



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 03:02 PM UTC

PDB ID : 9EH2 / pdb_00009eh2
EMDB ID : EMD-48044
Title : RNA polymerase II-DSIF-SPT6-PAF1c-TFIIS-IWS1-SETD2-FACT nucleosome upstream
Authors : Markert, J.; Farnung, L.
Deposited on : 2024-11-21
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

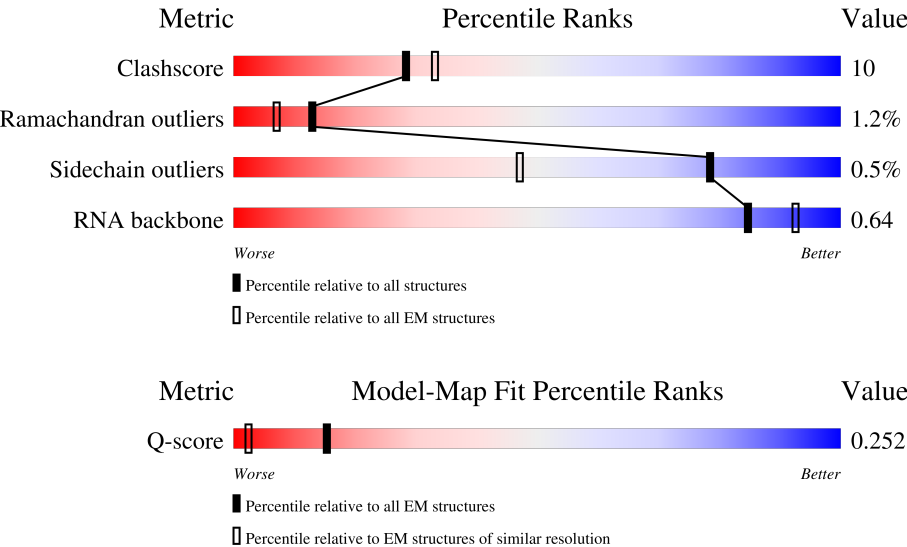
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.10 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	14724 (2.60 - 3.60)

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

Mol	Chain	Length	Quality of chain
1	A	1984	
2	B	1251	
3	C	275	

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Mol	Chain	Length	Quality of chain
4	D	142	
5	E	210	
6	F	127	
7	G	172	
8	H	150	
9	I	125	
10	J	67	
11	K	117	
12	L	58	
13	M	1729	
14	N	205	
15	O	821	
16	P	11	
17	Q	1179	
18	R	713	
19	S	304	
20	T	215	
21	U	666	
22	V	531	
23	W	305	
24	X	531	
25	Y	121	
26	Z	1087	
27	a	136	
27	e	136	

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Mol	Chain	Length	Quality of chain
28	b	103	58%17%24%
28	f	103	49%21%30%
29	g	130	60%9%31%
30	h	123	66%7%28%
31	l	1133	98%
32	x	1049	39%7%54%
33	y	709	8%52%7%40%

2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 148010 atoms, of which 72095 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 DNA-directed RNA polymerase subunit.

Mol	Chain	Residues	Atoms							AltConf	Trace
1	A	1426	Total	C	H	N	O	P	S	0	0
			22643	7074	11388	2014	2095	2	70		

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	1122	Total	C	H	N	O	S	0	0
			18007	5684	9027	1576	1656	64		

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	258	Total	C	H	N	O	S	0	0
			4096	1300	2024	356	410	6		

- Molecule 4 is a protein called RNA polymerase Rpb4/RPC9 core domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	D	126	Total	C	H	N	O	S	0	0
			1985	630	981	170	200	4		

- Molecule 5 is a protein called DNA-directed RNA polymerase II subunit E.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	E	209	Total	C	H	N	O	S	0	0
			3458	1089	1738	300	323	8		

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	F	78	Total	C	H	N	O	S	0	0
			1284	401	658	106	114	5		

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	G	171	Total	C	H	N	O	S	0	0
			2654	866	1321	214	245	8		

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	H	149	Total	C	H	N	O	S	0	0
			2354	759	1157	195	238	5		

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	I	116	Total	C	H	N	O	S	0	0
			1822	582	880	168	181	11		

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	J	66	Total	C	H	N	O	S	0	0
			1068	339	544	88	91	6		

- Molecule 11 is a protein called RNA polymerase II subunit J.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	K	115	Total	C	H	N	O	S	0	0
			1862	593	942	152	173	2		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
12	L	47	Total	C	H	N	O	S	0	0
			803	246	406	77	68	6		

- Molecule 13 is a protein called Transcription elongation factor SPT6.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	M	1172	Total	C	H	N	O	S	0	0
			18977	6063	9394	1658	1815	47		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	-2	SER	-	expression tag	UNP Q7KZ85
M	-1	ASN	-	expression tag	UNP Q7KZ85
M	0	ALA	-	expression tag	UNP Q7KZ85

- Molecule 14 is a DNA chain called non-template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	54	Total	C	N	O	P	0	0
			1106	526	182	344	54		

- Molecule 15 is a protein called Protein IWS1 homolog.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	O	132	Total	C	H	N	O	S	0	0
			2143	663	1097	181	196	6		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	-1	SER	-	expression tag	UNP Q96ST2
O	0	ASN	-	expression tag	UNP Q96ST2
O	1	ALA	-	expression tag	UNP Q96ST2

- Molecule 16 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	11	Total	C	N	O	P	0	0
			232	103	35	83	11		

- Molecule 17 is a protein called RNA polymerase-associated protein CTR9 homolog.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	Q	890	Total	C	H	N	O	S	0	0
			14396	4579	7170	1264	1352	31		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	1174	GLU	-	expression tag	UNP Q6PD62
Q	1175	ASN	-	expression tag	UNP Q6PD62
Q	1176	LEU	-	expression tag	UNP Q6PD62
Q	1177	TYR	-	expression tag	UNP Q6PD62

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	1178	PHE	-	expression tag	UNP Q6PD62
Q	1179	GLN	-	expression tag	UNP Q6PD62

- Molecule 18 is a protein called RNA polymerase-associated protein RTF1 homolog.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	R	283	Total	C	H	N	O	S	0	0
			4222	1349	2056	409	400	8		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	-2	SER	-	expression tag	UNP Q92541
R	-1	ASN	-	expression tag	UNP Q92541
R	0	ALA	-	expression tag	UNP Q92541

- Molecule 19 is a protein called Transcription elongation factor A protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	S	161	Total	C	H	N	O		0	0
			858	334	201	161	162			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	-2	SER	-	expression tag	UNP P23193
S	-1	ASN	-	expression tag	UNP P23193
S	0	ALA	-	expression tag	UNP P23193

- Molecule 20 is a DNA chain called Template DNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	T	65	Total	C	N	O	P		0	0
			1335	627	279	364	65			

- Molecule 21 is a protein called RNA polymerase-associated protein LEO1.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	U	125	Total	C	H	N	O	S	0	0
			1540	538	684	151	166	1		

- Molecule 22 is a protein called RNA polymerase II-associated factor 1 homolog.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	V	244	Total	C	H	N	O	S	0	0
			3150	1065	1443	305	333	4		

- Molecule 23 is a protein called WDR61.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	W	300	Total	C	H	N	O	S	0	0
			4582	1483	2249	392	454	4		

- Molecule 24 is a protein called Parafibromin.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	X	43	Total	C	H	N	O		0	0
			725	220	372	69	64			

- Molecule 25 is a protein called Transcription elongation factor SPT4.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	Y	116	Total	C	H	N	O	S	0	0
			1820	570	909	159	173	9		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	-3	GLY	-	expression tag	UNP P63272
Y	-2	PRO	-	expression tag	UNP P63272
Y	-1	GLY	-	expression tag	UNP P63272
Y	0	SER	-	expression tag	UNP P63272

- Molecule 26 is a protein called Transcription elongation factor SPT5.

Mol	Chain	Residues	Atoms							AltConf	Trace
26	Z	510	Total	C	H	N	O	P	S	0	0
			8071	2552	4046	709	745	1	18		

- Molecule 27 is a protein called Histone H3.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	a	76	Total	C	H	N	O	S	0	0
			1237	391	621	112	110	3		

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Mol	Chain	Residues	Atoms						AltConf	Trace
27	e	75	Total	C	H	N	O	S	0	0
			1225	387	617	111	107	3		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	36	MET	LYS	engineered mutation	UNP A0A310TTQ1
e	36	MET	LYS	engineered mutation	UNP A0A310TTQ1

- Molecule 28 is a protein called Histone H4.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	b	78	Total	C	H	N	O	S	0	0
			1283	393	661	120	108	1		
28	f	72	Total	C	H	N	O	S	0	0
			1195	361	619	114	100	1		

- Molecule 29 is a protein called Histone H2A type 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	g	90	Total	C	H	N	O		0	0
			1425	441	721	140	123			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
g	99	ARG	GLY	conflict	UNP P06897
g	123	SER	ALA	conflict	UNP P06897

- Molecule 30 is a protein called Histone H2B 1.1.

Mol	Chain	Residues	Atoms						AltConf	Trace
30	h	89	Total	C	H	N	O	S	0	0
			1387	438	693	122	132	2		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
h	3	MET	-	initiating methionine	UNP P02281
h	32	THR	SER	engineered mutation	UNP P02281

- Molecule 31 is a protein called Histone-lysine N-methyltransferase SETD2.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	l	23	Total	C	H	N	O	0	0
			395	119	200	35	41		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
l	1432	SER	-	expression tag	UNP Q9BYW2
l	1433	ASN	-	expression tag	UNP Q9BYW2
l	1434	ALA	-	expression tag	UNP Q9BYW2
l	1962	LEU	PRO	conflict	UNP Q9BYW2

- Molecule 32 is a protein called FACT complex subunit SPT16.

Mol	Chain	Residues	Atoms						AltConf	Trace
32	x	483	Total	C	H	N	O	S	0	0
			7818	2506	3870	682	743	17		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
x	-1	SER	-	expression tag	UNP Q9Y5B9
x	0	ASN	-	expression tag	UNP Q9Y5B9

- Molecule 33 is a protein called FACT complex subunit SSRP1.

Mol	Chain	Residues	Atoms						AltConf	Trace
33	y	422	Total	C	H	N	O	S	0	0
			6842	2201	3406	585	635	15		

- Molecule 34 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
34	A	2	Total	Zn	0
			2	2	
34	B	1	Total	Zn	0
			1	1	
34	C	1	Total	Zn	0
			1	1	
34	I	2	Total	Zn	0
			2	2	

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Mol	Chain	Residues	Atoms		AltConf
34	J	1	Total 1	Zn 1	0
34	L	1	Total 1	Zn 1	0
34	Y	1	Total 1	Zn 1	0

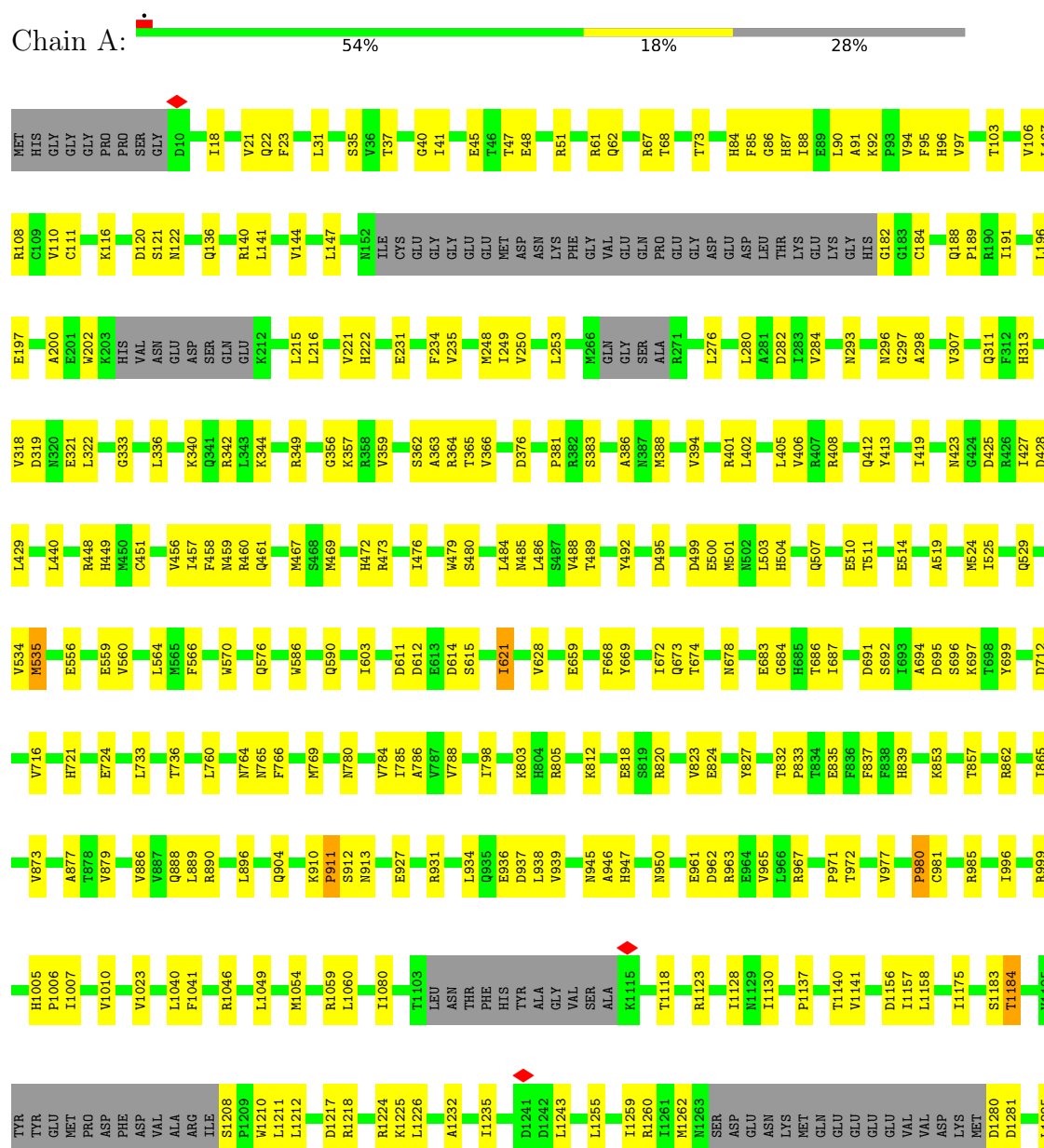
- Molecule 35 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

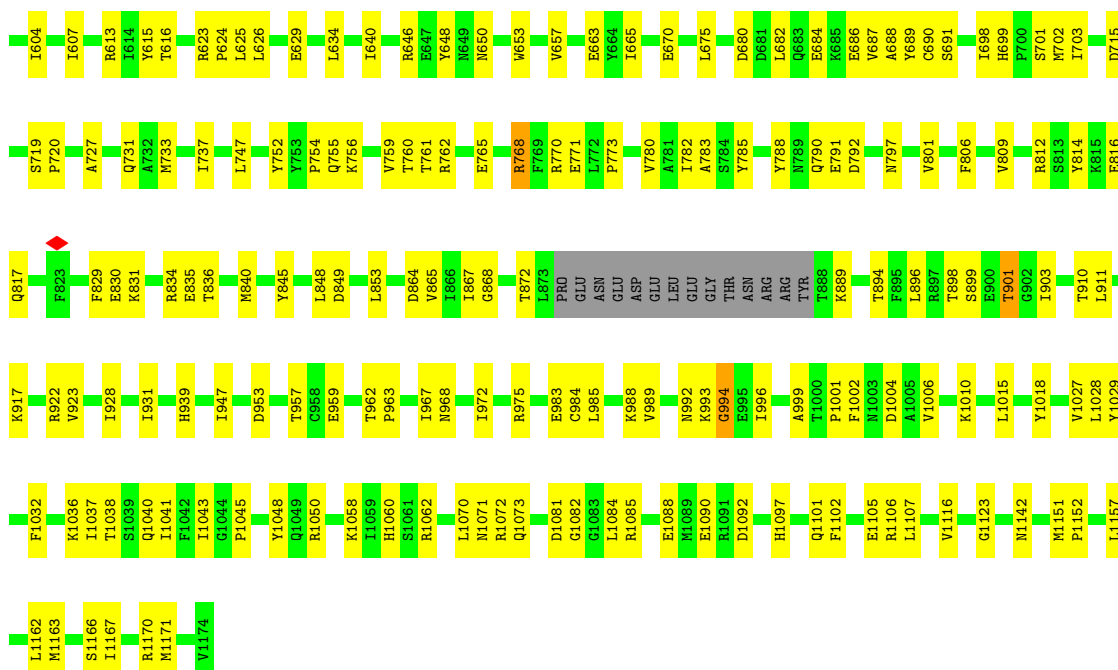
Mol	Chain	Residues	Atoms		AltConf
35	A	1	Total 1	Mg 1	0

3 Residue-property plots

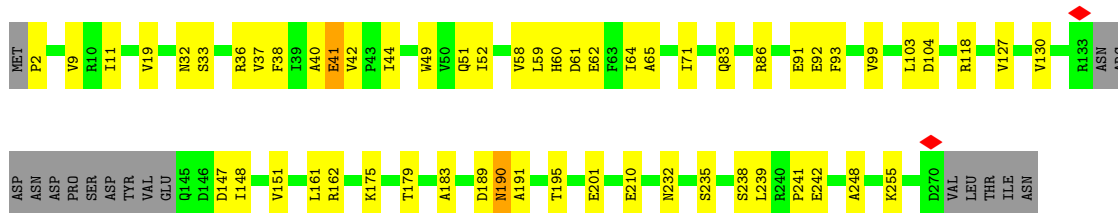
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: DNA-directed RNA polymerase subunit





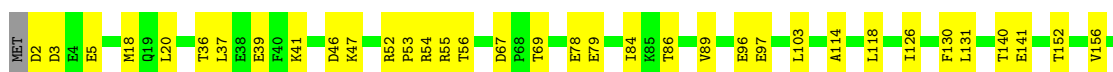
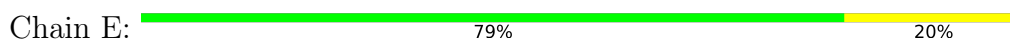
• Molecule 3: DNA-directed RNA polymerase II subunit RPB3



• Molecule 4: RNA polymerase Rpb4/PC9 core domain-containing protein

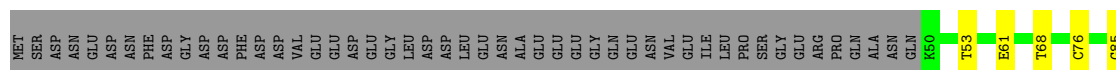


• Molecule 5: DNA-directed RNA polymerase II subunit E

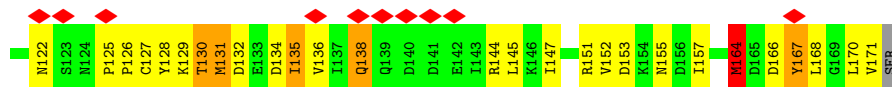




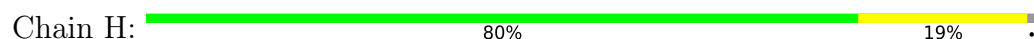
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2



- Molecule 7: DNA-directed RNA polymerase II subunit RPB7



- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



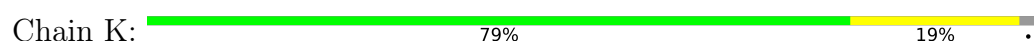
- Molecule 9: DNA-directed RNA polymerase II subunit RPB9



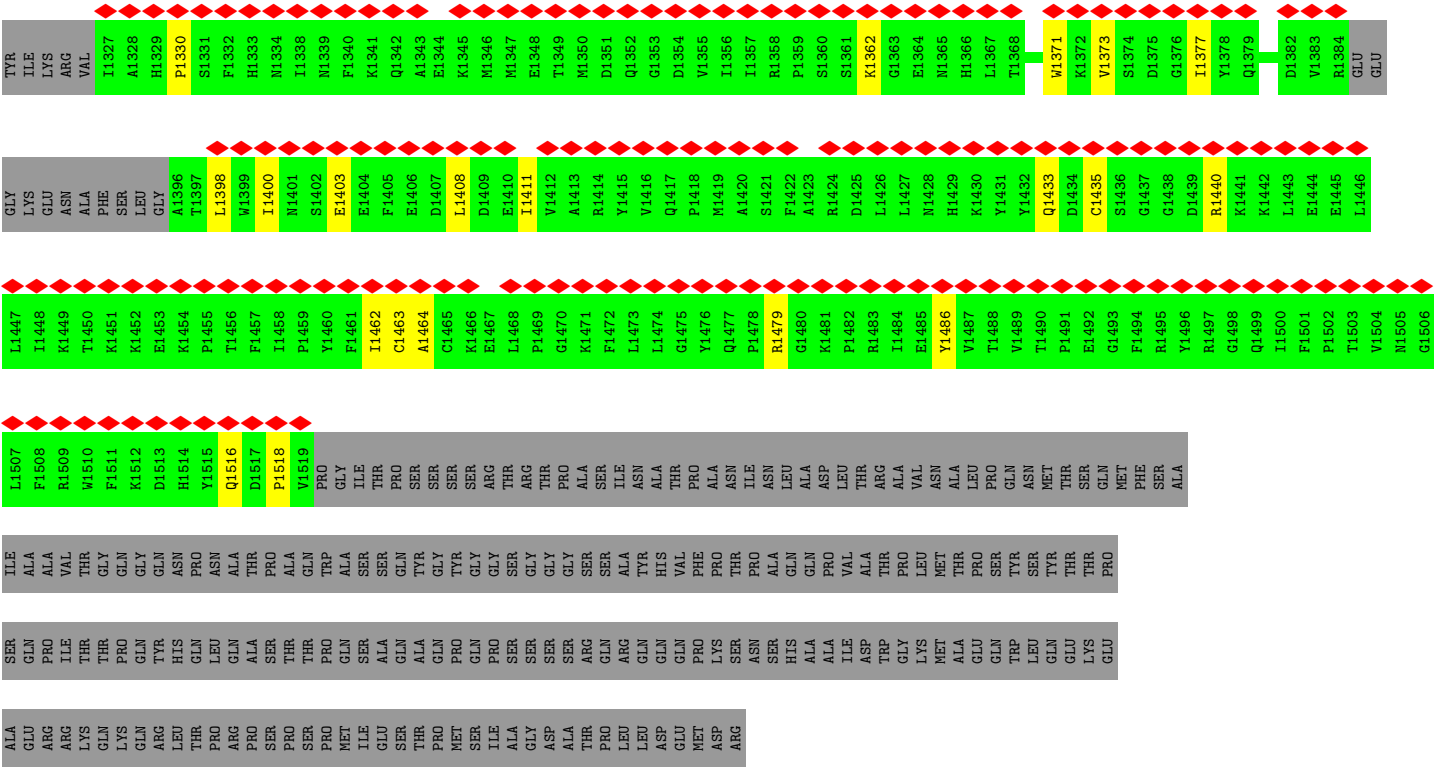
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5



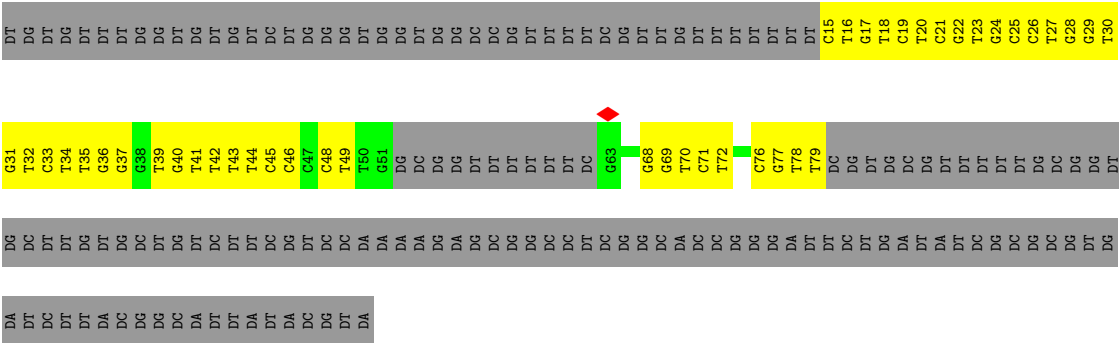
- Molecule 11: RNA polymerase II subunit J



