



Full wwPDB EM Validation Report ⓘ

Aug 8, 2026 – 08:02 am BST

PDB ID : 29VF / pdb_000029vf
EMDB ID : EMD-57390
Title : RNA polymerase II initially transcribing complex with a 2-nt RNA and the +1 nucleosome
Authors : Zhan, Y.; Abril-Garrido, J.; Dienemann, C.; Cramer, P.
Deposited on : 2026-04-09
Resolution : 7.50 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

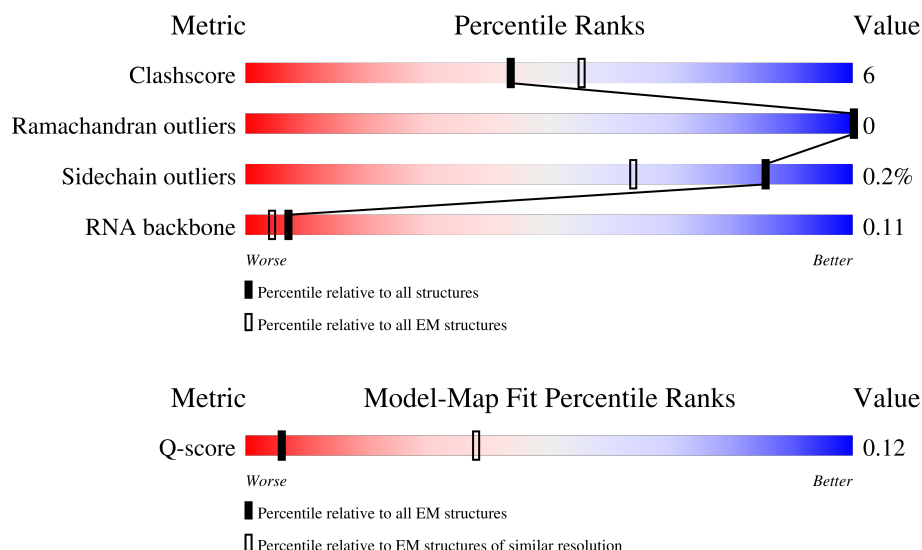
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.50

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 7.50 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	436 (7.00 - 8.00)

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

Mol	Chain	Length	Quality of chain
1	0	782	15% 67% 10% 23%
2	1	760	27% 75% 18% • 6%
3	2	548	32% 59% 8% 32%

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Mol	Chain	Length	Quality of chain
4	3	462	
5	4	395	
6	5	308	
7	6	71	
8	7	309	
9	A	1984	
10	B	1300	
11	C	275	
12	D	184	
13	E	210	
14	F	127	
15	G	172	
16	H	150	
17	I	125	
18	J	67	
19	K	117	
20	L	58	
21	M	316	
22	N	236	
23	O	339	
24	P	2	
25	Q	517	
26	R	249	
27	T	236	
28	U	376	

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Mol	Chain	Length	Quality of chain
29	V	109	
30	W	439	
31	X	291	
32	a	136	
32	e	136	
33	b	103	
33	f	103	
34	c	130	
34	g	130	
35	d	126	
35	h	126	

2 Entry composition [i](#)

There are 38 unique types of molecules in this entry. The entry contains 80190 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 General transcription and DNA repair factor IIIH helicase subunit XPB.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	605	Total	C	N	O	S	0	0
			4890	3127	848	885	30		

- Molecule 2 is a protein called TFIIH basal transcription factor complex helicase XPD subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	714	Total	C	N	O	S	0	0
			5751	3683	999	1040	29		

- Molecule 3 is a protein called General transcription factor IIIH subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	371	Total	C	N	O	S	0	0
			3016	1922	529	549	16		

- Molecule 4 is a protein called General transcription factor IIIH subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	421	Total	C	N	O	S	0	0
			3338	2154	584	587	13		

- Molecule 5 is a protein called General transcription factor IIIH subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	347	Total	C	N	O	S	0	0
			2732	1726	471	508	27		

- Molecule 6 is a protein called General transcription factor IIIH subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	5	263	Total	C	N	O	S	0	0
			2066	1323	344	380	19		

- Molecule 7 is a protein called General transcription factor IIIH subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	69	Total	C	N	O	S	0	0
			549	352	88	106	3		

- Molecule 8 is a protein called CDK-activating kinase assembly factor MAT1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	7	44	Total	C	N	O	S	0	0
			382	245	61	76			

- Molecule 9 is a protein called DNA-directed RNA polymerase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	A	1421	Total	C	N	O	S	0	0
			11257	7083	2013	2089	72		

- Molecule 10 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	B	1121	Total	C	N	O	S	0	0
			8971	5675	1574	1658	64		

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	C	257	Total	C	N	O	S	0	0
			2059	1294	351	408	6		

- Molecule 12 is a protein called RNA polymerase II subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	D	128	Total	C	N	O	S	0	0
			1050	656	178	212	4		

- Molecule 13 is a protein called DNA-directed RNA polymerase II subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	E	209	Total	C	N	O	S	0	0
			1721	1089	300	324	8		

- Molecule 14 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	F	79	Total	C	N	O	S	0	0
			636	406	108	117	5		

- Molecule 15 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	G	171	Total	C	N	O	S	0	0
			1351	875	219	249	8		

- Molecule 16 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	H	148	Total	C	N	O	S	0	0
			1186	750	194	237	5		

- Molecule 17 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	I	114	Total	C	N	O	S	0	0
			928	571	166	180	11		

- Molecule 18 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	J	64	Total	C	N	O	S	0	0
			507	328	86	87	6		

- Molecule 19 is a protein called DNA-directed RNA polymerase II subunit RPB11-a.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	K	115	Total	C	N	O	S	0	0
			920	593	152	173	2		

- Molecule 20 is a protein called RNA polymerase II subunit K.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	L	44	Total	C	N	O	S	0	0
			373	231	72	64	6		

- Molecule 21 is a protein called Transcription initiation factor IIB.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	M	298	Total	C	N	O	S	0	0
			2302	1435	409	440	18		

- Molecule 22 is a DNA chain called DNA (213-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
22	N	213	Total	C	N	O	P	0	0
			4375	2070	822	1270	213		

- Molecule 23 is a protein called TATA-box-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	O	179	Total	C	N	O	S	0	0
			1422	923	251	241	7		

- Molecule 24 is a RNA chain called RNA (5'-R(P*AP*C)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
24	P	2	Total	C	N	O	P	0	0
			42	19	8	13	2		

- Molecule 25 is a protein called General transcription factor IIF subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Q	138	Total	C	N	O	S	0	0
			1138	719	208	208	3		

- Molecule 26 is a protein called General transcription factor IIF subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	R	222	Total	C	N	O	S	0	0
			1788	1127	320	338	3		

- Molecule 27 is a DNA chain called DNA (227-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
27	T	227	Total	C	N	O	P	0	0
			4653	2205	855	1366	227		

- Molecule 28 is a protein called Transcription initiation factor IIA subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	U	113	Total	C	N	O	S	0	0
			931	585	152	190	4		

- Molecule 29 is a protein called Transcription initiation factor IIA subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	V	99	Total	C	N	O	S	0	0
			806	510	142	151	3		

- Molecule 30 is a protein called General transcription factor IIE subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	W	187	Total	C	N	O	S	0	0
			1535	964	275	285	11		

- Molecule 31 is a protein called Transcription initiation factor IIE subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	X	171	Total	C	N	O	S	0	0
			1403	895	243	261	4		

- Molecule 32 is a protein called Histone H3.2.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	a	97	Total	C	N	O	S	0	0
			801	505	155	138	3		
32	e	98	Total	C	N	O	S	0	0
			810	511	157	139	3		

- Molecule 33 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	b	82	Total	C	N	O	S	0	0
			653	412	127	113	1		
33	f	82	Total	C	N	O	S	0	0
			653	412	127	113	1		

- Molecule 34 is a protein called Histone H2A type 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	c	109	Total	C	N	O		0	0
			843	531	167	145			

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Mol	Chain	Residues	Atoms				AltConf	Trace
34	g	106	Total	C	N	O	0	0
			818	516	160	142		

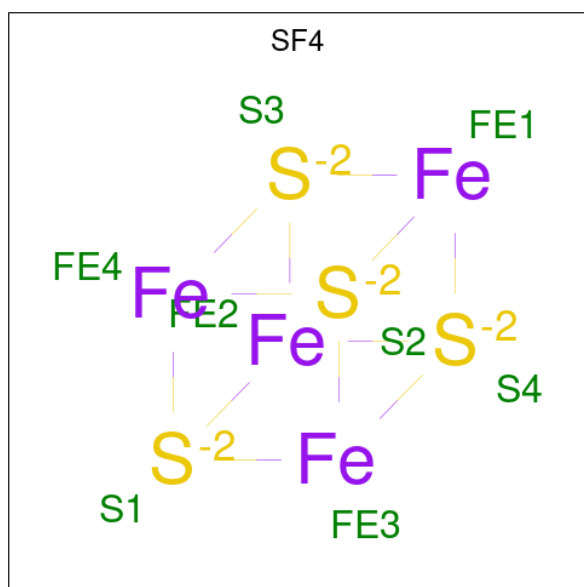
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
c	100	ARG	GLY	engineered mutation	UNP P06897
g	100	ARG	GLY	engineered mutation	UNP P06897

- Molecule 35 is a protein called Histone H2B 1.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	d	97	Total	C	N	O	S	0	0
			766	480	142	142	2		
35	h	95	Total	C	N	O	S	0	0
			744	468	134	140	2		

- Molecule 36 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
36	1	1	Total	Fe	S	0
			8	4	4	

- Molecule 37 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
37	4	4	Total 4	Zn 4	0
37	5	1	Total 1	Zn 1	0
37	A	2	Total 2	Zn 2	0
37	B	1	Total 1	Zn 1	0
37	C	1	Total 1	Zn 1	0
37	I	2	Total 2	Zn 2	0
37	J	1	Total 1	Zn 1	0
37	L	1	Total 1	Zn 1	0
37	M	1	Total 1	Zn 1	0
37	W	1	Total 1	Zn 1	0

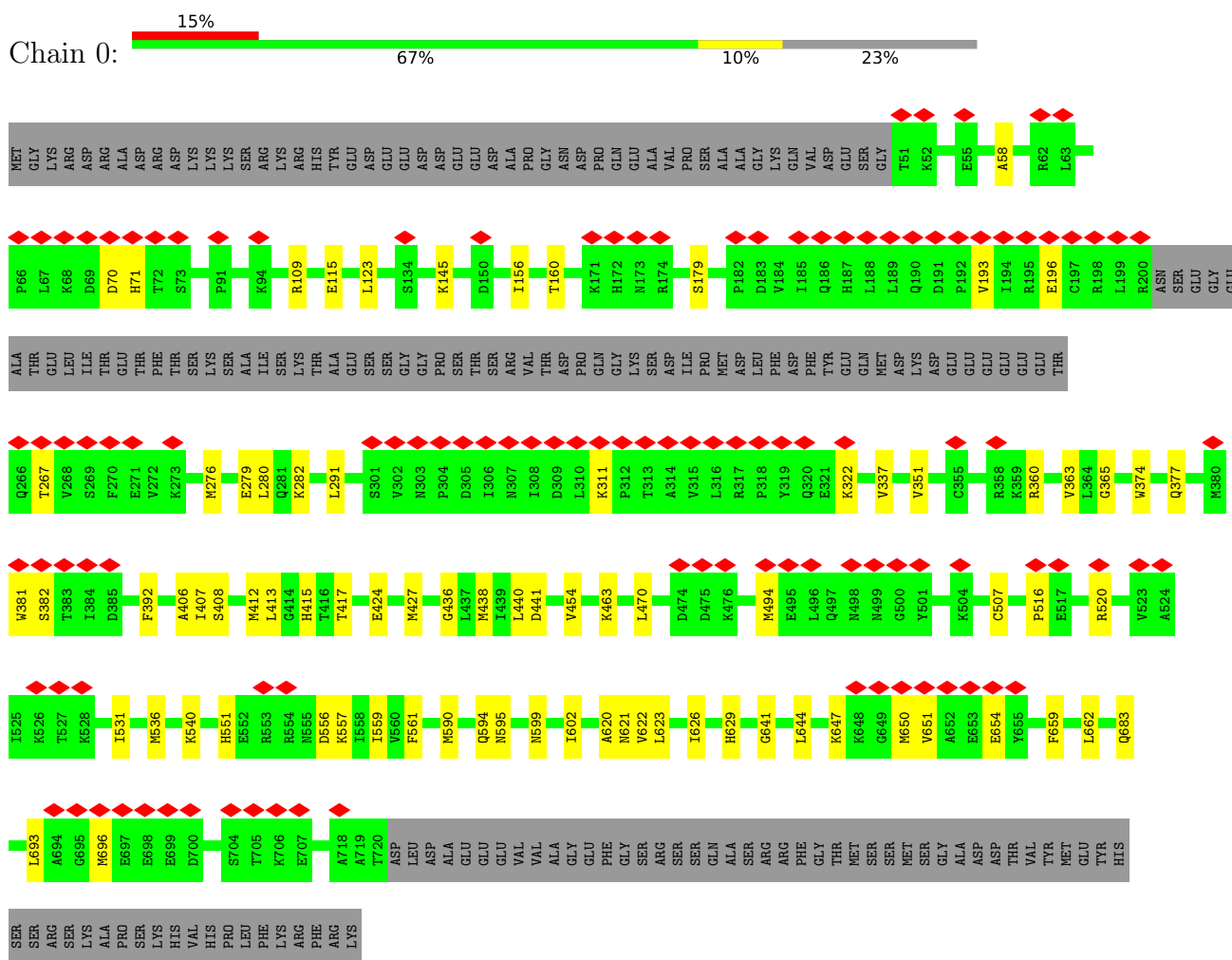
- Molecule 38 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
38	A	1	Total 1	Mg 1	0

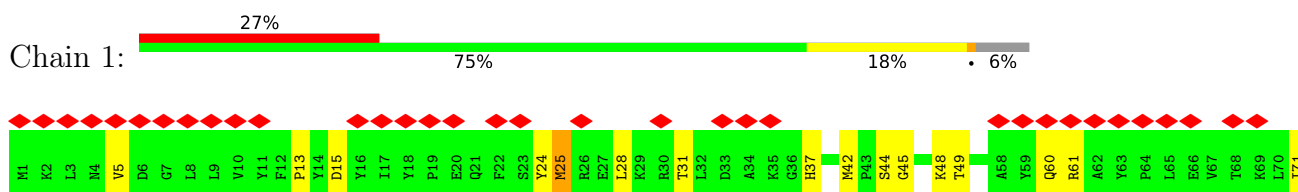
3 Residue-property plots

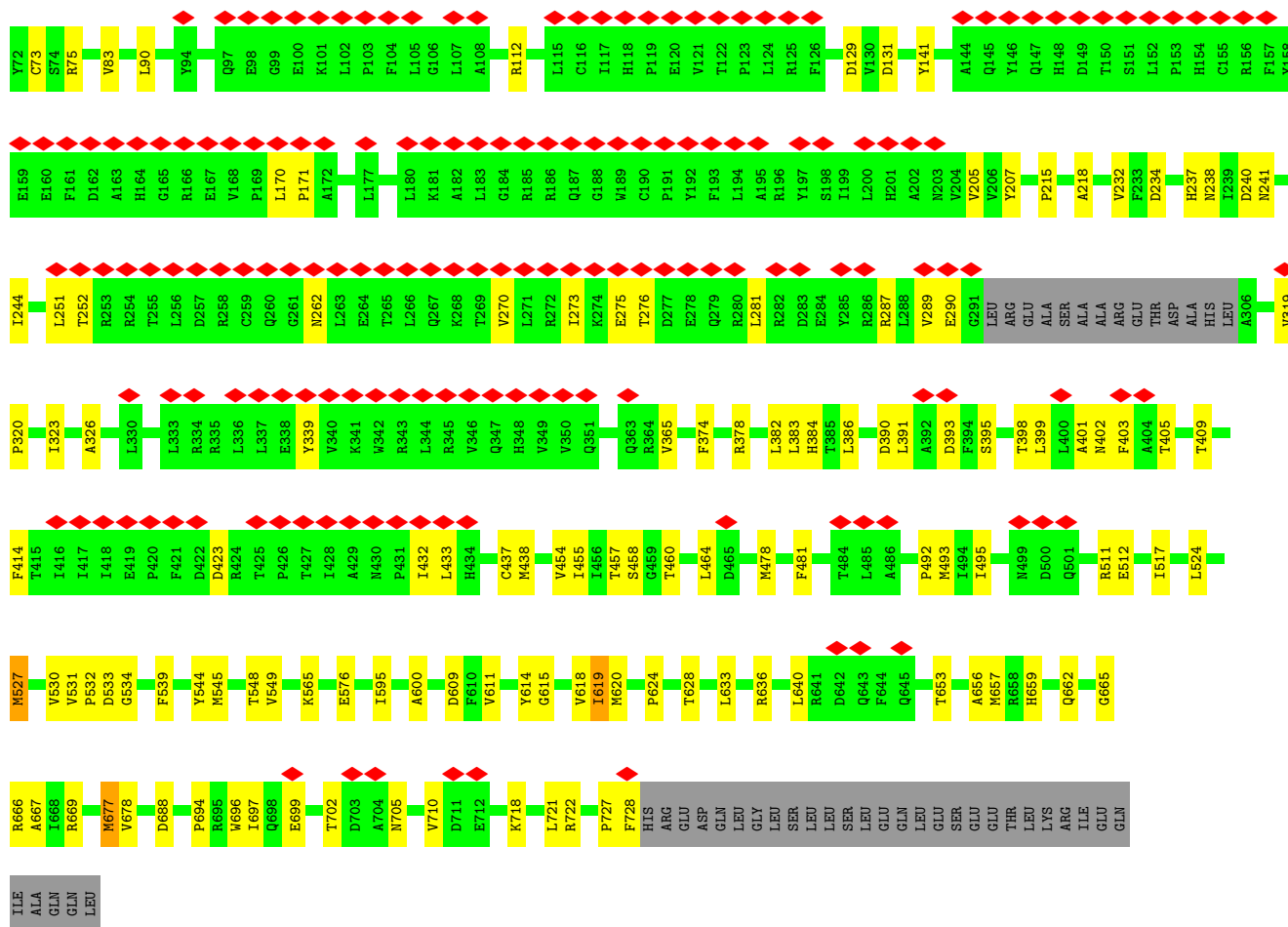
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: General transcription and DNA repair factor IIH helicase subunit XPB

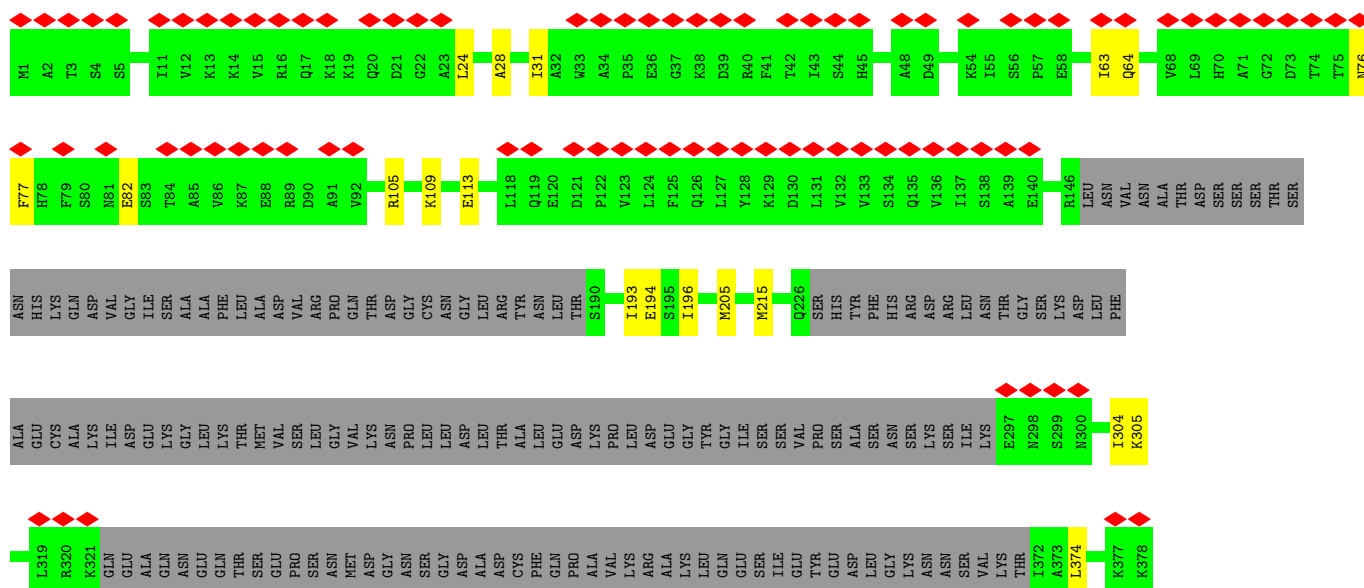


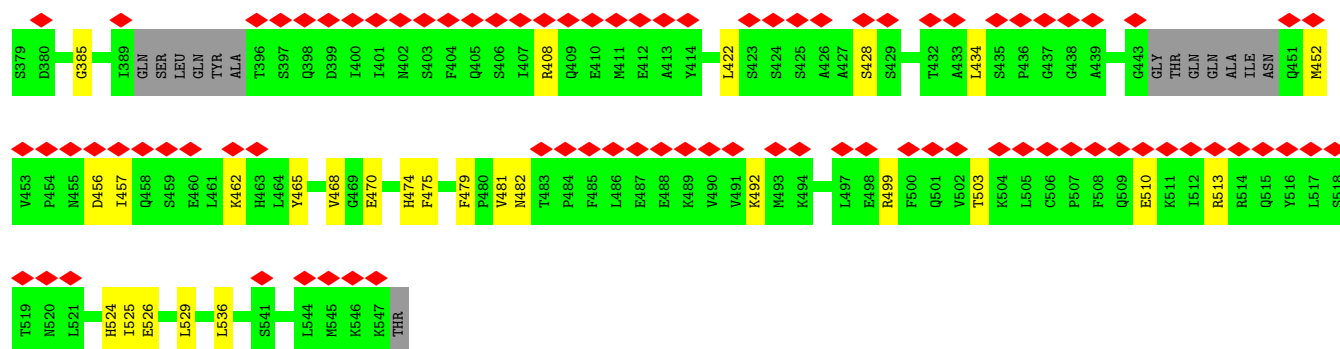
- Molecule 2: TFIIH basal transcription factor complex helicase XPD subunit



