



Full wwPDB EM Validation Report ⓘ

Dec 8, 2025 – 08:37 AM EST

PDB ID : 9YNW / pdb_00009ynw
EMDB ID : EMD-73236
Title : Tra1, Core and minimal HAT modules of ctSAGA, composite.
Authors : Mattoo, R.U.H.; Chen, D.H.; Bushnell, D.A.; Tamir, S.; Kornberg, R.D.
Deposited on : 2025-10-12
Resolution : 3.50 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:

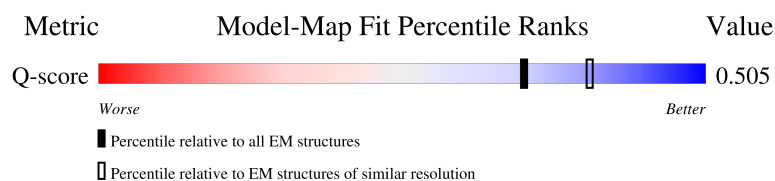
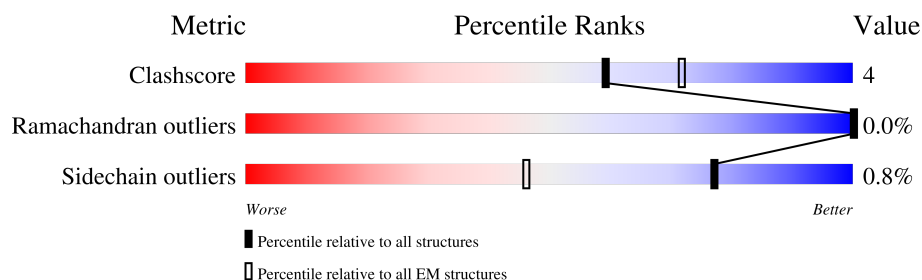
EMDB validation analysis : 0.0.1.dev129
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.47

1 Overall quality at a glance

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

The reported resolution of this entry is 3.50 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.





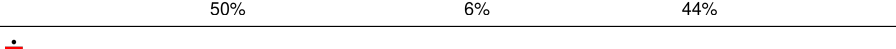




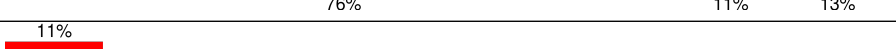


Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	13950 (3.00 - 4.00)

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	3893	
2	B	1192	
3	C	433	
4	D	767	

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Mol	Chain	Length	Quality of chain
5	E	480	
6	F	277	
7	G	204	
8	I	770	
9	K	1196	
10	Q	1273	
11	H	485	
12	M	519	
13	N	405	
14	O	730	

2 Entry composition [i](#)

There are 14 unique types of molecules in this entry. The entry contains 121271 atoms, of which 60418 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 Non-specific serine/threonine protein kinase.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	3619	Total	C	H	N	O	S	0	0
			58964	18811	29628	5111	5270	144		

- Molecule 2 is a protein called Spt20-like SEP domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	245	Total	C	H	N	O	S	0	0
			3987	1319	1952	341	368	7		

- Molecule 3 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	197	Total	C	H	N	O	S	0	0
			3225	1022	1607	287	303	6		

- Molecule 4 is a protein called Transcription initiation factor TFIID subunit 5.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	D	523	Total	C	H	N	O	S	0	0
			8240	2632	4096	730	762	20		

- Molecule 5 is a protein called Transcription initiation factor TFIID subunit 6.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	E	443	Total	C	H	N	O	S	0	0
			6959	2193	3519	598	639	10		

- Molecule 6 is a protein called Putative transcription initiation factor.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	F	121	Total	C	H	N	O	S	0	0
			1461	578	546	170	166	1		

- Molecule 7 is a protein called Transcription initiation factor TFIID subunit 10.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	G	114	Total	C	H	N	O	S	0	0
			1762	556	879	157	166	4		

- Molecule 8 is a protein called Transcription initiation factor TFIID subunit 12.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	I	154	Total	C	H	N	O	S	0	0
			2269	744	1084	215	220	6		

- Molecule 9 is a protein called Putative transcriptional activator protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	K	587	Total	C	H	N	O	S	0	0
			9498	2973	4741	858	908	18		

- Molecule 10 is a protein called SCA7 domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	Q	62	Total	C	H	N	O	S	0	0
			950	303	472	86	88	1		

- Molecule 11 is a protein called Putative transcriptional coactivator HFI1 protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	H	341	Total	C	H	N	O	S	0	0
			5279	1681	2613	463	509	13		

- Molecule 12 is a protein called Transcriptional adapter 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	M	464	Total	C	H	N	O	S	0	0
			7393	2333	3681	656	701	22		

- Molecule 13 is a protein called histone acetyltransferase.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	N	352	Total	C	H	N	O	S	0	0
			5764	1846	2874	498	530	16		

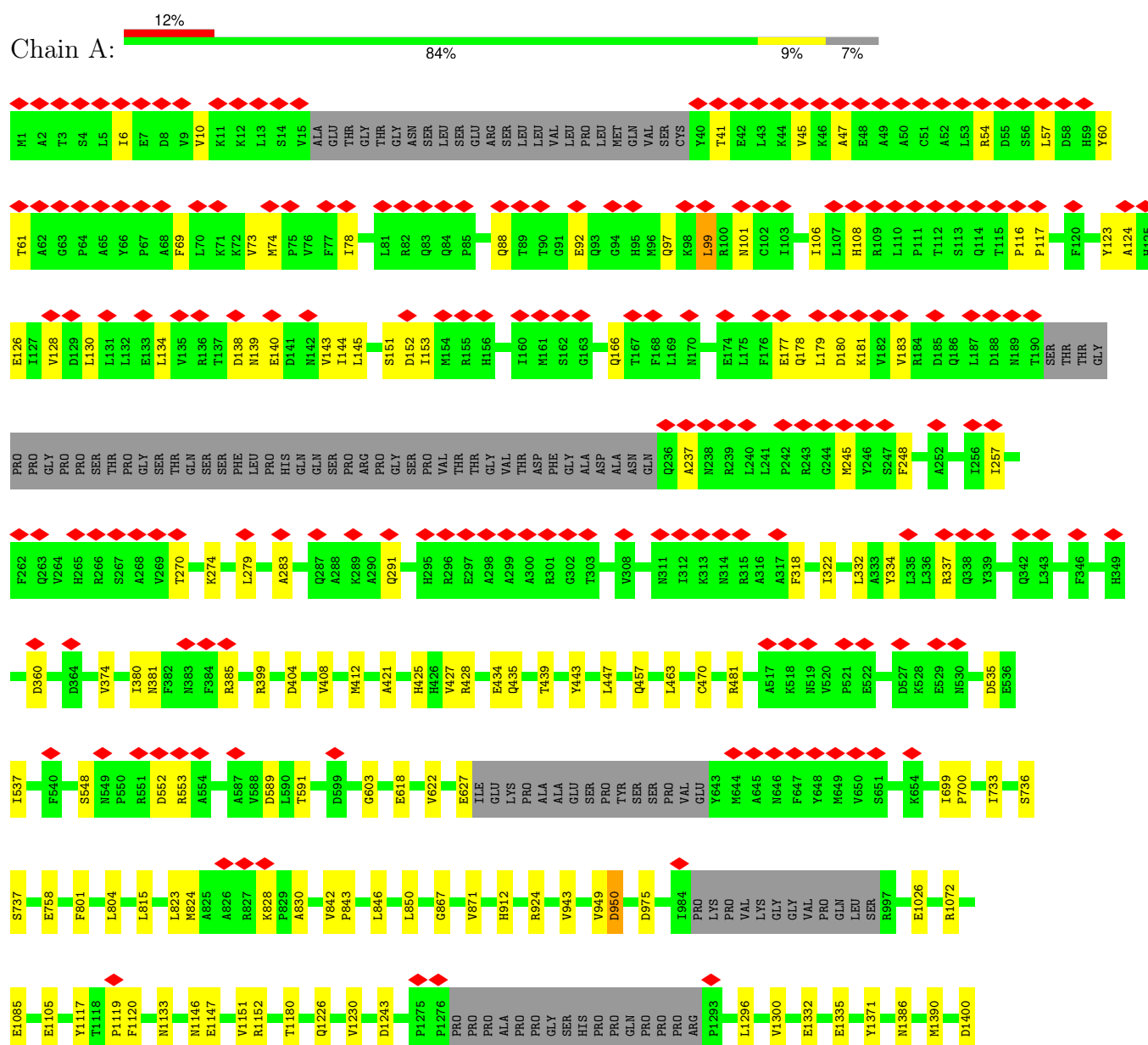
- Molecule 14 is a protein called Uncharacterized protein.

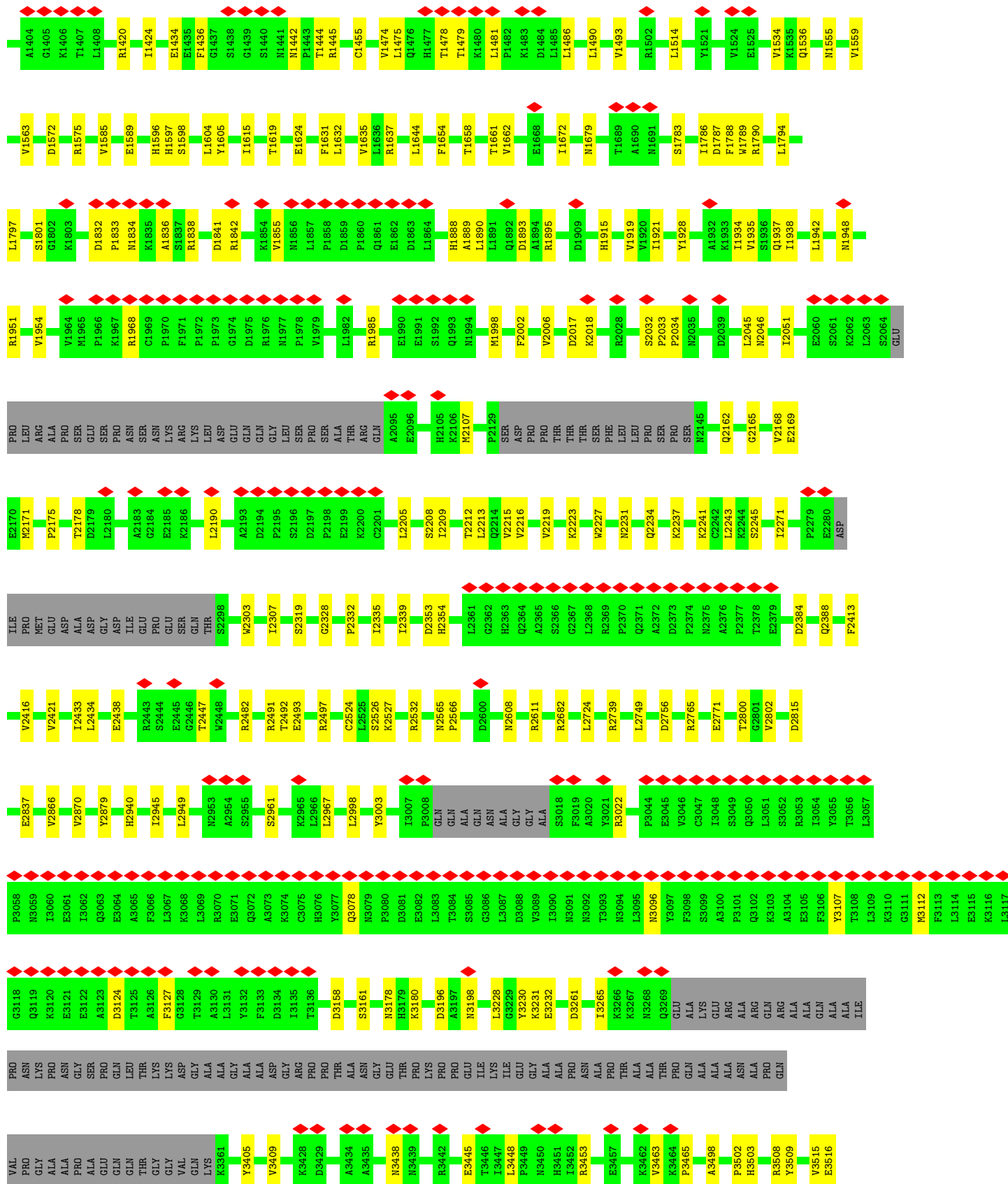
Mol	Chain	Residues	Atoms						AltConf	Trace
14	O	346	Total	C	H	N	O	S	0	0
			5520	1745	2726	491	546	12		

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.

