



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 03:05 PM UTC

PDB ID : 8H7G / pdb_00008h7g
EMDB ID : EMD-34520
Title : Cryo-EM structure of the human SAGA complex
Authors : Huang, J.; Zhang, Y.
Deposited on : 2022-10-20
Resolution : 3.70 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

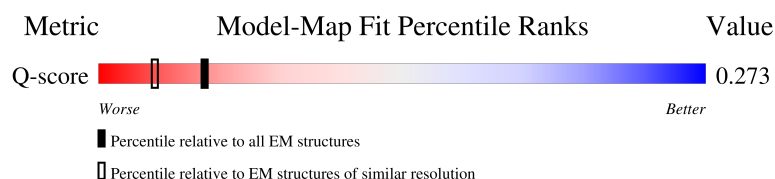
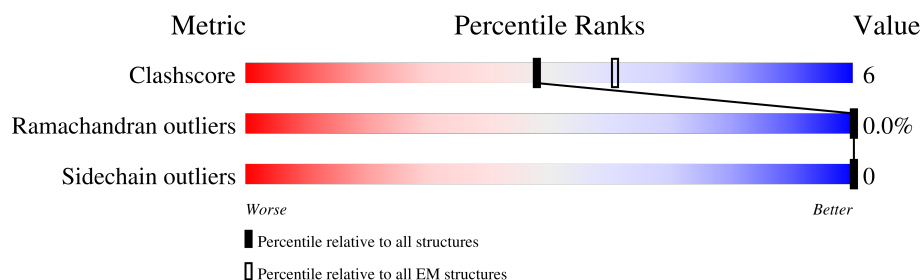
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.70 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11569 (3.20 - 4.20)

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	C	3859	
2	A	1217	
3	B	86	
4	D	779	

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Mol	Chain	Length	Quality of chain
5	E	317	
6	G	374	
7	H	589	
8	I	455	
9	K	622	
10	M	264	
11	O	218	
12	R	161	
13	X	19	
14	L	892	

2 Entry composition [i](#)

There are 14 unique types of molecules in this entry. The entry contains 52609 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 Transformation/transcription domain-associated protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	3261	Total	C	N	O	S	0	0
			26251	16890	4519	4654	188		

- Molecule 2 is a protein called Splicing factor 3B subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	1168	Total	C	N	O	S	0	0
			9158	5817	1558	1738	45		

- Molecule 3 is a protein called Splicing factor 3B subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	45	Total	C	N	O	S	0	0
			383	245	67	67	4		

- Molecule 4 is a protein called Transcription factor SPT20 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	318	Total	C	N	O	S	0	0
			2595	1641	448	490	16		

- Molecule 5 is a protein called Transcription initiation protein SPT3 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	225	Total	C	N	O	S	0	0
			1770	1116	324	318	12		

- Molecule 6 is a protein called Transcriptional adapter 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	188	Total	C	N	O	S	0	0
			1505	951	271	277	6		

There are 39 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-38	MET	-	initiating methionine	UNP Q96BN2
G	-37	ASP	-	expression tag	UNP Q96BN2
G	-36	TYR	-	expression tag	UNP Q96BN2
G	-35	LYS	-	expression tag	UNP Q96BN2
G	-34	ASP	-	expression tag	UNP Q96BN2
G	-33	HIS	-	expression tag	UNP Q96BN2
G	-32	ASP	-	expression tag	UNP Q96BN2
G	-31	GLY	-	expression tag	UNP Q96BN2
G	-30	ASP	-	expression tag	UNP Q96BN2
G	-29	TYR	-	expression tag	UNP Q96BN2
G	-28	LYS	-	expression tag	UNP Q96BN2
G	-27	ASP	-	expression tag	UNP Q96BN2
G	-26	HIS	-	expression tag	UNP Q96BN2
G	-25	ASP	-	expression tag	UNP Q96BN2
G	-24	ILE	-	expression tag	UNP Q96BN2
G	-23	ASP	-	expression tag	UNP Q96BN2
G	-22	TYR	-	expression tag	UNP Q96BN2
G	-21	LYS	-	expression tag	UNP Q96BN2
G	-20	ASP	-	expression tag	UNP Q96BN2
G	-19	ASP	-	expression tag	UNP Q96BN2
G	-18	ASP	-	expression tag	UNP Q96BN2
G	-17	ASP	-	expression tag	UNP Q96BN2
G	-16	LYS	-	expression tag	UNP Q96BN2
G	-15	GLY	-	expression tag	UNP Q96BN2
G	-14	GLY	-	expression tag	UNP Q96BN2
G	-13	SER	-	expression tag	UNP Q96BN2
G	-12	GLY	-	expression tag	UNP Q96BN2
G	-11	GLY	-	expression tag	UNP Q96BN2
G	-10	SER	-	expression tag	UNP Q96BN2
G	-9	LEU	-	expression tag	UNP Q96BN2
G	-8	GLU	-	expression tag	UNP Q96BN2
G	-7	VAL	-	expression tag	UNP Q96BN2
G	-6	LEU	-	expression tag	UNP Q96BN2
G	-5	PHE	-	expression tag	UNP Q96BN2
G	-4	GLN	-	expression tag	UNP Q96BN2
G	-3	GLY	-	expression tag	UNP Q96BN2
G	-2	PRO	-	expression tag	UNP Q96BN2
G	-1	LEU	-	expression tag	UNP Q96BN2
G	0	ASP	-	expression tag	UNP Q96BN2

- Molecule 7 is a protein called TAF5-like RNA polymerase II p300/CBP-associated factor-associated factor 65 kDa subunit 5L.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	514	Total	C	N	O	S	0	0
			4084	2580	706	778	20		

- Molecule 8 is a protein called STAGA complex 65 subunit gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	175	Total	C	N	O	S	0	0
			1419	901	253	260	5		

There are 41 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	415	GLY	-	expression tag	UNP O94864
I	416	SER	-	expression tag	UNP O94864
I	417	GLU	-	expression tag	UNP O94864
I	418	ASN	-	expression tag	UNP O94864
I	419	LEU	-	expression tag	UNP O94864
I	420	TYR	-	expression tag	UNP O94864
I	421	PHE	-	expression tag	UNP O94864
I	422	GLN	-	expression tag	UNP O94864
I	423	GLY	-	expression tag	UNP O94864
I	424	SER	-	expression tag	UNP O94864
I	425	GLY	-	expression tag	UNP O94864
I	426	THR	-	expression tag	UNP O94864
I	427	SER	-	expression tag	UNP O94864
I	428	THR	-	expression tag	UNP O94864
I	429	ALA	-	expression tag	UNP O94864
I	430	TRP	-	expression tag	UNP O94864
I	431	SER	-	expression tag	UNP O94864
I	432	HIS	-	expression tag	UNP O94864
I	433	PRO	-	expression tag	UNP O94864
I	434	GLN	-	expression tag	UNP O94864
I	435	PHE	-	expression tag	UNP O94864
I	436	GLU	-	expression tag	UNP O94864
I	437	LYS	-	expression tag	UNP O94864
I	438	THR	-	expression tag	UNP O94864
I	439	GLY	-	expression tag	UNP O94864
I	440	VAL	-	expression tag	UNP O94864
I	441	SER	-	expression tag	UNP O94864
I	442	ILE	-	expression tag	UNP O94864
I	443	THR	-	expression tag	UNP O94864
I	444	SER	-	expression tag	UNP O94864
I	445	SER	-	expression tag	UNP O94864

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Chain	Residue	Modelled	Actual	Comment	Reference
I	446	GLY	-	expression tag	UNP O94864
I	447	SER	-	expression tag	UNP O94864
I	448	TRP	-	expression tag	UNP O94864
I	449	SER	-	expression tag	UNP O94864
I	450	HIS	-	expression tag	UNP O94864
I	451	PRO	-	expression tag	UNP O94864
I	452	GLN	-	expression tag	UNP O94864
I	453	PHE	-	expression tag	UNP O94864
I	454	GLU	-	expression tag	UNP O94864
I	455	LYS	-	expression tag	UNP O94864

- Molecule 9 is a protein called TAF6-like RNA polymerase II p300/CBP-associated factor-associated factor 65 kDa subunit 6L.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	352	Total	C	N	O	S	0	0
			2703	1720	478	493	12		

- Molecule 10 is a protein called Transcription initiation factor TFIID subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	M	119	Total	C	N	O	S	0	0
			957	607	168	176	6		

- Molecule 11 is a protein called Transcription initiation factor TFIID subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	O	91	Total	C	N	O	S	0	0
			722	466	116	136	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	R	74	Total	C	N	O	S	0	0
			605	379	105	118	3		

- Molecule 13 is a protein called Unassigned sequence.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	X	19	Total	C	N	O	0	0
			95	57	19	19		

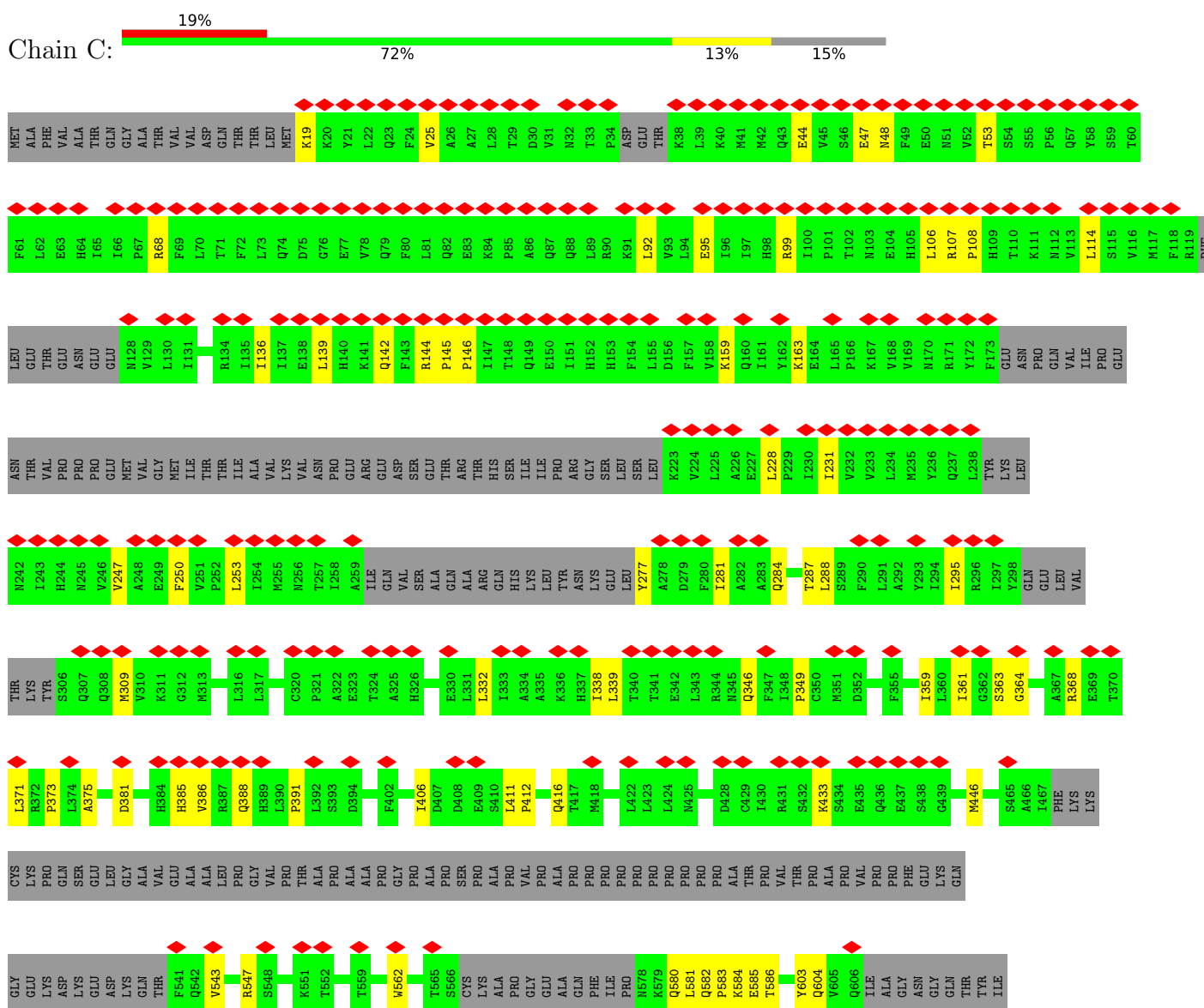
- Molecule 14 is a protein called Ataxin-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	L	44	Total	C	N	O	S	0	0
			362	228	70	60	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.

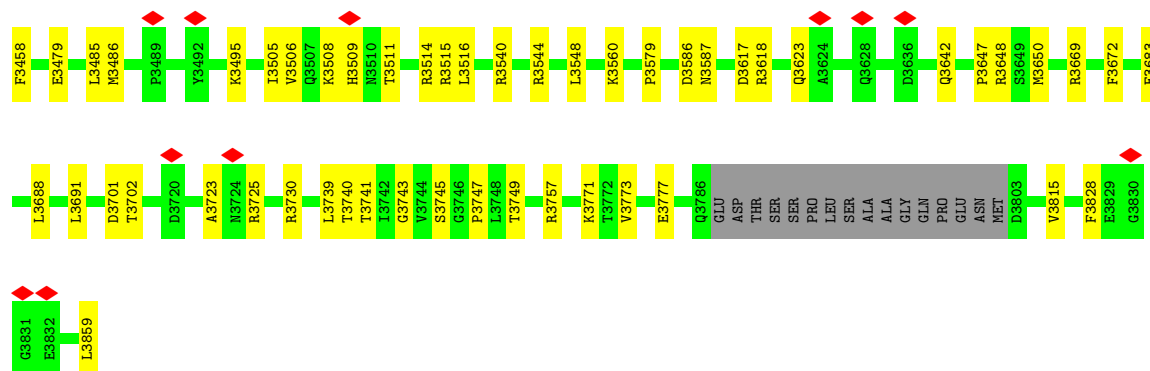
- Molecule 1: Transformation/transcription domain-associated protein



