



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 05:35 AM UTC

PDB ID : 7EGI / pdb_00007egi
EMDB ID : EMD-31118
Title : TFIID in rearranged conformation
Authors : Chen, X.; Wu, Z.; Li, J.; Zhao, D.; Xu, Y.
Deposited on : 2021-03-24
Resolution : 9.82 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:

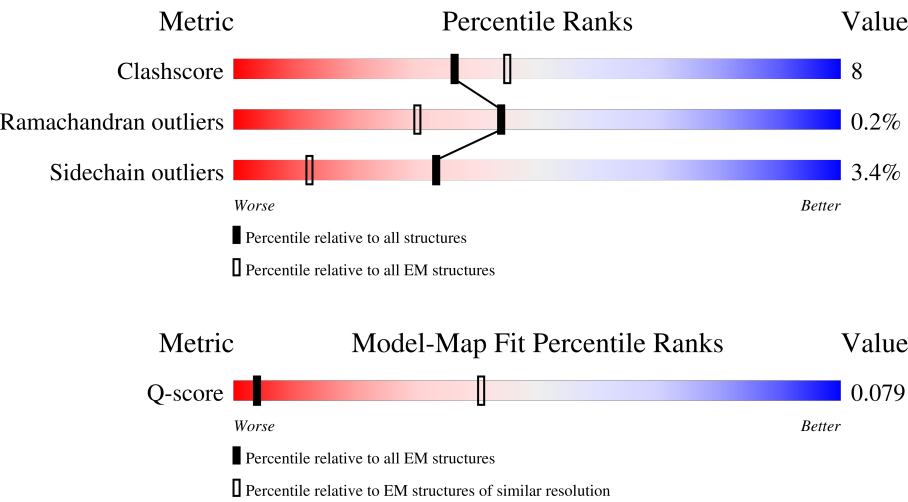
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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

The reported resolution of this entry is 9.82 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.



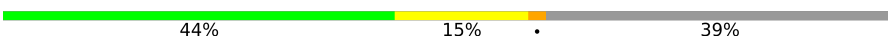
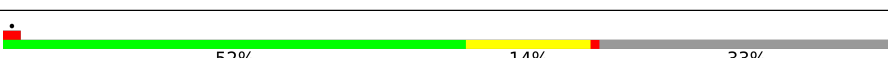
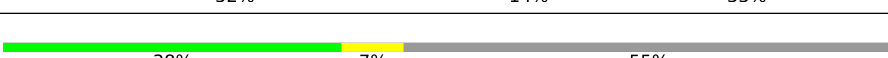
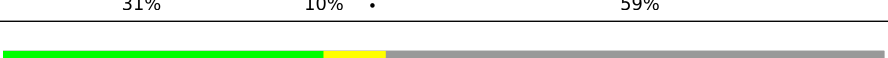
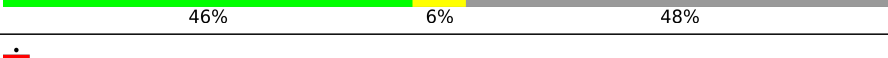
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	143 (9.40 - 10.31)

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

Mol	Chain	Length	Quality of chain
1	A	1872	
2	B	1199	
3	D	1085	
3	d	1085	

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Mol	Chain	Length	Quality of chain
4	E	800	
4	e	800	
5	F	677	
5	f	677	
6	G	349	
7	H	310	
8	I	264	
8	i	264	
9	J	218	
9	j	218	
10	L	161	
10	l	161	
11	O	109	
12	P	339	
13	Q	376	
14	c	929	
15	k	211	
16	m	124	

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 43358 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 initiation factor TFIID subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	549	Total	C	N	O	S	0	0
			4505	2879	781	818	27		

- Molecule 2 is a protein called Transcription initiation factor TFIID subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	963	Total	C	N	O	S	0	0
			7796	5011	1315	1412	58		

- Molecule 3 is a protein called Transcription initiation factor TFIID subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	197	Total	C	N	O	S	0	0
			1614	997	302	310	5		
3	d	158	Total	C	N	O	S	0	0
			1307	814	238	252	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	545	Total	C	N	O	S	0	0
			4359	2765	756	817	21		
4	e	539	Total	C	N	O	S	0	0
			4327	2746	748	814	19		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	412	Total	C	N	O	S	0	0
			3143	1994	548	583	18		
5	f	403	Total	C	N	O	S	0	0
			3081	1954	533	576	18		

- Molecule 6 is a protein called Transcription initiation factor TFIID subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	144	Total	C	N	O	S	0	0
			1171	742	215	210	4		

- Molecule 7 is a protein called Transcription initiation factor TFIID subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	209	Total	C	N	O	S	0	0
			1622	1026	281	310	5		

- Molecule 8 is a protein called Transcription initiation factor TFIID subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	120	Total	C	N	O	S	0	0
			959	610	166	177	6		
8	i	121	Total	C	N	O	S	0	0
			967	615	167	178	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	90	Total	C	N	O	S	0	0
			720	466	115	135	4		
9	j	95	Total	C	N	O	S	0	0
			759	488	124	143	4		

- Molecule 10 is a protein called Transcription initiation factor TFIID subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	76	Total	C	N	O	S	0	0
			622	388	109	122	3		
10	l	107	Total	C	N	O	S	0	0
			876	547	158	166	5		

- Molecule 11 is a protein called Transcription initiation factor IIA subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	O	97	Total	C	N	O	S	0	0
			771	491	133	145	2		

- Molecule 12 is a protein called TATA-box-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	P	177	Total	C	N	O	S	0	0
			1412	918	249	238	7		

- Molecule 13 is a protein called Transcription initiation factor IIA subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Q	101	Total	C	N	O	S	0	0
			827	524	139	160	4		

- Molecule 14 is a protein called Transcription initiation factor TFIID subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	c	127	Total	C	N	O	S	0	0
			1011	638	174	193	6		

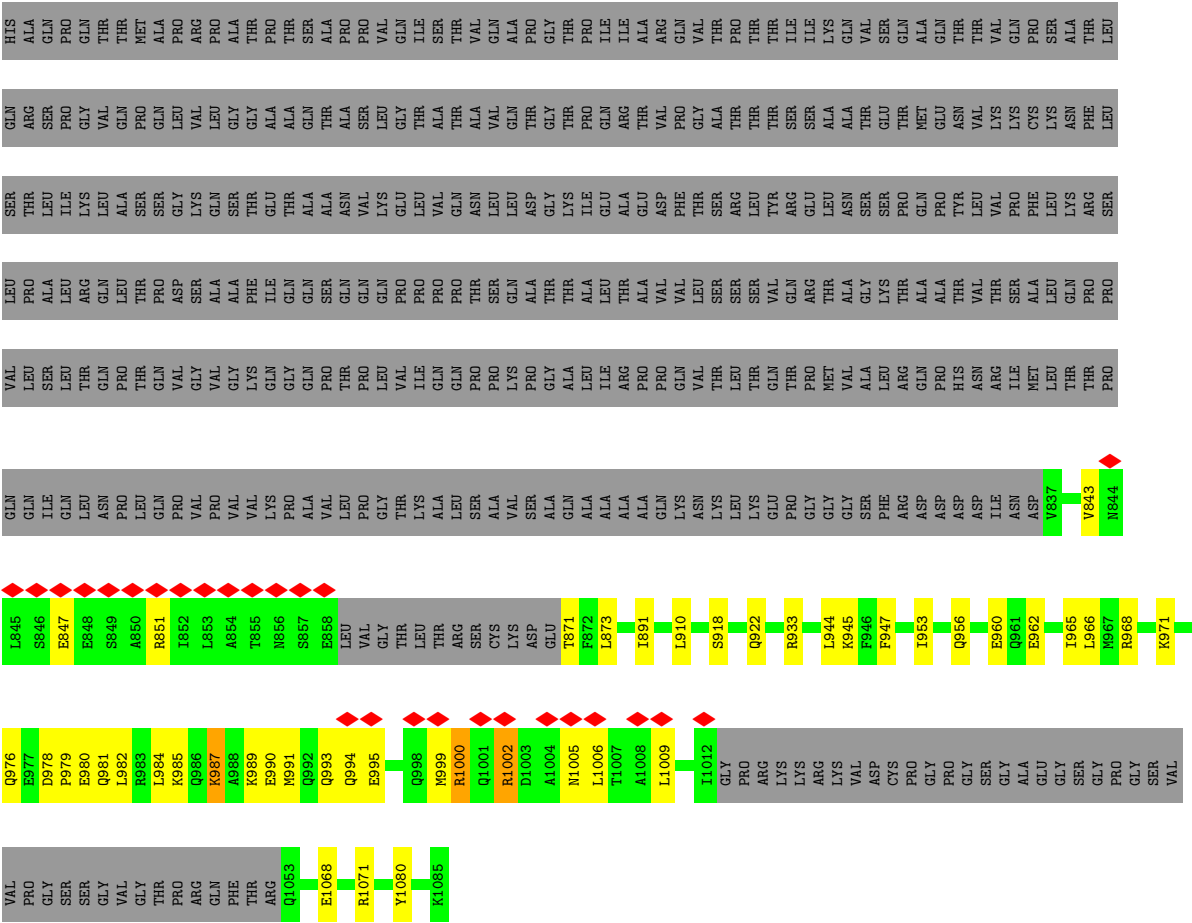
- Molecule 15 is a protein called Transcription initiation factor TFIID subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	k	98	Total	C	N	O	S	0	0
			785	499	142	139	5		

- Molecule 16 is a protein called Transcription initiation factor TFIID subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	m	87	Total	C	N	O	S	0	0
			724	456	131	131	6		