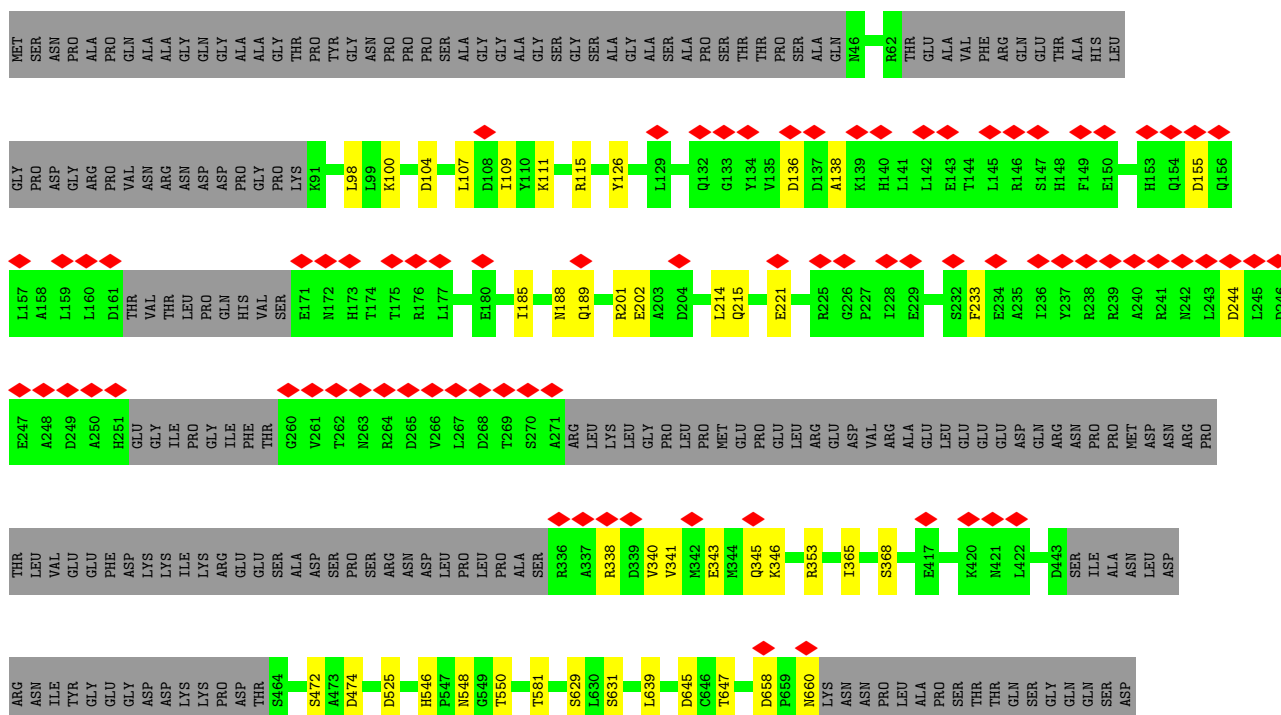
- Molecule 1: Non-specific serine/threonine protein kinase

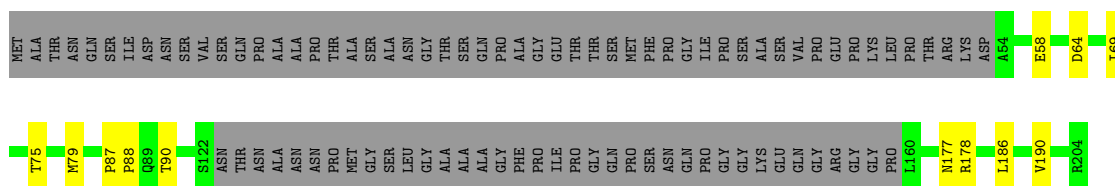
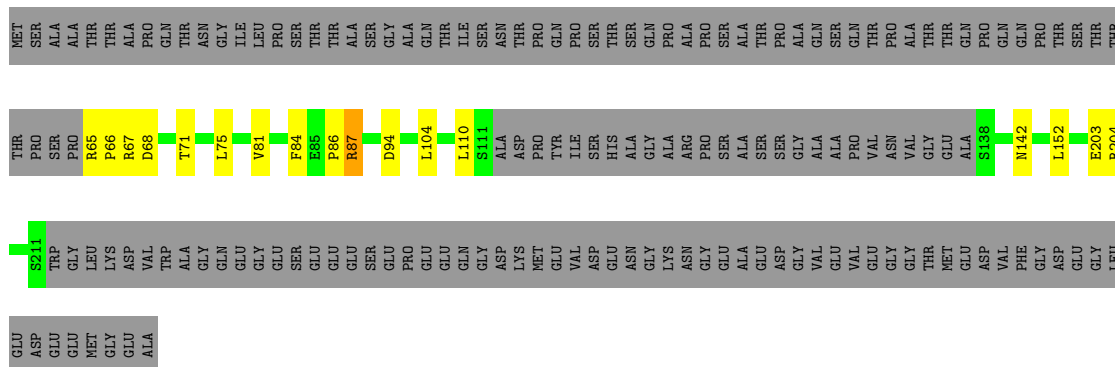
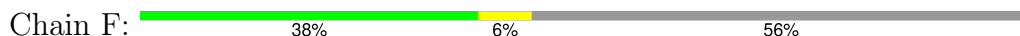
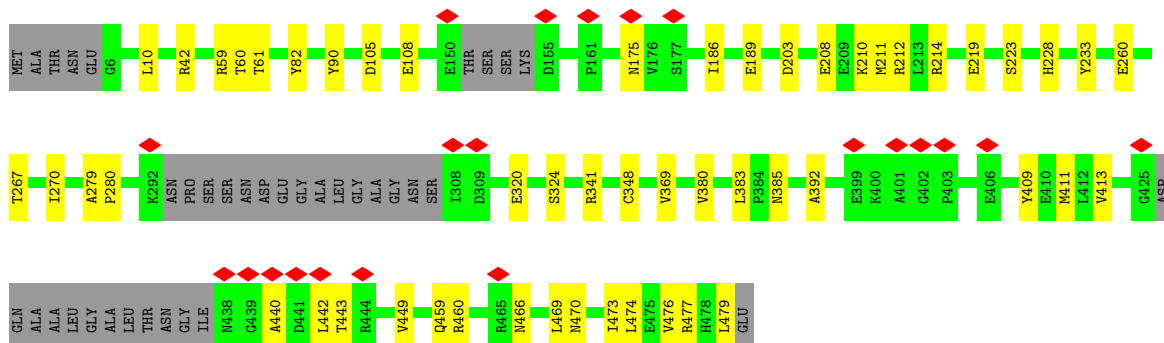
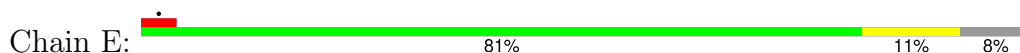
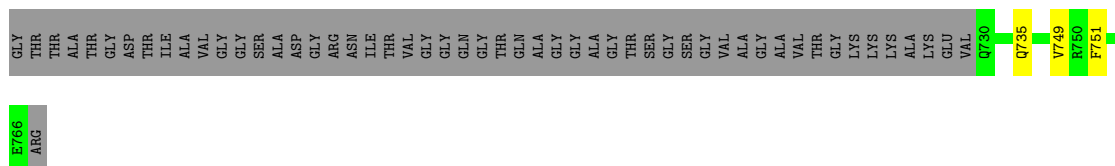


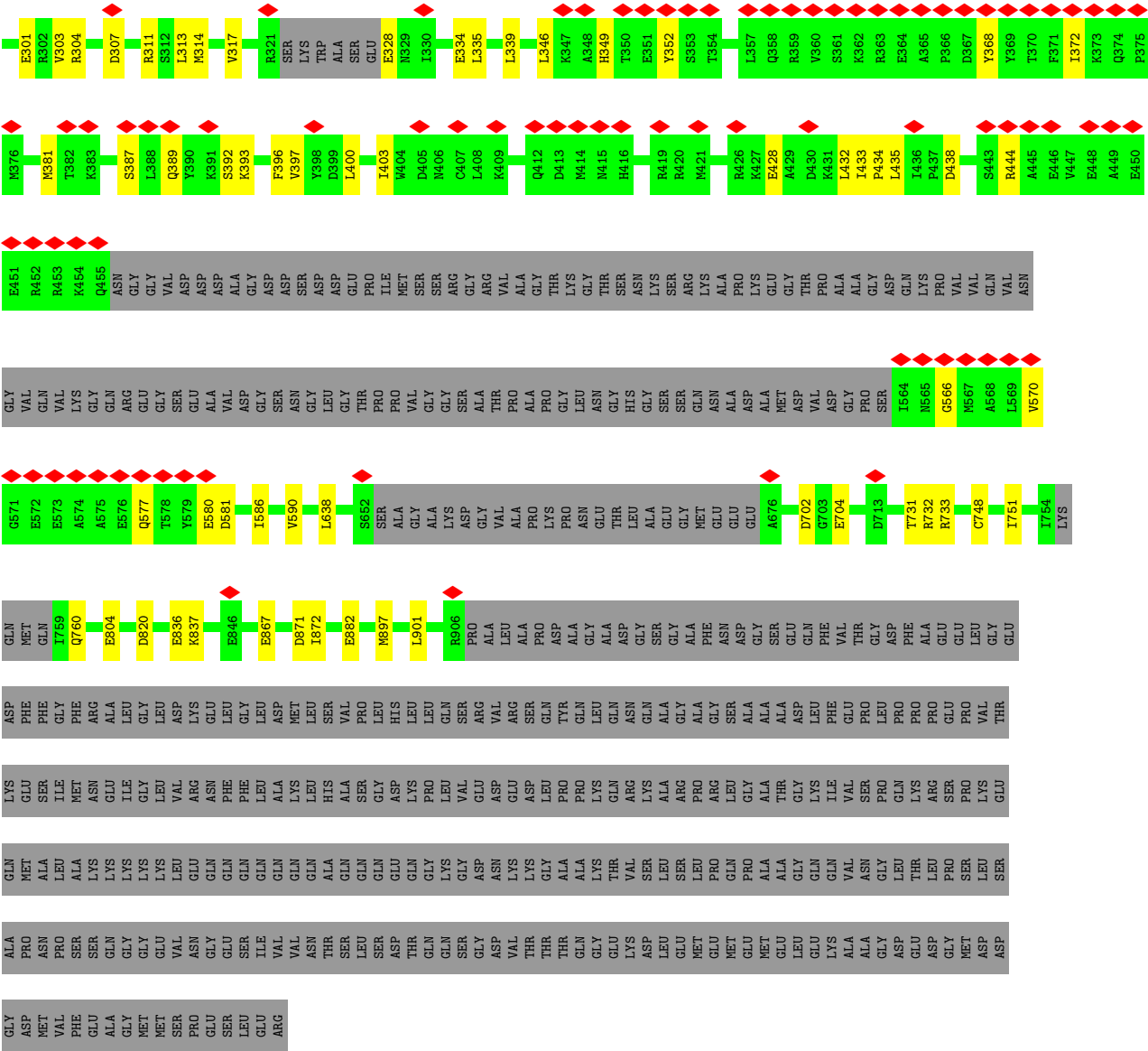




Chain C:  5% 38% 7% 50%

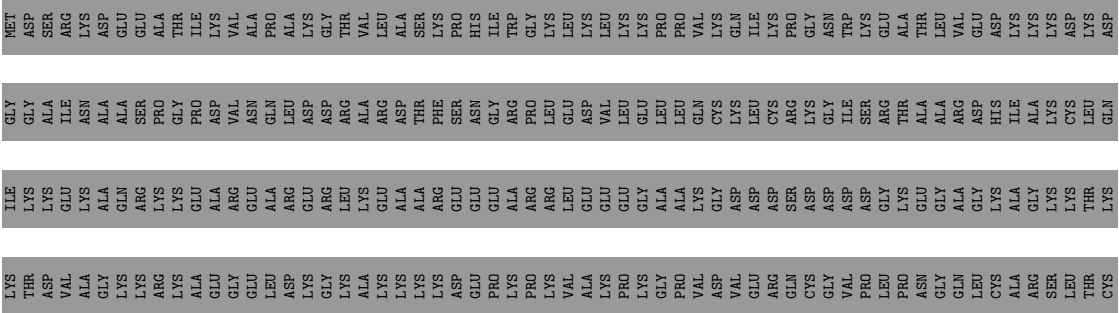


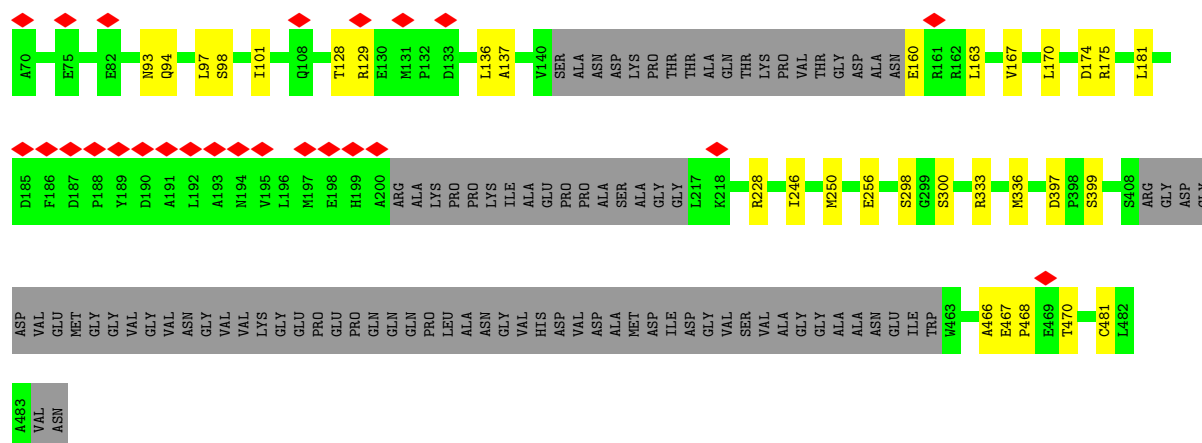




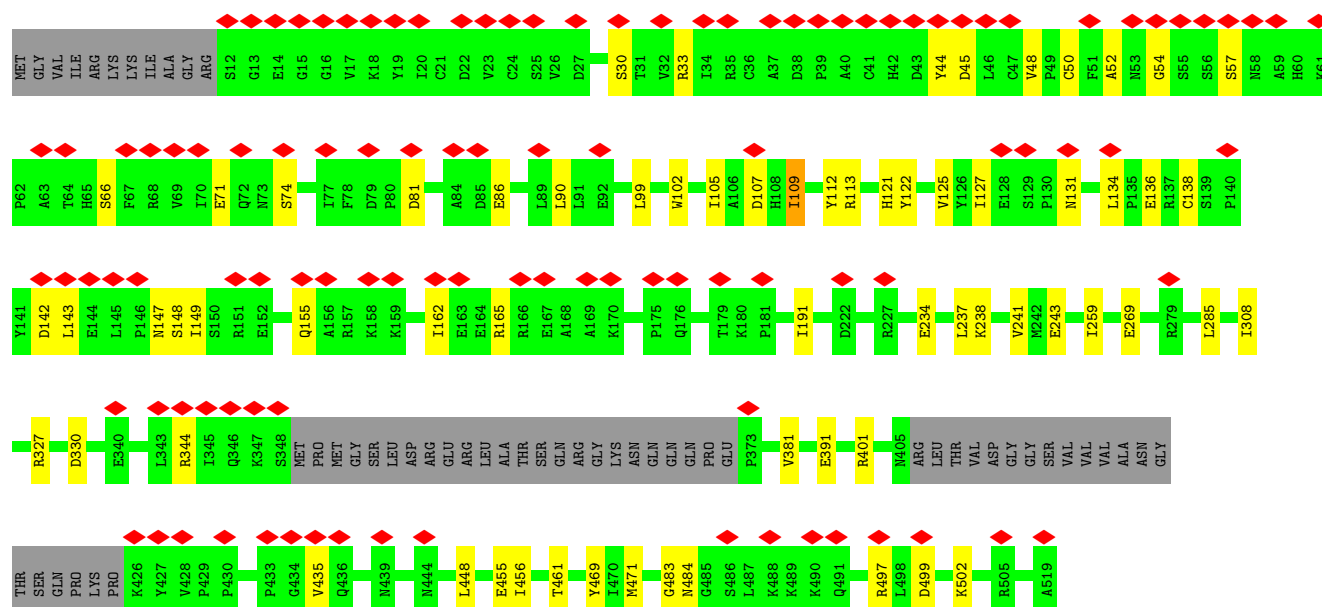
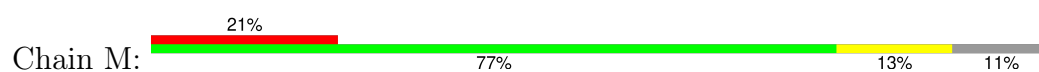
● Molecule 10: SCA7 domain-containing protein

