



Full wwPDB EM Validation Report ⓘ

Mar 28, 2026 – 02:15 PM UTC

PDB ID : 6T9I / pdb_00006t9i
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.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

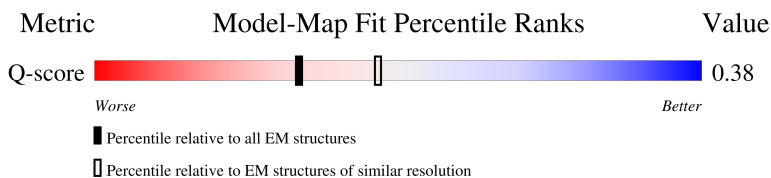
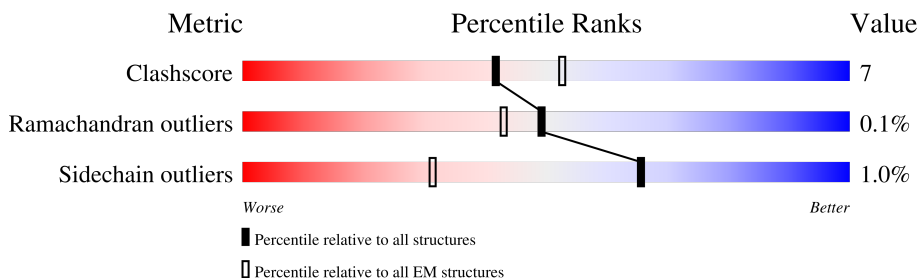
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	8855 (3.40 - 4.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	B	604	
2	C	337	
3	D	798	
4	E	516	

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Mol	Chain	Length	Quality of chain
5	F	157	
6	G	206	
7	H	488	
8	I	539	
9	K	1332	
10	Q	657	
11	T	3744	
12	U	155	

2 Entry composition

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
1	B	224	Total	C	N	O	S	0	0
			1891	1207	318	358	8		

- Molecule 2 is a protein called Protein SPT3.

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

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

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

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

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

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

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

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

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

- 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.

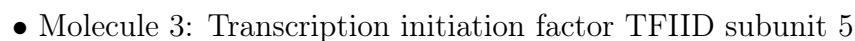
Mol	Chain	Residues	Atoms					AltConf	Trace
10	Q	84	Total	C	N	O	S	0	0
			675	426	119	127	3		

- 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		

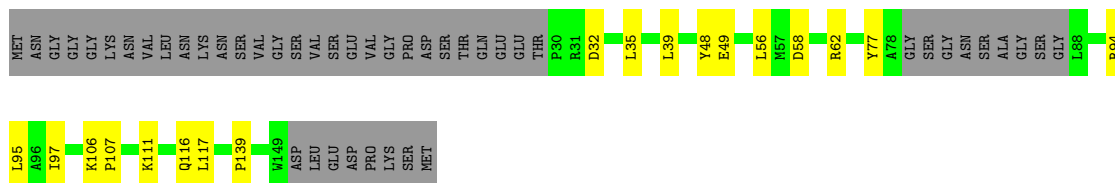
- Molecule 12 is a protein called unassigned sequence.

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



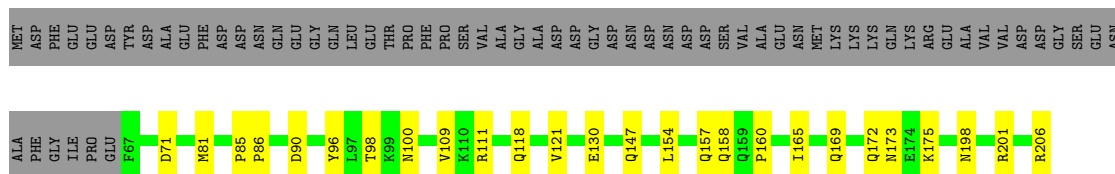
- Molecule 5: Transcription initiation factor TFIID subunit 9

Chain F:



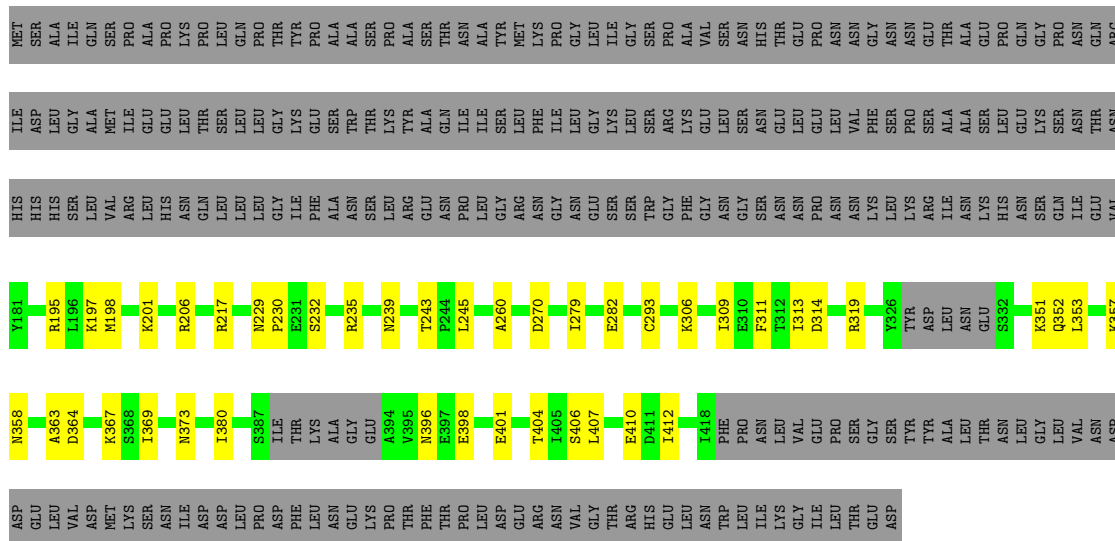
- Molecule 6: Transcription initiation factor TFIID subunit 10

Chain G:



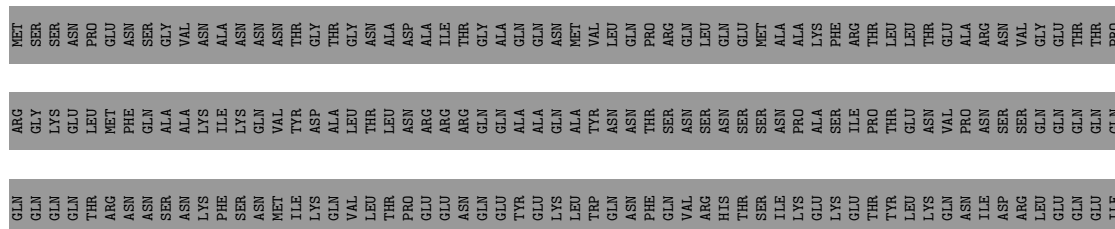
- Molecule 7: Transcriptional coactivator HFI1/ADA1

