



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 05:04 AM UTC

PDB ID : 4V1O / pdb_00004v1o
EMDB ID : EMD-2786
Title : Architecture of the RNA polymerase II-Mediator core transcription initiation complex
Authors : Plaschka, C.; Lariviere, L.; Wenzek, L.; Hemann, M.; Tegunov, D.; Petrotchenko, E.V.; Borchers, C.H.; Baumeister, W.; Herzog, F.; Villa, E.; Cramer, P.
Deposited on : 2014-09-29
Resolution : 9.70 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

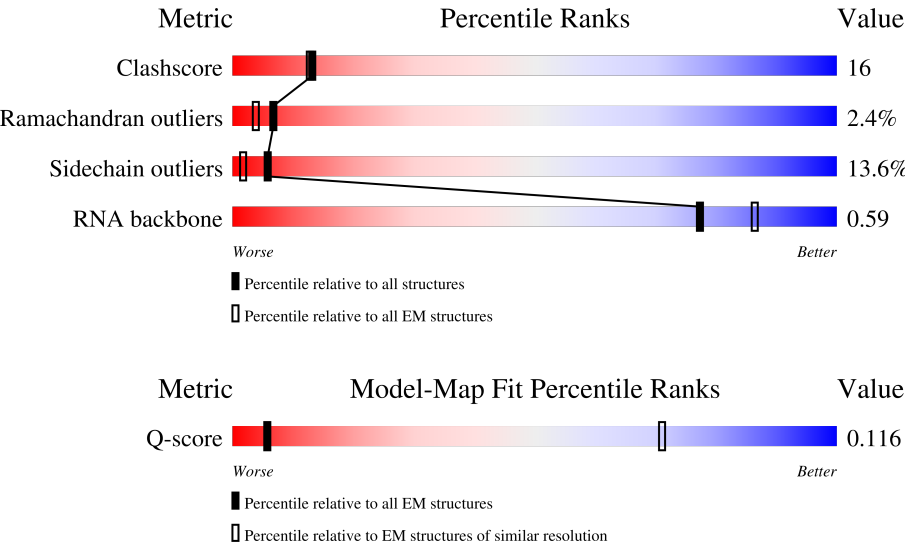
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 9.70 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	165 (9.20 - 10.20)

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

Mol	Chain	Length	Quality of chain
1	A	1733	
2	B	1224	
3	C	318	

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Mol	Chain	Length	Quality of chain
4	D	221	
5	E	215	
6	F	155	
7	G	171	
8	H	146	
9	I	122	
10	J	70	
11	K	120	
12	L	70	
13	M	345	
14	N	50	
15	O	181	
16	P	6	
17	Q	734	
18	R	331	
19	S	295	
20	T	58	
21	U	222	
22	V	115	
23	W	687	
24	X	307	
25	Y	209	
26	Z	120	

2 Entry composition

There are 28 unique types of molecules in this entry. The entry contains 45091 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1422	Total	C	N	O	S	0	0
			11174	7036	1954	2122	62		

- Molecule 2 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1156	Total	C	N	O	S	0	0
			9140	5781	1606	1697	56		

- Molecule 3 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	266	Total	C	N	O	S	0	0
			2095	1317	348	417	13		

- Molecule 4 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	178	Total	C	N	O	S	0	0
			1434	887	257	288	2		

- Molecule 5 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	214	Total	C	N	O	S	0	0
			1752	1111	309	321	11		

- Molecule 6 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	84	Total	C	N	O	S	0	0
			679	434	115	127	3		

- Molecule 7 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	171	Total	C	N	O	S	0	0
			1340	861	222	249	8		

- Molecule 8 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	133	Total	C	N	O	S	0	0
			1068	673	180	211	4		

- Molecule 9 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	119	Total	C	N	O	S	0	0
			971	596	179	186	10		

- Molecule 10 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	65	Total	C	N	O	S	0	0
			532	339	93	94	6		

- Molecule 11 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	115	Total	C	N	O	S	0	1
			920	590	157	171	2		

- Molecule 12 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	46	Total	C	N	O	S	0	0
			363	224	72	63	4		

- Molecule 13 is a protein called TRANSCRIPTION INITIATION FACTOR IIB.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	300	Total	C	N	O	S	0	1
			2202	1384	380	423	15		

- Molecule 14 is a DNA chain called NONTEMPLATE DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	50	Total	C	N	O	P	0	0
			975	490	191	246	48		

- Molecule 15 is a protein called TATA-BOX-BINDING PROTEIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	180	Total	C	N	O	S	0	0
			1416	921	242	247	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	60	MET	-	expression tag	UNP P13393

- Molecule 16 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	6	Total	C	N	O	P	0	0
			123	57	22	39	5		

- Molecule 17 is a protein called TRANSCRIPTION INITIATION FACTOR IIF SUBUNIT ALPHA.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	Q	122	Total	C	N	O	0	0
			606	362	122	122		

- Molecule 18 is a protein called TRANSCRIPTION INITIATION FACTOR IIF SUBUNIT BETA.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	R	105	Total	C	N	O	0	0
			521	311	105	105		

- Molecule 19 is a protein called MEDIATOR OF RNA POLYMERASE II TRANSCRIPTION SUBUNIT 6.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	S	139	Total	C	N	O	0	0
			691	413	139	139		

- Molecule 20 is a DNA chain called TEMPLATE DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	58	Total	C	N	O	P	0	0
			1125	568	206	294	57		

- Molecule 21 is a protein called MEDIATOR OF RNA POLYMERASE II TRANSCRIPTION SUBUNIT 8.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	U	158	Total	C	N	O	0	0
			787	471	158	158		

- Molecule 22 is a protein called MEDIATOR OF RNA POLYMERASE II TRANSCRIPTION SUBUNIT 20.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	V	99	Total	C	N	O	0	0
			491	293	99	99		

- Molecule 23 is a protein called MEDIATOR OF RNA POLYMERASE II TRANSCRIPTION SUBUNIT 11.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	W	419	Total	C	N	O	0	0
			2085	1247	419	419		

- Molecule 24 is a protein called MEDIATOR OF RNA POLYMERASE II TRANSCRIPTION SUBUNIT 18.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	X	232	Total	C	N	O	0	0
			1146	682	232	232		

- Molecule 25 is a protein called MEDIATOR OF RNA POLYMERASE II TRANSCRIPTION SUBUNIT 20.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	Y	203	Total	C	N	O	0	0
			1003	597	203	203		

- Molecule 26 is a protein called MEDIATOR OF RNA POLYMERASE II TRANSCRIPTION SUBUNIT 22.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	Z	88	Total	C	N	O	1	0
			442	266	88	88		

- Molecule 27 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
27	A	2	Total	Zn	0
			2	2	
27	B	1	Total	Zn	0
			1	1	
27	C	1	Total	Zn	0
			1	1	
27	I	2	Total	Zn	0
			2	2	
27	J	1	Total	Zn	0
			1	1	
27	L	1	Total	Zn	0
			1	1	
27	M	1	Total	Zn	0
			1	1	

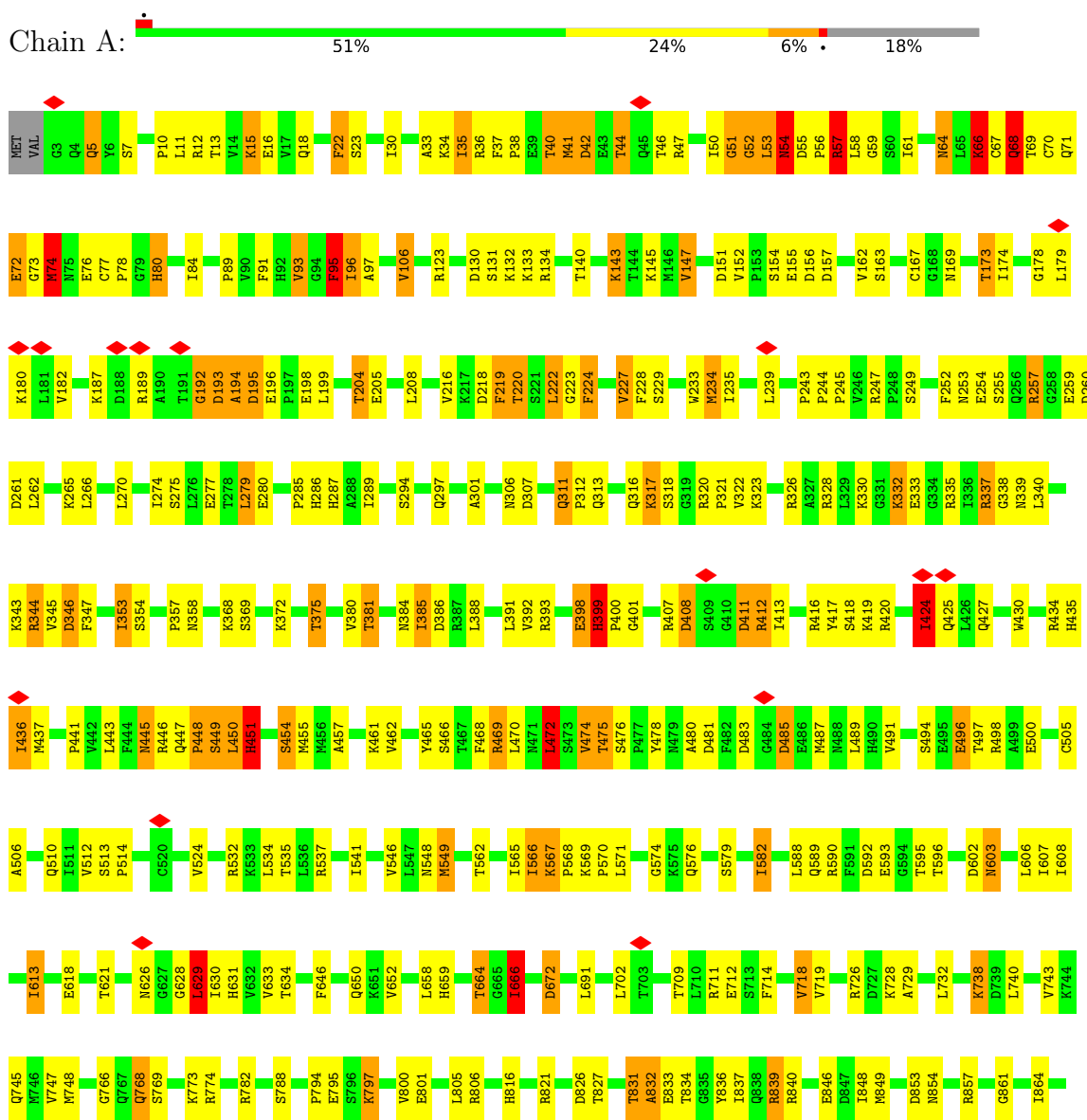
- Molecule 28 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

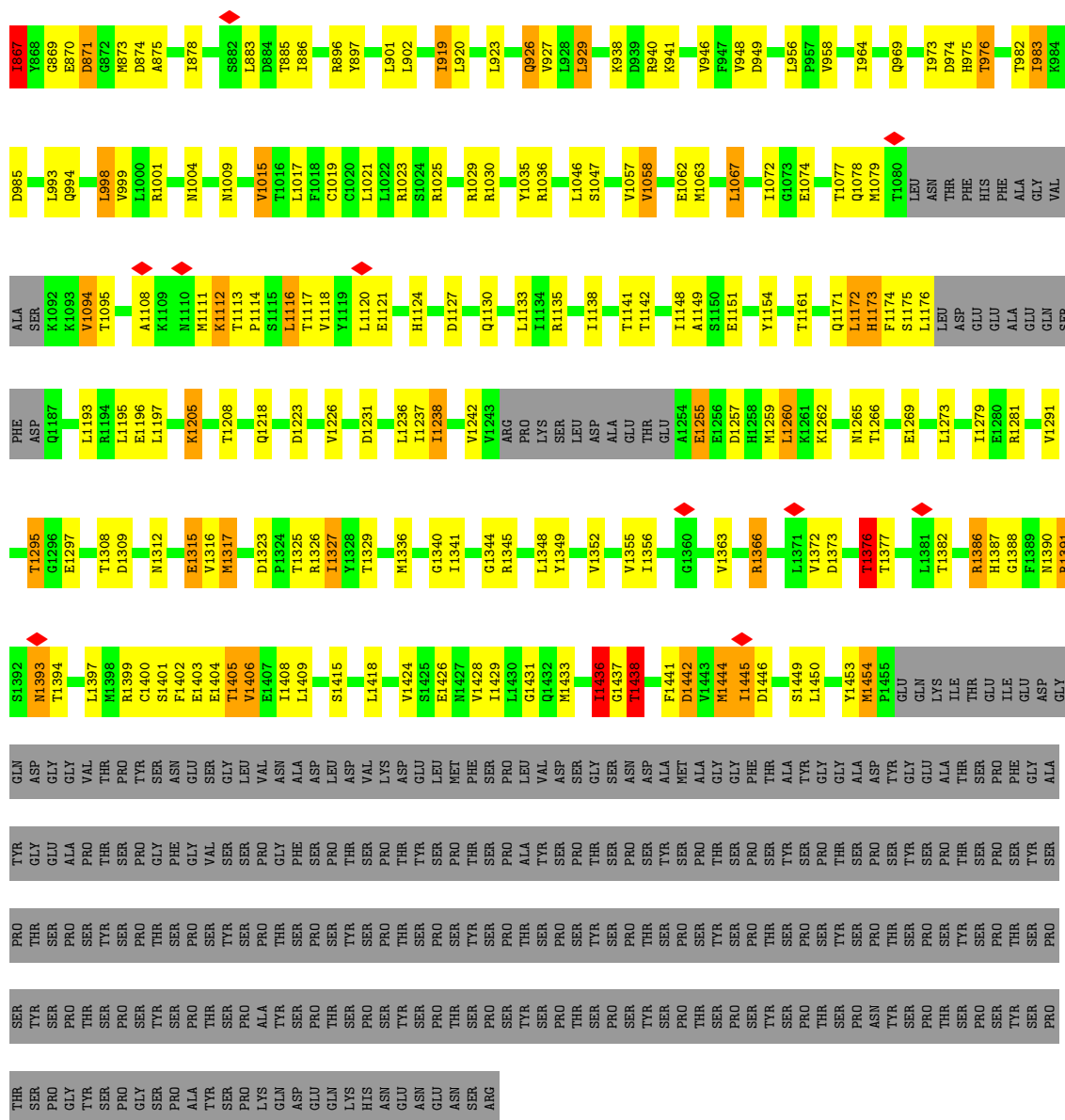
Mol	Chain	Residues	Atoms		AltConf
28	A	1	Total	Mg	0
			1	1	

3 Residue-property plots

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

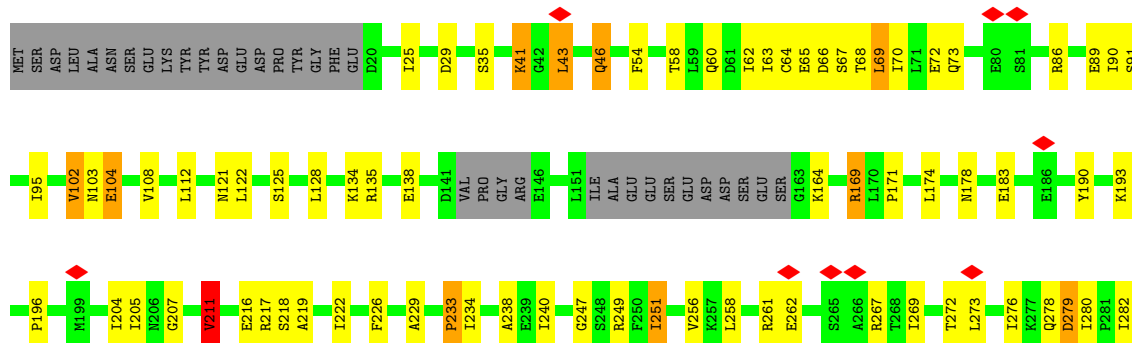
• Molecule 1: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB1

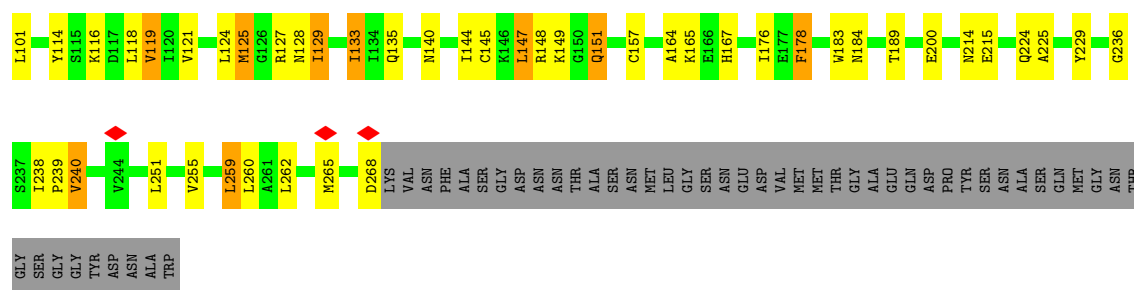




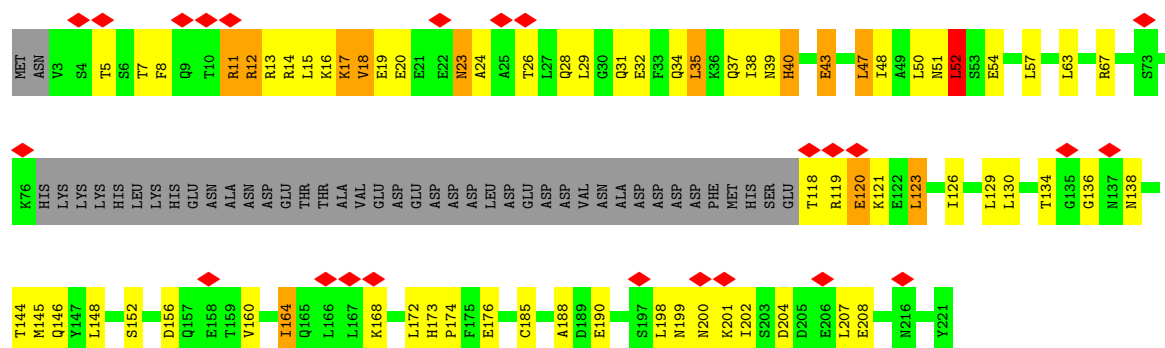
• Molecule 2: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB2

Chain B: 59% 28% 6% • 6%

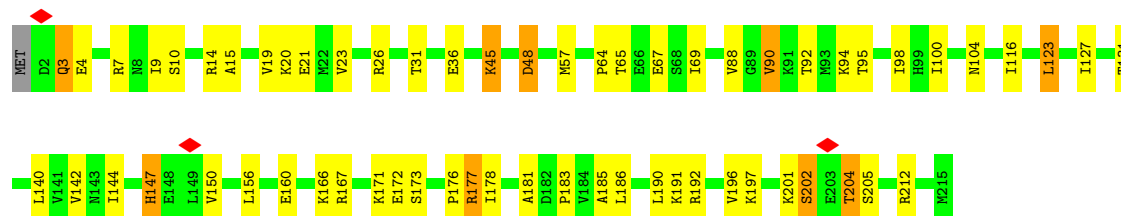




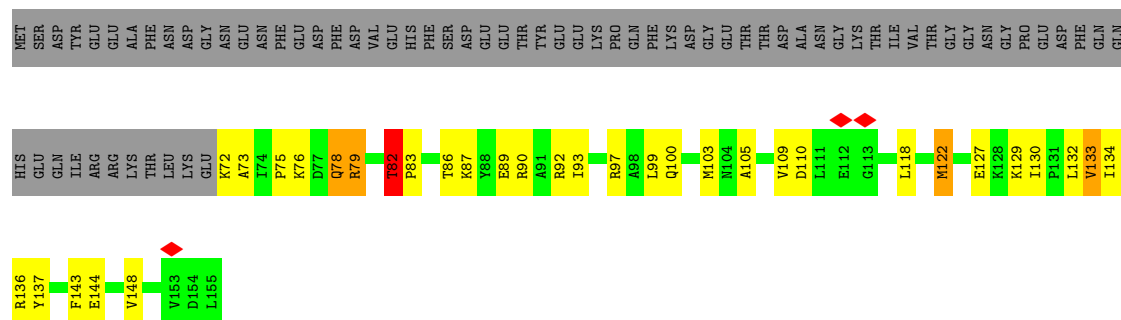
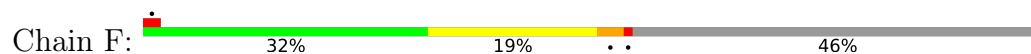
• Molecule 4: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB4



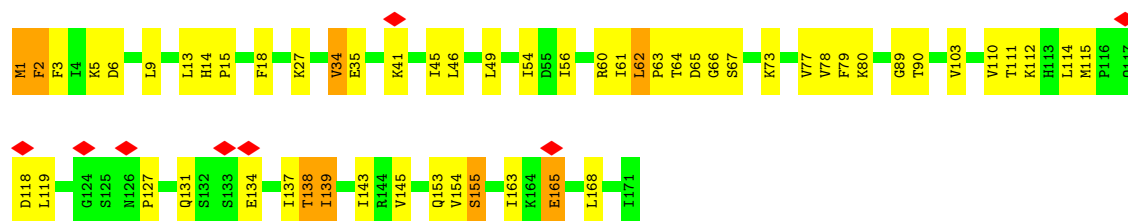
• Molecule 5: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 1



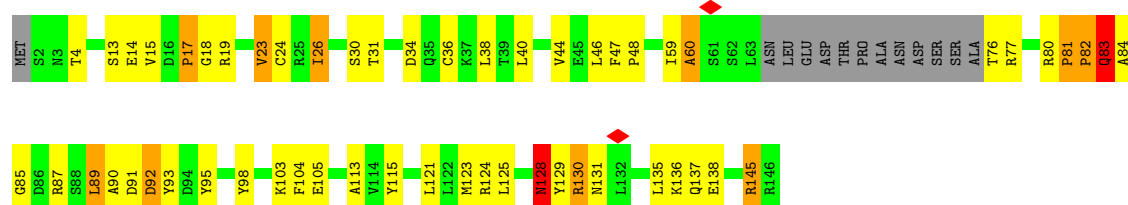
• Molecule 6: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 2



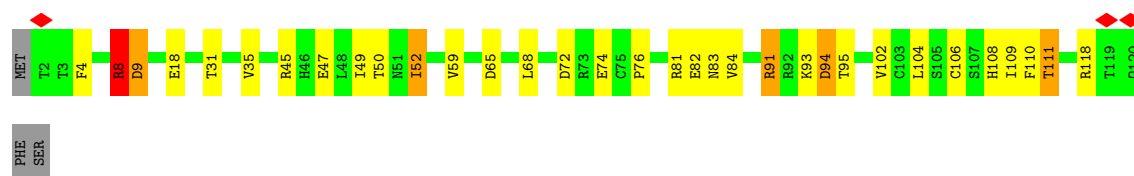
• Molecule 7: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB7



- Molecule 8: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 3



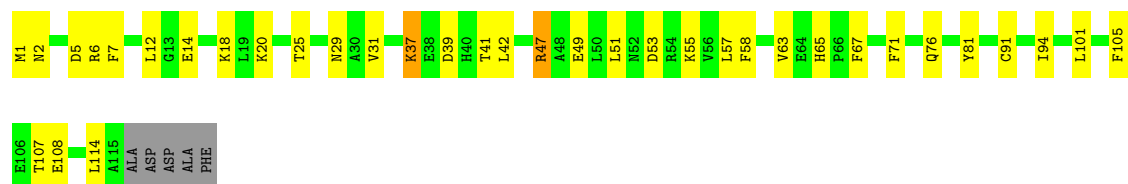
- Molecule 9: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB9



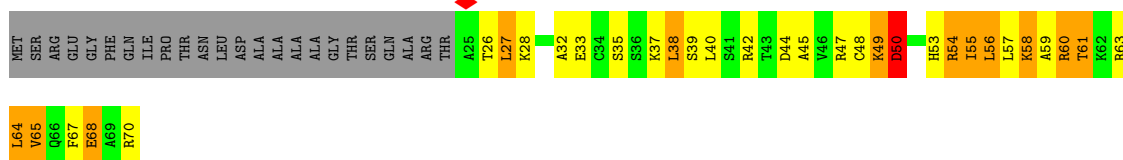
- Molecule 10: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 5



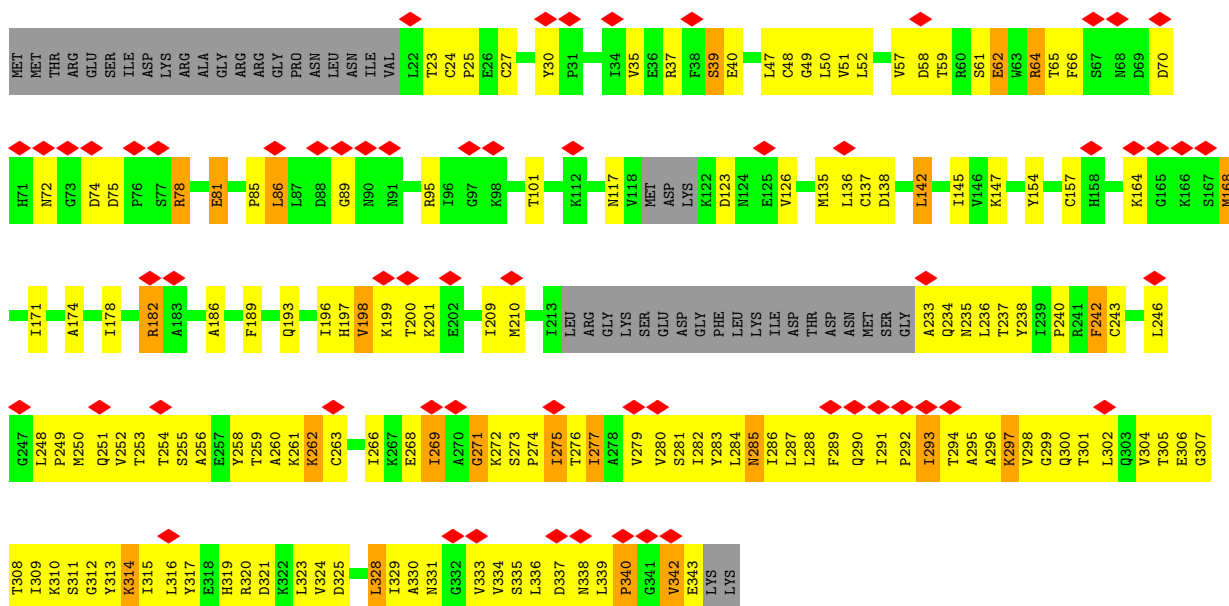
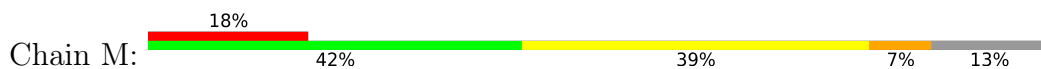
- Molecule 11: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB11



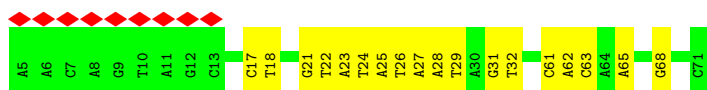
- Molecule 12: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 4



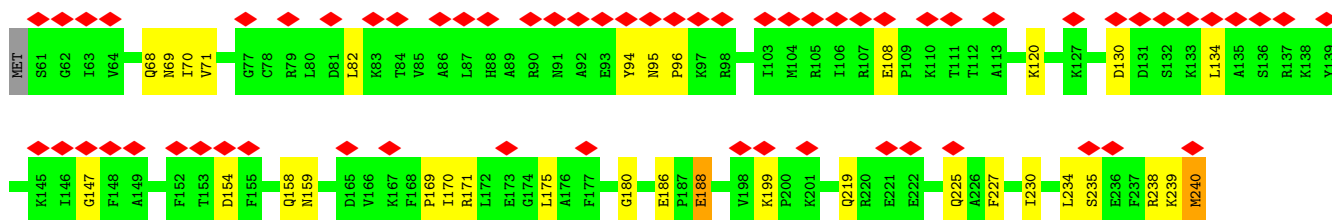
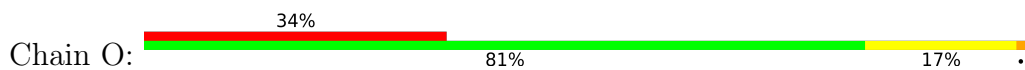
• Molecule 13: TRANSCRIPTION INITIATION FACTOR IIB