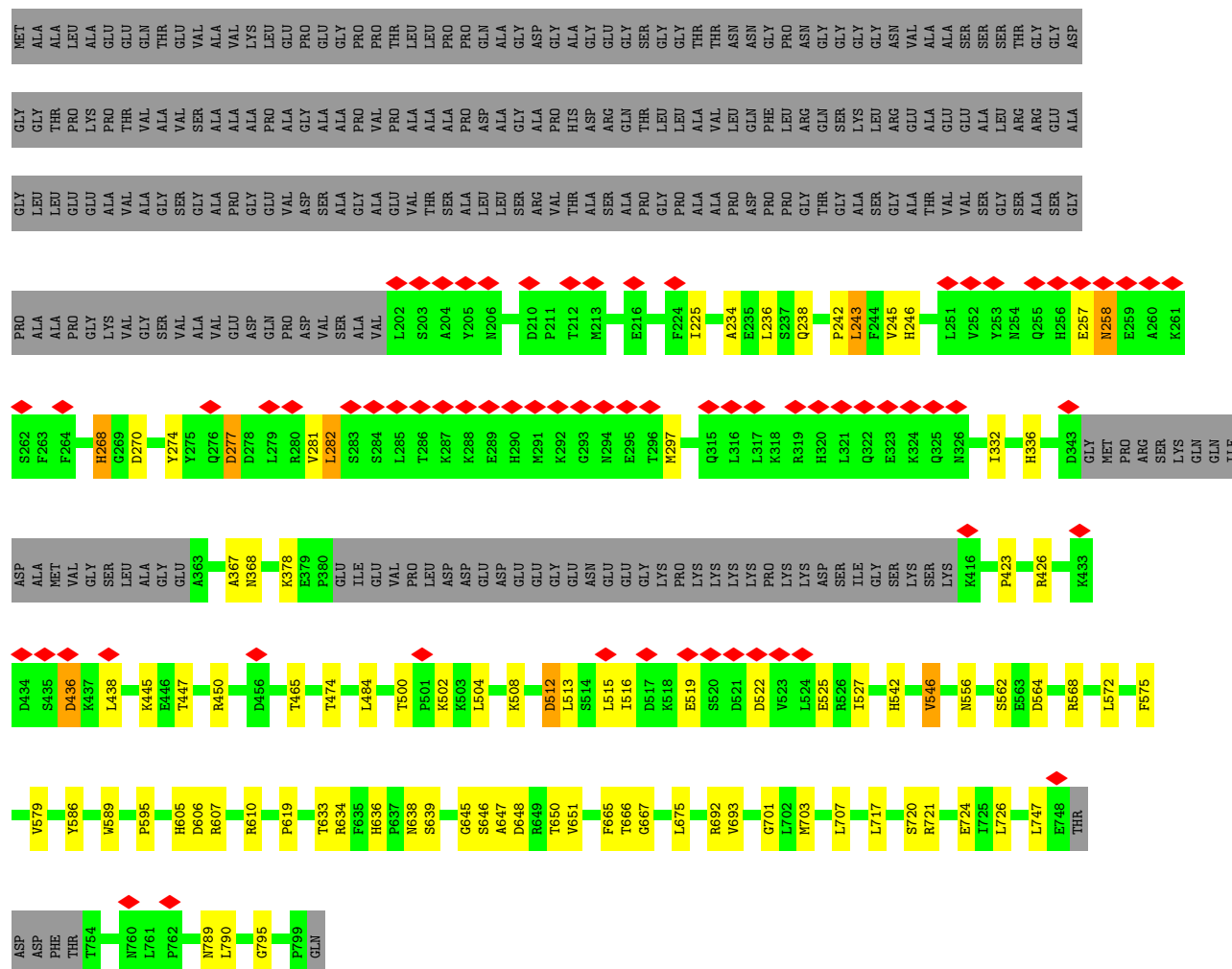


● Molecule 3: Transcription initiation factor TFIID subunit 4

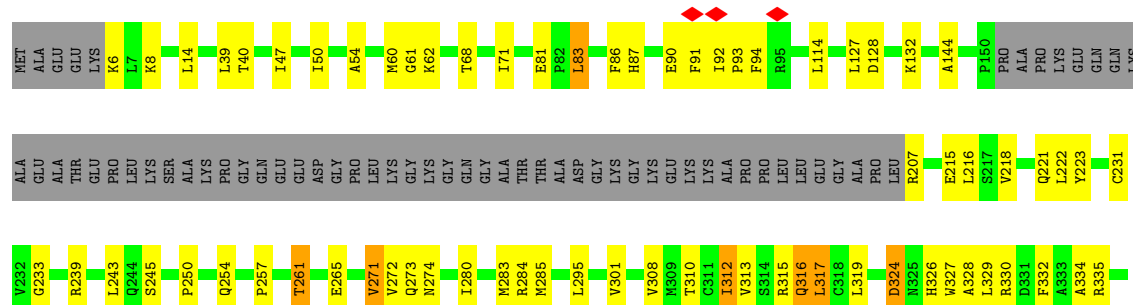


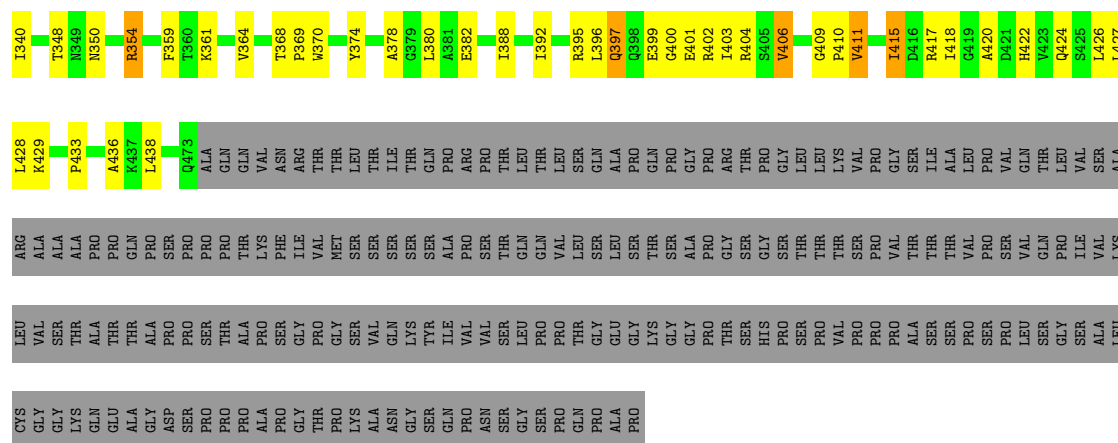


• Molecule 4: Transcription initiation factor TFIID subunit 5

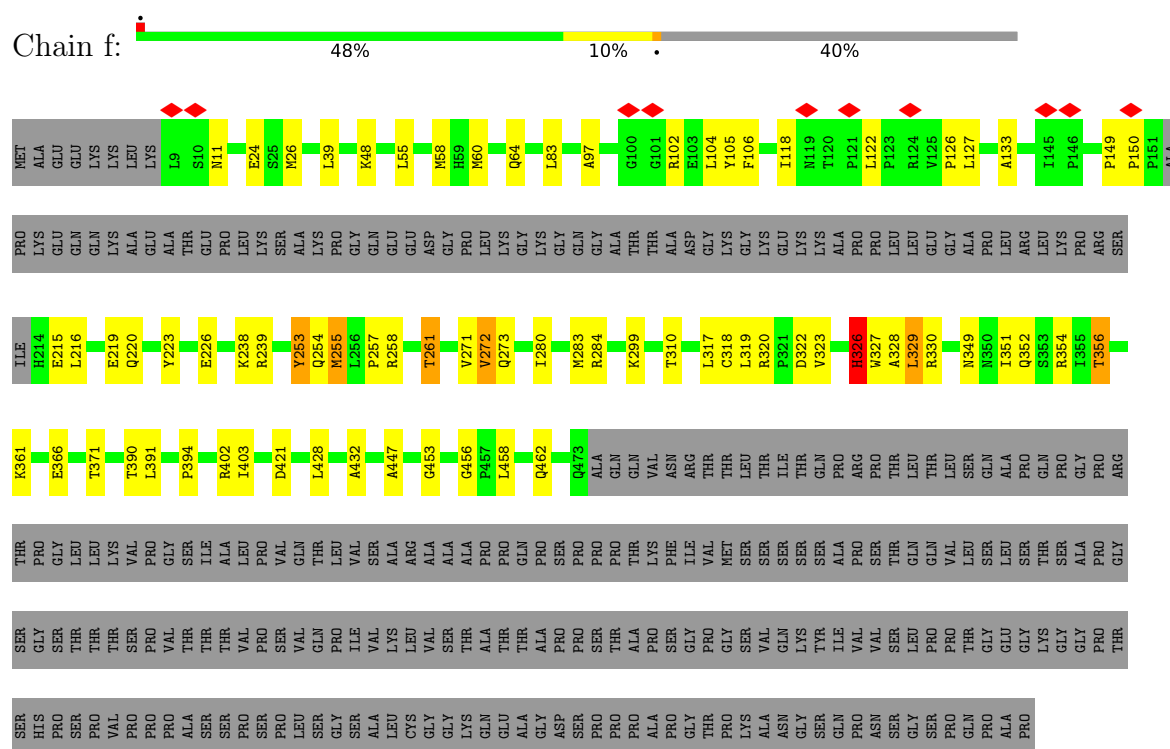


• Molecule 5: Transcription initiation factor TFIID subunit 6

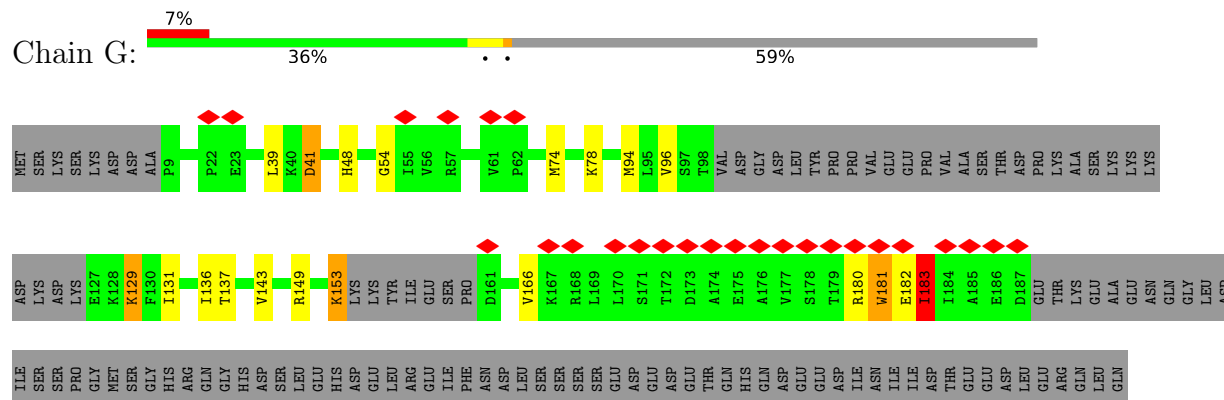


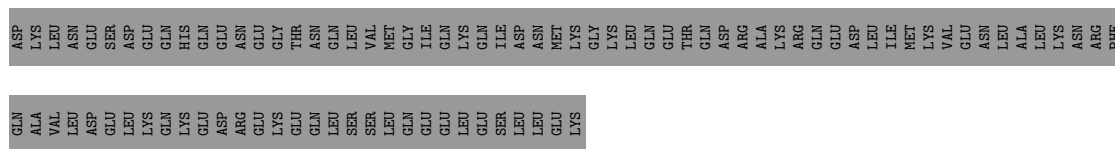


• Molecule 5: Transcription initiation factor TFIID subunit 6

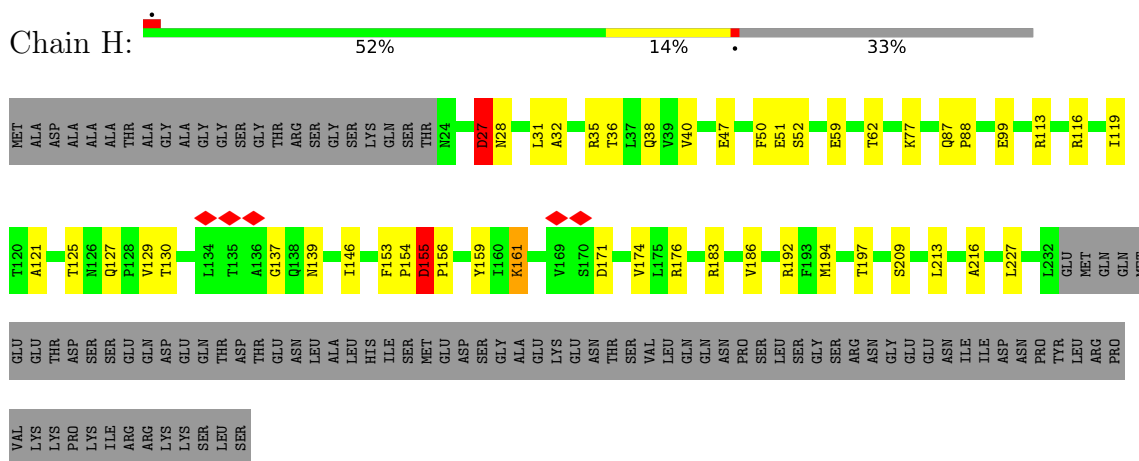


• Molecule 6: Transcription initiation factor TFIID subunit 7

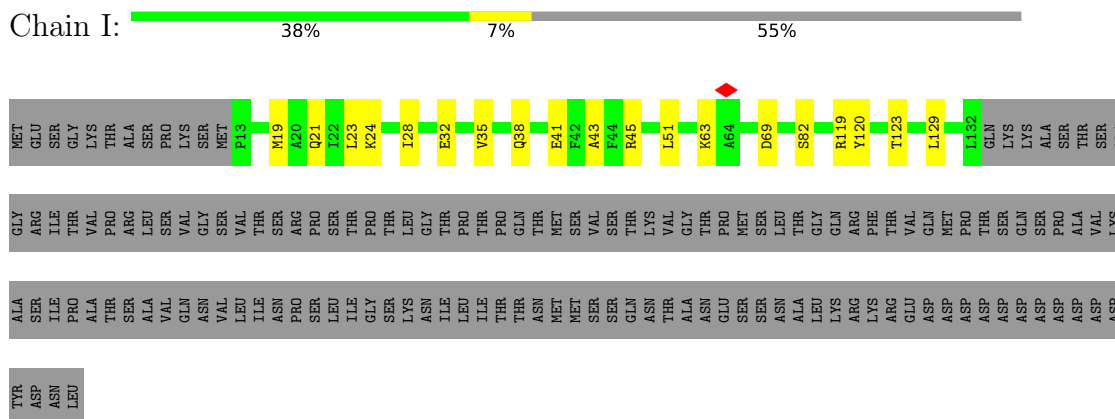




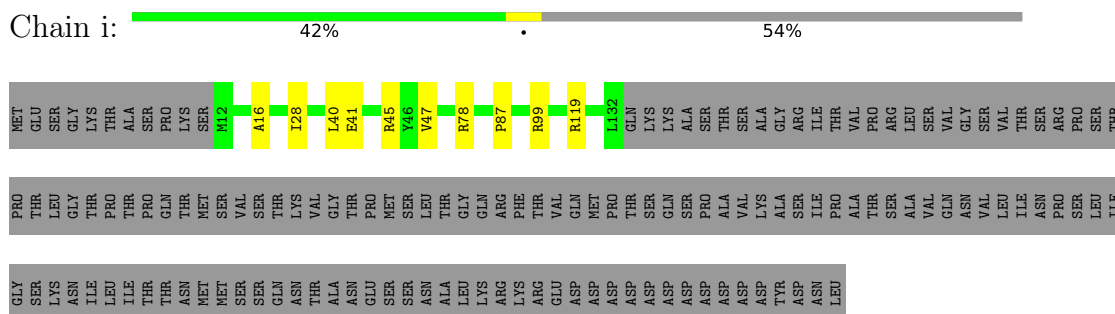
- Molecule 7: Transcription initiation factor TFIID subunit 8



- Molecule 8: Transcription initiation factor TFIID subunit 9

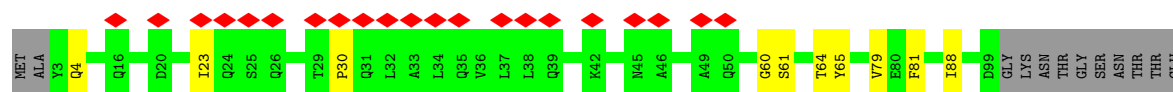


- Molecule 8: Transcription initiation factor TFIID subunit 9



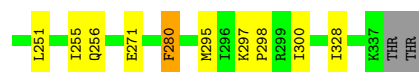
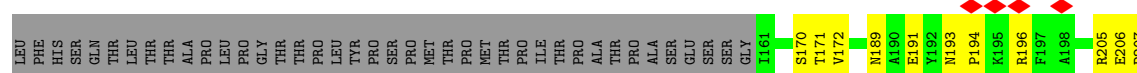
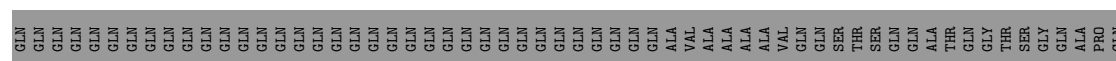
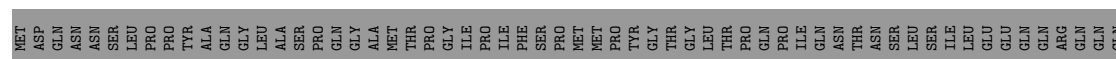
- Molecule 9: Transcription initiation factor TFIID subunit 10





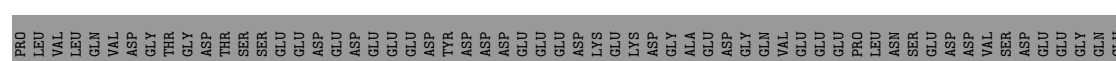
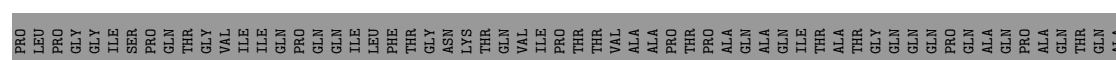
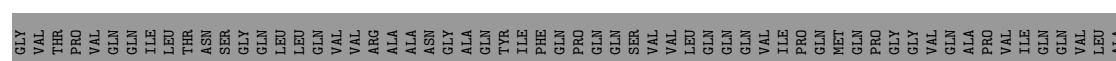
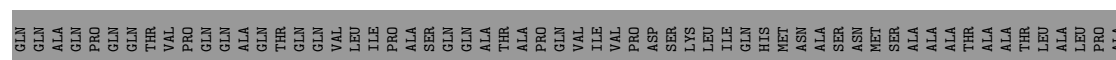
- Molecule 12: TATA-box-binding protein

Chain P: 46% 6% 48%



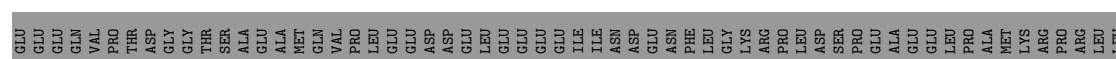
- Molecule 13: Transcription initiation factor IIA subunit 1

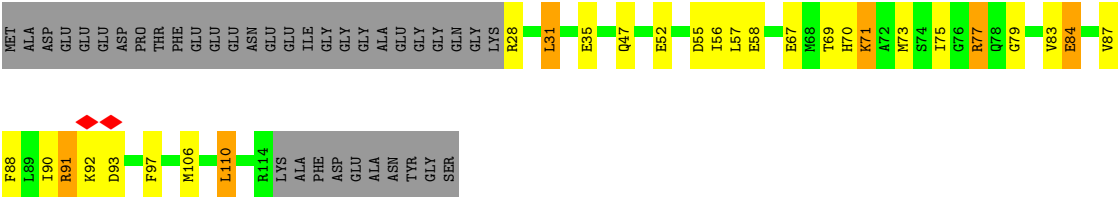
Chain Q: 22% 5% 73%



- Molecule 14: Transcription initiation factor TFIID subunit 3

Chain c: 12% 86%





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	64496	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 ($e^-/\text{\AA}^2$)	50	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	0.040	Depositor
Minimum map value	-0.012	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	432.0, 432.0, 432.0	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.35, 1.35, 1.35	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.62	0/4621	0.95	7/6240 (0.1%)
2	B	0.46	2/7993 (0.0%)	0.68	7/10836 (0.1%)
3	D	0.58	0/1628	0.83	0/2178
3	d	0.47	0/1321	0.71	2/1772 (0.1%)
4	E	0.45	1/4465 (0.0%)	0.72	3/6045 (0.0%)
4	e	0.54	1/4433 (0.0%)	0.77	0/6004
5	F	0.63	1/3201 (0.0%)	1.00	7/4347 (0.2%)
5	f	0.46	0/3140	0.80	6/4268 (0.1%)
6	G	0.68	0/1190	0.94	1/1601 (0.1%)
7	H	0.70	3/1662 (0.2%)	0.93	8/2272 (0.4%)
8	I	0.20	0/981	0.41	0/1332
8	i	0.20	0/989	0.40	0/1343
9	J	0.83	0/736	1.15	4/998 (0.4%)
9	j	0.73	0/775	0.97	0/1049
10	L	0.68	0/630	1.13	1/852 (0.1%)
10	l	0.58	0/888	0.88	0/1194
11	O	0.30	0/781	0.73	0/1061
12	P	0.55	0/1438	0.78	1/1935 (0.1%)
13	Q	0.34	0/842	0.69	0/1134
14	c	0.48	0/1035	0.67	0/1406
15	k	0.28	0/799	0.53	1/1070 (0.1%)
16	m	0.84	0/733	1.18	1/977 (0.1%)
All	All	0.54	8/44281 (0.0%)	0.81	49/59914 (0.1%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	H	28	ASN	C-O	-7.56	1.15	1.24
7	H	27	ASP	C-O	-7.14	1.15	1.24
7	H	31	LEU	C-O	-6.34	1.16	1.24
2	B	61	ASN	C-O	-6.02	1.18	1.24
4	e	445	LYS	C-O	5.71	1.30	1.24
5	F	395	ARG	C-O	5.64	1.31	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	524	LEU	C-O	5.63	1.30	1.24
2	B	903	SER	CA-CB	-5.06	1.45	1.53