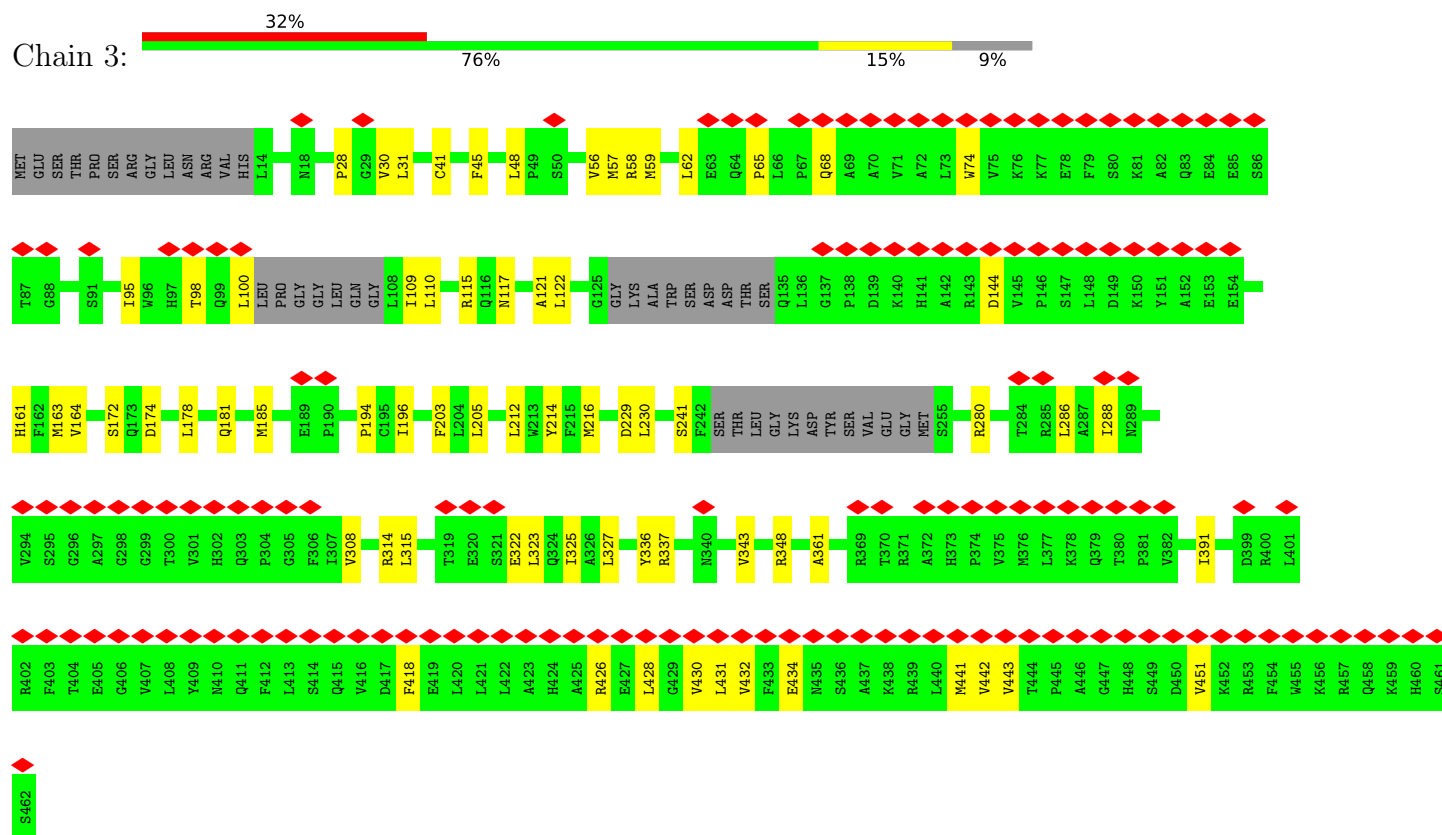


• Molecule 3: General transcription factor IIH subunit 1

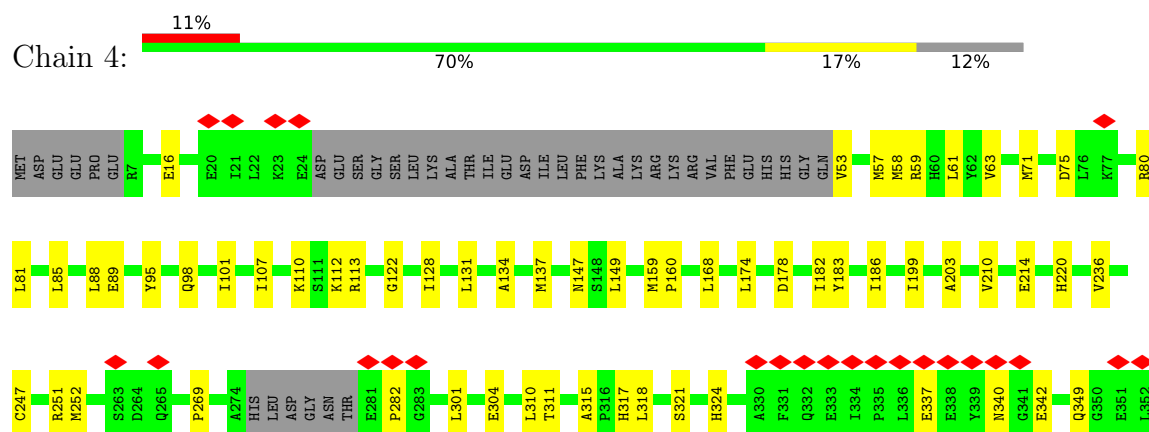




• Molecule 4: General transcription factor IIH subunit 4



• Molecule 5: General transcription factor IIH subunit 2



Chain A: 58% 13% 28%

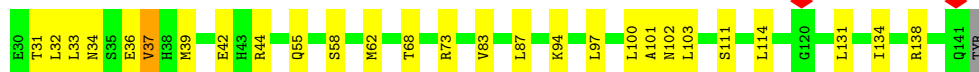
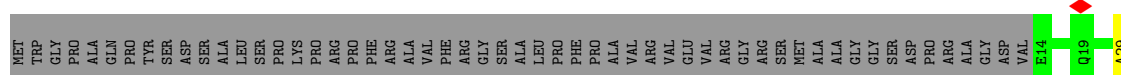






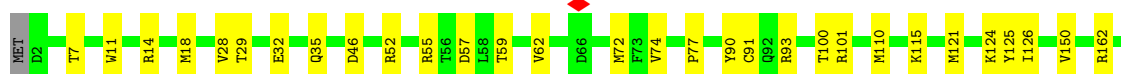
• Molecule 12: RNA polymerase II subunit D

Chain D:  54% 15% 30%



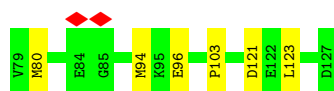
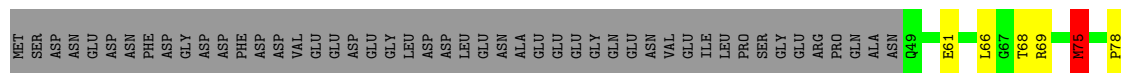
• Molecule 13: DNA-directed RNA polymerase II subunit E

Chain E:  84% 16%



• Molecule 14: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F:  53% 9% 38%



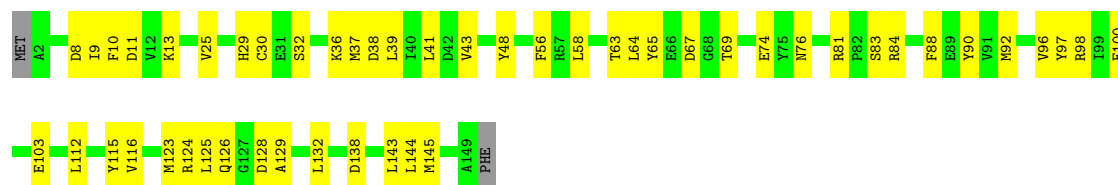
• Molecule 15: DNA-directed RNA polymerase II subunit RPB7

Chain G:  74% 25%

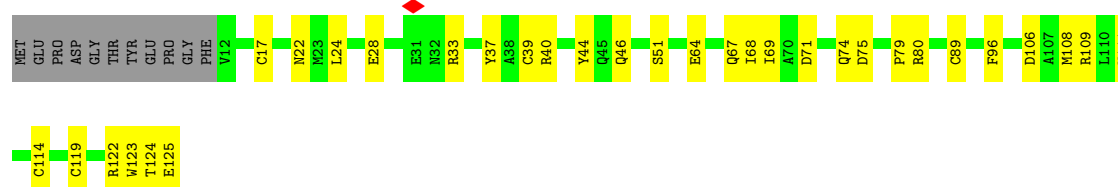


• Molecule 16: DNA-directed RNA polymerases I, II, and III subunit RPABC3

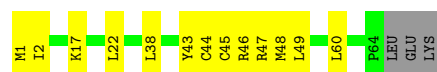
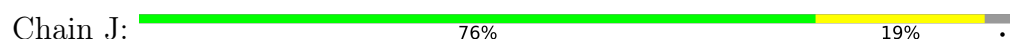
Chain H:  65% 33%



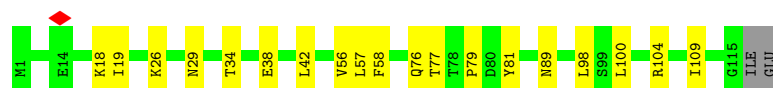
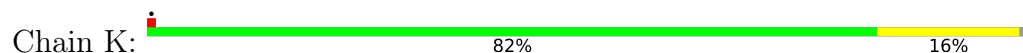
- Molecule 17: DNA-directed RNA polymerase II subunit RPB9



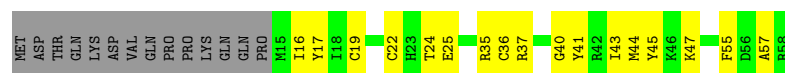
- Molecule 18: DNA-directed RNA polymerases I, II, and III subunit RPABC5



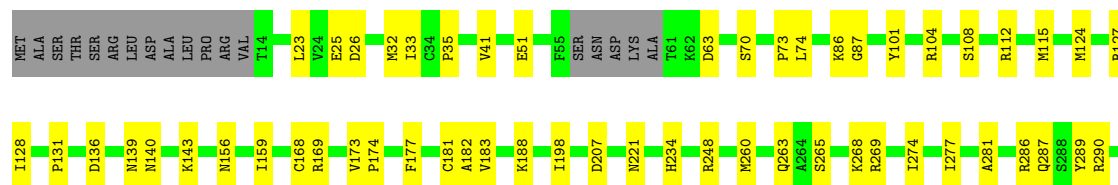
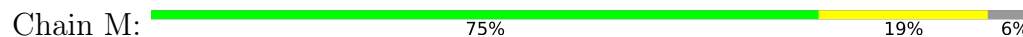
- Molecule 19: DNA-directed RNA polymerase II subunit RPB11-a



- Molecule 20: RNA polymerase II subunit K

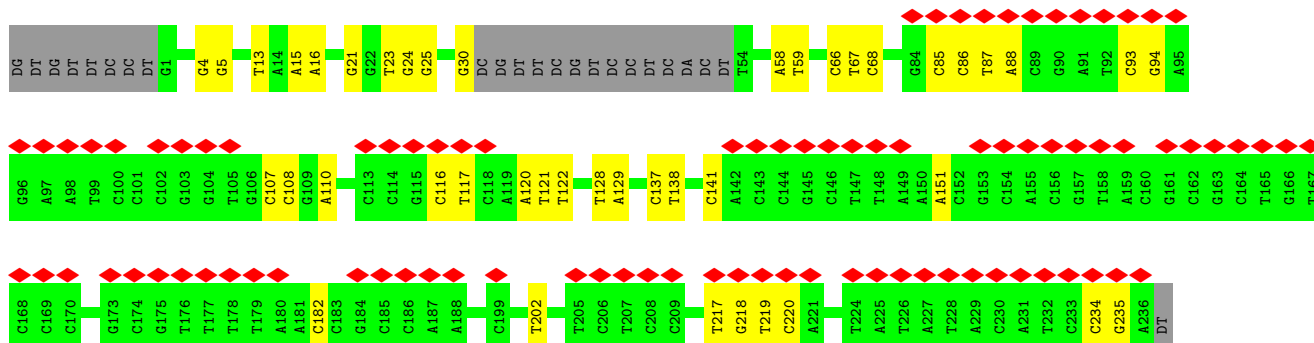
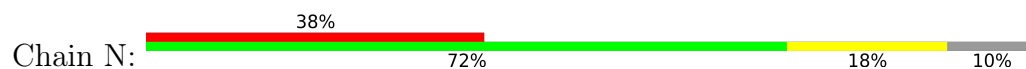


- Molecule 21: Transcription initiation factor IIB

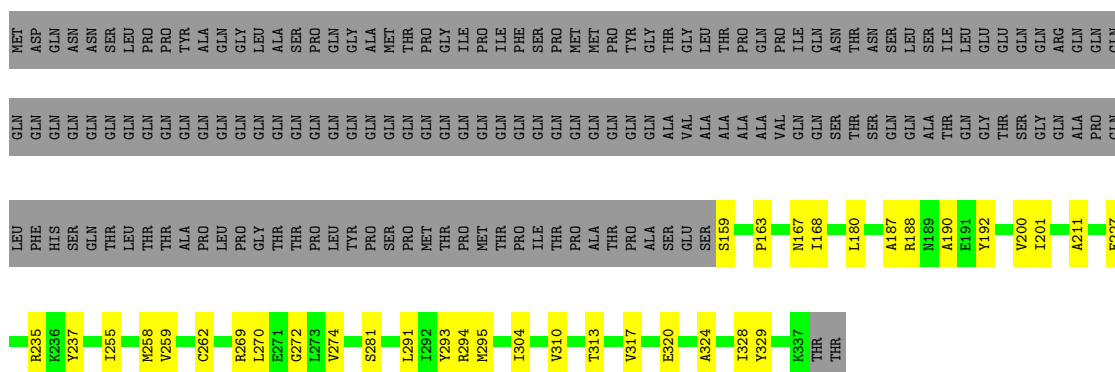




• Molecule 22: DNA (213-MER)



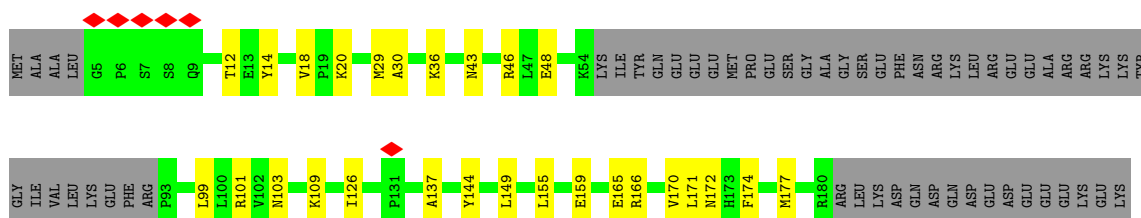
• Molecule 23: TATA-box-binding protein

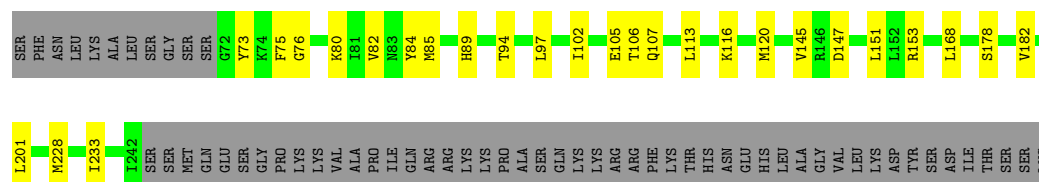


• Molecule 24: RNA (5'-R(P*AP*C)-3')



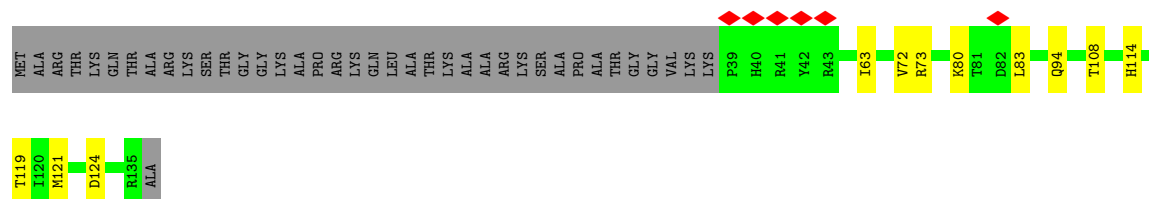
• Molecule 25: General transcription factor IIF subunit 1





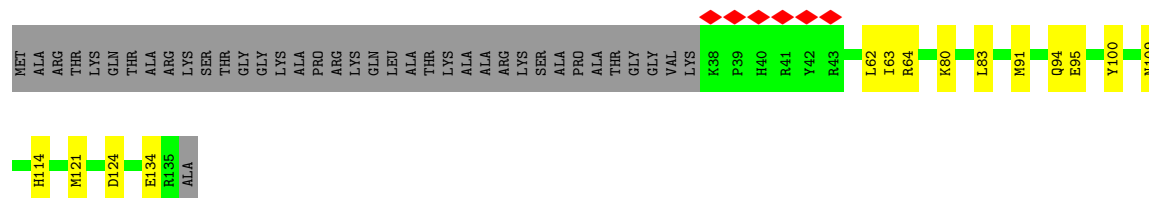
- Molecule 32: Histone H3.2

Chain a: 63% 8% 29%



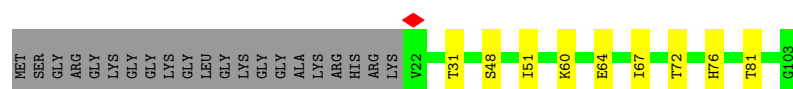
- Molecule 32: Histone H3.2

Chain e: 62% 10% 28%



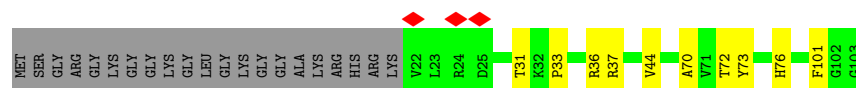
- Molecule 33: Histone H4

Chain b: 71% 9% 20%



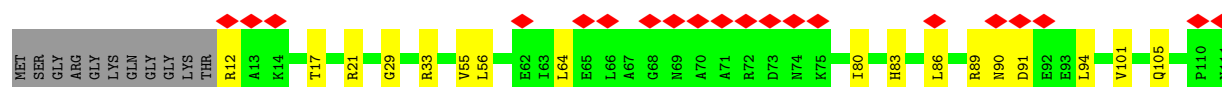
- Molecule 33: Histone H4

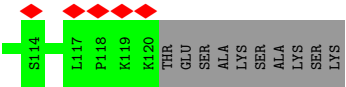
Chain f: 70% 10% 20%



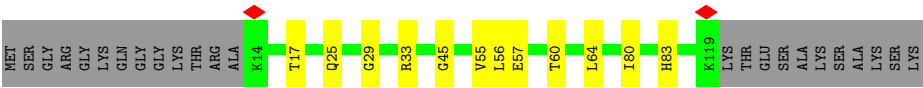
- Molecule 34: Histone H2A type 1

Chain c: 19% 71% 13% 16%

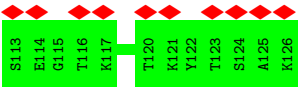
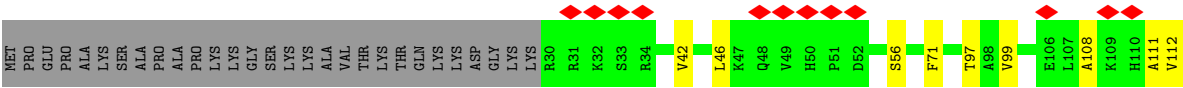




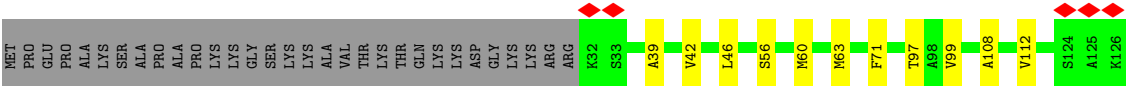
• Molecule 34: Histone H2A type 1



• Molecule 35: Histone H2B 1.1



• Molecule 35: Histone H2B 1.1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	5015	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	1700	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.019	Depositor
Minimum map value	-0.002	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.00432	Depositor
Map size (Å)	503.99997, 503.99997, 503.99997	wwPDB
Map dimensions	480, 480, 480	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

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, ZN, MG

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	0	0.18	0/4994	0.49	1/6745 (0.0%)
2	1	0.23	0/5875	0.57	3/7955 (0.0%)
3	2	0.20	0/3073	0.50	0/4132
4	3	0.20	0/3412	0.54	6/4622 (0.1%)
5	4	0.20	0/2793	0.53	0/3780
6	5	0.18	0/2103	0.46	0/2846
7	6	0.18	0/555	0.48	0/747
8	7	0.15	0/387	0.38	0/519
9	A	0.20	0/11462	0.53	9/15473 (0.1%)
10	B	0.21	0/9149	0.54	6/12349 (0.0%)
11	C	0.23	0/2102	0.47	0/2857
12	D	0.18	0/1064	0.48	0/1428
13	E	0.21	0/1752	0.51	1/2366 (0.0%)
14	F	0.25	0/646	0.61	1/871 (0.1%)
15	G	0.19	0/1382	0.52	0/1874
16	H	0.22	0/1207	0.55	0/1628
17	I	0.20	0/949	0.55	0/1284
18	J	0.20	0/516	0.46	0/696
19	K	0.19	0/939	0.40	0/1271
20	L	0.22	0/378	0.54	0/500
21	M	0.21	0/2338	0.55	4/3154 (0.1%)
22	N	0.21	0/4911	0.48	0/7576
23	O	0.20	0/1448	0.50	0/1948
24	P	0.16	0/46	0.95	0/69
25	Q	0.17	0/1167	0.45	1/1576 (0.1%)
26	R	0.15	0/1817	0.41	0/2445
27	T	0.21	0/5218	0.47	0/8052
28	U	0.20	0/946	0.52	0/1274
29	V	0.15	0/816	0.39	0/1105
30	W	0.20	0/1560	0.48	0/2097
31	X	0.20	0/1427	0.55	1/1916 (0.1%)
32	a	0.18	0/813	0.43	0/1090

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	e	0.19	0/822	0.42	0/1102
33	b	0.16	0/660	0.38	0/883
33	f	0.16	0/660	0.46	0/883
34	c	0.15	0/853	0.36	0/1149
34	g	0.16	0/828	0.40	0/1117
35	d	0.16	0/777	0.41	0/1041
35	h	0.16	0/755	0.38	0/1013
All	All	0.20	0/82600	0.50	33/113433 (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
2	1	0	1
14	F	0	1
All	All	0	2

There are no bond length outliers.

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	M	115	MET	CA-CB-CG	7.32	128.75	114.10
9	A	1292	MET	CB-CG-SD	7.00	133.70	112.70
4	3	59	MET	CB-CG-SD	6.95	133.54	112.70
21	M	115	MET	CB-CG-SD	6.51	132.24	112.70
10	B	368	MET	CA-CB-CG	6.22	126.53	114.10
21	M	124	MET	CA-CB-CG	5.96	126.02	114.10
14	F	75	MET	CA-CB-CG	5.83	125.75	114.10
2	1	544	TYR	CA-CB-CG	5.80	124.33	113.90
4	3	144	ASP	CA-C-N	5.70	123.83	120.24
4	3	144	ASP	C-N-CA	5.70	123.83	120.24
21	M	124	MET	CB-CG-SD	5.64	129.62	112.70
31	X	120	MET	CA-CB-CG	-5.58	102.93	114.10
1	0	276	MET	CA-CB-CG	5.50	125.11	114.10
10	B	976	MET	CA-CB-CG	5.44	124.99	114.10
4	3	59	MET	CA-CB-CG	5.44	124.98	114.10
9	A	524	MET	CB-CA-C	5.40	119.71	111.02
10	B	1075	MET	CA-CB-CG	5.31	124.72	114.10
2	1	677	MET	CA-CB-CG	5.28	124.66	114.10
10	B	53	MET	CB-CG-SD	5.22	128.38	112.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1	533	ASP	CB-CA-C	-5.21	110.59	116.63
4	3	58	ARG	CA-C-N	-5.20	114.36	122.73
4	3	58	ARG	C-N-CA	-5.20	114.36	122.73
9	A	768	SER	CA-C-N	-5.17	112.09	121.14
9	A	768	SER	C-N-CA	-5.17	112.09	121.14
9	A	266	MET	CB-CG-SD	5.17	128.20	112.70
9	A	524	MET	CA-CB-CG	5.16	124.42	114.10
25	Q	29	MET	CA-CB-CG	5.15	124.40	114.10
9	A	1405	MET	N-CA-CB	5.05	117.54	110.56
9	A	520	MET	CA-C-N	5.05	125.28	120.43
9	A	520	MET	C-N-CA	5.05	125.28	120.43
10	B	368	MET	N-CA-CB	5.04	118.76	110.39
13	E	57	ASP	N-CA-C	-5.04	108.17	114.56
10	B	840	MET	CB-CG-SD	5.01	127.73	112.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	1	619	ILE	Peptide
14	F	75	MET	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	4890	0	4949	49	0
2	1	5751	0	5798	86	0
3	2	3016	0	3065	33	0
4	3	3338	0	3343	45	0
5	4	2732	0	2704	47	0
6	5	2066	0	2102	21	0
7	6	549	0	558	8	0
8	7	382	0	380	1	0
9	A	11257	0	11398	185	0
10	B	8971	0	8999	149	0
11	C	2059	0	2007	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	D	1050	0	1033	21	0
13	E	1721	0	1737	24	0
14	F	636	0	665	9	0
15	G	1351	0	1358	30	0
16	H	1186	0	1147	38	0
17	I	928	0	861	27	0
18	J	507	0	523	8	0
19	K	920	0	942	15	0
20	L	373	0	378	12	0
21	M	2302	0	2316	40	0
22	N	4375	0	2386	38	0
23	O	1422	0	1514	28	0
24	P	42	0	22	1	0
25	Q	1138	0	1103	19	0
26	R	1788	0	1819	26	0
27	T	4653	0	2548	33	0
28	U	931	0	888	15	0
29	V	806	0	818	14	0
30	W	1535	0	1539	24	0
31	X	1403	0	1428	21	0
32	a	801	0	839	9	0
32	e	810	0	851	11	0
33	b	653	0	696	7	0
33	f	653	0	696	8	0
34	c	843	0	908	15	0
34	g	818	0	877	11	0
35	d	766	0	797	9	0
35	h	744	0	771	11	0
36	1	8	0	0	0	0
37	4	4	0	0	0	0
37	5	1	0	0	0	0
37	A	2	0	0	0	0
37	B	1	0	0	0	0
37	C	1	0	0	0	0
37	I	2	0	0	0	0
37	J	1	0	0	0	0
37	L	1	0	0	0	0
37	M	1	0	0	0	0
37	W	1	0	0	0	0
38	A	1	0	0	0	0
All	All	80190	0	76763	1017	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 6.

