Full wwPDB EM Validation Report ⓘ

Dec 11, 2022 – 07:17 pm GMT

PDB ID	:	6T9I
EMDB ID	:	EMD-10412
Title	:	cryo-EM structure of transcription coactivator SAGA
Authors	:	Wang, H.; Cheung, A.; Cramer, P.
Deposited on	:	2019-10-28
Resolution	:	3.90 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

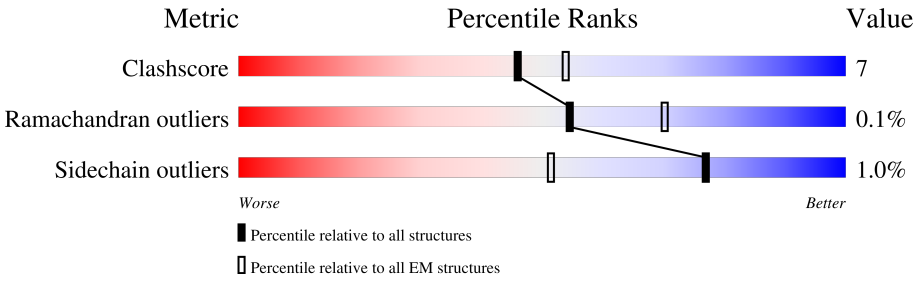
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance

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

The reported resolution of this entry is 3.90 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	B	604	30% 6% 63%
2	C	337	53% 11% 36%
3	D	798	60% 11% 29%
4	E	516	70% 14% 16%
5	F	157	60% 11% 29%
6	G	206	56% 12% 32%
7	H	488	38% 8% 53%
8	I	539	23% 8% 68%

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Mol	Chain	Length	Quality of chain
9	K	1332	
10	Q	657	
11	T	3744	
12	U	155	

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 48821 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Transcription factor SPT20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	B	224	1891	1207	318	358	8	0	0

- Molecule 2 is a protein called Protein SPT3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	214	1774	1130	319	318	7	0	0

- Molecule 3 is a protein called Transcription initiation factor TFIID subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	D	566	4474	2830	772	854	18	0	0

- Molecule 4 is a protein called Transcription initiation factor TFIID subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	E	433	3441	2207	572	657	5	0	0

- Molecule 5 is a protein called Transcription initiation factor TFIID subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	F	111	902	581	158	159	4	0	0

- Molecule 6 is a protein called Transcription initiation factor TFIID subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	G	140	1108	689	199	218	2	0	0

- Molecule 7 is a protein called Transcriptional coactivator HFI1/ADA1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	227	Total	C	N	O	S	0	0
			1803	1121	314	359	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	173	Total	C	N	O	S	0	0
			1351	836	243	268	4		

- Molecule 9 is a protein called Transcriptional activator SPT7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	279	Total	C	N	O	S	0	0
			2258	1427	392	428	11		

- Molecule 10 is a protein called SAGA-associated factor 73.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	Q	84	Total	C	N	O	S	0	0
			675	426	119	127	3		

- Molecule 11 is a protein called Transcription-associated protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	T	3513	Total	C	N	O	S	0	0
			28729	18596	4776	5237	120		

- Molecule 12 is a protein called unassigned sequence.

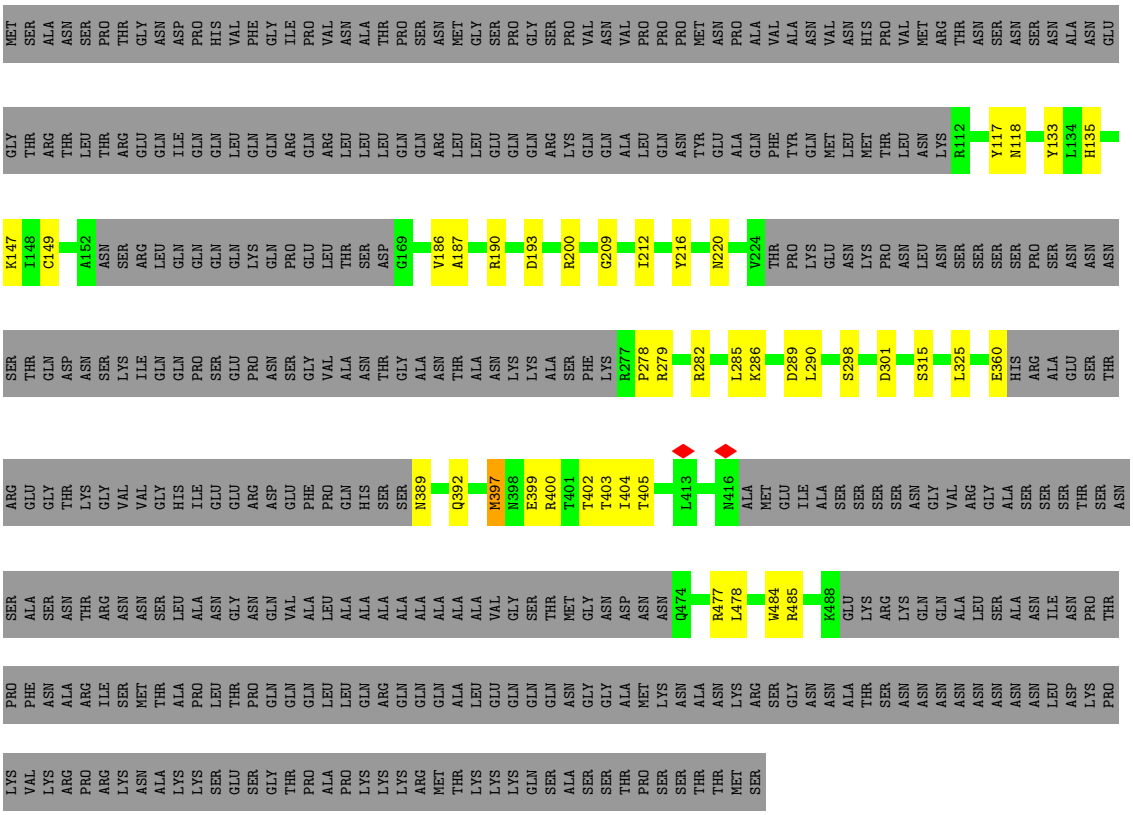
Mol	Chain	Residues	Atoms				AltConf	Trace
12	U	83	Total	C	N	O	0	0
			415	249	83	83		

3 Residue-property plots (i)

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

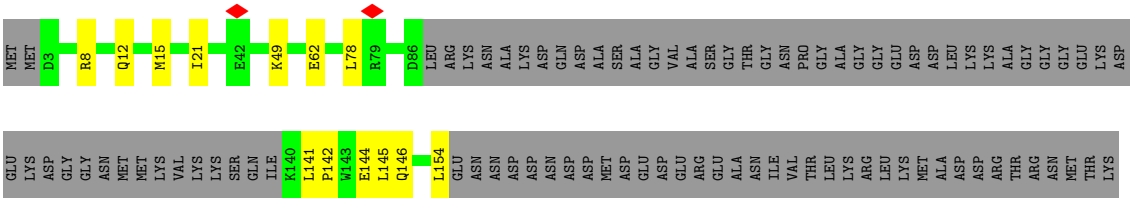
• Molecule 1: Transcription factor SPT20

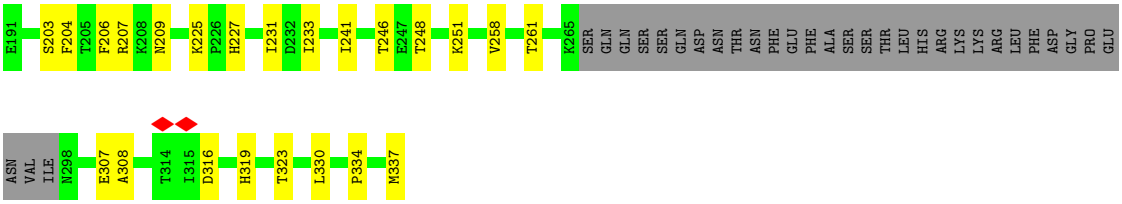
Chain B:



• Molecule 2: Protein SPT3

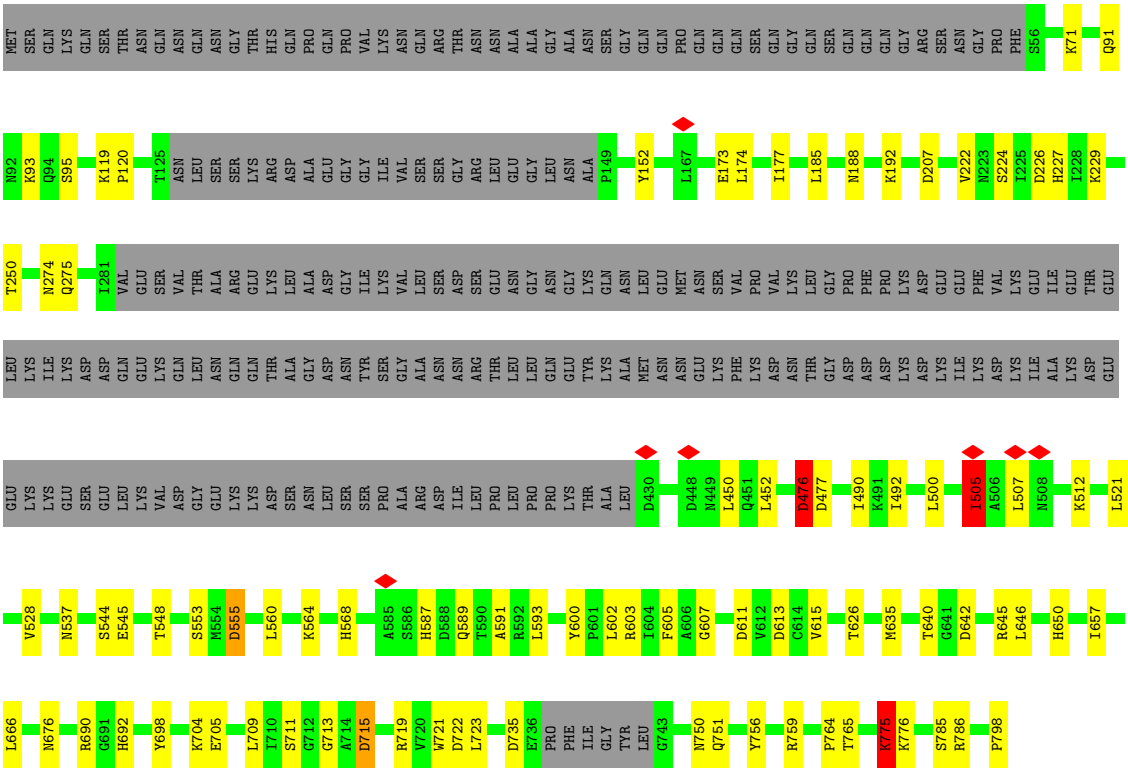
Chain C:





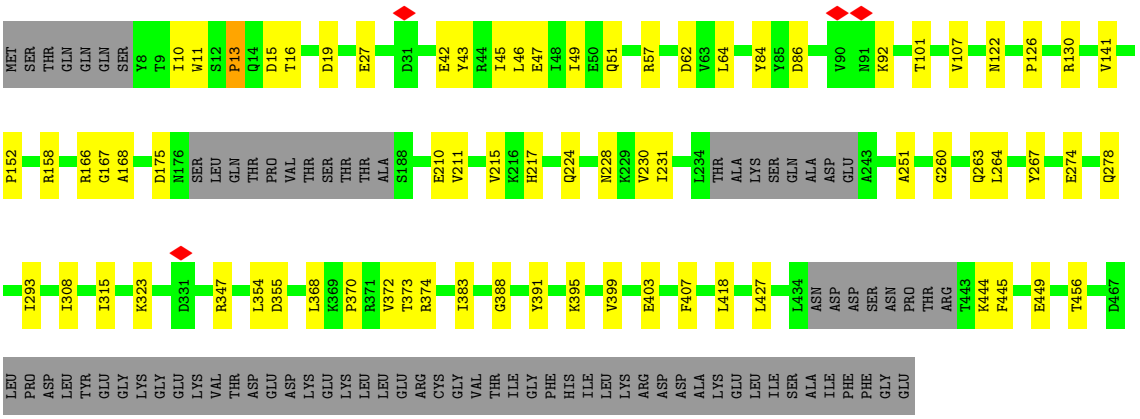
• Molecule 3: Transcription initiation factor TFIID subunit 5

Chain D:



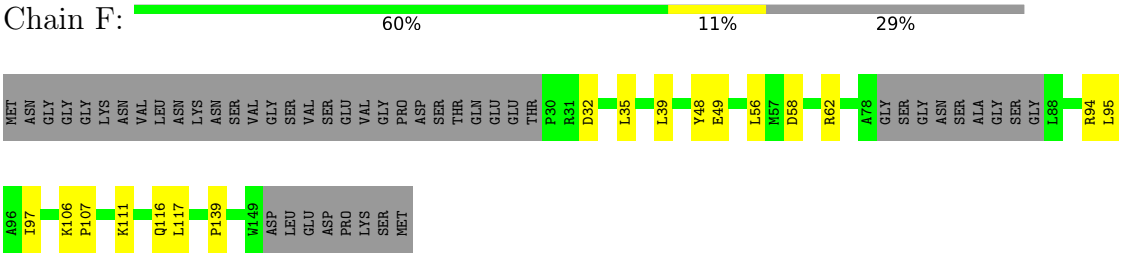
• Molecule 4: Transcription initiation factor TFIID subunit 6

Chain E:



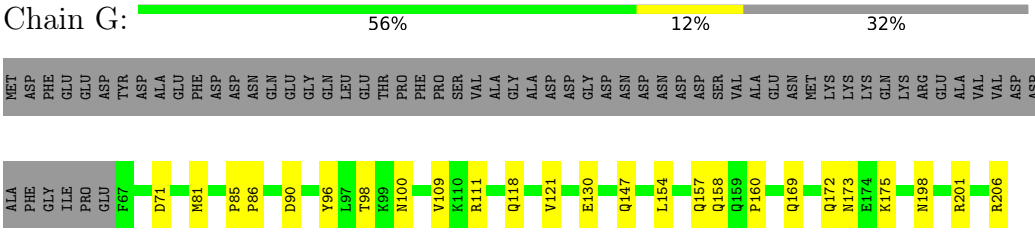
• Molecule 5: Transcription initiation factor TFIID subunit 9

Chain F:



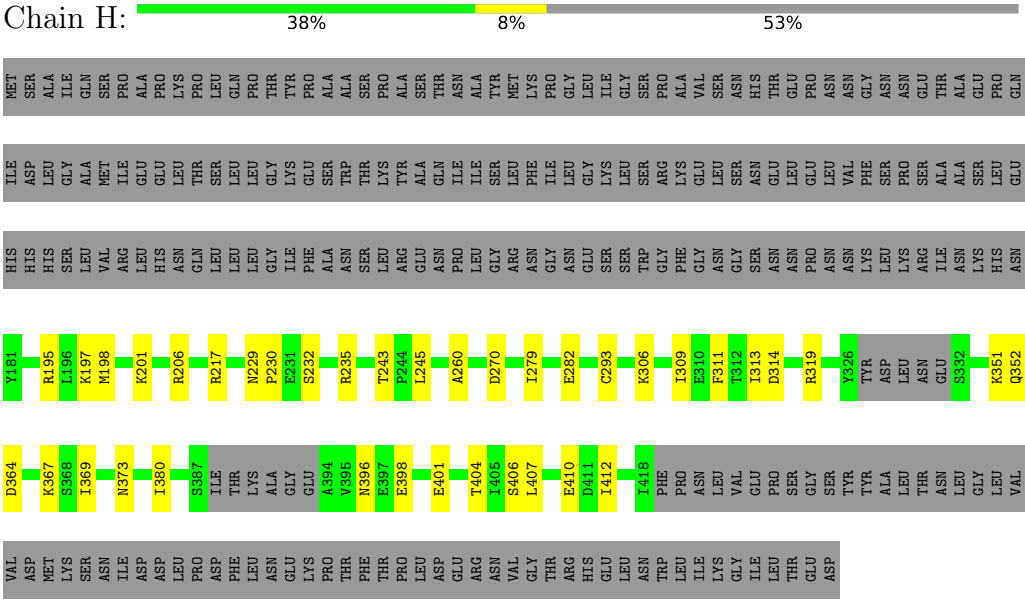
• Molecule 6: Transcription initiation factor TFIID subunit 10

