



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 11:33 AM UTC

PDB ID : 7VPX / pdb_00007vpx
EMDB ID : EMD-32074
Title : The cryo-EM structure of the human pre-A complex
Authors : Zhang, X.; Zhan, X.; Shi, Y.
Deposited on : 2021-10-18
Resolution : 3.00 Å(reported)

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<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

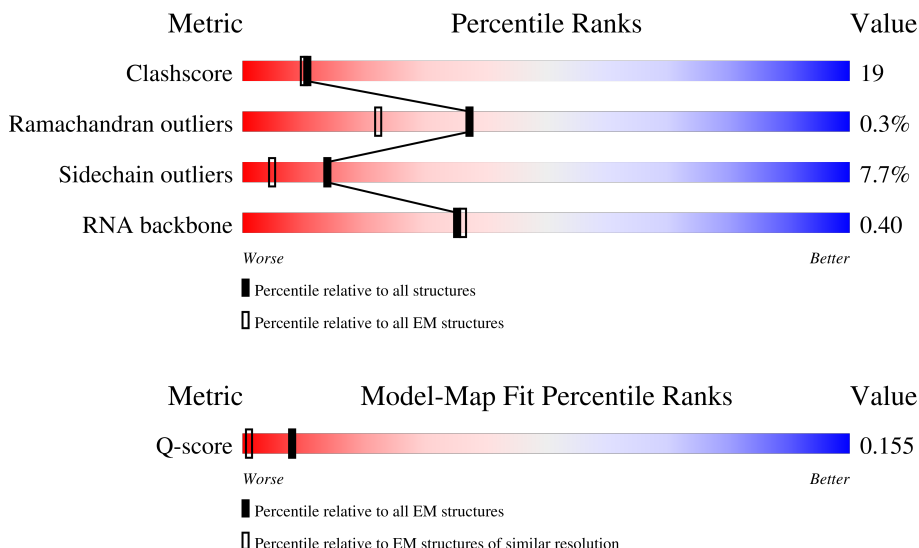
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 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	14081 (2.50 - 3.50)

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

Mol	Chain	Length	Quality of chain
1	B	464	23% 28% 68%
2	D	639	14% 19% 81%
3	J	253	5% 17% 79%

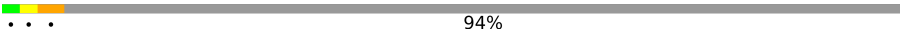
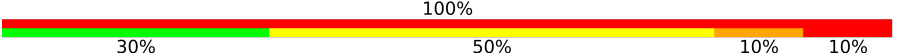
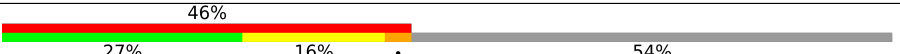
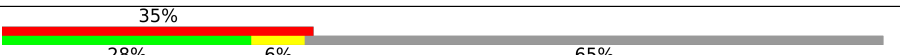
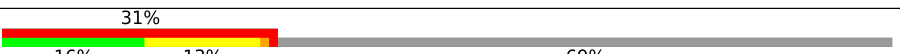
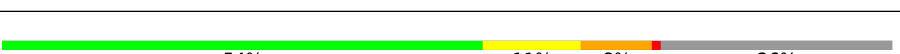
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Mol	Chain	Length	Quality of chain
4	H	188	
5	1	1304	
6	2	895	
7	3	1217	
8	4	424	
9	5	86	
10	A	793	
11	C	501	
12	E	1031	
13	F	255	
14	G	225	
15	a	118	
15	i	118	
16	b	86	
16	m	86	
17	c	92	
17	l	92	
18	d	76	
18	n	76	
19	e	126	
19	j	126	
20	f	240	
20	k	240	
21	g	119	
21	h	119	

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Mol	Chain	Length	Quality of chain
22	I	259	 . . . 94%
23	K	10	 30% 100% 50% 10% 10%
24	L	164	 40% 100% 37% 21% .
25	O	437	 46% 27% 16% . 54%
26	M	282	 35% 28% 6% 65%
27	N	159	 31% 16% 13% .. 69%
28	6	110	 54% 11% 8% . 26%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	SJT	6	204	X	-	-	-

2 Entry composition [i](#)

There are 30 unique types of molecules in this entry. The entry contains 43240 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 Splicing factor 3A subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	147	Total	C	N	O	S	0	0
			799	455	173	168	3		

- Molecule 2 is a protein called Splicing factor 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	D	122	Total	C	N	O	0	0
			604	360	122	122		

- Molecule 3 is a protein called DnaJ homolog subfamily C member 8.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	J	54	Total	C	N	O	0	0
			369	224	73	72		

- Molecule 4 is a RNA chain called U2 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	130	Total	C	N	O	P	0	0
			2754	1233	478	915	128		

- Molecule 5 is a protein called Splicing factor 3B subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	1	815	Total	C	N	O	S	0	0
			6487	4163	1121	1164	39		

- Molecule 6 is a protein called Splicing factor 3B subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	2	187	Total	C	N	O	S	0	0
			1325	835	245	243	2		

- Molecule 7 is a protein called Splicing factor 3B subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	3	1180	Total	C	N	O	S	0	0
			9247	5872	1571	1759	45		

- Molecule 8 is a protein called Splicing factor 3B subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	4	160	Total	C	N	O	0	0
			664	344	160	160		

- Molecule 9 is a protein called Splicing factor 3B subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	5	66	Total	C	N	O	S	0	0
			539	342	93	99	5		

- Molecule 10 is a protein called Splicing factor 3A subunit 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	A	123	Total	C	N	O	0	0
			504	258	123	123		

- Molecule 11 is a protein called Splicing factor 3A subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	C	425	Total	C	N	O	S	0	0
			2127	1191	470	462	4		

- Molecule 12 is a protein called Probable ATP-dependent RNA helicase DDX46.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	E	455	Total	C	N	O	S	0	0
			2153	1157	487	507	2		

- Molecule 13 is a protein called U2 small nuclear ribonucleoprotein A'.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	F	162	Total	C	N	O	0	0
			666	342	162	162		

- Molecule 14 is a protein called U2 small nuclear ribonucleoprotein B'.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	G	166	Total	C	N	O	0	0
			685	353	166	166		

- Molecule 15 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	a	90	Total	C	N	O	0	0
			372	192	90	90		
15	i	94	Total	C	N	O	S	0
			764	478	139	141	6	0

- Molecule 16 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	b	74	Total	C	N	O	0	0
			308	160	74	74		
16	m	74	Total	C	N	O	S	0
			576	373	95	103	5	0

- Molecule 17 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	c	79	Total	C	N	O	0	0
			319	161	79	79		
17	l	77	Total	C	N	O	S	0
			638	405	113	115	5	0

- Molecule 18 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	d	74	Total	C	N	O	0	0
			305	157	74	74		
18	n	73	Total	C	N	O	S	0
			568	358	102	102	6	0

- Molecule 19 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	e	83	Total	C	N	O	0	0
			341	175	83	83		
19	j	81	Total	C	N	O	S	0
			637	400	112	119	6	0

- Molecule 20 is a protein called Small nuclear ribonucleoprotein-associated proteins B and B'.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	f	71	Total	C	N	O		0	0
			293	151	71	71			
20	k	86	Total	C	N	O	S	0	0
			692	435	126	124	7		

- Molecule 21 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	g	82	Total	C	N	O		0	0
			337	173	82	82			
21	h	81	Total	C	N	O	S	0	0
			641	408	112	118	3		

- Molecule 22 is a RNA chain called pre-mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	I	15	Total	C	N	O	P	0	0
			314	141	51	107	15		

- Molecule 23 is a RNA chain called 5SS.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	K	10	Total	C	N	O	P	0	0
			216	97	42	68	9		

- Molecule 24 is a RNA chain called U1 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	L	164	Total	C	N	O	P	0	0
			3485	1555	607	1159	164		

- Molecule 25 is a protein called U1 small nuclear ribonucleoprotein 70 kDa.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	O	201	Total	C	N	O	S	0	0
			1643	1030	317	291	5		

- Molecule 26 is a protein called U1 small nuclear ribonucleoprotein A.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	M	98	Total	C	N	O	S	0	0
			787	506	134	143	4		

- Molecule 27 is a protein called U1 small nuclear ribonucleoprotein C.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	N	50	Total	C	N	O	S	0	0
			425	266	73	82	4		

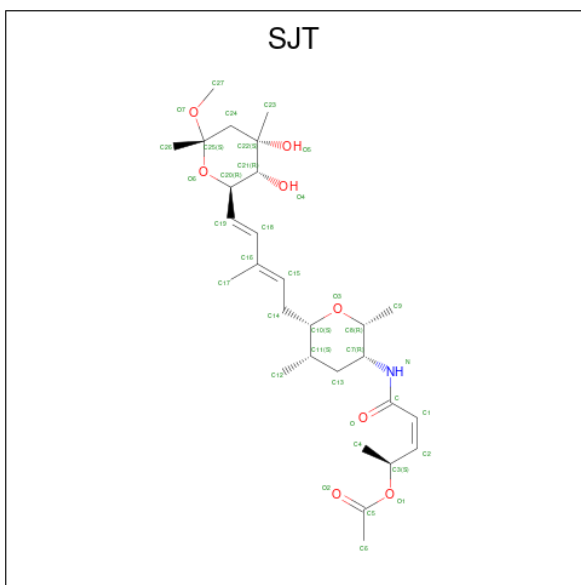
- Molecule 28 is a protein called PHD finger-like domain-containing protein 5A.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	6	81	Total	C	N	O	S	0	0
			613	376	109	115	13		

- Molecule 29 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
29	B	1	Total	Zn	0
			1	1	
29	C	1	Total	Zn	0
			1	1	
29	N	1	Total	Zn	0
			1	1	
29	6	3	Total	Zn	0
			3	3	

- Molecule 30 is spliceostatin A (form II) (CCD ID: SJT) (formula: C₂₈H₄₅NO₈) (labeled as "Ligand of Interest" by depositor).

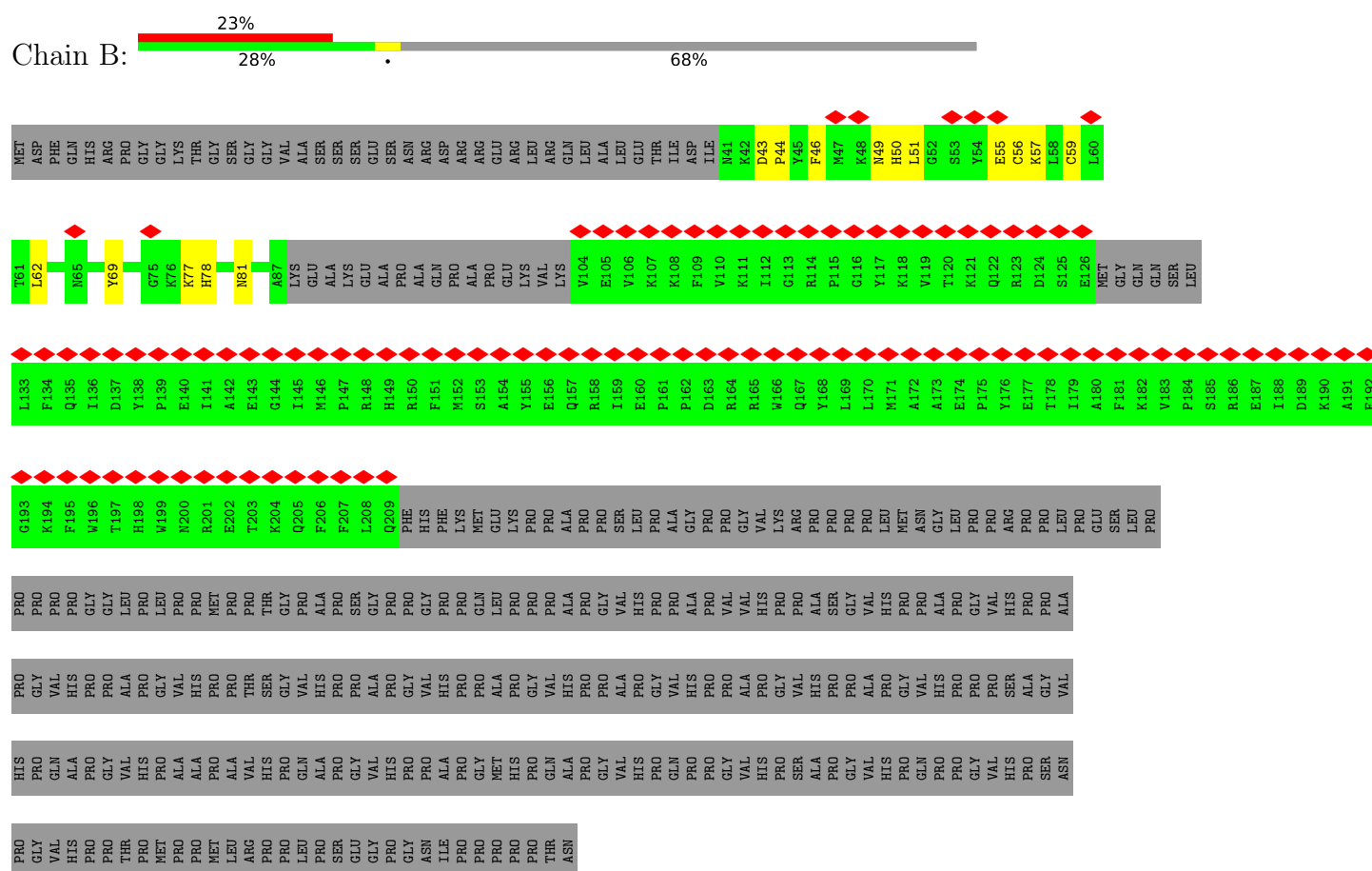


Mol	Chain	Residues	Atoms				AltConf
30	6	1	Total	C	N	O	0
			37	28	1	8	

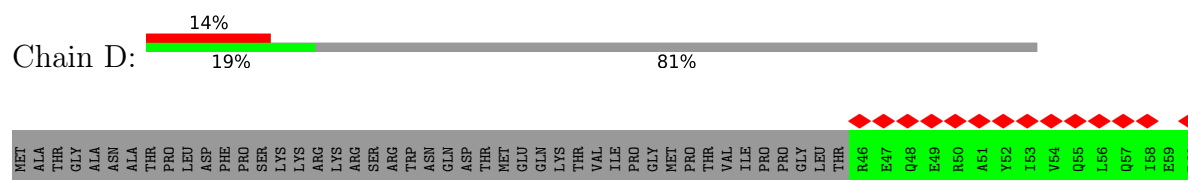
3 Residue-property plots

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: Splicing factor 3A subunit 2

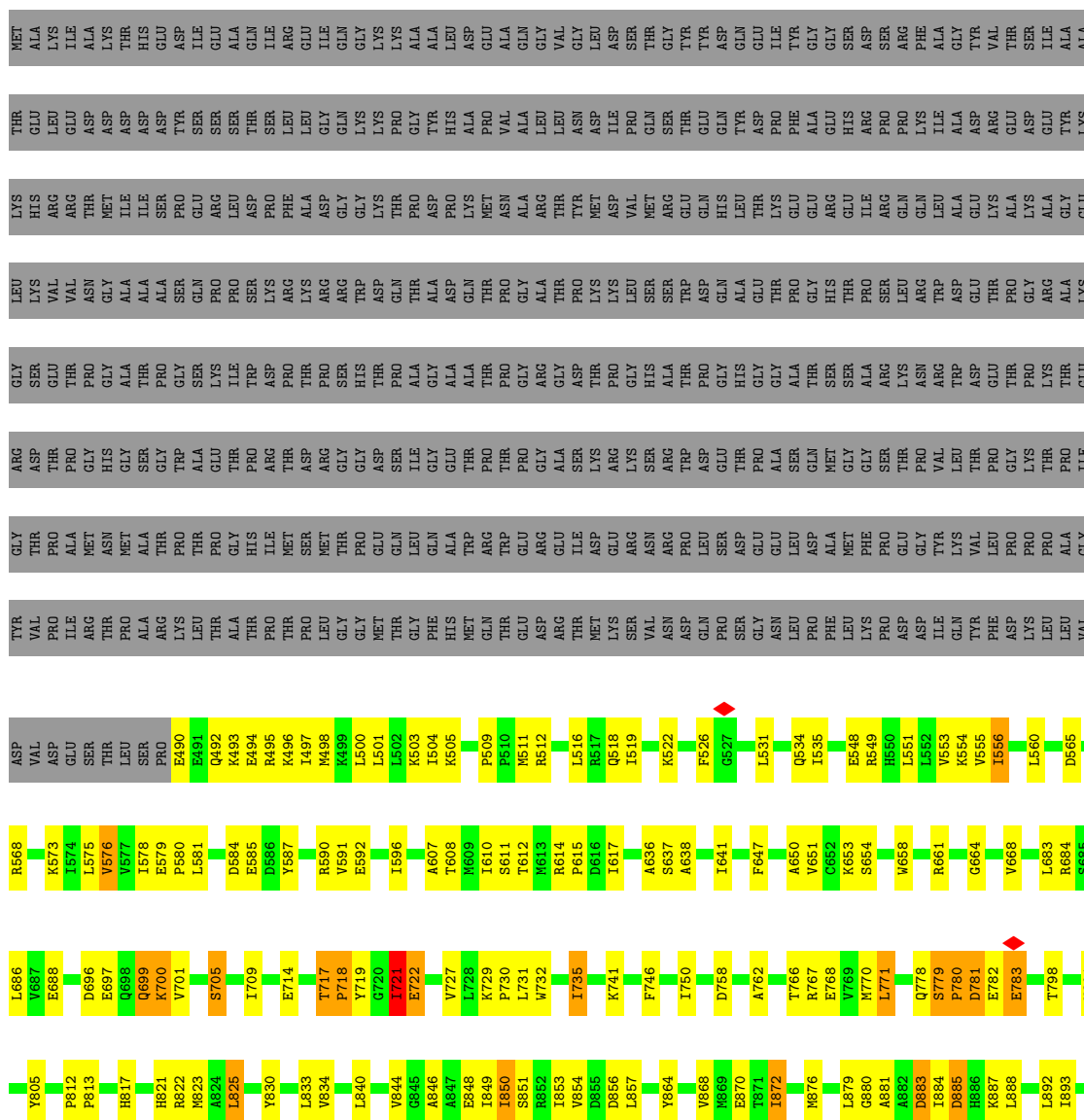
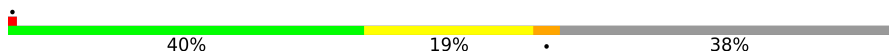


• Molecule 2: Splicing factor 1



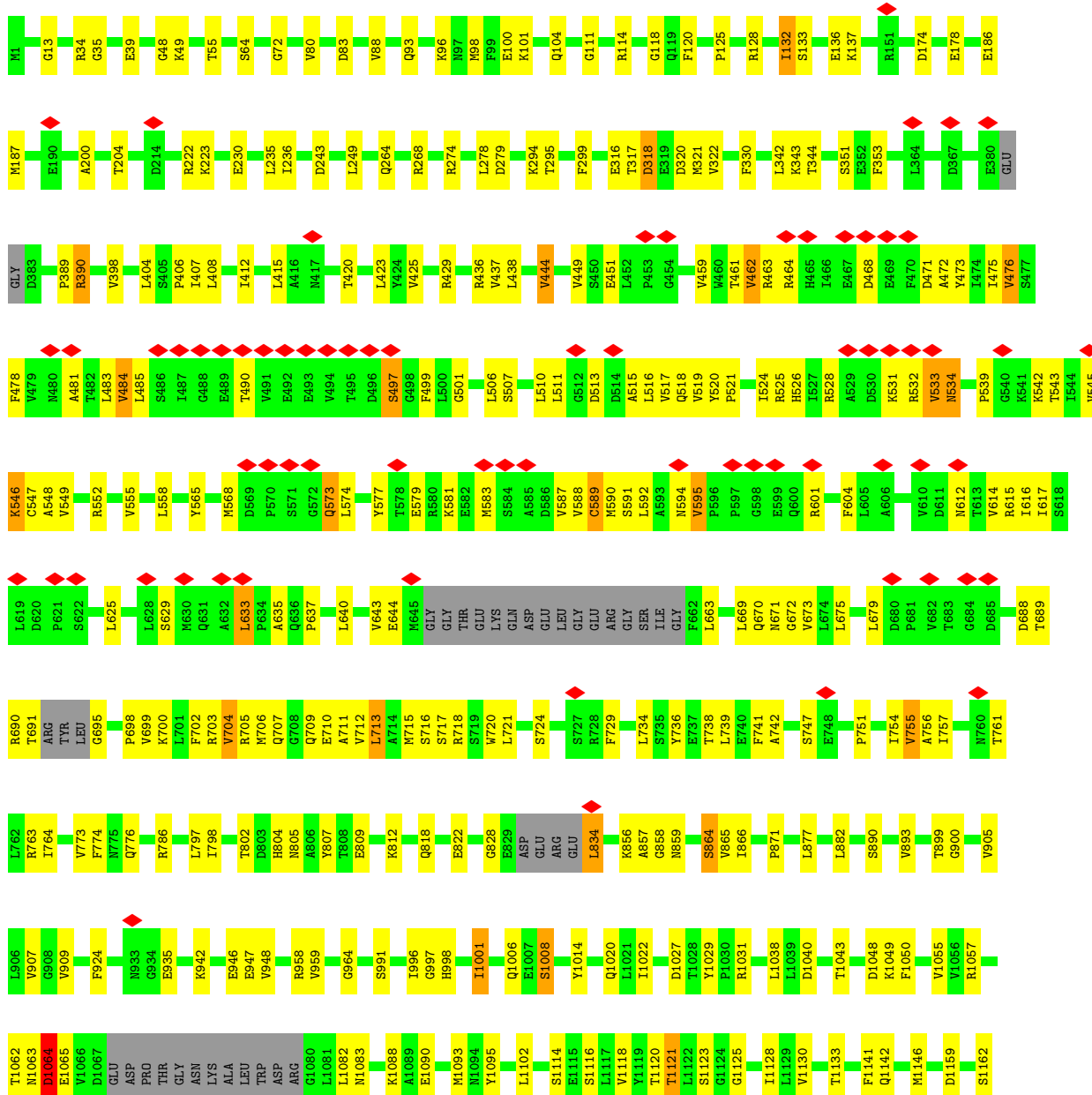
- Molecule 5: Splicing factor 3B subunit 1

Chain 1:

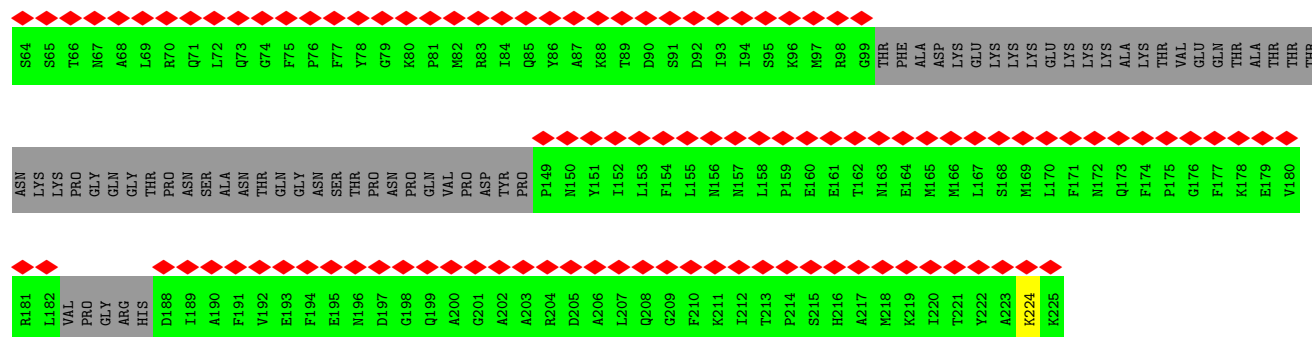




- Molecule 7: Splicing factor 3B subunit 3



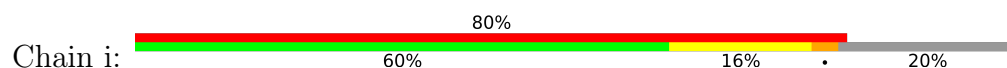




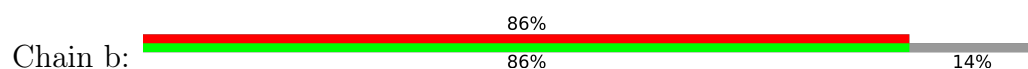
• Molecule 15: Small nuclear ribonucleoprotein Sm D2



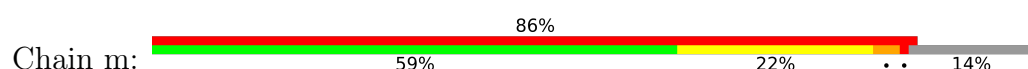
• Molecule 15: Small nuclear ribonucleoprotein Sm D2



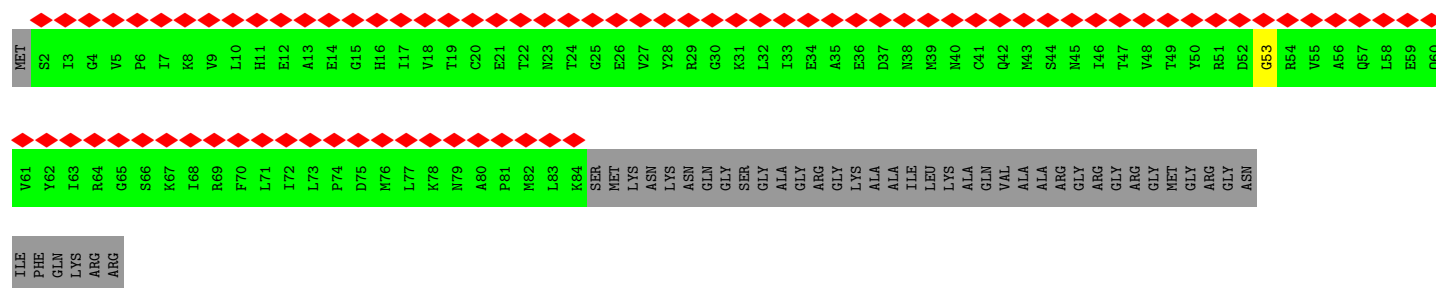
• Molecule 16: Small nuclear ribonucleoprotein F