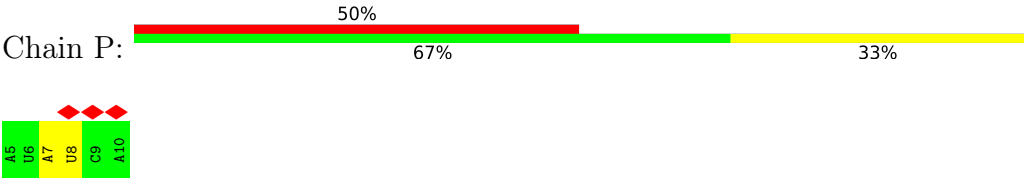
• Molecule 14: NONTEMPLATE DNA



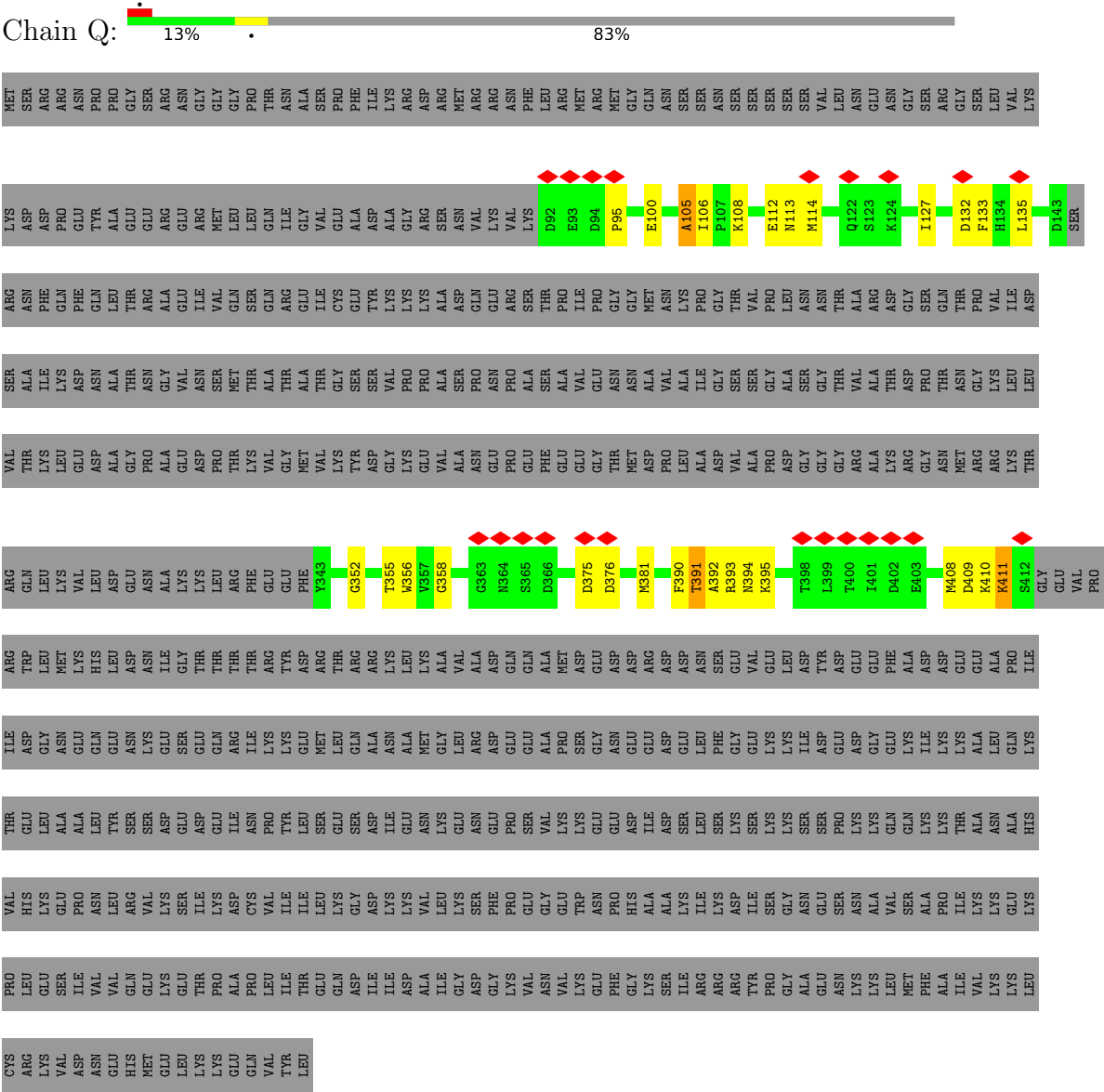
• Molecule 15: TATA-BOX-BINDING PROTEIN



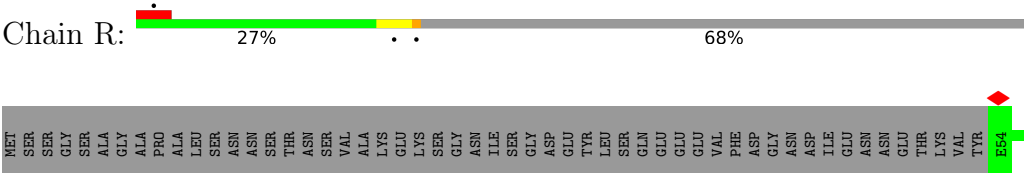
• Molecule 16: RNA



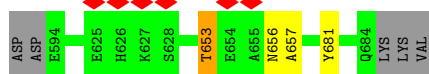
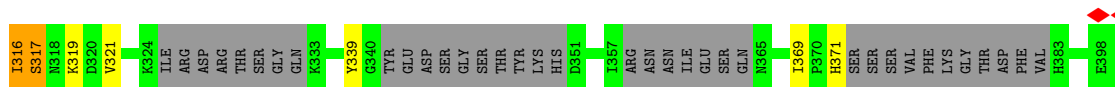
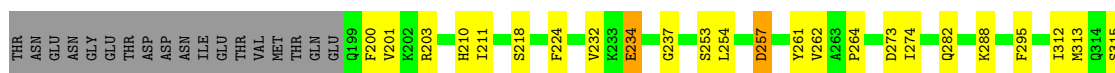
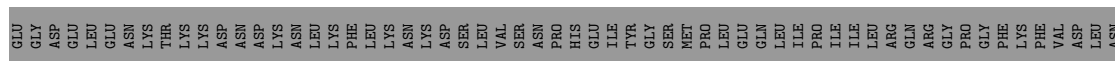
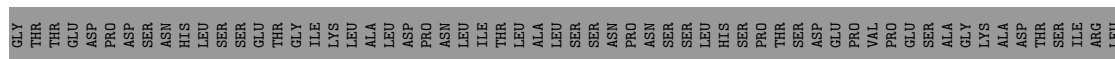
• Molecule 17: TRANSCRIPTION INITIATION FACTOR IIF SUBUNIT ALPHA



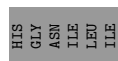
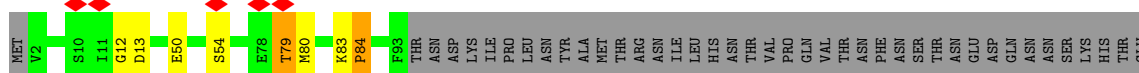
• Molecule 18: TRANSCRIPTION INITIATION FACTOR IIF SUBUNIT BETA



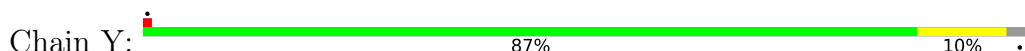
● Molecule 23: MEDIATOR OF RNA POLYMERASE II TRANSCRIPTION SUBUNIT 11



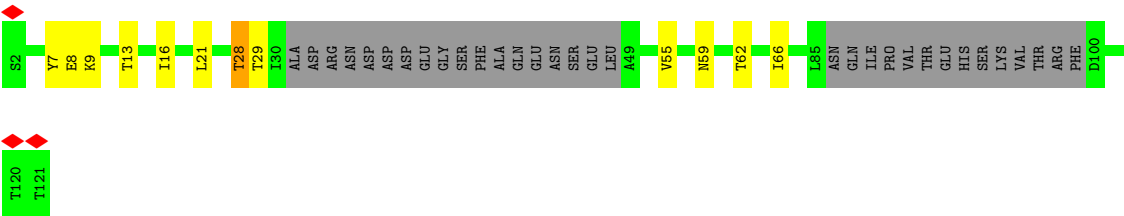
● Molecule 24: MEDIATOR OF RNA POLYMERASE II TRANSCRIPTION SUBUNIT 18



● Molecule 25: MEDIATOR OF RNA POLYMERASE II TRANSCRIPTION SUBUNIT 20



• Molecule 26: MEDIATOR OF RNA POLYMERASE II TRANSCRIPTION SUBUNIT 22



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	3267	Depositor
Resolution determination method	Not provided	
CTF correction method	EACH PARTICLE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	25	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	37169	Depositor
Image detector	GATAN K2 (4k x 4k)	Depositor
Maximum map value	0.055	Depositor
Minimum map value	-0.022	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0135	Depositor
Map size ($\text{\AA}$)	378.0, 378.0, 378.0	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.35, 1.35, 1.35	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, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.93	10/11374 (0.1%)	1.47	103/15384 (0.7%)
2	B	0.80	8/9316 (0.1%)	1.32	71/12564 (0.6%)
3	C	0.84	0/2133	1.43	14/2891 (0.5%)
4	D	0.49	0/1444	0.89	3/1935 (0.2%)
5	E	0.83	0/1788	1.41	13/2406 (0.5%)
6	F	1.00	1/691 (0.1%)	1.41	5/933 (0.5%)
7	G	0.52	0/1368	0.92	0/1844
8	H	0.86	0/1086	1.43	14/1470 (1.0%)
9	I	0.82	0/989	1.37	7/1331 (0.5%)
10	J	0.91	0/541	1.60	8/727 (1.1%)
11	K	0.77	0/938	1.34	1/1267 (0.1%)
12	L	0.92	0/365	1.51	5/485 (1.0%)
13	M	0.91	1/2232 (0.0%)	1.17	12/3031 (0.4%)
14	N	0.58	0/1100	1.08	2/1625 (0.1%)
15	O	0.70	0/1443	1.09	8/1942 (0.4%)
16	P	0.18	0/137	0.31	0/211
17	Q	1.59	2/604 (0.3%)	1.88	15/840 (1.8%)
18	R	1.54	0/520	1.82	7/724 (1.0%)
19	S	0.79	1/688 (0.1%)	1.97	30/956 (3.1%)
20	T	0.64	2/1265 (0.2%)	1.09	5/1866 (0.3%)
21	U	0.65	0/785	1.65	22/1094 (2.0%)
22	V	0.64	1/489 (0.2%)	1.43	7/679 (1.0%)
23	W	0.64	2/2077 (0.1%)	1.38	35/2889 (1.2%)
24	X	0.62	0/1143	1.25	9/1587 (0.6%)
25	Y	0.51	0/1001	1.24	7/1391 (0.5%)
26	Z	0.62	0/442	1.58	11/614 (1.8%)
All	All	0.83	28/45959 (0.1%)	1.37	414/62686 (0.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a

sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
2	B	0	1
17	Q	0	1
19	S	0	1
21	U	0	2
23	W	0	4
All	All	0	11

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	95	PHE	C-N	-24.15	1.00	1.33
1	A	234	MET	C-N	-21.97	1.07	1.33
1	A	1436	ILE	C-N	18.17	1.60	1.33
1	A	1394	THR	C-N	-9.76	1.21	1.33
1	A	867	ILE	CG1-CD1	8.15	1.83	1.51
2	B	973	ILE	C-N	7.72	1.51	1.33
2	B	851	PHE	C-N	7.70	1.43	1.33
1	A	549	MET	SD-CE	-7.53	1.60	1.79
2	B	218	SER	C-N	7.33	1.43	1.33
17	Q	411	LYS	C-N	-7.15	1.23	1.33
1	A	1454	MET	CA-C	6.93	1.61	1.52
20	T	47	DA	C1'-N9	-6.93	1.32	1.46
1	A	346	ASP	C-N	-6.88	1.24	1.33
23	W	321	VAL	CA-CB	6.74	1.61	1.54
20	T	53	DA	P-O5'	-6.25	1.48	1.60
6	F	122	MET	SD-CE	6.19	1.95	1.79
2	B	43	LEU	C-N	-5.83	1.25	1.33
19	S	200	VAL	CA-CB	-5.75	1.47	1.54
2	B	839	MET	SD-CE	-5.71	1.65	1.79
1	A	437	MET	SD-CE	5.50	1.93	1.79
2	B	1017	ILE	CA-C	5.34	1.58	1.52
2	B	465	ASN	C-N	-5.33	1.26	1.33
22	V	6	ILE	CA-CB	5.31	1.61	1.54
1	A	1057	VAL	C-N	5.21	1.39	1.33
17	Q	411	LYS	CA-C	5.19	1.59	1.52
23	W	543	ARG	C-N	5.15	1.41	1.34
2	B	1169	MET	SD-CE	-5.09	1.66	1.79
13	M	342	VAL	C-N	-5.03	1.26	1.33

All (414) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	234	MET	O-C-N	-18.93	99.26	122.17
19	S	192	ILE	CB-CA-C	-17.69	87.22	111.63
22	V	52	VAL	CB-CA-C	-14.33	92.44	112.22
1	A	1394	THR	CA-C-N	13.98	133.38	120.10
1	A	1394	THR	C-N-CA	13.98	133.38	120.10
25	Y	65	HIS	N-CA-C	-13.81	91.68	112.54
1	A	234	MET	CA-C-N	12.68	138.22	120.98
1	A	234	MET	C-N-CA	12.68	138.22	120.98
20	T	6	DA	O3'-P-O5'	-11.54	86.69	104.00
18	R	60	ASP	CA-C-N	11.52	143.54	121.54
18	R	60	ASP	C-N-CA	11.52	143.54	121.54
1	A	95	PHE	CA-C-N	-11.25	101.71	121.97
1	A	95	PHE	C-N-CA	-11.25	101.71	121.97
17	Q	411	LYS	N-CA-C	10.94	126.68	110.48
22	V	30	VAL	N-CA-CB	10.49	122.15	110.51
25	Y	53	VAL	N-CA-C	-9.89	93.04	107.78
13	M	285	ASN	CA-CB-CG	-9.88	102.72	112.60
24	X	54	SER	N-CA-C	-9.86	100.67	112.89
8	H	92	ASP	N-CA-C	-9.78	101.57	112.72
17	Q	114	MET	CA-C-N	-9.76	109.00	122.86
17	Q	114	MET	C-N-CA	-9.76	109.00	122.86
17	Q	411	LYS	CA-C-O	9.76	132.69	121.47
2	B	296	GLU	N-CA-C	-9.72	99.73	111.69
26	Z	8	GLU	CB-CA-C	-9.64	95.74	110.88
23	W	274	ILE	CB-CA-C	-9.58	99.71	111.97
3	C	39	ALA	N-CA-C	9.53	125.70	112.45
10	J	5	VAL	N-CA-C	-9.41	97.44	109.58
2	B	628	THR	CA-C-N	9.38	135.29	121.31
2	B	628	THR	C-N-CA	9.38	135.29	121.31
21	U	79	VAL	CB-CA-C	-9.36	99.30	112.22
1	A	346	ASP	O-C-N	-9.36	110.59	122.20
26	Z	7	TYR	CB-CA-C	-9.31	96.26	110.88
25	Y	67	ARG	N-CA-C	-9.17	100.50	112.24
19	S	166	ILE	N-CA-CB	9.13	126.30	111.23
19	S	200	VAL	N-CA-CB	-8.91	100.79	111.21
18	R	61	LEU	N-CA-C	8.86	129.67	110.80
23	W	369	ILE	CA-C-N	8.83	130.88	119.84
23	W	369	ILE	C-N-CA	8.83	130.88	119.84
21	U	145	ILE	CB-CA-C	-8.79	100.27	112.14
8	H	81	PRO	N-CA-C	8.76	121.39	110.70
21	U	137	THR	CB-CA-C	8.74	123.95	109.53
21	U	110	VAL	CB-CA-C	-8.73	100.17	112.22
26	Z	16	ILE	CB-CA-C	-8.60	100.53	112.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	S	161	TYR	CB-CA-C	8.51	123.79	109.75
2	B	1122	ARG	CA-C-N	8.42	131.91	120.54
2	B	1122	ARG	C-N-CA	8.42	131.91	120.54
18	R	89	GLY	N-CA-C	-8.41	103.41	115.27
21	U	122	VAL	CB-CA-C	-8.33	98.76	112.26
19	S	156	ILE	CB-CA-C	-8.31	98.81	110.12
8	H	129	TYR	N-CA-C	8.17	119.81	111.07
4	D	26	THR	N-CA-C	-8.15	101.81	112.41
25	Y	55	LYS	N-CA-C	-8.14	102.39	113.30
19	S	17	ILE	CB-CA-C	-8.06	101.09	112.22
19	S	13	SER	CA-C-N	7.93	129.76	119.84
19	S	13	SER	C-N-CA	7.93	129.76	119.84
21	U	94	VAL	CB-CA-C	7.90	122.76	110.28
21	U	171	ASP	CB-CA-C	7.87	123.33	109.72
23	W	295	PHE	CB-CA-C	7.84	123.18	110.88
1	A	194	ALA	CA-C-N	7.83	135.79	121.70
1	A	194	ALA	C-N-CA	7.83	135.79	121.70
13	M	340	PRO	CA-C-N	-7.72	110.78	122.28
13	M	340	PRO	C-N-CA	-7.72	110.78	122.28
1	A	143	LYS	CA-C-N	7.65	130.53	120.28
1	A	143	LYS	C-N-CA	7.65	130.53	120.28
1	A	485	ASP	CA-CB-CG	7.58	120.18	112.60
2	B	340	ALA	CA-C-N	7.55	135.97	121.54
2	B	340	ALA	C-N-CA	7.55	135.97	121.54
19	S	130	LYS	N-CA-CB	7.53	122.18	110.21
19	S	115	TYR	CB-CA-C	-7.52	98.11	110.14
2	B	629	ASP	CA-CB-CG	7.50	120.10	112.60
17	Q	105	ALA	N-CA-C	-7.47	99.40	110.23
1	A	399	HIS	N-CA-CB	7.42	123.58	110.37
1	A	998	LEU	N-CA-C	7.34	120.63	108.96
26	Z	55	VAL	CB-CA-C	-7.33	102.24	112.14
2	B	736	THR	N-CA-C	-7.31	104.22	113.72
2	B	1169	MET	CA-C-N	7.27	130.99	120.38
2	B	1169	MET	C-N-CA	7.27	130.99	120.38
6	F	87	LYS	CA-C-N	7.24	129.98	120.28
6	F	87	LYS	C-N-CA	7.24	129.98	120.28
4	D	24	ALA	N-CA-C	7.22	117.51	108.19
3	C	62	PHE	CA-C-N	7.17	129.60	120.56
3	C	62	PHE	C-N-CA	7.17	129.60	120.56
19	S	168	LYS	CB-CA-C	7.14	122.65	110.79
8	H	128	ASN	CA-C-N	7.13	129.71	120.44
8	H	128	ASN	C-N-CA	7.13	129.71	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	J	9	SER	N-CA-C	7.13	118.70	111.07
24	X	233	GLN	N-CA-C	7.13	120.58	109.52
19	S	133	ARG	CB-CA-C	-7.12	97.78	109.53
18	R	214	ILE	N-CA-CB	-7.09	104.52	111.89
3	C	183	TRP	N-CA-C	-7.02	97.79	109.24
17	Q	376	ASP	N-CA-C	-7.01	100.61	110.50
23	W	653	THR	N-CA-C	-6.97	97.04	108.41
23	W	232	VAL	CB-CA-C	-6.91	99.96	111.29
18	R	101	GLY	N-CA-C	-6.84	103.01	112.18
17	Q	113	ASN	N-CA-C	-6.83	103.92	111.36
19	S	31	PHE	N-CA-CB	6.80	120.12	110.12
19	S	16	TRP	N-CA-CB	6.78	120.79	110.28
23	W	542	ILE	N-CA-C	6.77	117.52	110.62
26	Z	9	LYS	CB-CA-C	-6.70	99.68	110.79
2	B	1181	GLU	N-CA-C	6.64	124.95	110.80
23	W	254	LEU	N-CA-C	6.61	120.13	109.02
24	X	79	THR	N-CA-C	-6.61	96.72	110.80
10	J	18	TRP	N-CA-C	6.58	118.34	111.03
20	T	47	DA	C4'-C3'-O3'	-6.58	100.13	110.00
3	C	40	GLU	N-CA-C	6.57	121.44	113.17
1	A	219	PHE	CA-CB-CG	6.56	120.36	113.80
1	A	897	TYR	N-CA-C	6.54	121.39	113.41
21	U	50	ILE	CB-CA-C	6.54	120.34	111.97
2	B	339	THR	CA-C-N	6.52	133.99	121.54
2	B	339	THR	C-N-CA	6.52	133.99	121.54
15	O	95	ASN	CA-C-N	6.51	127.98	119.84
15	O	95	ASN	C-N-CA	6.51	127.98	119.84
3	C	178	PHE	CA-CB-CG	6.51	120.31	113.80
20	T	53	DA	P-O5'-C5'	6.50	129.75	120.00
2	B	790	ASP	CA-CB-CG	6.49	119.09	112.60
17	Q	408	MET	CA-C-N	6.47	129.48	120.29
17	Q	408	MET	C-N-CA	6.47	129.48	120.29
1	A	223	GLY	CA-C-N	6.46	133.87	121.54
1	A	223	GLY	C-N-CA	6.46	133.87	121.54
2	B	294	ASP	CA-CB-CG	6.46	119.06	112.60
2	B	1156	ASP	N-CA-C	6.45	124.53	110.80
1	A	472	LEU	N-CA-C	6.44	119.11	111.71
23	W	200	PHE	CB-CA-C	6.41	120.95	110.88
2	B	1219	ASP	CA-CB-CG	6.41	119.01	112.60
22	V	58	ARG	CB-CA-C	-6.38	100.01	110.85
13	M	242	PHE	CA-CB-CG	-6.37	107.43	113.80
3	C	200	GLU	N-CA-C	6.36	118.29	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	89	GLU	N-CA-C	-6.35	96.72	108.02
3	C	135	GLN	CA-C-N	6.34	131.46	121.56
3	C	135	GLN	C-N-CA	6.34	131.46	121.56
26	Z	21	LEU	N-CA-CB	6.33	119.19	110.01
2	B	818	PRO	N-CA-C	6.33	120.08	111.22
2	B	1177	HIS	N-CA-C	-6.33	105.60	113.38
25	Y	37	ILE	N-CA-C	6.26	116.07	108.06
4	D	38	ILE	N-CA-C	6.25	116.86	108.11
19	S	34	SER	CA-C-N	6.25	125.93	119.56
19	S	34	SER	C-N-CA	6.25	125.93	119.56
21	U	145	ILE	N-CA-CB	6.23	119.02	110.54
23	W	234	GLU	CB-CA-C	6.23	121.94	110.10
1	A	398	GLU	CA-C-O	-6.21	114.79	121.56
1	A	408	ASP	CA-C-N	6.21	130.62	120.63
1	A	408	ASP	C-N-CA	6.21	130.62	120.63
1	A	411	ASP	CA-C-N	6.19	130.35	121.50
1	A	411	ASP	C-N-CA	6.19	130.35	121.50
1	A	123	ARG	CA-C-N	6.19	128.86	120.44
1	A	123	ARG	C-N-CA	6.19	128.86	120.44
1	A	169	ASN	N-CA-C	6.19	119.01	110.35
14	N	65	DA	C5'-C4'-C3'	-6.18	105.63	114.90
10	J	14	VAL	CB-CA-C	6.17	117.28	110.62
23	W	371	HIS	N-CA-CB	-6.16	100.02	110.50
2	B	1180	PHE	CA-CB-CG	-6.16	107.64	113.80
2	B	363	HIS	N-CA-C	-6.16	102.55	110.19
20	T	46	DT	C5'-C4'-C3'	-6.12	105.73	114.90
1	A	1112	LYS	N-CA-C	6.08	119.17	111.69
10	J	14	VAL	N-CA-C	-6.07	107.34	113.47
19	S	34	SER	CB-CA-C	6.06	120.72	109.51
19	S	113	THR	CB-CA-C	-6.05	98.41	109.54
23	W	211	ILE	CB-CA-C	-6.03	104.00	112.14
11	K	53	ASP	CA-CB-CG	6.03	118.63	112.60
9	I	8	ARG	N-CA-C	-6.02	100.18	109.76
8	H	131	ASN	N-CA-C	-6.01	104.80	111.36
2	B	338	GLY	CA-C-N	6.00	132.51	121.70
2	B	338	GLY	C-N-CA	6.00	132.51	121.70
21	U	73	LEU	CB-CA-C	5.99	120.29	110.88
1	A	1376	THR	CB-CA-C	5.98	120.89	111.39
23	W	540	LEU	N-CA-C	5.96	118.47	107.99
2	B	642	ASP	N-CA-C	-5.95	105.12	112.38
9	I	94	ASP	CA-C-N	5.93	132.87	121.54
9	I	94	ASP	C-N-CA	5.93	132.87	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	853	ASP	CA-CB-CG	5.93	118.53	112.60
2	B	707	PRO	CA-C-N	5.93	128.54	120.54
2	B	707	PRO	C-N-CA	5.93	128.54	120.54
19	S	51	GLN	CB-CA-C	-5.91	100.81	110.85
1	A	794	PRO	CA-C-N	5.89	128.76	120.28
1	A	794	PRO	C-N-CA	5.89	128.76	120.28
1	A	30	ILE	CB-CA-C	-5.87	104.33	112.02
15	O	186	GLU	CA-C-N	5.87	127.17	119.84
15	O	186	GLU	C-N-CA	5.87	127.17	119.84
2	B	791	THR	N-CA-C	-5.86	100.97	109.59
19	S	166	ILE	CB-CA-C	5.86	120.91	111.29
5	E	123	LEU	CA-C-N	5.86	125.02	120.33
5	E	123	LEU	C-N-CA	5.86	125.02	120.33
21	U	172	PHE	CB-CA-C	5.84	121.20	110.10
23	W	282	GLN	CB-CA-C	-5.84	101.71	110.88
1	A	424	ILE	CA-C-N	-5.84	115.25	122.84
1	A	424	ILE	C-N-CA	-5.84	115.25	122.84
5	E	171	LYS	N-CA-C	-5.83	100.78	110.17
2	B	211	VAL	CB-CA-C	-5.83	102.44	110.96
23	W	210	HIS	CB-CA-C	-5.82	101.50	110.81
5	E	95	THR	CA-C-N	5.81	128.06	120.28
5	E	95	THR	C-N-CA	5.81	128.06	120.28
23	W	313	MET	N-CA-C	-5.80	104.55	111.69
1	A	871	ASP	CA-CB-CG	5.80	118.40	112.60
21	U	119	ILE	N-CA-CB	5.79	119.32	111.21
1	A	718	VAL	CA-C-N	5.78	128.68	120.53
1	A	718	VAL	C-N-CA	5.78	128.68	120.53
1	A	462	VAL	N-CA-CB	5.78	117.42	110.31
12	L	44	ASP	CA-C-N	5.77	132.56	121.54
12	L	44	ASP	C-N-CA	5.77	132.56	121.54
9	I	52	ILE	N-CA-CB	5.77	118.24	111.66
19	S	113	THR	N-CA-CB	-5.77	101.87	110.17
1	A	833	GLU	CA-C-N	5.75	127.99	120.28
1	A	833	GLU	C-N-CA	5.75	127.99	120.28
13	M	30	TYR	CA-C-N	-5.75	114.45	120.38
13	M	30	TYR	C-N-CA	-5.75	114.45	120.38
19	S	162	GLN	N-CA-CB	5.75	118.43	109.97
1	A	800	VAL	CA-C-N	5.75	127.98	120.28
1	A	800	VAL	C-N-CA	5.75	127.98	120.28
2	B	703	ILE	N-CA-C	5.74	117.27	108.71
26	Z	28	THR	N-CA-CB	5.74	119.78	110.77
9	I	93	LYS	CA-C-N	5.72	129.40	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	93	LYS	C-N-CA	5.72	129.40	120.82
2	B	825	VAL	N-CA-C	5.72	116.09	107.80
17	Q	352	GLY	N-CA-C	-5.72	107.43	115.32
1	A	938	LYS	CA-C-N	5.71	128.25	120.54
1	A	938	LYS	C-N-CA	5.71	128.25	120.54
1	A	728	LYS	CA-C-N	5.71	128.20	120.38
1	A	728	LYS	C-N-CA	5.71	128.20	120.38
22	V	70	ILE	CB-CA-C	-5.70	104.35	112.22
20	T	47	DA	C5'-C4'-C3'	-5.70	106.36	114.90
25	Y	93	PHE	N-CA-C	5.68	117.47	111.28
22	V	32	PHE	N-CA-CB	-5.67	101.78	110.12
23	W	526	SER	N-CA-C	5.67	119.94	112.35
1	A	832	ALA	CA-C-N	5.66	127.80	120.44
1	A	832	ALA	C-N-CA	5.66	127.80	120.44
12	L	49	LYS	CA-C-N	5.66	132.34	121.54
12	L	49	LYS	C-N-CA	5.66	132.34	121.54
15	O	180	GLY	N-CA-C	5.66	119.73	112.83
24	X	80	MET	N-CA-C	-5.66	105.49	112.90
21	U	140	LEU	CA-C-N	5.64	131.86	121.70
21	U	140	LEU	C-N-CA	5.64	131.86	121.70
15	O	147	GLY	N-CA-C	5.64	122.90	114.95
1	A	537	ARG	CA-C-N	5.64	128.61	120.38
1	A	537	ARG	C-N-CA	5.64	128.61	120.38
19	S	175	MET	CB-CA-C	-5.63	101.97	110.92
18	R	215	VAL	N-CA-C	5.62	115.81	110.53
2	B	343	ILE	CA-C-N	5.62	132.27	121.54
2	B	343	ILE	C-N-CA	5.62	132.27	121.54
19	S	190	ASP	CB-CA-C	-5.60	98.50	110.32
21	U	113	LEU	CB-CA-C	-5.59	99.93	110.67
2	B	1013	ASN	N-CA-C	5.59	117.72	109.50
2	B	732	SER	N-CA-C	5.59	116.74	108.86
1	A	1138	ILE	N-CA-C	5.58	116.42	111.90
23	W	288	LYS	CB-CA-C	-5.58	102.13	110.88
23	W	681	TYR	N-CA-C	5.57	118.54	111.69
13	M	277	ILE	CB-CA-C	-5.57	104.84	111.97
1	A	346	ASP	CA-C-N	5.56	130.02	122.07
1	A	346	ASP	C-N-CA	5.56	130.02	122.07
1	A	602	ASP	CA-CB-CG	5.56	118.16	112.60
2	B	1155	SER	CA-C-N	5.54	132.12	121.54
2	B	1155	SER	C-N-CA	5.54	132.12	121.54
1	A	218	ASP	CA-CB-CG	5.54	118.14	112.60
1	A	1344	GLY	CA-C-N	5.53	127.63	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1344	GLY	C-N-CA	5.53	127.63	120.44
1	A	229	SER	N-CA-C	5.53	117.72	107.60
2	B	1017	ILE	N-CA-C	5.52	120.81	108.88
24	X	232	LEU	N-CA-C	-5.52	98.22	107.99
1	A	496	GLU	CA-C-N	5.52	127.68	120.28
1	A	496	GLU	C-N-CA	5.52	127.68	120.28
1	A	222	LEU	N-CA-C	-5.51	103.63	110.41
17	Q	132	ASP	N-CA-C	-5.51	105.27	111.28
23	W	543	ARG	CA-C-N	-5.51	112.94	119.05
23	W	543	ARG	C-N-CA	-5.51	112.94	119.05
1	A	629	LEU	N-CA-C	-5.50	105.29	111.28
2	B	41	LYS	N-CA-C	5.50	117.35	111.36
2	B	755	ILE	N-CA-C	-5.50	107.44	113.43
2	B	1009	ASP	N-CA-C	-5.48	105.72	112.90
1	A	399	HIS	CA-CB-CG	-5.48	108.32	113.80
2	B	733	HIS	CA-C-N	5.48	127.89	120.38
2	B	733	HIS	C-N-CA	5.48	127.89	120.38
1	A	332	LYS	N-CA-C	-5.48	102.29	110.23
1	A	1001	ARG	N-CA-C	5.48	120.62	113.88
1	A	173	THR	CB-CA-C	5.47	120.51	111.31
24	X	171	ILE	N-CA-C	-5.47	103.94	109.02
1	A	1231	ASP	CA-C-N	5.46	128.06	120.63
1	A	1231	ASP	C-N-CA	5.46	128.06	120.63
23	W	262	VAL	N-CA-C	-5.45	105.06	111.00
26	Z	59	ASN	CB-CA-C	-5.45	102.09	110.81
1	A	1072	ILE	N-CA-C	-5.44	107.49	111.90
2	B	1180	PHE	N-CA-C	5.44	119.58	112.13
1	A	1269	GLU	N-CA-C	5.44	118.38	111.69
2	B	1185	CYS	N-CA-C	-5.43	106.78	113.41
13	M	328	LEU	CA-C-N	-5.43	115.85	123.13
13	M	328	LEU	C-N-CA	-5.43	115.85	123.13
21	U	98	LEU	CA-C-N	5.43	126.63	119.84
21	U	98	LEU	C-N-CA	5.43	126.63	119.84
6	F	82	THR	CB-CA-C	-5.43	100.94	109.52
2	B	43	LEU	N-CA-C	5.43	119.89	113.16
14	N	68	DG	P-O3'-C3'	5.43	128.34	120.20
5	E	172	GLU	CA-C-N	5.43	127.87	120.54
5	E	172	GLU	C-N-CA	5.43	127.87	120.54
23	W	218	SER	CB-CA-C	-5.42	102.37	110.88
1	A	874	ASP	CA-CB-CG	5.42	118.02	112.60
2	B	218	SER	O-C-N	-5.42	116.70	123.04
22	V	5	TYR	CB-CA-C	-5.41	101.66	110.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	Z	62	THR	CB-CA-C	-5.40	102.41	110.88
3	C	87	PHE	N-CA-C	5.39	119.85	113.16
25	Y	27	SER	N-CA-C	-5.39	107.96	114.75
10	J	8	PHE	CA-CB-CG	5.38	119.18	113.80
24	X	50	GLU	N-CA-C	-5.38	103.79	110.41
1	A	1295	THR	CB-CA-C	5.38	121.14	110.17
19	S	18	GLN	N-CA-CB	5.37	118.60	110.28
13	M	337	ASP	CA-CB-CG	-5.35	107.25	112.60
17	Q	127	ILE	N-CA-CB	5.35	116.55	110.72
12	L	40	LEU	N-CA-C	5.35	117.59	110.53
21	U	74	SER	N-CA-CB	5.35	117.77	110.01
23	W	531	ILE	CB-CA-C	-5.35	104.34	111.13
2	B	1186	ASP	CA-CB-CG	5.34	117.94	112.60
10	J	16	ASP	CA-CB-CG	5.34	117.94	112.60
23	W	545	ILE	N-CA-C	5.34	116.07	110.62
1	A	1161	THR	N-CA-C	5.34	118.18	109.59
1	A	224	PHE	CA-CB-CG	-5.33	108.47	113.80
1	A	510	GLN	N-CA-C	5.33	119.40	113.01
23	W	273	ASP	CB-CA-C	-5.32	101.81	110.85
8	H	137	GLN	CA-C-N	5.32	127.94	120.28
8	H	137	GLN	C-N-CA	5.32	127.94	120.28
15	O	82	LEU	N-CA-C	5.32	117.83	111.71
8	H	128	ASN	CA-CB-CG	5.31	117.91	112.60
1	A	1205	LYS	N-CA-C	-5.30	98.18	107.73
26	Z	66	ILE	N-CA-CB	5.30	116.75	110.55
2	B	1099	VAL	N-CA-CB	5.29	116.38	110.51
1	A	664	THR	CB-CA-C	5.29	118.82	109.89
2	B	1065	GLN	CB-CA-C	5.29	118.96	110.29
2	B	628	THR	N-CA-C	-5.28	106.84	113.28
5	E	21	GLU	CA-C-N	5.28	127.36	120.28
5	E	21	GLU	C-N-CA	5.28	127.36	120.28
23	W	339	TYR	CB-CA-C	-5.27	99.63	110.38
2	B	973	ILE	O-C-N	5.26	125.57	121.46
17	Q	112	GLU	N-CA-C	-5.26	103.70	111.81
1	A	1117	THR	CB-CA-C	5.26	120.07	111.23
8	H	83	GLN	CA-C-N	5.26	130.77	120.99
8	H	83	GLN	C-N-CA	5.26	130.77	120.99
1	A	592	ASP	CA-CB-CG	5.26	117.86	112.60
23	W	203	ARG	CB-CA-C	-5.25	102.07	110.79
1	A	1266	THR	N-CA-C	-5.25	105.46	111.07
1	A	451	HIS	N-CA-CB	-5.23	101.79	111.52
5	E	147	HIS	CA-C-N	5.23	129.50	121.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	147	HIS	C-N-CA	5.23	129.50	121.19
24	X	168	ILE	N-CA-C	-5.23	100.59	108.12
1	A	535	THR	N-CA-C	5.21	118.49	112.97
19	S	107	LEU	CB-CA-C	5.21	121.19	110.31
2	B	233	PRO	CA-C-N	5.20	128.84	121.66
2	B	233	PRO	C-N-CA	5.20	128.84	121.66
5	E	177	ARG	N-CA-C	5.19	117.43	109.07
1	A	666	ILE	N-CA-CB	5.19	119.52	110.65
3	C	262	LEU	CA-C-N	5.18	127.23	120.28
3	C	262	LEU	C-N-CA	5.18	127.23	120.28
1	A	969	GLN	N-CA-CB	5.17	117.81	110.16
3	C	225	ALA	N-CA-C	5.16	116.67	108.67
23	W	253	SER	CB-CA-C	5.16	118.82	109.37
13	M	269	ILE	CA-C-N	5.16	127.71	120.28
13	M	269	ILE	C-N-CA	5.16	127.71	120.28
2	B	222	ILE	CA-C-N	5.16	128.92	121.18
2	B	222	ILE	C-N-CA	5.16	128.92	121.18
21	U	125	TRP	N-CA-CB	5.16	118.56	110.46
23	W	224	PHE	CB-CA-C	-5.15	102.56	110.81
2	B	810	GLU	CA-C-N	5.15	129.43	120.68
2	B	810	GLU	C-N-CA	5.15	129.43	120.68
1	A	1079	MET	N-CA-C	5.15	116.91	108.52
21	U	48	ARG	CB-CA-C	-5.15	102.25	110.79
6	F	122	MET	CA-C-N	5.14	127.13	120.44
6	F	122	MET	C-N-CA	5.14	127.13	120.44
2	B	366	GLN	N-CA-C	-5.14	105.90	113.61
21	U	59	LEU	CA-C-N	5.13	125.34	120.31
21	U	59	LEU	C-N-CA	5.13	125.34	120.31
1	A	244	PRO	N-CA-C	5.12	116.95	110.70
22	V	75	GLU	CB-CA-C	-5.12	99.29	109.99
9	I	110	PHE	CA-CB-CG	5.12	118.92	113.80
24	X	301	ALA	N-CA-C	5.12	125.32	111.00
23	W	321	VAL	CB-CA-C	5.11	118.95	111.33
10	J	64	ASN	N-CA-C	5.11	121.09	109.81
19	S	9	LEU	N-CA-CB	-5.10	102.94	111.20
1	A	106	VAL	N-CA-CB	-5.10	106.53	112.34
1	A	1315	GLU	N-CA-C	5.09	116.64	111.14
1	A	192	GLY	CA-C-N	5.08	131.25	121.54
1	A	192	GLY	C-N-CA	5.08	131.25	121.54
2	B	681	TRP	N-CA-C	-5.08	105.82	111.36
23	W	316	ILE	CB-CA-C	5.08	117.59	110.99
17	Q	375	ASP	N-CA-C	-5.07	105.65	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	408	ASP	CA-CB-CG	5.07	117.67	112.60
2	B	472	ALA	CA-C-N	5.07	131.22	121.54
2	B	472	ALA	C-N-CA	5.07	131.22	121.54
19	S	191	LEU	N-CA-C	5.06	117.92	111.69
1	A	193	ASP	CA-C-N	5.06	130.81	121.70
1	A	193	ASP	C-N-CA	5.06	130.81	121.70
8	H	145	ARG	CA-C-N	5.06	130.80	121.70
8	H	145	ARG	C-N-CA	5.06	130.80	121.70
1	A	5	GLN	N-CA-C	5.05	117.05	110.43
1	A	1127	ASP	CA-CB-CG	5.05	117.65	112.60
15	O	154	ASP	N-CA-C	5.05	118.56	111.90
1	A	478	TYR	CA-C-N	5.05	129.72	122.35
1	A	478	TYR	C-N-CA	5.05	129.72	122.35
19	S	21	GLY	N-CA-C	-5.04	105.11	111.72
1	A	147	VAL	N-CA-C	5.04	115.18	108.27
1	A	474	VAL	CA-C-N	5.04	127.31	120.65
1	A	474	VAL	C-N-CA	5.04	127.31	120.65
23	W	495	LYS	N-CA-C	5.04	115.69	108.74
19	S	119	SER	N-CA-C	5.04	116.08	108.07
17	Q	95	PRO	N-CA-C	-5.03	107.84	114.03
2	B	222	ILE	N-CA-C	5.03	115.09	107.75
2	B	998	ASP	CA-CB-CG	5.03	117.63	112.60
2	B	296	GLU	CA-C-N	5.03	126.89	120.56
2	B	296	GLU	C-N-CA	5.03	126.89	120.56
1	A	466	SER	N-CA-C	5.02	120.30	113.37
23	W	257	ASP	CB-CA-C	5.02	120.08	109.79
2	B	276	ILE	CA-C-N	5.01	127.31	120.54
2	B	276	ILE	C-N-CA	5.01	127.31	120.54
2	B	648	HIS	CA-C-N	5.01	129.46	121.99
2	B	648	HIS	C-N-CA	5.01	129.46	121.99
5	E	48	ASP	CA-CB-CG	5.01	117.61	112.60
26	Z	13	THR	N-CA-CB	5.01	117.58	110.16
2	B	663	ALA	N-CA-C	-5.01	105.29	111.40
8	H	85	GLY	N-CA-C	-5.01	106.69	112.50
23	W	201	VAL	CB-CA-C	-5.00	105.39	112.14

