



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 09:48 PM UTC

PDB ID : 8RDJ / pdb_00008rdj
EMDB ID : EMD-19023
Title : Plastid-encoded RNA polymerase transcription elongation complex (Integrated model)
Authors : Webster, M.W.; Pramanick, I.; Vergara-Cruces, A.
Deposited on : 2023-12-08
Resolution : 2.62 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
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

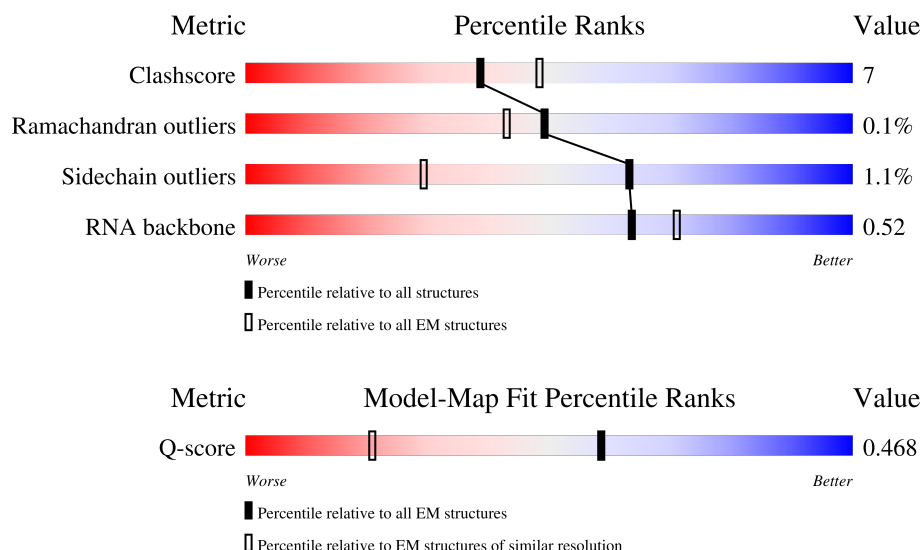
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.62 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	8810 (2.12 - 3.12)

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	327	 22% 80% 11% • 8%
1	B	327	 28% 77% 9% • 13%
2	C	1072	 22% 78% 18% • •

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Mol	Chain	Length	Quality of chain
3	D	680	
4	E	1373	
5	F	911	
6	G	862	
7	H	675	
8	I	263	
9	J	529	
10	K	460	
11	L	483	
12	M	334	
13	N	297	
14	O	185	
14	P	185	
15	Q	768	
16	R	162	
17	S	611	
18	T	140	
19	U	187	
20	X	81	
21	Y	81	
22	Z	40	

2 Entry composition

There are 27 unique types of molecules in this entry. The entry contains 70206 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	301	Total	C	N	O	S	0	0
			2449	1571	422	446	10		
1	B	283	Total	C	N	O	S	0	0
			2292	1461	395	425	11		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	67	PHE	SER	conflict	UNP A0A6C0M610
B	67	PHE	SER	conflict	UNP A0A6C0M610

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	1040	Total	C	N	O	S	0	0
			8287	5278	1462	1517	30		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	113	PHE	SER	conflict	UNP A0A6C0M5W1
C	657	VAL	ILE	conflict	UNP A0A6C0M5W1

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	611	Total	C	N	O	S	0	0
			4983	3200	880	876	27		

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit beta''.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	1091	Total	C	N	O	S	0	0
			8758	5612	1554	1561	31		

- Molecule 5 is a protein called PAP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	660	Total	C	N	O	S	0	0
			5307	3355	929	990	33		

- Molecule 6 is a protein called PAP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	748	Total	C	N	O	S	0	0
			5887	3723	994	1131	39		

- Molecule 7 is a protein called PAP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	549	Total	C	N	O	S	0	0
			4607	2937	799	854	17		

- Molecule 8 is a protein called PAP4.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	215	Total	C	N	O	S	0	0
			1771	1141	300	324	6		

- Molecule 9 is a protein called PAP5.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	234	Total	C	N	O	S	0	0
			1970	1247	350	363	10		

- Molecule 10 is a protein called PAP6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	384	Total	C	N	O	S	0	0
			3103	1985	520	583	15		

- Molecule 11 is a protein called PAP7.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	416	Total	C	N	O	S	0	0
			3403	2183	580	620	20		

- Molecule 12 is a protein called PAP8.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	215	Total	C	N	O	S	0	0
			1803	1142	312	341	8		

- Molecule 13 is a protein called PAP9.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	224	Total	C	N	O	S	0	0
			1819	1168	309	338	4		

- Molecule 14 is a protein called PAP10.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	114	Total	C	N	O	S	0	0
			923	588	148	178	9		
14	P	108	Total	C	N	O	S	0	0
			865	550	139	167	9		

- Molecule 15 is a protein called PAP11.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Q	539	Total	C	N	O	S	0	0
			4148	2584	706	833	25		

- Molecule 16 is a protein called PAP12.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	R	128	Total	C	N	O	S	0	0
			1069	672	193	201	3		

- Molecule 17 is a protein called FLN2.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	S	386	Total	C	N	O	S	0	0
			3056	1941	516	578	21		

- Molecule 18 is a protein called PTAC18.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	T	104	Total	C	N	O	S	0	0
			881	572	148	157	4		

- Molecule 19 is a protein called PRIN2.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	U	109	Total	C	N	O	S	0	0
			877	561	144	169	3		

- Molecule 20 is a DNA chain called DNA (81-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
20	X	31	Total	C	N	O	P	0	0
			638	304	122	182	30		

- Molecule 21 is a DNA chain called DNA (81-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Y	40	Total	C	N	O	P	0	0
			813	386	145	242	40		

- Molecule 22 is a RNA chain called RNA (40-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Z	10	Total	C	N	O	P	0	0
			215	95	40	70	10		

- Molecule 23 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
23	D	1	Total	Mg	0
			1	1	

- Molecule 24 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

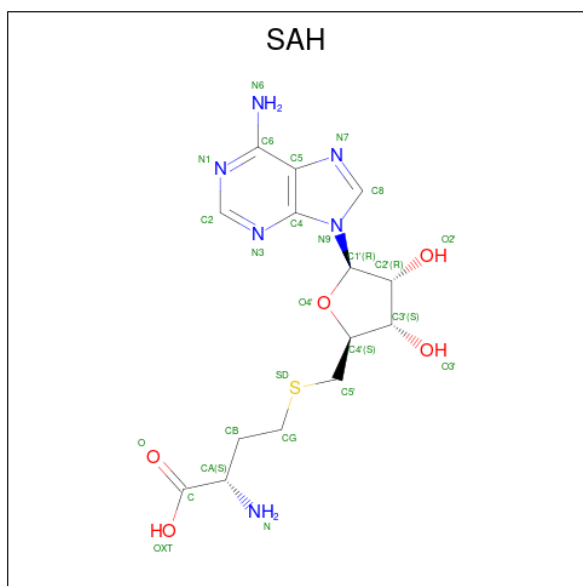
Mol	Chain	Residues	Atoms		AltConf
24	E	1	Total	Zn	0
			1	1	

- Molecule 25 is FE (III) ION (CCD ID: FE) (formula: Fe) (labeled as "Ligand of Interest"

by depositor).

Mol	Chain	Residues	Atoms		AltConf
25	I	1	Total	Fe	0
			1	1	
25	N	1	Total	Fe	0
			1	1	

- Molecule 26 is S-ADENOSYL-L-HOMOCYSTEINE (CCD ID: SAH) (formula: $C_{14}H_{20}N_6O_5S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
26	L	1	Total	C	N	O	S	0
			26	14	6	5	1	

- Molecule 27 is water.

Mol	Chain	Residues	Atoms		AltConf
27	A	17	Total	O	0
			17	17	
27	B	12	Total	O	0
			12	12	
27	C	54	Total	O	0
			54	54	
27	D	17	Total	O	0
			17	17	
27	E	24	Total	O	0
			24	24	

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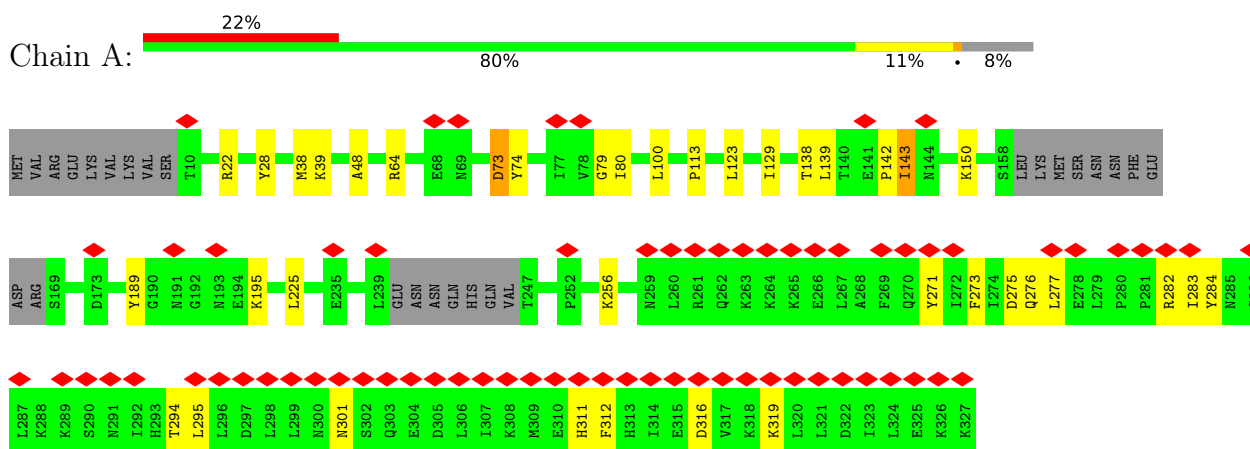
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Mol	Chain	Residues	Atoms		AltConf
27	F	2	Total 2	O 2	0
27	H	6	Total 6	O 6	0
27	I	3	Total 3	O 3	0
27	J	31	Total 31	O 31	0
27	K	17	Total 17	O 17	0
27	L	19	Total 19	O 19	0
27	M	16	Total 16	O 16	0
27	N	4	Total 4	O 4	0
27	O	2	Total 2	O 2	0
27	P	2	Total 2	O 2	0
27	R	3	Total 3	O 3	0
27	S	23	Total 23	O 23	0

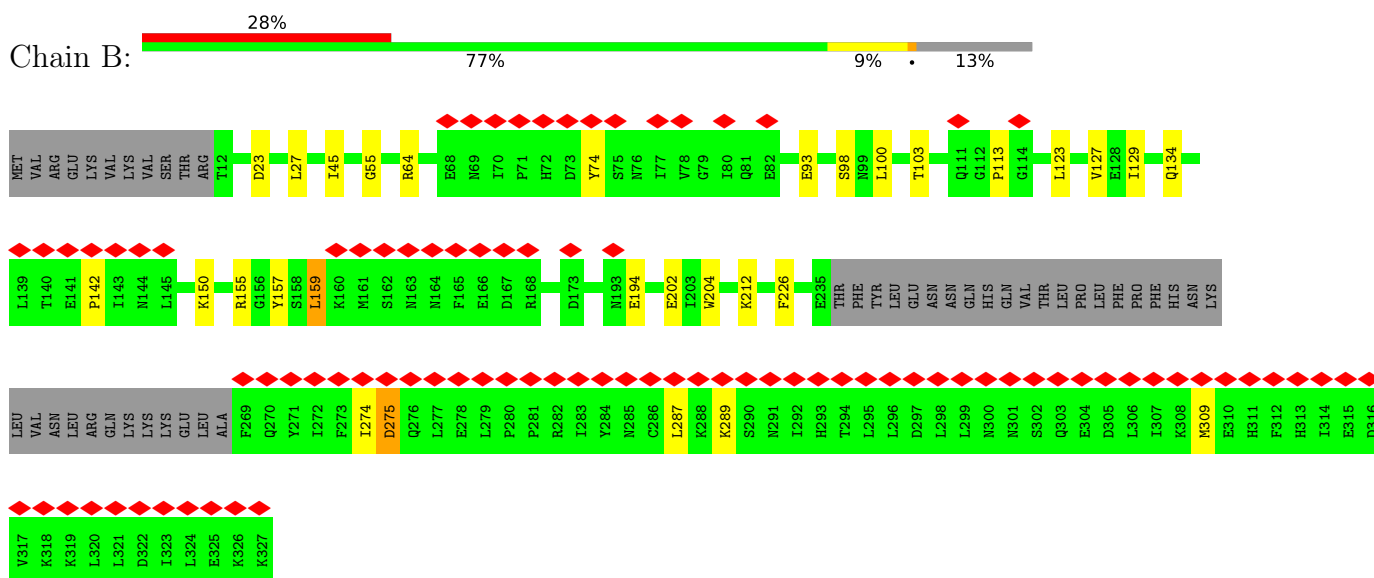
3 Residue-property plots

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.

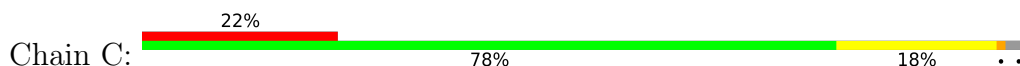
- Molecule 1: DNA-directed RNA polymerase subunit alpha

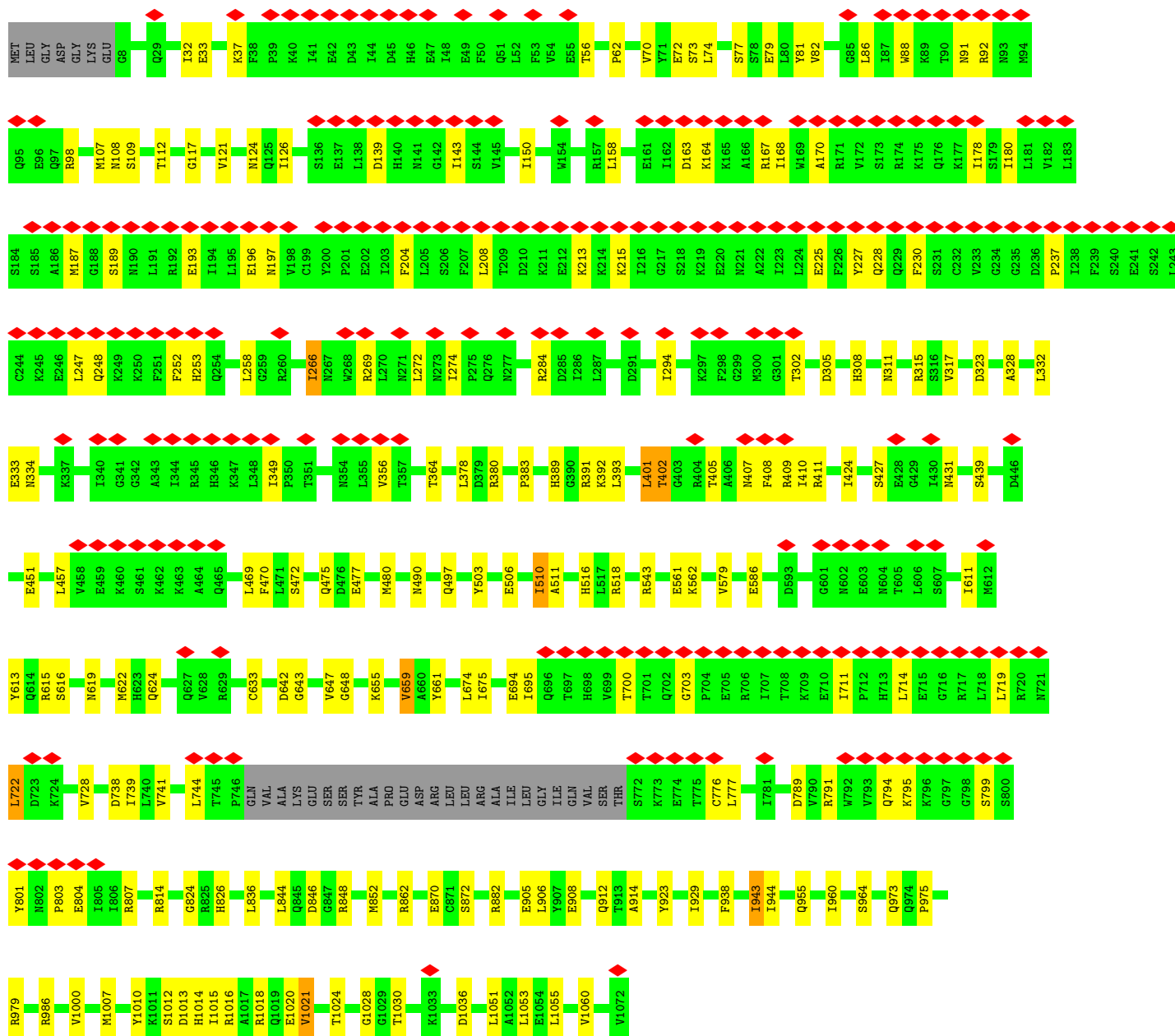


- Molecule 1: DNA-directed RNA polymerase subunit alpha

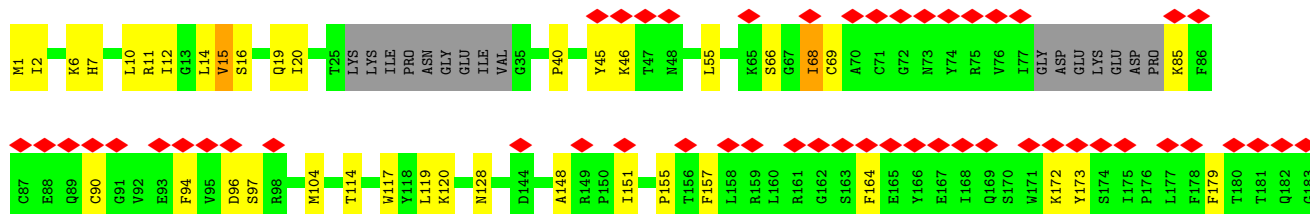


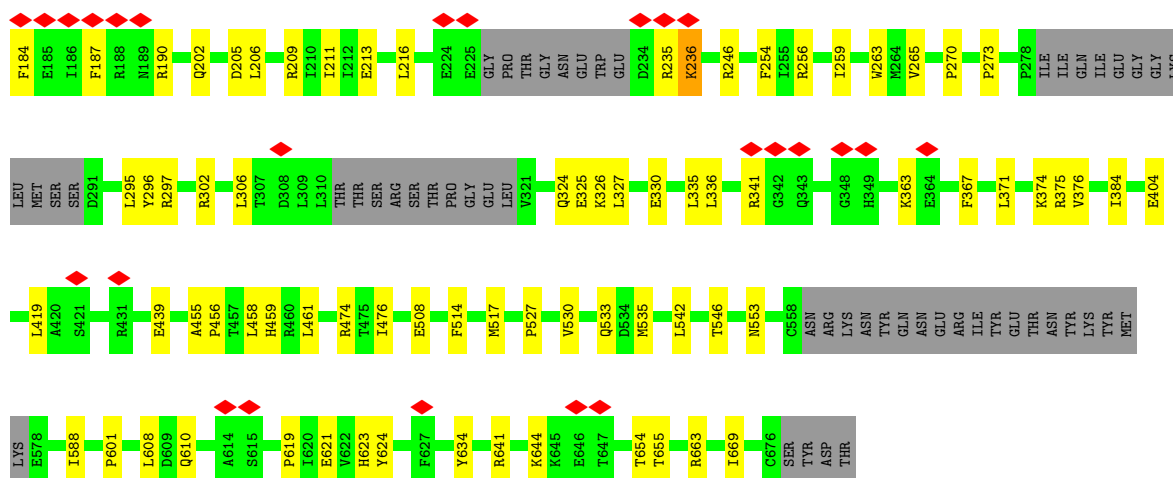
- Molecule 2: DNA-directed RNA polymerase subunit beta



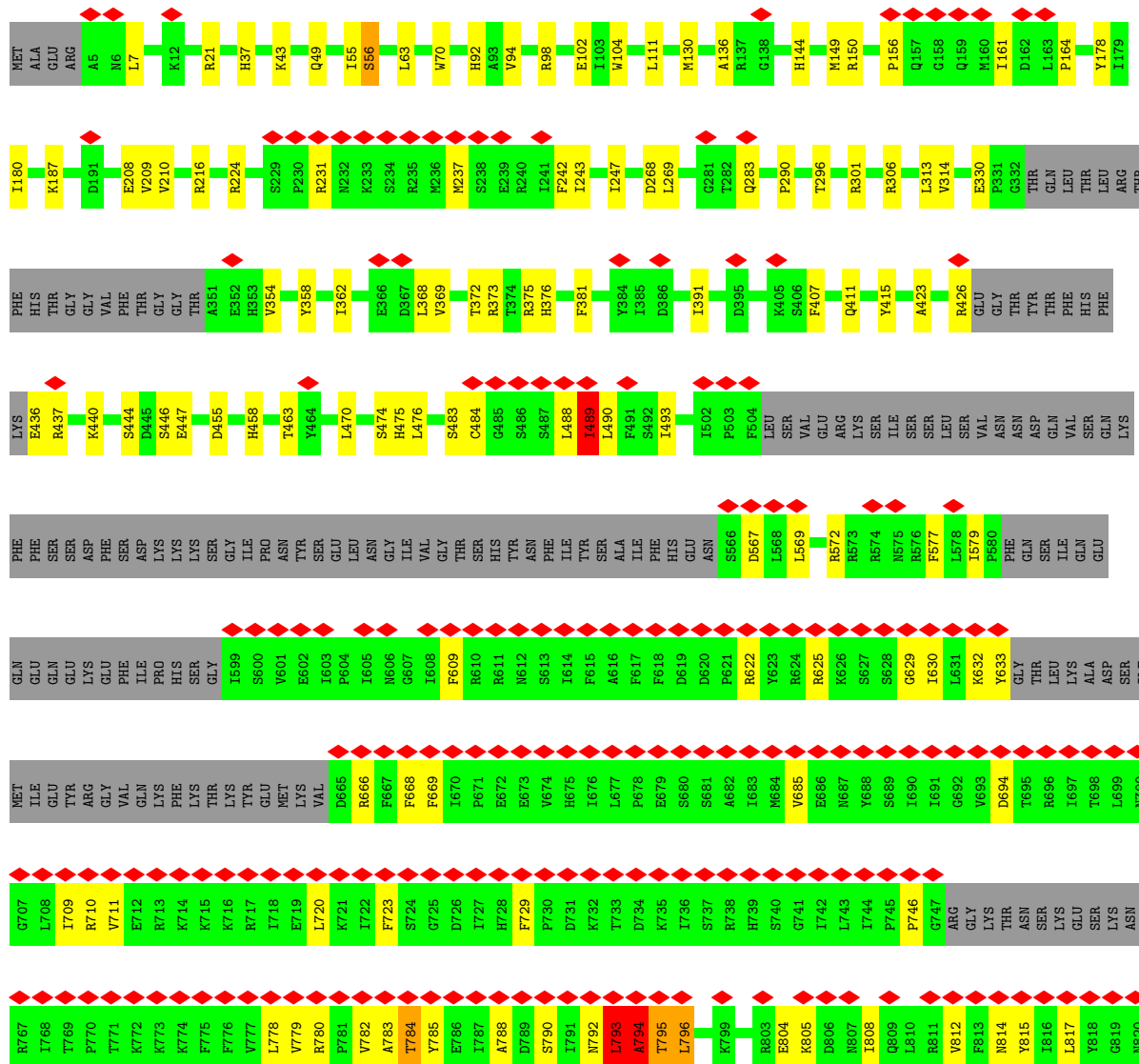


• Molecule 3: DNA-directed RNA polymerase subunit beta'