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	491	HIS	N-CA-C	-9.51	100.91	111.28
5	f	149	PRO	O-C-N	9.18	125.53	121.31
4	E	756	THR	N-CA-C	-8.38	103.19	113.50
7	H	32	ALA	N-CA-C	-8.20	102.29	111.07
1	A	356	PRO	N-CA-C	7.90	124.79	114.68
7	H	27	ASP	N-CA-C	-7.86	102.79	111.36
4	E	762	PRO	N-CA-C	7.40	124.25	114.27
5	F	271	VAL	N-CA-C	-7.21	105.98	112.90
1	A	715	PRO	N-CA-C	-7.14	100.03	111.03
2	B	495	GLN	N-CA-C	-7.08	104.64	113.28
15	k	180	PRO	N-CA-C	6.78	118.97	110.70
1	A	396	LEU	N-CA-C	-6.71	104.83	113.16
5	f	326	HIS	N-CA-C	-6.63	104.28	112.38
5	f	319	LEU	N-CA-C	-6.55	103.97	112.68
1	A	467	ILE	N-CA-C	-6.42	104.00	111.00
1	A	1205	PHE	CA-CB-CG	-6.23	107.57	113.80
9	J	148	ASP	CA-C-N	6.00	125.71	119.05
9	J	148	ASP	C-N-CA	6.00	125.71	119.05
12	P	207	PRO	N-CA-C	-5.99	100.14	112.47
5	f	255	MET	N-CA-C	-5.99	104.81	114.09
7	H	27	ASP	CA-C-O	-5.92	114.15	120.42
2	B	181	GLY	CA-C-O	-5.86	118.09	122.37
2	B	583	GLU	CB-CA-C	-5.77	101.21	110.79
5	F	316	GLN	CB-CA-C	5.77	120.19	110.79
5	F	310	THR	CB-CA-C	5.75	120.34	110.79
5	F	330	ARG	N-CA-C	-5.65	105.12	111.28
2	B	264	GLU	N-CA-C	-5.55	106.18	113.17
7	H	156	PRO	N-CA-C	-5.54	107.55	114.20
5	f	150	PRO	N-CA-C	5.51	117.42	110.70
5	F	324	ASP	N-CA-C	-5.48	105.41	111.71
7	H	137	GLY	CA-C-O	-5.45	115.74	121.57
4	E	270	ASP	CB-CA-C	5.45	119.19	110.09
16	m	71	LYS	CB-CA-C	5.45	119.83	110.79
7	H	127	GLN	N-CA-C	-5.42	105.37	112.75
5	F	272	VAL	N-CA-C	-5.31	105.20	110.62
5	f	329	LEU	N-CA-C	-5.30	106.51	112.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	183	ILE	N-CA-C	-5.28	102.70	109.30
1	A	498	PRO	N-CA-CB	5.24	108.76	103.25
2	B	491	HIS	CB-CA-C	5.23	119.47	110.79
1	A	1067	GLN	CB-CA-C	5.19	119.41	110.79
10	L	106	ARG	N-CA-C	-5.17	107.00	113.15
3	d	942	ALA	CA-C-N	-5.10	113.44	120.28
3	d	942	ALA	C-N-CA	-5.10	113.44	120.28
7	H	156	PRO	CA-C-O	-5.07	112.30	118.99
2	B	541	ARG	CB-CA-C	-5.05	101.66	110.09
7	H	51	GLU	CB-CA-C	-5.05	100.47	109.71
5	F	438	LEU	N-CA-C	5.04	118.50	111.30
9	J	151	ILE	CA-C-N	-5.00	113.61	120.46
9	J	151	ILE	C-N-CA	-5.00	113.61	120.46

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4505	0	4424	109	0
2	B	7796	0	7751	84	0
3	D	1614	0	1634	42	0
3	d	1307	0	1318	15	0
4	E	4359	0	4245	76	0
4	e	4327	0	4197	59	0
5	F	3143	0	3093	101	0
5	f	3081	0	3012	64	0
6	G	1171	0	1222	17	0
7	H	1622	0	1595	37	0
8	I	959	0	969	15	0
8	i	967	0	977	9	0
9	J	720	0	719	14	0
9	j	759	0	759	14	0
10	L	622	0	620	22	0
10	l	876	0	893	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	O	771	0	764	11	0
12	P	1412	0	1506	18	0
13	Q	827	0	794	12	0
14	c	1011	0	975	17	0
15	k	785	0	818	9	0
16	m	724	0	744	25	0
All	All	43358	0	43029	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 8.

