



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 09:09 PM UTC

PDB ID : 8WAK / pdb_00008wak
EMDB ID : EMD-37395
Title : Structure of transcribing complex 2 (TC2), the initially transcribing complex with Pol II positioned 2nt downstream of TSS.
Authors : Chen, X.; Liu, W.; Wang, Q.; Wang, X.; Ren, Y.; Qu, X.; Li, W.; Xu, Y.
Deposited on : 2023-09-07
Resolution : 5.47 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

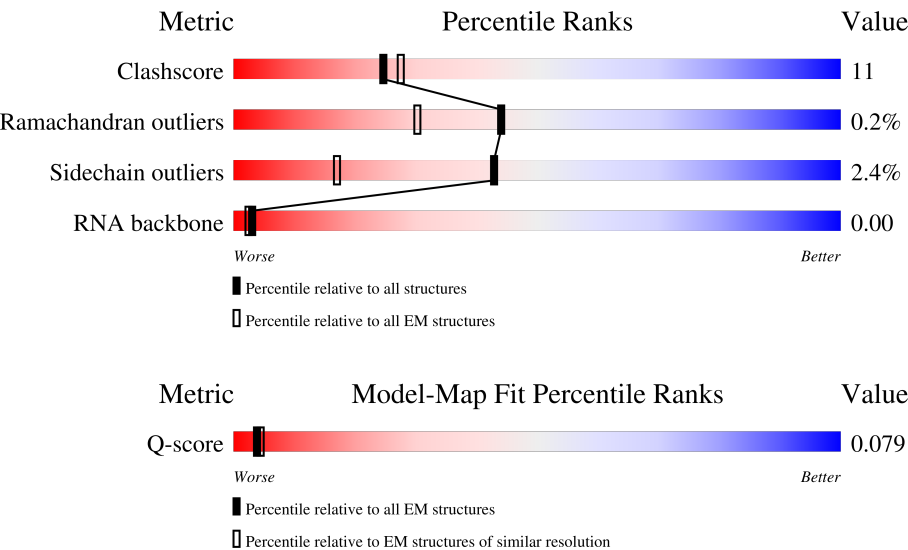
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 5.47 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	470 (4.97 - 5.97)

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

Mol	Chain	Length	Quality of chain
1	0	309	
2	1	548	
3	2	395	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	3	308	
5	4	462	
6	5	71	
7	6	782	
8	7	760	
9	N	8	
10	Z	2	
11	A	1872	
12	B	1199	
13	D	1085	
13	d	1085	
14	E	800	
14	e	800	
15	F	677	
15	f	677	
16	G	349	
17	H	310	
18	I	264	
18	i	264	
19	J	218	
19	j	218	
20	L	161	
20	l	161	
21	O	109	
22	P	339	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
23	Q	376	
24	R	316	
25	S	517	
26	T	249	
27	U	439	
28	V	291	
29	X	99	
30	Y	99	
31	c	929	
32	k	211	
33	m	124	
34	o	1970	
35	p	1174	
36	q	275	
37	r	142	
38	s	210	
39	t	127	
40	u	172	
41	v	150	
42	w	125	
43	x	67	
44	y	117	
45	z	58	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
48	W0F	Z	2500	-	-	X	-

2 Entry composition

There are 49 unique types of molecules in this entry. The entry contains 108642 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 CDK-activating kinase assembly factor MAT1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	171	Total	C	N	O	S	0	0
			1420	882	249	279	10		

- Molecule 2 is a protein called General transcription factor IIH subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	265	Total	C	N	O	S	0	0
			2167	1382	378	395	12		

- Molecule 3 is a protein called General transcription factor IIH subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	329	Total	C	N	O	S	0	0
			2567	1621	440	479	27		

- Molecule 4 is a protein called General transcription factor IIH subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	263	Total	C	N	O	S	0	0
			2066	1323	344	380	19		

- Molecule 5 is a protein called General transcription factor IIH subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	394	Total	C	N	O	S	0	0
			3189	2068	552	557	12		

- Molecule 6 is a protein called General transcription factor IIH subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	5	54	Total	C	N	O	S	0	0
			428	277	67	82	2		

- Molecule 7 is a protein called General transcription and DNA repair factor IIIH helicase subunit XPB.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	605	Total	C	N	O	S	0	0
			4890	3127	848	885	30		

- Molecule 8 is a protein called General transcription and DNA repair factor IIIH helicase subunit XPD.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	7	714	Total	C	N	O	S	0	0
			5751	3683	999	1040	29		

- Molecule 9 is a protein called Alpha-amanitin.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	N	8	Total	C	N	O	S	0	0
			64	39	10	14	1		

- Molecule 10 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	Z	2	Total	C	N	O	P	0	0
			55	21	10	20	4		

- Molecule 11 is a protein called Transcription initiation factor TFIID subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	A	559	Total	C	N	O	S	0	0
			4580	2924	795	834	27		

- Molecule 12 is a protein called Transcription initiation factor TFIID subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	B	963	Total	C	N	O	S	0	0
			7796	5011	1315	1412	58		

- Molecule 13 is a protein called Transcription initiation factor TFIID subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	D	164	Total	C	N	O	S	0	0
			1366	851	256	255	4		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
13	d	158	Total	C	N	O	S	0	0
			1307	814	238	252	3		

- Molecule 14 is a protein called Transcription initiation factor TFIID subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	E	547	Total	C	N	O	S	0	0
			4376	2774	759	822	21		
14	e	539	Total	C	N	O	S	0	0
			4327	2746	748	814	19		

- Molecule 15 is a protein called Transcription initiation factor TFIID subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	F	412	Total	C	N	O	S	0	0
			3143	1994	548	583	18		
15	f	403	Total	C	N	O	S	0	0
			3081	1954	533	576	18		

- Molecule 16 is a protein called Transcription initiation factor TFIID subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	G	144	Total	C	N	O	S	0	0
			1171	742	215	210	4		

- Molecule 17 is a protein called Transcription initiation factor TFIID subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	H	209	Total	C	N	O	S	0	0
			1633	1034	283	311	5		

- Molecule 18 is a protein called Transcription initiation factor TFIID subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	I	120	Total	C	N	O	S	0	0
			959	610	166	177	6		
18	i	121	Total	C	N	O	S	0	0
			967	615	167	178	7		

- Molecule 19 is a protein called Transcription initiation factor TFIID subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	J	90	Total	C	N	O	S	0	0
			720	466	115	135	4		
19	j	95	Total	C	N	O	S	0	0
			759	488	124	143	4		

- Molecule 20 is a protein called Transcription initiation factor TFIID subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	L	76	Total	C	N	O	S	0	0
			622	388	109	122	3		
20	l	107	Total	C	N	O	S	0	0
			876	547	158	166	5		

- Molecule 21 is a protein called Transcription initiation factor IIA subunit 2.

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

- Molecule 22 is a protein called TATA-box-binding protein.

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

- Molecule 23 is a protein called Transcription initiation factor IIA beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Q	113	Total	C	N	O	S	0	0
			930	585	152	189	4		

- Molecule 24 is a protein called Transcription initiation factor IIB.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	R	282	Total	C	N	O	S	0	0
			2167	1353	384	412	18		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
25	S	176	Total	C	N	O	S	0	0
			1461	921	268	268	4		

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

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

- Molecule 27 is a protein called General transcription factor IIE subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	U	184	Total	C	N	O	S	0	0
			1520	957	272	280	11		

- Molecule 28 is a protein called Transcription initiation factor IIE subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	V	165	Total	C	N	O	S	0	0
			1357	865	235	253	4		

- Molecule 29 is a DNA chain called non-template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	X	63	Total	C	N	O	P	0	0
			1301	616	245	377	63		

- Molecule 30 is a DNA chain called template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Y	77	Total	C	N	O	P	0	0
			1571	747	288	459	77		

- Molecule 31 is a protein called Transcription initiation factor TFIID subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	c	127	Total	C	N	O	S	0	0
			1011	638	174	193	6		

- Molecule 32 is a protein called Transcription initiation factor TFIID subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	k	98	Total	C	N	O	S	0	0
			785	499	142	139	5		

- Molecule 33 is a protein called Transcription initiation factor TFIID subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	m	87	Total	C	N	O	S	0	0
			724	456	131	131	6		

- Molecule 34 is a protein called DNA-directed RNA polymerase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	o	1452	Total	C	N	O	S	0	0
			11510	7235	2056	2146	73		

- Molecule 35 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	p	1149	Total	C	N	O	S	0	0
			9175	5796	1614	1701	64		

- Molecule 36 is a protein called DNA-directed RNA polymerase II subunit RPB3.

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

- Molecule 37 is a protein called DNA-directed RNA polymerase II subunit RPB4.

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

- Molecule 38 is a protein called DNA-directed RNA polymerase II subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	s	209	Total	C	N	O	S	0	0
			1720	1089	300	323	8		

- Molecule 39 is a protein called DNA-directed RNA polymerase II subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	t	82	Total	C	N	O	S	0	0
			657	418	113	121	5		

- Molecule 40 is a protein called DNA-directed RNA polymerase II subunit RPB7.

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

- Molecule 41 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

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

- Molecule 42 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	w	114	Total	C	N	O	S	0	0
			927	571	166	179	11		

- Molecule 43 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	x	67	Total	C	N	O	S	0	0
			533	345	90	92	6		

- Molecule 44 is a protein called DNA-directed RNA polymerase II subunit RPB11-a.

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

- Molecule 45 is a protein called RPB12.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	z	44	Total	C	N	O	S	0	0
			372	231	72	63	6		

- Molecule 46 is ZINC ION (CCD ID: ZN) (formula: Zn).

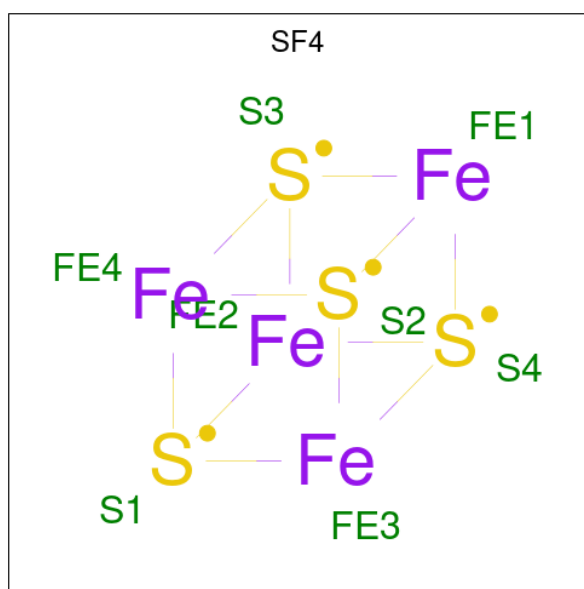
Mol	Chain	Residues	Atoms		AltConf
46	0	2	Total	Zn	0
			2	2	
46	2	3	Total	Zn	0
			3	3	
46	3	2	Total	Zn	0
			2	2	

Continued on next page...

Continued from previous page...

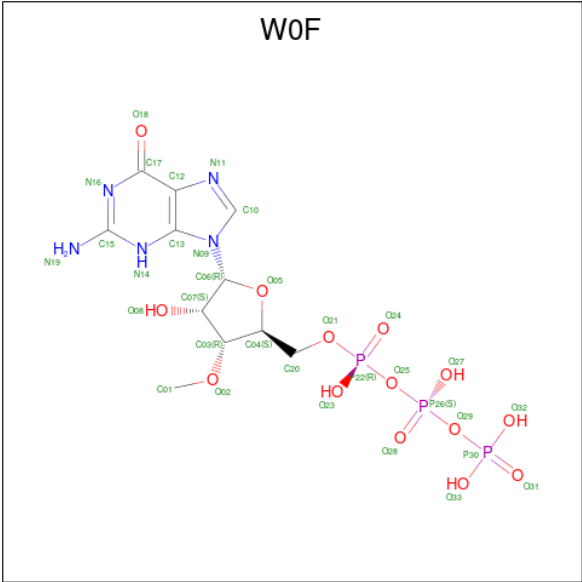
Mol	Chain	Residues	Atoms		AltConf
46	R	1	Total	Zn	0
			1	1	
46	U	1	Total	Zn	0
			1	1	
46	o	2	Total	Zn	0
			2	2	
46	p	1	Total	Zn	0
			1	1	
46	q	1	Total	Zn	0
			1	1	
46	w	2	Total	Zn	0
			2	2	
46	x	1	Total	Zn	0
			1	1	
46	z	1	Total	Zn	0
			1	1	

- Molecule 47 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
47	7	1	Total	Fe	S	0
			8	4	4	

- Molecule 48 is $[[(2 \text{ {S}}, 3 \text{ {R}}, 4 \text{ {S}}, 5 \text{ {R}}) - 5 - (2\text{-azanyl-6-oxidanylidene-3 {H}}) \text{-purin-9-y l}) - 3\text{-methoxy-4-oxidanyl-oxolan-2-yl}] \text{methoxy-oxidanyl-phosphoryl}] \text{phosphono hydrogen phosphate}$ (CCD ID: W0F) (formula: $\text{C}_{11}\text{H}_{18}\text{N}_5\text{O}_{14}\text{P}_3$).



Mol	Chain	Residues	Atoms					AltConf
48	Z	1	Total	C	N	O	P	0
			33	11	5	14	3	

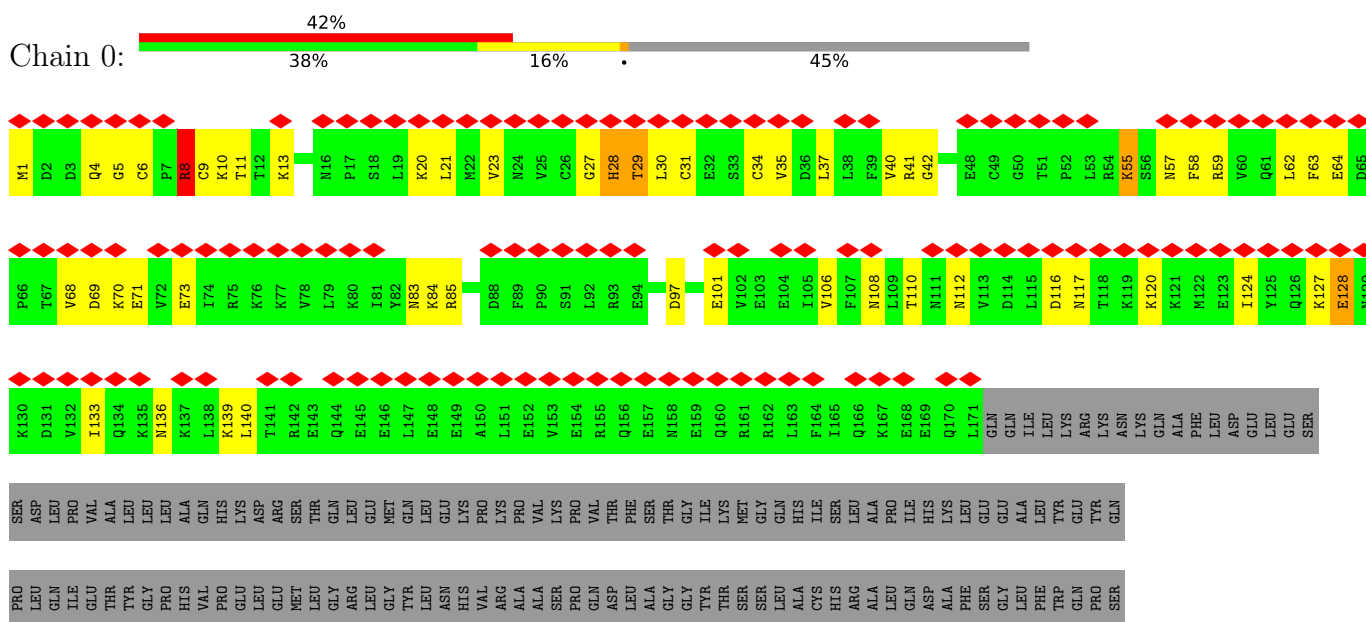
- Molecule 49 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
49	o	1	Total	Mg	0
			1	1	

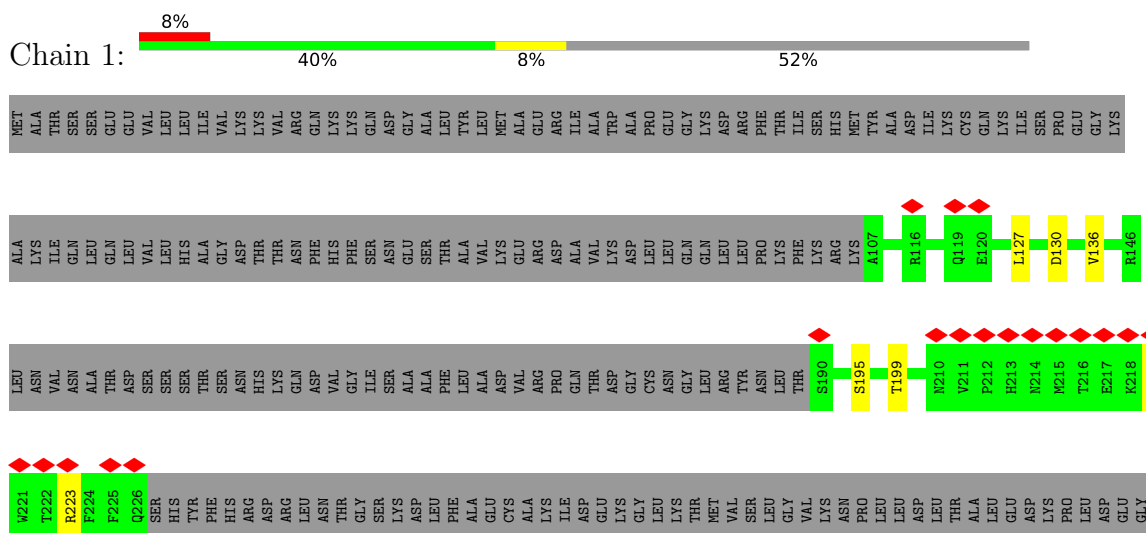
3 Residue-property plots

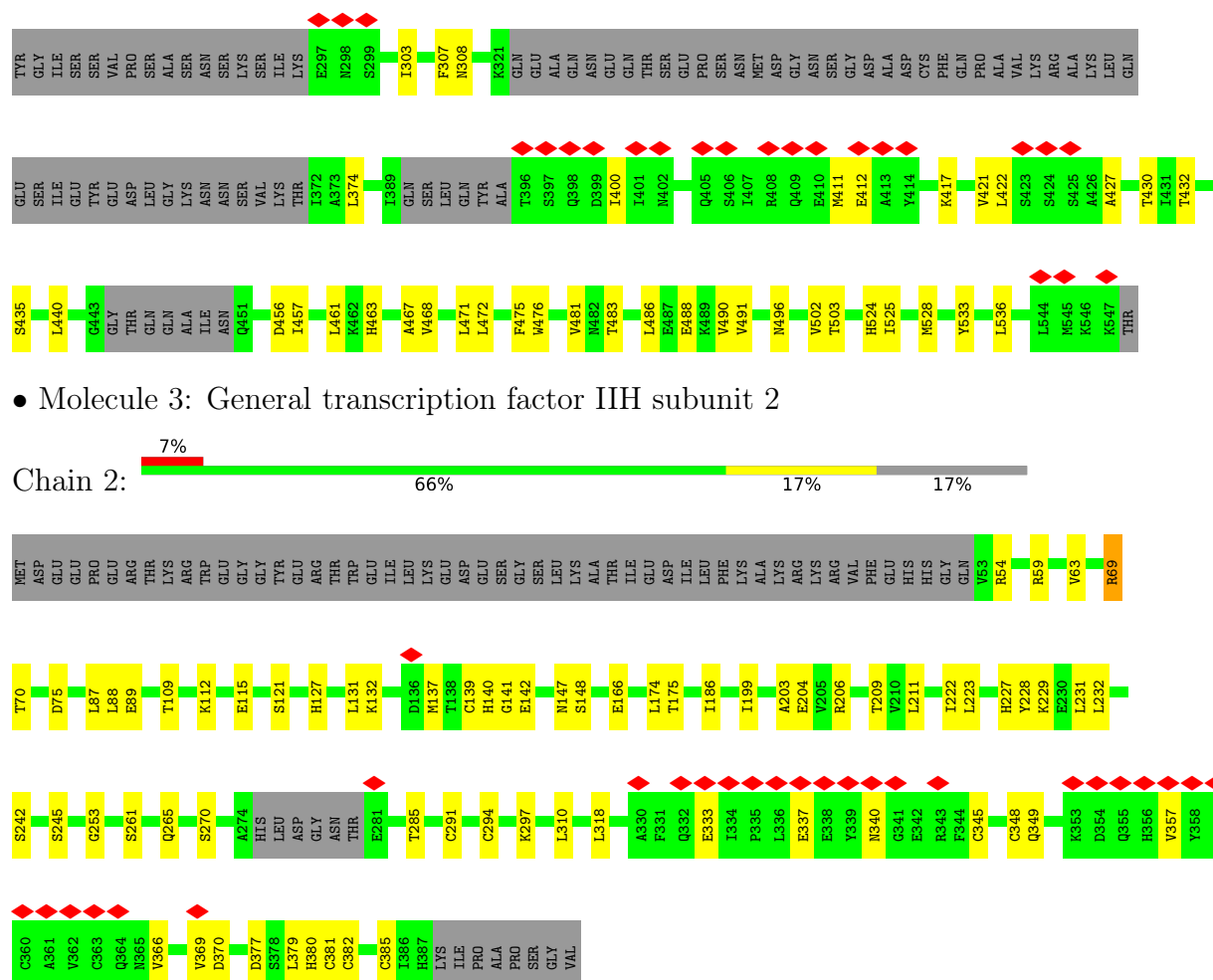
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: CDK-activating kinase assembly factor MAT1

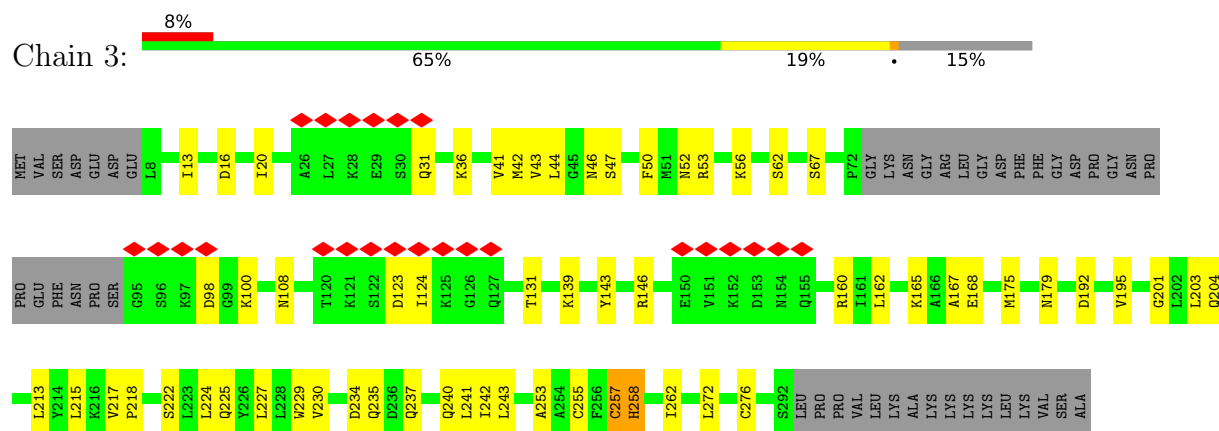


• Molecule 2: General transcription factor IIH subunit 1

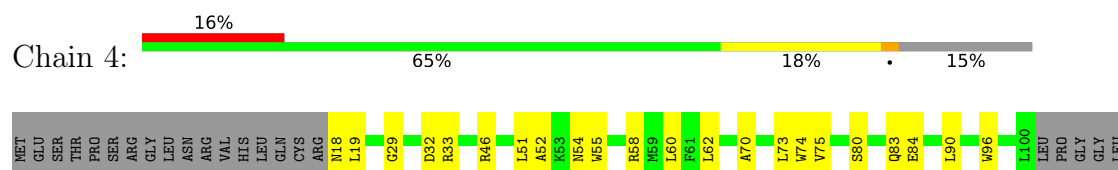




• Molecule 4: General transcription factor IIH subunit 3

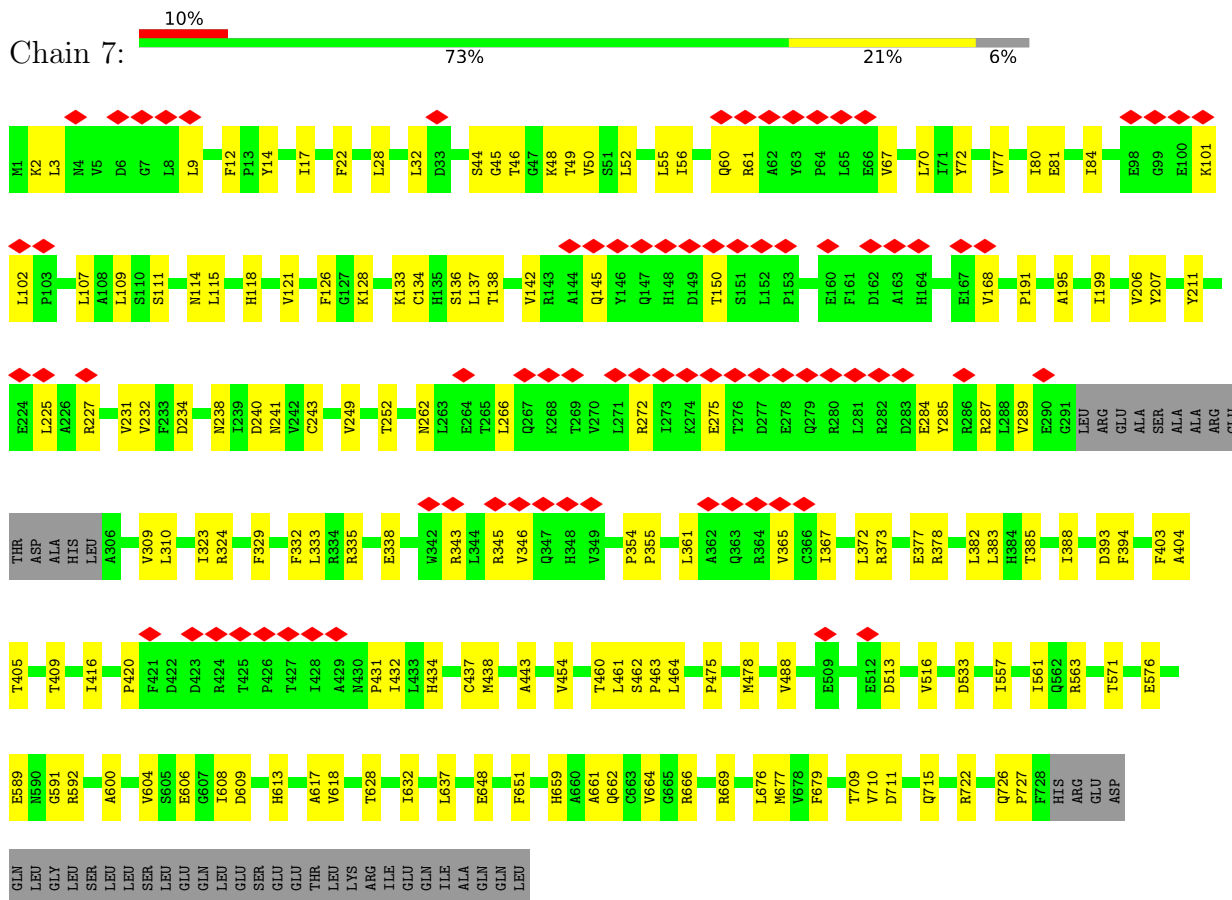


• Molecule 5: General transcription factor IIH subunit 4

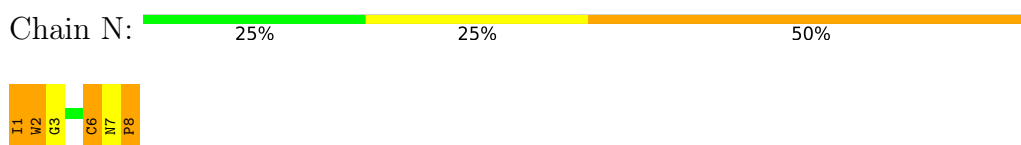


SER MET SER GLY ALA ASP THR VAL TVR MET GLU TVR HIS SER SER ARG SER LYS ALA PRO SER LYS VAL HIS HIS PRO PHE LEU LYS ARG PHE ARG ARG LYS