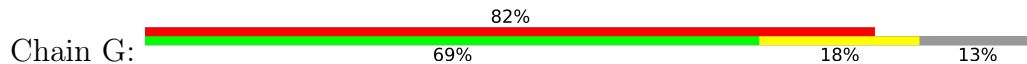


• Molecule 4: DNA-directed RNA polymerase subunit beta”



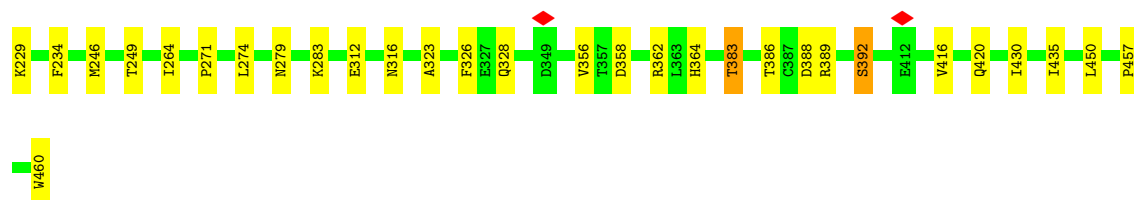
ASN	THR	L859	ASN	THR	L859
GLU	LEU	G860	GLU	LEU	G860
GLU	ASP	E861	ASP	ASP	E861
GLU	ASP	L862	ASP	ASP	L862
ALA	ALA	D863	ALA	ALA	D863
VAL	ASP	A864	ASP	ASP	A864
VAL	ASP	A865	ASP	ASP	A865
VAL	ASP	T866	ASP	ASP	T866
GLU	W740	A867	W740	W740	A867
PRO	E744	A868	E744	E744	A868
GLU	E747	A869	E747	E747	A869
ASN	A749	A870	A749	A749	A870
ARG	F749	D871	F749	F749	D871
ALA	ALA	D872	ALA	ALA	D872
GLU	GLY	E873	GLY	GLY	E873
GLY	M752	T874	M752	M752	T874
ASP	D762	G875	D762	D762	G875
LEU	Q788	G876	Q788	Q788	G876
ILE	PHE	L877	PHE	PHE	L877
LYS	L798	T878	L798	L798	T878
ASN	ASN	G879	ASN	ASN	G879
LYS	Y808	P880	Y808	Y808	P880
ALA	P809	D881	P809	P809	D881
ALA	ALA	Q882	ALA	ALA	Q882
ALA	ALA	T883	ALA	ALA	T883
ARG	V816	L818	V816	V816	L818
HIS	L817	R819	L817	L817	R819
LEU	L818	D885	L818	L818	D885
GLN	R819	K886	GLN	GLN	R819
ASP	A820	E887	ASP	ASP	A820
MET	ILE	S888	ILE	ILE	S888
ILE	A821	T888	A821	A821	T888
GLY	L822	G889	L822	L822	G889
VAL	R823	A890	R823	R823	A890
GLN	S828	R891	S828	S828	R891
LEU	L831	Q892	L831	L831	Q892
LYS	K832	S893	LYS	LYS	K832
GLU	L833	V894	GLU	GLU	L833
ASP	L834	E895	ASP	ASP	L834
GLU	Q835	ILE	GLU	GLU	Q835
ALA	ALA	PRO	ALA	ALA	PRO
ASN	ASN	LYS	ASN	ASN	LYS
ARG	ARG	THR	ARG	ARG	THR
THR	THR	LYS	THR	THR	LYS
LYS	LYS	GLY	LYS	LYS	GLY
ARG	ARG	GLU	ARG	ARG	GLU
GLY	GLY	HIS	GLY	GLY	HIS
LYS	LYS	GLU	LYS	LYS	GLU
ARG	ARG	PRO	ARG	ARG	PRO
ALA	ALA	VAL	ALA	ALA	VAL
ARG	ARG	LEU	ARG	ARG	LEU
MET	MET	GLY	MET	MET	GLY
		ASN			ASN

• Molecule 6: PAP2

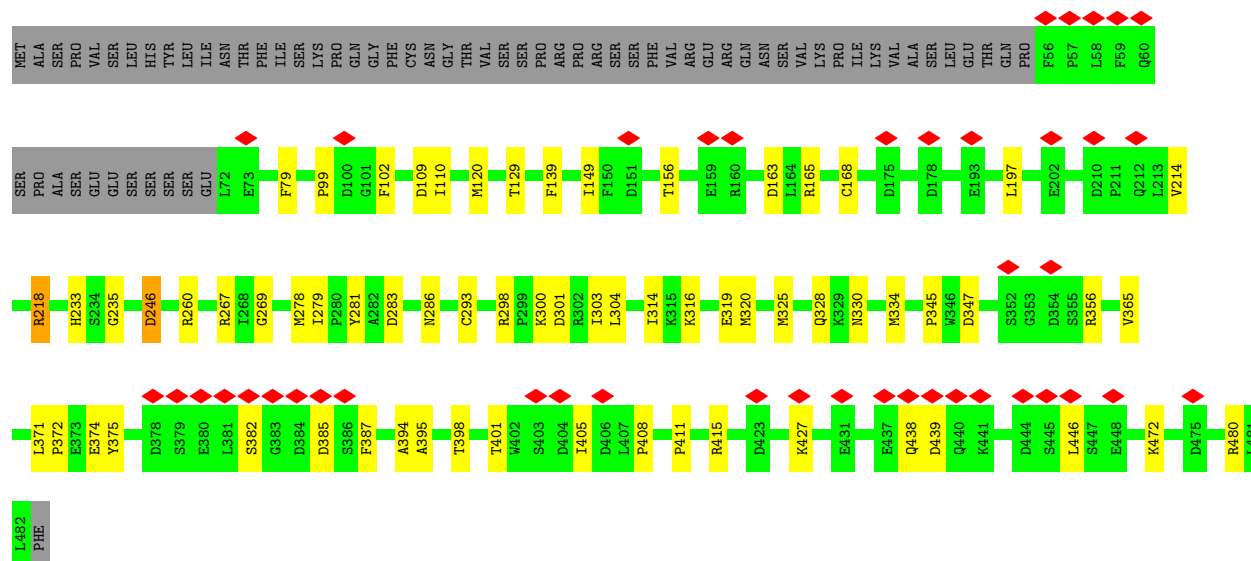


MET	PRO	R121	I181	I241	D301	G361	E421	G485	V545
ASN	SER	S122	N182	Q242	L302	Q362	T422	S486	K546
LEU	V63	L123	A183	P243	L303	R363	T423	M487	T547
ALA	S64	R124	Y184	D244	S304	G364	E424	P488	Y548
ILE	V65	L125	G185	I245	E305	R365	G425	S489	V549
ASN	E66	F126	R186	V246	M306	Y366	I426	D550	D550
PRO	K67	K127	N187	T247	A307	D367	I427	E491	M551
ASN	G68	Y128	G188	Y248	S308	D368	F428	T492	E552
SER	K69	Q130	R189	M249	G309	S369	A429	F493	K553
HIS	Y70	R131	Y190	T250	G310	R370	C430	H494	S554
GLU	S71	Q132	E191	L251	S311	Q371	G431	S495	R555
LEU	D73	Q133	T192	L252	L312	L372	K432	L496	C556
ILE	V74	W134	S193	S253	F313	F373	G433	L497	D557
GLY	E75	W135	L194	A254	D314	L374	A434	Y498	P558
ASN	E873	C135	E195	C255	I315	E375	L435	S499	D559
SER	T874	K136	L196	A256	T316	M376	H436	F500	E560
THR	L77	P137	L197	T257	S317	K377	E437	A501	R561
PHE	I78	N138	D198	R258	Y318	S378	D438	R502	T562
GLY	M79	E139	R199	G259	N319	S379	A439	G503	L563
ASN	K80	H140	K200	L260	V320	N380	R440	G504	E564
ARG	L81	I141	K201	G261	L321	T381	K441	F506	Y566
ALA	S82	Y142	E203	D262	L322	D382	L442	E508	L567
ALA	S83	T143	E203	E263	E323	F383	L443	E509	S568
ALA	L84	I144	K204	A264	A324	D384	Q444	E510	V570
SER	P85	M145	I205	E265	Y325	A385	Y445	V571	C572
ASN	P86	I146	S206	V267	K327	A386	M446	L512	L573
HIS	R87	S147	P207	D268	S328	S387	T447	S514	R574
LEU	G88	L148	S208	R269	G329	Y388	A448	L515	L575
SER	S89	L149	I209	L270	S330	N389	K449	L516	V576
LEU	T90	G150	L210	T271	I331	L391	D450	V517	D577
SER	A91	R151	T211	M271	K332	L392	V451	N518	E578
GLY	R92	E152	Y212	N272	E333	D393	P453	S519	C579
LYS	C93	G153	N213	D273	A334	V394	S454	E520	R580
PRO	L94	L154	T214	G274	K335	F395	S455	I521	E581
CYS	D95	L155	V215	G275	G336	G396	K456	P522	F583
SER	I96	D156	I216	D276	V337	E397	A457	R523	E584
VAL	F97	K157	N217	V277	F337	S398	T458	R524	E585
ALA	K98	C158	A218	P278	H339	G399	G460	R525	M586
LYS	N99	L159	C219	D279	Q340	Y400	V461	D526	K587
ASN	K100	E160	A220	L280	K341	F401	E462	F528	A588
ALA	L101	V161	R221	T281	Q342	K402	A463	N529	S589
THR	S102	F162	G222	D282	A343	E403	A464	D590	M600
LYS	L103	E163	G223	Y283	K344	V404	F465	T531	F541
ASP	N104	E164	L224	S284	A345	V405	G466	L532	L592
LEU	D105	M165	D225	H285	G346	T406	Q467	E533	P593
VAL	F106	P166	V226	L286	C347	L407	A468	A534	I595
SER	E107	S167	E227	V287	S347	F408	Y471	Y535	M596
SER	L108	Q168	G228	E288	H348	H409	E472	K536	Q537
GLU	V109	V170	L230	T289	A350	D410	A473	E537	Y598
SER	F110	A171	G231	P290	N351	M411	L475	G538	C599
ILE	E112	R172	L232	G291	T352	V412	V476	M601	L602
GLY	F113	S173	F233	L293	Y353	E413		S603	V604
GLY	A114	V174	F234	G294	S354	E414			
GLY	G115	F175	E235	R295	V355	M415			
GLY	R116	S176	W236	L296	V356	L416			
GLY	G117	Y177	R237	L297	L357	E417			
GLY	D118	T178	H238	K298	N358	F418			
GLY	W119	A179	E239	V299	L359	D419			
GLY	Q120	L180	G240	S300	F360	M420			