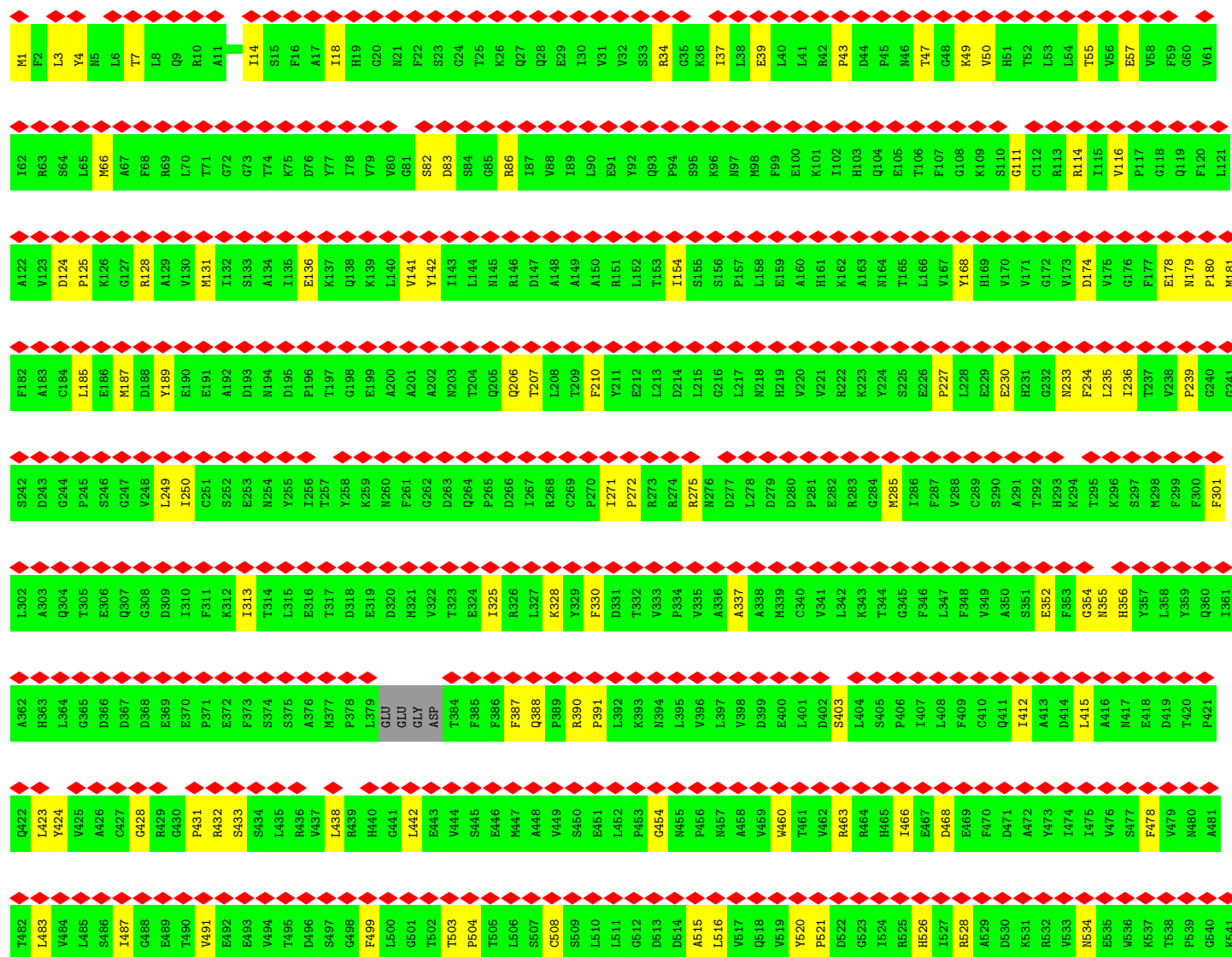
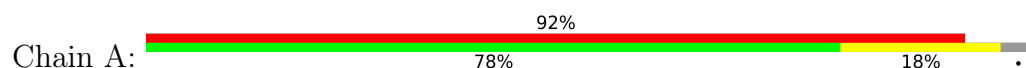




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PROTEIN DATA BANK

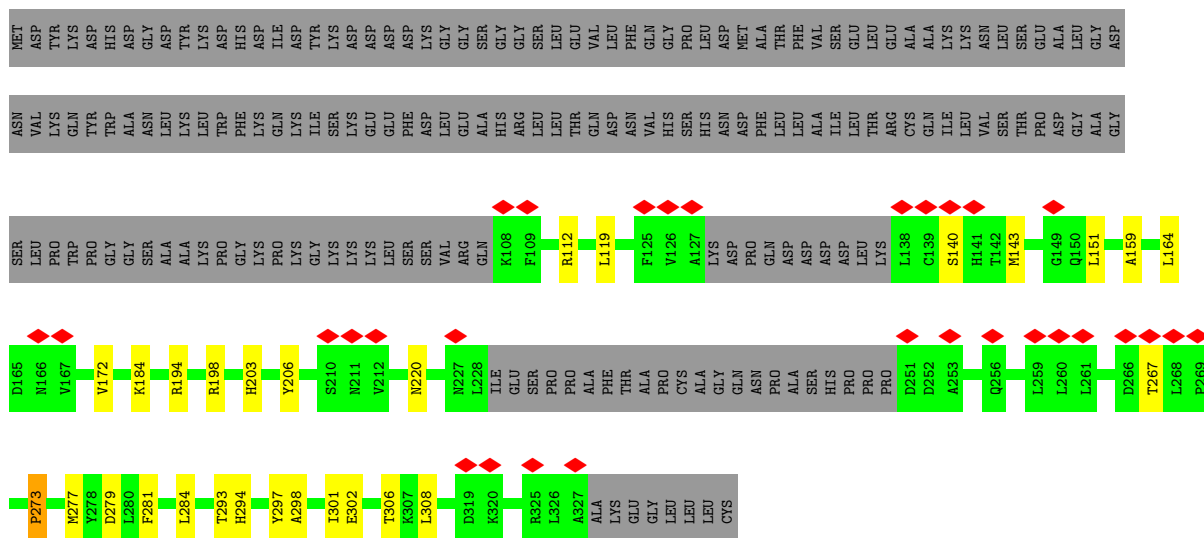


• Molecule 2: Splicing factor 3B subunit 3

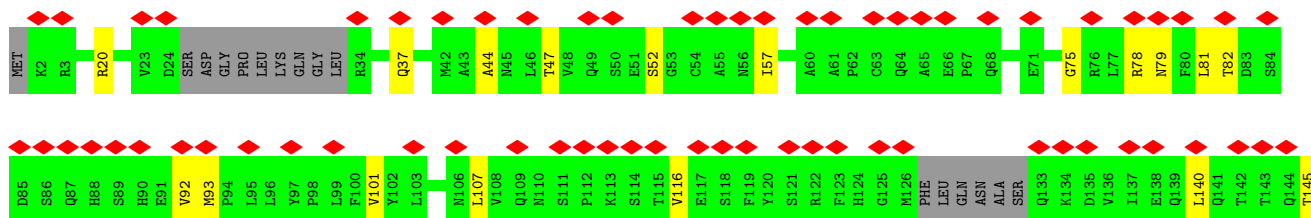


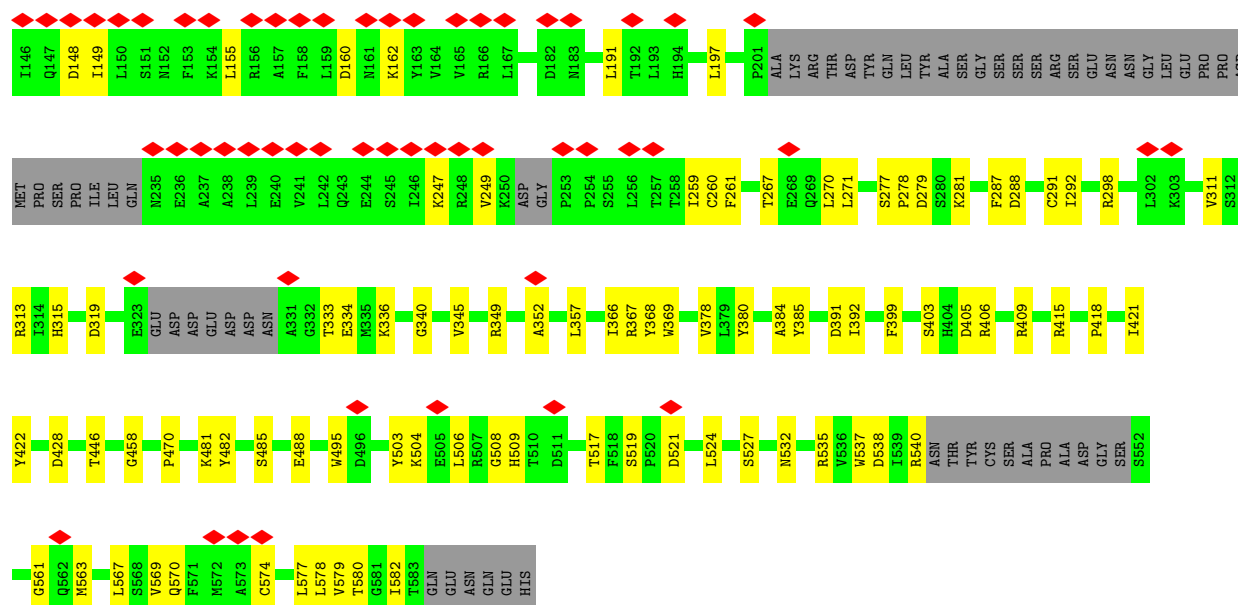


- Molecule 6: Transcriptional adapter 1

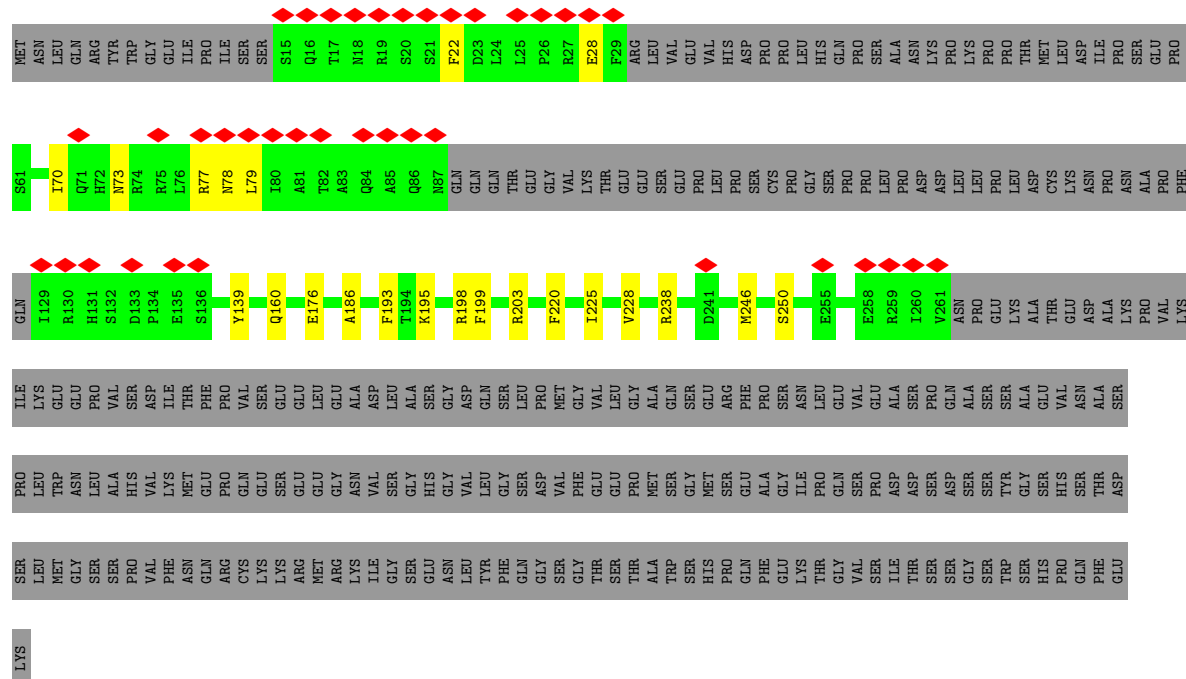


● Molecule 7: TAF5-like RNA polymerase II p300/CBP-associated factor-associated factor 65 kDa subunit 5L

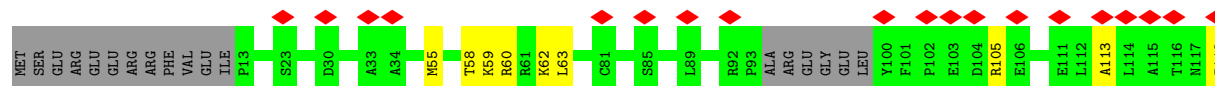




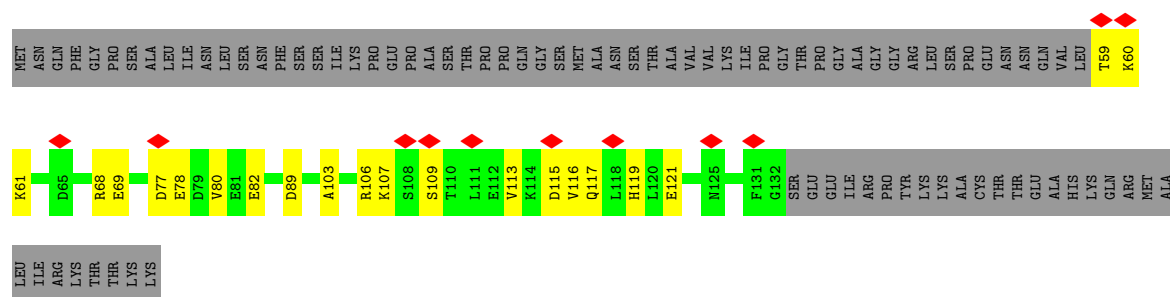
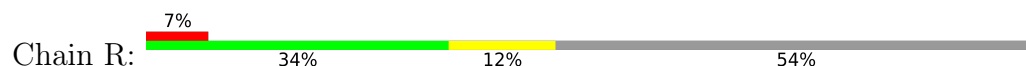
• Molecule 8: STAGA complex 65 subunit gamma



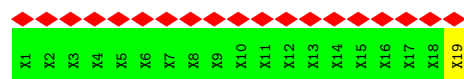
• Molecule 9: TAF6-like RNA polymerase II p300/CBP-associated factor-associated factor 65 kDa subunit 6L



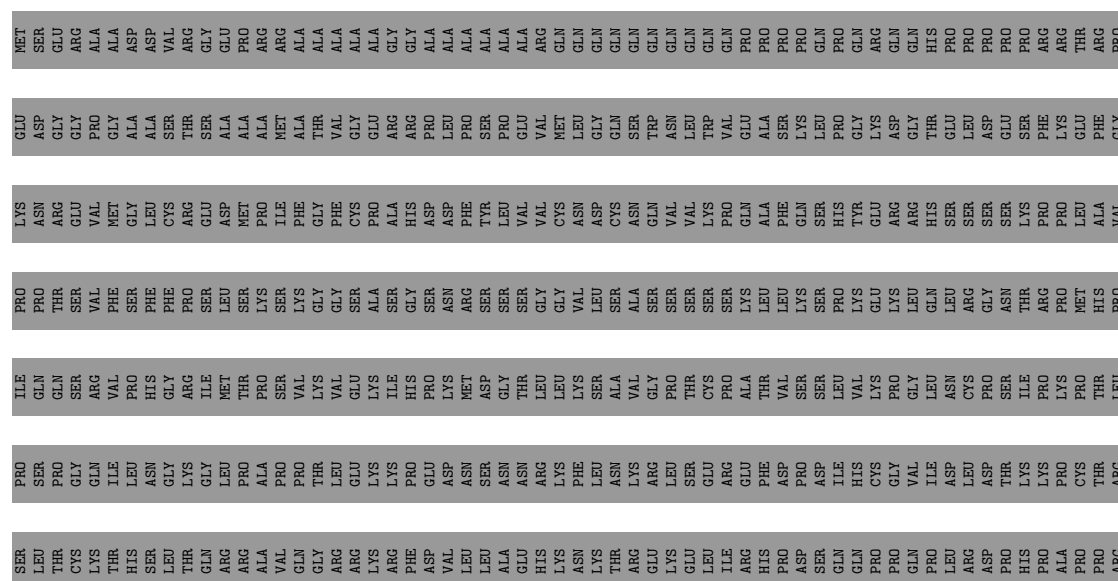
- Molecule 12: Transcription initiation factor TFIID subunit 12



- Molecule 13: Unassigned sequence



- Molecule 14: Ataxin-7



[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	378168	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)	800	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.115	Depositor
Minimum map value	-0.060	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.015	Depositor
Map size ($\text{\AA}$)	440.0, 440.0, 440.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.1, 1.1, 1.1	Depositor

5 Model quality

5.1 Standard geometry

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	C	0.11	0/26794	0.32	2/36236 (0.0%)
2	A	0.11	0/9345	0.29	1/12680 (0.0%)
3	B	0.07	0/393	0.25	0/528
4	D	0.12	0/2638	0.33	0/3559
5	E	0.10	0/1793	0.31	0/2408
6	G	0.15	0/1538	0.38	2/2089 (0.1%)
7	H	0.12	0/4167	0.34	1/5647 (0.0%)
8	I	0.08	0/1449	0.26	0/1959
9	K	0.12	0/2757	0.37	2/3745 (0.1%)
10	M	0.12	0/979	0.38	0/1328
11	O	0.12	0/737	0.37	0/998
12	R	0.12	0/614	0.39	0/829
14	L	0.13	0/374	0.39	0/504
All	All	0.11	0/53578	0.32	8/72510 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	273	PRO	N-CD-CG	-6.77	93.05	103.20
9	K	420	PRO	N-CA-CB	6.74	110.41	103.00
9	K	413	PRO	N-CA-CB	6.65	110.23	103.25
2	A	504	PRO	CA-N-CD	-6.47	102.94	112.00
6	G	273	PRO	CA-N-CD	-6.18	103.34	112.00
7	H	57	ILE	N-CA-C	-5.61	107.27	112.43
1	C	1032	LYS	CA-C-N	5.41	135.67	125.66
1	C	1032	LYS	C-N-CA	5.41	135.67	125.66

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	26251	0	26857	298	0
2	A	9158	0	9102	126	0
3	B	383	0	364	5	0
4	D	2595	0	2617	35	0
5	E	1770	0	1750	14	0
6	G	1505	0	1482	23	0
7	H	4084	0	4012	71	0
8	I	1419	0	1375	17	0
9	K	2703	0	2670	34	0
10	M	957	0	969	21	0
11	O	722	0	720	17	0
12	R	605	0	598	17	0
13	X	95	0	21	1	0
14	L	362	0	336	5	0
All	All	52609	0	52873	624	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 6.