All (1017) 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)
1:0:424:GLU:O	1:0:427:MET:HB2	1.80	0.81
9:A:74:CYS:SG	9:A:81:CYS:HB2	2.23	0.77
30:W:129:CYS:HB2	30:W:132:CYS:SG	2.28	0.74
10:B:407:MET:HE3	10:B:440:ILE:HA	1.70	0.73
9:A:1427:LEU:HD12	9:A:1456:GLU:HG3	1.71	0.73
11:C:37:VAL:HG23	11:C:41:GLU:HB2	1.70	0.73
13:E:59:THR:HA	13:E:74:VAL:O	1.88	0.72
10:B:297:MET:HA	10:B:300:MET:HG2	1.70	0.72
20:L:19:CYS:HB3	20:L:22:CYS:SG	2.30	0.70
23:O:167:ASN:HB2	23:O:259:VAL:HG12	1.73	0.70
9:A:457:ILE:HG23	9:A:469:MET:HE1	1.73	0.70
4:3:164:VAL:HA	4:3:196:ILE:HD11	1.74	0.69
2:1:73:CYS:HA	2:1:207:TYR:O	1.93	0.68
10:B:594:MET:HE1	10:B:658:ALA:HA	1.76	0.68
10:B:744:MET:HE1	10:B:922:ARG:HB2	1.76	0.68
10:B:261:PRO:HD2	10:B:347:MET:HE1	1.75	0.67
17:I:40:ARG:HB2	25:Q:177:MET:HE1	1.77	0.67
9:A:467:MET:HG3	9:A:534:VAL:HG11	1.76	0.67
1:0:647:LYS:HG2	1:0:650:MET:HE2	1.75	0.66
9:A:1030:SER:HB2	13:E:162:ARG:HE	1.60	0.66
10:B:1075:MET:HE3	10:B:1076:GLU:H	1.61	0.65
30:W:144:LEU:HD22	30:W:155:THR:H	1.62	0.65
9:A:838:PHE:HA	9:A:841:MET:HG2	1.77	0.65
3:2:452:MET:HE1	5:4:269:PRO:HG3	1.80	0.64
9:A:1183:SER:HA	9:A:1190:GLN:HE22	1.62	0.64
5:4:379:LEU:HD11	6:5:179:ASN:HB3	1.78	0.64
2:1:45:GLY:HA3	2:1:669:ARG:HD3	1.78	0.64
9:A:583:ARG:NH1	11:C:222:PRO:O	2.30	0.64
10:B:240:LEU:O	10:B:254:GLN:HA	1.97	0.64
23:O:201:ILE:HA	23:O:211:ALA:O	1.98	0.64
3:2:28:ALA:HB2	3:2:215:MET:HA	1.79	0.63
10:B:403:LEU:O	10:B:407:MET:HB2	1.98	0.63
10:B:954:MET:SD	10:B:954:MET:N	2.71	0.63
15:G:164:MET:N	15:G:164:MET:SD	2.71	0.63
27:T:-99:DA:H5"	34:g:17:THR:HA	1.79	0.63
2:1:42:MET:HB3	2:1:481:PHE:HB2	1.81	0.63
9:A:1218:ARG:NH2	9:A:1252:ALA:O	2.32	0.63
10:B:957:THR:HG23	10:B:959:GLU:H	1.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:H:41:LEU:HA	16:H:123:MET:HB3	1.80	0.63
9:A:1412:MET:SD	9:A:1412:MET:N	2.70	0.63
11:C:53:ASP:HB2	11:C:160:ARG:HG2	1.81	0.62
13:E:18:MET:HG3	13:E:32:GLU:HB3	1.81	0.62
10:B:343:LEU:HA	10:B:347:MET:HG2	1.80	0.62
10:B:910:THR:HG22	20:L:43:ILE:HA	1.80	0.62
15:G:18:PHE:HA	15:G:22:LEU:HD13	1.81	0.62
9:A:233:CYS:SG	9:A:244:ARG:NH1	2.72	0.62
13:E:110:MET:HB3	13:E:115:LYS:HE3	1.81	0.62
28:U:374:ALA:HB1	29:V:62:LEU:HB2	1.82	0.62
11:C:130:VAL:HG11	11:C:237:GLY:HA3	1.81	0.62
11:C:49:TRP:HB3	11:C:164:TYR:HB2	1.82	0.62
2:1:624:PRO:HD2	2:1:656:ALA:HB1	1.81	0.62
16:H:124:ARG:NH2	16:H:126:GLN:OE1	2.33	0.62
13:E:100:THR:HA	13:E:125:TYR:HD1	1.65	0.61
9:A:1141:VAL:HB	9:A:1336:LEU:HB2	1.81	0.61
34:g:55:VAL:HG21	35:h:99:VAL:HG21	1.83	0.61
30:W:107:LEU:HA	30:W:110:MET:HG2	1.82	0.61
2:1:576:GLU:HG3	3:2:305:LYS:HE3	1.82	0.61
11:C:7:PRO:O	19:K:104:ARG:NH1	2.33	0.61
30:W:55:ASP:H	30:W:58:GLN:HE21	1.48	0.61
10:B:502:HIS:H	10:B:505:LEU:HD12	1.65	0.61
10:B:1138:ARG:O	10:B:1141:ARG:NH1	2.34	0.61
2:1:460:THR:HG21	2:1:665:GLY:HA3	1.83	0.61
22:N:110:DA:H5"	35:d:56:SER:HA	1.83	0.61
9:A:71:CYS:SG	9:A:81:CYS:CB	2.88	0.60
9:A:1226:LEU:HD23	9:A:1298:LEU:HD22	1.83	0.60
10:B:529:MET:HE3	10:B:623:ARG:HB2	1.82	0.60
10:B:796:MET:HE3	10:B:945:CYS:HB2	1.84	0.60
9:A:790:GLN:HA	9:A:822:PHE:HA	1.84	0.60
9:A:1212:LEU:HB3	9:A:1259:ILE:HB	1.83	0.60
9:A:966:LEU:HD21	9:A:1043:ILE:HG21	1.82	0.60
10:B:155:MET:HB2	10:B:158:SER:HB3	1.83	0.60
11:C:117:SER:HG	11:C:131:THR:HG1	1.49	0.60
2:1:722:ARG:NH2	5:4:75:ASP:OD2	2.33	0.60
9:A:693:ILE:HD13	9:A:828:LEU:HD21	1.83	0.60
9:A:1239:PHE:O	9:A:1243:LEU:N	2.32	0.60
10:B:643:LEU:HD11	10:B:656:LEU:HD11	1.83	0.60
2:1:718:LYS:HA	2:1:721:LEU:HD12	1.84	0.60
9:A:916:PHE:O	9:A:920:PHE:HB2	2.02	0.60
9:A:1054:MET:SD	9:A:1054:MET:N	2.75	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:B:1036:LYS:HB2	11:C:194:HIS:HB3	1.84	0.59
9:A:1206:ARG:O	9:A:1263:ASN:ND2	2.35	0.59
10:B:102:ASP:HA	21:M:173:VAL:HG21	1.83	0.59
22:N:23:DT:H2'	22:N:24:DG:C8	2.36	0.59
23:O:281:SER:HB3	23:O:293:TYR:HD1	1.67	0.59
21:M:169:ARG:NH1	21:M:207:ASP:O	2.35	0.59
17:I:89:CYS:HB2	17:I:119:CYS:SG	2.42	0.59
10:B:701:SER:HB2	10:B:1001:PRO:HG2	1.84	0.59
23:O:259:VAL:HG23	23:O:313:THR:HB	1.83	0.59
2:1:611:VAL:HG12	2:1:614:TYR:HB2	1.85	0.59
9:A:393:ILE:HG21	14:F:75:MET:HB3	1.83	0.59
10:B:274:ARG:NH1	10:B:311:ILE:O	2.36	0.59
23:O:269:ARG:HG2	23:O:272:GLY:H	1.68	0.59
16:H:39:LEU:HD12	16:H:125:LEU:HD13	1.85	0.59
16:H:25:VAL:HA	16:H:43:VAL:O	2.03	0.58
23:O:168:ILE:HG12	23:O:227:GLU:HG3	1.84	0.58
2:1:112:ARG:NH1	2:1:131:ASP:OD1	2.34	0.58
26:R:12:ALA:HB2	26:R:106:LEU:HD22	1.84	0.58
23:O:255:ILE:HG22	23:O:258:MET:HE1	1.85	0.58
30:W:110:MET:SD	30:W:110:MET:N	2.76	0.58
34:c:64:LEU:HD11	35:d:42:VAL:HG13	1.85	0.58
9:A:11:SER:N	10:B:1135:TYR:HH	2.02	0.58
9:A:74:CYS:SG	9:A:81:CYS:CB	2.87	0.58
1:0:58:ALA:HB1	4:3:337:ARG:HB2	1.86	0.58
9:A:358:ARG:HA	10:B:1085:ARG:HA	1.86	0.58
11:C:88:CYS:SG	11:C:89:THR:N	2.77	0.58
15:G:91:GLN:HB3	15:G:98:PHE:HB2	1.85	0.58
31:X:85:MET:HB3	31:X:97:LEU:HD12	1.85	0.58
5:4:337:GLU:O	5:4:340:ASN:ND2	2.37	0.58
34:c:55:VAL:HG21	35:d:99:VAL:HG21	1.85	0.58
30:W:104:LYS:HG3	30:W:191:LEU:HD22	1.86	0.58
9:A:1484:MET:HE3	9:A:1484:MET:H	1.69	0.58
17:I:89:CYS:CB	17:I:119:CYS:SG	2.92	0.58
23:O:295:MET:SD	23:O:295:MET:N	2.77	0.58
28:U:339:TYR:HB3	29:V:97:ALA:HB1	1.84	0.58
32:e:63:ILE:O	32:e:94:GLN:NE2	2.37	0.58
9:A:620:HIS:ND1	16:H:100:GLU:OE2	2.36	0.58
9:A:1455:SER:HA	9:A:1458:ILE:HB	1.85	0.58
10:B:101:ARG:HG2	21:M:131:PRO:HG3	1.85	0.58
22:N:121:DT:O2	34:c:12:ARG:NH2	2.36	0.58
31:X:145:VAL:HG21	31:X:151:LEU:HD13	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:4:112:LYS:O	5:4:147:ASN:ND2	2.36	0.57
9:A:463:THR:HB	10:B:1089:MET:HG2	1.86	0.57
10:B:407:MET:HE1	10:B:443:GLY:HA3	1.85	0.57
15:G:97:LEU:HB2	15:G:108:ILE:HD12	1.85	0.57
5:4:375:VAL:HG21	5:4:383:PRO:HG3	1.85	0.57
9:A:21:VAL:HB	9:A:1449:ASP:HB3	1.86	0.57
9:A:320:ASN:ND2	9:A:336:LEU:O	2.34	0.57
9:A:457:ILE:O	9:A:503:LEU:HA	2.04	0.57
9:A:1024:ASN:O	13:E:162:ARG:NH2	2.37	0.57
28:U:9:THR:HG23	29:V:53:ARG:HH12	1.70	0.57
2:1:399:LEU:O	2:1:403:PHE:N	2.38	0.57
8:7:91:SER:OG	8:7:92:LEU:N	2.36	0.57
9:A:1139:LEU:HD21	9:A:1343:LEU:HA	1.85	0.57
15:G:89:VAL:HG22	15:G:99:THR:HG22	1.86	0.57
16:H:90:TYR:O	16:H:145:MET:HB3	2.04	0.57
29:V:54:ASN:ND2	29:V:83:GLU:OE2	2.37	0.57
10:B:1172:MET:SD	10:B:1172:MET:N	2.78	0.57
11:C:154:ARG:NH1	18:J:60:LEU:O	2.37	0.57
34:c:64:LEU:HD13	35:d:46:LEU:HB2	1.86	0.57
2:1:13:PRO:HD3	2:1:90:LEU:HD12	1.87	0.57
9:A:890:ARG:HH21	9:A:1023:VAL:HA	1.69	0.57
3:2:479:PHE:HB2	3:2:499:ARG:HH22	1.68	0.57
1:0:71:HIS:HB2	1:0:145:LYS:HD3	1.87	0.57
1:0:438:MET:HE3	1:0:440:LEU:HD21	1.86	0.57
4:3:109:ILE:HG13	4:3:115:ARG:HH22	1.68	0.57
9:A:576:GLN:NE2	16:H:74:GLU:O	2.38	0.56
10:B:1116:VAL:HB	10:B:1125:MET:HE1	1.87	0.56
3:2:113:GLU:OE1	5:4:110:LYS:NZ	2.39	0.56
9:A:270:ALA:HB1	21:M:70:SER:HB2	1.87	0.56
9:A:923:ASP:N	9:A:923:ASP:OD1	2.37	0.56
9:A:1206:ARG:HH22	17:I:33:ARG:HD3	1.70	0.56
9:A:1228:MET:HE2	9:A:1247:PHE:HB2	1.86	0.56
10:B:710:ILE:HA	10:B:764:MET:HE1	1.86	0.56
11:C:205:LYS:HE2	11:C:213:GLU:HA	1.88	0.56
21:M:248:ARG:NH2	21:M:287:GLN:OE1	2.38	0.56
23:O:188:ARG:NH2	29:V:63:ASN:O	2.38	0.56
28:U:15:ARG:HA	28:U:18:ILE:HD12	1.87	0.56
28:U:20:ASP:O	28:U:24:ASP:HB2	2.05	0.56
31:X:84:TYR:HD2	31:X:102:ILE:HG23	1.71	0.56
2:1:531:VAL:O	2:1:565:LYS:NZ	2.37	0.56
10:B:513:GLU:OE2	10:B:525:ASN:ND2	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:F:66:LEU:HB3	14:F:94:MET:HE1	1.87	0.56
1:0:360:ARG:O	1:0:436:GLY:N	2.38	0.56
5:4:75:ASP:HB2	5:4:80:ARG:HE	1.71	0.56
9:A:430:ARG:NH2	21:M:26:ASP:OD2	2.37	0.56
9:A:497:ASP:HA	10:B:943:GLY:HA2	1.87	0.56
10:B:1135:TYR:HB3	10:B:1146:ILE:HG12	1.88	0.56
4:3:57:MET:HE1	4:3:122:LEU:HD11	1.88	0.56
9:A:340:LYS:HG3	9:A:1436:VAL:HG21	1.88	0.56
9:A:921:ARG:O	9:A:1052:ARG:NH1	2.39	0.56
10:B:344:GLN:NE2	10:B:353:VAL:O	2.38	0.56
10:B:568:PHE:HB2	10:B:613:ARG:HG2	1.88	0.56
9:A:1086:MET:SD	9:A:1086:MET:N	2.78	0.56
27:T:57:DT:H2'	27:T:58:DG:H8	1.70	0.56
15:G:162:SER:HB2	15:G:164:MET:HE1	1.87	0.55
9:A:43:TYR:HB2	9:A:56:GLY:HA2	1.89	0.55
9:A:26:LEU:HD11	10:B:1163:MET:HE3	1.88	0.55
9:A:60:PRO:HB2	9:A:72:GLN:HG3	1.88	0.55
9:A:959:MET:SD	9:A:959:MET:N	2.79	0.55
15:G:79:PRO:HB2	15:G:147:ILE:HG13	1.87	0.55
28:U:358:MET:HE1	28:U:367:PHE:HD1	1.72	0.55
30:W:114:ILE:HG23	30:W:177:LEU:HB3	1.88	0.55
9:A:1221:MET:SD	9:A:1221:MET:N	2.79	0.55
2:1:270:VAL:HG22	2:1:326:ALA:HB1	1.88	0.55
16:H:63:THR:O	16:H:84:ARG:NH2	2.37	0.55
9:A:233:CYS:HB3	9:A:238:MET:HG3	1.88	0.55
23:O:167:ASN:HD21	27:T:84:DT:H1'	1.71	0.55
3:2:82:GLU:HB3	31:X:153:ARG:HE	1.72	0.55
3:2:462:LYS:HE3	5:4:282:PRO:HG2	1.89	0.55
9:A:293:ASN:ND2	9:A:306:ASP:OD2	2.37	0.55
9:A:402:LEU:HB3	9:A:446:VAL:HG21	1.89	0.55
2:1:628:THR:HA	2:1:633:LEU:HD22	1.89	0.55
9:A:18:ILE:HD13	10:B:1173:SER:HB3	1.88	0.55
10:B:343:LEU:O	10:B:361:LYS:NZ	2.40	0.55
33:b:72:THR:HG22	35:d:97:THR:HG23	1.88	0.55
13:E:46:ASP:OD1	13:E:52:ARG:NH2	2.40	0.54
16:H:67:ASP:N	16:H:67:ASP:OD1	2.39	0.54
9:A:416:ALA:HA	9:A:448:ARG:HA	1.88	0.54
10:B:65:ILE:HB	10:B:86:LEU:HB2	1.89	0.54
9:A:469:MET:HG3	10:B:1094:GLN:HE21	1.72	0.54
33:b:76:HIS:HB2	35:d:97:THR:HG21	1.88	0.54
1:0:693:LEU:HD22	1:0:696:MET:HE2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:527:MET:HA	2:1:530:VAL:HG22	1.89	0.54
3:2:193:ILE:HG13	3:2:196:ILE:HD12	1.89	0.54
6:5:45:GLY:HA3	6:5:57:LEU:HD13	1.88	0.54
15:G:131:MET:SD	15:G:131:MET:N	2.80	0.54
19:K:56:VAL:HG22	19:K:77:THR:HG22	1.89	0.54
32:a:124:ASP:OD1	32:e:114:HIS:NE2	2.40	0.54
16:H:97:TYR:HA	16:H:138:ASP:H	1.73	0.54
1:0:363:VAL:HB	1:0:407:ILE:HG12	1.88	0.54
9:A:457:ILE:HD11	9:A:515:ILE:HG13	1.89	0.54
9:A:1051:SER:HA	9:A:1054:MET:HG2	1.90	0.54
9:A:1130:ILE:HG22	9:A:1413:ALA:HB2	1.90	0.54
16:H:38:ASP:HB3	16:H:126:GLN:HB2	1.89	0.54
5:4:101:ILE:HA	5:4:311:THR:HB	1.89	0.53
13:E:121:MET:HE1	13:E:125:TYR:HD2	1.73	0.53
21:M:73:PRO:O	21:M:143:LYS:NZ	2.41	0.53
1:0:392:PHE:HE2	1:0:406:ALA:HB1	1.73	0.53
9:A:1228:MET:HA	9:A:1231:ILE:HD12	1.89	0.53
10:B:157:ARG:NH2	10:B:178:PRO:O	2.41	0.53
30:W:103:VAL:HG12	30:W:191:LEU:HD21	1.90	0.53
22:N:141:DC:H3'	32:a:73:ARG:HH22	1.73	0.53
5:4:88:LEU:HB3	5:4:131:LEU:HD13	1.91	0.53
9:A:936:GLU:OE1	9:A:940:LYS:NZ	2.40	0.53
10:B:455:ASP:OD2	21:M:86:LYS:NZ	2.41	0.53
1:0:337:VAL:HG11	1:0:470:LEU:HD21	1.91	0.53
4:3:56:VAL:HG13	4:3:110:LEU:HD11	1.90	0.53
9:A:1210:TRP:NE1	17:I:28:GLU:OE1	2.39	0.53
21:M:263:GLN:HA	21:M:268:LYS:HG2	1.90	0.53
33:f:72:THR:HG22	35:h:97:THR:HG23	1.90	0.53
1:0:322:LYS:NZ	5:4:16:GLU:OE2	2.41	0.53
2:1:383:LEU:HD21	2:1:391:LEU:HD11	1.90	0.53
29:V:29:THR:HG23	29:V:32:LEU:H	1.73	0.53
2:1:323:ILE:HD12	2:1:378:ARG:HD3	1.91	0.53
6:5:14:VAL:HG22	6:5:60:ILE:HD12	1.91	0.53
12:D:29:ALA:O	12:D:94:LYS:NZ	2.41	0.53
9:A:1178:ASP:OD1	9:A:1178:ASP:N	2.42	0.53
9:A:1197:TYR:HE2	9:A:1258:ARG:HH12	1.56	0.53
29:V:72:TRP:HB2	29:V:97:ALA:HB3	1.90	0.53
30:W:15:LYS:HG2	30:W:38:ILE:HG12	1.91	0.53
17:I:96:PHE:HA	17:I:111:TYR:O	2.08	0.53
21:M:156:ASN:HA	21:M:159:ILE:HD12	1.91	0.53
9:A:1420:ASN:ND2	9:A:1433:GLU:O	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:K:29:ASN:HD22	19:K:79:PRO:HA	1.73	0.52
25:Q:174:PHE:HA	25:Q:177:MET:HE3	1.92	0.52
9:A:1158:LEU:HG	9:A:1307:VAL:HB	1.91	0.52
10:B:584:MET:HA	10:B:587:LEU:HD12	1.91	0.52
34:c:89:ARG:NH2	34:c:101:VAL:O	2.41	0.52
30:W:121:SER:OG	30:W:174:ARG:NH1	2.42	0.52
9:A:889:LEU:O	9:A:890:ARG:NH1	2.42	0.52
10:B:1112:ASP:OD1	10:B:1112:ASP:N	2.42	0.52
4:3:428:LEU:HD12	4:3:451:VAL:HG23	1.91	0.52
10:B:823:PHE:HE2	21:M:143:LYS:HD3	1.75	0.52
11:C:74:THR:HA	11:C:238:SER:HA	1.92	0.52
2:1:15:ASP:HB3	2:1:728:PHE:HZ	1.74	0.52
2:1:492:PRO:HA	2:1:677:MET:HB3	1.91	0.52
5:4:71:MET:HG3	5:4:81:LEU:HD12	1.92	0.52
15:G:17:TYR:HB3	15:G:25:THR:HG21	1.92	0.52
17:I:114:CYS:CB	17:I:119:CYS:SG	2.91	0.52
20:L:36:CYS:HB3	20:L:41:TYR:H	1.75	0.52
1:0:494:MET:SD	1:0:494:MET:N	2.83	0.52
4:3:441:MET:HE3	4:3:442:VAL:H	1.75	0.52
9:A:1279:MET:HA	25:Q:172:ASN:HD21	1.75	0.52
21:M:221:ASN:HD22	21:M:277:ILE:HD11	1.75	0.52
22:N:120:DA:H3'	34:c:29:GLY:HA3	1.92	0.52
26:R:24:PRO:HD3	26:R:116:CYS:HB3	1.92	0.52
10:B:226:GLU:OE2	10:B:537:GLN:NE2	2.42	0.52
16:H:64:LEU:O	16:H:84:ARG:N	2.41	0.52
22:N:182:DC:H5''	32:e:64:ARG:HH21	1.75	0.52
3:2:428:SER:HA	4:3:62:LEU:HD21	1.91	0.52
2:1:339:TYR:HB2	2:1:365:VAL:HG21	1.92	0.51
2:1:517:ILE:HG23	2:1:548:THR:HG23	1.91	0.51
10:B:812:ARG:NH1	10:B:900:GLU:OE2	2.43	0.51
16:H:74:GLU:OE2	16:H:76:ASN:ND2	2.43	0.51
27:T:-110:DC:H5''	35:h:56:SER:HA	1.93	0.51
2:1:244:ILE:HG12	2:1:437:CYS:HB3	1.92	0.51
5:4:251:ARG:NH1	6:5:266:TYR:OH	2.43	0.51
12:D:55:GLN:HG2	15:G:32:THR:HA	1.92	0.51
12:D:73:ARG:NE	12:D:102:ASN:O	2.41	0.51
33:f:76:HIS:HB2	35:h:97:THR:HG21	1.91	0.51
1:0:507:CYS:HA	1:0:659:PHE:O	2.09	0.51
9:A:1178:ASP:HB3	9:A:1185:VAL:HG13	1.91	0.51
15:G:120:ASP:OD1	15:G:122:ASN:ND2	2.43	0.51
21:M:260:MET:HB3	21:M:289:TYR:HE1	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:601:ASN:HA	9:A:630:VAL:O	2.10	0.51
2:1:273:ILE:HD13	2:1:281:LEU:HD11	1.92	0.51
2:1:320:PRO:HA	2:1:374:PHE:HB3	1.93	0.51
9:A:355:MET:HA	9:A:1459:MET:HE1	1.93	0.51
9:A:1279:MET:HG2	25:Q:171:LEU:HD13	1.92	0.51
10:B:905:ASP:OD1	10:B:924:ARG:NH1	2.41	0.51
3:2:64:GLN:NE2	3:2:76:ASN:OD1	2.40	0.51
3:2:456:ASP:N	3:2:456:ASP:OD1	2.44	0.51
10:B:229:SER:HB2	10:B:409:LYS:HE2	1.91	0.51
10:B:743:ARG:NH2	10:B:745:ASP:OD1	2.38	0.51
15:G:36:GLY:H	15:G:46:ILE:HG12	1.76	0.51
2:1:619:ILE:HA	2:1:678:VAL:HG13	1.91	0.51
9:A:1190:GLN:HA	9:A:1193:VAL:HB	1.92	0.51
16:H:56:PHE:HE2	16:H:58:LEU:HB2	1.76	0.51
31:X:168:LEU:HD13	31:X:201:LEU:HD21	1.92	0.51
4:3:241:SER:HA	4:3:288:ILE:HA	1.93	0.51
4:3:418:PHE:HE1	4:3:441:MET:HB2	1.76	0.51
9:A:906:LEU:HB2	9:A:975:SER:HB2	1.91	0.51
10:B:674:MET:HG3	10:B:693:TYR:HA	1.93	0.51
22:N:23:DT:H2'	22:N:24:DG:H8	1.76	0.51
3:2:385:GLY:O	6:5:259:ARG:NH1	2.44	0.51
9:A:33:ARG:HB3	10:B:1139:GLY:HA2	1.92	0.51
9:A:998:PRO:O	9:A:1059:ARG:NH1	2.44	0.51
9:A:1454:VAL:HA	9:A:1465:PRO:HD2	1.92	0.51
17:I:71:ASP:OD1	17:I:74:GLN:NE2	2.43	0.51
21:M:23:LEU:HA	21:M:35:PRO:HD3	1.93	0.51
21:M:108:SER:O	21:M:112:ARG:N	2.42	0.51
9:A:734:ARG:NH1	17:I:106:ASP:O	2.43	0.51
10:B:42:GLN:HE22	10:B:483:ARG:HE	1.58	0.51
11:C:58:VAL:HG23	11:C:59:LEU:HD13	1.93	0.51
21:M:168:CYS:HB3	21:M:174:PRO:HA	1.92	0.51
29:V:79:VAL:HG21	29:V:93:VAL:HG12	1.93	0.51
30:W:49:LEU:HD23	30:W:59:LEU:HD23	1.92	0.51
1:0:280:LEU:HD21	1:0:291:LEU:HD22	1.92	0.50
9:A:902:GLU:OE2	9:A:985:ARG:NH2	2.42	0.50
10:B:34:PHE:HZ	10:B:528:LEU:HB3	1.76	0.50
10:B:759:VAL:HG12	10:B:999:ALA:HB2	1.93	0.50
12:D:31:THR:HG23	12:D:94:LYS:HD2	1.93	0.50
4:3:308:VAL:O	4:3:315:LEU:HA	2.11	0.50
5:4:61:LEU:HD21	5:4:168:LEU:HB3	1.93	0.50
11:C:52:ILE:HD12	11:C:61:ASP:HB3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:H:98:ARG:HB3	16:H:115:TYR:HB2	1.92	0.50
3:2:479:PHE:O	3:2:492:LYS:NZ	2.39	0.50
4:3:336:TYR:HB2	4:3:343:VAL:HB	1.93	0.50
4:3:432:VAL:HB	4:3:442:VAL:HG13	1.92	0.50
9:A:326:PRO:HG3	21:M:87:GLY:HA2	1.92	0.50
9:A:329:MET:SD	9:A:330:GLN:N	2.84	0.50
16:H:11:ASP:O	16:H:30:CYS:HA	2.12	0.50
16:H:32:SER:HB3	16:H:37:MET:H	1.75	0.50
22:N:137:DC:H4'	22:N:138:DT:H5'	1.92	0.50
30:W:22:ILE:HG21	30:W:34:LEU:HD22	1.92	0.50
2:1:532:PRO:HA	5:4:174:LEU:HD13	1.93	0.50
9:A:312:PHE:O	9:A:316:THR:OG1	2.24	0.50
9:A:447:GLU:OE2	10:B:1064:ARG:NH1	2.36	0.50
10:B:731:GLN:NE2	24:P:6:A:OP1	2.44	0.50
25:Q:46:ARG:HB2	25:Q:101:ARG:HB3	1.93	0.50
29:V:70:ASN:ND2	29:V:99:ASP:O	2.45	0.50
32:e:121:MET:SD	32:e:121:MET:N	2.85	0.50
5:4:210:VAL:O	5:4:214:GLU:HB2	2.12	0.50
28:U:34:VAL:HG21	29:V:32:LEU:HD22	1.94	0.50
6:5:34:LEU:HD12	6:5:37:CYS:HB3	1.94	0.50
10:B:347:MET:SD	10:B:347:MET:N	2.84	0.50
2:1:437:CYS:SG	2:1:438:MET:N	2.85	0.50
2:1:618:VAL:HG23	2:1:667:ALA:HB2	1.94	0.50
9:A:579:ILE:HG12	16:H:92:MET:HG3	1.94	0.50
15:G:39:THR:HG23	15:G:42:TYR:H	1.77	0.50
21:M:136:ASP:O	21:M:140:ASN:ND2	2.45	0.50
23:O:281:SER:HB2	23:O:291:LEU:HD11	1.93	0.50
2:1:539:PHE:HB2	2:1:545:MET:HE2	1.94	0.50
9:A:329:MET:SD	9:A:331:LYS:N	2.85	0.50
9:A:362:SER:HB2	10:B:1084:LEU:HD12	1.94	0.50
9:A:983:LEU:HB3	9:A:1048:THR:HG21	1.93	0.50
10:B:746:THR:HA	10:B:813:SER:HB2	1.92	0.50
22:N:21:DG:OP1	26:R:175:ARG:NE	2.37	0.50
22:N:120:DA:OP1	34:c:33:ARG:NH1	2.41	0.50
6:5:255:CYS:HA	6:5:274:ILE:HB	1.93	0.50
9:A:407:ARG:HA	9:A:438:LEU:HD23	1.93	0.50
22:N:24:DG:H2'	22:N:25:DG:C8	2.47	0.50
35:h:42:VAL:HG11	35:h:63:MET:HG2	1.92	0.50