• Molecule 8: General transcription and DNA repair factor IIH helicase subunit XPD



• Molecule 9: Alpha-amanitin



• Molecule 10: RNA



• Molecule 11: Transcription initiation factor TFIID subunit 1



MET GLY PRO GLY CYS ASP LEU LEU ARG THR ALA THR ILE THR ALA ALA ILE MET SER ASP THR ASP SER ASP GLU ASP SER ALA GLY GLY PRO PHE SER LEU ALA GLY PHE LEU PHE GLY ASN ILE ASN GLY ALA GLY GLN LEU LEU GLY GLY GLY VAL LEU ASP ASP

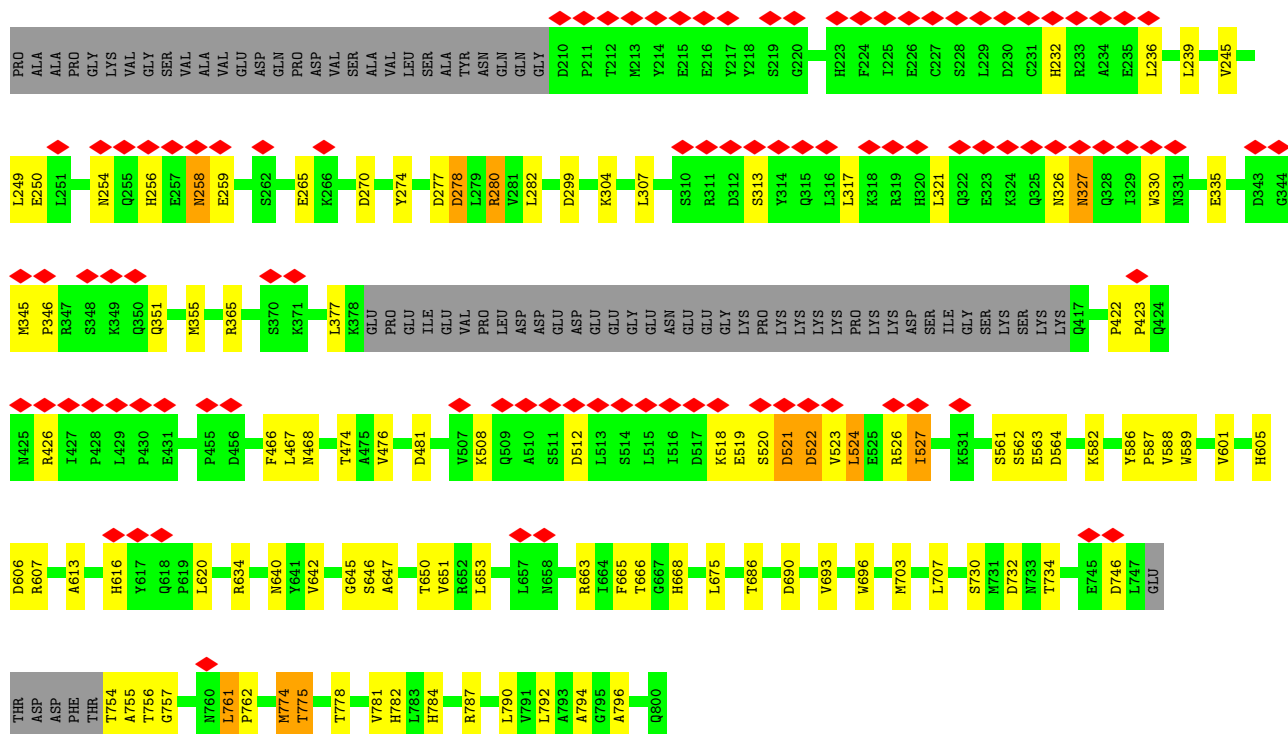


[illegible]

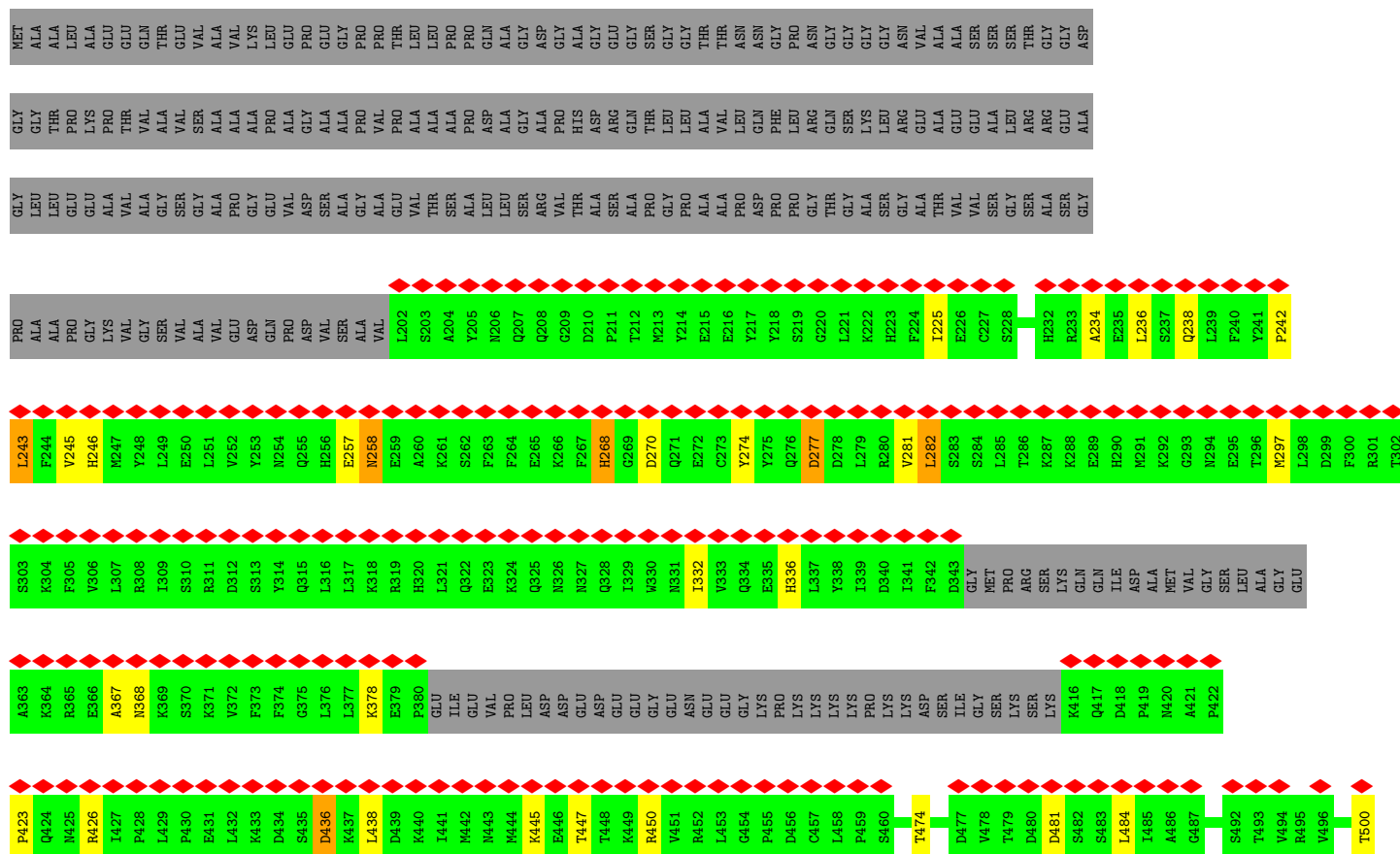
- Molecule 12: Transcription initiation factor TFIID subunit 2

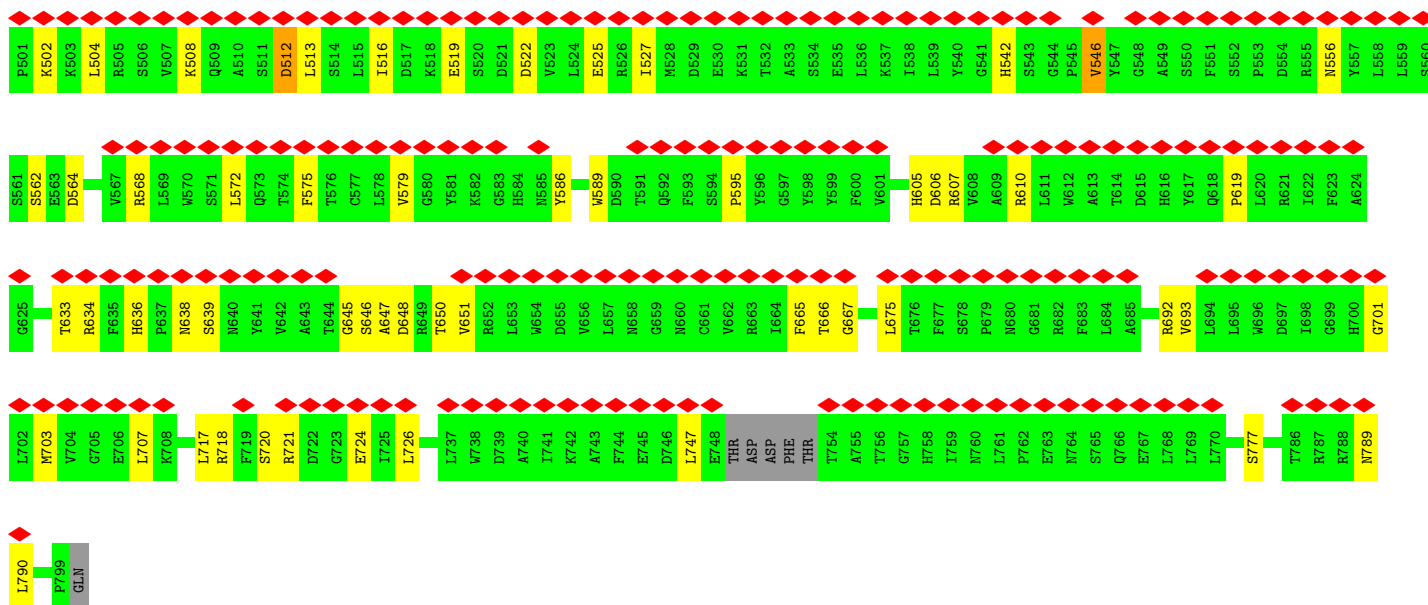
[illegible]



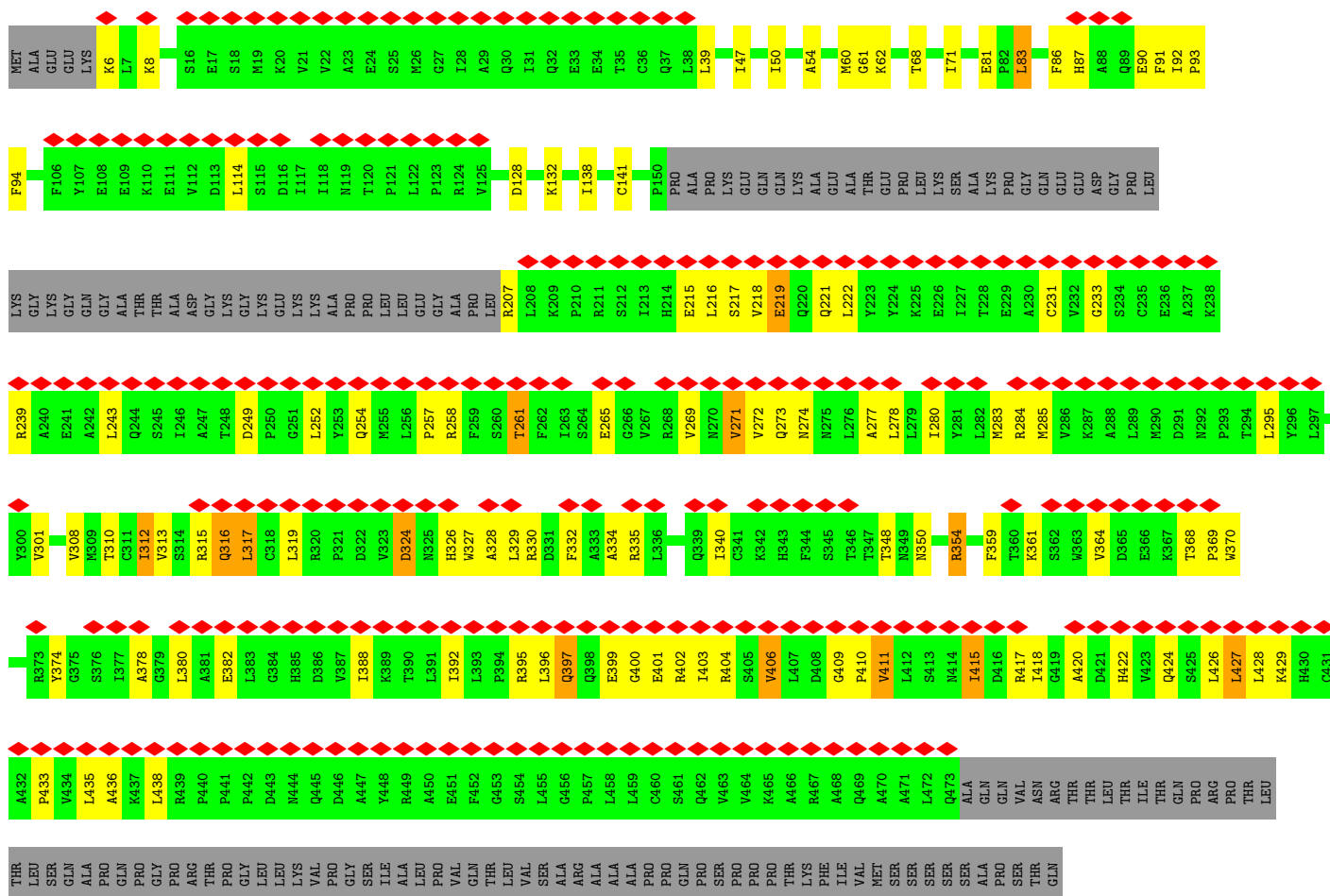
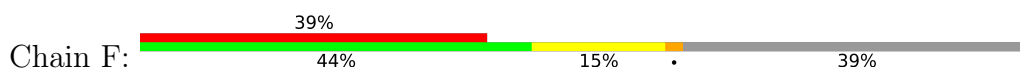


• Molecule 14: Transcription initiation factor TFIID subunit 5

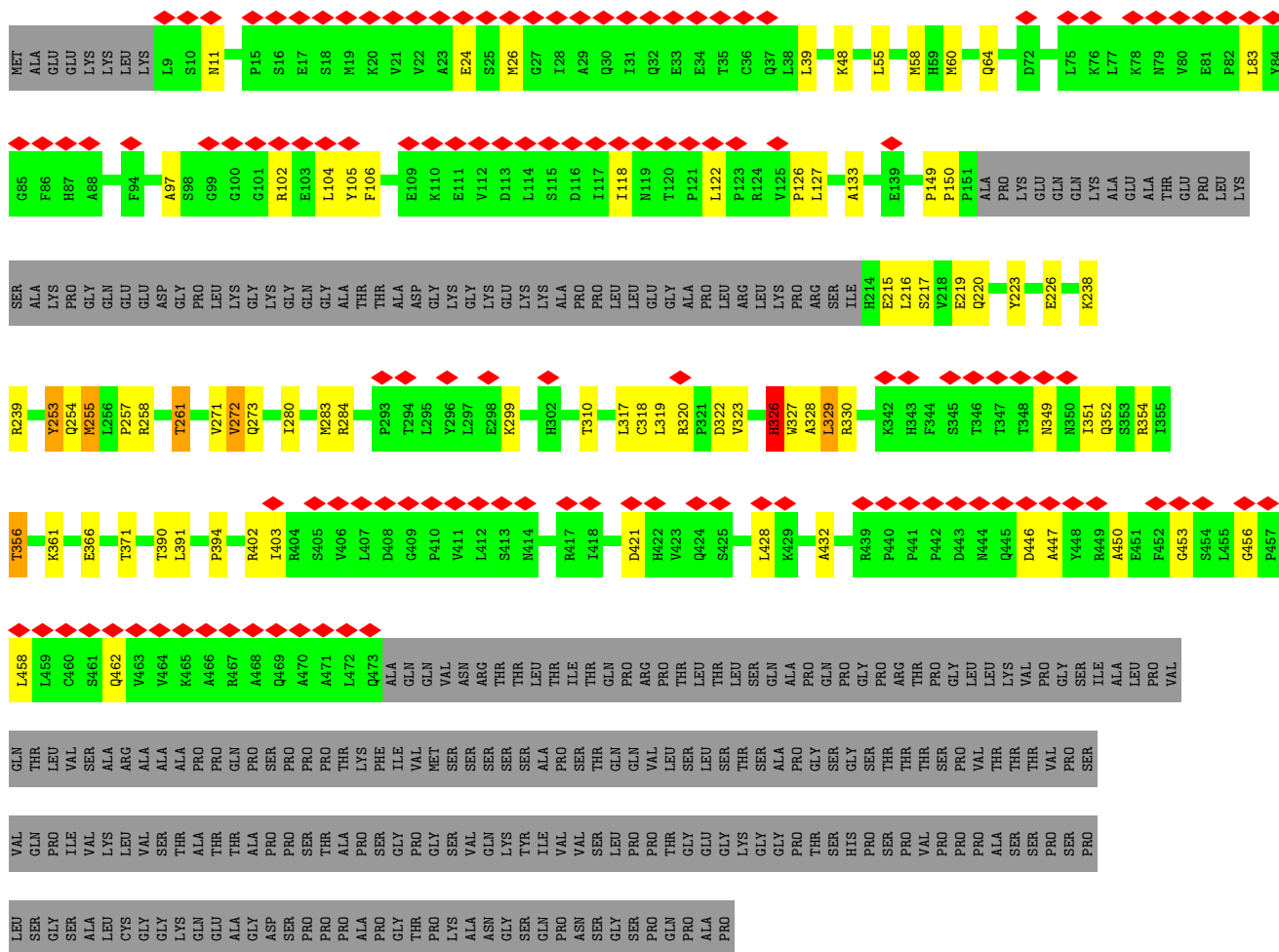




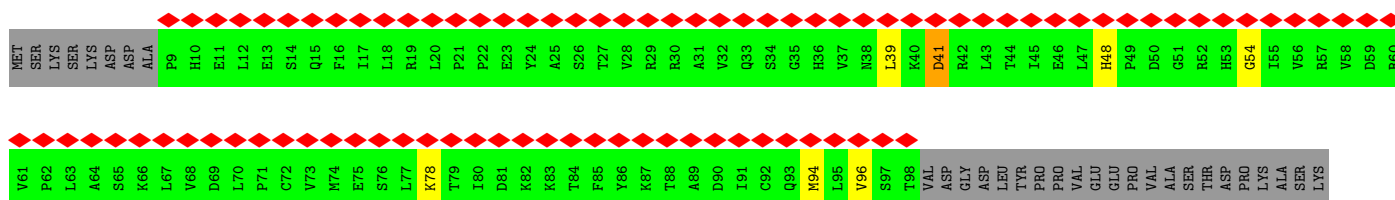
• Molecule 15: Transcription initiation factor TFIID subunit 6

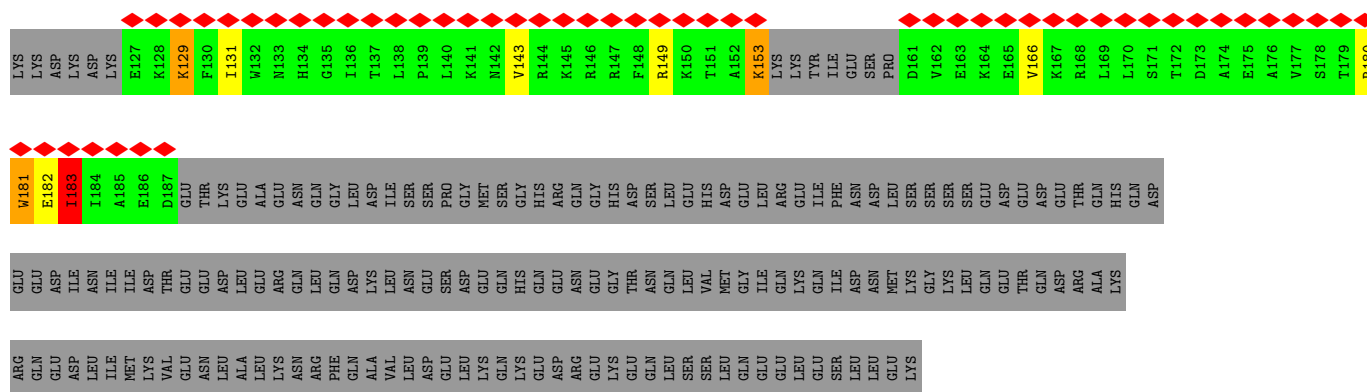


- Molecule 15: Transcription initiation factor TFIID subunit 6

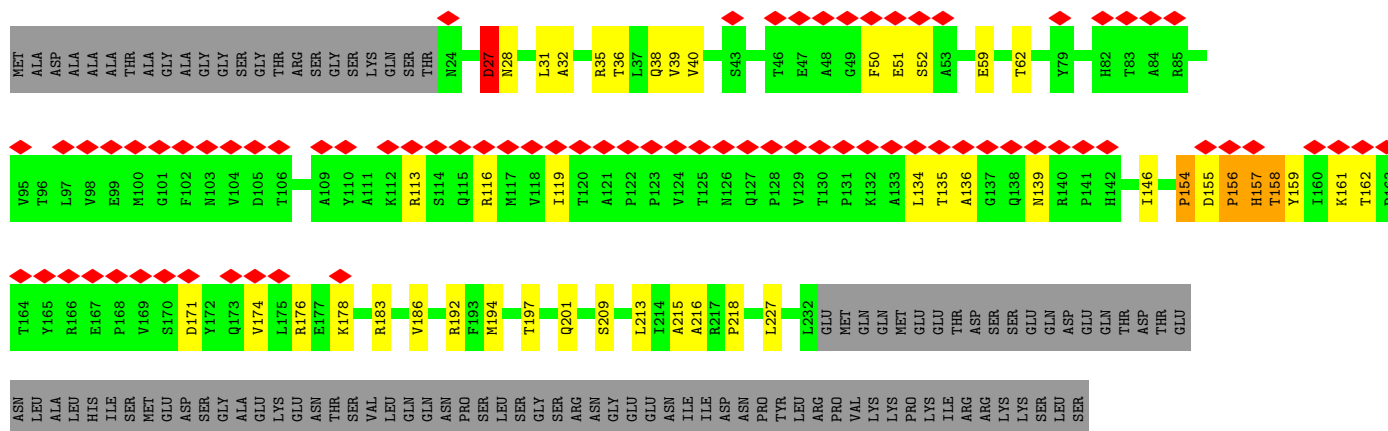


- Molecule 16: Transcription initiation factor TFIID subunit 7

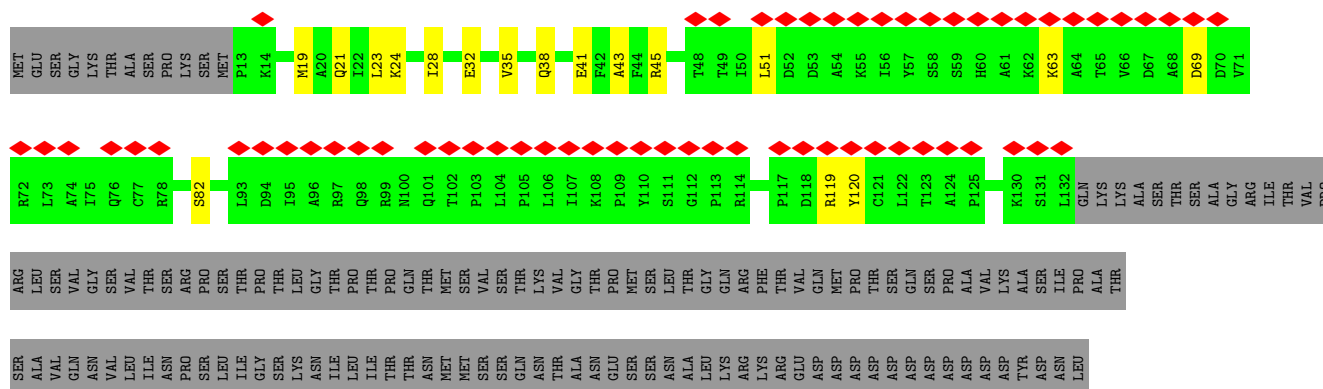
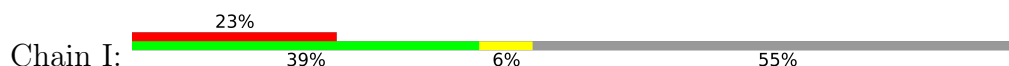




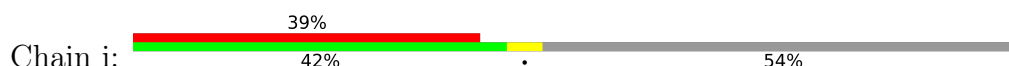
• Molecule 17: Transcription initiation factor TFIID subunit 8

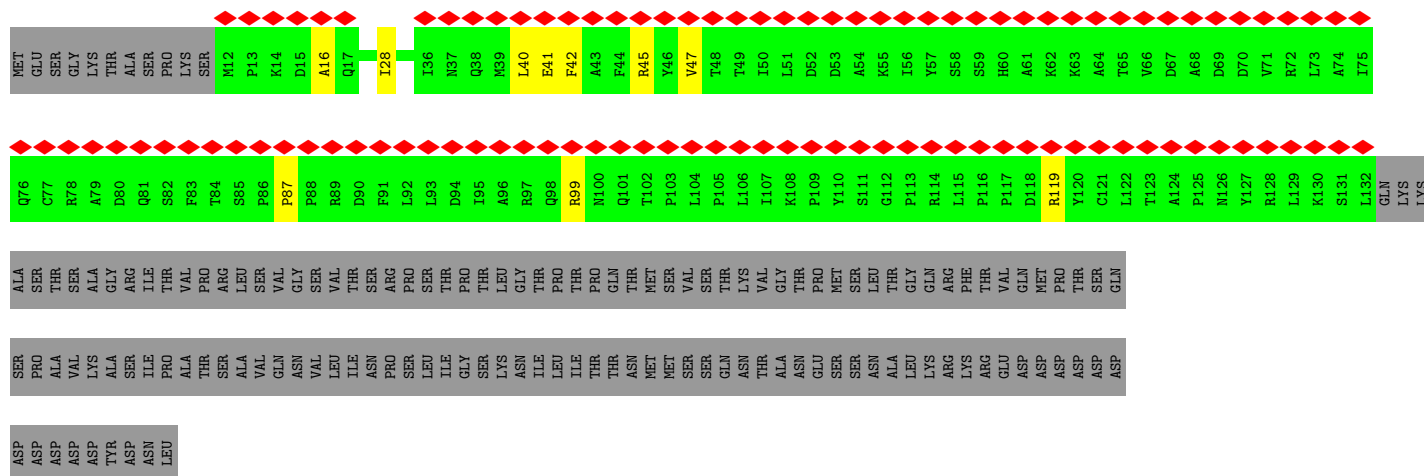


• Molecule 18: Transcription initiation factor TFIID subunit 9

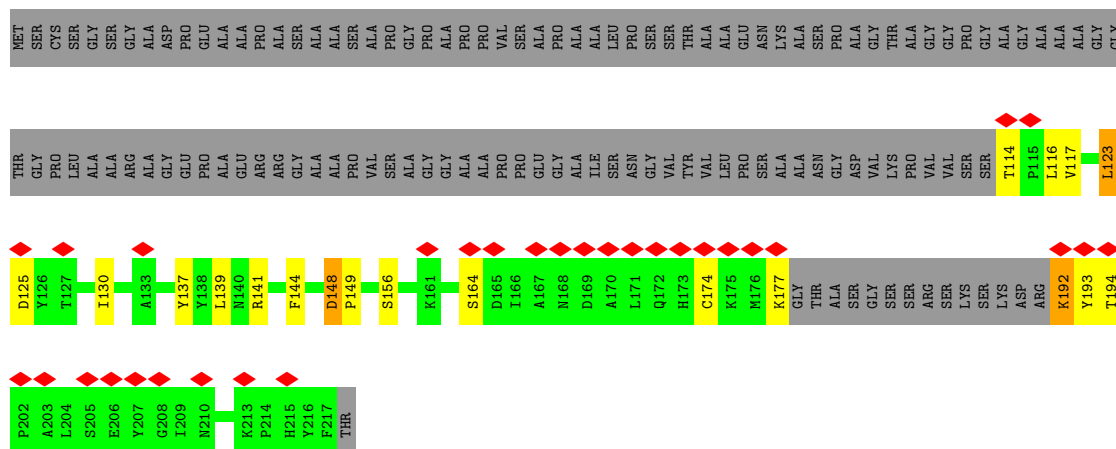


• Molecule 18: Transcription initiation factor TFIID subunit 9

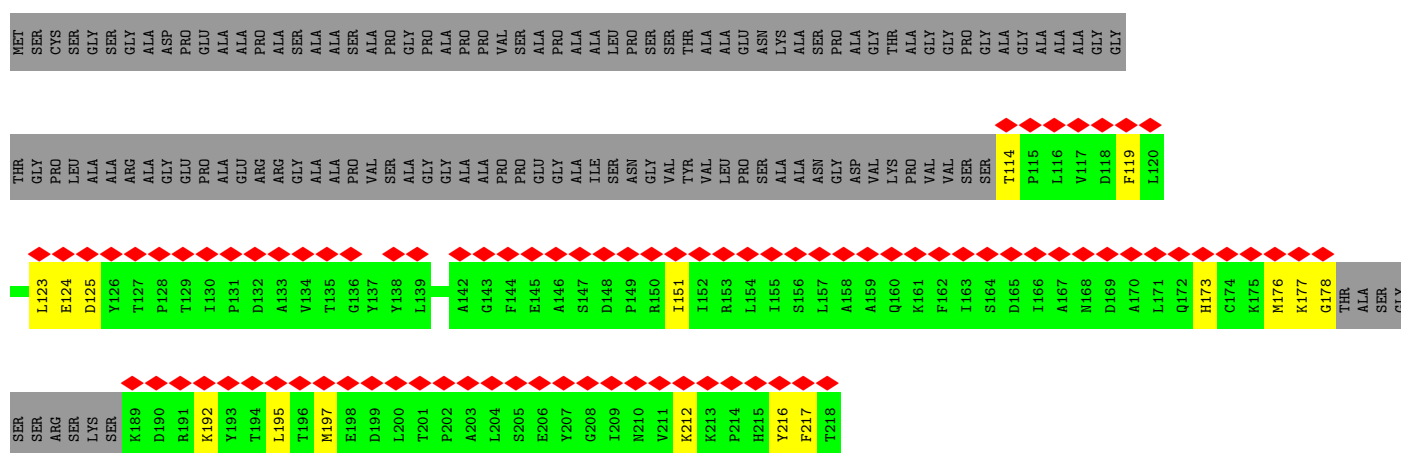
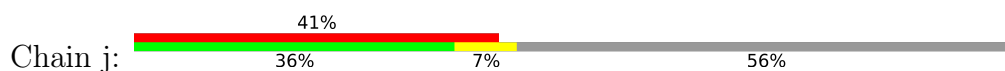