All (624) 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:O:139:LEU:HB3	11:O:144:PHE:HB2	1.61	0.82
1:C:411:LEU:HD12	1:C:412:PRO:HD2	1.61	0.81
2:A:701:LEU:HD11	2:A:712:VAL:HB	1.62	0.81
1:C:3455:LEU:HD12	1:C:3456:PRO:HD2	1.63	0.80
2:A:548:ALA:HB3	2:A:555:VAL:HB	1.68	0.74
1:C:1771:LYS:O	1:C:1775:HIS:ND1	2.22	0.72
1:C:373:PRO:HG3	1:C:411:LEU:HD21	1.71	0.72
2:A:18:ILE:HG21	2:A:66:MET:HA	1.72	0.72
7:H:333:THR:HG22	7:H:334:GLU:H	1.56	0.71
7:H:340:GLY:O	7:H:367:ARG:NH1	2.24	0.71
1:C:1575:MET:HE3	1:C:1577:ALA:HB3	1.73	0.70
11:O:204:LEU:HB3	11:O:209:ILE:HB	1.73	0.70
1:C:2797:MET:HE1	4:D:263:LEU:HB2	1.72	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:128:ARG:NH2	2:A:178:GLU:O	2.24	0.69
4:D:419:CYS:HB2	4:D:420:PRO:HD3	1.75	0.68
1:C:1752:LEU:HD22	1:C:1755:ARG:HE	1.57	0.68
7:H:535:ARG:HB3	7:H:537:TRP:HE1	1.60	0.67
7:H:532:ASN:HB3	7:H:561:GLY:HA3	1.74	0.67
1:C:2343:ARG:HG3	1:C:2347:ILE:HD12	1.77	0.66
1:C:1671:TRP:HE1	1:C:1718:LEU:HB3	1.61	0.66
2:A:719:SER:HB2	2:A:734:LEU:HB2	1.78	0.65
8:I:22:PHE:HB3	9:K:282:VAL:HG11	1.77	0.65
1:C:1889:HIS:HA	1:C:1926:ILE:HG21	1.79	0.65
2:A:415:LEU:HD11	2:A:790:ILE:HD13	1.79	0.65
2:A:428:GLY:HA3	2:A:433:SER:HA	1.77	0.65
1:C:1319:GLN:HG2	1:C:1320:PRO:HD3	1.78	0.64
2:A:3:LEU:HD23	2:A:1129:LEU:HD13	1.79	0.64
2:A:898:ASN:HD21	2:A:972:LEU:HD23	1.61	0.64
2:A:1050:PHE:HE1	3:B:49:LEU:HD13	1.63	0.64
1:C:2837:LEU:HD23	1:C:2851:LEU:HD11	1.80	0.64
5:E:305:ASN:O	5:E:308:ARG:NH1	2.30	0.64
9:K:168:VAL:O	9:K:215:ARG:NH2	2.30	0.64
7:H:357:LEU:HB3	7:H:369:TRP:HB2	1.80	0.63
9:K:60:ARG:HG2	9:K:62:LYS:H	1.63	0.63
1:C:1675:ASN:HA	1:C:1719:ARG:HH11	1.62	0.63
7:H:349:ARG:HG3	7:H:391:ASP:HA	1.81	0.63
2:A:354:GLY:HA3	2:A:432:ARG:HH12	1.62	0.63
7:H:319:ASP:OD1	11:O:150:ARG:NH2	2.26	0.63
4:D:60:ASN:ND2	7:H:160:ASP:O	2.32	0.62
2:A:791:HIS:HB3	2:A:796:ASN:H	1.64	0.62
1:C:1135:LEU:HD23	1:C:1137:LEU:H	1.64	0.62
1:C:391:PRO:HA	1:C:433:LYS:HE2	1.81	0.62
1:C:3167:PHE:O	1:C:3171:ARG:NH2	2.33	0.62
1:C:1149:CYS:O	1:C:1157:LYS:NZ	2.33	0.61
2:A:554:VAL:HB	2:A:566:PHE:HB2	1.82	0.61
2:A:663:LEU:HB2	2:A:679:LEU:HD22	1.82	0.61
2:A:996:ILE:HG23	2:A:998:HIS:H	1.65	0.61
2:A:1086:SER:O	9:K:221:ARG:NH2	2.33	0.61
8:I:238:ARG:NH1	11:O:168:ASN:OD1	2.34	0.60
1:C:737:HIS:NE2	1:C:778:GLU:OE2	2.32	0.60
1:C:562:TRP:HA	1:C:641:MET:HE1	1.83	0.60
1:C:916:VAL:HG23	1:C:917:THR:HG23	1.83	0.60
1:C:2002:GLN:HG3	1:C:2005:LEU:HD22	1.83	0.60
4:D:64:LEU:HD12	4:D:69:MET:HE3	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:960:LEU:HD12	2:A:969:VAL:HG12	1.84	0.60
7:H:259:ILE:HA	7:H:577:LEU:HB3	1.82	0.60
12:R:113:VAL:HG12	12:R:115:ASP:H	1.67	0.60
2:A:969:VAL:HG23	2:A:980:LYS:HB2	1.83	0.60
8:I:176:GLU:OE1	9:K:105:ARG:NH1	2.35	0.60
2:A:454:GLY:O	2:A:760:ASN:ND2	2.35	0.60
2:A:1105:GLN:HE22	2:A:1107:THR:HB	1.65	0.59
4:D:167:ARG:NH2	7:H:52:SER:OG	2.35	0.59
1:C:47:GLU:O	1:C:99:ARG:NH2	2.35	0.59
2:A:1106:LYS:HB2	2:A:1117:LEU:HD23	1.83	0.59
4:D:230:ASN:HD22	4:D:234:MET:HB2	1.67	0.59
2:A:124:ASP:HB2	2:A:180:PRO:HB3	1.85	0.59
7:H:563:MET:SD	7:H:563:MET:N	2.76	0.59
6:G:159:ALA:HB1	6:G:164:LEU:HB2	1.83	0.59
2:A:520:TYR:CD2	2:A:521:PRO:HD2	2.38	0.59
1:C:3135:SER:HG	1:C:3162:TYR:HH	1.48	0.59
1:C:1007:TYR:HE1	1:C:3456:PRO:HB3	1.68	0.58
4:D:209:LEU:HB2	7:H:37:GLN:HG3	1.84	0.58
1:C:869:ARG:NH1	1:C:901:SER:O	2.35	0.58
4:D:63:LEU:HD12	4:D:66:LYS:HD2	1.86	0.58
7:H:107:LEU:HD13	7:H:116:VAL:HA	1.86	0.58
1:C:2444:LEU:HD12	1:C:2486:MET:HE1	1.85	0.58
5:E:29:GLU:OE2	5:E:196:LYS:NZ	2.34	0.58
1:C:977:LEU:HB3	1:C:2603:ARG:HH21	1.69	0.58
1:C:2651:GLU:OE1	6:G:220:ASN:ND2	2.37	0.58
1:C:3544:ARG:NH1	1:C:3777:GLU:OE1	2.36	0.58
1:C:1145:LEU:HD13	1:C:1163:SER:HB3	1.84	0.57
1:C:2449:CYS:SG	1:C:2450:ALA:N	2.76	0.57
1:C:2698:LYS:HD3	1:C:2878:LYS:HD3	1.85	0.57
2:A:412:ILE:HG12	2:A:423:LEU:HG	1.86	0.57
2:A:903:TRP:HB2	2:A:930:LEU:HD23	1.86	0.57
1:C:1527:ALA:HB3	1:C:1564:ARG:HH12	1.69	0.57
2:A:932:ASN:ND2	2:A:935:GLU:OE1	2.38	0.57
4:D:177:VAL:HG11	4:D:196:GLU:OE2	2.03	0.57
5:E:62:LEU:HD12	5:E:314:PHE:HB2	1.87	0.57
1:C:1379:LEU:HD22	1:C:1381:GLN:HE22	1.69	0.57
1:C:1100:MET:SD	1:C:1163:SER:OG	2.62	0.57
1:C:838:SER:HB3	1:C:841:LEU:HB2	1.86	0.57
1:C:1171:LEU:HD23	1:C:1175:TRP:CE3	2.39	0.57
1:C:1657:LEU:HG	1:C:1661:HIS:HE1	1.68	0.57
1:C:721:VAL:HG23	1:C:728:ASN:HB3	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:125:PRO:HG2	2:A:174:ASP:HB2	1.87	0.57
2:A:463:ARG:NH1	2:A:468:ASP:O	2.37	0.57
1:C:3294:THR:HG22	1:C:3296:PRO:HD2	1.87	0.57
1:C:386:VAL:HG12	1:C:388:GLN:H	1.69	0.56
1:C:1318:LEU:HB3	1:C:1320:PRO:HD2	1.87	0.56
7:H:292:ILE:HD11	7:H:345:VAL:HG21	1.86	0.56
10:M:92:LEU:HD13	10:M:95:ILE:HD12	1.86	0.56
1:C:3485:LEU:O	1:C:3486:MET:HE2	2.05	0.56
2:A:805:ASN:ND2	2:A:858:GLY:O	2.38	0.56
1:C:2631:GLN:O	1:C:2635:ARG:NH1	2.34	0.56
7:H:101:VAL:HG13	7:H:140:LEU:HD11	1.87	0.56
1:C:583:PRO:O	1:C:586:THR:OG1	2.21	0.56
1:C:1253:ASN:HB3	1:C:1256:VAL:HG12	1.88	0.56
1:C:1903:GLN:HA	1:C:1906:HIS:CE1	2.41	0.56
2:A:1109:LEU:HD21	2:A:1118:VAL:HG21	1.88	0.56
7:H:287:PHE:HB2	7:H:291:CYS:HB3	1.87	0.56
7:H:278:PRO:HG2	7:H:352:ALA:HA	1.87	0.56
1:C:106:LEU:HD21	1:C:146:PRO:HG2	1.88	0.56
1:C:3672:PHE:HD2	1:C:3739:LEU:HD21	1.71	0.56
1:C:3683:GLU:HA	1:C:3688:LEU:HB2	1.88	0.56
2:A:956:GLN:HE22	2:A:997:GLY:HA2	1.70	0.56
14:L:535:VAL:HG23	14:L:540:TRP:HD1	1.71	0.56
1:C:3691:LEU:HD23	1:C:3730:ARG:HD3	1.88	0.55
2:A:801:GLU:HB2	2:A:865:VAL:HB	1.87	0.55
2:A:415:LEU:HD22	2:A:424:TYR:HE2	1.71	0.55
1:C:3505:ILE:HG12	1:C:3514:ARG:HG3	1.88	0.55
1:C:3739:LEU:O	1:C:3740:THR:OG1	2.21	0.55
8:I:220:PHE:HB3	8:I:225:ILE:HB	1.88	0.55
4:D:36:VAL:HA	4:D:40:LEU:HD13	1.89	0.55
8:I:160:GLN:NE2	9:K:113:ALA:O	2.39	0.55
1:C:136:ILE:HD12	1:C:139:LEU:HD21	1.88	0.55
2:A:717:SER:HA	2:A:738:THR:HG22	1.89	0.55
7:H:313:ARG:HB2	7:H:315:HIS:CD2	2.42	0.55
1:C:2493:LYS:HD3	1:C:2619:HIS:HA	1.87	0.55
9:K:55:MET:HE3	9:K:63:LEU:HD12	1.89	0.55
2:A:603:ARG:NH2	2:A:623:ASP:OD2	2.40	0.55
2:A:862:TRP:O	2:A:884:GLN:NE2	2.39	0.55
1:C:2989:SER:O	1:C:2993:MET:HG2	2.07	0.54
1:C:3163:LEU:HD13	1:C:3166:ILE:HD12	1.89	0.54
8:I:139:TYR:O	11:O:150:ARG:NH1	2.40	0.54
10:M:67:ASP:OD1	10:M:68:ALA:N	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1891:ILE:HG23	1:C:1895:ALA:HB3	1.88	0.54
1:C:835:LEU:HA	1:C:842:VAL:HG22	1.89	0.54
2:A:783:TYR:HB2	2:A:801:GLU:HB3	1.88	0.54
12:R:77:ASP:OD1	12:R:78:GLU:N	2.40	0.54
1:C:1063:LEU:HB2	1:C:1066:TYR:HD2	1.72	0.54
2:A:86:ARG:NH1	2:A:1157:GLY:O	2.38	0.54
1:C:228:LEU:HG	1:C:231:ILE:HD13	1.89	0.54
4:D:60:ASN:OD1	4:D:62:ASN:ND2	2.41	0.54
4:D:177:VAL:HG23	4:D:195:LEU:HD23	1.90	0.54
1:C:295:ILE:HG21	1:C:338:ILE:HG22	1.90	0.54
1:C:2272:LEU:HG	1:C:2328:LEU:HD11	1.88	0.54
1:C:2355:ILE:HD11	1:C:2363:ILE:HD11	1.88	0.54
1:C:2400:MET:HG3	1:C:2442:ALA:HB2	1.88	0.54
2:A:43:PRO:HA	2:A:50:VAL:HG22	1.90	0.54
2:A:700:LYS:O	2:A:715:MET:HG2	2.08	0.54
1:C:2982:SER:HA	1:C:3560:LYS:HG3	1.90	0.54
4:D:104:LEU:HD12	4:D:105:PRO:HD2	1.88	0.54
1:C:1811:PHE:CE1	1:C:1839:LEU:HD13	2.43	0.54
1:C:381:ASP:O	1:C:385:HIS:ND1	2.41	0.53
10:M:47:VAL:HA	10:M:50:ILE:HG22	1.90	0.53
1:C:339:LEU:O	1:C:385:HIS:NE2	2.41	0.53
8:I:78:ASN:OD1	8:I:79:LEU:N	2.41	0.53
2:A:136:GLU:OE2	2:A:189:TYR:OH	2.23	0.53
4:D:82:PRO:HG2	4:D:149:ARG:HB2	1.88	0.53
1:C:767:ILE:HG13	1:C:775:LEU:HB3	1.90	0.53
1:C:1035:ARG:HE	1:C:1039:LEU:HD11	1.74	0.53
2:A:168:TYR:HB2	2:A:185:LEU:HB2	1.89	0.53
7:H:446:THR:HG22	7:H:470:PRO:HB3	1.91	0.53
1:C:1397:THR:O	1:C:1443:ASN:ND2	2.41	0.53
1:C:2340:MET:HG2	1:C:2342:MET:H	1.72	0.53
12:R:77:ASP:HB3	12:R:80:VAL:HG23	1.91	0.53
2:A:337:ALA:HB2	2:A:352:GLU:HB3	1.91	0.53
7:H:78:ARG:O	7:H:82:THR:OG1	2.23	0.53
1:C:835:LEU:HD23	1:C:842:VAL:HA	1.91	0.53
7:H:75:GLY:O	7:H:79:ASN:ND2	2.42	0.53
1:C:25:VAL:HA	1:C:68:ARG:HH22	1.75	0.52
2:A:206:GLN:NE2	2:A:230:GLU:O	2.31	0.52
2:A:355:ASN:HA	2:A:403:SER:HB3	1.90	0.52
2:A:355:ASN:H	2:A:432:ARG:HH22	1.57	0.52
2:A:1199:ARG:HH12	2:A:1207:LYS:HG3	1.75	0.52
1:C:604:GLN:NE2	1:C:665:ASN:OD1	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1126:LEU:O	1:C:1131:ARG:NH1	2.42	0.52
1:C:2870:VAL:HG11	5:E:176:ILE:HA	1.91	0.52
2:A:181:MET:CE	2:A:210:PHE:HB3	2.39	0.52
9:K:58:THR:OG1	9:K:59:LYS:N	2.35	0.52
1:C:3338:ARG:HD3	1:C:3511:THR:HB	1.91	0.52
1:C:1829:ARG:NH1	1:C:1868:CYS:SG	2.82	0.52
2:A:423:LEU:HB2	2:A:438:LEU:HB2	1.90	0.52
2:A:592:LEU:HD13	2:A:605:LEU:HD13	1.90	0.52
4:D:236:ARG:HE	12:R:78:GLU:HG2	1.75	0.52
7:H:249:VAL:HA	7:H:540:ARG:HH12	1.75	0.52
1:C:580:GLN:NE2	1:C:581:LEU:O	2.42	0.52
2:A:1117:LEU:HB2	2:A:1129:LEU:HB2	1.92	0.52
2:A:1005:VAL:HG13	2:A:1006:GLN:HG2	1.92	0.52
7:H:403:SER:OG	7:H:405:ASP:OD1	2.28	0.52
9:K:193:LEU:O	9:K:197:VAL:HG23	2.09	0.52
1:C:859:ASP:OD1	1:C:860:PHE:N	2.43	0.52
2:A:1012:VAL:HG22	2:A:1023:ILE:HG12	1.91	0.52
7:H:415:ARG:HH12	10:M:105:PRO:HG3	1.75	0.52
1:C:1660:GLN:O	1:C:1660:GLN:HG2	2.10	0.52
2:A:37:ILE:HG12	2:A:57:GLU:HG2	1.90	0.52
7:H:247:LYS:HB3	9:K:186:ASN:HD22	1.75	0.52
1:C:2883:LYS:HE2	1:C:2887:TYR:CZ	2.45	0.51
2:A:313:ILE:HG23	2:A:325:ILE:HG23	1.91	0.51
11:O:126:TYR:O	11:O:153:ARG:NH2	2.42	0.51
11:O:161:LYS:NZ	11:O:165:ASP:OD2	2.43	0.51
1:C:1355:CYS:SG	1:C:3313:THR:OG1	2.62	0.51
2:A:548:ALA:HB2	2:A:590:MET:HG3	1.92	0.51
9:K:271:LEU:HD11	9:K:289:ILE:HD11	1.92	0.51
1:C:159:LYS:O	1:C:163:LYS:HG3	2.10	0.51
1:C:1824:MET:HG2	1:C:1828:LEU:HD22	1.93	0.51
2:A:637:PRO:HA	2:A:669:LEU:HA	1.92	0.51
6:G:140:SER:OG	12:R:89:ASP:OD1	2.29	0.51
7:H:311:VAL:HG12	8:I:198:ARG:HH12	1.75	0.51
1:C:1006:ARG:NH2	1:C:3458:PHE:O	2.44	0.51
10:M:104:LEU:HD12	10:M:105:PRO:HD2	1.93	0.51
1:C:1833:LEU:HD22	1:C:1886:LEU:HD13	1.93	0.50
1:C:1862:MET:HE2	1:C:1862:MET:HA	1.93	0.50
1:C:625:MET:HE3	1:C:628:GLU:HB2	1.93	0.50
1:C:1894:PHE:HA	1:C:1934:ARG:HH12	1.76	0.50
2:A:178:GLU:HG3	2:A:179:ASN:H	1.76	0.50
1:C:828:MET:HB3	1:C:868:VAL:HG21	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3191:ASN:ND2	4:D:398:SER:OG	2.44	0.50
4:D:177:VAL:O	4:D:181:THR:N	2.37	0.50
7:H:481:LYS:HG3	7:H:482:TYR:CD1	2.46	0.50
1:C:1194:LEU:HB3	1:C:1198:VAL:HG13	1.94	0.50
1:C:2098:VAL:HA	1:C:2144:LEU:HD12	1.93	0.50
1:C:2476:TYR:CE2	1:C:2481:GLN:HB2	2.46	0.50
1:C:3669:ARG:HD2	1:C:3739:LEU:HA	1.94	0.50
2:A:914:ILE:HG22	2:A:917:PRO:HD2	1.92	0.50
4:D:220:ASN:HD22	10:M:107:ILE:HD12	1.75	0.50
6:G:194:ARG:NH2	6:G:273:PRO:O	2.44	0.50
7:H:261:PHE:CE1	7:H:563:MET:HE2	2.47	0.50
7:H:508:GLY:HA3	7:H:537:TRP:HZ2	1.76	0.50
7:H:392:ILE:HD12	7:H:399:PHE:HB3	1.94	0.50
12:R:68:ARG:HB3	12:R:68:ARG:NH1	2.27	0.50
1:C:2813:ILE:HG13	1:C:2813:ILE:O	2.11	0.49
3:B:31:TRP:HH2	9:K:364:VAL:HG12	1.77	0.49
7:H:44:ALA:O	7:H:47:THR:OG1	2.29	0.49
7:H:517:THR:HG21	7:H:570:GLN:HA	1.93	0.49
1:C:95:GLU:OE2	1:C:99:ARG:NH2	2.36	0.49
1:C:1296:LEU:HB2	1:C:1299:HIS:HD2	1.77	0.49
1:C:3548:LEU:HD13	1:C:3773:VAL:HG21	1.94	0.49
4:D:103:ARG:HH11	4:D:103:ARG:HA	1.77	0.49
2:A:526:HIS:HB3	2:A:534:ASN:HB2	1.94	0.49
2:A:603:ARG:NH1	2:A:620:ASP:OD2	2.45	0.49
7:H:567:LEU:HD12	7:H:580:THR:HG22	1.95	0.49
1:C:359:ILE:HG22	1:C:363:SER:HB2	1.94	0.49
4:D:79:ASN:HB2	4:D:88:SER:HB3	1.92	0.49
6:G:279:ASP:OD2	8:I:203:ARG:NH2	2.43	0.49
1:C:696:ARG:NH2	1:C:710:TYR:OH	2.35	0.49
1:C:758:LEU:HD23	1:C:761:ARG:HH12	1.76	0.49
2:A:187:MET:HE2	2:A:206:GLN:HB3	1.93	0.49
2:A:390:ARG:HG2	2:A:391:PRO:HD2	1.95	0.49
1:C:1678:GLU:HG3	1:C:1725:PHE:HE1	1.77	0.49
2:A:272:PRO:HB2	2:A:387:PHE:HD1	1.78	0.49
2:A:1040:ASP:OD1	2:A:1043:THR:OG1	2.18	0.49
1:C:406:ILE:HA	1:C:416:GLN:HG2	1.94	0.49
1:C:1825:LEU:HD23	1:C:1825:LEU:O	2.12	0.49
2:A:142:TYR:HB3	2:A:154:ILE:HD11	1.94	0.49
9:K:58:THR:O	9:K:59:LYS:HG2	2.13	0.49
12:R:107:LYS:C	12:R:109:SER:H	2.20	0.49
1:C:371:LEU:HD23	1:C:371:LEU:H	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:799:LYS:HB2	1:C:802:MET:HB2	1.94	0.49
1:C:1005:HIS:HB3	1:C:1140:TYR:HE1	1.78	0.49
7:H:574:CYS:HA	9:K:228:HIS:HA	1.95	0.49
1:C:1771:LYS:O	1:C:1774:GLN:HG3	2.12	0.49
1:C:3617:ASP:OD1	1:C:3618:ARG:N	2.46	0.49
1:C:1422:GLN:O	1:C:1426:HIS:ND1	2.33	0.48
1:C:2276:LYS:HD2	1:C:2327:SER:HB3	1.95	0.48
1:C:3647:PRO:HD2	1:C:3650:MET:HE3	1.95	0.48
2:A:207:THR:HA	2:A:227:PRO:HA	1.95	0.48
2:A:515:ALA:HB2	2:A:528:ARG:HH11	1.78	0.48
1:C:3457:LYS:HA	1:C:3505:ILE:HD12	1.94	0.48
1:C:2490:PHE:HD2	1:C:2493:LYS:HG3	1.78	0.48
6:G:151:LEU:HD23	6:G:172:VAL:HG13	1.95	0.48
7:H:409:ARG:HD3	7:H:418:PRO:HG3	1.94	0.48
1:C:406:ILE:HD12	1:C:416:GLN:HG2	1.95	0.48
1:C:3508:LYS:HG2	1:C:3509:HIS:H	1.78	0.48
1:C:662:ILE:HG22	1:C:709:LEU:HD11	1.94	0.48
1:C:1215:MET:O	1:C:1219:THR:OG1	2.27	0.48
1:C:1527:ALA:HB3	1:C:1564:ARG:NH1	2.28	0.48
1:C:2372:GLU:HG3	1:C:2420:LEU:HD12	1.94	0.48
2:A:1086:SER:N	13:X:19:UNK:O	2.46	0.48
6:G:306:THR:HA	10:M:99:ARG:HH21	1.77	0.48
7:H:93:MET:HE3	7:H:93:MET:HA	1.94	0.48
9:K:299:ASP:N	9:K:299:ASP:OD1	2.45	0.48
1:C:1759:PHE:O	1:C:1762:PRO:HD3	2.12	0.48
1:C:2197:ILE:O	1:C:2197:ILE:HG22	2.14	0.48
1:C:2251:TYR:HB2	1:C:2271:THR:HG23	1.95	0.48
2:A:691:THR:HG22	2:A:716:SER:HB2	1.95	0.48
4:D:60:ASN:HB3	7:H:162:LYS:HG2	1.95	0.48
5:E:307:TYR:HE1	11:O:209:ILE:HD13	1.79	0.48
1:C:19:LYS:HE2	1:C:53:THR:HG22	1.94	0.48
1:C:2489:HIS:O	1:C:2664:GLN:NE2	2.47	0.48
1:C:2697:GLY:HA2	1:C:2702:LEU:HB2	1.95	0.48
1:C:3540:ARG:HH22	1:C:3579:PRO:HA	1.78	0.48
1:C:3340:LEU:HB3	1:C:3445:ILE:HD11	1.96	0.47
8:I:193:PHE:HE2	11:O:155:ILE:HG12	1.79	0.47
1:C:1750:ARG:HA	1:C:1753:PHE:HB2	1.94	0.47
2:A:612:ASN:HB3	2:A:633:LEU:HB2	1.96	0.47
4:D:234:MET:HA	4:D:237:CYS:SG	2.54	0.47
5:E:213:PRO:HB3	5:E:217:ALA:HB3	1.95	0.47
1:C:1355:CYS:HG	1:C:3313:THR:HG1	1.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2388:THR:OG1	1:C:2391:GLU:OE1	2.28	0.47
7:H:366:ILE:HB	7:H:380:TYR:HB2	1.97	0.47
1:C:2689:ARG:H	6:G:267:THR:HG22	1.78	0.47
1:C:1058:CYS:SG	1:C:1059:GLY:N	2.87	0.47
1:C:1289:MET:HA	1:C:1289:MET:HE2	1.97	0.47
12:R:59:THR:OG1	12:R:60:LYS:N	2.47	0.47
1:C:277:TYR:HB2	1:C:281:ILE:HG22	1.96	0.47
1:C:2361:ALA:O	1:C:2365:ARG:NH1	2.47	0.47
2:A:131:MET:SD	2:A:141:VAL:HG22	2.55	0.47
2:A:168:TYR:OH	2:A:187:MET:HG3	2.15	0.47
2:A:515:ALA:HB2	2:A:528:ARG:HD2	1.95	0.47
7:H:406:ARG:HH12	10:M:88:PRO:HB3	1.78	0.47
7:H:569:VAL:HG12	7:H:579:VAL:HG12	1.96	0.47
12:R:60:LYS:HG3	12:R:61:LYS:HG2	1.97	0.47
1:C:1598:ARG:HB3	1:C:1599:PRO:HD3	1.96	0.47
1:C:1657:LEU:HG	1:C:1661:HIS:CE1	2.48	0.47
1:C:1758:ASP:HA	1:C:1773:LEU:HD21	1.97	0.47
6:G:198:ARG:NE	6:G:206:TYR:OH	2.47	0.47
7:H:149:ILE:HG23	7:H:155:LEU:HB3	1.96	0.47
1:C:3168:VAL:HG12	1:C:3169:LYS:HD3	1.97	0.47
6:G:184:LYS:NZ	12:R:69:GLU:HG2	2.30	0.47