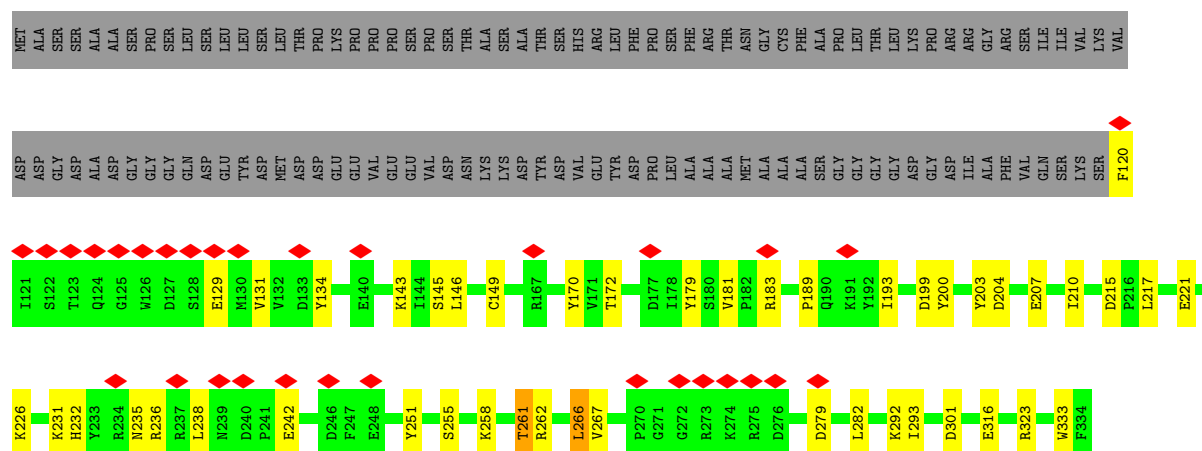




• Molecule 11: PAP7

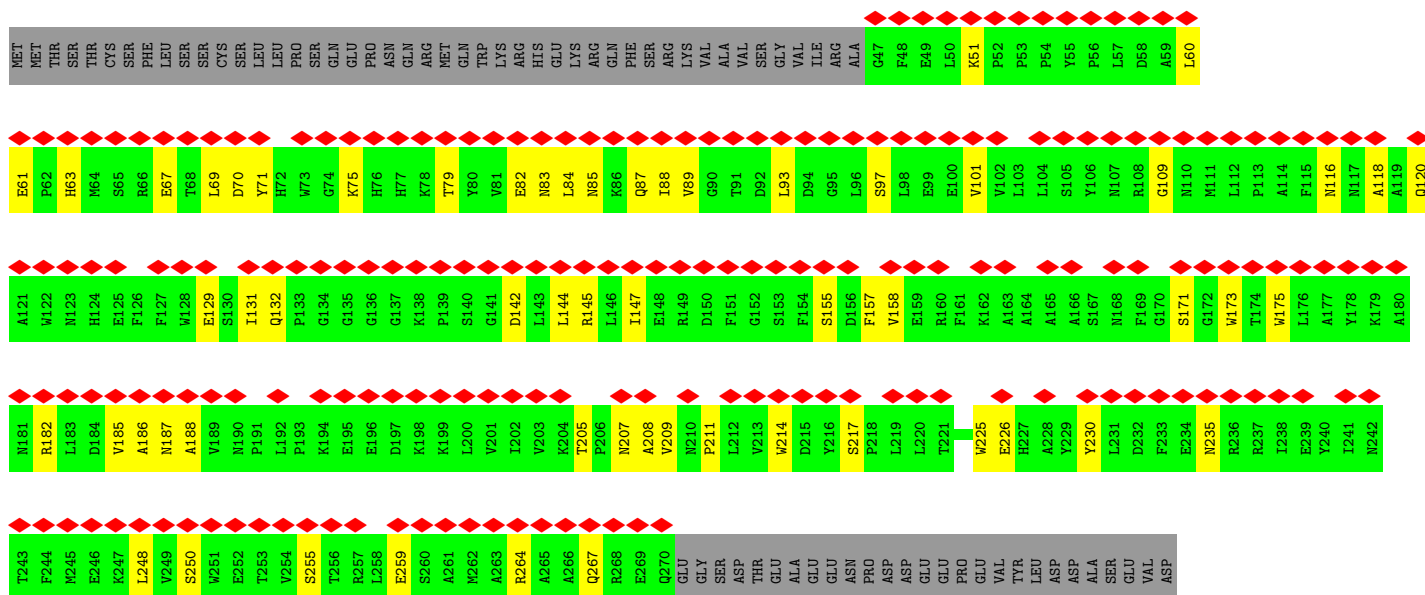


• Molecule 12: PAP8

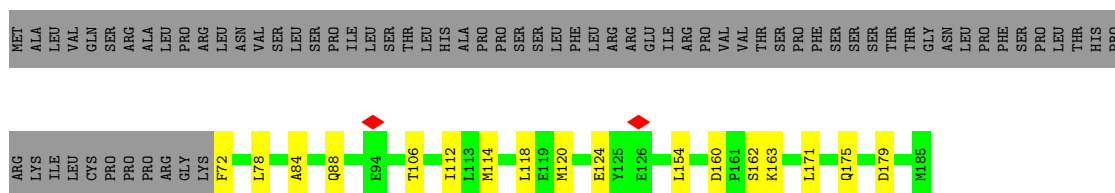


• Molecule 13: PAP9

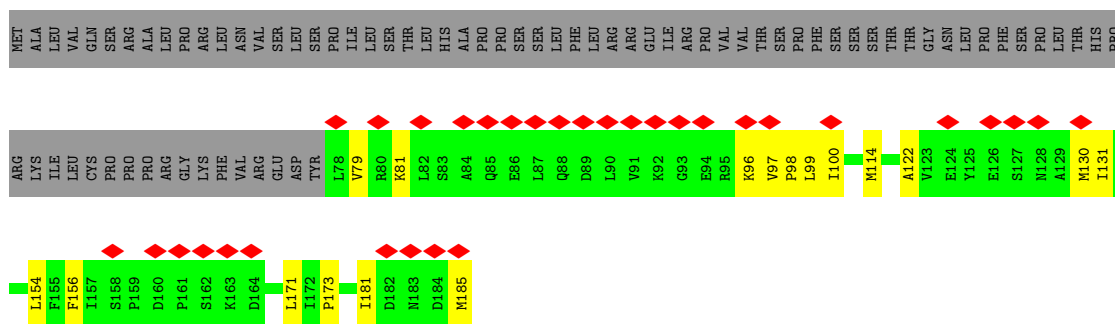




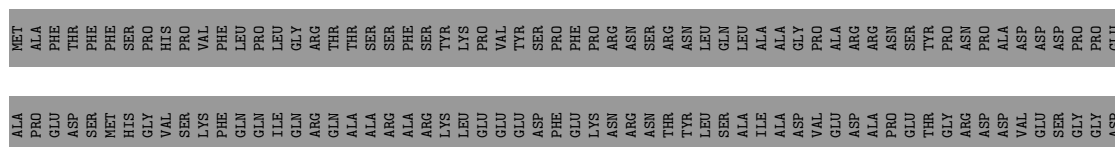
- Molecule 14: PAP10

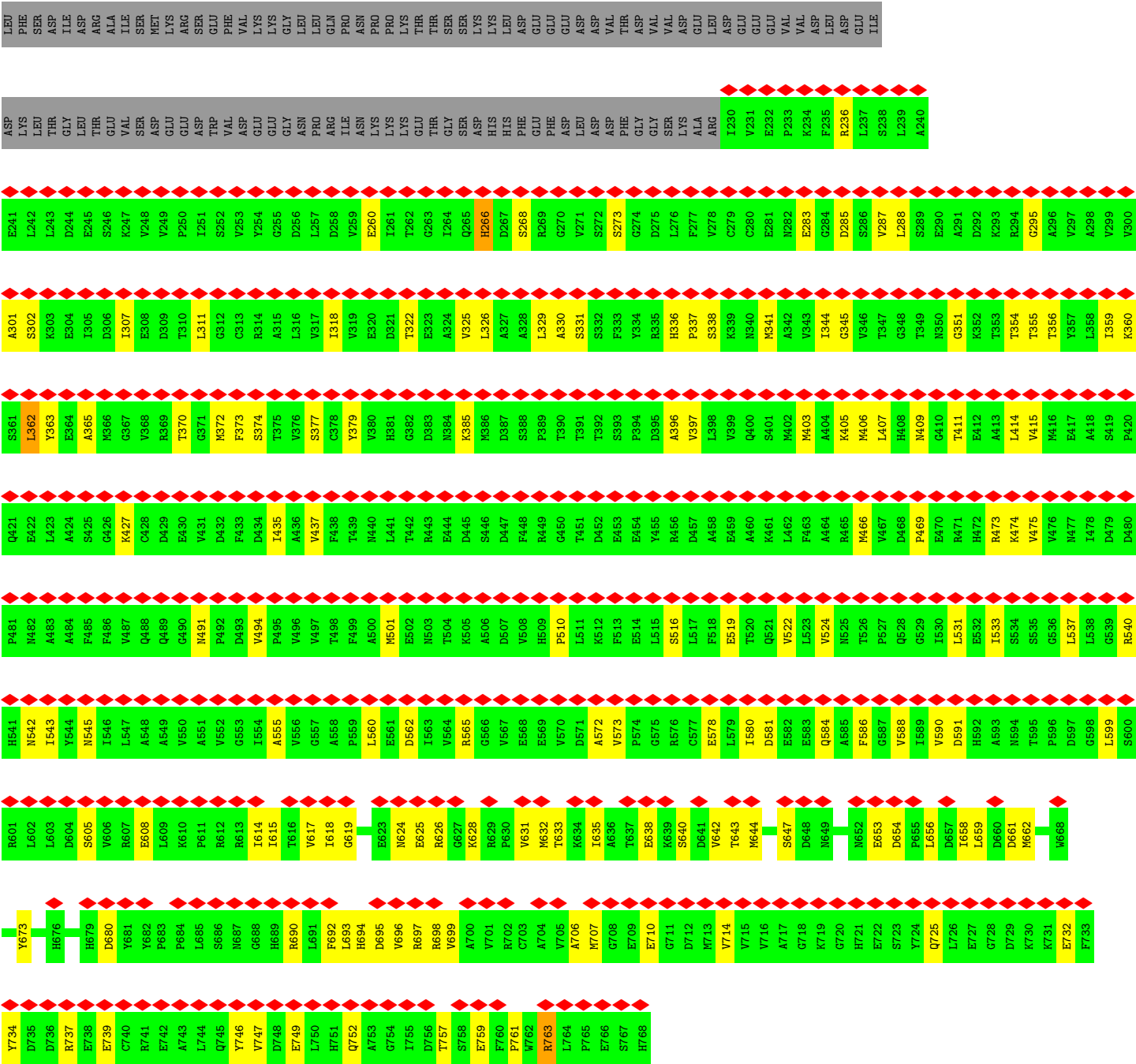


- Molecule 14: PAP10

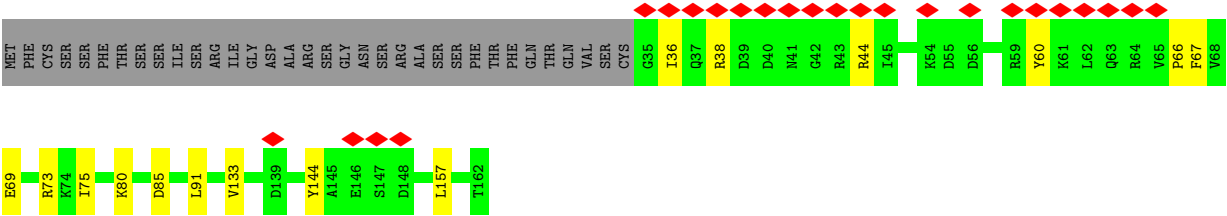


- Molecule 15: PAP11





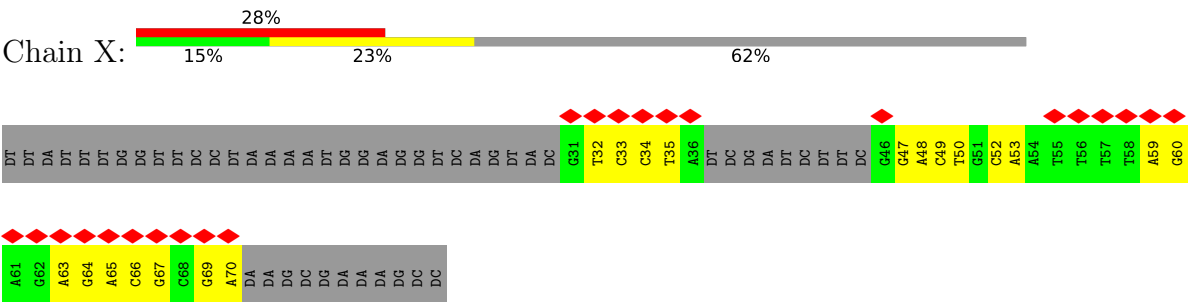
• Molecule 16: PAP12



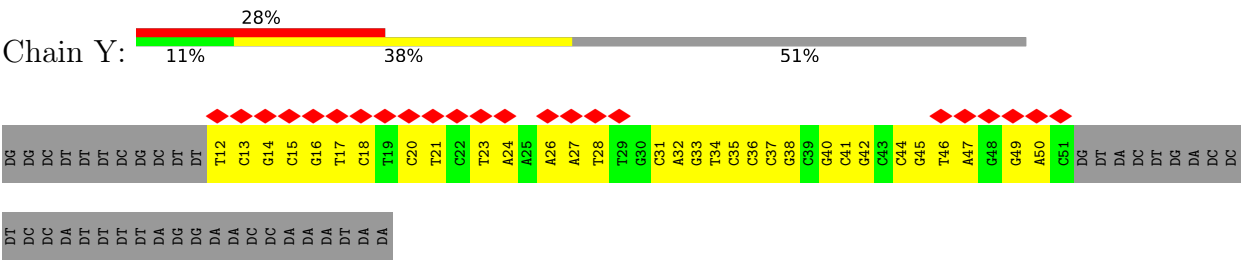
Chain S: 7% 56% 7% 37%



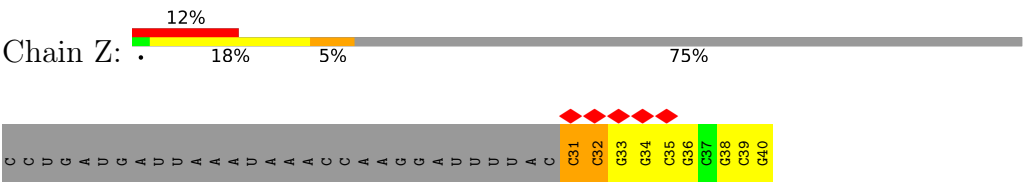
● Molecule 20: DNA (81-MER)



● Molecule 21: DNA (81-MER)



● Molecule 22: RNA (40-MER)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	417374	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40.48	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	5.127	Depositor
Minimum map value	-0.951	Depositor
Average map value	0.140	Depositor
Map value standard deviation	0.155	Depositor
Recommended contour level	0.8	Depositor
Map size (Å)	300.0, 300.0, 300.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.5, 0.5, 0.5	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.12	0/2498	0.25	0/3377
1	B	0.12	0/2336	0.28	0/3159
2	C	0.12	0/8458	0.26	0/11422
3	D	0.12	0/5093	0.26	0/6878
4	E	0.13	0/8932	0.27	1/12058 (0.0%)
5	F	0.11	0/5410	0.26	0/7306
6	G	0.08	0/5997	0.23	0/8096
7	H	0.10	0/4736	0.23	0/6386
8	I	0.09	0/1825	0.27	1/2481 (0.0%)
9	J	0.13	0/2021	0.25	0/2724
10	K	0.14	0/3184	0.27	0/4320
11	L	0.11	0/3492	0.23	0/4727
12	M	0.11	0/1848	0.23	0/2502
13	N	0.09	0/1873	0.26	0/2549
14	O	0.12	0/939	0.23	0/1268
14	P	0.10	0/879	0.22	0/1187
15	Q	0.11	0/4218	0.27	0/5720
16	R	0.12	0/1089	0.25	0/1462
17	S	0.11	0/3123	0.25	0/4226
18	T	0.10	0/906	0.29	0/1225
19	U	0.08	0/900	0.21	0/1219
20	X	0.16	0/716	0.34	0/1102
21	Y	0.18	0/909	0.37	0/1399
22	Z	0.12	0/239	0.31	0/371
All	All	0.11	0/71621	0.26	2/97164 (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
4	E	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	794	ALA	N-CA-C	-7.86	103.69	112.57
8	I	195	ASN	CB-CA-C	-5.31	110.47	116.63

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	E	1182	ILE	Peptide
4	E	794	ALA	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2449	0	2490	26	0
1	B	2292	0	2311	25	0
2	C	8287	0	8381	126	0
3	D	4983	0	5052	92	0
4	E	8758	0	8895	160	0
5	F	5307	0	5267	81	0
6	G	5887	0	5803	106	0
7	H	4607	0	4464	87	0
8	I	1771	0	1696	39	0
9	J	1970	0	1923	25	0
10	K	3103	0	3026	30	0
11	L	3403	0	3348	42	0
12	M	1803	0	1756	29	0
13	N	1819	0	1746	40	0
14	O	923	0	917	13	0
14	P	865	0	867	14	0
15	Q	4148	0	4046	101	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	R	1069	0	1058	16	0
17	S	3056	0	3042	31	0
18	T	881	0	860	18	0
19	U	877	0	840	12	0
20	X	638	0	351	26	0
21	Y	813	0	450	33	0
22	Z	215	0	111	10	0
23	D	1	0	0	0	0
24	E	1	0	0	0	0
25	I	1	0	0	0	0
25	N	1	0	0	0	0
26	L	26	0	19	1	0
27	A	17	0	0	0	0
27	B	12	0	0	0	0
27	C	54	0	0	1	0
27	D	17	0	0	1	0
27	E	24	0	0	1	0
27	F	2	0	0	0	0
27	H	6	0	0	0	0
27	I	3	0	0	1	0
27	J	31	0	0	1	0
27	K	17	0	0	0	0
27	L	19	0	0	0	0
27	M	16	0	0	0	0
27	N	4	0	0	0	0
27	O	2	0	0	0	0
27	P	2	0	0	0	0
27	R	3	0	0	0	0
27	S	23	0	0	3	0
All	All	70206	0	68719	1009	0