• Molecule 19: Transcription initiation factor TFIID subunit 10



• Molecule 19: Transcription initiation factor TFIID subunit 10



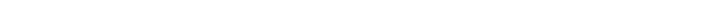
• Molecule 20: Transcription initiation factor TFIID subunit 12

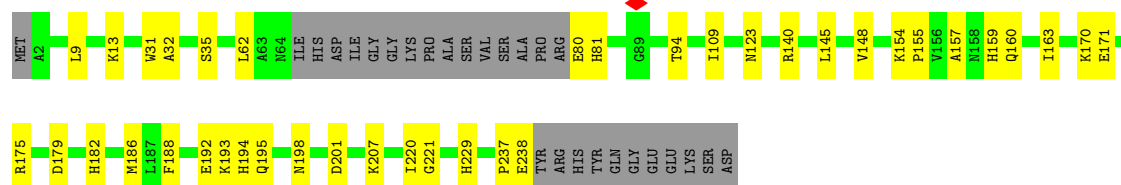
[illegible]

Chain R: 74% 15% 11%

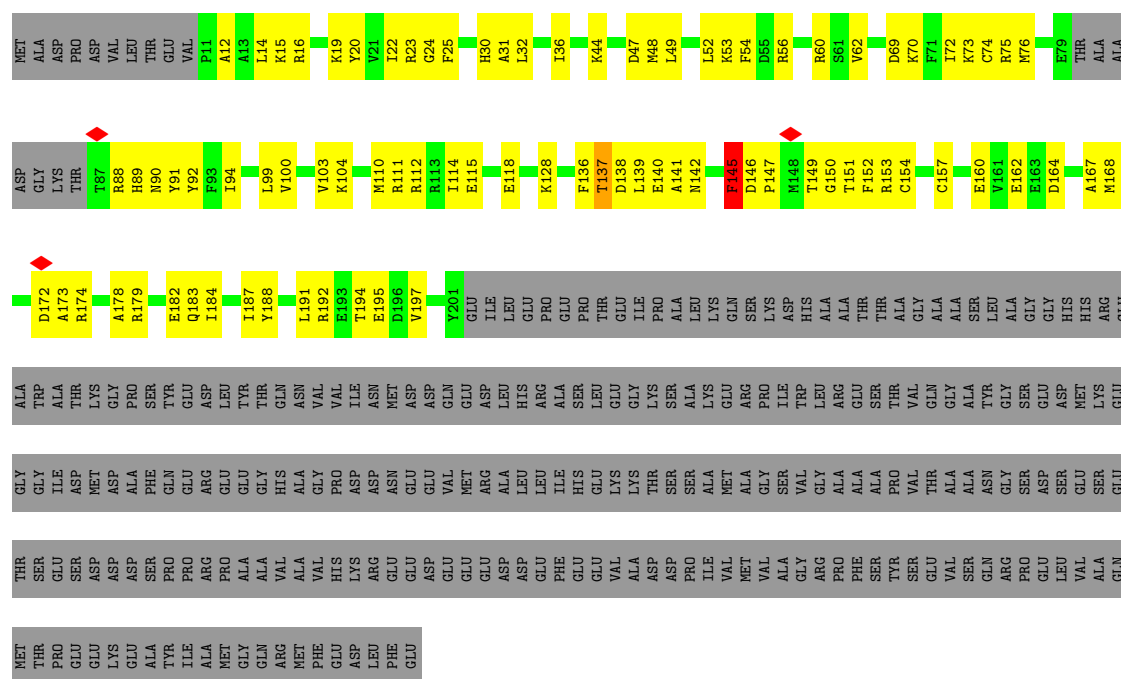
MET	ALA	SER	THR	SER	ARG	LEU	ASP	ALA	LEU	PRO	ARG	VAL	T14	L23	D31	M32	L39	I46	D47	V48	G49	S50	GLU	TRP	ARG	THR	PHE	SER	ASN	ASP	LYS	ALA	THR	LYS	ASP	PRO	SER	ARG	VAL	GLY	ASP	SER	GLN	N72	P73	L74	L75	M83	I84	G87	A90
F93	D94	E95	G96	G97	N98	S99	K100	Y101	Q102	N103	R104	R105	T106	M107	R112	I121	T122	T123	M124	P126	R127	I128	N129	P130	L131	R132	M133	I134	T138	E171	F177	K178	L179	A182	V183	K188	R248	I251	I277	Q287	L316										

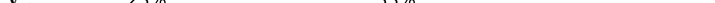
[illegible]

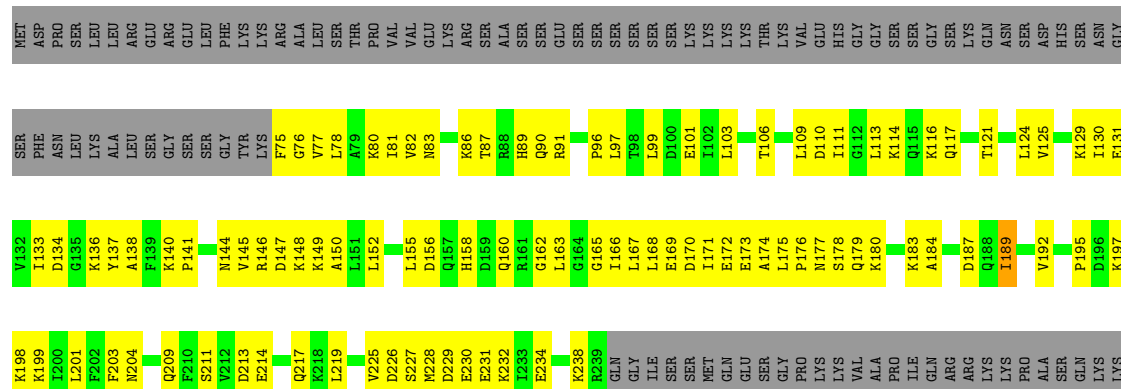
- Chain T:  73% 16% 11%



- Chain U: 22% 19% 58%

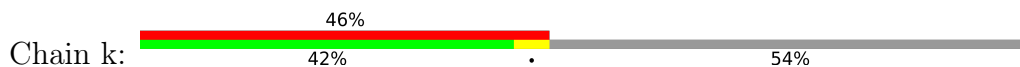


- Chain V:  23% 33% 43%



[illegible]

- Molecule 32: Transcription initiation factor TFIID subunit 11

[illegible]

- Molecule 33: Transcription initiation factor TFIID subunit 13



ASN	TYR	GLY	SER	V61	I62	E63	F64	I65	T66	E67	H68	T69	H70	K71	A72	M73	S74	I75	G76	R77	Q78	G79	R80	V81	Q82	V83	E84	D85	I86	V87	F88	L89	I90	R91	K92	D93	F94	R95	K96	F97	A98	R99	V100	K101	D102	L103	L104	T105	M106	N107	E108	E109	L110	K111	R112	A113	R114	LYS	ALA	PHE	ASP	GLU	VAL
				ASP	GLY	GLU	GLU	ASP	PRO	THR	PHE	GLU	GLU	ASN	GLU	ILE	GLY	GLY	ALA	GLU	GLY	GLN	LYS	R28	K29	R30	L31	F32	S33	K34	E35	L36	R37	C38	M39	M40	V41	C42	F43	C44	D45	D46	Q47	M48	P49	Y50	T51	E52	S53	V54	D55	I56	L57	E58	D59	L60							

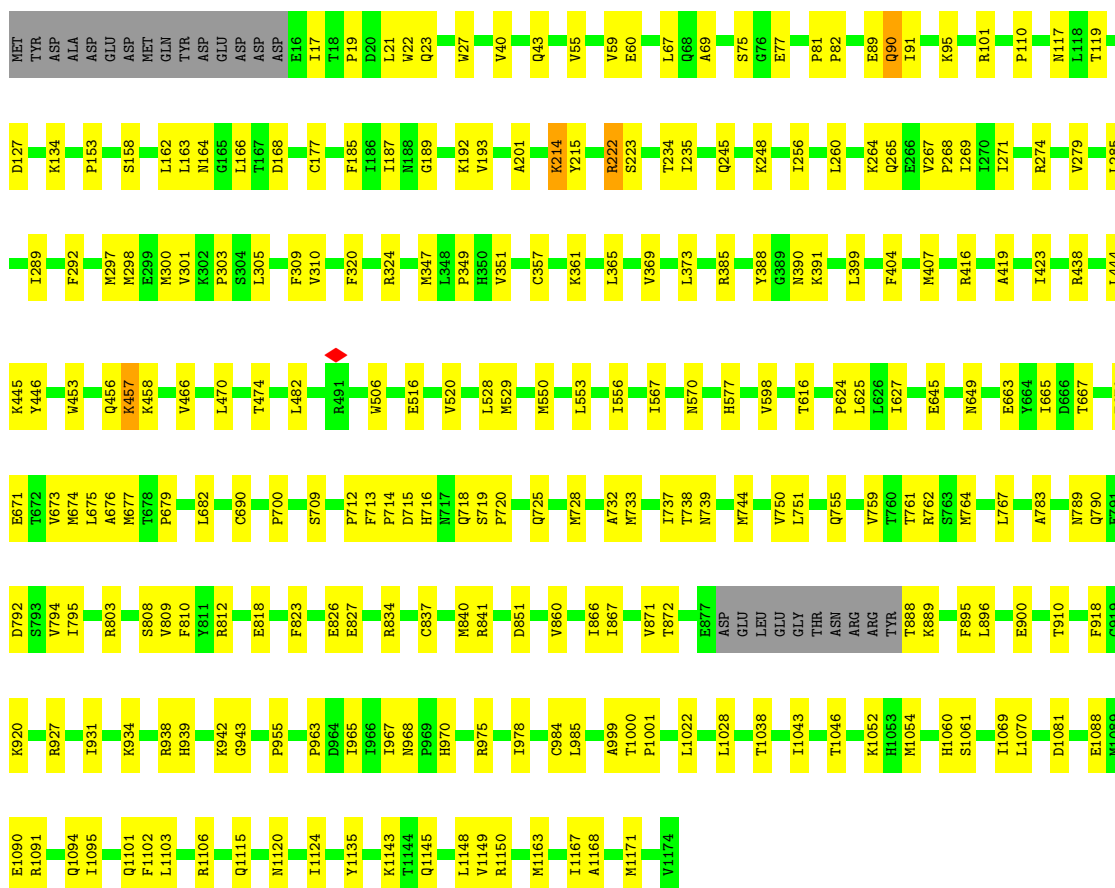
Chain o: 56% 17% 0 26%



[illegible]

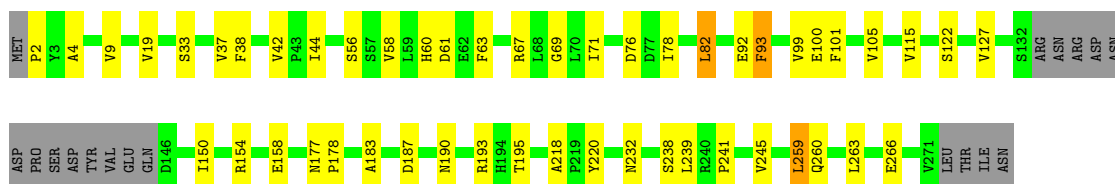
- Molecule 35: DNA-directed RNA polymerase subunit beta

Chain p: 77% 21% .



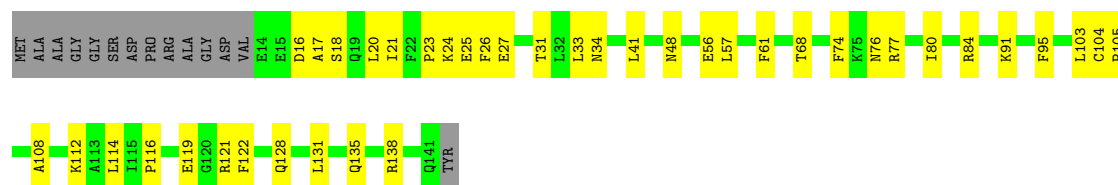
- Molecule 36: DNA-directed RNA polymerase II subunit RPB3

Chain q: 75% 17% • 7%



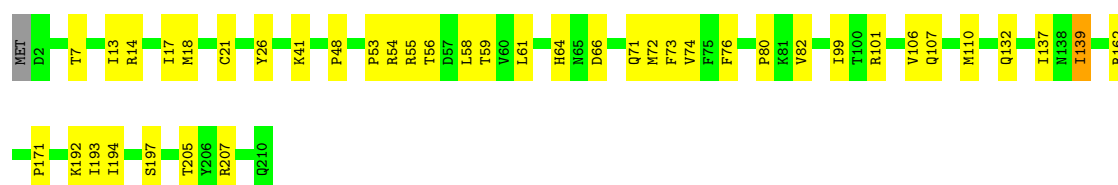
- Molecule 37: DNA-directed RNA polymerase II subunit RPB4

Chain r: 



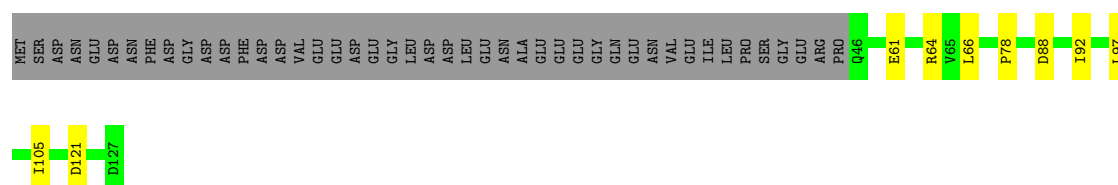
- Molecule 38: DNA-directed RNA polymerase II subunit E

Chain s: 



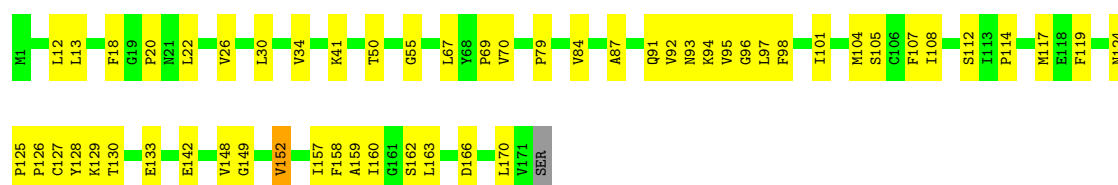
- Molecule 39: DNA-directed RNA polymerase II subunit F

Chain t: 



- Molecule 40: DNA-directed RNA polymerase II subunit RPB7

Chain u: 



- Molecule 41: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain v: 



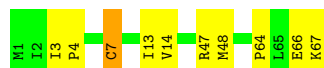
- Molecule 42: DNA-directed RNA polymerase II subunit RPB9

Chain w:  66% 23% 9%



- Molecule 43: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain x:  85% 13%



- Molecule 44: DNA-directed RNA polymerase II subunit RPB11-a

Chain y:  82% 15%



- Molecule 45: RPB12

Chain z:  57% 19% 24%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	6727	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.990	Depositor
Minimum map value	-0.875	Depositor
Average map value	0.041	Depositor
Map value standard deviation	0.187	Depositor
Recommended contour level	0.477	Depositor
Map size ($\text{\AA}$)	426.88, 426.88, 426.88	wwPDB
Map dimensions	160, 160, 160	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	2.668, 2.668, 2.668	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CSX, ILX, HYP, WOF, ATP, TRX, ZN, SF4, MG, G2L

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	0	0.41	0/1437	0.71	3/1926 (0.2%)
2	1	0.20	0/2210	0.34	0/2975
3	2	0.18	0/2624	0.33	1/3555 (0.0%)
4	3	0.24	0/2103	0.36	0/2846
5	4	0.31	0/3262	0.45	1/4418 (0.0%)
6	5	0.41	0/433	0.79	1/585 (0.2%)
7	6	0.19	0/4994	0.32	0/6745
8	7	0.17	0/5875	0.30	0/7955
9	N	0.42	0/22	0.98	0/26
11	A	0.63	0/4698	0.95	5/6345 (0.1%)
12	B	0.46	1/7993 (0.0%)	0.68	6/10836 (0.1%)
13	D	0.56	0/1379	0.88	3/1843 (0.2%)
13	d	0.47	0/1321	0.71	0/1772
14	E	0.45	1/4482 (0.0%)	0.72	3/6069 (0.0%)
14	e	0.55	1/4433 (0.0%)	0.77	0/6004
15	F	0.63	1/3201 (0.0%)	1.00	7/4347 (0.2%)
15	f	0.47	0/3140	0.80	6/4268 (0.1%)
16	G	0.68	0/1190	0.95	1/1601 (0.1%)
17	H	0.63	3/1673 (0.2%)	0.86	5/2285 (0.2%)
18	I	0.20	0/981	0.41	0/1332
18	i	0.22	0/989	0.40	0/1343
19	J	0.83	0/736	1.15	2/998 (0.2%)
19	j	0.74	0/775	0.97	0/1049
20	L	0.69	0/630	1.14	1/852 (0.1%)
20	l	0.59	0/888	0.88	0/1194
21	O	0.26	0/816	0.36	0/1105
22	P	0.12	0/1448	0.24	0/1948
23	Q	0.18	0/945	0.35	0/1274
24	R	0.19	0/2199	0.37	0/2967
25	S	0.16	0/1496	0.37	0/2013
26	T	0.13	0/1817	0.28	0/2445
27	U	0.35	0/1545	0.69	1/2075 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
28	V	0.24	0/1380	0.58	0/1854
29	X	0.28	0/1460	0.59	0/2251
30	Y	0.31	0/1761	0.53	0/2713
31	c	0.48	0/1035	0.67	0/1406
32	k	0.28	0/799	0.53	1/1070 (0.1%)
33	m	0.85	0/733	1.18	1/977 (0.1%)
34	o	0.26	1/11723 (0.0%)	0.37	0/15830
35	p	0.27	0/9358	0.35	0/12633
36	q	0.32	1/2102 (0.0%)	0.36	0/2857
37	r	0.11	0/1064	0.22	0/1428
38	s	0.22	0/1751	0.32	0/2366
39	t	0.23	0/667	0.30	0/901
40	u	0.15	0/1382	0.28	0/1874
41	v	0.24	0/1207	0.31	0/1628
42	w	0.18	0/948	0.30	0/1284
43	x	0.29	0/542	0.36	0/730
44	y	0.28	0/939	0.34	0/1271
45	z	0.20	0/377	0.31	0/500
All	All	0.38	9/110963 (0.0%)	0.58	48/150569 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
24	R	0	1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	H	28	ASN	C-O	-7.46	1.15	1.24
17	H	27	ASP	C-O	-7.05	1.15	1.24
36	q	187	ASP	C-O	7.04	1.27	1.23
17	H	31	LEU	C-O	-6.20	1.16	1.24
12	B	61	ASN	C-O	-6.13	1.18	1.24
14	E	524	LEU	C-O	5.77	1.30	1.24
14	e	445	LYS	C-O	5.62	1.30	1.24
15	F	395	ARG	C-O	5.61	1.31	1.24
34	o	1121	VAL	CA-CB	-5.53	1.51	1.54

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	55	LYS	CB-CA-C	-11.48	94.97	111.85
12	B	491	HIS	N-CA-C	-9.38	101.06	111.28
15	f	149	PRO	O-C-N	9.05	125.47	121.31
14	E	756	THR	N-CA-C	-8.38	103.19	113.50
17	H	32	ALA	N-CA-C	-8.26	102.23	111.07
17	H	27	ASP	N-CA-C	-7.89	102.76	111.36
14	E	762	PRO	N-CA-C	7.39	124.25	114.27
15	F	271	VAL	N-CA-C	-7.26	105.93	112.90
11	A	715	PRO	N-CA-C	-7.07	100.14	111.03
12	B	495	GLN	N-CA-C	-7.05	104.68	113.28
6	5	38	ILE	N-CA-CB	-6.92	102.45	110.55
11	A	396	LEU	N-CA-C	-6.79	104.75	113.16
1	0	8	ARG	N-CA-CB	-6.77	99.04	110.49
32	k	180	PRO	N-CA-C	6.76	118.95	110.70
15	f	326	HIS	N-CA-C	-6.67	104.24	112.38
15	f	319	LEU	N-CA-C	-6.58	103.93	112.68
11	A	467	ILE	N-CA-C	-6.40	104.03	111.00
3	2	70	THR	N-CA-C	-6.35	104.46	111.82
13	D	999	MET	N-CA-C	-6.29	104.34	111.07
11	A	1205	PHE	CA-CB-CG	-6.28	107.52	113.80
5	4	439	ARG	CB-CA-C	6.19	122.73	110.42
13	D	964	GLU	N-CA-C	-6.16	97.69	110.80
17	H	27	ASP	CA-C-O	-6.11	113.94	120.42
19	J	148	ASP	CA-C-N	6.11	125.83	119.05
19	J	148	ASP	C-N-CA	6.11	125.83	119.05
15	f	255	MET	N-CA-C	-5.88	104.98	114.09
15	F	316	GLN	CB-CA-C	5.77	120.19	110.79
27	U	145	PHE	CA-CB-CG	5.75	119.55	113.80
12	B	583	GLU	CB-CA-C	-5.73	101.28	110.79
1	0	8	ARG	CB-CG-CD	-5.71	98.17	111.30
15	F	310	THR	CB-CA-C	5.71	120.26	110.79
12	B	181	GLY	CA-C-O	-5.68	118.22	122.37
15	F	330	ARG	N-CA-C	-5.65	105.12	111.28
15	f	150	PRO	N-CA-C	5.62	117.56	110.70
15	F	324	ASP	N-CA-C	-5.57	105.31	111.71
13	D	1002	ARG	CB-CA-C	5.55	122.03	110.32
12	B	264	GLU	N-CA-C	-5.54	106.18	113.17
33	m	71	LYS	CB-CA-C	5.43	119.81	110.79
16	G	183	ILE	N-CA-C	-5.43	102.51	109.30
14	E	270	ASP	CB-CA-C	5.42	119.14	110.09
15	f	329	LEU	N-CA-C	-5.39	106.41	112.87
15	F	272	VAL	N-CA-C	-5.36	105.16	110.62
12	B	491	HIS	CB-CA-C	5.26	119.52	110.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	L	106	ARG	N-CA-C	-5.21	106.95	113.15
11	A	1067	GLN	CB-CA-C	5.15	119.35	110.79
17	H	134	LEU	CB-CA-C	-5.14	110.62	116.54
17	H	51	GLU	CB-CA-C	-5.04	100.48	109.71
15	F	438	LEU	N-CA-C	5.02	118.48	111.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
24	R	106	THR	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	1420	0	1420	122	0
2	1	2167	0	2175	39	0
3	2	2567	0	2539	96	0
4	3	2066	0	2097	102	0
5	4	3189	0	3243	142	0
6	5	428	0	434	43	0
7	6	4890	0	4949	93	0
8	7	5751	0	5794	141	0
9	N	64	0	51	7	0
10	Z	55	0	19	6	0
11	A	4580	0	4502	97	0
12	B	7796	0	7751	119	0
13	D	1366	0	1390	75	0
13	d	1307	0	1318	14	0
14	E	4376	0	4256	74	0
14	e	4327	0	4197	59	0
15	F	3143	0	3093	102	0
15	f	3081	0	3012	70	0
16	G	1171	0	1222	15	0
17	H	1633	0	1621	32	0
18	I	959	0	969	13	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	i	967	0	977	9	0
19	J	720	0	719	13	0
19	j	759	0	759	14	0
20	L	622	0	620	19	0
20	l	876	0	893	10	0
21	O	806	0	818	18	0
22	P	1422	0	1514	18	0
23	Q	930	0	888	12	0
24	R	2167	0	2193	38	0
25	S	1461	0	1429	41	0
26	T	1788	0	1819	54	0
27	U	1520	0	1520	213	0
28	V	1357	0	1381	90	0
29	X	1301	0	709	34	0
30	Y	1571	0	865	48	0
31	c	1011	0	975	18	0
32	k	785	0	818	8	0
33	m	724	0	744	24	0
34	o	11510	0	11615	246	0
35	p	9175	0	9196	180	0
36	q	2059	0	2007	34	0
37	r	1050	0	1033	24	0
38	s	1720	0	1737	25	0
39	t	657	0	684	7	0
40	u	1351	0	1358	129	0
41	v	1186	0	1147	14	0
42	w	927	0	860	26	0
43	x	533	0	553	8	0
44	y	920	0	942	17	0
45	z	372	0	378	10	0
46	0	2	0	0	0	0
46	2	3	0	0	0	0
46	3	2	0	0	0	0
46	R	1	0	0	0	0
46	U	1	0	0	0	0
46	o	2	0	0	0	0
46	p	1	0	0	0	0
46	q	1	0	0	0	0
46	w	2	0	0	0	0
46	x	1	0	0	0	0
46	z	1	0	0	0	0
47	7	8	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
48	Z	33	0	0	9	0
49	o	1	0	0	0	0
All	All	108642	0	107203	2283	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 11.