6:G:281:PHE:HZ	7:H:384:ALA:HB2	1.80	0.47
1:C:1430:LEU:HD21	1:C:1448:LEU:HD13	1.97	0.47
1:C:2656:LEU:HD13	1:C:2672:LEU:HD11	1.96	0.47
2:A:1:MET:HA	2:A:1:MET:HE2	1.96	0.47
2:A:114:ARG:NH1	3:B:37:ARG:HB3	2.30	0.47
2:A:548:ALA:HB2	2:A:590:MET:CG	2.45	0.47
3:B:39:SER:OG	9:K:416:GLY:O	2.30	0.47
5:E:232:LEU:HD21	5:E:286:ILE:HD11	1.97	0.47
7:H:421:ILE:HG13	10:M:95:ILE:HG22	1.97	0.47
10:M:126:ASN:HB3	10:M:129:LEU:HG	1.97	0.47
7:H:519:SER:OG	7:H:521:ASP:OD1	2.30	0.46
1:C:648:LYS:HB3	1:C:684:LEU:HD21	1.97	0.46
2:A:595:VAL:HG13	2:A:601:ARG:HA	1.96	0.46
2:A:952:ILE:HG12	2:A:961:ILE:HG12	1.98	0.46
7:H:270:LEU:HD13	7:H:288:ASP:H	1.79	0.46
7:H:485:SER:HG	7:H:495:TRP:HE1	1.63	0.46
2:A:1199:ARG:HG2	2:A:1200:THR:H	1.79	0.46
9:K:302:ARG:HB3	9:K:306:CYS:SG	2.56	0.46
9:K:311:VAL:HG13	9:K:312:VAL:HG13	1.98	0.46
1:C:48:ASN:OD1	1:C:1947:ARG:NH1	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2007:VAL:O	1:C:2010:SER:OG	2.25	0.46
1:C:2805:GLU:HG3	1:C:2806:ARG:HD2	1.96	0.46
2:A:478:PHE:HE2	2:A:483:LEU:HD22	1.81	0.46
10:M:118:ASP:CG	10:M:119:ARG:H	2.23	0.46
1:C:582:GLN:HB3	1:C:585:GLU:OE1	2.16	0.46
1:C:1888:ALA:HB1	1:C:1927:LEU:HD22	1.97	0.46
1:C:3701:ASP:OD1	1:C:3702:THR:N	2.49	0.46
1:C:1441:THR:HG23	1:C:1443:ASN:H	1.80	0.46
1:C:1914:MET:HE2	1:C:1914:MET:HA	1.97	0.46
2:A:1048:ASP:HB3	2:A:1052:ASN:H	1.81	0.46
1:C:979:ASP:HB2	1:C:983:ALA:HB3	1.96	0.46
7:H:191:LEU:HD12	7:H:197:LEU:HD11	1.98	0.46
7:H:503:TYR:CD2	7:H:504:LYS:HG2	2.51	0.46
9:K:337:LEU:HD11	9:K:357:LYS:HZ2	1.80	0.46
1:C:361:ILE:HD12	1:C:375:ALA:HB1	1.97	0.46
1:C:3723:ALA:HB1	1:C:3725:ARG:HH21	1.81	0.46
2:A:503:THR:HB	2:A:520:TYR:CE2	2.51	0.46
9:K:213:LEU:HD22	9:K:263:LEU:HD22	1.97	0.46
3:B:32:LEU:O	3:B:36:HIS:ND1	2.33	0.46
4:D:236:ARG:NH2	12:R:82:GLU:OE2	2.48	0.46
1:C:2254:LEU:HD11	1:C:2268:LEU:HG	1.98	0.46
2:A:487:ILE:HA	2:A:491:VAL:HG22	1.97	0.46
7:H:267:THR:HG21	9:K:125:THR:HG22	1.97	0.46
7:H:368:TYR:HB3	7:H:378:VAL:HB	1.98	0.46
7:H:385:TYR:CD2	7:H:405:ASP:HB3	2.51	0.46
1:C:2522:THR:HG23	1:C:2525:ILE:HD12	1.97	0.45
2:A:870:ASN:ND2	2:A:873:GLN:OE1	2.49	0.45
4:D:5:LEU:HD13	10:M:109:PRO:HB3	1.98	0.45
1:C:829:ASP:HB2	1:C:830:PRO:HD3	1.98	0.45
2:A:4:TYR:HB3	2:A:1130:VAL:HB	1.97	0.45
8:I:73:ASN:HD21	8:I:250:SER:HA	1.82	0.45
1:C:309:MET:SD	1:C:309:MET:N	2.89	0.45
1:C:1558:LEU:O	1:C:1562:LEU:N	2.48	0.45
4:D:183:ASP:HB3	4:D:187:TRP:HE1	1.81	0.45
1:C:253:LEU:HD23	1:C:288:LEU:HD23	1.99	0.45
1:C:1947:ARG:HA	1:C:1950:ILE:HG22	1.98	0.45
1:C:1986:VAL:HA	1:C:1989:MET:HG2	1.98	0.45
1:C:2202:THR:HG22	1:C:2246:VAL:HG13	1.98	0.45
2:A:887:ALA:HB3	2:A:910:ALA:HB3	1.97	0.45
6:G:119:LEU:HD11	14:L:534:TYR:CD2	2.52	0.45
11:O:196:THR:HG23	11:O:198:GLU:H	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:961:ARG:HG2	1:C:1034:LEU:HD11	1.98	0.45
1:C:2699:THR:HA	1:C:2921:ARG:HH21	1.81	0.45
1:C:2850:TYR:CZ	1:C:2872:VAL:HG13	2.51	0.45
1:C:338:ILE:HG13	1:C:339:LEU:HD22	1.98	0.45
1:C:1902:LEU:H	1:C:1902:LEU:HD23	1.82	0.45
2:A:239:PRO:HD2	2:A:301:PHE:HZ	1.81	0.45
1:C:727:GLU:O	1:C:727:GLU:HG3	2.17	0.45
6:G:294:HIS:CE1	10:M:84:THR:HG23	2.52	0.45
9:K:314:LEU:HD23	9:K:322:VAL:HG13	1.99	0.45
1:C:547:ARG:HB3	1:C:603:TYR:HE1	1.81	0.45
1:C:2858:ARG:NH1	1:C:2989:SER:OG	2.49	0.45
1:C:3086:TYR:CE1	1:C:3104:VAL:HG11	2.51	0.45
2:A:233:ASN:OD1	2:A:234:PHE:N	2.45	0.45
2:A:960:LEU:HD21	2:A:967:LEU:HD11	1.99	0.45
9:K:206:VAL:HG12	9:K:206:VAL:O	2.16	0.45
1:C:247:VAL:HA	1:C:250:PHE:CE2	2.52	0.45
1:C:857:GLN:O	1:C:859:ASP:N	2.50	0.45
1:C:2142:SER:OG	1:C:2143:GLU:OE1	2.34	0.45
1:C:2305:LEU:O	1:C:2357:LYS:NZ	2.48	0.45
1:C:2714:ALA:HB2	1:C:2744:ILE:HD12	1.98	0.45
1:C:2859:VAL:HG23	1:C:2861:ASN:H	1.81	0.45
1:C:3757:ARG:HH11	1:C:3828:PHE:HE2	1.64	0.45
9:K:146:VAL:HG13	9:K:150:VAL:HB	1.97	0.45
14:L:527:ARG:HE	14:L:535:VAL:HG13	1.82	0.45
1:C:1019:GLU:OE2	1:C:1098:ILE:HG13	2.17	0.44
1:C:2865:MET:HB2	1:C:2891:LEU:HD21	1.99	0.44
1:C:3330:GLU:HG3	1:C:3334:GLU:HB2	2.00	0.44
4:D:236:ARG:HH21	12:R:78:GLU:HG2	1.81	0.44
8:I:186:ALA:HB2	11:O:163:ILE:HD11	1.99	0.44
10:M:48:THR:HG21	11:O:212:LYS:HD2	1.99	0.44
1:C:446:MET:SD	1:C:585:GLU:HG2	2.57	0.44
1:C:2633:PHE:HB3	1:C:2634:PRO:HD3	1.99	0.44
2:A:235:LEU:HG	2:A:250:ILE:HG13	1.98	0.44
2:A:236:ILE:HB	2:A:249:LEU:HB2	1.99	0.44
5:E:297:ILE:HG22	5:E:297:ILE:O	2.17	0.44
1:C:3304:MET:O	1:C:3308:ARG:HG2	2.17	0.44
7:H:313:ARG:HB2	7:H:315:HIS:NE2	2.32	0.44
1:C:44:GLU:HG2	1:C:92:LEU:HD21	1.98	0.44
1:C:1283:LYS:O	1:C:1287:GLN:HG3	2.17	0.44
1:C:3586:ASP:OD1	1:C:3587:ASN:N	2.50	0.44
1:C:3730:ARG:NH2	1:C:3859:LEU:O	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3743:GLY:HA2	1:C:3747:PRO:HD2	2.00	0.44
5:E:99:LYS:HB3	5:E:104:ARG:HH12	1.82	0.44
7:H:509:HIS:NE2	7:H:527:SER:OG	2.38	0.44
1:C:744:MET:HE3	1:C:744:MET:HB3	1.91	0.44
6:G:112:ARG:NH1	7:H:488:GLU:OE2	2.50	0.44
9:K:55:MET:CE	9:K:63:LEU:HA	2.48	0.44
1:C:1168:MET:HE2	1:C:1168:MET:HB3	1.84	0.44
1:C:1920:VAL:HA	1:C:1923:ALA:HB3	2.00	0.44
1:C:2240:GLU:HA	1:C:2243:TYR:CE2	2.52	0.44
1:C:2476:TYR:HD2	1:C:2480:SER:HB2	1.82	0.44
5:E:189:ARG:HG2	5:E:190:GLN:HG2	2.00	0.44
1:C:907:LYS:HD2	1:C:907:LYS:HA	1.84	0.44
1:C:3516:LEU:H	1:C:3516:LEU:HD23	1.83	0.44
1:C:3745:SER:O	1:C:3749:THR:OG1	2.29	0.44
2:A:431:PRO:HG3	2:A:849:GLU:HG2	1.99	0.44
7:H:506:LEU:HB3	7:H:537:TRP:CZ3	2.53	0.44
10:M:61:ALA:C	12:R:106:ARG:HH22	2.26	0.44
1:C:139:LEU:HA	1:C:142:GLN:HG2	1.99	0.44
1:C:1514:CYS:HB3	1:C:1554:PHE:HE1	1.83	0.44
1:C:3302:ARG:O	1:C:3306:MET:HG3	2.18	0.44
2:A:645:MET:HB2	2:A:662:PHE:HB2	2.00	0.44
11:O:148:ASP:OD2	11:O:151:ILE:HG22	2.18	0.44
1:C:783:LEU:HD11	1:C:815:VAL:HG21	2.00	0.43
1:C:3357:ALA:O	1:C:3623:GLN:NE2	2.51	0.43
2:A:7:THR:HA	2:A:1127:GLY:HA2	1.99	0.43
1:C:346:GLN:C	1:C:349:PRO:HD2	2.44	0.43
1:C:1803:ASN:N	1:C:1804:PRO:HD2	2.33	0.43
1:C:3064:ILE:HG21	1:C:3078:LYS:HG3	1.99	0.43
1:C:3098:CYS:SG	1:C:3099:MET:HE2	2.58	0.43
4:D:131:SER:OG	14:L:552:GLU:OE2	2.35	0.43
2:A:577:TYR:CE2	2:A:579:GLU:HB3	2.53	0.43
1:C:2509:ILE:HG12	1:C:2607:THR:HB	2.00	0.43
2:A:14:ILE:HG12	2:A:34:ARG:HH12	1.83	0.43
2:A:275:ARG:HG3	2:A:388:GLN:HG2	2.00	0.43
2:A:328:LYS:HB3	2:A:330:PHE:CZ	2.53	0.43
7:H:260:CYS:HB2	7:H:578:LEU:HD23	1.99	0.43
1:C:903:ARG:HH22	1:C:2979:PRO:HB3	1.83	0.43
1:C:2815:PRO:HA	1:C:2818:GLN:HG2	2.01	0.43
2:A:111:GLY:O	2:A:116:VAL:HG11	2.19	0.43
2:A:816:LYS:HD3	2:A:843:LEU:HG	2.01	0.43
2:A:939:PHE:HZ	2:A:942:LYS:HG3	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:296:ILE:HD12	9:K:302:ARG:HH12	1.84	0.43
1:C:822:PRO:HB3	4:D:394:PHE:CD1	2.54	0.43
1:C:2741:GLN:HG2	1:C:2744:ILE:HD11	2.00	0.43
1:C:3238:LEU:HD22	1:C:3250:LEU:HD11	2.01	0.43
4:D:205:GLU:HG3	4:D:206:PRO:HD2	2.00	0.43
7:H:81:LEU:HD11	7:H:92:VAL:HG21	2.00	0.43
1:C:647:PHE:CZ	1:C:681:THR:HG23	2.54	0.43
1:C:2653:SER:HB2	1:C:2654:PRO:HD3	1.99	0.43
2:A:895:ARG:HD3	2:A:903:TRP:CZ3	2.54	0.43
9:K:285:LEU:HG	9:K:288:HIS:HB2	2.00	0.43
1:C:1829:ARG:HD2	1:C:1879:CYS:HB2	2.00	0.43
1:C:2278:ALA:HA	1:C:2281:ASN:HD22	1.83	0.43
1:C:2637:TRP:HZ3	1:C:2648:LEU:HD23	1.83	0.43
12:R:117:GLN:O	12:R:121:GLU:HG2	2.19	0.43
1:C:114:LEU:HD23	1:C:114:LEU:H	1.84	0.43
1:C:987:LEU:HD21	1:C:2525:ILE:HD11	2.00	0.43
1:C:2849:PRO:HB3	1:C:2871:GLN:HE21	1.84	0.43
1:C:3739:LEU:C	1:C:3740:THR:HG1	2.21	0.43
1:C:3771:LYS:HG2	1:C:3815:VAL:HG21	2.01	0.43
7:H:535:ARG:HB3	7:H:537:TRP:NE1	2.29	0.43
1:C:543:VAL:O	1:C:547:ARG:HG3	2.18	0.43
4:D:85:GLU:HB2	4:D:103:ARG:NH2	2.33	0.43
8:I:28:GLU:O	9:K:128:ARG:NH1	2.48	0.43
1:C:2173:VAL:HA	1:C:2176:PHE:CE1	2.53	0.42
1:C:3051:GLN:HE22	1:C:3560:LYS:HD2	1.84	0.42
1:C:3442:LYS:HE2	1:C:3442:LYS:HB3	1.87	0.42
4:D:16:ILE:HD11	4:D:222:LEU:HD21	2.01	0.42
1:C:1473:LYS:HE2	1:C:1473:LYS:HB3	1.84	0.42
11:O:192:LYS:HD2	11:O:192:LYS:HA	1.82	0.42
1:C:2887:TYR:HA	1:C:2890:TYR:HD2	1.84	0.42
1:C:3149:HIS:CD2	1:C:3151:VAL:HG22	2.55	0.42
2:A:271:ILE:HD13	2:A:285:MET:HG3	2.00	0.42
2:A:1118:VAL:HG22	2:A:1128:ILE:HG22	2.01	0.42
4:D:192:LYS:O	4:D:196:GLU:HG2	2.19	0.42
9:K:282:VAL:HG12	9:K:282:VAL:O	2.20	0.42
11:O:123:LEU:HD21	11:O:153:ARG:HD3	2.01	0.42
4:D:362:LEU:HD23	4:D:362:LEU:HA	1.95	0.42
1:C:284:GLN:O	1:C:287:THR:OG1	2.31	0.42
1:C:1927:LEU:H	1:C:1927:LEU:HD23	1.85	0.42
6:G:143:MET:SD	6:G:143:MET:N	2.92	0.42
7:H:336:LYS:HB3	7:H:336:LYS:HE2	1.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:642:MET:HE1	1:C:650:ILE:HD12	2.02	0.42
5:E:124:LEU:HA	11:O:175:LYS:NZ	2.35	0.42
5:E:201:ARG:HG2	5:E:218:MET:HE2	2.01	0.42
7:H:145:THR:HG23	7:H:148:ASP:H	1.84	0.42
7:H:428:ASP:OD1	7:H:428:ASP:N	2.52	0.42
1:C:231:ILE:H	1:C:231:ILE:HD12	1.84	0.42
1:C:3086:TYR:HE1	1:C:3104:VAL:HG11	1.85	0.42
2:A:355:ASN:OD1	2:A:356:HIS:N	2.53	0.42
2:A:790:ILE:HA	2:A:797:LEU:HD23	2.00	0.42
9:K:118:ILE:HD12	9:K:119:PRO:HD2	2.01	0.42
1:C:1409:MET:HG3	1:C:1454:LEU:HD11	2.02	0.42
2:A:1154:PRO:HG2	2:A:1158:ARG:O	2.19	0.42
1:C:647:PHE:HZ	1:C:681:THR:HG23	1.85	0.42
1:C:2007:VAL:HG21	1:C:2122:LEU:HB2	2.01	0.42
1:C:3740:THR:HG22	1:C:3741:THR:N	2.34	0.42
1:C:1803:ASN:N	1:C:1804:PRO:CD	2.83	0.42
1:C:1909:LEU:HD23	1:C:1909:LEU:H	1.85	0.42
1:C:2396:LEU:HB3	1:C:2439:LEU:HD11	2.02	0.42
1:C:2883:LYS:HA	1:C:2883:LYS:HD2	1.77	0.42
2:A:249:LEU:HD13	2:A:313:ILE:HD13	2.01	0.42
2:A:895:ARG:HD3	2:A:903:TRP:HZ3	1.85	0.42
10:M:57:TYR:CE1	12:R:119:HIS:HE1	2.38	0.42
1:C:956:GLU:H	1:C:956:GLU:CD	2.28	0.41
1:C:2275:LEU:HD22	1:C:2328:LEU:HD22	2.00	0.41
2:A:460:TRP:CG	2:A:508:CYS:HB2	2.55	0.41
4:D:123:ILE:HG21	14:L:543:LEU:HD21	2.02	0.41
7:H:271:LEU:O	9:K:59:LYS:HB2	2.19	0.41
1:C:584:LYS:HE3	1:C:1586:ARG:HG2	2.02	0.41
1:C:1330:VAL:C	1:C:1331:GLU:HG3	2.44	0.41
1:C:1753:PHE:HA	1:C:1756:PHE:CE1	2.55	0.41
1:C:2807:SER:OG	1:C:2808:ASN:N	2.53	0.41
1:C:3154:LYS:O	1:C:3158:MET:HG2	2.20	0.41
8:I:70:ILE:HG12	8:I:246:MET:HE2	2.02	0.41
9:K:314:LEU:HD11	9:K:325:VAL:HG11	2.01	0.41
1:C:2858:ARG:NH2	1:C:2990:SER:OG	2.54	0.41
11:O:121:MET:HA	11:O:124:GLU:HG2	2.01	0.41
1:C:1191:MET:HE1	1:C:1259:GLN:HG2	2.01	0.41
1:C:1812:ILE:HG12	1:C:1860:ARG:HH12	1.84	0.41
1:C:3295:ALA:HB3	1:C:3296:PRO:HD3	2.02	0.41
1:C:3440:LYS:O	1:C:3443:LYS:HG2	2.20	0.41
1:C:3642:GLN:HE21	1:C:3648:ARG:HG3	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:499:PHE:CE2	2:A:516:LEU:HD22	2.55	0.41
2:A:789:VAL:HB	2:A:798:ILE:HD11	2.01	0.41
4:D:139:GLY:HA2	7:H:20:ARG:NE	2.35	0.41
6:G:293:THR:HA	10:M:81:GLN:HG2	2.02	0.41
1:C:1188:LEU:HD11	1:C:1256:VAL:HG23	2.03	0.41
1:C:1811:PHE:HE1	1:C:1839:LEU:HD22	1.84	0.41
1:C:1860:ARG:O	1:C:1863:THR:OG1	2.36	0.41
1:C:2101:LEU:HA	1:C:2104:VAL:HG12	2.02	0.41
1:C:3163:LEU:HA	1:C:3166:ILE:HD12	2.01	0.41
2:A:442:LEU:HD23	2:A:767:LEU:HD11	2.02	0.41
2:A:463:ARG:NH1	2:A:466:ILE:O	2.54	0.41
7:H:277:SER:OG	7:H:279:ASP:OD1	2.34	0.41
7:H:298:ARG:HA	7:H:298:ARG:HD3	1.77	0.41
7:H:524:LEU:HD23	7:H:538:ASP:HA	2.02	0.41
10:M:26:MET:HE2	10:M:26:MET:HB2	1.98	0.41
1:C:1330:VAL:O	1:C:1332:HIS:N	2.53	0.41
1:C:1531:LEU:C	1:C:1534:PRO:HD2	2.46	0.41
2:A:1001:ILE:HG21	2:A:1044:VAL:HG11	2.02	0.41
6:G:164:LEU:HD11	12:R:103:ALA:HB1	2.03	0.41
1:C:144:ARG:HB3	1:C:145:PRO:HD3	2.03	0.41
1:C:3163:LEU:HD12	1:C:3175:LEU:HD21	2.03	0.41
7:H:508:GLY:HA3	7:H:537:TRP:CZ2	2.55	0.41
8:I:195:LYS:HG2	8:I:199:PHE:HE2	1.85	0.41
1:C:1459:PHE:HD2	1:C:1524:ILE:HD12	1.86	0.41
1:C:1985:MET:HE2	1:C:1985:MET:HB2	1.99	0.41
1:C:3111:LYS:HB2	1:C:3112:TYR:HD2	1.86	0.41
1:C:3266:TYR:OH	1:C:3319:GLU:OE2	2.38	0.41
1:C:3446:LYS:HD2	1:C:3446:LYS:HA	1.75	0.41
2:A:565:TYR:OH	2:A:617:ILE:HG21	2.21	0.41
2:A:1053:ILE:HG23	2:A:1104:LEU:HD21	2.03	0.41
6:G:277:MET:HG3	6:G:308:LEU:HD23	2.02	0.41
6:G:284:LEU:HB3	6:G:297:TYR:HE1	1.85	0.41
6:G:293:THR:HG22	10:M:81:GLN:HE21	1.86	0.41
6:G:302:GLU:HB2	10:M:91:PHE:HE2	1.84	0.41
8:I:220:PHE:HE2	8:I:228:VAL:HG12	1.86	0.41
1:C:107:ARG:HB2	1:C:108:PRO:HD3	2.03	0.41
1:C:1054:VAL:O	1:C:1058:CYS:HB2	2.21	0.41
1:C:1339:LEU:HD12	1:C:1340:LEU:HD22	2.01	0.41
1:C:3164:GLU:HA	1:C:3167:PHE:HD2	1.85	0.41
2:A:995:THR:HG22	2:A:1000:VAL:HG13	2.02	0.41
7:H:247:LYS:HB3	9:K:186:ASN:ND2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:271:LEU:HD23	7:H:582:ILE:HD11	2.03	0.41
10:M:115:LEU:HD23	10:M:115:LEU:HA	1.90	0.41
1:C:1242:THR:O	1:C:1246:VAL:HG23	2.21	0.41
1:C:1740:ILE:HB	1:C:1741:PRO:HD3	2.03	0.41
1:C:2668:GLN:NE2	1:C:2920:ARG:HD3	2.36	0.41
2:A:47:THR:HG23	2:A:49:LYS:H	1.85	0.41
8:I:73:ASN:O	8:I:77:ARG:N	2.46	0.41
1:C:1889:HIS:CD2	1:C:1926:ILE:HG13	2.56	0.40
1:C:3479:GLU:HG3	1:C:3495:LYS:HD3	2.02	0.40
1:C:3506:VAL:HG11	1:C:3515:ARG:HH12	1.86	0.40
2:A:39:GLU:HG2	2:A:55:THR:HG23	2.01	0.40
7:H:422:TYR:HE1	7:H:458:GLY:HA2	1.86	0.40
2:A:555:VAL:HG11	2:A:590:MET:HE2	2.01	0.40
6:G:298:ALA:O	6:G:301:ILE:HG22	2.21	0.40
7:H:281:LYS:NZ	7:H:298:ARG:HG3	2.36	0.40
9:K:118:ILE:HG13	9:K:120:LYS:H	1.85	0.40
1:C:1363:VAL:O	1:C:1367:ILE:HG12	2.22	0.40
1:C:1887:LEU:HD23	1:C:1904:VAL:HB	2.03	0.40
1:C:2871:GLN:HA	1:C:2874:VAL:HG12	2.03	0.40
2:A:630:MET:HE2	2:A:630:MET:HB3	2.00	0.40
1:C:364:GLY:O	1:C:368:ARG:NE	2.54	0.40
1:C:793:LEU:HD11	1:C:1197:GLU:HG3	2.04	0.40
1:C:1514:CYS:HA	1:C:1517:ILE:HG22	2.04	0.40
1:C:2668:GLN:HE21	1:C:2920:ARG:HB3	1.86	0.40
1:C:3054:VAL:HG21	1:C:3089:LEU:HB2	2.03	0.40
2:A:82:SER:OG	2:A:83:ASP:N	2.54	0.40
2:A:808:THR:HG23	2:A:811:THR:H	1.87	0.40
5:E:188:SER:HA	5:E:191:LEU:HD12	2.04	0.40
12:R:113:VAL:HB	12:R:116:VAL:HG22	2.02	0.40
1:C:332:LEU:HD12	1:C:371:LEU:HD12	2.03	0.40
1:C:1116:ALA:HB2	1:C:1166:PHE:HZ	1.85	0.40
1:C:1448:LEU:HG	1:C:1520:LEU:HD11	2.02	0.40
1:C:1876:ASP:HB3	1:C:1879:CYS:SG	2.61	0.40
1:C:2492:ILE:HD11	1:C:2671:ALA:O	2.22	0.40
1:C:3002:LYS:HB2	1:C:3003:PRO:HD3	2.02	0.40
2:A:916:ASN:HB2	2:A:917:PRO:HD3	2.03	0.40
5:E:296:ARG:HG3	6:G:203:HIS:ND1	2.37	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	C	3191/3859 (83%)	3008 (94%)	182 (6%)	1 (0%)	100	100
2	A	1156/1217 (95%)	1117 (97%)	39 (3%)	0	100	100
3	B	43/86 (50%)	43 (100%)	0	0	100	100
4	D	304/779 (39%)	282 (93%)	22 (7%)	0	100	100
5	E	215/317 (68%)	197 (92%)	18 (8%)	0	100	100
6	G	182/374 (49%)	176 (97%)	6 (3%)	0	100	100
7	H	500/589 (85%)	476 (95%)	24 (5%)	0	100	100
8	I	169/455 (37%)	166 (98%)	3 (2%)	0	100	100
9	K	342/622 (55%)	318 (93%)	24 (7%)	0	100	100
10	M	117/264 (44%)	111 (95%)	5 (4%)	1 (1%)	14	45
11	O	87/218 (40%)	83 (95%)	4 (5%)	0	100	100
12	R	72/161 (45%)	63 (88%)	9 (12%)	0	100	100
14	L	42/892 (5%)	35 (83%)	7 (17%)	0	100	100
All	All	6420/9833 (65%)	6075 (95%)	343 (5%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	M	118	ASP
1	C	773	ASP