Chain Q: . 95%

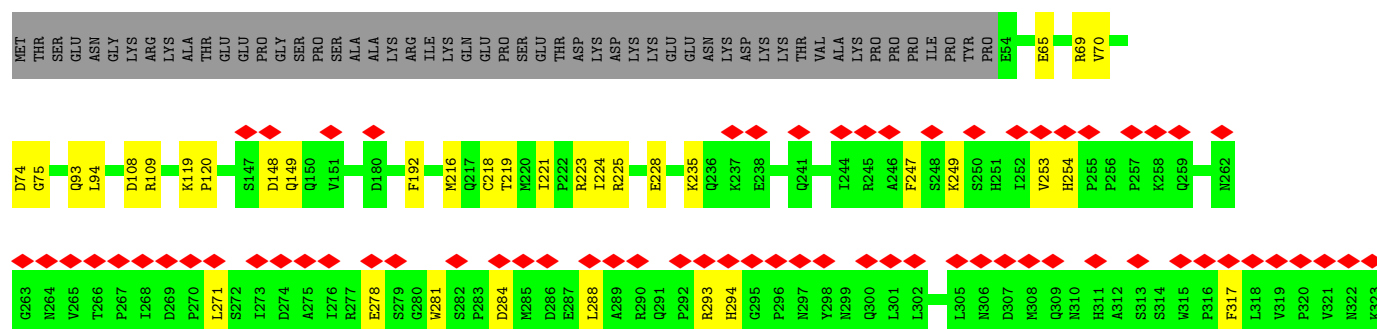
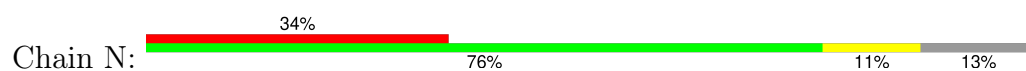


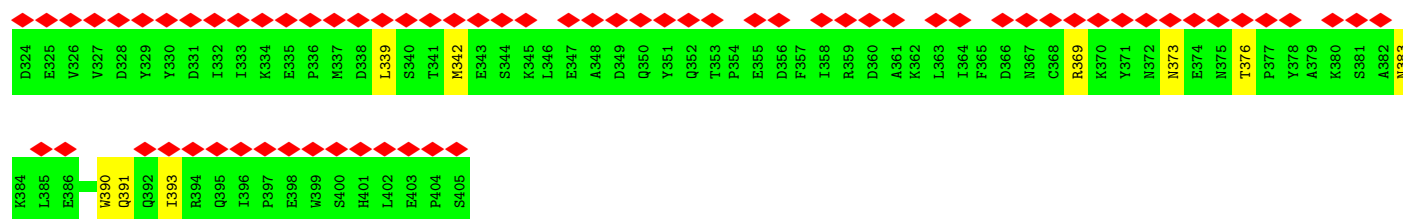


• Molecule 12: Transcriptional adapter 2

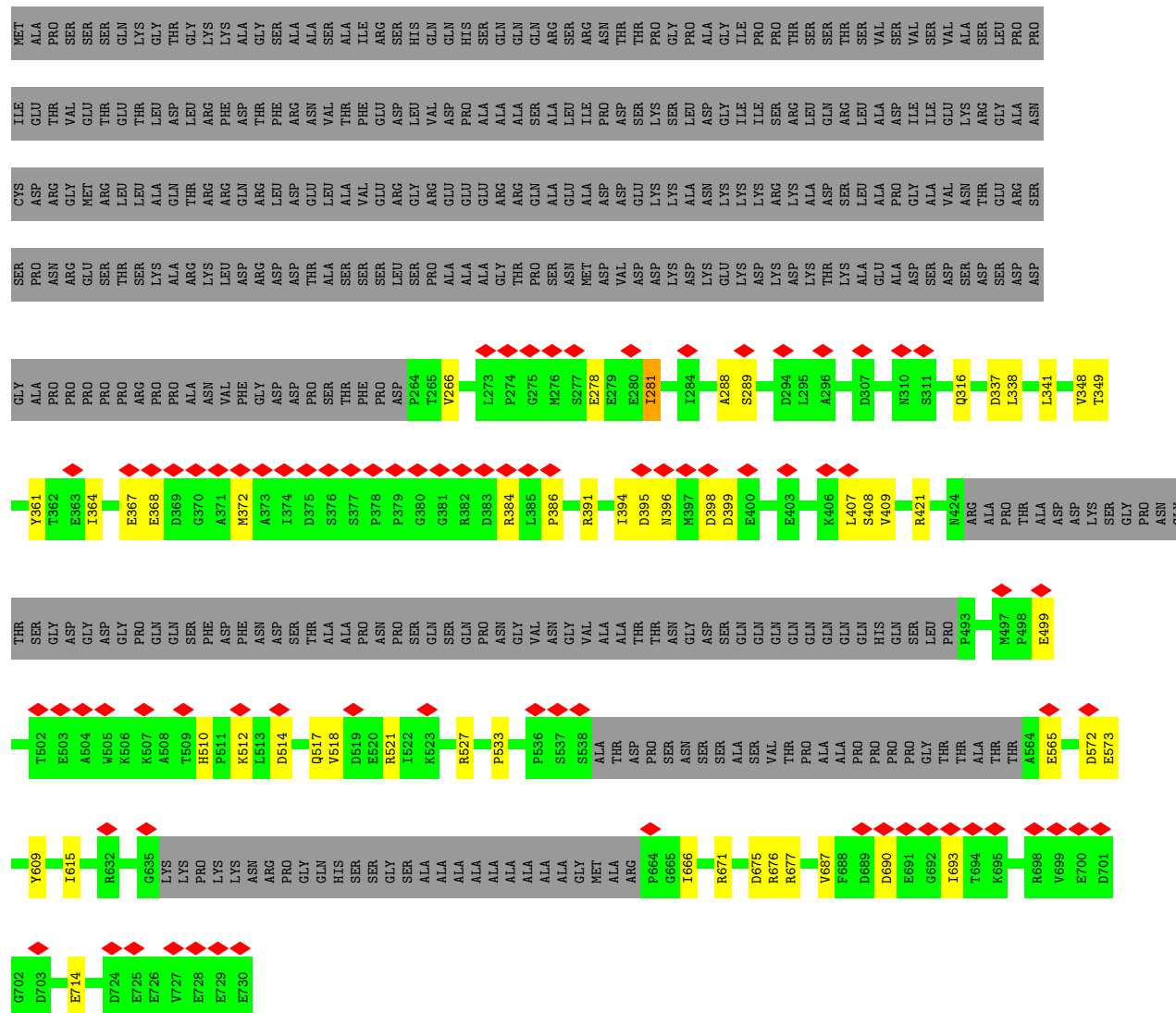
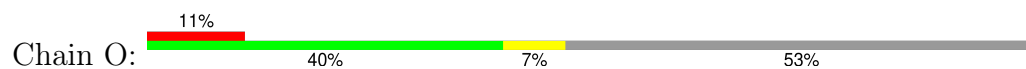


• Molecule 13: histone acetyltransferase





• Molecule 14: Uncharacterized protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	3566416	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	68.9	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	71.846	Depositor
Minimum map value	-0.910	Depositor
Average map value	0.421	Depositor
Map value standard deviation	1.062	Depositor
Recommended contour level	7	Depositor
Map size (Å)	503.844, 502.803, 521.541	wwPDB
Map dimensions	484, 483, 501	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.041, 1.041, 1.041	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	0.10	0/30011	0.26	0/40686
2	B	0.11	0/2094	0.23	0/2842
3	C	0.11	0/1649	0.24	0/2214
4	D	0.09	0/4235	0.26	0/5730
5	E	0.10	0/3505	0.25	0/4767
6	F	0.11	0/932	0.25	0/1259
7	G	0.12	0/899	0.25	0/1213
8	I	0.10	0/1203	0.26	0/1624
9	K	0.11	0/4832	0.25	0/6495
10	Q	0.11	0/489	0.22	0/667
11	H	0.09	0/2723	0.22	0/3686
12	M	0.08	0/3793	0.23	0/5121
13	N	0.08	0/2962	0.22	0/4003
14	O	0.09	0/2851	0.26	0/3848
All	All	0.10	0/62178	0.25	0/84155