All (2283) 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)
27:U:152:PHE:CE1	40:u:95:VAL:HB	1.24	1.65
27:U:139:LEU:HB2	40:u:160:ILE:CG1	1.22	1.57
1:0:41:ARG:CG	27:U:169:PRO:HG2	1.34	1.55
27:U:139:LEU:CB	40:u:160:ILE:HG12	1.41	1.50
6:5:33:PHE:CE1	6:5:49:LEU:HD12	1.44	1.48
27:U:139:LEU:CA	40:u:160:ILE:HG12	1.46	1.44
4:3:50:PHE:CZ	5:4:118:LEU:HD11	1.57	1.39
6:5:31:LYS:HB3	12:B:540:LYS:NZ	1.31	1.39
3:2:174:LEU:HD11	3:2:203:ALA:CB	1.51	1.39
1:0:41:ARG:HG3	27:U:169:PRO:CG	1.56	1.36
4:3:237:GLN:NE2	5:4:51:LEU:HD22	1.39	1.35
27:U:141:ALA:CB	40:u:107:PHE:CD1	2.08	1.34
27:U:139:LEU:CB	40:u:160:ILE:CG1	1.95	1.33
13:D:960:GLU:CG	13:D:983:ARG:HG2	1.59	1.30
27:U:139:LEU:HB2	40:u:160:ILE:CD1	1.63	1.28
1:0:85:ARG:HH22	1:0:139:LYS:C	1.40	1.28
27:U:138:ASP:OD1	40:u:160:ILE:HD13	1.15	1.27
27:U:142:ASN:ND2	40:u:105:SER:HB2	1.46	1.27
4:3:237:GLN:CD	5:4:51:LEU:CD2	2.08	1.27
6:5:31:LYS:CB	12:B:540:LYS:HZ3	1.47	1.26
1:0:85:ARG:NH1	1:0:140:LEU:HG	1.51	1.25
27:U:152:PHE:CE1	40:u:95:VAL:CB	2.21	1.23
1:0:42:GLY:N	27:U:168:MET:HE1	1.53	1.22
6:5:31:LYS:CB	12:B:540:LYS:NZ	2.01	1.21
7:6:528:LYS:CG	7:6:531:ILE:CD1	2.17	1.21
3:2:175:THR:HG23	8:7:592:ARG:CD	1.72	1.20
27:U:139:LEU:CD2	40:u:158:PHE:HD1	1.53	1.20
7:6:528:LYS:HG2	7:6:531:ILE:HD13	1.21	1.19
4:3:50:PHE:CZ	5:4:118:LEU:CD1	2.25	1.18
27:U:138:ASP:CG	40:u:160:ILE:HG21	1.69	1.17
3:2:174:LEU:CD1	3:2:203:ALA:CB	2.24	1.15

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:21:LEU:HD22	1:0:69:ASP:OD2	1.43	1.15
4:3:237:GLN:NE2	5:4:51:LEU:CD2	2.11	1.14
13:D:960:GLU:CG	13:D:983:ARG:CG	2.25	1.14
3:2:174:LEU:CD1	3:2:203:ALA:HB2	1.75	1.14
1:0:85:ARG:HH22	1:0:140:LEU:N	1.46	1.13
13:D:960:GLU:HG3	13:D:983:ARG:HG2	1.29	1.13
7:6:528:LYS:HG2	7:6:531:ILE:CD1	1.76	1.13
4:3:50:PHE:HZ	5:4:118:LEU:CD1	1.58	1.12
4:3:229:TRP:CZ3	5:4:58:ARG:NH1	2.17	1.12
27:U:152:PHE:CD1	40:u:95:VAL:HB	1.84	1.12
1:0:85:ARG:NH2	1:0:139:LYS:C	2.07	1.11
3:2:175:THR:HG23	8:7:592:ARG:HD2	1.17	1.11
3:2:175:THR:CG2	8:7:592:ARG:HD2	1.81	1.11
4:3:237:GLN:CD	5:4:51:LEU:HD22	1.71	1.10
6:5:33:PHE:CE1	6:5:49:LEU:CD1	2.34	1.10
11:A:1200:THR:O	11:A:1204:GLU:HG2	1.52	1.09
1:0:37:LEU:HD11	27:U:173:ALA:HA	1.34	1.09
27:U:139:LEU:HD21	40:u:158:PHE:C	1.77	1.09
27:U:152:PHE:CZ	40:u:95:VAL:HB	1.87	1.09
27:U:141:ALA:CB	40:u:107:PHE:CG	2.36	1.09
27:U:141:ALA:CB	40:u:107:PHE:CE1	2.35	1.09
4:3:237:GLN:CD	5:4:51:LEU:HD23	1.75	1.07
13:D:960:GLU:HG2	13:D:983:ARG:HG2	1.29	1.07
27:U:138:ASP:O	40:u:107:PHE:CD2	2.07	1.07
1:0:83:ASN:OD1	1:0:140:LEU:HD11	1.53	1.07
27:U:139:LEU:HD12	40:u:160:ILE:HG13	1.36	1.06
27:U:141:ALA:HB3	40:u:107:PHE:CD1	1.90	1.06
10:Z:1:ATP:C5'	10:Z:2:G2L:OP2	1.98	1.06
1:0:5:GLY:HA3	1:0:10:LYS:HB2	1.37	1.06
10:Z:1:ATP:H5'2	10:Z:2:G2L:OP2	1.51	1.05
27:U:139:LEU:HA	40:u:160:ILE:HG12	1.38	1.05
27:U:139:LEU:HB2	40:u:160:ILE:HG13	1.30	1.04
1:0:84:LYS:HA	1:0:136:ASN:ND2	1.73	1.04
3:2:174:LEU:HD21	3:2:203:ALA:HB1	1.36	1.04
27:U:139:LEU:HD11	40:u:159:ALA:HA	1.39	1.04
13:D:1006:LEU:HD13	21:O:69:ASP:OD2	1.56	1.04
3:2:175:THR:CG2	8:7:592:ARG:NE	2.21	1.02
6:5:33:PHE:HE1	6:5:49:LEU:CD1	1.66	1.02
27:U:139:LEU:CD2	40:u:158:PHE:CD1	2.42	1.02
3:2:175:THR:CG2	8:7:592:ARG:CD	2.35	1.02
11:A:339:ALA:HB3	11:A:355:VAL:HG21	1.42	1.01

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:U:141:ALA:HB1	40:u:107:PHE:CE1	1.96	1.01
26:T:238:GLU:HB3	28:V:130:ILE:HG12	1.42	1.00
19:J:192:LYS:N	19:J:192:LYS:HE3	1.77	0.99
27:U:141:ALA:HB3	40:u:107:PHE:CG	1.97	0.99
1:0:10:LYS:NZ	27:U:178:ALA:HB1	1.77	0.98
7:6:528:LYS:HG3	7:6:531:ILE:CD1	1.92	0.98
1:0:37:LEU:HD13	27:U:173:ALA:HB2	1.45	0.98
11:A:725:CYS:SG	11:A:725:CYS:O	2.22	0.98
1:0:8:ARG:CZ	27:U:173:ALA:HB2	1.94	0.97
3:2:174:LEU:CD2	3:2:203:ALA:HB1	1.93	0.97
27:U:138:ASP:OD1	40:u:160:ILE:CD1	2.11	0.97
27:U:145:PHE:CD1	27:U:149:THR:OG1	2.17	0.97
29:X:15:DT:H3	30:Y:-15:DA:H61	1.07	0.96
13:D:960:GLU:HG2	13:D:983:ARG:CG	1.92	0.96
3:2:174:LEU:HD21	3:2:203:ALA:CB	1.95	0.95
1:0:41:ARG:CG	27:U:169:PRO:CG	2.27	0.95
27:U:139:LEU:CD1	40:u:160:ILE:HG13	1.95	0.95
11:A:467:ILE:H	15:F:221:GLN:NE2	1.64	0.95
3:2:174:LEU:CG	3:2:203:ALA:CB	2.44	0.94
3:2:175:THR:HG23	8:7:592:ARG:NE	1.82	0.94
27:U:139:LEU:HB2	40:u:160:ILE:HD11	1.49	0.94
27:U:142:ASN:HD22	40:u:105:SER:HB2	1.13	0.94
1:0:37:LEU:HD13	27:U:173:ALA:CB	1.97	0.94
8:7:726:GLN:HG3	8:7:727:PRO:HD2	1.51	0.93
1:0:41:ARG:CD	27:U:169:PRO:HG2	1.99	0.93
27:U:139:LEU:HG	40:u:159:ALA:C	1.92	0.92
27:U:141:ALA:HB2	40:u:107:PHE:CD2	2.03	0.92
27:U:139:LEU:HD21	40:u:158:PHE:O	1.70	0.92
1:0:21:LEU:CD2	1:0:69:ASP:OD2	2.18	0.92
4:3:229:TRP:CE3	5:4:58:ARG:NE	2.38	0.92
25:S:65:SER:HA	25:S:81:ARG:HH12	1.32	0.92
13:D:960:GLU:HG3	13:D:983:ARG:CG	1.97	0.91
27:U:139:LEU:HD22	40:u:158:PHE:HD1	1.35	0.91
27:U:141:ALA:HB2	40:u:107:PHE:CD1	2.02	0.91
1:0:85:ARG:HH12	1:0:140:LEU:HG	1.34	0.91
16:G:153:LYS:HD3	16:G:153:LYS:H	1.36	0.91
5:4:442:VAL:HG21	6:5:44:PHE:HZ	1.35	0.91
27:U:141:ALA:HB1	40:u:107:PHE:CD1	2.01	0.91
27:U:140:GLU:OE2	40:u:158:PHE:HE1	1.53	0.91
1:0:27:GLY:HA3	1:0:70:LYS:HD3	1.51	0.90
8:7:726:GLN:CG	8:7:727:PRO:HD2	2.01	0.90