Chain H:



- Molecule 8: Transcription initiation factor TFIID subunit 12

Chain I:









4 Experimental information

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 ($e^-/\text{\AA}^2$)	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

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	B	0.21	0/1931	0.51	0/2607
2	C	0.20	0/1810	0.51	0/2435
3	D	0.24	0/4582	0.57	3/6211 (0.0%)
4	E	0.22	0/3504	0.55	0/4759
5	F	0.24	0/922	0.57	0/1249
6	G	0.21	0/1123	0.50	0/1518
7	H	0.24	0/1826	0.61	2/2456 (0.1%)
8	I	0.28	0/1373	0.61	0/1863
9	K	0.20	0/2288	0.52	0/3080
10	Q	0.22	0/692	0.52	0/937
11	T	0.33	0/29358	0.59	2/39779 (0.0%)
12	U	0.13	0/412	0.43	0/572
All	All	0.29	0/49821	0.57	7/67466 (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 (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	T	871	VAL	N-CA-C	-6.31	99.34	108.36
11	T	62	VAL	CA-CB-CG1	5.85	120.34	110.40
7	H	239	ASN	CA-C-N	5.82	131.69	122.61
7	H	239	ASN	C-N-CA	5.82	131.69	122.61
3	D	775	LYS	CA-CB-CG	5.51	125.12	114.10
3	D	476	ASP	CA-C-N	5.16	135.21	125.66
3	D	476	ASP	C-N-CA	5.16	135.21	125.66

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 ⓘ

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	25	0
3	D	4474	0	4377	61	0
4	E	3441	0	3493	51	0
5	F	902	0	919	23	0
6	G	1108	0	1110	20	0
7	H	1803	0	1800	38	0
8	I	1351	0	1351	76	0
9	K	2258	0	2308	29	0
10	Q	675	0	666	17	0
11	T	28729	0	29144	383	0
12	U	415	0	415	3	0
All	All	48821	0	49213	667	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 (667) 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
11:T:850:ARG:C	11:T:852:PRO:HD3	1.57	1.27
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
8:I:415:MET:HE3	8:I:415:MET:HA	1.43	1.01
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
11:T:850:ARG:C	11:T:852:PRO:CD	2.39	0.96
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:851:LEU:HG	11:T:1156:TYR:OH	1.69	0.90
8:I:418:ARG:HG3	8:I:421:ARG:CD	2.06	0.86
11:T:850:ARG:HB2	11:T:854:GLU:CD	2.00	0.85
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
8:I:415:MET:HA	8:I:415:MET:CE	2.04	0.80
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
8:I:415:MET:HE3	8:I:415:MET:CA	2.18	0.72
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
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:845:MET:HE2	11:T:1205:THR:HA	1.77	0.66
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
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:2469:LEU:HD12	11:T:2605:MET:HE2	1.85	0.58
11:T:2422:VAL:HA	11:T:2463:ILE:HD11	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:400:ARG:HA	8:I:381:ASN:HB3	1.85	0.58
2:C:15:MET:HE2	2:C:32:ILE:HD12	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
11:T:3028:MET:HE2	11:T:3059:GLN:HG3	1.86	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
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
8:I:415:MET:HE3	8:I:416:SER:H	1.71	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:D:555:ASP:OD1	3:D:555:ASP:N	2.39	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
7:H:406:SER:OG	7:H:407:LEU:N	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:363:ALA:O	7:H:367:LYS:NZ	2.40	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
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
11:T:465:MET:HE2	11:T:630:GLU:HB3	1.91	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
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
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:OD1	11:T:1852:ASP:N	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:3319:ARG:HH22	11:T:3476:LYS:HZ2	1.57	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: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:1775:ASN:N	11:T:1775:ASN:OD1	2.42	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:3597:LYS:HG2	11:T:3599:LEU:H	1.77	0.49
10:Q:373:LEU:O	10:Q:427:TYR:OH	2.29	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
3:D:640:THR:OG1	3:D:642:ASP:OD1	2.30	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
5:F:35:LEU:HD21	7:H:198:MET:HE1	1.94	0.48
11:T:1774:SER:O	11:T:1774:SER:OG	2.30	0.48
2:C:241:ILE:HG12	2:C:337:MET:HE2	1.95	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: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:850:ARG:O	11:T:852:PRO:HD3	2.05	0.47
11:T:1818:SER:OG	11:T:1819:GLY:N	2.43	0.47
11:T:2217:ILE:HD11	11:T:2266:ASN:HD22	1.80	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
11:T:3304:LYS:O	11:T:3309:THR:OG1	2.31	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
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:216:SER:HB3	11:T:218:MET:HE2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1098:ASP:N	11:T:1098:ASP:OD1	2.47	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
11:T:434:MET:HE3	11:T:434:MET:HB3	1.80	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
8:I:415:MET:HE3	8:I:416:SER:N	2.31	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:1139:MET:HE1	11:T:2500:LEU:HD21	1.97	0.46
11:T:2169:TYR:HA	11:T:2172:PHE:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:607:GLY:HA2	5:F:111:LYS:HE3	1.98	0.46
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:2571:ILE:O	11:T:2576:LYS:NZ	2.43	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
5:F:77:TYR:OH	8:I:477:ASP:OD1	2.31	0.45
11:T:1007:TYR:C	11:T:1014:ARG:HH22	2.25	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
11:T:1244:VAL:O	11:T:1248:THR:OG1	2.28	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:217:SER:O	11:T:217:SER:OG	2.36	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
11:T:850:ARG:CA	11:T:852:PRO:HD3	2.42	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
1:B:117:TYR:O	3:D:119:LYS:NZ	2.50	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
11:T:3306:ASP:OD1	11:T:3309:THR:OG1	2.35	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: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
11:T:928:LEU:HD22	11:T:945:VAL:HG13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:2294:GLN:HG2	11:T:2295:PRO:HD3	1.99	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:1038:ASN:OD1	11:T:1038:ASN:N	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
11:T:3609:PRO:HG3	11:T:3691:MET:HE2	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
11:T:2181:MET:HE3	11:T:2181:MET:HB3	1.86	0.42
11:T:3566:ASN:OD1	11:T:3566:ASN:N	2.50	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
8:I:394:SER:O	8:I:394:SER:OG	2.31	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
3:D:715:ASP:OD1	3:D:715:ASP:N	2.42	0.42
11:T:712:ARG:HD3	11:T:712:ARG:HA	1.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
3:D:628:SER:OG	3:D:630:ASP:OD1	2.31	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
11:T:1389:ASP:OD1	11:T:1389:ASP:N	2.51	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1137:ASN:OD1	11:T:1137:ASN:N	2.50	0.41
11:T:1861:ARG:HB3	11:T:1893:PHE:HE1	1.84	0.41
11:T:2762:CYS:SG	11:T:2904:TRP:NE1	2.93	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
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
10:Q:390:MET:HB2	10:Q:390:MET:HE2	1.85	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:1328:HIS:O	11:T:1331:GLN:NE2	2.54	0.41
11:T:1628:VAL:HG11	11:T:1676:MET:HE1	2.03	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
11:T:3685:ASN:OD1	11:T:3685:ASN:N	2.51	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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:1581:GLU:OE2	11:T:1590:SER:OG	2.32	0.40
11:T:1651:TYR:HD2	11:T:1669:MET:HE2	1.86	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
9:K:1032:ASN:OD1	9:K:1032:ASN:N	2.54	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
9:K:992:MET:HE3	9:K:992:MET:HB2	1.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	43	74
4	E	425/516 (82%)	393 (92%)	31 (7%)	1 (0%)	43	74
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%)	48	80
12	U	77/155 (50%)	73 (95%)	4 (5%)	0	100	100
All	All	5959/9533 (62%)	5511 (92%)	444 (8%)	4 (0%)	49	80