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	234	MET	Mainchain
1	A	95	PHE	Mainchain

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Mol	Chain	Res	Type	Group
2	B	43	LEU	Mainchain
17	Q	410	LYS	Peptide
19	S	165	THR	Peptide
21	U	135	VAL	Peptide
21	U	142	ASP	Peptide
23	W	316	ILE	Peptide
23	W	317	SER	Peptide
23	W	319	LYS	Peptide
23	W	540	LEU	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11174	0	11225	438	0
2	B	9140	0	9108	336	0
3	C	2095	0	2051	47	0
4	D	1434	0	1460	108	0
5	E	1752	0	1776	28	0
6	F	679	0	701	50	0
7	G	1340	0	1357	73	0
8	H	1068	0	1040	22	0
9	I	971	0	927	17	0
10	J	532	0	542	18	0
11	K	920	0	929	19	0
12	L	363	0	386	27	0
13	M	2202	0	2154	393	0
14	N	975	0	567	23	0
15	O	1416	0	1491	29	0
16	P	123	0	66	1	0
17	Q	606	0	256	32	0
18	R	521	0	216	5	0
19	S	691	0	279	6	0
20	T	1125	0	661	63	0
21	U	787	0	330	7	0
22	V	491	0	201	0	0
23	W	2085	0	871	13	0
24	X	1146	0	489	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	Y	1003	0	467	8	0
26	Z	442	0	190	1	0
27	A	2	0	0	0	0
27	B	1	0	0	0	0
27	C	1	0	0	0	0
27	I	2	0	0	0	0
27	J	1	0	0	0	0
27	L	1	0	0	0	0
27	M	1	0	0	0	0
28	A	1	0	0	0	0
All	All	45091	0	39740	1383	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 16.