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:174:LEU:HD11	3:2:203:ALA:HB2	0.93	0.90
27:U:141:ALA:HB2	40:u:107:PHE:CG	2.03	0.90
14:E:365:ARG:HD3	14:E:757:GLY:HA3	1.54	0.90
13:D:963:ARG:C	13:D:965:ILE:H	1.72	0.90
4:3:108:ASN:OD1	5:4:123:LEU:HD13	1.69	0.90
27:U:141:ALA:HB2	40:u:107:PHE:CE1	2.07	0.90
1:0:8:ARG:HH22	1:0:37:LEU:HB3	1.34	0.89
4:3:50:PHE:CG	5:4:122:LEU:HD12	2.07	0.89
10:Z:2:G2L:N1	30:Y:-1:DC:N3	2.20	0.89
7:6:528:LYS:CG	7:6:531:ILE:HD11	2.00	0.89
27:U:141:ALA:HB2	40:u:107:PHE:CE2	2.07	0.89
4:3:229:TRP:CE3	5:4:58:ARG:CZ	2.55	0.89
13:D:1006:LEU:HD13	21:O:69:ASP:CG	1.97	0.89
7:6:528:LYS:CE	7:6:531:ILE:HD11	2.03	0.88
4:3:237:GLN:HE21	5:4:51:LEU:HD22	1.37	0.88
4:3:229:TRP:CZ3	5:4:58:ARG:CZ	2.57	0.88
3:2:174:LEU:O	8:7:591:GLY:HA3	1.74	0.88
27:U:140:GLU:OE2	40:u:158:PHE:CE1	2.26	0.88
7:6:528:LYS:HG3	7:6:531:ILE:HD11	1.53	0.88
26:T:238:GLU:HB3	28:V:130:ILE:CG1	2.02	0.88
27:U:53:LYS:HD2	28:V:166:ILE:HD11	1.56	0.88
27:U:152:PHE:CD1	40:u:95:VAL:CB	2.52	0.88
13:D:1006:LEU:CD1	21:O:69:ASP:OD2	2.21	0.88
27:U:145:PHE:CE1	27:U:149:THR:OG1	2.27	0.88
1:0:83:ASN:CG	1:0:140:LEU:CD1	2.47	0.87
5:4:438:LYS:HE2	12:B:621:ALA:CB	2.04	0.87
5:4:442:VAL:HG21	6:5:44:PHE:CZ	2.09	0.87
27:U:141:ALA:HB2	40:u:107:PHE:CZ	2.09	0.87
29:X:5:DC:H4'	29:X:6:DT:H5'	1.55	0.87
11:A:475:LEU:HD11	15:f:351:ILE:HD11	1.57	0.87
6:5:35:ILE:O	12:B:539:ARG:HD3	1.75	0.86
7:6:528:LYS:HE3	7:6:531:ILE:HD11	1.57	0.86
26:T:238:GLU:CB	28:V:130:ILE:HG12	2.05	0.86
7:6:528:LYS:CG	7:6:531:ILE:HD13	1.90	0.86
48:Z:2500:W0F:O33	34:o:497:ASP:OD2	1.94	0.86
11:A:511:LEU:H	11:A:511:LEU:HD22	1.37	0.86
3:2:174:LEU:HD11	3:2:203:ALA:HB3	1.57	0.85
13:D:963:ARG:C	13:D:965:ILE:N	2.25	0.85
13:D:1006:LEU:HD11	21:O:69:ASP:HB3	1.58	0.85
4:3:100:LYS:HG2	5:4:124:GLY:O	1.76	0.85
9:N:1:ILX:HG23	34:o:791:GLN:HE22	1.42	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:55:LYS:HB2	40:u:166:ASP:OD2	1.78	0.84
1:0:37:LEU:CD1	27:U:173:ALA:HA	2.06	0.84
7:6:528:LYS:CE	7:6:531:ILE:CD1	2.55	0.84
6:5:31:LYS:CB	12:B:540:LYS:HZ1	1.88	0.84
27:U:138:ASP:O	40:u:107:PHE:HD2	1.61	0.84
14:e:508:LYS:HB3	14:e:512:ASP:HB2	1.59	0.84
4:3:50:PHE:CE2	5:4:118:LEU:HD11	2.12	0.84
9:N:3:GLY:HA3	34:o:749:ARG:NH1	1.93	0.84
5:4:448:HIS:O	5:4:452:LYS:HG2	1.78	0.83
27:U:56:ARG:O	27:U:60:ARG:HG3	1.78	0.83
3:2:175:THR:CG2	8:7:592:ARG:HE	1.92	0.83
3:2:174:LEU:CG	3:2:203:ALA:HB1	2.07	0.83
5:4:432:VAL:HG12	6:5:9:LEU:HD22	1.61	0.83
27:U:142:ASN:ND2	40:u:105:SER:CB	2.39	0.83
48:Z:2500:WOF:O32	35:p:975:ARG:NH2	2.11	0.83
6:5:31:LYS:HB3	12:B:540:LYS:HZ3	0.80	0.82
11:A:1065:GLU:OE1	11:A:1065:GLU:HA	1.78	0.82
1:0:83:ASN:ND2	1:0:140:LEU:CD1	2.43	0.82
11:A:821:ARG:CZ	11:A:821:ARG:HA	2.10	0.82
7:6:266:GLN:N	7:6:266:GLN:HE21	1.79	0.81
15:F:324:ASP:HA	15:F:327:TRP:HB3	1.63	0.81
15:f:447:ALA:HA	15:f:456:GLY:HA3	1.61	0.81
13:D:960:GLU:HB3	13:D:983:ARG:HG3	1.63	0.81
1:0:85:ARG:NH2	1:0:140:LEU:N	2.26	0.81
27:U:139:LEU:CG	40:u:160:ILE:HG13	2.11	0.81
33:m:77:ARG:HH11	33:m:77:ARG:HG2	1.45	0.81
1:0:8:ARG:HD2	27:U:173:ALA:H	1.44	0.80
5:4:438:LYS:CE	12:B:621:ALA:H	1.94	0.80
14:E:327:ASN:HD22	14:E:327:ASN:H	1.30	0.80
27:U:139:LEU:HD23	40:u:158:PHE:HD1	1.45	0.80
13:D:1006:LEU:CD1	21:O:69:ASP:CG	2.55	0.80
26:T:188:PHE:CD2	28:V:80:LYS:HB2	2.16	0.80
4:3:16:ASP:HA	4:3:62:SER:OG	1.82	0.80
27:U:56:ARG:NH1	27:U:60:ARG:NH1	2.30	0.80
27:U:138:ASP:OD1	40:u:160:ILE:HG21	1.81	0.80
2:1:430:THR:OG1	4:3:222:SER:OG	2.00	0.79
5:4:334:MET:SD	7:6:56:TYR:CD2	2.76	0.79
27:U:139:LEU:CA	40:u:160:ILE:CG1	2.42	0.79
1:0:8:ARG:NE	1:0:9:CYS:SG	2.54	0.79
1:0:83:ASN:OD1	1:0:140:LEU:CD1	2.31	0.79
40:u:142:GLU:HB2	40:u:170:LEU:HD22	1.64	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:42:GLY:N	27:U:168:MET:CE	2.44	0.79
27:U:139:LEU:CD1	40:u:159:ALA:HA	2.13	0.79
3:2:174:LEU:CD2	3:2:203:ALA:CB	2.57	0.79
6:5:33:PHE:CZ	6:5:49:LEU:HD12	2.17	0.79
34:o:1242:ASP:HA	34:o:1262:MET:HB2	1.64	0.79
1:0:83:ASN:CG	1:0:140:LEU:HD11	2.07	0.79
14:E:774:MET:HE2	14:E:774:MET:H	1.46	0.79
22:P:188:ARG:NH2	23:Q:321:SER:OG	2.16	0.79
15:F:273:GLN:NE2	15:F:273:GLN:H	1.81	0.78
27:U:139:LEU:HD22	40:u:158:PHE:CD1	2.16	0.78
27:U:151:THR:HG23	27:U:153:ARG:HD3	1.65	0.78
4:3:237:GLN:CG	5:4:51:LEU:CD2	2.60	0.78
15:F:274:ASN:ND2	15:F:316:GLN:HA	1.99	0.78
5:4:393:LEU:HD21	7:6:511:TRP:CZ3	2.19	0.78
33:m:31:LEU:HD23	33:m:31:LEU:H	1.47	0.78
14:e:747:LEU:HD23	14:e:747:LEU:H	1.47	0.78
4:3:56:LYS:NZ	4:3:143:TYR:OH	2.16	0.78
7:6:449:LYS:HD3	29:X:29:DA:OP1	1.84	0.78
3:2:69:ARG:HG2	3:2:140:HIS:HA	1.66	0.77
5:4:456:LYS:O	5:4:460:HIS:CD2	2.37	0.77
34:o:877:ALA:HB3	34:o:890:ARG:HH11	1.48	0.77
34:o:111:CYS:SG	34:o:188:GLN:NE2	2.57	0.77
1:0:37:LEU:CD1	27:U:173:ALA:CB	2.63	0.77
3:2:223:LEU:HD12	8:7:726:GLN:HB2	1.67	0.77
9:N:8:HYP:HD23	34:o:1108:HIS:CE1	2.19	0.76
1:0:37:LEU:HD11	27:U:173:ALA:CA	2.14	0.76
1:0:85:ARG:HH22	1:0:140:LEU:CA	1.98	0.76
13:D:963:ARG:C	13:D:982:LEU:HD11	2.10	0.76
34:o:1307:VAL:HG13	34:o:1338:THR:HG22	1.67	0.76
3:2:69:ARG:HD3	3:2:140:HIS:CD2	2.20	0.76
5:4:432:VAL:CG1	6:5:9:LEU:HD22	2.15	0.76
4:3:46:ASN:OD1	5:4:123:LEU:HD22	1.85	0.76
1:0:41:ARG:HG2	27:U:168:MET:HE3	1.68	0.76
30:Y:28:DT:H2'	30:Y:29:DA:C8	2.21	0.75
4:3:240:GLN:NE2	5:4:51:LEU:HD21	2.01	0.75
15:F:429:LYS:O	15:F:433:PRO:HD2	1.85	0.75
11:A:467:ILE:H	15:F:221:GLN:HE21	1.33	0.75
35:p:761:THR:H	35:p:764:MET:HE3	1.49	0.75
26:T:192:GLU:HG3	28:V:75:PHE:HB3	1.69	0.75
1:0:42:GLY:H	27:U:168:MET:HE1	1.49	0.75
27:U:141:ALA:HB1	40:u:98:PHE:HE1	1.51	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:84:LYS:CA	1:0:136:ASN:ND2	2.48	0.75
1:0:41:ARG:HB2	27:U:168:MET:SD	2.26	0.74
8:7:711:ASP:OD1	8:7:715:GLN:NE2	2.20	0.74
35:p:269:ILE:HD11	35:p:369:VAL:HG21	1.68	0.74
27:U:152:PHE:CD2	40:u:95:VAL:HG11	2.22	0.74
4:3:47:SER:HA	5:4:122:LEU:HD11	1.68	0.74
11:A:970:ASN:OD1	11:A:970:ASN:N	2.21	0.74
1:0:8:ARG:NH2	1:0:34:CYS:SG	2.61	0.74
27:U:48:MET:HE2	27:U:52:LEU:HB2	1.70	0.74
6:5:33:PHE:HE1	6:5:49:LEU:HD12	0.84	0.74
27:U:138:ASP:O	40:u:107:PHE:CE2	2.41	0.74
29:X:27:DA:H2''	29:X:28:DG:C8	2.23	0.74
5:4:438:LYS:HE2	12:B:621:ALA:HB3	1.70	0.74
6:5:31:LYS:HB3	12:B:540:LYS:CE	2.17	0.73
15:F:359:PHE:HB3	15:F:380:LEU:HG	1.68	0.73
11:A:639:LEU:HD11	11:A:774:ARG:HG2	1.70	0.73
1:0:41:ARG:C	27:U:168:MET:HE1	2.13	0.73
37:r:25:GLU:HG3	40:u:41:LYS:HE2	1.70	0.73
11:A:488:ALA:HB1	15:f:271:VAL:HG23	1.70	0.73
40:u:92:VAL:HB	40:u:126:PRO:HB2	1.70	0.73
6:5:31:LYS:CG	12:B:540:LYS:HZ3	2.01	0.73
7:6:371:VAL:HG23	7:6:407:ILE:HG22	1.69	0.73
8:7:231:VAL:HG13	8:7:454:VAL:HG23	1.70	0.73
6:5:34:ILE:O	12:B:539:ARG:NH2	2.22	0.72
36:q:2:PRO:HB3	44:y:54:PRO:HD2	1.70	0.72
25:S:64:GLU:O	25:S:81:ARG:NH2	2.19	0.72
1:0:10:LYS:HZ2	27:U:178:ALA:HB1	1.54	0.72
4:3:237:GLN:OE1	5:4:54:ASN:OD1	2.07	0.72
15:F:418:ILE:H	15:F:418:ILE:HD12	1.54	0.72
4:3:50:PHE:CD2	5:4:122:LEU:HD12	2.24	0.72
34:o:922:PHE:H	34:o:1052:ARG:HD2	1.53	0.72
26:T:188:PHE:HE2	28:V:80:LYS:HG3	1.55	0.72
27:U:152:PHE:CD1	40:u:95:VAL:CG2	2.72	0.72
27:U:147:PRO:HA	40:u:91:GLN:CD	2.14	0.72
28:V:131:GLU:HG3	28:V:140:LYS:HA	1.72	0.72
1:0:23:VAL:HG21	1:0:73:GLU:HG3	1.71	0.72
1:0:85:ARG:NH2	1:0:139:LYS:O	2.23	0.71
5:4:120:ILE:HG23	5:4:125:GLY:HA2	1.72	0.71
11:A:353:LEU:HD21	15:f:272:VAL:HG21	1.72	0.71
24:R:103:ASN:HB3	30:Y:12:DC:H5'	1.72	0.71
4:3:160:ARG:NH2	4:3:234:ASP:OD1	2.23	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:237:GLN:CG	5:4:51:LEU:HD22	2.19	0.71
14:e:274:TYR:HB3	14:e:367:ALA:HB2	1.72	0.71
23:Q:346:LYS:NZ	30:Y:29:DA:OP1	2.24	0.71
24:R:72:ASN:HB2	24:R:75:LEU:HG	1.72	0.71
27:U:139:LEU:CB	40:u:160:ILE:HG13	1.94	0.71
27:U:152:PHE:CZ	40:u:95:VAL:CB	2.63	0.71
36:q:67:ARG:NH2	43:x:3:ILE:O	2.24	0.71
35:p:69:ALA:HB3	35:p:81:PRO:HB3	1.71	0.71
4:3:272:LEU:O	4:3:272:LEU:HD23	1.90	0.71
5:4:29:GLY:O	5:4:33:ARG:NE	2.24	0.71
2:1:195:SER:O	2:1:199:THR:OG1	2.05	0.71
5:4:404:THR:HG22	6:5:9:LEU:H	1.56	0.71
6:5:31:LYS:HB2	12:B:540:LYS:NZ	2.06	0.71
1:0:8:ARG:HH22	1:0:37:LEU:CB	2.04	0.70
4:3:67:SER:O	4:3:139:LYS:NZ	2.24	0.70
13:D:960:GLU:HG2	13:D:983:ARG:CD	2.22	0.70
27:U:23:ARG:HD2	27:U:31:ALA:HB1	1.73	0.70
28:V:197:LYS:HG3	28:V:198:LYS:HG3	1.72	0.70
34:o:46:THR:HG22	34:o:57:LEU:HB2	1.73	0.70
36:q:190:ASN:ND2	36:q:195:THR:O	2.24	0.70
1:0:120:LYS:O	1:0:124:ILE:HD12	1.91	0.70
12:B:241:PRO:HG2	12:B:496:MET:HE1	1.72	0.70
34:o:585:LEU:HD22	41:v:47:ILE:HD11	1.73	0.70
14:E:258:ASN:H	14:E:258:ASN:ND2	1.89	0.70
4:3:237:GLN:HG3	5:4:51:LEU:CD2	2.21	0.70
7:6:528:LYS:HE2	7:6:531:ILE:CD1	2.22	0.70
24:R:102:GLN:HE21	34:o:305:GLU:HG2	1.57	0.70
9:N:3:GLY:HA3	34:o:749:ARG:HH12	1.54	0.70
28:V:234:GLU:OE1	28:V:238:LYS:NZ	2.25	0.70
13:D:961:GLN:HG3	13:D:983:ARG:HH12	1.56	0.70
27:U:75:ARG:H	27:U:91:TYR:HB2	1.55	0.70
35:p:910:THR:HG22	45:z:43:ILE:HA	1.73	0.70
3:2:206:ARG:HB3	8:7:589:GLU:O	1.91	0.70
11:A:339:ALA:CB	11:A:355:VAL:HG21	2.22	0.69
24:R:104:ARG:NH2	30:Y:10:DC:H42	1.91	0.69
34:o:877:ALA:HB3	34:o:890:ARG:NH1	2.06	0.69
7:6:191:ASP:O	7:6:195:ARG:NH1	2.25	0.69
8:7:252:THR:HG22	8:7:432:ILE:HG22	1.74	0.69
16:G:129:LYS:O	16:G:129:LYS:NZ	2.23	0.69
27:U:36:ILE:HD11	28:V:163:LEU:HD22	1.74	0.69
7:6:611:GLY:O	7:6:642:ARG:NH2	2.25	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:o:1158:LEU:HD11	34:o:1309:MET:HB2	1.75	0.69
15:f:447:ALA:CA	15:f:456:GLY:HA3	2.23	0.69
35:p:866:ILE:HG22	35:p:867:ILE:HG13	1.74	0.69
2:1:468:VAL:HG21	2:1:525:ILE:HD11	1.74	0.69
5:4:438:LYS:HE3	12:B:621:ALA:H	1.58	0.69
7:6:56:TYR:C	7:6:58:ALA:H	2.01	0.69
27:U:24:GLY:HA2	28:V:209:GLN:HG2	1.75	0.69
4:3:242:ILE:HD11	5:4:75:VAL:C	2.17	0.69
35:p:827:GLU:HG2	35:p:871:VAL:HG22	1.73	0.69
15:F:274:ASN:HB2	15:F:317:LEU:H	1.58	0.68
12:B:490:SER:HA	12:B:493:TRP:HB2	1.75	0.68
32:k:191:VAL:HG13	32:k:200:ILE:HD13	1.74	0.68
3:2:69:ARG:HD2	8:7:563:ARG:HH21	1.58	0.68
8:7:637:LEU:HD11	8:7:648:GLU:HA	1.74	0.68
9:N:1:ILX:HG23	34:o:791:GLN:NE2	2.08	0.68
34:o:577:PRO:HG2	34:o:580:LEU:HD23	1.76	0.68
3:2:75:ASP:OD2	8:7:722:ARG:NH2	2.26	0.68
15:F:83:LEU:CD1	15:F:83:LEU:H	2.06	0.68
27:U:56:ARG:HH11	27:U:60:ARG:NH1	1.89	0.68
11:A:568:SER:HB2	12:B:389:ASN:HB2	1.75	0.68
13:D:1002:ARG:HB2	26:T:182:HIS:CD2	2.29	0.68
27:U:138:ASP:OD2	40:u:160:ILE:HG21	1.91	0.68
8:7:72:TYR:OH	8:7:234:ASP:OD2	2.12	0.68
8:7:382:LEU:O	8:7:385:THR:OG1	2.11	0.68
13:D:998:GLN:NE2	26:T:186:MET:HA	2.07	0.68
14:e:645:GLY:H	14:e:675:LEU:HD11	1.59	0.68
34:o:1148:ALA:HB1	34:o:1333:GLU:HB2	1.74	0.68
1:0:85:ARG:NH1	1:0:140:LEU:CG	2.45	0.68
27:U:152:PHE:CE2	40:u:95:VAL:CG1	2.77	0.68
13:D:991:MET:HE2	26:T:193:LYS:HA	1.77	0.67
6:5:38:ILE:HG21	6:5:42:HIS:HB2	1.76	0.67
34:o:560:VAL:HG22	34:o:591:ILE:HD11	1.74	0.67
34:o:1286:ARG:HH21	42:w:53:ILE:HG22	1.59	0.67
35:p:457:LYS:HG2	35:p:458:LYS:HG3	1.76	0.67
27:U:48:MET:HA	27:U:48:MET:HE3	1.75	0.67
14:E:426:ARG:HH11	14:E:640:ASN:HD22	1.42	0.67
17:H:40:VAL:HG11	19:J:130:ILE:HG12	1.77	0.67
1:0:37:LEU:CD1	27:U:173:ALA:CA	2.72	0.67
11:A:396:LEU:HD21	15:f:394:PRO:HB2	1.77	0.67
30:Y:-15:DA:H1'	30:Y:-14:DG:H5'	1.76	0.67
1:0:10:LYS:NZ	27:U:178:ALA:CB	2.57	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:88:LEU:CD2	3:2:131:LEU:HD21	2.24	0.67
20:L:79:ASP:OD1	20:L:79:ASP:N	2.25	0.67
25:S:76:ARG:HH21	25:S:80:ARG:HD3	1.59	0.67
27:U:139:LEU:CG	40:u:160:ILE:CG1	2.67	0.67
4:3:46:ASN:OD1	5:4:123:LEU:CD2	2.42	0.67
27:U:20:TYR:O	27:U:23:ARG:NH2	2.27	0.67
15:f:239:ARG:HD3	15:f:284:ARG:HH11	1.60	0.67
14:E:365:ARG:HD3	14:E:757:GLY:CA	2.24	0.67
3:2:175:THR:HG23	8:7:592:ARG:HE	1.56	0.67
22:P:206:GLU:OE1	22:P:236:LYS:NZ	2.28	0.67
36:q:259:LEU:HD22	44:y:19:ILE:HD11	1.77	0.67
5:4:60:LEU:HD13	5:4:118:LEU:HD23	1.76	0.67
35:p:553:LEU:HA	35:p:556:ILE:HD12	1.77	0.67
4:3:237:GLN:OE1	5:4:51:LEU:HD23	1.94	0.66
28:V:141:PRO:HB2	28:V:144:ASN:HB3	1.76	0.66
3:2:75:ASP:OD1	8:7:722:ARG:NH2	2.28	0.66
3:2:174:LEU:CD1	3:2:203:ALA:HB3	2.17	0.66
4:3:43:VAL:HG11	4:3:224:LEU:HD21	1.78	0.66
5:4:409:TYR:HB2	5:4:412:PHE:CZ	2.30	0.66
28:V:227:SER:HB3	28:V:230:GLU:HB2	1.77	0.66
48:Z:2500:WOF:O32	35:p:975:ARG:NE	2.28	0.66
8:7:60:GLN:OE1	8:7:61:ARG:NH1	2.29	0.66
13:D:1006:LEU:HD11	21:O:69:ASP:CB	2.25	0.66
35:p:896:LEU:HD21	35:p:900:GLU:HB3	1.77	0.66
1:0:106:VAL:O	1:0:110:THR:HG23	1.95	0.66
5:4:438:LYS:HE3	12:B:621:ALA:N	2.10	0.66
27:U:141:ALA:HB1	40:u:98:PHE:CE1	2.31	0.66
30:Y:6:DA:H4'	30:Y:7:DG:H5'	1.76	0.66
4:3:229:TRP:CE3	5:4:58:ARG:HD2	2.31	0.66
26:T:237:PRO:HB3	28:V:83:ASN:HD21	1.60	0.66
33:m:79:GLY:HA2	20:l:141:LYS:HE2	1.76	0.66
19:j:123:LEU:C	19:j:125:ASP:H	2.03	0.66
4:3:229:TRP:CE3	5:4:58:ARG:CD	2.78	0.66
11:A:821:ARG:HA	11:A:821:ARG:NH1	2.11	0.66
34:o:98:GLY:HA3	34:o:1440:MET:HE2	1.77	0.66
8:7:238:ASN:ND2	8:7:662:GLN:OE1	2.29	0.66
21:O:51:ARG:NH2	23:Q:20:ASP:OD2	2.28	0.66
3:2:137:MET:SD	3:2:139:CYS:N	2.67	0.65
3:2:175:THR:HG22	8:7:592:ARG:CD	2.27	0.65
13:D:960:GLU:CB	13:D:983:ARG:HG3	2.26	0.65
29:X:15:DT:H3	30:Y:-15:DA:N6	1.88	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:p:407:MET:HE1	35:p:444:LEU:HG	1.77	0.65
37:r:103:LEU:HD13	37:r:114:LEU:HD13	1.76	0.65
24:R:23:LEU:HD12	24:R:32:MET:HE2	1.79	0.65
34:o:1146:GLN:HG2	34:o:1149:ARG:HH12	1.61	0.65
3:2:174:LEU:O	8:7:591:GLY:CA	2.43	0.65
38:s:192:LYS:HE3	38:s:194:ILE:HD11	1.78	0.65
37:r:77:ARG:HA	37:r:80:ILE:HD12	1.79	0.65
13:D:1006:LEU:CD1	21:O:69:ASP:CB	2.74	0.65
28:V:144:ASN:HA	28:V:173:GLU:HB2	1.78	0.65
30:Y:12:DC:H2"	30:Y:13:DA:C8	2.31	0.65
35:p:365:LEU:O	35:p:369:VAL:HG23	1.96	0.65
1:0:8:ARG:NE	27:U:173:ALA:HB2	2.10	0.65
4:3:229:TRP:HZ3	5:4:58:ARG:HH11	1.44	0.65
40:u:92:VAL:HG13	40:u:128:TYR:CE2	2.32	0.65
3:2:174:LEU:HG	3:2:203:ALA:CB	2.27	0.65
5:4:172:SER:OG	5:4:174:ASP:OD1	2.15	0.65
7:6:701:LEU:O	7:6:704:SER:OG	2.14	0.65
27:U:152:PHE:CD1	40:u:95:VAL:HG21	2.32	0.65
4:3:98:ASP:O	5:4:125:GLY:HA3	1.96	0.65
27:U:72:ILE:HG22	27:U:94:ILE:HA	1.78	0.65
33:m:77:ARG:HH11	33:m:77:ARG:CG	2.10	0.65
6:5:38:ILE:CG2	6:5:42:HIS:HB2	2.27	0.64
15:f:320:ARG:NH1	15:f:320:ARG:HB3	2.12	0.64
1:0:41:ARG:HG3	27:U:169:PRO:HG2	0.68	0.64
15:F:83:LEU:HD12	15:F:83:LEU:N	2.12	0.64
4:3:168:GLU:N	4:3:168:GLU:OE1	2.31	0.64
7:6:330:ASN:OD1	7:6:334:ARG:NH2	2.31	0.64
27:U:111:ARG:HD3	27:U:188:TYR:OH	1.97	0.64
6:5:31:LYS:HB2	12:B:540:LYS:HZ1	1.59	0.64
7:6:287:LEU:HD23	7:6:287:LEU:O	1.98	0.64
7:6:128:SER:HG	7:6:163:TYR:HH	1.42	0.64
48:Z:2500:W0F:N19	30:Y:-2:DC:O2	2.31	0.64
11:A:1168:TYR:HB2	16:G:180:ARG:HB3	1.78	0.64
27:U:139:LEU:HD12	40:u:149:GLY:O	1.98	0.64
35:p:193:VAL:HG21	35:p:470:LEU:HD13	1.78	0.64
3:2:377:ASP:O	3:2:380:HIS:NE2	2.30	0.64
5:4:335:LEU:O	7:6:58:ALA:HA	1.98	0.64
27:U:76:MET:HE3	27:U:88:ARG:HD2	1.80	0.64
27:U:139:LEU:N	40:u:160:ILE:HG12	2.11	0.64
34:o:733:LEU:HB3	42:w:106:ASP:HB2	1.80	0.64
19:j:123:LEU:O	19:j:125:ASP:N	2.30	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:41:ARG:CB	27:U:169:PRO:HG2	2.24	0.64
14:E:522:ASP:HB2	14:E:526:ARG:HG2	1.80	0.64
35:p:625:LEU:HD13	35:p:675:LEU:HD21	1.78	0.64
37:r:114:LEU:HD22	40:u:84:VAL:HG11	1.80	0.64
27:U:136:PHE:O	27:U:137:THR:OG1	2.13	0.64
34:o:760:LEU:HD11	34:o:781:ILE:HG21	1.79	0.64
7:6:517:GLU:O	7:6:521:GLU:OE1	2.16	0.63
8:7:513:ASP:OD1	8:7:516:VAL:N	2.29	0.63
27:U:145:PHE:HD1	27:U:149:THR:OG1	1.76	0.63
28:V:158:HIS:O	28:V:162:GLY:N	2.29	0.63
35:p:851:ASP:HB3	45:z:15:MET:HE1	1.80	0.63
5:4:55:TRP:CZ2	5:4:83:GLN:NE2	2.66	0.63
7:6:449:LYS:HB3	29:X:29:DA:OP1	1.98	0.63
3:2:175:THR:HG21	8:7:592:ARG:HE	1.63	0.63
4:3:229:TRP:HE3	5:4:58:ARG:NE	1.91	0.63
7:6:266:GLN:HG2	7:6:267:THR:HG23	1.81	0.63
27:U:138:ASP:CG	40:u:160:ILE:CG2	2.61	0.63
13:D:960:GLU:CB	13:D:983:ARG:CG	2.75	0.63
27:U:152:PHE:CG	40:u:95:VAL:HG11	2.34	0.63
1:0:27:GLY:CA	1:0:70:LYS:HD3	2.26	0.63
3:2:109:THR:OG1	3:2:148:SER:OG	2.06	0.63
3:2:242:SER:O	3:2:245:SER:OG	2.17	0.63
4:3:16:ASP:OD1	4:3:131:THR:OG1	2.16	0.63
3:2:75:ASP:CG	8:7:722:ARG:NH2	2.57	0.63
4:3:240:GLN:HE21	5:4:51:LEU:HD21	1.61	0.63
7:6:528:LYS:HG2	7:6:528:LYS:O	1.97	0.63
8:7:726:GLN:HG2	8:7:727:PRO:HD2	1.81	0.63
13:D:966:LEU:O	13:D:966:LEU:HD22	1.99	0.63
36:q:42:VAL:HB	36:q:178:PRO:HG3	1.81	0.63
14:e:277:ASP:OD1	14:e:277:ASP:N	2.32	0.63
3:2:175:THR:HG21	8:7:592:ARG:NE	2.13	0.63
13:D:1002:ARG:HE	26:T:182:HIS:CD2	2.17	0.63
28:V:78:LEU:HD21	28:V:124:LEU:HD22	1.79	0.63
12:B:361:ARG:HD2	12:B:367:GLU:HB2	1.80	0.63
17:H:50:PHE:HD1	19:J:193:TYR:O	1.82	0.63
1:0:71:GLU:OE2	8:7:335:ARG:NH1	2.32	0.62
3:2:87:LEU:HD22	3:2:232:LEU:HD12	1.81	0.62
27:U:139:LEU:CB	40:u:160:ILE:CD1	2.54	0.62
26:T:188:PHE:CE2	28:V:80:LYS:HG3	2.33	0.62
37:r:23:PRO:HG2	37:r:26:PHE:HB2	1.80	0.62
3:2:112:LYS:O	3:2:147:ASN:ND2	2.32	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:229:TRP:HE3	5:4:58:ARG:CD	2.12	0.62
15:F:92:ILE:HG13	15:F:93:PRO:HD3	1.81	0.62
1:0:83:ASN:ND2	1:0:140:LEU:HD12	2.14	0.62
7:6:528:LYS:HZ3	29:X:32:DT:H5"	1.64	0.62
11:A:342:ARG:HG2	11:A:342:ARG:O	1.99	0.62
27:U:152:PHE:CE2	40:u:95:VAL:HG12	2.35	0.62
3:2:223:LEU:HD13	8:7:726:GLN:OE1	1.99	0.62
8:7:343:ARG:O	8:7:346:VAL:HG12	1.99	0.62
12:B:583:GLU:CD	12:B:583:GLU:H	2.06	0.62
15:F:335:ARG:NE	15:F:382:GLU:OE1	2.33	0.62
7:6:371:VAL:HG23	7:6:407:ILE:CG2	2.30	0.62
13:D:960:GLU:CG	13:D:983:ARG:HG3	2.25	0.62
25:S:70:GLU:HA	25:S:74:LYS:HB2	1.82	0.62
27:U:100:VAL:O	27:U:104:LYS:HG2	1.99	0.62
1:0:41:ARG:HG3	27:U:169:PRO:CD	2.27	0.62
22:P:208:ARG:NH2	23:Q:346:LYS:O	2.33	0.62
8:7:2:LYS:HB3	8:7:9:LEU:HD11	1.81	0.61
34:o:784:VAL:HG22	35:p:978:ILE:HD11	1.81	0.61
36:q:56:SER:HB2	36:q:158:GLU:H	1.65	0.61
36:q:183:ALA:HB3	36:q:232:ASN:HB3	1.83	0.61
13:d:884:GLU:HA	13:d:887:LYS:HE3	1.82	0.61
3:2:379:LEU:HD22	3:2:381:CYS:O	1.99	0.61
35:p:570:ASN:ND2	35:p:616:THR:OG1	2.32	0.61
48:Z:2500:W0F:P30	35:p:975:ARG:HH21	2.23	0.61
27:U:147:PRO:HA	40:u:91:GLN:NE2	2.15	0.61
35:p:834:ARG:HA	35:p:840:MET:HG3	1.82	0.61
6:5:32:LYS:HD3	12:B:540:LYS:HA	1.80	0.61
14:E:613:ALA:HB2	14:E:620:LEU:HD11	1.81	0.61
34:o:460:ARG:HD2	34:o:494:ALA:HB2	1.83	0.61
36:q:19:VAL:HG23	36:q:241:PRO:HB2	1.83	0.61
7:6:189:LEU:O	7:6:195:ARG:NH1	2.33	0.61
8:7:609:ASP:OD1	8:7:669:ARG:NH2	2.34	0.61