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	T	851	LEU

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

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	B	212/536 (40%)	210 (99%)	2 (1%)	70	75
2	C	198/302 (66%)	198 (100%)	0	100	100
3	D	501/701 (72%)	497 (99%)	4 (1%)	73	77
4	E	391/464 (84%)	389 (100%)	2 (0%)	81	82
5	F	95/131 (72%)	95 (100%)	0	100	100
6	G	122/177 (69%)	120 (98%)	2 (2%)	55	69
7	H	206/434 (48%)	205 (100%)	1 (0%)	81	82
8	I	150/483 (31%)	142 (95%)	8 (5%)	20	46
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%)	3204 (99%)	34 (1%)	65	74
All	All	5447/8484 (64%)	5394 (99%)	53 (1%)	65	75

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	397	MET
1	B	404	ILE
3	D	95	SER
3	D	167	LEU
3	D	505	ILE
3	D	715	ASP
4	E	128	VAL
4	E	148	ILE

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Mol	Chain	Res	Type
6	G	130	GLU
6	G	165	ILE
7	H	353	LEU
8	I	382	ARG
8	I	385	ILE
8	I	413	ARG
8	I	414	VAL
8	I	415	MET
8	I	416	SER
8	I	417	LYS
8	I	437	VAL
11	T	16	ASP
11	T	106	VAL
11	T	291	TYR
11	T	295	ILE
11	T	296	LEU
11	T	299	ILE
11	T	300	LYS
11	T	576	THR
11	T	765	LEU
11	T	855	ARG
11	T	868	ARG
11	T	870	SER
11	T	871	VAL
11	T	907	ASN
11	T	908	LEU
11	T	909	THR
11	T	964	THR
11	T	997	ILE
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	1157	ILE
11	T	1775	ASN
11	T	1848	ILE
11	T	1849	LEU
11	T	1851	TYR
11	T	1852	ASP
11	T	1853	VAL

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Mol	Chain	Res	Type
11	T	2272	VAL
11	T	2276	THR
11	T	3307	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (134) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	145	ASN
1	B	218	HIS
1	B	311	GLN
1	B	336	HIS
2	C	13	GLN
2	C	46	GLN
2	C	227	HIS
2	C	319	HIS
3	D	113	ASN
3	D	161	ASN
3	D	274	ASN
3	D	275	GLN
3	D	463	GLN
3	D	537	ASN
3	D	598	HIS
4	E	51	GLN
4	E	127	GLN
4	E	145	GLN
4	E	199	HIS
4	E	228	ASN
4	E	249	GLN
4	E	275	GLN
4	E	337	HIS
5	F	51	GLN
5	F	128	GLN
6	G	118	GLN
6	G	142	ASN
6	G	144	ASN
6	G	147	GLN
6	G	157	GLN
6	G	168	GLN
6	G	169	GLN
7	H	219	ASN
7	H	303	GLN
7	H	307	ASN

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Mol	Chain	Res	Type
7	H	352	GLN
7	H	373	ASN
8	I	412	GLN
8	I	485	ASN
8	I	505	ASN
8	I	511	ASN
9	K	163	GLN
9	K	888	ASN
9	K	984	HIS
9	K	986	ASN
10	Q	435	GLN
11	T	45	HIS
11	T	57	ASN
11	T	73	GLN
11	T	77	ASN
11	T	84	ASN
11	T	93	GLN
11	T	114	ASN
11	T	134	GLN
11	T	150	ASN
11	T	153	ASN
11	T	157	GLN
11	T	258	ASN
11	T	400	HIS
11	T	441	ASN
11	T	510	ASN
11	T	565	ASN
11	T	639	HIS
11	T	695	ASN
11	T	760	ASN
11	T	794	ASN
11	T	840	GLN
11	T	843	ASN
11	T	853	HIS
11	T	938	ASN
11	T	1105	ASN
11	T	1109	HIS
11	T	1116	ASN
11	T	1126	ASN
11	T	1234	GLN
11	T	1287	ASN
11	T	1305	ASN

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Mol	Chain	Res	Type
11	T	1365	ASN
11	T	1479	GLN
11	T	1480	ASN
11	T	1493	GLN
11	T	1587	GLN
11	T	1619	GLN
11	T	1629	GLN
11	T	1646	ASN
11	T	1654	ASN
11	T	1659	GLN
11	T	1719	ASN
11	T	1781	ASN
11	T	1892	ASN
11	T	1968	ASN
11	T	2010	HIS
11	T	2163	ASN
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	2621	HIS
11	T	2668	ASN
11	T	2770	ASN
11	T	2792	GLN
11	T	2801	GLN
11	T	2802	ASN
11	T	2811	GLN
11	T	2822	GLN
11	T	2848	GLN
11	T	2882	GLN
11	T	2906	GLN
11	T	2910	GLN
11	T	2948	ASN
11	T	2952	HIS
11	T	2957	HIS
11	T	3040	ASN
11	T	3059	GLN
11	T	3064	ASN
11	T	3203	GLN