Chain G:



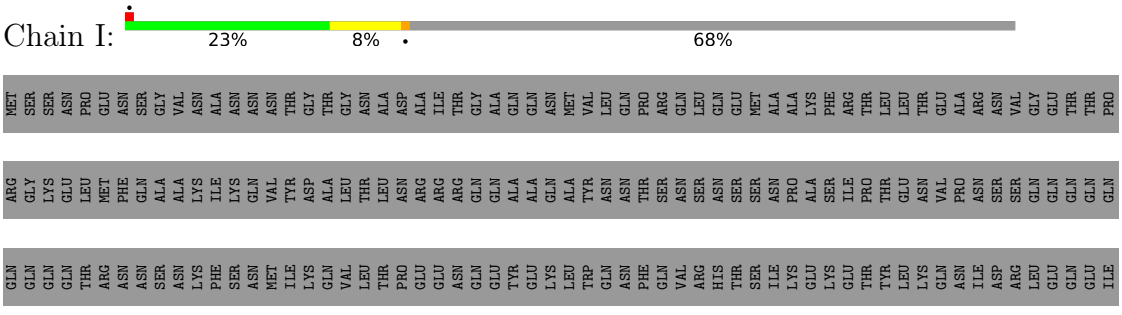
• Molecule 7: Transcriptional coactivator HFI1/ADA1

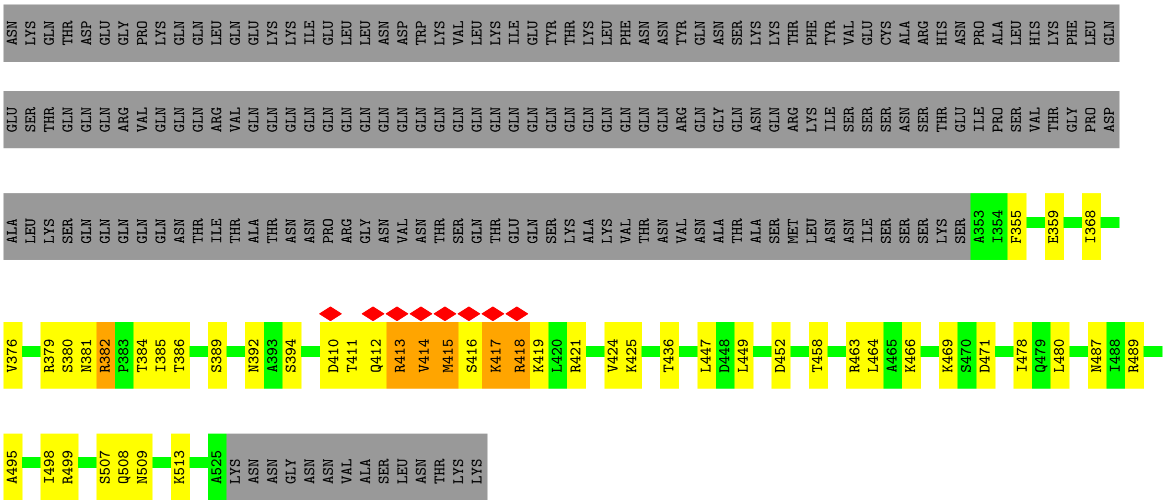
Chain H:



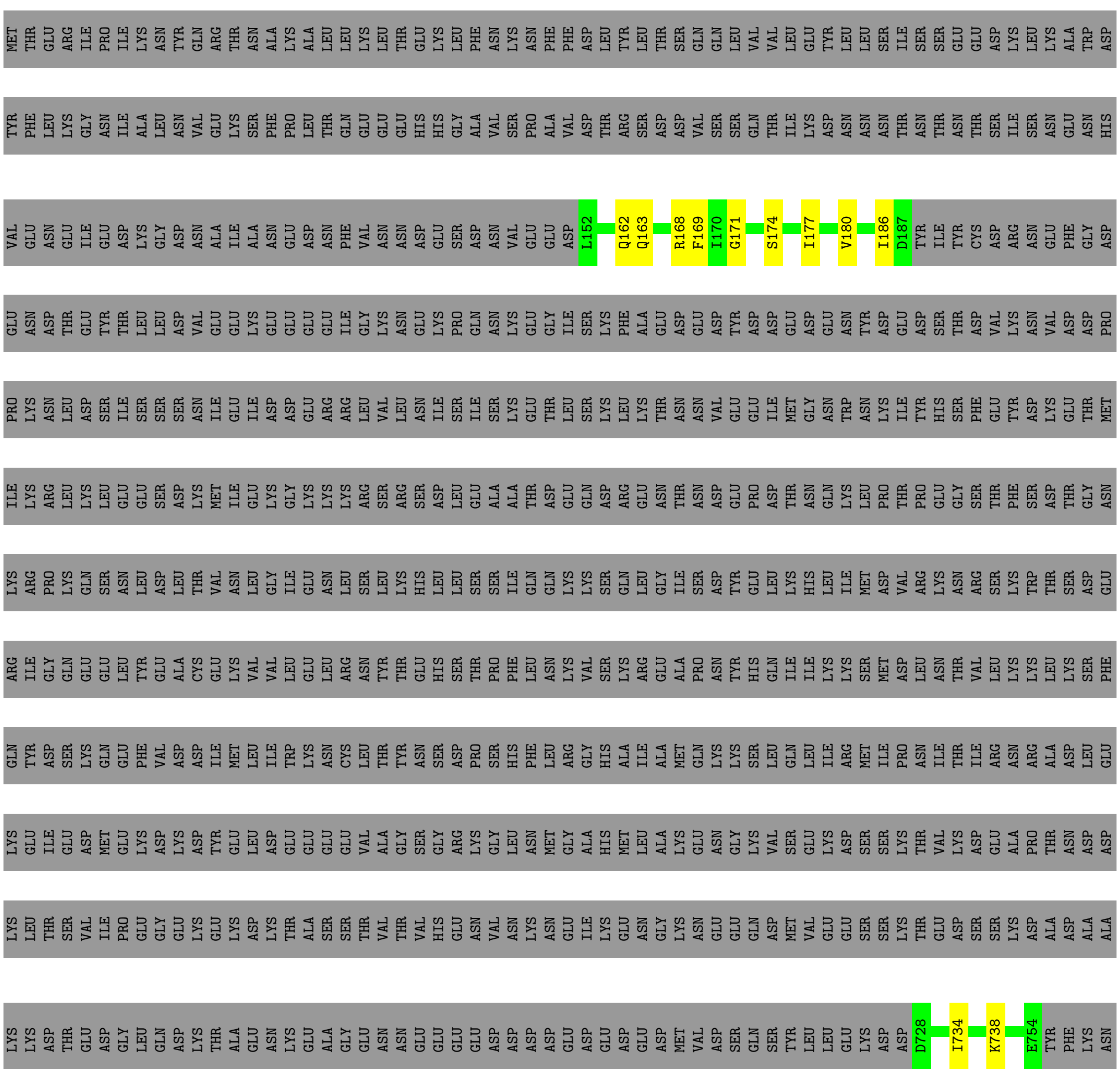
• Molecule 8: Transcription initiation factor TFIID subunit 12

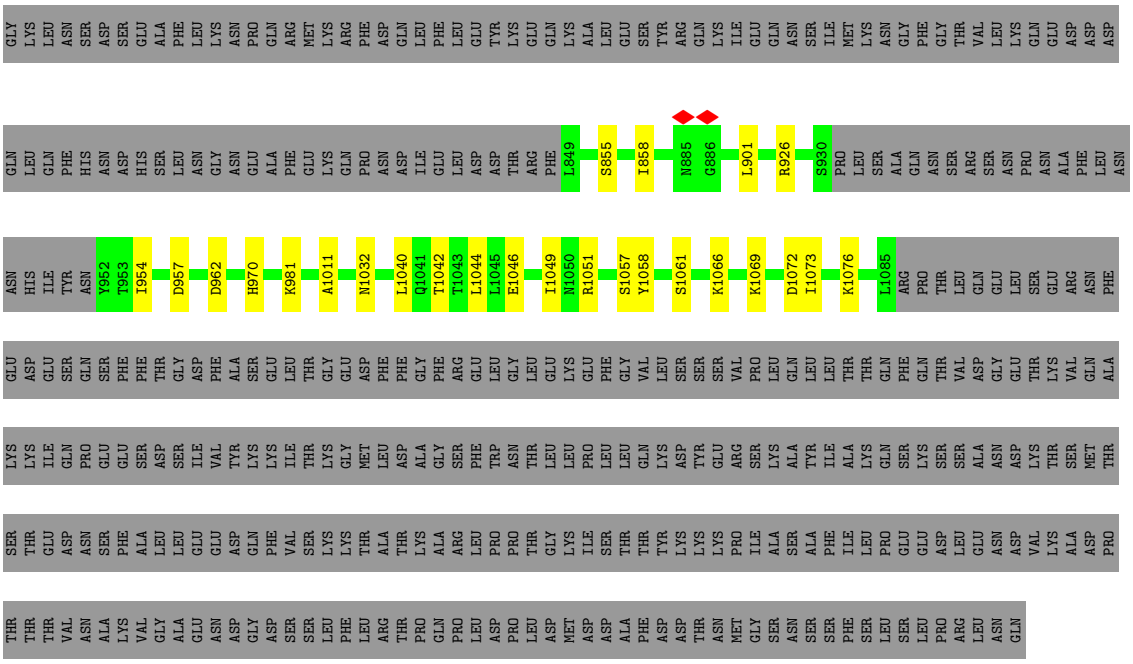
Chain I:





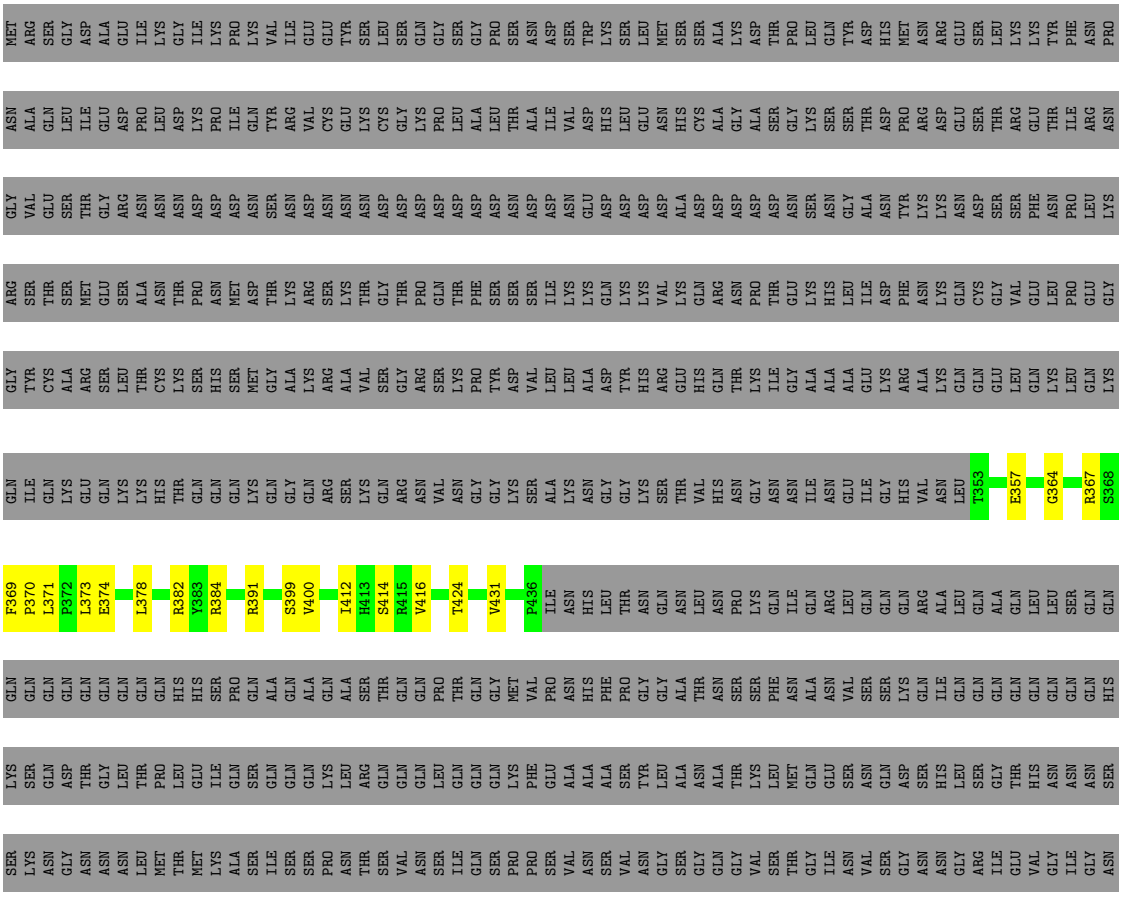
- Molecule 9: Transcriptional activator SPT7





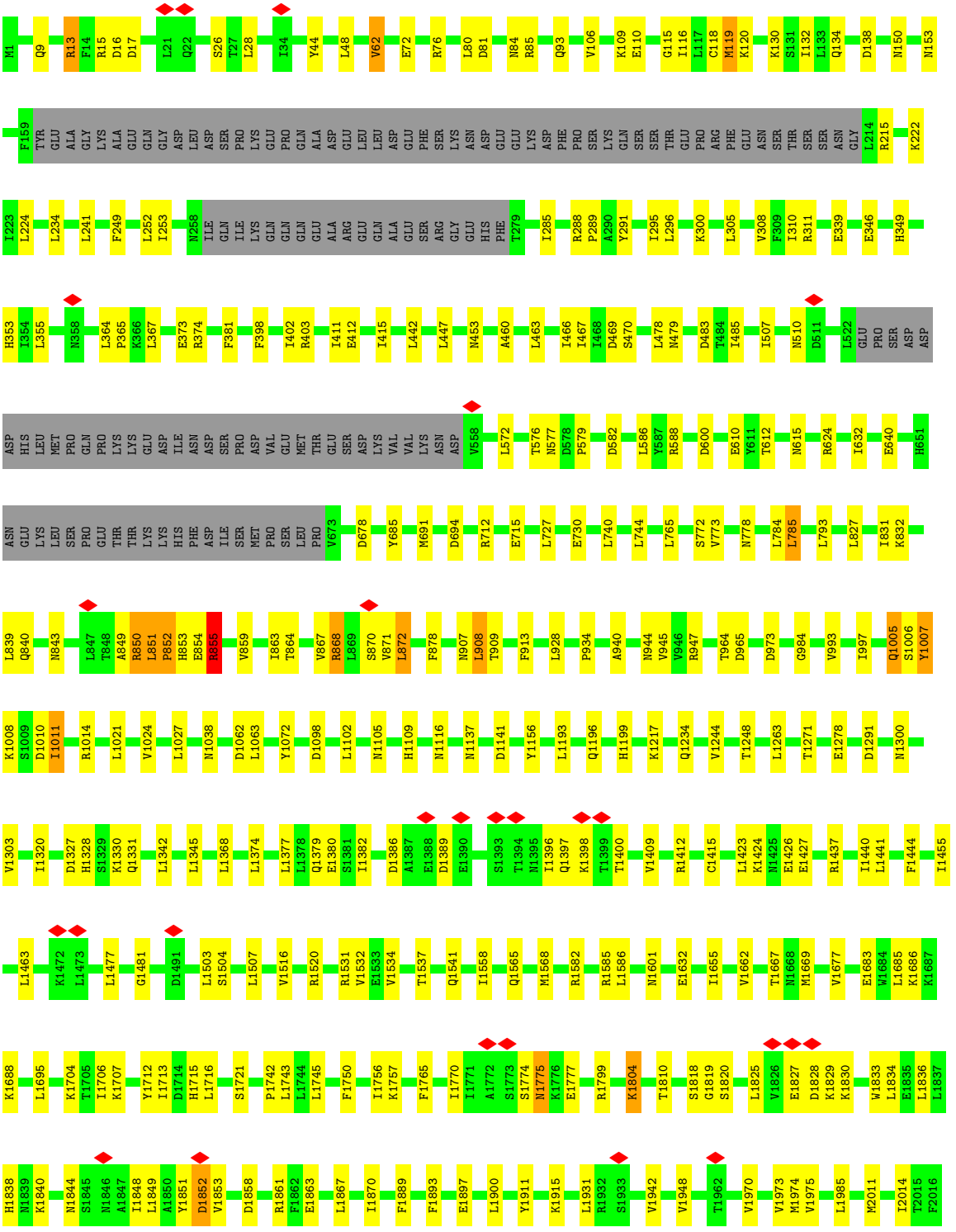
• Molecule 10: SAGA-associated factor 73