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	C	2918/3423 (85%)	2918 (100%)	0	100	100
2	A	1013/1051 (96%)	1013 (100%)	0	100	100
3	B	41/77 (53%)	41 (100%)	0	100	100
4	D	297/687 (43%)	297 (100%)	0	100	100
5	E	179/273 (66%)	179 (100%)	0	100	100
6	G	164/320 (51%)	164 (100%)	0	100	100
7	H	457/521 (88%)	457 (100%)	0	100	100
8	I	152/405 (38%)	152 (100%)	0	100	100
9	K	286/505 (57%)	286 (100%)	0	100	100
10	M	106/235 (45%)	106 (100%)	0	100	100
11	O	78/154 (51%)	78 (100%)	0	100	100
12	R	68/141 (48%)	68 (100%)	0	100	100
14	L	38/779 (5%)	38 (100%)	0	100	100
All	All	5797/8571 (68%)	5797 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	43	GLN
1	C	88	GLN
1	C	112	ASN
1	C	315	GLN
1	C	405	ASN
1	C	457	HIS
1	C	604	GLN
1	C	728	ASN
1	C	730	GLN
1	C	857	GLN
1	C	1071	GLN
1	C	1212	GLN
1	C	1259	GLN
1	C	1305	GLN
1	C	1424	HIS
1	C	1760	ASN
1	C	1842	HIS
1	C	2166	ASN