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)
1:A:576:LYS:HG2	1:A:943:LYS:CD	1.33	1.53
1:A:576:LYS:CG	1:A:943:LYS:HD3	1.38	1.51
1:A:1200:THR:O	1:A:1204:GLU:HG2	1.52	1.08
9:J:192:LYS:HE3	9:J:192:LYS:N	1.78	0.99
1:A:725:CYS:O	1:A:725:CYS:SG	2.22	0.97
12:P:271:GLU:CD	15:k:122:GLU:HG2	1.91	0.95
1:A:467:ILE:H	5:F:221:GLN:NE2	1.65	0.94
1:A:511:LEU:H	1:A:511:LEU:HD22	1.37	0.89
6:G:153:LYS:HD3	6:G:153:LYS:H	1.36	0.89
4:E:365:ARG:HD3	4:E:757:GLY:HA3	1.54	0.89
5:F:144:ALA:HB1	5:F:250:PRO:HG2	1.55	0.88
3:D:976:GLN:HB3	3:D:980:GLU:HG3	1.56	0.86
4:e:508:LYS:HB3	4:e:512:ASP:HB2	1.59	0.84
1:A:475:LEU:HD11	5:f:351:ILE:HD11	1.57	0.84
3:D:991:MET:O	3:D:995:GLU:HG3	1.79	0.83
1:A:576:LYS:HG2	1:A:943:LYS:CE	2.07	0.82
4:E:774:MET:H	4:E:774:MET:HE2	1.46	0.81
1:A:821:ARG:HA	1:A:821:ARG:CZ	2.10	0.81
3:D:990:GLU:O	3:D:994:GLN:HG3	1.81	0.81
1:A:1065:GLU:HA	1:A:1065:GLU:OE1	1.78	0.80
5:f:447:ALA:HA	5:f:456:GLY:HA3	1.61	0.80
16:m:77:ARG:HG2	16:m:77:ARG:HH11	1.45	0.80
3:D:968:ARG:HA	3:D:968:ARG:NH1	1.97	0.80
4:E:327:ASN:H	4:E:327:ASN:HD22	1.30	0.80
5:F:324:ASP:HA	5:F:327:TRP:HB3	1.63	0.79
16:m:31:LEU:H	16:m:31:LEU:HD23	1.47	0.79
4:e:747:LEU:HD23	4:e:747:LEU:H	1.47	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:273:GLN:H	5:F:273:GLN:NE2	1.81	0.78
5:F:274:ASN:ND2	5:F:316:GLN:HA	1.99	0.78
5:F:429:LYS:O	5:F:433:PRO:HD2	1.84	0.77
1:A:467:ILE:H	5:F:221:GLN:HE21	1.33	0.77
5:F:359:PHE:HB3	5:F:380:LEU:HG	1.68	0.75
2:B:241:PRO:HG2	2:B:496:MET:HE1	1.72	0.72
5:F:418:ILE:HD12	5:F:418:ILE:H	1.54	0.72
4:e:274:TYR:HB3	4:e:367:ALA:HB2	1.72	0.72
1:A:488:ALA:HB1	5:f:271:VAL:HG23	1.71	0.72
1:A:639:LEU:HD11	1:A:774:ARG:HG2	1.70	0.71
3:D:976:GLN:O	3:D:979:PRO:HD2	1.89	0.71
1:A:970:ASN:OD1	1:A:970:ASN:N	2.20	0.71
1:A:353:LEU:HD21	5:f:272:VAL:HG21	1.72	0.70
4:E:258:ASN:ND2	4:E:258:ASN:H	1.89	0.70
1:A:576:LYS:CG	1:A:943:LYS:CE	2.67	0.70
1:A:568:SER:HB2	2:B:389:ASN:HB2	1.74	0.69
1:A:576:LYS:CG	1:A:943:LYS:CD	2.23	0.69
5:F:274:ASN:HB2	5:F:317:LEU:H	1.58	0.69
6:G:129:LYS:O	6:G:129:LYS:NZ	2.23	0.69
15:k:191:VAL:HG13	15:k:200:ILE:HD13	1.74	0.69
5:f:447:ALA:CA	5:f:456:GLY:HA3	2.23	0.68
5:F:83:LEU:H	5:F:83:LEU:CD1	2.07	0.68
4:E:365:ARG:HD3	4:E:757:GLY:CA	2.24	0.68
10:l:141:LYS:HE2	16:m:79:GLY:HA2	1.76	0.67
7:H:40:VAL:HG11	9:J:130:ILE:HG12	1.77	0.67
4:e:645:GLY:H	4:e:675:LEU:HD11	1.59	0.67
9:j:123:LEU:C	9:j:125:ASP:H	2.03	0.67
2:B:490:SER:HA	2:B:493:TRP:HB2	1.75	0.67
5:F:127:LEU:HD21	7:H:129:VAL:HA	1.76	0.66
1:A:396:LEU:HD21	5:f:394:PRO:HB2	1.77	0.66
5:f:239:ARG:HD3	5:f:284:ARG:HH11	1.60	0.66
4:E:426:ARG:HH11	4:E:640:ASN:HD22	1.42	0.66
1:A:1168:TYR:HB2	6:G:180:ARG:HB3	1.78	0.65
3:D:978:ASP:O	3:D:982:LEU:HG	1.96	0.65
1:A:821:ARG:HA	1:A:821:ARG:NH1	2.11	0.65
3:D:999:MET:HE3	3:D:999:MET:HA	1.77	0.65
4:E:522:ASP:HB2	4:E:526:ARG:HG2	1.80	0.64
1:A:355:VAL:HG23	1:A:355:VAL:O	1.97	0.64
5:f:320:ARG:NH1	5:f:320:ARG:HB3	2.12	0.64
16:m:77:ARG:HH11	16:m:77:ARG:CG	2.11	0.64
5:F:83:LEU:HD12	5:F:83:LEU:N	2.13	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:361:ARG:HD2	2:B:367:GLU:HB2	1.80	0.64
9:j:123:LEU:O	9:j:125:ASP:N	2.30	0.63
5:F:92:ILE:HG13	5:F:93:PRO:HD3	1.81	0.63
4:E:613:ALA:HB2	4:E:620:LEU:HD11	1.81	0.63
10:L:79:ASP:OD1	10:L:79:ASP:N	2.25	0.62
2:B:583:GLU:CD	2:B:583:GLU:H	2.06	0.62
11:O:81:PHE:HB2	11:O:88:ILE:HB	1.80	0.62
7:H:50:PHE:HD1	9:J:193:TYR:O	1.82	0.62
3:d:884:GLU:HA	3:d:887:LYS:HE3	1.82	0.62
7:H:139:ASN:CB	7:H:153:PHE:O	2.47	0.62
3:D:1000:ARG:O	3:D:1000:ARG:NE	2.33	0.61
5:F:335:ARG:NE	5:F:382:GLU:OE1	2.33	0.61
7:H:192:ARG:NH1	7:H:209:SER:O	2.33	0.61
14:c:18:CYS:O	14:c:23:TRP:HB2	2.00	0.61
5:F:114:LEU:HB2	7:H:52:SER:H	1.66	0.61
1:A:1193:ALA:HB3	6:G:166:VAL:HG21	1.83	0.61
5:F:90:GLU:H	5:F:90:GLU:CD	2.08	0.61
9:j:176:MET:HE1	16:m:75:ILE:HD11	1.82	0.61
4:E:754:THR:O	4:E:755:ALA:HB3	2.01	0.60
7:H:194:MET:HE1	5:f:226:GLU:HG3	1.83	0.60
3:D:976:GLN:HB3	3:D:980:GLU:CG	2.29	0.60
1:A:576:LYS:CG	1:A:943:LYS:HE3	2.31	0.60
4:e:277:ASP:OD1	4:e:277:ASP:N	2.32	0.60
3:D:1005:ASN:O	3:D:1009:LEU:HG	2.01	0.60
5:f:330:ARG:HH22	5:f:371:THR:HB	1.66	0.60
1:A:475:LEU:HD13	5:f:349:ASN:OD1	2.02	0.60
16:m:67:GLU:HA	16:m:67:GLU:OE1	2.02	0.60
1:A:470:ILE:O	1:A:470:ILE:HG22	2.02	0.59
4:e:257:GLU:CD	4:e:257:GLU:H	2.10	0.59
2:B:203:LYS:HD3	2:B:237:MET:HE3	1.83	0.59
16:m:88:PHE:CD1	16:m:88:PHE:C	2.81	0.59
2:B:27:LYS:HE3	2:B:490:SER:HB3	1.84	0.59
14:c:99:PHE:HB2	14:c:100:PRO:HD3	1.83	0.59
16:m:31:LEU:HD23	16:m:31:LEU:N	2.16	0.59
2:B:769:LYS:HG3	2:B:769:LYS:O	2.03	0.58
14:c:21:LEU:HD12	14:c:21:LEU:C	2.29	0.58
5:F:312:ILE:HG13	5:F:334:ALA:CB	2.33	0.58
7:H:171:ASP:HB3	7:H:174:VAL:HG12	1.85	0.58
2:B:489:GLN:OE1	2:B:489:GLN:N	2.34	0.58
14:c:12:VAL:HG23	5:f:118:ILE:HA	1.86	0.58
4:e:513:LEU:HD21	4:e:527:ILE:HG23	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:576:LYS:HD3	1:A:943:LYS:HE3	1.86	0.58
3:d:967:MET:HA	3:d:967:MET:HE2	1.85	0.58
5:F:207:ARG:HD2	5:F:207:ARG:N	2.18	0.58
5:f:320:ARG:CB	5:f:320:ARG:HH11	2.17	0.57
4:e:562:SER:OG	4:e:564:ASP:OD1	2.21	0.57
3:D:981:GLN:O	3:D:985:LYS:HG3	2.05	0.57
5:f:349:ASN:HB3	5:f:351:ILE:HG13	1.84	0.57
3:D:989:LYS:O	3:D:993:GLN:HG3	2.03	0.57
13:Q:349:TRP:HB2	13:Q:374:ALA:HB3	1.85	0.57
1:A:1063:LYS:C	1:A:1063:LYS:HD3	2.29	0.57
5:F:335:ARG:HH21	5:F:378:ALA:HB1	1.69	0.57
7:H:161:LYS:HD2	7:H:161:LYS:H	1.68	0.57
2:B:560:TYR:CD2	2:B:581:ILE:HD11	2.40	0.57
5:F:83:LEU:CD1	5:F:83:LEU:N	2.67	0.57
1:A:402:PHE:HA	1:A:407:GLN:NE2	2.20	0.57
1:A:929:THR:HG22	1:A:954:ALA:HA	1.86	0.57
3:d:917:ILE:HD11	3:d:1063:LEU:HD13	1.87	0.57
5:F:81:GLU:HB3	5:F:83:LEU:HD13	1.85	0.57
3:d:910:LEU:HD11	10:l:88:ALA:HB2	1.87	0.57
4:e:636:HIS:HD2	4:e:638:ASN:H	1.53	0.57
4:E:522:ASP:O	4:E:524:LEU:N	2.37	0.56
2:B:27:LYS:CE	2:B:490:SER:HB3	2.35	0.56
4:E:586:TYR:HB3	4:E:605:HIS:HB3	1.85	0.56
4:e:484:LEU:HD21	4:e:504:LEU:HD21	1.86	0.56
5:f:280:ILE:O	5:f:284:ARG:HG3	2.05	0.56
1:A:401:ASN:HD22	1:A:401:ASN:H	1.53	0.56
2:B:61:ASN:O	2:B:130:VAL:HG23	2.06	0.56
3:D:847:GLU:OE2	3:D:851:ARG:NH2	2.38	0.56
10:L:113:VAL:O	10:L:114:LYS:C	2.49	0.56
1:A:355:VAL:O	1:A:355:VAL:CG2	2.54	0.56
5:F:406:VAL:HG11	5:F:420:ALA:HB2	1.88	0.56
12:P:205:ARG:HH21	13:Q:376:TRP:HE1	1.52	0.56
1:A:827:MET:HE2	1:A:862:TRP:HE1	1.69	0.56
2:B:837:LEU:HD22	7:H:213:LEU:HD22	1.86	0.56
3:d:960:GLU:HG2	3:d:963:ARG:HH21	1.70	0.56
1:A:851:ASP:OD1	1:A:851:ASP:N	2.38	0.56
4:E:345:MET:HE3	4:E:346:PRO:HD2	1.87	0.56
5:F:315:ARG:CZ	5:F:369:PRO:HB3	2.35	0.56
2:B:629:ARG:NH1	2:B:658:ASP:OD2	2.37	0.55
5:F:144:ALA:O	5:F:250:PRO:CG	2.54	0.55
5:F:265:GLU:HA	5:F:265:GLU:OE2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:468:ASN:ND2	5:F:128:ASP:O	2.39	0.55
10:l:99:ALA:HB1	10:l:111:LEU:HD11	1.87	0.55
4:e:257:GLU:CD	4:e:257:GLU:N	2.63	0.55
1:A:576:LYS:HD3	1:A:943:LYS:CE	2.37	0.55
2:B:259:ASP:HB3	2:B:262:MET:O	2.05	0.55
5:F:86:PHE:N	5:F:86:PHE:CD1	2.75	0.55
5:F:312:ILE:HG13	5:F:334:ALA:HB3	1.88	0.55
4:e:610:ARG:HD3	4:e:619:PRO:HG3	1.89	0.55
1:A:463:PRO:HD3	5:F:222:LEU:HB2	1.89	0.55
4:e:527:ILE:HG22	4:e:527:ILE:O	2.05	0.55
5:f:253:TYR:O	5:f:254:GLN:HB3	2.06	0.55
2:B:248:SER:OG	2:B:322:MET:SD	2.65	0.55
10:L:119:HIS:NE2	10:L:123:GLN:OE1	2.38	0.55
1:A:489:GLN:H	1:A:489:GLN:NE2	2.05	0.54
2:B:571:LEU:HD21	2:B:619:MET:HE1	1.89	0.54
4:E:561:SER:HB2	4:E:588:VAL:HB	1.88	0.54
5:f:223:TYR:HD2	5:f:255:MET:HE1	1.71	0.54
1:A:675:ASP:OD1	6:G:78:LYS:NZ	2.37	0.54
4:E:645:GLY:H	4:E:675:LEU:HD11	1.73	0.54
5:F:71:ILE:HD11	8:I:35:VAL:HG13	1.89	0.54
1:A:1052:ARG:HD2	1:A:1052:ARG:O	2.07	0.54
5:F:87:HIS:HB2	8:I:45:ARG:HE	1.71	0.54
3:d:911:GLN:NE2	10:l:69:GLU:OE2	2.40	0.54
3:D:976:GLN:CB	3:D:980:GLU:HG3	2.34	0.54
5:f:390:THR:HG23	5:f:391:LEU:HD22	1.89	0.54
2:B:345:CYS:HA	2:B:348:GLN:HE21	1.73	0.54
5:F:83:LEU:H	5:F:83:LEU:HD12	1.71	0.54
2:B:808:PRO:HA	2:B:864:ASN:HB3	1.90	0.54
4:E:474:THR:HG22	5:F:61:GLY:HA2	1.89	0.54
2:B:544:LEU:HD23	2:B:590:ILE:HD11	1.89	0.54
4:e:368:ASN:ND2	4:e:701:GLY:HA3	2.23	0.54
5:f:352:GLN:O	5:f:356:THR:OG1	2.25	0.54
3:D:968:ARG:HA	3:D:968:ARG:CZ	2.38	0.54
5:F:403:ILE:O	5:F:406:VAL:HG22	2.08	0.54
3:D:999:MET:HA	3:D:999:MET:CE	2.38	0.53
4:E:563:GLU:HG2	4:E:587:PRO:HG3	1.90	0.53
3:D:968:ARG:HA	3:D:968:ARG:HH11	1.70	0.53
5:F:335:ARG:HD2	5:F:382:GLU:HB2	1.90	0.53
4:E:653:LEU:HB2	4:E:663:ARG:HB2	1.90	0.53
2:B:66:ASN:HD21	2:B:119:PRO:HB3	1.73	0.53
5:F:273:GLN:H	5:F:273:GLN:CD	2.17	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:433:PRO:HA	5:F:436:ALA:HB3	1.89	0.53
5:f:283:MET:HG3	5:f:329:LEU:HD11	1.91	0.53
16:m:110:LEU:N	16:m:110:LEU:HD23	2.23	0.53
1:A:1200:THR:C	1:A:1204:GLU:HG2	2.30	0.53
6:G:149:ARG:O	6:G:149:ARG:HG3	2.08	0.53
3:D:873:LEU:HD21	10:L:92:ILE:HD11	1.91	0.53
4:E:781:VAL:HG13	5:F:62:LYS:HD3	1.90	0.53
4:E:524:LEU:O	4:E:527:ILE:HG12	2.08	0.53
2:B:937:THR:HG23	2:B:939:ASN:H	1.74	0.53
4:E:299:ASP:OD2	4:E:607:ARG:NH2	2.38	0.53
5:f:447:ALA:O	5:f:453:GLY:HA2	2.09	0.53
2:B:529:VAL:HG11	2:B:560:TYR:HB2	1.91	0.52
3:D:922:GLN:NE2	10:L:71:ASP:OD2	2.41	0.52
4:E:304:LYS:NZ	4:E:335:GLU:O	2.42	0.52
2:B:66:ASN:OD1	2:B:187:ARG:NH1	2.43	0.52
5:F:418:ILE:HD12	5:F:418:ILE:N	2.20	0.52
2:B:202:TRP:HB2	2:B:238:LEU:HB3	1.92	0.52
7:H:113:ARG:O	7:H:116:ARG:NH1	2.43	0.52
9:J:137:TYR:OH	9:J:141:ARG:NH2	2.43	0.52
5:f:318:CYS:SG	5:f:326:HIS:HB3	2.49	0.52
11:O:4:GLN:N	11:O:4:GLN:OE1	2.42	0.52
5:F:39:LEU:HD11	8:I:51:LEU:HD21	1.92	0.52
2:B:628:ILE:O	2:B:644:GLN:NE2	2.41	0.52
4:e:595:PRO:HD2	4:e:639:SER:HB3	1.91	0.52
1:A:576:LYS:CD	1:A:943:LYS:HE3	2.39	0.52
4:e:646:SER:OG	4:e:647:ALA:N	2.40	0.52
2:B:820:ASP:OD1	2:B:820:ASP:N	2.37	0.52
6:G:181:TRP:O	6:G:181:TRP:CE3	2.63	0.52
13:Q:358:MET:HB3	13:Q:360:LEU:HD23	1.92	0.52
14:c:33:LEU:HD13	9:j:197:MET:HE1	1.91	0.52
1:A:840:SER:HA	1:A:843:ARG:CZ	2.40	0.52
4:E:562:SER:OG	4:E:564:ASP:OD1	2.28	0.52
4:e:747:LEU:HG	4:e:747:LEU:O	2.10	0.52
1:A:511:LEU:HD22	1:A:511:LEU:N	2.11	0.51
1:A:828:GLU:HA	1:A:831:LYS:HB2	1.92	0.51
3:D:910:LEU:HD11	10:L:88:ALA:HB2	1.91	0.51
9:J:139:LEU:HB3	9:J:144:PHE:HB3	1.92	0.51
4:e:607:ARG:NH1	8:i:87:PRO:O	2.43	0.51
9:j:123:LEU:C	9:j:125:ASP:N	2.66	0.51
1:A:576:LYS:CB	1:A:943:LYS:HD3	2.28	0.51
1:A:1163:ARG:HB3	6:G:183:ILE:HG22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:e:423:PRO:HG2	4:e:426:ARG:HB2	1.91	0.51
2:B:780:LYS:O	7:H:183:ARG:NH1	2.44	0.51
5:F:243:LEU:HD21	5:F:284:ARG:HB3	1.92	0.51
4:E:690:ASP:OD1	4:E:690:ASP:N	2.43	0.51
14:c:21:LEU:HD12	14:c:21:LEU:O	2.11	0.51
2:B:656:GLU:HG2	2:B:661:ALA:HB3	1.92	0.51
4:E:601:VAL:HG21	4:E:642:VAL:HG11	1.92	0.51
1:A:395:ASP:N	1:A:395:ASP:OD1	2.41	0.51
2:B:90:THR:O	2:B:968:ARG:NH2	2.43	0.51
9:J:114:THR:HB	9:J:117:VAL:HB	1.92	0.51
4:E:278:ASP:OD1	4:E:278:ASP:N	2.43	0.51
10:L:126:MET:HE3	10:L:128:ILE:HD11	1.93	0.51
2:B:739:ASN:ND2	2:B:782:ASN:OD1	2.44	0.51
3:D:947:PHE:HZ	4:E:507:VAL:HG21	1.75	0.51
5:F:71:ILE:HD12	8:I:38:GLN:HE21	1.76	0.51
5:f:24:GLU:HG2	10:l:145:THR:HG21	1.93	0.51
1:A:510:ILE:HB	1:A:511:LEU:HD13	1.93	0.50
2:B:983:ARG:HG3	2:B:983:ARG:HH11	1.75	0.50
2:B:983:ARG:HG3	2:B:983:ARG:NH1	2.26	0.50
4:E:423:PRO:HG2	4:E:426:ARG:HB2	1.92	0.50
4:E:467:LEU:HD11	5:F:132:LYS:HD3	1.93	0.50
4:E:746:ASP:OD1	4:E:746:ASP:N	2.42	0.50
5:F:273:GLN:CD	5:F:273:GLN:N	2.70	0.50
7:H:52:SER:O	9:J:194:THR:HA	2.10	0.50
10:L:93:GLU:O	10:L:97:THR:HG23	2.11	0.50
11:O:64:THR:HA	12:P:189:ASN:HD21	1.76	0.50
4:e:258:ASN:OD1	4:e:258:ASN:N	2.38	0.50
4:e:474:THR:OG1	4:e:546:VAL:O	2.28	0.50
1:A:821:ARG:HA	1:A:821:ARG:NE	2.25	0.50
4:e:500:THR:HG22	4:e:502:LYS:H	1.76	0.50
16:m:28:ARG:HH21	16:m:31:LEU:HD21	1.75	0.50
4:E:256:HIS:HB3	4:E:259:GLU:HG2	1.93	0.50
3:D:843:VAL:HG21	5:F:93:PRO:HG3	1.94	0.50
5:F:257:PRO:O	5:F:261:THR:OG1	2.26	0.50
11:O:61:SER:OG	11:O:61:SER:O	2.30	0.50
4:e:586:TYR:HB3	4:e:605:HIS:HB3	1.94	0.50
4:E:522:ASP:N	4:E:522:ASP:OD1	2.42	0.50
7:H:125:THR:O	7:H:125:THR:HG22	2.12	0.50
11:O:4:GLN:CD	11:O:4:GLN:H	2.19	0.50
5:f:320:ARG:NH1	5:f:320:ARG:CB	2.73	0.50
14:c:1:MET:HG3	5:f:126:PRO:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:e:527:ILE:O	4:e:527:ILE:CG2	2.59	0.50
2:B:367:GLU:OE2	2:B:371:LYS:NZ	2.39	0.50
4:E:634:ARG:HG3	4:E:675:LEU:HB2	1.94	0.50
12:P:295:MET:HE1	12:P:328:ILE:HB	1.93	0.50
13:Q:353:LEU:HB2	13:Q:370:ALA:HB3	1.94	0.50
5:f:219:GLU:OE1	5:f:219:GLU:N	2.25	0.50
12:P:280:PHE:N	12:P:280:PHE:CD1	2.79	0.49
2:B:274:LEU:HG	2:B:278:LYS:HE2	1.93	0.49
2:B:598:ARG:HH11	2:B:619:MET:HE3	1.77	0.49
2:B:882:HIS:HE1	7:H:216:ALA:HB1	1.77	0.49
4:E:481:ASP:HB3	4:E:787:ARG:HH22	1.78	0.49
3:d:916:LYS:NZ	3:d:1070:GLU:OE2	2.42	0.49
2:B:152:LEU:HD23	2:B:155:PRO:HB3	1.94	0.49
2:B:818:THR:OG1	2:B:819:LEU:N	2.45	0.49
4:e:650:THR:HG22	4:e:666:THR:HG22	1.93	0.49
6:G:94:MET:HE3	6:G:96:VAL:HG22	1.94	0.49
13:Q:41:GLU:HG3	13:Q:45:LEU:HD23	1.95	0.49
1:A:468:PHE:CE1	5:F:216:LEU:HD12	2.47	0.49
12:P:170:SER:HA	12:P:255:ILE:HA	1.95	0.49
1:A:485:ILE:HB	5:f:310:THR:HG23	1.94	0.49
4:E:327:ASN:H	4:E:327:ASN:ND2	2.05	0.49
14:c:77:LEU:O	14:c:77:LEU:HD23	2.11	0.49
5:f:97:ALA:HB2	5:f:106:PHE:HE1	1.77	0.49
4:e:693:VAL:HB	4:e:707:LEU:HB2	1.94	0.49
16:m:69:THR:HG22	16:m:73:MET:HE2	1.94	0.49
1:A:927:VAL:O	1:A:933:ASN:ND2	2.45	0.49
15:k:191:VAL:HG13	15:k:200:ILE:CD1	2.41	0.49
4:E:589:TRP:CE3	5:F:60:MET:HG3	2.48	0.48
4:E:732:ASP:OD1	4:E:734:THR:OG1	2.31	0.48
2:B:135:TRP:HA	2:B:138:VAL:HG12	1.95	0.48
3:D:1068:GLU:OE2	4:E:582:LYS:NZ	2.45	0.48
10:L:113:VAL:O	10:L:116:VAL:N	2.46	0.48
1:A:638:PRO:HB3	6:G:39:LEU:HD23	1.95	0.48
2:B:560:TYR:HD2	2:B:581:ILE:HD11	1.78	0.48
4:E:256:HIS:HB3	4:E:259:GLU:CG	2.44	0.48
4:e:724:GLU:OE1	4:e:789:ASN:ND2	2.46	0.48
3:D:956:GLN:NE2	3:D:956:GLN:HA	2.28	0.48
3:D:1002:ARG:NH1	3:D:1002:ARG:HB2	2.28	0.48
4:E:693:VAL:HB	4:E:707:LEU:HB2	1.94	0.48
11:O:65:TYR:CE2	12:P:191:GLU:OE2	2.66	0.48
2:B:781:TYR:O	7:H:176:ARG:NH2	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:316:GLN:NE2	5:F:319:LEU:O	2.45	0.48
5:f:254:GLN:O	5:f:258:ARG:NH2	2.47	0.48
1:A:475:LEU:O	5:f:354:ARG:NH2	2.47	0.48
10:L:106:ARG:O	10:L:106:ARG:HG2	2.14	0.48
5:f:39:LEU:HD22	8:i:47:VAL:HG13	1.95	0.48
4:e:651:VAL:HG13	4:e:665:PHE:HB2	1.95	0.48
1:A:569:ASN:HB3	1:A:572:TYR:HD2	1.78	0.48
1:A:575:PRO:HD3	2:B:608:ASN:HD22	1.79	0.48
2:B:570:GLU:HA	2:B:625:LEU:HA	1.95	0.48
2:B:636:VAL:HG23	2:B:638:ARG:HB3	1.96	0.48
5:F:312:ILE:HG22	5:F:313:VAL:HG13	1.95	0.48
7:H:197:THR:HB	5:f:238:LYS:HG2	1.95	0.48
2:B:953:LEU:HD12	2:B:979:PHE:HE2	1.79	0.48
7:H:129:VAL:HG22	7:H:130:THR:HG23	1.94	0.48
11:O:23:ILE:HD11	11:O:30:PRO:HD3	1.96	0.48
12:P:298:PRO:HB2	12:P:300:ILE:HG12	1.95	0.48
5:f:102:ARG:HD3	10:l:151:ARG:HG3	1.95	0.48
15:k:173:CYS:SG	15:k:179:MET:O	2.72	0.48
4:E:651:VAL:HB	4:E:665:PHE:HB2	1.95	0.47
5:F:409:GLY:O	5:F:417:ARG:NH2	2.47	0.47
16:m:77:ARG:CG	16:m:77:ARG:NH1	2.73	0.47
1:A:639:LEU:O	1:A:643:ILE:HG13	2.13	0.47
1:A:824:ARG:HB3	1:A:863:VAL:HG12	1.95	0.47
4:E:703:MET:HE2	4:E:761:LEU:HD21	1.95	0.47
5:F:47:ILE:HD13	8:I:19:MET:HE1	1.97	0.47
5:F:317:LEU:N	5:F:317:LEU:HD23	2.30	0.47
4:e:234:ALA:HB2	4:e:648:ASP:HB2	1.96	0.47
4:e:589:TRP:HB3	5:f:60:MET:HE3	1.96	0.47
16:m:67:GLU:O	16:m:71:LYS:HG2	2.14	0.47
2:B:184:ASN:N	2:B:184:ASN:ND2	2.63	0.47
5:F:317:LEU:N	5:F:317:LEU:CD2	2.77	0.47
6:G:48:HIS:HD2	6:G:54:GLY:HA2	1.78	0.47
11:O:65:TYR:H	12:P:189:ASN:ND2	2.12	0.47
3:d:1061:ARG:NH1	8:i:119:ARG:O	2.48	0.47
5:f:326:HIS:O	5:f:330:ARG:HG2	2.15	0.47
9:j:176:MET:O	9:j:178:GLY:N	2.43	0.47
1:A:730:PHE:CD1	1:A:730:PHE:N	2.83	0.47
3:D:1000:ARG:NE	3:D:1000:ARG:C	2.73	0.47
4:E:774:MET:HE2	4:E:774:MET:N	2.22	0.47
4:e:556:ASN:HA	4:e:572:LEU:HB2	1.96	0.47
4:e:720:SER:OG	4:e:721:ARG:N	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:217:ASN:ND2	2:B:320:ALA:O	2.35	0.47
2:B:329:LEU:HB3	2:B:342:THR:HG23	1.95	0.47
14:c:80:LEU:HB3	9:j:119:PHE:CZ	2.50	0.47
14:c:119:GLU:HG3	4:e:790:LEU:HD11	1.96	0.47
5:f:330:ARG:NH1	5:f:371:THR:O	2.47	0.47
4:E:327:ASN:HD22	4:E:327:ASN:N	2.07	0.47
4:E:730:SER:OG	4:E:732:ASP:OD1	2.33	0.47
5:F:90:GLU:CD	5:F:90:GLU:N	2.72	0.47
8:I:63:LYS:NZ	8:I:69:ASP:OD1	2.47	0.47
10:L:104:ARG:HA	10:L:104:ARG:HH21	1.80	0.47
12:P:271:GLU:OE2	15:k:122:GLU:HG2	2.10	0.47
14:c:26:VAL:HG23	9:j:195:LEU:HB3	1.96	0.47
3:d:922:GLN:NE2	10:l:71:ASP:OD2	2.47	0.47
2:B:564:LEU:HB2	2:B:581:ILE:HD13	1.97	0.47
3:D:944:LEU:HD11	8:I:123:THR:HG21	1.97	0.47
11:O:60:GLY:HA2	11:O:79:VAL:HG23	1.96	0.47
5:F:144:ALA:O	5:F:250:PRO:HG3	2.15	0.47
5:F:415:ILE:HG12	5:F:415:ILE:O	2.14	0.47
7:H:121:ALA:HB2	9:J:131:PRO:HB3	1.96	0.47
1:A:397:LEU:HD21	5:f:361:LYS:HB3	1.97	0.46
1:A:1165:LEU:HB2	1:A:1191:ILE:HG12	1.97	0.46
5:f:58:MET:HE3	5:f:64:GLN:HA	1.98	0.46
4:E:369:LYS:HD3	4:E:369:LYS:HA	1.74	0.46
8:I:38:GLN:HA	8:I:41:GLU:HB2	1.97	0.46
3:d:1084:LEU:HB3	8:i:99:ARG:HH21	1.81	0.46
4:e:717:LEU:HD22	4:e:726:LEU:HD11	1.98	0.46
1:A:857:MET:HE3	1:A:858:ASP:H	1.81	0.46
2:B:559:LYS:HB2	2:B:559:LYS:NZ	2.31	0.46
7:H:27:ASP:OD1	7:H:27:ASP:N	2.48	0.46
10:L:106:ARG:NH1	10:L:115:ASP:OD2	2.48	0.46
1:A:819:LYS:H	1:A:819:LYS:HZ3	1.63	0.46
4:E:277:ASP:O	4:E:280:ARG:HG2	2.15	0.46
6:G:41:ASP:OD1	6:G:41:ASP:N	2.47	0.46
10:L:104:ARG:HA	10:L:104:ARG:HD2	1.49	0.46
13:Q:57:ASP:OD1	13:Q:57:ASP:N	2.34	0.46
3:D:847:GLU:HG3	7:H:99:GLU:HA	1.97	0.46
12:P:295:MET:HG2	12:P:298:PRO:HD2	1.97	0.46
3:d:860:VAL:HA	16:m:47:GLN:HG2	1.98	0.46
4:e:747:LEU:H	4:e:747:LEU:CD2	2.22	0.46
5:f:328:ALA:C	5:f:330:ARG:N	2.72	0.46
10:l:129:PRO:HB2	16:m:56:ILE:HG23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1080:TYR:OH	4:E:606:ASP:OD2	2.30	0.46
4:E:245:VAL:HG13	4:E:282:LEU:HD11	1.97	0.46
5:F:411:VAL:O	5:F:411:VAL:HG13	2.15	0.46
4:e:519:GLU:O	4:e:519:GLU:HG3	2.16	0.46
13:Q:25:VAL:HG13	13:Q:39:LEU:HD11	1.97	0.46
4:e:281:VAL:HG11	4:e:297:MET:HB3	1.98	0.46
1:A:401:ASN:HD22	1:A:401:ASN:N	2.14	0.46
4:E:321:LEU:HB3	4:E:330:TRP:HB2	1.97	0.46
8:I:119:ARG:NH1	8:I:120:TYR:OH	2.48	0.46
1:A:467:ILE:N	5:F:221:GLN:NE2	2.48	0.46
2:B:71:ARG:HD3	2:B:73:TYR:CE1	2.51	0.46
4:E:696:TRP:HA	4:E:703:MET:HA	1.96	0.46
5:F:47:ILE:HD11	8:I:43:ALA:HB2	1.98	0.46
7:H:186:VAL:HG21	5:f:220:GLN:HB3	1.97	0.46
1:A:404:MET:O	1:A:408:LEU:HB2	2.16	0.45
3:D:871:THR:HG21	3:D:910:LEU:HD12	1.98	0.45
10:L:83:MET:HE3	10:L:83:MET:HB3	1.61	0.45
4:e:525:GLU:OE1	4:e:525:GLU:N	2.41	0.45
2:B:568:VAL:HG22	2:B:628:ILE:HG23	1.98	0.45
6:G:181:TRP:CD2	6:G:181:TRP:C	2.87	0.45
1:A:345:PRO:HG3	1:A:500:LEU:HG	1.99	0.45
1:A:1063:LYS:HD3	1:A:1063:LYS:O	2.16	0.45
5:F:424:GLN:O	5:F:428:LEU:HG	2.15	0.45
7:H:59:GLU:HA	7:H:62:THR:HG22	1.99	0.45
13:Q:333:ASN:HB3	13:Q:360:LEU:HD13	1.98	0.45
16:m:57:LEU:HD23	16:m:57:LEU:HA	1.72	0.45
5:f:326:HIS:ND1	5:f:326:HIS:N	2.64	0.45
1:A:470:ILE:O	5:f:299:LYS:NZ	2.49	0.45
4:e:238:GLN:O	4:e:242:PRO:HD2	2.16	0.45
5:F:144:ALA:HB1	5:F:250:PRO:CG	2.37	0.45
5:F:215:GLU:O	5:F:254:GLN:NE2	2.39	0.45
9:J:124:GLU:O	9:J:125:ASP:HB3	2.17	0.45
1:A:576:LYS:CD	1:A:943:LYS:CE	2.95	0.45
5:f:327:TRP:O	5:f:330:ARG:HB2	2.16	0.45
5:F:361:LYS:HA	5:F:364:VAL:HG22	1.99	0.45
7:H:161:LYS:HD2	7:H:161:LYS:N	2.31	0.45
12:P:170:SER:HB3	12:P:255:ILE:HG12	1.99	0.45
5:f:26:MET:HE3	5:f:26:MET:HB3	1.77	0.45
5:f:257:PRO:O	5:f:261:THR:OG1	2.31	0.45
1:A:475:LEU:HD23	1:A:480:TRP:HE1	1.82	0.45
4:E:646:SER:OG	4:E:647:ALA:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:784:HIS:HB3	4:E:792:LEU:HB2	1.99	0.45
5:F:50:ILE:O	5:F:54:ALA:N	2.47	0.45
3:d:1080:TYR:OH	4:e:606:ASP:OD2	2.26	0.45
16:m:52:GLU:OE1	16:m:52:GLU:N	2.40	0.45
5:F:426:LEU:C	5:F:426:LEU:HD23	2.42	0.45
5:f:317:LEU:HD12	5:f:329:LEU:HD23	1.98	0.45
1:A:1053:PHE:HB2	1:A:1057:GLU:HB2	1.99	0.44
5:F:400:GLY:O	5:F:404:ARG:HG2	2.18	0.44
14:c:24:ASP:CB	9:j:192:LYS:HD2	2.48	0.44
4:e:268:HIS:O	4:e:268:HIS:CG	2.70	0.44
1:A:463:PRO:O	5:F:218:VAL:HG23	2.18	0.44
5:F:233:GLY:HA2	5:F:239:ARG:HE	1.82	0.44
5:f:83:LEU:HD22	8:i:41:GLU:HG2	1.99	0.44
1:A:690:LEU:HD22	1:A:747:LEU:HD22	1.99	0.44
1:A:1182:CYS:O	1:A:1182:CYS:SG	2.75	0.44
2:B:639:LYS:NZ	2:B:641:GLU:OE2	2.42	0.44
7:H:119:ILE:HD12	7:H:119:ILE:N	2.32	0.44
11:O:65:TYR:HE2	12:P:191:GLU:CG	2.30	0.44
1:A:592:SER:OG	1:A:695:GLY:O	2.31	0.44
13:Q:369:LYS:HD2	13:Q:369:LYS:HA	1.78	0.44
5:f:320:ARG:HH11	5:f:320:ARG:HB2	1.83	0.44
4:E:650:THR:HG22	4:E:666:THR:HG22	2.00	0.44
5:F:312:ILE:HG13	5:F:334:ALA:HB1	2.00	0.44
10:l:113:VAL:O	10:l:113:VAL:HG22	2.18	0.44
1:A:400:GLU:HG3	1:A:401:ASN:N	2.32	0.44
5:f:11:ASN:OD1	5:f:48:LYS:NZ	2.51	0.44
8:i:78:ARG:HD3	8:i:78:ARG:HA	1.77	0.44
1:A:645:LYS:HA	1:A:645:LYS:HD2	1.77	0.44
3:D:987:LYS:HE3	3:D:987:LYS:HB3	1.73	0.44
4:E:250:GLU:O	4:E:254:ASN:ND2	2.50	0.44
4:E:377:LEU:HD21	4:E:422:PRO:HG2	2.00	0.44
5:F:370:TRP:CZ3	5:F:420:ALA:HA	2.53	0.44
13:Q:15:ARG:HE	13:Q:59:PHE:HD2	1.66	0.44
8:i:16:ALA:HB2	8:i:40:LEU:HD11	2.00	0.44
2:B:414:LEU:HB2	2:B:523:VAL:HG13	1.99	0.44
3:D:945:LYS:HD2	3:D:945:LYS:C	2.43	0.44
12:P:171:THR:OG1	12:P:256:GLN:HG2	2.17	0.44
5:f:105:TYR:O	9:j:217:PHE:N	2.51	0.44
3:D:962:GLU:O	3:D:966:LEU:HG	2.18	0.43
3:D:971:LYS:O	3:D:971:LYS:HG3	2.18	0.43
14:c:124:ILE:HD11	5:f:133:ALA:HB1	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:e:245:VAL:HG12	4:e:282:LEU:HD11	1.99	0.43
4:E:518:LYS:C	4:E:520:SER:H	2.26	0.43
5:F:223:TYR:HH	5:F:245:SER:HG	1.63	0.43
7:H:119:ILE:HD13	9:J:129:THR:HG22	2.00	0.43
4:e:525:GLU:N	4:e:525:GLU:CD	2.76	0.43
4:e:542:HIS:CE1	4:e:568:ARG:HG3	2.53	0.43
2:B:766:LEU:HA	2:B:807:THR:HG21	2.00	0.43
5:F:328:ALA:O	5:F:332:PHE:N	2.51	0.43
1:A:843:ARG:HE	1:A:843:ARG:HB2	1.44	0.43
4:E:249:LEU:HD21	4:E:282:LEU:HD22	2.00	0.43
4:E:351:GLN:HG2	4:E:355:MET:HE2	2.01	0.43
4:e:436:ASP:OD1	4:e:436:ASP:N	2.49	0.43
3:D:891:ILE:HG21	10:L:111:LEU:HB2	2.01	0.43
3:D:933:ARG:HD2	9:J:117:VAL:HG11	2.00	0.43
4:E:476:VAL:HB	4:E:782:HIS:HB2	2.00	0.43
5:F:402:ARG:O	5:F:406:VAL:HG13	2.19	0.43
16:m:91:ARG:HG2	16:m:92:LYS:N	2.34	0.43
1:A:500:LEU:HD23	1:A:500:LEU:HA	1.81	0.43
1:A:639:LEU:O	1:A:639:LEU:CD1	2.67	0.43
1:A:727:THR:HG23	1:A:727:THR:O	2.19	0.43
4:E:466:PHE:HB2	4:E:796:ALA:HA	2.00	0.43
4:E:790:LEU:HD13	7:H:146:ILE:HG12	2.00	0.43
6:G:129:LYS:HD2	6:G:129:LYS:HA	1.77	0.43
2:B:594:SER:OG	2:B:595:LYS:N	2.52	0.43
2:B:653:LEU:HG	2:B:684:ILE:HG13	2.00	0.43
3:D:1071:ARG:HH22	8:I:82:SER:HA	1.83	0.43
5:F:401:GLU:CD	5:F:401:GLU:C	2.87	0.43
1:A:1052:ARG:O	1:A:1052:ARG:CG	2.67	0.43
2:B:219:ASP:OD1	2:B:219:ASP:N	2.52	0.43
4:E:651:VAL:HG21	4:E:686:THR:HG21	2.01	0.43
14:c:21:LEU:HD11	14:c:23:TRP:CD1	2.54	0.43
14:c:66:VAL:HG21	9:j:151:ILE:HG23	2.01	0.43
2:B:328:ASN:HA	7:H:227:LEU:HD21	2.00	0.43
1:A:968:ILE:HD12	1:A:968:ILE:HA	1.94	0.43
7:H:35:ARG:HA	7:H:35:ARG:HD3	1.59	0.43
8:i:45:ARG:HG3	9:j:212:LYS:HB3	2.01	0.43
1:A:925:ASP:N	1:A:925:ASP:OD1	2.52	0.42
4:E:613:ALA:HB3	4:E:616:HIS:HD2	1.83	0.42
8:I:21:GLN:HE22	8:I:24:LYS:HE2	1.84	0.42
8:I:23:LEU:HD22	8:I:28:ILE:HD12	2.00	0.42
5:f:317:LEU:HG	5:f:330:ARG:HE	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:216:SER:OG	2:B:217:ASN:N	2.52	0.42
3:D:918:SER:OG	10:L:74:GLU:OE1	2.37	0.42
5:F:283:MET:HE1	5:F:308:VAL:HG12	2.00	0.42
6:G:181:TRP:O	6:G:181:TRP:CD2	2.72	0.42
14:c:101:VAL:HG22	5:f:127:LEU:HA	2.00	0.42
5:f:428:LEU:HD13	5:f:458:LEU:CB	2.49	0.42
1:A:819:LYS:HE2	1:A:819:LYS:HB2	1.94	0.42
2:B:839:MET:HE1	2:B:843:LEU:HD13	2.00	0.42
3:D:1000:ARG:C	3:D:1000:ARG:HE	2.27	0.42
5:F:324:ASP:CG	5:F:327:TRP:HD1	2.27	0.42
7:H:155:ASP:OD1	7:H:155:ASP:N	2.38	0.42
14:c:94:HIS:CD2	5:f:122:LEU:HD22	2.54	0.42
4:e:703:MET:HB3	4:e:703:MET:HE2	1.83	0.42
5:F:14:LEU:O	5:F:40:THR:OG1	2.35	0.42
5:F:312:ILE:HG22	5:F:313:VAL:CG1	2.50	0.42
2:B:887:ARG:NH2	2:B:917:ASP:OD2	2.49	0.42
5:F:68:THR:OG1	8:I:32:GLU:OE1	2.35	0.42
5:F:410:PRO:O	5:F:411:VAL:C	2.63	0.42
10:L:120:LEU:HD23	10:L:128:ILE:HG12	2.01	0.42
15:k:179:MET:HB3	15:k:180:PRO:CD	2.50	0.42
2:B:496:MET:HB2	2:B:496:MET:HE3	1.84	0.42
2:B:831:GLU:OE1	2:B:835:ARG:NH2	2.52	0.42
4:E:521:ASP:N	4:E:521:ASP:OD1	2.53	0.42
4:E:754:THR:O	4:E:755:ALA:CB	2.67	0.42
5:F:6:LYS:HE2	5:F:8:LYS:HG3	2.01	0.42
4:e:513:LEU:CD2	4:e:527:ILE:HG23	2.49	0.42
5:f:223:TYR:CD2	5:f:255:MET:HE1	2.52	0.42
1:A:353:LEU:HD22	5:f:273:GLN:HE22	1.85	0.42
1:A:467:ILE:H	5:F:221:GLN:HE22	1.60	0.42
1:A:468:PHE:CE1	5:F:221:GLN:HG3	2.54	0.42
5:F:350:ASN:OD1	5:F:350:ASN:N	2.51	0.42
4:e:447:THR:O	4:e:450:ARG:HB2	2.19	0.42
4:e:667:GLY:O	4:e:692:ARG:NH2	2.52	0.42
5:f:447:ALA:CB	5:f:456:GLY:HA3	2.49	0.42
16:m:87:VAL:HG13	16:m:97:PHE:HE1	1.84	0.42
9:J:123:LEU:HD12	9:J:123:LEU:HA	1.74	0.42
10:L:113:VAL:C	10:L:115:ASP:N	2.75	0.42
12:P:194:PRO:C	12:P:196:ARG:H	2.27	0.42
4:e:504:LEU:HD23	4:e:504:LEU:HA	1.90	0.42
1:A:472:ASN:ND2	5:f:299:LYS:O	2.53	0.42
2:B:176:HIS:HE1	2:B:310:ASP:H	1.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:957:MET:O	2:B:968:ARG:NH1	2.53	0.42
11:O:23:ILE:HD12	11:O:23:ILE:HA	1.87	0.42
13:Q:350:LYS:HB3	13:Q:350:LYS:HE2	1.82	0.42
1:A:468:PHE:HE1	5:F:221:GLN:HG3	1.85	0.42
2:B:559:LYS:HB2	2:B:559:LYS:HZ3	1.84	0.42
2:B:882:HIS:CE1	7:H:216:ALA:HB1	2.54	0.42
7:H:38:GLN:HG2	7:H:62:THR:HG21	2.01	0.42
3:D:1002:ARG:HB2	3:D:1002:ARG:CZ	2.50	0.41
5:F:231:CYS:HB3	5:F:285:MET:HE2	2.02	0.41
3:d:955:LYS:HB3	3:d:955:LYS:HE2	1.90	0.41
4:e:636:HIS:CD2	4:e:638:ASN:H	2.36	0.41
5:f:432:ALA:HB1	5:f:462:GLN:CB	2.49	0.41
2:B:925:LYS:HA	2:B:925:LYS:HD3	1.78	0.41
4:e:332:ILE:HA	4:e:336:HIS:HD2	1.84	0.41
2:B:562:GLY:O	2:B:581:ILE:HG12	2.19	0.41
4:E:265:GLU:OE1	4:E:265:GLU:HA	2.20	0.41
4:E:743:ALA:HB2	4:E:768:LEU:HD13	2.02	0.41
5:F:426:LEU:O	5:F:429:LYS:HG2	2.21	0.41
7:H:77:LYS:HE3	7:H:77:LYS:HB3	1.93	0.41
10:L:62:LYS:HA	10:L:62:LYS:HD2	1.87	0.41
10:L:120:LEU:O	10:L:125:ASN:N	2.53	0.41
15:k:179:MET:HB3	15:k:180:PRO:HD2	2.01	0.41
1:A:463:PRO:HD2	5:F:218:VAL:HG22	2.03	0.41
1:A:706:ARG:HH12	2:B:296:THR:HB	1.86	0.41
5:F:388:ILE:HA	5:F:392:ILE:HG12	2.03	0.41
5:F:418:ILE:H	5:F:418:ILE:CD1	2.26	0.41
7:H:154:PRO:HD2	7:H:159:TYR:HE2	1.84	0.41
4:e:504:LEU:HD22	4:e:575:PHE:HZ	1.85	0.41
5:f:55:LEU:HD13	8:i:28:ILE:HG12	2.01	0.41
9:j:173:HIS:HA	9:j:176:MET:HE3	2.02	0.41
16:m:84:GLU:H	16:m:84:GLU:HG3	1.42	0.41
1:A:576:LYS:HD3	1:A:943:LYS:NZ	2.35	0.41
1:A:639:LEU:O	1:A:639:LEU:HD13	2.20	0.41
4:E:668:HIS:NE2	4:E:686:THR:OG1	2.42	0.41
4:E:703:MET:HE3	4:E:703:MET:HB2	1.77	0.41
12:P:193:ASN:C	12:P:193:ASN:HD22	2.27	0.41
1:A:825:ILE:HD12	1:A:830:ILE:HD11	2.01	0.41
1:A:846:LEU:HD13	1:A:862:TRP:NE1	2.36	0.41
2:B:55:PRO:HB3	2:B:60:LEU:HD22	2.03	0.41
2:B:684:ILE:HD13	2:B:684:ILE:HA	1.95	0.41
2:B:984:PRO:HG2	2:B:987:LEU:HD22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:236:LEU:HD21	4:E:317:LEU:HB2	2.03	0.41
4:E:508:LYS:HB3	4:E:512:ASP:HB2	2.02	0.41
10:L:110:THR:HG23	10:L:112:GLU:HG3	2.02	0.41
4:e:225:ILE:HD12	4:e:236:LEU:HB3	2.02	0.41
1:A:413:ASP:O	1:A:414:ILE:C	2.63	0.41
5:F:396:LEU:HA	5:F:399:GLU:OE1	2.20	0.41
7:H:87:GLN:HA	7:H:88:PRO:HD3	1.82	0.41
12:P:297:LYS:HB3	12:P:298:PRO:HD3	2.03	0.41
15:k:130:PRO:HD3	16:m:35:GLU:HG2	2.02	0.41
1:A:464:TRP:CD1	1:A:464:TRP:C	2.96	0.41
1:A:464:TRP:CD1	1:A:464:TRP:O	2.74	0.41
2:B:646:ASP:OD1	2:B:646:ASP:N	2.54	0.41
5:F:274:ASN:HB2	5:F:317:LEU:N	2.30	0.41
5:F:329:LEU:HA	5:F:332:PHE:HB3	2.02	0.41
5:F:397:GLN:H	5:F:397:GLN:HG3	1.60	0.41
13:Q:15:ARG:HH21	13:Q:59:PHE:H	1.67	0.41
5:f:216:LEU:HD21	5:f:254:GLN:O	2.21	0.41
5:f:402:ARG:HH22	5:f:403:ILE:HD12	1.86	0.41
16:m:70:HIS:HA	16:m:73:MET:HE3	2.02	0.41
16:m:77:ARG:HB3	16:m:77:ARG:CZ	2.51	0.41
1:A:352:MET:HB3	1:A:352:MET:HE3	1.81	0.41
1:A:511:LEU:N	1:A:511:LEU:CD2	2.80	0.41
2:B:203:LYS:HZ3	2:B:235:HIS:HB3	1.86	0.41
2:B:987:LEU:HG	2:B:988:PRO:HD2	2.03	0.41
4:E:564:ASP:OD1	4:E:564:ASP:N	2.51	0.41
5:F:233:GLY:CA	5:F:239:ARG:HE	2.34	0.41
6:G:74:MET:HE1	6:G:136:ILE:HD12	2.02	0.41
7:H:47:GLU:OE1	7:H:113:ARG:NH2	2.54	0.41
9:J:192:LYS:N	9:J:192:LYS:CE	2.66	0.41
4:e:378:LYS:HZ3	4:e:378:LYS:HG2	1.63	0.41
4:e:633:THR:O	4:e:634:ARG:NH2	2.45	0.41
16:m:106:MET:HE3	16:m:106:MET:HB3	1.88	0.41
1:A:604:PRO:O	1:A:889:TYR:OH	2.34	0.41
1:A:620:LEU:HD11	1:A:766:ARG:HD3	2.02	0.41
2:B:68:LYS:HE2	2:B:68:LYS:HB3	1.98	0.41
3:D:976:GLN:NE2	3:D:976:GLN:HA	2.36	0.41
4:E:306:VAL:HG21	4:E:363:ALA:HA	2.03	0.41
3:d:963:ARG:HH22	3:d:964:GLU:HG2	1.86	0.41
1:A:511:LEU:N	1:A:511:LEU:HD13	2.36	0.40
1:A:725:CYS:SG	1:A:734:LEU:HD12	2.61	0.40
2:B:464:ILE:HG12	2:B:513:LYS:HE2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:761:LEU:HA	4:E:762:PRO:HD3	1.92	0.40
2:B:560:TYR:CE2	2:B:581:ILE:HD11	2.57	0.40
5:F:370:TRP:CH2	5:F:402:ARG:HB3	2.56	0.40
5:f:104:LEU:HD22	9:j:216:TYR:HB2	2.02	0.40
1:A:781:VAL:HG22	6:G:137:THR:HG21	2.04	0.40
1:A:899:LYS:HE3	1:A:899:LYS:HB2	1.81	0.40
1:A:939:ILE:HG22	1:A:943:LYS:NZ	2.37	0.40
2:B:77:ILE:HG12	2:B:146:ILE:HG23	2.03	0.40
5:F:374:TYR:CE1	5:F:422:HIS:HB3	2.56	0.40
8:I:129:LEU:HD12	9:J:120:LEU:HD23	2.04	0.40
10:L:111:LEU:HG	10:L:111:LEU:O	2.21	0.40
4:e:243:LEU:HD13	4:e:243:LEU:HA	1.73	0.40
4:e:246:HIS:CD2	4:e:246:HIS:C	2.98	0.40
4:e:465:THR:HA	4:e:795:GLY:HA3	2.04	0.40
16:m:93:ASP:OD1	16:m:93:ASP:C	2.63	0.40
4:E:476:VAL:HG11	4:E:794:ALA:HB3	2.02	0.40
5:F:329:LEU:HA	5:F:332:PHE:CB	2.52	0.40
5:F:350:ASN:O	5:F:354:ARG:NH1	2.54	0.40
2:B:402:ILE:HD12	2:B:455:LEU:HD12	2.03	0.40
2:B:749:LEU:HA	2:B:752:THR:HG22	2.02	0.40
3:D:945:LYS:HB3	3:D:945:LYS:HE3	1.85	0.40
7:H:194:MET:HE2	7:H:194:MET:HB2	1.85	0.40
12:P:194:PRO:C	12:P:196:ARG:N	2.79	0.40
3:d:892:THR:OG1	3:d:893:GLU:OE1	2.33	0.40
15:k:142:THR:OG1	15:k:143:GLY:N	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	533/1872 (28%)	514 (96%)	18 (3%)	1 (0%)	43 78