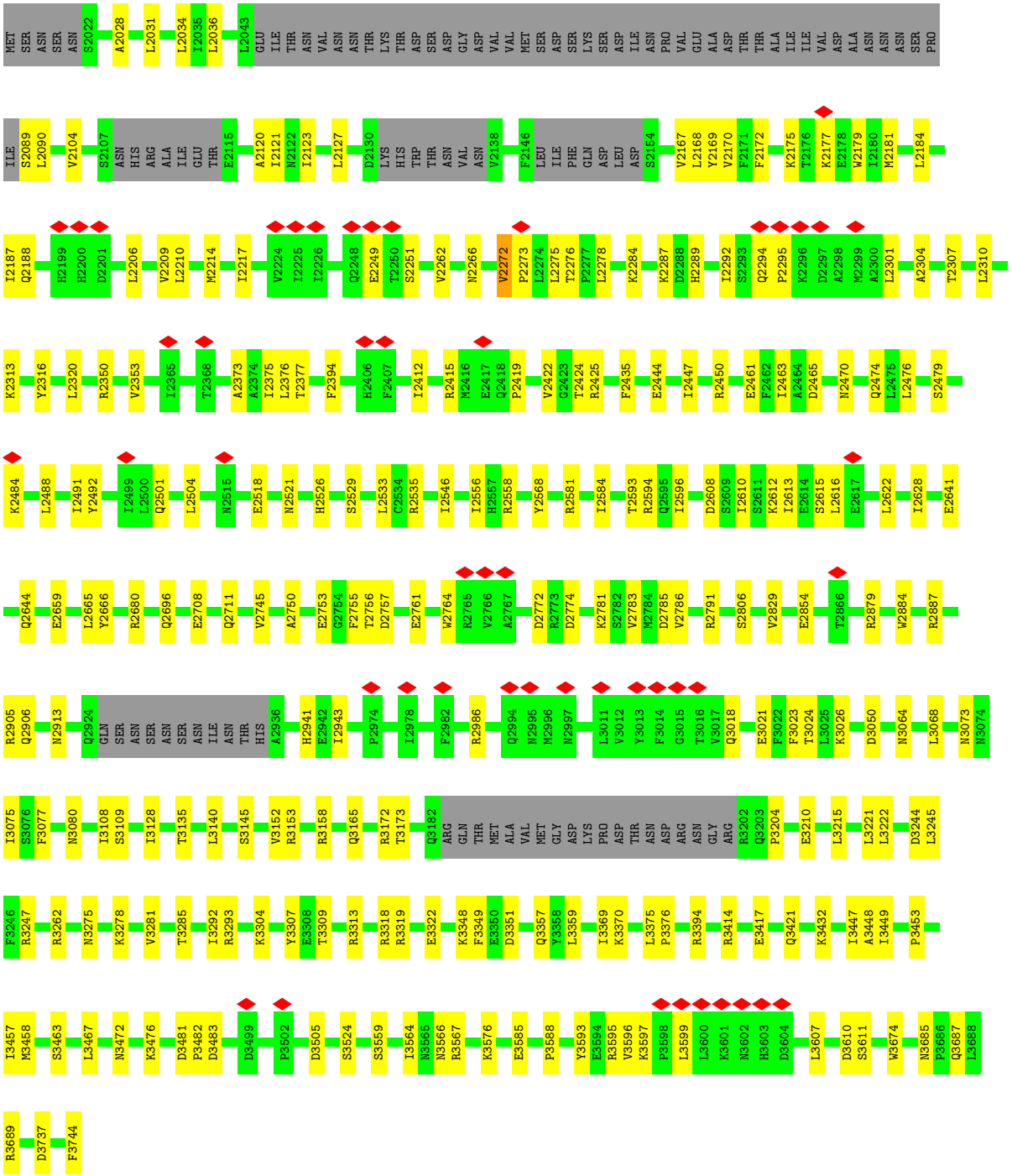
Chain Q:



• Molecule 11: Transcription-associated protein 1

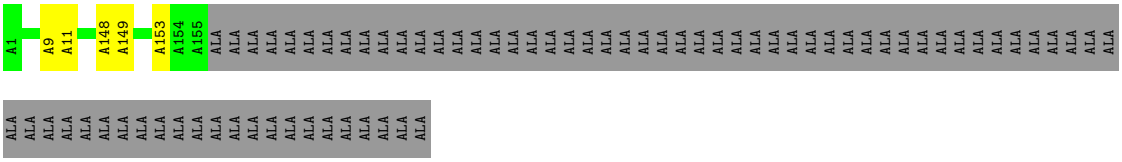
Chain T:





• Molecule 12: unassigned sequence

Chain U:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	27602	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	42.45	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.250	Depositor
Minimum map value	-0.106	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	419.99997, 419.99997, 419.99997	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	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	B	0.29	0/1931	0.53	0/2607
2	C	0.26	0/1810	0.48	0/2435
3	D	0.31	0/4582	0.58	3/6211 (0.0%)
4	E	0.29	0/3504	0.56	1/4759 (0.0%)
5	F	0.30	0/922	0.54	0/1249
6	G	0.29	0/1123	0.51	0/1518
7	H	0.29	0/1826	0.55	0/2456
8	I	0.33	0/1373	0.58	1/1863 (0.1%)
9	K	0.26	0/2288	0.54	1/3080 (0.0%)
10	Q	0.29	0/692	0.53	0/937
11	T	0.38	0/29358	0.60	12/39779 (0.0%)
12	U	0.28	0/412	0.46	0/572
All	All	0.35	0/49821	0.58	18/67466 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	D	0	1