5:4:122:GLY:HA3	5:4:304:GLU:H	1.77	0.49
9:A:1434:GLU:HG2	27:T:52:DA:H5''	1.94	0.49
10:B:82:PRO:HA	10:B:133:ILE:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:B:939:HIS:NE2	10:B:983:GLU:OE1	2.32	0.49
12:D:87:LEU:HD21	12:D:101:ALA:HB2	1.93	0.49
17:I:109:ARG:NE	17:I:124:THR:OG1	2.37	0.49
10:B:712:PRO:HD3	10:B:938:ARG:HG2	1.93	0.49
10:B:968:ASN:HD21	10:B:970:HIS:HB2	1.77	0.49
12:D:32:LEU:HB2	15:G:2:PHE:HB3	1.94	0.49
23:O:187:ALA:HB3	23:O:190:ALA:HB2	1.94	0.49
10:B:780:VAL:HA	10:B:965:ILE:O	2.11	0.49
21:M:265:SER:HA	21:M:307:ASP:HB3	1.94	0.49
27:T:-28:DA:OP1	33:b:81:THR:N	2.45	0.49
9:A:121:SER:HA	9:A:126:ILE:HG21	1.94	0.49
10:B:130:LYS:NZ	10:B:429:PHE:O	2.46	0.49
4:3:45:PHE:HZ	4:3:57:MET:HG2	1.78	0.49
9:A:1192:TRP:HZ3	9:A:1246:ILE:HG22	1.77	0.49
10:B:236:TRP:HB2	10:B:259:THR:HB	1.94	0.49
10:B:840:MET:HE1	10:B:845:TYR:CE2	2.48	0.49
22:N:13:DT:O5'	23:O:294:ARG:NH2	2.45	0.49
26:R:192:GLU:HB3	31:X:73:TYR:H	1.78	0.49
2:1:215:PRO:HA	2:1:218:ALA:HB3	1.94	0.49
4:3:348:ARG:NH1	7:6:62:ASP:OD1	2.44	0.49
12:D:39:MET:HA	12:D:42:GLU:HB2	1.93	0.49
10:B:295:PRO:HA	10:B:298:MET:HG2	1.93	0.49
23:O:168:ILE:HG21	23:O:227:GLU:HA	1.95	0.49
30:W:15:LYS:HE2	30:W:38:ILE:HG23	1.95	0.49
2:1:5:VAL:HG13	2:1:25:MET:HB3	1.94	0.49
3:2:24:LEU:HD21	3:2:31:ILE:HD11	1.95	0.49
9:A:351:ARG:HA	9:A:355:MET:HB3	1.94	0.49
13:E:14:ARG:NH2	13:E:32:GLU:OE2	2.46	0.49
23:O:235:ARG:NH2	28:U:316:SER:OG	2.46	0.49
26:R:16:THR:O	26:R:109:ILE:N	2.46	0.49
34:g:64:LEU:HD22	35:h:46:LEU:HD13	1.95	0.49
35:h:39:ALA:HA	35:h:60:MET:HE2	1.94	0.49
1:0:115:GLU:OE1	4:3:314:ARG:NH2	2.42	0.49
2:1:37:HIS:HA	2:1:454:VAL:O	2.12	0.49
3:2:481:VAL:HG12	5:4:159:MET:HB2	1.95	0.49
9:A:572:GLY:HA3	19:K:26:LYS:HB3	1.94	0.49
11:C:16:ASP:OD1	11:C:240:ARG:NH1	2.45	0.49
9:A:367:ILE:HG22	9:A:482:PHE:HB2	1.94	0.48
10:B:111:ASN:ND2	10:B:175:ASN:O	2.46	0.48
17:I:75:ASP:O	17:I:80:ARG:NH2	2.46	0.48
20:L:25:GLU:O	20:L:37:ARG:NH2	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:4:58:MET:HG2	6:5:269:SER:HA	1.93	0.48
5:4:89:GLU:HG2	5:4:128:ILE:HG12	1.95	0.48
9:A:660:MET:SD	9:A:660:MET:N	2.86	0.48
9:A:844:ARG:HG2	10:B:501:LEU:HB2	1.95	0.48
10:B:955:PRO:HB2	10:B:1028:LEU:HD13	1.95	0.48
28:U:51:MET:SD	28:U:51:MET:N	2.86	0.48
31:X:168:LEU:HD11	31:X:182:VAL:HG13	1.96	0.48
10:B:271:ILE:HD12	10:B:311:ILE:HD12	1.94	0.48
12:D:34:ASN:HA	12:D:37:VAL:HB	1.95	0.48
9:A:463:THR:HG23	9:A:468:SER:HB2	1.95	0.48
9:A:1197:TYR:CZ	9:A:1246:ILE:HG13	2.48	0.48
32:e:91:MET:HE3	33:f:101:PHE:HZ	1.78	0.48
2:1:141:TYR:H	2:1:384:HIS:CE1	2.31	0.48
2:1:600:ALA:O	2:1:659:HIS:NE2	2.41	0.48
16:H:96:VAL:O	16:H:138:ASP:N	2.47	0.48
23:O:167:ASN:ND2	27:T:85:DT:O2	2.46	0.48
32:e:62:LEU:HD22	33:f:37:ARG:HB3	1.96	0.48
4:3:178:LEU:HA	4:3:181:GLN:HE21	1.79	0.48
5:4:247:CYS:HB2	6:5:269:SER:HB3	1.96	0.48
9:A:61:ARG:O	9:A:84:HIS:ND1	2.43	0.48
26:R:96:PHE:HE2	26:R:104:LEU:HD12	1.78	0.48
32:a:119:THR:HB	32:a:121:MET:HE1	1.96	0.48
33:b:60:LYS:NZ	33:b:64:GLU:OE2	2.44	0.48
9:A:140:ARG:NH1	9:A:234:PHE:O	2.41	0.48
9:A:1173:THR:HB	9:A:1214:VAL:HG23	1.96	0.48
10:B:1125:MET:HE3	10:B:1126:ALA:H	1.78	0.48
34:c:80:ILE:HG12	34:c:83:HIS:CE1	2.49	0.48
31:X:113:LEU:HA	31:X:116:LYS:HD2	1.96	0.48
1:0:520:ARG:HB2	7:6:18:GLN:HB3	1.95	0.48
4:3:441:MET:HE3	4:3:442:VAL:N	2.28	0.48
9:A:1284:PHE:O	9:A:1288:ILE:HG12	2.14	0.48
21:M:128:ILE:HG23	21:M:183:VAL:HG11	1.96	0.48
27:T:48:DG:H2"	27:T:49:DA:H8	1.79	0.48
1:0:516:PRO:HB3	7:6:16:MET:HE2	1.95	0.48
2:1:287:ARG:HA	2:1:290:GLU:HG3	1.96	0.48
12:D:103:LEU:HD13	12:D:114:LEU:HD22	1.96	0.48
2:1:636:ARG:HE	2:1:640:LEU:HD12	1.78	0.47
10:B:715:ASP:N	10:B:715:ASP:OD1	2.42	0.47
15:G:95:VAL:HG13	15:G:110:ARG:HB2	1.94	0.47
16:H:116:VAL:HB	16:H:123:MET:SD	2.53	0.47
2:1:252:THR:HG22	2:1:432:ILE:HG22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:144:VAL:HG11	9:A:236:LEU:HD12	1.95	0.47
10:B:803:ARG:NH2	10:B:951:GLN:OE1	2.47	0.47
14:F:68:THR:HG23	15:G:59:ILE:HG21	1.96	0.47
17:I:17:CYS:HB3	17:I:22:ASN:H	1.79	0.47
13:E:29:THR:HG23	13:E:32:GLU:H	1.78	0.47
26:R:179:ASP:OD1	26:R:179:ASP:N	2.42	0.47
27:T:-121:DT:H2"	27:T:-120:DA:C8	2.49	0.47
1:0:415:HIS:NE2	1:0:417:THR:OG1	2.47	0.47
2:1:275:GLU:HG3	2:1:276:THR:HG23	1.96	0.47
9:A:1474:LEU:HA	15:G:58:VAL:HA	1.96	0.47
14:F:80:MET:HE1	14:F:103:PRO:HD3	1.96	0.47
31:X:105:GLU:O	31:X:107:GLN:NE2	2.47	0.47
1:0:179:SER:O	1:0:267:THR:HA	2.14	0.47
3:2:468:VAL:HG11	3:2:525:ILE:HD11	1.95	0.47
9:A:31:LEU:HD22	9:A:254:PRO:HB3	1.96	0.47
9:A:1375:ARG:HB2	9:A:1406:THR:HG21	1.96	0.47
10:B:203:ASN:OD1	10:B:224:CYS:N	2.40	0.47
11:C:45:ILE:HG13	11:C:79:VAL:HG23	1.95	0.47
1:0:408:SER:OG	1:0:412:MET:SD	2.72	0.47
2:1:251:LEU:HB2	2:1:433:LEU:HB3	1.97	0.47
3:2:408:ARG:O	3:2:408:ARG:NH1	2.45	0.47
5:4:63:VAL:O	5:4:107:ILE:N	2.43	0.47
9:A:390:PHE:HB2	9:A:505:LEU:HD21	1.97	0.47
9:A:1249:ASP:N	9:A:1249:ASP:OD1	2.45	0.47
16:H:10:PHE:HB3	16:H:30:CYS:HB3	1.95	0.47
1:0:412:MET:HA	1:0:415:HIS:HB2	1.96	0.47
4:3:426:ARG:HG2	4:3:431:LEU:HD22	1.95	0.47
4:3:441:MET:HE2	4:3:443:VAL:HG13	1.96	0.47
10:B:718:GLN:HG2	10:B:720:PRO:HD2	1.95	0.47
10:B:795:ILE:HG12	10:B:947:ILE:HG22	1.97	0.47
13:E:28:VAL:HG22	13:E:62:VAL:HG11	1.96	0.47
16:H:8:ASP:OD1	16:H:9:ILE:N	2.48	0.47
16:H:128:ASP:N	16:H:128:ASP:OD1	2.45	0.47
21:M:290:ARG:NE	21:M:316:LEU:OXT	2.47	0.47
32:e:109:ASN:HB2	33:f:44:VAL:HG22	1.97	0.47
15:G:38:CYS:SG	15:G:39:THR:N	2.87	0.47
30:W:107:LEU:HB3	30:W:188:TYR:HE1	1.79	0.47
31:X:147:ASP:OD1	31:X:147:ASP:N	2.48	0.47
34:c:91:ASP:HB3	34:c:94:LEU:HB2	1.96	0.47
2:1:390:ASP:N	2:1:390:ASP:OD1	2.46	0.47
4:3:98:THR:HG22	4:3:100:LEU:HG	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:442:VAL:HG11	7:6:9:LEU:HD13	1.97	0.47
5:4:375:VAL:HG22	5:4:379:LEU:HD23	1.97	0.47
11:C:259:LEU:HD22	19:K:42:LEU:HD13	1.96	0.47
22:N:116:DC:H2''	22:N:117:DT:C5	2.49	0.47
34:c:86:LEU:O	34:c:90:ASN:ND2	2.44	0.47
9:A:1002:SER:HB3	9:A:1059:ARG:HG3	1.97	0.47
13:E:121:MET:SD	13:E:125:TYR:HB2	2.55	0.47
17:I:111:TYR:HA	17:I:124:THR:HA	1.97	0.47
19:K:77:THR:OG1	19:K:81:TYR:O	2.30	0.47
25:Q:177:MET:H	25:Q:177:MET:HG2	1.58	0.47
28:U:22:ILE:HG21	28:U:43:LYS:HE2	1.97	0.47
32:a:63:ILE:O	32:a:94:GLN:NE2	2.48	0.47
2:1:620:MET:HE1	2:1:624:PRO:HD3	1.97	0.46
5:4:58:MET:HE1	5:4:101:ILE:HD11	1.96	0.46
32:a:80:LYS:HB3	32:a:83:LEU:HD11	1.97	0.46
5:4:381:CYS:SG	5:4:382:CYS:N	2.87	0.46
9:A:642:LYS:HG2	9:A:773:GLY:HA3	1.97	0.46
28:U:43:LYS:O	28:U:46:TRP:HB3	2.15	0.46
34:c:56:LEU:HD11	35:d:71:PHE:HB2	1.96	0.46
11:C:175:LYS:NZ	20:L:57:ALA:O	2.39	0.46
31:X:89:HIS:HE1	31:X:94:THR:HG23	1.81	0.46
34:g:25:GLN:N	34:g:57:GLU:OE1	2.47	0.46
34:g:64:LEU:HD13	35:h:46:LEU:HB2	1.96	0.46
1:0:590:MET:HE2	1:0:594:GLN:HE21	1.79	0.46
2:1:141:TYR:H	2:1:384:HIS:HE1	1.63	0.46
2:1:464:LEU:HB3	2:1:478:MET:HE2	1.96	0.46
2:1:565:LYS:HB3	2:1:595:ILE:HD11	1.97	0.46
5:4:134:ALA:HB1	5:4:137:MET:HE2	1.97	0.46
9:A:349:ARG:NH1	9:A:353:ASN:OD1	2.46	0.46
13:E:101:ARG:HA	13:E:126:ILE:HB	1.98	0.46
16:H:32:SER:HB3	16:H:37:MET:N	2.30	0.46
17:I:69:ILE:HG22	17:I:71:ASP:H	1.81	0.46
23:O:159:SER:HB2	23:O:329:TYR:HB3	1.97	0.46
23:O:293:TYR:HE2	23:O:328:ILE:HD12	1.80	0.46
28:U:342:ILE:HG12	28:U:351:PHE:HA	1.97	0.46
1:0:377:GLN:OE1	1:0:381:TRP:NE1	2.36	0.46
9:A:1263:ASN:OD1	9:A:1263:ASN:N	2.44	0.46
22:N:66:DC:H2'	22:N:67:DT:C6	2.50	0.46
25:Q:109:LYS:HG3	25:Q:149:LEU:HB2	1.96	0.46
31:X:228:MET:HE1	31:X:233:ILE:HG13	1.97	0.46
9:A:395:THR:HG23	9:A:397:PHE:H	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:B:298:MET:HA	10:B:301:VAL:HG22	1.98	0.46
10:B:331:THR:HG23	10:B:334:LYS:H	1.80	0.46
10:B:737:ILE:HG21	10:B:743:ARG:HD3	1.97	0.46
20:L:17:TYR:HB3	20:L:44:MET:SD	2.56	0.46
34:c:55:VAL:HG22	35:d:111:ALA:HB1	1.98	0.46
32:e:80:LYS:HB3	32:e:83:LEU:HD11	1.97	0.46
1:0:311:LYS:NZ	1:0:382:SER:O	2.44	0.46
5:4:183:TYR:HA	5:4:186:ILE:HB	1.98	0.46
6:5:70:LEU:HD21	6:5:115:ILE:HD13	1.97	0.46
9:A:71:CYS:SG	9:A:81:CYS:HB2	2.55	0.46
9:A:354:LEU:HD11	10:B:1155:CYS:HA	1.98	0.46
14:F:121:ASP:N	14:F:121:ASP:OD1	2.47	0.46
31:X:113:LEU:HD23	31:X:116:LYS:HE3	1.97	0.46
5:4:88:LEU:HD13	5:4:131:LEU:HD22	1.97	0.46
6:5:160:ARG:NH1	6:5:192:ASP:OD2	2.49	0.46
10:B:403:LEU:O	10:B:407:MET:CB	2.64	0.46
28:U:339:TYR:OH	29:V:70:ASN:OD1	2.27	0.46
32:a:108:THR:HG23	32:a:124:ASP:HB3	1.96	0.46
4:3:431:LEU:HD12	4:3:441:MET:HE1	1.98	0.46
10:B:818:GLU:HG2	10:B:917:LYS:HB3	1.98	0.46
10:B:865:VAL:HG22	10:B:895:PHE:HA	1.98	0.46
11:C:102:THR:N	11:C:121:ILE:O	2.45	0.46
16:H:58:LEU:HD11	16:H:143:LEU:HD11	1.97	0.46
18:J:47:ARG:NH1	18:J:48:MET:SD	2.89	0.46
19:K:77:THR:HB	19:K:81:TYR:HB3	1.98	0.46
20:L:44:MET:SD	20:L:45:TYR:N	2.88	0.46
21:M:182:ALA:HB2	26:R:155:PRO:HA	1.98	0.46
27:T:-100:DG:H3'	34:g:29:GLY:HA3	1.98	0.46
34:g:80:ILE:HG12	34:g:83:HIS:CE1	2.49	0.46
2:1:414:PHE:HA	2:1:437:CYS:HA	1.98	0.46
10:B:1087:GLY:N	10:B:1090:GLU:OE1	2.46	0.46
10:B:1129:ASN:O	10:B:1133:HIS:N	2.49	0.46
11:C:50:VAL:HB	20:L:55:PHE:HB2	1.98	0.46
16:H:64:LEU:HB3	16:H:83:SER:HB2	1.97	0.46
23:O:163:PRO:HA	23:O:262:CYS:HB3	1.98	0.46
9:A:1406:THR:O	13:E:207:ARG:NH1	2.42	0.45
9:A:1485:GLU:HG2	15:G:20:PRO:HD3	1.97	0.45
26:R:192:GLU:HG2	31:X:75:PHE:H	1.81	0.45
34:g:60:THR:HA	35:h:63:MET:HE1	1.97	0.45
5:4:342:GLU:HG2	5:4:349:GLN:HE22	1.81	0.45
5:4:356:HIS:HB2	5:4:369:VAL:HB	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:75:ALA:HB3	10:B:1129:ASN:HD21	1.81	0.45
9:A:450:MET:HE2	9:A:505:LEU:HD22	1.97	0.45
16:H:8:ASP:HB3	16:H:10:PHE:CE2	2.51	0.45
28:U:22:ILE:HA	28:U:39:LEU:HD11	1.99	0.45
9:A:485:ASN:OD1	9:A:673:GLN:NE2	2.36	0.45
17:I:37:TYR:O	17:I:46:GLN:N	2.48	0.45
18:J:44:CYS:SG	18:J:45:CYS:N	2.89	0.45
35:d:108:ALA:O	35:d:112:VAL:HG23	2.16	0.45
30:W:19:LYS:HA	30:W:22:ILE:HG22	1.99	0.45
2:1:129:ASP:N	2:1:129:ASP:OD1	2.49	0.45
9:A:351:ARG:O	10:B:1085:ARG:NH2	2.46	0.45
9:A:420:ILE:HB	9:A:445:LYS:HB2	1.98	0.45
11:C:82:LEU:HB3	11:C:97:CYS:HA	1.99	0.45
13:E:121:MET:HE2	13:E:124:LYS:HE3	1.97	0.45
15:G:9:HIS:NE2	15:G:33:GLU:OE2	2.39	0.45
1:0:365:GLY:HA2	1:0:441:ASP:HB3	1.99	0.45
2:1:262:ASN:ND2	2:1:393:ASP:O	2.45	0.45
3:2:109:LYS:HD2	5:4:113:ARG:HD3	1.99	0.45
6:5:270:VAL:HG21	6:5:285:CYS:HB2	1.98	0.45
9:A:1043:ILE:HD13	9:A:1046:ARG:HH21	1.82	0.45
10:B:228:SER:O	10:B:405:ARG:NH1	2.39	0.45
10:B:300:MET:SD	10:B:300:MET:N	2.90	0.45
10:B:783:ALA:O	10:B:789:ASN:ND2	2.49	0.45
11:C:20:LYS:HA	11:C:231:TYR:O	2.16	0.45
19:K:57:LEU:N	19:K:76:GLN:O	2.44	0.45
19:K:81:TYR:OH	19:K:89:ASN:OD1	2.34	0.45
20:L:16:ILE:HD12	20:L:47:LYS:HD3	1.98	0.45
22:N:85:DC:H2"	22:N:86:DC:C4	2.51	0.45
22:N:121:DT:H5"	34:c:17:THR:HA	1.99	0.45
32:a:114:HIS:NE2	32:e:124:ASP:OD1	2.39	0.45
3:2:63:ILE:HB	3:2:77:PHE:HB2	1.98	0.45
2:1:493:MET:SD	2:1:493:MET:N	2.90	0.45
2:1:511:ARG:NH1	2:1:512:GLU:OE1	2.45	0.45
6:5:162:LEU:HD21	6:5:227:LEU:HD22	1.98	0.45
9:A:62:GLN:HA	9:A:84:HIS:HB2	1.99	0.45
9:A:67:ARG:NH2	21:M:25:GLU:OE1	2.35	0.45
10:B:126:VAL:O	10:B:147:THR:N	2.46	0.45
14:F:69:ARG:NE	14:F:96:GLU:OE1	2.41	0.45
15:G:87:ALA:HB1	15:G:99:THR:HB	1.99	0.45
27:T:-69:DA:H5"	33:f:31:THR:HG21	1.98	0.45
9:A:274:ASP:OD1	9:A:275:ASP:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:H:69:THR:OG1	16:H:81:ARG:NH1	2.44	0.45
18:J:43:TYR:HA	18:J:46:ARG:HD3	1.98	0.45
1:0:156:ILE:O	1:0:160:THR:OG1	2.27	0.45
1:0:531:ILE:HG21	1:0:629:HIS:CD2	2.52	0.45
2:1:694:PRO:HG2	2:1:697:ILE:HD12	1.98	0.45
3:2:457:ILE:HD11	3:2:513:ARG:HG2	1.99	0.45
5:4:252:MET:HG2	5:4:310:LEU:HD11	1.99	0.45
9:A:612:ASP:OD1	9:A:612:ASP:N	2.48	0.45
9:A:1235:ILE:HG21	9:A:1245:CYS:HB3	1.98	0.45
10:B:229:SER:HA	10:B:405:ARG:HD2	1.99	0.45
11:C:27:ASP:HB2	11:C:30:VAL:HG23	1.99	0.45
22:N:218:DG:H2"	22:N:219:DT:C5	2.51	0.45
2:1:653:THR:HG22	2:1:657:MET:HE3	1.99	0.44
3:2:434:LEU:O	4:3:74:TRP:NE1	2.36	0.44
4:3:280:ARG:NH2	6:5:96:SER:OG	2.46	0.44
6:5:48:HIS:CD2	6:5:55:ASN:HB3	2.52	0.44
9:A:22:GLN:NE2	9:A:1446:GLY:O	2.47	0.44
9:A:1476:ASP:HB3	9:A:1479:LYS:HB2	1.98	0.44
10:B:581:GLU:HA	10:B:584:MET:HE1	1.99	0.44
10:B:714:PRO:HD2	10:B:1001:PRO:HB3	1.99	0.44
10:B:1075:MET:HE3	10:B:1076:GLU:N	2.29	0.44
15:G:79:PRO:HG2	15:G:150:THR:HG21	1.99	0.44
3:2:422:LEU:HD21	6:5:224:LEU:HD23	1.98	0.44
17:I:39:CYS:HB3	17:I:44:TYR:HB3	1.98	0.44
25:Q:20:LYS:HB2	26:R:35:SER:HB2	1.99	0.44
35:h:108:ALA:O	35:h:112:VAL:HG23	2.17	0.44
9:A:52:PRO:HB2	9:A:60:PRO:HG3	1.99	0.44
9:A:1372:GLU:HG3	13:E:193:ILE:HG21	1.99	0.44
10:B:65:ILE:O	10:B:85:LEU:HA	2.17	0.44
11:C:76:ASP:N	11:C:76:ASP:OD1	2.47	0.44
27:T:-100:DG:OP1	34:g:33:ARG:NH1	2.46	0.44
27:T:-22:DC:H2"	27:T:-21:DT:C5	2.52	0.44
34:g:56:LEU:HD11	35:h:71:PHE:HB2	1.99	0.44
9:A:790:GLN:NE2	9:A:791:GLN:O	2.49	0.44
9:A:1201:ASP:OD1	9:A:1201:ASP:N	2.50	0.44
10:B:195:ILE:HD12	10:B:484:ARG:HB3	1.98	0.44
10:B:761:THR:HG23	10:B:1000:THR:HA	1.99	0.44
13:E:150:VAL:HG22	13:E:191:VAL:HG22	1.99	0.44
16:H:48:TYR:HE2	16:H:145:MET:HE2	1.82	0.44
27:T:-114:DC:H2"	27:T:-113:DT:C5	2.52	0.44
31:X:84:TYR:CD2	31:X:102:ILE:HG23	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:499:ARG:HH11	3:2:536:LEU:HG	1.82	0.44
4:3:430:VAL:HG12	4:3:443:VAL:HB	1.99	0.44
9:A:727:PRO:HG3	9:A:733:LEU:HB2	1.99	0.44
10:B:85:LEU:O	10:B:130:LYS:HA	2.18	0.44
10:B:132:VAL:O	10:B:139:GLN:HA	2.17	0.44
10:B:380:ARG:NH1	10:B:611:GLU:OE2	2.50	0.44
10:B:1085:ARG:HD3	27:T:57:DT:H5"	1.99	0.44
10:B:1165:MET:SD	10:B:1165:MET:N	2.90	0.44
28:U:338:GLN:HB2	28:U:354:LYS:HG3	1.98	0.44
2:1:240:ASP:OD1	2:1:240:ASP:N	2.51	0.44
4:3:348:ARG:HD2	7:6:61:MET:HE3	2.00	0.44
9:A:916:PHE:HZ	9:A:959:MET:HB2	1.83	0.44
9:A:1364:GLU:HA	9:A:1367:THR:HG22	2.00	0.44
12:D:111:SER:HB3	12:D:131:LEU:HD11	2.00	0.44
26:R:183:VAL:O	26:R:187:LEU:HB2	2.17	0.44
30:W:54:PHE:HB2	30:W:59:LEU:HD22	2.00	0.44
4:3:68:GLN:HE22	4:3:100:LEU:HD11	1.82	0.44
4:3:216:MET:HE2	4:3:216:MET:HA	1.98	0.44
9:A:459:ASN:ND2	10:B:1090:GLU:OE2	2.49	0.44
10:B:782:ILE:HG23	10:B:967:ILE:HG13	2.00	0.44
12:D:36:GLU:HA	12:D:39:MET:SD	2.58	0.44
30:W:76:MET:SD	30:W:88:ARG:NH2	2.91	0.44
9:A:620:HIS:CE1	16:H:98:ARG:HH21	2.36	0.44
9:A:674:THR:O	9:A:678:ASN:ND2	2.51	0.44
9:A:956:PHE:HA	9:A:959:MET:HG2	1.99	0.44
10:B:710:ILE:HB	10:B:725:GLN:HE22	1.82	0.44
12:D:97:LEU:HD22	12:D:100:LEU:HD12	1.99	0.44
4:3:172:SER:OG	4:3:174:ASP:OD1	2.35	0.44
4:3:431:LEU:HD11	4:3:434:GLU:HB3	2.00	0.44
7:6:14:PRO:HD3	7:6:41:THR:HG22	2.00	0.44
9:A:97:VAL:HA	9:A:100:LEU:HB2	1.99	0.44
9:A:1477:ALA:HA	15:G:22:LEU:HD23	1.99	0.44
10:B:198:GLU:OE2	10:B:391:LYS:NZ	2.42	0.44
10:B:529:MET:SD	10:B:702:MET:HE1	2.58	0.44
13:E:59:THR:HG21	13:E:93:ARG:HH12	1.82	0.44
22:N:128:DT:H2"	22:N:129:DA:N7	2.33	0.44
25:Q:43:ASN:OD1	25:Q:103:ASN:ND2	2.44	0.44
26:R:22:LYS:HB3	26:R:115:GLU:HA	2.00	0.44
27:T:-104:DC:H2"	27:T:-103:DC:C5	2.53	0.44
32:a:72:VAL:HG22	33:b:67:ILE:HD11	1.99	0.44
33:f:70:ALA:HA	33:f:73:TYR:HD2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:251:LEU:HD13	2:1:433:LEU:HD22	2.00	0.43
9:A:276:LEU:O	9:A:280:LEU:HB2	2.18	0.43
10:B:665:ILE:HG23	10:B:669:GLU:HB3	2.00	0.43
18:J:1:MET:HB2	18:J:2:ILE:H	1.64	0.43
23:O:259:VAL:HG11	27:T:85:DT:H1'	2.00	0.43
1:0:279:GLU:HA	1:0:282:LYS:HG2	1.99	0.43
4:3:203:PHE:HE1	4:3:214:TYR:HB3	1.82	0.43
6:5:118:LEU:O	6:5:122:SER:OG	2.35	0.43
9:A:325:LEU:HD22	21:M:101:TYR:HE2	1.83	0.43
9:A:379:GLY:HA3	9:A:483:ARG:HG2	2.01	0.43
9:A:811:ILE:HD12	17:I:79:PRO:HG3	2.00	0.43
11:C:7:PRO:HD2	19:K:100:LEU:HD23	2.00	0.43
12:D:32:LEU:HD11	15:G:4:HIS:HB2	2.00	0.43
14:F:69:ARG:NH2	14:F:78:PRO:O	2.47	0.43
26:R:198:ASN:OD1	26:R:199:LEU:N	2.51	0.43
27:T:-74:DG:H2''	27:T:-73:DT:C5	2.52	0.43
5:4:363:CYS:SG	5:4:365:ASN:ND2	2.91	0.43
9:A:583:ARG:HB3	9:A:585:LEU:HD13	2.00	0.43
9:A:1177:TYR:HB3	17:I:51:SER:HB2	1.99	0.43
10:B:94:SER:OG	10:B:95:LYS:N	2.51	0.43
10:B:796:MET:HE1	10:B:935:PHE:CD1	2.53	0.43
17:I:123:TRP:NE1	17:I:125:GLU:OE1	2.46	0.43
30:W:132:CYS:SG	30:W:134:SER:OG	2.75	0.43
1:0:413:LEU:HD12	1:0:454:VAL:HG13	2.00	0.43
1:0:551:HIS:CG	1:0:622:VAL:HG21	2.54	0.43
1:0:595:ASN:O	1:0:599:ASN:N	2.45	0.43
4:3:117:ASN:O	4:3:121:ALA:HB2	2.19	0.43
4:3:229:ASP:OD1	4:3:229:ASP:N	2.47	0.43
6:5:238:ARG:HG3	6:5:243:LEU:HD13	2.00	0.43
9:A:435:PRO:HA	9:A:438:LEU:HB2	2.01	0.43
9:A:1471:PHE:CZ	14:F:61:GLU:HA	2.53	0.43
11:C:101:PHE:HD2	11:C:120:LEU:HG	1.83	0.43
16:H:112:LEU:HB2	16:H:132:LEU:HD12	2.00	0.43
17:I:114:CYS:HB3	17:I:119:CYS:SG	2.58	0.43