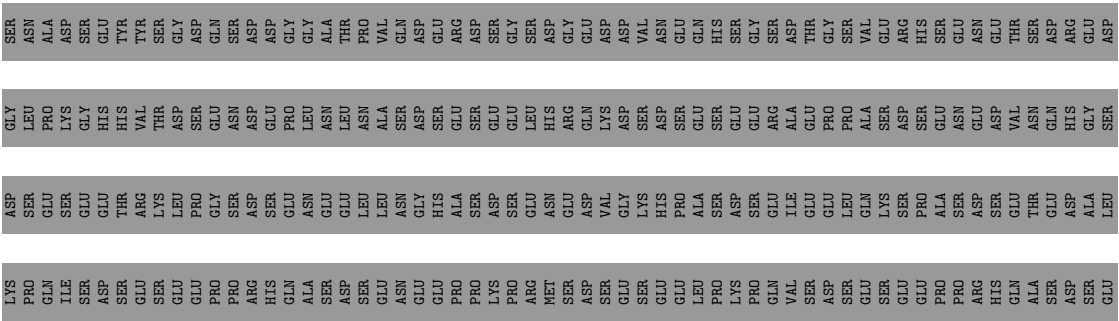


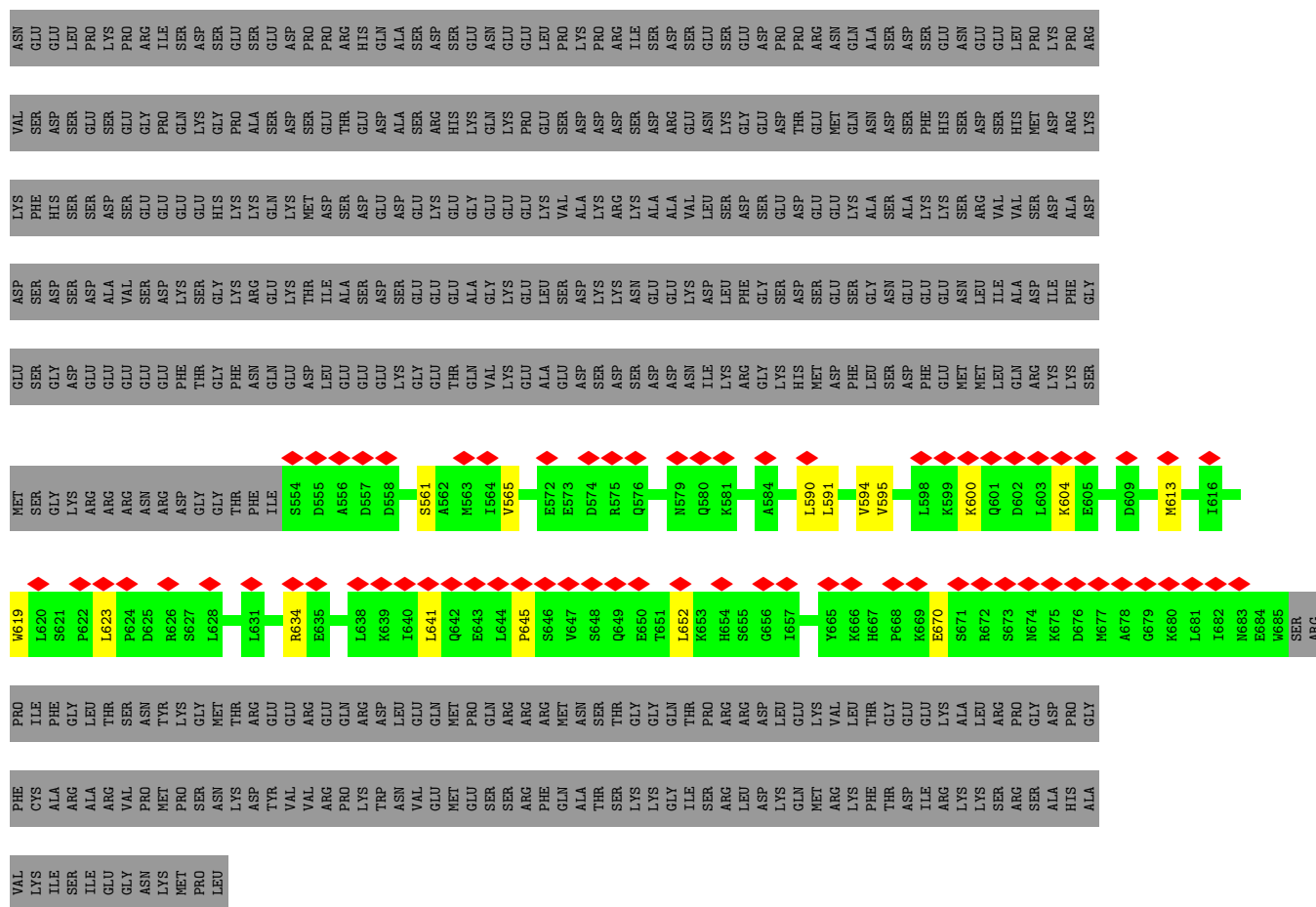


● Molecule 14: non-template DNA

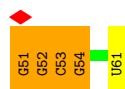


● Molecule 15: Protein IWS1 homolog

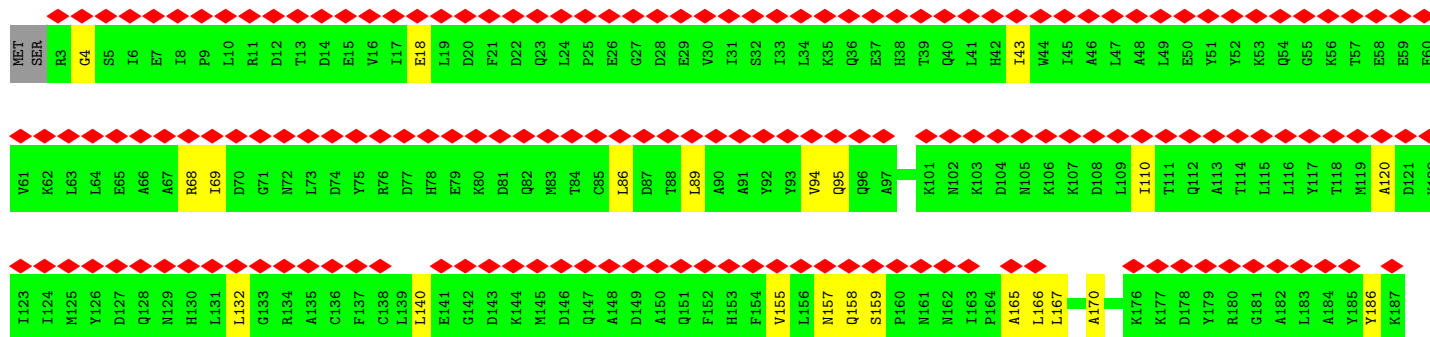


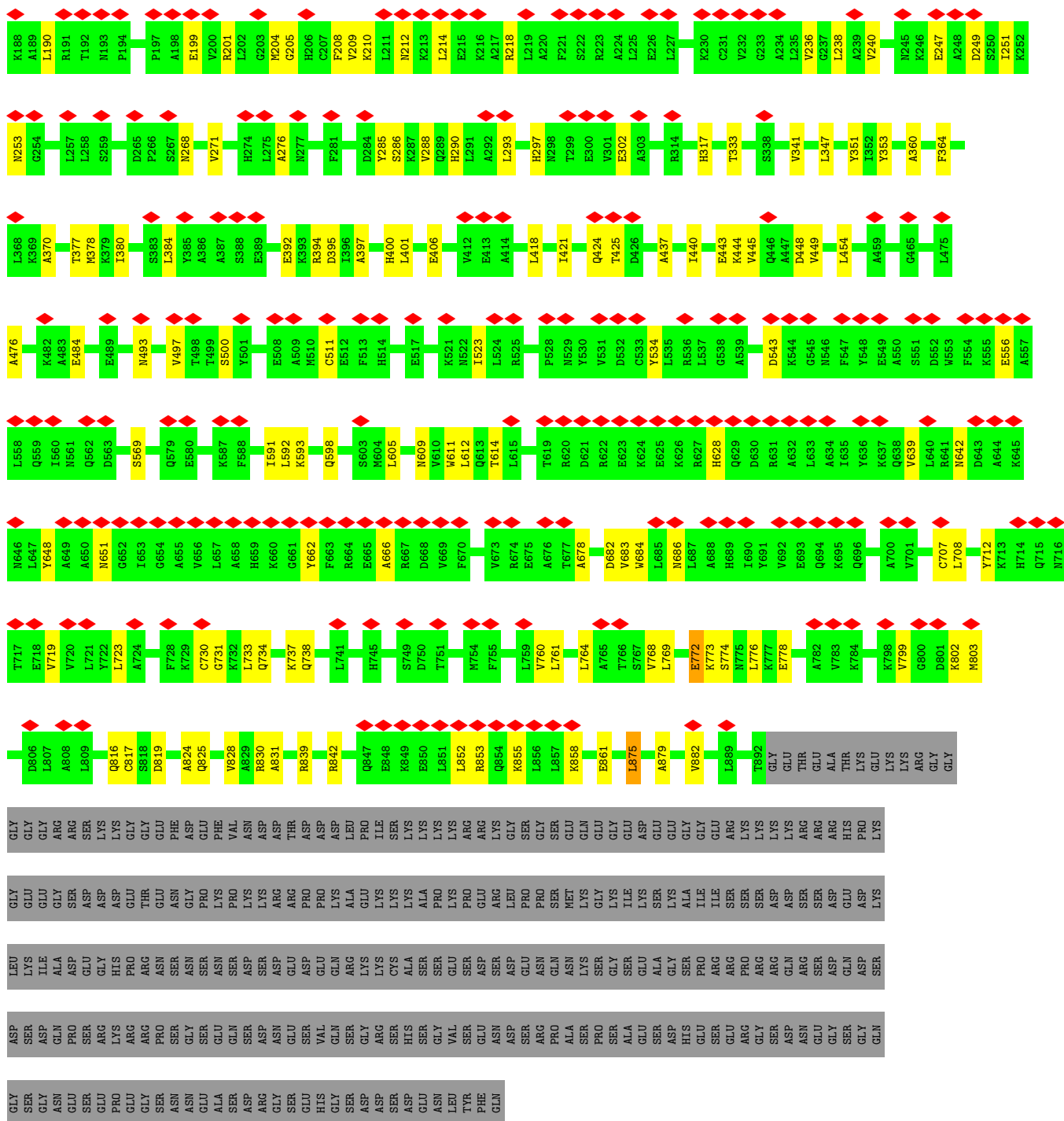


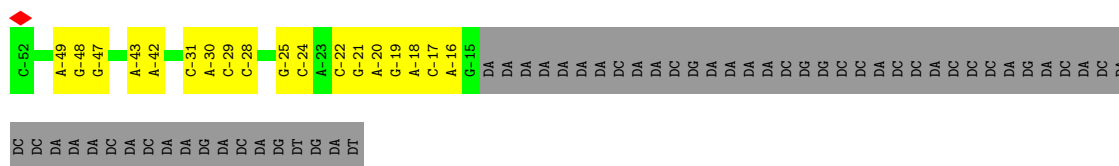
• Molecule 16: RNA



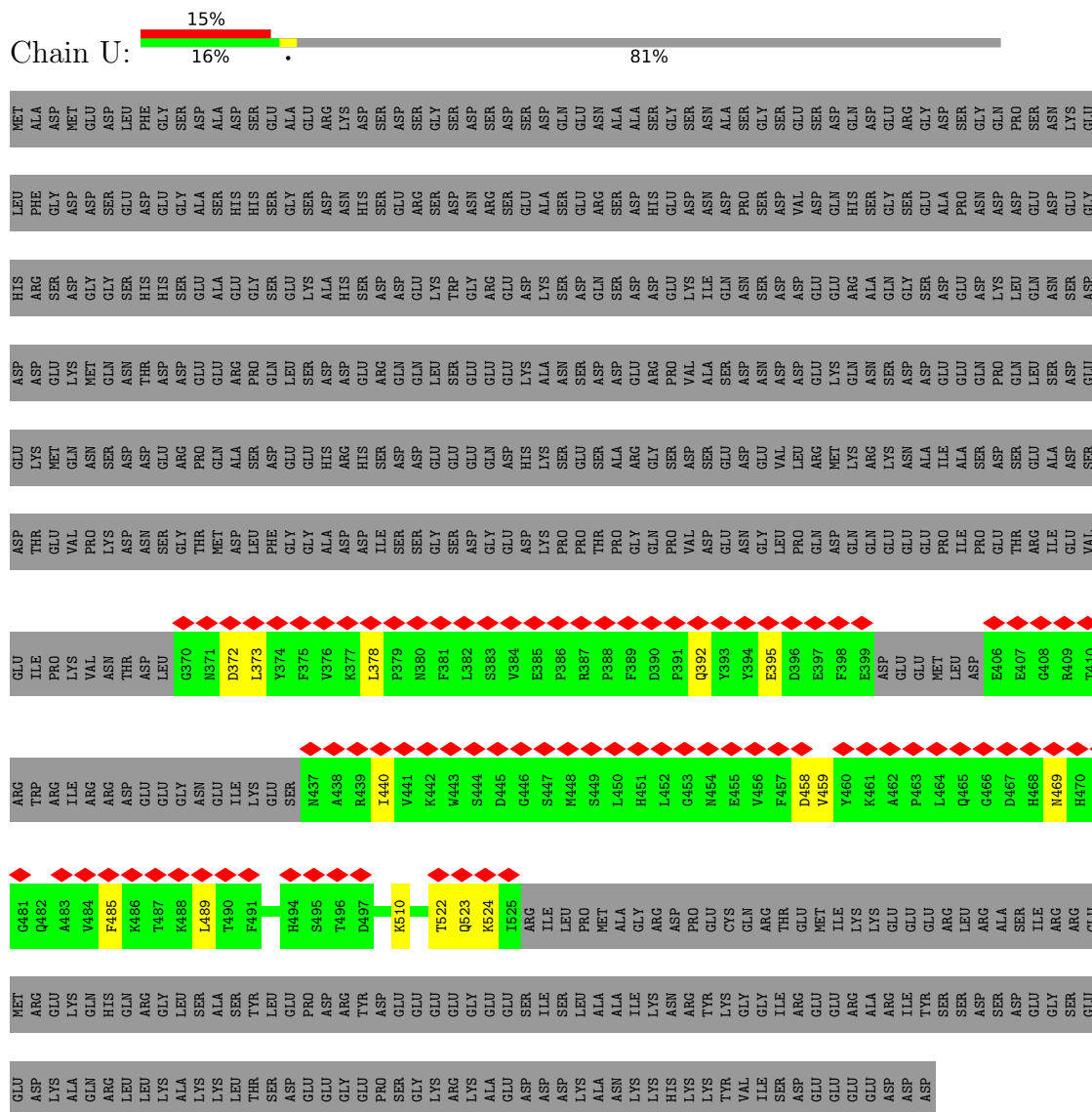
• Molecule 17: RNA polymerase-associated protein CTR9 homolog



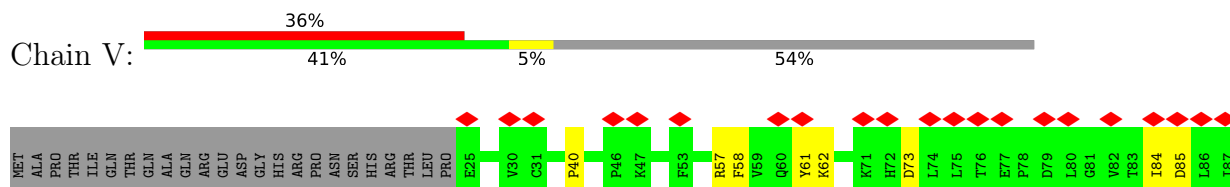


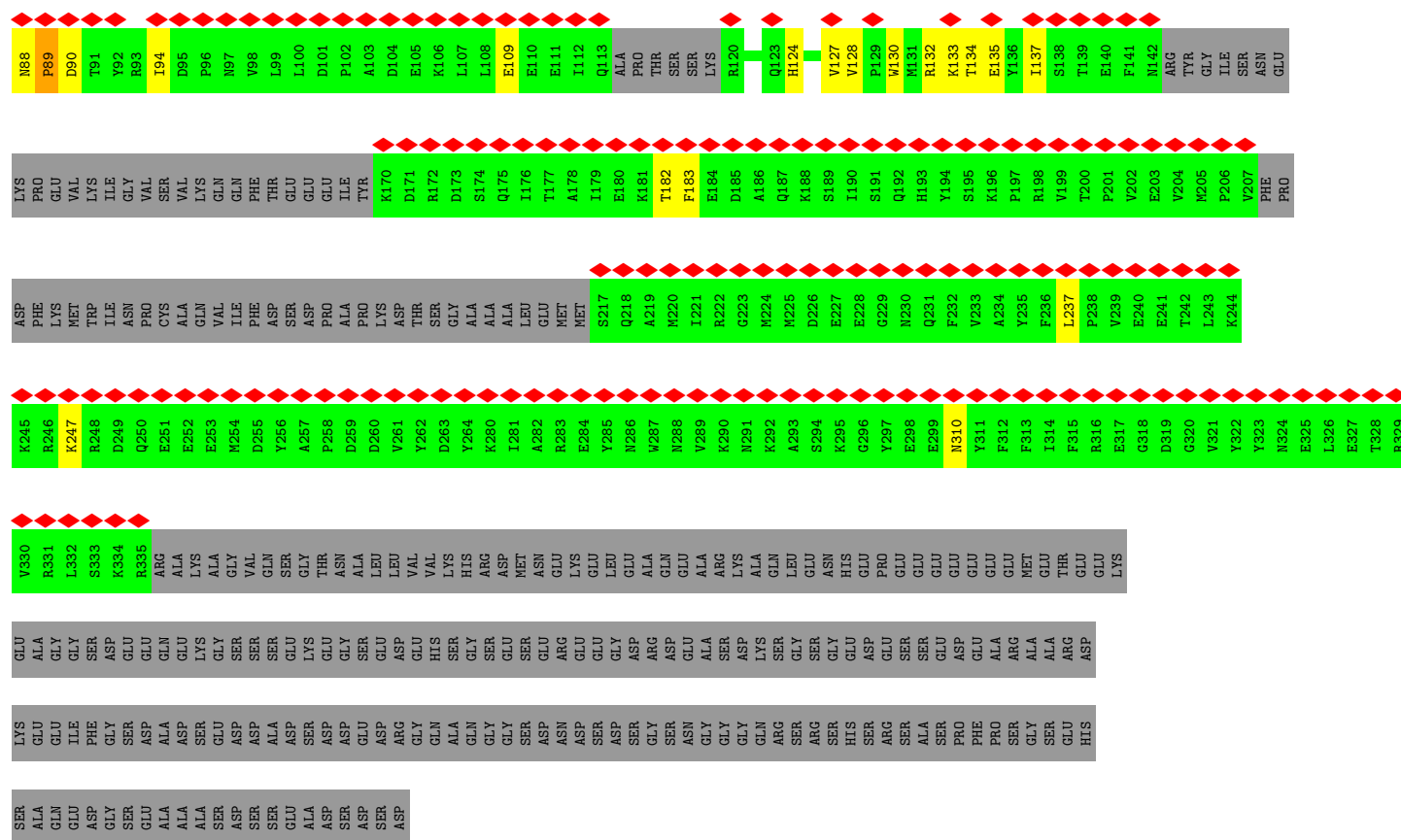


• Molecule 21: RNA polymerase-associated protein LEO1

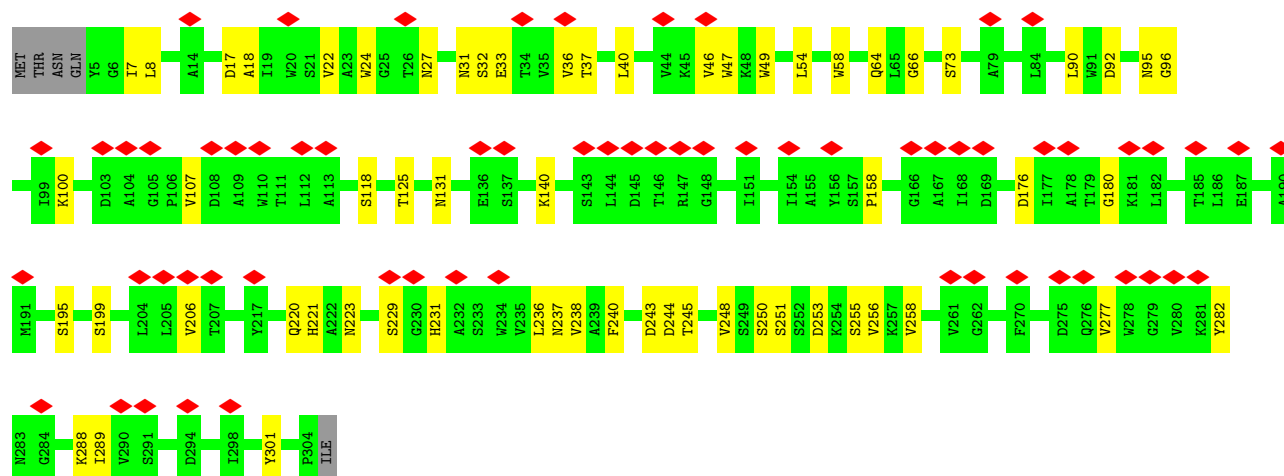
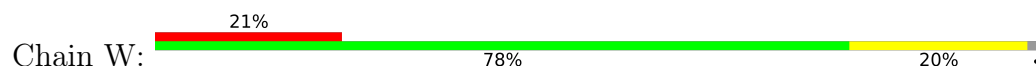


• Molecule 22: RNA polymerase II-associated factor 1 homolog



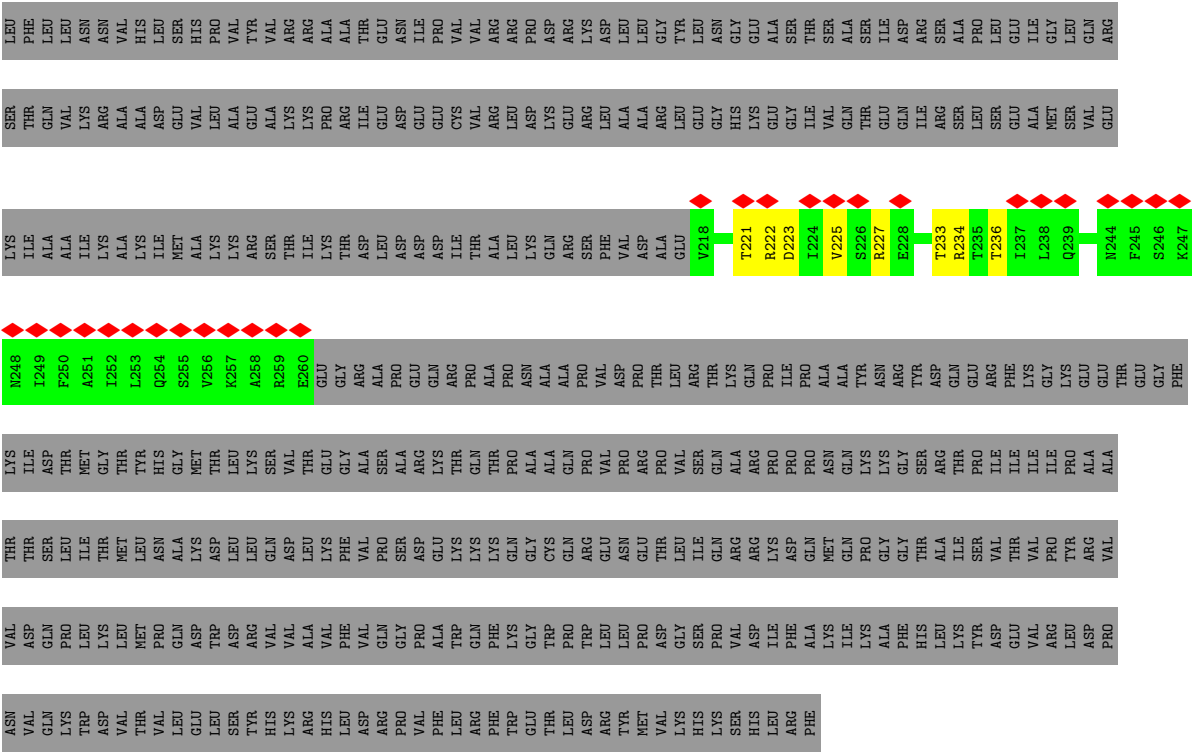


• Molecule 23: WDR61

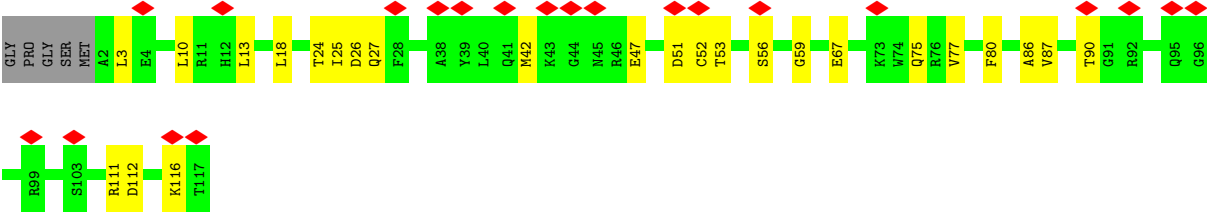
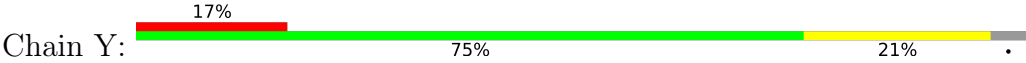


• Molecule 24: Parafibromin

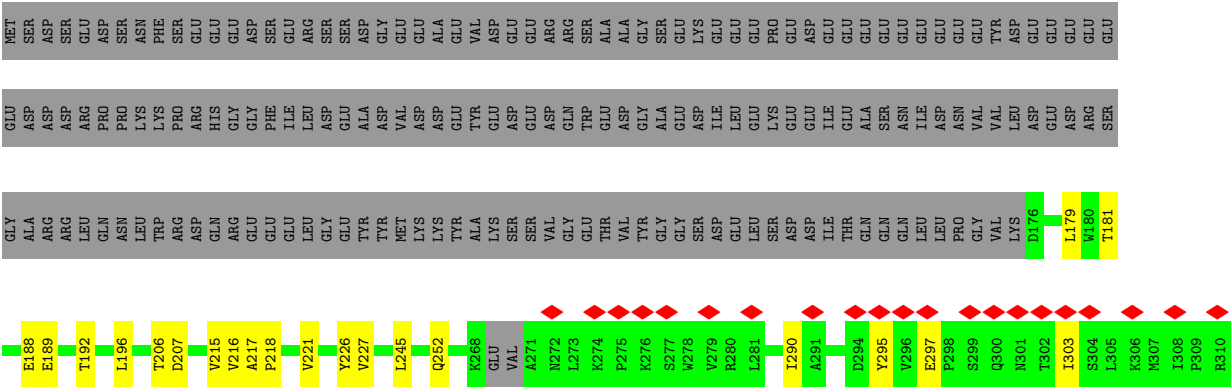
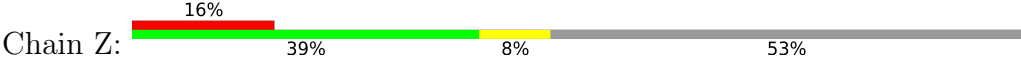


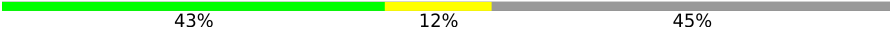


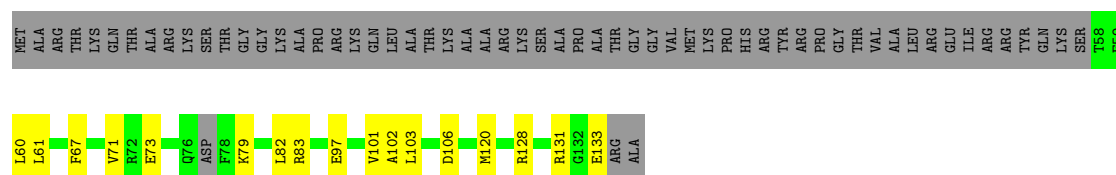
• Molecule 25: Transcription elongation factor SPT4



• Molecule 26: Transcription elongation factor SPT5



Chain e: 



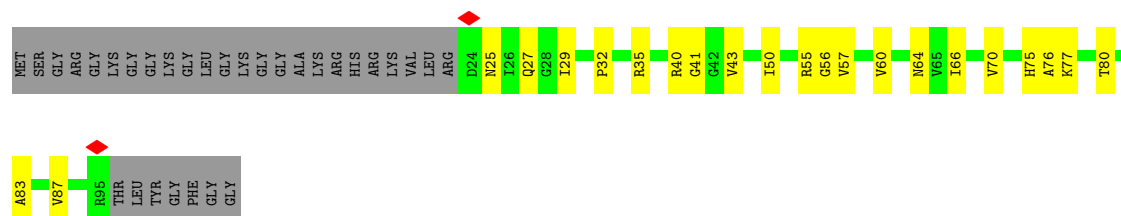
• Molecule 28: Histone H4

Chain b: 



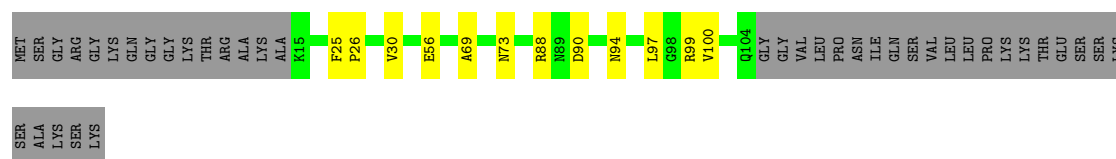
• Molecule 28: Histone H4

Chain f: 



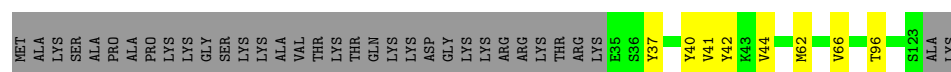
• Molecule 29: Histone H2A type 1

Chain g: 