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Mol	Chain	Res	Type
1	C	2281	ASN
1	C	2451	GLN
1	C	2489	HIS
1	C	2586	ASN
1	C	2662	GLN
1	C	2700	HIS
1	C	2756	GLN
1	C	2832	ASN
1	C	2924	HIS
1	C	2996	GLN
1	C	3088	GLN
1	C	3139	ASN
1	C	3174	HIS
1	C	3237	GLN
1	C	3435	HIS
1	C	3510	ASN
1	C	3610	ASN
1	C	3761	GLN
2	A	119	GLN
2	A	169	HIS
2	A	411	GLN
2	A	551	GLN
2	A	775	ASN
2	A	776	GLN
2	A	782	GLN
2	A	861	GLN
2	A	1160	HIS
3	B	34	ASN
4	D	84	ASN
4	D	150	GLN
4	D	220	ASN
4	D	225	ASN
5	E	295	HIS
6	G	162	HIS
6	G	220	ASN
7	H	8	GLN
7	H	109	GLN
7	H	139	GLN
7	H	315	HIS
7	H	404	HIS
7	H	562	GLN
8	I	73	ASN

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Mol	Chain	Res	Type
9	K	53	GLN
9	K	288	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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.

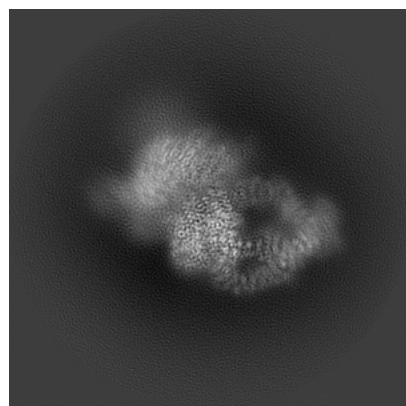
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-34520. These allow visual inspection of the internal detail of the map and identification of artifacts.

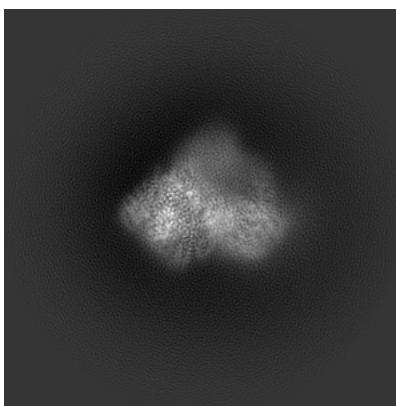
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

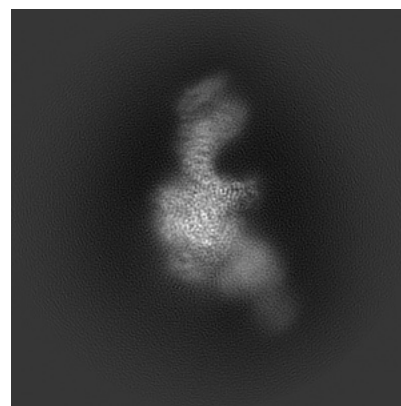
6.1.1 Primary map



X

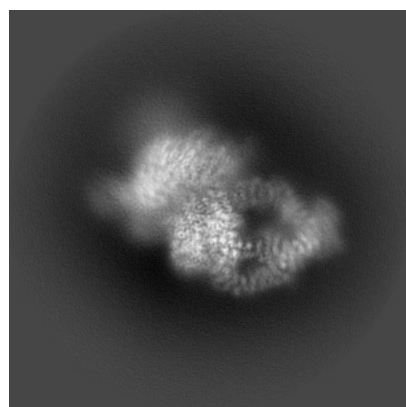


Y

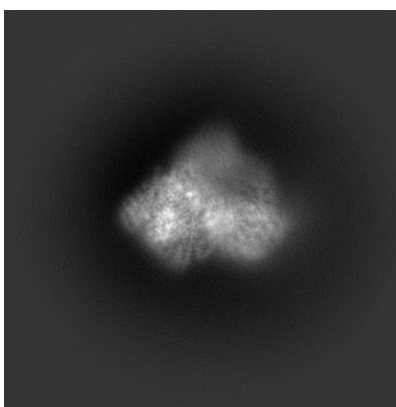


Z

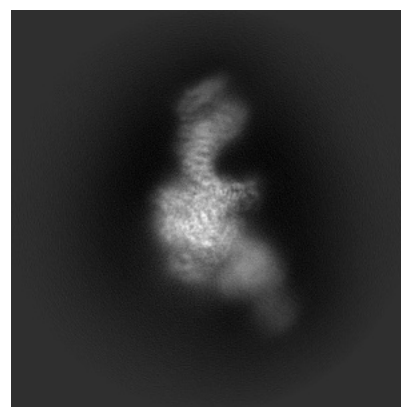
6.1.2 Raw map



X



Y

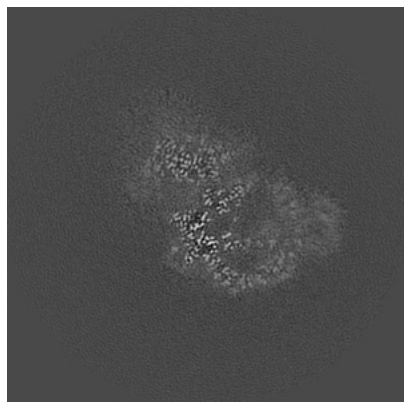


Z

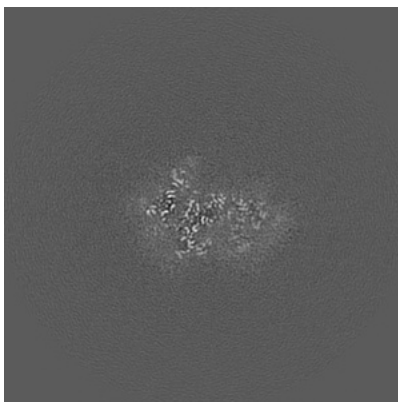
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