20:L:36:CYS:N	20:L:41:TYR:O	2.42	0.43
26:R:94:THR:OG1	26:R:108:GLY:O	2.32	0.43
27:T:-103:DC:H2''	27:T:-102:DT:C5	2.53	0.43
30:W:114:ILE:HD13	30:W:177:LEU:HD22	2.00	0.43
30:W:126:SER:HA	30:W:166:SER:HB3	2.01	0.43
9:A:26:LEU:HD12	10:B:1166:SER:HA	2.00	0.43
10:B:273:PHE:HB3	10:B:284:ILE:HG12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:B:828:VAL:HG13	10:B:830:GLU:HG2	2.00	0.43
11:C:103:LEU:HD23	11:C:161:LEU:HD21	1.99	0.43
14:F:75:MET:HG2	15:G:14:HIS:CE1	2.54	0.43
25:Q:30:ALA:N	25:Q:144:TYR:O	2.52	0.43
26:R:9:LEU:HG	26:R:13:LYS:HE3	1.99	0.43
2:1:60:GLN:OE1	2:1:61:ARG:NH1	2.52	0.43
2:1:524:LEU:HA	2:1:527:MET:HE2	2.01	0.43
2:1:609:ASP:OD1	2:1:666:ARG:NH1	2.49	0.43
3:2:374:LEU:HA	5:4:53:VAL:HG12	2.00	0.43
9:A:422:ASP:OD1	9:A:422:ASP:N	2.51	0.43
22:N:87:DT:H2"	22:N:88:DA:C5	2.54	0.43
26:R:7:LEU:HD21	26:R:106:LEU:HD12	2.00	0.43
3:2:475:PHE:HB3	3:2:499:ARG:HE	1.83	0.43
9:A:901:VAL:HA	9:A:980:PRO:HA	2.00	0.43
9:A:1116:ASN:OD1	9:A:1116:ASN:N	2.52	0.43
10:B:840:MET:HE2	10:B:840:MET:HA	2.01	0.43
11:C:7:PRO:HA	11:C:25:ASN:HB2	2.01	0.43
25:Q:12:THR:HB	26:R:45:ILE:HB	2.00	0.43
27:T:-42:DT:H2"	27:T:-41:DT:C5	2.54	0.43
21:M:32:MET:HG3	21:M:41:VAL:HG23	2.01	0.43
1:0:559:ILE:O	1:0:623:LEU:HA	2.19	0.43
1:0:561:PHE:HD2	1:0:623:LEU:HD21	1.84	0.43
2:1:493:MET:O	2:1:678:VAL:HA	2.18	0.43
3:2:482:ASN:HB2	5:4:160:PRO:HD3	2.00	0.43
4:3:48:LEU:HD11	4:3:95:ILE:HD13	2.00	0.43
10:B:1089:MET:H	10:B:1089:MET:HE3	1.84	0.43
11:C:256:LEU:HD23	11:C:256:LEU:HA	1.85	0.43
25:Q:14:TYR:HB2	26:R:43:LEU:HB3	2.01	0.43
26:R:58:LEU:HD11	26:R:62:LEU:HD23	2.01	0.43
27:T:-32:DC:H2"	27:T:-31:DT:C5	2.54	0.43
27:T:30:DT:H2"	27:T:31:DG:C8	2.54	0.43
31:X:189:ILE:HG21	31:X:201:LEU:HB3	2.01	0.43
2:1:696:TRP:HA	2:1:699:GLU:HG2	2.01	0.43
3:2:470:GLU:OE2	3:2:474:HIS:NE2	2.52	0.43
4:3:361:ALA:HB1	4:3:391:ILE:HG22	2.01	0.43
5:4:315:ALA:HA	5:4:318:LEU:HD12	2.00	0.43
9:A:100:LEU:HA	9:A:103:THR:HG22	2.00	0.43
16:H:103:GLU:H	16:H:103:GLU:HG3	1.66	0.43
21:M:289:TYR:OH	21:M:314:PRO:O	2.29	0.43
5:4:58:MET:HE3	5:4:58:MET:HA	2.01	0.42
6:5:39:ASP:HA	6:5:42:MET:HG2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:267:GLN:OE1	27:T:64:DG:N1	2.37	0.42
9:A:1004:LEU:HD13	9:A:1062:GLY:HA2	2.01	0.42
9:A:1186:VAL:HG12	9:A:1189:ASP:H	1.83	0.42
9:A:1228:MET:HE3	9:A:1257:LEU:HB2	1.99	0.42
9:A:1365:ILE:HG23	9:A:1369:LEU:HD12	2.01	0.42
16:H:56:PHE:CE2	16:H:58:LEU:HB2	2.54	0.42
27:T:20:DT:H2"	27:T:21:DA:C5	2.54	0.42
1:0:438:MET:HB3	1:0:463:LYS:HA	2.00	0.42
1:0:536:MET:HE3	1:0:536:MET:HA	2.01	0.42
2:1:398:THR:O	2:1:402:ASN:N	2.37	0.42
9:A:20:ARG:HB3	10:B:1172:MET:HE2	2.00	0.42
10:B:912:ASN:OD1	10:B:916:TYR:N	2.46	0.42
13:E:7:THR:HG21	13:E:46:ASP:HA	2.01	0.42
13:E:77:PRO:HB3	13:E:90:TYR:HE2	1.84	0.42
18:J:22:LEU:HD23	18:J:22:LEU:HA	1.93	0.42
2:1:237:HIS:HB3	2:1:458:SER:HB3	2.00	0.42
4:3:322:GLU:HA	4:3:325:ILE:HG22	2.02	0.42
9:A:23:PHE:HB3	9:A:1443:ALA:HA	2.00	0.42
10:B:845:TYR:HB3	10:B:848:LEU:HD12	2.02	0.42
11:C:33:SER:HA	11:C:36:ARG:HG2	2.01	0.42
17:I:68:ILE:HG22	17:I:122:ARG:HD2	2.01	0.42
17:I:109:ARG:NH2	17:I:125:GLU:O	2.53	0.42
19:K:19:ILE:HA	19:K:34:THR:O	2.19	0.42
21:M:74:LEU:HD13	21:M:139:ASN:HB3	1.99	0.42
22:N:234:DC:H2"	22:N:235:DG:C8	2.55	0.42
25:Q:165:GLU:OE1	25:Q:165:GLU:N	2.47	0.42
31:X:80:LYS:HE2	31:X:106:THR:HB	2.01	0.42
31:X:151:LEU:HD23	31:X:185:LEU:HD13	2.00	0.42
2:1:395:SER:O	2:1:398:THR:OG1	2.37	0.42
2:1:495:ILE:HD13	2:1:710:VAL:HA	2.01	0.42
2:1:549:VAL:HG11	3:2:304:ILE:HG12	2.01	0.42
2:1:688:ASP:N	2:1:688:ASP:OD1	2.51	0.42
4:3:65:PRO:HB2	4:3:100:LEU:HD23	2.02	0.42
5:4:85:LEU:HD11	5:4:134:ALA:HB3	2.02	0.42
10:B:59:VAL:HG21	10:B:91:ILE:HD11	2.01	0.42
12:D:83:VAL:O	12:D:87:LEU:HG	2.19	0.42
13:E:62:VAL:HG23	13:E:72:MET:HB3	2.00	0.42
23:O:304:ILE:HG12	23:O:310:VAL:HG13	2.00	0.42
26:R:202:LEU:HD22	26:R:217:LEU:HD22	2.02	0.42
1:0:392:PHE:HB2	1:0:408:SER:HA	2.01	0.42
2:1:534:GLY:HA3	2:1:615:GLY:H	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:41:CYS:O	4:3:45:PHE:HB2	2.20	0.42
10:B:53:MET:HA	10:B:53:MET:HE3	2.00	0.42
10:B:483:ARG:HB3	10:B:526:LEU:HD12	2.00	0.42
23:O:211:ALA:HB2	23:O:237:TYR:CZ	2.54	0.42
2:1:28:LEU:O	2:1:31:THR:OG1	2.32	0.42
11:C:212:ASP:HB2	11:C:215:GLU:HG2	2.00	0.42
13:E:91:CYS:SG	13:E:121:MET:HE3	2.60	0.42
20:L:35:ARG:NH1	20:L:40:GLY:HA2	2.35	0.42
21:M:269:ARG:HB2	21:M:274:ILE:HD11	2.01	0.42
1:0:374:TRP:HB3	1:0:407:ILE:HD13	2.01	0.42
1:0:556:ASP:OD1	1:0:621:ASN:ND2	2.47	0.42
2:1:24:TYR:CE2	2:1:48:LYS:HB2	2.55	0.42
2:1:702:THR:HG23	2:1:705:ASN:H	1.84	0.42
10:B:499:ARG:NH1	10:B:520:VAL:O	2.51	0.42
23:O:324:ALA:O	23:O:328:ILE:HG12	2.20	0.42
25:Q:36:LYS:HA	25:Q:36:LYS:HD2	1.84	0.42
31:X:178:SER:O	31:X:182:VAL:HG23	2.20	0.42
2:1:75:ARG:NH2	2:1:662:GLN:O	2.52	0.42
2:1:382:LEU:O	2:1:386:LEU:HG	2.20	0.42
5:4:98:GLN:HA	5:4:324:HIS:HE1	1.85	0.42
9:A:653:VAL:HG11	9:A:669:TYR:OH	2.19	0.42
10:B:605:ARG:NH2	17:I:71:ASP:OD2	2.53	0.42
10:B:713:PHE:HB3	10:B:716:HIS:CD2	2.54	0.42
12:D:34:ASN:O	12:D:68:THR:OG1	2.38	0.42
13:E:11:TRP:NE1	13:E:35:GLN:O	2.39	0.42
16:H:65:TYR:HA	16:H:83:SER:HA	2.01	0.42
21:M:286:ARG:HD2	22:N:4:DG:H3'	2.00	0.42
21:M:290:ARG:NH2	22:N:5:DG:OP2	2.53	0.42
21:M:308:THR:HG23	21:M:312:LYS:HD2	2.02	0.42
27:T:-102:DT:H2''	27:T:-101:DG:C8	2.55	0.42
4:3:161:HIS:CD2	4:3:323:LEU:HB2	2.55	0.42
4:3:205:LEU:HD23	4:3:327:LEU:HD22	2.00	0.42
6:5:223:LEU:O	6:5:227:LEU:N	2.48	0.42
10:B:109:MET:HG3	10:B:174:LEU:HD22	2.02	0.42
10:B:433:LEU:O	21:M:127:ARG:NH2	2.53	0.42
11:C:47:ILE:HG13	11:C:73:LEU:HD11	2.01	0.42
11:C:83:GLN:NE2	11:C:96:GLU:OE2	2.53	0.42
16:H:88:PHE:CG	16:H:144:LEU:HB3	2.55	0.42
18:J:49:LEU:HD23	18:J:49:LEU:HA	1.86	0.42
22:N:217:DT:H2''	22:N:218:DG:C8	2.54	0.42
27:T:-114:DC:H2''	27:T:-113:DT:C6	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:T:18:DC:H2"	27:T:19:DG:N7	2.35	0.42
1:0:109:ARG:NH2	1:0:683:GLN:OE1	2.52	0.42
1:0:651:VAL:HB	1:0:654:GLU:HG3	2.02	0.42
2:1:531:VAL:HG22	2:1:721:LEU:HD11	2.02	0.42
5:4:59:ARG:HG3	5:4:95:TYR:HE1	1.85	0.42
10:B:724:TYR:HB3	10:B:728:MET:HE3	2.02	0.42
15:G:123:SER:HB2	15:G:125:PRO:HD2	2.01	0.42
16:H:112:LEU:HD12	16:H:129:ALA:HA	2.02	0.42
22:N:58:DA:C8	22:N:59:DT:H72	2.55	0.42
22:N:107:DC:H2"	22:N:108:DC:C5	2.55	0.42
4:3:212:LEU:HD22	4:3:286:LEU:HD23	2.02	0.41
9:A:350:VAL:O	9:A:355:MET:N	2.43	0.41
18:J:17:LYS:HB3	18:J:38:LEU:HD13	2.02	0.41
19:K:18:LYS:NZ	19:K:38:GLU:OE2	2.48	0.41
21:M:159:ILE:HG23	21:M:198:ILE:HD11	2.01	0.41
26:R:188:PHE:HB3	31:X:76:GLY:HA3	2.02	0.41
29:V:16:GLN:NE2	29:V:20:ASP:OD2	2.52	0.41
29:V:59:ARG:HG2	29:V:82:ARG:HH12	1.85	0.41
31:X:82:VAL:HA	31:X:85:MET:SD	2.60	0.41
33:f:33:PRO:HA	33:f:36:ARG:HB2	2.02	0.41
2:1:49:THR:HG21	2:1:83:VAL:HG21	2.02	0.41
2:1:170:LEU:HA	2:1:171:PRO:HD3	1.97	0.41
2:1:234:ASP:HA	2:1:457:THR:HB	2.02	0.41
2:1:460:THR:O	2:1:460:THR:OG1	2.38	0.41
9:A:561:MET:HE2	19:K:58:PHE:CD1	2.55	0.41
10:B:286:GLU:HB3	10:B:558:PRO:HG2	2.01	0.41
11:C:103:LEU:HB3	11:C:161:LEU:HG	2.01	0.41
17:I:24:LEU:HD12	17:I:37:TYR:HB3	2.02	0.41
22:N:122:DT:OP1	34:c:21:ARG:NH2	2.50	0.41
4:3:28:PRO:HA	4:3:31:LEU:HB2	2.03	0.41
7:6:39:ASP:HB3	7:6:42:HIS:H	1.85	0.41
9:A:1170:THR:HA	9:A:1216:LEU:HA	2.01	0.41
26:R:55:SER:HA	26:R:82:PRO:HA	2.03	0.41
30:W:162:GLU:HG2	30:W:164:ASP:H	1.85	0.41
1:0:557:LYS:HB2	1:0:620:ALA:HA	2.03	0.41
2:1:398:THR:O	2:1:401:ALA:HB3	2.21	0.41
12:D:58:SER:O	12:D:62:MET:HE2	2.20	0.41
12:D:134:ILE:O	12:D:138:ARG:N	2.53	0.41
20:L:22:CYS:SG	20:L:24:THR:OG1	2.66	0.41
21:M:177:PHE:HB3	21:M:188:LYS:HG3	2.02	0.41
30:W:107:LEU:HB3	30:W:188:TYR:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:641:GLY:HA2	1:0:644:LEU:HB2	2.01	0.41
2:1:44:SER:O	2:1:48:LYS:HD3	2.21	0.41
6:5:44:LEU:HD22	6:5:227:LEU:HD13	2.03	0.41
9:A:535:MET:HG2	9:A:669:TYR:CE2	2.55	0.41
10:B:384:ASP:OD1	10:B:384:ASP:N	2.51	0.41
10:B:1067:ILE:HD12	10:B:1072:ARG:HG3	2.02	0.41
16:H:36:LYS:HD2	16:H:36:LYS:HA	1.82	0.41
19:K:56:VAL:HA	19:K:77:THR:HA	2.01	0.41
22:N:15:DA:H2'	22:N:16:DA:C8	2.56	0.41
22:N:93:DC:H2''	22:N:94:DG:C8	2.55	0.41
26:R:41:GLY:HA3	26:R:56:PHE:CZ	2.56	0.41
27:T:57:DT:H2'	27:T:58:DG:C8	2.54	0.41
3:2:465:TYR:OH	3:2:524:HIS:ND1	2.39	0.41
9:A:1161:LEU:HD12	9:A:1336:LEU:HD13	2.02	0.41
9:A:1210:TRP:CE2	9:A:1282:ASP:HB3	2.55	0.41
10:B:745:ASP:O	10:B:813:SER:OG	2.37	0.41
22:N:87:DT:H2''	22:N:88:DA:N7	2.36	0.41
22:N:151:DA:H5''	33:b:31:THR:HG21	2.02	0.41
22:N:219:DT:H2''	22:N:220:DC:C5	2.56	0.41
26:R:8:ASP:O	26:R:106:LEU:N	2.53	0.41
1:0:626:ILE:HA	1:0:662:LEU:HB2	2.03	0.41
2:1:232:VAL:HG22	2:1:455:ILE:HD13	2.03	0.41
2:1:238:ASN:HB3	2:1:241:ASN:HB2	2.02	0.41
7:6:13:ASP:OD1	7:6:16:MET:N	2.51	0.41
9:A:567:LEU:HB3	9:A:570:TRP:HB2	2.03	0.41
9:A:807:LEU:HD23	9:A:807:LEU:HA	1.91	0.41
10:B:645:GLU:HG2	10:B:649:ASN:HB2	2.03	0.41
10:B:1075:MET:HG2	21:M:51:GLU:HB2	2.02	0.41
17:I:106:ASP:OD1	17:I:106:ASP:N	2.54	0.41
22:N:4:DG:N2	27:T:96:DT:O2	2.54	0.41
23:O:317:VAL:HG23	23:O:320:GLU:H	1.86	0.41
4:3:30:VAL:HG21	4:3:230:LEU:HB3	2.03	0.41
5:4:199:ILE:HD11	5:4:236:VAL:HG11	2.02	0.41
10:B:194:LEU:HD23	10:B:194:LEU:HA	1.82	0.41
11:C:38:PHE:HE1	11:C:245:VAL:HA	1.86	0.41
15:G:50:THR:HG22	15:G:73:LYS:HB2	2.02	0.41
27:T:-112:DG:H4'	27:T:-111:DA:H5'	2.03	0.41
1:0:70:ASP:OD1	1:0:70:ASP:N	2.54	0.41
2:1:727:PRO:HD3	5:4:220:HIS:CD2	2.56	0.41
3:2:205:MET:HE2	3:2:205:MET:HA	2.02	0.41
3:2:503:THR:HG22	3:2:529:LEU:HD22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:185:MET:HG2	4:3:194:PRO:HG2	2.03	0.41
9:A:99:PHE:HB3	9:A:248:MET:HE2	2.02	0.41
9:A:906:LEU:HD13	9:A:966:LEU:HD13	2.03	0.41
9:A:1379:GLU:HG2	9:A:1398:LEU:HB3	2.03	0.41
10:B:399:LEU:HB3	10:B:453:TRP:CZ3	2.56	0.41
11:C:59:LEU:HD22	11:C:151:VAL:HG23	2.01	0.41
11:C:193:ARG:HD3	11:C:193:ARG:HA	1.85	0.41
12:D:44:ARG:HD3	15:G:48:VAL:H	1.86	0.41
16:H:13:LYS:N	16:H:29:HIS:O	2.41	0.41
17:I:64:GLU:HA	17:I:67:GLN:HG2	2.02	0.41
21:M:281:ALA:HB2	27:T:91:DC:H2'	2.03	0.41
25:Q:166:ARG:HH21	25:Q:170:VAL:HA	1.86	0.41
30:W:96:TYR:O	30:W:100:VAL:HG23	2.21	0.41
30:W:113:ARG:HA	30:W:116:THR:HG22	2.02	0.41
3:2:105:ARG:NH2	3:2:194:GLU:OE2	2.41	0.41
9:A:913:ASN:N	9:A:1325:ASP:O	2.54	0.41
9:A:1192:TRP:CD2	9:A:1248:ASN:HB3	2.56	0.41
10:B:365:LEU:HA	10:B:368:MET:SD	2.60	0.41
10:B:1138:ARG:HD3	10:B:1138:ARG:HA	1.94	0.41
25:Q:48:GLU:HG2	25:Q:99:LEU:HB3	2.03	0.41
1:0:351:VAL:HG11	1:0:381:TRP:HB2	2.03	0.40
10:B:1040:GLN:NE2	11:C:195:THR:OG1	2.54	0.40
13:E:55:ARG:HD3	13:E:55:ARG:HA	1.89	0.40
22:N:67:DT:H2'	22:N:68:DC:C6	2.55	0.40
22:N:85:DC:H2''	22:N:86:DC:C5	2.56	0.40
23:O:180:LEU:HD13	23:O:200:VAL:HG23	2.03	0.40
25:Q:126:ILE:HG21	26:R:95:VAL:HG11	2.03	0.40
34:c:105:GLN:H	32:e:95:GLU:CD	2.29	0.40
1:0:123:LEU:HD13	1:0:156:ILE:HA	2.02	0.40
1:0:540:LYS:HG3	1:0:662:LEU:HD23	2.04	0.40
2:1:289:VAL:HA	2:1:319:VAL:HG22	2.03	0.40
2:1:405:THR:O	2:1:409:THR:OG1	2.30	0.40
5:4:149:LEU:HD12	5:4:182:ILE:HD11	2.03	0.40
5:4:301:LEU:HD12	5:4:317:HIS:HE1	1.85	0.40
9:A:1242:ASP:C	9:A:1262:MET:HE3	2.46	0.40
10:B:87:LYS:NZ	10:B:88:PHE:O	2.45	0.40
11:C:252:LEU:HG	19:K:98:LEU:HD11	2.02	0.40
12:D:33:LEU:HD11	12:D:101:ALA:HB3	2.04	0.40
12:D:39:MET:SD	12:D:39:MET:N	2.92	0.40
21:M:181:CYS:O	26:R:159:HIS:NE2	2.54	0.40
23:O:192:TYR:HB2	23:O:200:VAL:HG22	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:O:211:ALA:HB2	23:O:237:TYR:CE2	2.56	0.40
23:O:270:LEU:O	23:O:274:VAL:HG12	2.22	0.40
27:T:-63:DG:H2''	27:T:-62:DG:C8	2.56	0.40
33:b:48:SER:HB3	33:b:51:ILE:HG12	2.03	0.40
32:e:100:TYR:OH	32:e:134:GLU:OE1	2.36	0.40
3:2:510:GLU:HG3	3:2:526:GLU:HG3	2.02	0.40
5:4:57:MET:SD	5:4:321:SER:OG	2.79	0.40
9:A:20:ARG:NH1	9:A:1448:SER:OG	2.51	0.40
10:B:260:LEU:HD22	10:B:347:MET:HE2	2.03	0.40
12:D:102:ASN:HB3	15:G:1:MET:HE3	2.03	0.40
15:G:96:GLY:HA2	15:G:113:ILE:HD11	2.03	0.40
21:M:63:ASP:OD1	21:M:63:ASP:N	2.49	0.40
1:0:193:VAL:O	1:0:196:GLU:HG3	2.21	0.40
2:1:423:ASP:OD1	2:1:423:ASP:N	2.54	0.40
2:1:532:PRO:HG3	5:4:203:ALA:HA	2.03	0.40
10:B:117:ASN:HA	10:B:189:GLY:HA3	2.04	0.40
10:B:794:VAL:HG13	10:B:965:ILE:HG23	2.02	0.40
10:B:1162:LEU:HD22	10:B:1167:ILE:HG21	2.02	0.40
17:I:108:MET:HE2	17:I:108:MET:HB2	1.99	0.40
21:M:104:ARG:HD3	22:N:30:DG:C6	2.57	0.40
22:N:86:DC:H2''	22:N:87:DT:C5	2.56	0.40
25:Q:155:LEU:HD23	25:Q:159:GLU:HG2	2.03	0.40
1:0:599:ASN:HB3	1:0:602:ILE:HG22	2.03	0.40
2:1:71:ILE:HA	2:1:205:VAL:HG22	2.04	0.40
9:A:42:LYS:O	9:A:288:ASN:ND2	2.43	0.40
9:A:461:GLN:HG2	27:T:57:DT:H1'	2.03	0.40
9:A:525:ILE:HG23	9:A:535:MET:HB3	2.04	0.40
9:A:1153:ARG:O	9:A:1157:ILE:HG12	2.21	0.40
9:A:1454:VAL:HG13	9:A:1464:ALA:HB1	2.03	0.40
10:B:109:MET:HE3	10:B:112:GLU:HG3	2.03	0.40
10:B:806:PHE:O	10:B:1050:ARG:NH1	2.54	0.40
21:M:234:HIS:ND1	21:M:299:LEU:O	2.52	0.40
22:N:141:DC:O5'	32:a:73:ARG:NH2	2.55	0.40
22:N:202:DT:H5''	34:g:45:GLY:HA2	2.04	0.40
25:Q:18:VAL:HA	25:Q:137:ALA:HB3	2.02	0.40
29:V:76:LEU:HB2	29:V:93:VAL:HG12	2.04	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	0	601/782 (77%)	574 (96%)	27 (4%)	0	100	100
2	1	710/760 (93%)	686 (97%)	24 (3%)	0	100	100
3	2	359/548 (66%)	352 (98%)	7 (2%)	0	100	100
4	3	413/462 (89%)	401 (97%)	12 (3%)	0	100	100
5	4	341/395 (86%)	321 (94%)	20 (6%)	0	100	100
6	5	259/308 (84%)	252 (97%)	7 (3%)	0	100	100
7	6	67/71 (94%)	65 (97%)	2 (3%)	0	100	100
8	7	42/309 (14%)	42 (100%)	0	0	100	100
9	A	1411/1984 (71%)	1365 (97%)	46 (3%)	0	100	100
10	B	1111/1300 (86%)	1077 (97%)	34 (3%)	0	100	100
11	C	253/275 (92%)	242 (96%)	11 (4%)	0	100	100
12	D	126/184 (68%)	124 (98%)	2 (2%)	0	100	100
13	E	207/210 (99%)	203 (98%)	4 (2%)	0	100	100
14	F	77/127 (61%)	73 (95%)	4 (5%)	0	100	100
15	G	169/172 (98%)	163 (96%)	6 (4%)	0	100	100
16	H	146/150 (97%)	138 (94%)	8 (6%)	0	100	100
17	I	112/125 (90%)	106 (95%)	6 (5%)	0	100	100
18	J	62/67 (92%)	61 (98%)	1 (2%)	0	100	100
19	K	113/117 (97%)	112 (99%)	1 (1%)	0	100	100
20	L	42/58 (72%)	41 (98%)	1 (2%)	0	100	100
21	M	294/316 (93%)	287 (98%)	7 (2%)	0	100	100
23	O	177/339 (52%)	172 (97%)	5 (3%)	0	100	100
25	Q	134/517 (26%)	130 (97%)	4 (3%)	0	100	100
26	R	218/249 (88%)	216 (99%)	2 (1%)	0	100	100
28	U	109/376 (29%)	103 (94%)	6 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	V	97/109 (89%)	93 (96%)	4 (4%)	0	100	100
30	W	185/439 (42%)	182 (98%)	3 (2%)	0	100	100
31	X	169/291 (58%)	164 (97%)	5 (3%)	0	100	100
32	a	95/136 (70%)	95 (100%)	0	0	100	100
32	e	96/136 (71%)	96 (100%)	0	0	100	100
33	b	80/103 (78%)	80 (100%)	0	0	100	100
33	f	80/103 (78%)	79 (99%)	1 (1%)	0	100	100
34	c	107/130 (82%)	107 (100%)	0	0	100	100
34	g	104/130 (80%)	104 (100%)	0	0	100	100
35	d	95/126 (75%)	93 (98%)	2 (2%)	0	100	100
35	h	93/126 (74%)	93 (100%)	0	0	100	100
All	All	8754/12030 (73%)	8492 (97%)	262 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	0	536/688 (78%)	536 (100%)	0	100	100
2	1	624/664 (94%)	622 (100%)	2 (0%)	86	86
3	2	333/484 (69%)	333 (100%)	0	100	100
4	3	351/399 (88%)	350 (100%)	1 (0%)	86	86
5	4	311/352 (88%)	310 (100%)	1 (0%)	86	86
6	5	234/272 (86%)	233 (100%)	1 (0%)	84	84
7	6	62/64 (97%)	62 (100%)	0	100	100
8	7	44/283 (16%)	44 (100%)	0	100	100
9	A	1252/1763 (71%)	1249 (100%)	3 (0%)	87	87
10	B	985/1127 (87%)	985 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	C	234/252 (93%)	234 (100%)	0	100	100
12	D	118/160 (74%)	117 (99%)	1 (1%)	73	80
13	E	191/192 (100%)	191 (100%)	0	100	100
14	F	69/111 (62%)	68 (99%)	1 (1%)	59	72
15	G	152/153 (99%)	152 (100%)	0	100	100
16	H	129/131 (98%)	129 (100%)	0	100	100
17	I	103/112 (92%)	103 (100%)	0	100	100
18	J	53/56 (95%)	53 (100%)	0	100	100
19	K	104/106 (98%)	103 (99%)	1 (1%)	68	78
20	L	41/55 (74%)	41 (100%)	0	100	100
21	M	253/268 (94%)	252 (100%)	1 (0%)	84	84
23	O	154/293 (53%)	154 (100%)	0	100	100
25	Q	121/448 (27%)	121 (100%)	0	100	100
26	R	196/218 (90%)	196 (100%)	0	100	100
28	U	105/324 (32%)	105 (100%)	0	100	100
29	V	90/98 (92%)	90 (100%)	0	100	100
30	W	169/373 (45%)	168 (99%)	1 (1%)	78	83
31	X	154/261 (59%)	154 (100%)	0	100	100
32	a	85/111 (77%)	85 (100%)	0	100	100
32	e	86/111 (78%)	86 (100%)	0	100	100
33	b	67/79 (85%)	67 (100%)	0	100	100
33	f	67/79 (85%)	67 (100%)	0	100	100
34	c	86/101 (85%)	86 (100%)	0	100	100
34	g	84/101 (83%)	84 (100%)	0	100	100
35	d	83/106 (78%)	83 (100%)	0	100	100
35	h	81/106 (76%)	81 (100%)	0	100	100
All	All	7807/10501 (74%)	7794 (100%)	13 (0%)	85	87