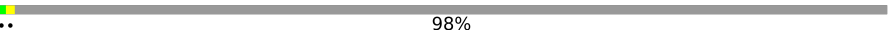


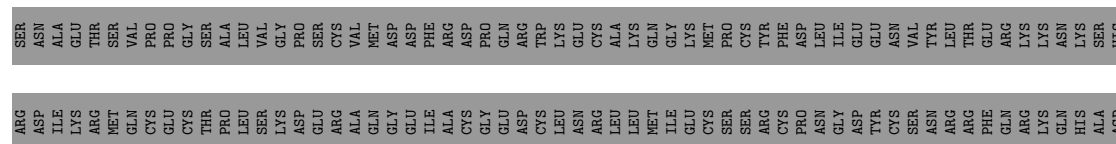
• Molecule 30: Histone H2B 1.1

Chain h: 



• Molecule 31: Histone-lysine N-methyltransferase SETD2

Chain i: 





[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	74820	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.008	Depositor
Minimum map value	-0.004	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.028	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	535.5, 535.5, 535.5	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.19, 1.19, 1.19	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.28	0/11437	0.46	0/15433
2	B	0.29	0/9158	0.46	0/12360
3	C	0.26	0/2115	0.43	0/2873
4	D	0.19	0/1017	0.36	0/1368
5	E	0.26	0/1751	0.46	0/2366
6	F	0.30	0/636	0.44	0/859
7	G	0.27	0/1364	0.51	0/1853
8	H	0.26	0/1219	0.46	0/1644
9	I	0.23	0/964	0.40	0/1305
10	J	0.28	0/533	0.41	0/719
11	K	0.26	0/939	0.41	0/1271
12	L	0.31	0/403	0.41	0/536
13	M	0.24	0/9783	0.37	0/13201
14	N	0.38	0/1232	0.60	0/1900
15	O	0.09	0/1062	0.19	0/1428
16	P	0.34	0/257	0.59	0/398
17	Q	0.13	0/7365	0.29	2/9927 (0.0%)
18	R	0.12	0/2195	0.23	0/2947
19	S	0.11	0/659	0.26	0/827
20	T	0.44	0/1506	0.61	0/2318
21	U	0.13	0/870	0.25	0/1183
22	V	0.11	0/1734	0.29	0/2367
23	W	0.12	0/2392	0.27	0/3257
24	X	0.12	0/356	0.18	0/478
25	Y	0.14	0/927	0.29	0/1250
26	Z	0.15	0/4084	0.29	0/5498
27	a	0.27	0/623	0.37	0/837
27	e	0.26	0/615	0.39	0/826
28	b	0.22	0/629	0.35	0/843
28	f	0.21	0/581	0.35	0/778
29	g	0.25	0/712	0.35	0/959
30	h	0.24	0/705	0.34	0/951

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	l	0.19	0/196	0.21	0/261
32	x	0.27	1/4033 (0.0%)	0.43	2/5438 (0.0%)
33	y	0.19	0/3513	0.33	0/4734
All	All	0.24	1/77565 (0.0%)	0.40	4/105193 (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
1	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	x	463	ARG	C-N	5.06	1.40	1.33

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	x	466	ASN	CA-C-N	5.51	132.06	121.54
32	x	466	ASN	C-N-CA	5.51	132.06	121.54
17	Q	772	GLU	CA-C-N	5.34	131.31	121.70
17	Q	772	GLU	C-N-CA	5.34	131.31	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1525	TPO	Mainchain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11255	11388	11374	283	0
2	B	8980	9027	9019	247	0
3	C	2072	2024	2020	52	0
4	D	1004	981	980	27	0
5	E	1720	1738	1737	33	0
6	F	626	658	657	7	0
7	G	1333	1321	1321	84	0
8	H	1197	1157	1156	24	0
9	I	942	880	872	24	0
10	J	524	544	541	23	0
11	K	920	942	942	14	0
12	L	397	406	405	20	0
13	M	9583	9394	9386	138	0
14	N	1106	0	616	79	0
15	O	1046	1097	1096	9	0
16	P	232	0	115	9	0
17	Q	7226	7170	7169	110	0
18	R	2166	2056	2053	31	0
19	S	657	201	199	4	0
20	T	1335	0	716	55	0
21	U	856	684	680	8	0
22	V	1707	1443	1438	27	0
23	W	2333	2249	2246	39	0
24	X	353	372	371	6	0
25	Y	911	909	907	20	0
26	Z	4025	4046	4041	74	0
27	a	616	621	645	13	0
27	e	608	617	641	16	0
28	b	622	661	660	10	0
28	f	576	619	618	22	0
29	g	704	721	745	10	0
30	h	694	693	709	6	0
31	l	195	200	199	5	0
32	x	3948	3870	3897	59	0
33	y	3436	3406	3405	42	0
34	A	2	0	0	0	0
34	B	1	0	0	0	0
34	C	1	0	0	0	0
34	I	2	0	0	0	0
34	J	1	0	0	0	0
34	L	1	0	0	0	0
34	Y	1	0	0	0	0
35	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	75915	72095	73576	1419	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 10.