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	T	1291	ASP	CB-CG-OD2	6.86	124.47	118.30
11	T	855	ARG	NE-CZ-NH1	6.79	123.69	120.30
3	D	477	ASP	CB-CG-OD1	6.78	124.40	118.30
11	T	2504	LEU	CA-CB-CG	6.39	130.01	115.30
11	T	785	LEU	CA-CB-CG	6.34	129.88	115.30
11	T	62	VAL	CA-CB-CG1	6.29	120.34	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	T	1368	LEU	CA-CB-CG	6.29	129.77	115.30
9	K	1072	ASP	CB-CG-OD1	5.93	123.64	118.30
4	E	427	LEU	CA-CB-CG	5.92	128.93	115.30
11	T	2301	LEU	CA-CB-CG	5.79	128.61	115.30
11	T	252	LEU	CA-CB-CG	5.75	128.52	115.30
11	T	1586	LEU	CA-CB-CG	5.56	128.08	115.30
11	T	872	LEU	CA-CB-CG	5.48	127.90	115.30
3	D	476	ASP	C-N-CA	5.40	135.21	121.70
3	D	775	LYS	CA-CB-CG	5.33	125.12	113.40
8	I	385	ILE	C-N-CA	5.15	134.57	121.70
11	T	2465	ASP	C-N-CA	5.15	134.57	121.70
11	T	241	LEU	CA-CB-CG	5.12	127.07	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	476	ASP	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1891	0	1840	34	0
2	C	1774	0	1790	23	0
3	D	4474	0	4377	60	0
4	E	3441	0	3493	52	0
5	F	902	0	919	22	0
6	G	1108	0	1110	20	0
7	H	1803	0	1800	37	0
8	I	1351	0	1351	72	0
9	K	2258	0	2308	28	0
10	Q	675	0	666	15	0
11	T	28729	0	29144	368	0
12	U	415	0	415	3	0
All	All	48821	0	49213	642	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (642) 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)
8:I:418:ARG:HG3	8:I:421:ARG:NE	1.08	1.39
8:I:418:ARG:NE	8:I:421:ARG:HH11	1.24	1.32
11:T:850:ARG:CB	11:T:854:GLU:OE2	1.80	1.29
8:I:418:ARG:CD	8:I:421:ARG:NH1	1.98	1.26
11:T:850:ARG:HB2	11:T:854:GLU:OE2	1.10	1.25
8:I:418:ARG:CG	8:I:421:ARG:NE	2.00	1.24
8:I:418:ARG:CD	8:I:421:ARG:HH11	1.48	1.23
11:T:850:ARG:C	11:T:852:PRO:HD3	1.57	1.22
8:I:418:ARG:HG3	8:I:421:ARG:CZ	1.68	1.21
8:I:418:ARG:HD2	8:I:421:ARG:NH1	1.52	1.19
8:I:413:ARG:H	8:I:413:ARG:HD3	1.11	1.08
8:I:411:THR:HG22	8:I:414:VAL:HG12	1.36	1.07
8:I:411:THR:CG2	8:I:414:VAL:HG12	1.83	1.06
11:T:867:VAL:CG2	11:T:872:LEU:HA	1.84	1.06
11:T:867:VAL:HG21	11:T:872:LEU:CA	1.88	1.03
11:T:851:LEU:HD23	11:T:1156:TYR:CE2	1.98	0.98
8:I:411:THR:HA	8:I:413:ARG:NH1	1.77	0.97
11:T:851:LEU:N	11:T:852:PRO:CD	2.28	0.97
8:I:418:ARG:NE	8:I:421:ARG:NH1	2.07	0.95
11:T:850:ARG:CG	11:T:854:GLU:OE2	2.15	0.95
8:I:418:ARG:CG	8:I:421:ARG:CZ	2.39	0.93
11:T:867:VAL:HG21	11:T:872:LEU:HA	0.96	0.93
8:I:418:ARG:HG3	8:I:421:ARG:HE	1.18	0.92
8:I:418:ARG:HE	8:I:421:ARG:HH11	0.98	0.92
11:T:851:LEU:CD2	11:T:1156:TYR:CZ	2.53	0.92
11:T:849:ALA:O	11:T:851:LEU:CD2	2.18	0.91
11:T:850:ARG:C	11:T:852:PRO:CD	2.39	0.91
11:T:851:LEU:HG	11:T:1156:TYR:OH	1.69	0.90
8:I:415:MET:CE	8:I:415:MET:HA	2.04	0.86
8:I:418:ARG:HG3	8:I:421:ARG:CD	2.06	0.86
11:T:850:ARG:O	11:T:851:LEU:HB2	1.77	0.84
8:I:411:THR:CG2	8:I:414:VAL:CG1	2.56	0.82
11:T:850:ARG:HB3	11:T:852:PRO:CD	2.09	0.81
8:I:418:ARG:CD	8:I:421:ARG:CZ	2.58	0.81
11:T:871:VAL:HG21	11:T:908:LEU:HD21	1.62	0.81
8:I:418:ARG:HE	8:I:421:ARG:NH1	1.70	0.81
11:T:850:ARG:HB2	11:T:854:GLU:CD	2.00	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:T:851:LEU:N	11:T:852:PRO:HD3	1.93	0.80
11:T:1007:TYR:HD1	11:T:1007:TYR:H	1.28	0.80
8:I:418:ARG:CG	8:I:421:ARG:HE	1.78	0.79
11:T:849:ALA:O	11:T:851:LEU:HD23	1.82	0.78
11:T:851:LEU:HD23	11:T:1156:TYR:CZ	2.17	0.78
11:T:1007:TYR:HA	11:T:1014:ARG:HH22	1.50	0.77
8:I:355:PHE:CE1	11:T:871:VAL:HB	2.20	0.76
8:I:355:PHE:HE1	11:T:871:VAL:HB	1.51	0.76
11:T:871:VAL:HG21	11:T:908:LEU:CD2	2.15	0.75
11:T:851:LEU:CG	11:T:1156:TYR:OH	2.35	0.75
8:I:411:THR:HA	8:I:413:ARG:CZ	2.17	0.74
8:I:413:ARG:HD3	8:I:413:ARG:N	1.95	0.74
11:T:3073:ASN:HD21	11:T:3689:ARG:HG2	1.53	0.73
11:T:851:LEU:HD21	11:T:1156:TYR:CZ	2.25	0.70
8:I:411:THR:HG23	8:I:414:VAL:HG12	1.73	0.70
11:T:850:ARG:HB3	11:T:852:PRO:CG	2.21	0.70
11:T:850:ARG:HB3	11:T:852:PRO:HD3	1.73	0.69
8:I:415:MET:HA	8:I:415:MET:HE3	1.77	0.67
11:T:2167:VAL:HA	11:T:2170:VAL:HG12	1.74	0.67
11:T:851:LEU:CD2	11:T:1156:TYR:OH	2.43	0.67
11:T:863:ILE:HG13	11:T:864:THR:HG23	1.78	0.64
11:T:851:LEU:N	11:T:852:PRO:HD2	2.13	0.64
11:T:843:ASN:O	11:T:855:ARG:NH1	2.31	0.64
8:I:411:THR:HA	8:I:413:ARG:HH12	1.60	0.64
11:T:1685:LEU:HB3	11:T:1688:LYS:HB3	1.80	0.63
11:T:2373:ALA:HA	11:T:2415:ARG:HH12	1.63	0.62
7:H:293:CYS:HB2	8:I:478:ILE:HD12	1.80	0.62
8:I:411:THR:HG23	8:I:414:VAL:CG1	2.30	0.62
11:T:2613:ILE:HG22	11:T:2615:SER:H	1.65	0.62
11:T:305:LEU:HA	11:T:308:VAL:HG22	1.81	0.62
11:T:1010:ASP:OD1	11:T:1011:ILE:N	2.33	0.62
2:C:15:MET:HG2	2:C:246:THR:HG21	1.82	0.61
1:B:399:GLU:OE1	8:I:379:ARG:NH1	2.33	0.61
11:T:3128:ILE:HD11	11:T:3158:ARG:HD2	1.83	0.61
11:T:612:THR:HB	11:T:1532:VAL:HG11	1.83	0.60
11:T:1504:SER:HB2	11:T:1558:ILE:HG22	1.83	0.60
11:T:2761:GLU:HB3	11:T:2764:TRP:HB3	1.83	0.60
2:C:141:LEU:HB2	2:C:144:GLU:HG2	1.82	0.60
3:D:568:HIS:HB3	3:D:587:HIS:HB3	1.83	0.60
1:B:200:ARG:NH2	1:B:298:SER:OG	2.34	0.60
3:D:505:ILE:O	3:D:505:ILE:HG23	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:410:ASP:HB3	8:I:412:GLN:HE21	1.67	0.60
8:I:466:LYS:HG2	10:Q:424:THR:HG21	1.84	0.59
11:T:850:ARG:HB3	11:T:852:PRO:HG3	1.83	0.59
7:H:401:GLU:HG2	7:H:404:THR:H	1.66	0.59
7:H:243:THR:HG23	7:H:245:LEU:H	1.68	0.59
11:T:81:ASP:HA	11:T:84:ASN:HD22	1.66	0.59
1:B:360:GLU:HG2	5:F:139:PRO:HG3	1.84	0.58
7:H:314:ASP:HB3	7:H:319:ARG:HH11	1.67	0.58
11:T:2422:VAL:HA	11:T:2463:ILE:HD11	1.86	0.58
1:B:400:ARG:HA	8:I:381:ASN:HB3	1.85	0.58
11:T:3145:SER:HA	11:T:3204:PRO:HG3	1.85	0.58
11:T:940:ALA:O	11:T:944:ASN:ND2	2.36	0.57
3:D:548:THR:HG22	3:D:564:LYS:HG2	1.86	0.57
3:D:776:LYS:HE2	3:D:798:PRO:HG3	1.86	0.57
7:H:206:ARG:NH2	10:Q:369:PHE:O	2.37	0.57
7:H:358:ASN:HB2	8:I:449:LEU:HD12	1.87	0.57
8:I:418:ARG:H	8:I:418:ARG:HD3	1.70	0.57
11:T:2272:VAL:HG23	11:T:2273:PRO:HD3	1.87	0.57
3:D:476:ASP:O	3:D:537:ASN:ND2	2.38	0.57
8:I:410:ASP:O	8:I:413:ARG:CZ	2.53	0.56
4:E:47:GLU:O	4:E:51:GLN:NE2	2.38	0.56
11:T:1750:PHE:O	11:T:1799:ARG:NH1	2.39	0.56
11:T:2175:LYS:HB3	11:T:2179:TRP:HB3	1.86	0.56
4:E:175:ASP:HB2	4:E:210:GLU:HB3	1.87	0.56
7:H:282:GLU:OE1	10:Q:384:ARG:NH2	2.39	0.56
11:T:2310:LEU:HA	11:T:2313:LYS:HD2	1.88	0.56
11:T:2474:GLN:HG2	11:T:2546:ILE:HD12	1.87	0.56
11:T:851:LEU:HG	11:T:1156:TYR:HH	1.68	0.56
2:C:12:GLN:HG2	2:C:21:ILE:HD11	1.88	0.56
3:D:452:LEU:HD21	3:D:722:ASP:HB2	1.86	0.56
11:T:3165:GLN:HG3	11:T:3222:LEU:HD21	1.88	0.56
11:T:3611:SER:HB3	11:T:3674:TRP:HE1	1.71	0.56
4:E:293:ILE:HG21	4:E:315:ILE:HD11	1.88	0.56
11:T:3285:THR:O	11:T:3293:ARG:NH2	2.39	0.56
1:B:389:ASN:N	1:B:392:GLN:OE1	2.39	0.55
3:D:490:ILE:HD11	3:D:528:VAL:HG11	1.88	0.55
11:T:3564:ILE:HA	11:T:3588:PRO:HA	1.89	0.55
11:T:1756:ILE:HG13	11:T:1757:LYS:HG2	1.87	0.55
11:T:2262:VAL:O	11:T:2266:ASN:ND2	2.38	0.55
11:T:2986:ARG:NH2	11:T:3018:GLN:OE1	2.39	0.55
4:E:445:PHE:HB3	4:E:449:GLU:HG3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:T:339:GLU:HB2	11:T:1897:GLU:HB2	1.87	0.55
11:T:1327:ASP:O	11:T:1330:LYS:NZ	2.39	0.55
1:B:477:ARG:NH2	11:T:2753:GLU:OE2	2.40	0.55
3:D:555:ASP:OD1	3:D:555:ASP:N	2.39	0.55
7:H:358:ASN:HD22	8:I:452:ASP:HB3	1.71	0.55
11:T:1706:ILE:HG12	11:T:1713:ILE:HG22	1.88	0.55
11:T:2628:ILE:HG13	11:T:2665:LEU:HD21	1.88	0.55
11:T:373:GLU:O	11:T:374:ARG:NH1	2.39	0.55
11:T:849:ALA:O	11:T:851:LEU:HD22	2.06	0.55
11:T:3481:ASP:OD1	11:T:3481:ASP:N	2.40	0.55
1:B:193:ASP:OD2	5:F:116:GLN:NE2	2.39	0.55
11:T:934:PRO:HD3	11:T:2829:VAL:HG21	1.88	0.55
11:T:2284:LYS:HA	11:T:2287:LYS:HG2	1.89	0.54
11:T:1386:ASP:OD2	11:T:1412:ARG:NH1	2.40	0.54
4:E:308:ILE:HD11	4:E:368:LEU:HD13	1.88	0.54
11:T:997:ILE:HD11	11:T:1024:VAL:HG11	1.89	0.54
11:T:3244:ASP:OD1	11:T:3247:ARG:NH1	2.41	0.54
11:T:1005:GLN:N	11:T:1005:GLN:OE1	2.40	0.54
2:C:307:GLU:OE2	7:H:306:LYS:NZ	2.39	0.54
11:T:2415:ARG:HE	11:T:2419:PRO:HG3	1.73	0.54
4:E:230:VAL:HG23	4:E:251:ALA:HB1	1.90	0.54
11:T:106:VAL:HG11	11:T:115:GLY:HA3	1.88	0.54
11:T:381:PHE:HB2	11:T:1858:ASP:H	1.73	0.54
7:H:195:ARG:HA	7:H:198:MET:HG2	1.89	0.54
11:T:415:ILE:HD11	11:T:463:LEU:HD22	1.89	0.54
11:T:2774:ASP:OD1	11:T:2774:ASP:N	2.41	0.54
11:T:2036:LEU:HD13	11:T:2123:ILE:HG13	1.89	0.54
11:T:2206:LEU:HA	11:T:2209:VAL:HG12	1.89	0.54
11:T:3153:ARG:NH1	11:T:3210:GLU:OE2	2.41	0.54
4:E:166:ARG:NH1	4:E:167:GLY:O	2.42	0.53
4:E:383:ILE:O	4:E:444:LYS:NZ	2.41	0.53
1:B:147:LYS:HE2	1:B:149:CYS:HB3	1.90	0.53
7:H:235:ARG:NH1	8:I:471:ASP:OD2	2.40	0.53
8:I:413:ARG:HH11	8:I:414:VAL:H	1.57	0.53
2:C:145:LEU:HD11	9:K:1066:LYS:HG3	1.90	0.53
11:T:1667:THR:HG22	11:T:1721:SER:HB3	1.90	0.53
4:E:19:ASP:OD2	8:I:513:LYS:NZ	2.41	0.53
11:T:85:ARG:NH2	11:T:1975:VAL:O	2.41	0.53
11:T:310:ILE:HG12	11:T:353:HIS:HB3	1.90	0.53
4:E:215:VAL:HG13	4:E:217:HIS:H	1.73	0.53
7:H:195:ARG:NH2	10:Q:357:GLU:OE2	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:406:SER:OG	7:H:407:LEU:N	2.42	0.53
11:T:1775:ASN:N	11:T:1775:ASN:OD1	2.42	0.53
11:T:2444:GLU:O	11:T:2450:ARG:NE	2.40	0.53
12:U:9:ALA:O	12:U:11:ALA:N	2.42	0.53
3:D:476:ASP:HB2	3:D:537:ASN:HD21	1.74	0.53
11:T:447:LEU:HD11	11:T:600:ASP:HB3	1.91	0.53
11:T:1770:ILE:HG12	11:T:1810:THR:HB	1.91	0.53
2:C:145:LEU:HD13	9:K:1069:LYS:HD3	1.91	0.52
11:T:840:GLN:NE2	11:T:878:PHE:O	2.42	0.52
11:T:850:ARG:CB	11:T:852:PRO:CD	2.86	0.52
11:T:1840:LYS:O	11:T:1840:LYS:NZ	2.35	0.52
8:I:508:GLN:NE2	8:I:509:ASN:OD1	2.42	0.52
11:T:1516:VAL:HG21	11:T:1565:GLN:HG2	1.89	0.52
11:T:2610:ILE:HD12	11:T:2616:LEU:HD11	1.90	0.52
8:I:376:VAL:HG11	11:T:2786:VAL:HG12	1.91	0.52
11:T:2488:LEU:HD12	11:T:2491:ILE:HD13	1.91	0.52
3:D:544:SER:OG	3:D:545:GLU:N	2.43	0.52
11:T:3318:ARG:NH1	11:T:3322:GLU:OE1	2.42	0.52
11:T:93:GLN:HE22	11:T:134:GLN:HB3	1.72	0.52
11:T:624:ARG:H	11:T:694:ASP:HB2	1.75	0.52
11:T:3021:GLU:HA	11:T:3024:THR:HG22	1.92	0.52
7:H:363:ALA:O	7:H:367:LYS:NZ	2.40	0.52
11:T:851:LEU:CD2	11:T:1156:TYR:CE2	2.76	0.52
11:T:1007:TYR:CA	11:T:1014:ARG:HH22	2.19	0.52
11:T:3610:ASP:OD1	11:T:3610:ASP:N	2.42	0.52
4:E:43:TYR:HB2	10:Q:370:PRO:HB2	1.92	0.52
4:E:92:LYS:HG2	5:F:49:GLU:HA	1.91	0.52
4:E:347:ARG:HH21	4:E:388:GLY:HA3	1.75	0.52
11:T:1827:GLU:HG2	11:T:1829:LYS:HG2	1.91	0.52
11:T:3075:ILE:HG22	11:T:3077:PHE:H	1.75	0.52
11:T:3221:LEU:HB3	11:T:3349:PHE:HE2	1.75	0.52
1:B:133:TYR:O	1:B:282:ARG:NH2	2.43	0.52
3:D:492:ILE:HG22	3:D:500:LEU:HD21	1.92	0.52
11:T:850:ARG:O	11:T:851:LEU:CB	2.53	0.52
11:T:1818:SER:OG	11:T:1819:GLY:N	2.43	0.52
3:D:589:GLN:HA	3:D:611:ASP:HA	1.92	0.51
11:T:412:GLU:HG2	11:T:463:LEU:HD21	1.91	0.51
2:C:203:SER:HB3	2:C:206:PHE:HB2	1.92	0.51
2:C:248:THR:HG23	2:C:308:ALA:HB1	1.93	0.51
8:I:480:LEU:HB2	8:I:498:ILE:HD12	1.91	0.51