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	1	25	MET
2	1	527	MET

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Mol	Chain	Res	Type
4	3	163	MET
5	4	178	ASP
6	5	189	ILE
9	A	469	MET
9	A	1139	LEU
9	A	1412	MET
12	D	37	VAL
14	F	123	LEU
19	K	109	ILE
21	M	33	ILE
30	W	43	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (108) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	71	HIS
1	0	373	GLN
1	0	576	ASN
1	0	629	HIS
1	0	714	GLN
2	1	114	ASN
2	1	203	ASN
2	1	555	GLN
2	1	560	ASN
2	1	585	GLN
2	1	612	HIS
2	1	613	HIS
3	2	78	HIS
3	2	115	ASN
3	2	298	ASN
3	2	402	ASN
3	2	496	ASN
3	2	540	GLN
4	3	68	GLN
4	3	161	HIS
4	3	181	GLN
4	3	211	GLN
4	3	390	GLN
4	3	435	ASN
5	4	98	GLN
5	4	99	ASN
5	4	158	HIS

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Mol	Chain	Res	Type
5	4	220	HIS
5	4	365	ASN
6	5	48	HIS
6	5	65	GLN
6	5	145	HIS
6	5	204	GLN
9	A	273	GLN
9	A	295	GLN
9	A	372	ASN
9	A	387	ASN
9	A	459	ASN
9	A	601	ASN
9	A	673	GLN
9	A	700	GLN
9	A	742	ASN
9	A	1093	GLN
9	A	1105	ASN
9	A	1180	ASN
9	A	1190	GLN
9	A	1194	ASN
9	A	1291	ASN
9	A	1410	HIS
9	A	1445	HIS
10	B	42	GLN
10	B	420	GLN
10	B	452	ASN
10	B	471	ASN
10	B	486	ASN
10	B	593	GLN
10	B	654	GLN
10	B	725	GLN
10	B	913	GLN
10	B	930	GLN
10	B	1009	GLN
10	B	1097	HIS
10	B	1117	HIS
10	B	1160	GLN
11	C	66	HIS
11	C	108	ASN
11	C	217	GLN
12	D	93	HIS
13	E	30	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	E	71	GLN
15	G	122	ASN
17	I	22	ASN
17	I	98	GLN
19	K	22	ASN
19	K	113	GLN
21	M	116	ASN
21	M	140	ASN
21	M	221	ASN
21	M	263	GLN
23	O	167	ASN
23	O	278	GLN
23	O	327	ASN
25	Q	129	GLN
25	Q	141	HIS
26	R	29	GLN
26	R	64	ASN
26	R	91	GLN
26	R	123	ASN
26	R	195	GLN
30	W	58	GLN
30	W	89	HIS
30	W	101	ASN
31	X	83	ASN
31	X	107	GLN
31	X	144	ASN
31	X	209	GLN
32	a	40	HIS
32	a	69	GLN
34	c	25	GLN
35	d	48	GLN
35	d	50	HIS
35	d	64	ASN
35	d	68	ASN
35	d	96	GLN
32	e	109	ASN
34	g	25	GLN
34	g	105	GLN
35	h	83	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
24	P	1/2 (50%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 16 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
36	SF4	1	1000	-	0,12,12	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	SF4	1	1000	-	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