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Mol	Chain	Res	Type
11	T	3234	ASN
11	T	3250	ASN
11	T	3259	ASN
11	T	3333	ASN
11	T	3340	HIS
11	T	3357	GLN
11	T	3361	ASN
11	T	3367	HIS
11	T	3421	GLN
11	T	3442	GLN
11	T	3472	ASN
11	T	3486	GLN
11	T	3537	GLN
11	T	3695	ASN
11	T	3710	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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

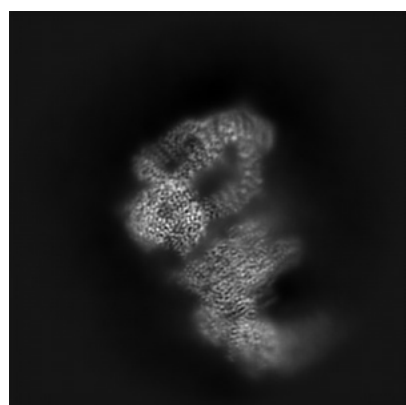
6 Map visualisation [i](#)

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.

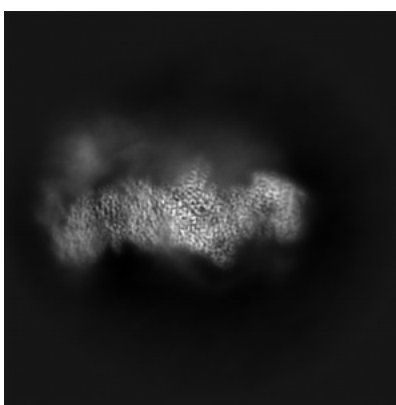
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

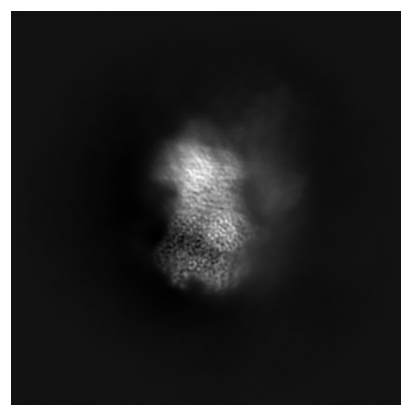
6.1.1 Primary map



X



Y

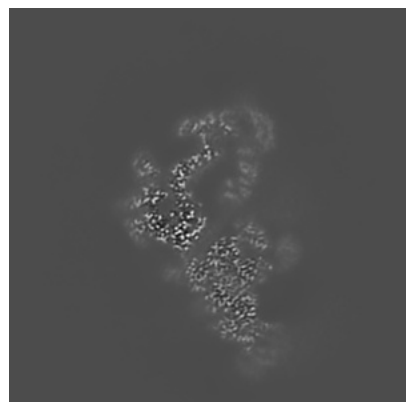


Z

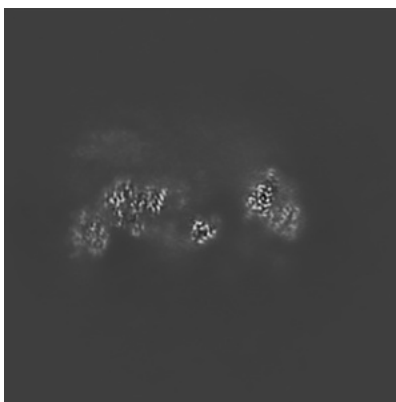
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 200



Y Index: 200

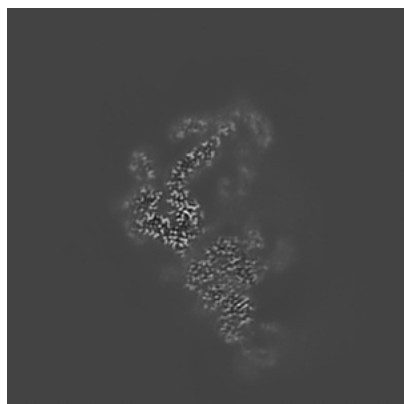


Z Index: 200

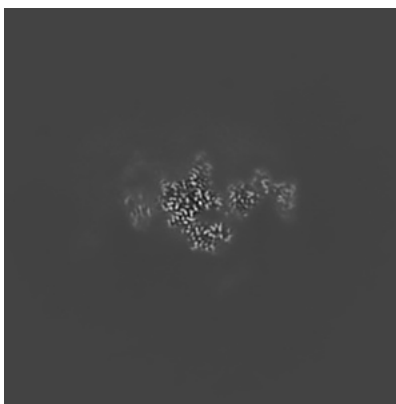
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

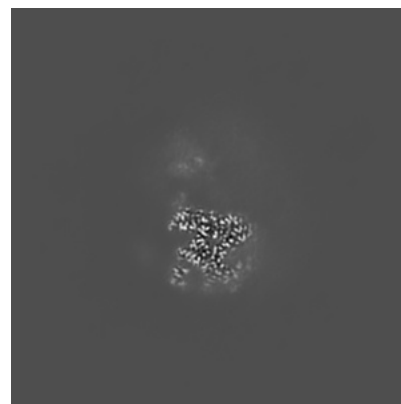
6.3.1 Primary map



X Index: 204



Y Index: 178

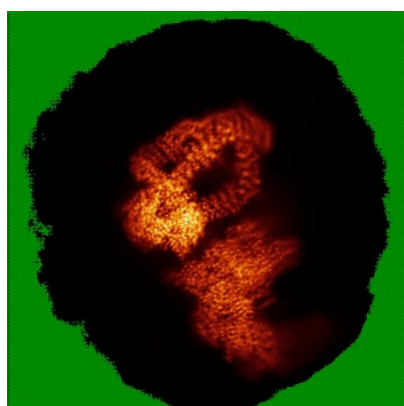


Z Index: 188

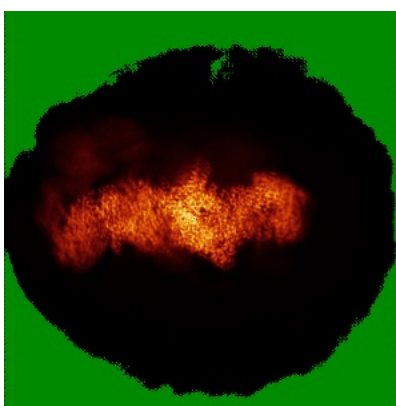
The images above show the largest variance slices of the map in three orthogonal directions.