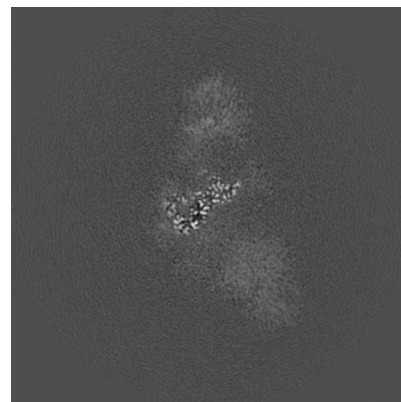
6.2.1 Primary map



X Index: 200

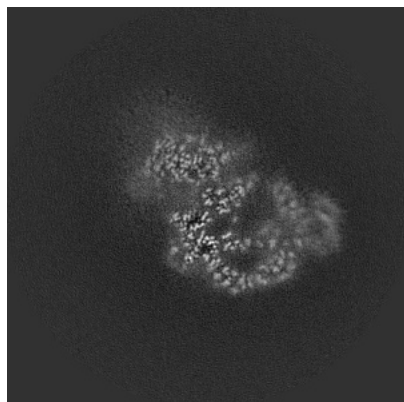


Y Index: 200

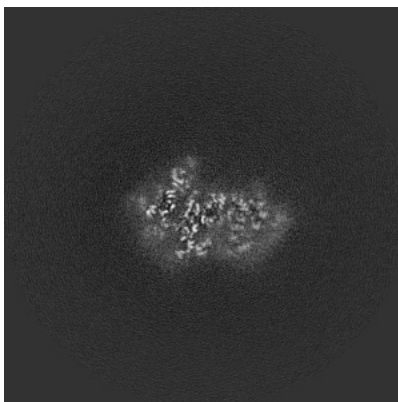


Z Index: 200

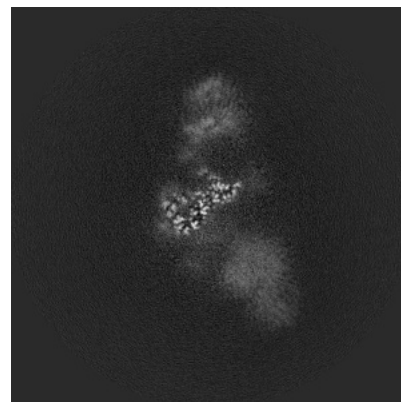
6.2.2 Raw map



X Index: 200



Y Index: 200

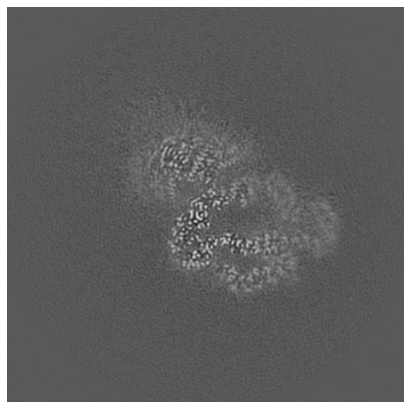


Z Index: 200

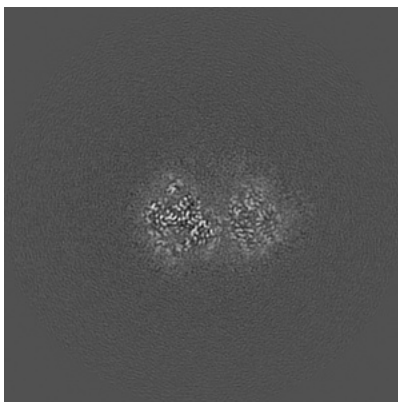
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

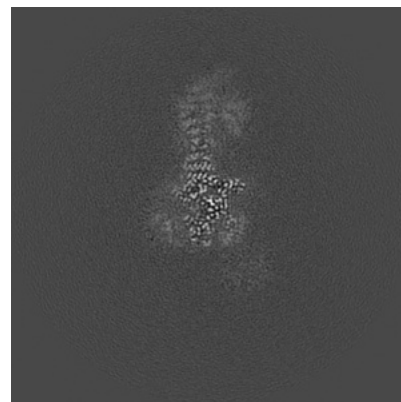
6.3.1 Primary map



X Index: 194

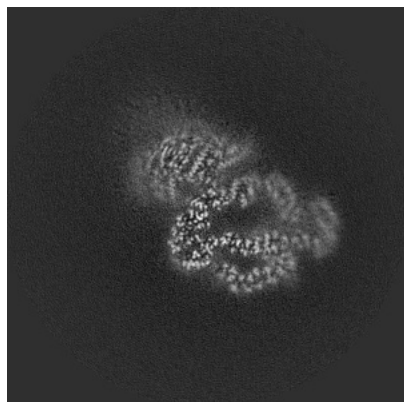


Y Index: 183

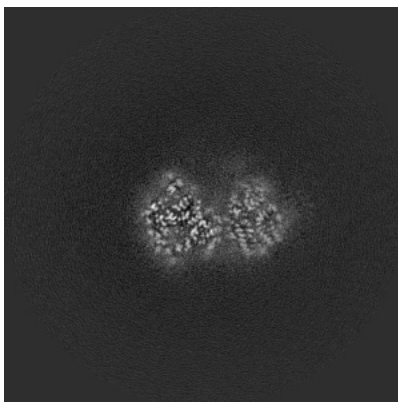


Z Index: 164

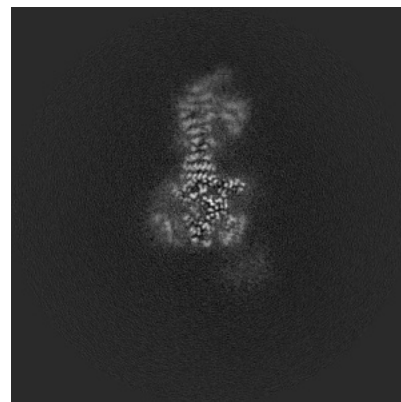
6.3.2 Raw map



X Index: 194



Y Index: 183

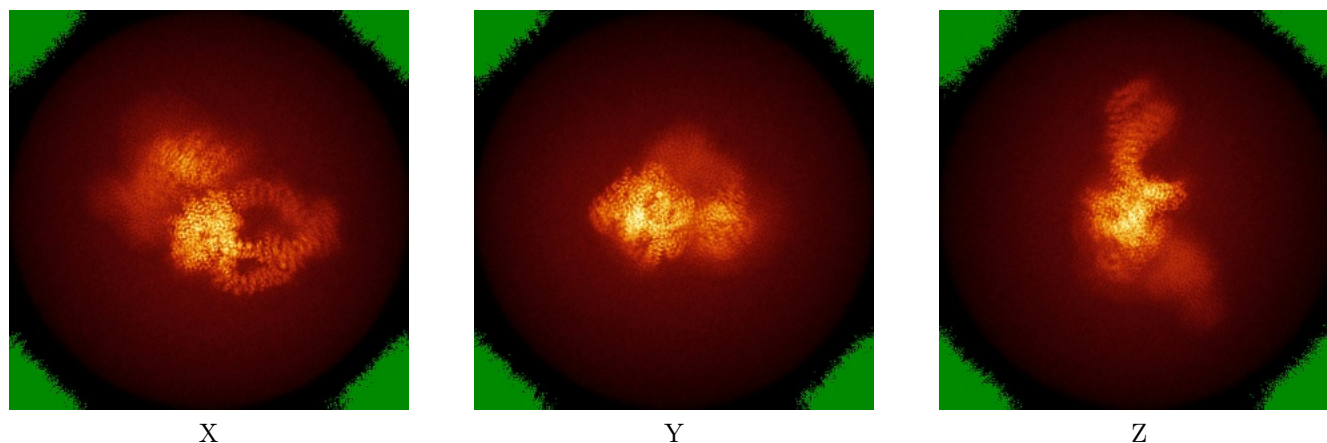


Z Index: 164

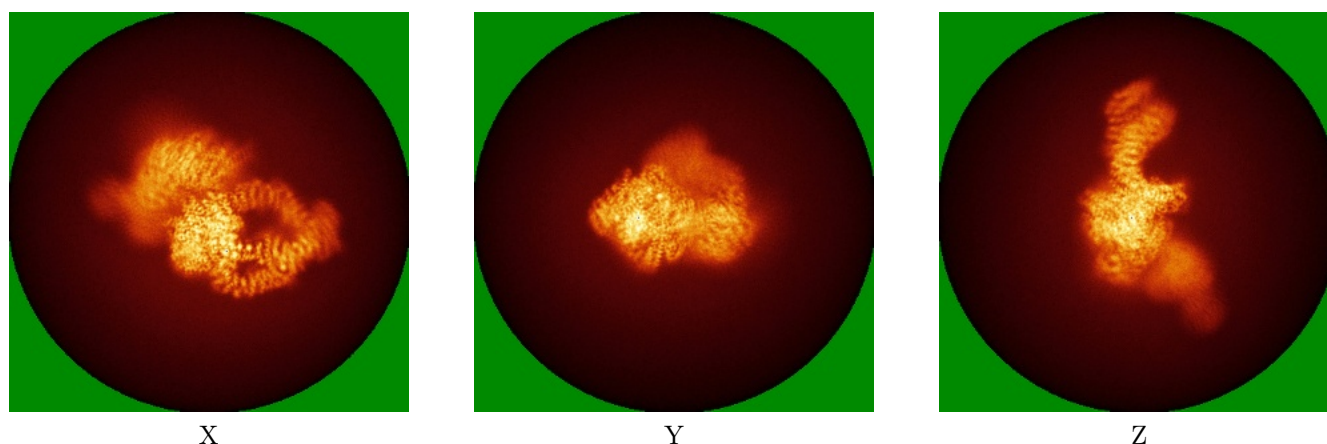
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

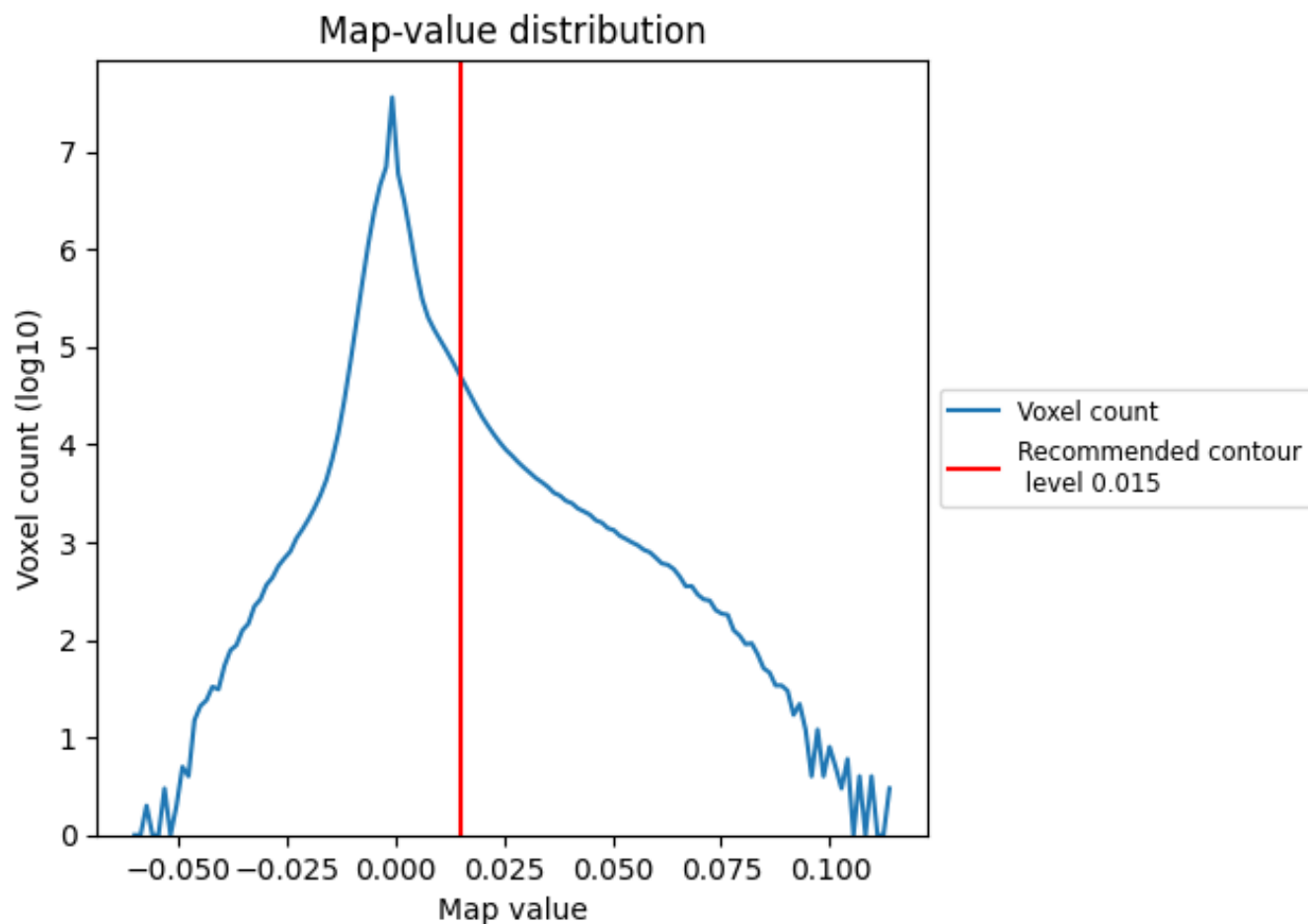
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

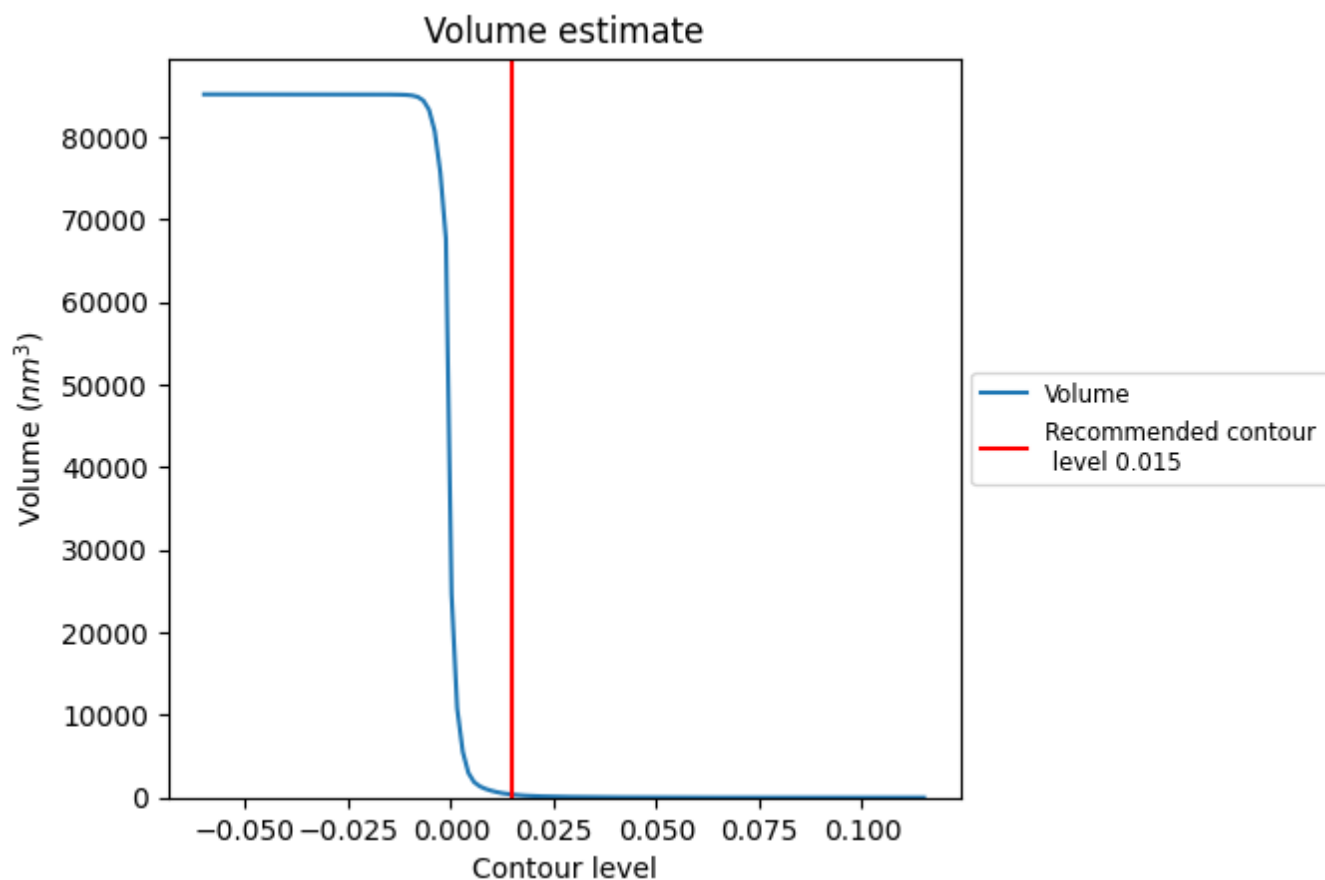
This section contains the results of statistical analysis of the map.