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [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	29336	29628	29619	227	0
2	B	2035	1952	2013	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1618	1607	1602	23	0
4	D	4144	4096	4088	32	0
5	E	3440	3519	3515	43	0
6	F	915	546	922	23	0
7	G	883	879	877	9	0
8	I	1185	1084	1220	22	0
9	K	4757	4741	4740	54	0
10	Q	478	472	471	5	0
11	H	2666	2613	2609	24	0
12	M	3712	3681	3679	52	0
13	N	2890	2874	2873	28	0
14	O	2794	2726	2725	42	0
All	All	60853	60418	60953	536	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (536) 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)
11:H:128:THR:HG1	14:O:510:HIS:HD1	1.11	0.88
1:A:2756:ASP:OD1	8:I:628:TYR:OH	1.90	0.87
1:A:1888:HIS:O	1:A:1928:TYR:OH	1.98	0.81
1:A:1400:ASP:OD1	1:A:1420:ARG:NH2	2.13	0.80
14:O:386:PRO:O	14:O:391:ARG:NH2	2.15	0.80
4:D:546:HIS:ND1	4:D:548:ASN:OD1	2.14	0.79
14:O:671:ARG:NE	14:O:671:ARG:O	2.17	0.78
6:F:203:GLU:O	9:K:837:LYS:NZ	2.15	0.78
13:N:69:ARG:NH1	14:O:288:ALA:O	2.17	0.78
2:B:400:ARG:NH2	8:I:684:GLU:OE1	2.16	0.78
5:E:10:LEU:HD13	11:H:181:LEU:HD11	1.65	0.78
2:B:143:ARG:NH1	2:B:144:PHE:O	2.17	0.77
4:D:645:ASP:OD1	4:D:647:THR:OG1	2.02	0.76
11:H:129:ARG:O	14:O:521:ARG:NH2	2.18	0.76
12:M:162:ILE:HG21	13:N:288:LEU:HD21	1.66	0.76
5:E:203:ASP:O	5:E:214:ARG:NH1	2.18	0.76
4:D:472:SER:OG	4:D:474:ASP:OD1	2.04	0.75
1:A:3261:ASP:O	1:A:3265:ILE:HG22	1.85	0.75
12:M:234:GLU:OE1	12:M:234:GLU:N	2.20	0.75
14:O:572:ASP:OD1	14:O:573:GLU:N	2.20	0.75
12:M:243:GLU:OE1	14:O:677:ARG:NH2	2.20	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:341:ARG:NH1	9:K:86:GLY:O	2.19	0.74
8:I:746:GLN:N	8:I:746:GLN:OE1	2.19	0.74
1:A:3445:GLU:O	1:A:3453:ARG:NH1	2.21	0.74
13:N:249:LYS:NZ	13:N:278:GLU:OE1	2.20	0.74
1:A:2526:SER:O	1:A:2532:ARG:NH1	2.21	0.74
2:B:157:MET:HE2	10:Q:338:LEU:HD21	1.68	0.73
3:C:313:VAL:HG23	3:C:314:THR:HG23	1.71	0.73
1:A:2765:ARG:NH1	2:B:220:ILE:O	2.22	0.73
3:C:144:VAL:O	3:C:276:ARG:NH2	2.22	0.73
13:N:369:ARG:NE	13:N:383:ASN:OD1	2.22	0.72
14:O:675:ASP:OD1	14:O:676:ARG:N	2.21	0.72
5:E:385:ASN:CG	9:K:70:LEU:HD21	2.14	0.72
12:M:71:GLU:N	12:M:71:GLU:OE1	2.23	0.72
1:A:2438:GLU:OE2	1:A:2482:ARG:NH1	2.23	0.72
1:A:435:GLN:O	1:A:439:THR:HG23	1.90	0.71
8:I:647:GLU:N	8:I:647:GLU:OE1	2.22	0.71
2:B:229:PRO:O	2:B:230:SER:HB3	1.89	0.71
6:F:67:ARG:HG2	6:F:68:ASP:OD1	1.90	0.71
5:E:442:LEU:HD12	5:E:443:THR:N	2.06	0.71
1:A:1637:ARG:NH2	1:A:1679:ASN:OD1	2.24	0.70
4:D:215:GLN:OE1	4:D:341:VAL:HG23	1.90	0.70
1:A:1596:HIS:O	1:A:1597:HIS:ND1	2.25	0.70
9:K:352:TYR:OH	9:K:577:GLN:OE1	2.09	0.70
1:A:2303:TRP:CE2	1:A:2307:ILE:HD11	2.27	0.70
6:F:68:ASP:O	6:F:71:THR:HG22	1.92	0.70
12:M:66:SER:OG	13:N:254:HIS:O	2.07	0.70
12:M:391:GLU:OE1	12:M:401:ARG:NE	2.25	0.70
11:H:170:LEU:O	11:H:175:ARG:NH1	2.24	0.70
1:A:126:GLU:N	1:A:126:GLU:OE1	2.24	0.69
14:O:714:GLU:OE1	14:O:714:GLU:N	2.24	0.69
1:A:1928:TYR:O	1:A:1968:ARG:NH2	2.26	0.69
9:K:387:SER:O	9:K:389:GLN:NE2	2.25	0.69
8:I:651:GLU:OE1	8:I:655:ASN:ND2	2.25	0.69
1:A:1146:ASN:O	1:A:1152:ARG:NH1	2.25	0.69
1:A:2162:GLN:N	1:A:2162:GLN:OE1	2.26	0.68
1:A:1085:GLU:OE1	1:A:1085:GLU:N	2.26	0.68
1:A:548:SER:O	1:A:553:ARG:NH2	2.26	0.68
13:N:65:GLU:N	13:N:65:GLU:OE1	2.26	0.68
9:K:301:GLU:OE2	9:K:301:GLU:N	2.25	0.68
12:M:112:TYR:O	12:M:165:ARG:NH1	2.27	0.68
6:F:142:ASN:ND2	8:I:708:GLU:OE1	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:882:GLU:OE1	9:K:882:GLU:N	2.27	0.67
5:E:203:ASP:OD2	5:E:210:LYS:NZ	2.21	0.67
1:A:2237:LYS:O	1:A:2241:LYS:NZ	2.27	0.67
3:C:319:SER:OG	3:C:321:ASP:OD1	2.12	0.66
9:K:580:GLU:N	9:K:580:GLU:OE1	2.28	0.66
4:D:201:ARG:NH1	5:E:219:GLU:OE2	2.28	0.66
1:A:589:ASP:OD1	1:A:591:THR:HG23	1.94	0.66
1:A:2739:ARG:NH1	2:B:217:PRO:O	2.29	0.66
1:A:627:GLU:N	1:A:627:GLU:OE1	2.28	0.66
3:C:135:TRP:CD1	3:C:156:THR:HG21	2.30	0.66
1:A:2171:MET:O	1:A:2223:LYS:NZ	2.29	0.65
1:A:2815:ASP:OD1	8:I:625:ARG:NH1	2.28	0.65
1:A:2493:GLU:OE2	1:A:2497:ARG:NH1	2.29	0.65
5:E:108:GLU:N	5:E:108:GLU:OE1	2.30	0.65
1:A:1026:GLU:OE1	1:A:1026:GLU:N	2.30	0.65
12:M:136:GLU:N	12:M:136:GLU:OE1	2.29	0.65
9:K:296:ILE:HD11	9:K:303:VAL:HG11	1.79	0.64
1:A:2447:THR:OG1	3:C:283:GLU:OE2	2.10	0.64
12:M:48:VAL:O	12:M:52:ALA:N	2.31	0.64
5:E:189:GLU:N	5:E:189:GLU:OE1	2.30	0.63
4:D:365:ILE:HD11	5:E:228:HIS:HB2	1.79	0.63
14:O:565:GLU:OE1	14:O:565:GLU:N	2.30	0.63
1:A:1478:THR:O	1:A:1479:THR:OG1	2.12	0.63
8:I:610:GLN:OE1	8:I:610:GLN:HA	1.97	0.63
9:K:392:SER:OG	9:K:438:ASP:OD1	2.13	0.63
13:N:70:VAL:N	14:O:289:SER:OG	2.25	0.63
1:A:1436:PHE:O	1:A:1445:ARG:NH1	2.31	0.62
6:F:68:ASP:HA	6:F:71:THR:HG22	1.81	0.62
9:K:871:ASP:OD1	9:K:872:ILE:N	2.32	0.62
12:M:269:GLU:N	12:M:269:GLU:OE1	2.32	0.62
12:M:344:ARG:NH2	14:O:368:GLU:OE1	2.33	0.62
1:A:2002:PHE:O	1:A:2006:VAL:HG23	1.99	0.62
1:A:912:HIS:CG	8:I:609:ILE:HG22	2.34	0.62
4:D:338:ARG:NH2	4:D:343:GLU:OE2	2.33	0.62
8:I:715:GLU:OE1	8:I:715:GLU:N	2.33	0.61
11:H:160:GLU:OE1	11:H:160:GLU:N	2.33	0.61
9:K:296:ILE:HD12	14:O:687:VAL:HG21	1.83	0.61
1:A:3178:ASN:OD1	1:A:3178:ASN:O	2.19	0.61
12:M:44:TYR:OH	12:M:57:SER:OG	2.08	0.61
1:A:1998:MET:SD	1:A:1998:MET:N	2.74	0.61
2:B:139:GLN:O	2:B:197:ARG:NH1	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1475:LEU:CD2	1:A:1481:LEU:HD21	2.31	0.60
1:A:2771:GLU:N	1:A:2771:GLU:OE1	2.35	0.60
3:C:137:GLU:N	3:C:137:GLU:OE1	2.35	0.60
4:D:109:ILE:HD13	5:E:320:GLU:OE1	2.02	0.60
5:E:449:VAL:HG21	5:E:470:ASN:OD1	2.01	0.60
1:A:2765:ARG:NH2	2:B:228:THR:O	2.36	0.59
9:K:69:ASP:OD1	9:K:72:ARG:NH1	2.35	0.59
11:H:298:SER:OG	11:H:333:ARG:NH2	2.35	0.59
1:A:457:GLN:N	1:A:457:GLN:OE1	2.35	0.59
1:A:2949:LEU:HD11	1:A:3003:TYR:CE1	2.37	0.59
12:M:50:CYS:O	12:M:54:GLY:N	2.35	0.59
1:A:1836:ALA:O	1:A:1838:ARG:NH2	2.35	0.59
1:A:180:ASP:OD1	1:A:181:LYS:N	2.36	0.59
1:A:434:GLU:N	1:A:434:GLU:OE1	2.35	0.59
6:F:86:PRO:O	6:F:87:ARG:HG2	2.03	0.59
9:K:586:ILE:O	9:K:590:VAL:HG23	2.03	0.59
3:C:321:ASP:OD1	3:C:321:ASP:N	2.35	0.59
11:H:397:ASP:OD1	11:H:399:SER:OG	2.21	0.59
1:A:1786:ILE:HD12	1:A:1786:ILE:H	1.69	0.58
5:E:348:CYS:HB3	5:E:369:VAL:HG23	1.85	0.58
12:M:86:GLU:OE2	12:M:113:ARG:NH1	2.36	0.58
1:A:2940:HIS:NE2	8:I:599:PRO:HD3	2.19	0.58
1:A:3760:PRO:HB2	1:A:3819:MET:HE1	1.84	0.58
1:A:3819:MET:HE3	1:A:3819:MET:HA	1.86	0.58
1:A:2945:ILE:HD11	1:A:2967:LEU:HD22	1.86	0.58
1:A:2608:ASN:OD1	1:A:2611:ARG:NH2	2.36	0.58
1:A:134:LEU:O	1:A:138:ASP:N	2.34	0.58
1:A:2245:SER:O	1:A:2319:SER:OG	2.23	0.57
1:A:3530:ASP:OD1	1:A:3530:ASP:N	2.36	0.57
12:M:30:SER:O	12:M:30:SER:OG	2.18	0.57
12:M:121:HIS:CE1	12:M:125:VAL:HG21	2.39	0.57
1:A:166:GLN:N	1:A:166:GLN:OE1	2.36	0.57
13:N:93:GLN:C	13:N:94:LEU:HD12	2.29	0.57
1:A:924:ARG:HG3	8:I:598:LEU:HD13	1.85	0.57
12:M:448:LEU:HD23	12:M:448:LEU:O	2.04	0.57
1:A:2384:ASP:O	1:A:2388:GLN:NE2	2.37	0.57
4:D:548:ASN:ND2	4:D:550:THR:OG1	2.37	0.57
3:C:247:GLU:OE1	3:C:247:GLU:N	2.33	0.57
2:B:235:TYR:CG	2:B:236:PRO:HD2	2.39	0.57
1:A:139:ASN:O	1:A:143:VAL:HG22	2.04	0.57
1:A:2205:LEU:O	1:A:2209:ILE:HG13	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:381:MET:HE3	9:K:403:ILE:HD11	1.86	0.57
1:A:1934:ILE:H	1:A:1934:ILE:HD12	1.68	0.56
1:A:1619:THR:HG21	1:A:1632:LEU:HD22	1.88	0.56
1:A:2384:ASP:OD1	1:A:2388:GLN:NE2	2.38	0.56
1:A:3228:LEU:HD12	1:A:3228:LEU:O	2.05	0.56
1:A:124:ALA:O	1:A:128:VAL:HG22	2.05	0.56
12:M:285:LEU:HD21	12:M:308:ILE:HD11	1.87	0.56
1:A:1797:LEU:O	1:A:1801:SER:N	2.38	0.56
1:A:1572:ASP:OD1	1:A:1575:ARG:NH2	2.38	0.56
2:B:410:ASP:OD1	2:B:410:ASP:N	2.38	0.56
1:A:828:LYS:O	1:A:830:ALA:N	2.37	0.56
3:C:147:GLU:OE1	3:C:393:ARG:NH2	2.38	0.56
11:H:136:LEU:HD23	11:H:137:ALA:N	2.21	0.56
1:A:950:ASP:OD2	1:A:3639:ARG:NH2	2.38	0.56
4:D:188:ASN:OD1	4:D:189:GLN:N	2.39	0.56
12:M:33:ARG:NH2	12:M:45:ASP:OD1	2.39	0.56
12:M:74:SER:OG	12:M:155:GLN:OE1	2.09	0.56
1:A:2492:THR:HG22	1:A:2493:GLU:H	1.70	0.55
5:E:279:ALA:HB3	5:E:280:PRO:HD3	1.88	0.55
5:E:469:LEU:O	5:E:473:ILE:HG13	2.07	0.55
1:A:3829:THR:OG1	1:A:3830:MET:N	2.39	0.55
12:M:330:ASP:N	12:M:330:ASP:OD1	2.39	0.55
1:A:2190:LEU:HD13	1:A:2205:LEU:HD23	1.89	0.55
1:A:270:THR:O	1:A:274:LYS:NZ	2.25	0.55
9:K:387:SER:OG	9:K:389:GLN:OE1	2.08	0.55
1:A:3158:ASP:O	1:A:3161:SER:OG	2.23	0.55
12:M:143:LEU:HD22	13:N:247:PHE:CE1	2.41	0.55
13:N:148:ASP:OD1	13:N:149:GLN:N	2.40	0.54
1:A:758:GLU:OE2	1:A:801:PHE:N	2.36	0.54
9:K:400:LEU:HA	9:K:403:ILE:HD12	1.88	0.54
6:F:68:ASP:HA	6:F:71:THR:CG2	2.37	0.54
14:O:408:SER:OG	14:O:409:VAL:N	2.41	0.54
1:A:1475:LEU:HD22	1:A:1481:LEU:HD21	1.90	0.54
14:O:690:ASP:OD1	14:O:690:ASP:N	2.38	0.54
4:D:346:LYS:HE2	5:E:212:ARG:CD	2.37	0.54
9:K:428:GLU:O	9:K:432:LEU:HD12	2.07	0.54
1:A:425:HIS:O	1:A:428:ARG:NH1	2.41	0.54
5:E:186:ILE:HD11	5:E:233:TYR:CE2	2.43	0.54
14:O:514:ASP:N	14:O:517:GLN:OE1	2.41	0.54
3:C:329:LEU:O	3:C:333:MET:HG3	2.06	0.53
12:M:191:ILE:N	14:O:316:GLN:OE1	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:760:GLN:N	9:K:760:GLN:OE1	2.37	0.53
4:D:98:LEU:HD21	4:D:202:GLU:OE2	2.08	0.53
7:G:186:LEU:O	7:G:190:VAL:HG22	2.09	0.53
12:M:122:TYR:CE2	12:M:127:ILE:HD11	2.43	0.53
1:A:2231:ASN:OD1	1:A:2234:GLN:NE2	2.42	0.53
3:C:413:LYS:NZ	9:K:867:GLU:OE1	2.41	0.53
5:E:409:TYR:O	5:E:413:VAL:HG23	2.09	0.53
1:A:1619:THR:HG21	1:A:1632:LEU:CD2	2.39	0.53
1:A:2332:PRO:O	1:A:2335:ILE:HD12	2.09	0.53
9:K:396:PHE:HE2	9:K:433:ILE:HD13	1.73	0.53
1:A:69:PHE:O	1:A:73:VAL:HG13	2.09	0.52
1:A:318:PHE:O	1:A:322:ILE:HG12	2.08	0.52
11:H:94:GLN:OE1	14:O:421:ARG:NH2	2.41	0.52
5:E:459:GLN:OE1	5:E:459:GLN:O	2.27	0.52
9:K:222:GLU:OE2	9:K:226:ARG:NH2	2.42	0.52
12:M:497:ARG:NH2	14:O:394:ILE:O	2.43	0.52
8:I:675:ASP:N	8:I:675:ASP:OD1	2.41	0.52
11:H:128:THR:HG1	14:O:510:HIS:CG	2.25	0.52
13:N:271:LEU:HD21	13:N:281:TRP:O	2.09	0.52
1:A:332:LEU:C	1:A:332:LEU:HD23	2.35	0.52
1:A:1654:PHE:HD1	1:A:1654:PHE:O	1.93	0.52
8:I:611:MET:O	8:I:611:MET:HG3	2.08	0.52
9:K:328:GLU:OE2	9:K:444:ARG:N	2.43	0.52
10:Q:300:GLU:OE2	11:H:175:ARG:NE	2.42	0.51
2:B:468:GLN:OE1	2:B:469:GLU:N	2.43	0.51
3:C:354:ARG:NH2	11:H:336:MET:SD	2.83	0.51
1:A:443:TYR:CE2	1:A:463:LEU:HD23	2.45	0.51
1:A:1434:GLU:N	1:A:1434:GLU:OE1	2.39	0.51
2:B:120:GLU:OE2	2:B:120:GLU:N	2.41	0.51
1:A:823:LEU:HD12	1:A:824:MET:O	2.10	0.51
9:K:210:ARG:NH2	9:K:435:LEU:O	2.44	0.51
14:O:572:ASP:OD1	14:O:572:ASP:C	2.54	0.51
9:K:334:GLU:OE1	9:K:334:GLU:N	2.44	0.51
12:M:448:LEU:HD21	12:M:456:ILE:HD11	1.91	0.51
9:K:260:ASP:OD1	9:K:260:ASP:N	2.44	0.51
1:A:152:ASP:OD1	1:A:153:ILE:N	2.43	0.51
1:A:2800:THR:HG22	1:A:2802:VAL:HG13	1.93	0.50
5:E:392:ALA:O	9:K:63:ARG:NH2	2.44	0.50
8:I:597:LYS:O	8:I:598:LEU:HD12	2.11	0.50
12:M:344:ARG:NH1	14:O:368:GLU:OE2	2.43	0.50
3:C:347:GLN:NE2	11:H:300:SER:O	2.35	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:H:97:LEU:HD11	11:H:101:ILE:HD12	1.92	0.50
12:M:112:TYR:HE2	12:M:162:ILE:HG23	1.77	0.50
14:O:395:ASP:OD1	14:O:396:ASN:N	2.45	0.50
1:A:183:VAL:HG22	1:A:248:PHE:CZ	2.46	0.50
1:A:1534:VAL:HG23	1:A:1563:VAL:HG11	1.94	0.50
5:E:474:LEU:O	5:E:477:ARG:NH1	2.37	0.50
1:A:2169:GLU:OE1	1:A:2169:GLU:N	2.44	0.50
2:B:234:PRO:O	2:B:235:TYR:HB2	2.12	0.50
12:M:121:HIS:O	12:M:125:VAL:HG23	2.11	0.50
1:A:3760:PRO:CB	1:A:3819:MET:HE1	2.41	0.49
12:M:81:ASP:O	12:M:113:ARG:NH2	2.44	0.49
1:A:334:TYR:O	1:A:337:ARG:NE	2.45	0.49
5:E:208:GLU:HG3	5:E:212:ARG:HE	1.77	0.49
12:M:471:MET:HE1	14:O:407:LEU:HD13	1.94	0.49
5:E:270:ILE:O	5:E:270:ILE:HG22	2.11	0.49
9:K:732:ARG:O	9:K:733:ARG:HB3	2.13	0.49
9:K:304:ARG:NH1	9:K:304:ARG:HA	2.27	0.49
9:K:751:ILE:HD11	9:K:901:LEU:HB2	1.93	0.49
1:A:408:VAL:HG13	1:A:412:MET:HE2	1.94	0.49
14:O:527:ARG:NH1	14:O:533:PRO:O	2.46	0.49
1:A:3802:GLU:CB	1:A:3803:PRO:HD3	2.43	0.49
12:M:237:LEU:HD22	14:O:666:ILE:HD11	1.95	0.49
1:A:2866:VAL:O	1:A:2870:VAL:HG22	2.12	0.49
5:E:380:VAL:HG12	5:E:380:VAL:O	2.13	0.49
12:M:90:LEU:O	12:M:105:ILE:HD11	2.13	0.49
1:A:427:VAL:O	1:A:427:VAL:HG13	2.12	0.49
1:A:3078:GLN:HG2	1:A:3112:MET:HE1	1.94	0.49
6:F:68:ASP:CA	6:F:71:THR:HG22	2.42	0.49
9:K:83:ASP:OD1	9:K:87:GLU:N	2.39	0.49
12:M:455:GLU:OE1	12:M:469:TYR:OH	2.21	0.49
1:A:179:LEU:C	1:A:179:LEU:HD12	2.38	0.49
1:A:1536:GLN:O	1:A:1536:GLN:NE2	2.43	0.49
1:A:1783:SER:OG	1:A:1789:TRP:NE1	2.45	0.49
5:E:90:TYR:CD2	6:F:66:PRO:HD3	2.48	0.49
12:M:448:LEU:HD21	12:M:456:ILE:CD1	2.42	0.49
1:A:2961:SER:O	1:A:3022:ARG:NH1	2.46	0.49