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

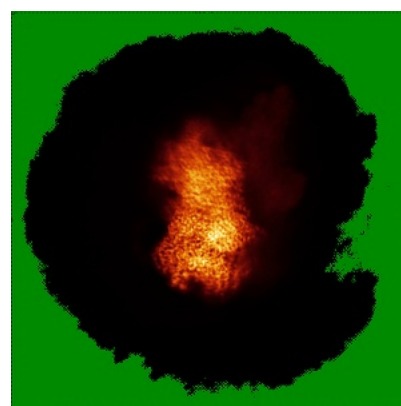
6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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

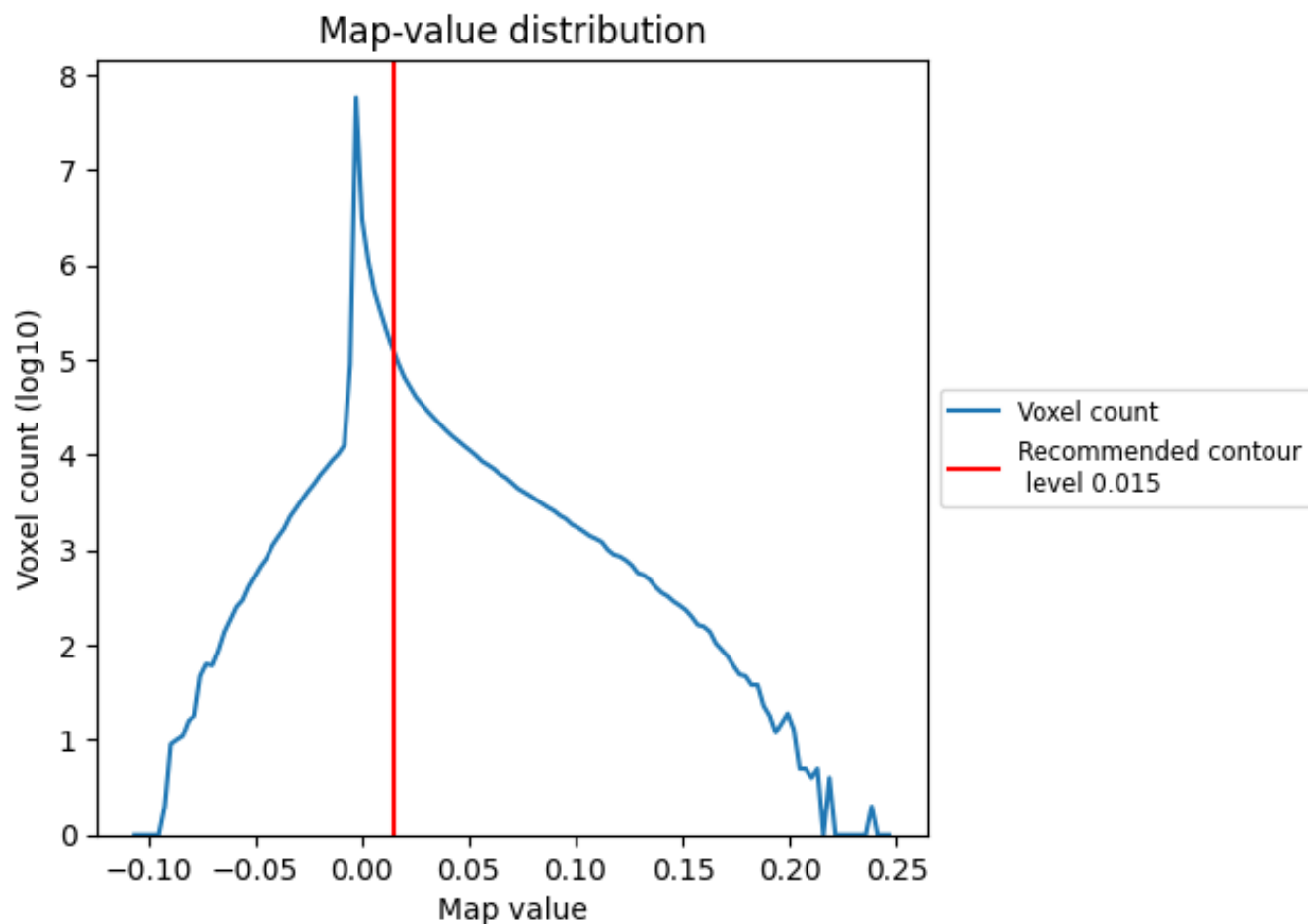
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

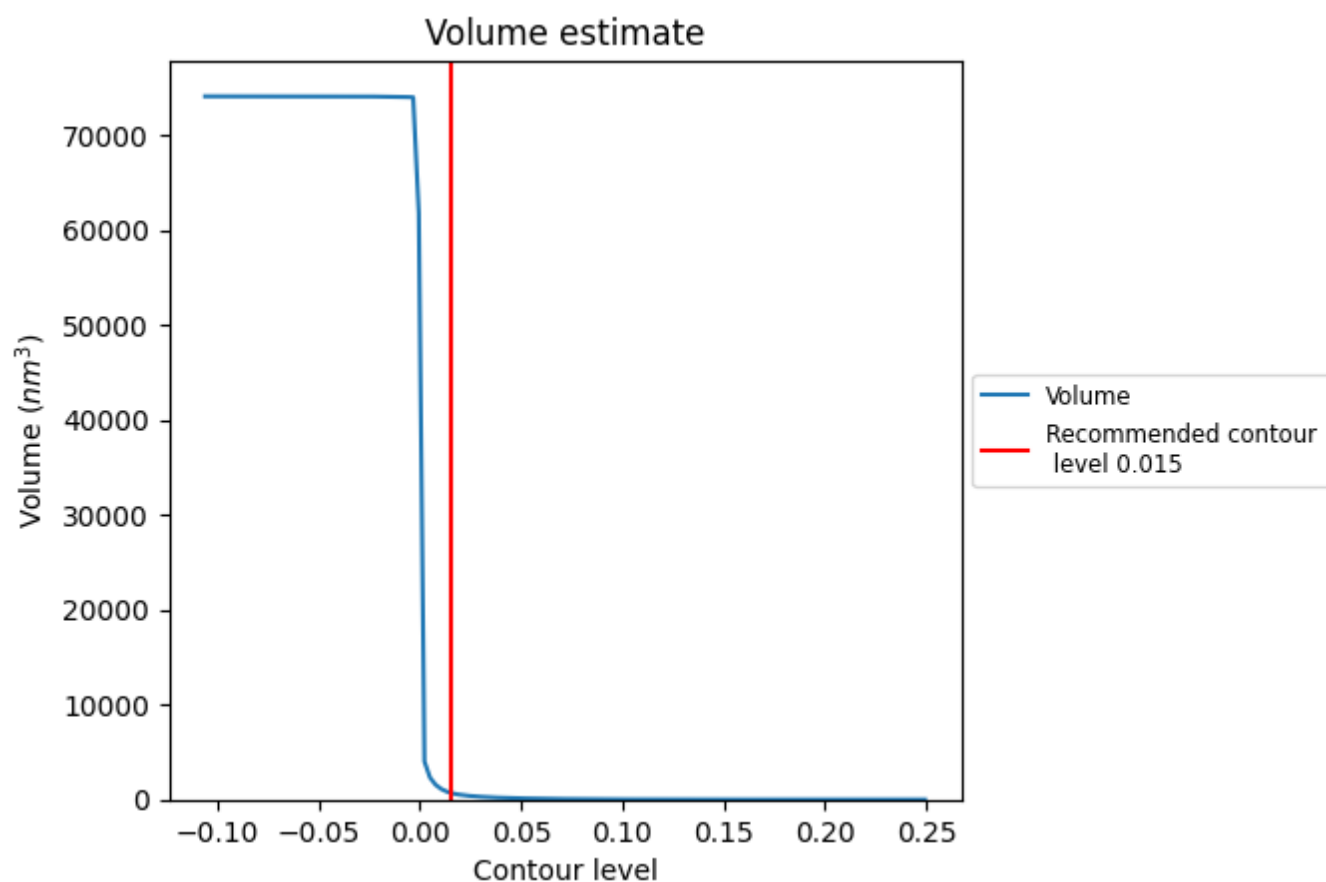
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