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	959/1199 (80%)	912 (95%)	47 (5%)	0	100	100
3	D	191/1085 (18%)	182 (95%)	9 (5%)	0	100	100
3	d	154/1085 (14%)	150 (97%)	4 (3%)	0	100	100
4	E	539/800 (67%)	515 (96%)	23 (4%)	1 (0%)	43	78
4	e	531/800 (66%)	482 (91%)	48 (9%)	1 (0%)	43	78
5	F	408/677 (60%)	390 (96%)	17 (4%)	1 (0%)	43	78
5	f	399/677 (59%)	383 (96%)	16 (4%)	0	100	100
6	G	138/349 (40%)	135 (98%)	3 (2%)	0	100	100
7	H	207/310 (67%)	193 (93%)	13 (6%)	1 (0%)	24	63
8	I	118/264 (45%)	115 (98%)	3 (2%)	0	100	100
8	i	119/264 (45%)	115 (97%)	4 (3%)	0	100	100
9	J	86/218 (39%)	82 (95%)	4 (5%)	0	100	100
9	j	91/218 (42%)	85 (93%)	4 (4%)	2 (2%)	5	29
10	L	74/161 (46%)	72 (97%)	2 (3%)	0	100	100
10	l	105/161 (65%)	100 (95%)	5 (5%)	0	100	100
11	O	95/109 (87%)	86 (90%)	9 (10%)	0	100	100
12	P	175/339 (52%)	165 (94%)	9 (5%)	1 (1%)	21	59
13	Q	97/376 (26%)	89 (92%)	8 (8%)	0	100	100
14	c	125/929 (14%)	116 (93%)	9 (7%)	0	100	100
15	k	96/211 (46%)	91 (95%)	5 (5%)	0	100	100
16	m	85/124 (68%)	82 (96%)	3 (4%)	0	100	100
All	All	5325/12228 (44%)	5054 (95%)	263 (5%)	8 (0%)	44	78