11:T:76:ARG:HH12	11:T:116:ILE:HG13	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:T:285:ILE:HG21	11:T:289:PRO:HD3	1.92	0.51
1:B:190:ARG:HA	1:B:286:LYS:H	1.75	0.51
11:T:1852:ASP:N	11:T:1852:ASP:OD1	2.43	0.51
5:F:97:ILE:HD11	10:Q:373:LEU:HB2	1.92	0.51
3:D:750:ASN:OD1	4:E:158:ARG:NH2	2.42	0.51
3:D:785:SER:OG	3:D:786:ARG:N	2.42	0.51
4:E:355:ASP:HB2	4:E:399:VAL:HB	1.93	0.51
11:T:773:VAL:HG21	11:T:784:LEU:HD22	1.93	0.51
4:E:49:ILE:HD11	5:F:56:LEU:HD11	1.93	0.51
11:T:17:ASP:OD1	11:T:26:SER:OG	2.29	0.51
11:T:1063:LEU:HD13	11:T:3319:ARG:HD3	1.92	0.51
11:T:93:GLN:NE2	11:T:134:GLN:OE1	2.44	0.51
11:T:678:ASP:OD1	11:T:678:ASP:N	2.43	0.51
11:T:850:ARG:O	11:T:852:PRO:HD3	2.05	0.51
11:T:1601:ASN:ND2	11:T:1632:GLU:O	2.44	0.51
11:T:2484:LYS:HE3	11:T:2535:ARG:HD2	1.92	0.51
11:T:2906:GLN:HG2	11:T:2943:ILE:HG23	1.92	0.51
3:D:91:GLN:O	3:D:93:LYS:NZ	2.43	0.51
11:T:507:ILE:HD12	11:T:2168:LEU:HD23	1.93	0.51
11:T:577:ASN:ND2	11:T:582:ASP:OD2	2.44	0.51
11:T:691:MET:HG2	11:T:730:GLU:HG3	1.93	0.51
9:K:957:ASP:OD1	9:K:957:ASP:N	2.45	0.50
11:T:793:LEU:HG	11:T:831:ILE:HD11	1.93	0.50
11:T:839:LEU:O	11:T:843:ASN:HB2	2.11	0.50
11:T:850:ARG:CB	11:T:852:PRO:HD3	2.40	0.50
11:T:727:LEU:HD13	11:T:772:SER:HB3	1.93	0.50
11:T:3109:SER:OG	11:T:3689:ARG:NH1	2.44	0.50
11:T:1300:ASN:HB3	11:T:1303:VAL:HG12	1.94	0.50
11:T:1531:ARG:HB2	11:T:1534:VAL:HG12	1.93	0.50
11:T:2089:SER:OG	11:T:2090:LEU:N	2.42	0.50
11:T:3140:LEU:HD22	11:T:3152:VAL:HG23	1.93	0.50
4:E:224:GLN:O	4:E:228:ASN:ND2	2.45	0.50
3:D:635:MET:HB3	3:D:645:ARG:HB2	1.94	0.50
8:I:411:THR:HG22	8:I:414:VAL:CG1	2.25	0.50
11:T:2011:MET:HA	11:T:2014:ILE:HG22	1.94	0.50
11:T:3505:ASP:OD1	11:T:3505:ASP:N	2.42	0.50
1:B:484:TRP:HE1	11:T:2745:VAL:HG22	1.77	0.50
11:T:1007:TYR:CD1	11:T:1007:TYR:N	2.73	0.50
11:T:2581:ARG:HA	11:T:2584:ILE:HD12	1.94	0.50
11:T:365:PRO:HB3	11:T:398:PHE:HZ	1.76	0.50
11:T:850:ARG:HG2	11:T:854:GLU:OE2	2.04	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:T:1007:TYR:O	11:T:1014:ARG:NH2	2.45	0.50
11:T:1105:ASN:ND2	11:T:2529:SER:OG	2.45	0.50
11:T:2289:HIS:HD2	11:T:2292:ILE:HD11	1.77	0.50
6:G:90:ASP:OD1	6:G:90:ASP:N	2.44	0.49
11:T:138:ASP:OD1	11:T:138:ASP:N	2.45	0.49
11:T:1342:LEU:HD12	11:T:1345:LEU:HD12	1.93	0.49
1:B:405:THR:HG21	11:T:2755:PHE:HA	1.94	0.49
3:D:735:ASP:OD1	3:D:735:ASP:N	2.45	0.49
4:E:86:ASP:N	4:E:86:ASP:OD1	2.45	0.49
8:I:382:ARG:HG2	8:I:384:THR:HG23	1.92	0.49
11:T:3559:SER:HA	11:T:3564:ILE:HG12	1.94	0.49
3:D:591:ALA:HB3	3:D:605:PHE:HB2	1.94	0.49
11:T:2887:ARG:O	11:T:2905:ARG:NH2	2.38	0.49
1:B:478:LEU:HD22	11:T:2711:GLN:HB3	1.93	0.49
11:T:851:LEU:HD21	11:T:1156:TYR:OH	2.12	0.49
11:T:1503:LEU:O	11:T:1507:LEU:HB2	2.13	0.49
6:G:96:TYR:O	6:G:100:ASN:ND2	2.44	0.49
11:T:479:ASN:ND2	11:T:640:GLU:OE1	2.45	0.49
4:E:370:PRO:HA	4:E:373:THR:HG22	1.93	0.49
4:E:418:LEU:HD11	9:K:171:GLY:HA3	1.93	0.49
9:K:168:ARG:HH22	9:K:169:PHE:HD2	1.61	0.49
4:E:141:VAL:HG21	9:K:858:ILE:HG22	1.95	0.49
9:K:162:GLN:OE1	9:K:163:GLN:NE2	2.45	0.49
11:T:9:GLN:O	11:T:13:ARG:NH2	2.44	0.49
11:T:2461:GLU:O	11:T:2594:ARG:NH2	2.46	0.49
11:T:3319:ARG:HH22	11:T:3476:LYS:HZ2	1.59	0.49
11:T:3597:LYS:HG2	11:T:3599:LEU:H	1.77	0.49
11:T:1062:ASP:N	11:T:1062:ASP:OD1	2.45	0.49
3:D:173:GLU:HG2	3:D:250:THR:HG21	1.95	0.49
11:T:3483:ASP:N	11:T:3483:ASP:OD1	2.43	0.49
3:D:553:SER:OG	3:D:555:ASP:OD1	2.31	0.49
8:I:413:ARG:H	8:I:413:ARG:CD	1.97	0.49
10:Q:391:ARG:NH1	10:Q:414:SER:OG	2.46	0.49
11:T:3359:LEU:HD12	11:T:3447:ILE:HG23	1.94	0.49
1:B:403:THR:OG1	1:B:404:ILE:N	2.44	0.48
11:T:3448:ALA:HB2	11:T:3458:MET:HG3	1.94	0.48
2:C:225:LYS:HD2	2:C:227:HIS:HE1	1.78	0.48
3:D:222:VAL:HA	3:D:227:HIS:HB3	1.95	0.48
11:T:2214:MET:HG2	11:T:2266:ASN:HD21	1.77	0.48
11:T:867:VAL:CB	11:T:872:LEU:HA	2.43	0.48
11:T:2184:LEU:HD23	11:T:2187:ILE:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:T:3357:GLN:HE22	11:T:3369:ILE:H	1.61	0.48
11:T:3467:LEU:HB3	11:T:3744:PHE:HE2	1.78	0.48
2:C:146:GLN:HG2	9:K:1073:ILE:HD11	1.96	0.48
3:D:640:THR:OG1	3:D:642:ASP:OD1	2.30	0.48
11:T:712:ARG:NH2	11:T:715:GLU:OE2	2.46	0.48
11:T:2641:GLU:OE2	11:T:2666:TYR:OH	2.31	0.48
5:F:32:ASP:HA	5:F:35:LEU:HB2	1.94	0.48
11:T:1931:LEU:HD13	11:T:1973:VAL:HG11	1.95	0.48
11:T:2104:VAL:HG21	11:T:2121:ILE:HD11	1.95	0.48
4:E:84:TYR:OH	5:F:58:ASP:OD2	2.31	0.48
4:E:228:ASN:HA	4:E:231:ILE:HG22	1.95	0.48
11:T:1774:SER:O	11:T:1774:SER:OG	2.30	0.48
5:F:97:ILE:HG13	10:Q:374:GLU:HB2	1.95	0.48
8:I:386:THR:HG22	8:I:392:ASN:HB3	1.95	0.48
11:T:1911:TYR:HE1	11:T:1948:VAL:HG21	1.79	0.48
3:D:174:LEU:HA	3:D:177:ILE:HG12	1.96	0.48
11:T:130:LYS:NZ	11:T:224:LEU:O	2.43	0.48
11:T:832:LYS:NZ	11:T:867:VAL:HB	2.27	0.48
4:E:13:PRO:HG3	7:H:197:LYS:HD3	1.96	0.48
11:T:1098:ASP:N	11:T:1098:ASP:OD1	2.47	0.48
11:T:850:ARG:CD	11:T:854:GLU:OE2	2.61	0.48
11:T:3135:THR:O	11:T:3421:GLN:NE2	2.47	0.48
11:T:1477:LEU:O	11:T:1481:GLY:N	2.46	0.47
11:T:1377:LEU:HA	11:T:1380:GLU:HG2	1.96	0.47
3:D:452:LEU:O	4:E:263:GLN:NE2	2.37	0.47
11:T:2316:TYR:O	11:T:2320:LEU:HB2	2.13	0.47
7:H:260:ALA:HB1	8:I:447:LEU:HD12	1.95	0.47
11:T:2217:ILE:HD11	11:T:2266:ASN:HD22	1.80	0.47
11:T:3304:LYS:O	11:T:3309:THR:OG1	2.31	0.47
2:C:258:VAL:HA	2:C:261:THR:HG22	1.96	0.47
11:T:110:GLU:O	11:T:215:ARG:NH2	2.43	0.47
11:T:1217:LYS:HB3	11:T:1263:LEU:HD11	1.97	0.47
2:C:209:ASN:HB3	2:C:231:ILE:HG21	1.96	0.47
3:D:274:ASN:ND2	3:D:275:GLN:OE1	2.47	0.47
4:E:211:VAL:HB	9:K:855:SER:HB3	1.96	0.47
6:G:154:LEU:O	6:G:157:GLN:NE2	2.48	0.47
11:T:610:GLU:OE2	11:T:1582:ARG:NH2	2.44	0.47
11:T:1426:GLU:OE1	11:T:1427:GLU:N	2.47	0.47
7:H:373:ASN:HD21	7:H:380:ILE:HG13	1.80	0.47
8:I:464:LEU:HD13	8:I:480:LEU:HD23	1.95	0.47
11:T:867:VAL:HG11	11:T:872:LEU:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:T:1327:ASP:OD1	11:T:1327:ASP:N	2.47	0.47
1:B:290:LEU:HD11	5:F:116:GLN:HA	1.97	0.47
6:G:169:GLN:O	6:G:173:ASN:HB2	2.15	0.47
11:T:1199:HIS:HE1	11:T:3376:PRO:HB2	1.79	0.47
1:B:289:ASP:OD1	1:B:289:ASP:N	2.47	0.47
3:D:690:ARG:HB2	3:D:765:THR:HG23	1.96	0.47
3:D:698:TYR:H	3:D:713:GLY:HA2	1.80	0.47
11:T:1537:THR:O	11:T:1541:GLN:NE2	2.47	0.47
11:T:2177:LYS:HG3	11:T:2179:TRP:HB2	1.97	0.47
11:T:2470:ASN:HB2	11:T:2556:ILE:HD13	1.96	0.47
11:T:3050:ASP:OD1	11:T:3050:ASP:N	2.48	0.47
8:I:411:THR:HG23	8:I:413:ARG:HH12	1.79	0.47
11:T:843:ASN:HD21	11:T:859:VAL:HG12	1.80	0.47
11:T:1382:ILE:HD12	11:T:1415:CYS:HB2	1.97	0.47
11:T:3414:ARG:NH1	11:T:3417:GLU:OE2	2.48	0.47
3:D:450:LEU:HD22	4:E:260:GLY:HA3	1.97	0.46
11:T:76:ARG:HH22	11:T:116:ILE:H	1.63	0.46
1:B:220:ASN:ND2	7:H:398:GLU:OE1	2.49	0.46
7:H:270:ASP:OD1	7:H:270:ASP:N	2.46	0.46
11:T:346:GLU:HA	11:T:349:HIS:HB2	1.98	0.46
11:T:1234:GLN:NE2	11:T:1271:THR:OG1	2.48	0.46
11:T:2476:LEU:O	11:T:2479:SER:OG	2.31	0.46
8:I:379:ARG:HE	8:I:379:ARG:HB2	1.57	0.46
11:T:355:LEU:HD21	11:T:364:LEU:HD23	1.97	0.46
11:T:2750:ALA:HB2	11:T:2757:ASP:HB3	1.97	0.46
1:B:187:ALA:HA	7:H:412:ILE:HG22	1.98	0.46
11:T:1844:ASN:HD22	11:T:1889:PHE:HA	1.80	0.46
6:G:81:MET:O	6:G:111:ARG:NH1	2.48	0.46
4:E:264:LEU:HA	4:E:267:TYR:HD2	1.80	0.46
1:B:301:ASP:OD2	7:H:217:ARG:NH1	2.46	0.46
11:T:1683:GLU:O	11:T:1686:LYS:NZ	2.35	0.46
11:T:3023:PHE:HA	11:T:3026:LYS:HD2	1.98	0.46
6:G:121:VAL:HG11	9:K:1011:ALA:HB2	1.97	0.46
7:H:311:PHE:HB2	7:H:352:GLN:HE22	1.80	0.46
11:T:868:ARG:HA	11:T:868:ARG:HD3	1.61	0.46
11:T:3685:ASN:ND2	11:T:3687:GLN:OE1	2.49	0.46
12:U:148:ALA:O	12:U:153:ALA:N	2.49	0.46
3:D:756:TYR:OH	4:E:158:ARG:O	2.31	0.46
11:T:249:PHE:O	11:T:288:ARG:NH1	2.49	0.46
11:T:2169:TYR:HA	11:T:2172:PHE:HB3	1.98	0.46
3:D:607:GLY:HA2	5:F:111:LYS:HE3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:615:VAL:HG23	3:D:626:THR:HG22	1.97	0.46
8:I:469:LYS:HA	8:I:469:LYS:HD3	1.81	0.46
11:T:2249:GLU:HG2	11:T:2251:SER:H	1.80	0.46
11:T:3524:SER:O	11:T:3524:SER:OG	2.30	0.46
2:C:323:THR:HG23	7:H:351:LYS:HE2	1.98	0.45
8:I:417:LYS:HA	8:I:417:LYS:HD3	1.65	0.45
11:T:3449:ILE:HG23	11:T:3457:ILE:HG13	1.96	0.45
4:E:27:GLU:OE2	8:I:507:SER:OG	2.32	0.45
11:T:740:LEU:HD21	11:T:765:LEU:HD12	1.98	0.45
3:D:650:HIS:NE2	3:D:676:ASN:OD1	2.50	0.45
3:D:719:ARG:NH1	4:E:168:ALA:O	2.41	0.45
3:D:704:LYS:HD3	3:D:705:GLU:HG2	1.99	0.45
5:F:62:ARG:NH2	6:G:198:ASN:O	2.47	0.45
11:T:2425:ARG:HD3	11:T:2463:ILE:HD12	1.98	0.45
3:D:709:LEU:HB2	3:D:723:LEU:HD11	1.97	0.45
4:E:10:ILE:HD11	5:F:39:LEU:HD13	1.98	0.45
4:E:354:LEU:HD11	4:E:372:VAL:HG11	1.98	0.45
9:K:1057:SER:O	9:K:1061:SER:N	2.49	0.45
11:T:62:VAL:HG23	11:T:72:GLU:HG3	1.98	0.45
11:T:1409:VAL:HG22	11:T:1455:ILE:HD11	1.96	0.45
1:B:209:GLY:HA2	3:D:71:LYS:HG3	1.99	0.45
1:B:279:ARG:NE	7:H:398:GLU:OE2	2.49	0.45
3:D:188:ASN:OD1	3:D:192:LYS:NZ	2.50	0.45
4:E:62:ASP:OD1	4:E:62:ASP:N	2.46	0.45
6:G:158:GLN:HG2	6:G:160:PRO:HD2	1.99	0.45
11:T:466:ILE:O	11:T:469:ASP:HB3	2.16	0.45
11:T:588:ARG:HG3	11:T:685:TYR:HE2	1.80	0.45
11:T:2680:ARG:NH2	11:T:2696:GLN:OE1	2.43	0.45
11:T:3245:LEU:HD22	11:T:3292:ILE:HD12	1.98	0.45
11:T:285:ILE:HG23	11:T:288:ARG:HH21	1.82	0.45
6:G:71:ASP:OD2	9:K:1051:ARG:NH2	2.50	0.45
11:T:80:LEU:O	11:T:84:ASN:ND2	2.50	0.45
11:T:478:LEU:HD22	11:T:586:LEU:HD23	1.99	0.45
11:T:485:ILE:HG23	11:T:579:PRO:HB2	1.99	0.45
11:T:1844:ASN:HA	11:T:1848:ILE:HG13	1.99	0.45
11:T:1915:LYS:HA	11:T:1915:LYS:HD3	1.84	0.45
7:H:396:ASN:HB2	7:H:410:GLU:HG3	1.99	0.45
11:T:1116:ASN:ND2	11:T:2501:GLN:OE1	2.50	0.45
6:G:169:GLN:HA	6:G:172:GLN:HE21	1.82	0.44
11:T:1774:SER:OG	11:T:1777:GLU:OE2	2.33	0.44
1:B:279:ARG:NH2	7:H:410:GLU:OE1	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:394:SER:O	8:I:394:SER:OG	2.31	0.44
11:T:850:ARG:CA	11:T:852:PRO:HD3	2.42	0.44
11:T:1244:VAL:O	11:T:1248:THR:OG1	2.28	0.44
11:T:1825:LEU:HD12	11:T:1828:ASP:HA	1.99	0.44
11:T:1829:LYS:HA	11:T:1829:LYS:HD3	1.79	0.44
3:D:152:TYR:HD2	3:D:185:LEU:HD22	1.81	0.44
11:T:106:VAL:HG13	11:T:109:LYS:HE3	2.00	0.44
11:T:460:ALA:O	11:T:463:LEU:HB2	2.17	0.44
11:T:1102:LEU:HD12	11:T:2533:LEU:HD21	2.00	0.44
3:D:188:ASN:O	3:D:192:LYS:NZ	2.47	0.44
8:I:359:GLU:OE2	11:T:2879:ARG:NH2	2.50	0.44
11:T:1396:ILE:HD12	11:T:1398:LYS:HG2	1.98	0.44
4:E:122:ASN:ND2	9:K:954:ILE:O	2.46	0.44
4:E:403:GLU:O	4:E:407:PHE:N	2.51	0.44
11:T:374:ARG:HA	11:T:374:ARG:HD3	1.85	0.44
11:T:744:LEU:HD11	11:T:765:LEU:HB3	2.00	0.44
11:T:1278:GLU:HG2	11:T:1320:ILE:HG12	1.99	0.44
4:E:46:LEU:HD21	5:F:39:LEU:HD11	2.00	0.44
9:K:1076:LYS:HA	9:K:1076:LYS:HD3	1.76	0.44
11:T:973:ASP:OD1	11:T:2558:ARG:NH2	2.48	0.44
11:T:2781:LYS:HA	11:T:2781:LYS:HD3	1.87	0.44
4:E:15:ASP:OD1	6:G:206:ARG:NH1	2.49	0.44
9:K:1044:LEU:HD13	9:K:1049:ILE:HD11	2.00	0.44