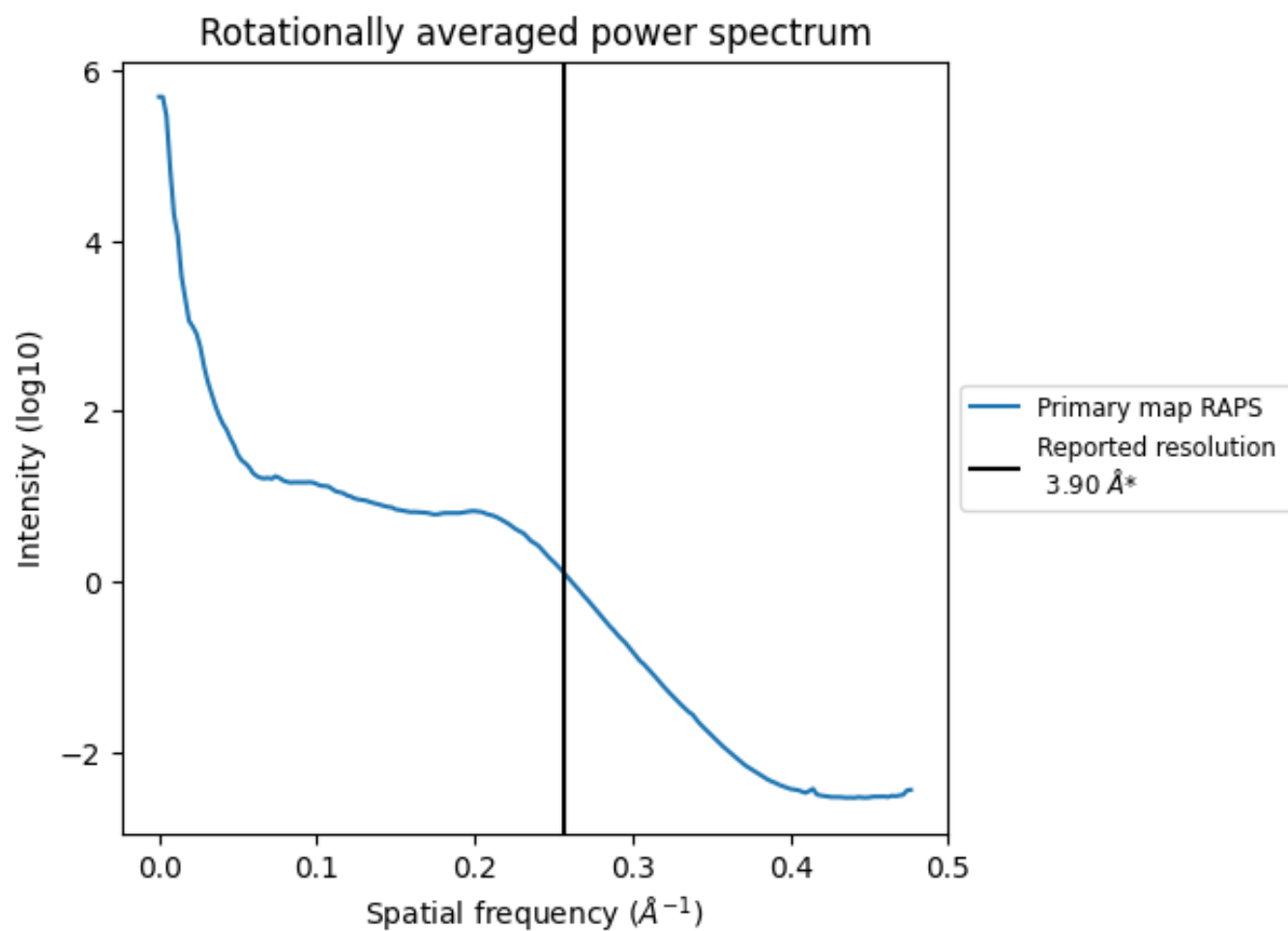
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 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 ⓘ