13:D:956:GLN:HA	13:D:956:GLN:NE2	2.15	0.61
34:o:863:ARG:HH21	34:o:1415:THR:HG22	1.65	0.61
34:o:1030:SER:HB3	38:s:162:ARG:HE	1.65	0.61
34:o:1208:SER:HA	34:o:1266:GLU:HG3	1.82	0.61
35:p:22:TRP:CE2	35:p:679:PRO:HG3	2.35	0.61
4:3:53:ARG:HG2	5:4:46:ARG:NH2	2.15	0.61
15:F:114:LEU:HB2	17:H:52:SER:H	1.66	0.61
27:U:152:PHE:CZ	40:u:95:VAL:CG1	2.84	0.61
34:o:581:LYS:HG2	34:o:582:PRO:HA	1.81	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:p:222:ARG:HB3	35:p:234:THR:HG22	1.82	0.61
35:p:267:VAL:HG13	35:p:320:PHE:HE2	1.65	0.61
35:p:404:PHE:HA	35:p:407:MET:HE2	1.83	0.61
3:2:206:ARG:HG2	8:7:589:GLU:HA	1.81	0.61
5:4:265:LEU:CD1	5:4:270:LEU:HD12	2.31	0.61
5:4:401:LEU:HD13	6:5:10:ILE:HD13	1.81	0.61
7:6:473:GLU:OE1	7:6:473:GLU:N	2.33	0.61
31:c:18:CYS:O	31:c:23:TRP:HB2	2.00	0.61
34:o:1004:LEU:HD13	34:o:1062:GLY:HA2	1.83	0.61
35:p:755:GLN:HE22	43:x:48:MET:HE2	1.66	0.61
25:S:58:GLN:C	25:S:60:GLU:H	2.08	0.61
27:U:139:LEU:CB	40:u:160:ILE:HD11	2.24	0.61
28:V:171:ILE:HD13	28:V:177:ASN:HB3	1.83	0.61
8:7:461:LEU:HD23	8:7:464:LEU:CD2	2.31	0.60
12:B:203:LYS:HD3	12:B:237:MET:HE3	1.83	0.60
13:D:996:LEU:O	13:D:1000:ARG:HG3	2.01	0.60
24:R:83:MET:HB2	24:R:104:ARG:HH11	1.66	0.60
29:X:-19:DT:H2''	29:X:-18:DG:C8	2.36	0.60
30:Y:10:DC:N3	30:Y:11:DT:H2'	2.16	0.60
17:H:192:ARG:NH1	17:H:209:SER:O	2.34	0.60
28:V:121:THR:O	28:V:125:VAL:HG23	2.01	0.60
28:V:174:ALA:HB1	28:V:180:LYS:HZ1	1.66	0.60
3:2:357:VAL:HG13	3:2:366:VAL:HG23	1.83	0.60
7:6:528:LYS:NZ	29:X:32:DT:H5''	2.15	0.60
8:7:628:THR:O	8:7:628:THR:HG22	2.02	0.60
27:U:25:PHE:O	28:V:217:GLN:NE2	2.33	0.60
33:m:75:ILE:HD11	19:j:176:MET:HE1	1.82	0.60
36:q:154:ARG:HD3	43:x:64:PRO:HD3	1.83	0.60
40:u:93:ASN:O	40:u:128:TYR:OH	2.11	0.60
1:0:55:LYS:HB2	40:u:166:ASP:CG	2.25	0.60
2:1:432:THR:O	2:1:435:SER:OG	2.10	0.60
5:4:18:ASN:OD1	5:4:19:LEU:N	2.35	0.60
14:e:257:GLU:H	14:e:257:GLU:CD	2.10	0.60
12:B:27:LYS:HE3	12:B:490:SER:HB3	1.84	0.60
14:E:754:THR:O	14:E:755:ALA:HB3	2.01	0.60
27:U:150:GLY:HA2	40:u:93:ASN:OD1	2.00	0.60
28:V:77:VAL:O	28:V:81:ILE:HG12	2.01	0.60
29:X:8:DC:H2''	29:X:9:DA:C8	2.37	0.60
31:c:99:PHE:HB2	31:c:100:PRO:HD3	1.83	0.60
33:m:31:LEU:HD23	33:m:31:LEU:N	2.16	0.60
34:o:433:PRO:HG2	34:o:438:LEU:HD21	1.83	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:o:689:ILE:HD12	35:p:985:LEU:HD22	1.82	0.60
15:F:90:GLU:H	15:F:90:GLU:CD	2.08	0.60
2:1:422:LEU:HD22	4:3:225:GLN:HE22	1.66	0.60
3:2:174:LEU:HG	3:2:203:ALA:HB1	1.83	0.60
3:2:175:THR:HG22	8:7:592:ARG:HD2	1.80	0.60
17:H:194:MET:HE1	15:f:226:GLU:HG3	1.83	0.60
34:o:203:LYS:HG2	34:o:212:LYS:HE3	1.84	0.60
34:o:420:ILE:HG12	34:o:426:ARG:HG3	1.84	0.60
7:6:707:GLU:O	7:6:711:GLN:OE1	2.20	0.60
1:0:55:LYS:HE2	40:u:166:ASP:OD2	2.02	0.59
5:4:438:LYS:HE2	12:B:621:ALA:HB2	1.82	0.59
4:3:242:ILE:HD13	5:4:74:TRP:C	2.27	0.59
34:o:347:GLU:HA	34:o:352:GLY:HA3	1.85	0.59
34:o:769:MET:HE1	35:p:970:HIS:HA	1.84	0.59
35:p:826:GLU:H	35:p:872:THR:HG22	1.66	0.59
14:e:562:SER:OG	14:e:564:ASP:OD1	2.21	0.59
1:0:10:LYS:HZ3	27:U:178:ALA:HB1	1.68	0.59
2:1:130:ASP:OD2	2:1:463:HIS:NE2	2.33	0.59
11:A:475:LEU:HD13	15:f:349:ASN:OD1	2.02	0.59
33:m:88:PHE:C	33:m:88:PHE:CD1	2.81	0.59
37:r:16:ASP:H	37:r:21:ILE:HB	1.67	0.59
1:0:83:ASN:HD21	1:0:140:LEU:HD13	1.66	0.59
3:2:88:LEU:HD22	3:2:131:LEU:HD21	1.83	0.59
5:4:401:LEU:HG	6:5:53:LEU:HD23	1.85	0.59
15:F:312:ILE:HG13	15:F:334:ALA:CB	2.33	0.59
7:6:266:GLN:N	7:6:266:GLN:NE2	2.49	0.59
7:6:528:LYS:HE2	7:6:531:ILE:HD13	1.83	0.59
8:7:462:SER:OG	8:7:463:PRO:HD2	2.02	0.59
11:A:1193:ALA:HB3	16:G:166:VAL:HG21	1.83	0.59
26:T:238:GLU:CG	28:V:130:ILE:HG12	2.32	0.59
40:u:108:ILE:HG21	40:u:163:LEU:HG	1.84	0.59
34:o:392:GLU:HB2	34:o:448:ARG:NH1	2.18	0.59
6:5:48:GLU:HG3	6:5:49:LEU:HG	1.84	0.59
8:7:372:LEU:HD11	8:7:404:ALA:HB1	1.84	0.59
15:f:349:ASN:HB3	15:f:351:ILE:HG13	1.84	0.59
1:0:84:LYS:HA	1:0:136:ASN:CG	2.28	0.58
4:3:98:ASP:HB2	4:3:100:LYS:HE3	1.84	0.58
25:S:73:ARG:CZ	25:S:76:ARG:HD2	2.32	0.58
27:U:15:LYS:NZ	27:U:94:ILE:O	2.31	0.58
34:o:1262:MET:HE2	34:o:1264:SER:HB3	1.84	0.58
15:f:330:ARG:HH22	15:f:371:THR:HB	1.66	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:195:VAL:HG12	4:3:203:LEU:HD23	1.85	0.58
8:7:262:ASN:O	8:7:266:LEU:HD23	2.03	0.58
8:7:405:THR:O	8:7:409:THR:OG1	2.16	0.58
1:0:35:VAL:HG13	1:0:58:PHE:CE2	2.39	0.58
2:1:417:LYS:HA	2:1:421:VAL:HG23	1.85	0.58
2:1:503:THR:HG1	2:1:533:TYR:HH	1.19	0.58
8:7:664:VAL:HG22	8:7:677:MET:HG2	1.83	0.58
11:A:470:ILE:O	11:A:470:ILE:HG22	2.02	0.58
5:4:404:THR:H	6:5:8:VAL:HG13	1.68	0.58
29:X:16:DT:H2"	29:X:17:DC:C6	2.38	0.58
38:s:73:PHE:HD2	38:s:99:ILE:HD13	1.68	0.58
2:1:422:LEU:HD22	4:3:225:GLN:NE2	2.19	0.58
17:H:171:ASP:HB3	17:H:174:VAL:HG12	1.85	0.58
27:U:137:THR:HB	27:U:140:GLU:OE1	2.04	0.58
34:o:11:SER:N	35:p:1135:TYR:HH	2.00	0.58
34:o:375:ILE:HG21	34:o:535:MET:HE1	1.85	0.58
3:2:69:ARG:CD	8:7:563:ARG:HH21	2.15	0.58
11:A:929:THR:HG22	11:A:954:ALA:HA	1.86	0.58
15:F:207:ARG:HD2	15:F:207:ARG:N	2.18	0.58
27:U:36:ILE:HG21	27:U:48:MET:HE1	1.84	0.58
34:o:890:ARG:HE	34:o:1023:VAL:HG22	1.68	0.58
34:o:938:LEU:HD22	34:o:1005:HIS:HD1	1.69	0.58
35:p:67:LEU:HD21	35:p:416:ARG:HG3	1.85	0.58
3:2:345:CYS:O	3:2:349:GLN:N	2.36	0.58
5:4:438:LYS:CE	12:B:621:ALA:N	2.65	0.58
15:F:83:LEU:CD1	15:F:83:LEU:N	2.67	0.58
27:U:145:PHE:HB2	27:U:153:ARG:HG2	1.85	0.58
31:c:12:VAL:HG23	15:f:118:ILE:HA	1.86	0.58
35:p:627:ILE:HD11	35:p:663:GLU:HB2	1.85	0.58
14:e:513:LEU:HD21	14:e:527:ILE:HG23	1.86	0.58
2:1:471:LEU:HD12	2:1:472:LEU:HD22	1.84	0.58
11:A:1063:LYS:HD3	11:A:1063:LYS:C	2.28	0.58
27:U:70:LYS:HE2	28:V:226:ASP:HA	1.86	0.58
33:m:67:GLU:HA	33:m:67:GLU:OE1	2.02	0.58
35:p:153:PRO:HB3	35:p:187:ILE:HD11	1.84	0.58
40:u:152:VAL:HB	40:u:157:ILE:HG12	1.85	0.58
1:0:8:ARG:O	27:U:178:ALA:HB2	2.04	0.58
4:3:241:LEU:HD23	4:3:243:LEU:HD11	1.86	0.58
25:S:71:PHE:CE2	26:T:194:HIS:HB3	2.39	0.58
28:V:163:LEU:HG	28:V:201:LEU:HD21	1.85	0.58
31:c:21:LEU:HD12	31:c:21:LEU:C	2.29	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:s:82:VAL:HG23	38:s:106:VAL:HG13	1.85	0.58
7:6:56:TYR:C	7:6:58:ALA:N	2.61	0.57
11:A:340:GLU:N	11:A:497:PRO:HG2	2.18	0.57
14:E:522:ASP:O	14:E:524:LEU:N	2.37	0.57
1:0:41:ARG:CD	27:U:169:PRO:CG	2.74	0.57
4:3:52:ASN:OD1	4:3:53:ARG:N	2.37	0.57
21:O:29:THR:HG23	21:O:32:LEU:H	1.70	0.57
22:P:299:ARG:NH2	29:X:-27:DA:OP1	2.36	0.57
34:o:1128:ILE:HG23	34:o:1414:ILE:HB	1.85	0.57
13:d:967:MET:HA	13:d:967:MET:HE2	1.84	0.57
14:e:484:LEU:HD21	14:e:504:LEU:HD21	1.86	0.57
15:f:219:GLU:OE1	15:f:219:GLU:N	2.25	0.57
4:3:215:LEU:HD22	4:3:230:VAL:HG21	1.87	0.57
43:x:3:ILE:HD12	43:x:4:PRO:HD2	1.85	0.57
1:0:1:MET:SD	8:7:345:ARG:HD3	2.45	0.57
7:6:528:LYS:CG	7:6:531:ILE:HD12	2.29	0.57
11:A:334:THR:HA	11:A:489:GLN:O	2.04	0.57
24:R:134:ILE:HG12	24:R:171:GLU:HG3	1.85	0.57
1:0:8:ARG:NH2	1:0:37:LEU:HB3	2.12	0.57
1:0:8:ARG:CD	27:U:173:ALA:H	2.14	0.57
7:6:625:GLN:OE1	7:6:639:ARG:NH1	2.36	0.57
12:B:629:ARG:NH1	12:B:658:ASP:OD2	2.37	0.57
14:E:586:TYR:HB3	14:E:605:HIS:HB3	1.85	0.57
15:F:81:GLU:HB3	15:F:83:LEU:HD13	1.85	0.57
28:V:148:LYS:HG3	28:V:149:LYS:HE2	1.86	0.57
8:7:240:ASP:OD1	8:7:241:ASN:N	2.37	0.57
30:Y:28:DT:H2'	30:Y:29:DA:N7	2.19	0.57
41:v:124:ARG:HD3	41:v:126:GLN:HG3	1.85	0.57
15:F:315:ARG:CZ	15:F:369:PRO:HB3	2.35	0.57
1:0:84:LYS:CB	1:0:136:ASN:ND2	2.68	0.57
34:o:1147:SER:HA	34:o:1153:ARG:HB2	1.86	0.57
34:o:1210:TRP:HZ3	42:w:53:ILE:HG13	1.70	0.57
35:p:55:VAL:HG12	35:p:91:ILE:HD13	1.86	0.57
41:v:37:MET:HE3	41:v:127:GLY:HA3	1.86	0.57
1:0:1:MET:SD	8:7:345:ARG:CD	2.93	0.57
1:0:41:ARG:CB	27:U:169:PRO:CG	2.81	0.57
27:U:160:GLU:OE2	27:U:162:GLU:N	2.38	0.57
14:e:257:GLU:CD	14:e:257:GLU:N	2.63	0.57
12:B:769:LYS:O	12:B:769:LYS:HG3	2.03	0.57
12:B:837:LEU:HD22	17:H:213:LEU:HD22	1.86	0.57
28:V:192:VAL:HG21	28:V:203:PHE:HB3	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:-20:DG:C8	29:X:-19:DT:H72	2.40	0.57
34:o:1366:PHE:HB2	34:o:1374:VAL:HG21	1.87	0.57
34:o:459:ASN:HD22	34:o:469:MET:HE3	1.69	0.56
8:7:664:VAL:HG21	8:7:679:PHE:CE1	2.40	0.56
15:F:335:ARG:HH21	15:F:378:ALA:HB1	1.69	0.56
25:S:73:ARG:NH1	25:S:76:ARG:HD2	2.20	0.56
28:V:148:LYS:HB3	28:V:183:LYS:HE3	1.87	0.56
35:p:82:PRO:HB3	35:p:134:LYS:HG2	1.87	0.56
3:2:223:LEU:CD1	8:7:726:GLN:OE1	2.53	0.56
7:6:281:GLN:NE2	7:6:482:PHE:O	2.37	0.56
11:A:851:ASP:OD1	11:A:851:ASP:N	2.38	0.56
13:D:960:GLU:HB3	13:D:983:ARG:CG	2.35	0.56
14:E:345:MET:HE3	14:E:346:PRO:HD2	1.88	0.56
21:O:62:LEU:HA	21:O:76:LEU:HD23	1.86	0.56
22:P:297:LYS:NZ	22:P:323:GLU:OE2	2.38	0.56
25:S:72:ASN:HB3	26:T:201:ASP:OD2	2.05	0.56
25:S:168:ASN:HA	35:p:248:LYS:HD2	1.87	0.56
30:Y:10:DC:N4	35:p:457:LYS:HZ1	2.03	0.56
34:o:628:VAL:HA	34:o:638:GLY:HA3	1.87	0.56
35:p:265:GLN:OE1	35:p:324:ARG:NH1	2.37	0.56
15:f:320:ARG:CB	15:f:320:ARG:HH11	2.17	0.56
5:4:433:PHE:CE2	6:5:38:ILE:HG23	2.41	0.56
7:6:54:ASP:HB2	7:6:58:ALA:HB3	1.87	0.56
12:B:259:ASP:HB3	12:B:262:MET:O	2.06	0.56
3:2:261:SER:OG	3:2:265:GLN:O	2.22	0.56
27:U:152:PHE:CD2	40:u:95:VAL:CG1	2.88	0.56
28:V:86:LYS:NZ	28:V:140:LYS:HD2	2.21	0.56
34:o:555:LEU:HD13	34:o:591:ILE:HD12	1.88	0.56
34:o:706:ILE:HD13	34:o:824:GLU:HG3	1.87	0.56
38:s:171:PRO:HB2	38:s:207:ARG:HD3	1.86	0.56
44:y:12:LEU:HD11	44:y:18:LYS:HE2	1.86	0.56
4:3:108:ASN:HD21	5:4:123:LEU:HD22	1.71	0.56
11:A:401:ASN:H	11:A:401:ASN:HD22	1.53	0.56
12:B:560:TYR:CD2	12:B:581:ILE:HD11	2.40	0.56
20:L:113:VAL:O	20:L:114:LYS:C	2.49	0.56
34:o:1230:GLN:HG2	34:o:1234:LYS:HE3	1.87	0.56
38:s:13:ILE:HD11	38:s:132:GLN:HG3	1.87	0.56
13:d:910:LEU:HD11	20:l:88:ALA:HB2	1.87	0.56
14:e:527:ILE:HG22	14:e:527:ILE:O	2.05	0.56
42:w:69:ILE:HG22	42:w:71:ASP:H	1.70	0.56
13:d:917:ILE:HD11	13:d:1063:LEU:HD13	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:e:636:HIS:HD2	14:e:638:ASN:H	1.53	0.56
15:F:265:GLU:OE2	15:F:265:GLU:HA	2.06	0.56
20:L:119:HIS:NE2	20:L:123:GLN:OE1	2.38	0.56
35:p:761:THR:HG23	35:p:1000:THR:HA	1.88	0.56
15:f:223:TYR:HD2	15:f:255:MET:HE1	1.71	0.56
15:f:280:ILE:O	15:f:284:ARG:HG3	2.05	0.56
1:0:8:ARG:CZ	1:0:34:CYS:SG	2.94	0.56
4:3:242:ILE:C	4:3:243:LEU:HD12	2.31	0.56
5:4:393:LEU:HD21	7:6:511:TRP:CH2	2.41	0.56
8:7:606:GLU:O	8:7:666:ARG:NH2	2.39	0.56
27:U:139:LEU:HD23	40:u:158:PHE:CD1	2.29	0.56
29:X:4:DA:H2''	29:X:5:DC:H2'	1.86	0.56
1:0:85:ARG:NH2	1:0:140:LEU:CA	2.69	0.56
12:B:27:LYS:CE	12:B:490:SER:HB3	2.35	0.56
30:Y:15:DA:H5''	30:Y:15:DA:H8	1.70	0.56
7:6:444:HIS:O	7:6:472:ARG:NH1	2.39	0.55
11:A:402:PHE:HA	11:A:407:GLN:NE2	2.20	0.55
12:B:61:ASN:O	12:B:130:VAL:HG23	2.06	0.55
26:T:194:HIS:CG	26:T:195:GLN:H	2.23	0.55
34:o:1386:ILE:HD12	34:o:1398:LEU:HD21	1.88	0.55
36:q:38:PHE:HE1	36:q:245:VAL:HA	1.71	0.55
2:1:456:ASP:OD1	2:1:457:ILE:HD12	2.06	0.55
3:2:59:ARG:NH2	3:2:166:GLU:OE1	2.38	0.55
5:4:407:VAL:N	5:4:443:VAL:O	2.37	0.55
13:D:956:GLN:HA	13:D:956:GLN:HE21	1.69	0.55
14:E:468:ASN:ND2	15:F:128:ASP:O	2.39	0.55
4:3:44:LEU:HD21	4:3:162:LEU:HD13	1.89	0.55
7:6:361:CYS:SG	7:6:405:VAL:HG13	2.46	0.55
15:F:312:ILE:HG13	15:F:334:ALA:HB3	1.88	0.55
28:V:149:LYS:HA	28:V:152:LEU:HD12	1.87	0.55
28:V:155:LEU:HD21	28:V:204:ASN:H	1.71	0.55
34:o:381:PRO:HB3	34:o:480:SER:HA	1.88	0.55
15:f:253:TYR:O	15:f:254:GLN:HB3	2.06	0.55
8:7:309:VAL:HG12	8:7:309:VAL:O	2.07	0.55
11:A:511:LEU:HD22	11:A:511:LEU:N	2.11	0.55
27:U:30:HIS:CD2	27:U:62:VAL:HG13	2.42	0.55
28:V:170:ASP:OD1	28:V:171:ILE:N	2.40	0.55
30:Y:10:DC:H1'	30:Y:11:DT:H5'	1.87	0.55
7:6:664:SER:O	7:6:667:THR:OG1	2.25	0.55
13:D:964:GLU:HA	13:D:982:LEU:HG	1.87	0.55
34:o:131:ALA:HA	34:o:134:LYS:HE2	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:o:1189:ASP:HA	34:o:1192:TRP:CE2	2.41	0.55
35:p:1120:ASN:HB2	35:p:1145:GLN:HB3	1.89	0.55
38:s:48:PRO:HA	38:s:53:PRO:HG2	1.87	0.55
13:d:960:GLU:HG2	13:d:963:ARG:HH21	1.70	0.55
1:0:20:LYS:HE3	1:0:62:LEU:HD13	1.87	0.55
7:6:528:LYS:CE	7:6:531:ILE:HD13	2.35	0.55
15:F:406:VAL:HG11	15:F:420:ALA:HB2	1.88	0.55
27:U:56:ARG:NH1	27:U:60:ARG:HH11	2.02	0.55
34:o:756:ALA:HB2	34:o:786:ALA:HB2	1.89	0.55
34:o:890:ARG:HH21	34:o:1023:VAL:HG13	1.71	0.55
34:o:1487:PRO:HG2	39:t:78:PRO:HA	1.88	0.55
38:s:59:THR:HB	38:s:73:PHE:HE1	1.72	0.55
7:6:83:HIS:ND1	7:6:115:GLU:OE2	2.39	0.55
48:Z:2500:W0F:O32	35:p:975:ARG:CZ	2.54	0.55
26:T:94:THR:HG22	26:T:109:ILE:HG22	1.89	0.55
29:X:5:DC:H1'	29:X:6:DT:C6	2.41	0.55
34:o:189:PRO:HA	34:o:205:VAL:HG21	1.87	0.55
20:l:99:ALA:HB1	20:l:111:LEU:HD11	1.87	0.55
8:7:114:ASN:C	8:7:114:ASN:HD22	2.15	0.55
11:A:1200:THR:C	11:A:1204:GLU:HG2	2.31	0.55
15:F:71:ILE:HD11	18:I:35:VAL:HG13	1.89	0.55
15:F:86:PHE:CD1	15:F:86:PHE:N	2.75	0.55
3:2:174:LEU:C	8:7:591:GLY:O	2.49	0.55
14:E:561:SER:HB2	14:E:588:VAL:HB	1.88	0.55
22:P:295:MET:HG2	22:P:298:PRO:HD2	1.88	0.55
28:V:213:ASP:O	28:V:217:GLN:N	2.39	0.55
34:o:769:MET:HE3	35:p:970:HIS:CD2	2.42	0.55
35:p:713:PHE:HB3	35:p:716:HIS:HD2	1.71	0.55
11:A:1052:ARG:HD2	11:A:1052:ARG:O	2.07	0.55
15:F:433:PRO:HA	15:F:436:ALA:HB3	1.89	0.55
24:R:90:ALA:HB3	34:o:324:GLY:HA2	1.88	0.55
27:U:14:LEU:HD11	27:U:194:THR:HG23	1.87	0.55
35:p:309:PHE:HE2	42:w:40:ARG:HB2	1.72	0.55
1:0:8:ARG:NH2	1:0:37:LEU:HD22	2.21	0.54
7:6:528:LYS:CD	7:6:531:ILE:CD1	2.85	0.54
11:A:463:PRO:HD3	15:F:222:LEU:HB2	1.89	0.54
13:D:963:ARG:O	13:D:982:LEU:HD11	2.07	0.54
14:E:474:THR:HG22	15:F:61:GLY:HA2	1.89	0.54
22:P:186:ARG:NH1	22:P:244:LEU:O	2.40	0.54
22:P:206:GLU:HB3	22:P:207:PRO:HD3	1.89	0.54
28:V:234:GLU:HB3	28:V:238:LYS:HZ3	1.72	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:8:DC:H2"	29:X:9:DA:H8	1.71	0.54
34:o:217:SER:HB3	34:o:220:ARG:HG3	1.89	0.54
7:6:87:GLU:OE2	7:6:145:LYS:NZ	2.40	0.54
8:7:17:ILE:HD11	8:7:22:PHE:CZ	2.42	0.54
15:F:87:HIS:HB2	18:I:45:ARG:HE	1.71	0.54
27:U:32:LEU:O	27:U:36:ILE:HG12	2.07	0.54
28:V:147:ASP:HB3	28:V:150:ALA:H	1.71	0.54
34:o:26:LEU:HD13	34:o:31:LEU:HD21	1.89	0.54
35:p:1115:GLN:HG2	35:p:1150:ARG:HG2	1.89	0.54
1:0:42:GLY:CA	27:U:168:MET:HE1	2.33	0.54
4:3:108:ASN:OD1	5:4:123:LEU:CD1	2.51	0.54
5:4:393:LEU:CD2	7:6:511:TRP:CH2	2.91	0.54
8:7:80:ILE:HD11	8:7:206:VAL:HB	1.89	0.54
35:p:665:ILE:HD13	35:p:673:VAL:HG21	1.89	0.54
35:p:841:ARG:HD2	35:p:895:PHE:CZ	2.42	0.54
1:0:85:ARG:NH2	1:0:140:LEU:HA	2.22	0.54
4:3:229:TRP:CZ3	5:4:58:ARG:HD2	2.42	0.54
5:4:80:SER:O	5:4:84:GLU:OE1	2.25	0.54
11:A:355:VAL:O	11:A:355:VAL:HG23	2.07	0.54
11:A:489:GLN:NE2	11:A:489:GLN:H	2.04	0.54
21:O:16:GLN:NE2	21:O:20:ASP:OD2	2.40	0.54
25:S:167:ARG:HH11	25:S:168:ASN:H	1.53	0.54
38:s:21:CYS:SG	38:s:26:TYR:HB2	2.47	0.54
41:v:113:SER:HB3	41:v:126:GLN:HG2	1.88	0.54
44:y:88:THR:O	44:y:92:THR:HG23	2.07	0.54
7:6:632:SER:OG	7:6:676:ARG:NH2	2.41	0.54
8:7:365:VAL:HG22	8:7:365:VAL:O	2.08	0.54
15:F:418:ILE:HD12	15:F:418:ILE:N	2.20	0.54
28:V:170:ASP:HA	28:V:173:GLU:HG2	1.89	0.54
38:s:26:TYR:HA	38:s:64:HIS:HA	1.89	0.54
15:f:390:THR:HG23	15:f:391:LEU:HD22	1.89	0.54
14:E:524:LEU:O	14:E:527:ILE:HG12	2.07	0.54
28:V:89:HIS:NE2	28:V:138:ALA:O	2.38	0.54
34:o:321:GLU:HG3	34:o:341:GLN:HE21	1.73	0.54
41:v:96:VAL:HG22	41:v:116:VAL:HG22	1.89	0.54
13:d:911:GLN:NE2	20:l:69:GLU:OE2	2.41	0.54
14:e:368:ASN:ND2	14:e:701:GLY:HA3	2.23	0.54
3:2:69:ARG:HB2	8:7:563:ARG:HH22	1.72	0.54
26:T:188:PHE:HB3	28:V:76:GLY:O	2.07	0.54
34:o:1005:HIS:HD2	34:o:1007:ILE:HG22	1.73	0.54
2:1:486:LEU:O	2:1:490:VAL:HG23	2.06	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:69:ARG:HB2	8:7:563:ARG:NH2	2.23	0.54
8:7:437:CYS:SG	8:7:438:MET:N	2.81	0.54
12:B:628:ILE:O	12:B:644:GLN:NE2	2.41	0.54
15:F:403:ILE:O	15:F:406:VAL:HG22	2.08	0.54
15:f:352:GLN:O	15:f:356:THR:OG1	2.25	0.54
4:3:242:ILE:CD1	5:4:75:VAL:C	2.81	0.54
12:B:544:LEU:HD23	12:B:590:ILE:HD11	1.88	0.54
23:Q:15:ARG:HA	23:Q:18:ILE:HD12	1.89	0.54
28:V:156:ASP:O	28:V:160:GLN:HG2	2.08	0.54
38:s:106:VAL:HG21	38:s:110:MET:HG3	1.90	0.54
42:w:17:CYS:HB2	42:w:24:LEU:HD21	1.90	0.54
19:j:123:LEU:C	19:j:125:ASP:N	2.66	0.54
1:0:85:ARG:HH12	1:0:140:LEU:N	2.06	0.54
5:4:265:LEU:HD12	5:4:270:LEU:HD12	1.90	0.54
12:B:571:LEU:HD21	12:B:619:MET:HE1	1.89	0.54
12:B:808:PRO:HA	12:B:864:ASN:HB3	1.90	0.54
33:m:110:LEU:N	33:m:110:LEU:HD23	2.23	0.54
4:3:195:VAL:CG1	4:3:203:LEU:HD23	2.38	0.53
5:4:408:LEU:HD21	5:4:440:LEU:HD22	1.89	0.53
12:B:248:SER:OG	12:B:322:MET:SD	2.65	0.53
14:E:653:LEU:HB2	14:E:663:ARG:HB2	1.90	0.53
27:U:76:MET:HG2	27:U:88:ARG:HB3	1.89	0.53
34:o:1173:THR:HG22	34:o:1214:VAL:HG22	1.90	0.53
34:o:1258:ARG:HH22	34:o:1260:ARG:HH21	1.54	0.53
35:p:529:MET:HE3	35:p:624:PRO:HG2	1.90	0.53
35:p:733:MET:HE3	35:p:1052:LYS:HA	1.90	0.53
13:D:998:GLN:HG3	13:D:1002:ARG:NH1	2.22	0.53
16:G:149:ARG:O	16:G:149:ARG:HG3	2.08	0.53
31:c:33:LEU:HD13	19:j:197:MET:HE1	1.91	0.53
34:o:538:VAL:HG22	34:o:539:GLN:HG2	1.91	0.53
35:p:783:ALA:O	35:p:789:ASN:ND2	2.41	0.53
1:0:85:ARG:HH22	1:0:140:LEU:HA	1.72	0.53
3:2:337:GLU:O	3:2:340:ASN:ND2	2.38	0.53
6:5:31:LYS:HB3	12:B:540:LYS:HZ1	1.44	0.53
7:6:377:GLN:OE1	7:6:381:TRP:NE1	2.40	0.53
8:7:420:PRO:HA	8:7:431:PRO:HB3	1.89	0.53
13:D:963:ARG:C	13:D:982:LEU:CD1	2.79	0.53
14:E:645:GLY:H	14:E:675:LEU:HD11	1.73	0.53
40:u:55:GLY:HA3	40:u:69:PRO:HG2	1.90	0.53
41:v:65:TYR:HD1	41:v:84:ARG:HG2	1.72	0.53
14:e:610:ARG:HD3	14:e:619:PRO:HG3	1.89	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:87:LEU:HD11	3:2:229:LYS:HG2	1.91	0.53
6:5:32:LYS:HB3	12:B:540:LYS:HG3	1.90	0.53
13:D:922:GLN:NE2	20:L:71:ASP:OD2	2.41	0.53
13:D:998:GLN:HG3	13:D:1002:ARG:HH12	1.73	0.53
14:E:563:GLU:HG2	14:E:587:PRO:HG3	1.90	0.53
3:2:88:LEU:HD23	3:2:131:LEU:HD21	1.91	0.53
4:3:44:LEU:HD22	4:3:227:LEU:HB3	1.90	0.53
8:7:289:VAL:HG22	8:7:324:ARG:NH1	2.23	0.53
48:Z:2500:WOF:C01	48:Z:2500:WOF:C20	2.85	0.53
12:B:937:THR:HG23	12:B:939:ASN:H	1.74	0.53
13:D:910:LEU:HD11	20:L:88:ALA:HB2	1.91	0.53
34:o:43:TYR:HB3	34:o:53:LYS:HE3	1.91	0.53
35:p:737:ILE:HG22	35:p:739:ASN:H	1.73	0.53
35:p:984:CYS:SG	35:p:1046:THR:OG1	2.56	0.53
14:e:646:SER:OG	14:e:647:ALA:N	2.40	0.53
7:6:528:LYS:CD	7:6:531:ILE:HD11	2.39	0.53
7:6:568:LEU:HD11	7:6:606:PHE:HB3	1.90	0.53
8:7:44:SER:OG	8:7:46:THR:O	2.16	0.53
8:7:133:LYS:O	8:7:137:LEU:HD23	2.07	0.53
10:Z:1:ATP:H5'1	10:Z:2:G2L:OP2	2.03	0.53