All (1419) 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)
14:N:17:DG:H2''	14:N:18:DT:C7	1.81	1.11
14:N:33:DC:H2'	14:N:34:DT:H71	1.35	1.08
7:G:36:GLY:O	26:Z:628:LYS:NZ	1.97	0.98
2:B:756:LYS:NZ	22:V:135:GLU:O	1.96	0.97
14:N:42:DT:H2'	14:N:43:DT:H71	1.49	0.94
14:N:41:DT:C2'	14:N:42:DT:H72	1.98	0.93
13:M:687:GLU:OE1	13:M:690:LYS:NZ	2.03	0.92
3:C:86:ARG:NH1	26:Z:716:PRO:O	2.03	0.92
3:C:190:ASN:ND2	3:C:195:THR:O	2.05	0.90
14:N:32:DT:H2''	14:N:33:DC:H5	1.36	0.89
7:G:118:GLU:OE2	7:G:129:LYS:NZ	2.05	0.89
28:b:27:GLN:OE1	28:b:55:ARG:NH1	2.06	0.88
5:E:36:THR:N	5:E:39:GLU:OE2	2.07	0.88
17:Q:353:TYR:OH	22:V:57:ARG:O	1.89	0.88
11:K:36:ASN:OD1	11:K:70:LYS:NZ	2.07	0.87
14:N:32:DT:H2''	14:N:33:DC:C5	2.11	0.86
29:g:99:ARG:H	29:g:99:ARG:HD2	1.37	0.86
14:N:17:DG:H2''	14:N:18:DT:H71	1.56	0.85
18:R:410:GLU:OE2	18:R:423:ASN:ND2	2.10	0.85
17:Q:605:LEU:O	17:Q:609:ASN:ND2	2.10	0.84
14:N:77:DG:C8	14:N:78:DT:H72	2.13	0.84
1:A:535:MET:O	1:A:669:TYR:OH	1.96	0.84
13:M:293:ASP:O	13:M:299:GLN:NE2	2.11	0.84
28:f:27:GLN:OE1	28:f:55:ARG:NH1	2.10	0.83
14:N:41:DT:H2''	14:N:42:DT:H72	1.59	0.82
3:C:36:ARG:NH1	11:K:41:THR:OG1	2.11	0.82
17:Q:276:ALA:HB1	17:Q:288:VAL:HG23	1.60	0.82
14:N:41:DT:H2''	14:N:42:DT:C7	2.10	0.82
1:A:96:HIS:HB2	1:A:250:VAL:HG23	1.62	0.81
7:G:135:ILE:O	13:M:464:TYR:OH	1.98	0.81
1:A:423:ASN:ND2	1:A:425:ASP:OD1	2.14	0.81
1:A:1314:THR:OG1	1:A:1316:ASN:OD1	1.96	0.81
2:B:1006:VAL:HG22	22:V:130:TRP:HB2	1.63	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:1255:GLU:N	13:M:1255:GLU:OE1	2.13	0.81
1:A:910:LYS:NZ	19:S:264:GLY:O	2.14	0.80
3:C:118:ARG:NH1	3:C:147:ASP:OD2	2.14	0.80
13:M:559:THR:O	13:M:695:ARG:NH1	2.15	0.80
14:N:34:DT:C6	14:N:35:DT:H72	2.17	0.80
17:Q:94:VAL:HG23	17:Q:140:LEU:HD11	1.62	0.80
29:g:88:ARG:NH2	32:x:850:PHE:O	2.13	0.80
1:A:461:GLN:HE21	20:T:-60:DA:H4'	1.47	0.80
23:W:73:SER:OG	23:W:118:SER:OG	1.99	0.79
7:G:101:ILE:N	7:G:104:MET:O	2.15	0.79
23:W:206:VAL:HG11	23:W:238:VAL:HG21	1.62	0.79
13:M:1110:GLU:OE1	13:M:1113:ARG:NH2	2.15	0.79
2:B:591:ARG:NH2	2:B:663:GLU:OE2	2.15	0.79
14:N:17:DG:H2''	14:N:18:DT:H73	1.64	0.79
1:A:1208:SER:O	1:A:1260:ARG:NH1	2.16	0.78
4:D:96:GLU:N	4:D:96:GLU:OE1	2.17	0.78
32:x:883:LYS:NZ	32:x:895:GLU:OE2	2.14	0.78
2:B:765:GLU:OE1	2:B:770:ARG:NE	2.17	0.77
13:M:570:ALA:O	13:M:572:ASP:N	2.17	0.77
1:A:111:CYS:SG	1:A:188:GLN:NE2	2.57	0.77
7:G:134:ASP:CB	13:M:475:ILE:HD13	2.16	0.76
18:R:388:ARG:NH1	18:R:446:GLU:O	2.18	0.76
14:N:69:DG:H2'	14:N:70:DT:H71	1.64	0.76
20:T:-56:DA:H2'	20:T:-55:DC:C6	2.20	0.76
2:B:992:ASN:O	10:J:46:ARG:NH1	2.18	0.76
13:M:889:LEU:HD11	13:M:930:VAL:HG21	1.67	0.76
27:e:128:ARG:NE	27:e:133:GLU:OE1	2.19	0.76
13:M:929:GLN:NE2	13:M:981:TYR:O	2.19	0.75
1:A:116:LYS:NZ	1:A:182:GLY:O	2.20	0.74
2:B:483:ARG:NH2	2:B:527:ALA:O	2.19	0.74
27:a:108:ASN:OD1	32:x:812:ARG:NH2	2.21	0.74
13:M:1076:TYR:O	31:l:2024:ARG:NH2	2.20	0.74
1:A:668:PHE:CE1	1:A:672:ILE:HD11	2.22	0.74
26:Z:563:MET:HA	26:Z:637:VAL:HG11	1.69	0.74
11:K:77:THR:OG1	11:K:81:TYR:O	2.03	0.73
4:D:112:LYS:NZ	4:D:124:ASP:OD1	2.21	0.73
1:A:140:ARG:NH2	1:A:234:PHE:O	2.21	0.73
2:B:836:THR:OG1	2:B:889:LYS:NZ	2.19	0.73
1:A:479:TRP:HB2	2:B:931:ILE:HD11	1.71	0.73
1:A:823:VAL:HG22	1:A:835:GLU:HB2	1.70	0.73
7:G:151:ARG:NE	7:G:153:ASP:OD1	2.22	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Z:541:GLN:NE2	26:Z:543:ASP:O	2.21	0.73
12:L:38:GLU:O	12:L:40:GLY:N	2.22	0.72
1:A:971:PRO:O	1:A:972:THR:OG1	2.03	0.72
5:E:2:ASP:OD1	5:E:3:ASP:N	2.21	0.72
26:Z:295:TYR:OH	32:x:754:HIS:NE2	2.22	0.72
2:B:727:ALA:O	2:B:731:GLN:NE2	2.22	0.72
17:Q:95:GLN:NE2	22:V:84:ILE:O	2.22	0.72
5:E:5:GLU:N	5:E:5:GLU:OE1	2.23	0.72
14:N:78:DT:H2'	14:N:79:DT:H72	1.71	0.71
16:P:53:C:O2'	16:P:54:G:OP1	2.08	0.71
17:Q:678:ALA:O	17:Q:684:TRP:NE1	2.23	0.71
14:N:42:DT:C2'	14:N:43:DT:H71	2.19	0.71
1:A:296:ASN:OD1	1:A:297:GLY:N	2.23	0.71
17:Q:406:GLU:N	17:Q:406:GLU:OE1	2.23	0.71
1:A:967:ARG:NH2	1:A:1326:GLY:O	2.24	0.71
2:B:388:TYR:H	2:B:504:THR:HG21	1.56	0.71
28:f:75:HIS:ND1	30:h:96:THR:OG1	2.22	0.71
5:E:55:ARG:O	5:E:56:THR:OG1	2.09	0.71
25:Y:51:ASP:OD1	32:x:755:GLN:NE2	2.23	0.71
14:N:69:DG:C2'	14:N:70:DT:H71	2.20	0.70
3:C:175:LYS:NZ	12:L:57:ALA:O	2.17	0.70
1:A:461:GLN:NE2	20:T:-60:DA:H4'	2.06	0.70
1:A:1370:GLY:O	1:A:1374:VAL:HG23	1.92	0.70
7:G:168:LEU:HD12	7:G:168:LEU:O	1.91	0.70
17:Q:534:TYR:OH	17:Q:556:GLU:OE1	2.08	0.70
2:B:600:GLU:N	2:B:600:GLU:OE1	2.25	0.70
5:E:96:GLU:OE1	5:E:96:GLU:N	2.25	0.70
2:B:1040:GLN:OE1	2:B:1040:GLN:N	2.25	0.70
14:N:41:DT:H2'	14:N:42:DT:H72	1.72	0.70
14:N:26:DC:H2''	14:N:27:DT:C7	2.21	0.69
18:R:366:ARG:NH2	26:Z:773:SER:OG	2.25	0.69
5:E:141:GLU:N	5:E:141:GLU:OE1	2.25	0.69
13:M:555:GLN:NE2	13:M:691:GLN:O	2.25	0.69
2:B:646:ARG:O	2:B:648:TYR:N	2.24	0.69
1:A:674:THR:O	1:A:678:ASN:ND2	2.26	0.69
15:O:634:ARG:NH1	15:O:670:GLU:OE2	2.25	0.69
14:N:26:DC:H2''	14:N:27:DT:C5	2.28	0.69
1:A:514:GLU:OE1	2:B:1101:GLN:NE2	2.26	0.69
14:N:43:DT:H2''	14:N:44:DT:H71	1.74	0.69
26:Z:729:GLU:O	26:Z:747:ARG:NH2	2.26	0.68
8:H:66:GLU:N	8:H:66:GLU:OE1	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:59:LEU:HD12	3:C:151:VAL:HG12	1.75	0.68
13:M:1026:LYS:O	13:M:1030:ASN:ND2	2.26	0.68
1:A:556:GLU:OE1	1:A:556:GLU:N	2.27	0.68
26:Z:417:GLU:O	26:Z:516:ARG:NH1	2.27	0.68
7:G:109:SER:HB3	26:Z:493:VAL:HG21	1.75	0.68
27:a:107:THR:HB	27:a:119:ILE:HD11	1.76	0.67
2:B:898:THR:O	2:B:899:SER:OG	2.11	0.67
2:B:1006:VAL:HG22	22:V:130:TRP:CB	2.24	0.67
11:K:63:VAL:HG22	11:K:71:ILE:HG22	1.76	0.67
12:L:39:CYS:SG	12:L:40:GLY:N	2.68	0.67
12:L:56:ASP:OD2	26:Z:720:TYR:OH	2.08	0.67
13:M:1180:GLN:OE1	13:M:1183:SER:OG	2.09	0.66
17:Q:772:GLU:N	17:Q:772:GLU:OE1	2.29	0.66
2:B:100:GLU:N	2:B:100:GLU:OE1	2.27	0.66
1:A:363:ALA:HB2	1:A:388:MET:HE3	1.76	0.66
23:W:27:ASN:O	23:W:32:SER:OG	2.09	0.66
2:B:613:ARG:NH1	2:B:615:TYR:OH	2.29	0.65
7:G:138:GLN:N	7:G:138:GLN:OE1	2.29	0.65
7:G:101:ILE:HD11	7:G:145:LEU:HD21	1.79	0.65
17:Q:401:LEU:HD11	17:Q:421:ILE:HD12	1.77	0.65
17:Q:500:SER:OG	17:Q:523:ILE:HD11	1.97	0.65
21:U:372:ASP:OD1	21:U:373:LEU:N	2.29	0.65
13:M:1159:GLU:N	13:M:1159:GLU:OE1	2.28	0.65
14:N:22:DG:H2'	14:N:23:DT:H71	1.79	0.65
2:B:1060:HIS:NE2	2:B:1082:GLY:O	2.25	0.64
18:R:404:GLU:N	18:R:404:GLU:OE1	2.30	0.64
3:C:64:ILE:CD1	3:C:151:VAL:HG11	2.27	0.64
8:H:116:VAL:CG1	8:H:123:MET:HE3	2.26	0.64
20:T:-28:DC:H41	32:x:579:LEU:HD13	1.62	0.64
27:e:103:LEU:HD22	28:f:57:VAL:HG11	1.78	0.64
14:N:40:DG:C8	14:N:41:DT:H72	2.32	0.64
1:A:1217:ASP:OD1	1:A:1218:ARG:N	2.30	0.64
1:A:576:GLN:O	1:A:590:GLN:NE2	2.28	0.64
1:A:691:ASP:OD2	1:A:765:ASN:ND2	2.29	0.64
2:B:342:VAL:HG23	2:B:346:GLU:HG3	1.79	0.64
17:Q:737:LYS:HZ3	17:Q:761:LEU:HD23	1.63	0.64
20:T:-29:DC:H2''	20:T:-28:DC:C5	2.32	0.64
17:Q:569:SER:OG	24:X:234:ARG:NH1	2.30	0.64
13:M:1516:GLN:N	13:M:1516:GLN:OE1	2.30	0.64
17:Q:394:ARG:NH1	17:Q:424:GLN:OE1	2.31	0.64
25:Y:47:GLU:N	25:Y:47:GLU:OE1	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:468:LEU:O	13:M:468:LEU:HD12	1.98	0.63
1:A:805:ARG:NH1	9:I:77:THR:OG1	2.30	0.63
17:Q:333:THR:HG21	17:Q:347:LEU:HD12	1.81	0.63
17:Q:799:VAL:O	17:Q:802:LYS:NZ	2.31	0.63
26:Z:775:TPO:O1P	26:Z:775:TPO:N	2.28	0.63
1:A:1467:GLY:O	1:A:1468:THR:OG1	2.17	0.63
26:Z:729:GLU:N	26:Z:729:GLU:OE1	2.31	0.63
14:N:20:DT:C2	20:T:-19:DG:N2	2.66	0.63
2:B:849:ASP:OD2	12:L:46:LYS:NZ	2.31	0.63
3:C:189:ASP:O	3:C:191:ALA:N	2.31	0.63
13:M:603:ARG:NH1	13:M:724:GLN:OE1	2.30	0.63
1:A:1302:GLU:OE1	1:A:1302:GLU:N	2.32	0.63
27:a:106:ASP:OD2	27:a:131:ARG:NH2	2.27	0.63
3:C:33:SER:O	3:C:37:VAL:HG23	1.98	0.63
12:L:25:GLU:N	12:L:25:GLU:OE1	2.32	0.63
17:Q:682:ASP:O	17:Q:686:ASN:ND2	2.32	0.63
26:Z:218:PRO:HB2	26:Z:221:VAL:HG12	1.81	0.63
26:Z:295:TYR:HH	32:x:754:HIS:CE1	2.17	0.63
1:A:507:GLN:N	2:B:1105:GLU:OE2	2.32	0.62
5:E:41:LYS:NZ	5:E:46:ASP:OD1	2.27	0.62
1:A:559:GLU:N	1:A:559:GLU:OE1	2.31	0.62
3:C:58:VAL:HG11	10:J:59:LEU:HB3	1.80	0.62
7:G:131:MET:SD	7:G:132:ASP:N	2.72	0.62
13:M:293:ASP:OD1	13:M:1027:VAL:HG23	1.99	0.62
5:E:140:THR:OG1	5:E:141:GLU:OE1	2.13	0.62
8:H:2:ALA:O	8:H:84:ARG:NH2	2.32	0.62
9:I:31:GLU:N	9:I:31:GLU:OE1	2.32	0.62
13:M:1440:ARG:NH1	13:M:1486:TYR:OH	2.32	0.62
26:Z:462:GLU:N	26:Z:462:GLU:OE1	2.33	0.62
17:Q:249:ASP:O	17:Q:253:ASN:ND2	2.33	0.62
10:J:44:CYS:O	10:J:47:ARG:NH1	2.33	0.62
17:Q:443:GLU:N	17:Q:443:GLU:OE1	2.32	0.62
25:Y:112:ASP:OD2	25:Y:116:LYS:NZ	2.33	0.62
12:L:21:GLU:OE1	12:L:21:GLU:N	2.33	0.62
2:B:1032:PHE:O	3:C:32:ASN:ND2	2.33	0.61
23:W:251:SER:OG	23:W:253:ASP:OD1	2.18	0.61
1:A:467:MET:SD	1:A:524:MET:HB3	2.40	0.61
1:A:818:GLU:OE1	1:A:818:GLU:N	2.32	0.61
30:h:37:TYR:O	30:h:41:VAL:HG23	2.01	0.61
1:A:357:LYS:NZ	2:B:1107:LEU:O	2.27	0.61
7:G:119:PHE:HE2	7:G:128:TYR:HH	1.47	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:x:829:GLU:N	32:x:829:GLU:OE1	2.33	0.61
13:M:949:VAL:HG23	13:M:951:LYS:H	1.64	0.61
13:M:1298:ASP:OD1	13:M:1299:THR:N	2.33	0.61
14:N:17:DG:H2"	14:N:18:DT:C5	2.35	0.61
25:Y:52:CYS:SG	25:Y:53:THR:N	2.73	0.61
1:A:200:ALA:HB2	1:A:216:LEU:HD21	1.82	0.61
9:I:67:GLN:N	9:I:67:GLN:OE1	2.33	0.61
2:B:309:PHE:O	2:B:312:GLN:NE2	2.34	0.61
5:E:97:GLU:N	5:E:97:GLU:OE1	2.33	0.61
13:M:1408:LEU:O	13:M:1411:ILE:HG22	2.01	0.61
14:N:39:DT:H2"	14:N:40:DG:C8	2.35	0.61
7:G:92:VAL:HG11	7:G:127:CYS:HA	1.82	0.61
25:Y:56:SER:OG	25:Y:90:THR:OG1	2.17	0.61
1:A:22:GLN:O	2:B:1170:ARG:N	2.34	0.60
2:B:953:ASP:OD1	3:C:36:ARG:NH2	2.32	0.60
7:G:129:LYS:O	7:G:131:MET:N	2.34	0.60
22:V:109:GLU:OE1	22:V:109:GLU:N	2.34	0.60
13:M:1046:THR:O	32:x:782:ASN:ND2	2.34	0.60
7:G:145:LEU:HD12	7:G:145:LEU:O	2.01	0.60
17:Q:247:GLU:OE1	17:Q:247:GLU:N	2.34	0.60
26:Z:523:GLU:N	26:Z:523:GLU:OE1	2.35	0.60
13:M:295:PRO:HB3	13:M:991:GLY:HA2	1.82	0.60
8:H:116:VAL:HG11	8:H:123:MET:HE3	1.84	0.60
17:Q:110:ILE:CD1	17:Q:140:LEU:HD13	2.31	0.60
17:Q:612:LEU:HD23	17:Q:612:LEU:O	2.01	0.60
13:M:629:ASP:OD2	26:Z:641:ARG:NH2	2.35	0.60
20:T:-18:DA:H2"	20:T:-17:DC:C5	2.37	0.60
32:x:465:ARG:O	32:x:466:ASN:CB	2.48	0.60
14:N:20:DT:H2"	14:N:21:DC:C6	2.36	0.60
26:Z:455:GLU:OE1	26:Z:455:GLU:N	2.35	0.60
1:A:108:ARG:NH2	1:A:191:ILE:O	2.35	0.60
1:A:402:LEU:O	1:A:406:VAL:HG23	2.02	0.60
17:Q:158:GLN:O	17:Q:159:SER:OG	2.16	0.60
23:W:40:LEU:HD12	23:W:66:GLY:HA3	1.84	0.60
13:M:977:ILE:HD11	13:M:1004:LEU:HD13	1.83	0.59
32:x:677:GLN:O	32:x:692:VAL:HG23	2.02	0.59
1:A:1372:GLU:OE2	5:E:195:ARG:NH1	2.36	0.59
2:B:40:VAL:HG11	2:B:482:LEU:HD13	1.85	0.59
12:L:56:ASP:O	12:L:58:ARG:N	2.35	0.59
20:T:-67:DC:H2"	20:T:-66:DC:C6	2.37	0.59
25:Y:26:ASP:OD1	25:Y:27:GLN:N	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:y:63:LYS:HE3	33:y:71:VAL:HG11	1.85	0.59
2:B:20:ASP:N	2:B:680:ASP:OD2	2.36	0.59
13:M:802:GLU:N	13:M:802:GLU:OE1	2.35	0.59
21:U:458:ASP:OD1	21:U:459:VAL:N	2.36	0.59
28:f:35:ARG:NE	32:x:751:LEU:HD23	2.17	0.59
2:B:529:MET:HG3	2:B:624:PRO:HD2	1.85	0.59
10:J:8:PHE:CD2	10:J:48:MET:HE1	2.38	0.59
1:A:357:LYS:HZ3	2:B:1152:PRO:HB3	1.66	0.59
1:A:1262:MET:SD	1:A:1262:MET:N	2.76	0.59
13:M:864:VAL:O	13:M:868:VAL:HG23	2.02	0.59
18:R:449:GLU:N	18:R:449:GLU:OE1	2.35	0.59
26:Z:592:ASN:OD1	26:Z:593:ASN:N	2.36	0.59
1:A:1302:GLU:O	1:A:1304:ILE:N	2.34	0.58
2:B:817:GLN:N	2:B:817:GLN:OE1	2.36	0.58
13:M:1463:CYS:SG	13:M:1464:ALA:N	2.76	0.58
14:N:27:DT:H72	32:x:579:LEU:HD23	1.85	0.58
17:Q:333:THR:HG21	17:Q:347:LEU:CD1	2.33	0.58
33:y:339:GLN:OE1	33:y:339:GLN:N	2.36	0.58
1:A:381:PRO:HB3	1:A:480:SER:HA	1.85	0.58
2:B:1062:ARG:NH1	2:B:1081:ASP:O	2.36	0.58
23:W:58:TRP:CZ2	23:W:95:ASN:HA	2.38	0.58
26:Z:437:GLN:OE1	26:Z:437:GLN:N	2.36	0.58
28:f:32:PRO:HA	32:x:751:LEU:HD21	1.86	0.58
2:B:993:LYS:HG2	2:B:1018:TYR:OH	2.02	0.58
5:E:152:THR:O	5:E:156:VAL:HG23	2.03	0.58
9:I:82:GLU:OE1	9:I:82:GLU:N	2.37	0.58
1:A:492:TYR:CD2	1:A:501:MET:HE1	2.39	0.58
26:Z:602:VAL:HG22	26:Z:643:LEU:HD23	1.85	0.58
1:A:479:TRP:CB	2:B:931:ILE:HD11	2.34	0.58
5:E:78:GLU:OE1	5:E:78:GLU:N	2.36	0.58
23:W:237:ASN:OD1	23:W:238:VAL:N	2.37	0.58
1:A:1484:MET:O	13:M:1362:LYS:NZ	2.37	0.58
2:B:809:VAL:HG11	3:C:60:HIS:CE1	2.39	0.58
20:T:-61:DA:H2'	20:T:-60:DA:O4'	2.04	0.58
26:Z:297:GLU:OE1	32:x:754:HIS:ND1	2.36	0.58
2:B:505:LEU:HD22	2:B:509:VAL:CG2	2.33	0.58
2:B:910:THR:OG1	12:L:42:ARG:O	2.16	0.58
31:l:2021:GLU:OE1	31:l:2021:GLU:N	2.35	0.58
25:Y:59:GLY:HA3	25:Y:87:VAL:HG22	1.86	0.58
1:A:376:ASP:OD2	1:A:473:ARG:NE	2.36	0.57
1:A:460:ARG:NH2	16:P:61:U:O2'	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1140:THR:HG22	1:A:1337:GLU:OE1	2.04	0.57
13:M:522:ASP:OD1	13:M:523:MET:N	2.32	0.57
22:V:127:VAL:HG23	22:V:128:VAL:H	1.69	0.57
26:Z:534:HIS:NE2	26:Z:575:VAL:O	2.37	0.57
2:B:988:LYS:O	2:B:992:ASN:ND2	2.37	0.57
27:a:107:THR:CG2	27:a:119:ILE:HD11	2.35	0.57
33:y:223:LEU:O	33:y:223:LEU:HD12	2.04	0.57
1:A:1342:SER:O	1:A:1344:MET:N	2.34	0.57
23:W:31:ASN:OD1	23:W:32:SER:N	2.38	0.57
7:G:116:GLU:N	7:G:116:GLU:OE1	2.37	0.57
26:Z:588:ASP:OD1	26:Z:592:ASN:N	2.37	0.57
33:y:370:ARG:NH2	33:y:373:GLU:OE2	2.34	0.57
26:Z:479:LYS:NZ	26:Z:521:CYS:O	2.24	0.57
23:W:17:ASP:OD1	23:W:18:ALA:N	2.37	0.57
27:a:129:ARG:NH2	27:e:106:ASP:OD1	2.37	0.57
1:A:668:PHE:CZ	1:A:672:ILE:HD11	2.40	0.57
2:B:19:PRO:O	2:B:21:LEU:N	2.36	0.57
2:B:30:ILE:HD11	2:B:698:ILE:HG21	1.85	0.57
2:B:626:LEU:HD11	2:B:698:ILE:HG12	1.87	0.57
13:M:387:GLU:OE1	13:M:387:GLU:N	2.38	0.57
17:Q:454:LEU:HD21	17:Q:476:ALA:HB3	1.86	0.57
28:b:89:ALA:O	28:b:93:GLN:NE2	2.37	0.57
1:A:103:THR:HG22	1:A:248:MET:HE3	1.86	0.57
17:Q:236:VAL:O	17:Q:240:VAL:HG23	2.05	0.57
18:R:493:GLU:OE1	18:R:493:GLU:N	2.38	0.57
1:A:144:VAL:HG11	1:A:235:VAL:HG12	1.87	0.56
2:B:23:GLN:N	2:B:23:GLN:OE1	2.38	0.56
2:B:686:GLU:N	2:B:686:GLU:OE1	2.37	0.56
14:N:16:DT:H2"	14:N:17:DG:C8	2.40	0.56
18:R:494:GLU:N	18:R:494:GLU:OE1	2.37	0.56
23:W:64:GLN:N	23:W:64:GLN:OE1	2.37	0.56
1:A:824:GLU:OE2	18:R:597:ARG:N	2.38	0.56
2:B:502:HIS:ND1	2:B:504:THR:HG22	2.20	0.56
2:B:806:PHE:O	2:B:1050:ARG:NH1	2.38	0.56
3:C:235:SER:OG	3:C:239:LEU:O	2.22	0.56
13:M:1164:GLY:O	13:M:1266:ARG:NH1	2.37	0.56
14:N:26:DC:H2"	14:N:27:DT:H71	1.86	0.56
21:U:392:GLN:OE1	21:U:392:GLN:N	2.38	0.56
2:B:1040:GLN:NE2	3:C:195:THR:OG1	2.39	0.56
4:D:62:MET:O	4:D:66:ASN:ND2	2.37	0.56
17:Q:774:SER:O	17:Q:830:ARG:NH1	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:GLU:HB2	1:A:215:LEU:HD11	1.87	0.56
17:Q:285:TYR:HA	17:Q:288:VAL:HG12	1.88	0.56
20:T:-64:DG:H2'	20:T:-63:DC:C6	2.40	0.56
24:X:233:THR:N	24:X:236:THR:OG1	2.37	0.56
18:R:285:LEU:HD21	18:R:289:ARG:NH1	2.21	0.56
32:x:842:LEU:HD12	32:x:842:LEU:C	2.30	0.56
1:A:428:ASP:OD1	1:A:429:LEU:N	2.39	0.56
1:A:485:ASN:OD1	1:A:673:GLN:NE2	2.39	0.56
1:A:486:LEU:HD21	2:B:790:GLN:HB2	1.87	0.56
1:A:1212:LEU:HD11	1:A:1285:LEU:HB3	1.86	0.56
2:B:814:TYR:OH	2:B:896:LEU:HD12	2.06	0.56
5:E:185:ILE:HD12	5:E:209:VAL:HG21	1.88	0.56
33:y:34:ASN:OD1	33:y:35:SER:N	2.39	0.56
13:M:820:ALA:O	13:M:826:ARG:NE	2.37	0.56
23:W:250:SER:OG	23:W:277:VAL:HG23	2.06	0.56
23:W:256:VAL:HG22	23:W:277:VAL:HG21	1.88	0.56
2:B:191:GLU:OE1	2:B:191:GLU:N	2.40	0.56
2:B:792:ASP:OD2	2:B:975:ARG:NH2	2.38	0.56
26:Z:745:VAL:HG11	26:Z:750:LEU:HD21	1.88	0.56
1:A:486:LEU:HD22	2:B:790:GLN:OE1	2.06	0.55
2:B:985:LEU:O	2:B:989:VAL:HG23	2.06	0.55
14:N:22:DG:H2''	14:N:23:DT:H6	1.71	0.55
18:R:470:ASP:OD1	18:R:471:GLU:N	2.39	0.55
2:B:1157:LEU:O	2:B:1157:LEU:HD23	2.06	0.55
13:M:925:ILE:HG13	13:M:985:LEU:HD11	1.89	0.55
27:e:103:LEU:CD2	28:f:57:VAL:HG11	2.37	0.55
1:A:687:ILE:HD12	1:A:769:MET:HE1	1.88	0.55
2:B:395:LEU:HD21	2:B:532:ILE:HD13	1.89	0.55
2:B:601:VAL:HG22	2:B:616:THR:HG22	1.87	0.55
7:G:92:VAL:HG13	7:G:97:LEU:HD23	1.88	0.55
7:G:109:SER:CB	26:Z:493:VAL:HG21	2.35	0.55
4:D:67:TYR:CE1	7:G:102:GLY:N	2.73	0.55
13:M:558:GLU:N	13:M:558:GLU:OE1	2.37	0.55
16:P:51:G:O2'	16:P:52:G:OP2	2.11	0.55
1:A:383:SER:HB3	11:K:2:ASN:HD21	1.71	0.55
2:B:581:GLU:O	2:B:585:ASN:ND2	2.38	0.55
26:Z:188:GLU:N	26:Z:188:GLU:OE1	2.40	0.55
2:B:139:GLN:OE1	2:B:139:GLN:N	2.40	0.55
2:B:388:TYR:CE2	2:B:505:LEU:HD21	2.42	0.55
13:M:617:ASN:OD1	13:M:642:ASN:N	2.39	0.55
1:A:459:ASN:OD1	1:A:460:ARG:N	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:695:ASP:O	1:A:697:LYS:N	2.37	0.55
3:C:64:ILE:HD11	3:C:151:VAL:HG11	1.89	0.55
6:F:90:LEU:HD23	6:F:90:LEU:O	2.07	0.55
1:A:1130:ILE:HD12	1:A:1362:ILE:HG21	1.87	0.55
1:A:803:LYS:O	1:A:812:LYS:NZ	2.40	0.54
13:M:443:LEU:HD12	13:M:471:TYR:OH	2.07	0.54
17:Q:879:ALA:O	17:Q:882:VAL:HG12	2.07	0.54
20:T:-21:DG:H2"	20:T:-20:DA:C8	2.42	0.54
25:Y:18:LEU:O	25:Y:111:ARG:NE	2.37	0.54
1:A:448:ARG:NH1	1:A:451:CYS:SG	2.80	0.54
2:B:114:ARG:NE	2:B:191:GLU:OE2	2.40	0.54
2:B:384:ASP:OD1	2:B:385:ARG:N	2.39	0.54
10:J:21:TYR:CE2	10:J:25:LEU:HD11	2.43	0.54
14:N:20:DT:O2	20:T:-19:DG:N2	2.40	0.54
17:Q:302:GLU:N	17:Q:302:GLU:OE1	2.41	0.54
27:a:129:ARG:HE	33:y:387:ARG:HD3	1.73	0.54
1:A:961:GLU:O	1:A:965:VAL:HG23	2.07	0.54
2:B:759:VAL:HG21	2:B:983:GLU:HG3	1.88	0.54
33:y:63:LYS:CE	33:y:71:VAL:HG11	2.38	0.54
1:A:977:VAL:HG21	1:A:1040:LEU:HD21	1.88	0.54
2:B:381:GLU:OE1	2:B:381:GLU:N	2.40	0.54
7:G:119:PHE:O	13:M:409:ARG:NH1	2.40	0.54
9:I:105:GLU:N	9:I:105:GLU:OE1	2.39	0.54
13:M:876:GLN:N	13:M:876:GLN:OE1	2.40	0.54
33:y:181:PHE:O	33:y:185:VAL:HG23	2.08	0.54
1:A:936:GLU:N	1:A:936:GLU:OE1	2.37	0.54
2:B:30:ILE:CD1	2:B:698:ILE:HG21	2.37	0.54
2:B:1071:ASN:O	2:B:1073:GLN:N	2.40	0.54
13:M:1177:ARG:N	13:M:1224:GLN:O	2.39	0.54
15:O:613:MET:HE1	15:O:641:LEU:HD22	1.90	0.54
17:Q:276:ALA:CB	17:Q:288:VAL:HG23	2.33	0.54
17:Q:493:ASN:O	17:Q:497:VAL:HG23	2.06	0.54
1:A:458:PHE:CD2	1:A:501:MET:HE2	2.43	0.54
2:B:989:VAL:HG22	2:B:1015:LEU:HB2	1.89	0.54
7:G:132:ASP:HB2	13:M:416:LEU:HD22	1.89	0.54
11:K:17:LYS:O	11:K:36:ASN:ND2	2.40	0.54
11:K:56:VAL:HG22	11:K:77:THR:HG22	1.90	0.54
27:e:101:VAL:HG13	33:y:383:THR:HB	1.90	0.54
6:F:53:THR:OG1	6:F:118:TRP:NE1	2.41	0.54
10:J:31:GLU:OE1	10:J:31:GLU:N	2.40	0.54
13:M:619:THR:OG1	13:M:666:THR:OG1	2.25	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:293:LEU:O	17:Q:297:HIS:ND1	2.40	0.54
1:A:293:ASN:O	1:A:298:ALA:N	2.41	0.54
1:A:461:GLN:HG2	20:T:-60:DA:H1'	1.90	0.54
1:A:721:HIS:CG	9:I:110:LEU:HD21	2.42	0.54
1:A:1456:GLU:N	1:A:1456:GLU:OE1	2.37	0.54
26:Z:295:TYR:HH	32:x:754:HIS:CD2	2.23	0.54
1:A:94:VAL:HG22	1:A:311:GLN:OE1	2.08	0.54
1:A:184:CYS:SG	15:O:600:LYS:NZ	2.79	0.54
1:A:457:ILE:HG23	1:A:504:HIS:HB2	1.89	0.54
1:A:489:THR:HG21	2:B:791:GLU:OE1	2.07	0.54
2:B:179:LEU:HD22	2:B:768:ARG:HD3	1.89	0.54
32:x:555:LYS:HA	32:x:573:TYR:CE2	2.43	0.54
33:y:12:GLN:N	33:y:19:ASN:O	2.39	0.54
5:E:185:ILE:HD13	5:E:191:VAL:HG21	1.90	0.54
6:F:112:ASP:OD1	6:F:113:GLY:N	2.39	0.53
18:R:379:ALA:O	18:R:383:THR:OG1	2.19	0.53
21:U:378:LEU:O	22:V:310:ASN:N	2.40	0.53
23:W:24:TRP:NE1	23:W:32:SER:O	2.40	0.53
25:Y:77:VAL:HG12	25:Y:80:PHE:CE2	2.42	0.53
1:A:67:ARG:O	1:A:68:THR:OG1	2.16	0.53
17:Q:155:VAL:HG11	17:Q:165:ALA:HB1	1.90	0.53
1:A:566:PHE:CZ	1:A:678:ASN:OD1	2.61	0.53
22:V:84:ILE:O	22:V:84:ILE:HG23	2.08	0.53
32:x:596:LYS:NZ	33:y:145:GLU:OE2	2.35	0.53
13:M:417:PHE:CZ	13:M:467:PHE:CD1	2.96	0.53
1:A:780:ASN:O	1:A:784:VAL:HG23	2.08	0.53
20:T:-77:DC:H2''	20:T:-76:DG:C8	2.42	0.53
31:l:2033:LYS:O	31:l:2037:THR:OG1	2.25	0.53
1:A:1525:TPO:O	1:A:1526:PRO:O	2.25	0.53
9:I:87:GLN:OE1	9:I:87:GLN:N	2.42	0.53
18:R:439:LEU:O	18:R:442:VAL:HG12	2.09	0.53
20:T:-21:DG:H2''	20:T:-20:DA:H8	1.73	0.53
27:e:101:VAL:HG12	33:y:384:THR:HG22	1.89	0.53
32:x:601:ARG:NH1	33:y:152:GLN:OE1	2.41	0.53
1:A:489:THR:HG21	2:B:791:GLU:CD	2.33	0.53
2:B:128:ILE:HG21	2:B:431:LEU:CD1	2.39	0.53
3:C:83:GLN:N	3:C:83:GLN:OE1	2.41	0.53
28:f:83:ALA:O	28:f:87:VAL:HG23	2.09	0.53
33:y:364:LYS:O	33:y:365:PRO:C	2.52	0.53
26:Z:477:HIS:O	26:Z:520:LEU:HD12	2.09	0.53
26:Z:489:THR:O	26:Z:505:ASP:N	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1408:ARG:O	1:A:1410:HIS:N	2.41	0.53
1:A:1427:LEU:HB2	1:A:1456:GLU:HG3	1.91	0.53
27:a:107:THR:CB	27:a:119:ILE:HD11	2.38	0.53
1:A:525:ILE:O	1:A:534:VAL:HG22	2.09	0.53
7:G:49:THR:OG1	7:G:73:LYS:O	2.23	0.53
17:Q:392:GLU:OE1	17:Q:392:GLU:N	2.41	0.53
26:Z:179:LEU:HD21	26:Z:226:TYR:HB3	1.91	0.53
1:A:45:GLU:N	1:A:45:GLU:OE1	2.41	0.52
1:A:1361:ASP:OD1	1:A:1362:ILE:N	2.41	0.52
1:A:1540:THR:O	1:A:1542:GLY:N	2.42	0.52
2:B:780:VAL:HG21	2:B:1048:TYR:CE1	2.44	0.52
20:T:-56:DA:H2'	20:T:-55:DC:H6	1.68	0.52
1:A:61:ARG:O	1:A:73:THR:OG1	2.25	0.52
6:F:86:GLU:N	6:F:86:GLU:OE1	2.42	0.52
32:x:719:VAL:HG22	32:x:741:TYR:HB3	1.92	0.52
2:B:86:LEU:HD11	2:B:128:ILE:HD11	1.89	0.52
1:A:937:ASP:C	1:A:938:LEU:HD12	2.34	0.52
1:A:1137:PRO:HB2	1:A:1341:VAL:HG23	1.90	0.52
1:A:1232:ALA:HA	1:A:1235:ILE:HG22	1.90	0.52
4:D:59:GLU:N	4:D:59:GLU:OE1	2.41	0.52
14:N:32:DT:C2'	14:N:33:DC:C5	2.90	0.52
1:A:524:MET:HA	1:A:524:MET:HE2	1.90	0.52
7:G:134:ASP:HB2	13:M:475:ILE:HD13	1.92	0.52
8:H:74:GLU:OE2	8:H:76:ASN:ND2	2.42	0.52
28:f:60:VAL:O	28:f:64:ASN:ND2	2.43	0.52
1:A:18:ILE:HD12	2:B:1171:MET:HB3	1.92	0.52
32:x:761:ASP:OD1	32:x:762:ASP:N	2.41	0.52
1:A:197:GLU:N	1:A:197:GLU:OE1	2.42	0.52
1:A:699:TYR:CD2	18:R:592:ASP:CB	2.93	0.52
2:B:829:PHE:CE1	2:B:867:ILE:HD11	2.44	0.52
6:F:118:TRP:CE3	6:F:123:LEU:HB3	2.45	0.52
7:G:134:ASP:CG	13:M:471:TYR:O	2.52	0.52
13:M:575:CYS:O	13:M:577:GLN:N	2.42	0.52
17:Q:803:MET:SD	17:Q:803:MET:N	2.80	0.52
1:A:890:ARG:CZ	1:A:1023:VAL:HG22	2.40	0.52
2:B:762:ARG:HG2	22:V:132:ARG:NH1	2.24	0.52
3:C:37:VAL:O	3:C:42:VAL:HG23	2.09	0.52
9:I:19:GLU:N	9:I:19:GLU:OE1	2.42	0.52
10:J:25:LEU:HB3	18:R:563:ILE:HD11	1.92	0.52
13:M:1256:ARG:HD2	13:M:1257:VAL:HG13	1.90	0.52
20:T:-31:DC:C2'	20:T:-30:DA:C8	2.93	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:687:ILE:HD13	2:B:972:ILE:HB	1.91	0.52
1:A:1158:LEU:C	1:A:1158:LEU:HD23	2.34	0.52
4:D:104:CYS:O	4:D:135:GLN:NE2	2.43	0.52
13:M:910:LEU:O	13:M:914:VAL:HG23	2.10	0.52
17:Q:401:LEU:HD22	17:Q:418:LEU:HG	1.91	0.52
32:x:541:PRO:O	32:x:600:TYR:OH	2.26	0.52
1:A:222:HIS:ND1	1:A:249:ILE:HD11	2.25	0.51
1:A:510:GLU:OE2	2:B:1101:GLN:NE2	2.38	0.51
1:A:694:ALA:HB3	1:A:699:TYR:CZ	2.46	0.51
2:B:44:LEU:HD22	2:B:157:ARG:O	2.10	0.51
2:B:446:TYR:CE1	2:B:450:THR:HG21	2.45	0.51
5:E:37:LEU:HD21	5:E:41:LYS:HZ3	1.73	0.51
14:N:77:DG:H2'	14:N:78:DT:H72	1.91	0.51
18:R:292:ARG:NH2	32:x:821:SER:OG	2.43	0.51
20:T:-17:DC:H2''	20:T:-16:DA:C8	2.44	0.51
23:W:176:ASP:O	23:W:180:GLY:N	2.39	0.51
26:Z:192:THR:HG23	26:Z:245:LEU:HD21	1.92	0.51
1:A:48:GLU:OE1	1:A:48:GLU:N	2.40	0.51
1:A:1141:VAL:HG13	1:A:1352:VAL:HG13	1.92	0.51
4:D:114:LEU:HD22	7:G:168:LEU:HD23	1.93	0.51
5:E:79:GLU:N	5:E:79:GLU:OE1	2.42	0.51
7:G:136:VAL:H	13:M:468:LEU:HD22	1.75	0.51
13:M:544:GLU:OE1	13:M:544:GLU:N	2.36	0.51
17:Q:341:VAL:O	17:Q:341:VAL:HG22	2.10	0.51
17:Q:768:VAL:HG21	17:Q:778:GLU:CG	2.39	0.51
28:b:41:GLY:O	32:x:847:ARG:NH1	2.44	0.51
1:A:413:TYR:O	1:A:449:HIS:CD2	2.63	0.51
4:D:87:LEU:O	4:D:87:LEU:HD23	2.10	0.51
5:E:67:ASP:OD1	5:E:69:THR:OG1	2.28	0.51
8:H:18:GLU:N	8:H:18:GLU:OE1	2.43	0.51
14:N:71:DC:C6	14:N:72:DT:H72	2.46	0.51
20:T:-31:DC:H2''	20:T:-30:DA:C8	2.45	0.51
1:A:873:VAL:HG22	1:A:879:VAL:HG22	1.93	0.51
1:A:1259:ILE:HD12	1:A:1259:ILE:N	2.26	0.51
13:M:413:LEU:O	13:M:417:PHE:HB2	2.11	0.51
1:A:980:PRO:HD2	1:A:1041:PHE:CD1	2.45	0.51
2:B:759:VAL:HG23	2:B:759:VAL:O	2.10	0.51
7:G:117:MET:SD	7:G:130:THR:N	2.84	0.51
14:N:78:DT:H2'	14:N:79:DT:C7	2.38	0.51
23:W:92:ASP:O	23:W:96:GLY:N	2.44	0.51
25:Y:3:LEU:N	25:Y:3:LEU:HD22	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:HIS:HB2	1:A:249:ILE:CD1	2.41	0.51
1:A:503:LEU:C	1:A:503:LEU:HD23	2.35	0.51
13:M:1403:GLU:OE1	13:M:1403:GLU:N	2.40	0.51
14:N:37:DG:O4'	32:x:674:LYS:NZ	2.43	0.51
27:a:67:PHE:CZ	27:a:93:GLN:HA	2.46	0.51
29:g:69:ALA:O	29:g:73:ASN:ND2	2.39	0.51
1:A:1183:SER:O	1:A:1184:THR:OG1	2.25	0.51
22:V:88:ASN:O	22:V:90:ASP:N	2.43	0.51
1:A:95:PHE:HE1	1:A:221:VAL:HG21	1.76	0.51
1:A:189:PRO:HB3	1:A:202:TRP:CZ2	2.46	0.51
25:Y:52:CYS:SG	25:Y:53:THR:HG23	2.50	0.51
14:N:22:DG:H2''	14:N:23:DT:C6	2.46	0.51
26:Z:746:ASP:OD1	26:Z:747:ARG:N	2.44	0.51
28:f:41:GLY:HA3	33:y:383:THR:N	2.26	0.51
32:x:843:ILE:HD12	32:x:886:LEU:HD22	1.93	0.51
1:A:896:LEU:HD13	1:A:980:PRO:HG3	1.92	0.50
1:A:1318:LYS:NZ	19:S:292:ASN:O	2.43	0.50
7:G:136:VAL:HB	13:M:468:LEU:CD2	2.41	0.50
17:Q:448:ASP:OD1	17:Q:449:VAL:N	2.44	0.50
2:B:269:ILE:HG21	2:B:369:VAL:HG21	1.93	0.50
4:D:108:ALA:N	4:D:128:GLN:OE1	2.44	0.50
7:G:112:SER:OG	26:Z:493:VAL:HG22	2.12	0.50
13:M:1076:TYR:OH	13:M:1091:GLU:OE1	2.29	0.50
17:Q:18:GLU:N	17:Q:18:GLU:OE1	2.44	0.50
1:A:1005:HIS:ND1	1:A:1007:ILE:HG22	2.26	0.50
8:H:27:ARG:C	8:H:28:LEU:HD22	2.36	0.50
10:J:7:CYS:HA	10:J:48:MET:HE3	1.92	0.50
14:N:15:DC:H2'	14:N:16:DT:H71	1.93	0.50
24:X:222:ARG:HA	24:X:225:VAL:HG22	1.92	0.50
25:Y:56:SER:HG	25:Y:90:THR:HG1	1.56	0.50
1:A:364:ARG:NH2	1:A:500:GLU:HB2	2.26	0.50
1:A:1212:LEU:HD11	1:A:1285:LEU:HD13	1.93	0.50
2:B:835:GLU:N	2:B:835:GLU:OE1	2.45	0.50
7:G:92:VAL:HG13	7:G:97:LEU:CD2	2.40	0.50
7:G:122:ASN:HB2	13:M:457:MET:HB2	1.93	0.50
14:N:43:DT:C2'	14:N:44:DT:H71	2.41	0.50
17:Q:268:ASN:HB3	17:Q:271:VAL:HG12	1.94	0.50
20:T:-22:DC:C2	20:T:-21:DG:N7	2.80	0.50
1:A:760:LEU:HD22	1:A:764:ASN:ND2	2.26	0.50
4:D:99:CYS:SG	4:D:100:LEU:N	2.84	0.50
26:Z:550:ILE:HD13	26:Z:558:PHE:HB3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:x:624:ILE:O	32:x:628:VAL:HG23	2.12	0.50
3:C:99:VAL:HG21	3:C:127:VAL:HG21	1.92	0.50
15:O:561:SER:O	15:O:565:VAL:HG23	2.12	0.50
23:W:195:SER:OG	23:W:236:LEU:O	2.26	0.50
29:g:90:ASP:OD2	32:x:465:ARG:NH2	2.39	0.50
1:A:231:GLU:OE1	1:A:231:GLU:N	2.42	0.50
3:C:62:GLU:N	3:C:62:GLU:OE1	2.45	0.50
3:C:242:GLU:OE1	3:C:242:GLU:N	2.41	0.50
5:E:173:ILE:O	5:E:173:ILE:HG23	2.12	0.50
11:K:24:ASP:OD1	11:K:25:THR:N	2.45	0.50
14:N:27:DT:H2'	32:x:583:GLU:OE1	2.11	0.50
20:T:-21:DG:C6	20:T:-20:DA:C6	2.99	0.50
26:Z:181:THR:HG22	26:Z:226:TYR:CD2	2.47	0.50
26:Z:550:ILE:HD11	26:Z:552:ARG:O	2.12	0.50
2:B:1038:THR:HA	3:C:195:THR:HA	1.94	0.50
13:M:889:LEU:CD1	13:M:930:VAL:HG21	2.38	0.50
16:P:51:G:H1'	16:P:52:G:OP2	2.12	0.50
27:e:60:LEU:HD23	27:e:97:GLU:OE1	2.12	0.50
27:e:101:VAL:HG13	33:y:383:THR:CB	2.41	0.50
1:A:88:ILE:O	1:A:90:LEU:N	2.44	0.49
23:W:243:ASP:OD1	23:W:245:THR:HG22	2.12	0.49
26:Z:602:VAL:HG22	26:Z:643:LEU:CD2	2.42	0.49
33:y:409:GLU:OE1	33:y:409:GLU:N	2.35	0.49
3:C:38:PHE:HB3	3:C:179:THR:HG21	1.94	0.49
7:G:113:ILE:HG22	7:G:117:MET:HB2	1.94	0.49
1:A:1211:LEU:C	1:A:1212:LEU:HD12	2.37	0.49
17:Q:205:GLY:O	17:Q:209:VAL:HG23	2.12	0.49
17:Q:612:LEU:HD23	17:Q:612:LEU:C	2.37	0.49
17:Q:875:LEU:C	17:Q:875:LEU:HD12	2.37	0.49
25:Y:13:LEU:HD23	25:Y:13:LEU:H	1.77	0.49
28:b:83:ALA:O	28:b:87:VAL:HG23	2.12	0.49
1:A:37:THR:HG21	1:A:41:ILE:HD11	1.93	0.49
1:A:1212:LEU:HD12	1:A:1212:LEU:N	2.26	0.49
1:A:1324:GLU:OE1	1:A:1324:GLU:N	2.38	0.49
1:A:1371:ILE:CD1	1:A:1409:GLY:O	2.60	0.49
2:B:47:PHE:HB2	2:B:155:MET:SD	2.53	0.49
7:G:12:LEU:N	7:G:12:LEU:HD12	2.28	0.49
1:A:1280:ASP:OD1	1:A:1281:ASP:N	2.45	0.49
2:B:302:LYS:HG3	9:I:14:ILE:HD11	1.94	0.49
7:G:129:LYS:HB3	13:M:464:TYR:CE2	2.47	0.49
7:G:164:MET:N	7:G:164:MET:SD	2.85	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:443:LEU:C	13:M:443:LEU:HD22	2.37	0.49
13:M:450:ARG:O	13:M:454:VAL:HG23	2.12	0.49
17:Q:852:LEU:HD12	17:Q:853:ARG:N	2.27	0.49
18:R:285:LEU:HD23	18:R:285:LEU:C	2.38	0.49
20:T:-28:DC:H41	32:x:579:LEU:HD22	1.77	0.49
1:A:946:ALA:O	1:A:950:ASN:ND2	2.46	0.49
1:A:1225:LYS:C	1:A:1226:LEU:HD12	2.38	0.49
7:G:136:VAL:N	13:M:468:LEU:HD22	2.28	0.49
14:N:68:DG:H2'	14:N:69:DG:C8	2.47	0.49
14:N:77:DG:H2'	14:N:78:DT:C7	2.42	0.49
22:V:127:VAL:HG23	22:V:128:VAL:N	2.27	0.49
23:W:33:GLU:O	23:W:49:TRP:N	2.45	0.49
2:B:755:GLN:NE2	10:J:48:MET:SD	2.86	0.49
13:M:287:ASN:OD1	13:M:290:ARG:NH2	2.43	0.49
13:M:618:ILE:HD12	13:M:640:LEU:HD12	1.95	0.49
13:M:653:PHE:CE2	13:M:657:CYS:SG	3.06	0.49
22:V:88:ASN:N	22:V:89:PRO:CD	2.76	0.49
14:N:17:DG:C2'	14:N:18:DT:H71	2.36	0.49
15:O:591:LEU:O	15:O:595:VAL:HG23	2.12	0.49
23:W:47:TRP:HB2	23:W:54:LEU:HD11	1.95	0.49
14:N:78:DT:C6	14:N:79:DT:H72	2.47	0.49
23:W:220:GLN:N	23:W:220:GLN:OE1	2.46	0.49
23:W:221:HIS:ND1	23:W:223:ASN:OD1	2.45	0.49
9:I:17:CYS:SG	9:I:18:GLN:N	2.86	0.48
1:A:386:ALA:O	1:A:449:HIS:ND1	2.46	0.48
1:A:1210:TRP:CD1	1:A:1285:LEU:HD11	2.48	0.48
2:B:1123:GLY:HA3	2:B:1170:ARG:HA	1.95	0.48
7:G:99:THR:OG1	7:G:100:GLU:N	2.42	0.48
29:g:99:ARG:HD2	29:g:99:ARG:N	2.15	0.48
3:C:91:GLU:N	3:C:91:GLU:OE1	2.47	0.48
13:M:898:LYS:NZ	13:M:929:GLN:OE1	2.38	0.48
14:N:44:DT:H2''	14:N:45:DC:C6	2.48	0.48
14:N:48:DC:H2'	14:N:49:DT:H72	1.95	0.48
32:x:836:THR:HG22	32:x:838:ASP:H	1.78	0.48
1:A:108:ARG:HG3	1:A:191:ILE:HD11	1.95	0.48
1:A:564:LEU:HD12	1:A:570:TRP:CD2	2.48	0.48
1:A:832:THR:HB	1:A:835:GLU:HG2	1.94	0.48
1:A:1471:PHE:CZ	6:F:61:GLU:HA	2.48	0.48
2:B:790:GLN:O	2:B:968:ASN:ND2	2.47	0.48
5:E:185:ILE:CD1	5:E:191:VAL:HG21	2.43	0.48
8:H:2:ALA:O	8:H:84:ARG:NH1	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:25:DC:H2''	14:N:26:DC:C6	2.48	0.48
16:P:53:C:O2'	16:P:54:G:P	2.71	0.48
33:y:118:LEU:HD23	33:y:132:PRO:HA	1.95	0.48
33:y:322:VAL:O	33:y:323:ASN:HB3	2.13	0.48
1:A:364:ARG:CD	20:T:-59:DA:H4'	2.43	0.48
3:C:210:GLU:N	3:C:210:GLU:OE1	2.47	0.48
17:Q:218:ARG:NH1	17:Q:238:LEU:HD22	2.29	0.48
23:W:107:VAL:HG22	23:W:107:VAL:O	2.13	0.48
2:B:910:THR:CB	12:L:42:ARG:O	2.62	0.48
12:L:21:GLU:HB2	12:L:41:TYR:CE2	2.49	0.48
1:A:321:GLU:C	1:A:322:LEU:HD22	2.38	0.48
2:B:715:ASP:OD2	2:B:1001:PRO:O	2.32	0.48
2:B:994:GLY:O	10:J:31:GLU:HB2	2.14	0.48
14:N:78:DT:H2''	14:N:79:DT:C6	2.49	0.48
17:Q:286:SER:O	17:Q:290:HIS:ND1	2.46	0.48
1:A:798:ILE:HB	1:A:820:ARG:O	2.14	0.48
2:B:388:TYR:CZ	2:B:505:LEU:HD21	2.49	0.48
7:G:101:ILE:N	7:G:101:ILE:HD12	2.28	0.48
7:G:130:THR:O	7:G:132:ASP:N	2.47	0.48
11:K:87:PHE:CE2	11:K:91:ILE:HD11	2.49	0.48
12:L:18:ILE:N	12:L:18:ILE:HD12	2.28	0.48
14:N:18:DT:H2''	14:N:19:DC:OP2	2.13	0.48
17:Q:593:LYS:O	17:Q:598:GLN:NE2	2.46	0.48
26:Z:466:GLN:OE1	26:Z:466:GLN:N	2.44	0.48
7:G:131:MET:SD	7:G:132:ASP:HB2	2.54	0.48
7:G:131:MET:HE3	13:M:412:ASN:OD1	2.13	0.48
8:H:136:GLU:N	8:H:136:GLU:OE1	2.47	0.48
9:I:14:ILE:HG23	9:I:23:MET:SD	2.53	0.48
24:X:223:ASP:OD1	24:X:227:ARG:NH2	2.43	0.48
26:Z:421:GLN:N	26:Z:421:GLN:OE1	2.47	0.48
1:A:107:LEU:HD23	1:A:107:LEU:O	2.14	0.48
1:A:408:ARG:NH2	1:A:412:GLN:OE1	2.47	0.48
1:A:457:ILE:HG21	2:B:1102:PHE:CZ	2.49	0.48
1:A:484:LEU:N	1:A:484:LEU:HD23	2.29	0.48
2:B:311:ILE:HG23	2:B:316:VAL:HG13	1.96	0.48
8:H:52:LEU:HD12	8:H:52:LEU:N	2.29	0.48
8:H:87:GLN:N	8:H:87:GLN:OE1	2.46	0.48
14:N:77:DG:N9	14:N:78:DT:H72	2.29	0.48
16:P:51:G:H1'	16:P:52:G:P	2.54	0.48
21:U:395:GLU:N	21:U:395:GLU:OE1	2.46	0.48
27:e:61:LEU:N	27:e:61:LEU:HD22	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:862:ARG:NH1	2:B:1088:GLU:OE1	2.47	0.47
2:B:516:GLU:N	2:B:516:GLU:OE1	2.46	0.47
2:B:754:PRO:O	10:J:53:VAL:HG12	2.14	0.47
18:R:289:ARG:NH2	32:x:889:CYS:SG	2.81	0.47
1:A:495:ASP:N	1:A:499:ASP:OD2	2.47	0.47
1:A:1443:ALA:HB2	2:B:1167:ILE:HG23	1.95	0.47
2:B:653:TRP:O	2:B:657:VAL:HG23	2.13	0.47
3:C:38:PHE:CD1	3:C:248:ALA:CB	2.97	0.47
13:M:906:TYR:CG	13:M:910:LEU:HD23	2.50	0.47
17:Q:317:HIS:HE2	22:V:58:PHE:HA	1.79	0.47
18:R:289:ARG:NH1	32:x:889:CYS:HA	2.28	0.47
1:A:488:VAL:O	1:A:488:VAL:HG12	2.14	0.47
2:B:1090:GLU:OE1	2:B:1090:GLU:N	2.42	0.47
7:G:131:MET:SD	7:G:131:MET:C	2.98	0.47
7:G:168:LEU:O	7:G:168:LEU:CD1	2.62	0.47
25:Y:42:MET:HE1	25:Y:53:THR:HG21	1.96	0.47
1:A:41:ILE:HB	1:A:88:ILE:CD1	2.45	0.47
1:A:196:LEU:HD12	1:A:196:LEU:N	2.30	0.47
1:A:282:ASP:HB3	1:A:313:HIS:ND1	2.29	0.47
1:A:500:GLU:OE2	2:B:1058:LYS:HD3	2.14	0.47
1:A:812:LYS:HE2	9:I:77:THR:HG23	1.96	0.47
1:A:971:PRO:C	1:A:972:THR:HG1	2.12	0.47
2:B:754:PRO:HB2	2:B:773:PRO:HG2	1.96	0.47
26:Z:290:ILE:N	26:Z:290:ILE:HD12	2.29	0.47
28:f:41:GLY:CA	33:y:383:THR:HG23	2.44	0.47
33:y:117:GLN:O	33:y:133:LEU:N	2.47	0.47
2:B:629:GLU:HG2	2:B:634:LEU:HD21	1.95	0.47
5:E:126:ILE:HD12	5:E:126:ILE:N	2.29	0.47
7:G:60:GLN:NE2	7:G:67:LEU:HD22	2.30	0.47
7:G:101:ILE:HG21	7:G:104:MET:HE2	1.96	0.47
7:G:131:MET:HG2	13:M:412:ASN:ND2	2.29	0.47
13:M:863:ASP:OD1	13:M:866:ARG:NH2	2.48	0.47
20:T:-71:DG:C2'	20:T:-70:DA:C8	2.97	0.47
32:x:645:ILE:HD11	32:x:729:MET:HE3	1.97	0.47
1:A:890:ARG:NH2	1:A:1023:VAL:HG22	2.29	0.47
1:A:1211:LEU:HD23	1:A:1260:ARG:NH2	2.30	0.47
1:A:1451:MET:SD	1:A:1456:GLU:HB3	2.54	0.47
2:B:407:MET:HB3	2:B:440:ILE:HD13	1.95	0.47
2:B:760:THR:O	22:V:132:ARG:NH2	2.48	0.47
2:B:771:GLU:HA	22:V:137:ILE:HD11	1.95	0.47
3:C:40:ALA:O	3:C:42:VAL:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:25:DC:C4	14:N:26:DC:N4	2.83	0.47