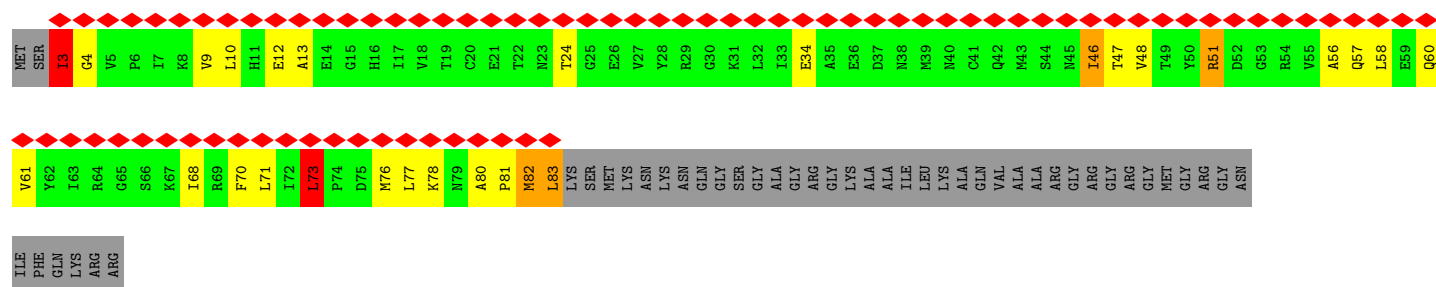
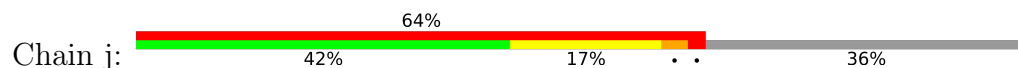
• Molecule 16: Small nuclear ribonucleoprotein F



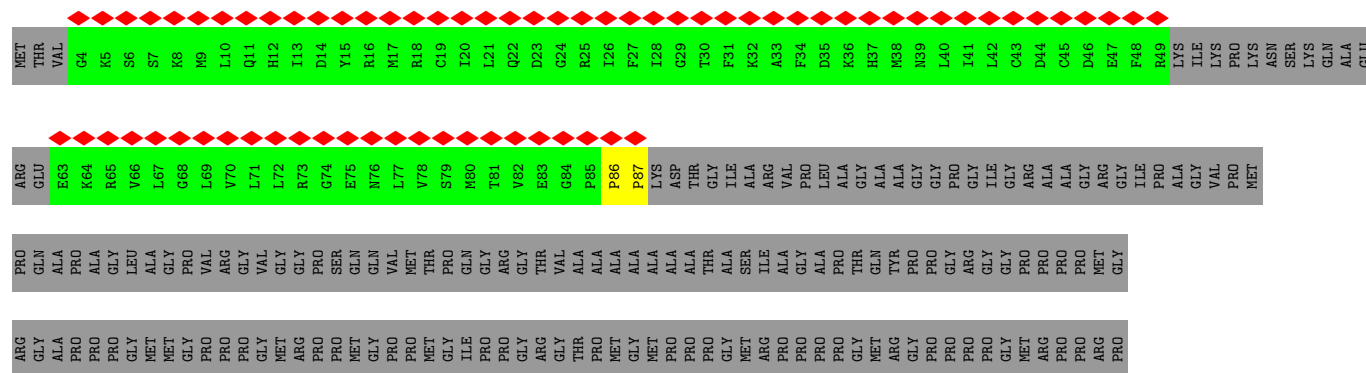




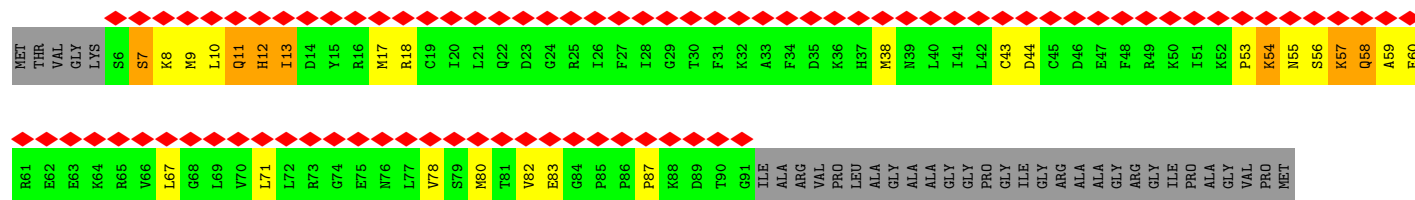
• Molecule 19: Small nuclear ribonucleoprotein Sm D3



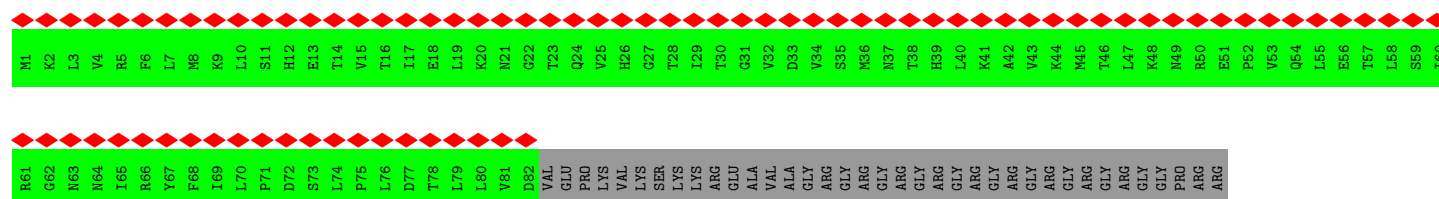
• Molecule 20: Small nuclear ribonucleoprotein-associated proteins B and B'



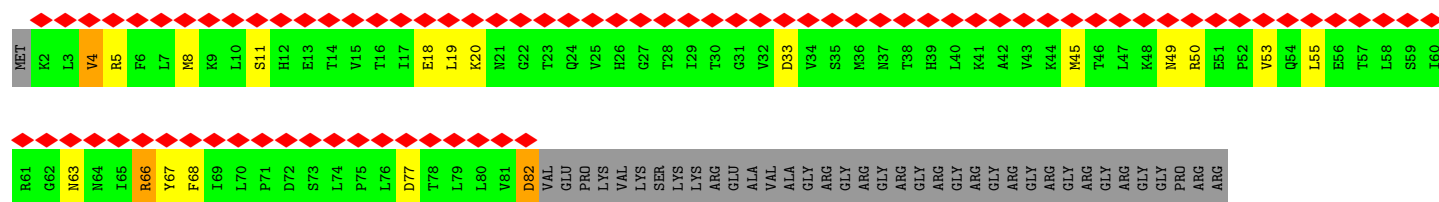
• Molecule 20: Small nuclear ribonucleoprotein-associated proteins B and B'



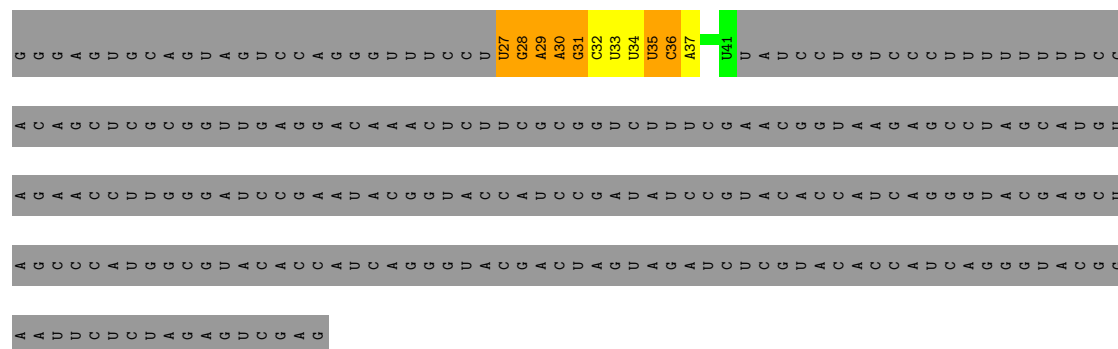
- Molecule 21: Small nuclear ribonucleoprotein Sm D1



- Molecule 21: Small nuclear ribonucleoprotein Sm D1



- Molecule 22: pre-mRNA



- Molecule 23: 5SS



- Molecule 24: U1 snRNA

Chain L:

Chain 0:

- Molecule 26: U1 small nuclear ribonucleoprotein A

Chain M:

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	419522	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.684	Depositor
Minimum map value	-2.084	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.043	Depositor
Recommended contour level	0.25	Depositor
Map size ($\text{\AA}$)	521.76, 521.76, 521.76	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.087, 1.087, 1.087	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	B	0.35	0/812	0.56	0/1060
2	D	0.64	0/600	1.25	0/830
3	J	1.02	0/374	1.38	0/507
4	H	0.19	0/3073	0.54	11/4779 (0.2%)
5	1	0.41	4/6609 (0.1%)	0.72	13/8946 (0.1%)
6	2	0.61	0/1364	0.81	0/1831
7	3	0.22	0/9435	0.54	2/12802 (0.0%)
8	4	0.15	0/670	0.36	0/850
9	5	0.46	1/555 (0.2%)	0.88	2/750 (0.3%)
10	A	0.17	0/507	0.37	0/640
11	C	0.51	2/2158 (0.1%)	0.71	5/2808 (0.2%)
12	E	0.53	0/2171	0.72	3/2779 (0.1%)
13	F	0.18	0/671	0.44	0/849
14	G	0.14	0/689	0.32	0/869
15	a	0.17	0/374	0.42	0/472
15	i	0.95	0/773	1.33	0/1039
16	b	0.17	0/311	0.42	0/395
16	m	0.83	1/588 (0.2%)	1.34	5/795 (0.6%)
17	c	0.16	0/319	0.41	0/399
17	l	0.82	0/646	1.42	6/867 (0.7%)
18	d	0.15	0/307	0.37	0/388
18	n	0.81	0/575	1.40	6/768 (0.8%)
19	e	0.18	0/343	0.37	0/433
19	j	0.72	0/645	1.22	4/870 (0.5%)
20	f	0.14	0/294	0.36	0/370
20	k	0.87	1/702 (0.1%)	1.33	5/936 (0.5%)
21	g	0.14	0/339	0.36	0/428
21	h	0.93	0/649	1.35	6/878 (0.7%)
22	I	0.50	2/349 (0.6%)	0.71	0/540
23	K	0.61	0/242	1.14	2/377 (0.5%)
24	L	0.53	1/3891 (0.0%)	0.83	15/6061 (0.2%)
25	O	1.47	13/1688 (0.8%)	1.33	12/2279 (0.5%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
26	M	1.32	1/801 (0.1%)	1.22	2/1074 (0.2%)
27	N	0.70	0/437	1.33	2/587 (0.3%)
28	6	0.94	3/621 (0.5%)	1.51	16/833 (1.9%)
All	All	0.58	29/44582 (0.1%)	0.83	117/61089 (0.2%)

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
5	1	0	1
15	i	0	1
25	O	0	1
All	All	0	3

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	C	419	PRO	N-CA	17.45	1.69	1.47
28	6	38	ARG	C-N	13.94	1.52	1.33
5	1	718	PRO	N-CA	11.30	1.66	1.47
28	6	30	CYS	C-O	-8.56	1.12	1.23
25	O	176	VAL	C-O	-7.94	1.15	1.24
9	5	78	PRO	C-N	7.24	1.50	1.33
25	O	142	LYS	CA-C	7.11	1.60	1.53
5	1	638	ALA	C-N	7.11	1.44	1.33
5	1	1140	GLU	C-O	-7.02	1.15	1.23
25	O	104	THR	C-O	-6.46	1.16	1.24
25	O	192	LEU	N-CA	-6.44	1.38	1.46
28	6	38	ARG	C-O	-6.16	1.16	1.24
25	O	129	ILE	C-O	-5.99	1.17	1.24
24	L	35	A	O3'-P	-5.82	1.52	1.61
25	O	110	VAL	CA-C	5.70	1.59	1.52
25	O	103	LYS	C-O	5.68	1.31	1.24
25	O	122	GLU	C-O	-5.65	1.17	1.24
26	M	54	GLN	CA-C	5.64	1.59	1.52
5	1	717	THR	C-N	5.57	1.44	1.34
25	O	72	ARG	C-O	-5.57	1.17	1.24
22	I	32	C	C1'-N1	5.43	1.56	1.48
22	I	34	U	C1'-N1	5.39	1.55	1.47
25	O	83	GLU	C-O	-5.36	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	O	125	VAL	C-O	-5.22	1.17	1.24
20	k	11	GLN	C-O	-5.22	1.17	1.24
25	O	165	ASP	C-O	-5.21	1.17	1.23
16	m	4	PRO	N-CD	5.16	1.54	1.47
25	O	180	ARG	CA-C	-5.08	1.46	1.52
11	C	418	GLY	C-N	5.04	1.45	1.33

All (117) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	3	1064	ASP	N-CA-CB	18.36	141.51	110.49
11	C	418	GLY	CA-C-N	16.07	139.93	119.84
11	C	418	GLY	C-N-CA	16.07	139.93	119.84
5	1	780	PRO	N-CA-C	14.94	133.41	113.40
28	6	38	ARG	CA-C-N	13.68	133.85	119.89
28	6	38	ARG	C-N-CA	13.68	133.85	119.89
4	H	69	U	C4'-C3'-O3'	11.93	130.89	113.00
7	3	1064	ASP	N-CA-C	-11.84	85.58	110.80
9	5	78	PRO	CA-C-N	11.59	134.33	119.84
9	5	78	PRO	C-N-CA	11.59	134.33	119.84
11	C	419	PRO	CA-N-CD	-10.37	97.48	112.00
5	1	1011	PRO	N-CA-C	-9.08	99.62	110.70
4	H	69	U	C1'-C2'-O2'	-8.92	95.02	108.40
24	L	2	U	C1'-C2'-O2'	-8.79	95.21	108.40
24	L	3	A	C1'-C2'-O2'	-8.51	95.64	108.40
5	1	1069	HIS	CA-CB-CG	8.46	122.26	113.80
5	1	718	PRO	CA-N-CD	-8.33	99.84	111.50
24	L	3	A	C4'-C3'-O3'	8.33	125.49	113.00
24	L	132	G	C2'-C3'-O3'	-8.09	101.57	113.70
24	L	3	A	N9-C1'-C2'	-8.07	99.89	112.00
21	h	67	TYR	N-CA-C	7.70	120.78	109.07
5	1	1069	HIS	CB-CA-C	7.65	123.98	110.37
24	L	79	G	C1'-C2'-O2'	-7.64	96.95	108.40
4	H	70	C	C1'-C2'-O2'	-7.41	97.28	108.40
20	k	7	SER	CA-CB-OG	7.40	125.91	111.10
4	H	45	C	C4'-C3'-O3'	-7.34	98.38	109.40
27	N	3	LYS	CB-CG-CD	7.30	128.09	111.30
4	H	70	C	N1-C1'-C2'	-7.27	101.09	112.00
4	H	69	U	C2'-C3'-O3'	-7.22	102.87	113.70
18	n	47	GLU	N-CA-C	7.21	119.14	111.28
28	6	27	ASP	CA-C-N	-6.97	111.43	122.10
28	6	27	ASP	C-N-CA	-6.97	111.43	122.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	O	96	ASN	N-CA-C	6.95	119.70	111.71
27	N	48	SER	N-CA-C	6.91	118.50	110.97
4	H	44	U	N1-C1'-C2'	-6.89	101.66	112.00
4	H	70	C	C3'-C2'-O2'	6.82	120.93	110.70
16	m	3	LEU	CA-C-N	-6.77	111.38	119.84
16	m	3	LEU	C-N-CA	-6.77	111.38	119.84
25	O	56	PRO	N-CA-C	6.67	118.83	110.70
4	H	44	U	C2'-C3'-O3'	6.51	123.47	113.70
20	k	87	PRO	CB-CA-C	6.50	119.89	111.64
12	E	198	TRP	CA-CB-CG	6.46	125.86	113.60
19	j	3	ILE	CA-CB-CG2	6.45	121.47	110.50
24	L	3	A	C2'-C3'-O3'	-6.42	104.08	113.70
21	h	66	ARG	N-CA-C	-6.41	102.92	111.96
20	k	78	VAL	O-C-N	6.38	126.70	121.85
17	l	83	ASN	N-CA-C	6.33	118.18	111.28
25	O	191	ARG	CG-CD-NE	-6.31	98.12	112.00
5	1	1069	HIS	N-CA-CB	-6.27	101.38	110.47
16	m	73	ARG	NE-CZ-NH1	-6.24	115.26	121.50
24	L	71	C	C2'-C3'-O3'	-6.17	104.44	113.70
26	M	8	PRO	N-CA-C	6.14	120.87	111.11
28	6	29	LYS	CB-CA-C	6.12	122.17	109.38
18	n	51	SER	N-CA-C	-6.09	102.07	110.35
28	6	27	ASP	CB-CA-C	-6.04	100.14	110.16
16	m	73	ARG	NE-CZ-NH2	6.01	124.61	119.20
28	6	38	ARG	CB-CG-CD	6.01	125.13	111.30
28	6	38	ARG	O-C-N	-6.01	114.41	121.32
4	H	45	C	C2'-C3'-O3'	-6.01	100.49	109.50
25	O	188	ARG	CA-C-N	-6.00	114.45	120.21
25	O	188	ARG	C-N-CA	-6.00	114.45	120.21
17	l	59	ASP	N-CA-CB	5.99	119.13	110.20
5	1	783	GLU	N-CA-C	-5.96	105.68	113.12
25	O	186	GLY	N-CA-C	5.93	123.23	115.47
5	1	1139	PRO	N-CA-CB	-5.91	98.63	102.65
19	j	73	LEU	CB-CG-CD2	5.89	128.39	110.70
28	6	35	SER	CA-C-N	5.80	131.93	122.65
28	6	35	SER	C-N-CA	5.80	131.93	122.65
25	O	117	SER	N-CA-C	5.76	117.23	111.07
28	6	36	TYR	CB-CA-C	-5.71	100.92	110.56
28	6	38	ARG	CA-C-O	-5.70	112.35	120.16
5	1	779	SER	CA-C-N	5.69	125.05	118.85
5	1	779	SER	C-N-CA	5.69	125.05	118.85
23	K	1	G	C3'-C2'-O2'	5.68	119.22	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	k	55	ASN	N-CA-C	5.67	117.46	111.28
18	n	75	ARG	N-CA-C	5.66	119.36	111.90
19	j	51	ARG	NE-CZ-NH2	5.65	124.28	119.20
24	L	79	G	N9-C1'-C2'	-5.63	103.55	112.00
25	O	121	ARG	N-CA-C	5.54	117.76	111.11
23	K	0	G	C3'-C2'-O2'	5.53	119.00	110.70
17	l	66	SER	N-CA-C	5.49	117.27	111.28
17	l	59	ASP	N-CA-C	5.45	118.39	111.69
28	6	33	CYS	O-C-N	5.43	128.71	122.25
24	L	37	G	C2'-C3'-O3'	-5.42	105.57	113.70
4	H	70	C	C4'-C3'-O3'	5.42	121.13	113.00
28	6	12	ARG	CB-CG-CD	-5.41	98.85	111.30
18	n	33	GLY	N-CA-C	5.41	118.62	110.18
5	1	885	ASP	CB-CA-C	-5.39	100.40	109.83
16	m	15	THR	N-CA-CB	5.39	117.97	109.83
24	L	133	G	C1'-C2'-O2'	-5.38	103.73	111.80
21	h	66	ARG	CG-CD-NE	5.35	123.77	112.00
21	h	45	MET	CG-SD-CE	-5.34	89.15	100.90
11	C	397	TYR	CA-C-N	-5.28	113.40	122.79
11	C	397	TYR	C-N-CA	-5.28	113.40	122.79
24	L	73	C	C2'-C3'-O3'	-5.26	105.81	113.70
28	6	33	CYS	CA-C-N	5.25	131.57	121.54
28	6	33	CYS	C-N-CA	5.25	131.57	121.54
24	L	63	C	C3'-C2'-O2'	5.21	118.52	110.70
21	h	4	VAL	CB-CA-C	-5.21	104.08	112.16
25	O	56	PRO	CA-C-N	-5.21	114.30	119.56
25	O	56	PRO	C-N-CA	-5.21	114.30	119.56
25	O	62	THR	N-CA-C	-5.20	101.39	109.24
17	l	73	GLN	CA-CB-CG	5.20	124.49	114.10
5	1	721	ILE	N-CA-C	5.16	117.54	111.09
18	n	51	SER	CA-C-O	-5.15	116.09	121.55
19	j	51	ARG	CA-CB-CG	5.15	124.39	114.10
18	n	53	GLN	N-CA-C	5.14	117.54	110.35
12	E	197	LYS	CA-C-N	5.11	129.95	122.39
12	E	197	LYS	C-N-CA	5.11	129.95	122.39
17	l	39	VAL	CB-CA-C	5.08	117.19	110.84
20	k	78	VAL	CB-CA-C	-5.07	107.40	111.71
5	1	1142	ASN	CB-CA-C	5.07	120.51	110.42
24	L	131	U	P-O5'-C5'	-5.06	113.31	120.90
26	M	98	LYS	N-CA-C	5.05	118.70	112.54
24	L	131	U	C2'-C3'-O3'	5.05	117.08	109.50
21	h	66	ARG	NE-CZ-NH2	5.04	123.74	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	O	78	ARG	N-CA-C	5.00	117.11	111.11

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	1	1002	ASN	Mainchain
25	O	56	PRO	Peptide
15	i	17	GLN	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	799	0	514	31	0
2	D	604	0	261	2	0
3	J	369	0	275	23	0
4	H	2754	0	1398	22	0
5	1	6487	0	6699	513	0
6	2	1325	0	1184	139	0
7	3	9247	0	9179	203	0
8	4	664	0	230	0	0
9	5	539	0	505	41	0
10	A	504	0	150	0	0
11	C	2127	0	1138	78	0
12	E	2153	0	1054	144	0
13	F	666	0	209	0	0
14	G	685	0	226	7	0
15	a	372	0	118	1	0
15	i	764	0	783	30	0
16	b	308	0	115	0	0
16	m	576	0	589	18	0
17	c	319	0	92	0	0
17	l	638	0	657	42	0
18	d	305	0	105	0	0
18	n	568	0	590	22	0
19	e	341	0	112	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	j	637	0	652	29	0
20	f	293	0	99	1	0
20	k	692	0	717	23	0
21	g	337	0	110	0	0
21	h	641	0	680	18	0
22	I	314	0	160	33	0
23	K	216	0	110	6	0
24	L	3485	0	1759	289	0
25	O	1643	0	1605	159	0
26	M	787	0	797	10	0
27	N	425	0	392	20	0
28	6	613	0	596	21	0
29	6	3	0	0	0	0
29	B	1	0	0	0	0
29	C	1	0	0	0	0
29	N	1	0	0	0	0
30	6	37	0	0	16	0
All	All	43240	0	33860	1429	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 19.

All (1429) 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)
6:2:574:ALA:HA	6:2:578:TRP:CE3	1.40	1.51
5:1:1114:VAL:HG21	30:6:204:SJT:C1	1.40	1.51
25:O:61:GLU:CB	25:O:65:GLU:HG2	1.41	1.50
24:L:92:C:H2'	24:L:93:G:C8	1.44	1.48
24:L:32:A:N3	25:O:135:VAL:HG22	1.22	1.47
24:L:29:A:C8	25:O:200:ARG:NH1	1.80	1.46
5:1:1299:GLU:HB3	9:5:53:PHE:CZ	1.46	1.44
11:C:419:PRO:N	11:C:419:PRO:CA	1.69	1.44
24:L:50:G:H1'	24:L:91:G:N2	1.15	1.44
5:1:1299:GLU:HB3	9:5:53:PHE:CE1	1.51	1.43
28:6:26:CYS:SG	30:6:204:SJT:C23	2.08	1.42
1:B:50:HIS:NE2	6:2:519:LYS:HD3	1.28	1.40
24:L:33:C:C4'	25:O:137:SER:HA	1.52	1.40
24:L:29:A:N3	25:O:200:ARG:HD2	1.32	1.39
5:1:885:ASP:OD2	5:1:888:LEU:CB	1.72	1.37
6:2:574:ALA:CA	6:2:578:TRP:HE3	1.37	1.35