12:B:345:CYS:HA	12:B:348:GLN:HE21	1.73	0.53
34:o:894:ASP:O	34:o:1022:ILE:HD13	2.08	0.53
35:p:810:PHE:CB	35:p:927:ARG:HE	2.22	0.53
36:q:260:GLN:HE22	44:y:92:THR:HG22	1.74	0.53
38:s:17:ILE:HD13	38:s:74:VAL:HG11	1.90	0.53
1:0:8:ARG:HB2	27:U:172:ASP:OD2	2.09	0.53
8:7:488:VAL:HG23	8:7:488:VAL:O	2.09	0.53
11:A:395:ASP:OD1	11:A:395:ASP:N	2.41	0.53
14:e:423:PRO:HG2	14:e:426:ARG:HB2	1.91	0.53
2:1:127:LEU:HD12	2:1:467:ALA:HA	1.91	0.53
7:6:528:LYS:HG3	7:6:531:ILE:HD12	1.88	0.53
8:7:28:LEU:HD22	8:7:55:LEU:HD23	1.90	0.53
15:F:335:ARG:HD2	15:F:382:GLU:HB2	1.90	0.53
30:Y:29:DA:H2'	30:Y:30:DT:C6	2.44	0.53
15:f:283:MET:HG3	15:f:329:LEU:HD11	1.91	0.53
6:5:38:ILE:HG22	6:5:39:ASP:N	2.24	0.53
12:B:66:ASN:HD21	12:B:119:PRO:HB3	1.73	0.53
34:o:1436:VAL:O	34:o:1440:MET:HG2	2.09	0.53
4:3:108:ASN:CG	5:4:123:LEU:HD13	2.33	0.53
13:D:960:GLU:HG2	13:D:983:ARG:HD3	1.91	0.53
16:G:181:TRP:CE3	16:G:181:TRP:O	2.62	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:T:238:GLU:HB3	28:V:130:ILE:CD1	2.39	0.53
27:U:146:ASP:HB2	27:U:147:PRO:HD2	1.90	0.53
11:A:675:ASP:OD1	16:G:78:LYS:NZ	2.37	0.52
14:E:304:LYS:NZ	14:E:335:GLU:O	2.42	0.52
27:U:183:GLN:NE2	28:V:211:SER:O	2.42	0.52
34:o:479:TRP:HB2	34:o:483:ARG:HH21	1.73	0.52
13:D:998:GLN:HB2	13:D:1002:ARG:HH22	1.73	0.52
27:U:139:LEU:CD1	40:u:149:GLY:O	2.57	0.52
34:o:1294:THR:HG21	35:p:245:GLN:NE2	2.24	0.52
35:p:709:SER:HB2	35:p:767:LEU:HD11	1.91	0.52
5:4:32:ASP:OD1	5:4:33:ARG:N	2.42	0.52
5:4:438:LYS:HE2	12:B:621:ALA:H	1.74	0.52
13:D:873:LEU:HD21	20:L:92:ILE:HD11	1.91	0.52
14:E:562:SER:OG	14:E:564:ASP:OD1	2.28	0.52
28:V:117:GLN:O	28:V:121:THR:OG1	2.18	0.52
34:o:863:ARG:NH2	34:o:1415:THR:HG22	2.25	0.52
40:u:148:VAL:N	40:u:160:ILE:O	2.43	0.52
1:0:83:ASN:CG	1:0:140:LEU:HD12	2.34	0.52
3:2:174:LEU:HD21	3:2:203:ALA:HB2	1.89	0.52
7:6:340:LEU:HD23	7:6:491:ALA:HB2	1.92	0.52
8:7:393:ASP:OD1	8:7:394:PHE:N	2.42	0.52
26:T:188:PHE:HB3	28:V:76:GLY:C	2.35	0.52
27:U:184:ILE:HG23	27:U:187:ILE:HB	1.91	0.52
34:o:392:GLU:HB2	34:o:448:ARG:HH11	1.74	0.52
15:f:447:ALA:O	15:f:453:GLY:HA2	2.09	0.52
4:3:50:PHE:HZ	5:4:118:LEU:HD13	1.61	0.52
12:B:202:TRP:HB2	12:B:238:LEU:HB3	1.92	0.52
15:F:39:LEU:HD11	18:I:51:LEU:HD21	1.92	0.52
22:P:203:ARG:NH1	30:Y:27:DT:OP1	2.42	0.52
25:S:174:PHE:HD1	42:w:40:ARG:HA	1.75	0.52
26:T:160:GLN:O	26:T:163:ILE:HG12	2.10	0.52
15:f:318:CYS:SG	15:f:326:HIS:HB3	2.49	0.52
14:E:522:ASP:OD1	14:E:522:ASP:N	2.42	0.52
15:F:273:GLN:H	15:F:273:GLN:CD	2.17	0.52
26:T:238:GLU:OE1	28:V:82:VAL:HG11	2.09	0.52
35:p:75:SER:O	35:p:77:GLU:HG2	2.10	0.52
5:4:172:SER:OG	5:4:267:GLU:OE2	2.13	0.52
7:6:181:HIS:O	7:6:184:VAL:HG12	2.10	0.52
8:7:571:THR:OG1	8:7:576:GLU:OE1	2.08	0.52
12:B:66:ASN:OD1	12:B:187:ARG:NH1	2.43	0.52
25:S:115:LYS:NZ	25:S:117:GLY:O	2.37	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:U:139:LEU:CG	40:u:159:ALA:C	2.76	0.52
28:V:175:LEU:HB2	28:V:180:LYS:HE2	1.91	0.52
30:Y:10:DC:H1'	30:Y:11:DT:C5'	2.40	0.52
34:o:62:GLN:HG3	34:o:84:HIS:O	2.10	0.52
34:o:1143:LEU:HD21	34:o:1336:LEU:HD11	1.92	0.52
14:e:607:ARG:NH1	18:i:87:PRO:O	2.43	0.52
5:4:413:LEU:HB2	12:B:672:PHE:HE1	1.75	0.52
11:A:339:ALA:HA	11:A:497:PRO:HG3	1.92	0.52
14:E:601:VAL:HG21	14:E:642:VAL:HG11	1.92	0.52
15:F:219:GLU:HG2	17:H:156:PRO:C	2.35	0.52
15:F:257:PRO:O	15:F:261:THR:OG1	2.26	0.52
34:o:1158:LEU:HD23	34:o:1336:LEU:HD13	1.92	0.52
35:p:934:LYS:HZ1	35:p:942:LYS:HD2	1.75	0.52
14:e:595:PRO:HD2	14:e:639:SER:HB3	1.91	0.52
14:e:747:LEU:HG	14:e:747:LEU:O	2.09	0.52
8:7:115:LEU:HD13	8:7:191:PRO:HB2	1.92	0.52
12:B:529:VAL:HG11	12:B:560:TYR:HB2	1.91	0.52
14:E:278:ASP:OD1	14:E:278:ASP:N	2.43	0.52
19:J:137:TYR:OH	19:J:141:ARG:NH2	2.43	0.52
24:R:177:PHE:HB3	24:R:188:LYS:HG3	1.91	0.52
34:o:597:PRO:HD2	34:o:600:ILE:HD12	1.90	0.52
34:o:1381:GLU:O	34:o:1385:VAL:HG13	2.10	0.52
36:q:38:PHE:CE1	36:q:245:VAL:HA	2.45	0.52
3:2:54:ARG:NH2	3:2:245:SER:O	2.42	0.51
19:J:114:THR:HB	19:J:117:VAL:HB	1.92	0.51
27:U:48:MET:O	27:U:52:LEU:N	2.42	0.51
27:U:110:MET:O	27:U:114:ILE:HG12	2.10	0.51
28:V:97:LEU:HG	28:V:101:GLU:CD	2.35	0.51
34:o:927:GLU:O	34:o:931:ARG:HG2	2.09	0.51
2:1:136:VAL:HG11	2:1:502:VAL:HG12	1.92	0.51
11:A:828:GLU:HA	11:A:831:LYS:HB2	1.92	0.51
13:D:960:GLU:HB3	13:D:983:ARG:HH11	1.74	0.51
15:F:243:LEU:HD21	15:F:284:ARG:HB3	1.92	0.51
27:U:139:LEU:CD1	40:u:159:ALA:CA	2.86	0.51
15:f:320:ARG:NH1	15:f:320:ARG:CB	2.73	0.51
1:0:8:ARG:NE	27:U:173:ALA:CB	2.73	0.51
1:0:41:ARG:C	27:U:168:MET:CE	2.81	0.51
4:3:165:LYS:NZ	4:3:167:ALA:O	2.38	0.51
8:7:709:THR:HG22	8:7:710:VAL:N	2.25	0.51
12:B:656:GLU:HG2	12:B:661:ALA:HB3	1.92	0.51
14:E:423:PRO:HG2	14:E:426:ARG:HB2	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:R:50:SER:C	35:p:1069:ILE:HG13	2.36	0.51
24:R:248:ARG:NH2	24:R:287:GLN:OE1	2.43	0.51
27:U:128:LYS:O	27:U:162:GLU:HB3	2.10	0.51
33:m:28:ARG:HH21	33:m:31:LEU:HD21	1.76	0.51
35:p:201:ALA:N	35:p:390:ASN:O	2.43	0.51
35:p:298:MET:HB3	42:w:14:ILE:HD12	1.92	0.51
2:1:471:LEU:HD13	2:1:475:PHE:HE2	1.75	0.51
5:4:266:ARG:HE	5:4:277:LYS:HZ2	1.56	0.51
7:6:463:LYS:O	7:6:484:ILE:HG23	2.10	0.51
8:7:126:PHE:CE2	8:7:128:LYS:HB2	2.45	0.51
14:E:781:VAL:HG13	15:F:62:LYS:HD3	1.90	0.51
24:R:87:GLY:HA3	34:o:326:PRO:HA	1.92	0.51
42:w:12:VAL:HG23	42:w:50:ASN:HD21	1.74	0.51
14:e:650:THR:HG22	14:e:666:THR:HG22	1.93	0.51
7:6:363:VAL:HG21	7:6:378:PHE:HE2	1.75	0.51
24:R:105:ARG:NH1	30:Y:13:DA:N7	2.50	0.51
31:c:21:LEU:HD12	31:c:21:LEU:O	2.11	0.51
34:o:110:VAL:HG13	34:o:115:SER:HA	1.93	0.51
3:2:204:GLU:OE1	3:2:209:THR:OG1	2.28	0.51
12:B:780:LYS:O	17:H:183:ARG:NH1	2.44	0.51
12:B:983:ARG:HH11	12:B:983:ARG:HG3	1.76	0.51
17:H:52:SER:O	19:J:194:THR:HA	2.10	0.51
21:O:57:ASN:OD1	21:O:58:PHE:N	2.44	0.51
34:o:349:ARG:HH21	35:p:1070:LEU:HD21	1.76	0.51
11:A:338:VAL:HG12	11:A:497:PRO:HD3	1.91	0.51
11:A:1163:ARG:HB3	16:G:183:ILE:HG22	1.92	0.51
16:G:181:TRP:CD2	16:G:181:TRP:C	2.87	0.51
25:S:73:ARG:CZ	26:T:229:HIS:HB2	2.41	0.51
42:w:59:THR:HB	42:w:61:GLU:HG3	1.93	0.51
12:B:90:THR:O	12:B:968:ARG:NH2	2.43	0.51
27:U:139:LEU:CD2	40:u:158:PHE:O	2.53	0.51
4:3:100:LYS:HG2	5:4:124:GLY:C	2.35	0.51
8:7:3:LEU:O	8:7:9:LEU:HD12	2.11	0.51
12:B:489:GLN:OE1	12:B:489:GLN:N	2.34	0.51
12:B:739:ASN:ND2	12:B:782:ASN:OD1	2.44	0.51
14:E:746:ASP:OD1	14:E:746:ASP:N	2.42	0.51
27:U:74:CYS:HA	27:U:91:TYR:O	2.11	0.51
30:Y:10:DC:C2	30:Y:11:DT:H2'	2.46	0.51
31:c:1:MET:HG3	15:f:126:PRO:HB3	1.93	0.51
37:r:33:LEU:HG	37:r:84:ARG:NH2	2.25	0.51
8:7:45:GLY:O	8:7:48:LYS:NZ	2.44	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:E:256:HIS:HB3	14:E:259:GLU:HG2	1.93	0.51
28:V:227:SER:O	28:V:231:GLU:HG2	2.11	0.51
44:y:41:THR:O	44:y:45:ILE:HG13	2.11	0.51
3:2:121:SER:OG	3:2:127:HIS:NE2	2.39	0.50
8:7:637:LEU:HD13	8:7:651:PHE:CD2	2.46	0.50
8:7:726:GLN:CG	8:7:727:PRO:CD	2.84	0.50
34:o:456:VAL:HG21	34:o:503:LEU:HD11	1.93	0.50
34:o:458:PHE:HE2	34:o:484:LEU:HD23	1.76	0.50
35:p:918:PHE:HE2	35:p:920:LYS:HE3	1.75	0.50
15:f:24:GLU:HG2	20:l:145:THR:HG21	1.93	0.50
5:4:390:GLN:HE21	5:4:394:TRP:NE1	2.09	0.50
7:6:274:GLN:OE1	7:6:459:GLN:NE2	2.44	0.50
27:U:164:ASP:HB2	27:U:167:ALA:HA	1.93	0.50
28:V:179:GLN:O	28:V:183:LYS:HB2	2.10	0.50
13:d:1080:TYR:OH	14:e:606:ASP:OD2	2.26	0.50
14:e:500:THR:HG22	14:e:502:LYS:H	1.76	0.50
5:4:409:TYR:HB2	5:4:412:PHE:HZ	1.74	0.50
8:7:284:GLU:HA	8:7:287:ARG:HG2	1.94	0.50
8:7:377:GLU:OE1	8:7:377:GLU:N	2.44	0.50
20:L:126:MET:HE3	20:L:128:ILE:HD11	1.93	0.50
22:P:169:VAL:HG21	29:X:-27:DA:C2	2.46	0.50
24:R:127:ARG:HD2	24:R:183:VAL:HB	1.93	0.50
2:1:412:GLU:OE1	2:1:412:GLU:N	2.44	0.50
27:U:139:LEU:HD11	40:u:158:PHE:O	2.11	0.50
40:u:97:LEU:HD23	40:u:108:ILE:HD13	1.94	0.50
1:0:8:ARG:HD3	1:0:34:CYS:SG	2.52	0.50
2:1:471:LEU:HD13	2:1:475:PHE:CE2	2.47	0.50
4:3:108:ASN:ND2	5:4:123:LEU:HD22	2.26	0.50
7:6:369:VAL:HG11	7:6:615:PHE:HA	1.93	0.50
11:A:510:ILE:HB	11:A:511:LEU:HD13	1.93	0.50
12:B:274:LEU:HG	12:B:278:LYS:HE2	1.93	0.50
13:D:998:GLN:NE2	26:T:186:MET:SD	2.85	0.50
20:L:93:GLU:O	20:L:97:THR:HG23	2.11	0.50
22:P:297:LYS:HB3	22:P:298:PRO:HD3	1.94	0.50
34:o:495:ASP:OD1	34:o:495:ASP:N	2.43	0.50
34:o:1311:LEU:HD11	34:o:1332:GLN:HB3	1.94	0.50
14:e:527:ILE:O	14:e:527:ILE:CG2	2.59	0.50
2:1:524:HIS:ND1	3:2:270:SER:OG	2.39	0.50
12:B:983:ARG:HG3	12:B:983:ARG:NH1	2.26	0.50
15:F:316:GLN:NE2	15:F:319:LEU:O	2.45	0.50
22:P:227:GLU:OE1	22:P:318:ARG:NH2	2.43	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:c:77:LEU:HD23	31:c:77:LEU:O	2.11	0.50
34:o:367:ILE:HG21	34:o:501:MET:HG3	1.94	0.50
34:o:631:GLU:HG2	34:o:988:TRP:HZ2	1.77	0.50
34:o:1443:ALA:HB2	35:p:1167:ILE:HG23	1.94	0.50
35:p:117:ASN:HA	35:p:189:GLY:HA3	1.92	0.50
35:p:713:PHE:HB3	35:p:716:HIS:CD2	2.47	0.50
40:u:94:LYS:HA	40:u:119:PHE:HB3	1.94	0.50
1:0:27:GLY:HA3	1:0:70:LYS:CD	2.34	0.50
12:B:882:HIS:HE1	17:H:216:ALA:HB1	1.77	0.50
17:H:113:ARG:O	17:H:116:ARG:NH1	2.44	0.50
34:o:1243:LEU:HD21	34:o:1288:ILE:HD13	1.93	0.50
36:q:99:VAL:HG21	36:q:127:VAL:HG21	1.94	0.50
27:U:30:HIS:CE1	27:U:62:VAL:HG22	2.47	0.50
27:U:145:PHE:HB2	27:U:153:ARG:CG	2.41	0.50
34:o:490:THR:OG1	34:o:491:PRO:HD3	2.11	0.50
34:o:1294:THR:HG21	35:p:245:GLN:HE22	1.76	0.50
42:w:14:ILE:HG21	42:w:23:MET:HE2	1.94	0.50
7:6:650:MET:SD	7:6:656:ASN:ND2	2.82	0.50
8:7:118:HIS:HB3	8:7:121:VAL:HG22	1.94	0.50
12:B:152:LEU:HD23	12:B:155:PRO:HB3	1.94	0.50
28:V:87:THR:O	28:V:91:ARG:HG2	2.11	0.50
34:o:602:CYS:HB2	34:o:655:ILE:HD12	1.94	0.50
35:p:759:VAL:HG12	35:p:999:ALA:HB2	1.92	0.50
42:w:113:VAL:HG22	42:w:122:ARG:HG2	1.94	0.50
3:2:285:THR:O	3:2:297:LYS:NZ	2.45	0.49
5:4:406:GLY:HA2	5:4:444:THR:HA	1.94	0.49
7:6:578:PRO:HG3	7:6:602:ILE:HD11	1.94	0.49
14:E:327:ASN:H	14:E:327:ASN:ND2	2.05	0.49
15:F:71:ILE:HD12	18:I:38:GLN:HE21	1.76	0.49
21:O:73:THR:O	21:O:73:THR:HG22	2.12	0.49
25:S:73:ARG:NH1	26:T:229:HIS:HB2	2.27	0.49
25:S:142:ASN:OD1	25:S:143:TRP:N	2.44	0.49
28:V:113:LEU:HA	28:V:116:LYS:HE2	1.94	0.49
29:X:-18:DG:C2	29:X:-17:DG:C6	3.00	0.49
33:m:69:THR:HG22	33:m:73:MET:HE2	1.94	0.49
5:4:438:LYS:CE	12:B:621:ALA:HB2	2.42	0.49
8:7:284:GLU:HG2	8:7:385:THR:HG21	1.94	0.49
10:Z:2:G2L:H2'	48:Z:2500:W0F:C10	2.42	0.49
12:B:820:ASP:OD1	12:B:820:ASP:N	2.37	0.49
13:D:965:ILE:C	13:D:965:ILE:HD13	2.37	0.49
14:E:232:HIS:HD1	14:E:313:SER:HG	1.57	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:u:13:LEU:HD11	40:u:26:VAL:HG22	1.94	0.49
14:e:586:TYR:HB3	14:e:605:HIS:HB3	1.94	0.49
14:E:481:ASP:HB3	14:E:787:ARG:HH22	1.77	0.49
15:F:312:ILE:HG22	15:F:313:VAL:HG13	1.94	0.49
24:R:104:ARG:HH21	30:Y:10:DC:H42	1.60	0.49
34:o:802:PHE:HD2	35:p:671:GLU:HG2	1.77	0.49
34:o:1481:LYS:HG2	40:u:20:PRO:HA	1.93	0.49
15:f:97:ALA:HB2	15:f:106:PHE:HE1	1.77	0.49
2:1:374:LEU:HD12	2:1:374:LEU:O	2.13	0.49
3:2:87:LEU:HD11	3:2:229:LYS:CG	2.43	0.49
19:J:139:LEU:HB3	19:J:144:PHE:HB3	1.93	0.49
27:U:139:LEU:HD11	40:u:159:ALA:CA	2.27	0.49
34:o:93:PRO:HD2	34:o:219:GLU:HG2	1.95	0.49
34:o:1228:MET:HE3	34:o:1247:PHE:HB2	1.93	0.49
3:2:69:ARG:CG	3:2:141:GLY:H	2.23	0.49
7:6:449:LYS:HB3	29:X:29:DA:P	2.52	0.49
11:A:821:ARG:HA	11:A:821:ARG:NE	2.25	0.49
24:R:39:LEU:HD11	34:o:425:ASP:HB3	1.93	0.49
44:y:84:GLN:O	44:y:88:THR:HG23	2.12	0.49
16:G:48:HIS:HD2	16:G:54:GLY:HA2	1.78	0.49
29:X:27:DA:H2"	29:X:28:DG:N7	2.27	0.49
34:o:26:LEU:HG	35:p:1168:ALA:HB2	1.94	0.49
34:o:95:PHE:HB2	34:o:311:GLN:HE22	1.77	0.49
4:3:237:GLN:HG3	5:4:51:LEU:HD21	1.94	0.49
12:B:818:THR:OG1	12:B:819:LEU:N	2.44	0.49
16:G:94:MET:HE3	16:G:96:VAL:HG22	1.94	0.49
34:o:463:THR:HG21	35:p:1090:GLU:HG3	1.94	0.49
35:p:168:ASP:N	35:p:168:ASP:OD1	2.46	0.49
35:p:567:ILE:HD11	35:p:577:HIS:HB2	1.94	0.49
35:p:789:ASN:HB3	35:p:795:ILE:HG13	1.94	0.49
35:p:1088:GLU:O	35:p:1091:ARG:HG2	2.12	0.49
41:v:17:PRO:HG3	41:v:29:HIS:NE2	2.28	0.49
5:4:405:GLU:O	5:4:444:THR:HG22	2.11	0.49
11:A:468:PHE:CE1	15:F:216:LEU:HD12	2.47	0.49
11:A:927:VAL:O	11:A:933:ASN:ND2	2.45	0.49
14:E:693:VAL:HB	14:E:707:LEU:HB2	1.94	0.49
27:U:99:LEU:O	27:U:103:VAL:HG23	2.13	0.49
34:o:48:GLU:HB2	34:o:53:LYS:HD2	1.94	0.49
34:o:455:ILE:HD13	34:o:516:GLN:HB2	1.93	0.49
34:o:486:LEU:HD13	35:p:790:GLN:CD	2.38	0.49
35:p:715:ASP:OD1	35:p:715:ASP:N	2.44	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:e:633:THR:O	14:e:634:ARG:NH2	2.45	0.49
1:0:4:GLN:OE1	1:0:10:LYS:HD3	2.13	0.49
5:4:338:PHE:N	5:4:341:MET:O	2.44	0.49
8:7:243:CYS:SG	8:7:443:ALA:HB3	2.53	0.49
14:E:589:TRP:CE3	15:F:60:MET:HG3	2.48	0.49
15:F:273:GLN:CD	15:F:273:GLN:N	2.70	0.49
35:p:1038:THR:HA	36:q:195:THR:HA	1.95	0.49
2:1:440:LEU:HD11	4:3:218:PRO:CD	2.43	0.49
3:2:63:VAL:HG11	3:2:88:LEU:HD11	1.95	0.49
8:7:134:CYS:O	8:7:138:THR:HG22	2.13	0.49
14:E:299:ASP:OD2	14:E:607:ARG:NH2	2.38	0.49
27:U:139:LEU:HD21	40:u:158:PHE:CD1	2.43	0.49
36:q:105:VAL:HG11	36:q:115:VAL:HG22	1.94	0.49
40:u:92:VAL:HG12	40:u:119:PHE:CD1	2.48	0.49
14:e:651:VAL:HG13	14:e:665:PHE:HB2	1.95	0.49
3:2:69:ARG:HG2	3:2:141:GLY:H	1.78	0.48
3:2:69:ARG:HD2	8:7:563:ARG:NH2	2.28	0.48
3:2:348:CYS:O	4:3:146:ARG:NH2	2.45	0.48
8:7:136:SER:O	8:7:142:VAL:HG21	2.13	0.48
11:A:337:ARG:HH11	11:A:338:VAL:H	1.61	0.48
14:E:651:VAL:HB	14:E:665:PHE:HB2	1.95	0.48
15:F:409:GLY:O	15:F:417:ARG:NH2	2.46	0.48
22:P:174:LEU:HD12	22:P:178:LEU:HD11	1.93	0.48
24:R:123:THR:O	24:R:127:ARG:HG3	2.13	0.48
25:S:71:PHE:CZ	26:T:194:HIS:HB3	2.48	0.48
28:V:234:GLU:HB3	28:V:238:LYS:NZ	2.28	0.48
30:Y:-29:DT:H2"	30:Y:-28:DC:C6	2.47	0.48
32:k:191:VAL:HG13	32:k:200:ILE:CD1	2.42	0.48
34:o:733:LEU:HA	34:o:736:THR:HG22	1.95	0.48
37:r:108:ALA:HB2	37:r:128:GLN:HB2	1.95	0.48
14:e:720:SER:OG	14:e:721:ARG:N	2.46	0.48
5:4:174:ASP:OD1	5:4:175:LEU:N	2.45	0.48
8:7:81:GLU:O	8:7:84:ILE:HG22	2.13	0.48
11:A:569:ASN:HB3	11:A:572:TYR:HD2	1.78	0.48
12:B:329:LEU:HB3	12:B:342:THR:HG23	1.95	0.48
13:D:991:MET:HE1	26:T:192:GLU:HG2	1.94	0.48
14:E:256:HIS:HB3	14:E:259:GLU:CG	2.43	0.48
14:E:467:LEU:HD11	15:F:132:LYS:HD3	1.94	0.48
24:R:102:GLN:NE2	34:o:305:GLU:HG2	2.28	0.48
34:o:478:PRO:O	44:y:4:PRO:HD3	2.13	0.48
40:u:93:ASN:N	40:u:128:TYR:OH	2.42	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:456:ASP:OD1	2:1:456:ASP:N	2.47	0.48
13:D:1068:GLU:OE2	14:E:582:LYS:NZ	2.45	0.48
17:H:197:THR:HB	15:f:238:LYS:HG2	1.95	0.48
20:L:113:VAL:O	20:L:116:VAL:N	2.46	0.48
34:o:18:ILE:HG12	35:p:1171:MET:HB2	1.95	0.48
36:q:101:PHE:CE2	36:q:122:SER:HB3	2.48	0.48
7:6:575:LEU:O	7:6:576:ASN:OD1	2.32	0.48
8:7:115:LEU:HD12	8:7:115:LEU:O	2.13	0.48
12:B:560:TYR:HD2	12:B:581:ILE:HD11	1.78	0.48
12:B:598:ARG:HH11	12:B:619:MET:HE3	1.77	0.48
20:L:106:ARG:O	20:L:106:ARG:HG2	2.14	0.48
23:Q:18:ILE:HD11	23:Q:46:TRP:CZ3	2.48	0.48
25:S:65:SER:HA	25:S:81:ARG:NH1	2.13	0.48
27:U:30:HIS:NE2	27:U:62:VAL:HA	2.28	0.48
28:V:110:ASP:OD1	28:V:114:LYS:HD3	2.12	0.48
34:o:51:ARG:HB2	34:o:52:PRO:HD3	1.96	0.48
34:o:330:GLN:HE21	34:o:334:ARG:HE	1.60	0.48
1:0:8:ARG:NH2	1:0:34:CYS:HA	2.29	0.48
4:3:13:ILE:HD13	4:3:41:VAL:HG13	1.94	0.48
7:6:363:VAL:HG21	7:6:378:PHE:CE2	2.47	0.48
12:B:559:LYS:HZ3	12:B:559:LYS:HB2	1.79	0.48
26:T:80:GLU:OE1	26:T:81:HIS:N	2.45	0.48
27:U:150:GLY:C	40:u:93:ASN:OD1	2.57	0.48
30:Y:19:DA:H2''	30:Y:20:DC:H5'	1.95	0.48
34:o:1440:MET:SD	35:p:1167:ILE:HD11	2.54	0.48
35:p:309:PHE:CE2	42:w:40:ARG:HB2	2.49	0.48
40:u:12:LEU:HD11	40:u:67:LEU:HD12	1.95	0.48
40:u:114:PRO:HD3	40:u:163:LEU:HB2	1.95	0.48
3:2:175:THR:HG23	8:7:592:ARG:HA	1.96	0.48
8:7:52:LEU:HD21	8:7:232:VAL:HG11	1.96	0.48
12:B:953:LEU:HD12	12:B:979:PHE:HE2	1.79	0.48
27:U:141:ALA:O	40:u:98:PHE:CZ	2.66	0.48
28:V:176:PRO:O	28:V:178:SER:N	2.46	0.48
30:Y:7:DG:O6	30:Y:8:DA:N6	2.47	0.48
35:p:789:ASN:O	35:p:968:ASN:HB2	2.13	0.48
37:r:112:LYS:HB3	37:r:119:GLU:HG2	1.95	0.48
14:e:525:GLU:OE1	14:e:525:GLU:N	2.41	0.48
1:0:8:ARG:CD	1:0:34:CYS:SG	3.01	0.48
1:0:63:PHE:HB2	1:0:69:ASP:OD1	2.13	0.48
2:1:427:ALA:HB1	5:4:62:LEU:CD1	2.44	0.48
8:7:310:LEU:HG	8:7:409:THR:HG21	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:338:VAL:HG13	11:A:360:SER:HB2	1.96	0.48
17:H:39:VAL:HG12	17:H:119:ILE:HG12	1.96	0.48
27:U:44:LYS:HG3	27:U:89:HIS:CD2	2.48	0.48
31:c:119:GLU:HG3	14:e:790:LEU:HD11	1.96	0.48
34:o:557:ARG:O	34:o:561:MET:HG2	2.13	0.48
14:e:693:VAL:HB	14:e:707:LEU:HB2	1.94	0.48
2:1:481:VAL:HG23	2:1:483:THR:HG23	1.94	0.48
12:B:570:GLU:HA	12:B:625:LEU:HA	1.95	0.48
12:B:636:VAL:HG23	12:B:638:ARG:HB3	1.96	0.48
14:E:703:MET:HE2	14:E:761:LEU:HD21	1.95	0.48
37:r:105:PRO:HG2	37:r:131:LEU:HD22	1.96	0.48
15:f:257:PRO:O	15:f:261:THR:OG1	2.31	0.48
11:A:638:PRO:HB3	16:G:39:LEU:HD23	1.95	0.48
34:o:597:PRO:HB3	34:o:664:ILE:HG22	1.95	0.48
34:o:1292:MET:O	34:o:1296:MET:HB2	2.14	0.48
35:p:320:PHE:HE1	35:p:324:ARG:HE	1.62	0.48
13:d:922:GLN:NE2	20:l:71:ASP:OD2	2.47	0.48
5:4:433:PHE:CE2	6:5:38:ILE:CG2	2.97	0.48
11:A:824:ARG:HB3	11:A:863:VAL:HG12	1.95	0.48
14:E:634:ARG:HG3	14:E:675:LEU:HB2	1.95	0.48
15:F:415:ILE:O	15:F:415:ILE:HG12	2.14	0.48
27:U:114:ILE:O	27:U:174:ARG:NH2	2.47	0.48
29:X:7:DT:H4'	34:o:1417:HIS:CG	2.49	0.48
15:f:254:GLN:O	15:f:258:ARG:NH2	2.47	0.48
5:4:360:THR:HG22	5:4:363:GLN:OE1	2.13	0.47
5:4:398:ARG:HA	5:4:398:ARG:HE	1.79	0.47
5:4:438:LYS:CE	12:B:621:ALA:CB	2.86	0.47
11:A:485:ILE:HB	15:f:310:THR:HG23	1.94	0.47
13:D:998:GLN:HG2	13:D:999:MET:N	2.29	0.47
14:E:774:MET:HE2	14:E:774:MET:N	2.22	0.47
26:T:238:GLU:OE1	28:V:130:ILE:HG13	2.14	0.47
29:X:-33:DC:C2	29:X:-32:DC:C5	3.01	0.47
30:Y:8:DA:OP1	35:p:445:LYS:HD2	2.13	0.47
34:o:201:GLU:HG3	34:o:213:LYS:HG3	1.96	0.47
35:p:289:ILE:HD11	35:p:301:VAL:HG21	1.96	0.47
3:2:253:GLY:N	3:2:310:LEU:HD21	2.29	0.47
5:4:261:PHE:O	5:4:265:LEU:HD23	2.14	0.47
7:6:605:ILE:HD12	7:6:607:ILE:HD11	1.96	0.47
11:A:639:LEU:O	11:A:643:ILE:HG13	2.13	0.47
12:B:135:TRP:HA	12:B:138:VAL:HG12	1.95	0.47
18:I:63:LYS:NZ	18:I:69:ASP:OD1	2.47	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:S:169:LYS:HD2	25:S:173:HIS:CD2	2.49	0.47
27:U:76:MET:HB2	27:U:90:ASN:OD1	2.14	0.47
34:o:971:PRO:O	34:o:972:THR:OG1	2.29	0.47
35:p:75:SER:OG	35:p:77:GLU:OE2	2.28	0.47
35:p:269:ILE:HD11	35:p:369:VAL:CG2	2.41	0.47
35:p:860:VAL:HG12	35:p:896:LEU:HD22	1.96	0.47
14:e:474:THR:OG1	14:e:546:VAL:O	2.28	0.47