12:M:148:SER:OG	12:M:149:ILE:HD12	2.13	0.49
1:A:399:ARG:NH1	1:A:404:ASP:OD1	2.46	0.48
4:D:221:GLU:N	4:D:221:GLU:OE1	2.46	0.48
1:A:1534:VAL:CG2	1:A:1563:VAL:HG11	2.42	0.48
12:M:147:ASN:C	12:M:147:ASN:OD1	2.56	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1951:ARG:HH21	1:A:1954:VAL:HG11	1.78	0.48
1:A:179:LEU:O	1:A:183:VAL:HG23	2.13	0.48
1:A:2682:ARG:HA	1:A:2682:ARG:NE	2.27	0.48
1:A:867:GLY:O	1:A:871:VAL:HG23	2.13	0.48
1:A:92:GLU:N	1:A:92:GLU:OE1	2.46	0.48
1:A:2212:THR:HA	1:A:2215:VAL:HG12	1.96	0.48
1:A:2353:ASP:OD1	1:A:2354:HIS:N	2.47	0.48
4:D:104:ASP:N	4:D:104:ASP:OD1	2.45	0.48
14:O:348:VAL:HG13	14:O:349:THR:N	2.29	0.48
1:A:2017:ASP:OD1	1:A:2018:LYS:N	2.47	0.48
1:A:3124:ASP:HA	1:A:3127:PHE:CE1	2.48	0.48
6:F:86:PRO:O	6:F:87:ARG:CG	2.62	0.48
3:C:138:LEU:O	3:C:142:MET:HG3	2.14	0.48
3:C:345:LYS:NZ	3:C:395:PRO:O	2.46	0.48
8:I:605:HIS:CD2	8:I:607:LYS:HB3	2.49	0.48
9:K:296:ILE:CD1	14:O:687:VAL:HG21	2.44	0.48
13:N:70:VAL:H	14:O:289:SER:HG	1.57	0.48
1:A:1332:GLU:N	1:A:1335:GLU:OE1	2.43	0.47
1:A:3755:MET:HE1	1:A:3819:MET:SD	2.54	0.47
6:F:68:ASP:C	6:F:71:THR:HG22	2.39	0.47
12:M:381:VAL:O	12:M:381:VAL:HG12	2.14	0.47
14:O:398:ASP:OD1	14:O:399:ASP:N	2.47	0.47
1:A:1296:LEU:O	1:A:1300:VAL:HG23	2.14	0.47
4:D:136:ASP:OD1	4:D:136:ASP:N	2.45	0.47
8:I:709:ARG:NH2	8:I:715:GLU:OE2	2.47	0.47
1:A:421:ALA:HB1	1:A:463:LEU:HD22	1.95	0.47
1:A:421:ALA:CB	1:A:463:LEU:HD22	2.44	0.47
6:F:75:LEU:HD21	10:Q:311:TRP:CE3	2.48	0.47
1:A:1855:VAL:O	1:A:1855:VAL:HG13	2.13	0.47
3:C:353:GLU:OE1	3:C:354:ARG:N	2.47	0.47
9:K:286:SER:O	9:K:290:LYS:N	2.48	0.47
1:A:1146:ASN:OD1	1:A:1147:GLU:N	2.47	0.47
1:A:2335:ILE:HD12	1:A:2335:ILE:H	1.80	0.47
4:D:340:VAL:O	4:D:341:VAL:HB	2.14	0.47
5:E:385:ASN:ND2	9:K:70:LEU:HD21	2.28	0.47
1:A:1226:GLN:O	1:A:1230:VAL:HG23	2.15	0.47
1:A:3196:ASP:OD1	1:A:3198:ASN:N	2.47	0.47
4:D:98:LEU:HD21	4:D:202:GLU:CD	2.39	0.47
8:I:599:PRO:O	8:I:601:PRO:HD3	2.14	0.47
9:K:566:GLY:O	9:K:570:VAL:HG23	2.15	0.47
5:E:476:VAL:HG12	5:E:476:VAL:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:O:514:ASP:O	14:O:518:VAL:HG23	2.15	0.47
1:A:3498:ALA:HB1	1:A:3502:PRO:HD3	1.97	0.47
6:F:86:PRO:O	6:F:87:ARG:CB	2.63	0.47
13:N:74:ASP:OD1	13:N:75:GLY:N	2.48	0.47
1:A:3730:ASP:OD1	1:A:3730:ASP:N	2.39	0.46
1:A:2227:TRP:O	1:A:2231:ASN:ND2	2.36	0.46
1:A:47:ALA:HB2	1:A:99:LEU:HD12	1.96	0.46
5:E:466:ASN:O	5:E:470:ASN:ND2	2.48	0.46
7:G:178:ARG:NE	9:K:804:GLU:OE1	2.36	0.46
11:H:98:SER:OG	14:O:421:ARG:NH2	2.48	0.46
1:A:1893:ASP:N	1:A:1893:ASP:OD1	2.48	0.46
4:D:233:PHE:HA	5:E:411:MET:HE1	1.98	0.46
12:M:99:LEU:CD2	13:N:221:ILE:HD12	2.45	0.46
13:N:218:CYS:SG	13:N:219:THR:N	2.88	0.46
14:O:499:GLU:OE1	14:O:499:GLU:N	2.42	0.46
1:A:842:VAL:HG22	1:A:843:PRO:HD2	1.97	0.46
2:B:235:TYR:CD1	2:B:236:PRO:HD2	2.50	0.46
12:M:435:VAL:HG11	12:M:461:THR:O	2.16	0.46
1:A:78:ILE:HG23	1:A:130:LEU:HD13	1.98	0.46
1:A:3508:ARG:O	1:A:3509:TYR:CD1	2.68	0.46
11:H:466:ALA:O	11:H:470:THR:HG22	2.16	0.46
1:A:97:GLN:O	1:A:101:ASN:ND2	2.45	0.46
3:C:348:GLU:OE1	3:C:400:HIS:NE2	2.43	0.46
9:K:368:TYR:O	9:K:372:ILE:N	2.43	0.46
1:A:1948:ASN:OD1	1:A:1948:ASN:N	2.49	0.46
4:D:109:ILE:HD11	5:E:324:SER:HB2	1.98	0.46
1:A:140:GLU:HA	1:A:143:VAL:HG22	1.99	0.45
1:A:2491:ARG:NH1	3:C:387:ASP:O	2.48	0.45
4:D:631:SER:O	4:D:639:LEU:HD12	2.16	0.45
1:A:1585:VAL:HG21	1:A:1604:LEU:HD13	1.98	0.45
1:A:2205:LEU:O	1:A:2208:SER:OG	2.25	0.45
1:A:2328:GLY:HA2	1:A:2335:ILE:HD11	1.98	0.45
1:A:1631:PHE:O	1:A:1635:VAL:HG23	2.16	0.45
1:A:2216:VAL:HA	1:A:2219:VAL:HG12	1.98	0.45
4:D:107:LEU:HD11	5:E:260:GLU:CD	2.42	0.45
4:D:346:LYS:HE2	5:E:212:ARG:NH1	2.31	0.45
1:A:47:ALA:HB2	1:A:99:LEU:CD1	2.46	0.45
1:A:3823:PHE:HB3	1:A:3829:THR:HG22	1.98	0.45
1:A:1119:PRO:C	1:A:1120:PHE:HD1	2.24	0.45
1:A:108:HIS:ND1	1:A:152:ASP:OD2	2.46	0.45
1:A:2967:LEU:C	1:A:2967:LEU:HD23	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:374:ASN:OD1	2:B:376:GLU:N	2.49	0.45
7:G:69:ILE:HG22	9:K:731:THR:HG22	1.98	0.45
12:M:127:ILE:HD12	13:N:224:ILE:HD11	1.98	0.45
1:A:699:ILE:HB	1:A:700:PRO:HD3	1.99	0.45
1:A:2837:GLU:OE1	2:B:459:ARG:NH1	2.50	0.45
4:D:111:LYS:O	4:D:115:ARG:HG3	2.17	0.45
11:H:93:ASN:OD1	11:H:93:ASN:N	2.50	0.45
1:A:3574:ARG:C	1:A:3574:ARG:HD2	2.42	0.45
5:E:228:HIS:NE2	5:E:267:THR:O	2.50	0.45
12:M:102:TRP:HA	12:M:105:ILE:HG22	1.99	0.45
1:A:1589:GLU:OE2	1:A:1598:SER:OG	2.19	0.45
1:A:183:VAL:HG22	1:A:248:PHE:CE1	2.52	0.44
1:A:548:SER:OG	1:A:553:ARG:NH2	2.40	0.44
1:A:3231:LYS:O	1:A:3231:LYS:HG2	2.17	0.44
4:D:100:LYS:O	4:D:104:ASP:OD1	2.34	0.44
12:M:241:VAL:HG22	12:M:241:VAL:O	2.16	0.44
1:A:69:PHE:O	1:A:73:VAL:HG22	2.17	0.44
1:A:1105:GLU:OE1	1:A:1133:ASN:ND2	2.40	0.44
11:H:246:ILE:O	11:H:250:MET:HG3	2.17	0.44
1:A:535:ASP:OD1	1:A:535:ASP:N	2.51	0.44
14:O:609:TYR:CD1	14:O:693:ILE:HG21	2.53	0.44
1:A:177:GLU:HG3	1:A:279:LEU:HD21	1.99	0.44
1:A:2243:LEU:HD21	1:A:2271:ILE:HD11	1.99	0.44
1:A:2724:LEU:CD1	1:A:2749:LEU:HD12	2.47	0.44
6:F:67:ARG:HD3	11:H:174:ASP:OD2	2.17	0.44
12:M:66:SER:OG	13:N:253:VAL:HG12	2.16	0.44
12:M:134:LEU:HD21	13:N:235:LYS:HG3	1.98	0.44
1:A:950:ASP:OD1	1:A:950:ASP:N	2.49	0.44
6:F:104:LEU:HD12	6:F:104:LEU:HA	1.82	0.44
1:A:1486:LEU:O	1:A:1490:LEU:HD13	2.17	0.44
4:D:353:ARG:O	4:D:353:ARG:HG2	2.17	0.44
8:I:598:LEU:HA	8:I:599:PRO:HD3	1.88	0.44
9:K:346:LEU:HD23	9:K:346:LEU:O	2.18	0.44
3:C:157:GLY:O	3:C:161:ASP:OD2	2.36	0.44
5:E:440:ALA:O	5:E:443:THR:OG1	2.29	0.44
13:N:223:ARG:O	13:N:223:ARG:HG2	2.17	0.44
6:F:204:ARG:NE	9:K:836:GLU:OE2	2.45	0.44
6:F:81:VAL:HB	6:F:84:PHE:HE1	1.83	0.44
12:M:238:LYS:O	12:M:241:VAL:HG12	2.18	0.44
12:M:327:ARG:NH2	14:O:384:ARG:O	2.49	0.44
5:E:383:LEU:HD13	5:E:473:ILE:HG23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:442:LEU:HD12	5:E:443:THR:HG23	2.00	0.43
7:G:75:THR:HG22	7:G:79:MET:SD	2.58	0.43
6:F:87:ARG:HG2	6:F:87:ARG:HH11	1.83	0.43
9:K:296:ILE:HD11	9:K:303:VAL:CG1	2.47	0.43
1:A:1832:ASP:O	1:A:1834:ASN:N	2.44	0.43
5:E:59:ARG:NH1	5:E:61:THR:O	2.50	0.43
12:M:86:GLU:O	12:M:109:ILE:HD11	2.18	0.43
1:A:2413:PHE:O	1:A:2416:VAL:HG12	2.18	0.43
9:K:90:LEU:N	9:K:90:LEU:HD23	2.33	0.43
13:N:108:ASP:OD1	13:N:109:ARG:N	2.50	0.43
9:K:313:LEU:O	9:K:317:VAL:HG22	2.18	0.43
2:B:349:PRO:O	2:B:352:ILE:HG22	2.19	0.43
4:D:658:ASP:OD1	4:D:660:ASN:N	2.49	0.43
13:N:317:PHE:HB3	13:N:339:LEU:HD13	2.01	0.43
1:A:144:ILE:HG23	1:A:145:LEU:N	2.32	0.43
1:A:179:LEU:HD21	1:A:283:ALA:HB2	2.00	0.43
1:A:178:GLN:NE2	1:A:245:MET:O	2.45	0.43
1:A:447:LEU:HD23	1:A:447:LEU:O	2.19	0.43
1:A:949:VAL:O	1:A:949:VAL:HG12	2.17	0.43
1:A:443:TYR:CD2	1:A:463:LEU:HD23	2.54	0.43
1:A:815:LEU:HD13	1:A:1243:ASP:HB2	2.00	0.43
1:A:1493:VAL:HG21	1:A:1514:LEU:HD12	2.00	0.43
1:A:2421:VAL:CG1	1:A:2433:ILE:HG21	2.49	0.43
11:H:97:LEU:CD1	11:H:101:ILE:HD12	2.49	0.43
13:N:373:ASN:O	13:N:376:THR:OG1	2.31	0.43
1:A:380:ILE:HD11	1:A:385:ARG:HB3	2.01	0.43
1:A:1895:ARG:HB2	1:A:1895:ARG:NH1	2.34	0.43
1:A:3405:TYR:O	1:A:3409:VAL:HG23	2.19	0.43
7:G:177:ASN:OD1	7:G:177:ASN:O	2.37	0.43
9:K:259:MET:SD	9:K:260:ASP:N	2.92	0.43
9:K:393:LYS:O	9:K:397:VAL:HG23	2.17	0.43
14:O:512:LYS:HE3	14:O:512:LYS:HA	2.01	0.43
1:A:88:GLN:NE2	1:A:237:ALA:O	2.52	0.42
1:A:291:GLN:NE2	1:A:360:ASP:OD1	2.48	0.42
1:A:2526:SER:OG	1:A:2527:LYS:N	2.52	0.42
1:A:3096:ASN:ND2	1:A:3107:TYR:OH	2.52	0.42
3:C:137:GLU:O	3:C:141:MET:HG3	2.19	0.42
6:F:65:ARG:HA	6:F:66:PRO:HD3	1.89	0.42
10:Q:316:VAL:HG12	10:Q:317:VAL:HG13	2.01	0.42
1:A:1787:ASP:O	1:A:1788:PHE:HB3	2.18	0.42
1:A:1942:LEU:HD22	1:A:1954:VAL:HG13	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:82:TYR:OH	6:F:94:ASP:OD2	2.24	0.42
5:E:223:SER:O	5:E:223:SER:OG	2.35	0.42
9:K:702:ASP:OD1	9:K:704:GLU:N	2.52	0.42
13:N:225:ARG:NH1	13:N:228:GLU:OE1	2.52	0.42
14:O:266:VAL:O	14:O:266:VAL:HG13	2.18	0.42
1:A:552:ASP:N	1:A:552:ASP:OD1	2.52	0.42
1:A:1615:ILE:HG21	1:A:1644:LEU:HD21	2.01	0.42
1:A:1889:ALA:C	1:A:1890:LEU:HD12	2.44	0.42
1:A:2033:PRO:N	1:A:2034:PRO:CD	2.82	0.42
9:K:253:LYS:HE2	9:K:253:LYS:HA	2.01	0.42
14:O:338:LEU:HD12	14:O:341:LEU:HD11	2.01	0.42
1:A:116:PRO:N	1:A:117:PRO:HD2	2.35	0.42
1:A:1146:ASN:HD22	1:A:1151:VAL:HG11	1.85	0.42
1:A:1442:ASN:O	1:A:1444:THR:N	2.51	0.42
1:A:3178:ASN:O	1:A:3180:LYS:N	2.52	0.42
4:D:341:VAL:O	4:D:345:GLN:HG2	2.19	0.42
14:O:337:ASP:OD1	14:O:337:ASP:C	2.62	0.42
9:K:748:CYS:SG	9:K:897:MET:HE3	2.59	0.42
11:H:163:LEU:O	11:H:167:VAL:HG23	2.19	0.42
1:A:6:ILE:O	1:A:10:VAL:HG23	2.19	0.42
1:A:381:ASN:OD1	1:A:381:ASN:C	2.62	0.42
12:M:483:GLY:O	12:M:484:ASN:HB3	2.19	0.42
1:A:41:THR:O	1:A:45:VAL:HG23	2.19	0.42
1:A:1841:ASP:OD1	1:A:1842:ARG:N	2.48	0.42
1:A:2335:ILE:O	1:A:2339:ILE:HG12	2.19	0.42
2:B:229:PRO:O	2:B:230:SER:CB	2.60	0.42
1:A:151:SER:HB3	1:A:257:ILE:HG23	2.01	0.42
1:A:3667:LYS:HG2	1:A:3672:VAL:HA	2.02	0.42
7:G:64:ASP:OD2	7:G:64:ASP:C	2.63	0.42
1:A:1654:PHE:CD1	1:A:1654:PHE:C	2.98	0.42
1:A:2724:LEU:HD12	1:A:2749:LEU:HD12	2.01	0.42
5:E:175:ASN:OD1	5:E:175:ASN:C	2.63	0.42
7:G:87:PRO:O	7:G:90:THR:O	2.38	0.42
1:A:139:ASN:O	1:A:143:VAL:HG13	2.20	0.42
3:C:276:ARG:O	3:C:280:MET:HG3	2.19	0.41
11:H:228:ARG:NH2	11:H:256:GLU:OE2	2.39	0.41
11:H:467:GLU:N	11:H:468:PRO:HD2	2.35	0.41
1:A:1424:ILE:HD11	1:A:1455:CYS:SG	2.61	0.41
2:B:304:VAL:HG13	2:B:304:VAL:O	2.19	0.41
12:M:131:ASN:O	12:M:134:LEU:O	2.38	0.41
13:N:192:PHE:HB3	13:N:216:MET:HE2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:LEU:O	1:A:61:THR:N	2.52	0.41
1:A:618:GLU:O	1:A:622:VAL:HG23	2.21	0.41
1:A:1937:GLN:O	1:A:1937:GLN:OE1	2.39	0.41
1:A:3515:VAL:HG12	1:A:3516:GLU:N	2.36	0.41
4:D:629:SER:OG	4:D:749:VAL:HG22	2.20	0.41
5:E:413:VAL:HG11	5:E:460:ARG:NE	2.35	0.41
9:K:84:GLU:OE2	9:K:85:ARG:NH2	2.49	0.41
9:K:335:LEU:HD12	9:K:339:LEU:HD13	2.03	0.41
14:O:367:GLU:HA	14:O:372:MET:HE1	2.03	0.41
1:A:332:LEU:HD23	1:A:332:LEU:O	2.20	0.41
1:A:975:ASP:OD1	1:A:1072:ARG:NH2	2.46	0.41
9:K:433:ILE:N	9:K:434:PRO:CD	2.83	0.41
13:N:390:TRP:CZ3	13:N:393:ILE:HD13	2.55	0.41
1:A:537:ILE:HG22	1:A:537:ILE:O	2.21	0.41
2:B:396:GLU:OE1	2:B:396:GLU:N	2.50	0.41
12:M:107:ASP:OD1	13:N:293:ARG:NH2	2.53	0.41
13:N:284:ASP:N	13:N:284:ASP:OD1	2.52	0.41
1:A:481:ARG:NH2	1:A:603:GLY:O	2.54	0.41
6:F:110:LEU:HD23	6:F:110:LEU:HA	1.80	0.41
4:D:126:TYR:CE1	4:D:138:ALA:HB1	2.55	0.41
12:M:499:ASP:OD2	12:M:502:LYS:NZ	2.53	0.41
14:O:361:TYR:HA	14:O:364:ILE:HD11	2.03	0.41
8:I:697:ASN:OD1	8:I:727:TYR:OH	2.39	0.41
1:A:54:ARG:HB2	1:A:106:ILE:HD11	2.02	0.41
1:A:733:ILE:O	1:A:737:SER:OG	2.30	0.41
1:A:1605:TYR:CE1	1:A:1635:VAL:HG22	2.55	0.41
1:A:1624:GLU:O	1:A:1672:ILE:HG21	2.20	0.41
1:A:2051:ILE:CG2	1:A:2107:MET:HE1	2.50	0.41
5:E:479:LEU:HD21	9:K:77:ARG:NH2	2.35	0.41
8:I:674:GLN:OE1	8:I:675:ASP:N	2.54	0.41
13:N:119:LYS:HB3	13:N:120:PRO:HD3	2.03	0.41
1:A:1481:LEU:HD22	1:A:1486:LEU:HD21	2.03	0.41
1:A:1790:ARG:O	1:A:1794:LEU:HD23	2.21	0.41
1:A:2175:PRO:HA	1:A:2178:THR:HG22	2.02	0.41
1:A:1833:PRO:O	1:A:1834:ASN:C	2.64	0.40
1:A:3230:TYR:O	1:A:3232:GLU:N	2.54	0.40
1:A:3463:VAL:HG13	1:A:3465:PRO:HD3	2.03	0.40
1:A:1915:HIS:O	1:A:1919:VAL:HG23	2.21	0.40
1:A:1921:ILE:HG21	1:A:1938:ILE:HD13	2.02	0.40
1:A:1985:ARG:O	1:A:1985:ARG:NH1	2.54	0.40
1:A:2051:ILE:HG21	1:A:2107:MET:HE1	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2565:ASN:N	1:A:2566:PRO:CD	2.84	0.40
4:D:340:VAL:HG12	4:D:341:VAL:N	2.36	0.40
5:E:42:ARG:NH2	6:F:152:LEU:HD21	2.35	0.40
11:H:61:LEU:O	11:H:61:LEU:HG	2.20	0.40
1:A:74:MET:HE1	1:A:123:TYR:O	2.21	0.40
1:A:1555:ASN:O	1:A:1559:VAL:HG23	2.21	0.40
1:A:3498:ALA:HB1	1:A:3502:PRO:CD	2.51	0.40
3:C:135:TRP:CD1	3:C:139:CYS:HG	2.40	0.40
7:G:87:PRO:HA	7:G:90:THR:O	2.21	0.40
7:G:87:PRO:N	7:G:88:PRO:CD	2.84	0.40
8:I:606:ASP:OD1	8:I:606:ASP:N	2.54	0.40
1:A:1658:THR:O	1:A:1662:VAL:HG23	2.22	0.40
1:A:2524:CYS:CB	3:C:385:LEU:HD12	2.52	0.40
6:F:75:LEU:HD21	10:Q:311:TRP:CZ3	2.57	0.40
1:A:1386:ASN:O	1:A:1390:MET:HG2	2.22	0.40
1:A:2165:GLY:O	1:A:2168:VAL:HG22	2.21	0.40
1:A:2213:LEU:HA	1:A:2216:VAL:HG22	2.04	0.40
2:B:227:ILE:HG22	2:B:228:THR:O	2.21	0.40
4:D:155:ASP:OD1	4:D:155:ASP:N	2.53	0.40
4:D:345:GLN:HG2	4:D:345:GLN:H	1.77	0.40
9:K:226:ARG:HH11	9:K:638:LEU:HD21	1.87	0.40
9:K:307:ASP:OD2	9:K:311:ARG:NH2	2.54	0.40
14:O:278:GLU:O	14:O:281: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	3597/3893 (92%)	3442 (96%)	155 (4%)	0	100	100
2	B	233/1192 (20%)	223 (96%)	9 (4%)	1 (0%)	30	64