30:h:62:MET:O	30:h:66:VAL:HG23	2.15	0.47
1:A:359:VAL:HG23	1:A:362:SER:OG	2.15	0.47
2:B:313:GLU:HG3	2:B:316:VAL:HG12	1.97	0.47
2:B:604:ILE:N	2:B:604:ILE:HD12	2.29	0.47
2:B:957:THR:HG22	2:B:1028:LEU:HD23	1.96	0.47
4:D:107:THR:HG23	4:D:110:GLU:H	1.79	0.47
5:E:140:THR:HG21	5:E:182:TYR:CE1	2.50	0.47
7:G:101:ILE:O	7:G:101:ILE:HG22	2.15	0.47
13:M:1400:ILE:HG21	13:M:1411:ILE:HD13	1.95	0.47
27:a:107:THR:HG22	27:a:119:ILE:CG1	2.45	0.47
28:b:31:LYS:HE3	28:b:51:TYR:OH	2.15	0.47
27:e:106:ASP:OD2	27:e:131:ARG:NH2	2.46	0.47
28:f:66:ILE:O	28:f:70:VAL:HG23	2.14	0.47
1:A:40:GLY:N	1:A:87:HIS:CE1	2.83	0.47
1:A:529:GLN:HA	1:A:1397:HIS:NE2	2.29	0.47
2:B:771:GLU:O	10:J:55:LEU:HD21	2.14	0.47
17:Q:110:ILE:HD11	17:Q:140:LEU:HD13	1.96	0.47
17:Q:825:GLN:O	17:Q:828:VAL:HG12	2.14	0.47
2:B:67:LEU:HD12	2:B:84:TYR:OH	2.14	0.47
3:C:38:PHE:CE1	3:C:248:ALA:HB3	2.50	0.47
5:E:86:THR:O	5:E:89:VAL:HG12	2.14	0.47
13:M:1377:ILE:N	13:M:1377:ILE:HD12	2.30	0.47
14:N:48:DC:C6	14:N:49:DT:H72	2.50	0.47
1:A:936:GLU:HA	1:A:939:VAL:HG22	1.97	0.47
1:A:1286:ARG:O	1:A:1289:GLU:HG3	2.14	0.47
2:B:834:ARG:HH11	2:B:840:MET:HE3	1.80	0.47
10:J:54:ASP:OD1	10:J:56:ILE:HG22	2.15	0.47
13:M:532:LEU:HD21	13:M:584:VAL:HG13	1.96	0.47
13:M:1479:ARG:NH2	13:M:1518:PRO:O	2.47	0.47
14:N:77:DG:C5	14:N:78:DT:C4	3.03	0.47
17:Q:170:ALA:HB1	17:Q:186:TYR:CE2	2.50	0.47
17:Q:772:GLU:HA	17:Q:773:LYS:HB2	1.97	0.47
27:a:61:LEU:N	27:a:61:LEU:HD12	2.30	0.47
28:f:41:GLY:N	33:y:383:THR:HG23	2.30	0.47
1:A:837:PHE:HB2	2:B:506:TRP:HZ3	1.80	0.46
2:B:109:MET:HE2	2:B:174:LEU:HD13	1.97	0.46
2:B:831:LYS:HG2	2:B:848:LEU:CD1	2.45	0.46
17:Q:768:VAL:HG21	17:Q:778:GLU:HG2	1.97	0.46
26:Z:587:LEU:H	26:Z:587:LEU:HD23	1.79	0.46
28:b:53:GLU:O	28:b:57:VAL:HG23	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:497:LYS:N	2:B:498:PRO:CD	2.79	0.46
2:B:690:CYS:SG	2:B:691:SER:N	2.87	0.46
2:B:782:ILE:HG12	2:B:967:ILE:HD11	1.97	0.46
5:E:20:LEU:C	5:E:20:LEU:HD23	2.41	0.46
7:G:132:ASP:HB2	13:M:416:LEU:HB3	1.97	0.46
1:A:733:LEU:HG	9:I:108:MET:HE1	1.97	0.46
2:B:733:MET:CE	2:B:1050:ARG:HD3	2.45	0.46
17:Q:210:LYS:NZ	22:V:73:ASP:OD1	2.43	0.46
26:Z:598:ASP:OD1	26:Z:599:ILE:N	2.48	0.46
28:f:40:ARG:HB3	33:y:383:THR:HG22	1.97	0.46
1:A:511:THR:HG21	2:B:1105:GLU:OE1	2.16	0.46
1:A:912:SER:O	1:A:913:ASN:C	2.58	0.46
7:G:134:ASP:OD1	13:M:471:TYR:O	2.33	0.46
7:G:152:VAL:HG22	7:G:157:ILE:HG22	1.98	0.46
13:M:1050:ILE:N	13:M:1050:ILE:HD12	2.30	0.46
13:M:1198:CYS:SG	13:M:1200:PHE:N	2.81	0.46
17:Q:511:CYS:O	23:W:229:SER:OG	2.27	0.46
17:Q:708:LEU:HD11	17:Q:719:VAL:HG21	1.96	0.46
26:Z:196:LEU:CD2	26:Z:215:VAL:HG11	2.45	0.46
1:A:85:PHE:CE1	2:B:1163:MET:HE3	2.51	0.46
1:A:276:LEU:CD1	1:A:342:ARG:NH2	2.79	0.46
2:B:388:TYR:CD2	2:B:505:LEU:HD21	2.51	0.46
2:B:903:ILE:C	2:B:923:VAL:HG13	2.40	0.46
5:E:36:THR:HG1	5:E:39:GLU:CD	2.23	0.46
7:G:134:ASP:HB3	13:M:475:ILE:HD13	1.97	0.46
13:M:294:LEU:HD22	13:M:370:HIS:CD2	2.50	0.46
16:P:53:C:H4'	16:P:54:G:OP1	2.16	0.46
21:U:469:ASN:O	21:U:489:LEU:N	2.49	0.46
25:Y:75:GLN:NE2	25:Y:86:ALA:O	2.48	0.46
31:l:2022:VAL:HG12	31:l:2023:TYR:N	2.31	0.46
1:A:611:ASP:OD1	1:A:612:ASP:N	2.49	0.46
1:A:1415:THR:O	1:A:1419:VAL:HG22	2.16	0.46
2:B:252:ILE:HD12	2:B:252:ILE:N	2.30	0.46
2:B:756:LYS:O	10:J:51:ALA:HB1	2.16	0.46
14:N:20:DT:H2''	14:N:21:DC:H6	1.80	0.46
14:N:29:DG:C2'	14:N:30:DT:H72	2.45	0.46
17:Q:69:ILE:N	17:Q:69:ILE:HD12	2.31	0.46
17:Q:591:ILE:HG22	17:Q:592:LEU:HD12	1.96	0.46
20:T:-69:DC:H2'	20:T:-68:DC:H6	1.79	0.46
1:A:106:VAL:O	1:A:110:VAL:HG12	2.16	0.46
2:B:1004:ASP:OD1	18:R:596:ARG:NH2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:11:ILE:N	3:C:11:ILE:HD12	2.30	0.46
13:M:637:PHE:CD1	13:M:656:ILE:HG12	2.51	0.46
14:N:36:DG:H2"	14:N:37:DG:H8	1.80	0.46
14:N:70:DT:H2"	14:N:71:DC:C6	2.51	0.46
15:O:594:VAL:HG11	15:O:619:TRP:CH2	2.51	0.46
32:x:493:LEU:HD12	32:x:917:PHE:CE2	2.51	0.46
32:x:761:ASP:O	32:x:765:ALA:N	2.43	0.46
1:A:614:ASP:OD1	1:A:615:SER:N	2.49	0.46
1:A:659:GLU:OE2	1:A:985:ARG:HD2	2.16	0.46
1:A:824:GLU:OE2	18:R:596:ARG:C	2.59	0.46
1:A:896:LEU:CD2	1:A:1080:ILE:HD13	2.46	0.46
2:B:594:MET:SD	2:B:657:VAL:HG12	2.56	0.46
5:E:162:ARG:C	5:E:162:ARG:HD3	2.40	0.46
7:G:134:ASP:CG	13:M:475:ILE:HD13	2.41	0.46
14:N:70:DT:H2"	14:N:71:DC:H6	1.81	0.46
17:Q:648:TYR:CZ	22:V:40:PRO:HD3	2.51	0.46
17:Q:737:LYS:HE3	17:Q:760:VAL:HG22	1.97	0.46
23:W:248:VAL:HG12	23:W:258:VAL:HG22	1.96	0.46
26:Z:303:ILE:N	26:Z:376:PHE:O	2.49	0.46
1:A:276:LEU:HD13	1:A:342:ARG:HH22	1.81	0.46
1:A:853:LYS:O	1:A:857:THR:HG22	2.16	0.46
1:A:910:LYS:HB3	1:A:1328:PHE:HE1	1.80	0.46
1:A:1175:ILE:HG22	9:I:54:TYR:HB3	1.98	0.46
4:D:67:TYR:O	4:D:71:PHE:HD2	1.99	0.46
7:G:54:ILE:HD13	7:G:70:VAL:HG23	1.98	0.46
13:M:417:PHE:CZ	13:M:467:PHE:CE1	3.03	0.46
17:Q:364:PHE:HB3	17:Q:380:ILE:HD11	1.98	0.46
1:A:427:ILE:N	1:A:427:ILE:HD12	2.31	0.46
2:B:52:GLN:OE1	2:B:160:TYR:OH	2.28	0.46
17:Q:611:TRP:HZ2	17:Q:628:HIS:CD2	2.33	0.46
23:W:36:VAL:HG22	23:W:46:VAL:HG13	1.97	0.46
26:Z:481:ILE:N	26:Z:481:ILE:HD12	2.31	0.46
27:e:83:ARG:HG2	28:f:80:THR:HG23	1.98	0.46
1:A:280:LEU:O	1:A:284:VAL:HG23	2.16	0.45
1:A:1224:ARG:HB3	1:A:1226:LEU:HD13	1.98	0.45
2:B:193:VAL:HG11	2:B:470:LEU:HD13	1.97	0.45
2:B:1018:TYR:HE1	22:V:124:HIS:CE1	2.34	0.45
13:M:1166:LEU:HD21	13:M:1266:ARG:NH2	2.31	0.45
26:Z:424:ASP:HB2	26:Z:440:ILE:HD12	1.99	0.45
29:g:99:ARG:H	29:g:99:ARG:CD	2.18	0.45
1:A:886:VAL:HG21	1:A:889:LEU:HD23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:414:GLU:HG3	2:B:439:ILE:HD11	1.98	0.45
9:I:42:CYS:SG	9:I:43:ASP:N	2.89	0.45
10:J:21:TYR:OH	10:J:31:GLU:HG3	2.16	0.45
17:Q:276:ALA:HB1	17:Q:288:VAL:CG2	2.39	0.45
26:Z:553:LEU:N	26:Z:553:LEU:HD12	2.30	0.45
31:l:2018:ASP:OD1	31:l:2019:LEU:N	2.48	0.45
1:A:92:LYS:HD2	1:A:307:VAL:HG11	1.98	0.45
1:A:1243:LEU:N	1:A:1243:LEU:HD12	2.30	0.45
20:T:-71:DG:C2'	20:T:-70:DA:H8	2.29	0.45
26:Z:366:TYR:O	26:Z:373:PHE:N	2.44	0.45
29:g:26:PRO:O	29:g:30:VAL:HG23	2.17	0.45
33:y:53:TRP:CZ2	33:y:60:HIS:CB	2.99	0.45
33:y:243:PHE:HB2	33:y:256:VAL:HB	1.97	0.45
1:A:911:PRO:HG2	1:A:963:ARG:HE	1.81	0.45
1:A:1358:THR:OG1	1:A:1359:SER:N	2.42	0.45
2:B:1151:MET:HE1	2:B:1171:MET:SD	2.57	0.45
5:E:52:ARG:O	5:E:54:ARG:N	2.49	0.45
7:G:11:ILE:HD11	7:G:26:VAL:HG13	1.98	0.45
13:M:950:VAL:HG12	13:M:950:VAL:O	2.16	0.45
13:M:1061:GLU:HG3	13:M:1062:THR:HG23	1.98	0.45
17:Q:132:LEU:C	17:Q:132:LEU:HD23	2.41	0.45
28:f:75:HIS:CE1	30:h:96:THR:HG1	2.23	0.45
32:x:463:ARG:O	32:x:464:THR:O	2.34	0.45
33:y:369:ILE:HD11	33:y:401:TYR:CD1	2.51	0.45
3:C:49:TRP:CE2	12:L:54:VAL:HG11	2.50	0.45
4:D:88:LEU:C	4:D:88:LEU:HD12	2.42	0.45
12:L:19:CYS:SG	12:L:20:GLY:N	2.89	0.45
13:M:554:TYR:O	13:M:556:ARG:N	2.49	0.45
23:W:248:VAL:HG13	23:W:282:TYR:CZ	2.51	0.45
1:A:394:VAL:HG22	1:A:402:LEU:HD23	1.98	0.45
2:B:281:ASP:OD1	2:B:285:LEU:HD13	2.17	0.45
3:C:19:VAL:HG23	3:C:241:PRO:CG	2.46	0.45
13:M:469:LEU:HD23	13:M:470:TYR:CE2	2.52	0.45
20:T:-69:DC:H2'	20:T:-68:DC:C6	2.51	0.45
21:U:440:ILE:HD12	21:U:440:ILE:N	2.32	0.45
26:Z:626:CYS:SG	26:Z:627:LYS:N	2.90	0.45
1:A:486:LEU:N	1:A:486:LEU:HD12	2.32	0.45
2:B:86:LEU:CD1	2:B:128:ILE:HD11	2.46	0.45
2:B:550:MET:HE2	2:B:575:GLY:HA3	1.99	0.45
2:B:829:PHE:CZ	2:B:867:ILE:HD11	2.52	0.45
7:G:60:GLN:HE21	7:G:67:LEU:HD22	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:91:VAL:HG22	8:H:144:LEU:HD23	1.99	0.45
11:K:105:PHE:CE2	11:K:109:ILE:HG13	2.52	0.45
13:M:561:GLN:HE22	13:M:702:VAL:HG13	1.82	0.45
13:M:689:ILE:HD11	13:M:717:LEU:HD11	1.98	0.45
13:M:813:HIS:N	13:M:832:ASP:OD2	2.49	0.45
13:M:1074:LEU:HD13	13:M:1076:TYR:OH	2.16	0.45
1:A:120:ASP:O	1:A:122:ASN:N	2.49	0.45
1:A:1371:ILE:HD13	1:A:1409:GLY:O	2.16	0.45
7:G:38:CYS:SG	7:G:155:ASN:HA	2.57	0.45
9:I:110:LEU:N	9:I:110:LEU:HD22	2.31	0.45
14:N:42:DT:C4'	14:N:43:DT:OP1	2.65	0.45
27:e:67:PHE:O	27:e:71:VAL:HG23	2.17	0.45
32:x:719:VAL:HG22	32:x:741:TYR:CB	2.46	0.45
1:A:519:ALA:HB2	2:B:1097:HIS:CD2	2.52	0.45
1:A:603:ILE:HA	1:A:628:VAL:O	2.17	0.45
2:B:584:MET:HG3	2:B:588:ARG:NH1	2.31	0.45
14:N:31:DG:H2'	14:N:32:DT:H72	1.99	0.45
17:Q:651:ASN:ND2	17:Q:682:ASP:OD2	2.49	0.45
17:Q:733:LEU:HD22	17:Q:760:VAL:HG23	1.99	0.45
18:R:391:ILE:HD12	18:R:391:ILE:N	2.32	0.45
26:Z:705:LEU:HD12	26:Z:705:LEU:C	2.42	0.45
27:a:129:ARG:HE	33:y:387:ARG:CD	2.29	0.45
27:e:79:LYS:CG	27:e:82:LEU:HD11	2.47	0.45
28:f:41:GLY:HA3	33:y:383:THR:H	1.82	0.45
32:x:947:THR:HB	32:x:949:ASN:ND2	2.32	0.45
1:A:495:ASP:O	2:B:791:GLU:O	2.35	0.45
1:A:686:THR:OG1	1:A:687:ILE:N	2.50	0.45
1:A:904:GLN:NE2	1:A:981:CYS:O	2.48	0.45
2:B:484:ARG:C	2:B:485:LEU:HD12	2.42	0.45
2:B:528:LEU:HB2	2:B:702:MET:SD	2.57	0.45
3:C:52:ILE:HD12	3:C:61:ASP:OD1	2.16	0.45
3:C:71:ILE:HG12	3:C:148:ILE:HG21	1.99	0.45
7:G:117:MET:SD	7:G:129:LYS:C	3.00	0.45
13:M:593:ALA:HA	13:M:716:ALA:HB2	1.99	0.45
13:M:1433:GLN:NE2	13:M:1435:CYS:SG	2.90	0.45
17:Q:444:LYS:HG3	17:Q:445:VAL:HG22	1.99	0.45
18:R:505:ALA:N	18:R:506:PRO:HD2	2.32	0.45
20:T:-22:DC:H2''	20:T:-21:DG:H8	1.81	0.45
23:W:58:TRP:CZ3	23:W:95:ASN:O	2.70	0.45
25:Y:77:VAL:HG12	25:Y:80:PHE:CD2	2.52	0.45
28:b:66:ILE:O	28:b:70:VAL:HG23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1473:LEU:N	1:A:1473:LEU:HD12	2.32	0.44
2:B:166:LEU:HG	2:B:170:ASP:HB2	1.99	0.44
2:B:177:CYS:SG	2:B:737:ILE:HD11	2.57	0.44
2:B:283:ASP:O	2:B:287:HIS:ND1	2.45	0.44
2:B:371:ARG:HH22	2:B:380:ARG:NH2	2.15	0.44
2:B:682:LEU:N	2:B:682:LEU:HD12	2.32	0.44
3:C:9:VAL:HG11	11:K:105:PHE:HD1	1.81	0.44
7:G:109:SER:CB	26:Z:493:VAL:HG11	2.47	0.44
1:A:47:THR:OG1	1:A:51:ARG:O	2.32	0.44
1:A:336:LEU:N	1:A:336:LEU:HD22	2.32	0.44
1:A:687:ILE:HD11	1:A:766:PHE:CZ	2.52	0.44
2:B:719:SER:N	2:B:720:PRO:CD	2.80	0.44
8:H:27:ARG:HD3	8:H:42:ASP:OD1	2.17	0.44
17:Q:190:LEU:HD11	17:Q:201:ARG:HB3	1.99	0.44
17:Q:768:VAL:HG21	17:Q:778:GLU:HG3	1.99	0.44
28:f:35:ARG:CD	32:x:751:LEU:HD23	2.47	0.44
32:x:514:ASN:C	33:y:104:VAL:HG21	2.42	0.44
1:A:692:SER:O	1:A:785:ILE:HG12	2.17	0.44
3:C:148:ILE:N	3:C:148:ILE:HD12	2.33	0.44
4:D:103:LEU:O	7:G:144:ARG:NH2	2.51	0.44
5:E:114:ALA:O	5:E:118:LEU:HD13	2.17	0.44
13:M:1074:LEU:HD13	13:M:1076:TYR:CZ	2.53	0.44
20:T:-43:DA:C6	20:T:-42:DA:C6	3.05	0.44
28:f:56:GLY:O	28:f:60:VAL:HG23	2.17	0.44
14:N:24:DG:H2"	14:N:25:DC:H6	1.82	0.44
17:Q:648:TYR:OH	22:V:40:PRO:HD3	2.16	0.44
18:R:369:LEU:C	18:R:369:LEU:HD12	2.43	0.44
33:y:322:VAL:HG12	33:y:324:ARG:HG2	1.99	0.44
1:A:695:ASP:O	1:A:696:SER:OG	2.29	0.44
1:A:938:LEU:HD12	1:A:938:LEU:N	2.32	0.44
2:B:591:ARG:NH1	2:B:601:VAL:O	2.46	0.44
10:J:10:CYS:SG	10:J:42:ARG:NH2	2.90	0.44
11:K:57:LEU:N	11:K:76:GLN:O	2.50	0.44
17:Q:839:ARG:HA	17:Q:842:ARG:HH11	1.83	0.44
23:W:8:LEU:HD23	23:W:8:LEU:C	2.41	0.44
26:Z:189:GLU:HB2	26:Z:217:ALA:HB1	1.98	0.44
1:A:621:ILE:HG23	1:A:621:ILE:O	2.17	0.44
2:B:623:ARG:NH2	2:B:670:GLU:OE2	2.50	0.44
2:B:625:LEU:HD13	2:B:675:LEU:HD13	1.98	0.44
2:B:957:THR:HG22	2:B:1028:LEU:CD2	2.47	0.44
13:M:451:LEU:C	13:M:451:LEU:HD12	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:1240:ILE:HD12	13:M:1240:ILE:N	2.32	0.44
14:N:48:DC:C2'	14:N:49:DT:H72	2.47	0.44
22:V:61:TYR:N	22:V:62:LYS:HA	2.33	0.44
23:W:158:PRO:HG3	23:W:199:SER:O	2.18	0.44
32:x:683:HIS:O	32:x:701:TYR:OH	2.27	0.44
1:A:1540:THR:OG1	13:M:1479:ARG:NE	2.45	0.44
2:B:959:GLU:N	2:B:959:GLU:OE1	2.51	0.44
13:M:860:LEU:O	13:M:864:VAL:HG23	2.17	0.44
13:M:908:PRO:N	13:M:911:ARG:HH21	2.16	0.44
17:Q:682:ASP:OD1	17:Q:683:VAL:N	2.50	0.44
20:T:-48:DG:C6	20:T:-47:DG:C6	3.05	0.44
26:Z:428:VAL:HG13	26:Z:467:GLU:HG2	2.00	0.44
26:Z:481:ILE:HD11	26:Z:519:GLN:CG	2.47	0.44
27:e:102:ALA:HA	33:y:384:THR:CG2	2.48	0.44
30:h:42:TYR:CE1	32:x:950:PRO:HD3	2.52	0.44
1:A:440:LEU:HD23	1:A:440:LEU:H	1.81	0.44
1:A:865:ILE:HG21	2:B:1092:ASP:OD2	2.18	0.44
1:A:1006:PRO:O	1:A:1010:VAL:HG23	2.18	0.44
1:A:1049:LEU:N	1:A:1049:LEU:HD12	2.33	0.44
2:B:1123:GLY:HA3	2:B:1170:ARG:CA	2.48	0.44
7:G:92:VAL:O	7:G:126:PRO:HB2	2.17	0.44
17:Q:730:CYS:SG	17:Q:731:GLY:N	2.91	0.44
32:x:555:LYS:N	32:x:571:ASN:O	2.45	0.44
1:A:564:LEU:HD12	1:A:570:TRP:CE2	2.53	0.44
2:B:207:VAL:HG21	2:B:371:ARG:HG2	2.00	0.44
2:B:962:THR:O	10:J:9:THR:HG23	2.17	0.44
3:C:183:ALA:HB3	3:C:232:ASN:HB3	2.00	0.44
13:M:618:ILE:CD1	13:M:640:LEU:HD12	2.48	0.44
13:M:1051:GLU:CD	13:M:1067:ARG:HH21	2.26	0.44
14:N:16:DT:H2''	14:N:17:DG:N7	2.31	0.44
17:Q:214:LEU:HD23	17:Q:214:LEU:O	2.18	0.44
27:a:112:ILE:HG12	32:x:812:ARG:HG3	2.00	0.44
32:x:641:GLU:O	32:x:734:ARG:NH1	2.48	0.44
1:A:21:VAL:HG12	1:A:1449:ASP:HB3	1.98	0.43
1:A:440:LEU:HD23	1:A:440:LEU:N	2.33	0.43
1:A:1411:LEU:N	1:A:1411:LEU:HD22	2.33	0.43
2:B:228:SER:O	2:B:405:ARG:NH1	2.51	0.43
2:B:542:LEU:HD21	2:B:569:VAL:HG11	2.00	0.43
8:H:7:GLU:HG2	8:H:59:VAL:HG22	1.99	0.43
14:N:76:DC:C4	14:N:77:DG:C6	3.06	0.43
21:U:522:THR:O	21:U:524:LYS:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Z:575:VAL:O	26:Z:575:VAL:HG13	2.17	0.43
2:B:431:LEU:N	2:B:431:LEU:HD23	2.32	0.43
2:B:607:ILE:HG21	9:I:72:VAL:HA	2.00	0.43
3:C:65:ALA:O	12:L:57:ALA:HB1	2.18	0.43
5:E:84:ILE:HD12	14:N:78:DT:H5''	1.99	0.43
9:I:108:MET:SD	9:I:108:MET:N	2.92	0.43
28:b:56:GLY:O	28:b:60:VAL:HG23	2.19	0.43
1:A:1322:ILE:N	1:A:1322:ILE:HD12	2.32	0.43
2:B:46:SER:OG	2:B:397:GLY:N	2.48	0.43
4:D:38:HIS:HA	4:D:68:THR:HG21	1.99	0.43
10:J:31:GLU:OE1	22:V:133:LYS:NZ	2.51	0.43
13:M:571:LYS:HG2	13:M:581:PRO:HG3	2.00	0.43
17:Q:218:ARG:HH11	17:Q:238:LEU:HD22	1.83	0.43
20:T:-57:DA:H2'	20:T:-56:DA:H8	1.83	0.43
1:A:1255:LEU:N	1:A:1255:LEU:HD12	2.33	0.43
2:B:128:ILE:HG21	2:B:431:LEU:HD12	2.00	0.43
2:B:910:THR:OG1	2:B:911:LEU:N	2.51	0.43
20:T:-66:DC:H2''	20:T:-65:DC:H6	1.83	0.43
20:T:-49:DA:H2''	20:T:-48:DG:C8	2.54	0.43
33:y:387:ARG:HG3	33:y:407:GLU:HA	2.00	0.43
1:A:486:LEU:CD2	2:B:790:GLN:OE1	2.66	0.43
2:B:928:ILE:HD12	2:B:928:ILE:N	2.34	0.43
5:E:131:LEU:N	5:E:131:LEU:HD12	2.34	0.43
12:L:38:GLU:OE1	12:L:38:GLU:N	2.51	0.43
20:T:-77:DC:H2''	20:T:-76:DG:H8	1.82	0.43
20:T:-65:DC:H2'	20:T:-64:DG:C8	2.53	0.43
20:T:-62:DG:C2	20:T:-61:DA:C5	3.06	0.43
20:T:-56:DA:C6	20:T:-55:DC:N4	2.86	0.43
22:V:94:ILE:HD12	22:V:94:ILE:N	2.33	0.43
2:B:634:LEU:HD22	2:B:634:LEU:N	2.33	0.43
2:B:665:ILE:N	2:B:665:ILE:HD12	2.34	0.43
2:B:719:SER:OG	2:B:720:PRO:HD3	2.18	0.43
3:C:103:LEU:HD23	3:C:104:ASP:N	2.33	0.43
4:D:71:PHE:CD1	7:G:86:ASP:OD2	2.71	0.43
8:H:58:LEU:C	8:H:58:LEU:HD23	2.43	0.43
13:M:1052:VAL:HG11	13:M:1093:LEU:CD1	2.49	0.43
23:W:125:THR:OG1	23:W:131:ASN:ND2	2.51	0.43
26:Z:252:GLN:OE1	26:Z:252:GLN:N	2.52	0.43
1:A:683:GLU:O	2:B:1038:THR:OG1	2.35	0.43
1:A:1156:ASP:OD1	1:A:1157:ILE:N	2.52	0.43
5:E:103:LEU:HD21	5:E:130:PHE:HD1	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:60:HIS:O	9:I:60:HIS:ND1	2.51	0.43
10:J:8:PHE:CG	10:J:48:MET:HE1	2.54	0.43
13:M:893:TYR:HD1	13:M:930:VAL:HG12	1.83	0.43
13:M:916:LEU:C	13:M:916:LEU:HD23	2.44	0.43
13:M:965:ARG:O	13:M:969:VAL:HG23	2.18	0.43
17:Q:86:LEU:HD23	17:Q:120:ALA:HA	2.01	0.43
17:Q:190:LEU:HD23	17:Q:204:MET:SD	2.58	0.43
17:Q:214:LEU:HD23	17:Q:214:LEU:C	2.44	0.43
17:Q:351:TYR:HB2	17:Q:360:ALA:HB2	2.00	0.43
18:R:292:ARG:HH21	32:x:798:GLU:HG2	1.83	0.43
26:Z:215:VAL:HG12	26:Z:227:VAL:HG23	1.99	0.43
29:g:25:PHE:CE1	29:g:56:GLU:HA	2.53	0.43
33:y:219:TYR:O	33:y:236:TYR:OH	2.32	0.43
1:A:1439:LEU:HD13	2:B:1162:LEU:HD21	2.00	0.43
5:E:103:LEU:C	5:E:103:LEU:HD23	2.43	0.43
7:G:101:ILE:HD13	7:G:106:CYS:SG	2.59	0.43
8:H:27:ARG:NH1	8:H:42:ASP:OD1	2.51	0.43
10:J:13:ILE:HD12	10:J:13:ILE:N	2.33	0.43
14:N:77:DG:C4	14:N:78:DT:C5	3.07	0.43
17:Q:384:LEU:HD22	17:Q:397:ALA:CB	2.49	0.43
18:R:483:LEU:C	18:R:483:LEU:HD23	2.44	0.43
26:Z:493:VAL:HG12	26:Z:501:ILE:HG23	2.01	0.43
26:Z:540:VAL:HG21	26:Z:575:VAL:CG2	2.49	0.43
29:g:88:ARG:NH1	29:g:94:ASN:OD1	2.52	0.43
1:A:833:PRO:HG3	2:B:1002:PHE:CG	2.54	0.43
1:A:996:ILE:HG23	1:A:1059:ARG:O	2.19	0.43
1:A:1140:THR:OG1	1:A:1358:THR:HG22	2.19	0.43
1:A:1158:LEU:HD23	1:A:1158:LEU:O	2.19	0.43
1:A:1211:LEU:C	1:A:1211:LEU:HD12	2.44	0.43
2:B:187:ILE:HG23	2:B:445:LYS:HG3	2.01	0.43
2:B:565:THR:O	2:B:565:THR:HG23	2.19	0.43
9:I:106:ASP:OD1	9:I:106:ASP:N	2.51	0.43
17:Q:852:LEU:HD12	17:Q:852:LEU:C	2.44	0.43
20:T:-57:DA:H2'	20:T:-56:DA:C8	2.54	0.43
33:y:197:ASP:HB2	33:y:288:ASN:ND2	2.34	0.43
1:A:340:LYS:O	1:A:344:LYS:HB2	2.18	0.43
1:A:461:GLN:HG2	20:T:-60:DA:H2''	2.01	0.43
1:A:724:GLU:OE1	1:A:724:GLU:N	2.51	0.43
2:B:227:ASN:ND2	2:B:227:ASN:O	2.51	0.43
2:B:275:ALA:CB	2:B:321:ILE:HD12	2.49	0.43
8:H:41:LEU:HD13	8:H:123:MET:HG3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:52:LEU:HD22	12:L:52:LEU:N	2.34	0.43
14:N:44:DT:C2'	14:N:45:DC:C6	3.02	0.43
17:Q:251:ILE:HD12	17:Q:251:ILE:H	1.84	0.43
20:T:-20:DA:C6	20:T:-19:DG:C6	3.07	0.43
33:y:375:SER:HB2	33:y:396:LYS:HA	1.99	0.43
1:A:560:VAL:HG21	1:A:586:TRP:CD2	2.54	0.42
1:A:1118:THR:O	1:A:1123:ARG:HB2	2.19	0.42
1:A:1128:ILE:CG2	1:A:1414:ILE:HB	2.49	0.42
2:B:51:ILE:HG23	2:B:93:LEU:HD13	2.00	0.42
7:G:31:PHE:CD1	7:G:48:VAL:HG11	2.53	0.42
7:G:108:ILE:N	7:G:108:ILE:HD12	2.34	0.42
9:I:72:VAL:HG11	9:I:97:PHE:CE1	2.54	0.42
10:J:8:PHE:H	10:J:48:MET:HE3	1.84	0.42
13:M:573:TYR:HB2	13:M:584:VAL:HG11	2.00	0.42
18:R:577:LYS:HA	18:R:580:VAL:HG22	2.00	0.42
26:Z:206:THR:OG1	26:Z:207:ASP:N	2.52	0.42
33:y:360:ILE:HG23	33:y:360:ILE:O	2.19	0.42
1:A:35:SER:OG	1:A:86:GLY:HA2	2.19	0.42
1:A:141:LEU:C	1:A:141:LEU:HD23	2.44	0.42
1:A:456:VAL:HG11	1:A:503:LEU:HD21	2.00	0.42
1:A:913:ASN:OD1	1:A:963:ARG:NH2	2.49	0.42
2:B:168:ASP:OD1	2:B:169:ARG:N	2.52	0.42
2:B:569:VAL:HG13	2:B:569:VAL:O	2.19	0.42
2:B:587:LEU:CD1	2:B:597:ILE:HD11	2.50	0.42
2:B:788:TYR:HB2	2:B:947:ILE:HG22	2.01	0.42
2:B:1029:TYR:CE2	2:B:1036:LYS:HG2	2.54	0.42
2:B:1084:LEU:N	2:B:1084:LEU:HD22	2.33	0.42
4:D:81:ALA:HA	4:D:84:ARG:HG2	2.01	0.42
7:G:110:ARG:NH1	7:G:114:PRO:O	2.51	0.42
10:J:21:TYR:CZ	10:J:25:LEU:HD11	2.54	0.42
13:M:962:PHE:O	13:M:966:VAL:HG23	2.20	0.42
14:N:36:DG:O3'	32:x:674:LYS:HD2	2.19	0.42
17:Q:166:LEU:HD12	17:Q:167:LEU:N	2.34	0.42
17:Q:377:THR:HG23	17:Q:378:MET:N	2.34	0.42
23:W:288:LYS:HA	23:W:301:TYR:O	2.19	0.42
26:Z:540:VAL:HG21	26:Z:575:VAL:HG21	2.01	0.42
1:A:92:LYS:HD2	1:A:307:VAL:CG1	2.50	0.42
2:B:265:GLN:OE1	2:B:265:GLN:N	2.48	0.42
2:B:984:CYS:HA	2:B:1045:PRO:O	2.19	0.42
3:C:201:GLU:OE1	3:C:201:GLU:N	2.44	0.42
5:E:103:LEU:HD21	5:E:130:PHE:CD1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:26:DC:H4'	14:N:27:DT:OP1	2.19	0.42
22:V:182:THR:HG23	22:V:183:PHE:N	2.35	0.42
23:W:90:LEU:HD13	23:W:100:LYS:HG3	2.01	0.42
1:A:457:ILE:HD11	1:A:469:MET:HB3	2.01	0.42
2:B:42:GLN:OE1	2:B:42:GLN:N	2.44	0.42
2:B:140:LEU:N	2:B:140:LEU:HD23	2.34	0.42
2:B:733:MET:HE2	2:B:1050:ARG:HG2	2.02	0.42
3:C:195:THR:O	3:C:195:THR:HG23	2.19	0.42
13:M:902:GLU:O	26:Z:316:ILE:HD11	2.19	0.42
13:M:1153:LEU:HD12	13:M:1154:THR:HG23	2.01	0.42
17:Q:157:ASN:OD1	17:Q:158:GLN:N	2.53	0.42
17:Q:251:ILE:HD12	17:Q:251:ILE:N	2.34	0.42
25:Y:13:LEU:HD23	25:Y:13:LEU:N	2.33	0.42
1:A:31:LEU:C	1:A:31:LEU:HD23	2.44	0.42
1:A:712:ASP:O	1:A:716:VAL:HG23	2.20	0.42
1:A:945:ASN:OD1	1:A:947:HIS:N	2.52	0.42
1:A:1419:VAL:HG21	1:A:1432:PHE:CE2	2.54	0.42
2:B:529:MET:CG	2:B:624:PRO:HD2	2.50	0.42
2:B:699:HIS:CE1	2:B:701:SER:HG	2.33	0.42
2:B:845:TYR:HA	2:B:865:VAL:HG11	2.01	0.42
5:E:47:LYS:H	5:E:53:PRO:HG3	1.85	0.42
17:Q:611:TRP:HE1	17:Q:628:HIS:HA	1.85	0.42
17:Q:723:LEU:HD23	17:Q:723:LEU:C	2.44	0.42
20:T:-29:DC:H4'	20:T:-28:DC:OP1	2.20	0.42
23:W:7:ILE:HG23	23:W:7:ILE:O	2.19	0.42
26:Z:216:VAL:HG12	26:Z:218:PRO:HD3	2.02	0.42
2:B:515:PRO:O	2:B:520:VAL:HG23	2.18	0.42
2:B:783:ALA:HB2	2:B:1041:ILE:HG23	2.01	0.42
14:N:40:DG:OP1	32:x:753:LYS:NZ	2.47	0.42
20:T:-67:DC:H2''	20:T:-66:DC:H6	1.82	0.42
25:Y:67:GLU:OE1	25:Y:67:GLU:N	2.42	0.42
26:Z:181:THR:HG22	26:Z:226:TYR:HD2	1.85	0.42
2:B:812:ARG:O	2:B:922:ARG:HA	2.20	0.42
2:B:1027:VAL:HG22	2:B:1040:GLN:HG3	2.02	0.42
8:H:72:ASP:OD1	8:H:73:GLY:N	2.53	0.42
14:N:31:DG:C8	14:N:32:DT:H72	2.54	0.42
17:Q:437:ALA:HA	17:Q:440:ILE:HG22	2.01	0.42
20:T:-76:DG:H2'	20:T:-75:DC:C6	2.55	0.42
1:A:349:ARG:HH22	2:B:1070:LEU:HD21	1.85	0.42
1:A:413:TYR:OH	1:A:476:ILE:HD12	2.20	0.42
1:A:934:LEU:N	1:A:934:LEU:HD12	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:607:ILE:CG2	9:I:72:VAL:HA	2.49	0.42
3:C:38:PHE:HD1	3:C:248:ALA:CB	2.33	0.42
7:G:92:VAL:HG11	7:G:127:CYS:CA	2.48	0.42
8:H:96:VAL:HA	8:H:116:VAL:HA	2.01	0.42
9:I:26:PRO:HB3	9:I:53:ILE:HD12	2.02	0.42
13:M:1265:CYS:SG	13:M:1281:CYS:HB3	2.60	0.42
18:R:505:ALA:O	18:R:506:PRO:C	2.63	0.42
20:T:-71:DG:H2'	20:T:-70:DA:C8	2.55	0.42
20:T:-69:DC:C2'	20:T:-68:DC:H6	2.32	0.42
20:T:-22:DC:H2''	20:T:-21:DG:C8	2.55	0.42
23:W:248:VAL:HG11	23:W:289:ILE:HD13	2.01	0.42
23:W:289:ILE:N	23:W:301:TYR:O	2.47	0.42
32:x:465:ARG:CB	32:x:465:ARG:HH11	2.32	0.42
1:A:962:ASP:OD2	1:A:1046:ARG:NH2	2.51	0.42
2:B:872:THR:O	2:B:872:THR:HG23	2.20	0.42
3:C:41:GLU:OE1	3:C:255:LYS:HD2	2.20	0.42
3:C:51:GLN:OE1	3:C:162:ARG:NH2	2.53	0.42
4:D:87:LEU:HD23	4:D:87:LEU:C	2.45	0.42
4:D:103:LEU:HD22	7:G:144:ARG:NH1	2.35	0.42
4:D:115:ILE:N	4:D:115:ILE:HD12	2.34	0.42
7:G:147:ILE:HD12	7:G:147:ILE:N	2.34	0.42
14:N:45:DC:H2''	14:N:46:DC:H6	1.85	0.42
17:Q:734:GLN:OE1	17:Q:738:GLN:NE2	2.53	0.42
17:Q:776:LEU:HD22	17:Q:831:ALA:HB1	2.02	0.42
25:Y:10:LEU:O	25:Y:13:LEU:HD22	2.20	0.42
26:Z:745:VAL:CG1	26:Z:750:LEU:HD21	2.49	0.42
28:b:61:PHE:O	28:b:65:VAL:HG23	2.20	0.42
32:x:474:ARG:O	32:x:478:GLN:HG2	2.20	0.42
32:x:815:CYS:SG	32:x:826:ASN:ND2	2.93	0.42
1:A:31:LEU:HD23	1:A:31:LEU:O	2.19	0.42
1:A:107:LEU:HD23	1:A:107:LEU:C	2.44	0.42
1:A:1374:VAL:HG11	1:A:1411:LEU:HD11	2.02	0.42
2:B:27:TRP:CD1	2:B:762:ARG:HE	2.38	0.42
2:B:163:LEU:HD22	2:B:163:LEU:N	2.34	0.42
2:B:864:ASP:OD1	26:Z:725:LYS:NZ	2.51	0.42
7:G:171:VAL:HG13	7:G:171:VAL:O	2.19	0.42
13:M:443:LEU:HD13	13:M:443:LEU:N	2.35	0.42
13:M:1150:PHE:O	13:M:1154:THR:OG1	2.17	0.42
23:W:253:ASP:OD1	23:W:255:SER:OG	2.32	0.42
33:y:205:LEU:HD12	33:y:216:ILE:HD12	2.02	0.42
1:A:136:GLN:OE1	1:A:136:GLN:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:48:ASP:OD2	2:B:159:THR:HG21	2.19	0.41
2:B:144:HIS:CD2	2:B:431:LEU:HD21	2.54	0.41
2:B:996:ILE:HD12	22:V:134:THR:HA	2.02	0.41
3:C:52:ILE:CD1	3:C:61:ASP:OD1	2.68	0.41
4:D:63:LYS:HA	4:D:66:ASN:HD21	1.84	0.41
8:H:38:ASP:OD1	8:H:39:LEU:N	2.53	0.41
13:M:444:ASP:OD1	13:M:444:ASP:N	2.51	0.41
14:N:78:DT:C2'	14:N:79:DT:H72	2.45	0.41
27:e:73:GLU:OE1	28:f:25:ASN:ND2	2.47	0.41
1:A:97:VAL:CG1	1:A:318:VAL:HG23	2.50	0.41
1:A:733:LEU:O	1:A:736:THR:HG22	2.20	0.41
1:A:910:LYS:N	1:A:911:PRO:HD3	2.35	0.41
2:B:67:LEU:CD1	2:B:84:TYR:OH	2.68	0.41
2:B:547:GLU:OE2	2:B:548:TRP:NE1	2.53	0.41
2:B:752:TYR:CE1	3:C:60:HIS:CE1	3.08	0.41
2:B:959:GLU:HA	3:C:183:ALA:CB	2.50	0.41
3:C:2:PRO:HB3	11:K:54:PRO:HD2	2.02	0.41
13:M:468:LEU:HD12	13:M:468:LEU:C	2.44	0.41
15:O:590:LEU:HG	15:O:594:VAL:HG13	2.02	0.41
17:Q:43:ILE:N	17:Q:43:ILE:HD12	2.35	0.41
17:Q:662:TYR:O	17:Q:666:ALA:N	2.53	0.41
18:R:366:ARG:NH2	26:Z:775:TPO:O2P	2.52	0.41
20:T:-71:DG:H2'	20:T:-70:DA:H8	1.84	0.41
1:A:356:GLY:O	2:B:1085:ARG:NH1	2.52	0.41
1:A:419:ILE:O	1:A:419:ILE:HG23	2.21	0.41
1:A:1054:MET:SD	1:A:1060:LEU:HD12	2.60	0.41
2:B:473:LEU:HD23	2:B:731:GLN:HA	2.02	0.41
2:B:830:GLU:N	2:B:868:GLY:O	2.34	0.41
13:M:999:HIS:CE1	13:M:1003:ILE:HD11	2.56	0.41
13:M:1371:TRP:CZ3	13:M:1373:VAL:HG22	2.55	0.41
13:M:1398:LEU:HD23	13:M:1411:ILE:HD11	2.01	0.41
15:O:591:LEU:C	15:O:591:LEU:HD13	2.45	0.41
17:Q:94:VAL:CG2	17:Q:140:LEU:HD11	2.41	0.41
17:Q:816:GLN:HA	17:Q:819:ASP:OD2	2.20	0.41
1:A:23:PHE:CE1	1:A:1427:LEU:HD21	2.55	0.41
1:A:489:THR:HG21	2:B:791:GLU:OE2	2.19	0.41
1:A:499:ASP:OD1	16:P:61:U:H4'	2.20	0.41
2:B:294:ASP:N	2:B:294:ASP:OD1	2.52	0.41
2:B:853:LEU:O	12:L:46:LYS:NZ	2.53	0.41
2:B:1010:LYS:HE3	22:V:130:TRP:CZ3	2.55	0.41
4:D:80:ILE:O	4:D:83:VAL:HG22	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:15:ILE:O	8:H:16:ASP:C	2.64	0.41
13:M:950:VAL:O	13:M:952:GLU:N	2.48	0.41
17:Q:611:TRP:CZ2	17:Q:628:HIS:CD2	3.09	0.41
20:T:-21:DG:C2'	20:T:-20:DA:C8	3.04	0.41
32:x:675:ARG:NH1	32:x:743:GLU:OE2	2.48	0.41
33:y:200:CYS:CB	33:y:285:LEU:HD21	2.50	0.41
1:A:365:THR:HG22	1:A:366:VAL:N	2.35	0.41
2:B:433:LEU:HD22	2:B:433:LEU:N	2.36	0.41
3:C:38:PHE:HE1	3:C:248:ALA:HB3	1.85	0.41
3:C:44:ILE:HD11	3:C:238:SER:CB	2.50	0.41
14:N:28:DG:H2''	14:N:29:DG:C8	2.55	0.41
14:N:33:DC:H2''	14:N:34:DT:H6	1.85	0.41
17:Q:611:TRP:O	17:Q:614:THR:OG1	2.31	0.41
29:g:97:LEU:HD22	29:g:100:VAL:HG21	2.02	0.41
30:h:40:TYR:O	30:h:44:VAL:HG23	2.21	0.41
32:x:470:ALA:O	32:x:473:LYS:N	2.53	0.41
1:A:253:LEU:HD23	1:A:253:LEU:C	2.45	0.41
1:A:927:GLU:HG2	1:A:931:ARG:NE	2.35	0.41
2:B:761:THR:HG22	2:B:999:ALA:O	2.20	0.41
9:I:72:VAL:HG11	9:I:97:PHE:CZ	2.55	0.41
10:J:26:GLN:HA	18:R:566:ARG:HD2	2.03	0.41
13:M:443:LEU:HD13	13:M:443:LEU:H	1.86	0.41
14:N:24:DG:H2''	14:N:25:DC:C6	2.56	0.41
17:Q:212:ASN:O	17:Q:212:ASN:ND2	2.54	0.41
17:Q:764:LEU:HD23	17:Q:764:LEU:C	2.46	0.41
26:Z:497:GLU:OE1	26:Z:497:GLU:N	2.47	0.41
33:y:391:PHE:CE2	33:y:393:ILE:HD11	2.55	0.41
1:A:147:LEU:HD23	1:A:147:LEU:C	2.45	0.41
1:A:458:PHE:HB2	1:A:472:HIS:CD2	2.55	0.41
2:B:140:LEU:HD23	2:B:140:LEU:H	1.85	0.41
2:B:506:TRP:CH2	2:B:703:ILE:HD13	2.55	0.41
2:B:595:ASP:OD1	2:B:595:ASP:N	2.52	0.41
2:B:598:VAL:CG2	2:B:601:VAL:HG23	2.51	0.41
2:B:816:GLU:HG2	2:B:867:ILE:HD13	2.03	0.41
3:C:49:TRP:NE1	12:L:54:VAL:HG11	2.36	0.41
3:C:161:LEU:HD12	3:C:161:LEU:C	2.45	0.41
13:M:1010:ARG:NH2	13:M:1042:LEU:O	2.54	0.41
14:N:39:DT:H2''	14:N:40:DG:H8	1.82	0.41
17:Q:204:MET:HG2	17:Q:208:PHE:CE2	2.56	0.41
24:X:221:THR:O	24:X:225:VAL:HG22	2.21	0.41
28:f:41:GLY:N	33:y:383:THR:CG2	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:y:313:MET:O	33:y:317:VAL:HG23	2.20	0.41
1:A:189:PRO:HB3	1:A:202:TRP:CE2	2.56	0.41
1:A:684:GLY:HA3	2:B:1037:ILE:CG2	2.51	0.41
1:A:1330:ALA:HB3	19:S:294:CYS:CA	2.50	0.41
1:A:1427:LEU:N	1:A:1427:LEU:HD22	2.36	0.41
2:B:395:LEU:N	2:B:395:LEU:HD22	2.35	0.41
4:D:57:LEU:HD12	4:D:57:LEU:H	1.85	0.41
7:G:131:MET:SD	13:M:416:LEU:CB	3.09	0.41
7:G:131:MET:CE	13:M:412:ASN:C	2.94	0.41
7:G:134:ASP:O	13:M:472:GLY:HA2	2.21	0.41
11:K:104:ARG:HA	11:K:107:VAL:HG22	2.02	0.41
20:T:-61:DA:H2'	20:T:-60:DA:C1'	2.50	0.41
20:T:-49:DA:H2''	20:T:-48:DG:H8	1.86	0.41
20:T:-43:DA:H2''	20:T:-42:DA:H8	1.86	0.41
20:T:-28:DC:N4	32:x:579:LEU:HD22	2.34	0.41
20:T:-25:DG:H2''	20:T:-24:DC:C6	2.56	0.41
23:W:206:VAL:HG23	23:W:240:PHE:CZ	2.56	0.41
1:A:40:GLY:CA	1:A:87:HIS:CE1	3.04	0.41
1:A:110:VAL:HG22	1:A:111:CYS:N	2.36	0.41
1:A:359:VAL:HG12	2:B:1106:ARG:O	2.20	0.41
1:A:510:GLU:OE1	6:F:68:THR:N	2.53	0.41
1:A:827:TYR:OH	1:A:839:HIS:NE2	2.48	0.41
1:A:980:PRO:HD2	1:A:1041:PHE:HD1	1.86	0.41
2:B:206:TYR:O	2:B:219:GLY:HA2	2.21	0.41
2:B:567:ILE:N	2:B:567:ILE:HD12	2.36	0.41
2:B:626:LEU:CD1	2:B:698:ILE:HG12	2.51	0.41
2:B:797:ASN:O	2:B:801:VAL:HG23	2.21	0.41
2:B:836:THR:OG1	2:B:889:LYS:CE	2.68	0.41
2:B:867:ILE:CG2	2:B:894:THR:HG22	2.50	0.41
2:B:917:LYS:HG2	12:L:34:ILE:HD11	2.02	0.41
2:B:963:PRO:HG3	2:B:1043:ILE:HD12	2.03	0.41
2:B:1116:VAL:HG21	2:B:1151:MET:HE3	2.03	0.41
3:C:19:VAL:HG23	3:C:241:PRO:HG2	2.01	0.41
4:D:31:THR:HA	7:G:3:TYR:CE2	2.55	0.41
7:G:58:VAL:C	7:G:66:VAL:HG23	2.46	0.41
7:G:170:LEU:HD23	7:G:171:VAL:N	2.35	0.41
8:H:59:VAL:O	8:H:143:LEU:O	2.39	0.41
13:M:469:LEU:HD21	13:M:595:GLN:HG2	2.03	0.41
13:M:576:SER:OG	13:M:577:GLN:N	2.53	0.41
13:M:936:ASP:HA	26:Z:571:ARG:HH21	1.86	0.41
17:Q:380:ILE:HD12	17:Q:400:HIS:HE1	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:231:HIS:HB3	23:W:253:ASP:OD2	2.20	0.41
26:Z:529:ASP:OD1	26:Z:533:GLN:NE2	2.53	0.41
32:x:864:TYR:CD1	32:x:906:MET:HE1	2.56	0.41
2:B:260:LEU:N	2:B:260:LEU:HD12	2.36	0.41
2:B:583:LEU:O	2:B:587:LEU:HD23	2.22	0.41
4:D:60:VAL:O	4:D:64:THR:HG23	2.21	0.41
4:D:70:ARG:NH1	7:G:88:VAL:HG21	2.36	0.41
7:G:38:CYS:HB3	7:G:155:ASN:HA	2.03	0.41
16:P:51:G:C1'	16:P:52:G:P	3.07	0.41
17:Q:395:ASP:OD1	17:Q:395:ASP:N	2.54	0.41
17:Q:639:VAL:O	17:Q:642:ASN:OD1	2.40	0.41
27:e:120:MET:C	28:f:50:ILE:HD11	2.46	0.41
1:A:62:GLN:HG3	1:A:84:HIS:O	2.21	0.40
1:A:276:LEU:HD13	1:A:342:ARG:NH2	2.35	0.40
1:A:865:ILE:HG21	2:B:1092:ASP:CG	2.45	0.40
1:A:877:ALA:HB3	1:A:890:ARG:NH1	2.36	0.40
1:A:1312:PRO:HD3	1:A:1333:GLU:O	2.20	0.40
1:A:1315:ASP:N	19:S:295:GLY:O	2.45	0.40
2:B:20:ASP:O	2:B:22:TRP:N	2.54	0.40
2:B:279:VAL:O	2:B:279:VAL:HG22	2.20	0.40
2:B:565:THR:O	2:B:576:ILE:HD12	2.21	0.40
7:G:116:GLU:HB3	7:G:131:MET:CB	2.51	0.40
7:G:118:GLU:CD	7:G:129:LYS:HZ1	2.21	0.40
7:G:170:LEU:HD23	7:G:170:LEU:C	2.45	0.40
8:H:14:ASP:OD1	8:H:15:ILE:N	2.54	0.40
13:M:339:LEU:C	13:M:339:LEU:HD13	2.46	0.40
17:Q:769:LEU:HD13	17:Q:824:ALA:HB2	2.03	0.40
20:T:-18:DA:H2''	20:T:-17:DC:C6	2.55	0.40
26:Z:189:GLU:N	26:Z:189:GLU:OE1	2.54	0.40
1:A:458:PHE:CE2	1:A:501:MET:HE2	2.56	0.40
13:M:1036:LYS:HG2	13:M:1134:TYR:CE2	2.56	0.40
13:M:1150:PHE:HB2	13:M:1272:ILE:CG2	2.51	0.40
13:M:1462:ILE:HG23	13:M:1462:ILE:O	2.21	0.40
15:O:623:LEU:HD22	15:O:623:LEU:N	2.36	0.40
17:Q:68:ARG:HE	17:Q:89:LEU:HD12	1.85	0.40
17:Q:166:LEU:HD12	17:Q:166:LEU:C	2.46	0.40
20:T:-28:DC:N4	32:x:579:LEU:HD13	2.33	0.40
1:A:21:VAL:CG1	1:A:1449:ASP:HB3	2.51	0.40
1:A:560:VAL:HG21	1:A:586:TRP:CG	2.55	0.40
2:B:25:ALA:HB1	2:B:640:ILE:HD12	2.04	0.40
2:B:474:THR:HG23	2:B:477:SER:H	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:57:LEU:HD12	4:D:57:LEU:N	2.36	0.40
7:G:116:GLU:CA	7:G:131:MET:HB2	2.52	0.40
13:M:781:VAL:HG12	13:M:782:LEU:N	2.37	0.40
13:M:884:LEU:CD2	13:M:1152:MET:HE3	2.51	0.40
13:M:918:ARG:HD3	13:M:981:TYR:CE1	2.57	0.40
13:M:926:GLU:O	13:M:930:VAL:HG22	2.21	0.40
14:N:36:DG:H2''	14:N:37:DG:C8	2.55	0.40
14:N:37:DG:H5'	32:x:674:LYS:NZ	2.37	0.40
17:Q:384:LEU:HD22	17:Q:397:ALA:HB2	2.03	0.40
17:Q:855:LYS:O	17:Q:858:LYS:HG3	2.21	0.40
22:V:94:ILE:O	22:V:94:ILE:HG22	2.20	0.40
1:A:401:ARG:O	1:A:405:LEU:HD13	2.20	0.40
1:A:888:GLN:NE2	1:A:1403:ASP:OD2	2.50	0.40
2:B:154:ILE:HD12	2:B:154:ILE:N	2.36	0.40
2:B:901:THR:CG2	26:Z:740:CYS:HB2	2.52	0.40
7:G:67:LEU:H	7:G:67:LEU:HD23	1.87	0.40
7:G:136:VAL:HG12	7:G:138:GLN:H	1.85	0.40
13:M:1111:LEU:HD12	13:M:1123:LEU:HD11	2.04	0.40
18:R:575:SER:O	18:R:579:LEU:HD13	2.20	0.40
23:W:22:VAL:HG23	23:W:37:THR:HG22	2.03	0.40
25:Y:24:THR:HG22	25:Y:25:ILE:N	2.36	0.40
33:y:56:VAL:HG22	33:y:60:HIS:C	2.47	0.40
1:A:832:THR:HG23	18:R:596:ARG:NH1	2.37	0.40
2:B:155:MET:HG3	2:B:185:PHE:CE1	2.56	0.40
2:B:270:ILE:CG2	2:B:274:ARG:NH1	2.85	0.40
2:B:687:VAL:O	2:B:689:TYR:N	2.54	0.40
2:B:939:HIS:NE2	2:B:983:GLU:OE1	2.50	0.40
7:G:110:ARG:HH22	7:G:115:SER:HA	1.86	0.40
8:H:96:VAL:O	8:H:96:VAL:HG13	2.22	0.40
13:M:373:VAL:HG13	13:M:393:LEU:CB	2.51	0.40
24:X:233:THR:OG1	24:X:234:ARG:N	2.53	0.40
27:a:96:SER:OG	28:b:62:LEU:HD21	2.22	0.40
28:f:76:ALA:O	28:f:77:LYS:HB2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1408/1984 (71%)	1244 (88%)	148 (10%)	16 (1%)	11	39
2	B	1112/1251 (89%)	972 (87%)	123 (11%)	17 (2%)	8	32
3	C	254/275 (92%)	221 (87%)	28 (11%)	5 (2%)	6	25
4	D	124/142 (87%)	111 (90%)	12 (10%)	1 (1%)	16	47
5	E	207/210 (99%)	187 (90%)	19 (9%)	1 (0%)	24	57
6	F	76/127 (60%)	69 (91%)	5 (7%)	2 (3%)	4	21
7	G	169/172 (98%)	143 (85%)	20 (12%)	6 (4%)	2	16
8	H	147/150 (98%)	125 (85%)	22 (15%)	0	100	100
9	I	114/125 (91%)	98 (86%)	16 (14%)	0	100	100
10	J	64/67 (96%)	55 (86%)	6 (9%)	3 (5%)	2	11
11	K	113/117 (97%)	105 (93%)	7 (6%)	1 (1%)	14	44
12	L	45/58 (78%)	39 (87%)	3 (7%)	3 (7%)	1	6
13	M	1154/1729 (67%)	1045 (91%)	93 (8%)	16 (1%)	9	34
15	O	130/821 (16%)	124 (95%)	5 (4%)	1 (1%)	16	47
17	Q	888/1179 (75%)	804 (90%)	78 (9%)	6 (1%)	18	49
18	R	277/713 (39%)	256 (92%)	21 (8%)	0	100	100
19	S	157/304 (52%)	149 (95%)	6 (4%)	2 (1%)	9	35
21	U	117/666 (18%)	95 (81%)	18 (15%)	4 (3%)	3	16
22	V	234/531 (44%)	194 (83%)	37 (16%)	3 (1%)	9	35
23	W	298/305 (98%)	259 (87%)	37 (12%)	2 (1%)	18	49
24	X	41/531 (8%)	38 (93%)	3 (7%)	0	100	100
25	Y	114/121 (94%)	98 (86%)	16 (14%)	0	100	100
26	Z	497/1087 (46%)	422 (85%)	70 (14%)	5 (1%)	12	41
27	a	74/136 (54%)	71 (96%)	3 (4%)	0	100	100
27	e	73/136 (54%)	70 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	b	76/103 (74%)	73 (96%)	3 (4%)	0	100	100
28	f	70/103 (68%)	65 (93%)	3 (4%)	2 (3%)	3	19
29	g	88/130 (68%)	85 (97%)	3 (3%)	0	100	100
30	h	87/123 (71%)	81 (93%)	6 (7%)	0	100	100
31	l	21/1133 (2%)	19 (90%)	2 (10%)	0	100	100
32	x	479/1049 (46%)	427 (89%)	40 (8%)	12 (2%)	4	21
33	y	418/709 (59%)	386 (92%)	29 (7%)	3 (1%)	18	49
All	All	9126/16287 (56%)	8130 (89%)	885 (10%)	111 (1%)	13	37