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

All (1009) 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)
5:F:565:GLN:NE2	20:X:65:DA:OP1	1.65	1.27
4:E:729:PHE:HE1	19:U:147:ILE:HD11	1.42	0.84
3:D:45:TYR:CG	20:X:34:DC:H3'	2.15	0.82
21:Y:45:DG:H1	22:Z:32:C:H42	1.29	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:45:TYR:HD1	20:X:34:DC:H5'	1.45	0.81
4:E:567:ASP:HB3	4:E:795:THR:C	2.07	0.79
4:E:729:PHE:CE1	19:U:147:ILE:CD1	2.67	0.78
4:E:790:SER:HB2	7:H:607:ALA:HA	1.66	0.77
15:Q:531:LEU:HD21	15:Q:560:LEU:HB3	1.66	0.76
1:B:202:GLU:OE2	16:R:73:ARG:NH2	2.22	0.73
5:F:131:LYS:NZ	6:G:472:GLU:OE1	2.21	0.73
4:E:729:PHE:CE1	19:U:147:ILE:HD11	2.24	0.73
8:I:119:ASN:OD1	27:I:8101:HOH:O	2.06	0.73
3:D:302:ARG:HD3	3:D:327:LEU:HB3	1.71	0.72
3:D:45:TYR:CD1	20:X:34:DC:H3'	2.24	0.72
7:H:519:ARG:NH1	7:H:522:GLU:OE2	2.23	0.72
11:L:99:PRO:HB2	16:R:44:ARG:NH1	2.03	0.72
11:L:446:LEU:O	16:R:38:ARG:NH1	2.23	0.72
5:F:413:VAL:HG21	5:F:809:PRO:HB3	1.72	0.72
1:A:195:LYS:HG3	1:B:159:LEU:HD13	1.71	0.71
4:E:792:ASN:O	4:E:794:ALA:N	2.22	0.71
4:E:792:ASN:C	4:E:794:ALA:H	1.97	0.71
9:J:251:ARG:NH1	9:J:276:PRO:O	2.23	0.71
13:N:182:ARG:NH1	13:N:188:ALA:O	2.23	0.71
6:G:359:LEU:O	6:G:363:ASN:ND2	2.23	0.71
3:D:45:TYR:CD1	20:X:34:DC:H5'	2.25	0.71
15:Q:647:SER:O	15:Q:697:ARG:NH1	2.24	0.70
3:D:179:PHE:HA	15:Q:698:ARG:HH12	1.55	0.70
4:E:793:LEU:HD12	7:H:604:TYR:CE1	2.27	0.70
4:E:455:ASP:HB2	4:E:474:SER:HB2	1.74	0.69
15:Q:510:PRO:HA	15:Q:524:VAL:HA	1.74	0.69
3:D:46:LYS:HD3	20:X:34:DC:OP1	1.93	0.69
15:Q:268:SER:HB3	15:Q:287:VAL:HG13	1.73	0.69
8:I:77:LYS:HB3	13:N:235:ASN:HD21	1.56	0.68
4:E:1006:TYR:CB	8:I:247:ALA:HB2	2.24	0.68
15:Q:759:GLU:OE2	15:Q:763:ARG:NH2	2.27	0.68
21:Y:15:DC:H2''	21:Y:16:DG:C8	2.28	0.68
4:E:208:GLU:OE1	4:E:1313:LYS:NZ	2.22	0.68
2:C:92:ARG:HH12	4:E:817:LEU:HB3	1.58	0.68
2:C:305:ASP:O	2:C:311:ASN:ND2	2.27	0.68
17:S:481:THR:HG22	17:S:483:PHE:H	1.58	0.68
21:Y:20:DC:H2''	21:Y:21:DT:H5'	1.75	0.68
3:D:455:ALA:HB1	21:Y:38:DG:H1'	1.75	0.67
4:E:1182:ILE:O	4:E:1184:TRP:N	2.27	0.67
4:E:1096:ARG:HH21	7:H:283:THR:HG22	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:272:LEU:HB3	2:C:274:ILE:HD13	1.77	0.67
1:A:39:LYS:O	1:B:155:ARG:NH2	2.27	0.66
2:C:960:ILE:HG21	3:D:474:ARG:HD3	1.77	0.66
3:D:45:TYR:HB2	20:X:34:DC:H5"	1.78	0.66
6:G:341:MET:HE1	6:G:348:PRO:HG3	1.77	0.66
7:H:433:LEU:HB3	7:H:474:LEU:HD13	1.78	0.66
19:U:99:ARG:HA	19:U:102:MET:HE3	1.77	0.65
4:E:761:ASN:HA	4:E:784:THR:HG21	1.79	0.65
2:C:228:GLN:HE21	2:C:237:PRO:HD2	1.61	0.65
4:E:209:VAL:HG13	4:E:210:VAL:HG13	1.78	0.65
6:G:265:GLU:HG3	6:G:302:LEU:HD21	1.79	0.65
20:X:70:DA:N1	21:Y:12:DT:O4	2.30	0.65
18:T:50:GLU:HB3	18:T:111:LEU:HB3	1.79	0.65
3:D:179:PHE:CA	15:Q:698:ARG:HH12	2.10	0.64
4:E:415:TYR:HB2	9:J:227:THR:HG21	1.79	0.64
1:B:289:LYS:HE2	10:K:88:ASP:HB3	1.79	0.64
2:C:112:THR:HG21	2:C:378:LEU:HD22	1.79	0.64
4:E:778:LEU:HD13	4:E:780:ARG:HE	1.63	0.64
15:Q:696:VAL:HG22	15:Q:698:ARG:H	1.62	0.64
1:B:123:LEU:HD11	1:B:129:ILE:HG13	1.78	0.64
2:C:163:ASP:OD1	2:C:167:ARG:N	2.30	0.64
4:E:290:PRO:O	4:E:1226:ARG:NH1	2.31	0.64
15:Q:331:SER:HG	15:Q:336:HIS:HD1	1.45	0.64
15:Q:372:MET:HB2	15:Q:379:TYR:H	1.63	0.64
15:Q:617:VAL:HG22	15:Q:644:MET:HB2	1.80	0.64
17:S:291:ARG:NH2	17:S:339:GLU:OE1	2.30	0.64
10:K:388:ASP:HB2	10:K:435:ILE:HD13	1.78	0.64
8:I:77:LYS:HB3	13:N:235:ASN:ND2	2.13	0.63
4:E:567:ASP:HB3	4:E:795:THR:HA	1.80	0.63
5:F:819:ARG:HH22	5:F:848:LEU:HD11	1.63	0.63
13:N:93:LEU:HD11	13:N:101:VAL:HG13	1.79	0.63
3:D:236:LYS:NZ	21:Y:24:DA:OP2	2.32	0.63
15:Q:642:VAL:HG22	15:Q:690:ARG:HB2	1.81	0.63
5:F:138:ARG:NH2	5:F:170:LEU:O	2.31	0.62
6:G:377:LYS:NZ	6:G:410:ASP:OD2	2.31	0.62
5:F:832:LYS:HA	5:F:835:GLN:HE21	1.63	0.62
3:D:157:PHE:HD2	15:Q:694:HIS:HE2	1.45	0.62
4:E:358:TYR:HD1	12:M:323:ARG:HE	1.47	0.62
21:Y:45:DG:H1	22:Z:32:C:N4	1.97	0.62
2:C:738:ASP:OD1	2:C:739:ILE:N	2.32	0.62
11:L:279:ILE:HD13	11:L:304:LEU:HD22	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:P:96:LYS:H	14:P:96:LYS:HD3	1.63	0.62
15:Q:360:LYS:NZ	15:Q:370:THR:O	2.31	0.62
1:A:123:LEU:HD11	1:A:129:ILE:HG12	1.81	0.62
4:E:224:ARG:NH2	5:F:762:ASP:OD2	2.32	0.62
15:Q:405:LYS:O	15:Q:409:ASN:ND2	2.32	0.62
4:E:437:ARG:HH21	4:E:1133:ILE:HG21	1.64	0.62
2:C:586:GLU:HG3	14:O:78:LEU:HD11	1.81	0.62
18:T:80:TRP:O	18:T:117:TRP:N	2.33	0.62
15:Q:344:ILE:HB	15:Q:415:VAL:HG22	1.82	0.61
2:C:480:MET:H	2:C:516:HIS:HD2	1.48	0.61
1:A:73:ASP:OD1	1:A:73:ASP:N	2.33	0.61
2:C:659:VAL:HG22	2:C:852:MET:HB2	1.82	0.61
10:K:88:ASP:OD1	10:K:88:ASP:N	2.32	0.61
3:D:259:ILE:O	5:F:455:LYS:NZ	2.26	0.61
3:D:206:LEU:HD22	3:D:211:ILE:HD11	1.83	0.61
6:G:503:GLY:HA2	6:G:715:ARG:HG2	1.81	0.61
13:N:217:SER:OG	13:N:264:ARG:NH2	2.32	0.61
4:E:63:LEU:HD11	9:J:285:ARG:HD2	1.82	0.61
2:C:794:GLN:HG3	2:C:804:GLU:HG2	1.82	0.61
5:F:225:ASP:OD2	5:F:228:ASN:ND2	2.34	0.60
14:P:99:LEU:HD13	14:P:130:MET:HE3	1.83	0.60
3:D:439:GLU:HG2	16:R:157:LEU:HD21	1.83	0.60
10:K:323:ALA:HB1	10:K:328:GLN:HB3	1.83	0.60
15:Q:283:GLU:HB3	15:Q:287:VAL:HG21	1.83	0.60
17:S:284:ASN:ND2	17:S:290:THR:OG1	2.35	0.60
19:U:102:MET:HE1	19:U:120:VAL:HG13	1.83	0.60
20:X:34:DC:H2''	20:X:35:DT:H5'	1.83	0.60
2:C:139:ASP:OD1	2:C:143:ILE:N	2.34	0.60
4:E:685:VAL:HG21	4:E:709:ILE:HG13	1.84	0.60
15:Q:615:ILE:HB	15:Q:714:VAL:HG12	1.84	0.60
16:R:75:ILE:HG23	16:R:80:LYS:HB2	1.83	0.60
7:H:188:GLU:HB3	7:H:221:ARG:HE	1.67	0.60
5:F:218:GLU:HG2	5:F:222:LYS:HE2	1.84	0.60
12:M:172:THR:HG22	12:M:179:TYR:HA	1.83	0.60
5:F:389:ASP:OD1	5:F:392:ARG:NH2	2.35	0.60
7:H:81:TRP:O	7:H:308:ASN:ND2	2.35	0.60
7:H:436:LEU:O	7:H:470:LYS:NZ	2.35	0.60
7:H:73:ARG:NH2	8:I:257:GLU:OE1	2.35	0.59
5:F:66:LEU:HD21	6:G:793:MET:CE	2.33	0.59
5:F:83:ARG:NH1	11:L:408:PRO:O	2.36	0.59
20:X:49:DC:H2'	20:X:50:DT:H71	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:624:TYR:HB3	12:M:282:LEU:HB3	1.84	0.59
15:Q:356:THR:HG23	15:Q:415:VAL:HB	1.83	0.59
15:Q:379:TYR:OH	15:Q:385:LYS:NZ	2.35	0.59
15:Q:537:LEU:HD13	15:Q:542:ASN:HB3	1.84	0.59
21:Y:33:DG:H2'	21:Y:34:DT:H71	1.84	0.59
21:Y:31:DC:H2''	21:Y:32:DA:H5'	1.83	0.59
2:C:694:GLU:HG2	2:C:807:ARG:HG2	1.84	0.59
8:I:180:VAL:HG11	8:I:199:PRO:HG2	1.85	0.59
15:Q:466:MET:HG3	15:Q:494:VAL:HG21	1.83	0.59
1:A:113:PRO:HD3	1:A:142:PRO:HG3	1.85	0.59
11:L:99:PRO:HB2	16:R:44:ARG:HH12	1.65	0.59
15:Q:325:VAL:HG12	15:Q:329:LEU:HG	1.85	0.59
21:Y:41:DC:H2'	21:Y:42:DG:H8	1.68	0.59
1:B:274:ILE:HD13	1:B:287:LEU:HD13	1.85	0.59
2:C:391:ARG:NH2	2:C:439:SER:O	2.36	0.59
14:O:114:MET:HE2	14:O:171:LEU:HD23	1.85	0.59
15:Q:351:GLY:HA3	15:Q:545:ASN:HD21	1.67	0.59
15:Q:354:THR:HG23	15:Q:573:VAL:HG21	1.84	0.59
6:G:213:ASN:O	6:G:217:ASN:ND2	2.36	0.58
6:G:742:LEU:HD21	6:G:799:LEU:HB3	1.84	0.58
14:O:175:GLN:NE2	14:O:179:ASP:OD1	2.36	0.58
2:C:332:LEU:HD11	2:C:356:VAL:HG13	1.85	0.58
4:E:793:LEU:HB3	4:E:796:LEU:HB2	1.84	0.58
3:D:45:TYR:CD1	20:X:34:DC:C5'	2.86	0.58
4:E:567:ASP:HB3	4:E:795:THR:CA	2.32	0.58
6:G:326:ALA:HA	6:G:359:LEU:HD13	1.85	0.58
1:A:282:ARG:NH1	1:A:311:HIS:O	2.37	0.58
2:C:383:PRO:HG3	2:C:579:VAL:HG21	1.85	0.58
6:G:642:ASP:OD2	6:G:684:ARG:NH2	2.33	0.58
1:B:113:PRO:HD3	1:B:142:PRO:HA	1.84	0.58
2:C:661:TYR:HB2	2:C:943:ILE:HG23	1.86	0.58
6:G:419:ASP:OD1	6:G:420:MET:N	2.37	0.58
8:I:180:VAL:HG12	8:I:206:PRO:HA	1.84	0.58
12:M:231:LYS:NZ	12:M:235:ASN:OD1	2.32	0.58
1:A:48:ALA:HB3	1:B:226:PHE:HZ	1.69	0.58
3:D:2:ILE:HA	5:F:270:ASN:HD21	1.68	0.58
3:D:588:ILE:HD12	3:D:663:ARG:HH11	1.68	0.58
4:E:632:LYS:HB2	4:E:668:PHE:HB2	1.84	0.58
6:G:583:PHE:HB2	6:G:601:MET:HE3	1.86	0.58
8:I:126:ASN:HD21	8:I:198:ASN:HB3	1.68	0.58
2:C:72:GLU:HG3	2:C:74:LEU:HD13	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:150:ILE:HB	2:C:158:LEU:HB3	1.85	0.58
4:E:150:ARG:NH1	27:E:8105:HOH:O	2.37	0.58
5:F:416:TRP:HB2	5:F:475:PHE:H	1.68	0.58
4:E:766:GLN:HB3	4:E:778:LEU:HD11	1.86	0.58
2:C:108:ASN:OD1	2:C:109:SER:N	2.37	0.57
10:K:119:TYR:HB2	14:O:112:ILE:HG23	1.85	0.57
3:D:10:LEU:HD21	4:E:1318:LEU:HD11	1.85	0.57
5:F:126:MET:HE3	5:F:159:ARG:HD2	1.85	0.57
6:G:224:LEU:O	6:G:258:ARG:NH2	2.37	0.57
11:L:325:MET:HE2	11:L:328:GLN:HG3	1.86	0.57
3:D:644:LYS:HG2	12:M:238:LEU:HD22	1.85	0.57
5:F:98:ILE:O	6:G:791:ARG:NH1	2.36	0.57
9:J:367:ARG:NH2	27:J:605:HOH:O	2.36	0.57
15:Q:331:SER:OG	15:Q:336:HIS:ND1	2.37	0.57
17:S:287:GLN:O	27:S:701:HOH:O	2.18	0.57
2:C:960:ILE:O	2:C:979:ARG:NH1	2.37	0.57
9:J:239:LYS:HD2	9:J:240:PRO:HD2	1.86	0.57
10:K:389:ARG:O	10:K:392:SER:OG	2.20	0.57
15:Q:659:LEU:HG	15:Q:693:LEU:HD11	1.85	0.57
3:D:11:ARG:HB3	4:E:1306:ILE:HG12	1.85	0.57
3:D:254:PHE:O	5:F:455:LYS:NZ	2.24	0.57
5:F:66:LEU:HD21	6:G:793:MET:HE1	1.85	0.57
5:F:175:ARG:NH1	11:L:374:GLU:OE2	2.38	0.56
6:G:86:PRO:O	6:G:124:ARG:NH1	2.38	0.56
4:E:111:LEU:HB2	4:E:144:HIS:HE1	1.69	0.56
3:D:66:SER:HB3	3:D:96:ASP:HA	1.87	0.56
4:E:814:ASN:HB3	7:H:599:TRP:HB3	1.87	0.56
13:N:205:THR:HB	13:N:209:VAL:HB	1.86	0.56
18:T:97:PRO:HA	18:T:120:ALA:HA	1.86	0.56
21:Y:31:DC:H2''	21:Y:32:DA:H8	1.70	0.56
5:F:556:THR:O	21:Y:13:DC:H5'	2.06	0.56
8:I:129:PHE:HD2	8:I:209:ASN:HB2	1.71	0.56
3:D:45:TYR:HD1	20:X:34:DC:C5'	2.16	0.56
22:Z:32:C:H2'	22:Z:33:G:C8	2.41	0.56
5:F:461:ASP:OD2	5:F:469:ASN:ND2	2.39	0.56
6:G:586:MET:HE1	6:G:593:PRO:HB3	1.87	0.56
6:G:602:LEU:HB3	6:G:679:LEU:HD11	1.87	0.56
6:G:514:SER:O	6:G:518:ASN:ND2	2.38	0.56
8:I:89:GLN:OE1	8:I:120:ASN:ND2	2.32	0.56
8:I:79:HIS:HD2	8:I:131:TRP:HE1	1.53	0.56
2:C:193:GLU:O	2:C:197:ASN:ND2	2.33	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:633:CYS:SG	14:O:124:GLU:HG2	2.46	0.56
7:H:187:ARG:NH2	8:I:94:ASP:OD2	2.39	0.56
11:L:387:PHE:HE1	11:L:472:LYS:HE2	1.71	0.56
15:Q:345:GLY:N	15:Q:435:ILE:O	2.29	0.56
7:H:196:ARG:HH11	8:I:53:LYS:HG2	1.70	0.55
20:X:66:DC:H2"	20:X:67:DG:N7	2.20	0.55
1:A:100:LEU:HD13	17:S:575:SER:HB3	1.88	0.55
2:C:248:GLN:HG3	2:C:252:PHE:HB3	1.89	0.55
4:E:763:ILE:HG23	4:E:779:VAL:HG13	1.87	0.55
2:C:180:ILE:HD13	2:C:204:PHE:HE2	1.69	0.55
8:I:208:ILE:HD11	8:I:242:ALA:HB2	1.89	0.55
12:M:129:GLU:OE2	12:M:183:ARG:NH1	2.40	0.55
15:Q:285:ASP:HA	15:Q:288:LEU:HD12	1.87	0.55
2:C:333:GLU:HG3	2:C:334:ASN:HD22	1.71	0.55
5:F:448:ARG:NH1	15:Q:661:ASP:OD2	2.39	0.55
13:N:142:ASP:HA	13:N:145:ARG:HG2	1.88	0.55
2:C:579:VAL:HG12	2:C:643:GLY:HA3	1.89	0.55
2:C:795:LYS:HB2	2:C:803:PRO:HG2	1.89	0.55
1:A:195:LYS:HB2	1:B:159:LEU:HD22	1.89	0.55
4:E:793:LEU:HD13	4:E:796:LEU:HG	1.88	0.55
6:G:785:THR:OG1	6:G:788:ASN:O	2.24	0.55
12:M:134:TYR:HH	12:M:170:TYR:HH	1.50	0.55
5:F:809:PRO:O	5:F:842:TYR:OH	2.21	0.55
17:S:378:ASN:OD1	27:S:702:HOH:O	2.18	0.55
6:G:286:LEU:HD13	6:G:302:LEU:HD13	1.87	0.54
15:Q:236:ARG:NH1	15:Q:260:GLU:OE2	2.39	0.54
18:T:66:TRP:O	18:T:131:ARG:NH2	2.40	0.54
21:Y:31:DC:H2"	21:Y:32:DA:C8	2.42	0.54
4:E:625:ARG:NH1	4:E:785:TYR:OH	2.41	0.54
6:G:798:GLN:O	6:G:801:GLN:NE2	2.41	0.54
13:N:88:ILE:HG21	13:N:93:LEU:HD22	1.90	0.54
16:R:36:ILE:HG23	16:R:44:ARG:HH21	1.72	0.54
15:Q:365:ALA:O	15:Q:565:ARG:NH2	2.40	0.54
4:E:569:LEU:HD21	7:H:415:GLN:HG3	1.89	0.54
6:G:755:LEU:HB3	6:G:761:ALA:HB2	1.90	0.54
7:H:196:ARG:NH1	8:I:53:LYS:HG2	2.23	0.54
1:B:103:THR:HG21	1:B:150:LYS:HE3	1.89	0.54
2:C:112:THR:HG22	2:C:121:VAL:HG22	1.88	0.54
2:C:1055:LEU:HD13	3:D:12:ILE:HG23	1.90	0.54
4:E:805:LYS:HE3	13:N:186:ALA:HB3	1.89	0.54
4:E:812:VAL:N	7:H:602:MET:O	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:227:TYR:HD1	2:C:247:LEU:HD21	1.73	0.54
2:C:1024:THR:O	2:C:1028:GLY:N	2.40	0.54
3:D:363:LYS:NZ	21:Y:36:DC:OP1	2.30	0.54
4:E:102:GLU:OE1	4:E:376:HIS:NE2	2.34	0.54
4:E:778:LEU:HD22	4:E:780:ARG:HH21	1.72	0.54
15:Q:580:ILE:HB	15:Q:588:VAL:HB	1.90	0.54
1:B:275:ASP:N	1:B:275:ASP:OD1	2.41	0.54
2:C:562:LYS:HG3	2:C:647:VAL:HB	1.90	0.54
21:Y:49:DG:H2"	21:Y:50:DA:N7	2.23	0.54
4:E:887:ARG:NH2	7:H:523:GLU:OE2	2.41	0.54
4:E:1006:TYR:HB2	8:I:247:ALA:HB2	1.90	0.54
15:Q:618:ILE:HD13	15:Q:632:MET:HB3	1.90	0.54
4:E:1038:ASN:HB2	4:E:1051:LEU:HB2	1.88	0.54
7:H:474:LEU:HD12	7:H:475:GLU:HG2	1.89	0.54
3:D:46:LYS:HD2	20:X:34:DC:OP2	2.08	0.53
3:D:533:GLN:HA	4:E:136:ALA:HB1	1.89	0.53
4:E:98:ARG:NH1	4:E:375:ARG:O	2.41	0.53
4:E:493:ILE:O	7:H:380:ARG:NH1	2.41	0.53
4:E:1080:ALA:HB3	4:E:1083:GLU:HG3	1.90	0.53
11:L:260:ARG:HB2	11:L:278:MET:HE1	1.90	0.53
17:S:380:PRO:HD2	17:S:383:LEU:HD22	1.89	0.53
4:E:440:LYS:HB3	4:E:1132:PHE:HB2	1.89	0.53
6:G:574:ARG:HE	6:G:607:LYS:HB3	1.73	0.53
11:L:356:ARG:NH2	11:L:401:THR:O	2.40	0.53
15:Q:406:MET:HE1	15:Q:414:LEU:HD13	1.90	0.53
6:G:742:LEU:HD23	6:G:796:ARG:HG3	1.90	0.53
8:I:58:PRO:HG2	8:I:61:ALA:HB2	1.90	0.53
11:L:246:ASP:N	11:L:246:ASP:OD1	2.40	0.53
11:L:382:SER:HB2	11:L:385:ASP:HB2	1.91	0.53
2:C:70:VAL:HA	2:C:117:GLY:HA2	1.90	0.53
2:C:124:ASN:HB2	2:C:393:LEU:HD23	1.90	0.53
5:F:289:ILE:O	5:F:293:THR:HG23	2.09	0.53
16:R:38:ARG:HG2	16:R:44:ARG:HG2	1.90	0.53
4:E:231:ARG:HB2	4:E:283:GLN:HE21	1.74	0.53
14:P:114:MET:HE2	14:P:171:LEU:HD12	1.90	0.53
1:B:93:GLU:O	1:B:134:GLN:NE2	2.40	0.53
2:C:1000:VAL:HG12	3:D:508:GLU:HB3	1.91	0.53
15:Q:673:TYR:OH	15:Q:693:LEU:N	2.41	0.53
5:F:541:GLU:OE1	5:F:541:GLU:N	2.41	0.53
6:G:384:ASP:OD1	6:G:385:ALA:N	2.38	0.53
7:H:315:HIS:O	7:H:318:ARG:NH2	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:40:PRO:O	3:D:297:ARG:NH1	2.42	0.53
4:E:609:PHE:HB2	4:E:855:VAL:HB	1.90	0.53
17:S:387:LEU:HD11	17:S:391:LYS:HE3	1.91	0.53
3:D:20:ILE:HD13	3:D:270:PRO:HD3	1.91	0.53
15:Q:307:ILE:HG22	15:Q:311:LEU:HD12	1.89	0.53
15:Q:562:ASP:OD1	15:Q:565:ARG:NH2	2.42	0.53
1:A:277:LEU:HD11	1:A:295:LEU:HD13	1.90	0.52
2:C:107:MET:HE1	2:C:317:VAL:HG11	1.91	0.52
15:Q:584:GLN:HG2	15:Q:586:PHE:H	1.73	0.52
6:G:669:TYR:HD1	6:G:672:LEU:HD11	1.74	0.52
11:L:129:THR:OG1	11:L:139:PHE:O	2.24	0.52
6:G:459:THR:OG1	6:G:492:THR:OG1	2.20	0.52
10:K:383:THR:HG1	10:K:386:THR:HG1	1.44	0.52
18:T:63:VAL:HG22	18:T:131:ARG:HD3	1.91	0.52
4:E:21:ARG:NH1	12:M:207:GLU:OE1	2.27	0.52
7:H:370:ASN:HD22	7:H:373:GLU:HG3	1.75	0.52
8:I:79:HIS:CD2	8:I:131:TRP:HE1	2.28	0.52
9:J:216:ILE:HD11	12:M:323:ARG:HH12	1.74	0.52
11:L:330:ASN:ND2	11:L:347:ASP:OD2	2.43	0.52
2:C:1014:HIS:CE1	2:C:1036:ASP:HB2	2.45	0.52
5:F:66:LEU:HD22	6:G:795:GLN:HE21	1.75	0.52
6:G:603:SER:HB3	6:G:678:TRP:HE3	1.74	0.52
6:G:735:ILE:HG23	6:G:736:LEU:HD12	1.91	0.52
2:C:164:LYS:NZ	21:Y:28:DT:OP1	2.38	0.52
4:E:1033:LEU:HD23	4:E:1039:LEU:HD13	1.92	0.52
5:F:437:VAL:HG13	5:F:442:LEU:HD11	1.91	0.52
4:E:1182:ILE:HD13	5:F:606:GLY:H	1.74	0.52
8:I:230:ASN:OD1	8:I:234:ASN:ND2	2.43	0.52
11:L:120:MET:HE1	11:L:281:TYR:HB3	1.92	0.52
21:Y:41:DC:H2'	21:Y:42:DG:C8	2.43	0.52
3:D:306:LEU:HD21	3:D:325:GLU:HG2	1.90	0.52
3:D:619:PRO:HG3	3:D:634:TYR:CZ	2.44	0.52
6:G:579:CYS:HB3	6:G:601:MET:HE1	1.91	0.52
9:J:329:GLN:HE21	9:J:333:GLU:HG3	1.75	0.52
11:L:365:VAL:HG13	11:L:480:ARG:HE	1.75	0.52
15:Q:707:MET:HA	15:Q:707:MET:HE2	1.92	0.52
22:Z:33:G:H2'	22:Z:34:G:H8	1.73	0.52
1:A:275:ASP:OD2	1:A:284:TYR:OH	2.26	0.52
7:H:154:ASP:OD1	7:H:154:ASP:N	2.40	0.52
3:D:184:PHE:HA	3:D:187:PHE:CE1	2.44	0.52
5:F:237:GLU:HG2	5:F:242:PHE:HA	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:81:LEU:HD23	6:G:84:LEU:HD12	1.92	0.52
15:Q:599:LEU:HD13	15:Q:618:ILE:HD11	1.92	0.52
3:D:669:ILE:HD12	4:E:7:LEU:HD11	1.92	0.51
4:E:988:ASN:ND2	7:H:200:GLU:OE2	2.43	0.51
6:G:127:LYS:HA	6:G:130:GLN:HE21	1.75	0.51
15:Q:590:VAL:HG21	15:Q:737:ARG:HG3	1.92	0.51
2:C:91:ASN:OD1	4:E:825:ARG:NH1	2.42	0.51
4:E:815:TYR:CZ	7:H:593:VAL:HB	2.46	0.51
2:C:739:ILE:HD11	2:C:776:CYS:HB3	1.92	0.51
4:E:1006:TYR:HE2	8:I:250:GLU:HG3	1.75	0.51