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	189/433 (44%)	185 (98%)	4 (2%)	0	100	100
4	D	509/767 (66%)	488 (96%)	21 (4%)	0	100	100
5	E	435/480 (91%)	428 (98%)	7 (2%)	0	100	100
6	F	117/277 (42%)	110 (94%)	6 (5%)	1 (1%)	14	49
7	G	110/204 (54%)	107 (97%)	3 (3%)	0	100	100
8	I	148/770 (19%)	143 (97%)	5 (3%)	0	100	100
9	K	573/1196 (48%)	557 (97%)	16 (3%)	0	100	100
10	Q	60/1273 (5%)	60 (100%)	0	0	100	100
11	H	333/485 (69%)	327 (98%)	6 (2%)	0	100	100
12	M	458/519 (88%)	433 (94%)	25 (6%)	0	100	100
13	N	350/405 (86%)	348 (99%)	2 (1%)	0	100	100
14	O	338/730 (46%)	321 (95%)	17 (5%)	0	100	100
All	All	7450/12624 (59%)	7172 (96%)	276 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	87	ARG
2	B	230	SER

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	3197/3412 (94%)	3172 (99%)	25 (1%)	79	88
2	B	227/928 (24%)	227 (100%)	0	100	100
3	C	173/377 (46%)	173 (100%)	0	100	100
4	D	450/635 (71%)	442 (98%)	8 (2%)	54	74
5	E	375/401 (94%)	372 (99%)	3 (1%)	79	88
6	F	92/212 (43%)	92 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	G	90/157 (57%)	89 (99%)	1 (1%)	70	83
8	I	129/620 (21%)	127 (98%)	2 (2%)	58	76
9	K	507/999 (51%)	502 (99%)	5 (1%)	73	84
10	Q	50/1047 (5%)	50 (100%)	0	100	100
11	H	279/387 (72%)	277 (99%)	2 (1%)	81	89
12	M	404/449 (90%)	400 (99%)	4 (1%)	73	84
13	N	318/365 (87%)	315 (99%)	3 (1%)	75	86
14	O	301/609 (49%)	299 (99%)	2 (1%)	81	89
All	All	6592/10598 (62%)	6537 (99%)	55 (1%)	77	88