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:E:226:ASP:OD1	12:E:227:PRO:HD2	1.18	1.35
5:1:568:ARG:NH1	12:E:242:PHE:CD1	1.94	1.34
6:2:573:ASP:O	6:2:577:LYS:HG2	1.24	1.34
1:B:50:HIS:CD2	6:2:519:LYS:HD3	1.63	1.32
11:C:420:LYS:NZ	22:I:28:G:H21	1.29	1.31
5:1:650:ALA:O	12:E:227:PRO:HG2	1.22	1.31
5:1:1114:VAL:HG11	30:6:204:SJT:C2	1.62	1.29
24:L:32:A:C4	25:O:135:VAL:HG22	1.66	1.29
24:L:32:A:C4	25:O:135:VAL:CG2	2.15	1.28
24:L:32:A:O4'	25:O:135:VAL:CG1	1.80	1.27
11:C:400:HIS:CE1	22:I:29:A:C2'	2.17	1.27
5:1:885:ASP:OD2	5:1:888:LEU:HB2	1.16	1.26
6:2:573:ASP:OD2	6:2:577:LYS:CD	1.82	1.26
24:L:32:A:H5'	25:O:146:TYR:OH	1.32	1.25
5:1:610:ILE:O	12:E:232:MET:HE1	1.27	1.25
24:L:30:U:C2	25:O:175:LEU:HD22	1.71	1.25
6:2:573:ASP:OD2	6:2:577:LYS:HD2	1.14	1.24
24:L:30:U:H3	25:O:175:LEU:CD2	1.35	1.24
5:1:885:ASP:CG	5:1:888:LEU:H	1.48	1.22
11:C:400:HIS:CE1	22:I:29:A:O2'	1.93	1.22
20:k:8:LYS:O	20:k:12:HIS:NE2	1.70	1.21
3:J:205:GLU:O	3:J:209:GLN:NE2	1.75	1.20
24:L:118:A:N6	19:j:3:ILE:C	1.99	1.19
24:L:29:A:C4	25:O:200:ARG:HD2	1.77	1.19
24:L:32:A:N3	25:O:135:VAL:CG2	2.06	1.18
6:2:527:PHE:O	6:2:530:ARG:HG2	1.44	1.18
24:L:118:A:H62	19:j:3:ILE:C	1.50	1.18
3:J:212:PHE:CE1	5:1:1092:ASP:OD2	1.97	1.17
5:1:783:GLU:HB2	12:E:198:TRP:CZ3	1.78	1.17
24:L:32:A:O4'	25:O:135:VAL:HG11	0.99	1.17
5:1:647:PHE:HB2	12:E:231:TYR:CE1	1.78	1.17
11:C:393:PRO:HG2	11:C:396:LEU:HD23	1.22	1.17
24:L:28:G:C2	25:O:112:TYR:CE2	2.34	1.16
5:1:610:ILE:O	12:E:232:MET:CE	1.95	1.14
24:L:50:G:C1'	24:L:91:G:N2	2.08	1.14
11:C:420:LYS:NZ	22:I:28:G:N2	1.96	1.14
24:L:29:A:C5'	25:O:200:ARG:NH2	2.02	1.14
24:L:164:G:O3'	21:h:50:ARG:O	1.64	1.14
5:1:1299:GLU:CB	9:5:53:PHE:CZ	2.31	1.13
2:D:213:GLU:CB	3:J:195:GLU:CB	2.27	1.13
24:L:30:U:N3	25:O:175:LEU:HD22	1.54	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1:783:GLU:HB2	12:E:198:TRP:HZ3	0.99	1.12
5:1:650:ALA:O	12:E:227:PRO:CG	1.98	1.12
5:1:901:GLN:OE1	12:E:163:ARG:NH1	1.81	1.12
5:1:610:ILE:C	12:E:232:MET:HE1	1.76	1.11
1:B:50:HIS:NE2	6:2:519:LYS:CD	2.12	1.11
5:1:614:ARG:HB2	12:E:232:MET:CE	1.81	1.11
24:L:28:G:N2	25:O:112:TYR:CE2	2.17	1.11
24:L:29:A:N3	25:O:200:ARG:CD	2.13	1.11
5:1:611:SER:HB3	12:E:236:LYS:NZ	1.65	1.11
24:L:92:C:O2	24:L:93:G:N7	1.83	1.11
24:L:32:A:N7	25:O:148:PHE:CE1	2.20	1.10
24:L:33:C:C2	25:O:139:ARG:NE	2.19	1.10
24:L:32:A:C5	25:O:148:PHE:CE1	2.22	1.10
5:1:651:VAL:HG23	12:E:228:LEU:HG	1.13	1.09
11:C:400:HIS:CE1	22:I:29:A:H2'	1.83	1.09
24:L:92:C:C2'	24:L:93:G:C8	2.34	1.09
5:1:1067:LYS:HD2	5:1:1107:GLN:NE2	1.68	1.09
5:1:614:ARG:HD2	12:E:232:MET:HG2	1.31	1.08
5:1:611:SER:HB3	12:E:236:LYS:HZ3	0.99	1.07
5:1:1278:ASP:OD2	7:3:1166:TYR:HE2	1.35	1.07
24:L:29:A:C4	25:O:200:ARG:CD	2.36	1.07
24:L:29:A:N9	25:O:200:ARG:NH1	2.01	1.07
5:1:650:ALA:HB1	12:E:227:PRO:O	1.54	1.07
24:L:33:C:H4'	25:O:137:SER:HA	1.13	1.07
5:1:614:ARG:HG3	12:E:232:MET:SD	1.94	1.06
11:C:392:ILE:HD11	11:C:397:TYR:HB2	1.34	1.06
18:n:66:SER:OG	17:l:85:THR:HG23	1.55	1.06
6:2:573:ASP:CG	6:2:577:LYS:HD2	1.80	1.06
5:1:610:ILE:HD13	12:E:231:TYR:HE1	1.16	1.05
5:1:1126:PHE:O	6:2:571:LEU:HD21	1.55	1.05
24:L:33:C:C5'	25:O:137:SER:HA	1.85	1.05
24:L:29:A:H5'	25:O:200:ARG:HH21	1.16	1.05
24:L:33:C:N3	25:O:139:ARG:NH2	2.05	1.05
1:B:50:HIS:CD2	6:2:519:LYS:CD	2.40	1.05
11:C:400:HIS:HE1	22:I:29:A:C2'	1.57	1.04
5:1:1137:ARG:HH21	5:1:1137:ARG:HB2	1.18	1.04
5:1:568:ARG:NH1	12:E:242:PHE:CG	2.25	1.04
5:1:614:ARG:HB2	12:E:232:MET:HE2	1.33	1.04
5:1:1114:VAL:CG2	30:6:204:SJT:C1	2.34	1.04
5:1:1046:GLY:HA2	5:1:1048:GLU:OE1	1.58	1.03
12:E:226:ASP:OD1	12:E:227:PRO:CD	2.05	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:O:61:GLU:CB	25:O:65:GLU:CG	2.36	1.03
24:L:32:A:C1'	25:O:135:VAL:CG1	2.36	1.03
5:1:651:VAL:HG23	12:E:228:LEU:CG	1.87	1.03
5:1:1066:LEU:HD22	30:6:204:SJT:C4	1.87	1.03
5:1:1173:LEU:O	5:1:1177:LEU:HG	1.59	1.02
5:1:1299:GLU:CB	9:5:53:PHE:CE1	2.42	1.02
24:L:29:A:H5'	25:O:200:ARG:NH2	1.71	1.02
25:O:59:ARG:CZ	21:h:77:ASP:OD1	2.06	1.02
5:1:651:VAL:CG2	12:E:228:LEU:HG	1.88	1.02
24:L:17:G:O2'	24:L:18:G:H5'	1.57	1.01
5:1:1278:ASP:OD2	7:3:1166:TYR:CE2	2.13	1.01
28:6:29:LYS:HE3	30:6:204:SJT:C14	1.89	1.01
1:B:62:LEU:HD21	5:1:1180:ARG:HH22	1.17	1.00
5:1:1302:TYR:HB2	9:5:52:TYR:HE2	1.24	1.00
5:1:611:SER:OG	12:E:235:VAL:HG12	1.60	0.99
5:1:960:VAL:O	5:1:964:THR:HG23	1.62	0.99
11:C:390:LYS:HB3	11:C:391:PRO:HD2	1.44	0.99
24:L:33:C:H4'	25:O:137:SER:CA	1.92	0.99
24:L:30:U:N3	25:O:175:LEU:CD2	2.03	0.99
24:L:140:G:OP1	20:k:54:LYS:HD3	1.61	0.99
25:O:59:ARG:NH1	21:h:77:ASP:OD1	1.95	0.99
5:1:611:SER:CB	12:E:236:LYS:HZ3	1.75	0.98
24:L:135:A:N6	25:O:37:PRO:O	1.96	0.98
5:1:1302:TYR:HB2	9:5:52:TYR:CE2	1.98	0.98
24:L:33:C:N3	25:O:139:ARG:CZ	2.27	0.98
3:J:212:PHE:CZ	5:1:1092:ASP:OD2	2.16	0.97
5:1:966:GLN:HE21	5:1:966:GLN:HA	1.28	0.97
5:1:961:VAL:HA	5:1:964:THR:OG1	1.64	0.97
5:1:900:PHE:CD1	5:1:914:PHE:HD2	1.83	0.97
5:1:1001:VAL:HA	5:1:1004:ILE:HG22	1.45	0.97
5:1:779:SER:OG	5:1:780:PRO:HD2	1.66	0.96
24:L:32:A:C4	25:O:135:VAL:HG21	1.98	0.96
24:L:50:G:C1'	24:L:91:G:H22	1.73	0.96
5:1:1302:TYR:CB	9:5:52:TYR:HE2	1.78	0.96
11:C:392:ILE:CD1	11:C:397:TYR:HB2	1.96	0.96
1:B:50:HIS:CG	6:2:519:LYS:HG3	2.01	0.96
24:L:32:A:H1'	25:O:135:VAL:HG13	1.46	0.96
24:L:33:C:H5'	25:O:136:TYR:O	1.65	0.96
5:1:614:ARG:CB	12:E:232:MET:HE2	1.95	0.95
5:1:783:GLU:CB	12:E:198:TRP:CZ3	2.49	0.95
5:1:1220:PHE:CE2	6:2:501:PRO:HD2	2.00	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:L:33:C:C4'	25:O:137:SER:CA	2.45	0.95
11:C:393:PRO:CG	11:C:396:LEU:HD23	1.96	0.95
24:L:32:A:H5'	25:O:146:TYR:HH	1.25	0.95
4:H:69:U:N3	4:H:85:A:N1	2.14	0.94
5:1:1286:ARG:HB2	7:3:1006:GLN:OE1	1.67	0.94
5:1:1043:ALA:HB2	5:1:1055:TRP:CH2	2.03	0.93
5:1:900:PHE:HD1	5:1:914:PHE:HD2	1.09	0.93
6:2:574:ALA:CA	6:2:578:TRP:CE3	2.23	0.93
24:L:92:C:C2'	24:L:93:G:H8	1.73	0.93
6:2:574:ALA:O	6:2:578:TRP:HB2	1.69	0.93
24:L:123:A:C8	15:i:13:PRO:HA	2.04	0.93
5:1:741:LYS:HG3	12:E:198:TRP:HE1	1.32	0.93
24:L:32:A:C1'	25:O:135:VAL:HG13	1.98	0.93
5:1:1300:LEU:O	7:3:1049:LYS:CE	2.17	0.93
11:C:420:LYS:HZ1	22:I:28:G:H21	0.93	0.92
6:2:573:ASP:O	6:2:577:LYS:CG	2.16	0.92
5:1:614:ARG:CD	12:E:232:MET:HG2	2.00	0.92
5:1:783:GLU:CB	12:E:198:TRP:HZ3	1.82	0.92
7:3:1063:ASN:ND2	7:3:1065:GLU:O	2.03	0.92
5:1:1114:VAL:CG1	30:6:204:SJT:C2	2.48	0.91
24:L:30:U:O2	25:O:175:LEU:HD22	1.68	0.91
5:1:885:ASP:OD1	5:1:887:LYS:HB2	1.70	0.91
24:L:32:A:C4'	25:O:135:VAL:HG11	2.00	0.91
5:1:1185:ARG:HD3	6:2:511:LEU:CD1	2.00	0.91
5:1:610:ILE:HD13	12:E:231:TYR:CE1	2.05	0.91
5:1:647:PHE:HB2	12:E:231:TYR:CZ	2.06	0.91
24:L:123:A:N7	15:i:13:PRO:HB3	1.86	0.91
1:B:50:HIS:CG	6:2:519:LYS:CG	2.54	0.90
5:1:1248:GLN:O	6:2:497:SER:HA	1.70	0.90
6:2:531:THR:CG2	6:2:533:ILE:HG13	2.00	0.90
24:L:29:A:C5'	25:O:200:ARG:HH21	1.60	0.90
24:L:50:G:H1'	24:L:91:G:H22	1.08	0.90
5:1:991:GLY:HA3	5:1:1030:LYS:CE	2.02	0.89
24:L:92:C:O2	24:L:93:G:C8	2.24	0.89
25:O:61:GLU:C	25:O:65:GLU:HG3	1.97	0.89
6:2:573:ASP:OD2	6:2:577:LYS:CG	2.19	0.89
5:1:1067:LYS:HD2	5:1:1107:GLN:HE21	1.34	0.89
24:L:33:C:N3	25:O:139:ARG:NE	2.21	0.89
11:C:400:HIS:HE1	22:I:29:A:C1'	1.84	0.88
1:B:50:HIS:HB3	6:2:519:LYS:O	1.73	0.88
18:n:57:ILE:HG12	17:l:88:GLN:HG3	1.55	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:2:530:ARG:NH2	6:2:578:TRP:CD1	2.42	0.88
11:C:400:HIS:HB3	11:C:402:LEU:CD2	2.02	0.88
24:L:33:C:H5'	25:O:137:SER:HA	1.56	0.88
24:L:164:G:N2	21:h:49:ASN:OD1	1.83	0.88
1:B:50:HIS:CE1	6:2:519:LYS:HG2	2.08	0.87
5:1:1125:PRO:HG2	5:1:1165:TYR:CE2	2.09	0.87
25:O:47:GLU:HG2	15:i:112:ASN:OD1	1.74	0.87
5:1:885:ASP:CG	5:1:888:LEU:N	2.33	0.87
5:1:1006:MET:H	5:1:1006:MET:HE2	1.39	0.87
24:L:118:A:H61	19:j:4:GLY:HA2	1.39	0.87
5:1:654:SER:OG	12:E:226:ASP:OD2	1.93	0.86
5:1:900:PHE:CD1	5:1:914:PHE:CD2	2.62	0.86
11:C:501:LEU:C	14:G:224:LYS:H	1.83	0.86
5:1:1137:ARG:HH21	5:1:1137:ARG:CB	1.87	0.86
25:O:61:GLU:C	25:O:65:GLU:CG	2.48	0.86
24:L:118:A:N6	19:j:3:ILE:O	2.08	0.86
1:B:50:HIS:ND1	6:2:519:LYS:HG2	1.90	0.86
6:2:527:PHE:O	6:2:530:ARG:CG	2.23	0.86
6:2:573:ASP:CG	6:2:577:LYS:CD	2.45	0.86
24:L:29:A:C8	25:O:200:ARG:CZ	2.54	0.86
5:1:611:SER:C	12:E:236:LYS:HZ1	1.83	0.85
5:1:991:GLY:C	5:1:1030:LYS:HE3	2.00	0.85
11:C:393:PRO:HG2	11:C:396:LEU:CD2	2.06	0.85
24:L:92:C:H4'	24:L:93:G:OP1	1.75	0.85
24:L:118:A:N7	19:j:3:ILE:N	2.24	0.85
11:C:420:LYS:HZ1	22:I:28:G:N2	1.67	0.85
24:L:92:C:O2	24:L:93:G:C5	2.28	0.85
5:1:650:ALA:HA	12:E:227:PRO:HB2	1.59	0.85
5:1:611:SER:HA	12:E:232:MET:HE3	1.58	0.84
6:2:527:PHE:C	6:2:530:ARG:HG2	2.01	0.84
24:L:91:G:H4'	24:L:91:G:OP1	1.78	0.84
5:1:1185:ARG:NH1	6:2:511:LEU:HD12	1.92	0.84
6:2:573:ASP:C	6:2:577:LYS:HG2	2.03	0.83
24:L:92:C:H2'	24:L:93:G:H8	1.02	0.83
25:O:61:GLU:CA	25:O:65:GLU:HG2	2.08	0.83
11:C:400:HIS:CB	11:C:402:LEU:CD2	2.56	0.83
5:1:883:ASP:OD1	5:1:883:ASP:N	2.12	0.83
5:1:1046:GLY:CA	5:1:1048:GLU:OE1	2.26	0.83
5:1:1299:GLU:HB3	9:5:53:PHE:CE2	2.12	0.83
11:C:392:ILE:HD12	11:C:392:ILE:O	1.78	0.83
24:L:32:A:C5	25:O:148:PHE:HE1	1.93	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1:900:PHE:HD1	5:1:914:PHE:CD2	1.97	0.83
24:L:32:A:C1'	25:O:135:VAL:HG11	2.04	0.83
24:L:123:A:N7	15:i:13:PRO:CB	2.41	0.83
11:C:420:LYS:HZ3	22:I:28:G:N2	1.73	0.83
5:1:611:SER:HB3	12:E:236:LYS:CE	2.07	0.83
24:L:50:G:H1'	24:L:91:G:H21	1.04	0.83
5:1:1066:LEU:CD2	30:6:204:SJT:C4	2.57	0.83
6:2:574:ALA:CB	6:2:578:TRP:CE3	2.61	0.83
5:1:610:ILE:HG22	12:E:232:MET:CE	2.10	0.82
1:B:56:CYS:SG	1:B:78:HIS:HE1	2.02	0.82
5:1:741:LYS:HG3	12:E:198:TRP:NE1	1.94	0.82
7:3:264:GLN:HE22	7:3:322:VAL:H	1.24	0.82
18:n:71:GLU:OE1	19:j:58:LEU:HD22	1.79	0.82
5:1:885:ASP:OD2	5:1:888:LEU:N	2.12	0.82
5:1:607:ALA:O	12:E:235:VAL:CG1	2.27	0.81
5:1:885:ASP:OD1	5:1:888:LEU:N	2.13	0.81
24:L:33:C:O3'	25:O:144:ARG:HD3	1.79	0.81
5:1:885:ASP:OD2	5:1:888:LEU:HB3	1.79	0.81
5:1:650:ALA:HB1	12:E:227:PRO:C	2.04	0.81
11:C:400:HIS:HB3	11:C:402:LEU:HD22	1.62	0.81
1:B:50:HIS:CD2	6:2:519:LYS:CG	2.64	0.80
5:1:938:TRP:CE3	12:E:160:MET:HE3	2.16	0.80
5:1:1007:HIS:CD2	5:1:1007:HIS:H	1.96	0.80
24:L:73:C:H2'	24:L:74:C:H6	1.45	0.80
5:1:991:GLY:HA3	5:1:1030:LYS:HE2	1.63	0.80
24:L:33:C:O2	25:O:139:ARG:NE	2.14	0.80
1:B:62:LEU:HD21	5:1:1180:ARG:NH2	1.97	0.80
5:1:1300:LEU:O	7:3:1049:LYS:NZ	2.15	0.80
24:L:73:C:H2'	24:L:74:C:C6	2.16	0.80
5:1:846:ALA:HB2	5:1:879:LEU:HD13	1.63	0.80
5:1:647:PHE:HD1	12:E:231:TYR:CD1	1.99	0.80
24:L:37:G:OP1	25:O:74:LYS:NZ	2.13	0.80
5:1:650:ALA:CA	12:E:227:PRO:HB2	2.11	0.80
24:L:22:U:H5''	24:L:22:U:H6	1.46	0.80
24:L:28:G:N2	25:O:112:TYR:CZ	2.50	0.79
24:L:32:A:N9	25:O:135:VAL:HG21	1.98	0.79
5:1:611:SER:O	12:E:236:LYS:NZ	2.14	0.79
5:1:1137:ARG:HB2	5:1:1137:ARG:NH2	1.97	0.79
5:1:614:ARG:CG	12:E:232:MET:SD	2.70	0.79
5:1:1174:GLU:O	5:1:1178:MET:HG3	1.83	0.79
5:1:1304:LEU:HD12	7:3:1102:LEU:HD11	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:HIS:HE2	6:2:519:LYS:HD3	1.43	0.79
24:L:92:C:O2'	24:L:93:G:O4'	2.00	0.79
24:L:123:A:C8	15:i:13:PRO:CA	2.65	0.79
28:6:12:ARG:NH1	28:6:83:ASP:OD2	2.16	0.79
24:L:30:U:H3	25:O:175:LEU:HD21	1.42	0.79
5:1:611:SER:CB	12:E:236:LYS:NZ	2.40	0.78
11:C:400:HIS:NE2	22:I:29:A:H2'	1.96	0.78
5:1:1070:LYS:HB2	5:1:1070:LYS:NZ	1.97	0.78
24:L:73:C:C2	24:L:74:C:C5	2.70	0.78
20:k:53:PRO:HG3	20:k:58:GLN:O	1.83	0.78
24:L:15:G:H2'	24:L:16:G:C8	2.19	0.78
5:1:781:ASP:N	5:1:781:ASP:OD2	2.17	0.78
24:L:118:A:H2'	27:N:2:PRO:HD3	1.66	0.78
5:1:1125:PRO:HG2	5:1:1165:TYR:CZ	2.19	0.78
5:1:1114:VAL:HG21	30:6:204:SJT:C2	2.12	0.77
17:l:48:ILE:HD11	17:l:59:ASP:CB	2.14	0.77
5:1:1006:MET:HG3	5:1:1013:ILE:HD11	1.66	0.77
5:1:1300:LEU:C	7:3:1049:LYS:HE2	2.09	0.77
3:J:212:PHE:HE1	5:1:1092:ASP:OD2	1.61	0.77
5:1:1302:TYR:CB	9:5:52:TYR:CE2	2.63	0.77
5:1:1299:GLU:HB3	9:5:53:PHE:CD1	2.19	0.77
24:L:119:C:H2'	24:L:120:U:C6	2.20	0.77
7:3:579:GLU:HB3	7:3:625:LEU:HD11	1.65	0.77
24:L:17:G:N2	24:L:47:C:O2	2.16	0.77
24:L:32:A:N9	25:O:135:VAL:CG2	2.48	0.76
16:m:19:VAL:HG11	16:m:72:ILE:HD11	1.66	0.76
24:L:32:A:C5'	25:O:146:TYR:HH	1.97	0.76
5:1:1006:MET:H	5:1:1006:MET:CE	1.98	0.76
5:1:1006:MET:HE1	5:1:1045:ARG:CZ	2.14	0.76
25:O:30:HIS:HB3	17:l:37:GLU:OE2	1.85	0.76
20:k:8:LYS:O	20:k:12:HIS:CD2	2.38	0.76
17:l:48:ILE:HD11	17:l:59:ASP:CG	2.09	0.76
1:B:50:HIS:CE1	6:2:519:LYS:CG	2.68	0.76
1:B:50:HIS:CE1	6:2:519:LYS:CD	2.67	0.76
5:1:565:ASP:HB3	12:E:242:PHE:CZ	2.20	0.76
5:1:885:ASP:OD1	5:1:887:LYS:N	2.19	0.76
5:1:966:GLN:HA	5:1:966:GLN:NE2	2.00	0.76
12:E:177:LYS:HB2	12:E:177:LYS:NZ	2.01	0.76
3:J:226:PHE:CD2	6:2:568:TYR:CB	2.69	0.76
5:1:1052:ALA:O	5:1:1055:TRP:N	2.19	0.76
1:B:59:CYS:SG	1:B:78:HIS:ND1	2.59	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1:1067:LYS:HG3	5:1:1111:CYS:SG	2.26	0.75
17:l:33:VAL:HG12	17:l:87:LEU:CD2	2.16	0.75
28:6:12:ARG:CZ	28:6:83:ASP:OD2	2.35	0.75
4:H:150:U:H3	4:H:181:G:H1	1.31	0.75
5:1:654:SER:OG	12:E:226:ASP:CG	2.30	0.75
5:1:1299:GLU:O	9:5:53:PHE:HE1	1.69	0.75
24:L:33:C:C2	25:O:139:ARG:CZ	2.68	0.75
5:1:1006:MET:SD	5:1:1006:MET:N	2.60	0.75
5:1:1185:ARG:CZ	6:2:511:LEU:HD12	2.17	0.75
5:1:614:ARG:HB2	12:E:232:MET:SD	2.27	0.75
5:1:1220:PHE:HE2	6:2:501:PRO:HD2	1.47	0.75
24:L:33:C:H5'	25:O:137:SER:CA	2.16	0.75
5:1:651:VAL:HG23	12:E:228:LEU:CD1	2.17	0.75
5:1:885:ASP:OD2	5:1:888:LEU:CA	2.34	0.74
24:L:32:A:N7	25:O:148:PHE:HE1	1.85	0.74
7:3:463:ARG:HB3	7:3:471:ASP:HA	1.70	0.74
11:C:405:ASN:HB2	11:C:415:THR:HG22	1.68	0.74
24:L:30:U:H3	25:O:175:LEU:HD22	1.20	0.74
5:1:1217:PRO:HB2	6:2:510:TYR:OH	1.86	0.74
11:C:420:LYS:HZ3	22:I:28:G:H21	1.23	0.74
6:2:527:PHE:HA	6:2:530:ARG:HG2	1.70	0.74
26:M:33:ILE:HG23	26:M:72:MET:HE2	1.70	0.74
24:L:33:C:O2	25:O:139:ARG:CD	2.36	0.74
24:L:118:A:H61	19:j:4:GLY:CA	2.01	0.73
28:6:26:CYS:HG	30:6:204:SJT:C23	1.99	0.73
24:L:28:G:N1	25:O:112:TYR:CD2	2.57	0.73
5:1:611:SER:OG	12:E:235:VAL:CG1	2.35	0.73
24:L:123:A:C8	15:i:13:PRO:HB3	2.23	0.73
3:J:226:PHE:CD2	6:2:568:TYR:HB2	2.22	0.73
5:1:611:SER:HA	12:E:232:MET:CE	2.18	0.73
5:1:1206:ASP:HB3	6:2:584:LEU:HD13	1.69	0.73
5:1:610:ILE:C	12:E:232:MET:CE	2.51	0.72
12:E:241:LYS:HA	12:E:241:LYS:HE3	1.69	0.72
5:1:647:PHE:CD1	12:E:231:TYR:CD1	2.76	0.72
24:L:33:C:O2	25:O:139:ARG:HD2	1.88	0.72
12:E:166:ARG:NH1	12:E:166:ARG:HB3	2.04	0.72
11:C:400:HIS:CB	11:C:402:LEU:HD22	2.18	0.72
24:L:28:G:C2	25:O:112:TYR:HE2	2.03	0.72
1:B:55:GLU:HG3	6:2:515:ARG:HB2	1.70	0.72
7:3:583:MET:SD	7:3:615:ARG:NH1	2.62	0.72
5:1:610:ILE:HG22	12:E:232:MET:HE1	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1:1178:MET:HE2	5:1:1214:TYR:HE1	1.54	0.72
7:3:1121:THR:HG22	7:3:1125:GLY:H	1.55	0.72
24:L:118:A:N6	19:j:4:GLY:N	2.37	0.72
24:L:15:G:H2'	24:L:16:G:N9	2.04	0.72
5:1:647:PHE:CB	12:E:231:TYR:CE1	2.69	0.72
5:1:945:ALA:HB1	5:1:989:VAL:HG21	1.72	0.72
11:C:396:LEU:O	11:C:402:LEU:HD23	1.90	0.72
24:L:48:C:O2	24:L:49:A:N7	2.22	0.72
28:6:12:ARG:NH1	28:6:83:ASP:CG	2.48	0.72
5:1:885:ASP:OD1	5:1:887:LYS:CB	2.38	0.71
24:L:32:A:C5'	25:O:146:TYR:OH	2.25	0.71
3:J:216:ARG:NH1	5:1:1056:MET:HG3	2.06	0.71
25:O:53:ASP:OD1	25:O:54:ALA:N	2.22	0.71
5:1:961:VAL:CA	5:1:964:THR:OG1	2.37	0.71
6:2:517:ILE:HD12	6:2:517:ILE:O	1.91	0.71
24:L:138:G:N1	24:L:163:U:O2	2.20	0.71
7:3:1121:THR:HG23	7:3:1123:SER:H	1.54	0.71
24:L:94:A:N1	24:L:115:U:C4	2.59	0.71
5:1:1137:ARG:O	5:1:1137:ARG:HG2	1.89	0.71
5:1:876:MET:SD	5:1:881:ALA:HB2	2.30	0.71
11:C:420:LYS:CE	22:I:28:G:N2	2.53	0.71
5:1:1067:LYS:CG	5:1:1111:CYS:SG	2.79	0.70
5:1:1006:MET:HE1	5:1:1045:ARG:NH1	2.06	0.70
23:K:3:G:H1	24:L:6:U:H3	1.38	0.70
24:L:118:A:H3'	24:L:118:A:N3	2.07	0.70
6:2:527:PHE:HA	6:2:530:ARG:CD	2.20	0.70
1:B:51:LEU:O	5:1:1140:GLU:HA	1.91	0.70
24:L:123:A:N3	24:L:123:A:H2'	2.05	0.70
24:L:123:A:OP1	24:L:124:U:H5''	1.91	0.70
5:1:1129:LEU:HD12	5:1:1165:TYR:CD1	2.26	0.70
11:C:501:LEU:HA	14:G:224:LYS:O	1.90	0.70
24:L:48:C:H4'	24:L:48:C:OP1	1.90	0.70
3:J:219:ARG:NH2	5:1:1092:ASP:OD1	2.24	0.70
24:L:90:U:O2'	24:L:91:G:C4'	2.39	0.70
11:C:396:LEU:O	11:C:400:HIS:HB2	1.92	0.70
6:2:571:LEU:C	6:2:571:LEU:HD23	2.16	0.70
7:3:698:PRO:O	7:3:700:LYS:NZ	2.24	0.70
5:1:1141:LEU:C	5:1:1143:VAL:H	1.99	0.69
5:1:1300:LEU:O	7:3:1049:LYS:HE2	1.89	0.69
6:2:527:PHE:CA	6:2:530:ARG:HG2	2.22	0.69
24:L:29:A:C4	25:O:200:ARG:HD3	2.23	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:CYS:SG	1:B:78:HIS:CE1	2.85	0.69
7:3:703:ARG:NH1	7:3:711:ALA:O	2.23	0.69
18:n:57:ILE:HG12	17:l:88:GLN:CG	2.22	0.69
5:1:885:ASP:OD1	5:1:887:LYS:CA	2.40	0.69
11:C:400:HIS:HE1	22:I:29:A:N9	1.89	0.69
24:L:12:G:OP1	27:N:15:HIS:CD2	2.44	0.69
5:1:1048:GLU:CD	5:1:1048:GLU:H	1.98	0.69
7:3:547:CYS:SG	7:3:548:ALA:N	2.65	0.69
28:6:61:CYS:O	28:6:63:GLY:N	2.26	0.69
24:L:32:A:C4'	25:O:135:VAL:CG1	2.66	0.69
5:1:607:ALA:O	12:E:235:VAL:HG13	1.90	0.69
5:1:607:ALA:CA	12:E:235:VAL:HG13	2.22	0.69
12:E:166:ARG:HB3	12:E:166:ARG:HH11	1.58	0.69
5:1:900:PHE:CE1	5:1:954:LEU:HD22	2.27	0.69
5:1:945:ALA:HA	5:1:948:ARG:HB2	1.74	0.69
5:1:925:VAL:HG23	5:1:928:TYR:HB2	1.74	0.69
5:1:608:THR:HA	12:E:239:VAL:HG21	1.75	0.68
5:1:778:GLN:HA	5:1:778:GLN:NE2	2.09	0.68
5:1:991:GLY:HA3	5:1:1030:LYS:HG2	1.73	0.68
25:O:47:GLU:HG2	15:i:112:ASN:CG	2.17	0.68
18:n:42:ILE:HD11	18:n:45:CYS:SG	2.33	0.68
1:B:50:HIS:ND1	6:2:519:LYS:CG	2.54	0.68
7:3:805:ASN:ND2	7:3:858:GLY:O	2.25	0.68
5:1:969:LYS:O	5:1:972:GLY:N	2.27	0.68
7:3:186:GLU:OE1	7:3:222:ARG:NH2	2.27	0.68
24:L:29:A:O5'	25:O:200:ARG:NH2	2.25	0.68
25:O:45:ILE:N	25:O:45:ILE:HD12	2.09	0.68
20:k:58:GLN:HG3	20:k:59:ALA:N	2.08	0.68
7:3:499:PHE:HD2	7:3:518:GLN:HE21	1.41	0.68
5:1:1185:ARG:HD3	6:2:511:LEU:HD11	1.75	0.68
24:L:123:A:N7	15:i:13:PRO:HA	2.08	0.68
24:L:164:G:O3'	21:h:50:ARG:C	2.36	0.68
5:1:614:ARG:CG	12:E:232:MET:HG2	2.23	0.67
16:m:20:MET:HE3	16:m:30:LYS:HB2	1.76	0.67
5:1:966:GLN:HE21	5:1:966:GLN:CA	2.05	0.67
5:1:991:GLY:CA	5:1:1030:LYS:HE3	2.24	0.67
3:J:226:PHE:CD2	6:2:569:GLN:N	2.63	0.67
5:1:721:ILE:HG13	5:1:721:ILE:O	1.93	0.67
24:L:28:G:C2	25:O:112:TYR:CD2	2.82	0.67
24:L:48:C:H2'	24:L:49:A:C8	2.30	0.67
19:j:46:ILE:HD11	19:j:61:VAL:HG21	1.74	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1:778:GLN:OE1	5:1:817:HIS:NE2	2.27	0.67
5:1:1299:GLU:C	9:5:53:PHE:CE1	2.72	0.67
7:3:893:VAL:HG22	7:3:905:VAL:HG22	1.77	0.67
11:C:390:LYS:HB3	11:C:391:PRO:CD	2.21	0.67
11:C:392:ILE:HD12	11:C:392:ILE:C	2.19	0.67
5:1:1185:ARG:HD3	6:2:511:LEU:HD12	1.74	0.67
24:L:29:A:N9	25:O:200:ARG:CD	2.58	0.67
5:1:611:SER:C	12:E:236:LYS:NZ	2.54	0.66
5:1:901:GLN:NE2	12:E:163:ARG:HD2	2.10	0.66
5:1:938:TRP:CD2	12:E:160:MET:HE3	2.30	0.66
5:1:1178:MET:HE2	5:1:1214:TYR:CE1	2.30	0.66
23:K:-1:G:H1	24:L:10:U:H3	1.40	0.66
5:1:991:GLY:HA3	5:1:1030:LYS:HE3	1.77	0.66
5:1:1286:ARG:N	7:3:1006:GLN:HE22	1.92	0.66
5:1:1303:ILE:HA	9:5:52:TYR:OH	1.94	0.66
6:2:591:TYR:HA	6:2:595:LYS:HD2	1.77	0.66
7:3:673:VAL:HG12	7:3:690:ARG:HA	1.77	0.66
5:1:647:PHE:CE1	12:E:228:LEU:HD21	2.31	0.66
5:1:1046:GLY:C	5:1:1048:GLU:OE1	2.39	0.66
5:1:1283:HIS:HE1	7:3:1168:PHE:CZ	2.14	0.66
6:2:595:LYS:O	6:2:595:LYS:HG3	1.95	0.66
12:E:177:LYS:HB2	12:E:177:LYS:HZ2	1.59	0.66
24:L:50:G:C1'	24:L:91:G:H21	1.92	0.66
24:L:119:C:H2'	24:L:120:U:H6	1.59	0.66
6:2:574:ALA:HA	6:2:578:TRP:HE3	0.55	0.66
24:L:140:G:O3'	20:k:57:LYS:HB2	1.96	0.66
25:O:61:GLU:O	25:O:65:GLU:CD	2.39	0.66
6:2:530:ARG:NH2	6:2:578:TRP:NE1	2.43	0.66
7:3:707:GLN:HG3	7:3:709:GLN:HE22	1.60	0.65
5:1:779:SER:OG	5:1:780:PRO:CD	2.43	0.65
24:L:117:G:H5''	24:L:118:A:O5'	1.96	0.65
7:3:101:LYS:HD3	7:3:104:GLN:HG3	1.77	0.65
7:3:511:LEU:HB2	7:3:517:VAL:HG23	1.78	0.65
7:3:672:GLY:HA3	7:3:695:GLY:HA3	1.76	0.65
5:1:1126:PHE:HD1	6:2:571:LEU:HD22	1.60	0.65
24:L:90:U:O2'	24:L:91:G:H4'	1.96	0.65
20:k:9:MET:HE2	20:k:38:MET:SD	2.36	0.65
5:1:1180:ARG:O	6:2:512:GLN:NE2	2.29	0.65
24:L:123:A:N7	15:i:13:PRO:CA	2.59	0.65
5:1:611:SER:HB3	12:E:236:LYS:CD	2.27	0.65
6:2:579:GLN:HA	6:2:579:GLN:OE1	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:C:501:LEU:C	14:G:224:LYS:N	2.52	0.65
26:M:92:ASP:O	26:M:96:LYS:HG3	1.97	0.65
5:1:699:GLN:O	5:1:699:GLN:HG3	1.95	0.65
24:L:20:G:H4'	25:O:67:MET:HE2	1.79	0.65
16:m:69:VAL:CG1	17:l:80:LYS:HD3	2.26	0.65
16:m:66:CYS:O	16:m:69:VAL:HG12	1.97	0.65
27:N:47:GLN:OE1	27:N:50:ILE:HD12	1.97	0.65
5:1:926:LYS:HG2	5:1:927:PRO:HD3	1.79	0.64
5:1:963:LYS:HD3	5:1:1003:VAL:HG22	1.78	0.64
24:L:29:A:C4	25:O:200:ARG:NH1	2.65	0.64
24:L:29:A:N7	25:O:200:ARG:NH1	2.42	0.64
11:C:395:TRP:O	11:C:399:LEU:HB3	1.96	0.64
5:1:614:ARG:CB	12:E:232:MET:CE	2.63	0.64
5:1:614:ARG:CB	12:E:232:MET:SD	2.84	0.64
5:1:778:GLN:HA	5:1:778:GLN:HE21	1.63	0.64
6:2:530:ARG:HH22	6:2:578:TRP:CD1	2.15	0.64
22:I:30:A:P	22:I:30:A:H3'	2.37	0.64
24:L:118:A:H62	19:j:3:ILE:CA	2.10	0.64
28:6:29:LYS:HA	28:6:35:SER:O	1.97	0.64
11:C:400:HIS:HB2	11:C:402:LEU:CD2	2.26	0.64
5:1:651:VAL:CB	12:E:228:LEU:HG	2.26	0.64
