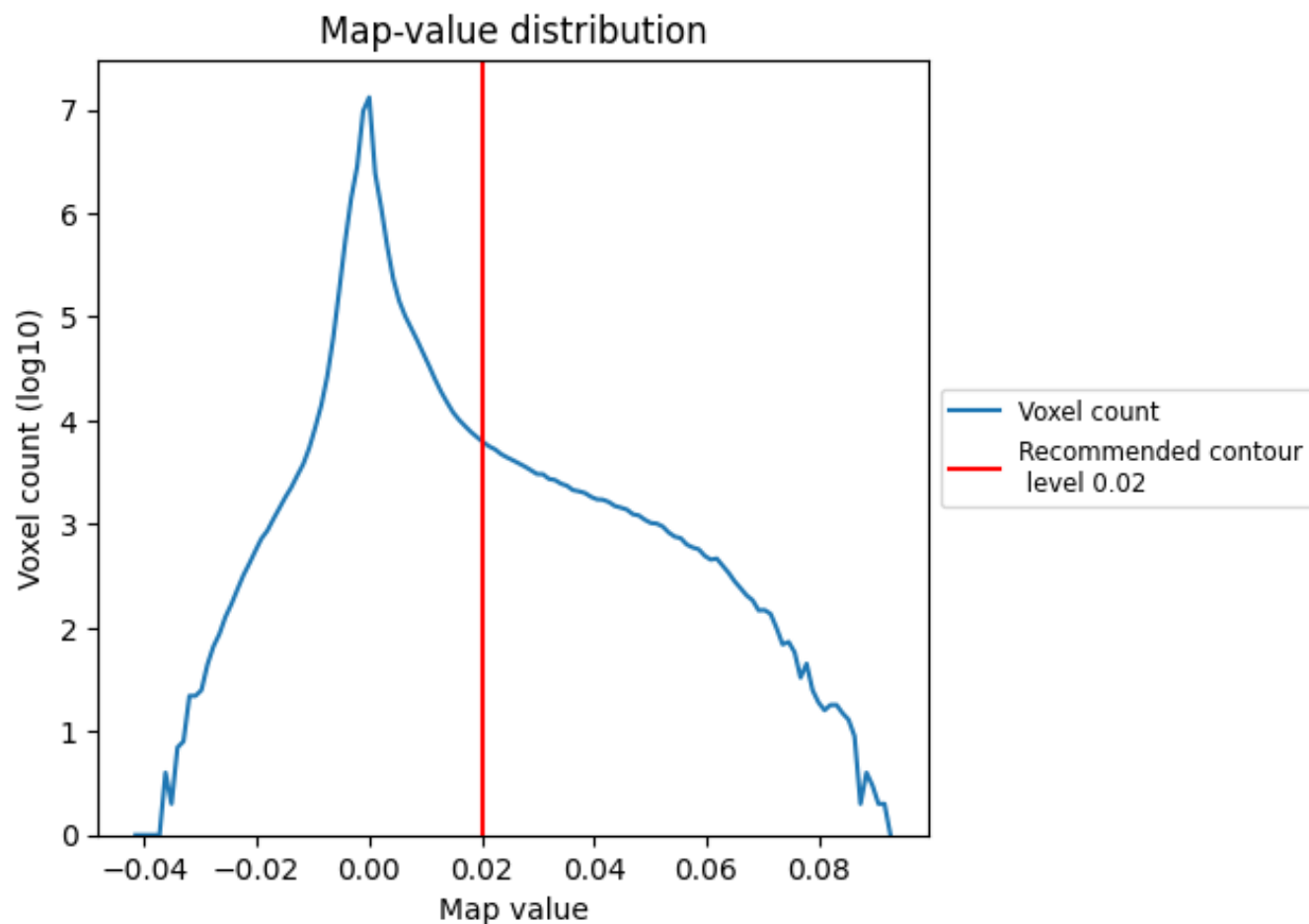
6.5 Mask visualisation

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

7 Map analysis [i](#)