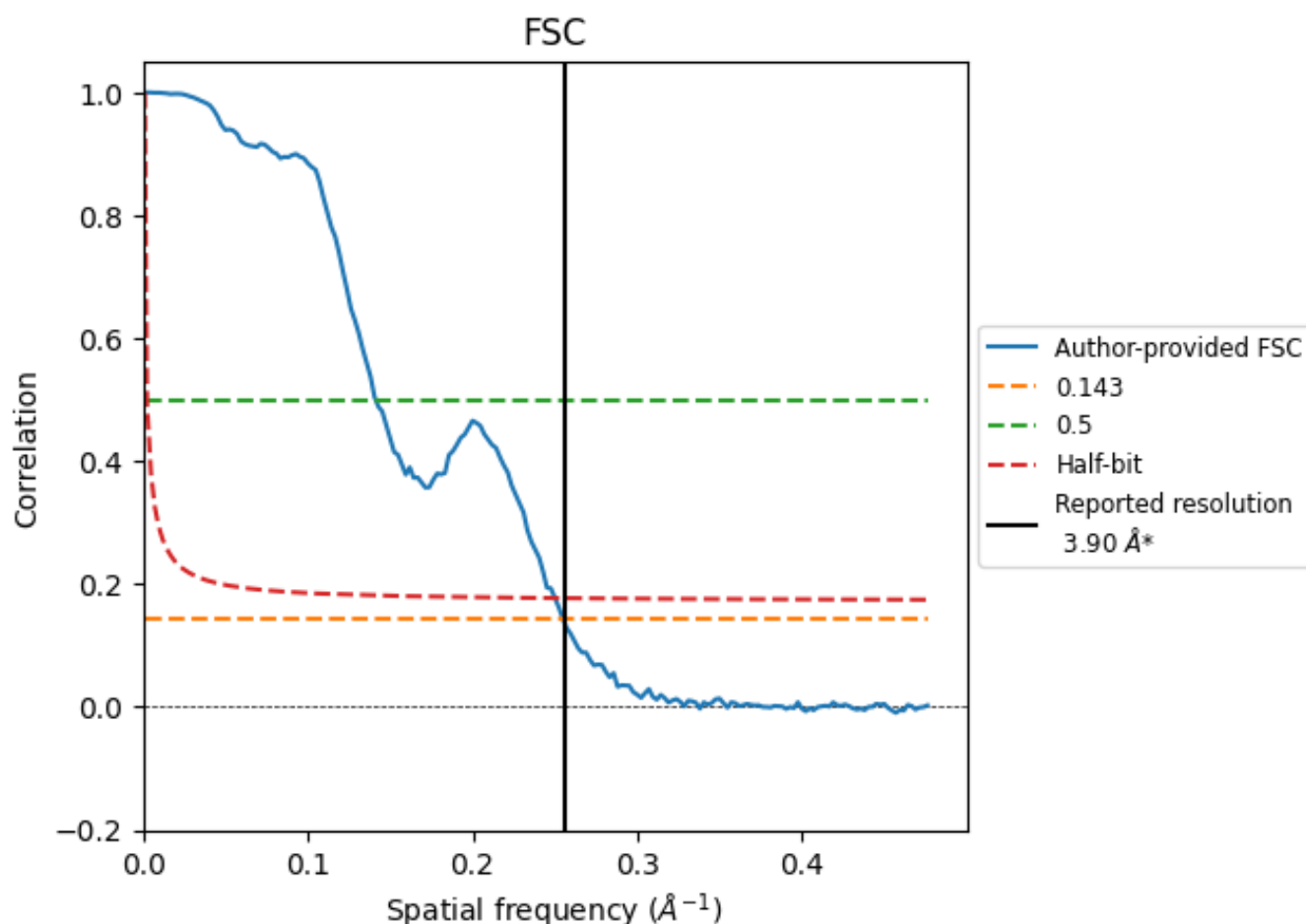


*Reported resolution corresponds to spatial frequency of 0.256 Å⁻¹

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 0.256 Å⁻¹

8.2 Resolution estimates [i](#)

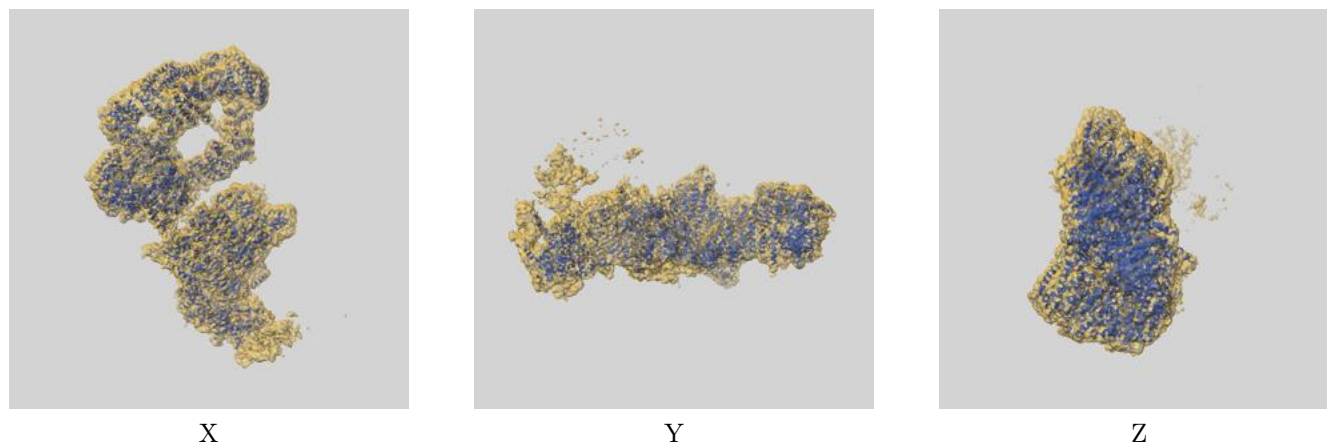
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	3.92	7.08	4.00
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

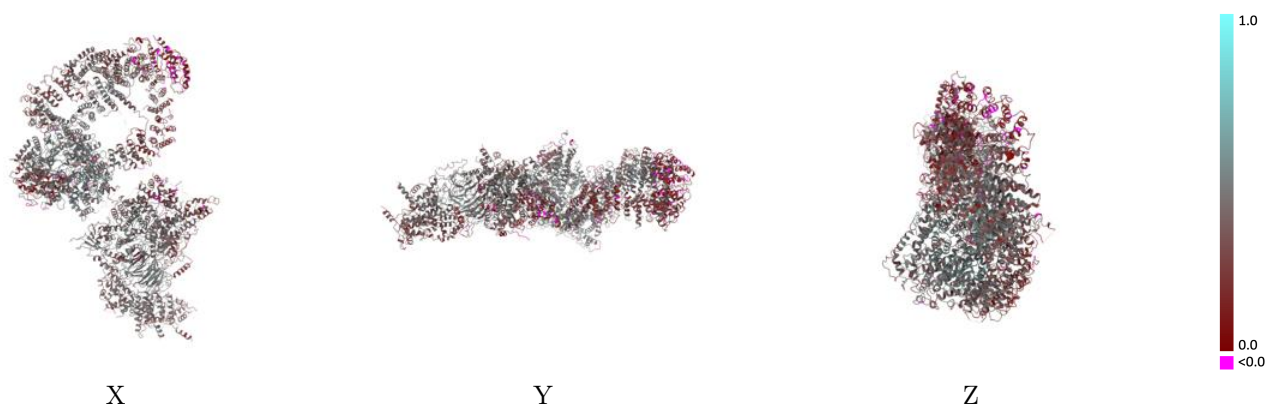
This section contains information regarding the fit between EMDB map EMD-10412 and PDB model 6T9I. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)