All (111) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	G	130	THR
7	G	167	TYR
12	L	39	CYS
13	M	570	ALA
13	M	1057	ARG
13	M	1257	VAL
19	S	181	ARG
22	V	237	LEU
32	x	464	THR
32	x	466	ASN
32	x	750	ASP
32	x	820	THR
33	y	365	PRO
1	A	91	ALA
1	A	1409	GLY
2	B	21	LEU
2	B	90	GLN
2	B	225	LEU
2	B	684	GLU
2	B	785	TYR
2	B	1072	ARG
2	B	1166	SER
3	C	41	GLU
3	C	93	PHE
3	C	190	ASN
7	G	131	MET
7	G	164	MET
12	L	57	ALA

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Mol	Chain	Res	Type
13	M	444	ASP
13	M	576	SER
13	M	1038	ASP
15	O	645	PRO
19	S	182	ASN
28	f	29	ILE
32	x	754	HIS
1	A	121	SER
1	A	786	ALA
1	A	1369	LEU
1	A	1467	GLY
2	B	20	ASP
2	B	650	ASN
2	B	688	ALA
2	B	747	LEU
10	J	28	GLU
13	M	1134	TYR
17	Q	425	THR
21	U	485	PHE
21	U	510	LYS
26	Z	429	CYS
26	Z	525	ALA
26	Z	774	GLN
1	A	319	ASP
1	A	999	ARG
1	A	1184	THR
2	B	901	THR
3	C	92	GLU
10	J	64	PRO
11	K	43	GLY
12	L	15	MET
13	M	571	LYS
13	M	628	VAL
13	M	683	GLN
13	M	807	ASP
13	M	879	SER
13	M	1330	PRO
21	U	523	GLN
23	W	140	LYS
26	Z	445	GLY
32	x	755	GLN
32	x	756	HIS