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	E	523	VAL
4	e	522	ASP
9	j	124	GLU
5	F	411	VAL
9	j	177	LYS
12	P	251	LEU
7	H	155	ASP
1	A	498	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	A	487/1665 (29%)	444 (91%)	43 (9%)	9	28
2	B	876/1083 (81%)	863 (98%)	13 (2%)	57	72
3	D	175/815 (22%)	167 (95%)	8 (5%)	24	45
3	d	146/815 (18%)	144 (99%)	2 (1%)	59	72
4	E	478/657 (73%)	465 (97%)	13 (3%)	39	61
4	e	475/657 (72%)	462 (97%)	13 (3%)	39	61
5	F	328/574 (57%)	309 (94%)	19 (6%)	18	40
5	f	322/574 (56%)	312 (97%)	10 (3%)	35	56
6	G	132/322 (41%)	124 (94%)	8 (6%)	17	38
7	H	178/270 (66%)	174 (98%)	4 (2%)	45	64
8	I	106/235 (45%)	106 (100%)	0	100	100
8	i	107/235 (46%)	107 (100%)	0	100	100
9	J	79/154 (51%)	72 (91%)	7 (9%)	9	28
9	j	83/154 (54%)	82 (99%)	1 (1%)	63	75
10	L	71/141 (50%)	66 (93%)	5 (7%)	14	35
10	l	98/141 (70%)	97 (99%)	1 (1%)	68	78
11	O	84/98 (86%)	84 (100%)	0	100	100
12	P	153/293 (52%)	150 (98%)	3 (2%)	48	66
13	Q	91/324 (28%)	89 (98%)	2 (2%)	45	64
14	c	113/833 (14%)	111 (98%)	2 (2%)	51	68
15	k	87/182 (48%)	87 (100%)	0	100	100
16	m	80/106 (76%)	71 (89%)	9 (11%)	5	19
All	All	4749/10328 (46%)	4586 (97%)	163 (3%)	33	54