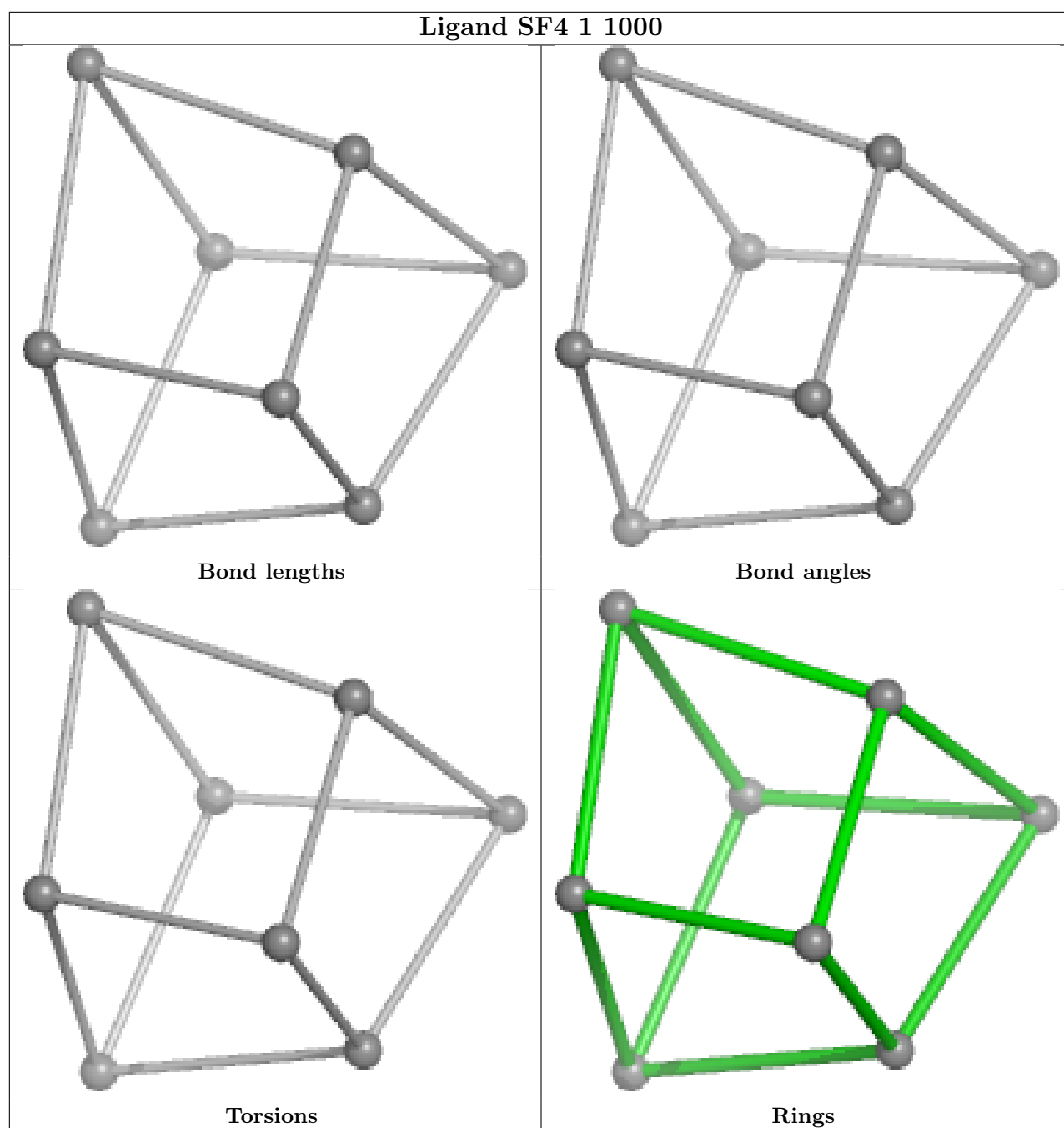
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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.

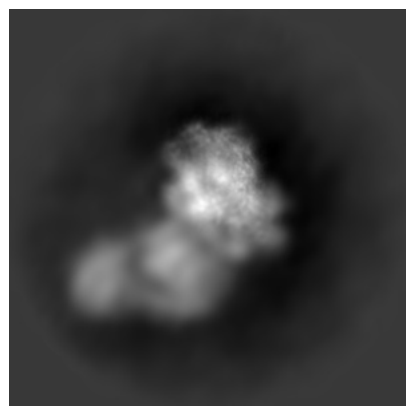
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-57390. These allow visual inspection of the internal detail of the map and identification of artifacts.

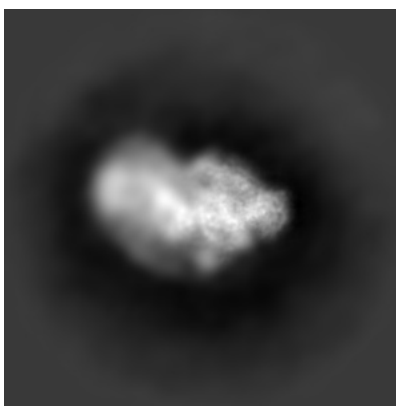
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

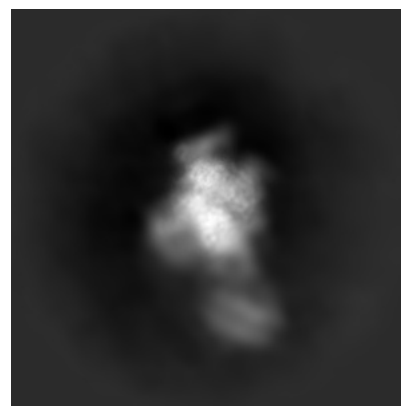
6.1.1 Primary map



X

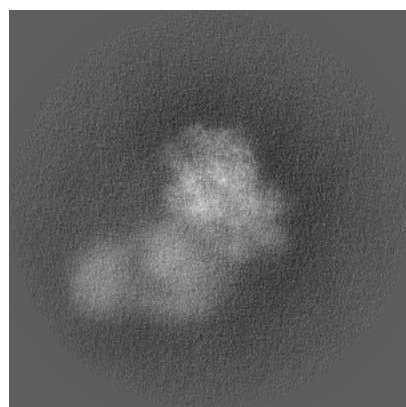


Y

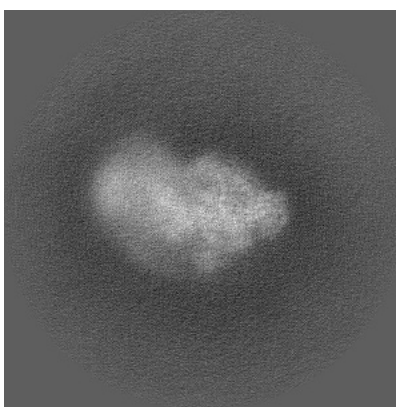


Z

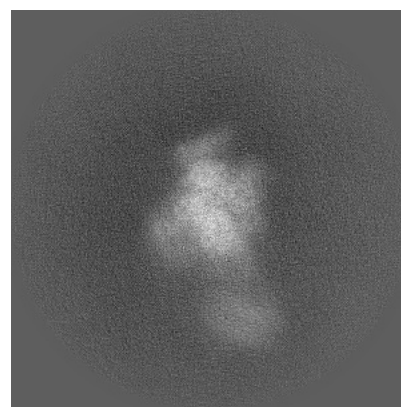
6.1.2 Raw map



X



Y

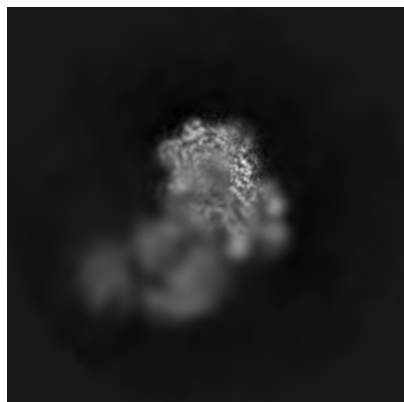


Z

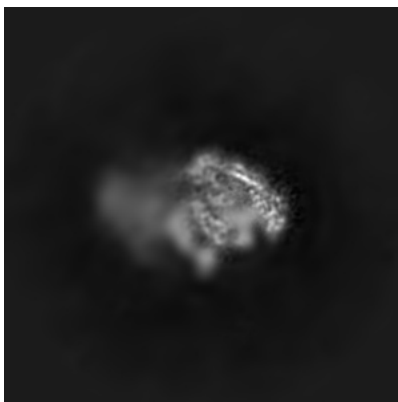
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

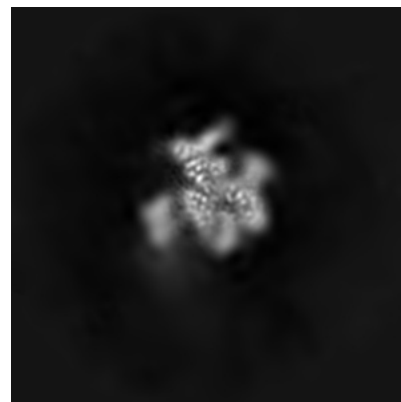
6.2.1 Primary map



X Index: 240

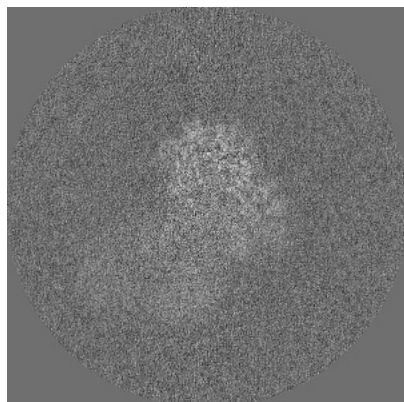


Y Index: 240

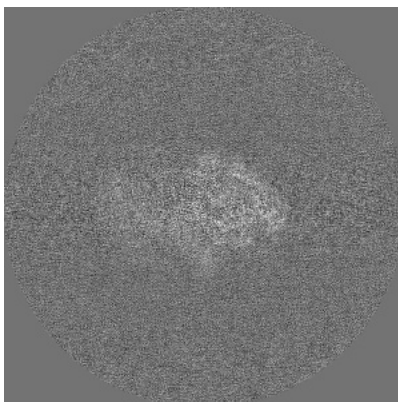


Z Index: 240

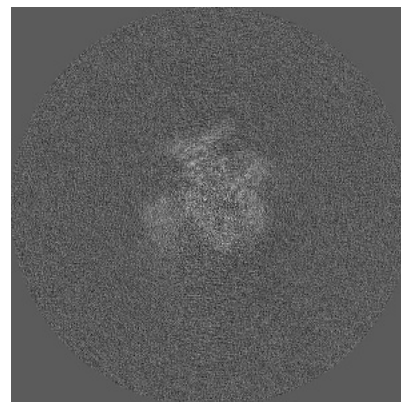
6.2.2 Raw map



X Index: 240



Y Index: 240

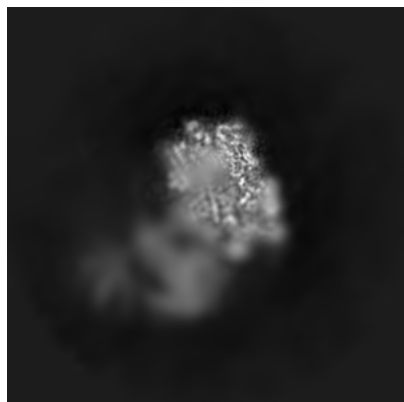


Z Index: 240

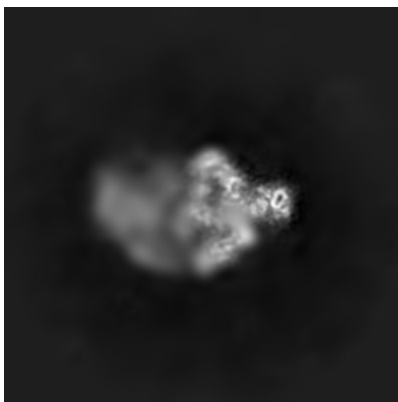
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

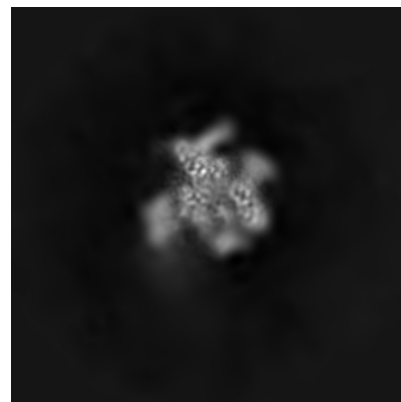
6.3.1 Primary map



X Index: 232

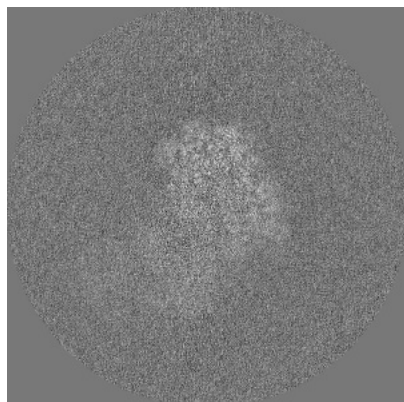


Y Index: 223

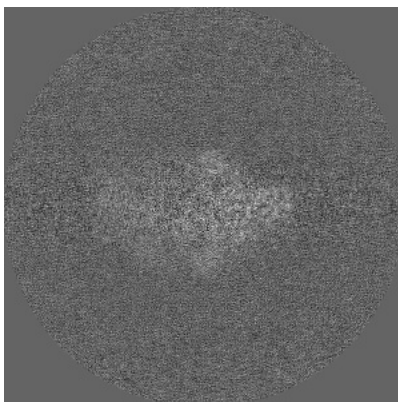


Z Index: 246

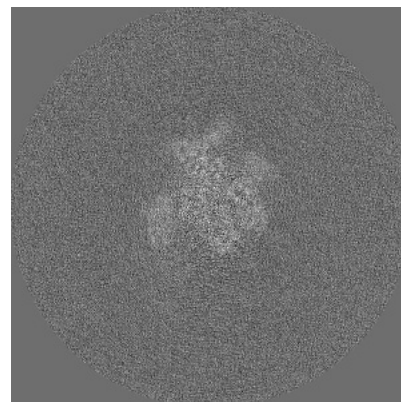
6.3.2 Raw map



X Index: 237



Y Index: 229

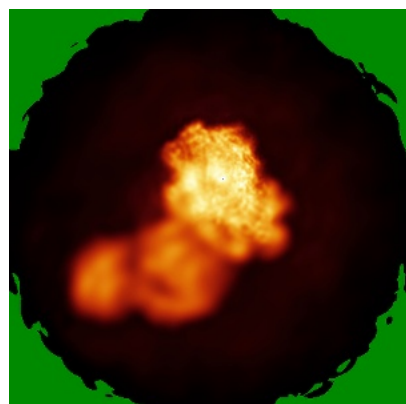


Z Index: 245

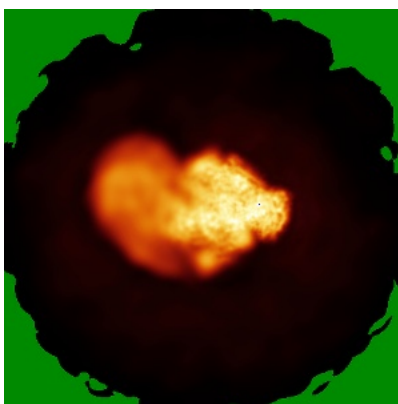
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

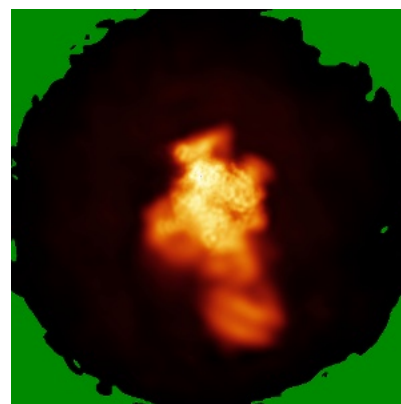
6.4.1 Primary map



X

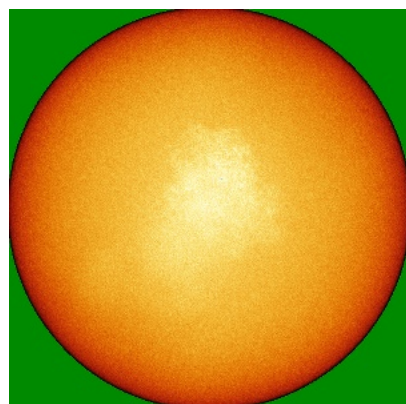


Y

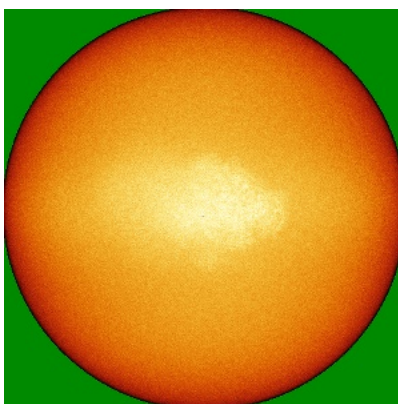


Z

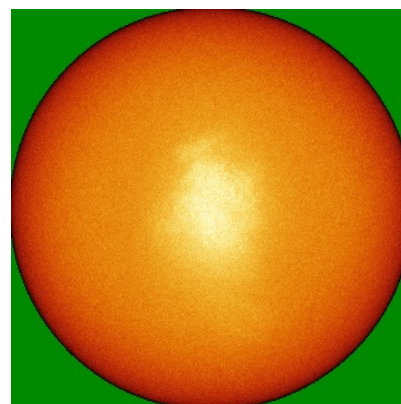
6.4.2 Raw map



X



Y

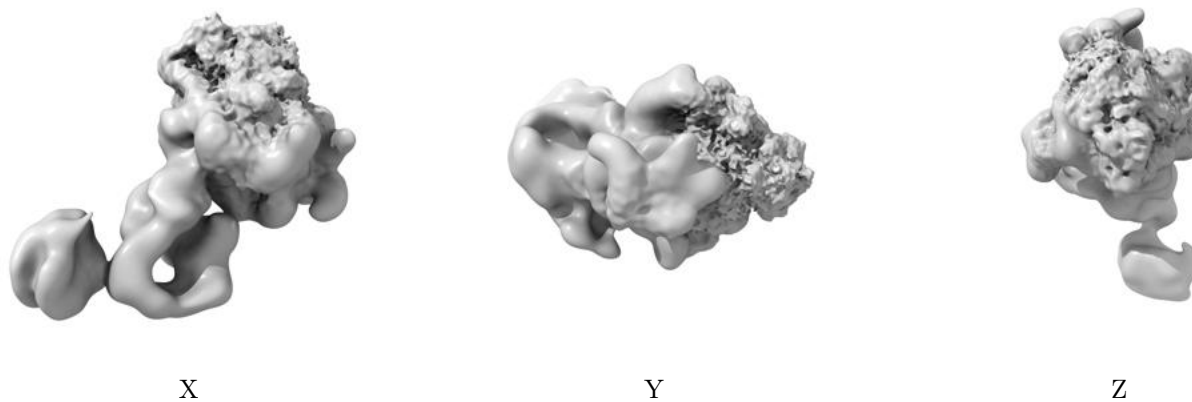


Z

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.

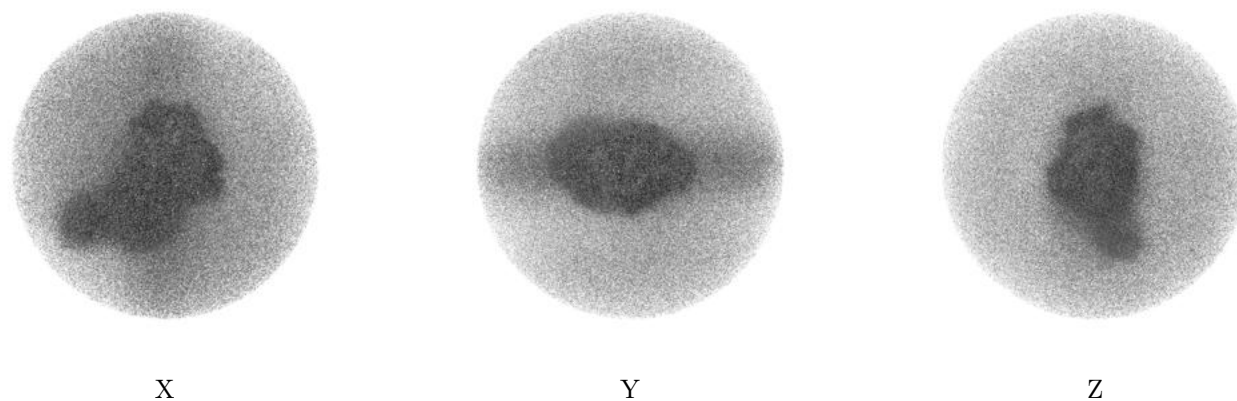
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.00432. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

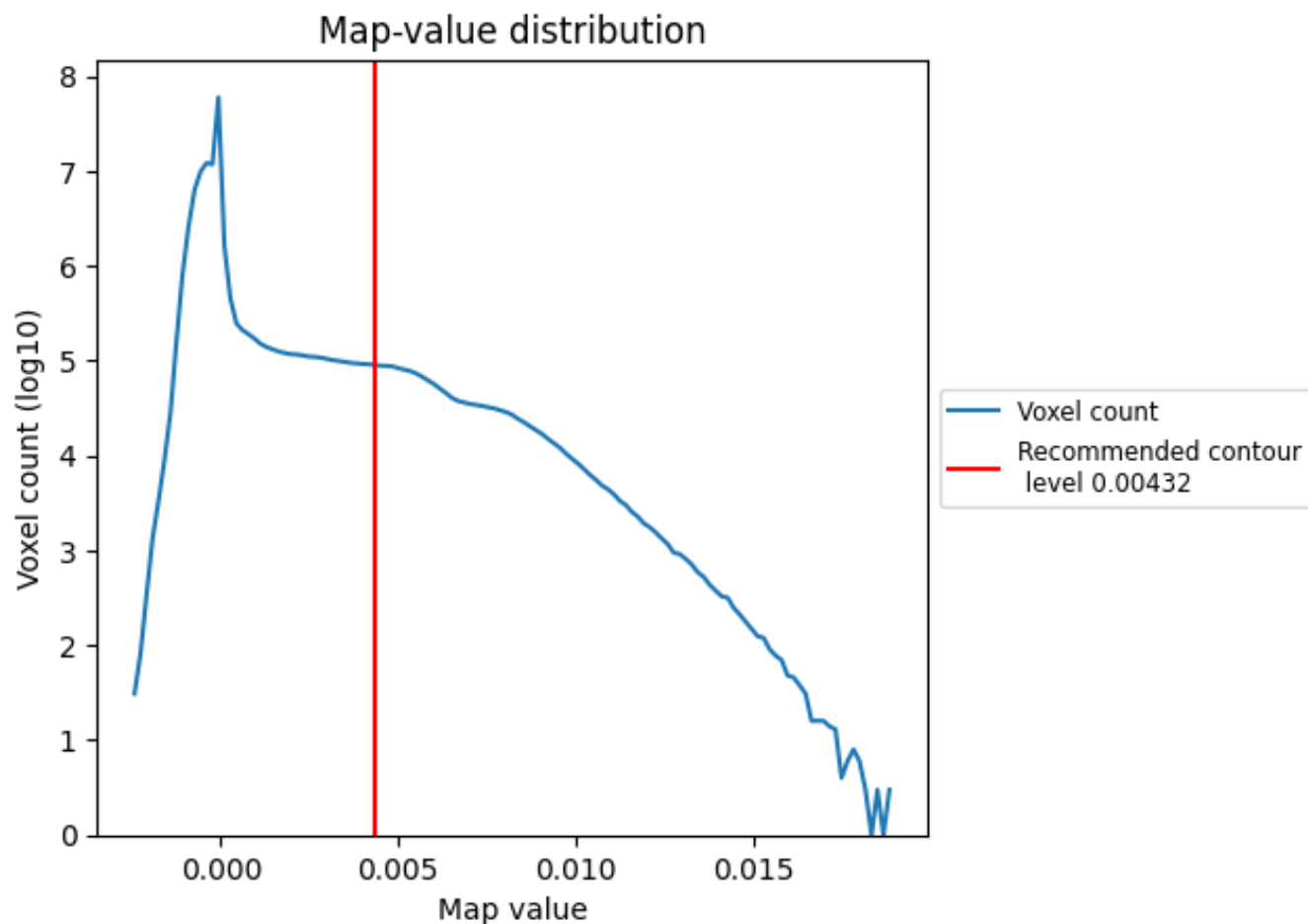
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