2:C:389:HIS:HD2	2:C:392:LYS:HE2	1.76	0.51
2:C:543:ARG:CZ	2:C:862:ARG:HG3	2.40	0.51
2:C:611:ILE:H	2:C:624:GLN:HE21	1.56	0.51
8:I:105:ILE:HD13	8:I:198:ASN:HD21	1.75	0.51
21:Y:34:DT:H2'	21:Y:35:DC:C6	2.46	0.51
2:C:126:ILE:HD11	2:C:393:LEU:HB3	1.91	0.51
3:D:6:LYS:HB2	4:E:1330:LYS:HD2	1.91	0.51
3:D:209:ARG:HD3	5:F:468:SER:HB3	1.92	0.51
9:J:415:ASN:HB3	9:J:418:SER:HB2	1.92	0.51
11:L:197:LEU:HD11	11:L:334:MET:HE3	1.91	0.51
14:P:100:ILE:HD11	14:P:181:ILE:HD11	1.91	0.51
4:E:407:PHE:HE1	4:E:426:ARG:HD3	1.76	0.51
4:E:569:LEU:HD22	7:H:412:VAL:HG12	1.93	0.51
5:F:126:MET:HE1	5:F:163:LEU:HD21	1.93	0.51
15:Q:580:ILE:N	15:Q:588:VAL:O	2.39	0.51
15:Q:658:ILE:HG22	15:Q:662:MET:HE2	1.93	0.51
2:C:1051:LEU:HD23	3:D:336:LEU:HD22	1.93	0.51
3:D:459:HIS:CD2	3:D:461:LEU:HB2	2.46	0.51
7:H:395:GLU:O	7:H:524:ARG:NH1	2.33	0.51
17:S:581:PRO:HA	17:S:586:VAL:HG11	1.93	0.51
6:G:603:SER:O	6:G:607:LYS:HG3	2.11	0.51
11:L:286:ASN:ND2	11:L:319:GLU:OE2	2.28	0.51
18:T:49:VAL:HG11	18:T:51:ARG:HH21	1.76	0.51
2:C:503:TYR:O	2:C:506:GLU:HG2	2.11	0.50
4:E:694:ASP:O	4:E:702:ARG:NH2	2.43	0.50
4:E:1311:GLY:O	4:E:1315:ASN:ND2	2.44	0.50
7:H:411:HIS:NE2	7:H:503:LEU:HD12	2.26	0.50
13:N:147:ILE:HD11	13:N:157:PHE:CD2	2.46	0.50
3:D:608:LEU:HD22	16:R:60:TYR:HB3	1.93	0.50
5:F:249:ASN:OD1	5:F:284:THR:OG1	2.23	0.50
7:H:196:ARG:NH2	8:I:132:GLU:OE2	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:97:SER:O	13:N:101:VAL:HG23	2.12	0.50
15:Q:540:ARG:HA	15:Q:543:ILE:HG12	1.94	0.50
15:Q:572:ALA:HB1	15:Q:578:GLU:HA	1.93	0.50
15:Q:680:ASP:HB2	15:Q:761:PRO:HG3	1.92	0.50
2:C:451:GLU:HB3	2:C:470:PHE:HB3	1.92	0.50
2:C:973:GLN:HG3	2:C:1015:ILE:HD11	1.92	0.50
3:D:96:ASP:OD1	3:D:97:SER:N	2.45	0.50
3:D:151:ILE:HD11	3:D:190:ARG:HG2	1.93	0.50
4:E:444:SER:OG	4:E:446:SER:O	2.30	0.50
5:F:175:ARG:NH1	11:L:371:LEU:HD23	2.26	0.50
3:D:542:LEU:HD13	4:E:49:GLN:HG3	1.93	0.50
20:X:69:DG:H2''	20:X:70:DA:C8	2.47	0.50
4:E:369:VAL:HB	4:E:381:PHE:HB3	1.92	0.50
4:E:694:ASP:OD2	4:E:702:ARG:NH2	2.44	0.50
11:L:110:ILE:HB	11:L:314:ILE:HB	1.92	0.50
15:Q:696:VAL:HG13	15:Q:699:VAL:HG12	1.93	0.50
17:S:459:SER:OG	17:S:476:GLU:OE1	2.25	0.50
18:T:81:GLN:O	18:T:116:LYS:NZ	2.43	0.50
2:C:642:ASP:OD2	2:C:648:GLY:N	2.38	0.50
5:F:78:LEU:HG	5:F:90:VAL:HG13	1.92	0.50
9:J:284:TYR:O	9:J:288:ARG:HB3	2.12	0.50
15:Q:374:SER:OG	15:Q:377:SER:O	2.30	0.50
15:Q:406:MET:HE2	15:Q:411:THR:HG21	1.94	0.50
2:C:1013:ASP:OD1	2:C:1013:ASP:N	2.43	0.50
4:E:484:CYS:HB3	4:E:938:LEU:HD22	1.94	0.50
4:E:1065:THR:OG1	4:E:1066:ILE:N	2.35	0.50
6:G:501:ALA:HB1	6:G:533:GLU:HG3	1.93	0.50
1:B:23:ASP:HB2	1:B:27:LEU:HD23	1.94	0.50
2:C:929:ILE:HG13	2:C:938:PHE:HD2	1.77	0.50
6:G:114:ALA:HA	6:G:148:LEU:HD13	1.93	0.50
8:I:164:PHE:HA	8:I:190:VAL:HG11	1.94	0.50
15:Q:635:ILE:HA	15:Q:638:GLU:HG2	1.94	0.50
17:S:501:MET:HB2	17:S:518:THR:HG23	1.94	0.50
1:A:79:GLY:HA3	1:A:143:ILE:HD11	1.94	0.49
5:F:342:ILE:HD13	5:F:383:GLU:HG2	1.93	0.49
15:Q:273:SER:HA	15:Q:295:GLY:HA3	1.93	0.49
21:Y:26:DA:H2''	21:Y:27:DA:H5'	1.92	0.49
2:C:427:SER:OG	2:C:431:ASN:O	2.29	0.49
4:E:622:ARG:HH22	4:E:788:ALA:HB2	1.77	0.49
11:L:267:ARG:NH1	11:L:269:GLY:O	2.45	0.49
12:M:204:ASP:HB3	12:M:221:GLU:HG2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:T:76:LEU:HD23	18:T:122:LEU:HD12	1.95	0.49
11:L:156:THR:OG1	11:L:165:ARG:NH1	2.41	0.49
12:M:143:LYS:NZ	12:M:145:SER:OG	2.45	0.49
17:S:227:GLU:OE1	17:S:227:GLU:N	2.44	0.49
19:U:105:LYS:HG2	19:U:171:TRP:HZ2	1.77	0.49
5:F:272:GLU:O	5:F:279:LYS:NZ	2.31	0.49
5:F:346:ARG:HA	5:F:349:LYS:HD3	1.93	0.49
6:G:548:TYR:O	6:G:552:GLU:HG2	2.13	0.49
12:M:210:ILE:HG23	12:M:215:ASP:HB2	1.93	0.49
5:F:77:GLU:OE1	5:F:81:ARG:NE	2.43	0.49
7:H:480:GLU:OE2	7:H:484:HIS:NE2	2.46	0.49
6:G:648:GLN:HA	6:G:651:GLU:HG2	1.93	0.49
1:A:316:ASP:HA	1:A:319:LYS:HG2	1.95	0.49
2:C:695:ILE:HG21	2:C:741:VAL:HG11	1.95	0.49
5:F:145:ILE:HA	5:F:148:VAL:HG22	1.93	0.49
5:F:811:ILE:HD13	5:F:842:TYR:HB3	1.95	0.49
7:H:196:ARG:NH1	8:I:54:THR:O	2.46	0.49
10:K:271:PRO:HD2	10:K:274:LEU:HD12	1.95	0.49
14:O:160:ASP:HB3	14:O:163:LYS:HE3	1.95	0.49
3:D:546:THR:HG21	3:D:601:PRO:HB3	1.94	0.49
6:G:577:ASP:OD1	6:G:577:ASP:N	2.33	0.49
4:E:928:PHE:HZ	4:E:1122:ILE:HD11	1.78	0.49
6:G:178:THR:OG1	6:G:211:THR:OG1	2.25	0.49
15:Q:338:SER:HB2	15:Q:403:MET:HE1	1.94	0.49
15:Q:516:SER:OG	15:Q:519:GLU:O	2.24	0.49
1:A:80:ILE:HG12	1:A:139:LEU:HD23	1.95	0.48
11:L:372:PRO:HA	11:L:375:TYR:CZ	2.48	0.48
11:L:438:GLN:NE2	11:L:439:ASP:OD1	2.45	0.48
15:Q:466:MET:HE3	15:Q:474:LYS:HG2	1.94	0.48
1:A:276:GLN:CD	17:S:280:LEU:HD21	2.38	0.48
4:E:723:PHE:HB3	4:E:780:ARG:NH2	2.29	0.48
6:G:672:LEU:HD12	6:G:673:LEU:N	2.28	0.48
7:H:385:ARG:HE	7:H:546:ARG:HD2	1.78	0.48
20:X:59:DA:H2'	20:X:60:DG:H8	1.78	0.48
2:C:1010:TYR:CD1	2:C:1021:VAL:HG21	2.48	0.48
4:E:411:GLN:HE22	9:J:234:TRP:H	1.60	0.48
4:E:1021:SER:OG	4:E:1039:LEU:O	2.30	0.48
19:U:143:VAL:HA	19:U:146:PHE:HD2	1.77	0.48
21:Y:36:DC:H2'	21:Y:37:DC:C6	2.48	0.48
1:A:189:TYR:O	9:J:308:PRO:HB3	2.14	0.48
3:D:371:LEU:HD13	4:E:1317:VAL:HG13	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:778:LEU:HD13	4:E:780:ARG:NE	2.26	0.48
4:E:793:LEU:C	4:E:796:LEU:H	2.22	0.48
5:F:408:LYS:HB3	5:F:423:GLU:HG2	1.95	0.48
7:H:148:ASP:OD1	7:H:149:LYS:N	2.46	0.48
15:Q:359:ILE:HG23	15:Q:363:TYR:CE1	2.48	0.48
2:C:308:HIS:NE2	2:C:477:GLU:OE2	2.41	0.48
4:E:630:ILE:HD12	4:E:821:GLY:HA2	1.95	0.48
2:C:561:GLU:HG2	2:C:655:LYS:HD3	1.95	0.48
2:C:616:SER:HB3	2:C:622:MET:HE3	1.94	0.48
7:H:205:ASP:OD1	7:H:207:LYS:NZ	2.36	0.48
10:K:124:MET:HG2	10:K:127:TRP:CZ2	2.48	0.48
20:X:32:DT:H2''	20:X:33:DC:C4	2.48	0.48
21:Y:17:DT:H2''	21:Y:18:DC:H5	1.79	0.48
1:A:273:PHE:HA	1:A:294:THR:HA	1.95	0.48
6:G:137:PRO:HA	6:G:141:ILE:HD12	1.95	0.48
6:G:279:ASP:O	6:G:282:THR:OG1	2.31	0.48
13:N:185:VAL:HG23	13:N:188:ALA:HB2	1.94	0.48
18:T:63:VAL:HA	18:T:66:TRP:CD2	2.48	0.48
2:C:170:ALA:N	2:C:178:ILE:O	2.40	0.48
3:D:114:THR:HA	3:D:265:VAL:HA	1.95	0.48
5:F:323:LYS:HE2	5:F:327:LEU:HD11	1.94	0.48
13:N:132:GLN:HG2	13:N:250:SER:HB2	1.94	0.48
17:S:448:ASN:OD1	17:S:448:ASN:N	2.45	0.48
2:C:975:PRO:HD3	2:C:1012:SER:O	2.13	0.48
4:E:746:PRO:HD3	4:E:762:TRP:HA	1.96	0.48
13:N:60:LEU:HD12	13:N:69:LEU:HD11	1.96	0.48
4:E:488:LEU:O	4:E:489:ILE:HG13	2.13	0.48
5:F:749:PHE:HA	5:F:752:MET:HE2	1.95	0.48
6:G:774:LEU:HD13	6:G:792:ILE:HG21	1.94	0.48
7:H:82:ALA:HB2	7:H:308:ASN:HD22	1.79	0.48
11:L:233:HIS:HD2	11:L:235:GLY:H	1.62	0.48
15:Q:330:ALA:HB2	15:Q:397:VAL:HG22	1.96	0.48
19:U:87:ILE:HG22	19:U:90:PHE:H	1.77	0.48
21:Y:46:DT:O3'	21:Y:47:DA:H8	1.97	0.48
2:C:92:ARG:NH2	4:E:817:LEU:O	2.46	0.47
7:H:559:ASP:OD1	7:H:559:ASP:N	2.41	0.47
10:K:81:ASP:O	10:K:229:LYS:HE3	2.14	0.47
15:Q:734:TYR:OH	15:Q:739:GLU:OE1	2.22	0.47
1:A:64:ARG:HB3	1:A:150:LYS:HB2	1.95	0.47
6:G:631:GLN:O	6:G:635:GLN:HG2	2.13	0.47
11:L:79:PHE:O	11:L:281:TYR:OH	2.18	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:83:ASN:O	13:N:87:GLN:HG2	2.13	0.47
3:D:155:PRO:HD2	15:Q:695:ASP:OD2	2.14	0.47
3:D:179:PHE:HD1	15:Q:698:ARG:HH11	1.63	0.47
4:E:470:LEU:HD13	4:E:1113:ALA:HB3	1.97	0.47
4:E:792:ASN:C	4:E:794:ALA:N	2.65	0.47
4:E:804:GLU:OE2	7:H:399:SER:N	2.45	0.47
4:E:904:PHE:CE1	18:T:94:ARG:HD2	2.49	0.47
2:C:248:GLN:O	2:C:253:HIS:N	2.42	0.47
2:C:711:ILE:HG23	2:C:744:LEU:HD21	1.96	0.47
4:E:710:ARG:HB3	4:E:723:PHE:HE2	1.80	0.47
4:E:1000:GLN:HB3	7:H:154:ASP:OD1	2.14	0.47
6:G:618:LEU:HD13	6:G:638:LYS:HE2	1.94	0.47
17:S:445:TRP:NE1	17:S:466:LYS:HD3	2.29	0.47
2:C:872:SER:HB3	2:C:906:LEU:HD11	1.95	0.47
3:D:621:GLU:OE2	3:D:623:HIS:NE2	2.34	0.47
4:E:458:HIS:HE1	7:H:81:TRP:CE2	2.32	0.47
8:I:181:LEU:HD11	8:I:255:LEU:HD21	1.95	0.47
11:L:411:PRO:O	11:L:415:ARG:HG2	2.15	0.47
20:X:69:DG:H1	21:Y:13:DC:H42	1.60	0.47
6:G:595:ILE:HG21	6:G:668:PHE:HE1	1.79	0.47
22:Z:33:G:H2'	22:Z:34:G:C8	2.50	0.47
2:C:33:GLU:O	2:C:37:LYS:NZ	2.33	0.47
3:D:235:ARG:HD2	21:Y:26:DA:C8	2.50	0.47
5:F:417:ILE:HG21	5:F:820:ALA:HB2	1.97	0.47
5:F:833:ILE:HG23	5:F:834:LEU:HD12	1.96	0.47
6:G:637:ILE:O	6:G:684:ARG:NH1	2.47	0.47
7:H:137:GLU:O	7:H:141:LYS:N	2.48	0.47
7:H:518:ARG:HA	7:H:521:LEU:HD23	1.96	0.47
14:P:173:PRO:HA	17:S:562:ASN:HD21	1.79	0.47
1:B:64:ARG:HB3	1:B:150:LYS:HB2	1.95	0.47
2:C:73:SER:HA	2:C:117:GLY:HA3	1.96	0.47
3:D:553:ASN:ND2	27:D:804:HOH:O	2.47	0.47
4:E:161:ILE:HD12	4:E:180:ILE:HG23	1.96	0.47
6:G:424:GLU:HG2	6:G:456:LYS:HD2	1.96	0.47
8:I:156:SER:OG	8:I:159:ASN:OD1	2.21	0.47
8:I:172:PHE:CE1	13:N:116:ASN:HB3	2.50	0.47
3:D:120:LYS:HE2	3:D:341:ARG:HA	1.97	0.47
4:E:243:ILE:O	4:E:247:ILE:HG12	2.15	0.47
5:F:208:ALA:HB1	5:F:212:LEU:HD23	1.97	0.47
6:G:514:SER:HA	6:G:517:VAL:HG12	1.96	0.47
2:C:986:ARG:HA	3:D:375:ARG:HA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:148:ALA:HB2	3:D:164:PHE:HE1	1.80	0.47
11:L:300:LYS:HD2	16:R:91:LEU:HA	1.97	0.47
15:Q:266:HIS:HB3	15:Q:326:LEU:HD11	1.97	0.47
15:Q:591:ASP:N	15:Q:591:ASP:OD1	2.47	0.47
20:X:65:DA:H1'	20:X:66:DC:H5'	1.97	0.47
2:C:88:TRP:CE2	2:C:349:ILE:HG23	2.50	0.46
2:C:227:TYR:HD2	2:C:237:PRO:HG3	1.80	0.46
4:E:301:ARG:NE	4:E:314:VAL:O	2.41	0.46
12:M:267:VAL:HG22	12:M:293:ILE:HD12	1.96	0.46
20:X:47:DG:H2''	20:X:48:DA:C8	2.50	0.46
6:G:177:TYR:HB3	6:G:200:MET:HE2	1.96	0.46
7:H:70:GLU:OE1	7:H:74:ARG:NH2	2.48	0.46
15:Q:581:ASP:HA	15:Q:584:GLN:HE22	1.81	0.46
2:C:661:TYR:O	4:E:56:SER:OG	2.29	0.46
5:F:359:HIS:ND1	5:F:366:ASP:OD1	2.47	0.46
5:F:384:LEU:HD23	5:F:798:LEU:HD11	1.97	0.46
5:F:401:ARG:NH2	5:F:461:ASP:O	2.49	0.46
6:G:712:ASP:OD1	6:G:714:HIS:ND1	2.33	0.46
10:K:80:ASP:OD1	10:K:80:ASP:N	2.48	0.46
14:P:79:VAL:HG12	14:P:133:LYS:HG2	1.97	0.46
15:Q:710:GLU:CD	15:Q:710:GLU:H	2.24	0.46
19:U:99:ARG:HH11	19:U:120:VAL:HG12	1.80	0.46
3:D:295:LEU:HD13	3:D:335:LEU:HA	1.97	0.46
4:E:633:TYR:OH	7:H:597:ASN:OD1	2.32	0.46
6:G:358:ASN:OD1	6:G:362:GLN:NE2	2.48	0.46
6:G:463:GLU:O	6:G:467:GLN:HG2	2.16	0.46
7:H:385:ARG:HH21	7:H:546:ARG:HD2	1.79	0.46
1:A:225:LEU:HD22	1:B:45:ILE:HD11	1.97	0.46
2:C:86:LEU:HD23	2:C:88:TRP:CZ2	2.50	0.46
4:E:982:THR:HB	7:H:166:ILE:HD12	1.98	0.46
7:H:508:GLU:O	7:H:511:GLU:HG2	2.15	0.46
16:R:85:ASP:HB3	16:R:133:VAL:HG21	1.98	0.46
7:H:207:LYS:HD2	7:H:211:ASP:HB3	1.96	0.46
15:Q:302:SER:HB3	15:Q:322:THR:HG23	1.98	0.46
15:Q:605:SER:O	15:Q:608:GLU:HG2	2.16	0.46
18:T:92:GLU:HG3	18:T:107:LEU:HD13	1.97	0.46
2:C:611:ILE:HB	2:C:624:GLN:HE21	1.81	0.46
7:H:141:LYS:HE3	7:H:141:LYS:HB3	1.81	0.46
10:K:358:ASP:HB3	10:K:362:ARG:HB2	1.98	0.46
10:K:416:VAL:O	10:K:420:GLN:HG2	2.15	0.46
14:P:81:LYS:HA	14:P:133:LYS:HG3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:819:ARG:HA	5:F:819:ARG:HH11	1.80	0.46
6:G:655:ASP:OD1	6:G:695:ARG:NH2	2.48	0.46
15:Q:673:TYR:CZ	15:Q:693:LEU:HB3	2.51	0.46
5:F:552:PRO:HG2	5:F:563:ARG:HD3	1.98	0.46
7:H:133:ILE:HB	7:H:137:GLU:OE2	2.16	0.46
7:H:331:ARG:NH1	7:H:341:GLU:OE1	2.45	0.46
13:N:144:LEU:O	13:N:147:ILE:HG22	2.16	0.46
13:N:173:TRP:HB2	13:N:175:TRP:NE1	2.31	0.46
16:R:66:PRO:HG2	16:R:67:PHE:CE2	2.51	0.46
1:A:74:TYR:HB3	2:C:613:TYR:CD2	2.51	0.46
2:C:799:SER:OG	2:C:801:TYR:O	2.31	0.46
4:E:55:ILE:HD12	4:E:130:MET:HE3	1.98	0.46
4:E:1109:ALA:HA	4:E:1132:PHE:HZ	1.81	0.46
5:F:378:GLU:HB3	5:F:478:ARG:HH21	1.81	0.46
5:F:411:THR:O	5:F:415:SER:OG	2.28	0.46
18:T:135:LYS:HE2	18:T:140:ASP:HB2	1.98	0.46
6:G:563:LEU:HA	6:G:566:VAL:HG12	1.97	0.45
8:I:148:GLU:HA	8:I:151:GLU:HG2	1.98	0.45
21:Y:49:DG:H2''	21:Y:50:DA:C5	2.51	0.45
2:C:215:LYS:HD3	2:C:225:GLU:HB2	1.97	0.45
7:H:125:LYS:O	7:H:128:ILE:HG13	2.15	0.45
13:N:226:GLU:O	13:N:230:TYR:HB2	2.16	0.45
1:A:283:ILE:HG23	1:A:312:PHE:HE1	1.81	0.45
2:C:490:ASN:OD1	2:C:497:GLN:NE2	2.44	0.45
3:D:128:ASN:HD22	3:D:246:ARG:HD2	1.82	0.45
4:E:447:GLU:OE1	4:E:483:SER:HB2	2.16	0.45
11:L:102:PHE:N	26:L:8001:SAH:OXT	2.37	0.45
15:Q:626:ARG:HH12	15:Q:653:GLU:CD	2.23	0.45
17:S:242:TYR:OH	17:S:476:GLU:OE2	2.33	0.45
4:E:102:GLU:OE2	4:E:375:ARG:NH2	2.50	0.45
4:E:729:PHE:CE1	19:U:147:ILE:HD13	2.47	0.45
6:G:389:ASN:ND2	6:G:421:GLU:OE2	2.49	0.45
6:G:618:LEU:O	6:G:622:LEU:HG	2.16	0.45
12:M:189:PRO:HG3	12:M:251:TYR:OH	2.16	0.45
15:Q:626:ARG:NH1	15:Q:653:GLU:OE1	2.49	0.45
1:B:204:TRP:HE1	16:R:69:GLU:CD	2.24	0.45
2:C:457:LEU:HD11	2:C:518:ARG:HG3	1.99	0.45
6:G:561:ARG:HH22	6:G:667:ARG:HD3	1.81	0.45
5:F:446:ARG:NH1	15:Q:661:ASP:OD1	2.49	0.45
2:C:380:ARG:CZ	2:C:622:MET:HE1	2.47	0.45
3:D:202:GLN:O	3:D:206:LEU:HG	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:812:VAL:HG21	7:H:607:ALA:HB2	1.99	0.45
6:G:145:MET:HE1	6:G:161:VAL:HG21	1.98	0.45
11:L:233:HIS:CD2	11:L:235:GLY:H	2.33	0.45
13:N:71:TYR:O	13:N:75:LYS:HB2	2.17	0.45
13:N:211:PRO:HA	13:N:214:TRP:CE3	2.51	0.45
21:Y:36:DC:H2'	21:Y:37:DC:H6	1.81	0.45
4:E:354:VAL:HB	4:E:423:ALA:HB3	1.98	0.45
4:E:1053:GLN:C	4:E:1055:TYR:H	2.25	0.45
6:G:260:LEU:O	6:G:289:THR:OG1	2.34	0.45
7:H:187:ARG:HH22	8:I:94:ASP:CG	2.24	0.45
12:M:193:ILE:HA	12:M:235:ASN:HD21	1.82	0.45
13:N:264:ARG:O	13:N:267:GLN:HG2	2.17	0.45
20:X:47:DG:H2''	20:X:48:DA:H8	1.82	0.45
20:X:63:DA:H2''	20:X:64:DG:N7	2.32	0.45
22:Z:35:C:H2'	22:Z:36:G:H8	1.82	0.45
3:D:55:LEU:HD21	3:D:296:TYR:HB3	1.99	0.45
5:F:142:GLU:O	5:F:145:ILE:HG13	2.17	0.45
7:H:534:ARG:O	7:H:538:GLY:N	2.49	0.45
14:P:98:PRO:HB3	14:P:185:MET:HG2	1.99	0.45
15:Q:355:THR:OG1	15:Q:545:ASN:ND2	2.50	0.45
2:C:674:LEU:HD11	2:C:836:LEU:HG	1.99	0.45
4:E:98:ARG:HD3	4:E:375:ARG:NH2	2.32	0.45
6:G:245:ILE:HA	6:G:248:TYR:HB2	1.99	0.45
7:H:535:GLN:HE22	7:H:541:LEU:HD11	1.82	0.45
11:L:149:ILE:HD11	11:L:168:CYS:HB3	1.97	0.45
22:Z:31:C:H4'	22:Z:32:C:O5'	2.17	0.45
2:C:424:ILE:HD11	4:E:178:TYR:HE2	1.82	0.44
9:J:212:PRO:HA	12:M:333:TRP:O	2.16	0.44
9:J:305:LYS:HE3	9:J:305:LYS:HB3	1.85	0.44
14:O:118:LEU:HD11	14:O:154:LEU:HD21	2.00	0.44
17:S:372:VAL:HG11	17:S:509:MET:HE1	1.99	0.44
2:C:408:PHE:HD2	2:C:409:ARG:HH21	1.65	0.44
3:D:69:CYS:HB3	3:D:90:CYS:SG	2.57	0.44
4:E:98:ARG:HD3	4:E:375:ARG:HH21	1.82	0.44
4:E:668:PHE:HB3	4:E:782:VAL:HG11	1.99	0.44
4:E:793:LEU:O	4:E:796:LEU:HB2	2.17	0.44
6:G:515:ARG:HA	6:G:518:ASN:HD21	1.80	0.44
6:G:742:LEU:HD12	6:G:743:PRO:HD2	1.99	0.44
15:Q:501:MET:SD	15:Q:510:PRO:HG2	2.58	0.44
17:S:534:ALA:HB2	27:S:712:HOH:O	2.17	0.44
19:U:112:PHE:HE1	19:U:160:GLY:HA3	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:MET:HE2	1:B:155:ARG:HE	1.80	0.44
2:C:472:SER:H	2:C:475:GLN:HE21	1.65	0.44
6:G:684:ARG:HA	6:G:687:ARG:HG2	1.99	0.44
12:M:200:TYR:HB3	12:M:226:LYS:HB2	1.99	0.44
15:Q:469:PRO:HG3	15:Q:491:ASN:ND2	2.33	0.44
6:G:214:THR:HA	6:G:217:ASN:HD21	1.83	0.44
7:H:85:GLU:OE2	7:H:314:ARG:NH2	2.50	0.44
7:H:343:ARG:NH2	7:H:350:ASP:OD2	2.49	0.44
8:I:113:ASN:HB2	18:T:117:TRP:CZ3	2.52	0.44
9:J:397:ALA:HB3	9:J:400:ALA:HB2	1.99	0.44
15:Q:654:ASP:OD2	15:Q:656:LEU:HB2	2.18	0.44
17:S:438:PRO:HA	17:S:441:VAL:HG22	1.98	0.44
2:C:1060:VAL:HB	3:D:7:HIS:HB2	1.99	0.44
3:D:641:ARG:NH1	12:M:199:ASP:OD1	2.47	0.44
4:E:1006:TYR:HB3	8:I:247:ALA:HB2	2.00	0.44
4:E:1248:LEU:HD21	4:E:1272:LEU:HD11	1.99	0.44
2:C:675:ILE:HG22	2:C:852:MET:HG2	2.00	0.44
4:E:711:VAL:HG22	4:E:720:LEU:HG	2.00	0.44
5:F:744:GLU:HB3	5:F:747:GLU:HB2	1.99	0.44
6:G:360:PHE:HA	6:G:363:ASN:HD21	1.82	0.44
6:G:467:GLN:CD	6:G:502:ARG:HH12	2.26	0.44
6:G:508:GLU:OE1	6:G:508:GLU:N	2.46	0.44
7:H:76:TRP:CZ2	7:H:308:ASN:HB3	2.53	0.44
9:J:421:LYS:HE2	14:O:72:PHE:CE1	2.53	0.44
16:R:85:ASP:OD2	16:R:144:TYR:OH	2.32	0.44
1:A:22:ARG:HG3	1:A:28:TYR:CE1	2.53	0.44
2:C:74:LEU:O	2:C:117:GLY:N	2.46	0.44
2:C:168:ILE:HD11	2:C:294:ILE:HD11	1.98	0.44
2:C:882:ARG:NH1	2:C:905:GLU:OE1	2.50	0.44