All (1383) 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)
2:B:868:MET:CE	13:M:182:ARG:HG2	1.34	1.57
1:A:867:ILE:CG1	1:A:867:ILE:CD1	1.83	1.52
17:Q:356:TRP:CA	17:Q:392:ALA:HA	1.06	1.51
13:M:274:PRO:HD2	15:O:188:GLU:CD	1.38	1.44
17:Q:356:TRP:HA	17:Q:392:ALA:CA	0.93	1.39
2:B:1215:ARG:CD	4:D:15:LEU:HD13	1.19	1.39
3:C:85:ASP:OD1	25:Y:146:THR:CB	1.73	1.36
17:Q:390:PHE:HA	17:Q:391:THR:CB	1.44	1.35
13:M:274:PRO:CD	15:O:188:GLU:OE2	1.75	1.34
13:M:274:PRO:CD	15:O:188:GLU:CD	2.01	1.34
2:B:1217:TYR:CD2	4:D:13:ARG:NH1	1.97	1.32
17:Q:355:THR:O	17:Q:393:ARG:N	1.61	1.31
1:A:344:ARG:NH2	2:B:1120:GLU:HG3	1.48	1.26
17:Q:356:TRP:CB	17:Q:392:ALA:HB2	1.65	1.25
13:M:273:SER:HB2	15:O:188:GLU:OE2	1.32	1.24
1:A:317:LYS:O	2:B:471:LYS:NZ	1.73	1.21
2:B:868:MET:CE	13:M:182:ARG:CG	2.19	1.21
13:M:274:PRO:CD	15:O:188:GLU:OE1	1.89	1.20
23:W:528:HIS:O	24:X:227:GLY:HA2	1.41	1.19
13:M:248:LEU:HD11	13:M:286:ILE:HD12	1.22	1.18
1:A:420:ARG:NH2	24:X:174:ALA:H	1.44	1.16
1:A:420:ARG:NH1	24:X:174:ALA:HB2	1.60	1.15
2:B:1215:ARG:HD3	4:D:15:LEU:CD1	1.29	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:PHE:CZ	4:D:12:ARG:NH1	2.14	1.14
2:B:104:GLU:OE2	12:L:54:ARG:HD3	1.44	1.13
14:N:24:DT:H2''	14:N:25:DA:H5'	1.25	1.13
1:A:496:GLU:CD	7:G:63:PRO:O	1.92	1.12
2:B:1217:TYR:CD2	4:D:13:ARG:CZ	2.17	1.12
1:A:419:LYS:NZ	13:M:48:CYS:HB3	1.65	1.12
17:Q:390:PHE:CA	17:Q:391:THR:CB	2.27	1.11
2:B:1166:CYS:HB2	4:D:15:LEU:HD12	1.23	1.11
1:A:420:ARG:HH22	24:X:174:ALA:N	1.48	1.10
1:A:227:VAL:HG13	4:D:14:ARG:NH2	1.64	1.09
13:M:295:ALA:HB1	13:M:309:ILE:HD11	1.28	1.09
1:A:89:PRO:HG2	1:A:204:THR:HB	1.35	1.08
2:B:1185:CYS:HA	4:D:17:LYS:HD3	1.32	1.08
1:A:836:TYR:OH	1:A:1403:GLU:OE2	1.69	1.08
6:F:100:GLN:HG3	7:G:66:GLY:HA3	1.32	1.07
6:F:103:MET:HE1	7:G:65:ASP:HB2	1.35	1.07
1:A:78:PRO:O	2:B:1201:LYS:NZ	1.89	1.06
13:M:311:SER:HA	13:M:314:LYS:HE2	1.32	1.05
1:A:89:PRO:CG	1:A:204:THR:HB	1.88	1.04
1:A:317:LYS:O	2:B:471:LYS:CE	2.06	1.04
13:M:279:VAL:HG23	13:M:298:VAL:HG22	1.39	1.03
13:M:288:LEU:HD21	13:M:339:LEU:HD11	1.35	1.03
2:B:1166:CYS:CB	4:D:15:LEU:HD12	1.89	1.02
17:Q:356:TRP:HA	17:Q:392:ALA:CB	1.88	1.02
2:B:451:LYS:HD2	13:M:138:ASP:OD2	1.59	1.02
2:B:1165:ILE:HG21	4:D:17:LYS:HA	1.35	1.02
17:Q:356:TRP:CB	17:Q:392:ALA:CB	2.37	1.02
1:A:228:PHE:HZ	4:D:12:ARG:NH1	1.56	1.02
6:F:99:LEU:HD21	7:G:65:ASP:HA	1.42	1.02
13:M:279:VAL:HB	13:M:302:LEU:HD22	1.39	1.01
1:A:344:ARG:CZ	2:B:1120:GLU:HG3	1.88	1.01
1:A:227:VAL:HG11	4:D:14:ARG:NE	1.75	1.01
2:B:868:MET:HE3	13:M:182:ARG:CD	1.90	1.01
2:B:868:MET:HE3	13:M:182:ARG:HG2	1.39	1.01
13:M:272:LYS:HE3	20:T:53:DA:P	2.01	1.01
17:Q:356:TRP:CA	17:Q:392:ALA:CA	1.86	1.01
2:B:1166:CYS:HB3	4:D:15:LEU:O	1.61	1.00
23:W:535:VAL:O	23:W:539:ILE:N	1.93	1.00
2:B:902:GLY:O	12:L:65:VAL:HG11	1.59	1.00
1:A:1386:ARG:NH1	1:A:1403:GLU:OE1	1.95	0.99
17:Q:356:TRP:CA	17:Q:392:ALA:CB	2.40	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1444:MET:HE1	6:F:135:ARG:HB2	1.46	0.98
1:A:344:ARG:HD2	2:B:1118:PRO:O	1.64	0.97
2:B:868:MET:HE3	13:M:182:ARG:CG	1.89	0.97
1:A:496:GLU:OE2	7:G:63:PRO:O	1.80	0.97
6:F:99:LEU:HD21	7:G:65:ASP:CA	1.95	0.96
6:F:132:LEU:HD22	7:G:61:ILE:HD12	1.47	0.96
13:M:274:PRO:HD3	15:O:188:GLU:OE1	1.62	0.96
13:M:259:THR:HG23	13:M:323:LEU:HB3	1.43	0.96
1:A:419:LYS:HB3	13:M:47:LEU:O	1.64	0.96
2:B:868:MET:HE1	13:M:182:ARG:CG	1.87	0.96
2:B:583:ASN:HD21	2:B:628:THR:HG22	1.27	0.94
13:M:242:PHE:CE1	13:M:302:LEU:HA	2.01	0.94
13:M:274:PRO:HD2	15:O:188:GLU:OE2	0.78	0.94
13:M:186:ALA:HB1	13:M:237:THR:OG1	1.65	0.94
2:B:1185:CYS:CA	4:D:17:LYS:HD3	1.98	0.94
13:M:269:ILE:HG12	13:M:315:ILE:HG21	1.48	0.94
13:M:283:TYR:CZ	13:M:287:LEU:HD11	2.04	0.93
6:F:99:LEU:CD2	7:G:64:THR:O	2.17	0.93
2:B:1215:ARG:CD	4:D:15:LEU:HB2	1.98	0.92
1:A:228:PHE:CE2	4:D:12:ARG:NH1	2.35	0.92
13:M:320:ARG:HE	13:M:336:LEU:HB3	1.32	0.92
17:Q:105:ALA:HB2	18:R:92:LEU:CB	1.98	0.92
17:Q:355:THR:O	17:Q:392:ALA:C	2.12	0.92
1:A:420:ARG:NH1	24:X:174:ALA:CB	2.32	0.92
13:M:286:ILE:HD13	13:M:293:ILE:CG2	1.98	0.92
13:M:279:VAL:CB	13:M:302:LEU:HD22	2.00	0.91
1:A:1438:THR:HG22	2:B:1144:ALA:HB3	1.52	0.91
1:A:419:LYS:HZ1	13:M:48:CYS:HB3	1.31	0.91
2:B:451:LYS:CE	13:M:138:ASP:OD2	2.19	0.90
13:M:238:TYR:HB3	13:M:242:PHE:CE2	2.06	0.90
13:M:248:LEU:CD1	13:M:286:ILE:HD12	2.00	0.90
13:M:248:LEU:HD13	13:M:252:VAL:HG11	1.54	0.90
2:B:1184:GLY:O	4:D:17:LYS:HD3	1.71	0.90
1:A:420:ARG:HH12	24:X:174:ALA:N	1.70	0.89
2:B:868:MET:HE1	13:M:182:ARG:HG2	0.91	0.89
2:B:451:LYS:CD	13:M:138:ASP:OD2	2.20	0.89
13:M:273:SER:CB	15:O:188:GLU:OE2	2.20	0.89
23:W:528:HIS:O	24:X:227:GLY:CA	2.20	0.89
2:B:1217:TYR:HD2	4:D:13:ARG:NH1	1.69	0.89
13:M:298:VAL:HG22	13:M:302:LEU:HD13	1.54	0.89
1:A:832:ALA:HA	20:T:15:DA:O4'	1.73	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:420:ARG:HH22	24:X:174:ALA:H	0.89	0.88
13:M:288:LEU:CD2	13:M:339:LEU:HD11	2.02	0.88
6:F:76:LYS:HA	6:F:79:ARG:HD3	1.56	0.88
1:A:417:TYR:CZ	13:M:37:ARG:HD3	2.09	0.88
2:B:1166:CYS:HB2	4:D:15:LEU:CD1	2.04	0.88
13:M:274:PRO:CG	15:O:188:GLU:OE1	2.21	0.88
1:A:420:ARG:HH12	24:X:174:ALA:CA	1.85	0.88
1:A:417:TYR:CE2	13:M:37:ARG:HD3	2.09	0.87
1:A:496:GLU:OE1	7:G:63:PRO:O	1.93	0.87
13:M:242:PHE:HD1	13:M:301:THR:HG22	1.36	0.87
13:M:339:LEU:HB3	13:M:340:PRO:HD2	1.57	0.87
15:O:69:ASN:HB2	20:T:48:DT:O4'	1.74	0.87
6:F:100:GLN:CG	7:G:66:GLY:HA3	2.05	0.87
20:T:49:DA:C2'	20:T:50:DT:H5'	2.03	0.87
13:M:288:LEU:HG	13:M:339:LEU:HD21	1.56	0.87
2:B:104:GLU:OE2	12:L:54:ARG:CD	2.22	0.86
13:M:279:VAL:CG1	13:M:309:ILE:HG22	2.06	0.86
13:M:295:ALA:HB1	13:M:306:GLU:HG3	1.56	0.86
1:A:91:PHE:HB3	1:A:96:ILE:HG13	1.56	0.86
2:B:1215:ARG:HD3	4:D:15:LEU:HD12	1.55	0.86
1:A:344:ARG:HA	2:B:1129:ARG:HA	1.57	0.85
1:A:11:LEU:HD11	2:B:1195:HIS:CD2	2.11	0.85
13:M:295:ALA:CB	13:M:309:ILE:HD11	2.06	0.85
2:B:1185:CYS:HA	4:D:17:LYS:CD	1.99	0.85
13:M:234:GLN:HB2	13:M:236:LEU:CD2	2.07	0.85
1:A:836:TYR:HH	1:A:1403:GLU:CD	1.83	0.84
13:M:293:ILE:HD13	13:M:297:LYS:HG3	1.60	0.84
1:A:419:LYS:HZ2	13:M:48:CYS:HB3	1.41	0.84
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.59	0.84
13:M:248:LEU:HD21	13:M:286:ILE:HD11	1.58	0.84
1:A:68:GLN:O	1:A:68:GLN:NE2	2.11	0.83
2:B:451:LYS:CE	13:M:138:ASP:CG	2.50	0.83
2:B:1215:ARG:HD2	4:D:15:LEU:HB2	1.59	0.83
1:A:420:ARG:NH2	24:X:174:ALA:N	2.15	0.83
13:M:295:ALA:CB	13:M:306:GLU:HG3	2.09	0.83
2:B:416:LEU:HD23	2:B:457:LEU:HD23	1.61	0.83
13:M:279:VAL:HG23	13:M:298:VAL:CG2	2.09	0.83
13:M:311:SER:HA	13:M:314:LYS:CE	2.09	0.83
2:B:451:LYS:HE3	13:M:138:ASP:CG	2.04	0.83
13:M:66:PHE:O	13:M:78:ARG:NH2	2.12	0.83
13:M:269:ILE:HG23	13:M:272:LYS:HG2	1.61	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:310:LYS:HE3	13:M:342:VAL:HG22	1.58	0.83
13:M:312:GLY:O	13:M:315:ILE:HG22	1.78	0.83
6:F:99:LEU:HD21	7:G:64:THR:O	1.78	0.83
1:A:53:LEU:HD23	1:A:54:ASN:H	1.44	0.83
13:M:266:ILE:CD1	13:M:268:GLU:HB2	2.09	0.82
2:B:792:MET:HE2	20:T:21:DT:OP1	1.79	0.82
1:A:344:ARG:NH2	2:B:1120:GLU:CG	2.40	0.82
13:M:269:ILE:HD11	13:M:316:LEU:HD11	1.60	0.82
13:M:273:SER:O	13:M:276:THR:HG22	1.79	0.82
3:C:148:ARG:H	3:C:151:GLN:HG3	1.43	0.82
13:M:275:ILE:HD11	13:M:302:LEU:HB3	1.61	0.82
20:T:49:DA:H2''	20:T:50:DT:H5'	1.61	0.82
2:B:451:LYS:NZ	13:M:138:ASP:CG	2.37	0.82
23:W:534:ASN:O	23:W:538:ASP:CB	2.28	0.82
1:A:95:PHE:O	1:A:96:ILE:C	2.13	0.82
13:M:310:LYS:CE	13:M:342:VAL:HG22	2.09	0.82
3:C:148:ARG:HD3	3:C:149:LYS:HG2	1.61	0.81
13:M:315:ILE:CG2	13:M:316:LEU:HD12	2.10	0.81
17:Q:356:TRP:CB	17:Q:392:ALA:CA	2.58	0.81
13:M:269:ILE:HG21	13:M:272:LYS:HB2	1.62	0.81
13:M:238:TYR:HB3	13:M:242:PHE:CD2	2.14	0.81
14:N:24:DT:C2'	14:N:25:DA:H5'	2.09	0.81
2:B:1217:TYR:CE1	4:D:13:ARG:HB2	2.16	0.81
23:W:535:VAL:O	23:W:539:ILE:CA	2.27	0.81
2:B:849:GLY:HA2	2:B:852:ARG:HD2	1.62	0.81
13:M:234:GLN:O	13:M:237:THR:HG22	1.81	0.81
13:M:305:THR:HG23	13:M:308:THR:H	1.46	0.81
1:A:22:PHE:HB2	2:B:1211:ASN:CG	2.06	0.80
13:M:186:ALA:CB	13:M:237:THR:OG1	2.28	0.80
6:F:103:MET:CE	7:G:65:ASP:HB2	2.10	0.80
13:M:279:VAL:CA	13:M:302:LEU:HD22	2.11	0.80
13:M:269:ILE:CD1	13:M:316:LEU:HD11	2.12	0.80
13:M:279:VAL:HG11	13:M:309:ILE:HG22	1.63	0.80
13:M:336:LEU:HA	13:M:339:LEU:CD1	2.12	0.80
17:Q:356:TRP:C	17:Q:392:ALA:HA	2.03	0.80
6:F:100:GLN:HG3	7:G:66:GLY:CA	2.10	0.79
1:A:420:ARG:NH1	24:X:174:ALA:N	2.31	0.79
1:A:89:PRO:HB2	1:A:204:THR:CG2	2.13	0.79
13:M:286:ILE:HD13	13:M:293:ILE:HG22	1.64	0.79
13:M:325:ASP:OD1	13:M:328:LEU:HB2	1.81	0.79
2:B:1165:ILE:CG2	4:D:17:LYS:HA	2.12	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:248:LEU:HD23	13:M:291:ILE:CD1	2.12	0.79
6:F:132:LEU:HD22	7:G:61:ILE:CD1	2.13	0.79
2:B:29:ASP:HB3	2:B:658:ILE:HG12	1.64	0.79
2:B:451:LYS:NZ	13:M:138:ASP:OD1	2.15	0.79
13:M:286:ILE:HG21	13:M:293:ILE:HG22	1.65	0.79
1:A:228:PHE:HZ	4:D:12:ARG:CZ	1.95	0.79
23:W:535:VAL:O	23:W:539:ILE:CB	2.31	0.78
1:A:418:SER:HA	13:M:48:CYS:C	2.07	0.78
1:A:55:ASP:HA	1:A:58:LEU:HB2	1.63	0.78
2:B:900:ALA:HB3	12:L:61:THR:HG23	1.64	0.78
13:M:277:ILE:O	13:M:280:VAL:HG22	1.83	0.78
3:C:147:LEU:HB3	3:C:151:GLN:HB2	1.66	0.78
13:M:290:GLN:CD	13:M:291:ILE:HG23	2.08	0.78
13:M:296:ALA:O	13:M:300:GLN:HG3	1.83	0.78
13:M:310:LYS:CD	13:M:342:VAL:HG22	2.13	0.78
13:M:248:LEU:HD21	13:M:286:ILE:CD1	2.14	0.77
13:M:315:ILE:HG23	13:M:316:LEU:HD12	1.64	0.77
2:B:108:VAL:HG13	13:M:240:PRO:HB2	1.64	0.77
13:M:287:LEU:HD13	13:M:340:PRO:HG3	1.65	0.77
6:F:99:LEU:HD22	7:G:64:THR:O	1.83	0.77
13:M:330:ALA:HB1	13:M:334:VAL:O	1.84	0.77
2:B:1189:ILE:HG21	7:G:41:LYS:HB2	1.65	0.77
2:B:1166:CYS:HA	4:D:15:LEU:HA	1.65	0.77
13:M:269:ILE:HG21	13:M:277:ILE:CD1	2.14	0.77
13:M:249:PRO:HD3	13:M:291:ILE:HD11	1.66	0.76
13:M:274:PRO:CG	15:O:188:GLU:CD	2.57	0.76
13:M:311:SER:CA	13:M:314:LYS:HE2	2.13	0.76
1:A:1116:LEU:HD12	1:A:1329:THR:HB	1.67	0.76
1:A:1433:MET:CE	2:B:1145:SER:OG	2.33	0.76
6:F:93:ILE:HD11	6:F:134:ILE:HD11	1.66	0.76
20:T:47:DA:N7	20:T:48:DT:O4	2.19	0.76
6:F:132:LEU:CD2	7:G:61:ILE:CD1	2.62	0.76
2:B:1215:ARG:CG	4:D:15:LEU:HD13	2.14	0.76
2:B:1217:TYR:HB2	4:D:13:ARG:CZ	2.16	0.76
2:B:449:ASN:ND2	13:M:135:MET:HG3	1.99	0.75
13:M:320:ARG:NE	13:M:336:LEU:HB3	2.00	0.75
2:B:1184:GLY:C	4:D:17:LYS:HD3	2.11	0.75
2:B:1184:GLY:O	4:D:17:LYS:CD	2.34	0.75
20:T:48:DT:H2'	20:T:49:DA:C8	2.21	0.75
1:A:368:LYS:HE2	1:A:399:HIS:HB2	1.66	0.75
1:A:497:THR:HG22	2:B:1146:PHE:HD1	1.52	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1390:ASN:O	1:A:1399:ARG:CD	2.34	0.75
2:B:902:GLY:O	12:L:65:VAL:CG1	2.36	0.74
13:M:286:ILE:HD13	13:M:293:ILE:CB	2.16	0.74
1:A:419:LYS:HG2	13:M:48:CYS:HA	1.68	0.74
13:M:272:LYS:CE	20:T:53:DA:P	2.76	0.74
1:A:420:ARG:NH1	24:X:174:ALA:CA	2.50	0.74
13:M:248:LEU:HA	13:M:291:ILE:HD11	1.69	0.74
2:B:451:LYS:HZ1	13:M:138:ASP:CG	1.96	0.74
1:A:836:TYR:CZ	1:A:1403:GLU:OE2	2.41	0.74
1:A:89:PRO:HG2	1:A:204:THR:CB	2.16	0.74
13:M:249:PRO:CD	13:M:291:ILE:HD11	2.18	0.73
12:L:50:ASP:HA	13:M:250:MET:HE1	1.70	0.73
13:M:293:ILE:HD11	13:M:297:LYS:HB2	1.67	0.73
1:A:418:SER:CA	13:M:49:GLY:HA3	2.17	0.73
13:M:290:GLN:NE2	13:M:291:ILE:HG23	2.03	0.73
13:M:321:ASP:OD1	13:M:336:LEU:HD13	1.89	0.73
1:A:16:GLU:HB2	4:D:13:ARG:NH2	2.03	0.73
2:B:1217:TYR:CE2	4:D:13:ARG:NH1	2.47	0.73
13:M:275:ILE:CD1	13:M:302:LEU:HB3	2.19	0.73
1:A:227:VAL:HG13	4:D:14:ARG:HH21	1.50	0.73
1:A:419:LYS:NZ	13:M:27:CYS:SG	2.62	0.72
1:A:228:PHE:HE2	4:D:12:ARG:HH12	1.35	0.72
2:B:1125:ASP:OD2	13:M:39:SER:O	2.07	0.72
1:A:50:ILE:O	1:A:52:GLY:N	2.23	0.72
13:M:233:ALA:HB1	13:M:237:THR:HG21	1.70	0.72
2:B:868:MET:O	13:M:182:ARG:NH2	2.21	0.72
8:H:38:LEU:HD11	8:H:123:MET:HE2	1.70	0.72
1:A:91:PHE:HB2	1:A:96:ILE:HD11	1.72	0.72
1:A:726:ARG:HD3	1:A:766:GLY:HA3	1.72	0.72
1:A:91:PHE:HB3	1:A:96:ILE:CG1	2.18	0.72
1:A:419:LYS:HE3	13:M:47:LEU:C	2.15	0.72
13:M:335:SER:O	13:M:339:LEU:HD12	1.89	0.72
1:A:227:VAL:HG11	4:D:14:ARG:HB3	1.70	0.72
2:B:952:VAL:O	12:L:58:LYS:HB2	1.88	0.72
1:A:317:LYS:O	2:B:471:LYS:HE3	1.89	0.72
8:H:84:ALA:HA	8:H:87:ARG:HB2	1.71	0.72
13:M:275:ILE:HD12	13:M:304:VAL:CG2	2.20	0.72
2:B:1198:TYR:CE2	2:B:1201:LYS:HE3	2.25	0.72
11:K:58:PHE:HB3	11:K:76:GLN:HB3	1.71	0.72
19:S:23:ARG:O	19:S:27:VAL:N	2.23	0.72
13:M:287:LEU:CD1	13:M:340:PRO:HG3	2.20	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:ILE:HA	1:A:52:GLY:O	1.89	0.71
4:D:123:LEU:HD11	4:D:146:GLN:HG2	1.72	0.71
7:G:1:MET:CE	7:G:80:LYS:H	2.02	0.71
13:M:286:ILE:HD13	13:M:293:ILE:HB	1.72	0.71
6:F:75:PRO:HG2	6:F:78:GLN:HB2	1.72	0.71
4:D:134:THR:HG23	4:D:136:GLY:H	1.56	0.71
1:A:418:SER:HA	13:M:48:CYS:O	1.90	0.70
12:L:50:ASP:CA	13:M:250:MET:HE1	2.17	0.70
1:A:418:SER:HA	13:M:49:GLY:HA3	1.72	0.70
3:C:66:ARG:NH2	10:J:3:VAL:O	2.23	0.70
1:A:831:THR:HG23	20:T:15:DA:C5	2.27	0.70
20:T:46:DT:H2'	20:T:47:DA:O5'	1.91	0.70
1:A:346:ASP:OD1	2:B:1106:ARG:NE	2.21	0.70
1:A:417:TYR:CE2	13:M:37:ARG:CD	2.75	0.70
17:Q:355:THR:O	17:Q:392:ALA:CA	2.39	0.70
13:M:242:PHE:CD1	13:M:301:THR:HG22	2.24	0.69
2:B:1133:MET:SD	20:T:16:DT:H4'	2.32	0.69
5:E:185:ALA:HA	5:E:190:LEU:HD12	1.74	0.69
1:A:420:ARG:NH2	24:X:173:ALA:HA	2.07	0.69
13:M:286:ILE:CD1	13:M:293:ILE:HB	2.22	0.69
1:A:53:LEU:CD2	1:A:54:ASN:H	2.06	0.69
1:A:140:THR:HA	1:A:143:LYS:HE2	1.75	0.69
1:A:227:VAL:CG1	4:D:14:ARG:NE	2.36	0.69
13:M:342:VAL:HG13	13:M:343:GLU:N	2.06	0.69
1:A:1197:LEU:HD11	1:A:1238:ILE:HD11	1.74	0.69
1:A:831:THR:CG2	20:T:15:DA:C5	2.75	0.69
4:D:12:ARG:HD3	4:D:14:ARG:HG2	1.74	0.69
13:M:243:CYS:SG	13:M:253:THR:HG22	2.32	0.69
13:M:274:PRO:HG3	15:O:188:GLU:OE1	1.92	0.69
1:A:344:ARG:HA	2:B:1128:LEU:O	1.93	0.69
2:B:868:MET:O	13:M:182:ARG:CZ	2.40	0.69
17:Q:356:TRP:N	17:Q:392:ALA:HA	2.02	0.69
1:A:16:GLU:OE1	4:D:13:ARG:NH2	2.26	0.68
1:A:412:ARG:HB3	13:M:51:VAL:CG1	2.23	0.68
13:M:334:VAL:HA	13:M:338:ASN:HD21	1.58	0.68
1:A:320:ARG:NH2	13:M:81:GLU:HG3	2.08	0.68
13:M:294:THR:H	13:M:297:LYS:HG3	1.57	0.68
13:M:235:ASN:HD22	13:M:260:ALA:HB3	1.58	0.68
13:M:261:LYS:HG3	13:M:262:LYS:N	2.09	0.68
13:M:283:TYR:O	13:M:287:LEU:HG	1.93	0.68
3:C:18:VAL:HG23	3:C:240:VAL:HB	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:334:VAL:HA	13:M:338:ASN:ND2	2.09	0.68
17:Q:355:THR:O	17:Q:392:ALA:HB1	1.94	0.68
7:G:45:ILE:HA	7:G:78:VAL:HG12	1.76	0.68
1:A:445:ASN:HB2	1:A:455:MET:HG2	1.75	0.68
1:A:870:GLU:HB2	5:E:204:THR:HG21	1.75	0.68
5:E:4:GLU:HB3	5:E:7:ARG:HE	1.59	0.67
13:M:306:GLU:HA	13:M:309:ILE:HG12	1.76	0.67
2:B:1217:TYR:HD2	4:D:13:ARG:CZ	1.93	0.67
13:M:324:VAL:CG2	13:M:328:LEU:HD22	2.24	0.67
1:A:420:ARG:HH22	24:X:173:ALA:HA	1.59	0.67
17:Q:358:GLY:HA2	17:Q:391:THR:CB	2.22	0.67
20:T:47:DA:C8	20:T:48:DT:O4	2.47	0.67
13:M:269:ILE:HG21	13:M:277:ILE:HD11	1.76	0.67
1:A:420:ARG:CZ	24:X:174:ALA:N	2.57	0.67
1:A:496:GLU:OE1	7:G:64:THR:HA	1.94	0.67
13:M:269:ILE:HD11	13:M:316:LEU:CD1	2.23	0.67
13:M:70:ASP:HB3	13:M:78:ARG:HD2	1.75	0.67
1:A:420:ARG:CZ	24:X:174:ALA:H	2.06	0.67
20:T:48:DT:H2'	20:T:49:DA:N7	2.08	0.67
13:M:284:LEU:CD1	13:M:339:LEU:HD22	2.24	0.66
2:B:563:MET:HE1	2:B:587:HIS:HB2	1.77	0.66
2:B:1215:ARG:CD	4:D:15:LEU:CD1	2.05	0.66
2:B:429:PHE:HA	2:B:432:MET:HE2	1.77	0.66
4:D:8:PHE:HD2	7:G:6:ASP:HB2	1.61	0.66
1:A:388:LEU:O	1:A:392:VAL:HG23	1.96	0.66
1:A:871:ASP:HB3	5:E:204:THR:HG23	1.76	0.66
13:M:242:PHE:O	13:M:246:LEU:HG	1.96	0.66
21:U:86:PHE:O	21:U:90:LEU:N	2.28	0.66
1:A:347:PHE:HE1	1:A:375:THR:HG22	1.60	0.66
13:M:290:GLN:HB3	13:M:331:ASN:ND2	2.11	0.66
1:A:1442:ASP:HB2	6:F:137:TYR:HE1	1.61	0.66
13:M:293:ILE:HG12	13:M:297:LYS:HD3	1.78	0.66
2:B:1165:ILE:HB	4:D:17:LYS:HB3	1.78	0.66
3:C:259:LEU:HD22	11:K:91:CYS:HB3	1.75	0.66
1:A:419:LYS:HZ2	13:M:48:CYS:CB	2.08	0.65
13:M:283:TYR:CE2	13:M:287:LEU:HD11	2.31	0.65
1:A:46:THR:HG22	1:A:47:ARG:H	1.61	0.65
1:A:316:GLN:O	1:A:318:SER:N	2.30	0.65
13:M:243:CYS:CB	13:M:253:THR:HG22	2.26	0.65
1:A:311:GLN:HG3	1:A:312:PRO:HD2	1.77	0.65
2:B:296:GLU:O	2:B:300:HIS:HD2	1.80	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:272:LYS:HB3	13:M:276:THR:HG21	1.77	0.65
13:M:269:ILE:CG1	13:M:315:ILE:HG21	2.25	0.65
14:N:24:DT:H2''	14:N:25:DA:C5'	2.17	0.65
1:A:15:LYS:NZ	2:B:1220:ARG:HE	1.93	0.65
2:B:872:GLU:HG2	2:B:916:THR:HG22	1.78	0.65
12:L:61:THR:CG2	12:L:63:ARG:HG2	2.26	0.65
17:Q:409:ASP:HA	17:Q:411:LYS:O	1.97	0.65
2:B:879:ARG:HG3	2:B:885:MET:HE2	1.78	0.65
13:M:311:SER:O	13:M:314:LYS:HD3	1.97	0.65
1:A:57:ARG:O	1:A:68:GLN:HG2	1.96	0.65
2:B:857:ARG:NH1	2:B:945:GLU:OE2	2.29	0.65
2:B:996:ARG:HG3	2:B:1007:VAL:HG11	1.79	0.65
3:C:56:THR:HG21	3:C:145:CYS:SG	2.37	0.65
13:M:269:ILE:HD12	13:M:277:ILE:HD12	1.79	0.65
13:M:275:ILE:HD13	13:M:275:ILE:O	1.97	0.65
1:A:832:ALA:HB2	20:T:15:DA:C8	2.32	0.65
4:D:51:ASN:ND2	4:D:54:GLU:OE1	2.30	0.64
13:M:255:SER:OG	13:M:328:LEU:HD13	1.96	0.64
1:A:204:THR:HG22	1:A:235:ILE:HG21	1.79	0.64
13:M:286:ILE:HG12	13:M:292:PRO:HA	1.78	0.64
2:B:68:THR:HG22	2:B:91:SER:HA	1.80	0.64
13:M:269:ILE:CD1	13:M:277:ILE:HD12	2.28	0.64
2:B:773:MET:HE1	2:B:985:GLY:HA2	1.79	0.64
2:B:917:PRO:HA	2:B:934:LYS:HB3	1.80	0.64
1:A:416:ARG:NH2	13:M:40:GLU:HG2	2.13	0.64
19:S:125:PHE:HA	19:S:155:ILE:O	1.98	0.64
8:H:82:PRO:C	8:H:84:ALA:H	2.05	0.64
13:M:275:ILE:HD12	13:M:304:VAL:HG21	1.80	0.64
1:A:1409:LEU:HD13	2:B:1207:LEU:HD21	1.79	0.63
2:B:806:THR:HG22	2:B:808:ALA:H	1.63	0.63
6:F:99:LEU:HD23	7:G:66:GLY:N	2.13	0.63
1:A:420:ARG:HH22	24:X:173:ALA:C	2.05	0.63
13:M:235:ASN:ND2	13:M:260:ALA:HB3	2.13	0.63
21:U:143:GLU:O	21:U:146:GLU:N	2.31	0.63
1:A:447:GLN:NE2	20:T:17:DG:H4'	2.13	0.63
12:L:28:LYS:HB2	12:L:39:SER:HA	1.80	0.63
17:Q:356:TRP:HA	17:Q:392:ALA:C	2.12	0.63
23:W:534:ASN:O	23:W:538:ASP:N	2.30	0.63
11:K:49:GLU:HG3	11:K:94:ILE:HG13	1.81	0.63
1:A:340:LEU:HD13	1:A:1429:ILE:HG23	1.81	0.63
2:B:868:MET:HE3	13:M:182:ARG:HD2	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:417:TYR:HE2	13:M:37:ARG:HG3	1.64	0.63
2:B:1185:CYS:HA	4:D:17:LYS:HB2	1.81	0.63
13:M:242:PHE:CG	13:M:302:LEU:HG	2.34	0.63
13:M:288:LEU:O	13:M:334:VAL:HG23	1.98	0.63
13:M:335:SER:H	13:M:338:ASN:ND2	1.96	0.63
1:A:1433:MET:HE2	2:B:1145:SER:OG	1.97	0.63
3:C:10:ILE:HD12	11:K:108:GLU:HB3	1.81	0.63
2:B:841:MET:HB3	2:B:846:ILE:HD11	1.81	0.62
1:A:16:GLU:HB3	1:A:1418:LEU:HD11	1.79	0.62
13:M:313:TYR:HD2	13:M:343:GLU:N	1.97	0.62
2:B:1184:GLY:O	4:D:17:LYS:CE	2.48	0.62
18:R:60:ASP:CB	18:R:213:ALA:HA	2.29	0.62
13:M:287:LEU:O	13:M:334:VAL:HG21	2.00	0.62
13:M:319:HIS:O	13:M:323:LEU:HG	2.00	0.62
20:T:49:DA:H2'	20:T:50:DT:H5'	1.80	0.62
3:C:67:LEU:HA	3:C:70:ILE:HD12	1.82	0.62
1:A:89:PRO:CB	1:A:204:THR:HB	2.29	0.62
1:A:95:PHE:C	1:A:97:ALA:N	2.54	0.62
13:M:291:ILE:O	13:M:291:ILE:HG13	1.99	0.62
20:T:21:DT:H2''	20:T:22:DT:H5'	1.81	0.62
1:A:5:GLN:HG3	2:B:1175:LEU:HD11	1.82	0.62
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.80	0.62
1:A:420:ARG:CZ	24:X:174:ALA:HB2	2.28	0.62
2:B:1215:ARG:HD3	4:D:15:LEU:HD13	0.62	0.62
13:M:271:GLY:O	20:T:52:DC:H4'	1.99	0.62
1:A:11:LEU:CD1	2:B:1195:HIS:CD2	2.82	0.62
6:F:99:LEU:CD2	7:G:65:ASP:C	2.73	0.62
13:M:269:ILE:CG2	13:M:272:LYS:HB2	2.30	0.62
13:M:304:VAL:HG12	13:M:305:THR:N	2.15	0.62
13:M:310:LYS:HD3	13:M:342:VAL:HG22	1.82	0.61
17:Q:394:ASN:CB	17:Q:395:LYS:HA	2.30	0.61
1:A:344:ARG:CZ	2:B:1120:GLU:CG	2.74	0.61
1:A:22:PHE:N	2:B:1211:ASN:O	2.32	0.61
2:B:486:TYR:HB3	2:B:1096:ARG:CZ	2.31	0.61
7:G:27:LYS:HE2	7:G:54:ILE:HB	1.82	0.61
1:A:1130:GLN:HA	1:A:1133:LEU:HD12	1.83	0.61
13:M:279:VAL:HG13	13:M:309:ILE:HG22	1.78	0.61
1:A:1111:MET:HG3	1:A:1114:PRO:HG3	1.83	0.61
13:M:256:ALA:HA	13:M:285:ASN:HD22	1.65	0.61
13:M:266:ILE:HD11	13:M:268:GLU:HB2	1.80	0.61
13:M:294:THR:N	13:M:297:LYS:HG3	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:420:ARG:HH22	24:X:173:ALA:CA	2.14	0.61
1:A:1390:ASN:O	1:A:1399:ARG:HG2	2.01	0.61
4:D:12:ARG:NH2	4:D:13:ARG:O	2.34	0.61
13:M:294:THR:H	13:M:297:LYS:CG	2.13	0.61
1:A:91:PHE:CB	1:A:96:ILE:HD11	2.30	0.61
2:B:249:ARG:HH12	2:B:418:LYS:HD2	1.66	0.61
2:B:269:ILE:HD11	2:B:386:LEU:HD21	1.82	0.61
3:C:11:ARG:HH21	3:C:229:TYR:HD2	1.48	0.61
1:A:66:LYS:HE2	1:A:68:GLN:H	1.65	0.61
13:M:324:VAL:HG22	13:M:325:ASP:N	2.15	0.61
1:A:419:LYS:NZ	13:M:48:CYS:CB	2.52	0.61
1:A:1428:VAL:HG13	2:B:1151:LEU:HD21	1.83	0.61
13:M:262:LYS:O	13:M:266:ILE:HG12	2.01	0.61
1:A:51:GLY:HA2	1:A:56:PRO:HA	1.83	0.60
1:A:72:GLU:HB3	1:A:76:GLU:HB3	1.83	0.60
1:A:132:LYS:NZ	1:A:1415:SER:CB	2.64	0.60
1:A:1193:LEU:HB2	1:A:1260:LEU:HD21	1.81	0.60
13:M:280:VAL:HG12	13:M:309:ILE:O	2.01	0.60
1:A:448:PRO:O	1:A:449:SER:HB2	2.01	0.60
2:B:843:GLN:HA	2:B:846:ILE:HD12	1.82	0.60
13:M:293:ILE:HD13	13:M:297:LYS:CG	2.29	0.60
1:A:326:ARG:HG3	1:A:1406:VAL:HG21	1.83	0.60
2:B:1185:CYS:N	4:D:17:LYS:HD3	2.16	0.60
2:B:1215:ARG:CD	4:D:15:LEU:CB	2.65	0.60
2:B:205:ILE:HD11	2:B:461:LEU:HD13	1.82	0.60
1:A:89:PRO:HB2	1:A:204:THR:HG21	1.83	0.60
13:M:293:ILE:HD11	13:M:297:LYS:CB	2.31	0.60
1:A:380:VAL:HG13	1:A:385:ILE:HG12	1.83	0.60
4:D:52:LEU:O	4:D:54:GLU:N	2.34	0.60
1:A:946:VAL:HG22	5:E:201:LYS:HD2	1.82	0.60
13:M:336:LEU:HA	13:M:339:LEU:HD13	1.83	0.60
2:B:911:ILE:HD11	2:B:941:LEU:HD12	1.82	0.60
5:E:202:SER:HB3	5:E:205:SER:H	1.66	0.60
13:M:324:VAL:HG23	13:M:328:LEU:HD22	1.83	0.60
1:A:372:LYS:HA	1:A:435:HIS:CD2	2.36	0.60
17:Q:105:ALA:HB3	18:R:90:GLN:O	2.01	0.60
2:B:976:ILE:O	2:B:990:ILE:HB	2.02	0.60
1:A:419:LYS:HE3	13:M:48:CYS:N	2.17	0.59
2:B:839:MET:HE3	2:B:1010:LEU:HD21	1.83	0.59
13:M:255:SER:HB3	13:M:285:ASN:OD1	2.01	0.59
19:S:17:ILE:O	19:S:21:GLY:N	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:792:MET:HE1	20:T:20:DA:O3'	2.01	0.59
1:A:418:SER:HA	13:M:49:GLY:CA	2.32	0.59
1:A:629:LEU:O	1:A:633:VAL:HG23	2.02	0.59
1:A:839:ARG:NH2	1:A:1401:SER:O	2.35	0.59
1:A:1063:MET:SD	1:A:1436:ILE:HB	2.41	0.59
1:A:871:ASP:OD1	1:A:1366:ARG:NH2	2.34	0.59
2:B:363:HIS:O	2:B:364:ILE:HB	2.02	0.59
2:B:1184:GLY:O	4:D:17:LYS:HE2	2.02	0.59
3:C:184:ASN:HD21	3:C:189:THR:H	1.50	0.59
5:E:4:GLU:HB3	5:E:7:ARG:NE	2.16	0.59
12:L:61:THR:HG21	12:L:63:ARG:HG2	1.84	0.59
1:A:1387:HIS:O	1:A:1391:ARG:HG2	2.02	0.59
7:G:1:MET:HE1	7:G:80:LYS:H	1.67	0.59
12:L:47:ARG:HH21	12:L:54:ARG:HH21	1.50	0.59
20:T:48:DT:C2'	20:T:49:DA:C8	2.86	0.59
1:A:53:LEU:HD23	1:A:54:ASN:N	2.15	0.59
2:B:868:MET:HE3	13:M:182:ARG:NE	2.18	0.59
20:T:47:DA:H2'	20:T:48:DT:C5	2.38	0.59
21:U:129:VAL:O	21:U:133:SER:N	2.36	0.59
1:A:22:PHE:CB	2:B:1211:ASN:OD1	2.50	0.59
1:A:412:ARG:HB3	13:M:51:VAL:HG11	1.83	0.59
1:A:857:ARG:HD3	1:A:861:GLY:O	2.03	0.59
2:B:451:LYS:HZ2	13:M:147:LYS:HZ3	1.51	0.59
2:B:950:ASP:HB3	2:B:967:ARG:HG2	1.84	0.59
13:M:197:HIS:H	13:M:198:VAL:HA	1.67	0.59
1:A:901:LEU:HD22	1:A:919:ILE:HG23	1.85	0.59
13:M:248:LEU:HD23	13:M:291:ILE:HD12	1.85	0.59
6:F:132:LEU:CD2	7:G:61:ILE:HD12	2.24	0.58
8:H:47:PHE:HB3	8:H:95:TYR:CD2	2.38	0.58
1:A:483:ASP:HB2	2:B:987:LYS:HE3	1.84	0.58
2:B:653:VAL:HG22	2:B:689:LEU:HB3	1.84	0.58
14:N:22:DT:C2'	14:N:23:DA:H5'	2.33	0.58
1:A:56:PRO:HD2	1:A:58:LEU:HG	1.86	0.58
13:M:320:ARG:HE	13:M:336:LEU:CB	2.13	0.58
1:A:566:ILE:HD11	8:H:98:TYR:HB2	1.85	0.58
1:A:588:LEU:HD23	1:A:607:ILE:HD12	1.86	0.58
1:A:836:TYR:CE1	1:A:1403:GLU:OE2	2.57	0.58
4:D:148:LEU:O	4:D:152:SER:OG	2.17	0.58
1:A:68:GLN:O	1:A:70:CYS:N	2.31	0.58
1:A:831:THR:CG2	20:T:15:DA:C6	2.87	0.58
5:E:147:HIS:HB3	5:E:150:VAL:HG23	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1217:TYR:CE1	4:D:13:ARG:CB	2.86	0.58
1:A:590:ARG:NH2	1:A:621:THR:OG1	2.36	0.58
4:D:67:ARG:HH21	4:D:129:LEU:HD13	1.68	0.58
1:A:228:PHE:CZ	4:D:12:ARG:NH2	2.71	0.57
1:A:417:TYR:CZ	13:M:37:ARG:CD	2.85	0.57
4:D:23:ASN:N	4:D:23:ASN:OD1	2.36	0.57
2:B:810:GLU:HA	2:B:815:ARG:HH12	1.69	0.57
4:D:8:PHE:CZ	4:D:37:GLN:HB2	2.40	0.57
14:N:61:DC:H2'	14:N:62:DA:C8	2.40	0.57
1:A:93:VAL:HA	1:A:96:ILE:HD12	1.86	0.57
1:A:436:ILE:HD11	1:A:491:VAL:HG11	1.85	0.57
1:A:344:ARG:CD	2:B:1118:PRO:O	2.47	0.57
13:M:269:ILE:HG23	13:M:272:LYS:CG	2.33	0.57
13:M:310:LYS:HE3	13:M:342:VAL:CG2	2.32	0.57
13:M:329:ILE:HG23	13:M:329:ILE:O	2.05	0.57
13:M:334:VAL:CA	13:M:338:ASN:HD21	2.17	0.57
17:Q:356:TRP:CB	17:Q:391:THR:C	2.74	0.57
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.87	0.57
8:H:44:VAL:HG13	8:H:48:PRO:HA	1.87	0.57
2:B:313:MET:HE2	2:B:386:LEU:HD22	1.87	0.57
6:F:105:ALA:HB2	7:G:15:PRO:CB	2.34	0.57
13:M:334:VAL:HA	13:M:338:ASN:OD1	2.05	0.57
2:B:542:MET:HE1	2:B:743:ILE:HD12	1.87	0.56
4:D:52:LEU:HB3	4:D:148:LEU:HD23	1.85	0.56
13:M:288:LEU:CG	13:M:339:LEU:HD21	2.30	0.56
20:T:50:DT:H2''	20:T:51:DA:H5'	1.87	0.56
1:A:1390:ASN:O	1:A:1399:ARG:HD3	2.04	0.56
2:B:519:TRP:HZ2	2:B:705:MET:HE1	1.70	0.56
13:M:284:LEU:HD11	13:M:339:LEU:HD22	1.87	0.56
21:U:140:LEU:CB	21:U:141:LYS:HA	2.35	0.56
2:B:65:GLU:OE1	2:B:247:GLY:HA2	2.04	0.56
2:B:226:PHE:HA	2:B:395:GLN:HG3	1.87	0.56
2:B:911:ILE:HG22	2:B:912:ILE:HG13	1.87	0.56
13:M:263:CYS:SG	13:M:316:LEU:HG	2.45	0.56
13:M:284:LEU:HD12	13:M:339:LEU:CD2	2.36	0.56
13:M:290:GLN:O	13:M:292:PRO:HD3	2.05	0.56
1:A:228:PHE:CZ	4:D:12:ARG:CZ	2.78	0.56
2:B:792:MET:CE	20:T:21:DT:P	2.94	0.56
13:M:324:VAL:HG21	13:M:328:LEU:CD2	2.36	0.56
8:H:89:LEU:C	8:H:91:ASP:H	2.14	0.56
11:K:57:LEU:HB2	11:K:76:GLN:HG2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:248:LEU:HD23	13:M:291:ILE:HD11	1.85	0.56
17:Q:355:THR:O	17:Q:392:ALA:CB	2.53	0.56
1:A:346:ASP:HB3	2:B:1108:ARG:H	1.70	0.56
1:A:419:LYS:CB	13:M:47:LEU:O	2.48	0.56
6:F:99:LEU:HD21	7:G:65:ASP:C	2.31	0.56
13:M:276:THR:O	13:M:280:VAL:HG13	2.06	0.56
1:A:74:MET:O	2:B:1116:ARG:NH2	2.39	0.56
1:A:388:LEU:HA	1:A:391:LEU:HD12	1.88	0.56
1:A:417:TYR:HE2	13:M:37:ARG:CG	2.18	0.56
1:A:418:SER:CA	13:M:48:CYS:O	2.53	0.56
13:M:242:PHE:CD2	13:M:302:LEU:HG	2.41	0.56
13:M:242:PHE:CZ	13:M:302:LEU:HA	2.40	0.56
26:Z:28:THR:HA	26:Z:29:THR:C	2.31	0.56
1:A:768:GLN:HG2	1:A:816:HIS:HA	1.88	0.56
2:B:54:PHE:HA	2:B:58:THR:HB	1.88	0.56
13:M:305:THR:CG2	13:M:308:THR:HG23	2.36	0.56
13:M:266:ILE:HD12	13:M:268:GLU:HB2	1.88	0.55
13:M:295:ALA:HA	13:M:298:VAL:HG12	1.87	0.55
1:A:5:GLN:HG3	2:B:1175:LEU:CD1	2.35	0.55
1:A:416:ARG:HH22	13:M:40:GLU:HG2	1.71	0.55
2:B:1217:TYR:HB2	4:D:13:ARG:NH2	2.21	0.55
13:M:334:VAL:HA	13:M:338:ASN:CG	2.30	0.55
23:W:234:GLU:HA	23:W:237:GLY:H	1.71	0.55
1:A:67:CYS:SG	1:A:77:CYS:SG	3.04	0.55
2:B:121:ASN:HA	2:B:207:GLY:HA3	1.87	0.55
2:B:789:MET:HE2	2:B:953:LEU:CD2	2.36	0.55
2:B:1124:ARG:HD3	13:M:61:SER:HB3	1.87	0.55
4:D:188:ALA:HB2	4:D:208:GLU:HG3	1.87	0.55
23:W:653:THR:O	23:W:657:ALA:N	2.39	0.55
1:A:993:LEU:HD22	1:A:1046:LEU:HD22	1.88	0.55
6:F:89:GLU:O	6:F:93:ILE:HD12	2.06	0.55
1:A:257:ARG:HH11	1:A:257:ARG:HB2	1.71	0.55
1:A:608:ILE:HD12	1:A:613:ILE:HD13	1.89	0.55
1:A:1015:VAL:HG13	1:A:1019:CYS:SG	2.47	0.55
3:C:260:LEU:HD13	25:Y:14:PRO:CB	2.37	0.55
13:M:273:SER:HB2	13:M:274:PRO:HD2	1.86	0.55
13:M:279:VAL:HB	13:M:302:LEU:CD2	2.27	0.55
1:A:18:GLN:HG2	1:A:1418:LEU:HD13	1.89	0.55
1:A:64:ASN:H	1:A:74:MET:HE1	1.72	0.55
1:A:228:PHE:HZ	4:D:12:ARG:NH2	2.03	0.55
13:M:284:LEU:HD12	13:M:339:LEU:HD22	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:LYS:HZ2	1:A:1415:SER:CB	2.20	0.55
1:A:344:ARG:CA	2:B:1128:LEU:O	2.55	0.55
6:F:100:GLN:NE2	7:G:66:GLY:O	2.37	0.55
6:F:109:VAL:HG23	6:F:127:GLU:OE1	2.07	0.55
10:J:1:MET:HB2	10:J:56:LEU:HB2	1.89	0.55
13:M:272:LYS:HE3	20:T:53:DA:OP1	2.06	0.55
13:M:304:VAL:HG12	13:M:305:THR:H	1.72	0.55
1:A:10:PRO:HG2	2:B:1192:TYR:HA	1.89	0.55
1:A:497:THR:HG23	2:B:1146:PHE:HA	1.89	0.55
2:B:486:TYR:HB3	2:B:1096:ARG:NH2	2.22	0.55
13:M:279:VAL:HA	13:M:302:LEU:HD22	1.88	0.55
13:M:294:THR:H	13:M:297:LYS:CD	2.20	0.55
2:B:280:ILE:HD13	2:B:334:ILE:HG12	1.89	0.55
10:J:3:VAL:HG11	10:J:18:TRP:HB2	1.88	0.55
1:A:228:PHE:CZ	4:D:14:ARG:HA	2.42	0.54
2:B:952:VAL:HG22	2:B:966:VAL:HG13	1.88	0.54
6:F:105:ALA:HB2	7:G:15:PRO:HB3	1.89	0.54
10:J:48:ARG:HE	10:J:49:MET:CE	2.20	0.54
23:W:312:ILE:HA	23:W:315:SER:CB	2.36	0.54
1:A:1349:TYR:HA	1:A:1372:VAL:HG21	1.90	0.54
2:B:217:ARG:NH1	2:B:407:ASP:OD1	2.40	0.54
2:B:1100:ASP:OD2	11:K:1:MET:HB3	2.08	0.54
15:O:169:PRO:HG2	15:O:240:MET:SD	2.47	0.54
2:B:405:ARG:NH2	2:B:629:ASP:OD2	2.40	0.54
3:C:85:ASP:CG	25:Y:146:THR:CB	2.72	0.54
17:Q:394:ASN:CB	17:Q:395:LYS:CA	2.86	0.54
4:D:35:LEU:HA	4:D:47:LEU:HB2	1.90	0.54
13:M:237:THR:HG23	13:M:238:TYR:N	2.21	0.54
13:M:269:ILE:HG22	13:M:269:ILE:O	2.06	0.54
1:A:418:SER:CB	13:M:48:CYS:O	2.55	0.54
5:E:94:LYS:HE2	5:E:98:ILE:HD11	1.90	0.54
1:A:22:PHE:CB	2:B:1211:ASN:CG	2.78	0.54
1:A:42:ASP:OD1	1:A:46:THR:N	2.41	0.54
2:B:338:GLY:CA	2:B:339:THR:HB	2.38	0.54
6:F:118:LEU:O	6:F:122:MET:HG3	2.06	0.54
13:M:58:ASP:O	13:M:62:GLU:HB2	2.08	0.54
13:M:268:GLU:HG2	13:M:316:LEU:HA	1.89	0.54
13:M:272:LYS:HD2	20:T:52:DC:H3'	1.89	0.54
1:A:666:ILE:HD11	2:B:1030:LEU:HD13	1.90	0.54
6:F:79:ARG:HG2	6:F:144:GLU:HB3	1.88	0.54
6:F:99:LEU:HD21	7:G:64:THR:C	2.33	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:75:ASP:HB3	13:M:78:ARG:HB3	1.89	0.54
13:M:243:CYS:HB3	13:M:253:THR:HG22	1.89	0.54
25:Y:48:ASN:O	25:Y:49:LEU:C	2.51	0.54
1:A:411:ASP:CG	13:M:50:LEU:HD11	2.33	0.54
2:B:356:LEU:HA	2:B:360:PHE:HB3	1.89	0.54
13:M:254:THR:CG2	13:M:258:TYR:HE2	2.19	0.54
1:A:33:ALA:HA	1:A:57:ARG:HD3	1.89	0.54
1:A:338:GLY:HA2	2:B:1129:ARG:NH2	2.23	0.54
1:A:1376:THR:HG23	5:E:212:ARG:HH22	1.72	0.54
1:A:1397:LEU:HB3	1:A:1429:ILE:HD12	1.90	0.54
1:A:1399:ARG:HB3	1:A:1408:ILE:HD13	1.89	0.54
7:G:153:GLN:O	7:G:155:SER:N	2.41	0.54
13:M:315:ILE:HG22	13:M:316:LEU:HD12	1.88	0.54
1:A:1004:ASN:CG	5:E:167:ARG:HD2	2.33	0.54
5:E:19:VAL:O	5:E:23:VAL:HG23	2.09	0.54
10:J:24:LEU:O	10:J:30:LEU:HB2	2.08	0.54
1:A:34:LYS:H	1:A:57:ARG:HH11	1.55	0.53
1:A:179:LEU:HD13	1:A:297:GLN:HG3	1.91	0.53
1:A:204:THR:HG22	1:A:235:ILE:CG2	2.37	0.53
1:A:320:ARG:HG2	1:A:321:PRO:HD2	1.89	0.53
1:A:338:GLY:HA2	2:B:1129:ARG:HH22	1.73	0.53
1:A:658:LEU:HD23	1:A:659:HIS:NE2	2.23	0.53
3:C:73:GLN:O	3:C:129:ILE:HA	2.08	0.53
2:B:343:ILE:O	2:B:344:LYS:HB2	2.07	0.53
7:G:1:MET:HE1	7:G:79:PHE:HA	1.91	0.53
13:M:236:LEU:HD23	13:M:237:THR:N	2.23	0.53
1:A:541:ILE:HG22	1:A:546:VAL:HG23	1.90	0.53
3:C:37:MET:HE3	3:C:176:ILE:HD13	1.90	0.53
13:M:289:PHE:HA	13:M:331:ASN:OD1	2.07	0.53
1:A:345:VAL:N	2:B:1128:LEU:O	2.39	0.53
1:A:22:PHE:HB2	2:B:1211:ASN:OD1	2.08	0.53
6:F:99:LEU:HD23	7:G:65:ASP:C	2.33	0.53
2:B:1103:ILE:O	2:B:1122:ARG:NH1	2.42	0.53
13:M:286:ILE:HG23	13:M:287:LEU:N	2.24	0.53
1:A:228:PHE:CE1	4:D:15:LEU:HB3	2.44	0.53
13:M:293:ILE:HD11	13:M:297:LYS:C	2.34	0.53
1:A:22:PHE:HB3	2:B:1211:ASN:OD1	2.09	0.53
6:F:132:LEU:CD2	7:G:61:ILE:HD11	2.39	0.53
13:M:249:PRO:HD2	13:M:291:ILE:HD11	1.91	0.53
13:M:269:ILE:HG12	13:M:315:ILE:CG2	2.31	0.53
1:A:23:SER:HB2	1:A:233:TRP:CE2	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:ARG:HH22	13:M:81:GLU:HG3	1.74	0.53
1:A:412:ARG:CB	13:M:51:VAL:HG11	2.38	0.53
1:A:1116:LEU:H	1:A:1308:THR:HB	1.73	0.53
1:A:1390:ASN:O	1:A:1399:ARG:CG	2.57	0.53
1:A:1444:MET:HG3	7:G:60:ARG:HA	1.90	0.53
2:B:174:LEU:HD11	2:B:204:ILE:HG13	1.91	0.53
2:B:295:GLY:HA2	2:B:298:LEU:HB2	1.91	0.53
3:C:164:ALA:HA	3:C:167:HIS:O	2.09	0.53
13:M:294:THR:H	13:M:297:LYS:HD2	1.74	0.53
1:A:253:ASN:O	1:A:255:SER:N	2.38	0.53
2:B:438:GLU:HG3	2:B:440:HIS:HB2	1.91	0.53
1:A:12:ARG:NH1	2:B:1218:THR:OG1	2.43	0.52
1:A:340:LEU:HD21	2:B:1199:ALA:HB3	1.91	0.52
2:B:249:ARG:HH12	2:B:418:LYS:CD	2.22	0.52
13:M:312:GLY:O	13:M:316:LEU:HD13	2.09	0.52
1:A:54:ASN:HB3	1:A:247:ARG:HH12	1.74	0.52
1:A:91:PHE:HD2	1:A:179:LEU:O	1.92	0.52
10:J:48:ARG:HE	10:J:49:MET:HE2	1.74	0.52
1:A:357:PRO:HD2	2:B:833:TYR:CZ	2.44	0.52
2:B:510:LYS:HB2	2:B:513:GLN:OE1	2.08	0.52
2:B:815:ARG:HG3	2:B:815:ARG:HH11	1.72	0.52
13:M:317:TYR:HE1	13:M:339:LEU:HB2	1.73	0.52