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Mol	Chain	Res	Type
32	x	822	SER
33	y	204	GLU
1	A	621	ILE
1	A	980	PRO
2	B	120	TYR
2	B	594	MET
4	D	51	ALA
7	G	125	PRO
10	J	10	CYS
13	M	1058	VAL
13	M	1136	ASP
17	Q	199	GLU
17	Q	484	GLU
17	Q	712	TYR
21	U	416	VAL
28	f	43	VAL
32	x	658	SER
32	x	659	ASN
32	x	873	ALA
1	A	788	VAL
1	A	1548	PRO
2	B	1142	ASN
3	C	130	VAL
6	F	76	CYS
13	M	637	PHE
17	Q	370	ALA
22	V	247	LYS
23	W	244	ASP
26	Z	362	GLU
33	y	151	HIS
5	E	201	GLY
7	G	135	ILE
17	Q	4	GLY
2	B	288	ILE
2	B	994	GLY
6	F	85	GLY
22	V	89	PRO
1	A	333	GLY
1	A	911	PRO
1	A	1541	PRO
32	x	608	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1245/1761 (71%)	1244 (100%)	1 (0%)	88	90
2	B	986/1084 (91%)	984 (100%)	2 (0%)	87	89
3	C	235/252 (93%)	235 (100%)	0	100	100
4	D	109/126 (86%)	109 (100%)	0	100	100
5	E	191/192 (100%)	190 (100%)	1 (0%)	81	85
6	F	68/111 (61%)	67 (98%)	1 (2%)	57	75
7	G	146/153 (95%)	142 (97%)	4 (3%)	39	67
8	H	130/131 (99%)	130 (100%)	0	100	100
9	I	104/112 (93%)	103 (99%)	1 (1%)	68	79
10	J	55/56 (98%)	55 (100%)	0	100	100
11	K	104/106 (98%)	104 (100%)	0	100	100
12	L	44/55 (80%)	44 (100%)	0	100	100
13	M	1037/1524 (68%)	1020 (98%)	17 (2%)	55	75
15	O	118/737 (16%)	116 (98%)	2 (2%)	53	74
17	Q	761/1011 (75%)	756 (99%)	5 (1%)	76	82
18	R	205/625 (33%)	204 (100%)	1 (0%)	81	85
19	S	4/268 (2%)	4 (100%)	0	100	100
21	U	65/590 (11%)	65 (100%)	0	100	100
22	V	146/462 (32%)	145 (99%)	1 (1%)	76	82
23	W	255/260 (98%)	255 (100%)	0	100	100
24	X	40/467 (9%)	40 (100%)	0	100	100
25	Y	102/105 (97%)	102 (100%)	0	100	100
26	Z	435/939 (46%)	435 (100%)	0	100	100
27	a	66/111 (60%)	66 (100%)	0	100	100
27	e	65/111 (59%)	65 (100%)	0	100	100
28	b	64/79 (81%)	63 (98%)	1 (2%)	55	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	f	60/79 (76%)	60 (100%)	0	100	100
29	g	71/102 (70%)	71 (100%)	0	100	100
30	h	76/103 (74%)	76 (100%)	0	100	100
31	l	23/1017 (2%)	23 (100%)	0	100	100
32	x	431/929 (46%)	426 (99%)	5 (1%)	63	78
33	y	379/631 (60%)	379 (100%)	0	100	100
All	All	7820/14289 (55%)	7778 (100%)	42 (0%)	78	85

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	535	MET
2	B	422	PHE
2	B	768	ARG
5	E	18	MET
6	F	123	LEU
7	G	138	GLN
7	G	164	MET
7	G	166	ASP
7	G	167	TYR
9	I	56	ASN
13	M	381	LYS
13	M	413	LEU
13	M	416	LEU
13	M	417	PHE
13	M	443	LEU
13	M	451	LEU
13	M	457	MET
13	M	468	LEU
13	M	475	ILE
13	M	538	LYS
13	M	550	LEU
13	M	585	LEU
13	M	837	LYS
13	M	1198	CYS
13	M	1243	LYS
13	M	1256	ARG
13	M	1258	LYS
15	O	604	LYS
15	O	652	LEU

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Mol	Chain	Res	Type
17	Q	543	ASP
17	Q	707	CYS
17	Q	817	CYS
17	Q	861	GLU
17	Q	875	LEU
18	R	576	GLU
22	V	85	ASP
28	b	93	GLN
32	x	465	ARG
32	x	469	THR
32	x	497	LYS
32	x	760	ARG
32	x	828	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (90) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	GLN
1	A	122	ASN
1	A	188	GLN
1	A	273	GLN
1	A	301	HIS
1	A	531	ASN
1	A	700	GLN
1	A	711	GLN
1	A	790	GLN
1	A	791	GLN
1	A	991	GLN
1	A	1036	ASN
1	A	1044	HIS
1	A	1190	GLN
1	A	1313	GLN
1	A	1332	GLN
1	A	1384	HIS
1	A	1422	GLN
2	B	197	GLN
2	B	227	ASN
2	B	254	GLN
2	B	642	GLN
2	B	725	GLN
2	B	731	GLN
2	B	968	ASN

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Mol	Chain	Res	Type
2	B	1053	HIS
2	B	1071	ASN
3	C	60	HIS
3	C	111	GLN
4	D	47	GLN
5	E	30	GLN
5	E	148	HIS
5	E	169	GLN
7	G	9	HIS
7	G	91	GLN
9	I	32	ASN
10	J	26	GLN
11	K	69	HIS
12	L	13	GLN
12	L	26	ASN
13	M	370	HIS
13	M	466	HIS
13	M	701	GLN
13	M	846	HIS
13	M	912	GLN
13	M	979	HIS
13	M	1176	HIS
13	M	1205	ASN
13	M	1264	HIS
13	M	1433	GLN
17	Q	129	ASN
17	Q	130	HIS
17	Q	373	ASN
17	Q	455	ASN
17	Q	461	HIS
17	Q	527	HIS
17	Q	628	HIS
17	Q	651	ASN
17	Q	659	HIS
17	Q	714	HIS
17	Q	738	GLN
17	Q	745	HIS
17	Q	756	ASN
17	Q	775	ASN
17	Q	816	GLN
17	Q	827	HIS
18	R	264	ASN

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Mol	Chain	Res	Type
18	R	432	ASN
18	R	588	ASN
23	W	27	ASN
23	W	131	ASN
23	W	223	ASN
23	W	273	HIS
25	Y	12	HIS
26	Z	234	HIS
26	Z	272	ASN
26	Z	301	ASN
26	Z	446	ASN
26	Z	545	GLN
26	Z	737	HIS
30	h	67	ASN
32	x	514	ASN
32	x	617	ASN
32	x	721	HIS
32	x	739	GLN
32	x	826	ASN
32	x	849	GLN
32	x	887	ASN
33	y	60	HIS
33	y	224	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
16	P	11/11 (100%)	2 (18%)	2 (18%)

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
16	P	52	G
16	P	54	G

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
16	P	51	G
16	P	53	C

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

3 non-standard protein/DNA/RNA residues are modelled in this entry.

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$
1	SEP	A	1547	1	8,9,10	1.61	1 (12%)	7,12,14	1.35	1 (14%)
1	TPO	A	1525	1	8,10,11	1.09	0	10,14,16	2.97	3 (30%)
26	TPO	Z	775	26	8,10,11	1.13	0	10,14,16	1.91	1 (10%)

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
1	SEP	A	1547	1	-	0/6/8/10	-
1	TPO	A	1525	1	-	1/9/11/13	-
26	TPO	Z	775	26	-	2/9/11/13	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1547	SEP	P-O1P	3.52	1.61	1.50

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1525	TPO	CG2-CB-CA	-6.50	100.60	113.26
1	A	1525	TPO	P-OG1-CB	-5.65	107.96	123.33
26	Z	775	TPO	P-OG1-CB	-5.29	108.96	123.33
1	A	1525	TPO	O-C-CA	-3.11	116.77	124.77
1	A	1547	SEP	OG-CB-CA	2.97	111.04	108.14

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1525	TPO	O-C-CA-CB
26	Z	775	TPO	C-CA-CB-CG2
26	Z	775	TPO	CB-OG1-P-O2P

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1525	TPO	1	0
26	Z	775	TPO	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 10 are monoatomic - leaving 0 for Mogul analysis.

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.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
21	U	1
22	V	1
13	M	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	U	497:ASP	C	505:SER	N	27.05
1	V	299:GLU	C	310:ASN	N	12.58
1	M	1334:ASN	C	1338:ILE	N	9.04

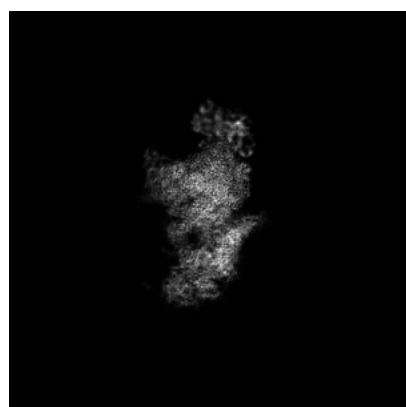
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-48044. These allow visual inspection of the internal detail of the map and identification of artifacts.