3:D:85:LYS:O	3:D:94:PHE:N	2.51	0.44
6:G:382:ASP:OD1	6:G:382:ASP:N	2.44	0.44
13:N:84:LEU:HD22	13:N:118:ALA:HA	1.99	0.44
15:Q:469:PRO:HA	15:Q:494:VAL:HG22	1.99	0.44
2:C:208:LEU:HB3	2:C:213:LYS:HE3	2.00	0.44
5:F:169:LYS:HE3	5:F:169:LYS:HB2	1.84	0.44
13:N:71:TYR:HA	13:N:75:LYS:HG3	1.98	0.44
13:N:171:SER:HB3	13:N:225:TRP:CE2	2.53	0.44
13:N:255:SER:O	13:N:259:GLU:HG2	2.18	0.44
14:P:156:PHE:HB3	14:P:185:MET:HE1	2.00	0.44
2:C:1013:ASP:OD2	3:D:374:LYS:NZ	2.47	0.44
2:C:1016:ARG:O	2:C:1020:GLU:HG2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:157:PHE:HD2	15:Q:694:HIS:NE2	2.15	0.44
4:E:903:PRO:HB2	18:T:94:ARG:HD3	1.99	0.44
5:F:144:MET:HB3	5:F:167:MET:HE2	2.00	0.44
5:F:818:LEU:O	5:F:822:ILE:HG12	2.17	0.44
11:L:293:CYS:SG	11:L:320:MET:HE3	2.58	0.44
15:Q:725:GLN:O	15:Q:732:GLU:N	2.51	0.44
15:Q:749:GLU:HA	15:Q:752:GLN:HG3	2.00	0.44
17:S:386:SER:O	17:S:389:GLU:HG2	2.17	0.44
2:C:269:ARG:NH2	2:C:302:THR:O	2.49	0.43
2:C:328:ALA:HB2	2:C:364:THR:HG21	2.00	0.43
8:I:79:HIS:NE2	8:I:128:ASP:OD1	2.51	0.43
9:J:186:PHE:CG	12:M:262:ARG:HD3	2.53	0.43
13:N:70:ASP:OD1	13:N:71:TYR:N	2.51	0.43
21:Y:13:DC:H2"	21:Y:14:DG:H8	1.83	0.43
1:B:74:TYR:OH	12:M:279:ASP:OD1	2.30	0.43
2:C:722:LEU:HD12	2:C:728:VAL:HA	2.00	0.43
2:C:1053:LEU:HD11	3:D:117:TRP:HZ3	1.83	0.43
4:E:630:ILE:HG22	4:E:823:PRO:HA	1.99	0.43
4:E:808:ILE:HA	4:E:843:TRP:HB3	1.99	0.43
10:K:110:HIS:CD2	10:K:130:PRO:HB3	2.53	0.43
2:C:81:TYR:HB3	2:C:98:ARG:HE	1.82	0.43
4:E:458:HIS:N	7:H:68:GLU:OE2	2.33	0.43
5:F:95:TYR:OH	6:G:472:GLU:OE2	2.32	0.43
6:G:181:ILE:HD13	6:G:215:VAL:HB	2.00	0.43
6:G:535:TYR:HD1	6:G:540:LYS:HB2	1.84	0.43
6:G:700:GLU:OE1	6:G:715:ARG:NH2	2.51	0.43
9:J:319:TRP:CG	9:J:346:MET:HG3	2.54	0.43
15:Q:522:VAL:HG23	15:Q:533:ILE:HB	1.99	0.43
2:C:914:ALA:HB3	9:J:356:ARG:HH21	1.82	0.43
4:E:268:ASP:OD1	4:E:268:ASP:N	2.51	0.43
4:E:572:ARG:HG3	4:E:577:PHE:HB3	2.00	0.43
4:E:864:THR:HG21	7:H:413:ALA:HB1	2.00	0.43
5:F:138:ARG:NH1	5:F:172:TYR:OH	2.51	0.43
6:G:669:TYR:HA	6:G:672:LEU:HG	2.00	0.43
11:L:427:LYS:HE3	11:L:427:LYS:HB3	1.75	0.43
13:N:131:ILE:HA	13:N:248:LEU:O	2.18	0.43
2:C:700:THR:OG1	2:C:703:GLY:O	2.31	0.43
4:E:92:HIS:CE1	4:E:94:VAL:HB	2.54	0.43
4:E:579:ILE:HD11	4:E:796:LEU:HD22	1.99	0.43
15:Q:473:ARG:NH1	15:Q:555:ALA:O	2.51	0.43
2:C:407:ASN:HB3	2:C:410:ILE:HG13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:410:ILE:HG22	2:C:411:ARG:H	1.82	0.43
3:D:419:LEU:HD12	3:D:419:LEU:HA	1.85	0.43
4:E:296:THR:HG21	4:E:1230:SER:HB2	1.99	0.43
4:E:306:ARG:HA	4:E:313:LEU:HA	2.00	0.43
5:F:131:LYS:HG2	6:G:476:VAL:HG21	2.01	0.43
5:F:248:PHE:HB3	5:F:271:MET:SD	2.59	0.43
6:G:797:SER:HA	6:G:800:LYS:HE2	2.00	0.43
13:N:79:THR:O	13:N:82:GLU:HG2	2.19	0.43
15:Q:396:ALA:HB2	15:Q:427:LYS:HA	2.01	0.43
15:Q:725:GLN:HB2	15:Q:734:TYR:HB3	2.01	0.43
17:S:481:THR:HG21	17:S:538:GLY:O	2.18	0.43
18:T:67:SER:HB2	18:T:132:TYR:HE1	1.83	0.43
1:A:256:LYS:HE2	1:A:271:TYR:CE2	2.54	0.43
1:B:55:GLY:HA3	1:B:157:TYR:CZ	2.54	0.43
4:E:70:TRP:CZ2	9:J:278:LEU:HD12	2.54	0.43
4:E:216:ARG:HG2	4:E:1328:PHE:HE1	1.84	0.43
5:F:788:GLN:NE2	5:F:820:ALA:HB1	2.33	0.43
7:H:318:ARG:HG2	7:H:321:MET:HE3	2.01	0.43
8:I:62:LEU:HB3	8:I:66:MET:HB3	2.01	0.43
12:M:261:THR:HG22	12:M:262:ARG:H	1.83	0.43
2:C:284:ARG:NH1	7:H:556:ASP:OD1	2.52	0.43
2:C:964:SER:HB2	3:D:404:GLU:O	2.19	0.43
4:E:156:PRO:HA	4:E:187:LYS:NZ	2.34	0.43
5:F:175:ARG:HH12	11:L:371:LEU:HD23	1.84	0.43
12:M:236:ARG:NH1	12:M:242:GLU:O	2.47	0.43
13:N:61:GLU:OE1	13:N:61:GLU:N	2.52	0.43
14:P:96:LYS:HG2	14:P:97:VAL:HG13	1.99	0.43
15:Q:337:PRO:HG2	15:Q:403:MET:HE2	2.00	0.43
21:Y:44:DC:H2''	21:Y:45:DG:O4'	2.18	0.43
2:C:315:ARG:NH2	2:C:323:ASP:OD2	2.51	0.43
2:C:615:ARG:NH2	2:C:619:ASN:OD1	2.51	0.43
4:E:104:TRP:CD1	4:E:164:PRO:HG3	2.53	0.43
4:E:362:ILE:HD13	4:E:391:ILE:HG12	1.99	0.43
4:E:783:ALA:HB1	4:E:785:TYR:CD2	2.54	0.43
4:E:1035:PRO:HG2	4:E:1036:TYR:CE2	2.54	0.43
5:F:74:PHE:CZ	6:G:707:LEU:HB3	2.54	0.43
6:G:615:ASN:O	6:G:619:GLU:HG2	2.19	0.43
9:J:203:PHE:C	9:J:205:LEU:H	2.27	0.43
10:K:312:GLU:OE1	10:K:316:ASN:ND2	2.51	0.43
12:M:146:LEU:HB3	12:M:255:SER:HB3	1.99	0.43
15:Q:618:ILE:HG12	15:Q:619:GLY:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:Y:23:DT:H2''	21:Y:24:DA:C8	2.52	0.43
2:C:739:ILE:HD11	2:C:776:CYS:CB	2.48	0.43
2:C:1014:HIS:O	2:C:1018:ARG:HG3	2.19	0.43
4:E:625:ARG:O	4:E:832:ILE:N	2.51	0.43
4:E:927:MET:HE3	4:E:938:LEU:HD12	1.99	0.43
7:H:276:MET:HB2	7:H:327:ILE:HD12	2.00	0.43
7:H:368:ASP:HB3	7:H:374:ILE:HD11	2.01	0.43
8:I:246:MET:O	8:I:250:GLU:HG2	2.18	0.43
10:K:205:MET:HB2	14:O:88:GLN:HG2	2.00	0.43
13:N:155:SER:HA	13:N:158:VAL:HG22	2.01	0.43
3:D:256:ARG:HA	3:D:256:ARG:HD2	1.83	0.42
4:E:1006:TYR:CE2	8:I:250:GLU:HG3	2.53	0.42
7:H:137:GLU:HA	7:H:140:ALA:HB3	2.01	0.42
9:J:232:GLU:OE1	9:J:232:GLU:N	2.51	0.42
3:D:114:THR:HG21	3:D:119:LEU:HD22	2.01	0.42
6:G:162:PHE:CG	6:G:180:LEU:HD22	2.54	0.42
11:L:109:ASP:OD1	11:L:316:LYS:N	2.50	0.42
14:P:122:ALA:HB2	14:P:131:ILE:HD12	2.00	0.42
15:Q:372:MET:HB2	15:Q:379:TYR:N	2.33	0.42
17:S:267:MET:HE1	17:S:337:LEU:HD21	2.01	0.42
1:B:212:LYS:HB2	1:B:212:LYS:HE3	1.82	0.42
3:D:306:LEU:HD13	3:D:324:GLN:HB3	2.00	0.42
3:D:514:PHE:HB2	3:D:517:MET:HE3	2.02	0.42
6:G:458:TYR:HA	6:G:461:VAL:HG22	2.01	0.42
7:H:535:GLN:HG2	13:N:109:GLY:O	2.19	0.42
10:K:136:PRO:HD2	10:K:389:ARG:O	2.19	0.42
12:M:200:TYR:N	12:M:226:LYS:O	2.51	0.42
15:Q:737:ARG:H	15:Q:737:ARG:HD3	1.84	0.42
21:Y:37:DC:H2''	21:Y:38:DG:C8	2.54	0.42
1:B:55:GLY:HA3	1:B:157:TYR:CE2	2.54	0.42
4:E:629:GLY:O	4:E:824:THR:N	2.34	0.42
4:E:1164:ASN:HB3	4:E:1168:ARG:NH1	2.35	0.42
4:E:1314:GLU:OE1	4:E:1314:GLU:N	2.50	0.42
5:F:405:MET:HG2	5:F:409:TYR:HA	2.01	0.42
6:G:601:MET:HA	6:G:604:VAL:HG12	2.01	0.42
6:G:650:VAL:O	6:G:653:VAL:HG12	2.19	0.42
7:H:370:ASN:ND2	7:H:373:GLU:HG3	2.35	0.42
11:L:283:ASP:N	11:L:283:ASP:OD1	2.52	0.42
20:X:52:DC:H2''	20:X:53:DA:C8	2.54	0.42
2:C:187:MET:SD	2:C:189:SER:OG	2.61	0.42
2:C:908:GLU:OE2	2:C:912:GLN:NE2	2.42	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:476:LEU:HD11	4:E:1115:VAL:HG22	2.01	0.42
5:F:81:ARG:NH1	5:F:92:GLU:OE1	2.50	0.42
6:G:235:GLU:O	6:G:239:GLU:HG2	2.19	0.42
6:G:793:MET:HE3	6:G:793:MET:HB3	1.98	0.42
11:L:163:ASP:OD1	11:L:163:ASP:N	2.51	0.42
11:L:345:PRO:HA	11:L:394:ALA:HB2	2.01	0.42
15:Q:624:ASN:C	15:Q:625:GLU:HG3	2.45	0.42
15:Q:673:TYR:CE2	15:Q:693:LEU:HB3	2.54	0.42
20:X:59:DA:H2"	20:X:60:DG:C8	2.54	0.42
3:D:172:LYS:HE3	3:D:173:TYR:CE2	2.55	0.42
5:F:482:ASP:HA	5:F:485:VAL:HG22	2.00	0.42
9:J:256:GLU:OE1	9:J:256:GLU:N	2.47	0.42
10:K:457:PRO:HA	10:K:460:TRP:CE2	2.54	0.42
13:N:85:ASN:O	13:N:89:VAL:HG23	2.19	0.42
2:C:979:ARG:N	21:Y:40:DG:OP1	2.53	0.42
4:E:1093:ILE:HG12	7:H:286:HIS:CD2	2.55	0.42
7:H:401:HIS:HB3	7:H:404:VAL:HG23	2.01	0.42
15:Q:341:MET:HG3	15:Q:407:LEU:HD13	2.02	0.42
15:Q:628:LYS:O	15:Q:631:VAL:HG22	2.20	0.42
17:S:445:TRP:CD2	17:S:449:LEU:HD23	2.55	0.42
18:T:58:LEU:HD22	18:T:63:VAL:HG11	2.02	0.42
18:T:85:LEU:HD23	18:T:113:ARG:HB2	2.00	0.42
2:C:510:ILE:HD12	2:C:511:ALA:O	2.20	0.42
4:E:904:PHE:CD1	18:T:94:ARG:HD2	2.54	0.42
6:G:472:GLU:H	6:G:472:GLU:HG3	1.64	0.42
10:K:279:ASN:O	10:K:283:LYS:HG2	2.20	0.42
12:M:210:ILE:HD11	12:M:217:LEU:HD23	2.02	0.42
13:N:120:GLN:HG2	13:N:208:ALA:HB2	2.00	0.42
15:Q:345:GLY:O	15:Q:437:VAL:N	2.50	0.42
17:S:446:HIS:CE1	17:S:449:LEU:HB2	2.55	0.42
19:U:130:PHE:CD1	19:U:134:GLU:HB2	2.54	0.42
2:C:789:ASP:OD2	2:C:791:ARG:NE	2.48	0.42
3:D:458:LEU:HB3	4:E:330:GLU:HG2	2.02	0.42
6:G:459:THR:HG23	6:G:492:THR:HA	2.02	0.42
10:K:122:TRP:CE2	14:O:106:THR:HG22	2.55	0.42
17:S:484:THR:HG22	17:S:537:ARG:HD2	2.01	0.42
1:B:309:MET:HE2	1:B:309:MET:HB2	1.75	0.42
2:C:402:THR:H	2:C:405:THR:HB	1.84	0.42
2:C:844:LEU:HB2	2:C:846:ASP:OD1	2.19	0.42
4:E:1110:THR:HG22	7:H:99:LEU:HD13	2.01	0.42
10:K:234:PHE:HB3	10:K:264:ILE:HD13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:Y:26:DA:H2''	21:Y:27:DA:C8	2.55	0.42
21:Y:37:DC:H2'	21:Y:38:DG:H8	1.84	0.42
1:B:194:GLU:N	1:B:194:GLU:OE1	2.52	0.41
4:E:1087:LYS:HE2	10:K:326:PHE:CG	2.54	0.41
6:G:528:PHE:O	6:G:532:ILE:HG12	2.20	0.41
6:G:691:GLU:OE1	6:G:695:ARG:NH1	2.48	0.41
15:Q:615:ILE:HA	15:Q:642:VAL:O	2.20	0.41
3:D:326:LYS:O	3:D:330:GLU:HG2	2.20	0.41
3:D:527:PRO:HB2	3:D:530:VAL:HG23	2.02	0.41
4:E:1204:LYS:HD3	4:E:1204:LYS:HA	1.91	0.41
7:H:337:ARG:HA	7:H:363:PHE:CE2	2.55	0.41
2:C:1007:MET:HB3	3:D:376:VAL:HG11	2.02	0.41
4:E:237:MET:SD	4:E:242:PHE:HB2	2.61	0.41
8:I:86:LEU:HD22	8:I:121:ALA:HA	2.02	0.41
11:L:395:ALA:HA	11:L:398:THR:HG22	2.02	0.41
15:Q:692:PHE:CZ	15:Q:759:GLU:HB2	2.55	0.41
17:S:505:GLN:HB2	17:S:514:TYR:CZ	2.55	0.41
20:X:32:DT:H2''	20:X:33:DC:C5	2.55	0.41
22:Z:39:C:H2'	22:Z:40:G:C8	2.55	0.41
1:A:48:ALA:HB3	1:B:226:PHE:CZ	2.53	0.41
4:E:104:TRP:CG	4:E:164:PRO:HG3	2.55	0.41
4:E:860:VAL:O	4:E:871:PHE:N	2.52	0.41
4:E:1231:LYS:HD3	4:E:1250:GLY:HA2	2.03	0.41
5:F:413:VAL:HA	5:F:798:LEU:HD22	2.02	0.41
7:H:399:SER:HB3	7:H:517:TRP:HD1	1.86	0.41
8:I:106:LYS:HE2	8:I:106:LYS:HB3	1.89	0.41
10:K:218:LEU:O	10:K:249:THR:OG1	2.32	0.41
12:M:149:CYS:HB3	12:M:258:LYS:HE2	2.02	0.41
15:Q:359:ILE:HG21	15:Q:415:VAL:HG21	2.02	0.41
17:S:498:LEU:HD23	17:S:518:THR:HG22	2.02	0.41
2:C:826:HIS:NE2	2:C:870:GLU:OE1	2.47	0.41
3:D:68:ILE:HD12	3:D:69:CYS:O	2.21	0.41
3:D:508:GLU:OE2	4:E:1326:THR:OG1	2.33	0.41
4:E:269:LEU:HD23	4:E:269:LEU:HA	1.89	0.41
5:F:542:LEU:HD21	5:F:564:VAL:HG11	2.03	0.41
6:G:77:LEU:HD23	6:G:109:VAL:HG21	2.02	0.41
6:G:225:ASP:HA	6:G:258:ARG:HH22	1.86	0.41
6:G:574:ARG:HE	6:G:607:LYS:HE2	1.85	0.41
6:G:796:ARG:HG2	6:G:800:LYS:NZ	2.36	0.41
7:H:273:TYR:OH	8:I:98:GLY:O	2.30	0.41
10:K:356:VAL:HB	10:K:364:HIS:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:334:MET:HE3	11:L:334:MET:HB3	1.98	0.41
13:N:51:LYS:NZ	13:N:129:GLU:OE2	2.38	0.41
15:Q:362:LEU:O	15:Q:365:ALA:N	2.53	0.41
2:C:32:ILE:HD13	2:C:32:ILE:HA	1.96	0.41
2:C:407:ASN:OD1	2:C:408:PHE:N	2.54	0.41
2:C:714:LEU:HD13	2:C:719:LEU:HD21	2.02	0.41
3:D:205:ASP:HB3	5:F:453:ARG:CZ	2.50	0.41
3:D:384:ILE:HG22	3:D:476:ILE:HB	2.02	0.41
4:E:372:THR:OG1	4:E:373:ARG:N	2.53	0.41
6:G:458:TYR:HE2	6:G:484:VAL:HG21	1.84	0.41
8:I:110:ASN:HB3	8:I:113:ASN:O	2.20	0.41
13:N:217:SER:HG	13:N:264:ARG:HH21	1.65	0.41
14:P:146:MET:SD	17:S:314:LEU:HB3	2.60	0.41
15:Q:706:ALA:HA	15:Q:747:VAL:HG23	2.03	0.41
2:C:824:GLY:O	27:C:1101:HOH:O	2.22	0.41
4:E:111:LEU:HD12	4:E:149:MET:HG2	2.03	0.41
4:E:666:ARG:N	7:H:599:TRP:HZ2	2.19	0.41
4:E:1180:LEU:HD13	4:E:1188:ILE:HD12	2.02	0.41
6:G:201:LYS:NZ	6:G:235:GLU:OE2	2.48	0.41
6:G:644:ASP:OD1	6:G:644:ASP:N	2.51	0.41
7:H:170:ASP:OD1	7:H:170:ASP:N	2.48	0.41
7:H:414:GLU:HG3	7:H:472:LEU:HD22	2.02	0.41
22:Z:39:C:H2'	22:Z:40:G:H8	1.86	0.41
3:D:367:PHE:HA	3:D:371:LEU:HD12	2.03	0.41
4:E:669:PHE:H	4:E:782:VAL:HG12	1.86	0.41
7:H:298:VAL:HG13	7:H:299:HIS:CD2	2.56	0.41
7:H:536:ALA:O	13:N:207:ASN:ND2	2.53	0.41
10:K:197:LYS:HG3	10:K:210:VAL:HG21	2.01	0.41
11:L:298:ARG:HD2	11:L:301:ASP:OD1	2.21	0.41
1:B:98:SER:HB3	1:B:127:VAL:HA	2.03	0.41
2:C:178:ILE:HD11	2:C:230:PHE:HB2	2.03	0.41
2:C:258:LEU:HD13	2:C:266:ILE:HD12	2.03	0.41
2:C:846:ASP:OD2	2:C:848:ARG:NE	2.52	0.41
3:D:15:VAL:HG22	3:D:19:GLN:HB3	2.03	0.41
3:D:120:LYS:HB3	3:D:120:LYS:HE3	1.85	0.41
3:D:213:GLU:CD	5:F:471:ILE:HG21	2.46	0.41
5:F:314:ASP:O	5:F:318:VAL:HG12	2.21	0.41
5:F:488:ARG:HA	5:F:488:ARG:HD3	1.76	0.41
6:G:467:GLN:O	6:G:715:ARG:NH1	2.35	0.41
6:G:617:LEU:HD23	6:G:617:LEU:HA	1.93	0.41
7:H:126:LYS:HA	7:H:126:LYS:HD3	1.81	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:236:ASN:CG	7:H:239:ARG:HH12	2.29	0.41
7:H:449:GLU:N	7:H:466:LYS:HZ1	2.19	0.41
10:K:383:THR:OG1	10:K:386:THR:OG1	2.16	0.41
10:K:430:ILE:HG13	10:K:450:LEU:HD22	2.03	0.41
13:N:60:LEU:HD12	13:N:69:LEU:HD21	2.03	0.41
14:O:84:ALA:O	14:O:88:GLN:HG3	2.20	0.41
14:O:120:MET:HE3	14:O:120:MET:HA	2.03	0.41
14:P:114:MET:SD	14:P:154:LEU:HD11	2.61	0.41
15:Q:437:VAL:HA	15:Q:475:VAL:HB	2.03	0.41
17:S:446:HIS:ND1	17:S:448:ASN:OD1	2.52	0.41
22:Z:35:C:H2'	22:Z:36:G:C8	2.55	0.41
1:A:150:LYS:HD3	1:A:150:LYS:HA	1.82	0.41
3:D:104:MET:SD	3:D:273:PRO:HD3	2.61	0.41
3:D:455:ALA:HB3	3:D:456:PRO:HD3	2.03	0.41
4:E:475:HIS:ND1	7:H:96:ARG:HD2	2.36	0.41
4:E:579:ILE:HD13	4:E:579:ILE:HA	1.95	0.41
7:H:528:LEU:HB3	13:N:214:TRP:CD1	2.56	0.41
15:Q:301:ALA:O	15:Q:318:ILE:HA	2.20	0.41
15:Q:614:ILE:O	15:Q:640:SER:OG	2.28	0.41
4:E:43:LYS:HE2	4:E:43:LYS:HB3	1.87	0.40
5:F:410:ARG:HD3	5:F:816:VAL:HG21	2.04	0.40
6:G:162:PHE:CD1	6:G:180:LEU:HD22	2.56	0.40
6:G:299:VAL:HA	6:G:302:LEU:HD12	2.03	0.40
9:J:415:ASN:HD22	9:J:416:MET:N	2.19	0.40
10:K:124:MET:HA	10:K:127:TRP:CE2	2.56	0.40
10:K:157:MET:HE1	10:K:228:LEU:HG	2.03	0.40
15:Q:614:ILE:HB	15:Q:640:SER:HA	2.02	0.40
7:H:121:PRO:HB3	7:H:124:ARG:NH2	2.36	0.40
10:K:85:PHE:HD2	10:K:87:TYR:H	1.69	0.40
12:M:266:LEU:HD22	12:M:292:LYS:HE2	2.04	0.40
14:P:173:PRO:CA	17:S:562:ASN:HD21	2.35	0.40
16:R:66:PRO:HG2	16:R:67:PHE:CD2	2.56	0.40
2:C:814:ARG:HH11	2:C:955:GLN:HE21	1.70	0.40
5:F:164:LEU:HD22	5:F:174:ILE:HB	2.04	0.40
7:H:164:ARG:HG2	7:H:166:ILE:HG13	2.03	0.40
7:H:415:GLN:OE1	7:H:481:ARG:NH2	2.51	0.40
7:H:502:LYS:HE2	7:H:502:LYS:HB3	1.83	0.40
7:H:517:TRP:NE1	13:N:187:ASN:O	2.44	0.40
15:Q:659:LEU:HD12	15:Q:659:LEU:HA	1.80	0.40
20:X:47:DG:OP1	20:X:47:DG:H8	2.04	0.40
2:C:62:PRO:HB3	2:C:77:SER:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:695:ILE:HB	2:C:777:LEU:HD22	2.02	0.40
3:D:16:SER:HB3	3:D:263:TRP:CZ2	2.56	0.40
3:D:610:GLN:HG2	12:M:203:TYR:CD2	2.56	0.40
3:D:654:THR:OG1	3:D:655:THR:N	2.53	0.40
5:F:182:VAL:HG21	5:F:212:LEU:HD21	2.02	0.40
5:F:418:GLU:HG2	5:F:419:PRO:HD3	2.03	0.40
5:F:557:ARG:C	5:F:559:VAL:H	2.28	0.40
6:G:78:ILE:HD13	6:G:112:GLU:HG2	2.02	0.40
6:G:365:ARG:HD3	6:G:365:ARG:HA	1.89	0.40
6:G:785:THR:HG22	6:G:793:MET:HB2	2.02	0.40
2:C:401:LEU:H	2:C:401:LEU:HG	1.74	0.40
3:D:12:ILE:HD11	4:E:1300:ALA:HB3	2.02	0.40
4:E:37:HIS:CE1	16:R:75:ILE:HD11	2.57	0.40
4:E:436:GLU:OE1	4:E:436:GLU:N	2.55	0.40
6:G:314:ASP:O	6:G:317:SER:OG	2.36	0.40
7:H:590:LYS:HD3	7:H:590:LYS:HA	1.87	0.40
9:J:212:PRO:HB2	9:J:270:LYS:HG2	2.03	0.40
9:J:291:PHE:O	9:J:295:ARG:HG3	2.21	0.40
11:L:214:VAL:HG12	11:L:218:ARG:NE	2.37	0.40
12:M:231:LYS:HG2	12:M:232:HIS:O	2.21	0.40
14:O:160:ASP:OD2	14:O:162:SER:OG	2.39	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	295/327 (90%)	284 (96%)	11 (4%)	0	100	100
1	B	279/327 (85%)	273 (98%)	6 (2%)	0	100	100
2	C	1036/1072 (97%)	1016 (98%)	19 (2%)	1 (0%)	48	69
3	D	597/680 (88%)	571 (96%)	26 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	E	1057/1373 (77%)	1011 (96%)	44 (4%)	2 (0%)	43	64
5	F	650/911 (71%)	631 (97%)	18 (3%)	1 (0%)	43	64
6	G	744/862 (86%)	730 (98%)	14 (2%)	0	100	100
7	H	547/675 (81%)	536 (98%)	11 (2%)	0	100	100
8	I	213/263 (81%)	204 (96%)	9 (4%)	0	100	100
9	J	230/529 (44%)	224 (97%)	6 (3%)	0	100	100
10	K	382/460 (83%)	370 (97%)	11 (3%)	1 (0%)	36	56
11	L	412/483 (85%)	400 (97%)	11 (3%)	1 (0%)	43	64
12	M	213/334 (64%)	210 (99%)	3 (1%)	0	100	100
13	N	222/297 (75%)	216 (97%)	6 (3%)	0	100	100
14	O	112/185 (60%)	110 (98%)	2 (2%)	0	100	100
14	P	106/185 (57%)	105 (99%)	1 (1%)	0	100	100
15	Q	537/768 (70%)	522 (97%)	15 (3%)	0	100	100
16	R	126/162 (78%)	121 (96%)	5 (4%)	0	100	100
17	S	382/611 (62%)	369 (97%)	13 (3%)	0	100	100
18	T	102/140 (73%)	96 (94%)	6 (6%)	0	100	100
19	U	107/187 (57%)	106 (99%)	1 (1%)	0	100	100
All	All	8349/10831 (77%)	8105 (97%)	238 (3%)	6 (0%)	49	69