1:A:982:THR:HB	1:A:985:ASP:H	1.73	0.52
1:A:1108:ALA:HA	14:N:63:DC:OP1	2.09	0.52
1:A:1172:LEU:C	1:A:1174:PHE:H	2.16	0.52
2:B:291:ILE:HD12	2:B:291:ILE:H	1.74	0.52
13:M:298:VAL:HG13	13:M:299:GLY:N	2.24	0.52
15:O:69:ASN:HB2	20:T:48:DT:C4'	2.40	0.52
13:M:310:LYS:HE3	13:M:342:VAL:O	2.09	0.52
7:G:15:PRO:HD3	7:G:67:SER:HA	1.92	0.52
1:A:831:THR:HG23	20:T:15:DA:C4	2.45	0.52
2:B:773:MET:CE	2:B:985:GLY:HA2	2.40	0.52
2:B:1122:ARG:HB2	20:T:19:DT:OP1	2.10	0.52
15:O:69:ASN:CB	20:T:48:DT:O4'	2.54	0.52
2:B:449:ASN:HD22	13:M:135:MET:HG3	1.72	0.52
13:M:266:ILE:HG13	13:M:268:GLU:H	1.75	0.52
1:A:446:ARG:HD2	1:A:480:ALA:HB2	1.92	0.52
1:A:494:SER:HB3	1:A:497:THR:OG1	2.10	0.52
2:B:90:ILE:HD11	2:B:134:LYS:HE2	1.91	0.52
1:A:33:ALA:HB2	1:A:57:ARG:HB2	1.90	0.52
1:A:228:PHE:HZ	4:D:14:ARG:HA	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1431:GLY:HA3	2:B:1197:PRO:HD3	1.91	0.52
4:D:198:LEU:O	4:D:200:ASN:N	2.44	0.52
1:A:418:SER:OG	13:M:48:CYS:O	2.25	0.51
1:A:832:ALA:HB2	20:T:15:DA:H8	1.74	0.51
1:A:870:GLU:HB2	5:E:204:THR:CG2	2.40	0.51
3:C:52:GLU:HA	12:L:64:LEU:HD22	1.91	0.51
5:E:156:LEU:HD11	5:E:197:LYS:HB2	1.90	0.51
1:A:940:ARG:HB3	1:A:941:LYS:HE2	1.92	0.51
1:A:1095:THR:HG23	1:A:1113:THR:HG23	1.92	0.51
6:F:73:ALA:HB2	6:F:143:PHE:CZ	2.45	0.51
13:M:157:CYS:HB3	13:M:210:MET:HE2	1.92	0.51
13:M:271:GLY:HA3	20:T:52:DC:H5''	1.92	0.51
14:N:22:DT:H2''	14:N:23:DA:H5'	1.93	0.51
1:A:412:ARG:CB	13:M:51:VAL:CG1	2.88	0.51
1:A:646:PHE:O	1:A:650:GLN:HG2	2.10	0.51
2:B:710:LEU:HA	2:B:733:HIS:HB3	1.93	0.51
11:K:49:GLU:HG3	11:K:94:ILE:CG1	2.40	0.51
13:M:246:LEU:CD1	13:M:282:ILE:HG21	2.40	0.51
13:M:249:PRO:HD3	13:M:291:ILE:CD1	2.39	0.51
13:M:269:ILE:CG2	13:M:272:LYS:HG2	2.35	0.51
1:A:1149:ALA:HB2	9:I:47:GLU:HA	1.92	0.51
2:B:451:LYS:HZ2	13:M:147:LYS:NZ	2.08	0.51
6:F:134:ILE:HG22	6:F:136:ARG:HG3	1.91	0.51
11:K:5:ASP:HB3	11:K:7:PHE:CE2	2.45	0.51
13:M:334:VAL:O	13:M:334:VAL:HG23	2.10	0.51
13:M:342:VAL:CG1	13:M:343:GLU:N	2.74	0.51
1:A:67:CYS:C	1:A:68:GLN:HG3	2.34	0.51
1:A:228:PHE:CE1	4:D:14:ARG:C	2.88	0.51
1:A:472:LEU:O	1:A:475:THR:HB	2.10	0.51
2:B:1217:TYR:CZ	4:D:13:ARG:HB2	2.45	0.51
1:A:1444:MET:HB2	6:F:133:VAL:HG12	1.92	0.51
2:B:471:LYS:HG2	13:M:95:ARG:NH2	2.26	0.51
7:G:1:MET:SD	7:G:2:PHE:N	2.62	0.51
5:E:64:PRO:HB2	5:E:69:ILE:HD11	1.93	0.51
23:W:653:THR:O	23:W:656:ASN:N	2.44	0.51
2:B:238:ALA:HB3	2:B:256:VAL:HB	1.93	0.51
13:M:320:ARG:HG3	13:M:321:ASP:N	2.26	0.51
5:E:15:ALA:O	5:E:19:VAL:HG23	2.10	0.51
1:A:412:ARG:HB3	13:M:51:VAL:HG12	1.92	0.51
1:A:67:CYS:O	1:A:70:CYS:HB3	2.11	0.50
2:B:530:GLY:O	2:B:532:ALA:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1201:LYS:HD3	2:B:1205:GLN:OE1	2.11	0.50
13:M:283:TYR:CE2	13:M:287:LEU:CD1	2.94	0.50
1:A:417:TYR:HE2	13:M:37:ARG:CD	2.22	0.50
2:B:70:ILE:HG22	2:B:89:GLU:HG2	1.93	0.50
11:K:55:LYS:HB3	11:K:81:TYR:CD2	2.45	0.50
13:M:333:VAL:HG12	13:M:333:VAL:O	2.11	0.50
14:N:23:DA:N6	20:T:51:DA:N6	2.60	0.50
20:T:19:DT:H2'	20:T:20:DA:C8	2.46	0.50
24:X:83:LYS:O	24:X:84:PRO:C	2.55	0.50
2:B:60:GLN:OE1	2:B:95:ILE:HG22	2.12	0.50
2:B:373:ARG:HG2	2:B:566:LEU:HD23	1.92	0.50
13:M:306:GLU:O	13:M:309:ILE:HG12	2.12	0.50
20:T:51:DA:H2''	20:T:52:DC:C5	2.47	0.50
1:A:55:ASP:HA	1:A:58:LEU:H	1.76	0.50
1:A:343:LYS:HB2	2:B:1117:GLN:OE1	2.11	0.50
13:M:237:THR:CG2	13:M:238:TYR:CD2	2.95	0.50
1:A:714:PHE:O	1:A:718:VAL:HG23	2.12	0.50
1:A:919:ILE:HG12	1:A:983:ILE:HD13	1.94	0.50
2:B:701:ILE:HD11	2:B:703:ILE:HD11	1.94	0.50
2:B:806:THR:HB	2:B:809:MET:HG3	1.94	0.50
2:B:1008:PRO:HB3	2:B:1087:PHE:HE1	1.77	0.50
4:D:126:ILE:HD13	4:D:145:MET:HE3	1.93	0.50
13:M:254:THR:CG2	13:M:258:TYR:CE2	2.94	0.50
13:M:263:CYS:HA	13:M:266:ILE:HG12	1.94	0.50
1:A:228:PHE:HE1	4:D:15:LEU:HB3	1.77	0.50
1:A:347:PHE:H	2:B:1107:ALA:HA	1.77	0.50
8:H:17:PRO:HB3	8:H:24:CYS:SG	2.52	0.50
2:B:1072:MET:HB3	2:B:1081:LEU:HD12	1.94	0.50
14:N:26:DT:H4'	15:O:158:GLN:O	2.12	0.50
15:O:71:VAL:HG21	20:T:47:DA:H2	1.77	0.50
4:D:118:THR:HG21	4:D:121:LYS:HE3	1.94	0.50
1:A:12:ARG:O	2:B:1194:ILE:HG22	2.12	0.49
1:A:245:PRO:O	2:B:1114:LEU:HD12	2.12	0.49
2:B:211:VAL:HG13	2:B:495:LEU:HD23	1.93	0.49
2:B:684:LEU:HA	2:B:689:LEU:HD12	1.93	0.49
9:I:65:ASP:HB3	9:I:68:LEU:HD12	1.93	0.49
13:M:307:GLY:O	13:M:310:LYS:HB3	2.11	0.49
1:A:40:THR:HG21	1:A:259:GLU:OE2	2.12	0.49
1:A:275:SER:OG	13:M:117:ASN:OD1	2.24	0.49
1:A:1436:ILE:HD13	2:B:1139:ILE:HG23	1.93	0.49
2:B:948:ILE:HD13	12:L:67:PHE:HE2	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:26:DT:H1'	15:O:159:ASN:HB2	1.93	0.49
1:A:1095:THR:HG21	1:A:1112:LYS:HB2	1.93	0.49
1:A:1312:ASN:O	1:A:1316:VAL:HG23	2.12	0.49
1:A:1348:LEU:O	1:A:1352:VAL:HG23	2.11	0.49
3:C:114:TYR:HB2	3:C:116:LYS:HG2	1.94	0.49
13:M:262:LYS:O	13:M:266:ILE:HG23	2.13	0.49
1:A:228:PHE:HE1	4:D:14:ARG:C	2.20	0.49
2:B:899:ILE:HD11	2:B:911:ILE:HA	1.94	0.49
2:B:1135:ARG:HG2	2:B:1139:ILE:HD11	1.94	0.49
4:D:173:HIS:CG	4:D:174:PRO:HD2	2.47	0.49
1:A:497:THR:CG2	2:B:1146:PHE:HD1	2.23	0.49
7:G:1:MET:HE3	7:G:80:LYS:H	1.76	0.49
13:M:249:PRO:HG2	13:M:252:VAL:HG23	1.94	0.49
13:M:283:TYR:CE1	13:M:287:LEU:HD11	2.47	0.49
15:O:171:ARG:HG3	15:O:239:LYS:HD3	1.95	0.49
1:A:89:PRO:HB2	1:A:204:THR:HB	1.93	0.49
1:A:418:SER:N	13:M:49:GLY:HA3	2.28	0.49
2:B:338:GLY:HA2	2:B:339:THR:HB	1.93	0.49
13:M:196:ILE:HG13	13:M:197:HIS:HB3	1.92	0.49
13:M:234:GLN:HB2	13:M:236:LEU:HD22	1.91	0.49
19:S:165:THR:CB	19:S:168:LYS:H	2.26	0.49
1:A:1193:LEU:HB2	1:A:1260:LEU:CD2	2.42	0.49
2:B:35:SER:HA	2:B:811:TYR:HE1	1.77	0.49
2:B:249:ARG:NH1	2:B:418:LYS:CD	2.76	0.49
1:A:216:VAL:O	1:A:220:THR:HB	2.12	0.49
2:B:574:SER:HB3	2:B:591:ARG:HE	1.77	0.49
2:B:693:ILE:HG21	2:B:701:ILE:HD13	1.95	0.49
4:D:144:THR:HG21	7:G:46:LEU:HD13	1.93	0.49
13:M:237:THR:HG23	13:M:238:TYR:CD2	2.48	0.49
1:A:228:PHE:HE2	4:D:12:ARG:NH1	1.99	0.49
1:A:1402:PHE:CE1	1:A:1403:GLU:HG3	2.48	0.49
2:B:104:GLU:CD	12:L:54:ARG:NE	2.71	0.49
13:M:276:THR:HA	13:M:279:VAL:HG12	1.94	0.49
1:A:418:SER:HA	13:M:49:GLY:N	2.27	0.48
2:B:451:LYS:NZ	13:M:138:ASP:OD2	2.40	0.48
3:C:75:MET:HB3	3:C:128:ASN:HB3	1.95	0.48
4:D:118:THR:O	4:D:120:GLU:N	2.42	0.48
6:F:100:GLN:HE22	7:G:61:ILE:HG21	1.77	0.48
2:B:62:ILE:HG21	2:B:417:PHE:HD2	1.78	0.48
8:H:80:ARG:HG2	11:K:57:LEU:HD22	1.95	0.48
13:M:294:THR:OG1	13:M:297:LYS:HG2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:ASP:OD1	1:A:328:ARG:NH2	2.42	0.48
1:A:1279:ILE:HG23	1:A:1308:THR:HG23	1.96	0.48
2:B:449:ASN:HD21	13:M:135:MET:HG3	1.75	0.48
2:B:705:MET:H	2:B:710:LEU:HD12	1.79	0.48
3:C:116:LYS:HD3	3:C:140:ASN:HA	1.93	0.48
8:H:40:LEU:HD13	8:H:123:MET:HG3	1.96	0.48
15:O:68:GLN:O	20:T:48:DT:H4'	2.12	0.48
1:A:11:LEU:HA	2:B:1193:GLN:HG2	1.95	0.48
2:B:640:VAL:HG22	2:B:651:LEU:HG	1.95	0.48
3:C:99:LEU:HB2	3:C:157:CYS:HB2	1.94	0.48
13:M:286:ILE:HG13	13:M:291:ILE:O	2.13	0.48
1:A:261:ASP:HB3	1:A:322:VAL:HG13	1.95	0.48
2:B:441:ASP:O	2:B:443:ASN:N	2.47	0.48
2:B:1113:VAL:HG22	13:M:57:VAL:HG11	1.96	0.48
6:F:100:GLN:NE2	7:G:61:ILE:HG21	2.29	0.48
13:M:246:LEU:HD22	13:M:293:ILE:HG13	1.96	0.48
19:S:23:ARG:H	19:S:26:ASN:CB	2.27	0.48
1:A:1116:LEU:HG	1:A:1327:ILE:HD11	1.95	0.48
2:B:451:LYS:NZ	13:M:147:LYS:NZ	2.61	0.48
13:M:250:MET:HG3	13:M:251:GLN:N	2.27	0.48
2:B:486:TYR:HB3	2:B:1096:ARG:NE	2.28	0.48
4:D:130:LEU:O	4:D:134:THR:HG22	2.13	0.48
4:D:168:LYS:HD2	4:D:168:LYS:HA	1.53	0.48
13:M:72:ASN:ND2	13:M:74:ASP:OD2	2.47	0.48
13:M:234:GLN:HB2	13:M:236:LEU:HD21	1.91	0.48
1:A:71:GLN:O	1:A:73:GLY:N	2.47	0.48
1:A:257:ARG:HB2	1:A:257:ARG:NH1	2.29	0.48
2:B:122:LEU:HD22	2:B:958:GLN:HG2	1.96	0.48
2:B:345:LYS:HA	2:B:348:ARG:HD2	1.96	0.48
2:B:542:MET:HG3	2:B:747:MET:HB3	1.96	0.48
2:B:840:ILE:HG21	2:B:994:TYR:HD2	1.79	0.48
13:M:259:THR:HG23	13:M:323:LEU:CB	2.30	0.48
13:M:280:VAL:O	13:M:283:TYR:HB3	2.14	0.48
1:A:832:ALA:CB	20:T:15:DA:C8	2.97	0.48
12:L:27:LEU:HD13	12:L:37:LYS:HG2	1.95	0.48
15:O:171:ARG:HD3	15:O:238:ARG:O	2.14	0.48
1:A:929:LEU:HD21	1:A:983:ILE:HG21	1.96	0.48
2:B:473:MET:SD	13:M:72:ASN:OD1	2.72	0.48
2:B:705:MET:HE2	2:B:745:PRO:HB3	1.94	0.48
5:E:176:PRO:O	5:E:212:ARG:HA	2.14	0.48
13:M:285:ASN:O	13:M:288:LEU:HB2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:SER:O	1:A:279:LEU:HD12	2.14	0.47
1:A:1450:LEU:HD21	7:G:18:PHE:O	2.15	0.47
2:B:219:ALA:HB2	2:B:405:ARG:HG2	1.95	0.47
8:H:115:TYR:CE1	8:H:124:ARG:HG3	2.49	0.47
13:M:136:LEU:HD21	13:M:196:ILE:HG22	1.96	0.47
1:A:89:PRO:HB2	1:A:204:THR:CB	2.44	0.47
1:A:154:SER:HB3	1:A:162:VAL:HG23	1.95	0.47
1:A:448:PRO:O	1:A:449:SER:CB	2.63	0.47
2:B:951:GLN:OE1	12:L:57:LEU:CD2	2.62	0.47
2:B:977:GLY:HA3	2:B:1099:VAL:HB	1.95	0.47
13:M:250:MET:HE2	13:M:251:GLN:NE2	2.30	0.47
15:O:170:ILE:HD13	15:O:234:LEU:HD22	1.96	0.47
1:A:132:LYS:HZ2	1:A:1415:SER:HB3	1.79	0.47
1:A:285:PRO:O	1:A:287:HIS:N	2.46	0.47
1:A:419:LYS:HE3	13:M:48:CYS:CA	2.44	0.47
1:A:831:THR:HG23	20:T:15:DA:C6	2.49	0.47
1:A:875:ALA:HB2	1:A:1366:ARG:HD2	1.95	0.47
1:A:1445:ILE:HG13	7:G:61:ILE:CG1	2.45	0.47
2:B:792:MET:CE	20:T:21:DT:OP1	2.57	0.47
3:C:38:ILE:HG13	3:C:176:ILE:HD12	1.95	0.47
7:G:118:ASP:OD1	7:G:118:ASP:N	2.42	0.47
13:M:196:ILE:HA	13:M:197:HIS:HA	1.65	0.47
1:A:280:GLU:HG2	1:A:289:ILE:HD13	1.96	0.47
3:C:58:LEU:HD21	10:J:57:ILE:HD12	1.97	0.47
4:D:8:PHE:CD2	7:G:6:ASP:HB2	2.45	0.47
12:L:68:GLU:HB2	12:L:70:ARG:HD2	1.96	0.47
13:M:271:GLY:O	20:T:52:DC:C4'	2.62	0.47
13:M:311:SER:HA	13:M:314:LYS:CD	2.44	0.47
13:M:335:SER:H	13:M:338:ASN:CG	2.23	0.47
14:N:24:DT:H3'	14:N:24:DT:H6	1.79	0.47
16:P:7:A:H2'	16:P:8:U:O4'	2.14	0.47
8:H:23:VAL:HG11	8:H:121:LEU:HD22	1.95	0.47
11:K:63:VAL:HG12	11:K:71:PHE:HB3	1.96	0.47
13:M:289:PHE:CD2	13:M:290:GLN:N	2.82	0.47
1:A:475:THR:HG21	2:B:836:GLU:OE2	2.14	0.47
1:A:1345:ARG:HG3	1:A:1376:THR:HG21	1.96	0.47
4:D:138:ASN:ND2	7:G:35:GLU:HG2	2.30	0.47
6:F:132:LEU:HD21	7:G:61:ILE:CD1	2.45	0.47
10:J:9:SER:HB2	10:J:45:CYS:HB2	1.95	0.47
13:M:306:GLU:CA	13:M:309:ILE:HG12	2.43	0.47
2:B:193:LYS:NZ	12:L:32:ALA:O	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:293:ILE:HD13	13:M:294:THR:N	2.29	0.47
20:T:50:DT:H3'	20:T:50:DT:H6	1.79	0.47
1:A:270:LEU:HD12	1:A:270:LEU:HA	1.69	0.47
1:A:568:PRO:HG2	8:H:46:LEU:HD12	1.95	0.47
1:A:832:ALA:HA	20:T:15:DA:C1'	2.45	0.47
2:B:901:PRO:HG2	12:L:60:ARG:HA	1.97	0.47
3:C:100:THR:HG22	3:C:119:VAL:HG22	1.97	0.47
13:M:293:ILE:CD1	13:M:297:LYS:CG	2.93	0.47
20:T:49:DA:C2'	20:T:50:DT:C5'	2.86	0.47
1:A:836:TYR:CE2	1:A:840:ARG:HD2	2.50	0.47
1:A:956:LEU:HD21	1:A:1017:LEU:HG	1.96	0.47
9:I:102:VAL:HG22	9:I:109:ILE:HG12	1.98	0.47
24:X:237:GLN:O	24:X:243:ASN:HA	2.15	0.47
1:A:353:ILE:HG21	1:A:487:MET:HE3	1.96	0.46
1:A:1345:ARG:HG2	1:A:1372:VAL:CG1	2.45	0.46
2:B:662:MET:HA	2:B:665:GLU:HB2	1.97	0.46
2:B:849:GLY:HA2	2:B:852:ARG:CD	2.39	0.46
4:D:7:THR:OG1	4:D:8:PHE:N	2.48	0.46
7:G:138:THR:HG22	7:G:139:ILE:H	1.80	0.46
9:I:106:CYS:SG	9:I:108:HIS:HB3	2.55	0.46
20:T:19:DT:H2'	20:T:20:DA:H8	1.80	0.46
1:A:709:THR:HG22	1:A:711:ARG:H	1.80	0.46
25:Y:66:GLY:C	25:Y:68:GLN:N	2.70	0.46
1:A:738:LYS:HA	8:H:19:ARG:HH12	1.79	0.46
4:D:40:HIS:CE1	7:G:73:LYS:HB3	2.51	0.46
13:M:186:ALA:HB1	13:M:237:THR:HG1	1.74	0.46
13:M:298:VAL:CG2	13:M:302:LEU:HD13	2.36	0.46
14:N:22:DT:H2'	14:N:23:DA:H5'	1.96	0.46
1:A:91:PHE:CD2	1:A:179:LEU:O	2.68	0.46
1:A:95:PHE:O	1:A:97:ALA:N	2.49	0.46
1:A:132:LYS:NZ	1:A:1415:SER:HB3	2.30	0.46
1:A:253:ASN:C	1:A:255:SER:H	2.22	0.46
6:F:99:LEU:CD2	7:G:66:GLY:N	2.78	0.46
7:G:1:MET:HE2	7:G:3:PHE:CD2	2.51	0.46
7:G:127:PRO:HD2	7:G:138:THR:HG21	1.96	0.46
13:M:237:THR:CG2	13:M:238:TYR:CE2	2.98	0.46
1:A:7:SER:HG	2:B:1161:HIS:CE1	2.22	0.46
1:A:34:LYS:N	1:A:57:ARG:HH11	2.13	0.46
2:B:258:LEU:HB2	2:B:385:LEU:HD21	1.96	0.46
7:G:1:MET:CE	7:G:2:PHE:H	2.27	0.46
13:M:272:LYS:HB2	13:M:277:ILE:HD11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:305:THR:HG22	13:M:308:THR:OG1	2.15	0.46
17:Q:355:THR:C	17:Q:392:ALA:HB1	2.39	0.46
17:Q:394:ASN:H	17:Q:395:LYS:HA	1.79	0.46
20:T:47:DA:C8	20:T:48:DT:C4	3.02	0.46
6:F:105:ALA:HB2	7:G:15:PRO:HB2	1.97	0.46
1:A:56:PRO:O	1:A:57:ARG:HG3	2.16	0.46
1:A:93:VAL:HG13	1:A:301:ALA:HB1	1.97	0.46
1:A:228:PHE:CE1	4:D:14:ARG:O	2.68	0.46
1:A:579:SER:HA	1:A:582:ILE:HG13	1.97	0.46
1:A:745:GLN:HA	1:A:748:MET:HE3	1.98	0.46
1:A:1446:ASP:HB3	1:A:1449:SER:OG	2.15	0.46
2:B:108:VAL:HG13	13:M:240:PRO:CB	2.42	0.46
2:B:756:ILE:O	2:B:759:PRO:HD3	2.15	0.46
3:C:18:VAL:HG12	3:C:20:PHE:HD1	1.81	0.46
8:H:30:SER:HB3	8:H:36:CYS:HB3	1.98	0.46
13:M:85:PRO:HA	13:M:89:GLY:O	2.15	0.46
13:M:193:GLN:HG2	13:M:198:VAL:HG12	1.96	0.46
13:M:276:THR:O	13:M:279:VAL:HG12	2.15	0.46
13:M:289:PHE:CG	13:M:290:GLN:N	2.82	0.46
1:A:58:LEU:HD22	1:A:80:HIS:O	2.16	0.46
1:A:78:PRO:C	2:B:1201:LYS:NZ	2.69	0.46
1:A:1074:GLU:O	1:A:1077:THR:HB	2.16	0.46
7:G:13:LEU:HA	7:G:13:LEU:HD23	1.64	0.46
1:A:227:VAL:HG13	4:D:16:LYS:HE3	1.98	0.46
2:B:291:ILE:HD12	2:B:291:ILE:N	2.30	0.46
2:B:951:GLN:CD	12:L:57:LEU:HD22	2.41	0.46
3:C:8:VAL:HG11	11:K:105:PHE:HD1	1.80	0.46
3:C:165:LYS:O	11:K:6:ARG:NH1	2.46	0.46
5:E:65:THR:O	5:E:69:ILE:HD12	2.16	0.46
1:A:565:ILE:O	1:A:570:PRO:HA	2.16	0.46
1:A:923:LEU:O	1:A:927:VAL:HG23	2.16	0.46
1:A:1428:VAL:HG13	2:B:1151:LEU:CD2	2.46	0.46
2:B:471:LYS:HE3	13:M:95:ARG:HE	1.80	0.46
2:B:800:GLN:HB2	2:B:821:GLN:HA	1.96	0.46
13:M:242:PHE:CD1	13:M:302:LEU:HA	2.50	0.46
2:B:468:GLU:HG2	2:B:469:GLN:HB2	1.99	0.45
13:M:258:TYR:O	13:M:261:LYS:HG2	2.17	0.45
13:M:293:ILE:CD1	13:M:298:VAL:N	2.79	0.45
14:N:24:DT:H2'	14:N:25:DA:C8	2.51	0.45
15:O:239:LYS:O	15:O:240:MET:HG3	2.16	0.45
1:A:11:LEU:HD13	2:B:1195:HIS:NE2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:HIS:O	1:A:401:GLY:N	2.48	0.45
9:I:72:ASP:O	9:I:81:ARG:HG2	2.16	0.45
25:Y:4:SER:HA	25:Y:155:LEU:O	2.16	0.45
2:B:64:CYS:HA	2:B:67:SER:HB3	1.98	0.45
2:B:365:THR:HG21	2:B:370:PHE:CG	2.51	0.45
4:D:39:ASN:ND2	4:D:43:GLU:OE2	2.49	0.45
7:G:49:LEU:HD21	7:G:77:VAL:HG23	1.99	0.45
7:G:119:LEU:HD21	7:G:137:ILE:HD12	1.97	0.45
13:M:282:ILE:O	13:M:286:ILE:HG22	2.16	0.45
1:A:420:ARG:CZ	24:X:174:ALA:CB	2.91	0.45
1:A:567:LYS:HA	1:A:568:PRO:C	2.41	0.45
2:B:1185:CYS:CA	4:D:17:LYS:HB2	2.41	0.45
3:C:70:ILE:HD11	3:C:144:ILE:HG12	1.97	0.45
5:E:167:ARG:HD3	5:E:167:ARG:HA	1.78	0.45
7:G:9:LEU:HD22	7:G:34:VAL:HG23	1.98	0.45
13:M:313:TYR:CD2	13:M:343:GLU:N	2.81	0.45
13:M:331:ASN:O	13:M:334:VAL:HG22	2.16	0.45
1:A:883:LEU:HD23	1:A:1021:LEU:HB2	1.97	0.45
1:A:1393:ASN:ND2	1:A:1393:ASN:H	2.15	0.45
2:B:86:ARG:HG2	2:B:138:GLU:HG3	1.98	0.45
2:B:582:VAL:HG22	2:B:626:ILE:HB	1.97	0.45
5:E:90:VAL:HG23	5:E:123:LEU:HD11	1.98	0.45
13:M:254:THR:HG22	13:M:258:TYR:CD2	2.51	0.45
13:M:286:ILE:HD11	13:M:293:ILE:HB	1.98	0.45
15:O:94:TYR:CZ	15:O:96:PRO:HG3	2.52	0.45
6:F:89:GLU:C	6:F:93:ILE:HD12	2.42	0.45
10:J:28:ASP:C	10:J:30:LEU:H	2.24	0.45
13:M:279:VAL:HG21	13:M:309:ILE:HG21	1.99	0.45
1:A:353:ILE:HG22	1:A:468:PHE:HB2	1.98	0.45
1:A:497:THR:HG22	2:B:1146:PHE:CD1	2.41	0.45
1:A:974:ASP:C	1:A:976:THR:H	2.25	0.45
2:B:89:GLU:HB2	2:B:135:ARG:HB2	1.99	0.45
2:B:900:ALA:CB	12:L:61:THR:HG23	2.42	0.45
13:M:248:LEU:HD13	13:M:252:VAL:CG1	2.37	0.45
13:M:269:ILE:CD1	13:M:277:ILE:CD1	2.94	0.45
17:Q:108:LYS:CB	18:R:86:ASN:CB	2.95	0.45
1:A:832:ALA:CB	20:T:15:DA:H8	2.29	0.45
2:B:394:ASP:OD2	9:I:91:ARG:HD2	2.17	0.45
2:B:563:MET:HE3	2:B:580:VAL:HB	1.99	0.45
2:B:803:LEU:HG	10:J:52:THR:HG21	1.98	0.45
13:M:238:TYR:HB3	13:M:242:PHE:HE2	1.75	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:280:VAL:HG11	13:M:312:GLY:HA3	1.98	0.45
14:N:23:DA:N6	20:T:51:DA:H61	2.15	0.45
20:T:47:DA:C5	20:T:48:DT:O4	2.70	0.45
1:A:457:ALA:HB3	1:A:506:ALA:HA	1.97	0.45
1:A:875:ALA:HA	1:A:878:ILE:HD12	1.99	0.45
2:B:1001:PHE:HE2	3:C:178:PHE:HB3	1.81	0.45
6:F:100:GLN:CG	7:G:66:GLY:CA	2.84	0.45
13:M:27:CYS:SG	13:M:48:CYS:HB3	2.57	0.45
13:M:269:ILE:CG2	13:M:272:LYS:CG	2.94	0.45
13:M:289:PHE:CE2	13:M:290:GLN:HG3	2.52	0.45
14:N:25:DA:C8	14:N:25:DA:O5'	2.70	0.45
20:T:55:DA:H2''	20:T:56:DG:C8	2.52	0.45
1:A:180:LYS:CE	1:A:294:SER:HB3	2.46	0.45
1:A:451:HIS:CD2	1:A:1074:GLU:HG3	2.52	0.45
13:M:193:GLN:HG2	13:M:198:VAL:CG1	2.47	0.45
13:M:289:PHE:CD2	13:M:290:GLN:HG3	2.52	0.45
13:M:295:ALA:HB3	13:M:306:GLU:HG3	1.96	0.45
14:N:17:DC:H2''	14:N:18:DT:H71	1.98	0.45
1:A:91:PHE:CB	1:A:96:ILE:CG1	2.90	0.44
1:A:151:ASP:HA	1:A:163:SER:HA	1.99	0.44
5:E:88:VAL:HB	5:E:116:ILE:HG12	1.97	0.44
8:H:93:TYR:HA	8:H:145:ARG:HB3	1.99	0.44
9:I:83:ASN:HA	9:I:104:LEU:HG	1.98	0.44
13:M:279:VAL:HG23	13:M:302:LEU:HD13	1.98	0.44
1:A:42:ASP:O	1:A:44:THR:N	2.50	0.44
1:A:589:GLN:HG2	1:A:606:LEU:HD13	1.99	0.44
1:A:743:VAL:O	1:A:747:VAL:HG23	2.17	0.44
2:B:451:LYS:HE3	13:M:138:ASP:OD2	1.99	0.44
7:G:89:GLY:HA3	7:G:103:VAL:HG22	2.00	0.44
13:M:236:LEU:HD23	13:M:237:THR:H	1.82	0.44
1:A:1154:TYR:CE1	9:I:18:GLU:HG3	2.53	0.44
1:A:1259:MET:HA	1:A:1262:LYS:HD2	1.99	0.44
2:B:792:MET:HE1	20:T:21:DT:P	2.57	0.44
9:I:50:THR:HG22	9:I:52:ILE:H	1.81	0.44
17:Q:394:ASN:N	17:Q:395:LYS:HA	2.29	0.44
1:A:317:LYS:C	2:B:471:LYS:HZ2	2.09	0.44
1:A:337:ARG:NH1	2:B:1132:GLU:OE1	2.49	0.44
1:A:1356:ILE:HG21	1:A:1363:VAL:HG23	1.99	0.44
2:B:233:PRO:HG2	2:B:234:ILE:HD12	1.99	0.44
10:J:1:MET:HE3	10:J:1:MET:HB3	1.87	0.44
13:M:293:ILE:CD1	13:M:297:LYS:CB	2.94	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:52:DC:H1'	20:T:53:DA:H5'	2.00	0.44
1:A:11:LEU:CD1	2:B:1195:HIS:NE2	2.80	0.44
1:A:66:LYS:CE	1:A:68:GLN:H	2.31	0.44
2:B:901:PRO:O	12:L:60:ARG:HA	2.18	0.44
3:C:55:THR:HB	3:C:151:GLN:HA	1.99	0.44
3:C:97:VAL:HG21	3:C:129:ILE:HG23	1.99	0.44
1:A:70:CYS:O	1:A:72:GLU:HG2	2.17	0.44
1:A:1148:ILE:HA	9:I:49:ILE:HD12	2.00	0.44
1:A:1436:ILE:O	2:B:1144:ALA:HB2	2.17	0.44
1:A:1441:PHE:CZ	6:F:89:GLU:HA	2.53	0.44
2:B:102:VAL:HG23	2:B:112:LEU:HD22	2.00	0.44
2:B:1158:PHE:HE2	2:B:1160:VAL:HG13	1.83	0.44
13:M:316:LEU:HD12	13:M:316:LEU:N	2.33	0.44
19:S:195:GLN:O	19:S:199:GLY:N	2.50	0.44
20:T:44:DA:H2'	20:T:45:DT:H71	1.99	0.44
1:A:22:PHE:HB2	2:B:1211:ASN:O	2.18	0.44
1:A:132:LYS:HZ1	1:A:1415:SER:HB2	1.83	0.44
1:A:449:SER:HA	1:A:454:SER:HB3	1.99	0.44
2:B:69:LEU:HD22	2:B:425:THR:HG23	2.00	0.44
2:B:125:SER:HA	2:B:171:PRO:HA	2.00	0.44
14:N:27:DA:H2'	14:N:28:DA:C8	2.52	0.44
20:T:49:DA:H2'	20:T:50:DT:C5'	2.48	0.44
1:A:548:ASN:HD21	11:K:47:ARG:HH21	1.65	0.44
1:A:1348:LEU:HG	1:A:1372:VAL:HG22	2.00	0.44
3:C:11:ARG:HE	3:C:21:ILE:HD11	1.83	0.44
4:D:11:ARG:HD3	4:D:12:ARG:N	2.33	0.44
6:F:92:ARG:HH21	7:G:63:PRO:HG3	1.83	0.44
11:K:65:HIS:HE1	11:K:67:PHE:CG	2.35	0.44
13:M:255:SER:HB3	13:M:285:ASN:CG	2.43	0.44
13:M:269:ILE:CG2	13:M:272:LYS:CB	2.95	0.44
1:A:33:ALA:HB1	1:A:56:PRO:HB2	2.00	0.44
2:B:998:ASP:OD1	3:C:35:ARG:NH2	2.46	0.44
7:G:165:GLU:HG2	7:G:168:LEU:HD12	1.99	0.44
1:A:514:PRO:HG2	1:A:1067:LEU:HD11	1.99	0.43
2:B:935:ARG:H	2:B:935:ARG:HD2	1.83	0.43
4:D:23:ASN:HA	4:D:28:GLN:O	2.18	0.43
4:D:172:LEU:HB3	4:D:176:GLU:OE1	2.18	0.43
13:M:24:CYS:HA	13:M:25:PRO:HD3	1.87	0.43
13:M:340:PRO:C	13:M:342:VAL:H	2.26	0.43
14:N:29:DT:OP1	15:O:120:LYS:HG3	2.18	0.43
1:A:358:ASN:HB2	11:K:65:HIS:HD2	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:407:ARG:HG2	1:A:430:TRP:CZ2	2.53	0.43
1:A:869:GLY:O	5:E:204:THR:HG21	2.18	0.43
2:B:521:LEU:HD22	2:B:633:VAL:HG12	2.01	0.43
8:H:4:THR:HA	8:H:60:ALA:HB2	2.00	0.43
8:H:105:GLU:HB3	8:H:113:ALA:HB3	2.00	0.43
13:M:62:GLU:O	13:M:65:THR:OG1	2.30	0.43
1:A:58:LEU:HB3	1:A:59:GLY:H	1.25	0.43
1:A:1345:ARG:HD2	1:A:1373:ASP:OD1	2.18	0.43
2:B:955:THR:HG22	2:B:956:THR:N	2.34	0.43
2:B:980:PHE:CD1	2:B:1094:ARG:HA	2.54	0.43
13:M:272:LYS:NZ	20:T:53:DA:P	2.91	0.43
20:T:48:DT:H2'	20:T:49:DA:C5	2.54	0.43
1:A:446:ARG:HB2	1:A:487:MET:SD	2.57	0.43
1:A:1323:ASP:CG	1:A:1326:ARG:HG3	2.44	0.43
1:A:1444:MET:HB2	1:A:1444:MET:HE2	1.62	0.43
2:B:860:MET:HE3	2:B:860:MET:HB3	1.86	0.43
13:M:269:ILE:HD13	13:M:277:ILE:CD1	2.48	0.43
1:A:91:PHE:HB3	1:A:96:ILE:CD1	2.48	0.43
1:A:187:LYS:HE3	1:A:198:GLU:HB2	1.99	0.43
1:A:449:SER:HA	1:A:454:SER:CB	2.49	0.43
1:A:875:ALA:HB2	1:A:1366:ARG:CD	2.48	0.43
1:A:1025:ARG:O	1:A:1035:TYR:HE2	2.01	0.43
1:A:1151:GLU:HG2	9:I:45:ARG:HG3	1.98	0.43
2:B:1165:ILE:HG21	4:D:17:LYS:CA	2.24	0.43
6:F:97:ARG:HA	6:F:97:ARG:HD2	1.82	0.43
13:M:263:CYS:CA	13:M:266:ILE:HG12	2.49	0.43
13:M:268:GLU:HG3	13:M:315:ILE:HG12	2.00	0.43
13:M:324:VAL:HG21	13:M:328:LEU:HD22	1.93	0.43
1:A:873:MET:HB3	1:A:878:ILE:HD11	2.01	0.43
1:A:1438:THR:HB	2:B:1142:GLY:O	2.19	0.43
2:B:915:THR:O	2:B:917:PRO:HD3	2.19	0.43
10:J:36:LEU:HD11	10:J:51:LEU:HB2	2.00	0.43
1:A:22:PHE:HD2	2:B:1211:ASN:HA	1.83	0.43
1:A:130:ASP:HB3	1:A:133:LYS:HB2	2.00	0.43
1:A:534:LEU:O	1:A:574:GLY:HA3	2.17	0.43
1:A:994:GLN:HE22	1:A:1023:ARG:HE	1.66	0.43
2:B:802:PRO:HA	2:B:822:ASN:HD21	1.84	0.43
2:B:1143:ALA:HB1	2:B:1146:PHE:HB3	2.01	0.43
1:A:41:MET:HE2	1:A:257:ARG:CZ	2.49	0.43
1:A:306:ASN:O	1:A:313:GLN:HG2	2.19	0.43
1:A:1340:GLY:HA2	5:E:183:PRO:HD2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:202:ILE:HD13	4:D:207:LEU:HB2	2.01	0.43
12:L:49:LYS:O	12:L:50:ASP:HB2	2.19	0.43
13:M:286:ILE:CG2	13:M:287:LEU:N	2.82	0.43
13:M:304:VAL:HG12	13:M:308:THR:OG1	2.19	0.43
1:A:89:PRO:C	1:A:204:THR:HG21	2.43	0.43
1:A:91:PHE:CB	1:A:96:ILE:CD1	2.96	0.43
1:A:339:ASN:HB3	2:B:1117:GLN:HE22	1.84	0.43
1:A:343:LYS:NZ	2:B:1156:ASP:HB2	2.33	0.43
2:B:169:ARG:HB2	2:B:454:THR:HG23	2.01	0.43
2:B:617:ARG:HG3	2:B:624:LEU:HD12	2.00	0.43
8:H:15:VAL:HG22	8:H:26:ILE:HG13	2.00	0.43
15:O:69:ASN:HB2	20:T:48:DT:H5'	2.00	0.43
1:A:413:ILE:HD13	1:A:424:ILE:HD11	2.01	0.43
2:B:171:PRO:HG2	2:B:461:LEU:HD12	2.01	0.43
2:B:583:ASN:ND2	2:B:628:THR:HG22	2.12	0.43
2:B:841:MET:HG2	2:B:1010:LEU:HD12	2.01	0.43
13:M:189:PHE:O	13:M:193:GLN:HG3	2.18	0.43
13:M:275:ILE:CG2	13:M:276:THR:N	2.82	0.43
2:B:509:ALA:C	2:B:511:PRO:HD3	2.43	0.42
2:B:766:ARG:NH2	2:B:1020:ARG:HD3	2.33	0.42
3:C:148:ARG:HG3	3:C:151:GLN:HG3	2.01	0.42
13:M:280:VAL:HG23	13:M:281:SER:N	2.33	0.42
17:Q:133:PHE:C	17:Q:135:LEU:H	2.27	0.42
24:X:12:GLY:O	24:X:13:ASP:C	2.62	0.42
1:A:332:LYS:O	1:A:333:GLU:HB2	2.19	0.42
1:A:709:THR:HB	1:A:712:GLU:H	1.83	0.42
1:A:774:ARG:HH21	1:A:797:LYS:HB2	1.83	0.42
1:A:1345:ARG:HG2	1:A:1372:VAL:HG12	2.01	0.42
2:B:983:ARG:HD2	2:B:1091:TYR:HD2	1.84	0.42
24:X:163:PRO:HA	24:X:190:ILE:O	2.18	0.42
1:A:11:LEU:HA	2:B:1193:GLN:O	2.19	0.42
1:A:332:LYS:HA	1:A:337:ARG:CB	2.50	0.42
1:A:481:ASP:OD1	1:A:485:ASP:OD1	2.37	0.42
2:B:65:GLU:HG3	2:B:66:ASP:H	1.85	0.42
2:B:792:MET:HE2	20:T:21:DT:P	2.57	0.42
6:F:103:MET:O	7:G:14:HIS:CE1	2.72	0.42
6:F:130:ILE:HB	6:F:148:VAL:HG21	1.99	0.42
13:M:236:LEU:HD23	13:M:236:LEU:N	2.34	0.42
14:N:31:DG:H2'	14:N:32:DT:C6	2.54	0.42
25:Y:22:ASP:C	25:Y:24:LEU:H	2.27	0.42
1:A:37:PHE:HA	1:A:38:PRO:HD3	1.93	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:LYS:HA	1:A:337:ARG:HB2	2.00	0.42
1:A:595:THR:OG1	1:A:603:ASN:HB3	2.20	0.42
3:C:251:LEU:O	3:C:255:VAL:HG23	2.19	0.42
5:E:10:SER:O	5:E:14:ARG:HG3	2.19	0.42
6:F:92:ARG:NH2	7:G:63:PRO:HG3	2.35	0.42
13:M:248:LEU:CD2	13:M:286:ILE:CD1	2.93	0.42
13:M:339:LEU:HB3	13:M:340:PRO:CD	2.38	0.42
1:A:469:ARG:NH2	2:B:991:GLY:O	2.52	0.42
1:A:832:ALA:HA	20:T:15:DA:C8	2.54	0.42
1:A:871:ASP:CG	1:A:1366:ARG:HH22	2.28	0.42
3:C:133:ILE:HG21	3:C:236:GLY:HA3	2.00	0.42
4:D:12:ARG:CZ	4:D:14:ARG:HA	2.48	0.42
7:G:34:VAL:HG13	7:G:45:ILE:HG21	2.00	0.42
15:O:227:PHE:HA	15:O:230:ILE:HG22	2.02	0.42
1:A:873:MET:C	1:A:1058:VAL:HG22	2.44	0.42
2:B:226:PHE:HA	2:B:395:GLN:CG	2.49	0.42
2:B:273:LEU:HD12	2:B:280:ILE:HD12	2.01	0.42
2:B:951:GLN:OE1	12:L:57:LEU:HD22	2.18	0.42
8:H:38:LEU:HD13	8:H:125:LEU:HD13	2.02	0.42
8:H:125:LEU:HG	8:H:130:ARG:HH22	1.85	0.42
13:M:269:ILE:HD12	13:M:277:ILE:HG23	2.02	0.42
13:M:339:LEU:HD12	13:M:339:LEU:H	1.84	0.42
1:A:399:HIS:HB3	1:A:400:PRO:HD3	2.02	0.42
1:A:1317:MET:HE2	5:E:142:VAL:HG11	2.02	0.42
2:B:311:LEU:HB3	9:I:4:PHE:HE2	1.85	0.42
3:C:184:ASN:ND2	3:C:189:THR:O	2.52	0.42
5:E:181:ALA:HA	5:E:186:LEU:HD21	2.01	0.42
7:G:1:MET:HE3	7:G:80:LYS:O	2.19	0.42
9:I:76:PRO:HD2	9:I:108:HIS:HD2	1.85	0.42
13:M:123:ASP:HA	13:M:126:VAL:HG23	2.02	0.42
14:N:25:DA:O5'	14:N:25:DA:H8	2.03	0.42
1:A:239:LEU:HD12	1:A:239:LEU:HA	1.77	0.42
1:A:420:ARG:HH11	24:X:174:ALA:HB2	1.68	0.42
1:A:729:ALA:HA	1:A:732:LEU:HD12	2.01	0.42
2:B:986:GLN:OE1	2:B:1016:ALA:HB1	2.20	0.42
2:B:1165:ILE:CG2	4:D:17:LYS:CA	2.93	0.42
6:F:82:THR:HG22	6:F:83:PRO:HD2	2.01	0.42
7:G:110:VAL:HG11	7:G:163:ILE:HG23	2.01	0.42
13:M:64:ARG:NH2	20:T:22:DT:O4	2.49	0.42
13:M:248:LEU:CD2	13:M:291:ILE:HG13	2.50	0.42
13:M:324:VAL:CG2	13:M:325:ASP:N	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:LEU:HD23	1:A:266:LEU:HA	1.92	0.42
1:A:541:ILE:HG21	1:A:549:MET:CE	2.49	0.42
2:B:279:ASP:OD1	2:B:279:ASP:N	2.53	0.42
2:B:383:ASN:O	2:B:387:LEU:HB2	2.19	0.42
4:D:8:PHE:CE1	4:D:37:GLN:HB2	2.55	0.42
17:Q:106:ILE:HA	17:Q:381:MET:O	2.20	0.42
21:U:134:GLY:HA2	21:U:135:VAL:C	2.45	0.42
1:A:194:ALA:HA	1:A:195:ASP:C	2.45	0.41
1:A:262:LEU:HG	1:A:328:ARG:NH2	2.35	0.41
1:A:270:LEU:O	1:A:274:ILE:HG13	2.20	0.41
1:A:1094:VAL:HG22	1:A:1113:THR:HB	2.02	0.41
2:B:190:TYR:CE2	2:B:196:PRO:HG3	2.55	0.41
2:B:216:GLU:OE2	2:B:404:LYS:HD2	2.20	0.41
2:B:854:LEU:HD23	2:B:854:LEU:HA	1.86	0.41
2:B:856:PHE:CE2	2:B:969:ARG:HG3	2.55	0.41
3:C:149:LYS:C	3:C:151:GLN:H	2.28	0.41
4:D:32:GLU:O	7:G:5:LYS:NZ	2.53	0.41
4:D:185:CYS:SG	4:D:190:GLU:HG2	2.60	0.41
13:M:263:CYS:SG	13:M:316:LEU:CG	3.08	0.41
1:A:11:LEU:HD21	2:B:1195:HIS:HD2	1.84	0.41
2:B:315:LYS:N	2:B:316:PRO:HD2	2.36	0.41
13:M:174:ALA:O	13:M:178:ILE:HG12	2.20	0.41
13:M:298:VAL:CG1	13:M:299:GLY:N	2.82	0.41
13:M:311:SER:C	13:M:314:LYS:HD3	2.46	0.41
2:B:789:MET:HG3	2:B:953:LEU:HD21	2.02	0.41
4:D:17:LYS:HD2	4:D:18:VAL:HG13	2.02	0.41
10:J:22:LEU:O	10:J:26:GLN:HG2	2.20	0.41
13:M:154:TYR:OH	13:M:168:MET:HE1	2.21	0.41
13:M:276:THR:HG23	13:M:277:ILE:N	2.35	0.41
1:A:1036:ARG:HH11	1:A:1036:ARG:HG2	1.85	0.41
5:E:3:GLN:HB2	5:E:4:GLU:H	1.74	0.41
10:J:32:GLU:CD	10:J:32:GLU:H	2.29	0.41
14:N:24:DT:C2'	14:N:25:DA:C5'	2.90	0.41
1:A:11:LEU:HD21	2:B:1195:HIS:CD2	2.55	0.41
1:A:243:PRO:HB2	1:A:245:PRO:HD2	2.02	0.41
2:B:211:VAL:CG1	2:B:495:LEU:HD23	2.51	0.41
2:B:955:THR:HG22	2:B:956:THR:H	1.85	0.41
13:M:283:TYR:HD2	13:M:313:TYR:CD1	2.38	0.41
21:U:93:THR:HA	23:W:257:ASP:O	2.19	0.41
1:A:562:THR:O	1:A:576:GLN:NE2	2.53	0.41
2:B:848:ARG:HD2	10:J:8:PHE:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:148:ARG:N	3:C:151:GLN:HG3	2.22	0.41
11:K:12:LEU:HA	11:K:37:LYS:HG3	2.03	0.41
13:M:237:THR:CG2	13:M:238:TYR:N	2.83	0.41
20:T:51:DA:H2'	20:T:52:DC:C6	2.55	0.41
1:A:420:ARG:HH12	24:X:174:ALA:HA	1.79	0.41
2:B:509:ALA:O	2:B:511:PRO:HD3	2.20	0.41
2:B:871:THR:HG22	2:B:872:GLU:O	2.21	0.41
3:C:75:MET:HE1	3:C:239:PRO:HG3	2.03	0.41
3:C:125:MET:HE3	3:C:125:MET:HA	2.02	0.41
4:D:57:LEU:HD12	4:D:160:VAL:HG21	2.03	0.41
5:E:156:LEU:HD23	5:E:160:GLU:HB3	2.03	0.41
9:I:111:THR:HG21	9:I:118:ARG:HD2	2.03	0.41
13:M:199:LYS:O	13:M:201:LYS:N	2.54	0.41
17:Q:100:GLU:HA	18:R:95:ILE:O	2.21	0.41
1:A:343:LYS:HA	2:B:1129:ARG:NH1	2.36	0.41
2:B:563:MET:CE	2:B:580:VAL:HB	2.51	0.41
2:B:1111:MET:O	13:M:57:VAL:HG12	2.21	0.41
3:C:99:LEU:HD12	3:C:118:LEU:HB3	2.02	0.41
3:C:99:LEU:HB3	3:C:118:LEU:HD22	2.02	0.41
13:M:279:VAL:HA	13:M:302:LEU:CD2	2.50	0.41
21:U:90:LEU:C	21:U:92:SER:H	2.28	0.41
1:A:16:GLU:HB2	4:D:13:ARG:HH21	1.83	0.41
1:A:34:LYS:HG2	1:A:36:ARG:NH1	2.36	0.41
1:A:227:VAL:HG11	4:D:14:ARG:CD	2.48	0.41
2:B:622:LYS:HE3	9:I:59:VAL:HG22	2.02	0.41
2:B:904:ARG:HG3	2:B:948:ILE:HG13	2.02	0.41
2:B:1166:CYS:O	2:B:1168:LEU:N	2.42	0.41
4:D:51:ASN:C	4:D:52:LEU:O	2.63	0.41
7:G:14:HIS:CD2	7:G:15:PRO:HD2	2.56	0.41
14:N:21:DG:C2'	14:N:22:DT:H5'	2.51	0.41
1:A:10:PRO:HG2	2:B:1192:TYR:HD1	1.85	0.41
1:A:369:SER:HB3	11:K:2:ASN:OD1	2.21	0.41
1:A:1196:GLU:HA	1:A:1236:LEU:O	2.21	0.41
2:B:642:ASP:HA	2:B:649:LYS:HA	2.02	0.41
6:F:99:LEU:CD2	7:G:64:THR:C	2.91	0.41
8:H:104:PHE:CE1	8:H:136:LYS:HG3	2.57	0.41
13:M:142:LEU:HD12	13:M:142:LEU:HA	1.89	0.41
13:M:293:ILE:CD1	13:M:297:LYS:HB2	2.43	0.41
14:N:26:DT:C1'	15:O:159:ASN:HB2	2.51	0.41
15:O:169:PRO:HB2	15:O:239:LYS:HB2	2.03	0.41
1:A:133:LYS:HE3	1:A:1391:ARG:HH12	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1404:GLU:HB3	1:A:1408:ILE:HG13	2.02	0.40
2:B:46:GLN:H	2:B:46:GLN:HG3	1.38	0.40
2:B:610:ASN:HB3	2:B:613:VAL:HG23	2.03	0.40
1:A:354:SER:O	1:A:469:ARG:HA	2.21	0.40
1:A:982:THR:H	1:A:985:ASP:HB2	1.86	0.40
2:B:1166:CYS:CA	4:D:15:LEU:HD12	2.50	0.40
4:D:54:GLU:OE1	4:D:164:ILE:HD11	2.21	0.40
7:G:62:LEU:HA	7:G:63:PRO:HD3	1.81	0.40
11:K:39:ASP:OD1	11:K:41:THR:HB	2.21	0.40
13:M:254:THR:O	13:M:258:TYR:CD2	2.75	0.40
2:B:341:LEU:HD11	2:B:343:ILE:HB	2.02	0.40
2:B:681:TRP:HA	2:B:684:LEU:HD12	2.03	0.40
2:B:1119:VAL:HG23	2:B:1126:GLY:HA2	2.03	0.40
4:D:12:ARG:NH1	4:D:14:ARG:HA	2.36	0.40
4:D:63:LEU:HD23	4:D:63:LEU:HA	1.88	0.40
7:G:168:LEU:HD23	7:G:168:LEU:HA	1.92	0.40
9:I:8:ARG:O	9:I:9:ASP:CB	2.69	0.40
10:J:43:ARG:O	10:J:47:ARG:HG3	2.21	0.40
13:M:254:THR:HG22	13:M:258:TYR:CE2	2.55	0.40
13:M:276:THR:CG2	13:M:277:ILE:N	2.82	0.40
13:M:282:ILE:HD12	13:M:302:LEU:HD21	2.03	0.40
1:A:7:SER:HB2	2:B:1175:LEU:HD22	2.03	0.40
1:A:255:SER:HB3	13:M:86:LEU:HD12	2.02	0.40
1:A:381:THR:HG22	1:A:384:ASN:CG	2.46	0.40
1:A:626:ASN:O	1:A:631:HIS:ND1	2.53	0.40
1:A:1141:THR:HG23	1:A:1205:LYS:HD3	2.04	0.40
2:B:577:ALA:HB1	2:B:589:VAL:HB	2.03	0.40
2:B:839:MET:HE1	2:B:980:PHE:HB2	2.04	0.40
2:B:979:LYS:HD3	2:B:1095:LEU:HD13	2.04	0.40
3:C:69:LEU:HD23	10:J:6:ARG:HB2	2.04	0.40
12:L:27:LEU:HD22	12:L:37:LYS:HE3	2.02	0.40
12:L:38:LEU:HD21	12:L:48:CYS:HA	2.02	0.40
13:M:242:PHE:CE1	13:M:301:THR:O	2.74	0.40
23:W:261:TYR:HA	23:W:264:PRO:CB	2.51	0.40
25:Y:71:LEU:O	25:Y:77:ALA:HA	2.22	0.40
1:A:420:ARG:HE	1:A:420:ARG:HB3	1.80	0.40
1:A:441:PRO:HD2	1:A:498:ARG:CZ	2.51	0.40
1:A:450:LEU:H	1:A:450:LEU:HG	1.71	0.40
1:A:497:THR:CG2	2:B:1146:PHE:CD1	3.02	0.40
1:A:1149:ALA:CB	9:I:47:GLU:HA	2.52	0.40
2:B:758:PHE:CE1	2:B:1044:ALA:HA	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:986:GLN:NE2	2:B:1022:THR:HG21	2.36	0.40
3:C:62:PHE:O	3:C:66:ARG:HG3	2.22	0.40
10:J:48:ARG:HH21	10:J:49:MET:HE1	1.85	0.40
13:M:137:CYS:SG	13:M:147:LYS:HG2	2.62	0.40
13:M:269:ILE:CG1	13:M:316:LEU:HD11	2.50	0.40
13:M:283:TYR:O	13:M:286:ILE:HG22	2.22	0.40
13:M:288:LEU:C	13:M:334:VAL:CG2	2.94	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1414/1733 (82%)	1248 (88%)	115 (8%)	51 (4%)	2	20
2	B	1140/1224 (93%)	1019 (89%)	85 (8%)	36 (3%)	3	21
3	C	264/318 (83%)	242 (92%)	20 (8%)	2 (1%)	16	54
4	D	174/221 (79%)	157 (90%)	12 (7%)	5 (3%)	3	23
5	E	212/215 (99%)	195 (92%)	13 (6%)	4 (2%)	6	32
6	F	82/155 (53%)	75 (92%)	7 (8%)	0	100	100
7	G	169/171 (99%)	152 (90%)	15 (9%)	2 (1%)	10	44
8	H	129/146 (88%)	106 (82%)	14 (11%)	9 (7%)	1	11
9	I	117/122 (96%)	98 (84%)	16 (14%)	3 (3%)	4	25
10	J	63/70 (90%)	51 (81%)	9 (14%)	3 (5%)	2	16
11	K	113/120 (94%)	109 (96%)	4 (4%)	0	100	100
12	L	44/70 (63%)	27 (61%)	9 (20%)	8 (18%)	0	2
13	M	294/345 (85%)	267 (91%)	24 (8%)	3 (1%)	12	49
15	O	178/181 (98%)	174 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	Q	118/734 (16%)	106 (90%)	11 (9%)	1 (1%)	16	54
18	R	103/331 (31%)	96 (93%)	3 (3%)	4 (4%)	2	19
19	S	133/295 (45%)	122 (92%)	9 (7%)	2 (2%)	8	40
21	U	154/222 (69%)	148 (96%)	5 (3%)	1 (1%)	21	59
22	V	95/115 (83%)	94 (99%)	1 (1%)	0	100	100
23	W	403/687 (59%)	382 (95%)	18 (4%)	3 (1%)	18	56
24	X	226/307 (74%)	210 (93%)	13 (6%)	3 (1%)	9	42
25	Y	199/209 (95%)	180 (90%)	17 (8%)	2 (1%)	12	49
26	Z	83/120 (69%)	82 (99%)	1 (1%)	0	100	100
All	All	5907/8111 (73%)	5340 (90%)	425 (7%)	142 (2%)	7	27