11:T:44:TYR:O	11:T:48:LEU:N	2.48	0.44
3:D:224:SER:H	3:D:227:HIS:HB2	1.82	0.44
3:D:709:LEU:HB3	3:D:721:TRP:HB2	2.00	0.44
11:T:222:LYS:HD3	11:T:234:LEU:HD22	1.99	0.44
11:T:1038:ASN:N	11:T:1038:ASN:OD1	2.51	0.44
11:T:2593:THR:HA	11:T:2596:ILE:HG13	2.00	0.44
11:T:1970:VAL:O	11:T:1974:MET:HB2	2.18	0.43
11:T:2518:GLU:HA	11:T:2521:ASN:HD21	1.82	0.43
11:T:3068:LEU:HD21	11:T:3073:ASN:HB3	2.00	0.43
11:T:3275:ASN:HA	11:T:3278:LYS:HG2	1.99	0.43
11:T:3304:LYS:HE2	11:T:3313:ARG:HG3	2.00	0.43
1:B:325:LEU:HB2	3:D:120:PRO:HG3	1.99	0.43
4:E:16:THR:OG1	5:F:32:ASP:OD2	2.28	0.43
11:T:928:LEU:HD22	11:T:945:VAL:HG13	2.00	0.43
11:T:2412:ILE:HD12	11:T:2412:ILE:HA	1.84	0.43
4:E:11:TRP:HB2	4:E:42:GLU:HB3	2.01	0.43
11:T:1389:ASP:N	11:T:1389:ASP:OD1	2.51	0.43
11:T:2294:GLN:HG2	11:T:2295:PRO:HD3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:T:3566:ASN:OD1	11:T:3566:ASN:N	2.50	0.43
11:T:3593:TYR:HB2	11:T:3596:VAL:HG12	2.00	0.43
6:G:118:GLN:NE2	9:K:1058:TYR:OH	2.51	0.43
11:T:1141:ASP:OD1	11:T:1141:ASP:N	2.38	0.43
11:T:2854:GLU:OE1	11:T:2884:TRP:NE1	2.49	0.43
1:B:216:TYR:HD2	1:B:278:PRO:HG2	1.84	0.43
8:I:418:ARG:CD	8:I:418:ARG:H	2.31	0.43
11:T:852:PRO:HB2	11:T:853:HIS:H	1.69	0.43
11:T:2031:LEU:O	11:T:2034:LEU:HB3	2.18	0.43
11:T:2275:LEU:HA	11:T:2278:LEU:HD13	1.99	0.43
3:D:613:ASP:OD2	4:E:57:ARG:NH2	2.52	0.43
8:I:368:ILE:HD12	8:I:368:ILE:HA	1.94	0.43
10:Q:412:ILE:HG21	10:Q:416:VAL:HB	2.01	0.43
11:T:1379:GLN:HA	11:T:1382:ILE:HG22	1.99	0.43
11:T:1911:TYR:HD1	11:T:1948:VAL:HG11	1.83	0.43
4:E:126:PRO:HD3	9:K:981:LYS:HG3	1.99	0.43
6:G:109:VAL:HG13	9:K:1040:LEU:HD21	2.01	0.43
11:T:1342:LEU:HD22	11:T:1374:LEU:HD11	2.00	0.43
11:T:3685:ASN:OD1	11:T:3685:ASN:N	2.51	0.43
4:E:395:LYS:HD3	4:E:395:LYS:HA	1.79	0.43
11:T:871:VAL:HG21	11:T:908:LEU:HD23	1.99	0.43
11:T:1397:GLN:NE2	11:T:1400:THR:O	2.39	0.43
11:T:1437:ARG:HH11	11:T:1441:LEU:HD11	1.84	0.43
11:T:1834:LEU:O	11:T:1838:HIS:ND1	2.43	0.43
1:B:212:ILE:HG21	1:B:282:ARG:HE	1.83	0.43
3:D:600:TYR:HB2	7:H:369:ILE:HG23	2.01	0.43
4:E:274:GLU:O	4:E:278:GLN:CB	2.67	0.43
11:T:851:LEU:N	11:T:851:LEU:CD2	2.81	0.43
11:T:1137:ASN:OD1	11:T:1137:ASN:N	2.50	0.43
11:T:1942:VAL:HG21	11:T:1985:LEU:HD21	2.01	0.43
11:T:3108:ILE:HD13	11:T:3108:ILE:HA	1.90	0.43
11:T:3262:ARG:NH2	11:T:3737:ASP:OD1	2.52	0.43
2:C:251:LYS:HD2	2:C:251:LYS:HA	1.86	0.43
7:H:232:SER:OG	7:H:235:ARG:NH2	2.44	0.43
11:T:785:LEU:HB2	11:T:827:LEU:HD21	2.00	0.43
11:T:944:ASN:OD1	11:T:947:ARG:NH2	2.52	0.43
11:T:1900:LEU:HD23	11:T:1900:LEU:HA	1.88	0.43
11:T:2377:THR:OG1	11:T:2415:ARG:NH2	2.52	0.43
11:T:2783:VAL:HG13	11:T:2791:ARG:HD2	2.00	0.43
11:T:3278:LYS:HA	11:T:3281:VAL:HG12	2.01	0.43
11:T:3348:LYS:HE2	11:T:3348:LYS:HB3	1.92	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:T:3472:ASN:ND2	11:T:3482:PRO:HG3	2.34	0.43
6:G:86:PRO:HA	9:K:901:LEU:HD22	2.00	0.42
7:H:367:LYS:HE2	7:H:367:LYS:HB2	1.90	0.42
11:T:467:ILE:O	11:T:470:SER:OG	2.27	0.42
11:T:851:LEU:N	11:T:851:LEU:HD22	2.34	0.42
11:T:2913:ASN:HD21	11:T:2941:HIS:HA	1.84	0.42
3:D:490:ILE:HB	3:D:521:LEU:HB2	2.00	0.42
3:D:602:LEU:O	3:D:603:ARG:NH1	2.52	0.42
9:K:1042:THR:OG1	9:K:1046:GLU:OE2	2.29	0.42
11:T:1072:TYR:HD1	11:T:2492:TYR:HE1	1.66	0.42
11:T:1444:PHE:HB3	11:T:1463:LEU:HD21	2.01	0.42
3:D:715:ASP:N	3:D:715:ASP:OD1	2.42	0.42
10:Q:364:GLY:HA2	10:Q:367:ARG:HH21	1.84	0.42
11:T:984:GLY:HA3	11:T:2447:ILE:HG22	2.01	0.42
11:T:2123:ILE:O	11:T:2127:LEU:HB2	2.19	0.42
11:T:2608:ASP:OD1	11:T:2612:LYS:NZ	2.53	0.42
6:G:85:PRO:HA	6:G:86:PRO:HD3	1.90	0.42
11:T:778:ASN:OD1	11:T:778:ASN:N	2.51	0.42
11:T:2350:ARG:HA	11:T:2353:VAL:HG22	2.01	0.42
11:T:2375:ILE:HD12	11:T:2375:ILE:HA	1.91	0.42
11:T:3567:ARG:NH2	11:T:3585:GLU:O	2.50	0.42
4:E:45:ILE:HG23	5:F:56:LEU:HD13	2.01	0.42
8:I:411:THR:O	8:I:415:MET:HB2	2.20	0.42
8:I:418:ARG:NE	8:I:421:ARG:CZ	2.80	0.42
9:K:174:SER:OG	12:U:149:ALA:O	2.36	0.42
11:T:1263:LEU:HD23	11:T:1263:LEU:HA	1.88	0.42
11:T:1655:ILE:HG12	11:T:1662:VAL:HG23	2.00	0.42
1:B:117:TYR:O	3:D:119:LYS:NZ	2.50	0.42
11:T:118:CYS:SG	11:T:119:MET:N	2.92	0.42
11:T:483:ASP:OD1	11:T:483:ASP:N	2.51	0.42
11:T:1804:LYS:HG3	11:T:1863:GLU:HB2	2.01	0.42
11:T:1844:ASN:N	11:T:1844:ASN:OD1	2.50	0.42
11:T:1867:LEU:HA	11:T:1870:ILE:HD12	2.02	0.42
11:T:3064:ASN:HD21	11:T:3080:ASN:HD22	1.68	0.42
11:T:3172:ARG:HH22	11:T:3215:LEU:HD23	1.84	0.42
2:C:62:GLU:HG2	2:C:142:PRO:HD3	2.02	0.42
11:T:712:ARG:HD3	11:T:712:ARG:HA	1.86	0.42
11:T:1423:LEU:HD22	11:T:1440:ILE:HD11	2.02	0.42
11:T:2184:LEU:O	11:T:2188:GLN:HB2	2.19	0.42
1:B:118:ASN:OD1	1:B:118:ASN:N	2.51	0.42
3:D:593:LEU:HB3	3:D:603:ARG:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:117:LEU:HD21	7:H:364:ASP:HB3	2.02	0.42
7:H:313:ILE:HG12	8:I:436:THR:HG21	2.02	0.42
8:I:414:VAL:O	8:I:414:VAL:HG13	2.20	0.42
11:T:868:ARG:HD2	11:T:868:ARG:O	2.20	0.42
11:T:2785:ASP:OD1	11:T:2785:ASP:N	2.51	0.42
11:T:3173:THR:HA	11:T:3453:PRO:HD3	2.02	0.42
3:D:207:ASP:OD1	3:D:207:ASP:N	2.53	0.42
3:D:522:VAL:HG11	6:G:98:THR:HB	2.02	0.42
4:E:374:ARG:HH21	9:K:186:ILE:HG21	1.84	0.42
5:F:95:LEU:HD11	8:I:463:ARG:HB3	2.02	0.42
7:H:206:ARG:HD3	10:Q:371:LEU:HD12	2.01	0.42
7:H:279:ILE:HG21	8:I:458:THR:HG23	2.02	0.42
11:T:80:LEU:HD11	11:T:120:LYS:HB2	2.01	0.42
11:T:2879:ARG:HA	11:T:2879:ARG:HD2	1.90	0.42
2:C:78:LEU:HD11	2:C:233:ILE:HG23	2.01	0.41
2:C:241:ILE:HG12	2:C:337:MET:HB2	2.02	0.41
5:F:94:ARG:HE	5:F:94:ARG:HB3	1.60	0.41
7:H:309:ILE:HD13	8:I:424:VAL:HG22	2.01	0.41
11:T:1327:ASP:OD1	11:T:1328:HIS:ND1	2.53	0.41
11:T:2028:ALA:O	11:T:2031:LEU:HB2	2.19	0.41
3:D:553:SER:HB2	3:D:560:LEU:HD11	2.03	0.41
6:G:175:LYS:HA	6:G:175:LYS:HD2	1.76	0.41
9:K:734:ILE:HG22	9:K:738:LYS:HE2	2.02	0.41
1:B:301:ASP:HB3	10:Q:431:VAL:HG21	2.02	0.41
6:G:172:GLN:OE1	9:K:926:ARG:NH1	2.53	0.41
11:T:150:ASN:HA	11:T:153:ASN:HD22	1.85	0.41
11:T:2304:ALA:HA	11:T:2307:THR:HG22	2.02	0.41
11:T:2450:ARG:HD2	11:T:2479:SER:HB3	2.01	0.41
11:T:2772:ASP:OD1	11:T:2772:ASP:N	2.52	0.41
11:T:3463:SER:HA	11:T:3576:LYS:HE2	2.02	0.41
3:D:775:LYS:HB3	4:E:152:PRO:HB3	2.02	0.41
5:F:106:LYS:HD3	5:F:107:PRO:HD2	2.03	0.41
11:T:1234:GLN:HG3	11:T:1271:THR:HG21	2.02	0.41
11:T:3375:LEU:HD21	11:T:3394:ARG:HB2	2.03	0.41
1:B:397:MET:HB2	11:T:2622:LEU:HB3	2.02	0.41
5:F:107:PRO:HB2	10:Q:378:LEU:HB2	2.02	0.41
11:T:1109:HIS:HD2	11:T:2526:HIS:HE1	1.67	0.41
11:T:1861:ARG:HB3	11:T:1893:PHE:HE1	1.84	0.41
2:C:203:SER:OG	2:C:204:PHE:N	2.52	0.41
2:C:330:LEU:O	8:I:487:ASN:ND2	2.49	0.41
11:T:411:ILE:HG23	11:T:442:LEU:HD23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:T:1520:ARG:HH12	11:T:1568:MET:HG3	1.85	0.41
11:T:1704:LYS:HA	11:T:1704:LYS:HD2	1.88	0.41
11:T:1820:SER:O	11:T:1820:SER:OG	2.39	0.41
11:T:2376:LEU:HG	11:T:2394:PHE:HE1	1.85	0.41
5:F:58:ASP:OD2	6:G:201:ARG:NE	2.52	0.41
9:K:177:ILE:HA	9:K:180:VAL:HG12	2.02	0.41
11:T:632:ILE:HD13	11:T:632:ILE:HA	1.92	0.41
11:T:1424:LYS:HE2	11:T:1424:LYS:HB3	1.90	0.41
3:D:692:HIS:NE2	3:D:711:SER:OG	2.49	0.41
11:T:76:ARG:HH22	11:T:116:ILE:N	2.19	0.41
11:T:615:ASN:OD1	11:T:615:ASN:N	2.54	0.41
11:T:965:ASP:OD1	11:T:965:ASP:N	2.54	0.41
11:T:1686:LYS:HA	11:T:1686:LYS:HD3	1.82	0.41
1:B:402:THR:HG22	1:B:403:THR:HG22	2.03	0.41
2:C:49:LYS:HE3	2:C:49:LYS:HB2	1.83	0.41
3:D:71:LYS:HD3	3:D:71:LYS:HA	1.84	0.41
3:D:751:GLN:HG3	3:D:764:PRO:HD3	2.03	0.41
4:E:130:ARG:HA	9:K:970:HIS:HA	2.01	0.41
4:E:391:TYR:HE1	4:E:456:THR:HG21	1.86	0.41
8:I:380:SER:O	8:I:380:SER:OG	2.34	0.41
8:I:419:LYS:HE2	8:I:419:LYS:HB3	1.74	0.41
9:K:962:ASP:N	9:K:962:ASP:OD1	2.53	0.41
11:T:1007:TYR:C	11:T:1014:ARG:HH22	2.25	0.41
11:T:1328:HIS:O	11:T:1331:GLN:NE2	2.54	0.41
11:T:1669:MET:HG3	11:T:1695:LEU:HD21	2.02	0.41
11:T:1707:LYS:HD3	11:T:1707:LYS:HA	1.88	0.41
11:T:1833:TRP:HA	11:T:1836:LEU:HD12	2.03	0.41
11:T:2424:THR:HG22	11:T:2435:PHE:HB3	2.03	0.41
1:B:186:VAL:HG12	1:B:285:LEU:HD21	2.03	0.41
7:H:357:LYS:NZ	10:Q:382:ARG:HE	2.19	0.41
8:I:421:ARG:O	8:I:425:LYS:HB2	2.20	0.41
8:I:495:ALA:O	8:I:499:ARG:NH2	2.54	0.41
11:T:132:ILE:O	11:T:134:GLN:NE2	2.53	0.41
11:T:1712:TYR:HB3	11:T:1715:HIS:NE2	2.35	0.41
11:T:2756:THR:HG21	11:T:2783:VAL:HG21	2.02	0.41
2:C:316:ASP:HB3	2:C:319:HIS:HD2	1.86	0.40
7:H:229:ASN:HA	7:H:230:PRO:HD3	1.95	0.40
9:K:1032:ASN:OD1	9:K:1032:ASN:N	2.54	0.40
11:T:28:LEU:H	11:T:28:LEU:HD23	1.86	0.40
11:T:572:LEU:HD12	11:T:572:LEU:HA	1.98	0.40
11:T:908:LEU:HB3	11:T:913:PHE:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:T:993:VAL:HG11	11:T:1027:LEU:HD12	2.02	0.40
11:T:1193:LEU:O	11:T:1196:GLN:HB2	2.21	0.40
11:T:1743:LEU:HD22	11:T:1765:PHE:HE2	1.85	0.40
11:T:2644:GLN:HE22	11:T:2659:GLU:HG2	1.86	0.40
1:B:135:HIS:CD2	1:B:135:HIS:H	2.38	0.40
11:T:402:ILE:HG13	11:T:403:ARG:H	1.85	0.40
11:T:2568:TYR:CE1	11:T:2616:LEU:HD23	2.56	0.40
11:T:3432:LYS:HA	11:T:3432:LYS:HD3	1.95	0.40
1:B:485:ARG:NH1	11:T:2708:GLU:OE2	2.51	0.40
2:C:154:LEU:O	6:G:147:GLN:NE2	2.55	0.40
3:D:226:ASP:HA	3:D:229:LYS:HE2	2.03	0.40
4:E:64:LEU:H	5:F:48:TYR:HA	1.86	0.40
4:E:101:THR:N	4:E:107:VAL:O	2.55	0.40
11:T:1677:VAL:HG23	11:T:1683:GLU:HA	2.03	0.40
11:T:1716:LEU:HD23	11:T:1716:LEU:HA	1.95	0.40
11:T:1742:PRO:HA	11:T:1745:LEU:HB2	2.03	0.40
11:T:2011:MET:HB3	11:T:2031:LEU:HD12	2.03	0.40
11:T:2120:ALA:HA	11:T:2123:ILE:HG22	2.03	0.40
11:T:3607:LEU:HD12	11:T:3607:LEU:HA	1.95	0.40
2:C:334:PRO:HG3	8:I:489:ARG:HD3	2.04	0.40
3:D:657:ILE:HD11	3:D:666:LEU:HD21	2.03	0.40
11:T:453:ASN:OD1	11:T:453:ASN:N	2.54	0.40
11:T:3351:ASP:HB3	11:T:3370:LYS:HG2	2.04	0.40
1:B:315:SER:HB2	3:D:646:LEU:HD23	2.03	0.40
3:D:507:LEU:HD13	3:D:507:LEU:HA	1.96	0.40
4:E:10:ILE:HG22	7:H:201:LYS:HE3	2.04	0.40
10:Q:399:SER:OG	10:Q:400:VAL:N	2.55	0.40
11:T:253:ILE:HD12	11:T:253:ILE:HA	1.93	0.40
11:T:367:LEU:HD23	11:T:367:LEU:HA	1.90	0.40
11:T:510:ASN:HD21	11:T:2210:LEU:HD13	1.86	0.40
11:T:2806:SER:O	11:T:2806:SER:OG	2.35	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	214/604 (35%)	202 (94%)	12 (6%)	0	100 100
2	C	206/337 (61%)	199 (97%)	7 (3%)	0	100 100
3	D	558/798 (70%)	515 (92%)	42 (8%)	1 (0%)	47 79
4	E	425/516 (82%)	393 (92%)	31 (7%)	1 (0%)	47 79
5	F	107/157 (68%)	104 (97%)	3 (3%)	0	100 100
6	G	138/206 (67%)	127 (92%)	11 (8%)	0	100 100
7	H	221/488 (45%)	204 (92%)	17 (8%)	0	100 100
8	I	171/539 (32%)	157 (92%)	14 (8%)	0	100 100
9	K	271/1332 (20%)	253 (93%)	18 (7%)	0	100 100
10	Q	82/657 (12%)	75 (92%)	7 (8%)	0	100 100
11	T	3489/3744 (93%)	3209 (92%)	278 (8%)	2 (0%)	51 84
12	U	77/155 (50%)	73 (95%)	4 (5%)	0	100 100
All	All	5959/9533 (62%)	5511 (92%)	444 (8%)	4 (0%)	54 84