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	E	489	ILE
4	E	793	LEU
11	L	405	ILE
2	C	1030	THR
5	F	553	ILE
10	K	87	TYR

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	275/301 (91%)	271 (98%)	4 (2%)	57	79
1	B	258/301 (86%)	255 (99%)	3 (1%)	63	82
2	C	905/931 (97%)	890 (98%)	15 (2%)	53	76
3	D	546/608 (90%)	539 (99%)	7 (1%)	61	81
4	E	969/1230 (79%)	956 (99%)	13 (1%)	61	81
5	F	565/782 (72%)	558 (99%)	7 (1%)	63	82
6	G	642/740 (87%)	639 (100%)	3 (0%)	81	91
7	H	489/609 (80%)	485 (99%)	4 (1%)	73	87
8	I	187/230 (81%)	185 (99%)	2 (1%)	65	83
9	J	212/469 (45%)	211 (100%)	1 (0%)	81	91
10	K	338/401 (84%)	333 (98%)	5 (2%)	57	79
11	L	369/431 (86%)	366 (99%)	3 (1%)	73	87
12	M	205/299 (69%)	198 (97%)	7 (3%)	32	58
13	N	192/259 (74%)	190 (99%)	2 (1%)	68	85
14	O	103/169 (61%)	103 (100%)	0	100	100
14	P	97/169 (57%)	97 (100%)	0	100	100
15	Q	458/661 (69%)	450 (98%)	8 (2%)	53	76
16	R	114/144 (79%)	114 (100%)	0	100	100
17	S	336/532 (63%)	336 (100%)	0	100	100
18	T	93/126 (74%)	92 (99%)	1 (1%)	65	83
19	U	91/160 (57%)	91 (100%)	0	100	100
All	All	7444/9552 (78%)	7359 (99%)	85 (1%)	63	83

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	73	ASP
1	A	138	THR
1	A	143	ILE
1	A	301	ASN
1	B	100	LEU
1	B	159	LEU
1	B	275	ASP
2	C	56	THR

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Mol	Chain	Res	Type
2	C	79	GLU
2	C	82	VAL
2	C	196	GLU
2	C	266	ILE
2	C	401	LEU
2	C	402	THR
2	C	469	LEU
2	C	510	ILE
2	C	659	VAL
2	C	722	LEU
2	C	923	TYR
2	C	943	ILE
2	C	944	ILE
2	C	1021	VAL
3	D	1	MET
3	D	14	LEU
3	D	15	VAL
3	D	68	ILE
3	D	216	LEU
3	D	236	LYS
3	D	535	MET
4	E	56	SER
4	E	368	LEU
4	E	463	THR
4	E	489	ILE
4	E	490	LEU
4	E	784	THR
4	E	793	LEU
4	E	795	THR
4	E	796	LEU
4	E	864	THR
4	E	945	ASN
4	E	990	TYR
4	E	997	THR
5	F	133	LEU
5	F	360	ASN
5	F	412	LEU
5	F	497	GLU
5	F	597	LEU
5	F	808	VAL
5	F	848	LEU
6	G	245	ILE

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Mol	Chain	Res	Type
6	G	577	ASP
6	G	776	ASP
7	H	113	ILE
7	H	474	LEU
7	H	532	SER
7	H	535	GLN
8	I	148	GLU
8	I	203	ASP
9	J	335	THR
10	K	88	ASP
10	K	99	VAL
10	K	246	MET
10	K	383	THR
10	K	392	SER
11	L	218	ARG
11	L	246	ASP
11	L	303	ILE
12	M	120	PHE
12	M	131	VAL
12	M	181	VAL
12	M	261	THR
12	M	266	LEU
12	M	301	ASP
12	M	316	GLU
13	N	63	HIS
13	N	67	GLU
15	Q	266	HIS
15	Q	362	LEU
15	Q	373	PHE
15	Q	633	THR
15	Q	643	THR
15	Q	746	TYR
15	Q	757	THR
15	Q	763	ARG
18	T	119	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (128) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	193	ASN
1	A	262	GLN
1	A	303	GLN

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Mol	Chain	Res	Type
1	B	14	GLN
1	B	180	GLN
1	B	196	GLN
1	B	303	GLN
2	C	16	ASN
2	C	17	GLN
2	C	19	GLN
2	C	93	ASN
2	C	124	ASN
2	C	135	GLN
2	C	228	GLN
2	C	278	ASN
2	C	307	ASN
2	C	322	GLN
2	C	334	ASN
2	C	441	HIS
2	C	475	GLN
2	C	516	HIS
2	C	524	GLN
2	C	538	HIS
2	C	542	ASN
2	C	624	GLN
2	C	713	HIS
2	C	812	GLN
2	C	867	GLN
2	C	883	HIS
2	C	954	HIS
2	C	974	GLN
2	C	1014	HIS
3	D	19	GLN
3	D	128	ASN
3	D	258	ASN
3	D	324	GLN
3	D	446	GLN
3	D	453	ASN
3	D	464	GLN
3	D	467	GLN
3	D	494	GLN
3	D	607	GLN
3	D	610	GLN
3	D	629	ASN
3	D	636	HIS

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Mol	Chain	Res	Type
3	D	674	GLN
4	E	41	GLN
4	E	78	GLN
4	E	113	GLN
4	E	118	ASN
4	E	144	HIS
4	E	283	GLN
4	E	310	HIS
4	E	326	GLN
4	E	739	HIS
4	E	792	ASN
4	E	922	HIS
4	E	1053	GLN
4	E	1054	ASN
4	E	1206	GLN
4	E	1291	GLN
4	E	1315	ASN
4	E	1365	HIS
5	F	84	ASN
5	F	270	ASN
5	F	360	ASN
5	F	363	ASN
5	F	788	GLN
5	F	835	GLN
6	G	130	GLN
6	G	182	ASN
6	G	217	ASN
6	G	351	ASN
6	G	362	GLN
6	G	363	ASN
6	G	409	HIS
6	G	518	ASN
6	G	624	ASN
6	G	628	ASN
6	G	640	ASN
7	H	228	GLN
7	H	249	GLN
7	H	289	GLN
7	H	322	HIS
7	H	588	HIS
8	I	68	GLN
8	I	123	GLN

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Mol	Chain	Res	Type
8	I	126	ASN
8	I	149	GLN
8	I	215	HIS
9	J	329	GLN
9	J	340	ASN
9	J	349	HIS
9	J	415	ASN
10	K	110	HIS
10	K	112	ASN
10	K	179	GLN
10	K	414	GLN
11	L	124	HIS
11	L	233	HIS
11	L	323	ASN
11	L	360	ASN
12	M	124	GLN
12	M	142	HIS
12	M	190	GLN
13	N	190	ASN
14	O	147	GLN
15	Q	440	ASN
15	Q	491	ASN
15	Q	509	HIS
15	Q	545	ASN
15	Q	676	HIS
15	Q	725	GLN
16	R	37	GLN
16	R	71	GLN
17	S	195	HIS
17	S	277	GLN
17	S	284	ASN
17	S	348	HIS
17	S	371	ASN
17	S	395	GLN
17	S	469	ASN
17	S	510	ASN
17	S	562	ASN
18	T	46	ASN
18	T	55	GLN
19	U	101	HIS
19	U	175	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
22	Z	10/40 (25%)	2 (20%)	1 (10%)

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
22	Z	32	C
22	Z	38	G

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
22	Z	31	C

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
26	SAH	L	8001	-	27,28,28	1.10	4 (14%)	36,40,40	2.12	11 (30%)

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
26	SAH	L	8001	-	-	3/15/31/31	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	L	8001	SAH	C2-N3	2.54	1.38	1.33
26	L	8001	SAH	C2-N1	2.46	1.38	1.33
26	L	8001	SAH	OXT-C	-2.28	1.23	1.30
26	L	8001	SAH	C5-N7	-2.11	1.35	1.39

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	L	8001	SAH	N3-C2-N1	-5.61	120.08	128.58
26	L	8001	SAH	C5-C4-N3	-4.82	120.08	126.72
26	L	8001	SAH	C5'-SD-CG	-3.85	90.83	102.26
26	L	8001	SAH	N9-C8-N7	-3.77	108.59	113.94
26	L	8001	SAH	C2-N3-C4	3.54	120.47	111.83
26	L	8001	SAH	C5-N7-C8	3.37	108.75	103.45
26	L	8001	SAH	N3-C4-N9	3.20	132.60	127.17
26	L	8001	SAH	OXT-C-O	-2.73	117.89	124.08
26	L	8001	SAH	C3'-C2'-C1'	2.37	105.94	101.46
26	L	8001	SAH	C4-C5-N7	-2.30	107.95	110.58
26	L	8001	SAH	C6-C5-C4	2.03	119.95	117.18

There are no chirality outliers.

All (3) torsion outliers are listed below:

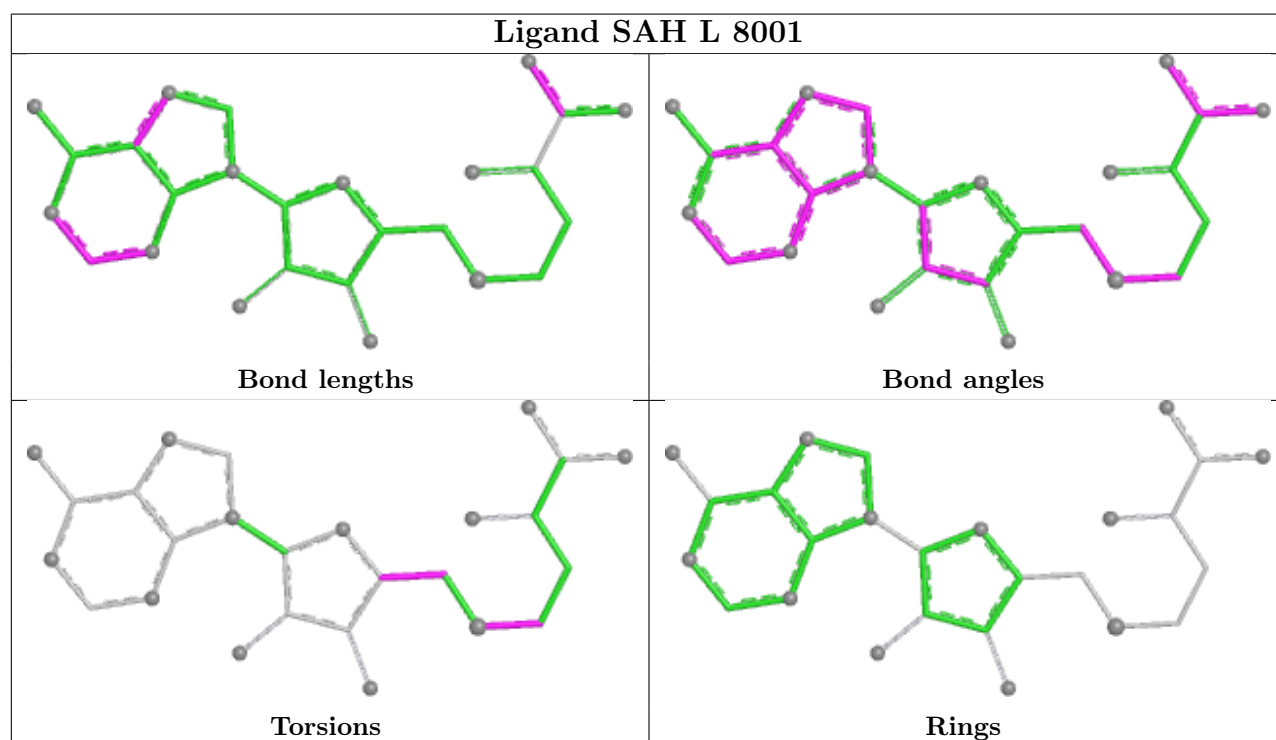
Mol	Chain	Res	Type	Atoms
26	L	8001	SAH	O4'-C4'-C5'-SD
26	L	8001	SAH	C3'-C4'-C5'-SD
26	L	8001	SAH	CB-CG-SD-C5'

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	L	8001	SAH	1	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

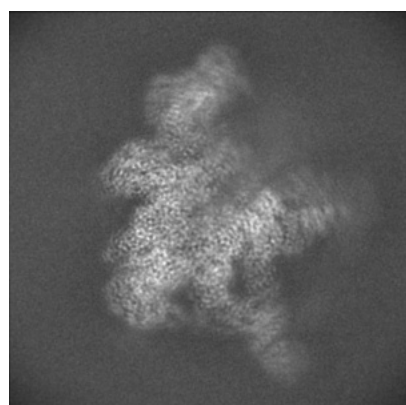
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19023. These allow visual inspection of the internal detail of the map and identification of artifacts.

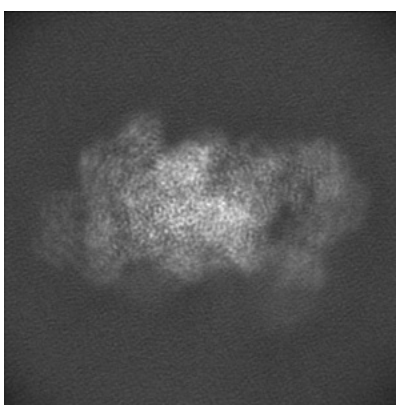
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

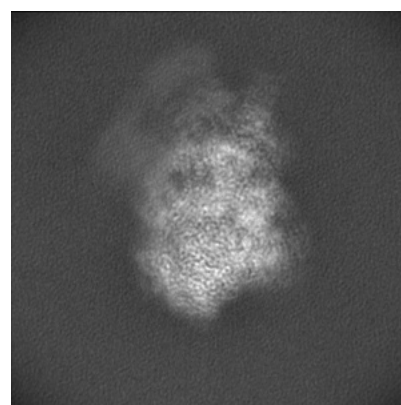
6.1.1 Primary map



X



Y

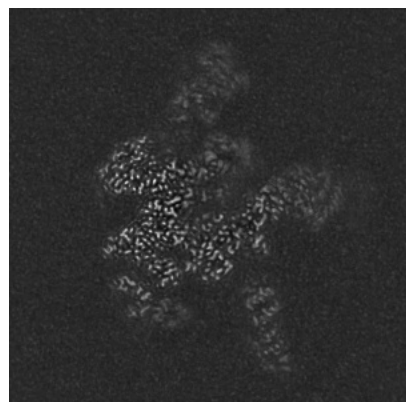


Z

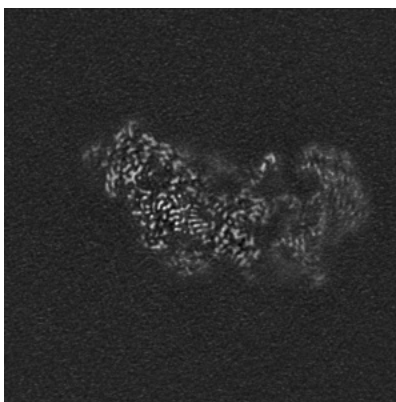
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

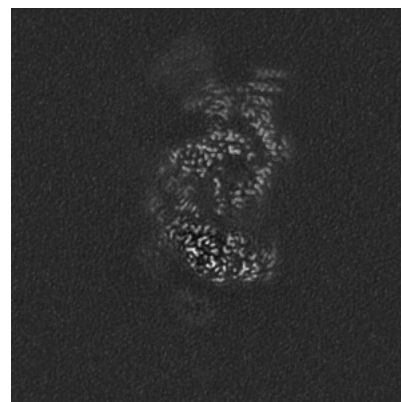
6.2.1 Primary map



X Index: 300



Y Index: 300

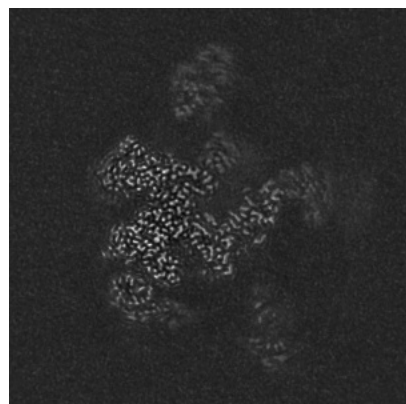


Z Index: 300

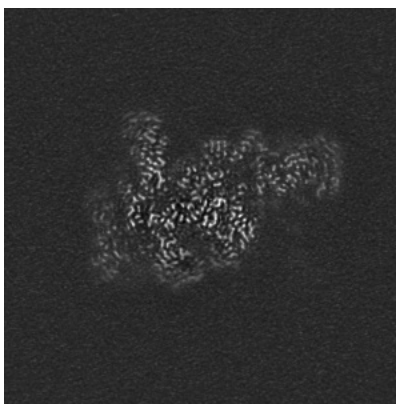
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

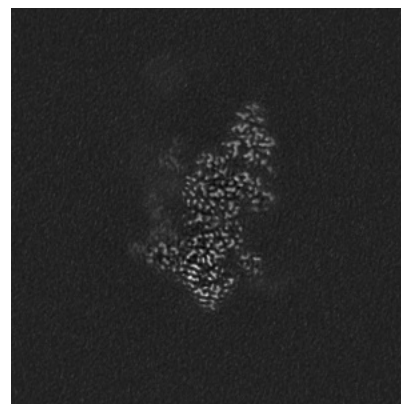
6.3.1 Primary map



X Index: 288



Y Index: 233

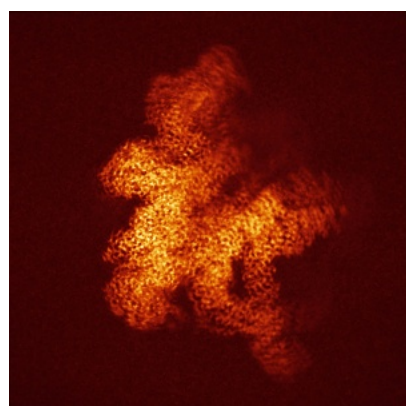


Z Index: 253

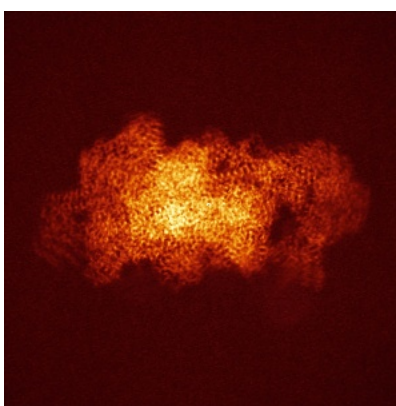
The images above show the largest variance slices of the map in three orthogonal directions.