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.

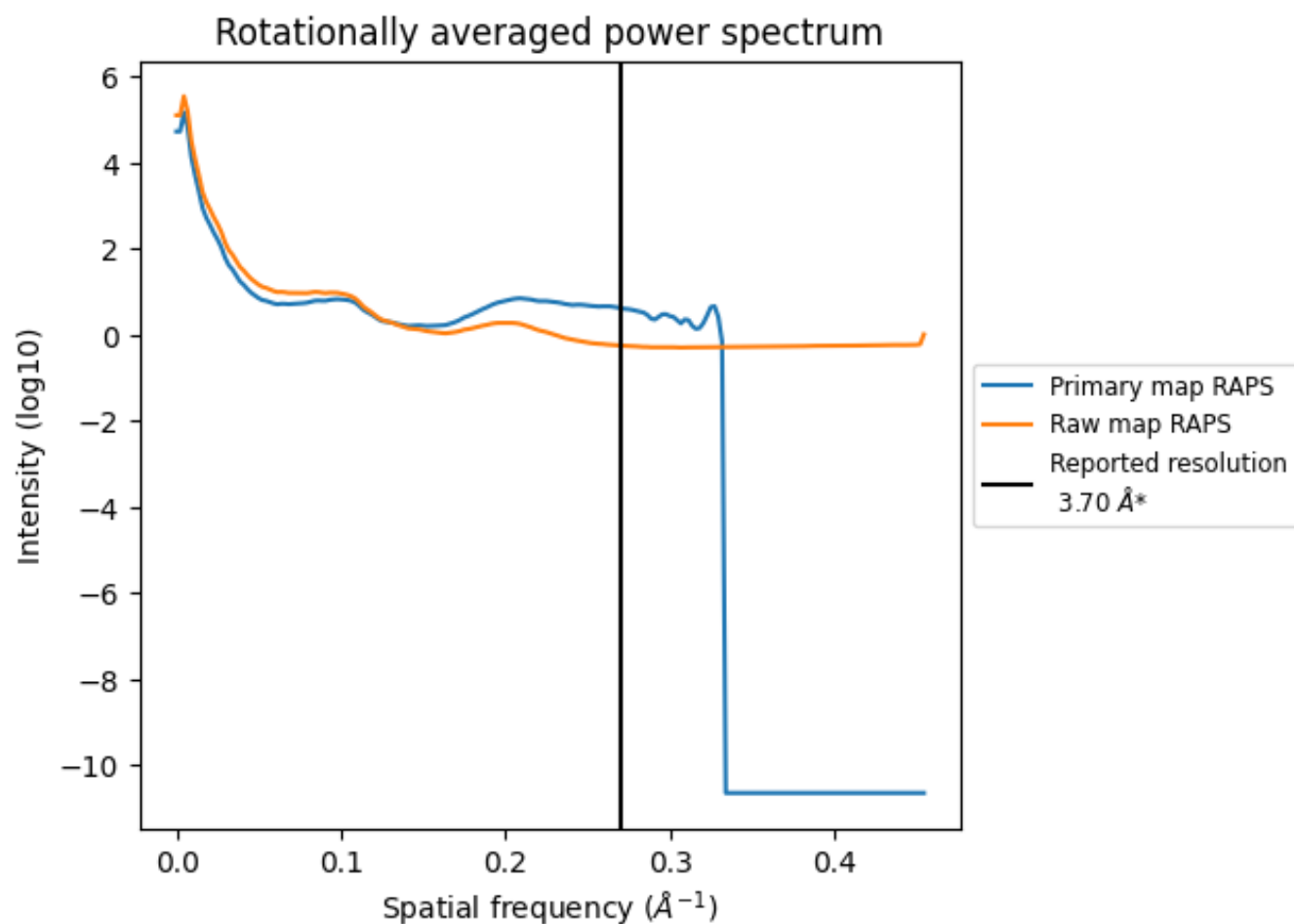
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 363 nm³; this corresponds to an approximate mass of 328 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 ⓘ

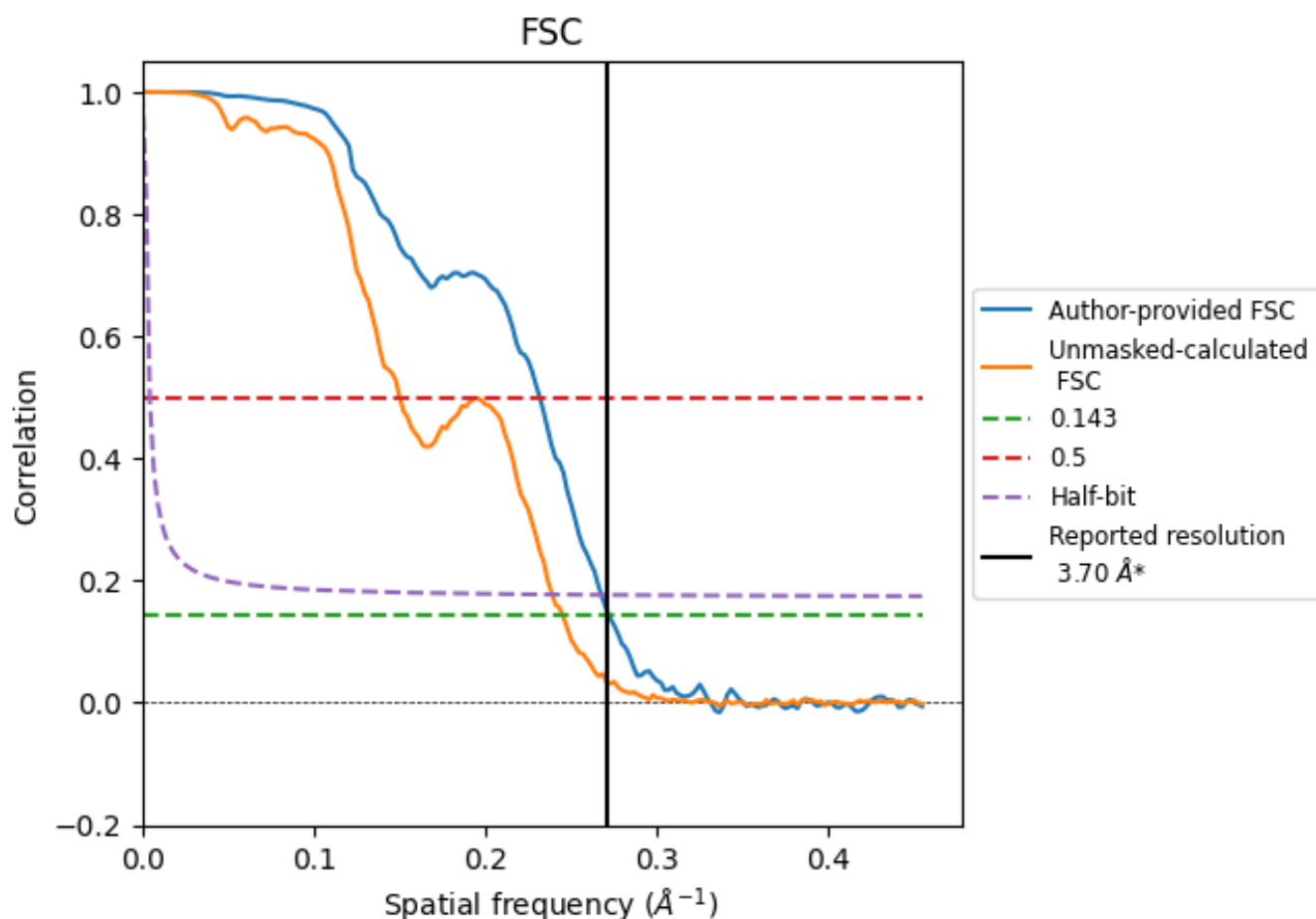


*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.270 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.68	4.32	3.74
Unmasked-calculated*	4.08	6.67	4.18

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.08 differs from the reported value 3.7 by more than 10 %

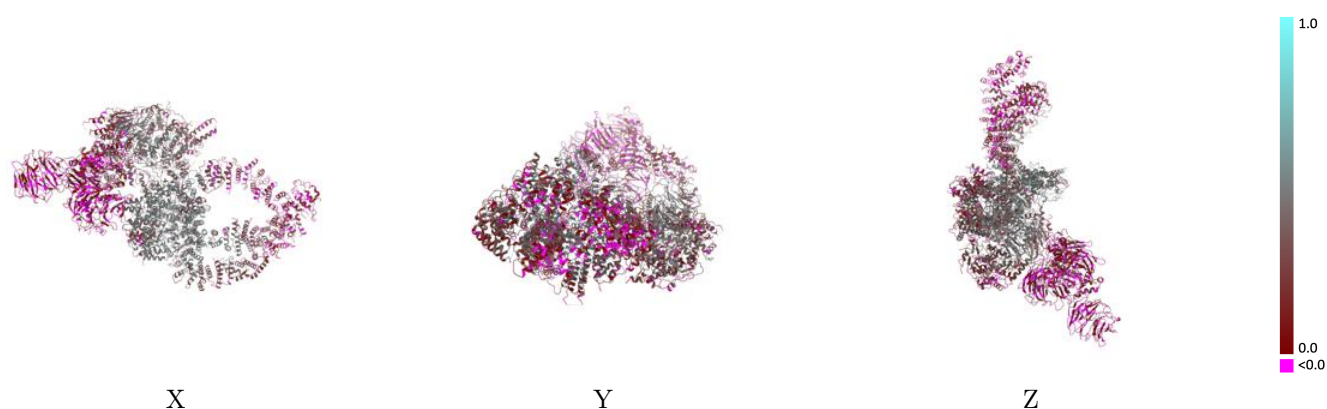
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-34520 and PDB model 8H7G. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)

This section was not generated.

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

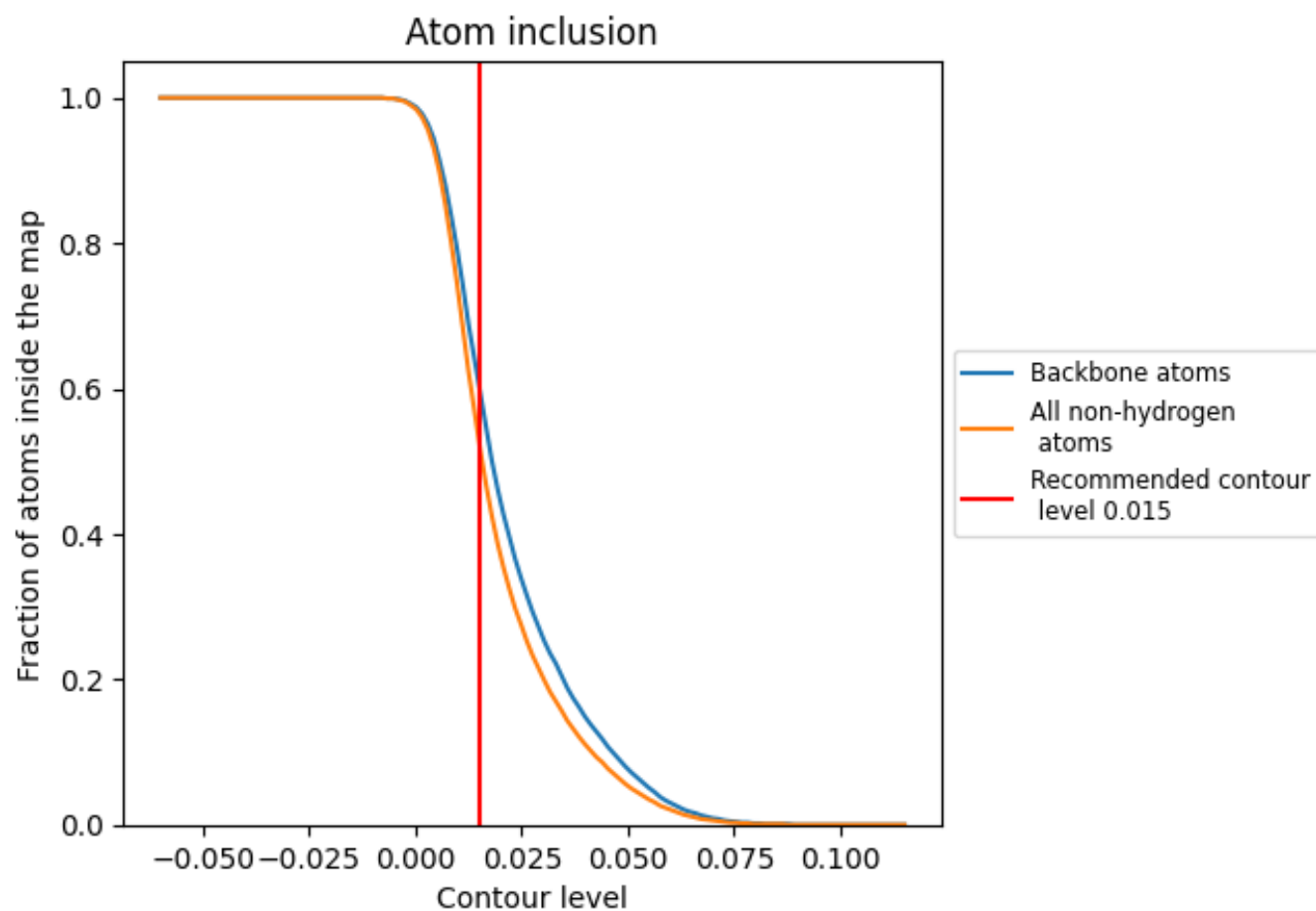


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 60% of all backbone atoms, 53% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5260	 0.2730
A	 0.0920	 0.0670
B	 0.1770	 0.0950
C	 0.6580	 0.3250
D	 0.5240	 0.2810
E	 0.4650	 0.2550
G	 0.6700	 0.3940
H	 0.6190	 0.3430
I	 0.6450	 0.3450
K	 0.3870	 0.2050
L	 0.5460	 0.2970
M	 0.6840	 0.3640
O	 0.7200	 0.3750
R	 0.6860	 0.3600
X	 0.2000	 0.1870