5:1:1137:ARG:HH21	5:1:1137:ARG:CG	2.09	0.64
5:1:1302:TYR:O	9:5:52:TYR:OH	2.13	0.64
6:2:517:ILE:HD12	6:2:517:ILE:C	2.21	0.64
5:1:901:GLN:CD	12:E:163:ARG:HH11	2.05	0.64
5:1:1133:MET:HE1	6:2:528:ILE:CD1	2.27	0.64
6:2:527:PHE:HA	6:2:530:ARG:CG	2.27	0.64
6:2:573:ASP:OD2	6:2:577:LYS:HG2	1.98	0.64
11:C:400:HIS:HB3	11:C:402:LEU:HD21	1.79	0.64
24:L:29:A:C5'	25:O:200:ARG:HH22	2.09	0.64
7:3:511:LEU:HD21	7:3:568:MET:HG3	1.78	0.64
5:1:1299:GLU:O	9:5:53:PHE:CE1	2.49	0.64
24:L:118:A:H2'	27:N:2:PRO:CD	2.28	0.64
24:L:30:U:C6	25:O:109:ARG:NE	2.46	0.64
5:1:731:LEU:HB3	5:1:750:ILE:HD11	1.80	0.63
17:l:36:TYR:N	17:l:83:ASN:O	2.30	0.63
5:1:611:SER:HB3	12:E:236:LYS:HD3	1.80	0.63
5:1:1067:LYS:CD	5:1:1107:GLN:NE2	2.53	0.63
5:1:1299:GLU:HG2	9:5:53:PHE:CD2	2.32	0.63
5:1:614:ARG:NH2	12:E:228:LEU:HD13	2.13	0.63
18:n:57:ILE:CG1	17:l:88:GLN:HG3	2.27	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1:568:ARG:HH11	12:E:242:PHE:HD1	1.44	0.63
5:1:994:LEU:HB3	5:1:1034:ASN:HB3	1.80	0.63
11:C:420:LYS:HE2	22:I:28:G:H22	1.63	0.63
24:L:90:U:O2'	24:L:91:G:O4'	2.16	0.63
7:3:828:GLY:O	7:3:834:LEU:N	2.31	0.63
24:L:90:U:H4'	24:L:91:G:OP1	1.99	0.63
25:O:48:PHE:CD1	15:i:41:GLN:OE1	2.51	0.63
9:5:51:ASN:OD1	9:5:61:LYS:NZ	2.30	0.63
20:k:12:HIS:CD2	20:k:12:HIS:H	2.16	0.63
5:1:1210:HIS:CE1	6:2:585:THR:HG23	2.33	0.63
5:1:1126:PHE:HD1	6:2:571:LEU:CD2	2.12	0.63
7:3:707:GLN:O	7:3:709:GLN:NE2	2.32	0.63
7:3:899:THR:HG22	7:3:900:GLY:H	1.64	0.63
5:1:654:SER:HA	12:E:227:PRO:HD2	1.81	0.62
5:1:610:ILE:CG2	12:E:232:MET:HE1	2.29	0.62
5:1:991:GLY:CA	5:1:1030:LYS:HG2	2.29	0.62
20:k:10:LEU:O	20:k:13:ILE:HG22	1.99	0.62
5:1:614:ARG:HG3	12:E:232:MET:CG	2.28	0.62
5:1:850:ILE:O	5:1:854:VAL:HB	2.00	0.62
5:1:1304:LEU:HD13	7:3:408:LEU:CD2	2.30	0.62
4:H:45:C:OP1	11:C:394:TYR:HB3	2.00	0.62
17:l:59:ASP:OD2	17:l:76:ARG:NH1	2.32	0.62
11:C:400:HIS:CE1	22:I:29:A:C4	2.88	0.62
11:C:392:ILE:HD11	11:C:397:TYR:CB	2.22	0.62
5:1:1304:LEU:CD1	7:3:1102:LEU:HD11	2.28	0.62
5:1:779:SER:HG	5:1:780:PRO:HD2	1.65	0.62
7:3:864:SER:HB3	7:3:882:LEU:HD12	1.82	0.62
24:L:15:G:O2'	24:L:16:G:O4'	2.13	0.62
5:1:900:PHE:HE1	5:1:954:LEU:HD22	1.65	0.61
6:2:531:THR:HG23	6:2:533:ILE:HG13	1.82	0.61
5:1:960:VAL:O	5:1:964:THR:CG2	2.44	0.61
5:1:1299:GLU:CB	9:5:53:PHE:CE2	2.80	0.61
5:1:1302:TYR:CD2	9:5:56:ALA:HB3	2.34	0.61
7:3:798:ILE:HD13	7:3:893:VAL:HG21	1.81	0.61
24:L:17:G:C2'	24:L:18:G:H5'	2.30	0.61
24:L:123:A:C8	15:i:13:PRO:CB	2.83	0.61
25:O:48:PHE:HE2	25:O:53:ASP:HA	1.65	0.61
5:1:1304:LEU:HD13	7:3:408:LEU:HD23	1.82	0.61
5:1:1004:ILE:HG21	5:1:1009:MET:HE2	1.82	0.61
2:D:65:LEU:CB	2:D:102:ARG:HA	2.30	0.61
7:3:614:VAL:HG23	7:3:633:LEU:HD21	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:L:73:C:C2'	24:L:74:C:C6	2.83	0.61
5:1:1145:ASN:OD1	5:1:1184:HIS:CD2	2.53	0.61
7:3:412:ILE:HG12	7:3:423:LEU:HG	1.83	0.61
7:3:1142:GLN:HG2	7:3:1146:MET:HE3	1.83	0.61
24:L:29:A:C2	25:O:200:ARG:HB2	2.36	0.61
15:i:61:ARG:HG3	15:i:62:HIS:CD2	2.36	0.61
5:1:568:ARG:CZ	12:E:242:PHE:CD1	2.80	0.61
25:O:45:ILE:HG22	25:O:45:ILE:O	2.01	0.61
25:O:61:GLU:O	25:O:65:GLU:OE1	2.19	0.61
7:3:958:ARG:NH2	7:3:1014:TYR:OH	2.33	0.60
24:L:72:U:H5''	24:L:73:C:OP1	2.01	0.60
6:2:593:GLU:OE2	6:2:593:GLU:N	2.24	0.60
24:L:17:G:HO2'	24:L:18:G:H5'	1.66	0.60
24:L:73:C:O2	24:L:74:C:C5	2.53	0.60
16:m:25:TRP:HB2	16:m:27:MET:CE	2.32	0.60
7:3:1055:VAL:HG23	7:3:1093:MET:HE3	1.82	0.60
5:1:565:ASP:HB3	12:E:242:PHE:HZ	1.66	0.60
5:1:1070:LYS:HB2	5:1:1070:LYS:HZ3	1.65	0.60
7:3:718:ARG:NH1	7:3:734:LEU:O	2.35	0.60
23:K:0:G:H2'	23:K:1:G:C8	2.36	0.60
5:1:610:ILE:CD1	12:E:231:TYR:HE1	2.03	0.60
24:L:12:G:OP1	27:N:15:HIS:NE2	2.35	0.60
3:J:226:PHE:CD2	6:2:568:TYR:HB3	2.37	0.60
16:m:65:ARG:NH1	15:i:62:HIS:O	2.33	0.60
16:m:3:LEU:HD23	16:m:4:PRO:HD2	1.83	0.60
18:n:57:ILE:HG21	17:l:88:GLN:OE1	2.02	0.60
5:1:1279:ALA:HB2	7:3:1166:TYR:O	2.01	0.59
5:1:611:SER:CA	12:E:236:LYS:NZ	2.65	0.59
7:3:93:GLN:NE2	7:3:100:GLU:OE1	2.35	0.59
7:3:1057:ARG:O	7:3:1090:GLU:HG2	2.02	0.59
24:L:15:G:C3'	24:L:16:G:C8	2.86	0.59
25:O:61:GLU:O	25:O:65:GLU:CG	2.49	0.59
7:3:294:LYS:HD2	7:3:299:PHE:HB3	1.84	0.59
27:N:9:CYS:HB2	27:N:11:THR:HG22	1.83	0.59
5:1:614:ARG:HB3	12:E:232:MET:HE2	1.84	0.59
25:O:61:GLU:O	25:O:65:GLU:HG3	2.01	0.59
5:1:610:ILE:O	12:E:232:MET:HE2	1.99	0.59
5:1:901:GLN:HE22	12:E:163:ARG:HD2	1.66	0.59
5:1:1126:PHE:CD1	6:2:571:LEU:HD22	2.37	0.59
6:2:530:ARG:HH22	6:2:578:TRP:NE1	1.99	0.59
11:C:467:ALA:HA	11:C:470:ARG:HD2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:L:46:C:H6	24:L:46:C:H5''	1.67	0.59
18:n:55:ASN:OD1	18:n:56:ASN:N	2.35	0.59
26:M:75:PHE:HB3	26:M:82:MET:HE3	1.83	0.59
24:L:33:C:O2	25:O:139:ARG:CZ	2.50	0.59
24:L:92:C:C2	24:L:93:G:N7	2.68	0.59
11:C:501:LEU:CA	14:G:224:LYS:O	2.51	0.59
24:L:83:U:H2'	24:L:84:G:O4'	2.03	0.59
7:3:343:LYS:O	7:3:344:THR:OG1	2.18	0.59
17:l:68:THR:OG1	17:l:70:SER:HB2	2.02	0.59
24:L:73:C:C2'	24:L:74:C:H6	2.13	0.59
16:m:69:VAL:HG13	17:l:80:LYS:HD3	1.85	0.59
24:L:91:G:C2'	24:L:92:C:O5'	2.51	0.58
24:L:138:G:H2'	24:L:139:G:C8	2.38	0.58
24:L:140:G:H1'	20:k:57:LYS:HE2	1.84	0.58
1:B:50:HIS:CD2	6:2:519:LYS:HG3	2.31	0.58
5:1:941:ASN:O	5:1:981:TYR:OH	2.20	0.58
5:1:1036:ILE:HD11	5:1:1065:LEU:HD13	1.84	0.58
7:3:856:LYS:NZ	9:5:58:ASN:O	2.36	0.58
12:E:207:GLU:OE1	12:E:207:GLU:HA	2.03	0.58
24:L:29:A:C1'	25:O:200:ARG:CD	2.76	0.58
25:O:86:LEU:HD12	25:O:192:LEU:HD13	1.85	0.58
5:1:607:ALA:C	12:E:235:VAL:HG13	2.26	0.58
5:1:938:TRP:HA	12:E:156:LEU:HD13	1.85	0.58
5:1:1070:LYS:HB2	5:1:1070:LYS:HZ2	1.69	0.58
6:2:574:ALA:HB2	6:2:578:TRP:CZ3	2.38	0.58
5:1:568:ARG:HH12	12:E:242:PHE:CB	2.16	0.58
5:1:650:ALA:CB	12:E:227:PRO:O	2.43	0.58
6:2:571:LEU:HD23	6:2:571:LEU:O	2.03	0.58
7:3:1001:ILE:HG13	7:3:1038:LEU:HD11	1.86	0.58
7:3:1183:ASN:OD1	7:3:1205:SER:OG	2.22	0.58
24:L:122:C:C2'	24:L:123:A:OP2	2.51	0.58
25:O:49:GLU:C	25:O:51:PRO:HD2	2.29	0.58
5:1:1217:PRO:O	6:2:503:HIS:HE1	1.85	0.58
4:H:46:U:C5	4:H:48:A:C8	2.92	0.58
24:L:15:G:C2'	24:L:16:G:C8	2.85	0.58
20:k:17:MET:HE3	20:k:82:VAL:HA	1.83	0.58
5:1:1302:TYR:CD2	9:5:56:ALA:CB	2.87	0.58
7:3:706:MET:HE1	7:3:754:ILE:HD11	1.86	0.58
24:L:31:C:O4'	25:O:146:TYR:CD1	2.32	0.58
24:L:93:G:N2	24:L:117:G:N3	2.52	0.58
24:L:138:G:H2'	24:L:139:G:H8	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1:647:PHE:CE1	12:E:228:LEU:CD2	2.86	0.58
5:1:1144:GLN:HB3	5:1:1184:HIS:HE1	1.68	0.58
7:3:675:LEU:HD13	7:3:688:ASP:HB3	1.86	0.58
24:L:32:A:N7	25:O:148:PHE:CZ	2.70	0.58
28:6:12:ARG:NH2	28:6:83:ASP:OD2	2.37	0.57
3:J:226:PHE:CE2	6:2:569:GLN:N	2.72	0.57
24:L:73:C:H3'	24:L:74:C:C5	2.39	0.57
25:O:42:ALA:O	25:O:45:ILE:HD13	2.04	0.57
7:3:118:GLY:HA2	7:3:132:ILE:HD11	1.86	0.57
24:L:93:G:C2	24:L:117:G:C2	2.93	0.57
5:1:553:VAL:HG22	5:1:596:ILE:HD11	1.85	0.57
5:1:611:SER:HG	12:E:235:VAL:HG12	1.69	0.57
5:1:961:VAL:C	5:1:964:THR:OG1	2.47	0.57
5:1:1126:PHE:CE1	6:2:572:HIS:HB2	2.39	0.57
7:3:755:VAL:HG13	7:3:764:ILE:HG12	1.87	0.57
15:i:30:SER:HA	15:i:33:THR:OG1	2.05	0.57
6:2:525:PRO:HD2	6:2:528:ILE:HD12	1.87	0.57
3:J:219:ARG:HH21	5:1:1092:ASP:CG	2.12	0.57
5:1:1283:HIS:CE1	7:3:1168:PHE:CZ	2.92	0.57
7:3:1008:SER:HB3	7:3:1031:ARG:HB2	1.87	0.57
24:L:29:A:N9	25:O:200:ARG:HD2	2.19	0.57
24:L:32:A:H1'	25:O:135:VAL:CG1	2.14	0.57
5:1:490:GLU:HB3	5:1:493:LYS:HB2	1.86	0.57
25:O:58:THR:O	25:O:59:ARG:HG2	2.03	0.57
24:L:118:A:H5'	24:L:119:C:OP2	2.05	0.57
7:3:120:PHE:HB2	7:3:133:SER:HB3	1.87	0.57
18:n:49:ALA:O	18:n:51:SER:O	2.22	0.57
5:1:952:ALA:HB3	5:1:992:SER:HB3	1.87	0.56
7:3:555:VAL:HG23	7:3:592:LEU:HD11	1.87	0.56
24:L:116:C:H6	24:L:116:C:O5'	1.87	0.56
19:j:71:LEU:HD12	19:j:71:LEU:N	2.20	0.56
3:J:226:PHE:HD2	6:2:569:GLN:N	2.02	0.56
5:1:976:VAL:O	5:1:980:GLU:HG2	2.05	0.56
24:L:33:C:H4'	25:O:137:SER:CB	2.35	0.56
24:L:90:U:O2'	24:L:91:G:OP1	2.24	0.56
24:L:123:A:O2'	24:L:124:U:OP2	2.20	0.56
5:1:823:MET:HG2	5:1:833:LEU:HD22	1.87	0.56
5:1:1300:LEU:O	7:3:1049:LYS:CD	2.53	0.56
24:L:94:A:O2'	24:L:95:U:H5'	2.05	0.56
20:k:9:MET:HE1	20:k:80:MET:CE	2.35	0.56
5:1:608:THR:OG1	12:E:239:VAL:HG22	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:3:786:ARG:NH1	7:3:802:THR:O	2.38	0.56
24:L:29:A:N3	25:O:200:ARG:HB2	2.20	0.56
24:L:135:A:H62	25:O:37:PRO:CA	2.18	0.56
24:L:33:C:C2	25:O:139:ARG:CD	2.86	0.56
5:1:701:VAL:O	5:1:705:SER:OG	2.24	0.56
5:1:778:GLN:HE22	5:1:817:HIS:CD2	2.23	0.56
24:L:32:A:C1'	25:O:135:VAL:CG2	2.83	0.56
24:L:86:C:H2'	24:L:87:C:O4'	2.06	0.56
28:6:36:TYR:CD1	28:6:36:TYR:N	2.73	0.56
5:1:1137:ARG:HG3	6:2:521:PRO:HB2	1.86	0.56
6:2:518:GLU:O	6:2:518:GLU:HG3	2.06	0.56
6:2:569:GLN:OE1	6:2:569:GLN:HA	2.04	0.56
17:l:48:ILE:HD13	17:l:76:ARG:NH2	2.21	0.56
3:J:226:PHE:CE2	6:2:568:TYR:C	2.84	0.56
5:1:991:GLY:CA	5:1:1030:LYS:CE	2.79	0.56
24:L:15:G:C2	24:L:16:G:C2	2.94	0.56
17:l:48:ILE:HD11	17:l:59:ASP:OD2	2.05	0.56
24:L:73:C:C2	24:L:74:C:C6	2.94	0.56
21:h:20:LYS:HE2	21:h:63:ASN:O	2.06	0.56
20:k:12:HIS:CD2	20:k:12:HIS:N	2.74	0.55
5:1:945:ALA:HB2	5:1:948:ARG:HH11	1.71	0.55
5:1:1213:ASN:ND2	6:2:586:ILE:O	2.39	0.55
11:C:400:HIS:CE1	22:I:29:A:N9	2.72	0.55
5:1:1141:LEU:HD23	5:1:1142:ASN:H	1.72	0.55
5:1:650:ALA:O	12:E:227:PRO:CB	2.54	0.55
24:L:33:C:H5'	25:O:136:TYR:C	2.31	0.55
1:B:55:GLU:OE2	6:2:515:ARG:O	2.23	0.55
11:C:424:ARG:NH1	11:C:428:GLU:OE1	2.39	0.55
24:L:29:A:C2	25:O:200:ARG:CB	2.89	0.55
24:L:46:C:H5''	24:L:46:C:C6	2.41	0.55
25:O:75:ILE:O	25:O:79:GLN:HG3	2.07	0.55
17:l:33:VAL:HG12	17:l:87:LEU:HD23	1.89	0.55
5:1:1217:PRO:HB2	6:2:510:TYR:CZ	2.41	0.55
11:C:400:HIS:NE2	22:I:29:A:C2'	2.62	0.55
25:O:32:LYS:HE2	25:O:34:HIS:HE2	1.70	0.55
7:3:507:SER:HB3	7:3:519:VAL:HB	1.88	0.55
5:1:783:GLU:HB3	12:E:198:TRP:CZ3	2.40	0.55
5:1:945:ALA:HB1	5:1:989:VAL:HG11	1.88	0.55
11:C:400:HIS:O	11:C:402:LEU:HD22	2.07	0.55
5:1:914:PHE:HZ	5:1:932:ILE:HG12	1.70	0.55
5:1:1295:TYR:HA	9:5:36:HIS:CE1	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:O:59:ARG:O	25:O:60:ALA:HB3	2.07	0.55
28:6:37:VAL:HG13	28:6:38:ARG:HG3	1.87	0.55
5:1:963:LYS:HD3	5:1:1003:VAL:CG2	2.36	0.55
24:L:48:C:O2	24:L:48:C:H2'	2.07	0.55
5:1:1302:TYR:CD2	9:5:53:PHE:HA	2.42	0.54
7:3:436:ARG:HH11	7:3:776:GLN:HE22	1.55	0.54
24:L:33:C:N4	25:O:139:ARG:HH21	2.05	0.54
18:n:42:ILE:CD1	18:n:45:CYS:SG	2.96	0.54
19:j:12:GLU:HB3	19:j:77:LEU:HD22	1.88	0.54
5:1:614:ARG:CG	12:E:232:MET:CG	2.84	0.54
5:1:1091:HIS:CD2	6:2:566:ILE:HD13	2.43	0.54
5:1:1220:PHE:CZ	6:2:501:PRO:HD2	2.42	0.54
11:C:501:LEU:C	14:G:224:LYS:CA	2.81	0.54
24:L:2:U:H2'	24:L:3:A:H8	1.71	0.54
24:L:31:C:H5'	25:O:146:TYR:CD2	2.15	0.54
5:1:782:GLU:N	5:1:782:GLU:OE1	2.40	0.54
7:3:804:HIS:O	9:5:58:ASN:ND2	2.32	0.54
3:J:226:PHE:CD1	3:J:226:PHE:C	2.85	0.54
4:H:46:U:C4	4:H:48:A:C8	2.96	0.54
5:1:1036:ILE:HG22	5:1:1080:THR:OG1	2.07	0.54
24:L:118:A:C2'	27:N:2:PRO:CD	2.86	0.54
17:l:48:ILE:CG1	17:l:59:ASP:HB2	2.38	0.54
7:3:407:ILE:HG23	7:3:425:VAL:HG13	1.90	0.54
12:E:241:LYS:HE3	12:E:241:LYS:CA	2.37	0.54
24:L:73:C:H2'	24:L:74:C:O4'	2.07	0.54
5:1:658:TRP:CH2	5:1:700:LYS:HE2	2.43	0.54
5:1:607:ALA:O	12:E:235:VAL:HG11	2.06	0.54
11:C:424:ARG:HH21	22:I:28:G:H1	1.55	0.54
24:L:33:C:O4'	25:O:138:LYS:N	2.41	0.54
7:3:612:ASN:O	7:3:633:LEU:N	2.42	0.54
7:3:804:HIS:NE2	7:3:859:ASN:O	2.39	0.54
24:L:118:A:C1'	27:N:2:PRO:CD	2.85	0.54
5:1:608:THR:O	5:1:612:THR:HG23	2.08	0.53
11:C:400:HIS:CE1	22:I:29:A:C1'	2.75	0.53
15:i:34:GLN:HB3	15:i:111:ARG:NH1	2.23	0.53
5:1:1008:LYS:HE3	5:1:1008:LYS:HA	1.90	0.53
5:1:1256:HIS:HD2	5:1:1258:ALA:H	1.55	0.53
5:1:1257:PRO:HG3	6:2:482:ALA:HB2	1.90	0.53
5:1:1185:ARG:CD	6:2:511:LEU:HD12	2.38	0.53
6:2:527:PHE:HA	6:2:530:ARG:HD2	1.91	0.53
25:O:59:ARG:NH1	21:h:77:ASP:CG	2.66	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1:1180:ARG:NH2	6:2:515:ARG:HB3	2.23	0.53
7:3:1118:VAL:HG22	7:3:1128:ILE:HG22	1.89	0.53
17:l:36:TYR:HB2	17:l:83:ASN:O	2.09	0.53
5:1:770:MET:HG2	5:1:805:TYR:OH	2.09	0.53
24:L:92:C:H2'	24:L:92:C:O2	2.09	0.53
16:m:5:LEU:HB3	17:l:48:ILE:CG2	2.38	0.53
24:L:132:G:H5''	15:i:104:ASP:HB2	1.91	0.53
25:O:2:THR:HG22	25:O:13:PHE:CZ	2.44	0.53
28:6:29:LYS:NZ	28:6:29:LYS:CB	2.72	0.53
4:H:151:C:H2'	4:H:152:G:H8	1.74	0.53
5:1:578:ILE:HD13	5:1:596:ILE:HG21	1.91	0.53
24:L:100:C:O2'	24:L:101:C:H5'	2.08	0.53
17:l:48:ILE:HD11	17:l:59:ASP:CA	2.38	0.53
5:1:494:GLU:HA	5:1:497:ILE:HG22	1.89	0.53
5:1:1174:GLU:CD	5:1:1210:HIS:HE2	2.17	0.53
5:1:1299:GLU:CA	9:5:53:PHE:CE1	2.92	0.53
5:1:1303:ILE:CD1	7:3:991:SER:HB2	2.39	0.53
22:I:30:A:H3'	22:I:30:A:OP2	2.09	0.53
28:6:15:ALA:HA	28:6:46:CYS:HA	1.91	0.53
28:6:61:CYS:C	28:6:63:GLY:H	2.16	0.53
7:3:947:GLU:HG2	7:3:964:GLY:HA3	1.91	0.53
24:L:1:A:H2'	24:L:2:U:C6	2.43	0.53
24:L:92:C:H2'	24:L:93:G:N7	2.10	0.53
25:O:61:GLU:CA	25:O:65:GLU:CG	2.77	0.53
3:J:216:ARG:HH11	5:1:1056:MET:HG3	1.73	0.52
5:1:1283:HIS:CE1	7:3:1168:PHE:CE1	2.97	0.52
7:3:463:ARG:HA	7:3:472:ALA:N	2.24	0.52
18:n:48:MET:SD	18:n:54:GLN:HG3	2.49	0.52
5:1:610:ILE:CD1	12:E:231:TYR:CE1	2.84	0.52
5:1:968:GLU:HB3	5:1:971:MET:SD	2.50	0.52
24:L:101:C:H2'	24:L:102:A:O4'	2.10	0.52
25:O:42:ALA:N	25:O:43:PRO:CD	2.71	0.52
28:6:29:LYS:CE	30:6:204:SJT:C14	2.77	0.52
5:1:1173:LEU:O	5:1:1177:LEU:CG	2.47	0.52
22:I:30:A:H4'	22:I:31:G:H8	1.73	0.52
16:m:49:GLU:HB2	16:m:59:LEU:HD11	1.91	0.52
5:1:830:TYR:O	5:1:834:VAL:HG23	2.09	0.52
7:3:478:PHE:N	7:3:481:ALA:O	2.42	0.52
24:L:29:A:C1'	25:O:200:ARG:HD2	2.39	0.52
24:L:118:A:N6	19:j:4:GLY:CA	2.71	0.52
24:L:118:A:N3	24:L:118:A:C3'	2.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1:1302:TYR:CD2	9:5:53:PHE:HD1	2.28	0.52
19:j:70:PHE:C	19:j:71:LEU:HD12	2.34	0.52
28:6:12:ARG:HH12	28:6:83:ASP:CG	2.15	0.52
4:H:120:A:N1	4:H:137:U:O4	2.43	0.52
5:1:611:SER:CB	12:E:236:LYS:CE	2.85	0.52
6:2:574:ALA:CA	6:2:578:TRP:CZ3	2.88	0.52
24:L:57:G:O2'	24:L:58:C:H5'	2.09	0.52
25:O:45:ILE:N	25:O:45:ILE:CD1	2.73	0.52
5:1:568:ARG:NH1	12:E:242:PHE:CE1	2.71	0.52
7:3:476:VAL:HG13	7:3:483:LEU:HG	1.91	0.52
7:3:528:ARG:HH22	7:3:573:GLN:NE2	2.08	0.52
7:3:1159:ASP:HB3	7:3:1162:SER:HB3	1.91	0.52
1:B:44:PRO:O	1:B:57:LYS:NZ	2.43	0.52
5:1:963:LYS:HG2	5:1:1003:VAL:HG21	1.91	0.52
24:L:17:G:H2'	24:L:18:G:H8	1.74	0.52
1:B:55:GLU:OE2	6:2:515:ARG:C	2.53	0.52
5:1:607:ALA:HA	12:E:235:VAL:HG13	1.91	0.52
7:3:462:VAL:HG23	7:3:510:LEU:HB2	1.92	0.52
26:M:33:ILE:CG2	26:M:72:MET:HE2	2.38	0.52
4:H:42:G:H1	22:I:33:U:H3	1.56	0.51
5:1:729:LYS:HB3	5:1:730:PRO:HD3	1.92	0.51
11:C:390:LYS:CB	11:C:391:PRO:HD2	2.28	0.51
5:1:1220:PHE:CE2	6:2:501:PRO:CD	2.84	0.51
26:M:33:ILE:O	26:M:36:GLN:HG2	2.09	0.51
11:C:400:HIS:NE2	22:I:29:A:O2'	2.39	0.51
17:l:68:THR:OG1	17:l:70:SER:N	2.42	0.51
17:l:80:LYS:O	17:l:83:ASN:ND2	2.38	0.51
7:3:534:ASN:OD1	7:3:534:ASN:N	2.43	0.51
7:3:797:LEU:HG	7:3:871:PRO:HG3	1.93	0.51
11:C:406:TYR:HB2	11:C:422:PHE:CD1	2.46	0.51
5:1:1220:PHE:HE2	6:2:501:PRO:CD	2.22	0.51
6:2:514:LYS:NZ	6:2:514:LYS:CB	2.73	0.51
24:L:73:C:N3	24:L:74:C:C4	2.79	0.51
11:C:405:ASN:HA	11:C:416:TYR:O	2.11	0.51
11:C:411:CYS:O	11:C:414:TYR:N	2.33	0.51
24:L:32:A:C2	25:O:135:VAL:CG2	2.88	0.51
7:3:236:ILE:HB	7:3:249:LEU:HB2	1.93	0.51
11:C:420:LYS:HE2	22:I:28:G:N2	2.22	0.51
24:L:28:G:N2	25:O:112:TYR:CD2	2.74	0.51
17:l:23:ARG:HD3	17:l:27:ASN:OD1	2.11	0.51
5:1:1302:TYR:CE2	9:5:53:PHE:HA	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:3:1133:THR:HG21	7:3:1214:ARG:HH22	1.75	0.50
5:1:961:VAL:O	5:1:964:THR:OG1	2.29	0.50
5:1:1006:MET:HE1	5:1:1045:ARG:NE	2.27	0.50
7:3:506:LEU:HD23	7:3:545:VAL:O	2.10	0.50
7:3:747:SER:H	7:3:751:PRO:HA	1.76	0.50
5:1:851:SER:HA	5:1:854:VAL:HG12	1.92	0.50
24:L:135:A:N6	25:O:37:PRO:C	2.68	0.50
17:l:86:LEU:HD12	17:l:87:LEU:N	2.26	0.50
5:1:495:ARG:HD2	5:1:534:GLN:HE21	1.77	0.50
5:1:821:HIS:O	5:1:825:LEU:HD23	2.12	0.50
23:K:7:A:C6	23:K:8:C:C4	2.99	0.50
24:L:30:U:C2	25:O:108:ALA:HB3	2.46	0.50
5:1:495:ARG:HD2	5:1:534:GLN:NE2	2.27	0.50
5:1:1187:THR:O	5:1:1191:VAL:HG23	2.12	0.50
7:3:573:GLN:CD	7:3:574:LEU:H	2.20	0.50
24:L:92:C:O2'	24:L:93:G:C8	2.64	0.50
25:O:46:ARG:CG	25:O:47:GLU:N	2.75	0.50
5:1:494:GLU:O	5:1:498:MET:HG3	2.12	0.50
5:1:498:MET:HE1	5:1:534:GLN:HB2	1.92	0.50
5:1:732:TRP:HA	5:1:735:ILE:HG12	1.93	0.50
5:1:1286:ARG:HB2	7:3:1006:GLN:CD	2.36	0.50
7:3:739:LEU:HD13	7:3:756:ALA:HB1	1.94	0.50
25:O:44:TYR:CE2	15:i:51:LYS:HG3	2.45	0.50
25:O:85:GLU:HA	25:O:88:MET:CE	2.41	0.50
6:2:508:ARG:HG3	6:2:508:ARG:O	2.12	0.50
7:3:34:ARG:NH1	7:3:39:GLU:OE1	2.45	0.50
7:3:663:LEU:HB3	7:3:679:LEU:HB3	1.94	0.50
17:l:59:ASP:OD2	17:l:76:ARG:CZ	2.59	0.50
5:1:610:ILE:HG22	12:E:232:MET:SD	2.51	0.50
11:C:397:TYR:CE2	11:C:403:ASN:CB	2.94	0.50
24:L:15:G:N2	24:L:16:G:N2	2.60	0.50
24:L:123:A:N3	24:L:123:A:C2'	2.73	0.50
24:L:123:A:H8	15:i:13:PRO:CA	2.20	0.50
20:k:58:GLN:HG3	20:k:59:ALA:H	1.76	0.50
26:M:66:THR:O	26:M:70:ARG:HG2	2.12	0.50
5:1:556:ILE:O	5:1:560:LEU:HB2	2.11	0.50
5:1:1141:LEU:C	5:1:1143:VAL:N	2.62	0.50
12:E:241:LYS:HE3	12:E:241:LYS:O	2.12	0.49
16:m:18:PRO:HG2	16:m:75:VAL:HG22	1.94	0.49
17:l:20:LEU:HD12	17:l:20:LEU:O	2.11	0.49
19:j:83:LEU:N	19:j:83:LEU:HD12	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:3:128:ARG:NH2	7:3:178:GLU:O	2.43	0.49
11:C:397:TYR:CE2	11:C:403:ASN:HB3	2.46	0.49
24:L:29:A:H1'	25:O:200:ARG:HD2	1.93	0.49
16:m:25:TRP:HB2	16:m:27:MET:HE1	1.93	0.49
5:1:647:PHE:HE1	12:E:228:LEU:CD2	2.23	0.49
5:1:968:GLU:HA	5:1:971:MET:SD	2.53	0.49
5:1:611:SER:HG	12:E:235:VAL:CG1	2.22	0.49
5:1:650:ALA:CB	12:E:227:PRO:HB2	2.42	0.49
5:1:1130:PRO:HB2	6:2:533:ILE:CD1	2.42	0.49
5:1:1137:ARG:CG	6:2:521:PRO:HB2	2.42	0.49
5:1:654:SER:OG	12:E:226:ASP:OD1	2.31	0.49
5:1:1043:ALA:HB2	5:1:1055:TRP:CZ2	2.44	0.49
7:3:353:PHE:HB3	7:3:406:PRO:HD3	1.94	0.49
5:1:575:LEU:O	5:1:579:GLU:N	2.46	0.49
9:5:29:TRP:O	9:5:33:VAL:HG13	2.12	0.49
11:C:438:LEU:HD21	11:C:452:ILE:HG23	1.94	0.49
12:E:177:LYS:NZ	12:E:177:LYS:CB	2.74	0.49
18:n:33:GLY:HA3	17:l:15:VAL:O	2.12	0.49
5:1:969:LYS:C	5:1:971:MET:N	2.69	0.49
6:2:473:ASP:OD1	6:2:473:ASP:N	2.46	0.49
7:3:604:PHE:HB3	7:3:616:ILE:HD11	1.95	0.49
24:L:22:U:H5''	24:L:22:U:C6	2.37	0.49
24:L:32:A:N1	25:O:133:HIS:HB3	2.28	0.49
24:L:124:U:OP1	24:L:124:U:H6	1.95	0.49
19:j:68:ILE:HG21	19:j:71:LEU:HD11	1.94	0.49
7:3:96:LYS:HB3	7:3:98:MET:HG2	1.94	0.49
7:3:187:MET:HE1	9:5:73:LEU:HD22	1.95	0.49
24:L:33:C:H42	25:O:139:ARG:HH21	1.59	0.49
16:m:3:LEU:CG	16:m:4:PRO:HD2	2.43	0.49
5:1:848:GLU:H	5:1:848:GLU:CD	2.21	0.49
7:3:463:ARG:H	7:3:463:ARG:HD2	1.78	0.49
22:I:29:A:H3'	22:I:30:A:C2	2.48	0.49
24:L:135:A:C2	24:L:136:G:O2'	2.59	0.49
20:k:11:GLN:HG2	20:k:12:HIS:CD2	2.48	0.49
27:N:13:LEU:HD23	27:N:20:VAL:HG12	1.95	0.49
1:B:77:LYS:O	1:B:81:ASN:ND2	2.44	0.49
5:1:551:LEU:O	5:1:555:VAL:HG23	2.13	0.49
7:3:473:TYR:HA	7:3:485:LEU:O	2.13	0.49
11:C:501:LEU:CB	14:G:224:LYS:N	2.76	0.49
5:1:719:TYR:CE1	7:3:72:GLY:O	2.66	0.48
7:3:539:PRO:O	7:3:542:LYS:HE2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:3:565:TYR:HD2	7:3:577:TYR:HB2	1.77	0.48
24:L:20:G:O3'	25:O:67:MET:HG3	2.12	0.48
25:O:50:ASP:N	25:O:51:PRO:HD2	2.28	0.48
5:1:509:PRO:HA	5:1:512:ARG:HB2	1.96	0.48
5:1:932:ILE:O	5:1:936:VAL:HG22	2.12	0.48
5:1:1052:ALA:O	5:1:1054:GLU:N	2.46	0.48
5:1:1114:VAL:CG2	30:6:204:SJT:C2	2.84	0.48
24:L:91:G:O2'	24:L:92:C:O5'	2.30	0.48
21:h:5:ARG:HA	21:h:8:MET:CE	2.43	0.48
5:1:968:GLU:CD	5:1:968:GLU:H	2.21	0.48
5:1:1278:ASP:OD2	7:3:1166:TYR:CZ	2.63	0.48
6:2:514:LYS:HB2	6:2:514:LYS:HZ2	1.78	0.48
7:3:671:ASN:HB2	7:3:673:VAL:HG22	1.96	0.48
5:1:968:GLU:CD	5:1:968:GLU:N	2.70	0.48
6:2:571:LEU:C	6:2:571:LEU:CD2	2.86	0.48
11:C:411:CYS:SG	11:C:430:ARG:HD3	2.53	0.48
5:1:1252:GLN:HG3	6:2:497:SER:OG	2.14	0.48
6:2:495:ARG:HG2	7:3:1083:ASN:O	2.14	0.48
7:3:274:ARG:HD2	7:3:389:PRO:HG3	1.94	0.48
7:3:742:ALA:HA	7:3:755:VAL:O	2.13	0.48
12:E:166:ARG:NH1	12:E:166:ARG:CB	2.75	0.48
24:L:15:G:H4'	24:L:16:G:OP1	2.14	0.48
5:1:1006:MET:CE	5:1:1006:MET:N	2.73	0.48
5:1:1007:HIS:CD2	5:1:1007:HIS:N	2.73	0.48
5:1:1043:ALA:HA	5:1:1055:TRP:CZ2	2.49	0.48
12:E:161:ARG:HD2	12:E:165:GLU:OE2	2.13	0.48
24:L:132:G:O6	21:h:66:ARG:NH1	2.46	0.48
26:M:93:ILE:O	26:M:97:MET:HG3	2.14	0.48
1:B:43:ASP:N	1:B:43:ASP:OD1	2.42	0.48
5:1:610:ILE:CG2	12:E:232:MET:SD	3.02	0.48
7:3:317:THR:HG22	7:3:318:ASP:O	2.14	0.48
11:C:392:ILE:CD1	11:C:392:ILE:C	2.86	0.48
7:3:1082:LEU:HD12	7:3:1088:LYS:HE3	1.96	0.48
25:O:47:GLU:OE2	15:i:112:ASN:HA	2.13	0.48
5:1:954:LEU:O	5:1:958:THR:OG1	2.23	0.48
6:2:574:ALA:HB2	6:2:578:TRP:CE3	2.48	0.48
24:L:143:A:C6	24:L:144:C:C2	3.02	0.48
5:1:1118:ILE:O	5:1:1122:THR:HG23	2.14	0.48
3:J:226:PHE:CE2	6:2:569:GLN:HA	2.49	0.47
4:H:45:C:OP2	4:H:45:C:H6	1.97	0.47
5:1:568:ARG:CZ	12:E:242:PHE:CE1	2.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:3:35:GLY:HA3	9:5:47:PHE:CZ	2.49	0.47
7:3:996:ILE:O	7:3:998:HIS:N	2.47	0.47
11:C:420:LYS:CE	22:I:28:G:H22	2.21	0.47