14:e:724:GLU:OE1	14:e:789:ASN:ND2	2.46	0.47
1:0:41:ARG:HD2	27:U:169:PRO:CG	2.44	0.47
11:A:475:LEU:O	15:f:354:ARG:NH2	2.46	0.47
11:A:501:THR:O	11:A:502:LEU:C	2.57	0.47
26:T:179:ASP:OD1	26:T:179:ASP:N	2.46	0.47
33:m:67:GLU:O	33:m:71:LYS:HG2	2.14	0.47
34:o:1143:LEU:HB2	34:o:1148:ALA:HB2	1.95	0.47
14:e:589:TRP:HB3	15:f:60:MET:HE3	1.96	0.47
15:f:39:LEU:HD22	18:i:47:VAL:HG13	1.95	0.47
2:1:422:LEU:HD13	4:3:225:GLN:NE2	2.29	0.47
11:A:730:PHE:CD1	11:A:730:PHE:N	2.82	0.47
15:F:90:GLU:CD	15:F:90:GLU:N	2.72	0.47
15:F:317:LEU:N	15:F:317:LEU:HD23	2.30	0.47
27:U:14:LEU:HD13	27:U:197:VAL:HG22	1.96	0.47
27:U:56:ARG:HD3	27:U:60:ARG:CZ	2.44	0.47
27:U:69:ASP:OD1	27:U:69:ASP:N	2.39	0.47
28:V:103:LEU:HA	28:V:106:THR:HG22	1.96	0.47
29:X:-19:DT:C2	29:X:-18:DG:C5	3.02	0.47
30:Y:-31:DC:H2"	30:Y:-30:DG:C8	2.50	0.47
32:k:173:CYS:SG	32:k:179:MET:O	2.72	0.47
35:p:297:MET:O	35:p:301:VAL:HG23	2.14	0.47
14:e:556:ASN:HA	14:e:572:LEU:HB2	1.96	0.47
15:f:330:ARG:NH1	15:f:371:THR:O	2.47	0.47
2:1:488:GLU:O	2:1:491:VAL:HG22	2.14	0.47
13:D:1003:ASP:HA	13:D:1006:LEU:HD23	1.96	0.47
14:E:696:TRP:HA	14:E:703:MET:HA	1.96	0.47
34:o:486:LEU:HD23	34:o:496:PHE:HE2	1.80	0.47
34:o:1429:LYS:HB2	34:o:1438:VAL:HG11	1.95	0.47
35:p:792:ASP:O	35:p:943:GLY:HA3	2.14	0.47
37:r:57:LEU:HD13	37:r:61:PHE:CE2	2.50	0.47
4:3:235:GLN:O	4:3:235:GLN:NE2	2.47	0.47
11:A:575:PRO:HD3	12:B:608:ASN:HD22	1.79	0.47
17:H:35:ARG:HD3	17:H:35:ARG:HA	1.59	0.47
26:T:238:GLU:CD	28:V:130:ILE:HG12	2.39	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:m:56:ILE:HG23	20:l:129:PRO:HB2	1.97	0.47
34:o:811:ILE:HG21	42:w:79:PRO:HB3	1.96	0.47
3:2:87:LEU:HD13	3:2:228:TYR:HD2	1.80	0.47
3:2:291:CYS:SG	3:2:294:CYS:N	2.82	0.47
4:3:50:PHE:CZ	5:4:118:LEU:HD12	2.38	0.47
7:6:297:PHE:O	7:6:359:LYS:NZ	2.38	0.47
12:B:217:ASN:ND2	12:B:320:ALA:O	2.35	0.47
14:E:732:ASP:OD1	14:E:734:THR:OG1	2.31	0.47
15:F:317:LEU:N	15:F:317:LEU:CD2	2.77	0.47
25:S:54:LYS:HG2	25:S:59:GLU:OE1	2.14	0.47
27:U:140:GLU:OE1	27:U:140:GLU:N	2.48	0.47
28:V:225:VAL:HG13	28:V:226:ASP:OD2	2.15	0.47
34:o:115:SER:OG	34:o:227:ARG:HB2	2.14	0.47
35:p:40:VAL:HG11	35:p:482:LEU:HD13	1.96	0.47
35:p:43:GLN:NE2	35:p:482:LEU:O	2.48	0.47
35:p:223:SER:HB2	35:p:349:PRO:HD2	1.96	0.47
35:p:271:ILE:HG21	35:p:320:PHE:CD2	2.49	0.47
35:p:955:PRO:HB2	35:p:1028:LEU:HD13	1.95	0.47
37:r:104:CYS:SG	37:r:138:ARG:HD2	2.55	0.47
13:d:916:LYS:NZ	13:d:1070:GLU:OE2	2.42	0.47
5:4:404:THR:O	6:5:8:VAL:HG22	2.15	0.47
8:7:617:ALA:HB2	8:7:676:LEU:HD21	1.97	0.47
11:A:1165:LEU:HB2	11:A:1191:ILE:HG12	1.97	0.47
12:B:71:ARG:HD3	12:B:73:TYR:CE1	2.50	0.47
18:I:119:ARG:NH1	18:I:120:TYR:OH	2.48	0.47
23:Q:321:SER:OG	23:Q:322:ASP:N	2.48	0.47
34:o:833:PRO:HB2	35:p:677:MET:HE2	1.97	0.47
34:o:1321:ILE:HD12	34:o:1331:LEU:HD12	1.96	0.47
37:r:74:PHE:HB2	37:r:80:ILE:HG12	1.97	0.47
37:r:131:LEU:O	37:r:135:GLN:HG2	2.15	0.47
40:u:124:ASN:HB2	40:u:125:PRO:HD3	1.97	0.47
1:0:28:HIS:HB3	1:0:30:LEU:HG	1.96	0.47
4:3:20:ILE:H	4:3:20:ILE:HD12	1.79	0.47
7:6:449:LYS:HD3	29:X:29:DA:P	2.54	0.47
15:F:418:ILE:H	15:F:418:ILE:CD1	2.26	0.47
15:F:424:GLN:O	15:F:428:LEU:HG	2.15	0.47
20:L:104:ARG:HH21	20:L:104:ARG:HA	1.80	0.47
27:U:49:LEU:O	27:U:53:LYS:HA	2.15	0.47
34:o:375:ILE:HD13	34:o:485:ASN:HD22	1.80	0.47
15:f:102:ARG:HD3	20:l:151:ARG:HG3	1.95	0.47
4:3:229:TRP:CH2	5:4:58:ARG:NH1	2.79	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:B:781:TYR:O	17:H:176:ARG:NH2	2.47	0.47
15:F:83:LEU:H	15:F:83:LEU:HD12	1.71	0.47
28:V:99:LEU:HD23	28:V:114:LYS:HZ2	1.80	0.47
38:s:14:ARG:O	38:s:18:MET:HG2	2.13	0.47
42:w:115:THR:HG22	42:w:116:ALA:H	1.80	0.47
4:3:44:LEU:HD21	4:3:162:LEU:CD1	2.45	0.46
11:A:397:LEU:HD21	15:f:361:LYS:HB3	1.97	0.46
12:B:564:LEU:HB2	12:B:581:ILE:HD13	1.97	0.46
15:F:411:VAL:HG13	15:F:411:VAL:O	2.15	0.46
25:S:73:ARG:HD2	25:S:73:ARG:HA	1.65	0.46
27:U:36:ILE:HG21	27:U:48:MET:CE	2.45	0.46
27:U:150:GLY:O	40:u:93:ASN:OD1	2.34	0.46
27:U:179:ARG:HA	27:U:182:GLU:HG2	1.96	0.46
29:X:-20:DG:H2''	29:X:-19:DT:OP2	2.15	0.46
30:Y:-2:DC:H2'	30:Y:-1:DC:C6	2.50	0.46
34:o:575:PRO:HG3	34:o:594:LEU:HD11	1.97	0.46
34:o:916:PHE:HE2	34:o:960:ARG:HG2	1.81	0.46
35:p:794:VAL:HG13	35:p:965:ILE:HG23	1.96	0.46
15:f:326:HIS:O	15:f:330:ARG:HG2	2.15	0.46
14:E:321:LEU:HB3	14:E:330:TRP:HB2	1.97	0.46
15:F:47:ILE:HD13	18:I:19:MET:HE1	1.96	0.46
27:U:150:GLY:CA	40:u:93:ASN:OD1	2.63	0.46
34:o:1171:ALA:HA	42:w:59:THR:HG23	1.96	0.46
44:y:49:GLN:HB2	44:y:94:LEU:HD21	1.97	0.46
15:f:326:HIS:ND1	15:f:326:HIS:N	2.64	0.46
15:f:328:ALA:C	15:f:330:ARG:N	2.72	0.46
1:0:8:ARG:CZ	1:0:9:CYS:SG	3.02	0.46
13:D:963:ARG:O	13:D:966:LEU:N	2.48	0.46
13:D:965:ILE:HD13	13:D:965:ILE:O	2.15	0.46
15:F:215:GLU:O	15:F:254:GLN:NE2	2.39	0.46
27:U:112:ARG:O	27:U:115:GLU:HG2	2.16	0.46
29:X:14:DC:H4'	29:X:15:DT:H5'	1.97	0.46
31:c:26:VAL:HG23	19:j:195:LEU:HB3	1.96	0.46
34:o:459:ASN:HD21	34:o:463:THR:HG21	1.80	0.46
34:o:525:ILE:HG12	34:o:535:MET:HE2	1.97	0.46
35:p:728:MET:SD	35:p:942:LYS:HB3	2.55	0.46
38:s:80:PRO:HA	38:s:107:GLN:HB2	1.97	0.46
44:y:45:ILE:HG22	44:y:94:LEU:HD22	1.98	0.46
2:1:427:ALA:HB1	5:4:62:LEU:HD11	1.97	0.46
3:2:382:CYS:HB3	3:2:385:CYS:HB3	1.96	0.46
6:5:32:LYS:HB2	12:B:540:LYS:O	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:7:28:LEU:O	8:7:32:LEU:HD23	2.16	0.46
11:A:470:ILE:O	15:f:299:LYS:NZ	2.48	0.46
14:E:277:ASP:O	14:E:280:ARG:HG2	2.16	0.46
29:X:7:DT:H4'	34:o:1417:HIS:CD2	2.50	0.46
31:c:80:LEU:HB3	19:j:119:PHE:CZ	2.50	0.46
34:o:36:VAL:HG11	34:o:73:THR:HG21	1.97	0.46
34:o:920:PHE:CD1	34:o:959:MET:HE1	2.51	0.46
35:p:163:LEU:HA	35:p:166:LEU:HD12	1.98	0.46
13:d:1061:ARG:NH1	18:i:119:ARG:O	2.48	0.46
4:3:13:ILE:HG21	4:3:41:VAL:HG13	1.97	0.46
4:3:31:GLN:OE1	4:3:36:LYS:NZ	2.42	0.46
20:L:106:ARG:NH1	20:L:115:ASP:OD2	2.48	0.46
25:S:43:ASN:OD1	25:S:44:GLN:N	2.48	0.46
26:T:188:PHE:CE2	28:V:80:LYS:HB2	2.49	0.46
30:Y:22:DC:H2''	30:Y:23:DC:C6	2.50	0.46
34:o:457:ILE:HD11	34:o:515:ILE:HG12	1.96	0.46
36:q:263:LEU:HD22	44:y:87:PHE:HD2	1.80	0.46
15:f:58:MET:HE3	15:f:64:GLN:HA	1.98	0.46
1:0:8:ARG:HH21	1:0:37:LEU:HD22	1.80	0.46
7:6:294:GLU:OE2	7:6:334:ARG:NH1	2.49	0.46
14:E:646:SER:OG	14:E:647:ALA:N	2.49	0.46
16:G:41:ASP:OD1	16:G:41:ASP:N	2.48	0.46
18:I:38:GLN:HA	18:I:41:GLU:HB2	1.98	0.46
21:O:64:THR:HG22	21:O:65:TYR:N	2.31	0.46
24:R:182:ALA:HB2	26:T:155:PRO:HA	1.97	0.46
26:T:31:TRP:HD1	26:T:62:LEU:HD21	1.80	0.46
33:m:84:GLU:H	33:m:84:GLU:HG3	1.42	0.46
34:o:551:ARG:HG2	41:v:121:LEU:HD23	1.98	0.46
34:o:811:ILE:HD11	35:p:690:CYS:HB2	1.96	0.46
34:o:1434:GLU:C	34:o:1435:THR:HG1	2.21	0.46
35:p:256:ILE:HD11	35:p:373:LEU:HD21	1.97	0.46
14:e:717:LEU:HD22	14:e:726:LEU:HD11	1.98	0.46
14:e:777:SER:O	14:e:777:SER:OG	2.34	0.46
1:0:8:ARG:CD	27:U:172:ASP:HB2	2.45	0.46
1:0:31:CYS:SG	1:0:34:CYS:HB2	2.56	0.46
1:0:128:GLU:HB3	1:0:133:ILE:HG12	1.98	0.46
4:3:53:ARG:HD2	5:4:46:ARG:HH12	1.80	0.46
8:7:77:VAL:HA	8:7:80:ILE:HG22	1.97	0.46
27:U:139:LEU:HD12	40:u:160:ILE:N	2.31	0.46
42:w:68:ILE:HB	42:w:122:ARG:HD2	1.98	0.46
14:e:238:GLN:O	14:e:242:PRO:HD2	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:e:519:GLU:O	14:e:519:GLU:HG3	2.16	0.46
14:e:747:LEU:H	14:e:747:LEU:CD2	2.22	0.46
15:f:327:TRP:O	15:f:330:ARG:HB2	2.15	0.46
1:0:37:LEU:O	1:0:40:VAL:HG12	2.16	0.46
11:A:404:MET:O	11:A:408:LEU:HB2	2.16	0.46
27:U:152:PHE:CZ	40:u:96:GLY:N	2.84	0.46
28:V:168:LEU:O	28:V:172:GLU:HG2	2.16	0.46
34:o:1153:ARG:O	34:o:1157:ILE:HG12	2.15	0.46
37:r:34:ASN:O	37:r:68:THR:OG1	2.33	0.46
14:e:234:ALA:HB2	14:e:648:ASP:HB2	1.96	0.46
14:e:718:ARG:HD3	14:e:718:ARG:HA	1.76	0.46
3:2:357:VAL:CG1	3:2:366:VAL:HG23	2.45	0.46
9:N:2:TRX:CE3	34:o:749:ARG:HD2	2.46	0.46
30:Y:15:DA:H5"	30:Y:15:DA:C8	2.48	0.46
34:o:890:ARG:NE	34:o:1023:VAL:HG22	2.30	0.46
40:u:96:GLY:O	40:u:128:TYR:OH	2.34	0.46
40:u:112:SER:HB3	40:u:162:SER:HA	1.98	0.46
7:6:656:ASN:OD1	7:6:657:ALA:N	2.49	0.46
24:R:31:ASP:OD1	24:R:31:ASP:N	2.49	0.46
28:V:176:PRO:C	28:V:178:SER:H	2.24	0.46
35:p:809:VAL:HG21	36:q:60:HIS:CE1	2.51	0.46
35:p:1090:GLU:N	35:p:1090:GLU:OE1	2.49	0.46
4:3:98:ASP:CB	4:3:100:LYS:HE3	2.47	0.45
8:7:137:LEU:O	8:7:142:VAL:HG11	2.15	0.45
8:7:329:PHE:O	8:7:333:LEU:HD23	2.17	0.45
12:B:559:LYS:HB2	12:B:559:LYS:NZ	2.31	0.45
12:B:568:VAL:HG22	12:B:628:ILE:HG23	1.98	0.45
14:E:245:VAL:HG13	14:E:282:LEU:HD11	1.97	0.45
15:F:141:CYS:SG	17:H:158:THR:HB	2.56	0.45
17:H:27:ASP:OD1	17:H:27:ASP:N	2.48	0.45
23:Q:22:ILE:HG22	23:Q:39:LEU:HD11	1.98	0.45
24:R:128:ILE:HG23	24:R:183:VAL:HG11	1.99	0.45
24:R:133:ASN:OD1	24:R:134:ILE:N	2.49	0.45
27:U:54:PHE:CE1	28:V:195:PRO:HG3	2.51	0.45
42:w:64:GLU:O	42:w:68:ILE:HG12	2.16	0.45
2:1:472:LEU:HD12	2:1:476:TRP:CD1	2.52	0.45
5:4:334:MET:SD	7:6:56:TYR:CE2	3.09	0.45
8:7:361:LEU:O	8:7:365:VAL:HG12	2.16	0.45
15:F:426:LEU:C	15:F:426:LEU:HD23	2.41	0.45
30:Y:-25:DC:H2"	30:Y:-24:DT:H72	1.98	0.45
30:Y:11:DT:H2"	30:Y:12:DC:OP2	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:Y:19:DA:C8	30:Y:19:DA:H5"	2.51	0.45
35:p:516:GLU:HA	35:p:520:VAL:HG22	1.98	0.45
35:p:645:GLU:O	35:p:649:ASN:HB2	2.16	0.45
1:0:37:LEU:HD11	27:U:118:GLU:OE2	2.16	0.45
5:4:435:ASN:HB3	5:4:440:LEU:HB2	1.97	0.45
7:6:185:ILE:HG22	7:6:189:LEU:HD13	1.98	0.45
12:B:184:ASN:ND2	12:B:184:ASN:N	2.63	0.45
13:D:871:THR:HG21	13:D:910:LEU:HD12	1.98	0.45
17:H:186:VAL:HG21	15:f:220:GLN:HB3	1.97	0.45
24:R:131:PRO:HG3	35:p:101:ARG:HG3	1.98	0.45
26:T:220:ILE:HG13	26:T:221:GLY:H	1.80	0.45
34:o:1087:VAL:HG12	34:o:1400:LEU:HD22	1.98	0.45
14:e:243:LEU:HD13	14:e:243:LEU:HA	1.73	0.45
14:e:281:VAL:HG11	14:e:297:MET:HB3	1.98	0.45
1:0:55:LYS:C	1:0:57:ASN:H	2.24	0.45
2:1:308:ASN:ND2	8:7:576:GLU:OE2	2.49	0.45
8:7:109:LEU:HD12	8:7:207:TYR:CD2	2.52	0.45
26:T:194:HIS:CG	26:T:195:GLN:N	2.83	0.45
28:V:97:LEU:O	28:V:137:TYR:HE1	2.00	0.45
35:p:1094:GLN:HB2	35:p:1103:LEU:HD13	1.99	0.45
36:q:44:ILE:HD13	36:q:238:SER:HB2	1.99	0.45
38:s:54:ARG:C	38:s:56:THR:H	2.23	0.45
38:s:64:HIS:HD2	38:s:66:ASP:H	1.64	0.45
11:A:467:ILE:N	15:F:221:GLN:NE2	2.48	0.45
11:A:690:LEU:HD22	11:A:747:LEU:HD22	1.99	0.45
11:A:857:MET:HE3	11:A:858:ASP:H	1.81	0.45
14:E:730:SER:OG	14:E:732:ASP:OD1	2.33	0.45
15:F:68:THR:OG1	18:I:32:GLU:OE1	2.35	0.45
19:J:123:LEU:HD12	19:J:123:LEU:HA	1.73	0.45
26:T:170:LYS:HE3	26:T:170:LYS:HB3	1.71	0.45
30:Y:-8:DG:H2"	30:Y:-7:DA:C8	2.52	0.45
34:o:18:ILE:HD11	35:p:1149:VAL:HG11	1.99	0.45
34:o:530:SER:O	34:o:532:ARG:HG3	2.16	0.45
34:o:1175:ILE:HD12	34:o:1286:ARG:HG2	1.99	0.45
36:q:9:VAL:HG11	44:y:105:PHE:CD1	2.52	0.45
43:x:66:GLU:HA	45:z:23:HIS:HB3	1.97	0.45
15:f:317:LEU:HD12	15:f:329:LEU:HD23	1.98	0.45
15:F:217:SER:HB3	17:H:157:HIS:HB2	1.99	0.45
30:Y:10:DC:H41	35:p:457:LYS:HE2	1.81	0.45
35:p:119:THR:HG23	35:p:187:ILE:HA	1.98	0.45
35:p:764:MET:HE1	35:p:938:ARG:NH1	2.32	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:21:LEU:HD21	1:0:29:THR:HG23	1.98	0.45
2:1:457:ILE:HG22	2:1:461:LEU:HD13	1.98	0.45
11:A:401:ASN:HD22	11:A:401:ASN:N	2.14	0.45
13:D:960:GLU:CB	13:D:983:ARG:HH11	2.29	0.45
30:Y:3:DA:N3	30:Y:4:DG:C8	2.85	0.45
34:o:96:HIS:HB2	34:o:250:VAL:HG23	1.98	0.45
34:o:931:ARG:NH1	34:o:936:GLU:HG3	2.32	0.45
34:o:1099:ALA:HA	34:o:1102:MET:HG2	1.99	0.45
35:p:714:PRO:HD2	35:p:1001:PRO:HA	1.98	0.45
15:f:83:LEU:HD22	18:i:41:GLU:HG2	1.99	0.45
5:4:406:GLY:O	6:5:7:GLY:N	2.49	0.45
5:4:411:GLN:HE22	12:B:534:SER:HB2	1.82	0.45
11:A:475:LEU:HD23	11:A:480:TRP:HE1	1.82	0.45
14:E:690:ASP:N	14:E:690:ASP:OD1	2.43	0.45
24:R:93:PHE:HB2	24:R:97:GLY:HA2	1.98	0.45
25:S:175:SER:O	25:S:179:GLN:HG2	2.17	0.45
27:U:76:MET:CG	27:U:88:ARG:HB3	2.46	0.45
27:U:179:ARG:HH21	27:U:183:GLN:HG3	1.81	0.45
33:m:47:GLN:HG2	13:d:860:VAL:HA	1.98	0.45
34:o:153:ILE:HG12	34:o:187:TYR:CD1	2.52	0.45
34:o:906:LEU:HD13	34:o:966:LEU:HD22	1.99	0.45
35:p:357:CYS:SG	35:p:361:LYS:NZ	2.90	0.45
36:q:92:GLU:HG3	36:q:93:PHE:H	1.81	0.45
37:r:20:LEU:HD12	37:r:121:ARG:HH22	1.81	0.45
13:d:1084:LEU:HB3	18:i:99:ARG:HH21	1.81	0.45
15:f:219:GLU:H	15:f:219:GLU:CD	2.21	0.45
1:0:5:GLY:HA3	1:0:10:LYS:CB	2.25	0.45
3:2:199:ILE:CG2	3:2:222:ILE:HD11	2.47	0.45
4:3:201:GLY:O	4:3:204:GLN:HG2	2.17	0.45
7:6:133:THR:HB	7:6:160:THR:HG21	1.99	0.45
8:7:373:ARG:O	8:7:405:THR:OG1	2.24	0.45
11:A:1182:CYS:O	11:A:1182:CYS:SG	2.75	0.45
13:D:966:LEU:HD22	13:D:966:LEU:C	2.42	0.45
24:R:107:MET:O	24:R:112:ARG:NH2	2.48	0.45
26:T:140:ARG:HH21	35:p:90:GLN:HG2	1.82	0.45
34:o:413:TYR:O	34:o:449:HIS:HD2	2.00	0.45
34:o:1206:ARG:H	34:o:1263:ASN:HB3	1.82	0.45
35:p:385:ARG:O	35:p:391:LYS:HE3	2.16	0.45
35:p:667:THR:HA	35:p:670:GLU:HB2	1.98	0.45
1:0:1:MET:SD	8:7:345:ARG:HD2	2.57	0.45
3:2:242:SER:N	3:2:245:SER:OG	2.50	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:7:285:TYR:O	8:7:289:VAL:HG23	2.17	0.45
8:7:460:THR:HB	8:7:661:ALA:HB1	1.98	0.45
10:Z:1:ATP:H2'	10:Z:1:ATP:N3	2.32	0.45
13:D:947:PHE:HE1	14:E:527:ILE:HD12	1.82	0.45
24:R:50:SER:O	34:o:264:VAL:HA	2.17	0.45
24:R:102:GLN:HE21	34:o:305:GLU:CG	2.29	0.45
27:U:12:ALA:O	27:U:16:ARG:HG2	2.18	0.45
28:V:86:LYS:HZ2	28:V:140:LYS:HD2	1.81	0.45
28:V:130:ILE:HD12	28:V:140:LYS:HG3	1.99	0.45
29:X:29:DA:N6	30:Y:-30:DG:O6	2.50	0.45
30:Y:19:DA:H8	30:Y:19:DA:OP2	2.00	0.45
34:o:34:MET:SD	35:p:1124:ILE:HG21	2.57	0.45
34:o:733:LEU:CB	42:w:106:ASP:HB2	2.47	0.45
34:o:1160:ARG:O	34:o:1300:GLY:HA2	2.16	0.45
35:p:1163:MET:HA	35:p:1167:ILE:O	2.16	0.45
41:v:65:TYR:HE1	41:v:84:ARG:HH11	1.65	0.45
14:e:245:VAL:HG12	14:e:282:LEU:HD11	1.99	0.45
14:e:436:ASP:N	14:e:436:ASP:OD1	2.49	0.45
1:0:6:CYS:O	1:0:10:LYS:HE3	2.17	0.44
3:2:175:THR:HA	8:7:591:GLY:C	2.42	0.44
7:6:528:LYS:CD	7:6:531:ILE:HD13	2.47	0.44
14:E:250:GLU:O	14:E:254:ASN:ND2	2.51	0.44
27:U:112:ARG:HA	27:U:115:GLU:OE2	2.16	0.44
34:o:618:TYR:HA	34:o:621:ILE:HG13	2.00	0.44
40:u:92:VAL:HG11	40:u:127:CYS:N	2.31	0.44
14:e:258:ASN:OD1	14:e:258:ASN:N	2.39	0.44
19:j:176:MET:O	19:j:178:GLY:N	2.43	0.44
3:2:174:LEU:O	8:7:591:GLY:C	2.60	0.44
5:4:325:ILE:H	5:4:325:ILE:HD12	1.82	0.44
8:7:107:LEU:HD12	8:7:195:ALA:HB1	1.98	0.44
8:7:475:PRO:HG3	8:7:478:MET:HE2	1.99	0.44
23:Q:332:GLU:OE1	23:Q:332:GLU:N	2.49	0.44
27:U:145:PHE:HB3	27:U:153:ARG:H	1.82	0.44
30:Y:-10:DA:H2''	30:Y:-9:DT:OP2	2.17	0.44
33:m:57:LEU:HA	33:m:57:LEU:HD23	1.73	0.44
34:o:211:GLU:H	34:o:211:GLU:HG3	1.47	0.44
34:o:436:SER:HA	34:o:439:HIS:HD2	1.80	0.44
34:o:508:SER:HB3	34:o:511:THR:HG22	1.98	0.44
34:o:1485:GLU:HG2	40:u:20:PRO:HD3	2.00	0.44
37:r:76:ASN:O	37:r:80:ILE:HG13	2.17	0.44
39:t:66:LEU:HD21	39:t:97:LEU:HB2	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:t:121:ASP:OD1	39:t:121:ASP:N	2.50	0.44
40:u:129:LYS:HD2	40:u:133:GLU:HG2	2.00	0.44
4:3:42:MET:SD	4:3:108:ASN:ND2	2.86	0.44
4:3:242:ILE:CD1	5:4:75:VAL:N	2.80	0.44
8:7:434:HIS:CB	8:7:632:ILE:HD11	2.48	0.44
8:7:613:HIS:ND1	8:7:613:HIS:O	2.50	0.44
11:A:1063:LYS:HD3	11:A:1063:LYS:O	2.16	0.44
14:E:249:LEU:HD21	14:E:282:LEU:HD22	2.00	0.44
14:E:784:HIS:HB3	14:E:792:LEU:HB2	2.00	0.44
15:F:328:ALA:O	15:F:332:PHE:N	2.50	0.44
15:F:361:LYS:HA	15:F:364:VAL:HG22	1.99	0.44
15:F:427:LEU:HD12	15:F:427:LEU:HA	1.72	0.44
30:Y:19:DA:C2'	30:Y:20:DC:H5'	2.48	0.44
34:o:526:VAL:HA	34:o:533:PRO:HA	2.00	0.44
34:o:784:VAL:HG13	35:p:978:ILE:HD11	2.00	0.44
35:p:399:LEU:HB3	35:p:453:TRP:NE1	2.32	0.44
1:0:8:ARG:CG	27:U:172:ASP:HB2	2.47	0.44
4:3:123:ASP:OD1	4:3:124:ILE:N	2.45	0.44
11:A:1053:PHE:HB2	11:A:1057:GLU:HB2	2.00	0.44
16:G:129:LYS:HA	16:G:129:LYS:HD2	1.77	0.44
25:S:70:GLU:CA	25:S:74:LYS:HB2	2.47	0.44
25:S:73:ARG:NE	25:S:76:ARG:HH11	2.15	0.44
28:V:96:PRO:HB3	28:V:136:LYS:HD2	1.98	0.44
28:V:129:LYS:HA	28:V:129:LYS:HE3	1.97	0.44
35:p:446:TYR:CG	35:p:456:GLN:HG2	2.52	0.44
35:p:927:ARG:HD3	35:p:1054:MET:SD	2.58	0.44
14:e:525:GLU:N	14:e:525:GLU:CD	2.76	0.44
2:1:400:ILE:H	2:1:400:ILE:HD12	1.82	0.44
5:4:52:ALA:HB1	5:4:90:LEU:HD21	1.99	0.44
6:5:35:ILE:C	12:B:539:ARG:HD3	2.43	0.44
7:6:415:HIS:HD2	7:6:419:ARG:HH22	1.65	0.44
11:A:463:PRO:O	15:F:218:VAL:HG23	2.17	0.44
14:E:650:THR:HG22	14:E:666:THR:HG22	2.00	0.44
15:F:47:ILE:HD11	18:I:43:ALA:HB2	1.98	0.44
25:S:47:LEU:HD11	25:S:98:TRP:HB3	1.99	0.44
34:o:364:ARG:NH1	34:o:502:ASN:OD1	2.50	0.44
34:o:417:LYS:HG3	34:o:449:HIS:HE1	1.81	0.44
34:o:1282:ASP:N	34:o:1282:ASP:OD1	2.50	0.44
1:0:97:ASP:O	1:0:101:GLU:OE1	2.36	0.44
4:3:229:TRP:HE3	5:4:58:ARG:HD2	1.76	0.44
4:3:242:ILE:CD1	5:4:74:TRP:C	2.91	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:4:157:GLU:O	5:4:161:HIS:ND1	2.51	0.44
8:7:726:GLN:HG2	8:7:727:PRO:CD	2.48	0.44
12:B:839:MET:HE1	12:B:843:LEU:HD13	2.00	0.44
13:D:1001:GLN:O	13:D:1004:ALA:HB3	2.18	0.44
17:H:59:GLU:HA	17:H:62:THR:HG22	1.99	0.44
17:H:194:MET:HE2	17:H:194:MET:HB2	1.85	0.44
24:R:46:ILE:O	24:R:49:GLY:N	2.51	0.44
28:V:111:ILE:O	28:V:114:LYS:N	2.51	0.44
28:V:214:GLU:HA	28:V:217:GLN:HB3	1.99	0.44
34:o:368:THR:HG21	35:p:931:ILE:O	2.18	0.44
34:o:1095:LEU:HD13	34:o:1401:LEU:HD22	2.00	0.44
35:p:17:ILE:O	35:p:19:PRO:HD3	2.17	0.44
5:4:288:ILE:H	5:4:288:ILE:HD12	1.83	0.44
8:7:600:ALA:HB1	8:7:659:HIS:HD2	1.82	0.44
12:B:653:LEU:HG	12:B:684:ILE:HG13	1.99	0.44
12:B:859:ARG:HA	12:B:859:ARG:HD2	1.80	0.44
12:B:925:LYS:HD3	12:B:925:LYS:HA	1.78	0.44
13:D:997:ALA:O	13:D:1001:GLN:N	2.48	0.44
14:E:481:ASP:N	14:E:481:ASP:OD1	2.41	0.44
15:F:400:GLY:O	15:F:404:ARG:HG2	2.18	0.44
21:O:65:TYR:OH	22:P:203:ARG:NE	2.51	0.44
25:S:173:HIS:HB2	42:w:40:ARG:HD3	1.98	0.44
27:U:53:LYS:O	28:V:199:LYS:HE2	2.18	0.44
33:m:90:ILE:HD12	33:m:90:ILE:HA	1.77	0.44
34:o:457:ILE:HD12	35:p:1102:PHE:CE2	2.53	0.44
36:q:76:ASP:HA	36:q:239:LEU:HD23	1.99	0.44
3:2:87:LEU:HD23	3:2:87:LEU:O	2.18	0.44
6:5:9:LEU:HD11	6:5:42:HIS:HD2	1.83	0.44
7:6:99:PHE:CZ	7:6:103:ILE:HD13	2.52	0.44
11:A:400:GLU:HG3	11:A:401:ASN:N	2.32	0.44
29:X:28:DG:H1	30:Y:-28:DC:H42	1.66	0.44
35:p:714:PRO:HG2	35:p:1001:PRO:HG3	1.99	0.44
14:e:542:HIS:CE1	14:e:568:ARG:HG3	2.53	0.44
15:f:447:ALA:CB	15:f:456:GLY:HA3	2.48	0.44
8:7:332:PHE:CZ	8:7:367:ILE:HG23	2.53	0.44
12:B:414:LEU:HB2	12:B:523:VAL:HG13	2.00	0.44
13:D:933:ARG:HD2	19:J:117:VAL:HG11	2.00	0.44
13:D:1071:ARG:HH22	18:I:82:SER:HA	1.83	0.44
14:E:564:ASP:OD1	14:E:564:