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

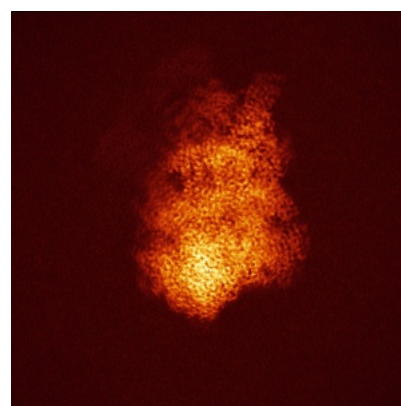
6.4.1 Primary map



X



Y

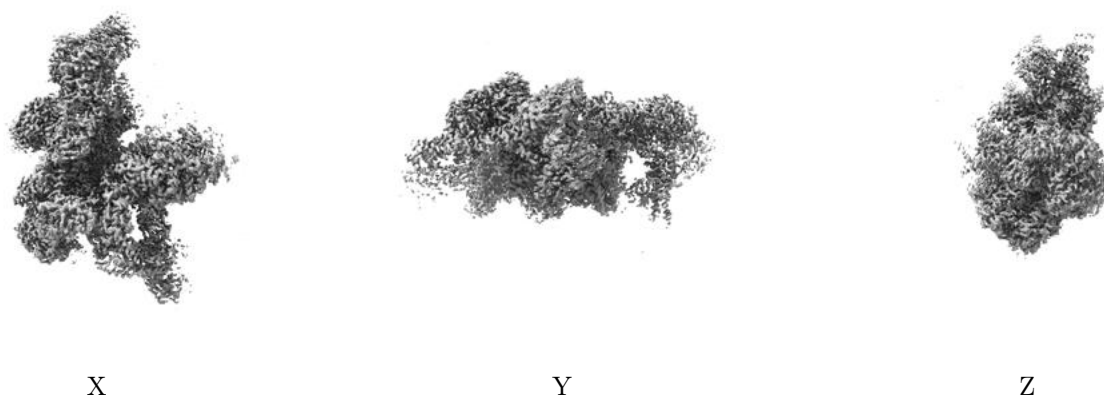


Z

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

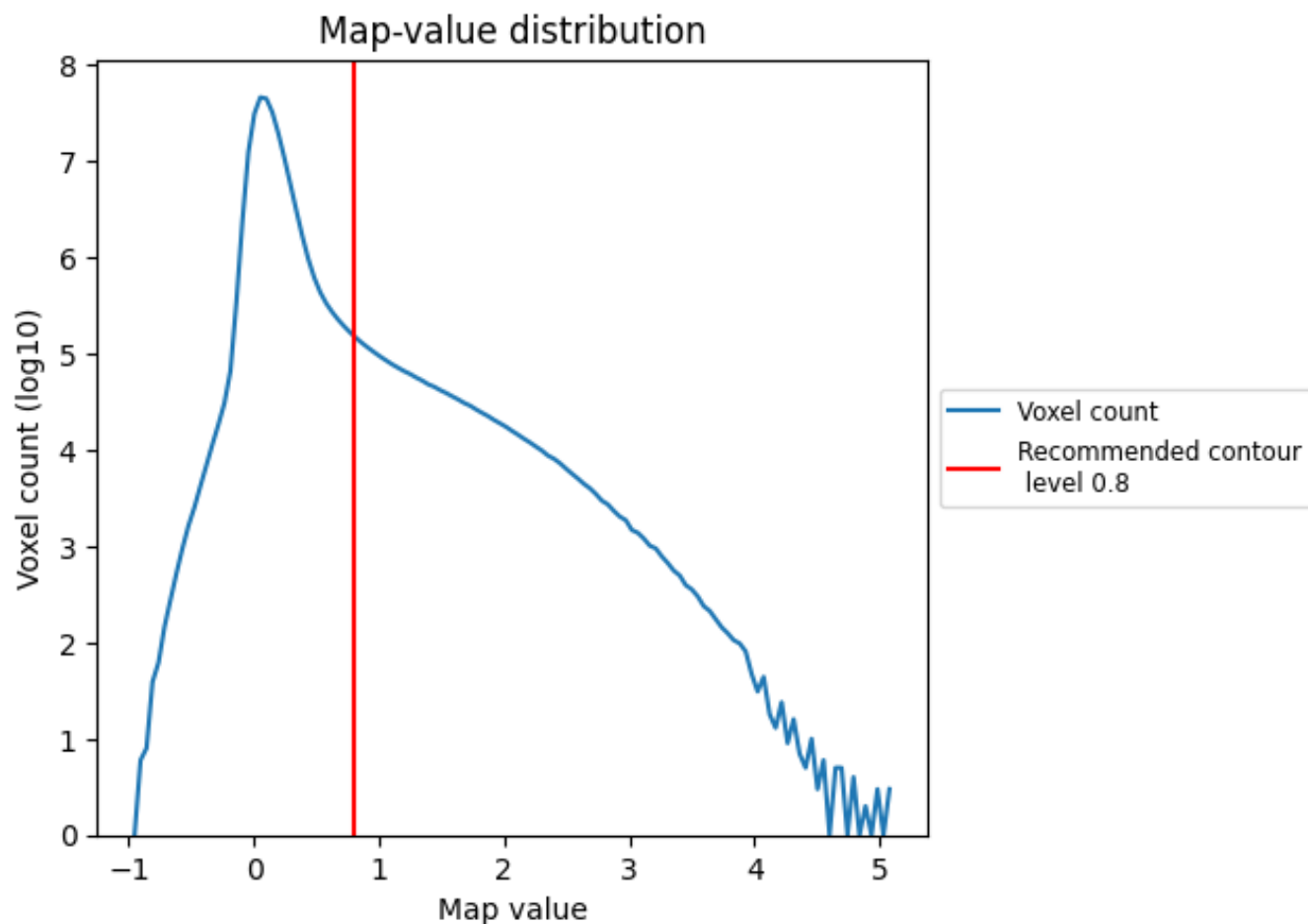
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

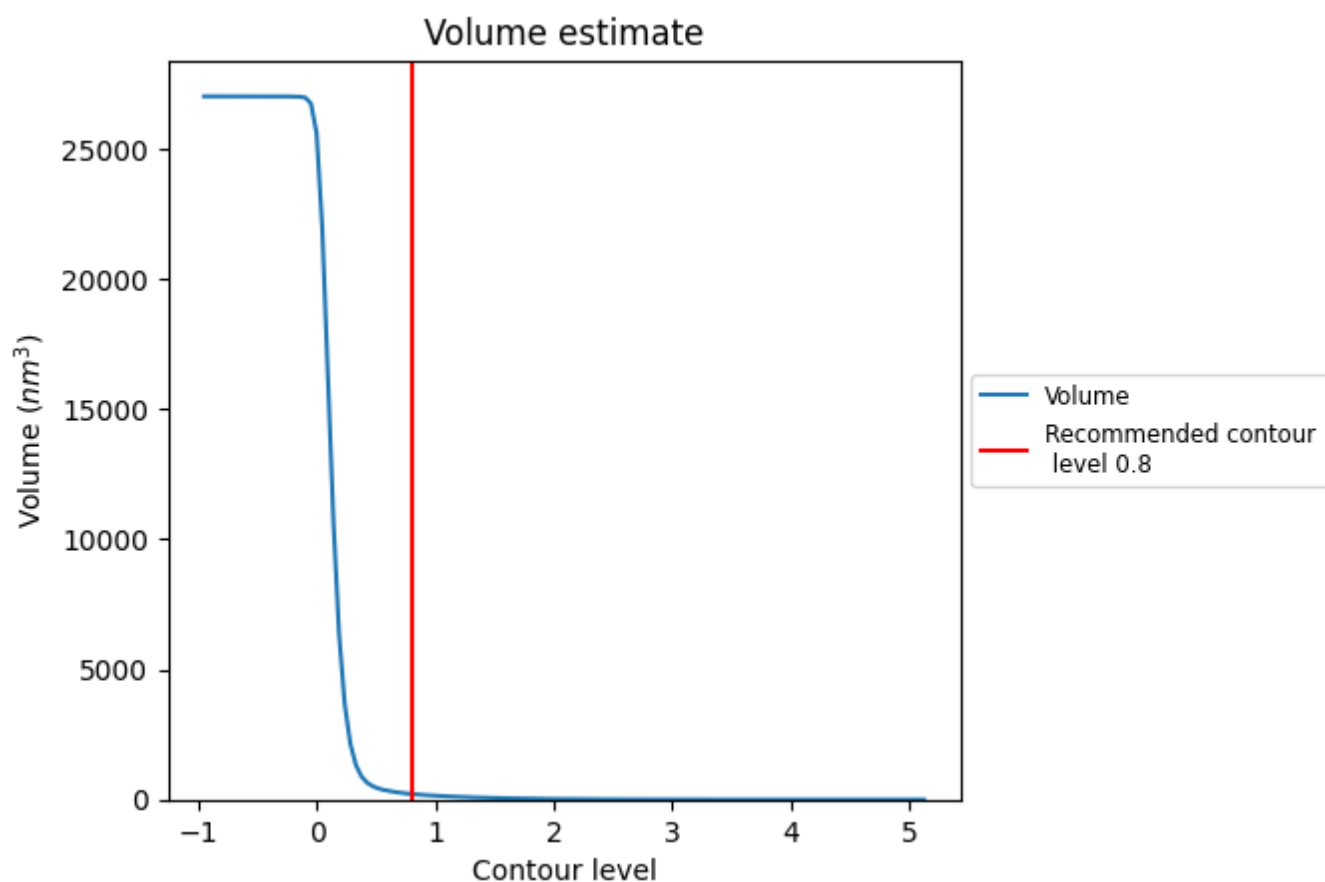
This section contains the results of statistical analysis of the map.

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.

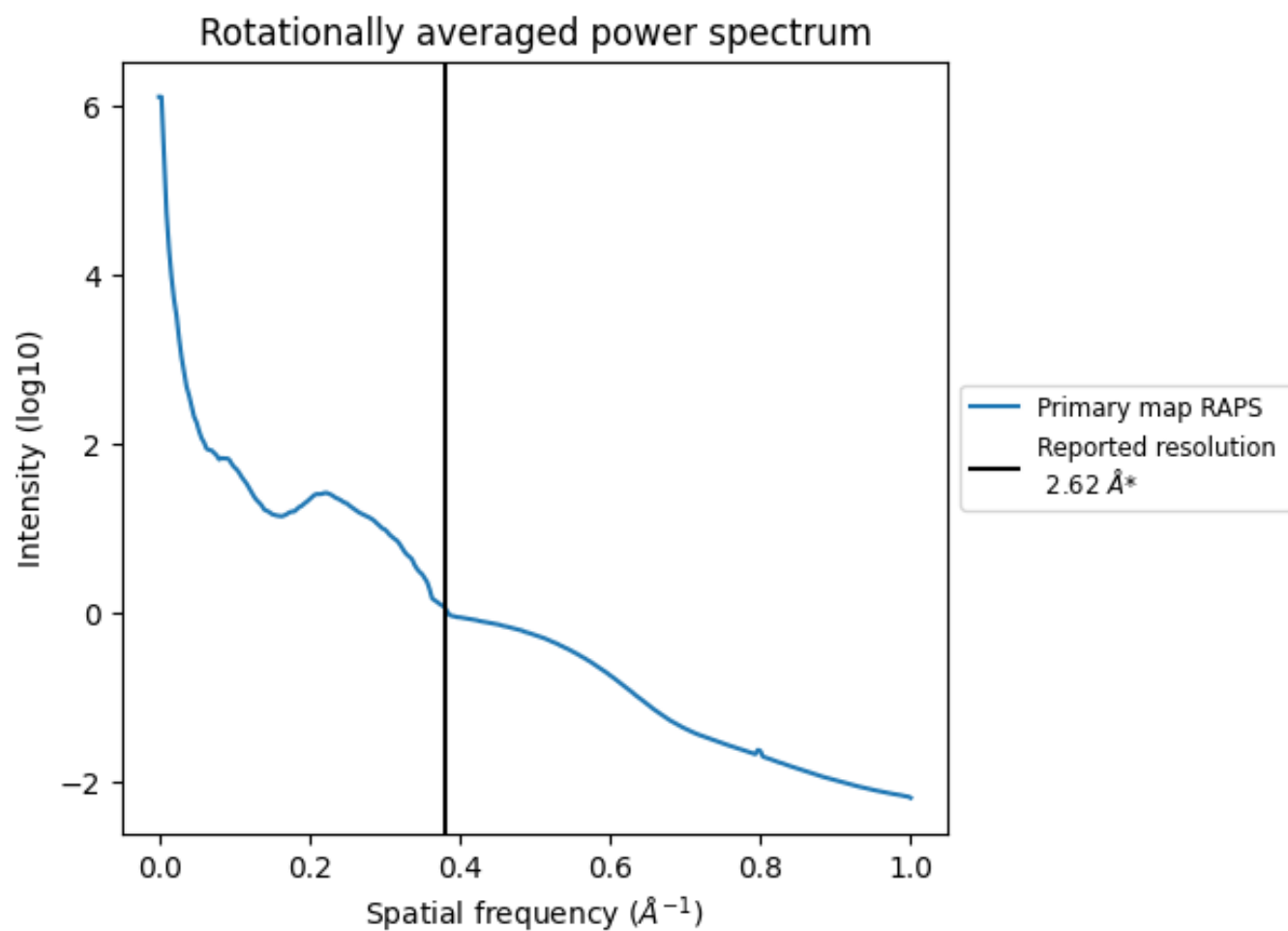
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 214 nm^3 ; this corresponds to an approximate mass of 193 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 0.382 Å⁻¹

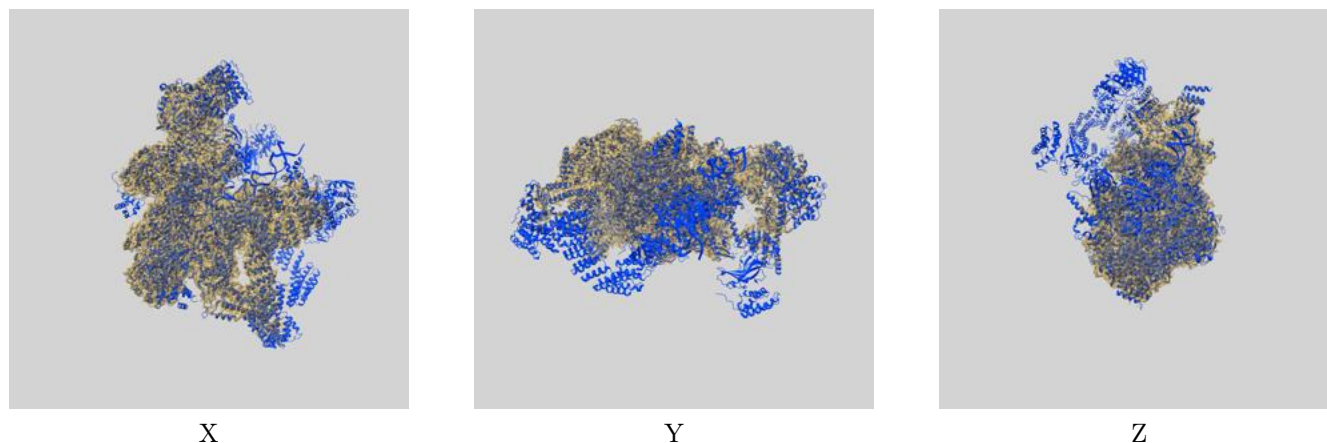
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

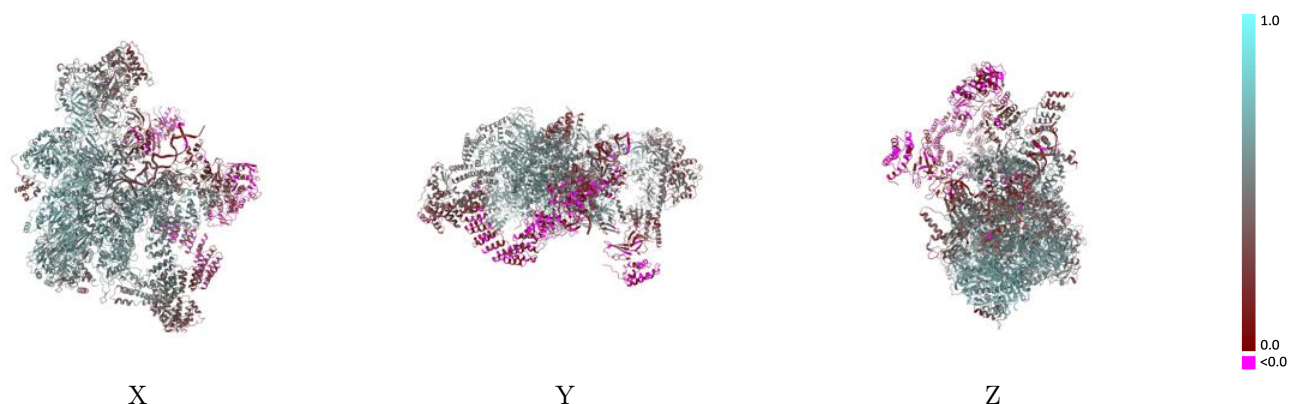
This section contains information regarding the fit between EMDB map EMD-19023 and PDB model 8RDJ. Per-residue inclusion information can be found in section [3](#) on page [10](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.8 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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

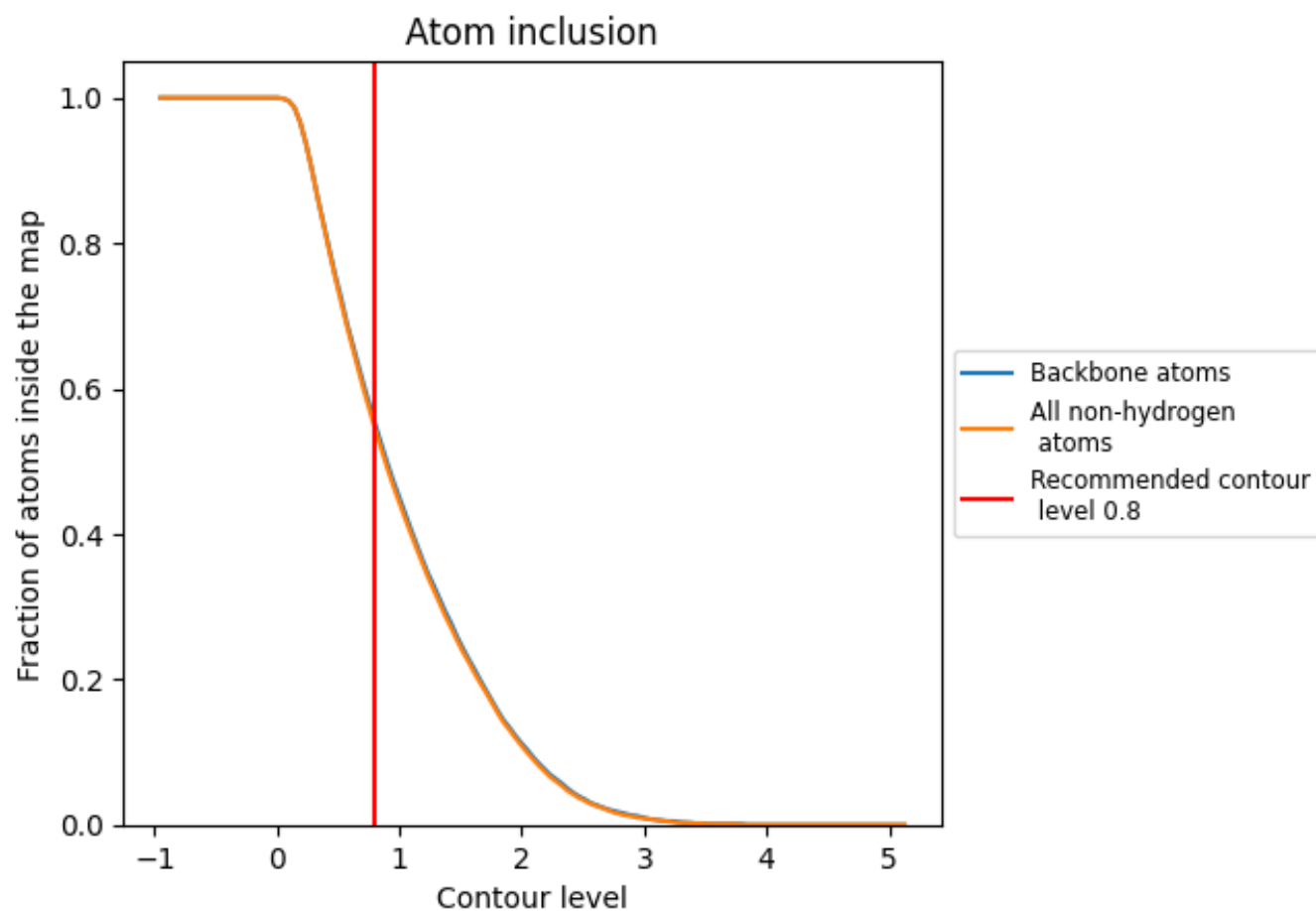


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 55% of all backbone atoms, 55% 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 (0.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5450	 0.4680
A	 0.6670	 0.5700
B	 0.5780	 0.5310
C	 0.6660	 0.5220
D	 0.7640	 0.5570
E	 0.6020	 0.4940
F	 0.6710	 0.4890
G	 0.0740	 0.2470
H	 0.4830	 0.4760
I	 0.4460	 0.4440
J	 0.8670	 0.6370
K	 0.8720	 0.6330
L	 0.7370	 0.5480
M	 0.6850	 0.5660
N	 0.1470	 0.3720
O	 0.8620	 0.6180
P	 0.5520	 0.5450
Q	 0.0710	 0.1330
R	 0.7050	 0.5630
S	 0.7540	 0.5930
T	 0.4670	 0.4500
U	 0.0000	 -0.0200
X	 0.1470	 0.1820
Y	 0.3530	 0.3440
Z	 0.4650	 0.3220