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	TYR
1	A	99	LEU
1	A	374	VAL
1	A	470	CYS
1	A	736	SER
1	A	804	LEU
1	A	846	LEU
1	A	850	LEU
1	A	943	VAL
1	A	950	ASP
1	A	1117	TYR
1	A	1180	THR
1	A	1371	TYR
1	A	1474	VAL
1	A	1661	THR
1	A	1935	VAL
1	A	2032	SER
1	A	2045	LEU
1	A	2046	ASN
1	A	2434	LEU
1	A	2879	TYR
1	A	2998	LEU
1	A	3438	ASN
1	A	3448	LEU
1	A	3503	HIS
4	D	185	ILE

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Mol	Chain	Res	Type
4	D	214	LEU
4	D	244	ASP
4	D	368	SER
4	D	525	ASP
4	D	581	THR
4	D	735	GLN
4	D	751	PHE
5	E	60	THR
5	E	105	ASP
5	E	211	MET
7	G	58	GLU
8	I	606	ASP
8	I	615	VAL
9	K	78	LEU
9	K	314	MET
9	K	349	HIS
9	K	581	ASP
9	K	820	ASP
11	H	59	ILE
11	H	481	CYS
12	M	109	ILE
12	M	138	CYS
12	M	142	ASP
12	M	259	ILE
13	N	294	HIS
13	N	342	MET
13	N	391	GLN
14	O	281	ILE
14	O	615	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	349	HIS
1	A	1067	GLN
1	A	1590	GLN
1	A	1596	HIS
1	A	1638	HIS
1	A	1701	HIS
1	A	2008	HIS
1	A	2705	HIS
1	A	2795	GLN

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Mol	Chain	Res	Type
1	A	2822	GLN
1	A	2882	GLN
1	A	2977	ASN
1	A	3269	GLN
1	A	3391	GLN
1	A	3524	HIS
1	A	3540	ASN
1	A	3631	GLN
1	A	3806	HIS
1	A	3844	ASN
2	B	171	HIS
2	B	196	HIS
2	B	223	HIS
2	B	293	GLN
4	D	46	ASN
4	D	197	HIS
4	D	217	HIS
5	E	131	HIS
5	E	139	GLN
5	E	240	ASN
5	E	241	GLN
5	E	315	GLN
5	E	385	ASN
8	I	635	GLN
9	K	237	HIS
9	K	349	HIS
9	K	687	GLN
9	K	737	ASN
9	K	740	GLN
10	Q	319	GLN
10	Q	335	HIS
11	H	313	HIS
12	M	189	HIS
12	M	270	ASN
12	M	512	ASN
13	N	157	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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.

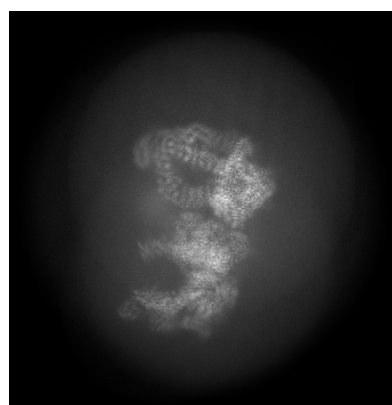
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-73236. These allow visual inspection of the internal detail of the map and identification of artifacts.

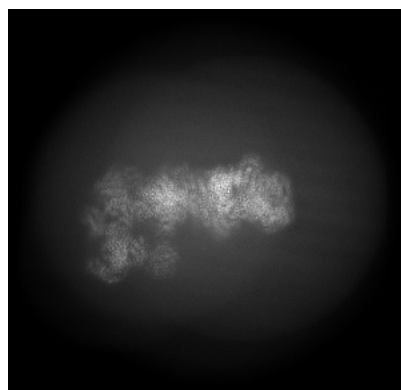
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

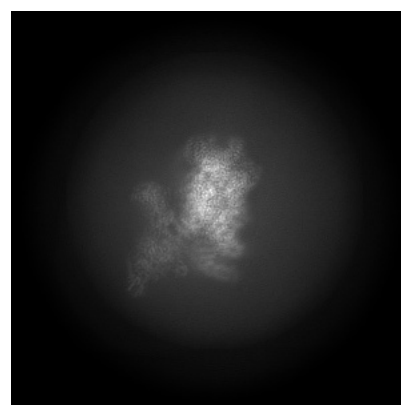
6.1.1 Primary map



X



Y

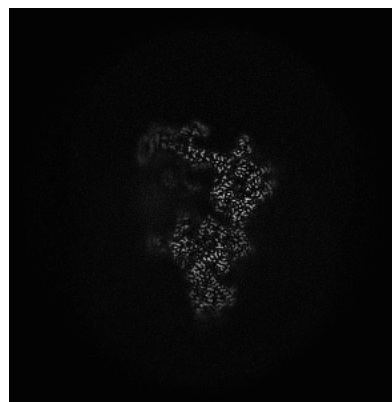


Z

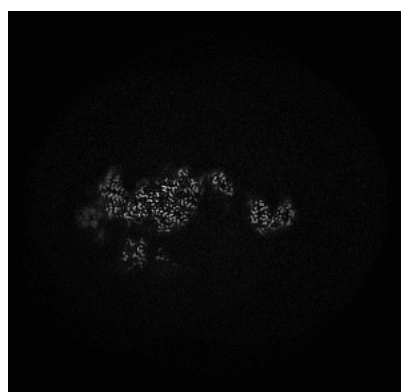
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 242



Y Index: 241

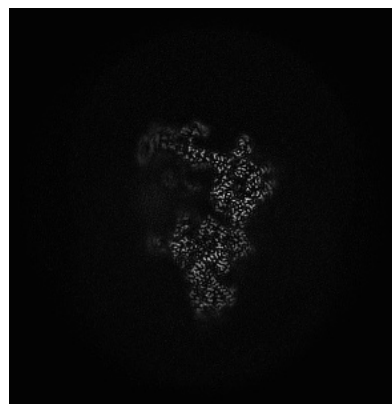


Z Index: 250

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: 242



Y Index: 264

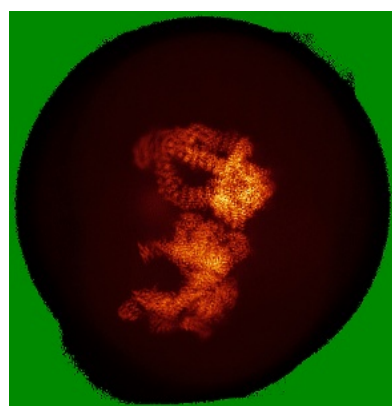


Z Index: 268

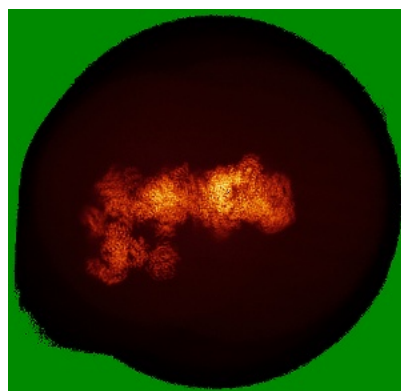
The images above show the largest variance slices of the map in three orthogonal directions.

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

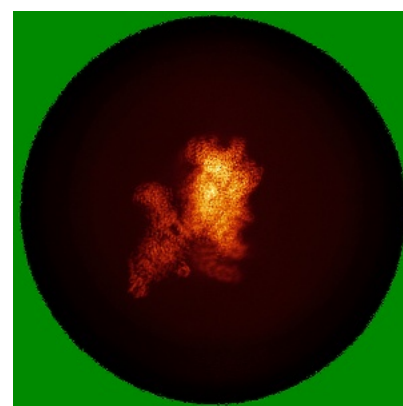
6.4.1 Primary map



X



Y

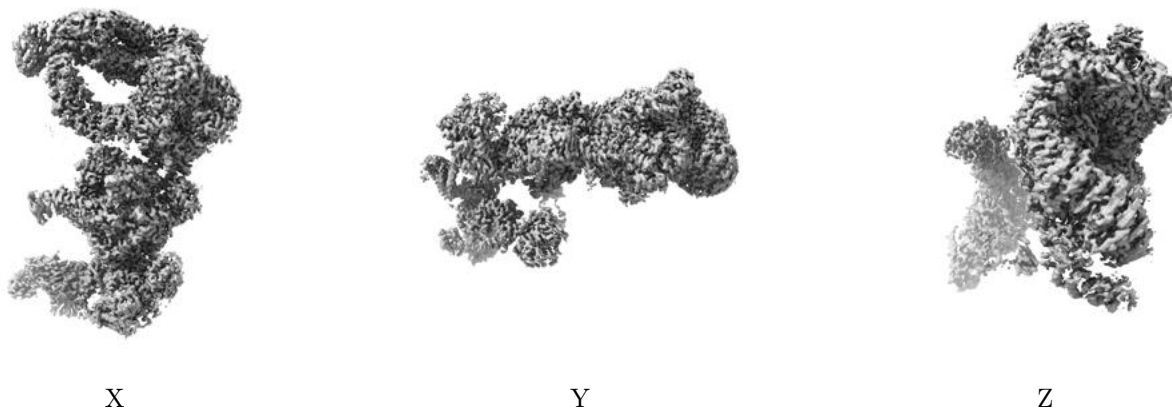


Z

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

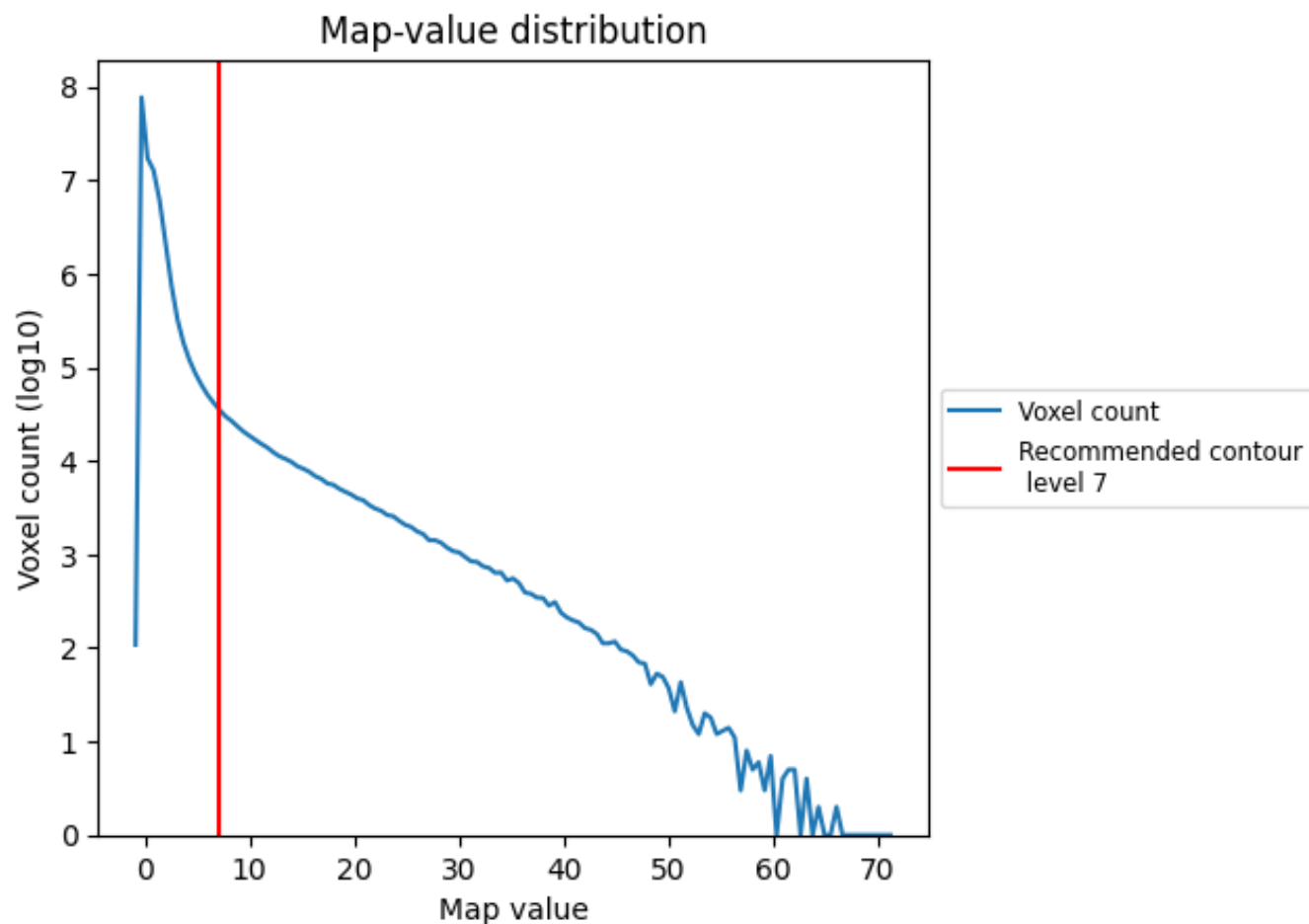
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