All (163) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	348	LEU
1	A	353	LEU
1	A	395	ASP
1	A	397	LEU
1	A	400	GLU
1	A	401	ASN
1	A	403	LEU
1	A	404	MET
1	A	408	LEU
1	A	415	ILE
1	A	416	TRP
1	A	419	GLU
1	A	470	ILE
1	A	475	LEU
1	A	481	GLU
1	A	483	ASN
1	A	491	MET
1	A	499	VAL
1	A	500	LEU
1	A	501	THR
1	A	502	LEU
1	A	505	ASN
1	A	511	LEU
1	A	639	LEU
1	A	661	GLU
1	A	667	THR
1	A	711	ASP
1	A	727	THR
1	A	730	PHE
1	A	819	LYS
1	A	821	ARG
1	A	828	GLU
1	A	843	ARG
1	A	925	ASP
1	A	943	LYS
1	A	970	ASN
1	A	1052	ARG
1	A	1058	HIS
1	A	1062	TYR
1	A	1068	ARG
1	A	1073	GLN
1	A	1165	LEU
1	A	1203	GLU

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Mol	Chain	Res	Type
2	B	21	GLU
2	B	71	ARG
2	B	140	GLU
2	B	184	ASN
2	B	262	MET
2	B	266	THR
2	B	559	LYS
2	B	603	LYS
2	B	640	VAL
2	B	746	SER
2	B	771	VAL
2	B	818	THR
2	B	987	LEU
3	D	953	ILE
3	D	960	GLU
3	D	965	ILE
3	D	984	LEU
3	D	987	LYS
3	D	1000	ARG
3	D	1002	ARG
3	D	1006	LEU
4	E	258	ASN
4	E	274	TYR
4	E	278	ASP
4	E	280	ARG
4	E	326	ASN
4	E	327	ASN
4	E	519	GLU
4	E	521	ASP
4	E	522	ASP
4	E	527	ILE
4	E	761	LEU
4	E	774	MET
4	E	775	THR
5	F	83	LEU
5	F	91	PHE
5	F	94	PHE
5	F	261	THR
5	F	271	VAL
5	F	280	ILE
5	F	295	LEU
5	F	301	VAL

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Mol	Chain	Res	Type
5	F	312	ILE
5	F	317	LEU
5	F	326	HIS
5	F	340	ILE
5	F	348	THR
5	F	354	ARG
5	F	368	THR
5	F	397	GLN
5	F	406	VAL
5	F	415	ILE
5	F	427	LEU
6	G	41	ASP
6	G	129	LYS
6	G	131	ILE
6	G	143	VAL
6	G	153	LYS
6	G	181	TRP
6	G	182	GLU
6	G	183	ILE
7	H	27	ASP
7	H	36	THR
7	H	155	ASP
7	H	161	LYS
9	J	116	LEU
9	J	123	LEU
9	J	156	SER
9	J	164	SER
9	J	174	CYS
9	J	177	LYS
9	J	192	LYS
10	L	79	ASP
10	L	104	ARG
10	L	108	SER
10	L	113	VAL
10	L	114	LYS
12	P	172	VAL
12	P	206	GLU
12	P	280	PHE
13	Q	57	ASP
13	Q	331	THR
14	c	24	ASP
14	c	106	VAL

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Mol	Chain	Res	Type
3	d	950	LEU
3	d	951	ASP
4	e	243	LEU
4	e	258	ASN
4	e	268	HIS
4	e	270	ASP
4	e	277	ASP
4	e	282	LEU
4	e	436	ASP
4	e	438	LEU
4	e	512	ASP
4	e	515	LEU
4	e	516	ILE
4	e	546	VAL
4	e	579	VAL
5	f	215	GLU
5	f	253	TYR
5	f	261	THR
5	f	272	VAL
5	f	322	ASP
5	f	323	VAL
5	f	326	HIS
5	f	356	THR
5	f	366	GLU
5	f	421	ASP
9	j	114	THR
10	l	114	LYS
16	m	31	LEU
16	m	55	ASP
16	m	58	GLU
16	m	77	ARG
16	m	83	VAL
16	m	84	GLU
16	m	90	ILE
16	m	91	ARG
16	m	110	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (116) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	401	ASN
1	A	472	ASN

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Mol	Chain	Res	Type
1	A	489	GLN
1	A	590	GLN
1	A	630	GLN
1	A	687	ASN
1	A	693	GLN
1	A	702	ASN
1	A	755	HIS
1	A	802	HIS
1	A	860	ASN
1	A	896	GLN
1	A	1073	GLN
2	B	30	HIS
2	B	36	ASN
2	B	39	ASN
2	B	137	HIS
2	B	176	HIS
2	B	183	GLN
2	B	235	HIS
2	B	348	GLN
2	B	439	HIS
2	B	450	GLN
2	B	509	ASN
2	B	577	HIS
2	B	644	GLN
2	B	652	GLN
2	B	750	GLN
2	B	813	ASN
2	B	864	ASN
2	B	882	HIS
2	B	908	GLN
2	B	912	ASN
2	B	963	HIS
3	D	875	GLN
3	D	912	ASN
3	D	925	ASN
3	D	936	GLN
3	D	943	GLN
3	D	956	GLN
3	D	976	GLN
3	D	1053	GLN
3	D	1075	HIS
4	E	254	ASN

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Mol	Chain	Res	Type
4	E	256	HIS
4	E	258	ASN
4	E	327	ASN
4	E	351	GLN
4	E	585	ASN
4	E	616	HIS
4	E	640	ASN
4	E	673	HIS
4	E	733	ASN
4	E	758	HIS
4	E	800	GLN
5	F	37	GLN
5	F	59	HIS
5	F	79	ASN
5	F	89	GLN
5	F	119	ASN
5	F	221	GLN
5	F	270	ASN
5	F	273	GLN
5	F	275	ASN
5	F	326	HIS
6	G	10	HIS
6	G	48	HIS
6	G	133	ASN
6	G	142	ASN
7	H	24	ASN
7	H	142	HIS
7	H	145	HIS
8	I	21	GLN
8	I	38	GLN
8	I	98	GLN
9	J	210	ASN
10	L	117	GLN
11	O	27	GLN
11	O	31	GLN
11	O	63	ASN
12	P	189	ASN
12	P	193	ASN
12	P	279	GLN
13	Q	23	ASN
13	Q	48	ASN
13	Q	333	ASN

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Mol	Chain	Res	Type
14	c	19	GLN
14	c	27	GLN
14	c	50	HIS
3	d	912	ASN
3	d	943	GLN
4	e	246	HIS
4	e	320	HIS
4	e	336	HIS
4	e	368	ASN
4	e	420	ASN
4	e	424	GLN
4	e	640	ASN
4	e	733	ASN
5	f	30	GLN
5	f	64	GLN
5	f	119	ASN
5	f	134	HIS
5	f	273	GLN
5	f	325	ASN
9	j	172	GLN
9	j	173	HIS
15	k	186	HIS
15	k	199	GLN
15	k	202	ASN
15	k	205	HIS
10	l	73	ASN
10	l	86	GLN
10	l	105	HIS
10	l	119	HIS
16	m	107	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

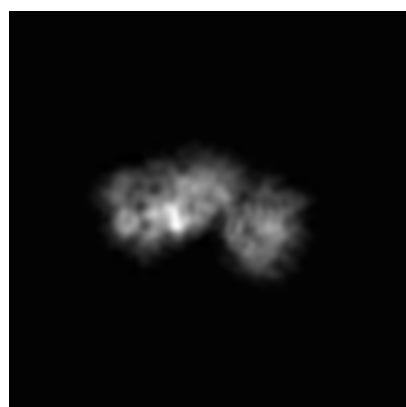
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31118. These allow visual inspection of the internal detail of the map and identification of artifacts.

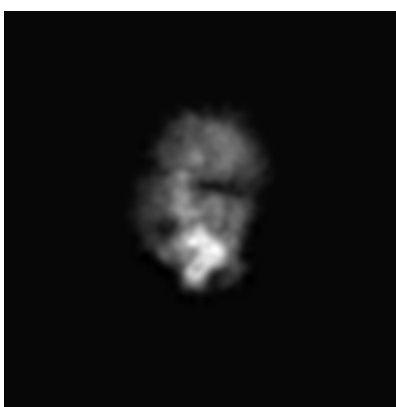
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

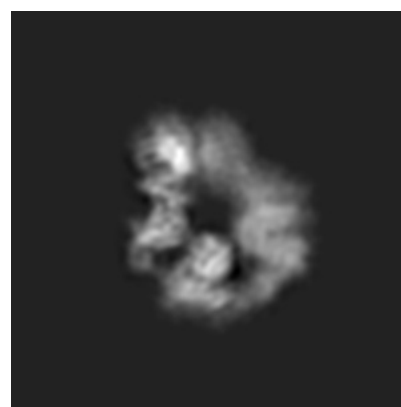
6.1.1 Primary map



X



Y

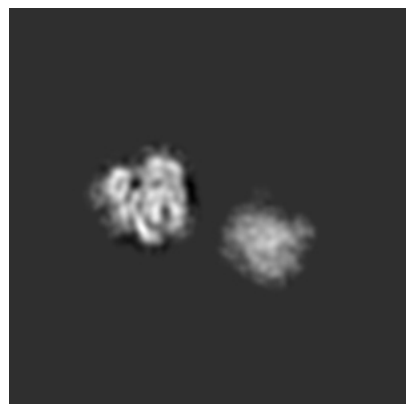


Z

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

6.2 Central slices [i](#)

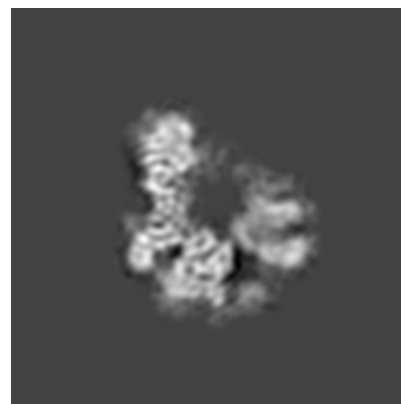
6.2.1 Primary map



X Index: 160



Y Index: 160



Z Index: 160

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

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 132



Y Index: 133

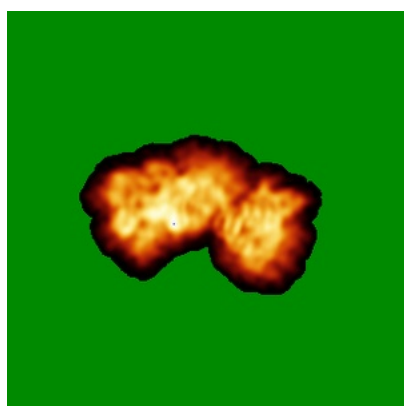


Z Index: 155

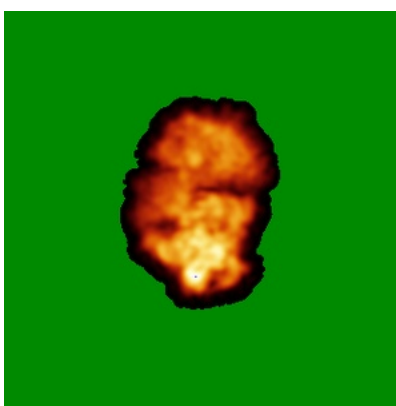
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



X



Y

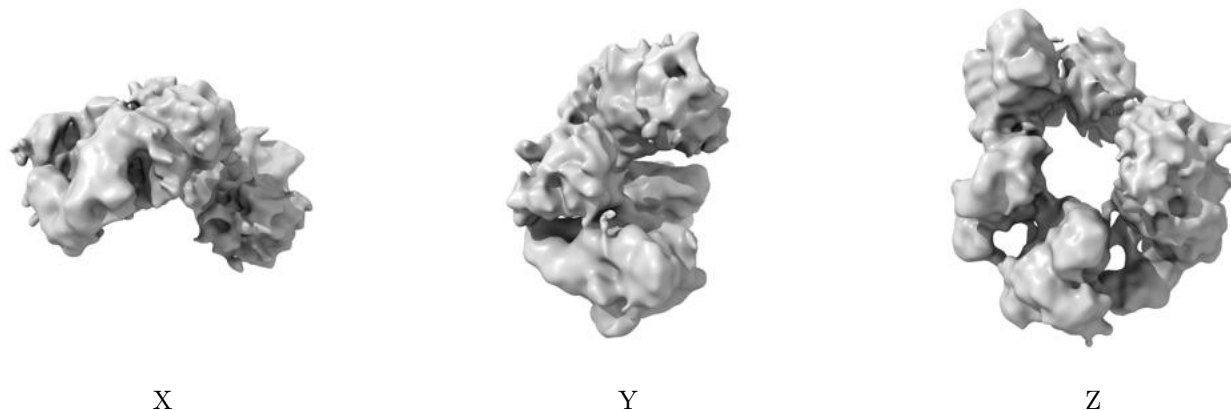


Z

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

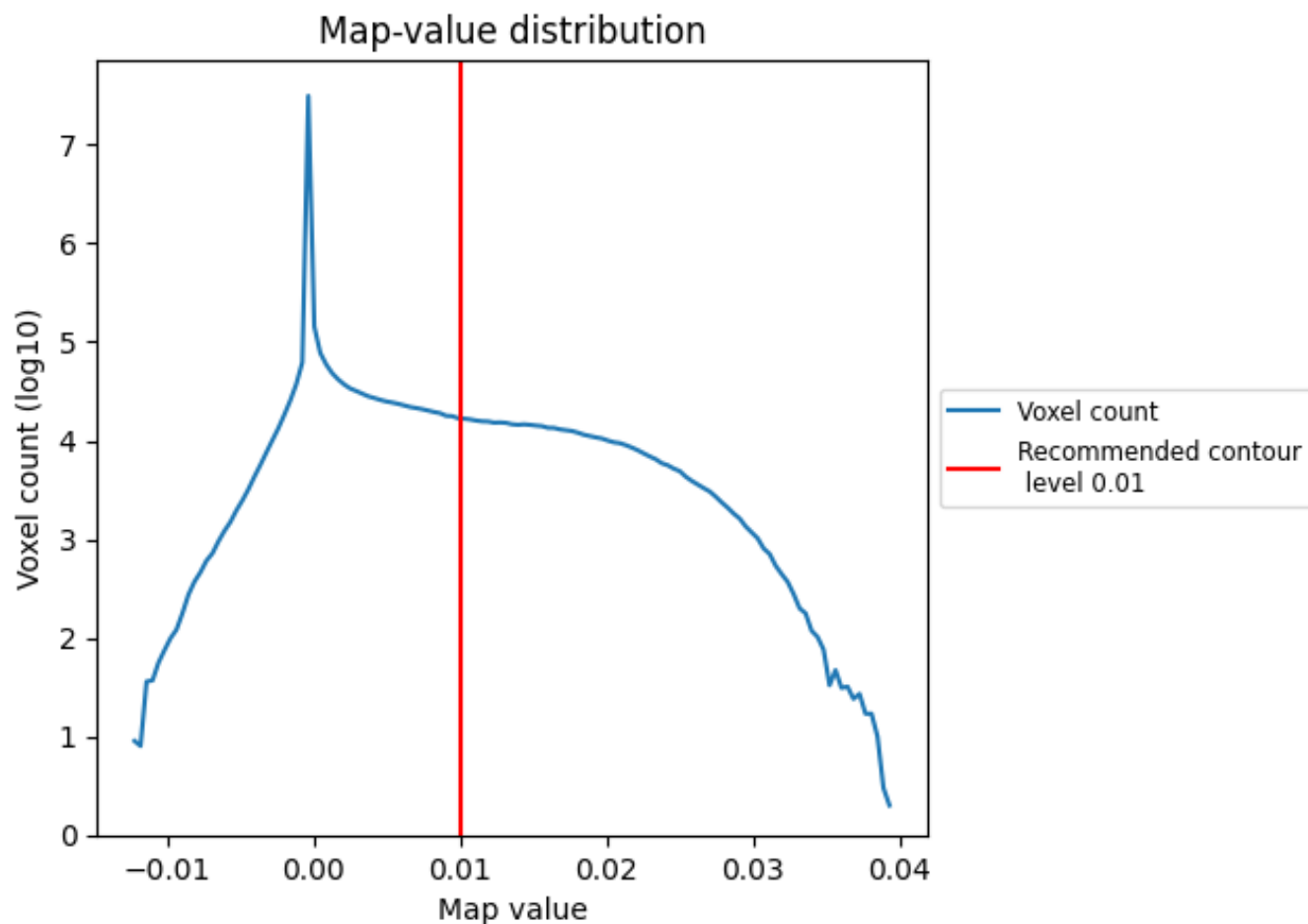
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