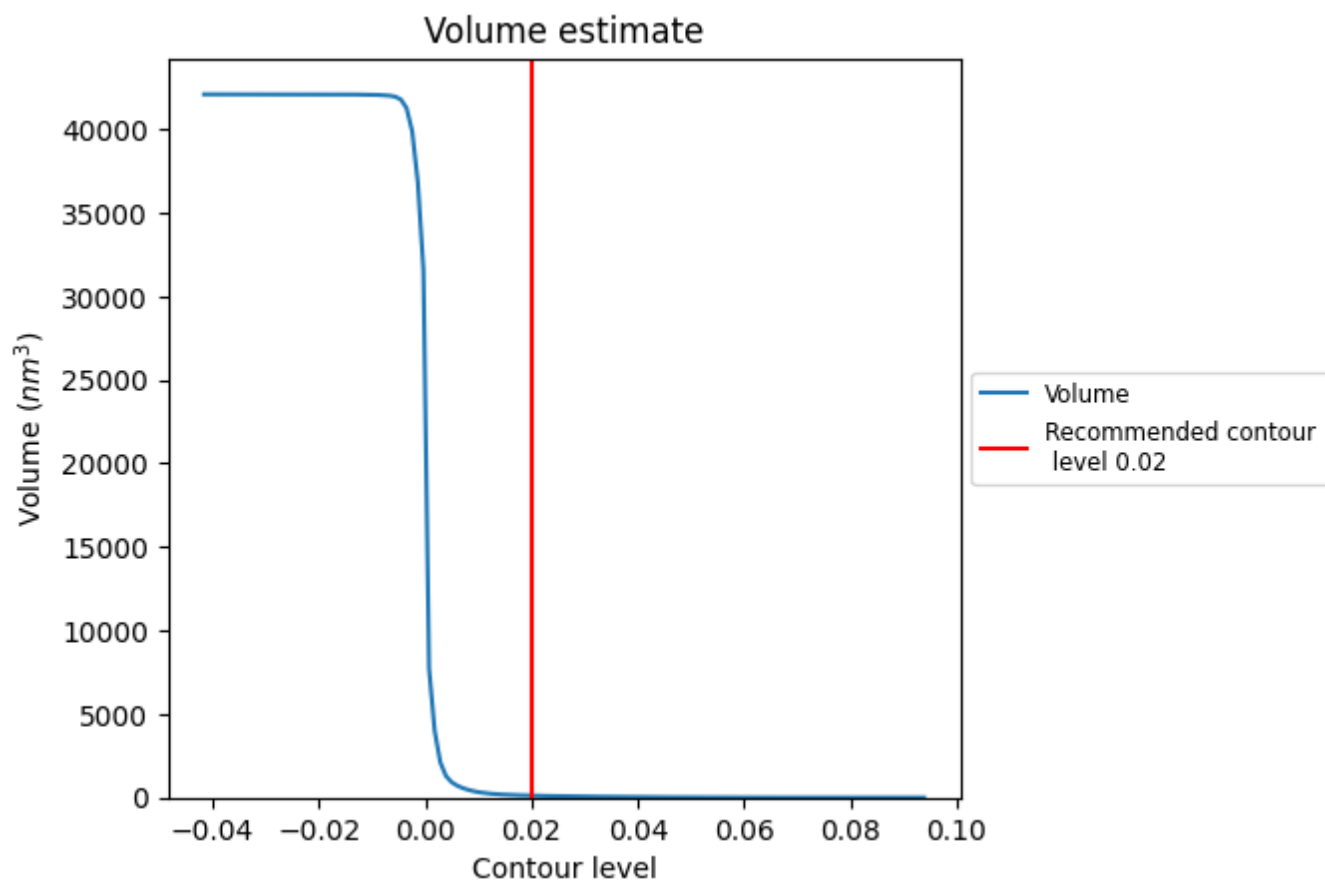
This section contains the results of statistical analysis of the map.

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.