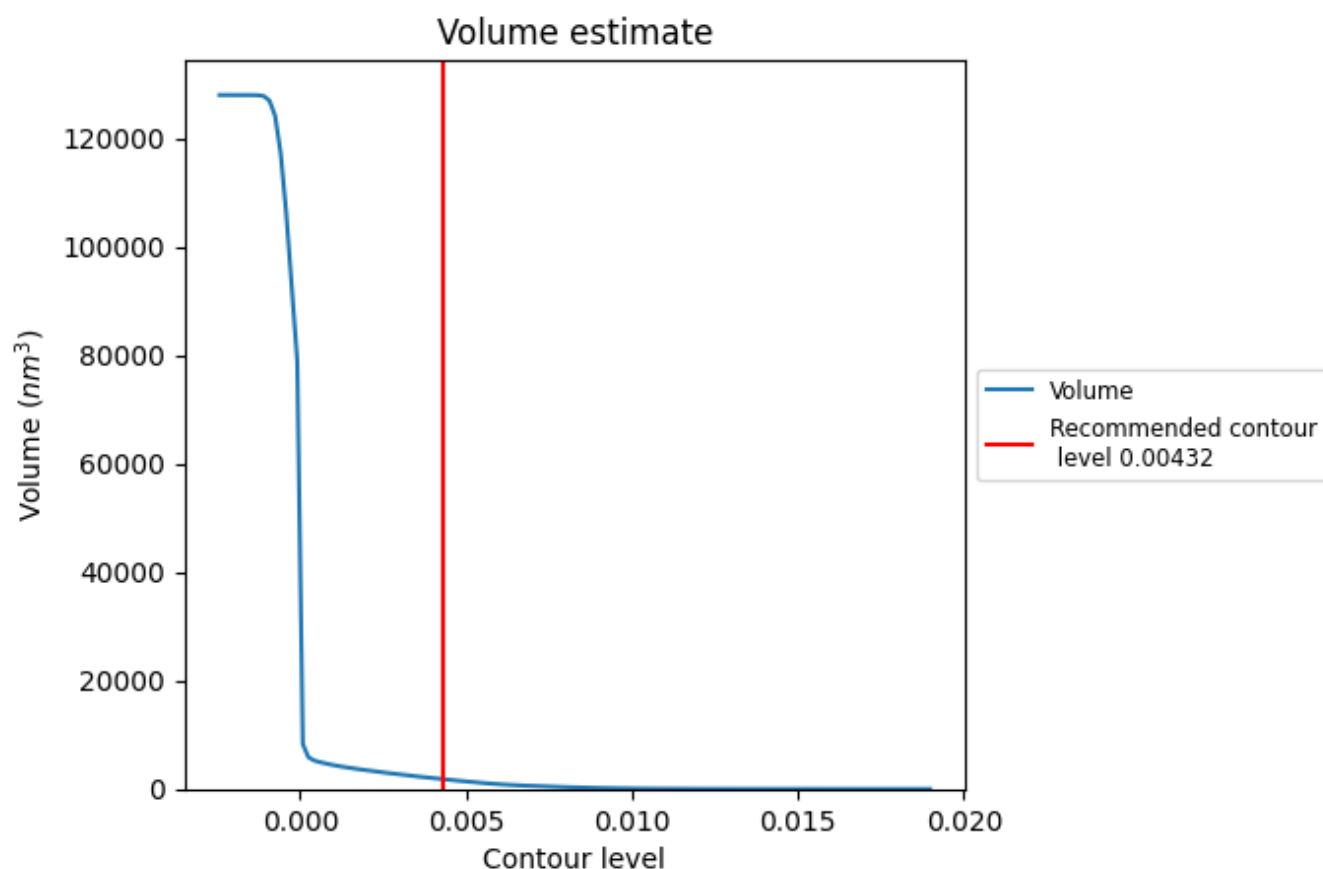
This section contains the results of statistical analysis of the map.

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.

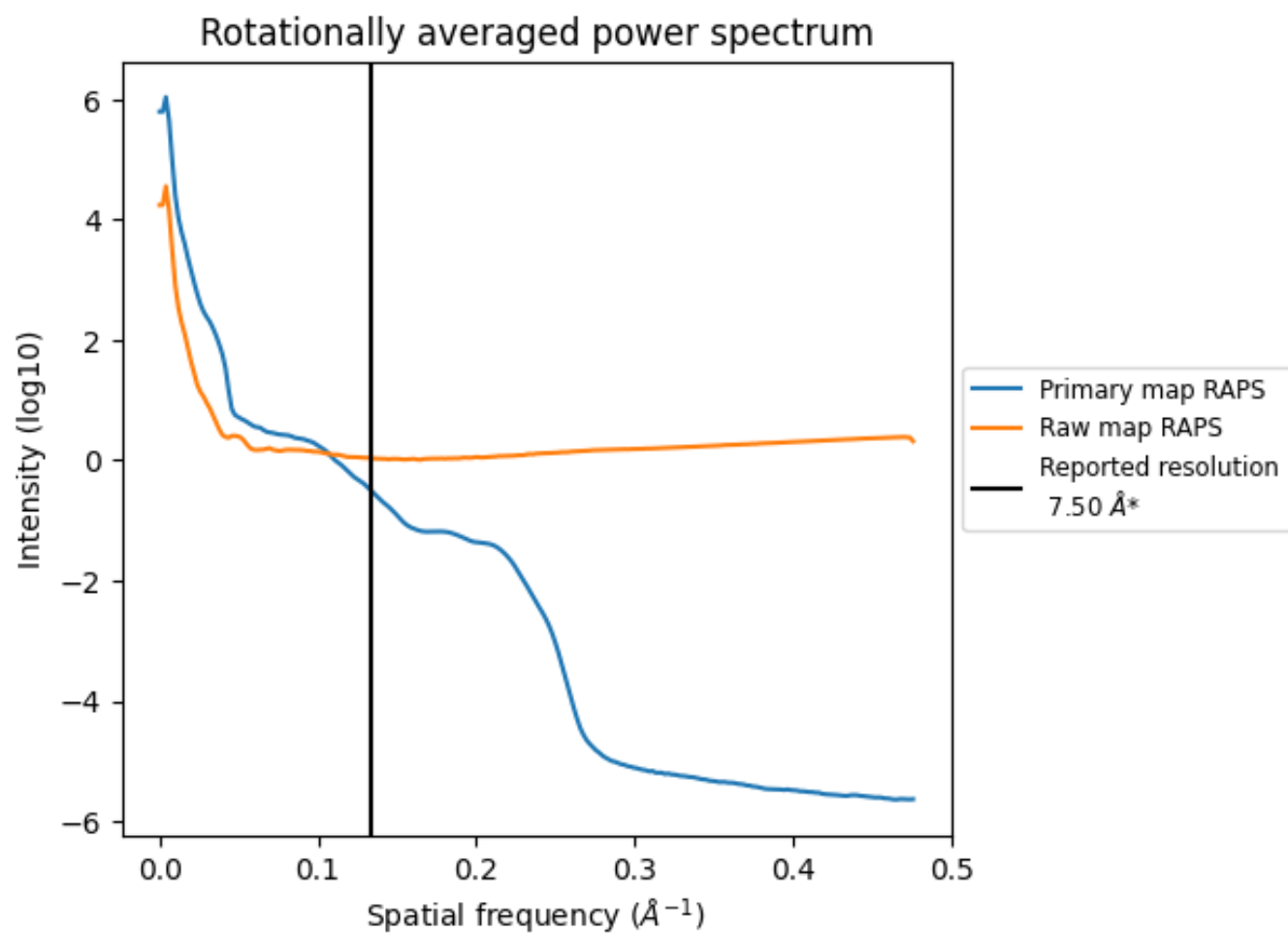
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1801 nm^3 ; this corresponds to an approximate mass of 1627 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 ⓘ

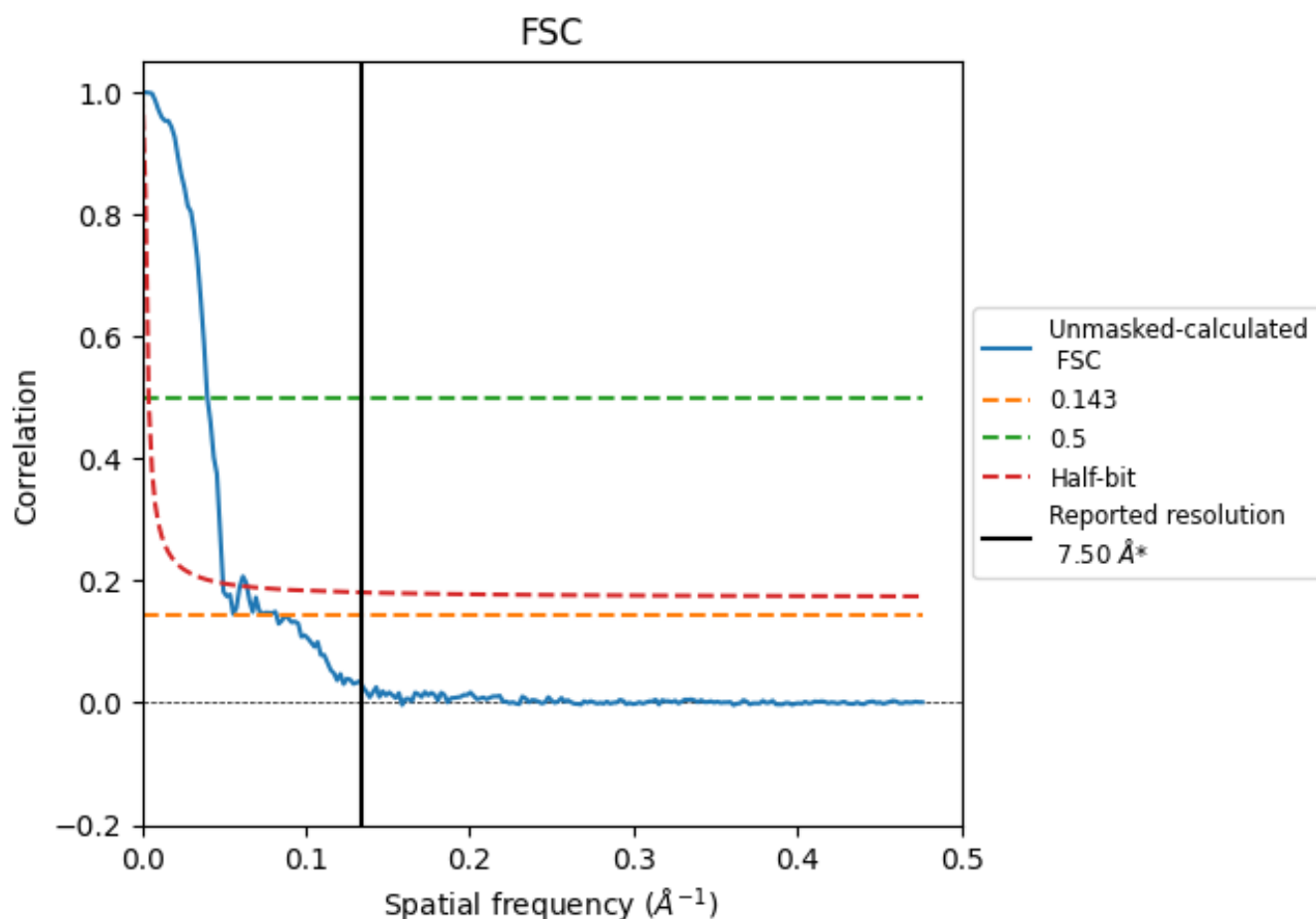


*Reported resolution corresponds to spatial frequency of 0.133 $\text{\AA}^{-1}$

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 0.133 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

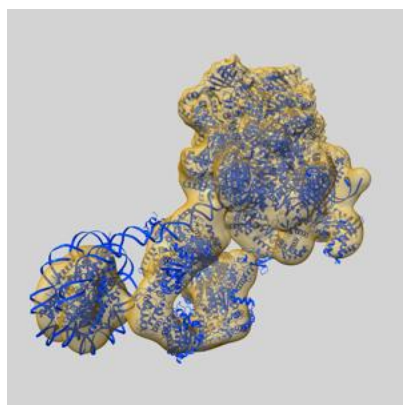
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	7.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	12.21	25.19	20.28

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 12.21 differs from the reported value 7.5 by more than 10 %

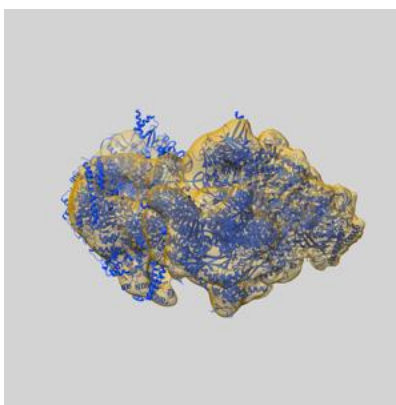
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-57390 and PDB model 29VF. Per-residue inclusion information can be found in section [3](#) on page [12](#).

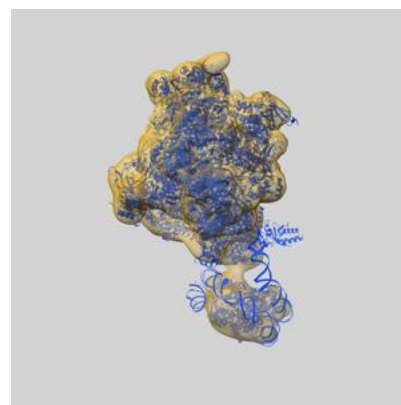
9.1 Map-model overlay [i](#)



X



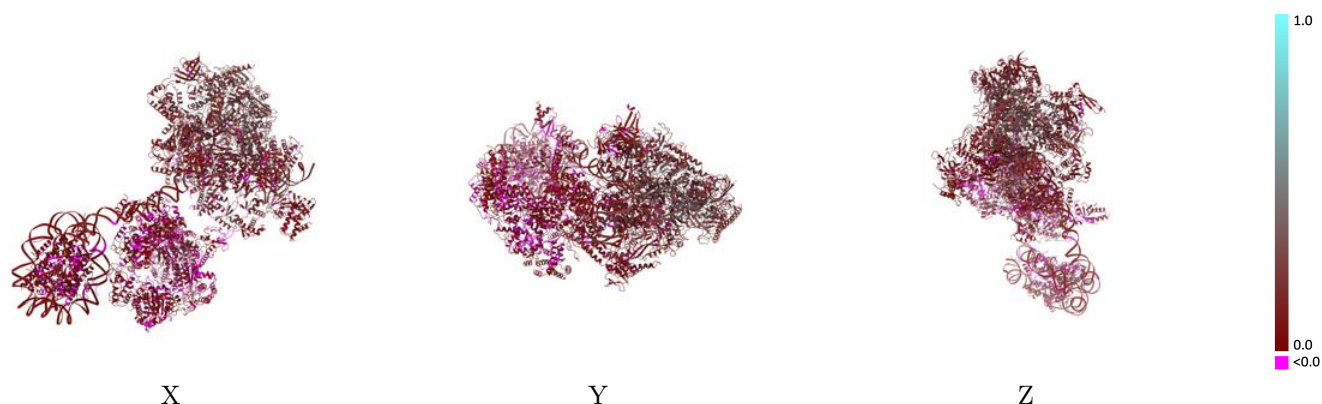
Y



Z

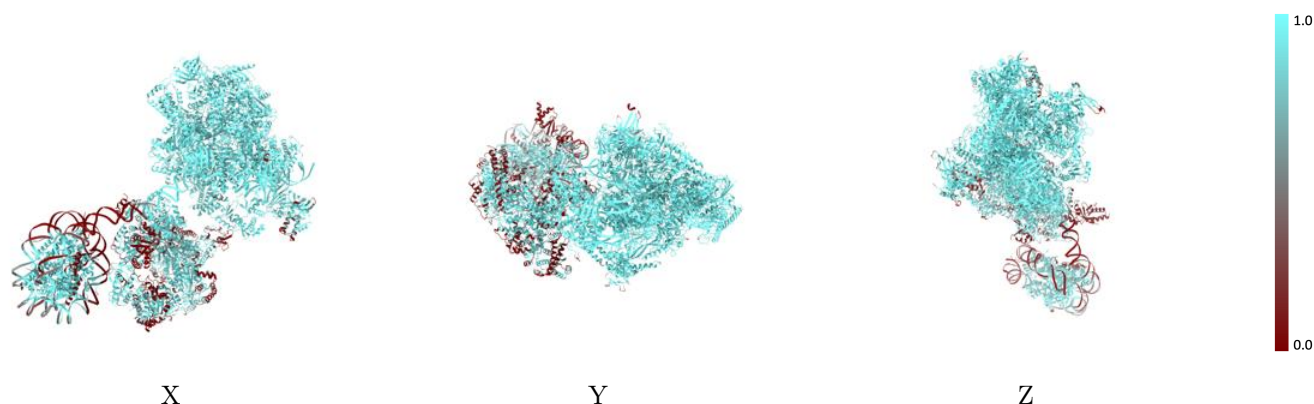
The images above show the 3D surface view of the map at the recommended contour level 0.00432 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



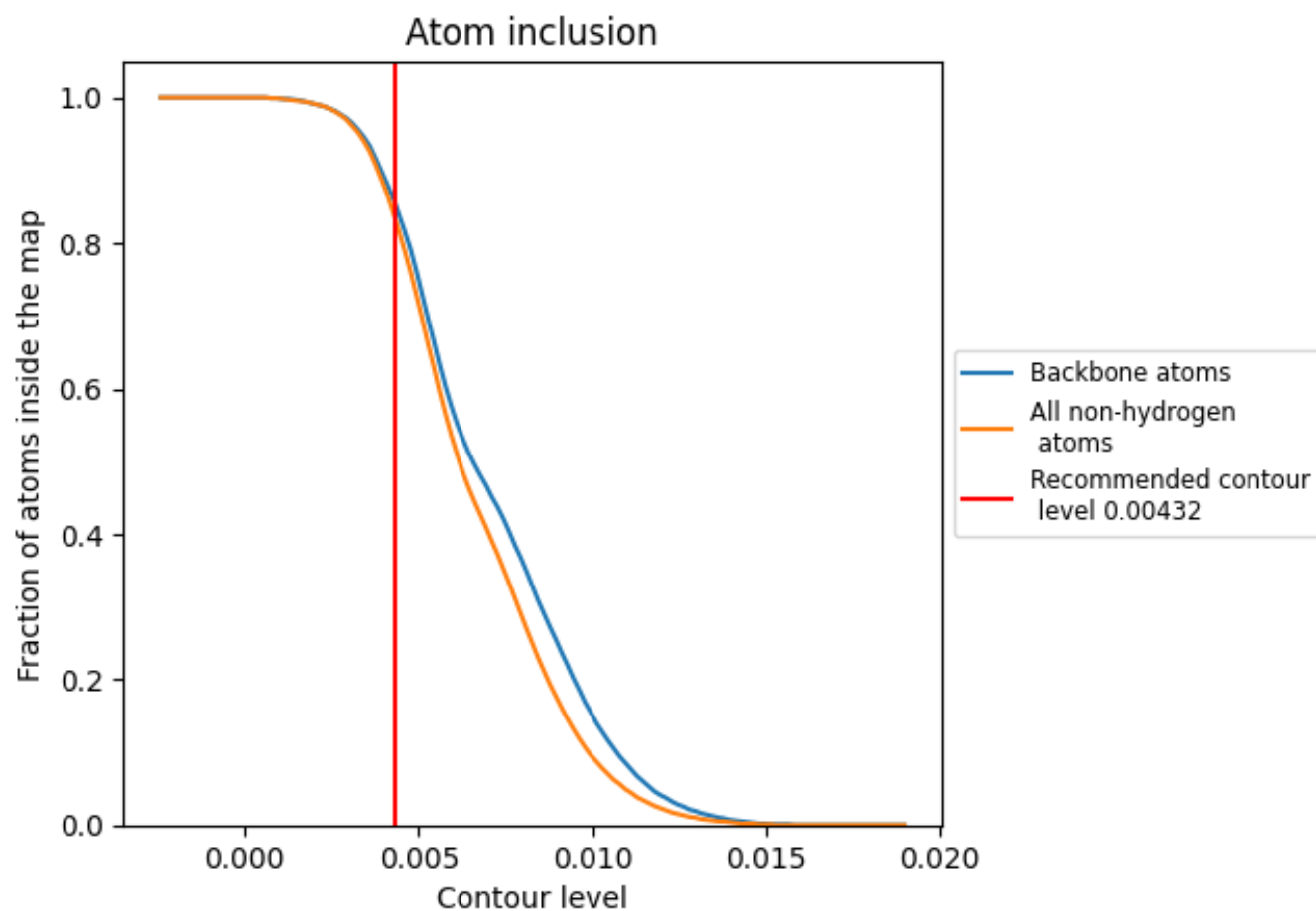
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.00432).

9.4 Atom inclusion ⓘ



At the recommended contour level, 86% of all backbone atoms, 84% 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 (0.00432) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8350	 0.1200
0	 0.7800	 0.0430
1	 0.6800	 0.0380
2	 0.5180	 0.0260
3	 0.6250	 0.0570
4	 0.8640	 0.0540
5	 0.5790	 0.0400
6	 0.1590	 0.0220
7	 0.4120	 0.0890
A	 0.9930	 0.1750
B	 0.9980	 0.2480
C	 0.9900	 0.2910
D	 0.9370	 0.0970
E	 0.9860	 0.1140
F	 0.9810	 0.1090
G	 0.9600	 0.0980
H	 0.9830	 0.1920
I	 0.9840	 0.1790
J	 0.9880	 0.2810
K	 0.9780	 0.2250
L	 0.9940	 0.2670
M	 0.9870	 0.1790
N	 0.5580	 0.0980
O	 0.9910	 0.1380
P	 1.0000	 -0.1100
Q	 0.9500	 0.0910
R	 0.9540	 0.1190
T	 0.5740	 0.0890
U	 0.8300	 0.0820
V	 0.7550	 0.0720
W	 0.9400	 0.0880
X	 0.9940	 0.0910
a	 0.9160	 0.0250
b	 0.9860	 0.0810
c	 0.7300	 0.0300



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Chain	Atom inclusion	Q-score
d	 0.7410	 0.0470
e	 0.9110	 0.0640
f	 0.9590	 0.0800
g	 0.9620	 0.0570
h	 0.9420	 0.0370