All (142) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	74	MET
1	A	96	ILE
1	A	189	ARG
1	A	195	ASP
1	A	286	HIS
1	A	317	LYS
1	A	399	HIS
1	A	449	SER
1	A	628	GLY
1	A	1377	THR
1	A	1405	THR
2	B	229	ALA
2	B	307	ASP
2	B	344	LYS
2	B	442	PHE
2	B	466	TRP
2	B	473	MET
2	B	531	GLN
2	B	772	ALA
2	B	1046	PRO
2	B	1181	GLU
4	D	5	THR
7	G	154	VAL
7	G	155	SER
9	I	9	ASP

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Mol	Chain	Res	Type
9	I	95	THR
12	L	50	ASP
12	L	53	HIS
13	M	200	THR
17	Q	391	THR
18	R	128	VAL
19	S	166	ILE
24	X	79	THR
1	A	40	THR
1	A	44	THR
1	A	51	GLY
1	A	52	GLY
1	A	57	ARG
1	A	66	LYS
1	A	68	GLN
1	A	167	CYS
1	A	178	GLY
1	A	193	ASP
1	A	224	PHE
1	A	252	PHE
1	A	254	GLU
1	A	330	LYS
1	A	672	ASP
1	A	1175	SER
1	A	1281	ARG
2	B	262	GLU
2	B	282	ILE
2	B	339	THR
2	B	341	LEU
2	B	707	PRO
2	B	731	VAL
2	B	792	MET
2	B	1175	LEU
2	B	1176	ASN
4	D	199	ASN
5	E	36	GLU
8	H	17	PRO
8	H	81	PRO
8	H	82	PRO
8	H	83	GLN
8	H	90	ALA
10	J	6	ARG