24:L:12:G:O6	24:L:122:C:N3	2.47	0.47
4:H:124:G:H2'	4:H:125:G:C8	2.50	0.47
5:1:741:LYS:CG	12:E:198:TRP:HE1	2.17	0.47
5:1:778:GLN:OE1	5:1:817:HIS:CE1	2.66	0.47
25:O:13:PHE:CE1	19:j:76:MET:HG3	2.49	0.47
16:m:3:LEU:CD2	16:m:4:PRO:HD2	2.44	0.47
5:1:580:PRO:O	5:1:581:LEU:HB2	2.15	0.47
5:1:914:PHE:CZ	5:1:932:ILE:HG12	2.49	0.47
5:1:963:LYS:CD	5:1:1003:VAL:CG2	2.92	0.47
19:j:10:LEU:HD13	19:j:71:LEU:HD22	1.97	0.47
19:j:13:ALA:HB2	19:j:77:LEU:HD11	1.96	0.47
6:2:467:GLN:HA	11:C:461:LYS:HE2	1.96	0.47
7:3:546:LYS:HD2	7:3:587:VAL:O	2.14	0.47
7:3:589:CYS:SG	7:3:637:PRO:HB2	2.54	0.47
24:L:97:U:H6	24:L:97:U:O5'	1.96	0.47
30:6:204:SJT:C15	30:6:204:SJT:C20	2.91	0.47
5:1:607:ALA:HB1	12:E:235:VAL:HG13	1.96	0.47
5:1:654:SER:HA	12:E:226:ASP:OD1	2.15	0.47
5:1:943:LYS:HE2	5:1:943:LYS:HB2	1.68	0.47
18:n:16:LYS:HG2	18:n:73:LEU:HD12	1.97	0.47
17:l:80:LYS:HE2	17:l:80:LYS:HB3	1.66	0.47
1:B:49:ASN:HD22	5:1:1180:ARG:NH1	2.12	0.47
1:B:51:LEU:O	5:1:1140:GLU:CA	2.59	0.47
4:H:120:A:N1	4:H:137:U:C4	2.82	0.47
5:1:661:ARG:NH1	5:1:696:ASP:OD2	2.47	0.47
5:1:1121:GLU:HG3	5:1:1161:MET:HE1	1.97	0.47
7:3:187:MET:CE	9:5:73:LEU:HD22	2.44	0.47
24:L:33:C:O4'	25:O:137:SER:HA	2.10	0.47
24:L:72:U:C5'	24:L:73:C:OP1	2.62	0.47
24:L:122:C:O2'	24:L:123:A:OP2	2.28	0.47
5:1:535:ILE:HG21	5:1:556:ILE:HD11	1.97	0.47
5:1:1303:ILE:HD13	7:3:991:SER:HB2	1.96	0.47
7:3:404:LEU:HD21	7:3:438:LEU:HD11	1.97	0.47
7:3:451:GLU:HG2	7:3:761:THR:HA	1.97	0.47
7:3:699:VAL:HA	7:3:715:MET:O	2.14	0.47
7:3:704:VAL:HB	7:3:706:MET:HE2	1.97	0.47
16:m:21:VAL:HG23	16:m:21:VAL:O	2.15	0.47
27:N:24:HIS:C	27:N:24:HIS:CD2	2.92	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1:1043:ALA:HB2	5:1:1055:TRP:CZ3	2.50	0.47
5:1:1278:ASP:CG	7:3:1166:TYR:HE2	2.15	0.47
7:3:501:GLY:HA2	7:3:525:ARG:HH22	1.80	0.47
18:n:57:ILE:CG1	18:n:57:ILE:O	2.63	0.47
17:l:23:ARG:O	17:l:27:ASN:OD1	2.33	0.47
4:H:151:C:O2'	19:e:53:GLY:O	2.31	0.47
23:K:-1:G:H2'	23:K:0:G:H8	1.79	0.47
24:L:106:G:C6	24:L:107:U:C2	3.02	0.47
21:h:82:ASP:OD1	21:h:82:ASP:N	2.47	0.47
27:N:41:TRP:O	27:N:44:GLU:HB3	2.15	0.47
5:1:611:SER:CA	12:E:236:LYS:HZ1	2.27	0.46
5:1:959:ALA:HA	5:1:962:MET:HB2	1.96	0.46
7:3:877:LEU:HD23	7:3:935:GLU:HG2	1.97	0.46
17:l:16:GLN:HG2	17:l:19:ASN:OD1	2.16	0.46
5:1:498:MET:C	5:1:500:LEU:N	2.74	0.46
5:1:746:PHE:O	5:1:750:ILE:HG12	2.15	0.46
7:3:532:ARG:HD3	7:3:533:VAL:H	1.79	0.46
24:L:164:G:H4'	21:h:50:ARG:CA	2.44	0.46
4:H:46:U:H5	4:H:48:A:H2'	1.80	0.46
5:1:830:TYR:OH	5:1:870:GLU:OE1	2.33	0.46
5:1:1106:ARG:HA	5:1:1106:ARG:HD2	1.74	0.46
5:1:1129:LEU:CD1	5:1:1165:TYR:CD1	2.97	0.46
5:1:1137:ARG:CB	5:1:1137:ARG:NH2	2.68	0.46
5:1:1180:ARG:HB2	6:2:512:GLN:CD	2.40	0.46
5:1:1185:ARG:HH11	6:2:511:LEU:HD12	1.76	0.46
7:3:520:TYR:HE1	7:3:525:ARG:HG2	1.79	0.46
24:L:116:C:H2'	24:L:117:G:O4'	2.15	0.46
21:h:66:ARG:NH2	15:i:48:ASN:HB3	2.30	0.46
5:1:505:LYS:NZ	5:1:548:GLU:OE1	2.48	0.46
7:3:475:ILE:HG23	7:3:484:VAL:HB	1.97	0.46
12:E:203:ASP:OD1	12:E:203:ASP:N	2.49	0.46
23:K:-1:G:H2'	23:K:0:G:C8	2.50	0.46
24:L:29:A:N3	25:O:200:ARG:CB	2.78	0.46
5:1:1283:HIS:HE1	7:3:1168:PHE:CE1	2.32	0.46
6:2:467:GLN:NE2	11:C:457:SER:OG	2.49	0.46
7:3:521:PRO:O	7:3:543:THR:HG23	2.16	0.46
24:L:22:U:H6	24:L:22:U:C5'	2.21	0.46
15:i:34:GLN:HB3	15:i:111:ARG:HH12	1.80	0.46
5:1:1256:HIS:CD2	5:1:1258:ALA:H	2.33	0.46
7:3:463:ARG:NH1	7:3:468:ASP:O	2.49	0.46
24:L:47:C:H2'	24:L:48:C:O4'	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1:912:ASN:O	5:1:916:THR:HG23	2.16	0.46
5:1:1004:ILE:O	5:1:1004:ILE:HG23	2.15	0.46
5:1:1177:LEU:HD21	5:1:1188:ALA:HB1	1.97	0.46
5:1:1210:HIS:ND1	6:2:585:THR:HG23	2.30	0.46
7:3:705:ARG:NH1	7:3:710:GLU:OE1	2.49	0.46
7:3:947:GLU:HG3	7:3:948:VAL:H	1.80	0.46
24:L:73:C:O2'	24:L:74:C:H5'	2.14	0.46
17:l:27:ASN:OD1	17:l:27:ASN:N	2.48	0.46
15:i:113:PRO:O	15:i:114:LEU:HD12	2.16	0.46
28:6:10:PHE:HB3	28:6:12:ARG:HG3	1.98	0.46
5:1:1067:LYS:HG2	5:1:1111:CYS:SG	2.56	0.46
5:1:1303:ILE:CA	9:5:52:TYR:OH	2.64	0.46
24:L:119:C:O2'	24:L:120:U:H5'	2.14	0.46
16:m:5:LEU:HB3	17:l:48:ILE:HG22	1.98	0.46
26:M:75:PHE:HB3	26:M:82:MET:CE	2.46	0.46
5:1:1302:TYR:HB3	9:5:52:TYR:CE2	2.49	0.46
7:3:330:PHE:O	7:3:390:ARG:NH2	2.49	0.46
5:1:492:GLN:OE1	5:1:496:LYS:HD3	2.15	0.46
5:1:500:LEU:O	5:1:503:LYS:HB3	2.16	0.46
7:3:88:VAL:HG12	7:3:104:GLN:HG2	1.98	0.46
11:C:466:LYS:O	11:C:470:ARG:HG3	2.16	0.46
24:L:135:A:H62	25:O:37:PRO:C	2.24	0.46
17:l:48:ILE:HD11	17:l:59:ASP:HA	1.96	0.46
4:H:120:A:C6	4:H:137:U:O4	2.69	0.45
5:1:636:ALA:HB1	5:1:641:ILE:HD13	1.98	0.45
5:1:850:ILE:HD13	5:1:872:ILE:HG12	1.97	0.45
5:1:1091:HIS:CG	6:2:566:ILE:HD13	2.51	0.45
5:1:1293:ASN:HB3	9:5:76:CYS:HB3	1.97	0.45
24:L:118:A:N3	24:L:118:A:H5''	2.31	0.45
28:6:29:LYS:HZ3	28:6:29:LYS:HB3	1.80	0.45
5:1:668:VAL:HG13	5:1:686:LEU:HD22	1.98	0.45
5:1:876:MET:O	5:1:880:GLY:N	2.46	0.45
5:1:1252:GLN:OE1	6:2:497:SER:O	2.35	0.45
5:1:1300:LEU:CA	7:3:1049:LYS:HE2	2.46	0.45
5:1:1300:LEU:HD11	7:3:1050:PHE:HZ	1.82	0.45
25:O:41:ILE:HG22	15:i:51:LYS:HD2	1.98	0.45
17:l:48:ILE:CD1	17:l:59:ASP:OD2	2.64	0.45
7:3:230:GLU:OE1	7:3:268:ARG:NH2	2.49	0.45
24:L:93:G:N2	24:L:117:G:C4	2.84	0.45
5:1:938:TRP:CA	12:E:156:LEU:HD13	2.46	0.45
5:1:1133:MET:CE	6:2:528:ILE:HD13	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1:1300:LEU:HA	7:3:1049:LYS:HE2	1.97	0.45
11:C:425:HIS:C	11:C:425:HIS:CD2	2.93	0.45
18:n:35:ASP:OD1	18:n:36:PRO:HD2	2.17	0.45
17:l:21:ILE:HG22	17:l:50:PHE:CE2	2.52	0.45
17:l:36:TYR:CB	17:l:83:ASN:O	2.65	0.45
5:1:1003:VAL:HG22	5:1:1003:VAL:O	2.16	0.45
24:L:48:C:H2'	24:L:49:A:H8	1.77	0.45
24:L:137:U:O5'	24:L:137:U:H6	2.00	0.45
3:J:226:PHE:HE2	6:2:569:GLN:HA	1.81	0.45
5:1:766:THR:O	5:1:770:MET:HB2	2.17	0.45
5:1:1193:GLN:HB2	5:1:1233:ALA:HA	1.99	0.45
21:h:68:PHE:HB2	15:i:100:PHE:HB3	1.98	0.45
4:H:166:G:N2	4:H:166:G:OP2	2.50	0.45
5:1:504:ILE:HD13	5:1:516:LEU:HG	1.98	0.45
5:1:925:VAL:CG2	5:1:928:TYR:HB2	2.44	0.45
7:3:444:VAL:HG11	7:3:736:TYR:HB2	1.98	0.45
24:L:74:C:H6	24:L:74:C:O5'	1.99	0.45
5:1:519:ILE:HA	5:1:522:LYS:HB2	1.99	0.45
5:1:611:SER:CB	12:E:236:LYS:HD3	2.46	0.45
5:1:647:PHE:HD1	12:E:231:TYR:HD1	1.55	0.45
5:1:722:GLU:H	5:1:722:GLU:CD	2.24	0.45
5:1:884:ILE:HD12	5:1:888:LEU:HG	1.98	0.45
5:1:1244:CYS:SG	7:3:1029:TYR:HD1	2.40	0.45
6:2:574:ALA:CB	6:2:578:TRP:CZ3	2.96	0.45
7:3:581:LYS:HG2	7:3:583:MET:HE2	1.98	0.45
7:3:998:HIS:CE1	7:3:1064:ASP:OD2	2.69	0.45
11:C:395:TRP:CD1	11:C:395:TRP:H	2.35	0.45
18:n:57:ILE:O	18:n:57:ILE:HD12	2.16	0.45
4:H:45:C:OP2	4:H:45:C:C6	2.70	0.45
5:1:522:LYS:HB3	5:1:526:PHE:CE2	2.52	0.45
5:1:696:ASP:OD1	5:1:697:GLU:N	2.50	0.45
5:1:822:ARG:H	5:1:822:ARG:HD2	1.82	0.45
5:1:849:ILE:O	5:1:853:ILE:HG12	2.17	0.45
5:1:901:GLN:NE2	12:E:163:ARG:HH11	2.15	0.45
7:3:13:GLY:O	7:3:34:ARG:HG3	2.16	0.45
7:3:80:VAL:HB	7:3:88:VAL:HG23	1.98	0.45
7:3:1116:SER:HB3	7:3:1130:VAL:HG12	1.99	0.45
5:1:778:GLN:NE2	5:1:778:GLN:CA	2.72	0.45
5:1:1006:MET:CE	5:1:1045:ARG:NE	2.80	0.45
24:L:28:G:N1	25:O:112:TYR:CE2	2.78	0.45
24:L:91:G:H2'	24:L:92:C:O5'	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:M:75:PHE:HD2	26:M:82:MET:HE2	1.82	0.45
5:1:1014:LYS:O	5:1:1018:PRO:CD	2.66	0.44
5:1:1213:ASN:CG	6:2:589:ASP:O	2.60	0.44
5:1:1260:LYS:HB2	5:1:1260:LYS:HE3	1.80	0.44
7:3:449:VAL:HG22	7:3:763:ARG:HG2	1.99	0.44
24:L:31:C:O2	25:O:148:PHE:CZ	2.70	0.44
24:L:127:U:C6	18:n:63:ARG:NH2	2.85	0.44
25:O:33:HIS:O	25:O:33:HIS:CD2	2.70	0.44
21:h:5:ARG:HA	21:h:8:MET:HE3	1.99	0.44
21:h:53:VAL:HG12	21:h:55:LEU:CD1	2.46	0.44
20:k:17:MET:HE3	20:k:82:VAL:CA	2.46	0.44
3:J:226:PHE:CE2	6:2:568:TYR:HB3	2.52	0.44
5:1:945:ALA:HB2	5:1:948:ARG:NH1	2.32	0.44
7:3:625:LEU:HD12	7:3:625:LEU:O	2.18	0.44
11:C:399:LEU:O	11:C:399:LEU:HD12	2.17	0.44
12:E:198:TRP:O	12:E:198:TRP:CE3	2.70	0.44
24:L:36:A:H2'	24:L:37:G:O4'	2.17	0.44
25:O:76:GLU:HA	25:O:79:GLN:CD	2.42	0.44
27:N:46:ALA:O	27:N:50:ILE:HG13	2.17	0.44
5:1:610:ILE:CG2	12:E:232:MET:CE	2.86	0.44
5:1:1137:ARG:NH2	5:1:1137:ARG:CG	2.72	0.44
6:2:681:PRO:HB2	6:2:682:LEU:H	1.64	0.44
7:3:318:ASP:N	7:3:321:MET:O	2.43	0.44
20:k:43:CYS:O	20:k:44:ASP:C	2.61	0.44
5:1:1255:PHE:O	6:2:488:LEU:HD23	2.16	0.44
7:3:294:LYS:HE3	7:3:295:THR:O	2.17	0.44
21:h:33:ASP:C	21:h:33:ASP:OD1	2.60	0.44
7:3:1114:SER:HB2	7:3:1215:TYR:CE1	2.53	0.44
12:E:166:ARG:CB	12:E:166:ARG:CZ	2.96	0.44
5:1:531:LEU:O	5:1:535:ILE:HG13	2.17	0.44
5:1:1302:TYR:HB2	9:5:52:TYR:CD2	2.47	0.44
7:3:49:LYS:HD3	7:3:49:LYS:HA	1.70	0.44
7:3:464:ARG:N	7:3:472:ALA:HB2	2.33	0.44
22:I:29:A:H3'	22:I:30:A:H2	1.82	0.44
1:B:62:LEU:CD2	5:1:1180:ARG:HH22	2.07	0.44
5:1:1006:MET:HE3	5:1:1045:ARG:HB3	1.99	0.44
24:L:15:G:N2	24:L:16:G:C2	2.86	0.44
24:L:118:A:N3	24:L:118:A:C5'	2.81	0.44
25:O:85:GLU:HA	25:O:88:MET:HE3	1.99	0.44
17:l:33:VAL:HG22	17:l:43:ILE:O	2.16	0.44
19:j:82:MET:HB2	19:j:83:LEU:HD12	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1:553:VAL:HG21	5:1:592:GLU:HG2	2.00	0.44
5:1:614:ARG:N	5:1:615:PRO:HD2	2.33	0.44
5:1:1121:GLU:CG	5:1:1161:MET:HE1	2.48	0.44
12:E:241:LYS:HA	12:E:241:LYS:CE	2.42	0.44
3:J:213:GLU:O	3:J:216:ARG:HB2	2.17	0.43
5:1:714:GLU:O	5:1:717:THR:HG22	2.18	0.43
5:1:758:ASP:O	5:1:762:ALA:CB	2.66	0.43
5:1:1174:GLU:HB3	5:1:1178:MET:HE3	1.99	0.43
6:2:522:PHE:O	6:2:522:PHE:CD1	2.71	0.43
6:2:573:ASP:CG	6:2:577:LYS:HD3	2.37	0.43
6:2:707:PRO:HA	7:3:1040:ASP:OD2	2.17	0.43
7:3:125:PRO:HG2	7:3:174:ASP:HA	1.99	0.43
7:3:1027:ASP:OD2	7:3:1031:ARG:NH1	2.50	0.43
12:E:357:MET:C	12:E:359:GLY:N	2.76	0.43
24:L:124:U:OP1	24:L:124:U:C6	2.70	0.43
18:n:43:ASP:CG	18:n:59:MET:CE	2.91	0.43
17:l:36:TYR:CD1	17:l:36:TYR:C	2.95	0.43
5:1:573:LYS:O	5:1:576:VAL:HG12	2.18	0.43
5:1:1180:ARG:HB2	6:2:512:GLN:OE1	2.17	0.43
7:3:899:THR:HG22	7:3:900:GLY:N	2.32	0.43
11:C:393:PRO:HG2	11:C:396:LEU:CG	2.48	0.43
24:L:132:G:C5'	15:i:104:ASP:HB2	2.47	0.43
15:i:62:HIS:CD2	15:i:62:HIS:N	2.86	0.43
5:1:549:ARG:NE	5:1:592:GLU:OE1	2.51	0.43
5:1:578:ILE:HG22	5:1:578:ILE:O	2.19	0.43
5:1:812:PRO:HB2	5:1:813:PRO:HD3	2.00	0.43
7:3:200:ALA:O	7:3:204:THR:OG1	2.35	0.43
7:3:706:MET:HG3	7:3:721:LEU:HD11	2.00	0.43
24:L:94:A:N1	24:L:115:U:C5	2.86	0.43
15:i:40:THR:HG21	15:i:111:ARG:HH21	1.83	0.43
5:1:611:SER:HA	12:E:236:LYS:HE2	1.99	0.43
5:1:611:SER:CA	12:E:232:MET:CE	2.93	0.43
5:1:617:ILE:HG21	12:E:228:LEU:HD11	2.01	0.43
5:1:1286:ARG:NE	7:3:1006:GLN:OE1	2.52	0.43
5:1:1299:GLU:C	9:5:53:PHE:HE1	2.14	0.43
6:2:591:TYR:CD1	6:2:595:LYS:HG2	2.53	0.43
7:3:588:VAL:HG23	7:3:589:CYS:SG	2.59	0.43
5:1:503:LYS:HE3	5:1:511:MET:HB2	1.99	0.43
5:1:607:ALA:CB	12:E:235:VAL:HG13	2.47	0.43
5:1:982:LEU:HD23	5:1:982:LEU:HA	1.86	0.43
5:1:1103:VAL:HG23	5:1:1103:VAL:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1:1185:ARG:NH1	6:2:511:LEU:CD1	2.75	0.43
5:1:1185:ARG:NE	6:2:511:LEU:HD12	2.33	0.43
20:k:53:PRO:CG	20:k:58:GLN:O	2.60	0.43
5:1:653:LYS:HB2	12:E:227:PRO:HG3	2.00	0.43
7:3:702:PHE:HE2	7:3:715:MET:HE2	1.83	0.43
9:5:49:LEU:HD12	9:5:49:LEU:HA	1.87	0.43
24:L:47:C:O5'	24:L:47:C:H6	2.01	0.43
24:L:73:C:C2	24:L:74:C:C4	3.06	0.43
7:3:478:PHE:CE2	7:3:483:LEU:HD23	2.52	0.43
7:3:534:ASN:HD21	7:3:573:GLN:NE2	2.16	0.43
7:3:1063:ASN:CG	7:3:1065:GLU:O	2.59	0.43
11:C:501:LEU:CB	14:G:224:LYS:H	2.31	0.43
24:L:46:C:N4	24:L:47:C:N4	2.66	0.43
24:L:49:A:C2	24:L:50:G:C5	3.07	0.43
24:L:58:C:O2'	24:L:59:U:H5'	2.19	0.43
24:L:118:A:N6	19:j:4:GLY:HA2	2.20	0.43
18:n:57:ILE:O	18:n:57:ILE:HG13	2.19	0.43
30:6:204:SJT:O	30:6:204:SJT:C13	2.66	0.43
5:1:1299:GLU:HG2	9:5:53:PHE:CE2	2.53	0.43
7:3:532:ARG:HE	7:3:532:ARG:HA	1.83	0.43
7:3:552:ARG:HG3	7:3:595:VAL:HG11	2.00	0.43
17:l:48:ILE:HD11	17:l:59:ASP:HB2	1.99	0.43
5:1:767:ARG:O	5:1:771:LEU:HD23	2.18	0.43
5:1:857:LEU:HD12	5:1:857:LEU:HA	1.86	0.43
5:1:1133:MET:CE	6:2:528:ILE:CD1	2.97	0.43
24:L:29:A:H1'	25:O:200:ARG:CD	2.49	0.43
18:n:48:MET:HE3	18:n:48:MET:HB3	1.75	0.43
5:1:495:ARG:HA	5:1:498:MET:HG3	2.01	0.43
5:1:614:ARG:HG3	12:E:232:MET:HG2	1.94	0.43
5:1:1021:THR:HG23	5:1:1022:PRO:HD3	2.01	0.43
6:2:531:THR:HG22	6:2:533:ILE:HG13	1.92	0.43
7:3:716:SER:OG	7:3:717:SER:N	2.51	0.43
7:3:807:TYR:HB2	7:3:812:LYS:HE3	2.01	0.43
24:L:94:A:C2	24:L:115:U:C5	3.07	0.43
20:k:18:ARG:HD2	20:k:83:GLU:OE1	2.19	0.43
5:1:608:THR:HA	12:E:239:VAL:CG2	2.45	0.42
5:1:684:ARG:O	5:1:688:GLU:HG3	2.18	0.42
5:1:709:ILE:HD12	5:1:727:VAL:HG11	2.00	0.42
7:3:515:ALA:HB1	7:3:526:HIS:NE2	2.34	0.42
9:5:53:PHE:O	9:5:57:GLU:HG2	2.19	0.42
22:I:35:U:H2'	22:I:36:C:H4'	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:N:25:CYS:HA	27:N:30:HIS:CD2	2.54	0.42
4:H:144:C:H2'	4:H:145:A:H2'	2.00	0.42
5:1:898:TYR:CE1	12:E:167:VAL:HG21	2.55	0.42
5:1:1010:THR:N	5:1:1011:PRO:HD2	2.34	0.42
6:2:514:LYS:CB	6:2:514:LYS:HZ2	2.31	0.42
7:3:866:ILE:HD13	7:3:907:VAL:HG21	2.00	0.42
25:O:78:ARG:HA	25:O:78:ARG:HD2	1.89	0.42
15:i:62:HIS:CD2	15:i:62:HIS:H	2.37	0.42
19:j:48:VAL:CG1	19:j:56:ALA:HB3	2.49	0.42
4:H:151:C:H2'	4:H:152:G:C8	2.53	0.42
5:1:963:LYS:HE2	5:1:1003:VAL:HG21	2.01	0.42
5:1:1220:PHE:HB2	6:2:503:HIS:NE2	2.34	0.42
5:1:1295:TYR:CE1	9:5:32:LEU:HB3	2.54	0.42
24:L:51:G:C2	24:L:52:G:C8	3.07	0.42
7:3:700:LYS:HB3	7:3:702:PHE:CZ	2.54	0.42
7:3:1128:ILE:HD13	7:3:1216:ALA:HB2	2.01	0.42
11:C:393:PRO:HB2	11:C:395:TRP:CD1	2.54	0.42
17:l:67:LYS:HG3	17:l:68:THR:N	2.34	0.42
19:j:80:ALA:HB1	19:j:81:PRO:HD2	2.01	0.42
5:1:735:ILE:HG22	5:1:746:PHE:HB3	2.02	0.42
7:3:565:TYR:OH	7:3:601:ARG:NH1	2.52	0.42
7:3:1141:PHE:HE1	7:3:1208:LEU:HD23	1.84	0.42
11:C:405:ASN:HB2	11:C:415:THR:CG2	2.44	0.42
24:L:102:A:O2'	24:L:103:A:C8	2.73	0.42
25:O:57:PRO:O	25:O:58:THR:C	2.62	0.42
18:n:59:MET:O	18:n:60:VAL:HG13	2.20	0.42
5:1:945:ALA:CB	5:1:989:VAL:HG21	2.43	0.42
6:2:570:LYS:O	6:2:574:ALA:CB	2.67	0.42
7:3:83:ASP:O	7:3:111:GLY:N	2.48	0.42
7:3:279:ASP:HA	7:3:857:ALA:HB2	2.01	0.42
7:3:635:ALA:HB3	7:3:669:LEU:HD13	2.01	0.42
11:C:400:HIS:HE1	22:I:29:A:C4	2.33	0.42
12:E:153:GLN:OE1	12:E:153:GLN:HA	2.20	0.42
16:m:3:LEU:HG	16:m:4:PRO:HD2	2.02	0.42
20:k:12:HIS:H	20:k:12:HIS:HD2	1.64	0.42
20:k:17:MET:HE3	20:k:82:VAL:CG2	2.49	0.42
27:N:17:SER:O	27:N:21:ARG:HG2	2.20	0.42
5:1:584:ASP:O	5:1:590:ARG:NH2	2.50	0.42
5:1:664:GLY:O	5:1:668:VAL:HG23	2.20	0.42
5:1:893:ILE:HG21	5:1:928:TYR:CG	2.55	0.42
5:1:926:LYS:O	5:1:929:LEU:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1:1133:MET:HE1	6:2:528:ILE:HD13	2.00	0.42
15:i:40:THR:HG21	15:i:111:ARG:NH2	2.35	0.42
5:1:900:PHE:CE1	5:1:954:LEU:CD2	2.99	0.42
5:1:998:LYS:O	5:1:1002:ASN:HB2	2.19	0.42
7:3:704:VAL:HG21	7:3:713:LEU:HB2	2.01	0.42
25:O:28:LEU:HD12	25:O:28:LEU:HA	1.96	0.42
19:j:9:VAL:HG12	19:j:73:LEU:HD23	2.01	0.42
28:6:61:CYS:C	28:6:63:GLY:N	2.74	0.42
5:1:560:LEU:HD12	5:1:560:LEU:HA	1.87	0.42
5:1:719:TYR:CZ	7:3:72:GLY:O	2.73	0.42
5:1:994:LEU:HD11	5:1:1031:VAL:HG13	2.02	0.42
24:L:104:A:H4'	24:L:106:G:C6	2.55	0.42
24:L:139:G:H2'	24:L:140:G:O4'	2.20	0.42
5:1:926:LYS:HG2	5:1:927:PRO:CD	2.48	0.42
5:1:1157:TYR:O	28:6:38:ARG:NH2	2.39	0.42
27:N:45:GLN:O	27:N:48:SER:HB3	2.19	0.42
27:N:46:ALA:O	27:N:49:LEU:HG	2.19	0.42
5:1:864:TYR:O	5:1:868:VAL:HG23	2.19	0.41
5:1:1004:ILE:HD12	5:1:1009:MET:HA	2.02	0.41
7:3:773:VAL:HG13	7:3:774:PHE:CD2	2.54	0.41
17:l:62:GLU:OE1	17:l:71:ARG:HD3	2.20	0.41
27:N:40:LYS:HE3	27:N:40:LYS:HA	2.02	0.41
5:1:952:ALA:O	5:1:956:SER:OG	2.37	0.41
5:1:1140:GLU:HB3	5:1:1143:VAL:HG21	2.02	0.41
7:3:437:VAL:O	7:3:776:GLN:HA	2.21	0.41
7:3:473:TYR:HB3	7:3:484:VAL:HG23	2.02	0.41
7:3:473:TYR:CZ	7:3:497:SER:HA	2.55	0.41
7:3:946:GLU:OE1	7:3:946:GLU:N	2.53	0.41
12:E:157:GLU:N	12:E:157:GLU:OE2	2.53	0.41
12:E:357:MET:C	12:E:359:GLY:H	2.28	0.41
24:L:54:G:N2	24:L:84:G:H2'	2.36	0.41
4:H:45:C:OP2	4:H:45:C:H2'	2.21	0.41
5:1:587:TYR:O	5:1:591:VAL:HG23	2.19	0.41
5:1:1021:THR:N	5:1:1022:PRO:HD2	2.34	0.41
6:2:522:PHE:CD1	6:2:522:PHE:C	2.99	0.41
7:3:48:GLY:HA3	7:3:398:VAL:HG11	2.02	0.41
7:3:703:ARG:NH1	7:3:703:ARG:HA	2.36	0.41
24:L:138:G:C6	24:L:164:G:C6	3.09	0.41
24:L:149:U:O2'	24:L:150:U:H2'	2.21	0.41
25:O:46:ARG:HG3	25:O:47:GLU:N	2.35	0.41
5:1:647:PHE:HB2	12:E:231:TYR:CD1	2.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1:1279:ALA:HB1	7:3:1167:TYR:HA	2.02	0.41
7:3:136:GLU:HB3	7:3:137:LYS:H	1.77	0.41
7:3:616:ILE:O	7:3:617:ILE:HD13	2.20	0.41
7:3:702:PHE:CE2	7:3:741:PHE:HA	2.55	0.41
7:3:724:SER:HA	7:3:729:PHE:HA	2.02	0.41
7:3:818:GLN:O	7:3:822:GLU:HG3	2.21	0.41
11:C:397:TYR:HE2	11:C:403:ASN:CB	2.33	0.41
12:E:155:LYS:N	12:E:155:LYS:HD2	2.35	0.41
24:L:15:G:H2'	24:L:16:G:C4	2.55	0.41
24:L:47:C:C5	24:L:48:C:C6	3.09	0.41
24:L:91:G:O2'	24:L:92:C:C5'	2.69	0.41
30:6:204:SJT:O3	30:6:204:SJT:C17	2.69	0.41
5:1:1036:ILE:HD11	5:1:1065:LEU:CD1	2.48	0.41
6:2:469:VAL:HG11	6:2:489:VAL:HG11	2.02	0.41
7:3:463:ARG:HA	7:3:472:ALA:H	1.86	0.41
24:L:135:A:N6	25:O:37:PRO:CA	2.83	0.41
25:O:50:ASP:N	25:O:51:PRO:CD	2.83	0.41
1:B:46:PHE:HB2	1:B:69:TYR:CZ	2.56	0.41
7:3:343:LYS:HE3	7:3:343:LYS:HB3	1.66	0.41
7:3:1165:SER:OG	7:3:1170:VAL:HG23	2.20	0.41
16:m:19:VAL:HG11	16:m:72:ILE:CD1	2.42	0.41
19:j:60:GLN:C	19:j:61:VAL:HG23	2.45	0.41
24:L:54:G:H22	24:L:84:G:H2'	1.85	0.41
25:O:89:TRP:CZ2	25:O:91:PRO:HG3	2.55	0.41
19:j:46:ILE:HG12	19:j:58:LEU:HB2	2.01	0.41
5:1:1178:MET:CE	5:1:1214:TYR:CE1	3.03	0.41
7:3:317:THR:HG22	7:3:318:ASP:N	2.36	0.41
7:3:691:THR:HB	7:3:720:TRP:CH2	2.55	0.41
11:C:400:HIS:C	11:C:402:LEU:HD22	2.45	0.41
24:L:15:G:H3'	24:L:16:G:C8	2.56	0.41
24:L:32:A:C2	25:O:133:HIS:O	2.73	0.41
24:L:33:C:O3'	25:O:144:ARG:CD	2.61	0.41
24:L:118:A:C2'	27:N:2:PRO:HD2	2.50	0.41
25:O:34:HIS:ND1	25:O:37:PRO:HB3	2.35	0.41
25:O:109:ARG:O	25:O:172:ARG:HD3	2.20	0.41
3:J:219:ARG:NH2	5:1:1092:ASP:CG	2.78	0.41
5:1:511:MET:HE2	5:1:511:MET:HB3	1.83	0.41
5:1:840:LEU:O	5:1:844:VAL:HG12	2.21	0.41
5:1:885:ASP:OD1	5:1:887:LYS:HE3	2.20	0.41
5:1:926:LYS:H	5:1:926:LYS:HD3	1.86	0.41
5:1:1137:ARG:HH21	5:1:1137:ARG:HG3	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1:1144:GLN:CB	5:1:1184:HIS:HE1	2.32	0.41
5:1:1177:LEU:CD2	5:1:1188:ALA:HB1	2.51	0.41
5:1:1302:TYR:C	9:5:52:TYR:OH	2.64	0.41
6:2:517:ILE:C	6:2:517:ILE:CD1	2.92	0.41
7:3:499:PHE:HE1	7:3:516:LEU:HD13	1.86	0.41
24:L:48:C:C6	24:L:48:C:H5'	2.56	0.41
24:L:120:U:O2'	24:L:121:G:H5'	2.20	0.41
24:L:164:G:C4'	21:h:49:ASN:C	2.93	0.41
21:h:18:GLU:OE1	15:i:94:ARG:NH2	2.37	0.41
20:k:60:GLU:O	20:k:60:GLU:HG2	2.20	0.41
26:M:50:LYS:HG2	26:M:51:MET:SD	2.60	0.41
19:j:57:GLN:O	19:j:58:LEU:HD23	2.20	0.41
19:j:73:LEU:N	19:j:73:LEU:CD1	2.84	0.41
5:1:823:MET:HE3	5:1:823:MET:HA	2.02	0.41
5:1:1066:LEU:HD23	30:6:204:SJT:C4	2.48	0.41
6:2:459:ARG:NH1	6:2:481:THR:HG22	2.36	0.41
7:3:1020:GLN:HB3	7:3:1022:ILE:HD11	2.03	0.41
24:L:17:G:H2'	24:L:18:G:C8	2.55	0.41
24:L:33:C:C5'	25:O:138:LYS:H	2.34	0.41
24:L:118:A:H8	27:N:3:LYS:N	2.01	0.41
24:L:122:C:H2'	24:L:123:A:OP2	2.21	0.41
3:J:227:GLN:O	3:J:231:LYS:HG3	2.22	0.40
4:H:45:C:P	11:C:394:TYR:HB3	2.59	0.40
7:3:531:LYS:HA	7:3:531:LYS:HD3	1.80	0.40
24:L:20:G:C2'	24:L:21:A:H5'	2.50	0.40
24:L:73:C:H3'	24:L:74:C:C6	2.55	0.40
24:L:73:C:H3'	24:L:74:C:H5	1.83	0.40
28:6:42:LEU:HD23	28:6:44:ARG:HH12	1.86	0.40
4:H:34:U:H6	4:H:34:U:H2'	1.76	0.40
4:H:51:A:H2'	4:H:52:G:H8	1.86	0.40
5:1:856:ASP:HB3	5:1:864:TYR:HE2	1.86	0.40
5:1:1009:MET:SD	5:1:1011:PRO:HD2	2.61	0.40
5:1:1016:LEU:CD2	5:1:1042:ILE:HD11	2.51	0.40
5:1:1206:ASP:HB3	6:2:584:LEU:CD1	2.46	0.40
7:3:594:ASN:H	7:3:594:ASN:ND2	2.18	0.40
15:a:78:PRO:HD3	15:a:89:PRO:HA	2.04	0.40
22:I:27:U:O2	22:I:27:U:C2'	2.70	0.40
5:1:1004:ILE:O	5:1:1004:ILE:CG2	2.69	0.40
7:3:511:LEU:HD11	7:3:568:MET:HG3	2.02	0.40
7:3:924:PHE:CG	7:3:942:LYS:HE2	2.57	0.40
7:3:1095:TYR:HB2	7:3:1173:VAL:HG21	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:I:27:U:H2'	22:I:28:G:C8	2.56	0.40
24:L:21:A:H2'	24:L:22:U:H5''	2.03	0.40
24:L:140:G:O2'	24:L:141:G:H5'	2.22	0.40
5:1:1129:LEU:HD12	5:1:1165:TYR:HD1	1.82	0.40
5:1:1137:ARG:NH2	5:1:1137:ARG:HG3	2.36	0.40
5:1:1286:ARG:HH21	7:3:1006:GLN:HB2	1.86	0.40
7:3:515:ALA:HB1	7:3:526:HIS:CE1	2.56	0.40
7:3:644:GLU:O	7:3:710:GLU:HB2	2.22	0.40
18:n:11:LYS:O	18:n:76:VAL:HG13	2.21	0.40
19:j:83:LEU:N	19:j:83:LEU:CD1	2.84	0.40
5:1:893:ILE:O	5:1:896:ILE:HG13	2.21	0.40
5:1:1004:ILE:HG21	5:1:1009:MET:CE	2.49	0.40
5:1:1056:MET:HE3	5:1:1056:MET:HB3	1.90	0.40
5:1:1177:LEU:HD23	5:1:1188:ALA:HB3	2.04	0.40
7:3:756:ALA:O	7:3:757:ILE:HD13	2.22	0.40
11:C:392:ILE:HD11	11:C:397:TYR:CD1	2.57	0.40
20:f:86:PRO:HA	20:f:87:PRO:HD3	1.92	0.40
24:L:118:A:C1'	27:N:2:PRO:HD2	2.50	0.40
24:L:140:G:O2'	20:k:57:LYS:CE	2.69	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	B	141/464 (30%)	139 (99%)	2 (1%)	0	100	100
2	D	114/639 (18%)	113 (99%)	1 (1%)	0	100	100
3	J	52/253 (21%)	51 (98%)	1 (2%)	0	100	100
5	1	813/1304 (62%)	776 (95%)	33 (4%)	4 (0%)	24	60
6	2	177/895 (20%)	162 (92%)	14 (8%)	1 (1%)	21	56