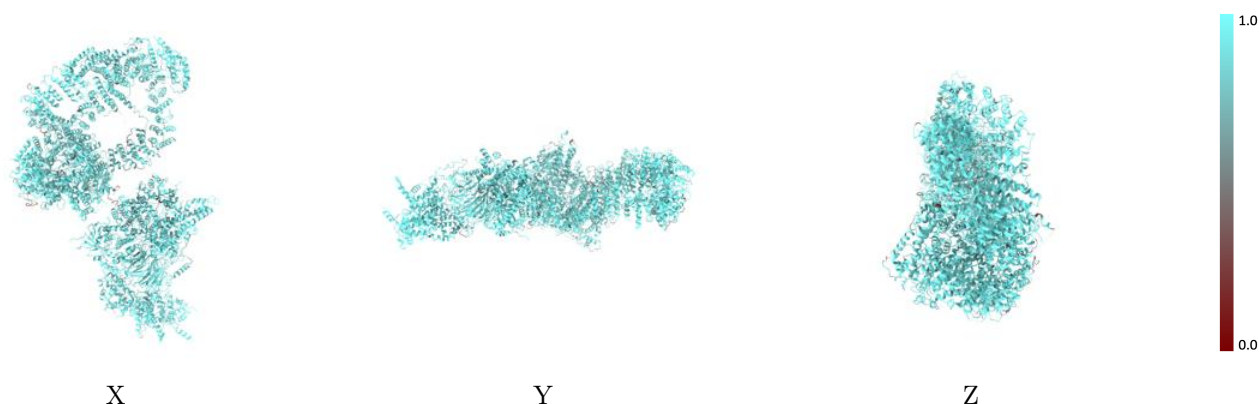
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



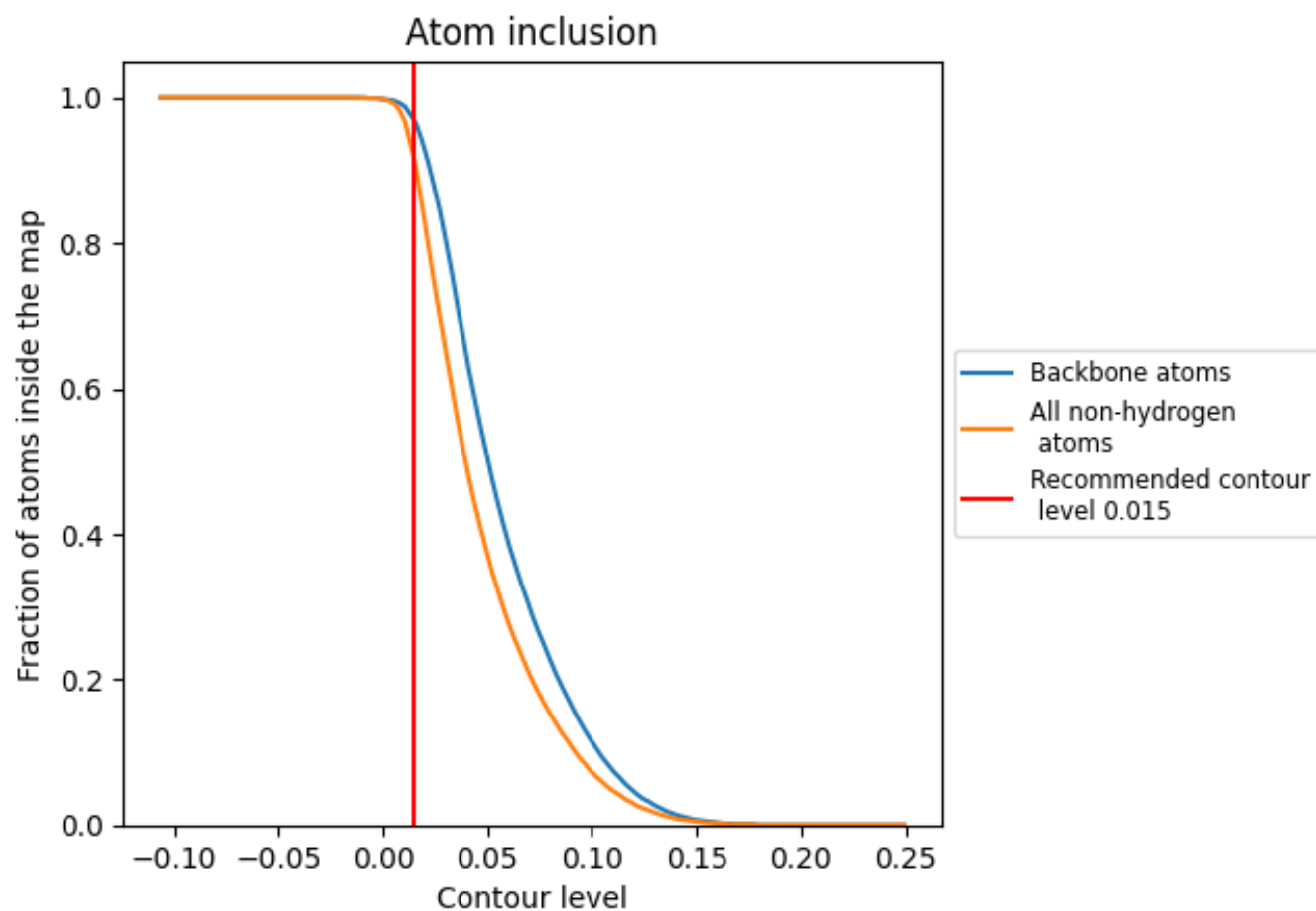
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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

9.4 Atom inclusion ⓘ



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	 0.9160	 0.3800
B	 0.9140	 0.4350
C	 0.8820	 0.2750
D	 0.9250	 0.4160
E	 0.9230	 0.3980
F	 0.9260	 0.4540
G	 0.9610	 0.3520
H	 0.9080	 0.4100
I	 0.8770	 0.4240
K	 0.9340	 0.3490
Q	 0.9480	 0.4250
T	 0.9130	 0.3710
U	 0.9980	 0.3980