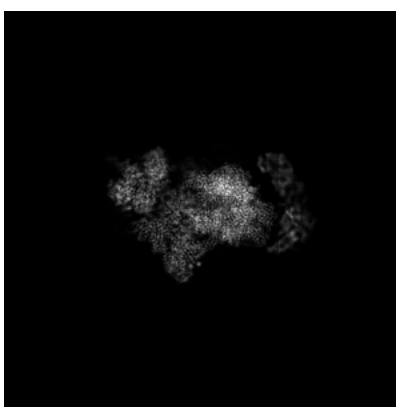
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

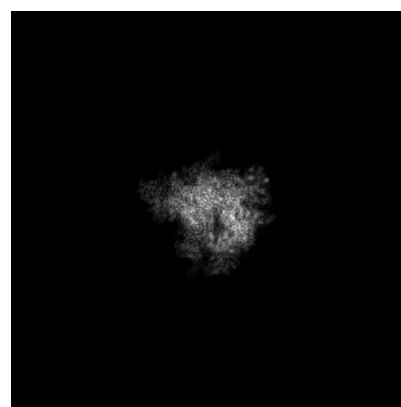
6.1.1 Primary map



X



Y



Z

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

6.2 Central slices [i](#)

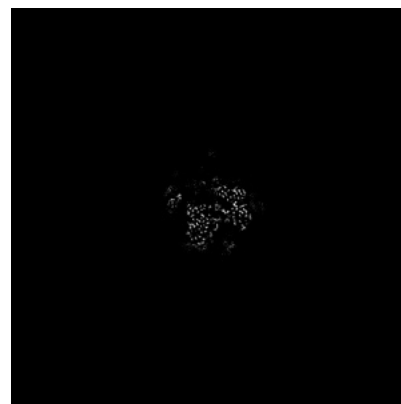
6.2.1 Primary map



X Index: 225



Y Index: 225



Z Index: 225

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: 251



Y Index: 238

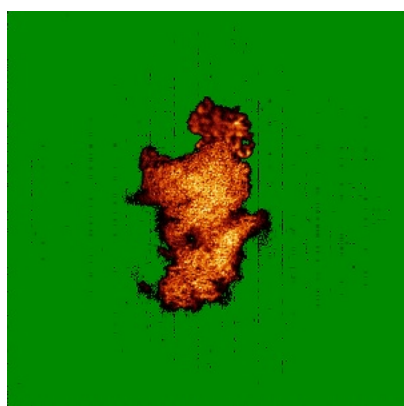


Z Index: 250

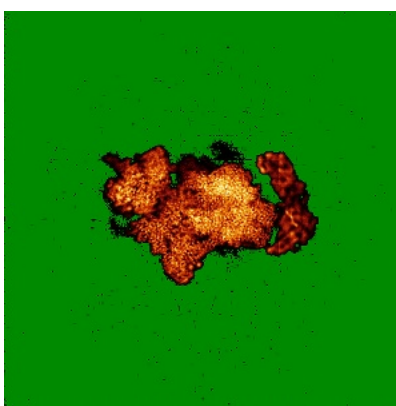
The images above show the largest variance slices of the map in three orthogonal directions.

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

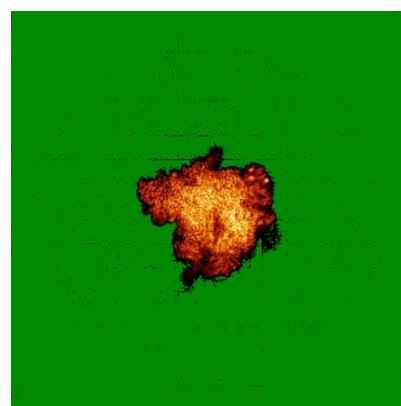
6.4.1 Primary map



X



Y

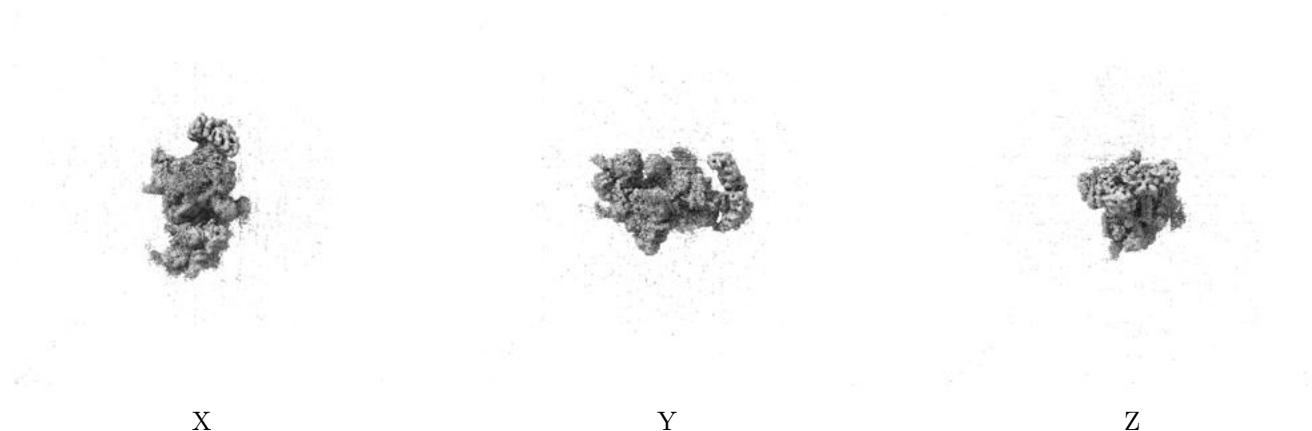


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

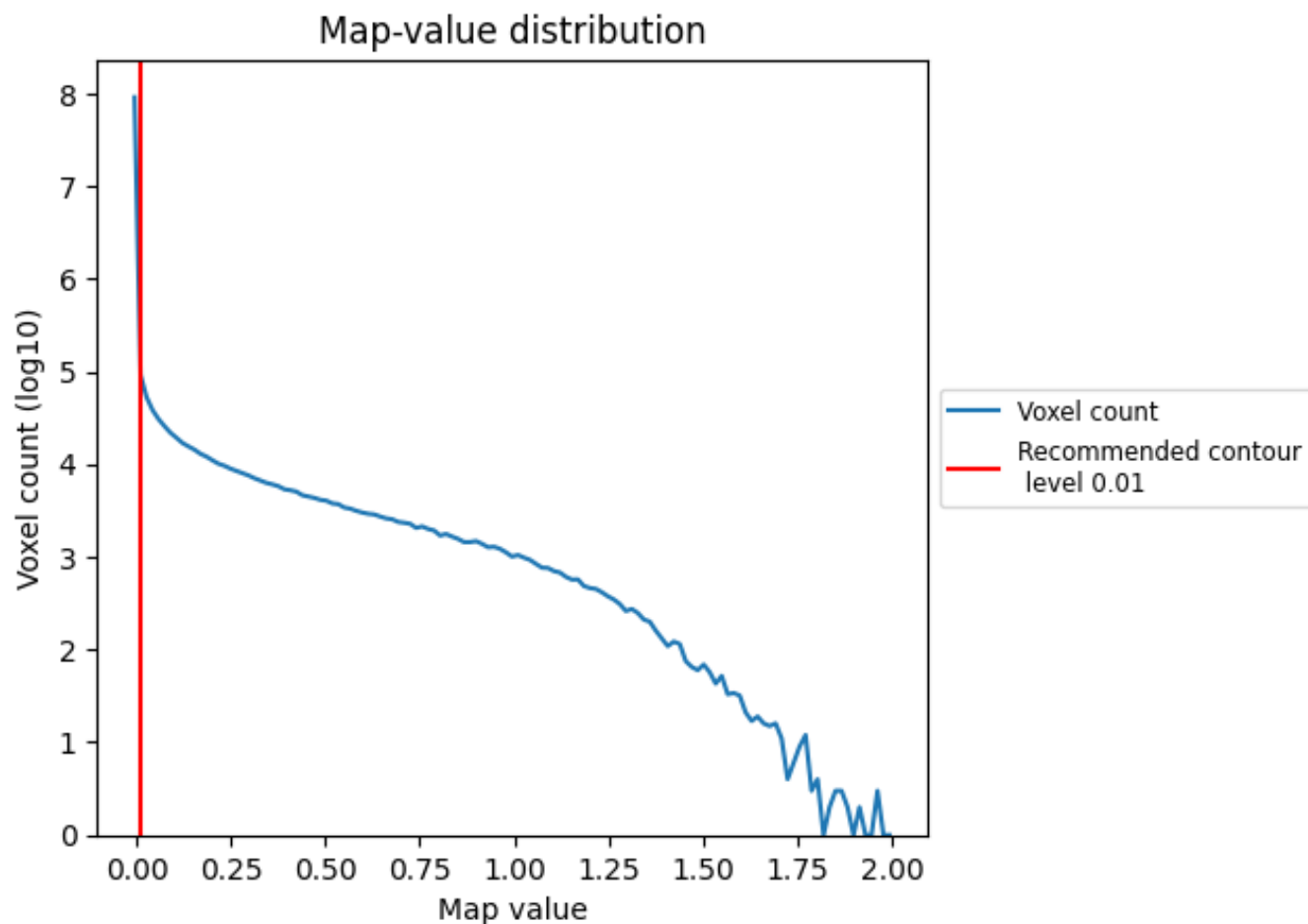
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

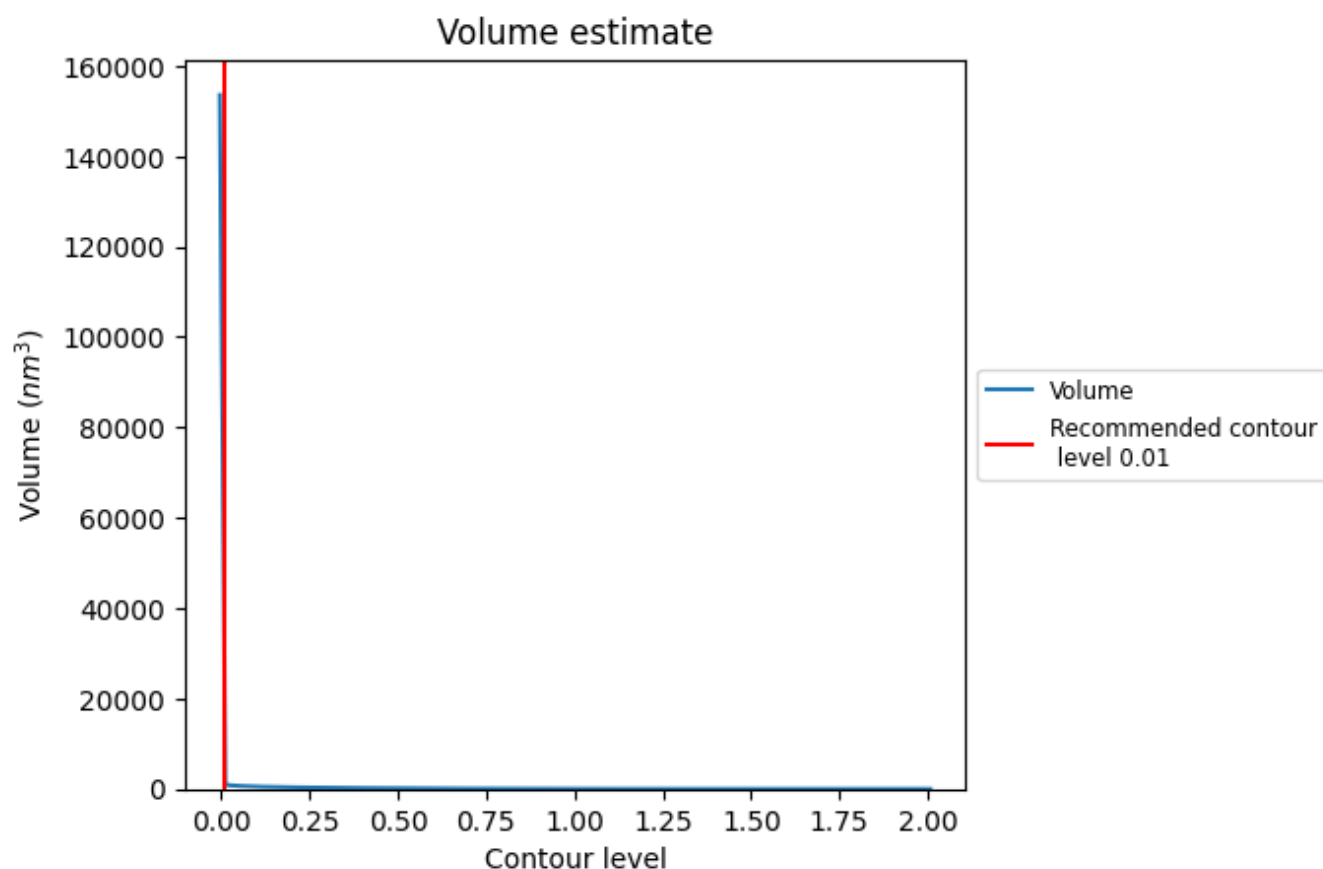
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

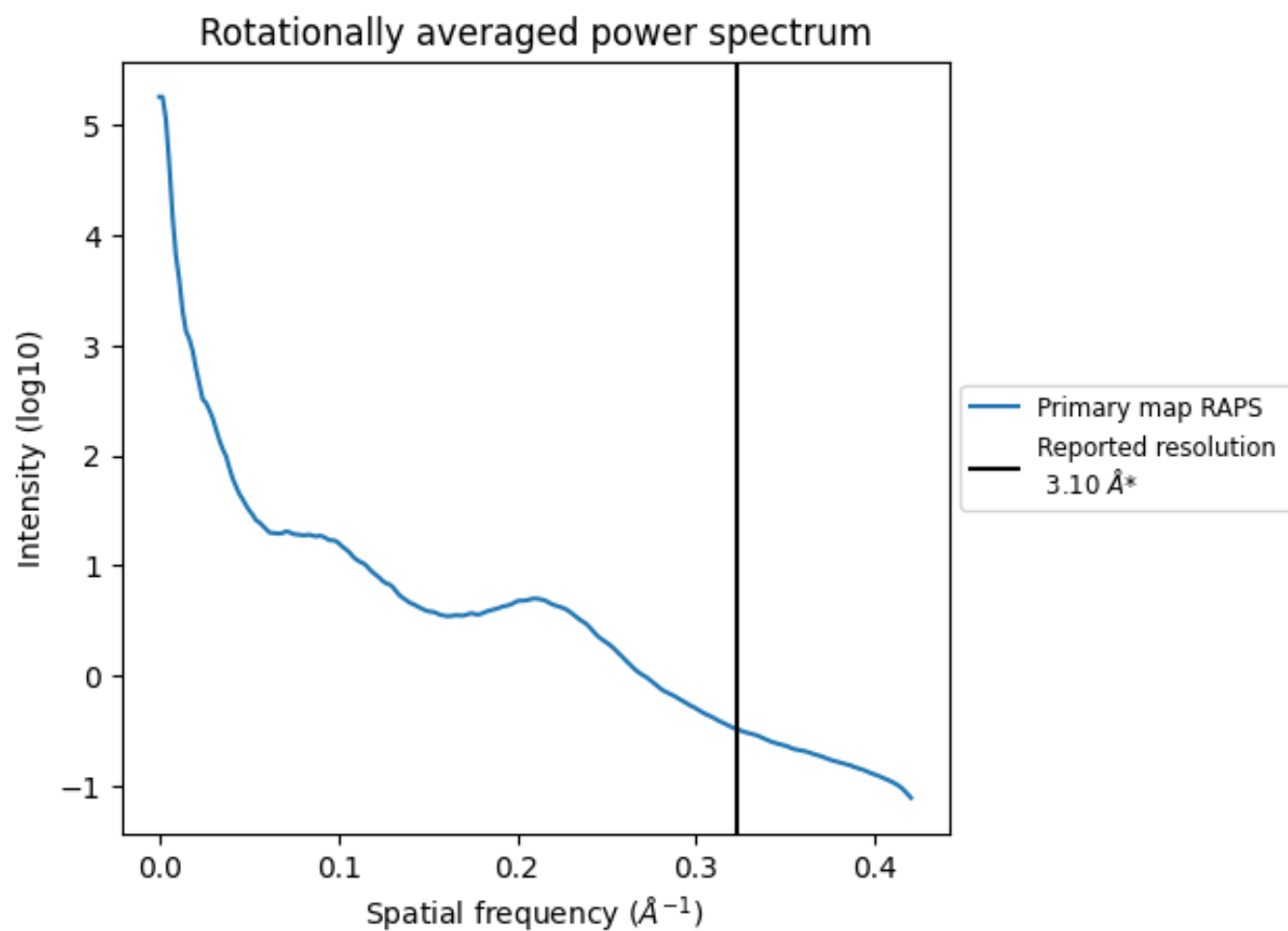
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 14275 nm^3 ; this corresponds to an approximate mass of 12895 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 0.323 Å⁻¹

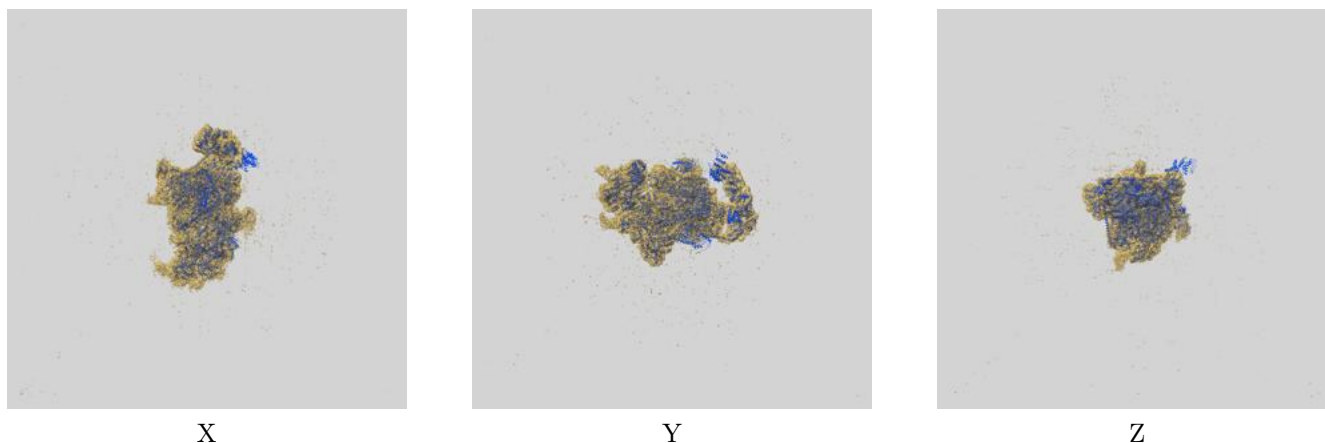
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

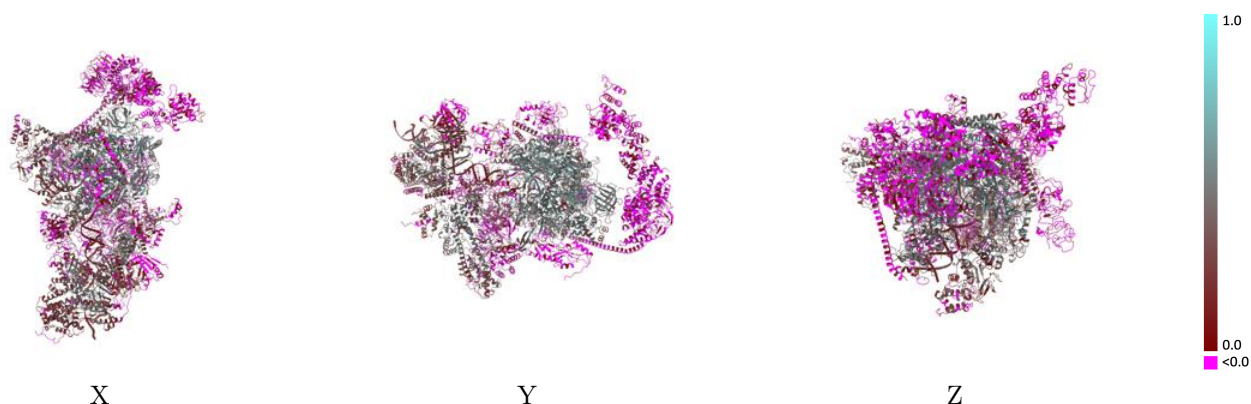
This section contains information regarding the fit between EMDB map EMD-48044 and PDB model 9EH2. Per-residue inclusion information can be found in section [3](#) on page [13](#).

9.1 Map-model overlay [i](#)



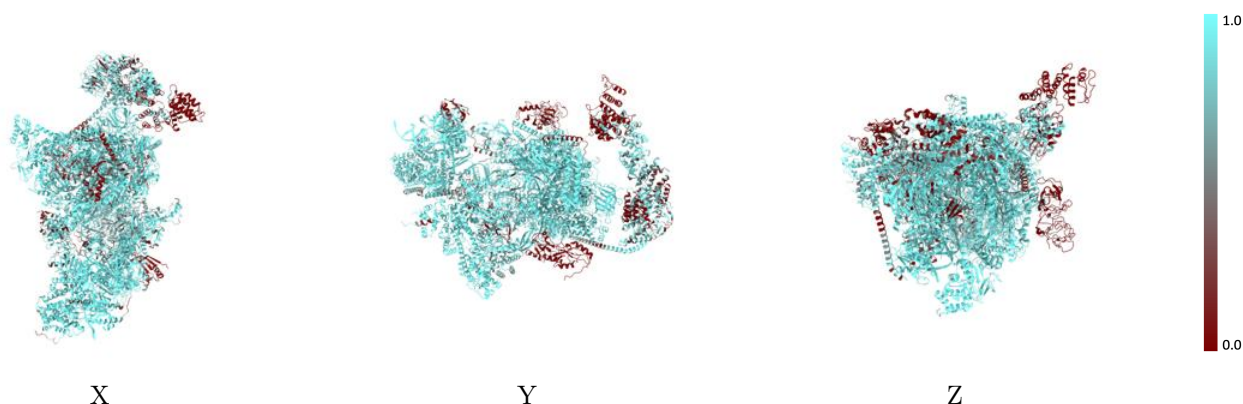
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



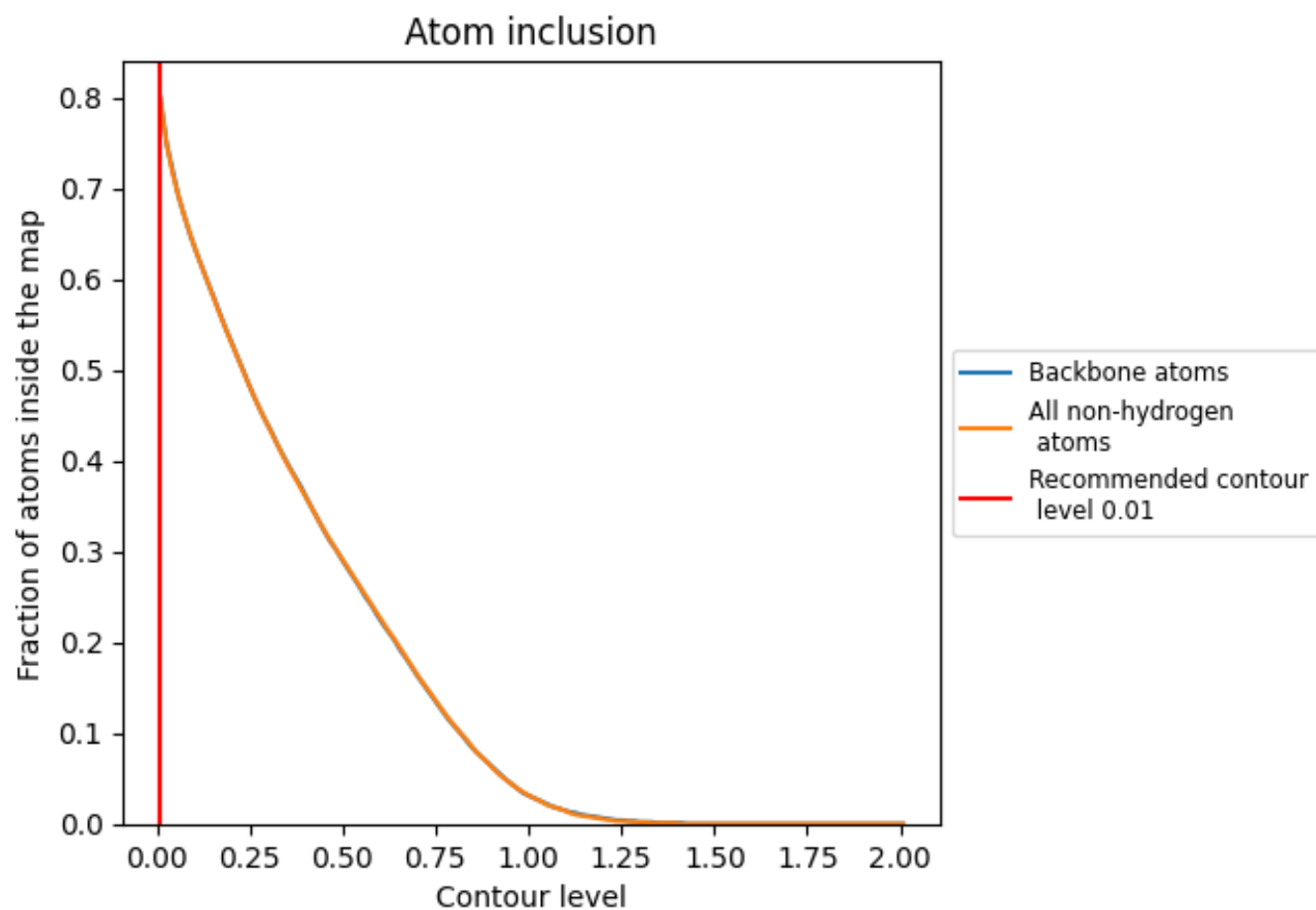
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.01).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 80% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7990	 0.2520
A	 0.9480	 0.4280
B	 0.9690	 0.4570
C	 0.9700	 0.4850
D	 0.7800	 0.0450
E	 0.9630	 0.3890
F	 0.9700	 0.4810
G	 0.8570	 0.1550
H	 0.9660	 0.4480
I	 0.9210	 0.3110
J	 0.9610	 0.4770
K	 0.9800	 0.4840
L	 0.9530	 0.3820
M	 0.8100	 0.2810
N	 0.9540	 0.2330
O	 0.3770	 -0.0500
P	 0.8970	 0.4270
Q	 0.5000	 -0.0160
R	 0.6270	 0.0260
S	 0.7320	 0.1500
T	 0.9550	 0.2770
U	 0.1730	 -0.0050
V	 0.2400	 -0.0400
W	 0.7210	 -0.0180
X	 0.3560	 -0.0690
Y	 0.7060	 -0.0260
Z	 0.5910	 0.0250
a	 0.9530	 0.3440
b	 0.9480	 0.3340
e	 0.9440	 0.3440
f	 0.9080	 0.2680
g	 0.9430	 0.2710
h	 0.9490	 0.2770
l	 0.6530	 0.1300
x	 0.8930	 0.2660
y	 0.8260	 0.2110