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	3	1168/1217 (96%)	1119 (96%)	47 (4%)	2 (0%)	43	76
8	4	156/424 (37%)	153 (98%)	3 (2%)	0	100	100
9	5	64/86 (74%)	63 (98%)	1 (2%)	0	100	100
10	A	121/793 (15%)	121 (100%)	0	0	100	100
11	C	419/501 (84%)	397 (95%)	20 (5%)	2 (0%)	24	60
12	E	447/1031 (43%)	430 (96%)	16 (4%)	1 (0%)	43	76
13	F	160/255 (63%)	160 (100%)	0	0	100	100
14	G	160/225 (71%)	158 (99%)	2 (1%)	0	100	100
15	a	86/118 (73%)	84 (98%)	2 (2%)	0	100	100
15	i	90/118 (76%)	84 (93%)	6 (7%)	0	100	100
16	b	72/86 (84%)	71 (99%)	1 (1%)	0	100	100
16	m	72/86 (84%)	69 (96%)	3 (4%)	0	100	100
17	c	77/92 (84%)	77 (100%)	0	0	100	100
17	l	75/92 (82%)	70 (93%)	5 (7%)	0	100	100
18	d	72/76 (95%)	72 (100%)	0	0	100	100
18	n	71/76 (93%)	69 (97%)	2 (3%)	0	100	100
19	e	81/126 (64%)	79 (98%)	2 (2%)	0	100	100
19	j	79/126 (63%)	75 (95%)	4 (5%)	0	100	100
20	f	67/240 (28%)	67 (100%)	0	0	100	100
20	k	84/240 (35%)	82 (98%)	2 (2%)	0	100	100
21	g	80/119 (67%)	79 (99%)	1 (1%)	0	100	100
21	h	79/119 (66%)	77 (98%)	2 (2%)	0	100	100
25	O	199/437 (46%)	182 (92%)	13 (6%)	4 (2%)	6	28
26	M	96/282 (34%)	94 (98%)	2 (2%)	0	100	100
27	N	48/159 (30%)	47 (98%)	1 (2%)	0	100	100
28	6	79/110 (72%)	71 (90%)	5 (6%)	3 (4%)	2	15
All	All	5499/10789 (51%)	5291 (96%)	191 (4%)	17 (0%)	37	70