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	T	851	LEU
3	D	505	ILE
11	T	852	PRO
4	E	13	PRO

5.3.2 Protein sidechains (i)

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	B	212/536 (40%)	211 (100%)	1 (0%)	88 93
2	C	198/302 (66%)	196 (99%)	2 (1%)	76 86
3	D	501/701 (72%)	494 (99%)	7 (1%)	67 81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	E	391/464 (84%)	390 (100%)	1 (0%)	92 95
5	F	95/131 (72%)	95 (100%)	0	100 100
6	G	122/177 (69%)	121 (99%)	1 (1%)	81 89
7	H	206/434 (48%)	206 (100%)	0	100 100
8	I	150/483 (31%)	142 (95%)	8 (5%)	22 52
9	K	257/1225 (21%)	257 (100%)	0	100 100
10	Q	77/579 (13%)	77 (100%)	0	100 100
11	T	3238/3452 (94%)	3201 (99%)	37 (1%)	73 84
All	All	5447/8484 (64%)	5390 (99%)	57 (1%)	77 86

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	397	MET
2	C	8	ARG
2	C	207	ARG
3	D	95	SER
3	D	505	ILE
3	D	512	LYS
3	D	555	ASP
3	D	715	ASP
3	D	759	ARG
3	D	775	LYS
4	E	323	LYS
6	G	130	GLU
8	I	382	ARG
8	I	389	SER
8	I	413	ARG
8	I	414	VAL
8	I	415	MET
8	I	416	SER
8	I	417	LYS
8	I	418	ARG
11	T	13	ARG
11	T	15	ARG
11	T	16	ASP
11	T	119	MET
11	T	291	TYR
11	T	295	ILE

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Mol	Chain	Res	Type
11	T	296	LEU
11	T	300	LYS
11	T	311	ARG
11	T	576	THR
11	T	850	ARG
11	T	855	ARG
11	T	868	ARG
11	T	870	SER
11	T	907	ASN
11	T	908	LEU
11	T	909	THR
11	T	964	THR
11	T	1005	GLN
11	T	1006	SER
11	T	1007	TYR
11	T	1008	LYS
11	T	1011	ILE
11	T	1021	LEU
11	T	1585	ARG
11	T	1775	ASN
11	T	1804	LYS
11	T	1830	LYS
11	T	1849	LEU
11	T	1851	TYR
11	T	1852	ASP
11	T	1853	VAL
11	T	2181	MET
11	T	2272	VAL
11	T	2276	THR
11	T	3307	TYR
11	T	3595	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (86) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	336	HIS
2	C	13	GLN
2	C	227	HIS
2	C	319	HIS
3	D	274	ASN
3	D	275	GLN
3	D	463	GLN

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Mol	Chain	Res	Type
3	D	486	GLN
3	D	537	ASN
4	E	127	GLN
4	E	228	ASN
5	F	51	GLN
6	G	118	GLN
7	H	219	ASN
7	H	240	ASN
7	H	303	GLN
7	H	307	ASN
7	H	352	GLN
7	H	373	ASN
8	I	412	GLN
8	I	505	ASN
9	K	163	GLN
9	K	888	ASN
10	Q	435	GLN
11	T	45	HIS
11	T	49	GLN
11	T	77	ASN
11	T	84	ASN
11	T	93	GLN
11	T	134	GLN
11	T	150	ASN
11	T	153	ASN
11	T	400	HIS
11	T	441	ASN
11	T	510	ASN
11	T	565	ASN
11	T	639	HIS
11	T	794	ASN
11	T	840	GLN
11	T	843	ASN
11	T	853	HIS
11	T	896	GLN
11	T	1105	ASN
11	T	1109	HIS
11	T	1116	ASN
11	T	1234	GLN
11	T	1298	ASN
11	T	1479	GLN
11	T	1587	GLN

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Mol	Chain	Res	Type
11	T	1619	GLN
11	T	1626	ASN
11	T	1629	GLN
11	T	1654	ASN
11	T	1659	GLN
11	T	1781	ASN
11	T	1856	HIS
11	T	1857	HIS
11	T	1892	ASN
11	T	1968	ASN
11	T	2203	GLN
11	T	2266	ASN
11	T	2289	HIS
11	T	2354	ASN
11	T	2441	ASN
11	T	2470	ASN
11	T	2521	ASN
11	T	2551	GLN
11	T	2668	ASN
11	T	2770	ASN
11	T	2792	GLN
11	T	2822	GLN
11	T	2906	GLN
11	T	2910	GLN
11	T	2952	HIS
11	T	3040	ASN
11	T	3064	ASN
11	T	3250	ASN
11	T	3259	ASN
11	T	3261	ASN
11	T	3340	HIS
11	T	3357	GLN
11	T	3421	GLN
11	T	3442	GLN
11	T	3472	ASN
11	T	3486	GLN
11	T	3537	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
12	U	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	U	29:ALA	C	101:ALA	N	57.64
1	U	9:ALA	C	11:ALA	N	3.53

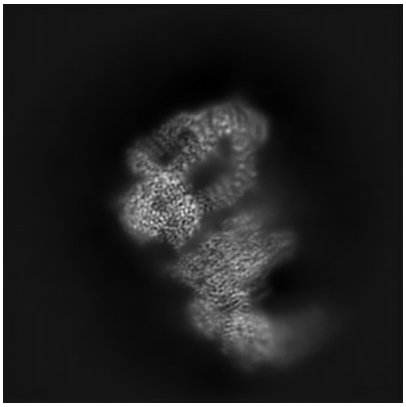
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-10412. These allow visual inspection of the internal detail of the map and identification of artifacts.

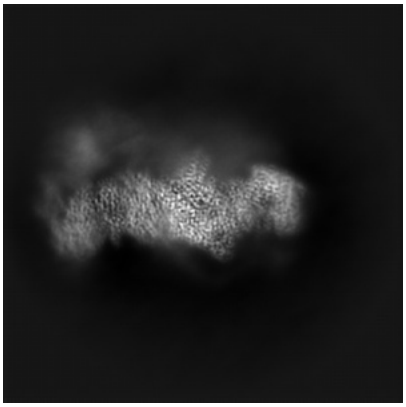
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

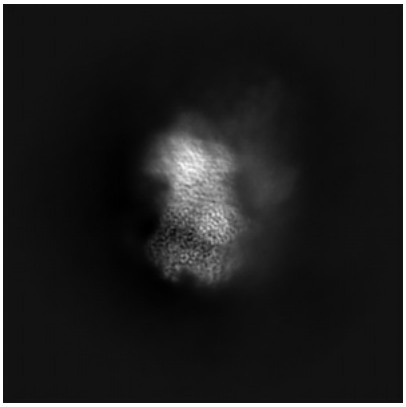
6.1.1 Primary map



X



Y

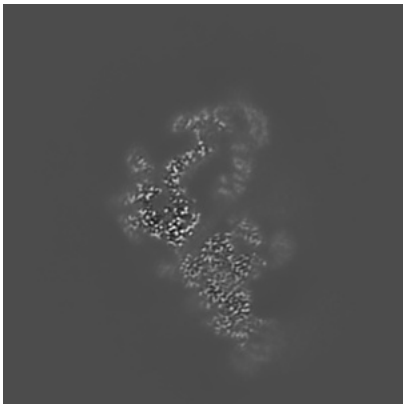


Z

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

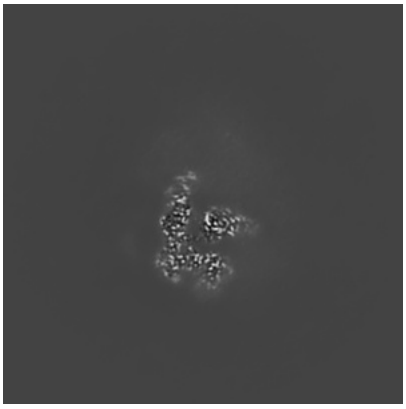
6.2 Central slices

6.2.1 Primary map



X Index: 200

Y Index: 200

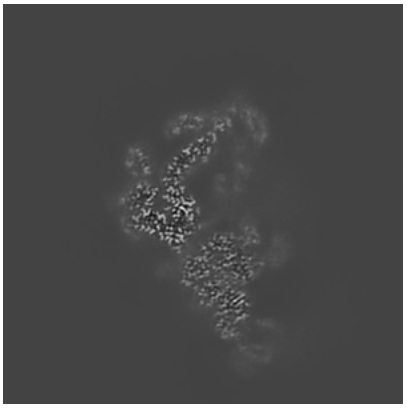


Z Index: 200

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

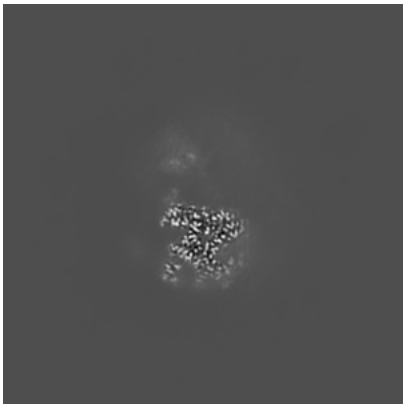
6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 204

Y Index: 178



Z Index: 188

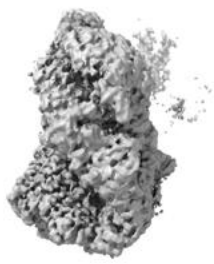
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X

Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

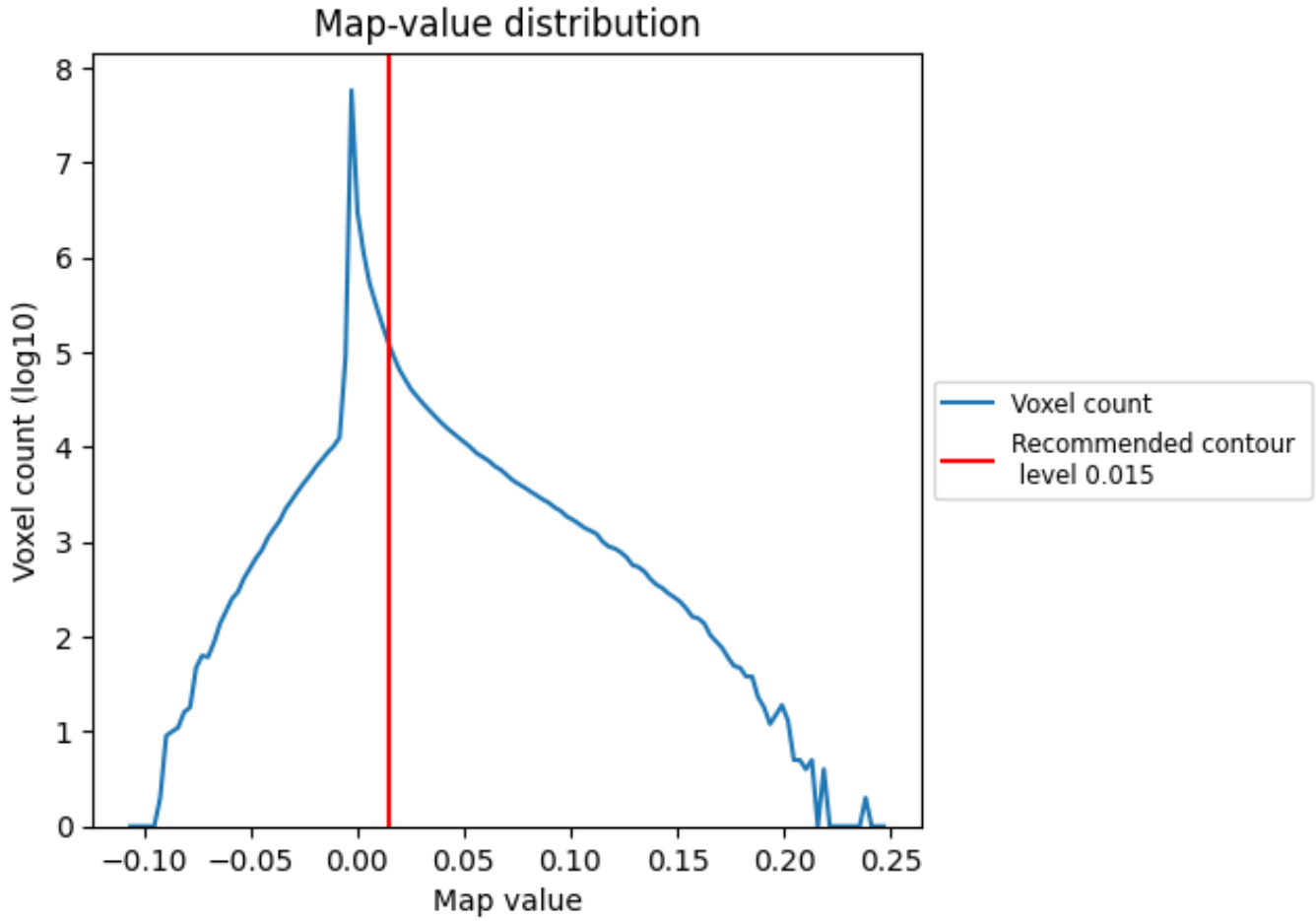
6.5 Mask visualisation (i)

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

7 Map analysis

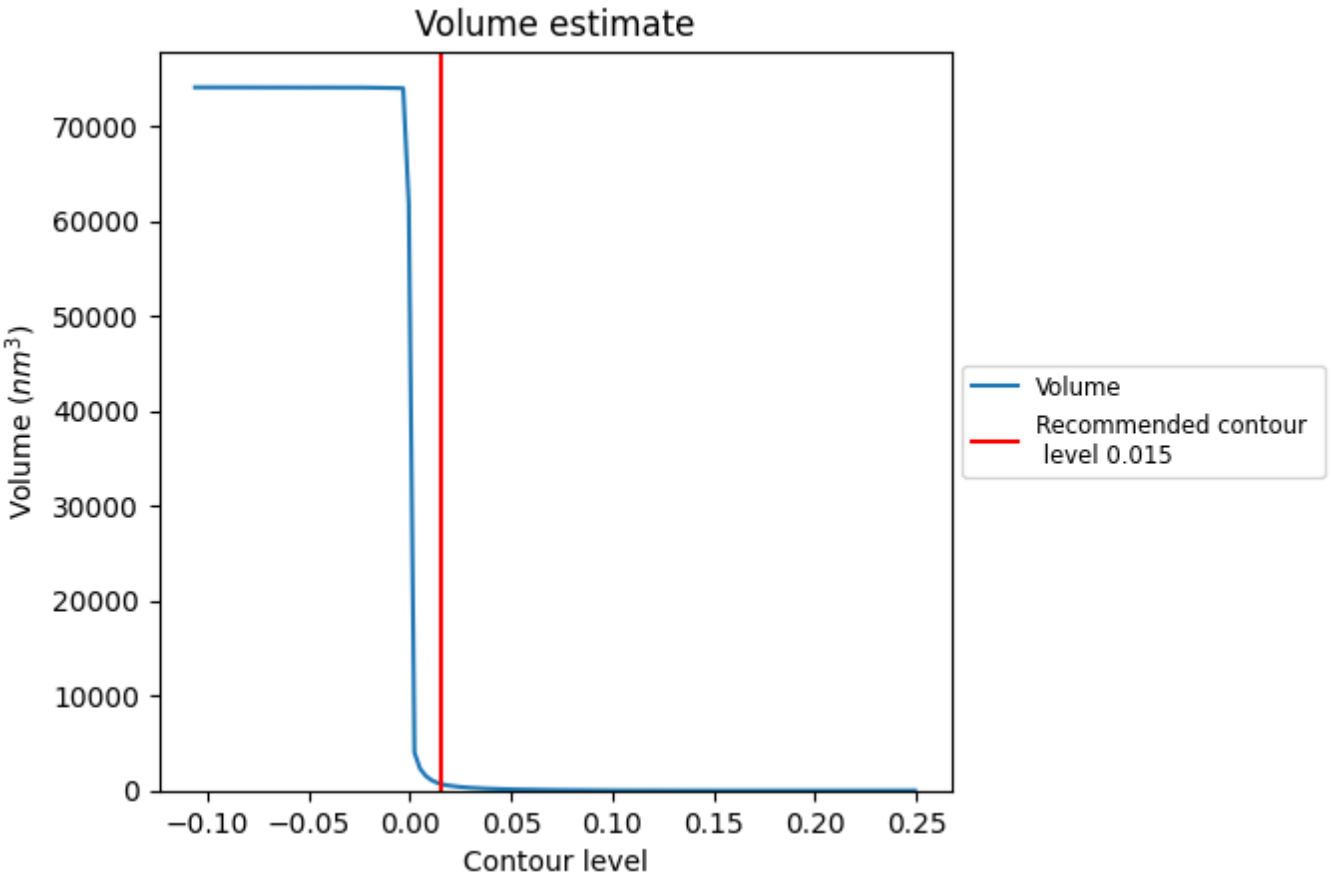
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