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Mol	Chain	Res	Type
12	L	45	ALA
12	L	56	LEU
18	R	61	LEU
18	R	62	GLU
25	Y	161	GLY
1	A	54	ASN
1	A	975	HIS
1	A	1173	HIS
2	B	340	ALA
2	B	343	ILE
2	B	711	GLU
2	B	1156	ASP
2	B	1157	ALA
2	B	1167	GLY
4	D	52	LEU
5	E	45	LYS
5	E	48	ASP
8	H	18	GLY
12	L	59	ALA
18	R	115	SER
21	U	143	GLU
23	W	317	SER
25	Y	159	GLU
1	A	69	THR
1	A	72	GLU
1	A	465	TYR
1	A	569	LYS
1	A	846	GLU
1	A	958	VAL
1	A	1255	GLU
1	A	1438	THR
2	B	441	ASP
2	B	648	HIS
2	B	1108	ARG
2	B	1155	SER
3	C	88	CYS
9	I	91	ARG
10	J	29	GLU
12	L	26	THR
12	L	55	ILE
12	L	64	LEU
23	W	547	GLY

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Mol	Chain	Res	Type
1	A	156	ASP
1	A	567	LYS
1	A	1171	GLN
1	A	1366	ARG
2	B	251	ILE
2	B	462	ALA
2	B	469	GLN
2	B	1223	ASP
4	D	119	ARG
8	H	60	ALA
8	H	128	ASN
10	J	2	ILE
1	A	35	ILE
1	A	155	GLU
1	A	885	THR
3	C	214	ASN
13	M	164	LYS
13	M	271	GLY
19	S	165	THR
24	X	196	LYS
1	A	196	GLU
1	A	1388	GLY
1	A	1437	GLY
5	E	90	VAL
2	B	364	ILE
1	A	192	GLY
2	B	1121	GLY
1	A	448	PRO
2	B	1214	PRO
4	D	18	VAL
8	H	59	ILE
24	X	84	PRO
23	W	541	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1240/1520 (82%)	1045 (84%)	195 (16%)	2	12
2	B	985/1061 (93%)	855 (87%)	130 (13%)	4	15
3	C	234/274 (85%)	204 (87%)	30 (13%)	4	15
4	D	160/200 (80%)	138 (86%)	22 (14%)	3	14
5	E	196/197 (100%)	172 (88%)	24 (12%)	5	17
6	F	74/137 (54%)	65 (88%)	9 (12%)	5	17
7	G	152/152 (100%)	135 (89%)	17 (11%)	6	19
8	H	117/128 (91%)	101 (86%)	16 (14%)	3	14
9	I	113/116 (97%)	105 (93%)	8 (7%)	13	35
10	J	60/65 (92%)	48 (80%)	12 (20%)	1	7
11	K	99/102 (97%)	86 (87%)	13 (13%)	4	15
12	L	40/57 (70%)	26 (65%)	14 (35%)	0	1
13	M	231/299 (77%)	208 (90%)	23 (10%)	7	24
15	O	152/153 (99%)	141 (93%)	11 (7%)	13	35
All	All	3853/4461 (86%)	3329 (86%)	524 (14%)	6	14

All (524) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	THR
1	A	15	LYS
1	A	22	PHE
1	A	41	MET
1	A	42	ASP
1	A	53	LEU
1	A	54	ASN
1	A	57	ARG
1	A	61	ILE
1	A	64	ASN
1	A	66	LYS
1	A	68	GLN
1	A	74	MET
1	A	80	HIS
1	A	84	ILE
1	A	93	VAL
1	A	106	VAL
1	A	131	SER
1	A	134	ARG

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Mol	Chain	Res	Type
1	A	145	LYS
1	A	147	VAL
1	A	152	VAL
1	A	157	ASP
1	A	173	THR
1	A	174	ILE
1	A	182	VAL
1	A	199	LEU
1	A	204	THR
1	A	205	GLU
1	A	208	LEU
1	A	219	PHE
1	A	220	THR
1	A	222	LEU
1	A	227	VAL
1	A	249	SER
1	A	257	ARG
1	A	265	LYS
1	A	277	GLU
1	A	279	LEU
1	A	307	ASP
1	A	311	GLN
1	A	323	LYS
1	A	335	ARG
1	A	337	ARG
1	A	344	ARG
1	A	353	ILE
1	A	375	THR
1	A	381	THR
1	A	385	ILE
1	A	386	ASP
1	A	393	ARG
1	A	398	GLU
1	A	408	ASP
1	A	412	ARG
1	A	424	ILE
1	A	425	GLN
1	A	427	GLN
1	A	434	ARG
1	A	436	ILE
1	A	443	LEU
1	A	445	ASN

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Mol	Chain	Res	Type
1	A	450	LEU
1	A	451	HIS
1	A	454	SER
1	A	461	LYS
1	A	469	ARG
1	A	470	LEU
1	A	472	LEU
1	A	474	VAL
1	A	475	THR
1	A	476	SER
1	A	489	LEU
1	A	500	GLU
1	A	505	CYS
1	A	512	VAL
1	A	513	SER
1	A	524	VAL
1	A	532	ARG
1	A	566	ILE
1	A	571	LEU
1	A	582	ILE
1	A	593	GLU
1	A	596	THR
1	A	603	ASN
1	A	613	ILE
1	A	618	GLU
1	A	629	LEU
1	A	630	ILE
1	A	634	THR
1	A	652	VAL
1	A	664	THR
1	A	666	ILE
1	A	672	ASP
1	A	691	LEU
1	A	702	LEU
1	A	719	VAL
1	A	738	LYS
1	A	740	LEU
1	A	768	GLN
1	A	769	SER
1	A	773	LYS
1	A	782	ARG
1	A	788	SER

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Mol	Chain	Res	Type
1	A	795	GLU
1	A	797	LYS
1	A	801	GLU
1	A	805	LEU
1	A	806	ARG
1	A	821	ARG
1	A	826	ASP
1	A	827	THR
1	A	831	THR
1	A	834	THR
1	A	837	ILE
1	A	839	ARG
1	A	848	ILE
1	A	849	MET
1	A	854	ASN
1	A	864	ILE
1	A	867	ILE
1	A	886	ILE
1	A	896	ARG
1	A	919	ILE
1	A	920	LEU
1	A	926	GLN
1	A	929	LEU
1	A	948	VAL
1	A	949	ASP
1	A	964	ILE
1	A	973	ILE
1	A	976	THR
1	A	983	ILE
1	A	998	LEU
1	A	999	VAL
1	A	1009	ASN
1	A	1015	VAL
1	A	1029	ARG
1	A	1030	ARG
1	A	1047	SER
1	A	1058	VAL
1	A	1062	GLU
1	A	1067	LEU
1	A	1078	GLN
1	A	1094	VAL
1	A	1116	LEU

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Mol	Chain	Res	Type
1	A	1118	VAL
1	A	1120	LEU
1	A	1121	GLU
1	A	1124	HIS
1	A	1135	ARG
1	A	1142	THR
1	A	1172	LEU
1	A	1173	HIS
1	A	1176	LEU
1	A	1195	LEU
1	A	1208	THR
1	A	1218	GLN
1	A	1223	ASP
1	A	1226	VAL
1	A	1237	ILE
1	A	1238	ILE
1	A	1242	VAL
1	A	1255	GLU
1	A	1257	ASP
1	A	1260	LEU
1	A	1265	ASN
1	A	1273	LEU
1	A	1291	VAL
1	A	1295	THR
1	A	1297	GLU
1	A	1309	ASP
1	A	1315	GLU
1	A	1317	MET
1	A	1325	THR
1	A	1327	ILE
1	A	1336	MET
1	A	1341	ILE
1	A	1355	VAL
1	A	1376	THR
1	A	1382	THR
1	A	1386	ARG
1	A	1391	ARG
1	A	1393	ASN
1	A	1400	CYS
1	A	1405	THR
1	A	1406	VAL
1	A	1424	VAL

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Mol	Chain	Res	Type
1	A	1426	GLU
1	A	1436	ILE
1	A	1438	THR
1	A	1442	ASP
1	A	1444	MET
1	A	1445	ILE
1	A	1453	TYR
1	A	1454	MET
2	B	25	ILE
2	B	41	LYS
2	B	46	GLN
2	B	63	ILE
2	B	69	LEU
2	B	72	GLU
2	B	73	GLN
2	B	102	VAL
2	B	103	ASN
2	B	104	GLU
2	B	128	LEU
2	B	164	LYS
2	B	169	ARG
2	B	178	ASN
2	B	183	GLU
2	B	211	VAL
2	B	240	ILE
2	B	251	ILE
2	B	261	ARG
2	B	267	ARG
2	B	272	THR
2	B	278	GLN
2	B	279	ASP
2	B	287	ARG
2	B	294	ASP
2	B	313	MET
2	B	324	ILE
2	B	325	GLN
2	B	337	ARG
2	B	341	LEU
2	B	343	ILE
2	B	344	LYS
2	B	348	ARG
2	B	357	GLN

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Mol	Chain	Res	Type
2	B	365	THR
2	B	393	LYS
2	B	408	LEU
2	B	419	THR
2	B	425	THR
2	B	440	HIS
2	B	442	PHE
2	B	470	LYS
2	B	476	ARG
2	B	482	VAL
2	B	485	ARG
2	B	487	THR
2	B	502	ILE
2	B	513	GLN
2	B	529	GLU
2	B	531	GLN
2	B	537	LYS
2	B	542	MET
2	B	547	VAL
2	B	552	MET
2	B	554	ILE
2	B	563	MET
2	B	570	VAL
2	B	574	SER
2	B	595	ARG
2	B	596	LEU
2	B	601	ARG
2	B	603	LEU
2	B	609	ILE
2	B	612	GLU
2	B	615	MET
2	B	616	ILE
2	B	620	ARG
2	B	644	GLU
2	B	651	LEU
2	B	653	VAL
2	B	658	ILE
2	B	680	THR
2	B	708	GLU
2	B	734	HIS
2	B	737	THR
2	B	766	ARG

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Mol	Chain	Res	Type
2	B	771	SER
2	B	776	GLN
2	B	786	ASN
2	B	790	ASP
2	B	791	THR
2	B	795	ILE
2	B	831	SER
2	B	835	GLN
2	B	839	MET
2	B	841	MET
2	B	844	SER
2	B	860	MET
2	B	933	SER
2	B	934	LYS
2	B	939	THR
2	B	942	ARG
2	B	944	THR
2	B	955	THR
2	B	956	THR
2	B	967	ARG
2	B	975	GLN
2	B	979	LYS
2	B	986	GLN
2	B	997	GLU
2	B	999	MET
2	B	1007	VAL
2	B	1028	GLU
2	B	1045	SER
2	B	1060	ARG
2	B	1065	GLN
2	B	1072	MET
2	B	1084	GLN
2	B	1094	ARG
2	B	1101	ASP
2	B	1106	ARG
2	B	1123	SER
2	B	1128	LEU
2	B	1138	MET
2	B	1145	SER
2	B	1147	LEU
2	B	1151	LEU
2	B	1156	ASP

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Mol	Chain	Res	Type
2	B	1159	ARG
2	B	1160	VAL
2	B	1165	ILE
2	B	1175	LEU
2	B	1179	GLN
2	B	1183	LYS
2	B	1188	LYS
2	B	1189	ILE
2	B	1193	GLN
2	B	1201	LYS
2	B	1202	LEU
2	B	1220	ARG
3	C	3	GLU
3	C	11	ARG
3	C	12	GLU
3	C	22	LEU
3	C	25	VAL
3	C	26	ASP
3	C	52	GLU
3	C	53	THR
3	C	54	ASN
3	C	55	THR
3	C	56	THR
3	C	81	GLU
3	C	100	THR
3	C	101	LEU
3	C	119	VAL
3	C	121	VAL
3	C	124	LEU
3	C	125	MET
3	C	127	ARG
3	C	129	ILE
3	C	133	ILE
3	C	147	LEU
3	C	151	GLN
3	C	215	GLU
3	C	224	GLN
3	C	238	ILE
3	C	240	VAL
3	C	259	LEU
3	C	265	MET
3	C	268	ASP

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Mol	Chain	Res	Type
4	D	11	ARG
4	D	12	ARG
4	D	17	LYS
4	D	19	GLU
4	D	20	GLU
4	D	23	ASN
4	D	29	LEU
4	D	31	GLN
4	D	34	GLN
4	D	35	LEU
4	D	40	HIS
4	D	43	GLU
4	D	47	LEU
4	D	48	ILE
4	D	50	LEU
4	D	52	LEU
4	D	120	GLU
4	D	123	LEU
4	D	156	ASP
4	D	164	ILE
4	D	201	LYS
4	D	204	ASP
5	E	3	GLN
5	E	9	ILE
5	E	20	LYS
5	E	26	ARG
5	E	31	THR
5	E	45	LYS
5	E	57	MET
5	E	67	GLU
5	E	92	THR
5	E	100	ILE
5	E	104	ASN
5	E	127	ILE
5	E	131	THR
5	E	140	LEU
5	E	144	ILE
5	E	166	LYS
5	E	173	SER
5	E	177	ARG
5	E	178	ILE
5	E	191	LYS

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Mol	Chain	Res	Type
5	E	192	ARG
5	E	196	VAL
5	E	202	SER
5	E	204	THR
6	F	72	LYS
6	F	78	GLN
6	F	79	ARG
6	F	82	THR
6	F	86	THR
6	F	90	ARG
6	F	110	ASP
6	F	129	LYS
6	F	133	VAL
7	G	1	MET
7	G	2	PHE
7	G	34	VAL
7	G	56	ILE
7	G	62	LEU
7	G	90	THR
7	G	111	THR
7	G	112	LYS
7	G	114	LEU
7	G	115	MET
7	G	131	GLN
7	G	134	GLU
7	G	138	THR
7	G	139	ILE
7	G	143	ILE
7	G	145	VAL
7	G	165	GLU
8	H	13	SER
8	H	14	GLU
8	H	23	VAL
8	H	26	ILE
8	H	31	THR
8	H	34	ASP
8	H	76	THR
8	H	77	ARG
8	H	83	GLN
8	H	89	LEU
8	H	92	ASP
8	H	103	LYS

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Mol	Chain	Res	Type
8	H	128	ASN
8	H	130	ARG
8	H	135	LEU
8	H	138	GLU
9	I	8	ARG
9	I	31	THR
9	I	35	VAL
9	I	74	GLU
9	I	82	GLU
9	I	84	VAL
9	I	94	ASP
9	I	111	THR
10	J	1	MET
10	J	2	ILE
10	J	3	VAL
10	J	7	CYS
10	J	12	LYS
10	J	13	VAL
10	J	14	VAL
10	J	22	LEU
10	J	29	GLU
10	J	42	LYS
10	J	48	ARG
10	J	52	THR
11	K	14	GLU
11	K	18	LYS
11	K	20	LYS
11	K	25	THR
11	K	29	ASN
11	K	31	VAL
11	K	37	LYS
11	K	42	LEU
11	K	47	ARG
11	K	51	LEU
11	K	101	LEU
11	K	107	THR
11	K	114	LEU
12	L	27	LEU
12	L	33	GLU
12	L	35	SER
12	L	38	LEU
12	L	42	ARG

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Mol	Chain	Res	Type
12	L	50	ASP
12	L	54	ARG
12	L	55	ILE
12	L	56	LEU
12	L	58	LYS
12	L	60	ARG
12	L	61	THR
12	L	65	VAL
12	L	68	GLU
13	M	23	THR
13	M	35	VAL
13	M	39	SER
13	M	52	LEU
13	M	59	THR
13	M	62	GLU
13	M	64	ARG
13	M	78	ARG
13	M	81	GLU
13	M	86	LEU
13	M	101	THR
13	M	142	LEU
13	M	145	ILE
13	M	168	MET
13	M	171	ILE
13	M	182	ARG
13	M	198	VAL
13	M	209	ILE
13	M	262	LYS
13	M	275	ILE
13	M	293	ILE
13	M	297	LYS
13	M	314	LYS
15	O	70	ILE
15	O	108	GLU
15	O	130	ASP
15	O	134	LEU
15	O	175	LEU
15	O	188	GLU
15	O	199	LYS
15	O	219	GLN
15	O	225	GLN
15	O	235	SER

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Mol	Chain	Res	Type
15	O	240	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (77) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	256	GLN
1	A	390	GLN
1	A	394	ASN
1	A	399	HIS
1	A	425	GLN
1	A	447	GLN
1	A	479	ASN
1	A	517	ASN
1	A	545	GLN
1	A	548	ASN
1	A	603	ASN
1	A	760	GLN
1	A	811	GLN
1	A	838	GLN
1	A	862	ASN
1	A	965	GLN
1	A	966	ASN
1	A	969	GLN
1	A	994	GLN
1	A	1106	ASN
1	A	1128	GLN
1	A	1140	HIS
1	A	1173	HIS
1	A	1232	ASN
1	A	1270	ASN
1	A	1393	ASN
2	B	300	HIS
2	B	350	GLN
2	B	357	GLN
2	B	449	ASN
2	B	538	ASN
2	B	786	ASN
2	B	842	ASN
2	B	881	ASN
2	B	887	HIS
2	B	1117	GLN

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Mol	Chain	Res	Type
2	B	1176	ASN
2	B	1177	HIS
2	B	1195	HIS
3	C	112	ASN
3	C	131	HIS
3	C	135	GLN
3	C	184	ASN
3	C	203	GLN
3	C	214	ASN
3	C	231	ASN
4	D	34	GLN
4	D	51	ASN
4	D	179	GLN
5	E	3	GLN
5	E	32	GLN
5	E	54	GLN
5	E	115	ASN
5	E	146	HIS
5	E	179	GLN
7	G	57	GLN
7	G	96	GLN
7	G	126	ASN
8	H	35	GLN
8	H	52	GLN
8	H	83	GLN
8	H	131	ASN
9	I	23	ASN
9	I	83	ASN
9	I	89	GLN
9	I	108	HIS
10	J	26	GLN
10	J	64	ASN
11	K	44	ASN
11	K	76	GLN
13	M	158	HIS
13	M	208	ASN
13	M	285	ASN
13	M	300	GLN
15	O	158	GLN
15	O	219	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
16	P	5/6 (83%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2
20	T	1
2	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	T	23:DT	O3'	33:DT	P	36.29
1	B	351:TYR	C	352:ALA	N	3.28
1	A	234:MET	C	235:ILE	N	1.07
1	A	95:PHE	C	96:ILE	N	1.00

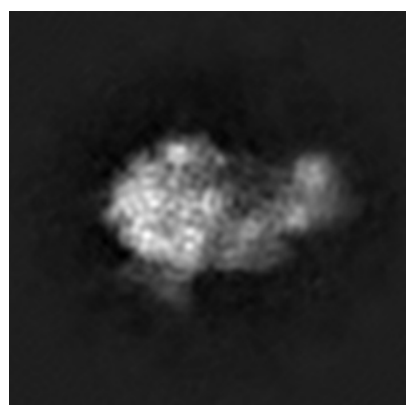
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-2786. These allow visual inspection of the internal detail of the map and identification of artifacts.