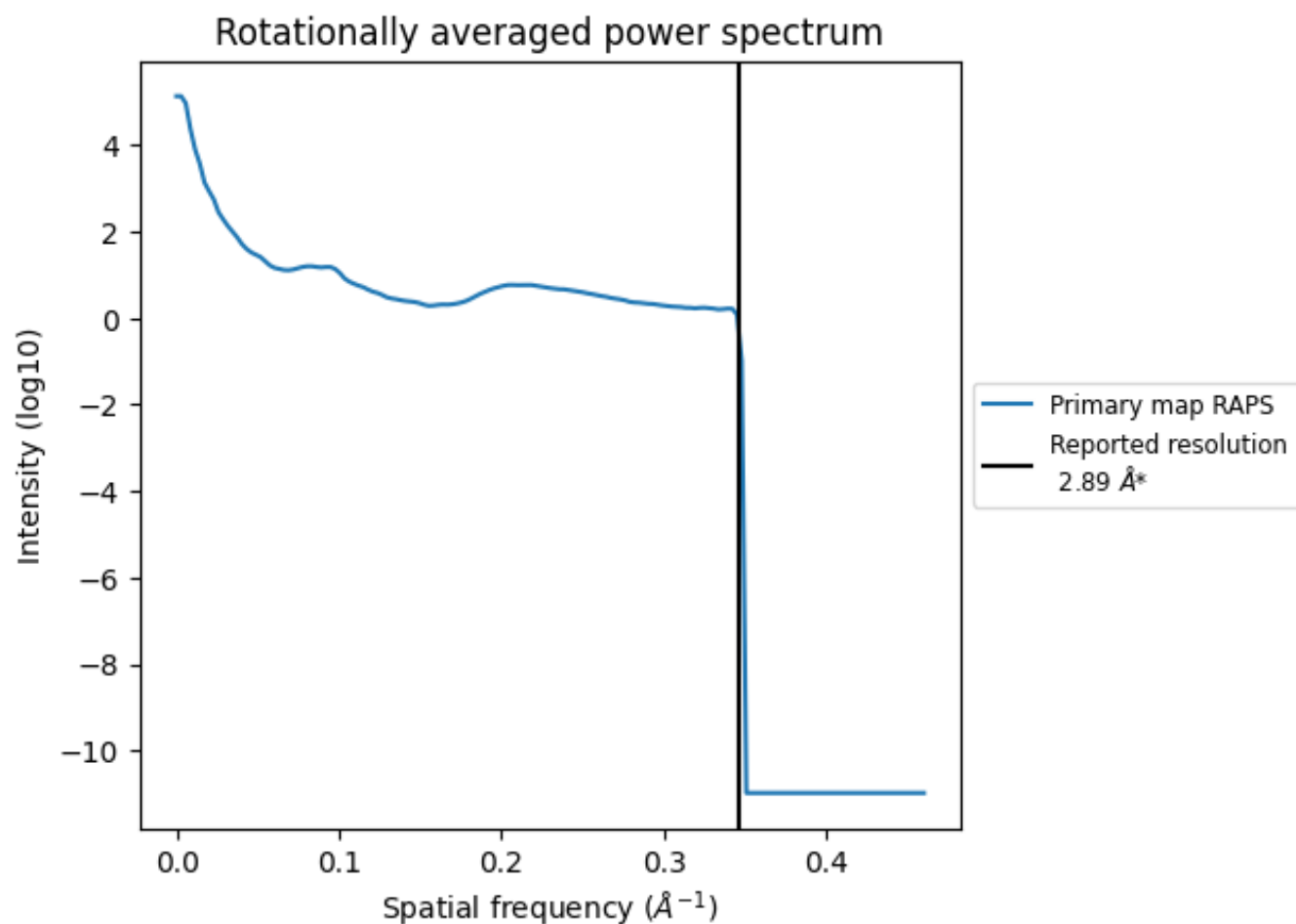
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 117 nm^3 ; this corresponds to an approximate mass of 106 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 0.346 Å⁻¹

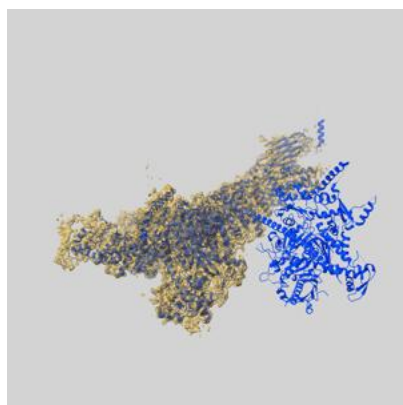
8 Fourier-Shell correlation

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

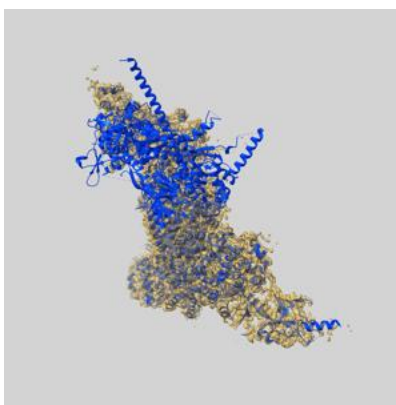
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-30285 and PDB model 7C4J. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