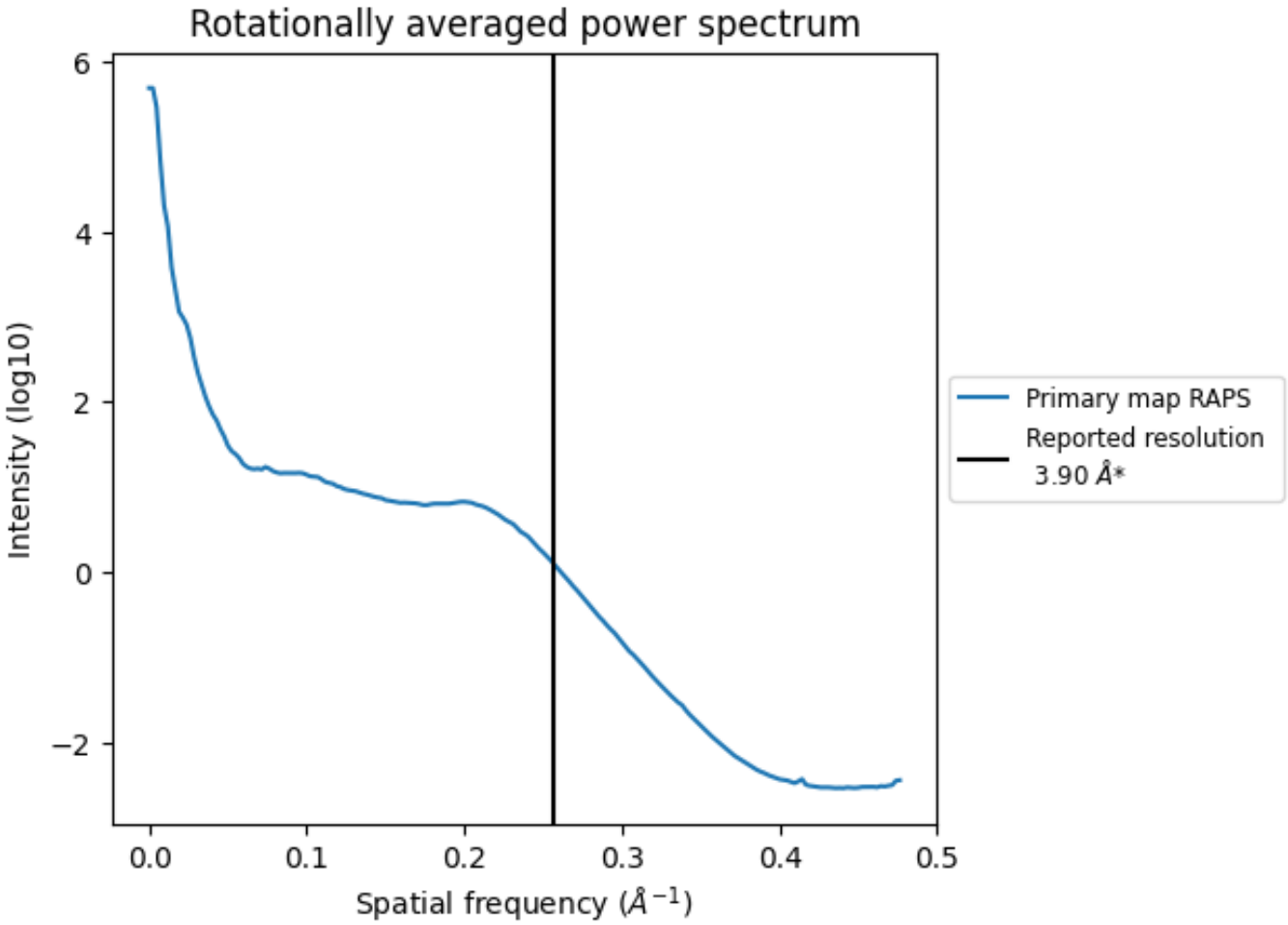
7.2 Volume estimate



The volume at the recommended contour level is 724 nm^3; this corresponds to an approximate mass of 654 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)

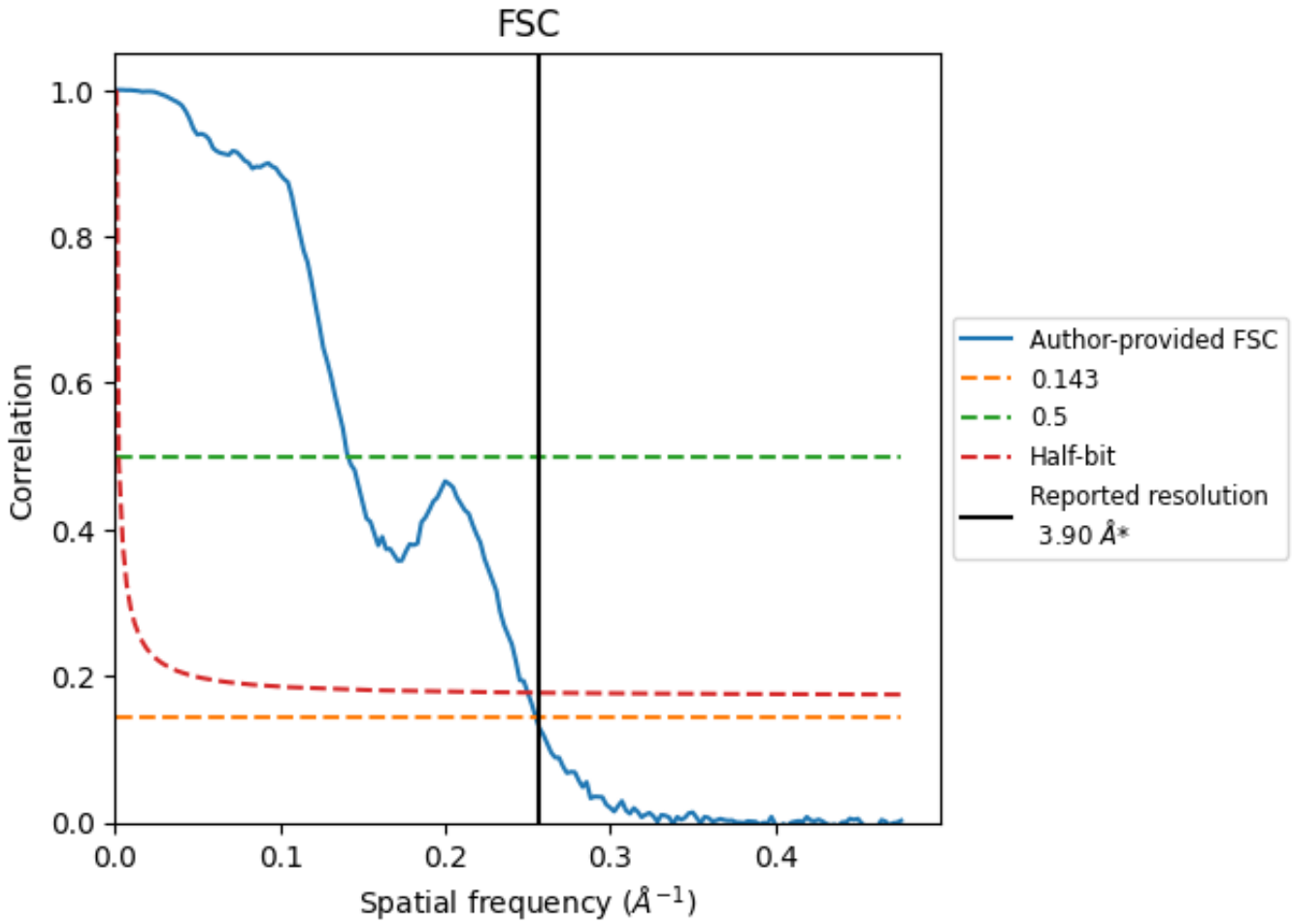


*Reported resolution corresponds to spatial frequency of 0.256 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.256 Å^{-1}

8.2 Resolution estimates (i)

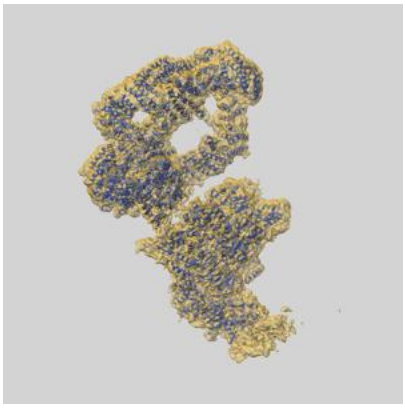
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	3.92	7.08	4.00
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

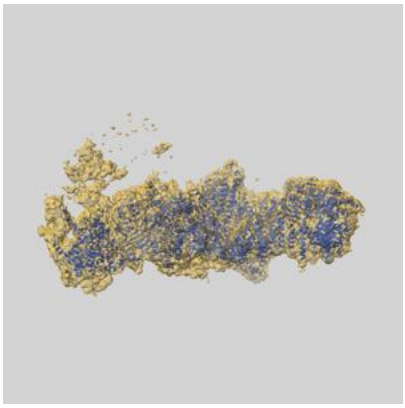
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-10412 and PDB model 6T9I. Per-residue inclusion information can be found in section 3 on page 6.

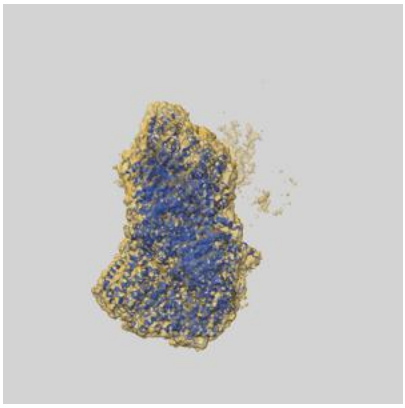
9.1 Map-model overlay



X



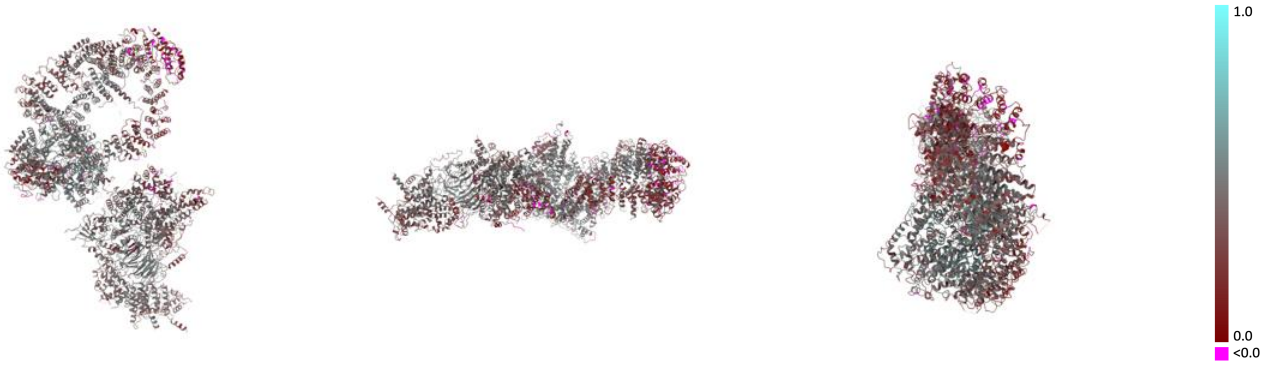
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.015 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.

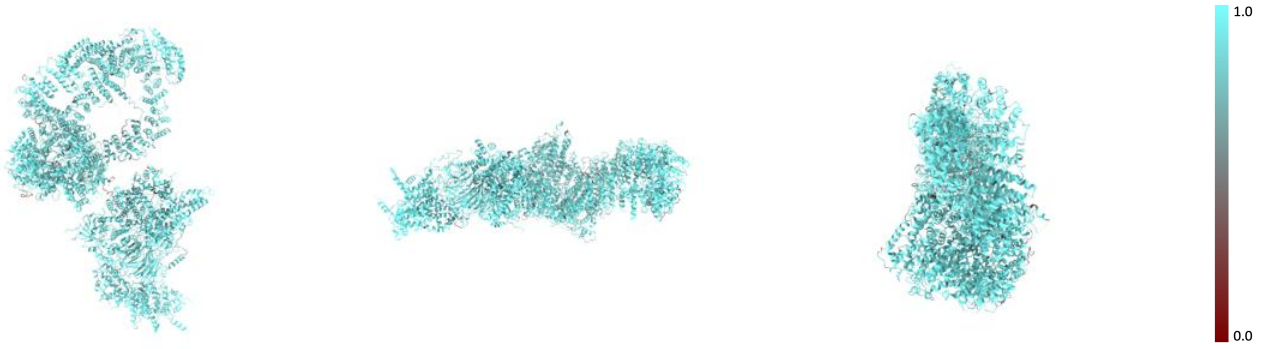
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

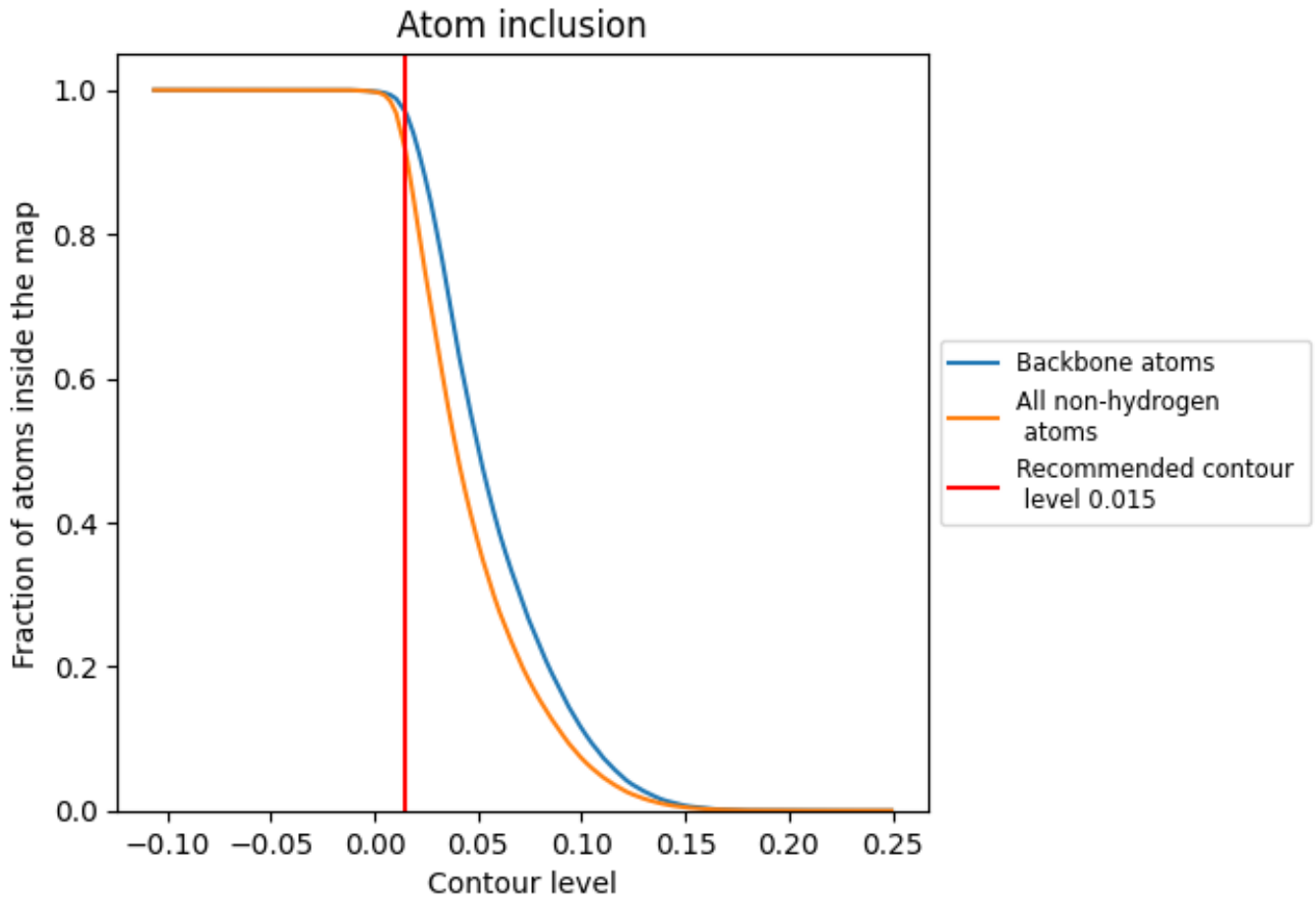
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.015).

9.4 Atom inclusion (i)



At the recommended contour level, 97% of all backbone atoms, 92% 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	0.9163	0.3800
B	0.9144	0.4350
C	0.8818	0.2750
D	0.9251	0.4160
E	0.9227	0.3980
F	0.9261	0.4540
G	0.9613	0.3520
H	0.9084	0.4100
I	0.8766	0.4240
K	0.9343	0.3490
Q	0.9479	0.4250
T	0.9134	0.3710
U	0.9976	0.3980