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	1	969	LYS
5	1	1052	ALA

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Mol	Chain	Res	Type
5	1	1053	ARG
7	3	1064	ASP
25	O	59	ARG
25	O	63	ARG
11	C	412	GLY
25	O	33	HIS
25	O	60	ALA
28	6	34	ASP
28	6	62	GLY
6	2	496	ASN
11	C	419	PRO
12	E	585	GLY
28	6	15	ALA
7	3	997	GLY
5	1	1003	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	47/382 (12%)	47 (100%)	0	100	100
3	J	24/226 (11%)	22 (92%)	2 (8%)	10	37
5	1	701/1104 (64%)	648 (92%)	53 (8%)	12	41
6	2	124/776 (16%)	116 (94%)	8 (6%)	15	47
7	3	1022/1051 (97%)	957 (94%)	65 (6%)	16	48
8	4	8/336 (2%)	8 (100%)	0	100	100
9	5	57/77 (74%)	56 (98%)	1 (2%)	51	77
10	A	4/709 (1%)	4 (100%)	0	100	100
11	C	83/446 (19%)	77 (93%)	6 (7%)	13	43
12	E	73/892 (8%)	64 (88%)	9 (12%)	4	21
13	F	6/218 (3%)	6 (100%)	0	100	100
14	G	7/195 (4%)	7 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	a	4/110 (4%)	4 (100%)	0	100	100
15	i	89/110 (81%)	80 (90%)	9 (10%)	7	29
16	b	4/74 (5%)	4 (100%)	0	100	100
16	m	63/74 (85%)	56 (89%)	7 (11%)	6	25
17	c	1/84 (1%)	1 (100%)	0	100	100
17	l	72/84 (86%)	61 (85%)	11 (15%)	3	14
18	d	3/66 (4%)	3 (100%)	0	100	100
18	n	63/66 (96%)	54 (86%)	9 (14%)	3	16
19	e	3/101 (3%)	3 (100%)	0	100	100
19	j	71/101 (70%)	61 (86%)	10 (14%)	3	16
20	f	3/177 (2%)	3 (100%)	0	100	100
20	k	78/177 (44%)	69 (88%)	9 (12%)	5	24
21	g	3/101 (3%)	3 (100%)	0	100	100
21	h	76/101 (75%)	72 (95%)	4 (5%)	20	54
25	O	169/373 (45%)	153 (90%)	16 (10%)	8	31
26	M	85/240 (35%)	81 (95%)	4 (5%)	23	58
27	N	48/135 (36%)	41 (85%)	7 (15%)	3	15
28	6	69/95 (73%)	62 (90%)	7 (10%)	7	29
All	All	3060/8681 (35%)	2823 (92%)	237 (8%)	14	40

All (237) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	J	209	GLN
3	J	230	THR
5	1	501	LEU
5	1	518	GLN
5	1	554	LYS
5	1	556	ILE
5	1	576	VAL
5	1	585	GLU
5	1	637	SER
5	1	683	LEU
5	1	699	GLN
5	1	700	LYS
5	1	705	SER

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Mol	Chain	Res	Type
5	1	718	PRO
5	1	721	ILE
5	1	722	GLU
5	1	735	ILE
5	1	768	GLU
5	1	771	LEU
5	1	781	ASP
5	1	798	THR
5	1	801	VAL
5	1	825	LEU
5	1	850	ILE
5	1	872	ILE
5	1	883	ASP
5	1	892	LEU
5	1	908	SER
5	1	925	VAL
5	1	926	LYS
5	1	946	LYS
5	1	956	SER
5	1	962	MET
5	1	965	CYS
5	1	966	GLN
5	1	967	GLU
5	1	968	GLU
5	1	1004	ILE
5	1	1007	HIS
5	1	1008	LYS
5	1	1009	MET
5	1	1010	THR
5	1	1013	ILE
5	1	1014	LYS
5	1	1016	LEU
5	1	1048	GLU
5	1	1050	VAL
5	1	1053	ARG
5	1	1069	HIS
5	1	1070	LYS
5	1	1105	GLU
5	1	1137	ARG
5	1	1141	LEU
5	1	1142	ASN
5	1	1160	GLU

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Mol	Chain	Res	Type
6	2	488	LEU
6	2	498	VAL
6	2	514	LYS
6	2	515	ARG
6	2	517	ILE
6	2	531	THR
6	2	587	HIS
6	2	595	LYS
7	3	55	THR
7	3	64	SER
7	3	114	ARG
7	3	132	ILE
7	3	223	LYS
7	3	235	LEU
7	3	243	ASP
7	3	278	LEU
7	3	316	GLU
7	3	318	ASP
7	3	320	ASP
7	3	342	LEU
7	3	351	SER
7	3	390	ARG
7	3	415	LEU
7	3	420	THR
7	3	429	ARG
7	3	444	VAL
7	3	459	VAL
7	3	461	THR
7	3	462	VAL
7	3	476	VAL
7	3	484	VAL
7	3	490	THR
7	3	497	SER
7	3	513	ASP
7	3	524	ILE
7	3	533	VAL
7	3	534	ASN
7	3	546	LYS
7	3	549	VAL
7	3	558	LEU
7	3	573	GLN
7	3	589	CYS

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Mol	Chain	Res	Type
7	3	590	MET
7	3	591	SER
7	3	595	VAL
7	3	629	SER
7	3	633	LEU
7	3	640	LEU
7	3	643	VAL
7	3	670	GLN
7	3	689	THR
7	3	704	VAL
7	3	712	VAL
7	3	713	LEU
7	3	738	THR
7	3	755	VAL
7	3	809	GLU
7	3	834	LEU
7	3	864	SER
7	3	865	VAL
7	3	890	SER
7	3	909	VAL
7	3	959	VAL
7	3	1001	ILE
7	3	1008	SER
7	3	1043	THR
7	3	1048	ASP
7	3	1062	THR
7	3	1120	THR
7	3	1121	THR
7	3	1191	LYS
7	3	1197	LEU
7	3	1217	PHE
9	5	49	LEU
11	C	395	TRP
11	C	399	LEU
11	C	403	ASN
11	C	425	HIS
11	C	472	GLN
11	C	475	THR
12	E	157	GLU
12	E	177	LYS
12	E	198	TRP
12	E	203	ASP

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Mol	Chain	Res	Type
12	E	207	GLU
12	E	225	LEU
12	E	228	LEU
12	E	239	VAL
12	E	241	LYS
25	O	3	GLN
25	O	19	ILE
25	O	28	LEU
25	O	45	ILE
25	O	47	GLU
25	O	48	PHE
25	O	50	ASP
25	O	70	LYS
25	O	82	VAL
25	O	86	LEU
25	O	124	GLU
25	O	140	SER
25	O	167	LYS
25	O	168	LYS
25	O	172	ARG
25	O	188	ARG
16	m	3	LEU
16	m	8	LYS
16	m	14	LEU
16	m	23	LEU
16	m	27	MET
16	m	51	ILE
16	m	65	ARG
21	h	4	VAL
21	h	11	SER
21	h	19	LEU
21	h	82	ASP
20	k	7	SER
20	k	12	HIS
20	k	13	ILE
20	k	54	LYS
20	k	56	SER
20	k	57	LYS
20	k	58	GLN
20	k	67	LEU
20	k	71	LEU
26	M	8	PRO

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Mol	Chain	Res	Type
26	M	39	GLN
26	M	61	GLU
26	M	103	GLU
18	n	21	LEU
18	n	27	VAL
18	n	28	GLN
18	n	46	VAL
18	n	50	THR
18	n	51	SER
18	n	57	ILE
18	n	59	MET
18	n	69	MET
17	l	25	LEU
17	l	27	ASN
17	l	60	ASP
17	l	62	GLU
17	l	63	GLU
17	l	68	THR
17	l	70	SER
17	l	79	LEU
17	l	80	LYS
17	l	82	ASP
17	l	86	LEU
15	i	20	GLU
15	i	37	LYS
15	i	42	VAL
15	i	51	LYS
15	i	61	ARG
15	i	75	THR
15	i	94	ARG
15	i	108	VAL
15	i	114	LEU
27	N	3	LYS
27	N	26	SER
27	N	29	LYS
27	N	39	GLN
27	N	44	GLU
27	N	45	GLN
27	N	48	SER
19	j	3	ILE
19	j	24	THR
19	j	34	GLU

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Mol	Chain	Res	Type
19	j	46	ILE
19	j	47	THR
19	j	51	ARG
19	j	73	LEU
19	j	78	LYS
19	j	82	MET
19	j	83	LEU
28	6	14	GLN
28	6	17	VAL
28	6	26	CYS
28	6	27	ASP
28	6	36	TYR
28	6	37	VAL
28	6	61	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (63) such sidechains are listed below:

Mol	Chain	Res	Type
3	J	209	GLN
5	1	506	ASN
5	1	533	ASN
5	1	534	GLN
5	1	662	HIS
5	1	737	GLN
5	1	763	ASN
5	1	817	HIS
5	1	919	ASN
5	1	950	GLN
5	1	966	GLN
5	1	1002	ASN
5	1	1007	HIS
5	1	1032	GLN
5	1	1091	HIS
5	1	1144	GLN
5	1	1184	HIS
5	1	1193	GLN
5	1	1256	HIS
5	1	1283	HIS
5	1	1293	ASN
6	2	458	ASN
6	2	467	GLN
6	2	478	HIS

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Mol	Chain	Res	Type
6	2	503	HIS
7	3	5	ASN
7	3	46	ASN
7	3	119	GLN
7	3	164	ASN
7	3	194	ASN
7	3	254	ASN
7	3	264	GLN
7	3	276	ASN
7	3	363	HIS
7	3	480	ASN
7	3	594	ASN
7	3	612	ASN
7	3	709	GLN
7	3	776	GLN
7	3	796	ASN
7	3	805	ASN
7	3	844	ASN
7	3	870	ASN
7	3	916	ASN
7	3	941	HIS
7	3	988	ASN
7	3	1017	ASN
7	3	1052	ASN
9	5	36	HIS
9	5	74	GLN
11	C	400	HIS
11	C	445	HIS
25	O	33	HIS
25	O	35	ASN
25	O	80	GLN
25	O	133	HIS
25	O	163	HIS
16	m	46	ASN
21	h	64	ASN
20	k	22	GLN
26	M	67	ASN
17	l	65	HIS
19	j	45	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
22	I	15/259 (5%)	7 (46%)	4 (26%)
23	K	9/10 (90%)	2 (22%)	0
24	L	163/164 (99%)	51 (31%)	6 (3%)
4	H	126/188 (67%)	29 (23%)	2 (1%)
All	All	313/621 (50%)	89 (28%)	12 (3%)

All (89) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	H	35	A
4	H	36	G
4	H	45	C
4	H	46	U
4	H	47	U
4	H	48	A
4	H	49	U
4	H	50	C
4	H	101	U
4	H	102	U
4	H	103	U
4	H	111	G
4	H	116	A
4	H	117	U
4	H	121	A
4	H	122	U
4	H	123	A
4	H	124	G
4	H	128	C
4	H	129	U
4	H	130	U
4	H	131	G
4	H	136	G
4	H	138	C
4	H	146	C
4	H	147	G
4	H	157	G
4	H	164	C
4	H	177	A
22	I	28	G
22	I	29	A
22	I	30	A
22	I	31	G
22	I	35	U

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Mol	Chain	Res	Type
22	I	36	C
22	I	37	A
23	K	0	G
23	K	5	G
24	L	3	A
24	L	10	U
24	L	12	G
24	L	15	G
24	L	16	G
24	L	17	G
24	L	20	G
24	L	21	A
24	L	22	U
24	L	23	A
24	L	28	G
24	L	29	A
24	L	35	A
24	L	41	G
24	L	47	C
24	L	48	C
24	L	50	G
24	L	51	G
24	L	55	A
24	L	62	U
24	L	72	U
24	L	73	C
24	L	75	G
24	L	78	U
24	L	88	C
24	L	90	U
24	L	91	G
24	L	92	C
24	L	93	G
24	L	94	A
24	L	103	A
24	L	105	U
24	L	108	G
24	L	112	A
24	L	114	C
24	L	115	U
24	L	117	G
24	L	118	A

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Mol	Chain	Res	Type
24	L	119	C
24	L	123	A
24	L	124	U
24	L	126	A
24	L	128	U
24	L	130	G
24	L	132	G
24	L	133	G
24	L	135	A
24	L	136	G
24	L	137	U
24	L	138	G
24	L	158	U

All (12) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	H	45	C
4	H	46	U
22	I	27	U
22	I	28	G
22	I	29	A
22	I	30	A
24	L	15	G
24	L	90	U
24	L	92	C
24	L	123	A
24	L	126	A
24	L	128	U

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 7 ligands modelled in this entry, 6 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
30	SJT	6	204	-	38,38,38	1.25	6 (15%)	51,55,55	1.77	11 (21%)

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
30	SJT	6	204	-	5/5/12/18	19/26/63/63	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	6	204	SJT	C17-C16	-3.21	1.44	1.50
30	6	204	SJT	C1-C	-3.09	1.41	1.48
30	6	204	SJT	O1-C3	-2.69	1.44	1.47
30	6	204	SJT	O1-C5	-2.50	1.29	1.35
30	6	204	SJT	C18-C16	-2.14	1.41	1.46
30	6	204	SJT	O-C	-2.02	1.20	1.24

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	6	204	SJT	C2-C1-C	-5.90	108.80	122.67
30	6	204	SJT	C19-C18-C16	-5.13	115.28	126.32
30	6	204	SJT	C26-C25-C24	-4.04	109.69	113.36
30	6	204	SJT	O7-C25-C26	-3.46	111.01	113.61
30	6	204	SJT	C21-C20-C19	-3.28	108.56	112.75
30	6	204	SJT	C13-C7-N	3.15	115.59	110.78
30	6	204	SJT	C22-C21-C20	-2.61	107.52	111.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	6	204	SJT	C13-C7-C8	2.35	114.03	109.53
30	6	204	SJT	C14-C10-C11	-2.17	110.33	115.30
30	6	204	SJT	O6-C25-C26	-2.16	103.97	106.94
30	6	204	SJT	C8-C7-N	2.02	112.93	110.09

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
30	6	204	SJT	C10
30	6	204	SJT	C22
30	6	204	SJT	C25
30	6	204	SJT	C8
30	6	204	SJT	C3

All (19) torsion outliers are listed below:

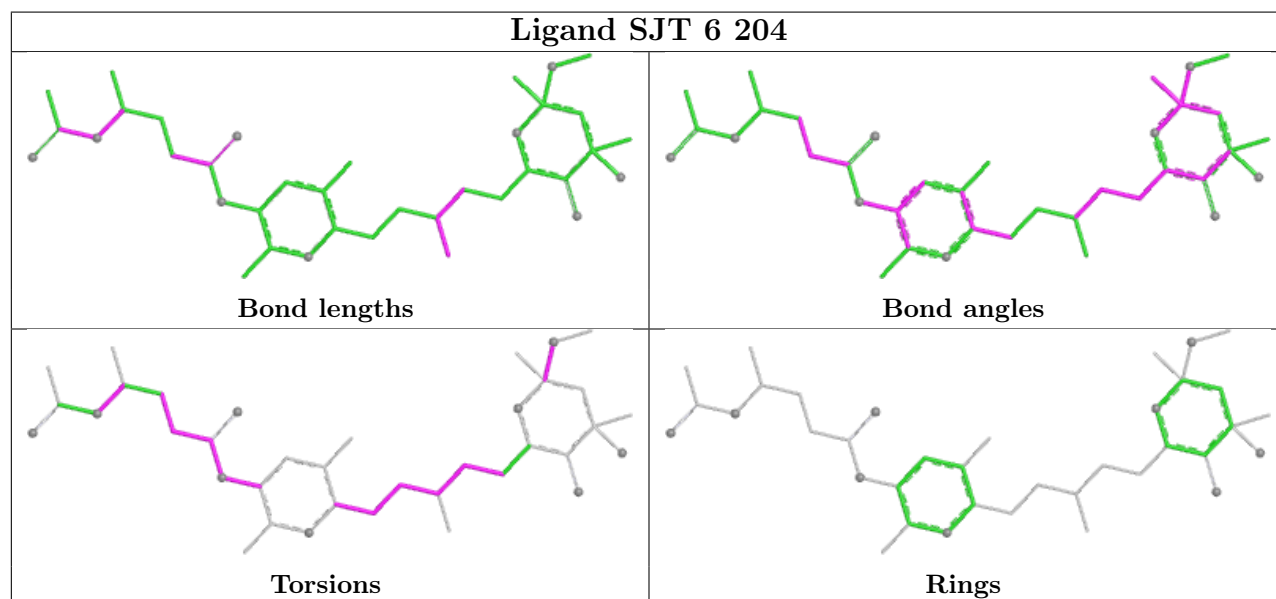
Mol	Chain	Res	Type	Atoms
30	6	204	SJT	C-C1-C2-C3
30	6	204	SJT	O-C-N-C7
30	6	204	SJT	C1-C-N-C7
30	6	204	SJT	C13-C7-N-C
30	6	204	SJT	O3-C10-C14-C15
30	6	204	SJT	C10-C14-C15-C16
30	6	204	SJT	C14-C15-C16-C17
30	6	204	SJT	C14-C15-C16-C18
30	6	204	SJT	C16-C18-C19-C20
30	6	204	SJT	C24-C25-O7-C27
30	6	204	SJT	C26-C25-O7-C27
30	6	204	SJT	O6-C25-O7-C27
30	6	204	SJT	O-C-C1-C2
30	6	204	SJT	N-C-C1-C2
30	6	204	SJT	C15-C16-C18-C19
30	6	204	SJT	C17-C16-C18-C19
30	6	204	SJT	C11-C10-C14-C15
30	6	204	SJT	C2-C3-O1-C5
30	6	204	SJT	C4-C3-O1-C5

There are no ring outliers.

1 monomer is involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	6	204	SJT	16	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.

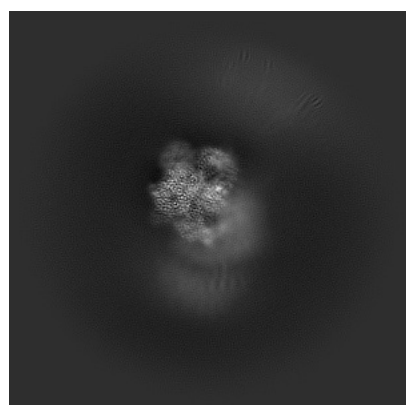
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32074. These allow visual inspection of the internal detail of the map and identification of artifacts.