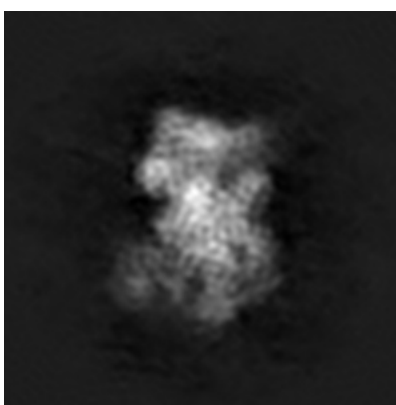
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

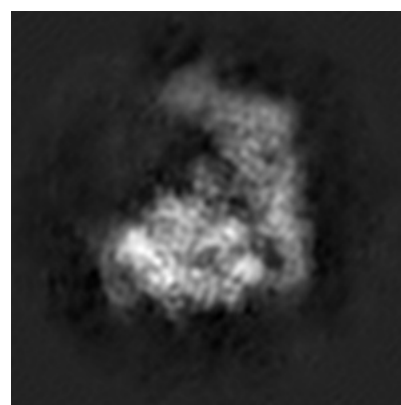
6.1.1 Primary map



X



Y

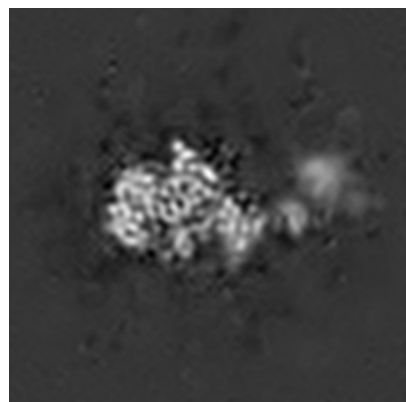


Z

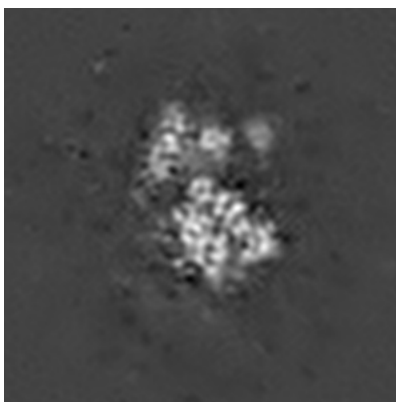
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

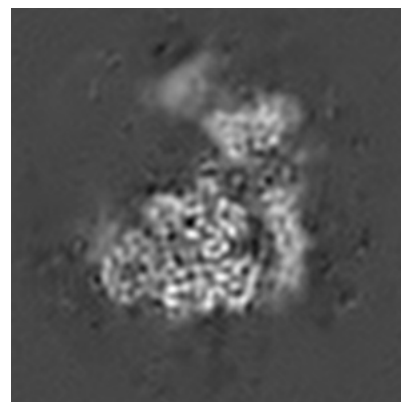
6.2.1 Primary map



X Index: 140



Y Index: 140

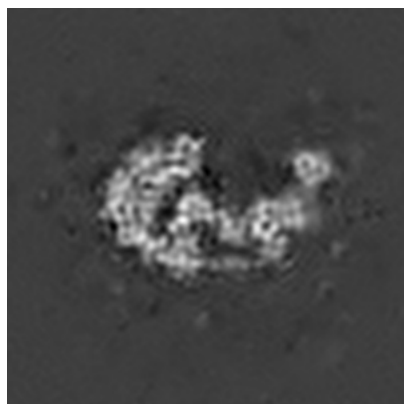


Z Index: 140

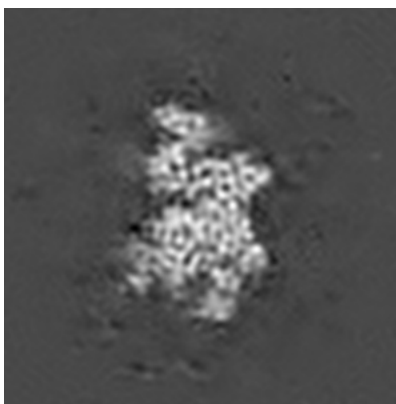
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

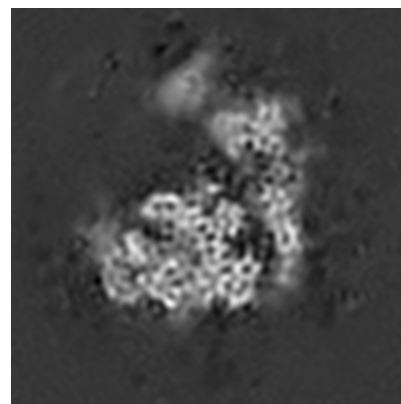
6.3.1 Primary map



X Index: 155



Y Index: 96

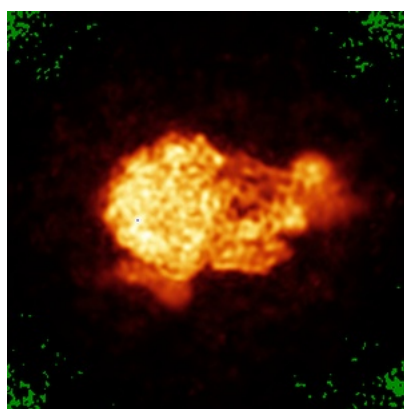


Z Index: 143

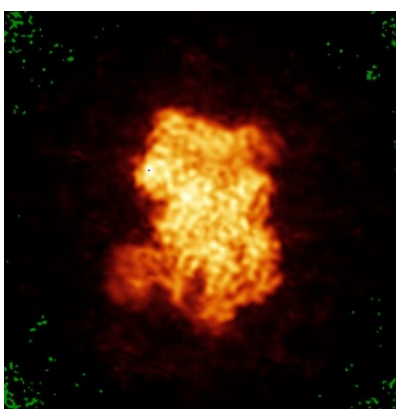
The images above show the largest variance slices of the map in three orthogonal directions.

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

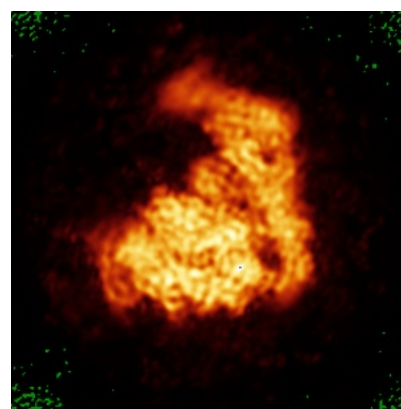
6.4.1 Primary map



X



Y

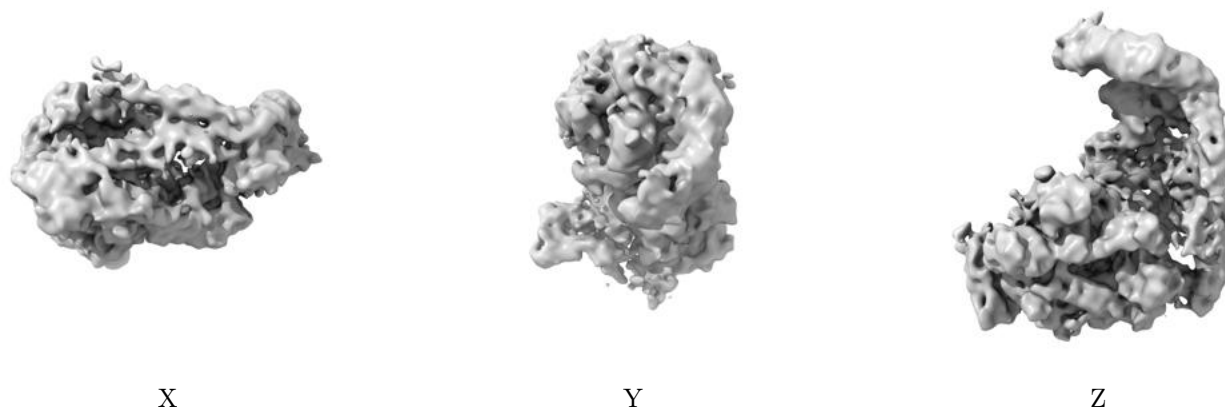


Z

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 0.0135. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

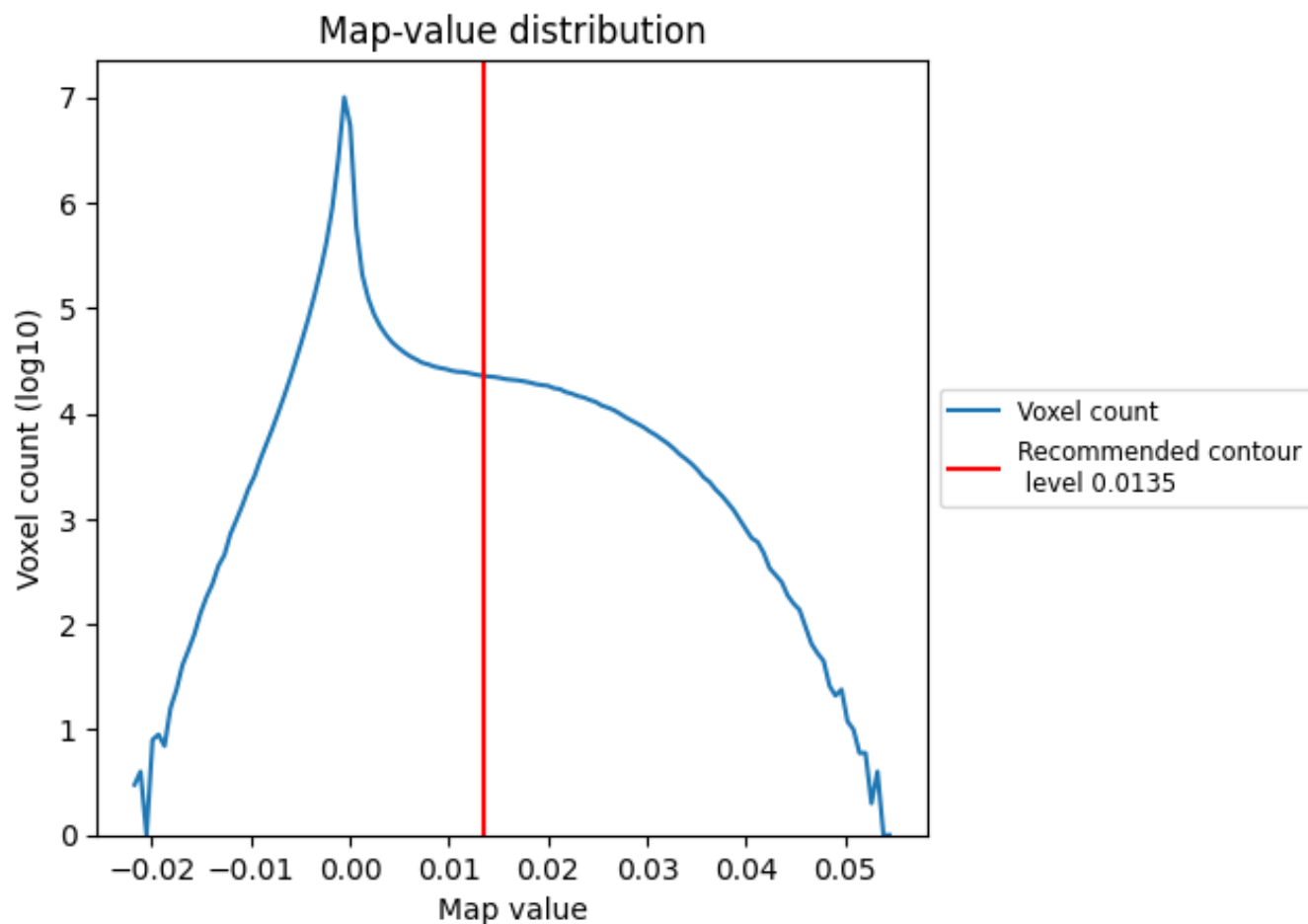
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

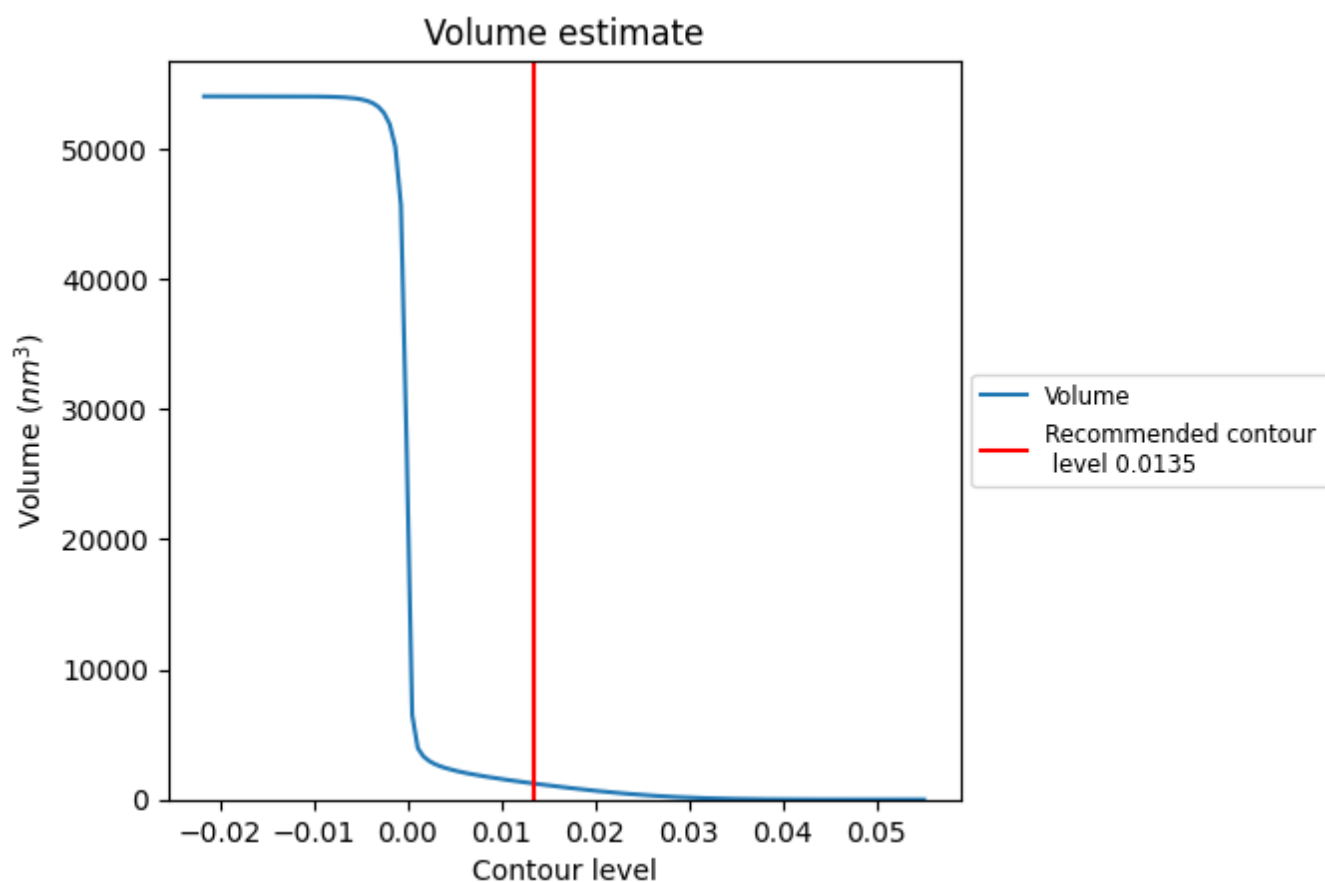
This section contains the results of statistical analysis of the map.

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.

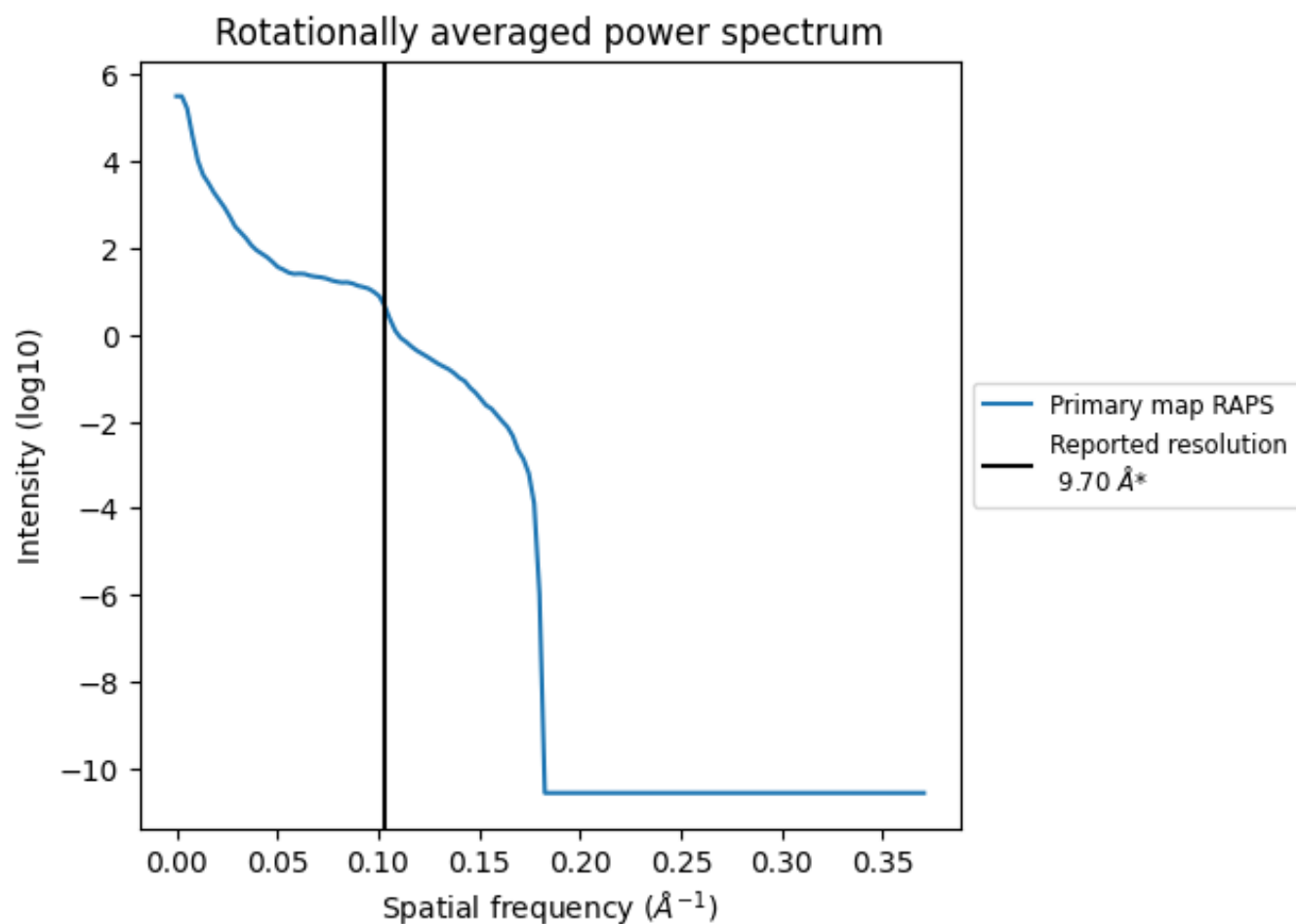
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1227 nm³; this corresponds to an approximate mass of 1108 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 0.103 Å⁻¹

8 Fourier-Shell correlation

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

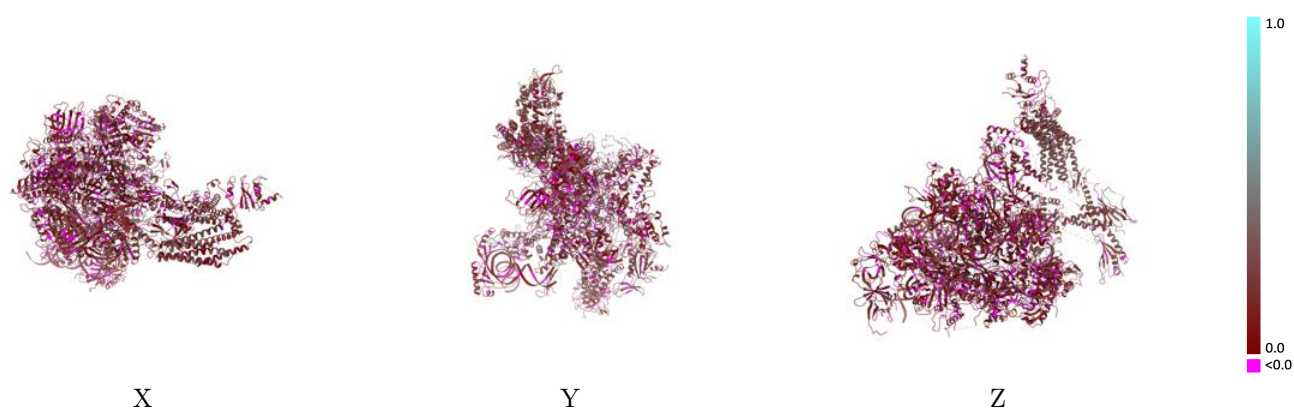
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-2786 and PDB model 4V1O. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)

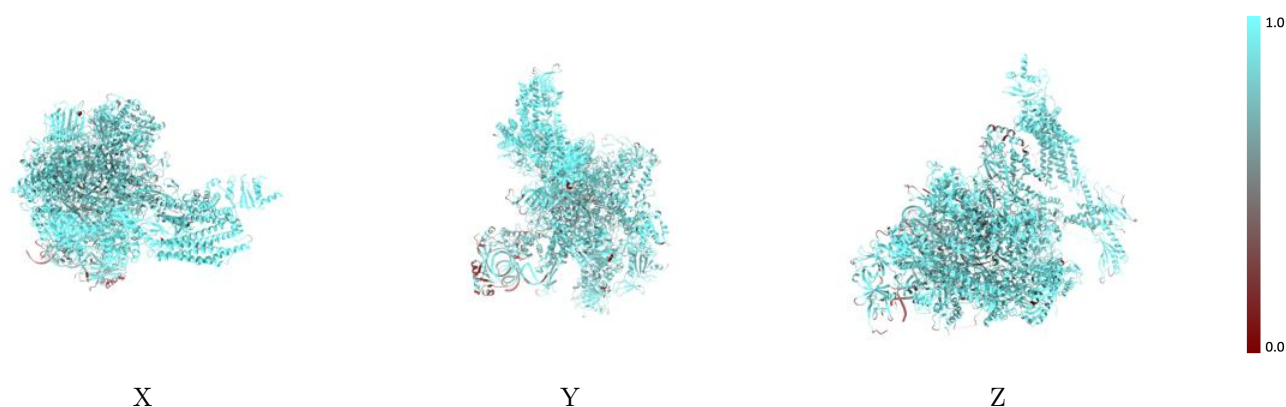
This section was not generated.

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



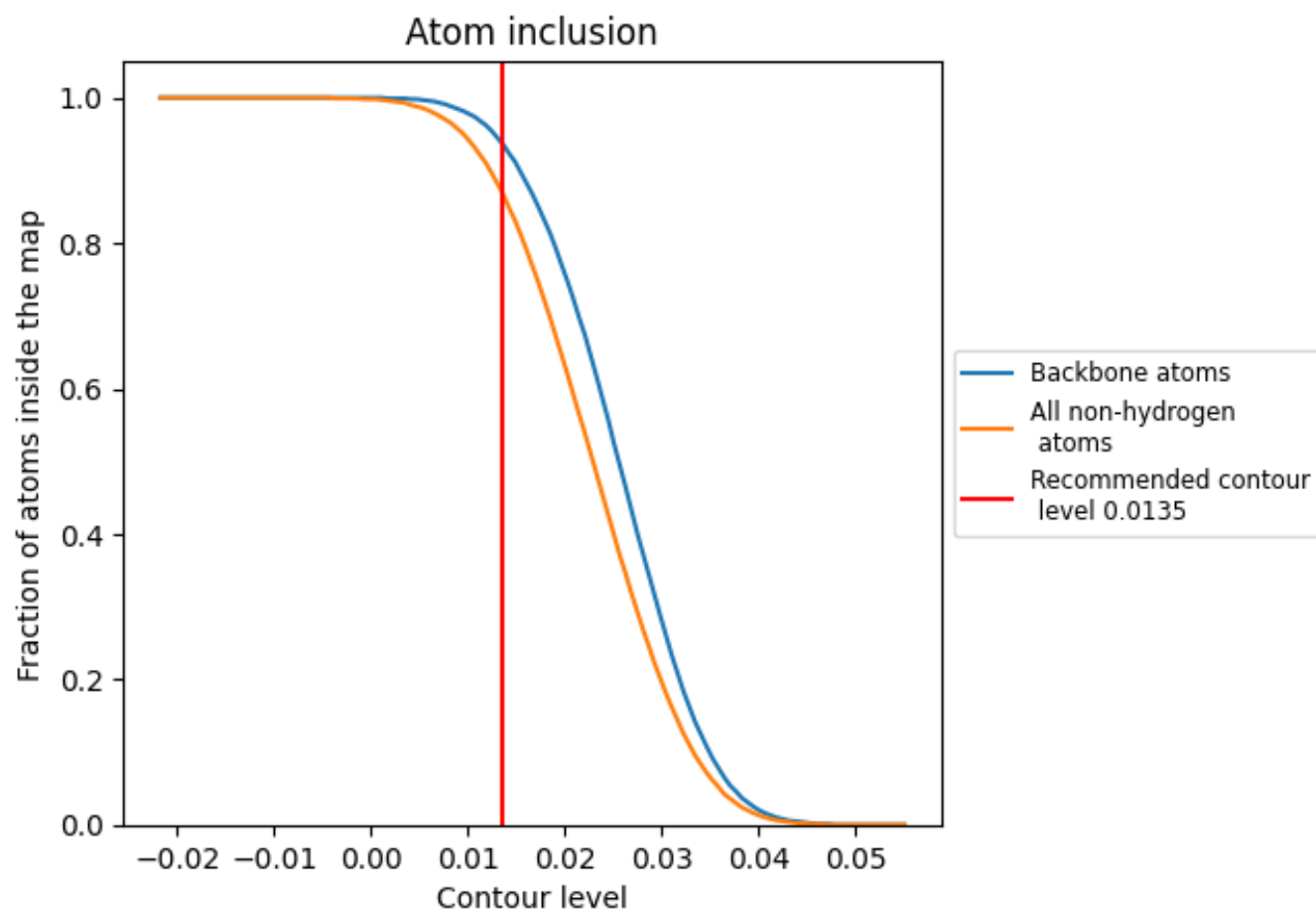
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0135).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 87% 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 (0.0135) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8710	 0.1160
A	 0.8940	 0.1140
B	 0.8820	 0.0970
C	 0.9170	 0.1140
D	 0.7990	 0.0810
E	 0.9070	 0.1100
F	 0.8910	 0.1220
G	 0.8680	 0.0910
H	 0.9070	 0.1220
I	 0.9080	 0.1040
J	 0.9030	 0.0950
K	 0.8820	 0.1240
L	 0.8750	 0.1000
M	 0.6800	 0.0870
N	 0.7760	 0.1280
O	 0.5990	 0.0670
P	 0.4310	 -0.0260
Q	 0.8190	 0.1300
R	 0.8220	 0.1360
S	 0.9940	 0.1600
T	 0.7090	 0.0970
U	 0.9820	 0.1990
V	 0.9980	 0.2100
W	 0.9590	 0.1880
X	 0.9530	 0.1730
Y	 0.9660	 0.1820
Z	 0.9680	 0.2060