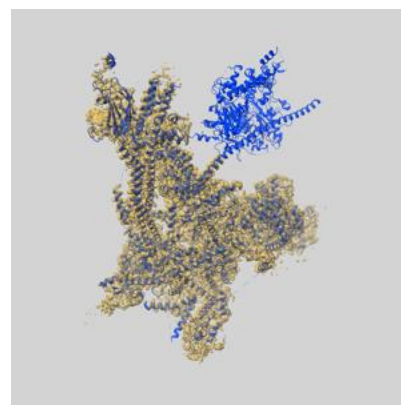
9.1 Map-model overlay [i](#)



X



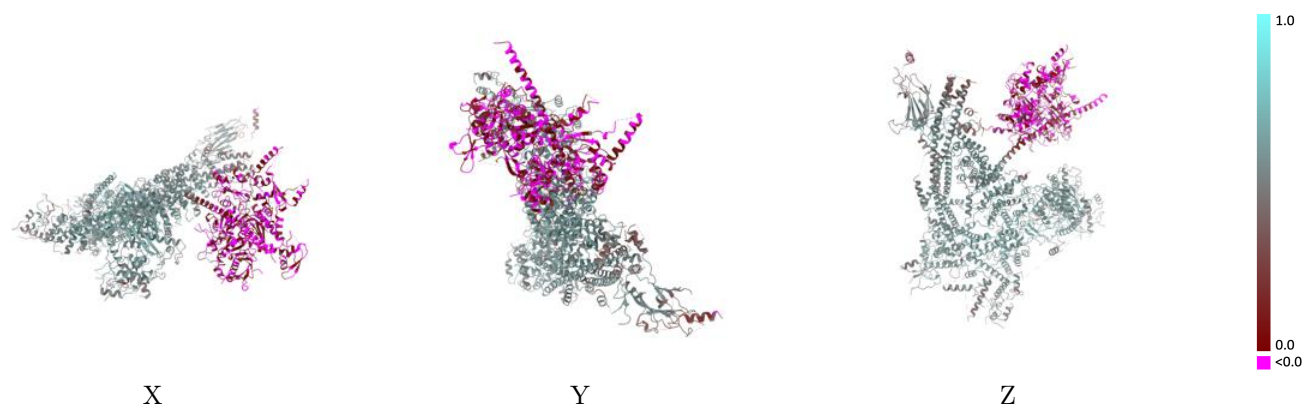
Y



Z

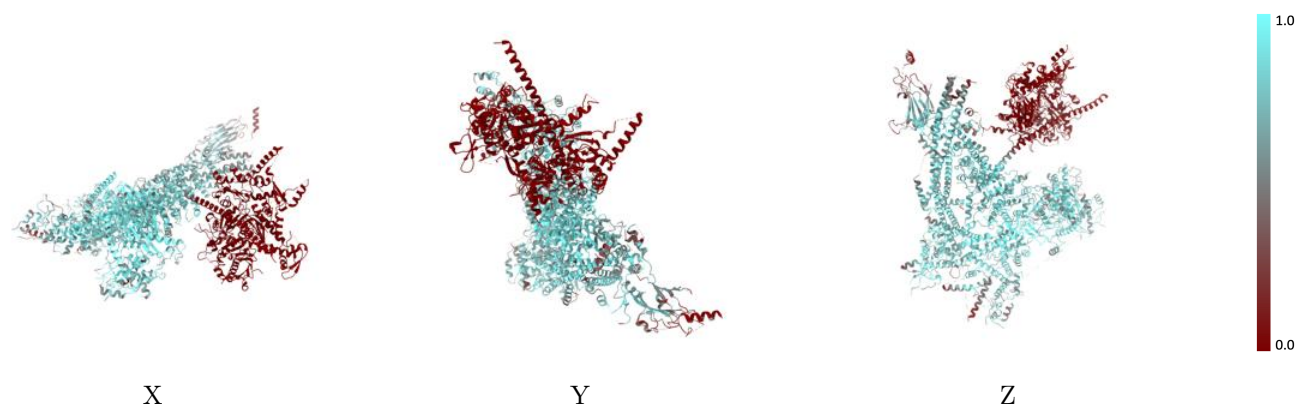
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