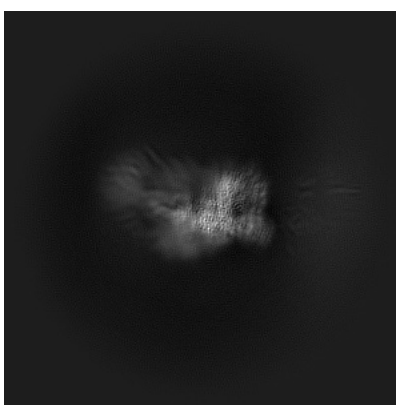
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

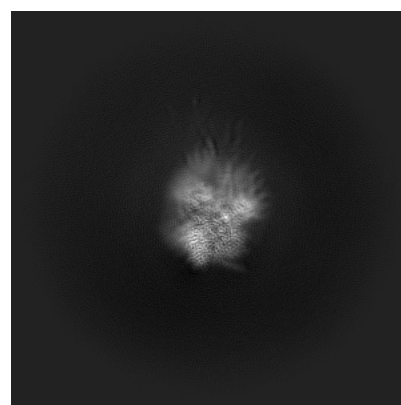
6.1.1 Primary map



X



Y

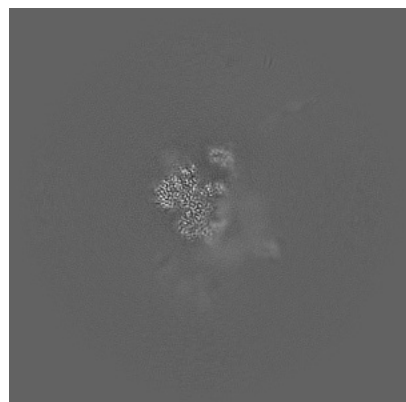


Z

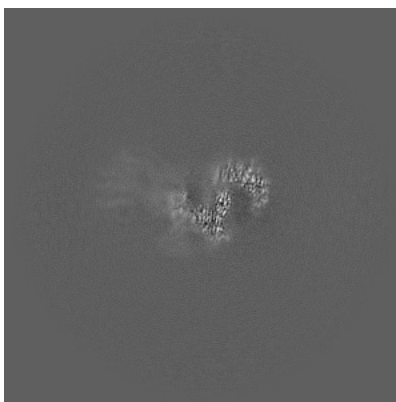
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 240



Y Index: 240



Z Index: 240

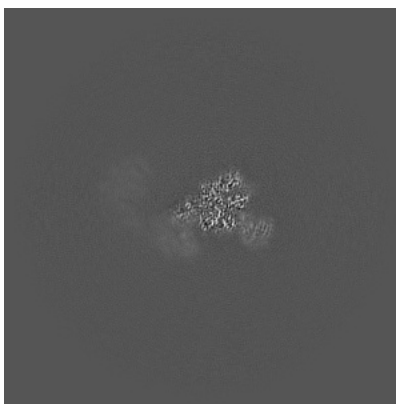
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

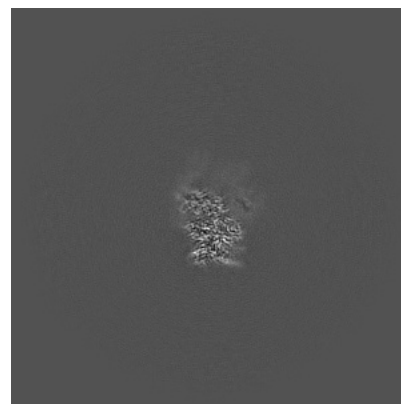
6.3.1 Primary map



X Index: 226



Y Index: 211

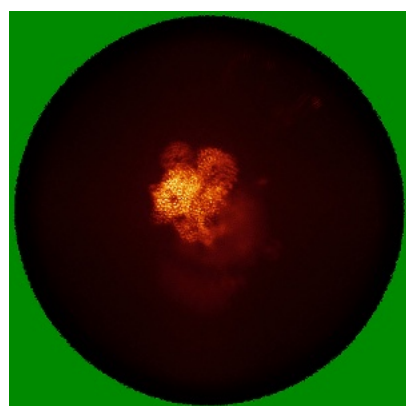


Z Index: 260

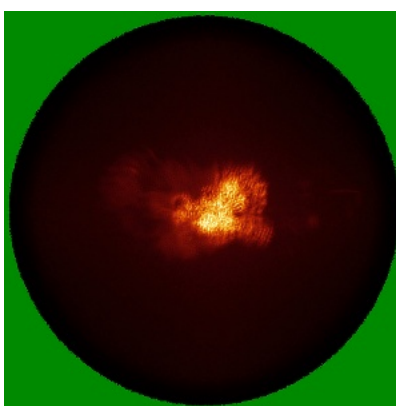
The images above show the largest variance slices of the map in three orthogonal directions.

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

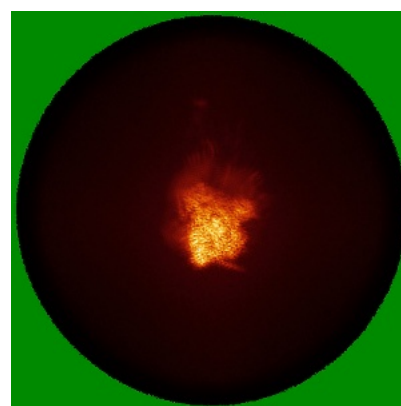
6.4.1 Primary map



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

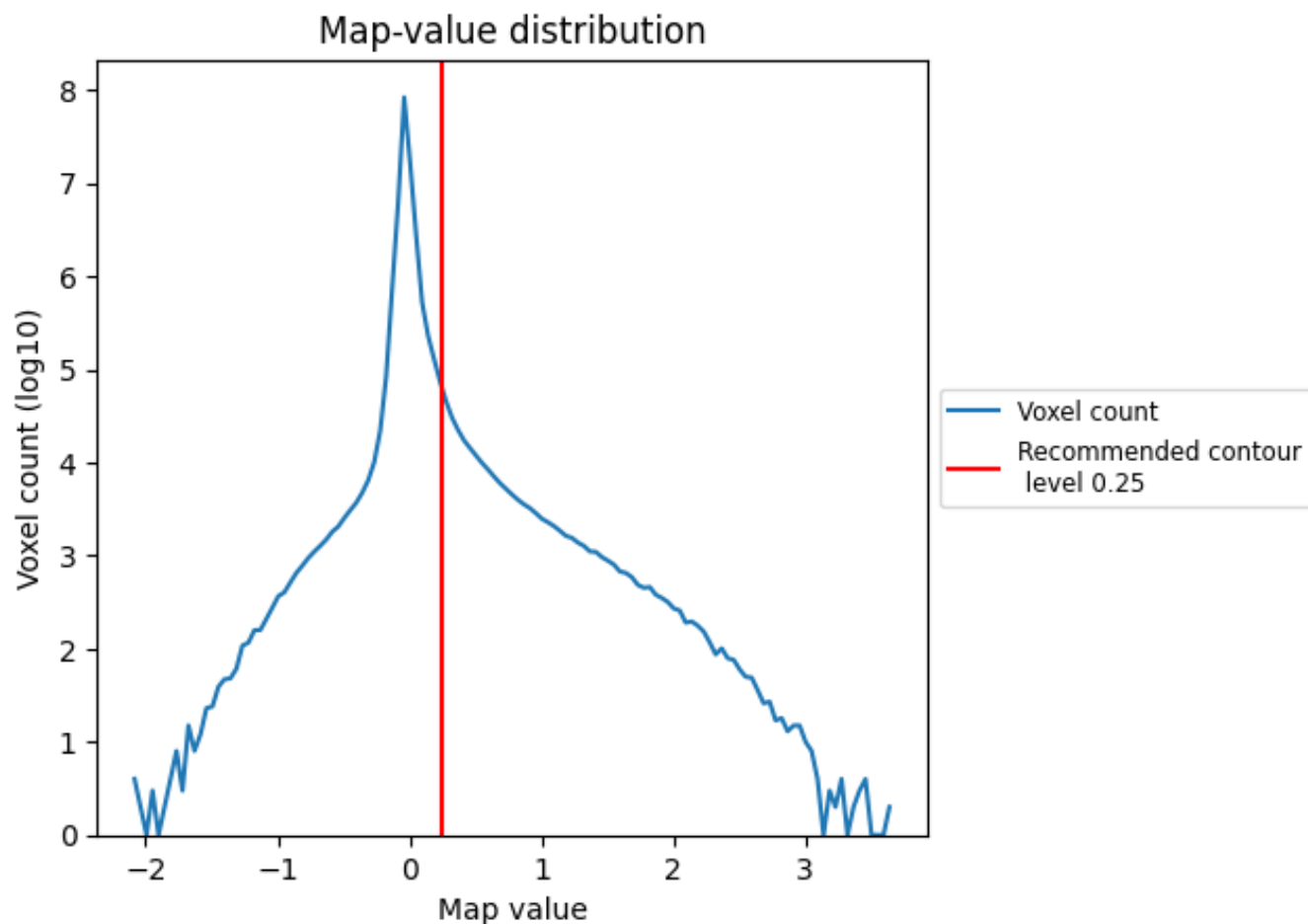
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

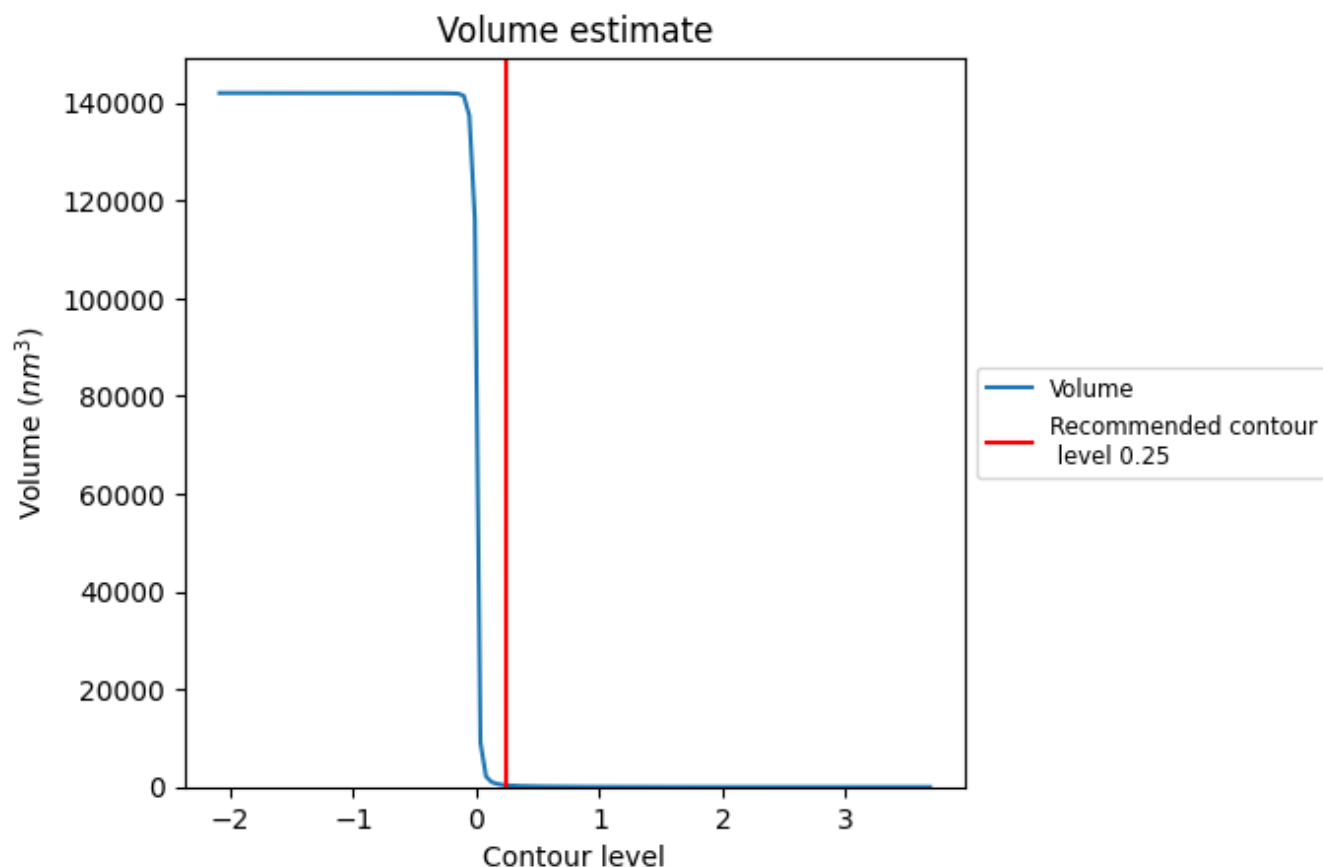
This section contains the results of statistical analysis of the map.

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.

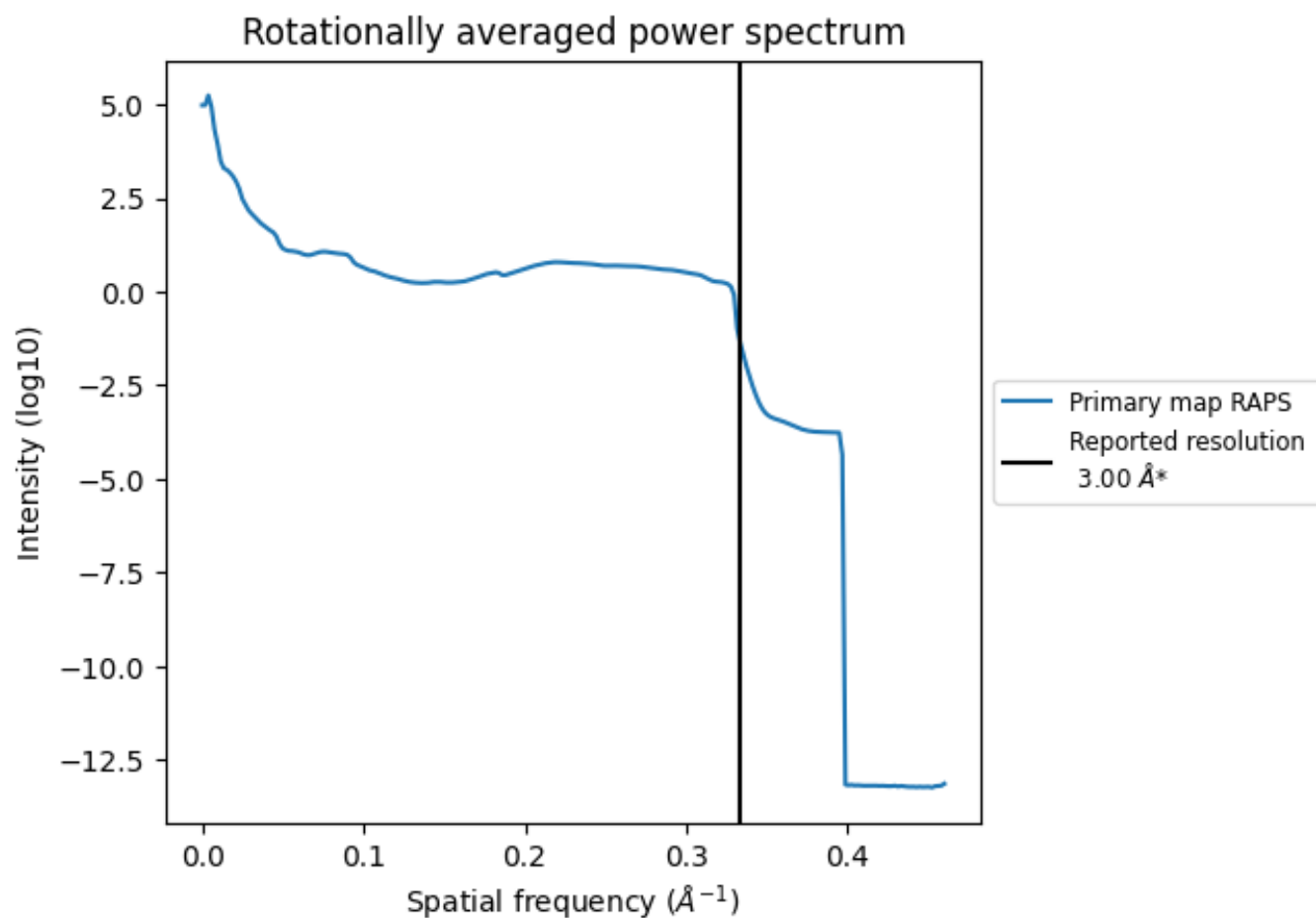
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 341 nm^3 ; this corresponds to an approximate mass of 308 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 0.333 Å⁻¹

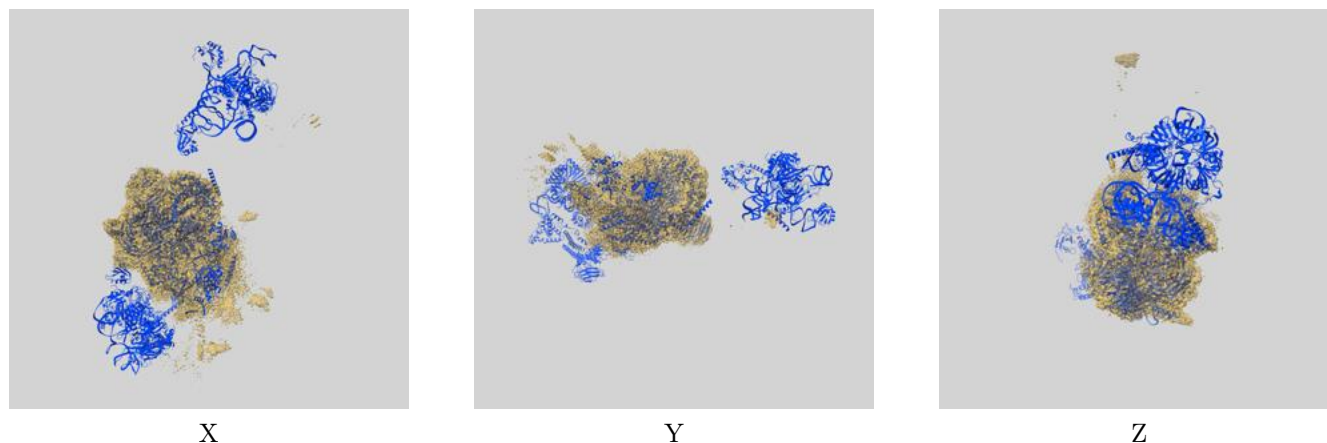
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

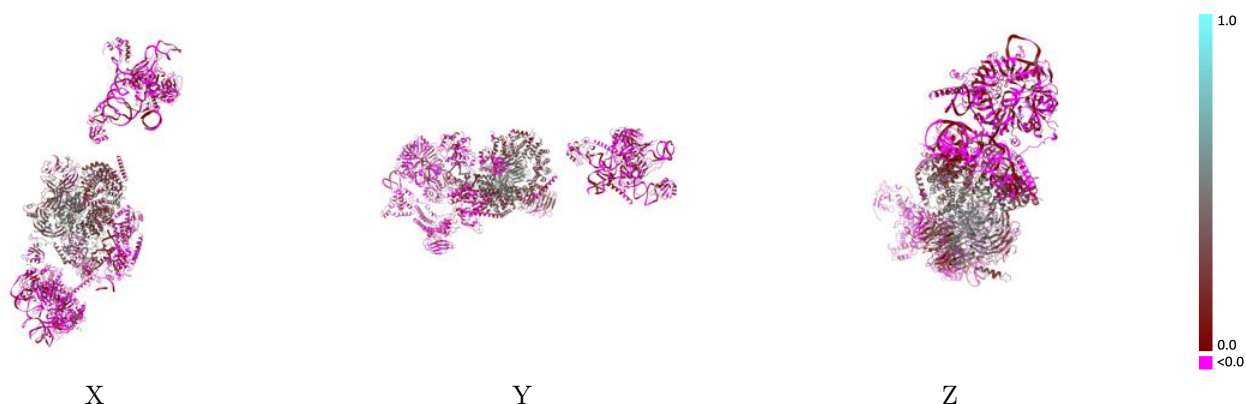
This section contains information regarding the fit between EMDB map EMD-32074 and PDB model 7VPX. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay [i](#)



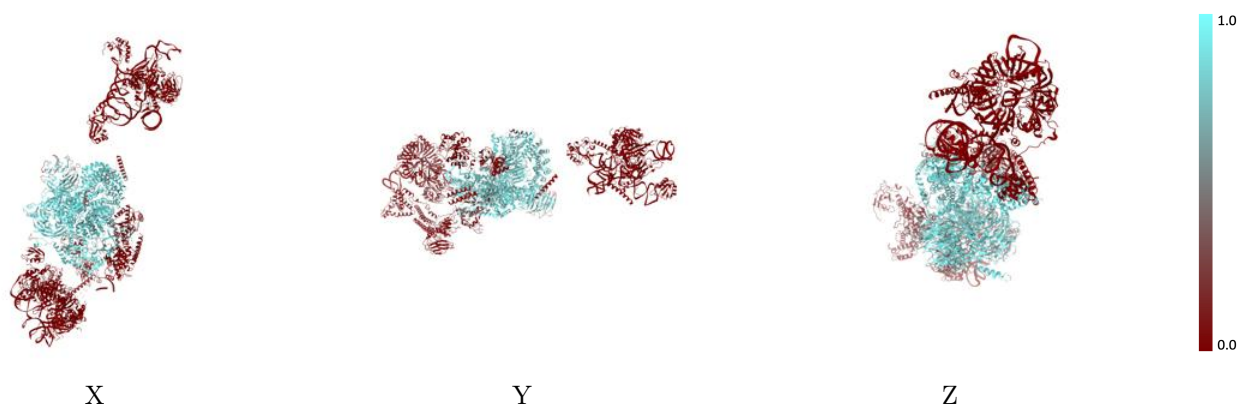
The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



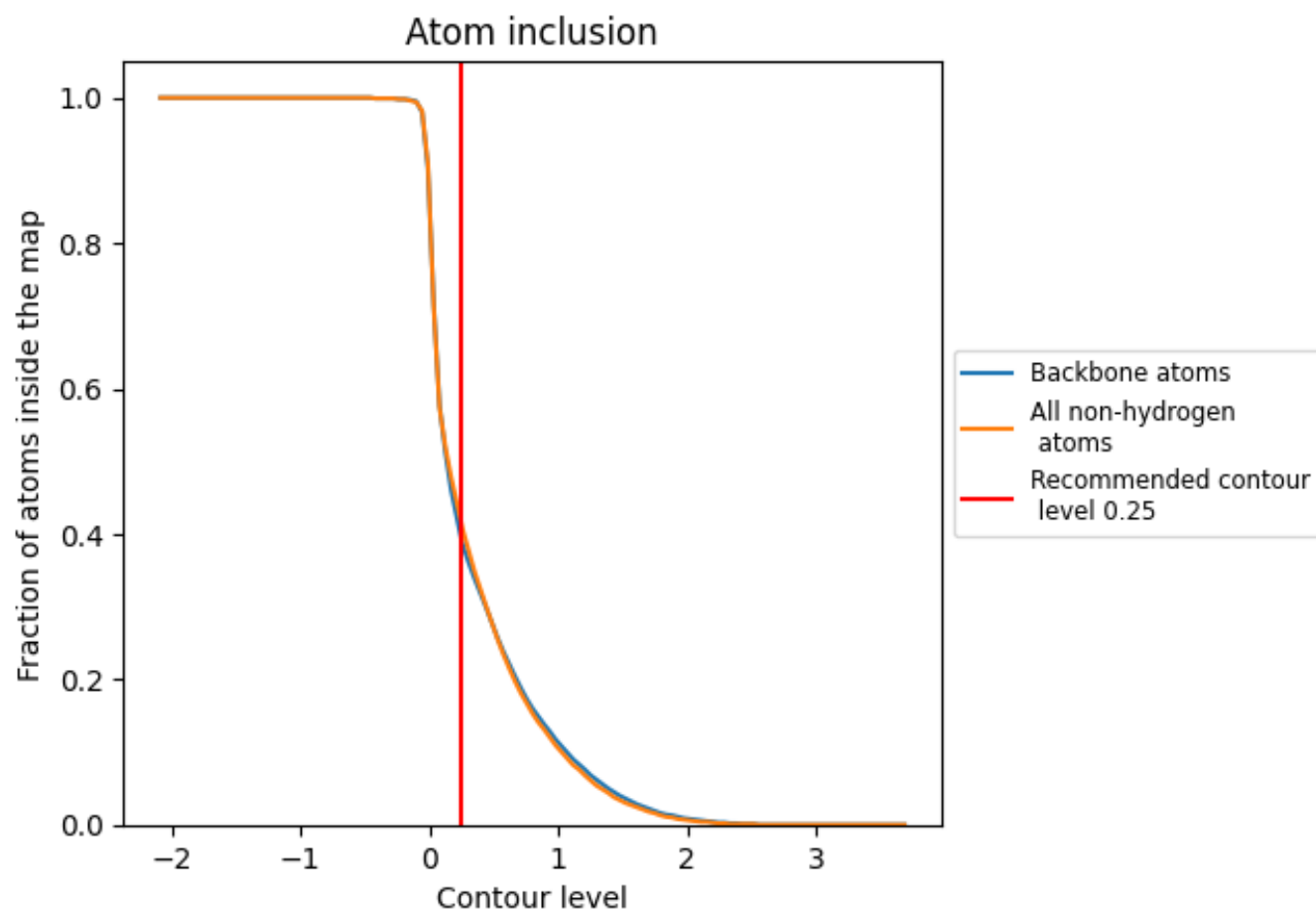
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.25).

9.4 Atom inclusion [i](#)



At the recommended contour level, 39% of all backbone atoms, 41% 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 (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4130	 0.1550
1	 0.8560	 0.3180
2	 0.6680	 0.2780
3	 0.8360	 0.3320
4	 0.1820	 -0.0130
5	 0.9150	 0.4810
6	 0.9070	 0.4080
A	 0.0000	 -0.0220
B	 0.3050	 0.0340
C	 0.3410	 0.1190
D	 0.3080	 0.0390
E	 0.1050	 0.0210
F	 0.0000	 0.0170
G	 0.0000	 -0.0200
H	 0.2320	 0.0690
I	 0.8540	 0.1490
J	 0.7150	 0.1100
K	 0.0000	 0.0440
L	 0.0000	 0.0100
M	 0.0000	 0.0120
N	 0.0000	 0.0110
O	 0.0000	 0.0030
a	 0.0000	 0.0040
b	 0.0000	 0.0060
c	 0.0000	 -0.0130
d	 0.0000	 0.0090
e	 0.0000	 0.0120
f	 0.0030	 -0.0260
g	 0.0030	 -0.0450
h	 0.0000	 -0.0010
i	 0.0000	 0.0050
j	 0.0000	 0.0260
k	 0.0000	 0.0060
l	 0.0000	 0.0120
m	 0.0000	 -0.0060
n	 0.0000	 -0.0180