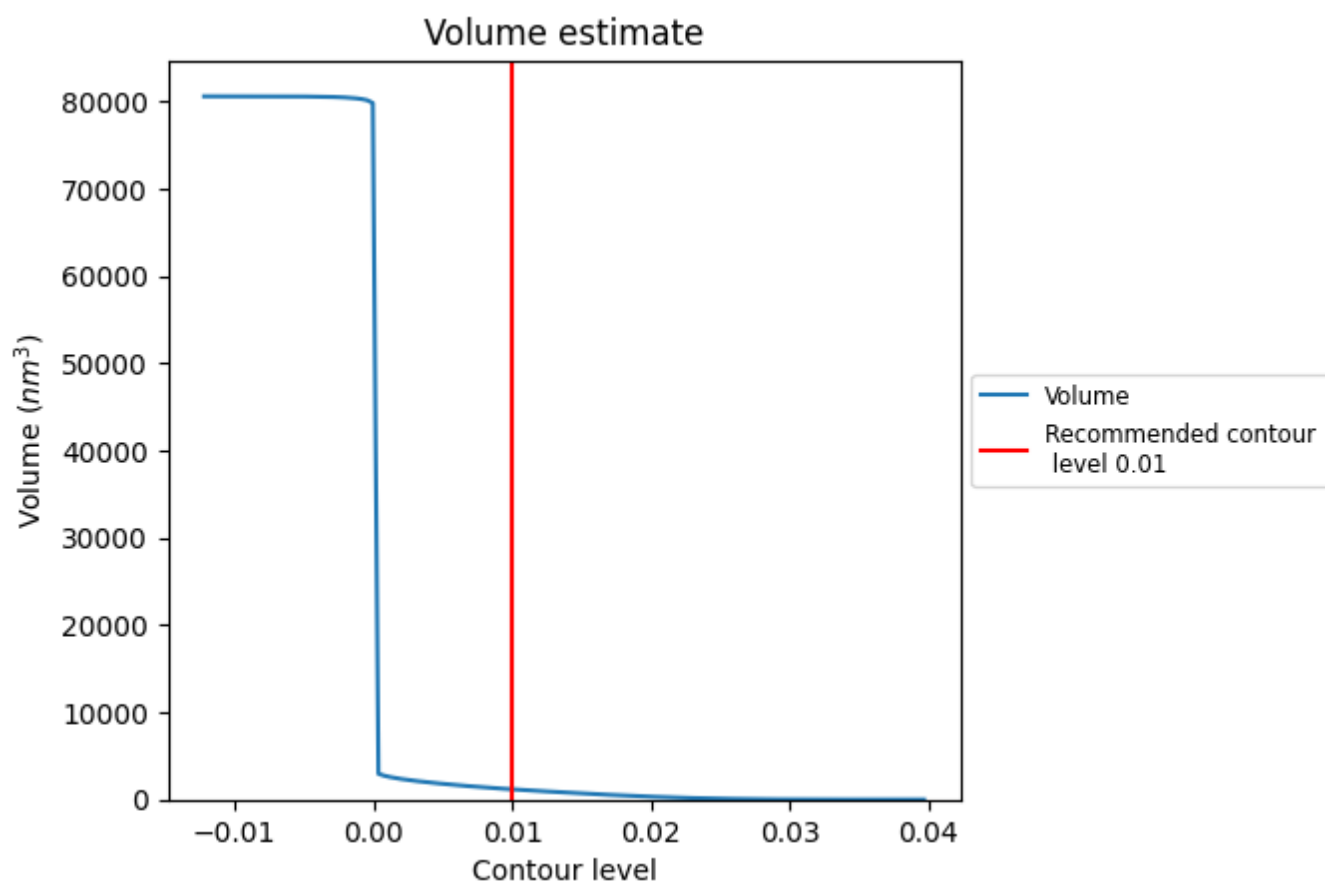
This section contains the results of statistical analysis of the map.

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.

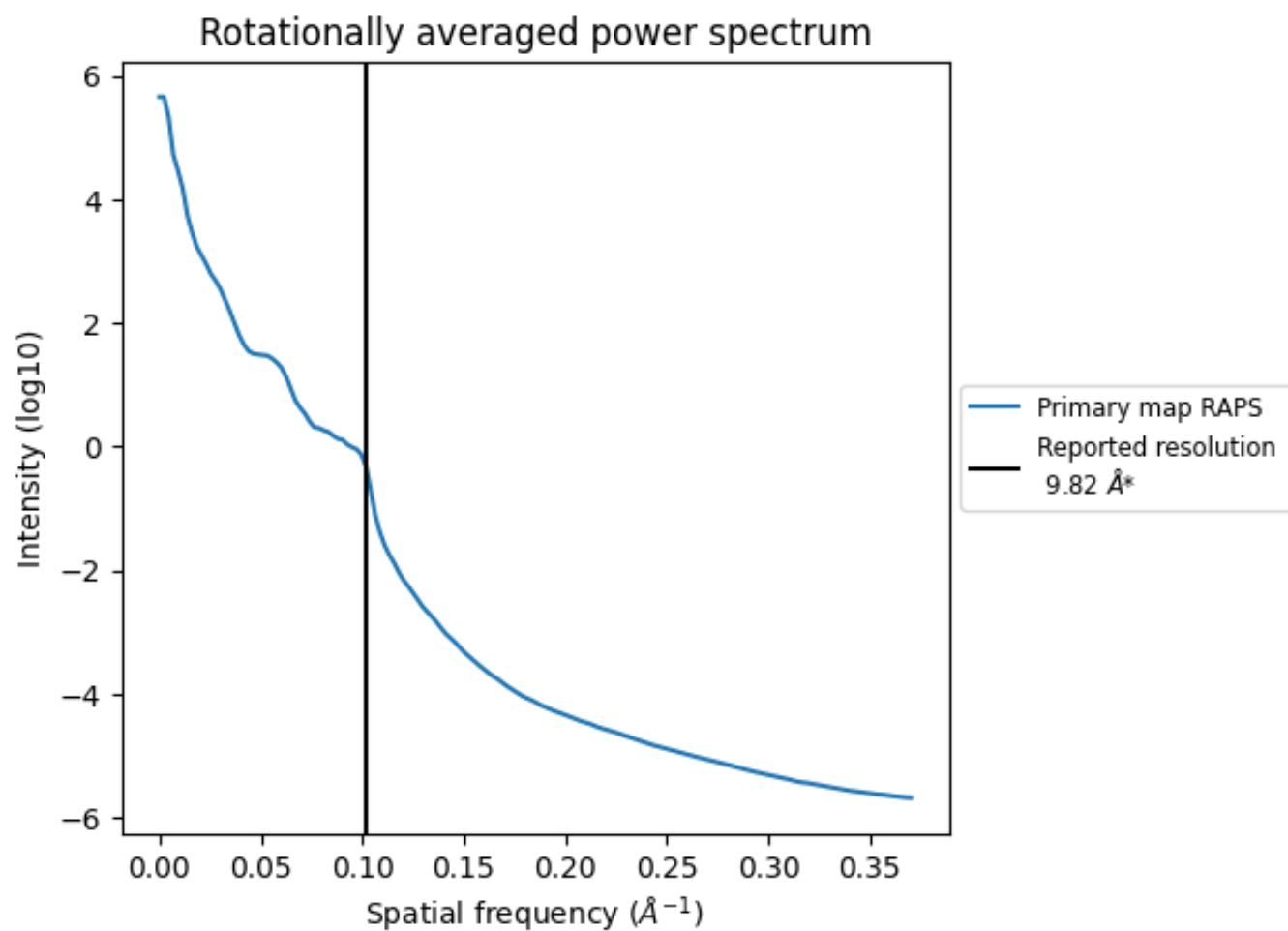
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1175 nm^3 ; this corresponds to an approximate mass of 1062 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 0.102 Å⁻¹

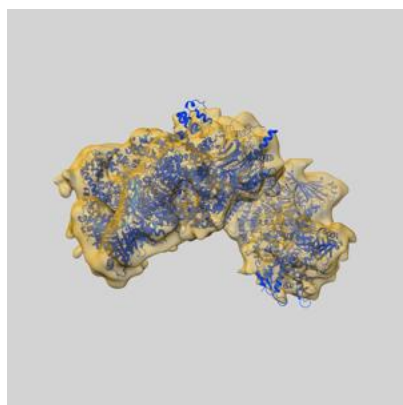
8 Fourier-Shell correlation

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

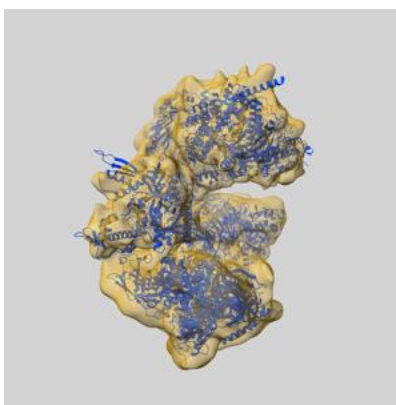
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-31118 and PDB model 7EGI. Per-residue inclusion information can be found in section [3](#) on page [7](#).

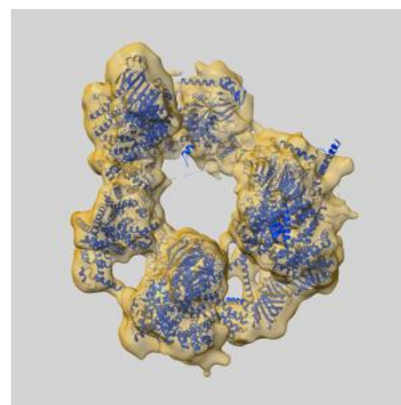
9.1 Map-model overlay [i](#)



X



Y



Z

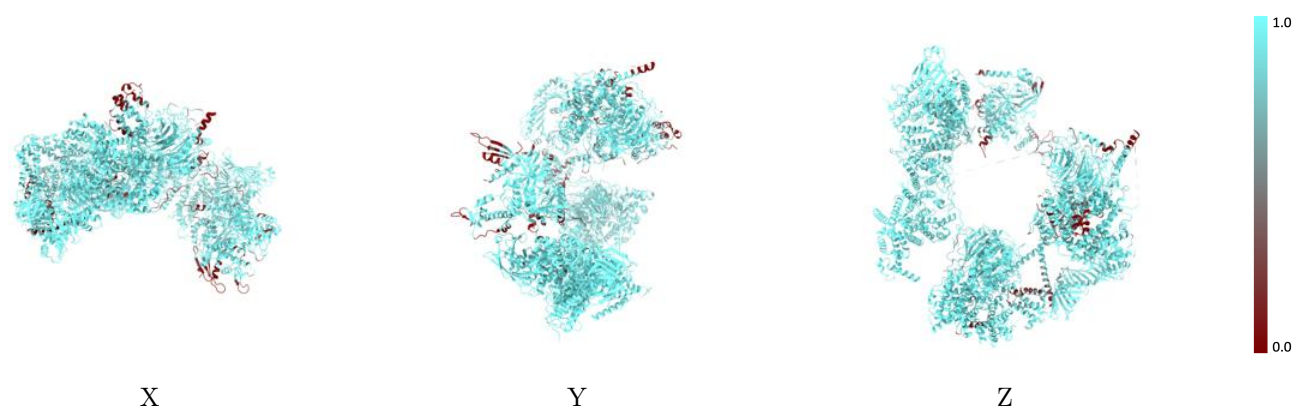
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



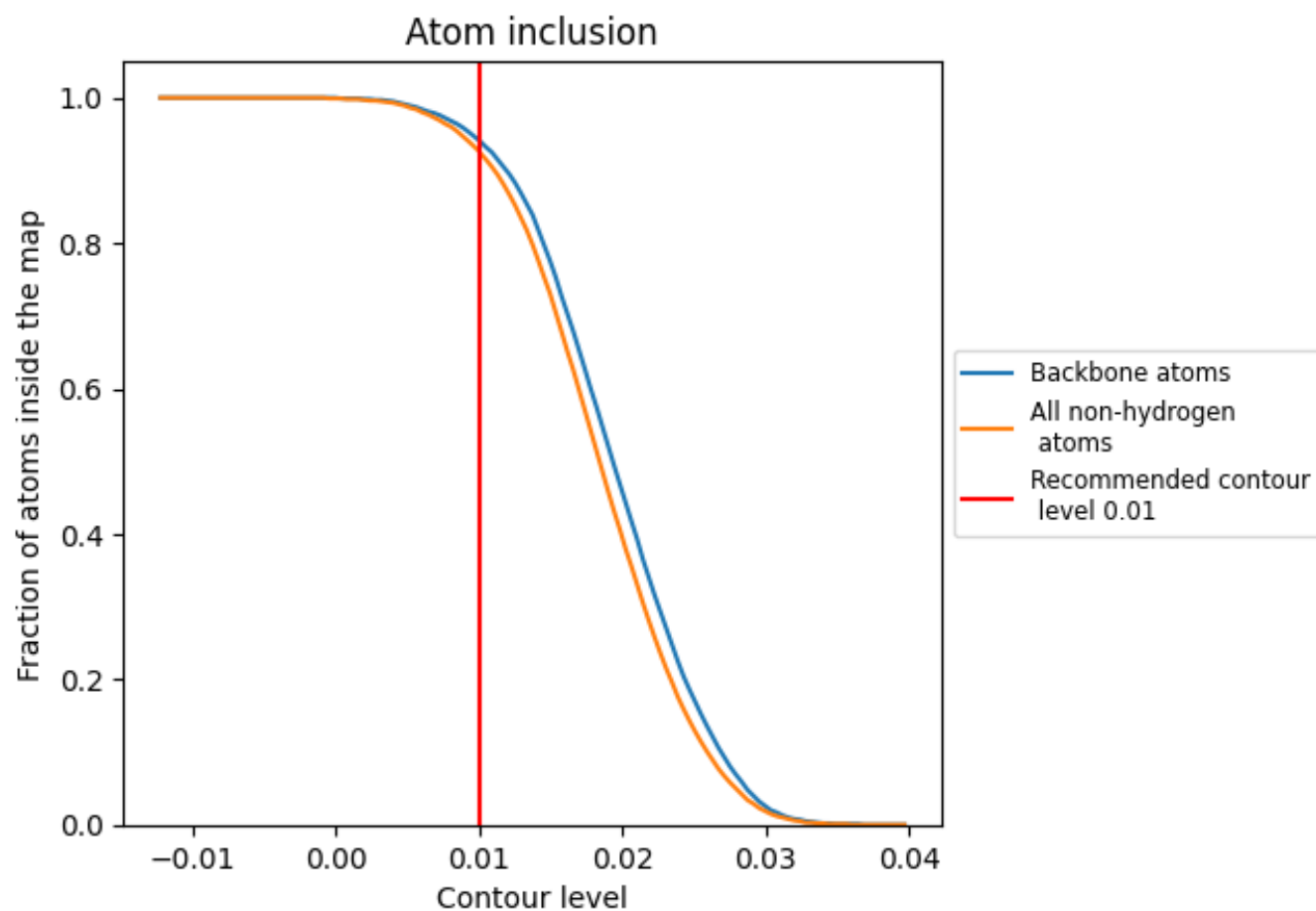
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 93% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9270	 0.0790
A	 0.8380	 0.0620
B	 0.9800	 0.0950
D	 0.8530	 0.0940
E	 0.9730	 0.0850
F	 0.9700	 0.1150
G	 0.8270	 0.0320
H	 0.9720	 0.1260
I	 0.9710	 0.1130
J	 0.9960	 0.1020
L	 0.9760	 0.1130
O	 0.7740	 0.0740
P	 0.9650	 0.0700
Q	 0.8870	 0.0520
c	 0.8690	 0.0420
d	 0.9030	 0.0490
e	 0.8480	 0.0310
f	 0.9590	 0.0980
i	 0.9780	 0.0700
j	 0.9660	 0.0590
k	 0.8960	 0.0510
l	 0.9700	 0.0740
m	 0.9500	 0.0700