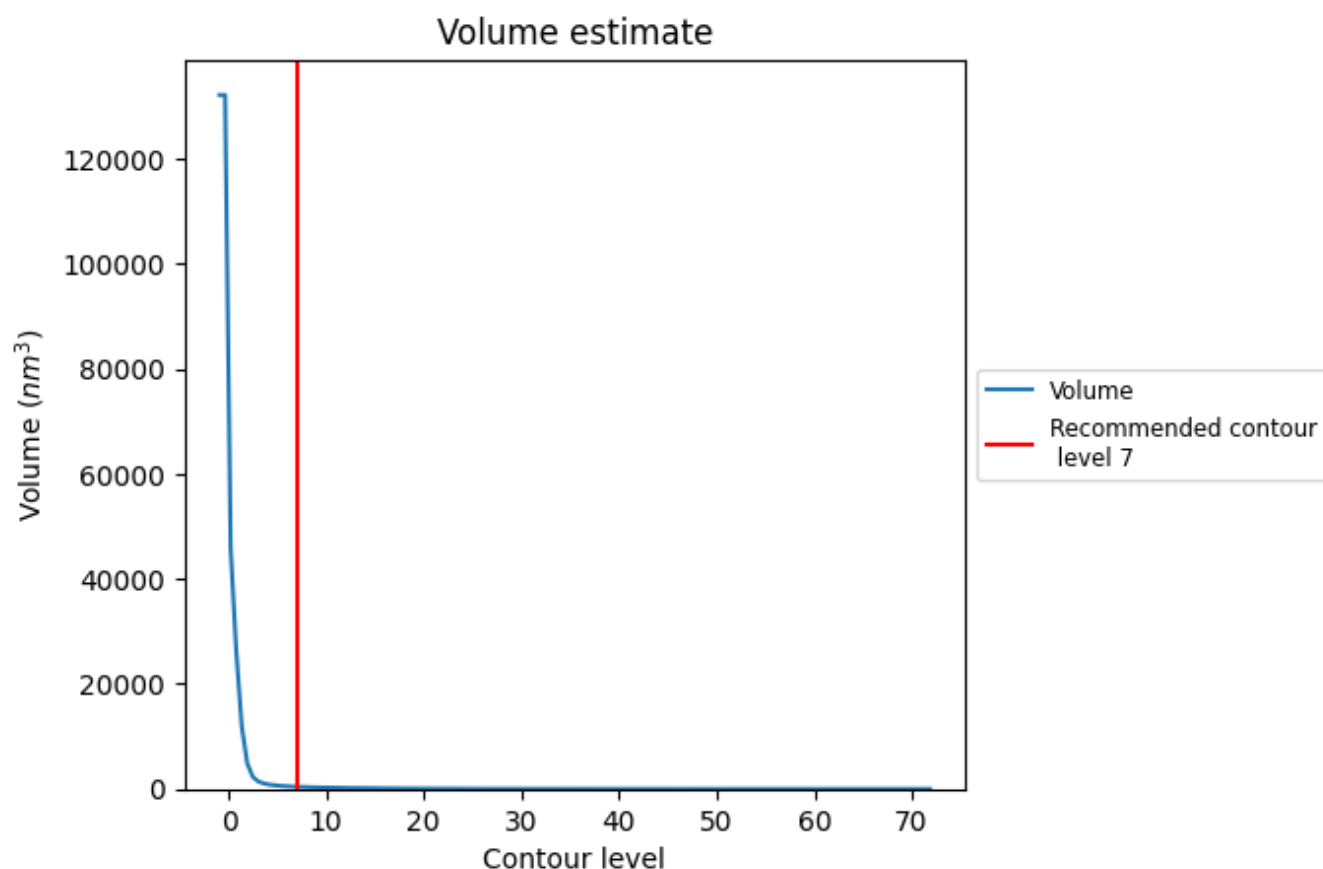
This section contains the results of statistical analysis of the map.

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 413 nm³; this corresponds to an approximate mass of 373 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 [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

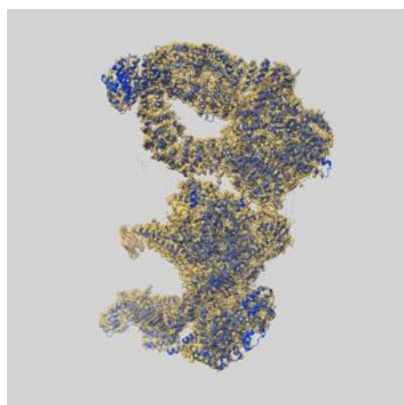
8 Fourier-Shell correlation ⓘ

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

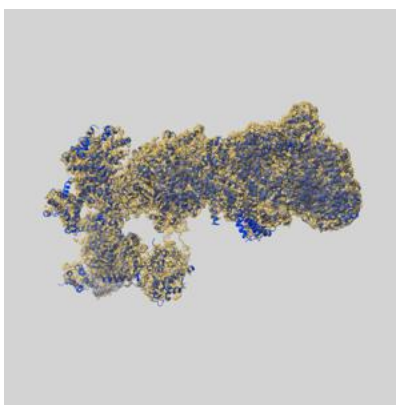
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-73236 and PDB model 9YNW. Per-residue inclusion information can be found in section [3](#) on page [7](#).

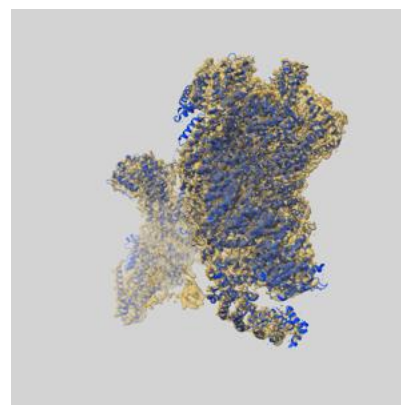
9.1 Map-model overlay [i](#)



X



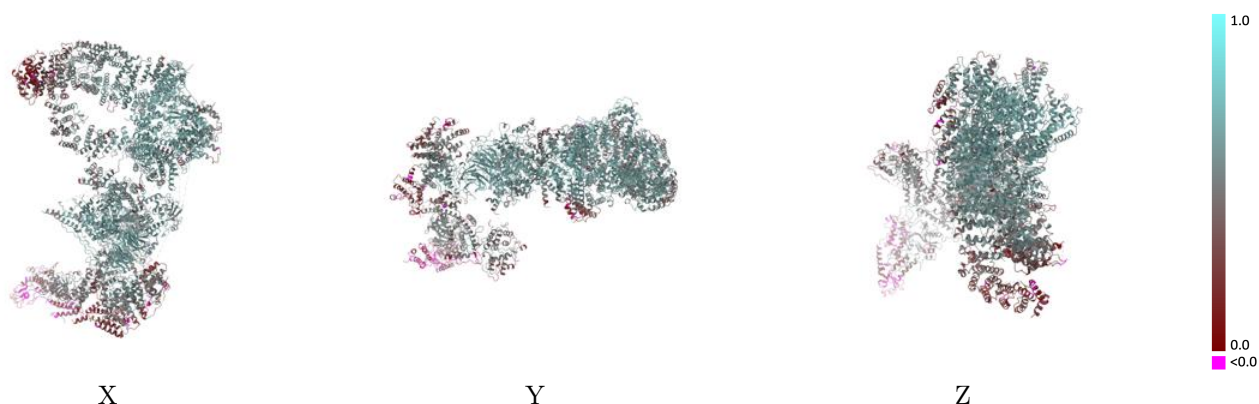
Y



Z

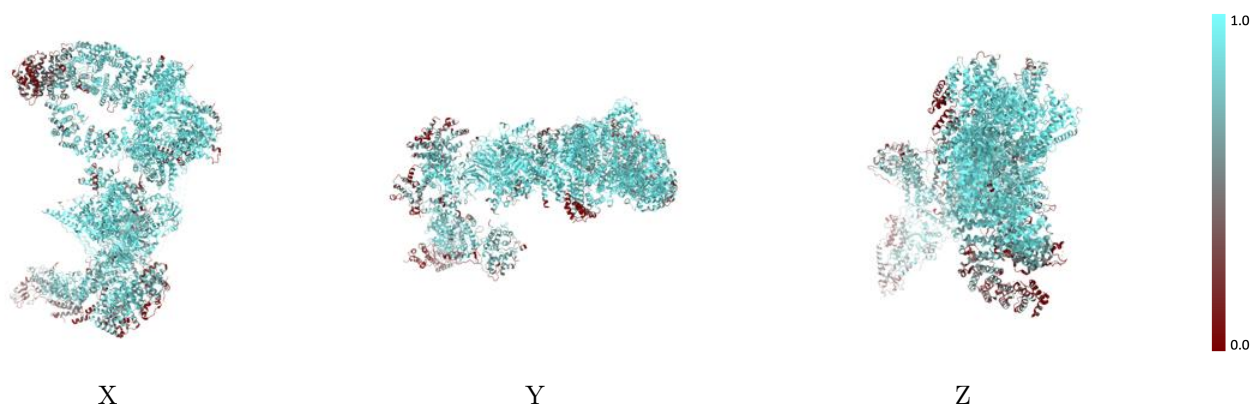
The images above show the 3D surface view of the map at the recommended contour level 7.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



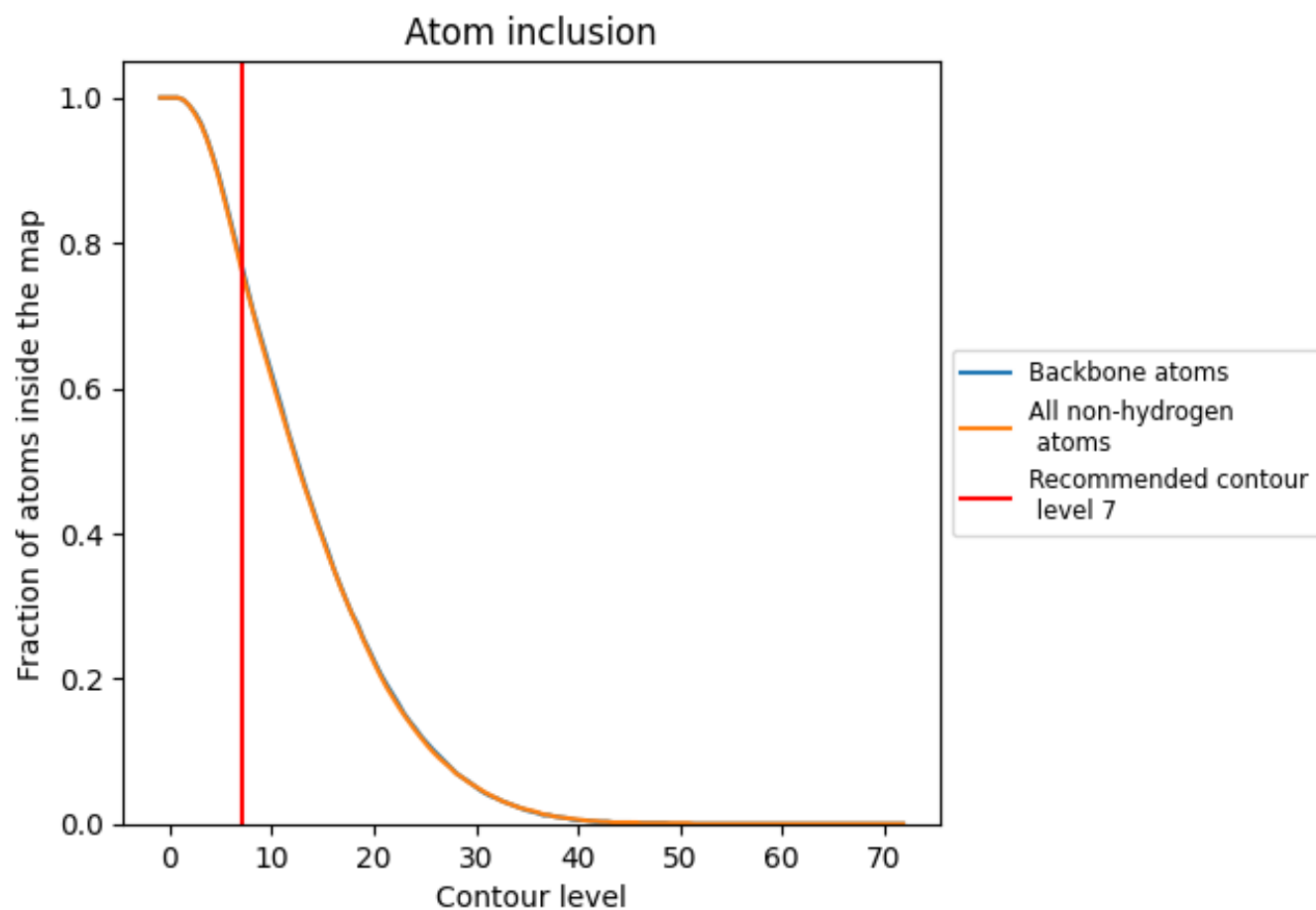
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (7).































9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 77% 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 (7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7660	 0.5050
A	 0.7970	 0.5360
B	 0.8710	 0.5830
C	 0.7930	 0.5370
D	 0.7820	 0.5460
E	 0.8670	 0.5490
F	 0.9650	 0.6170
G	 0.9460	 0.6210
H	 0.8180	 0.5420
I	 0.8350	 0.5730
K	 0.7080	 0.4360
M	 0.6160	 0.3470
N	 0.5280	 0.2730
O	 0.6440	 0.4070
Q	 0.9080	 0.5880