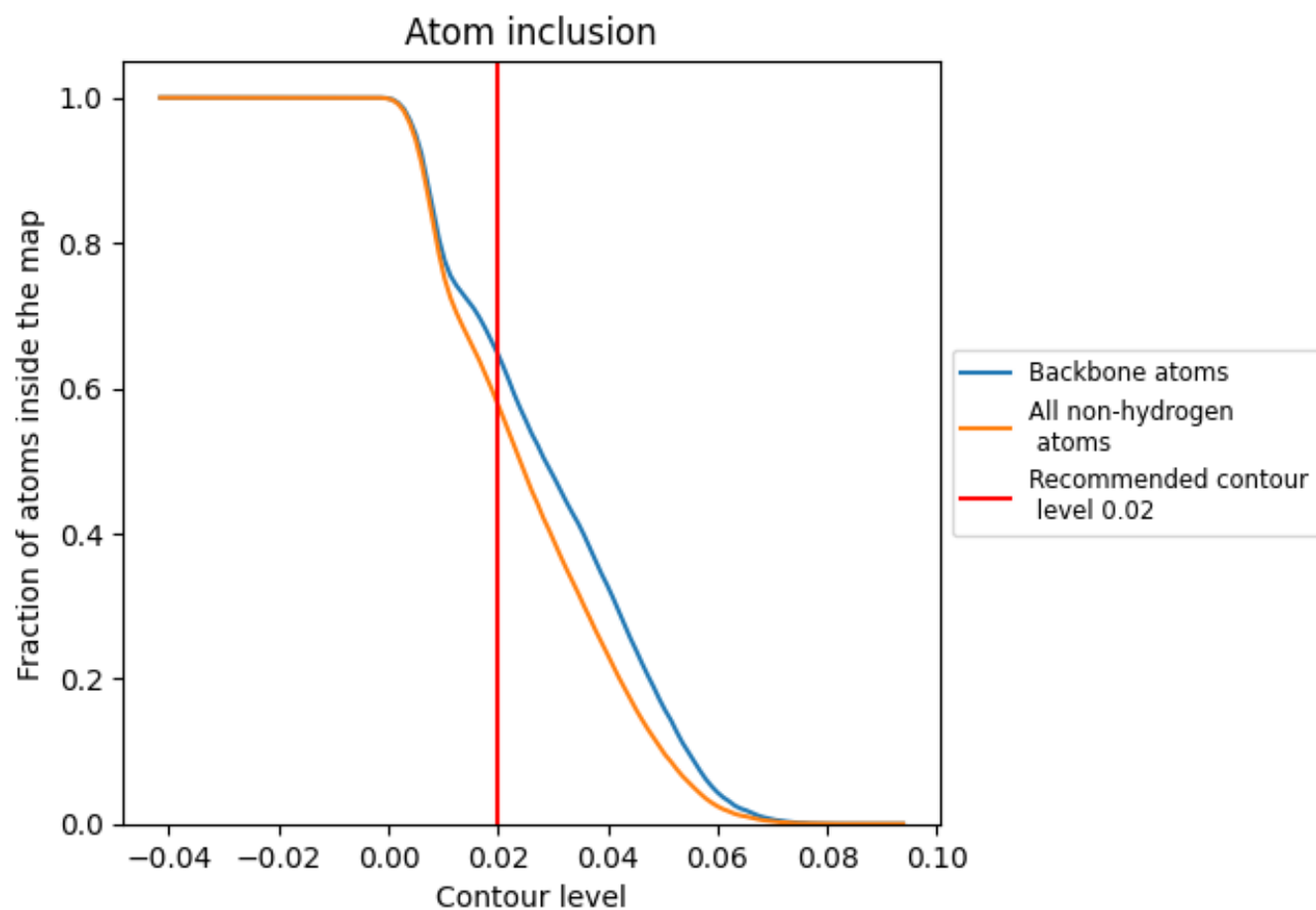
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).



























9.4 Atom inclusion [i](#)



At the recommended contour level, 65% of all backbone atoms, 58% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5773	 0.4210
A	 0.6749	 0.5210
B	 0.7748	 0.5570
C	 0.6392	 0.5020
D	 0.7583	 0.5560
E	 0.7078	 0.5270
F	 0.8218	 0.5720
G	 0.7985	 0.5180
H	 0.5779	 0.4090
I	 0.8424	 0.5850
J	 0.0000	 0.0470
K	 0.0000	 0.0130
L	 0.0000	 0.0160

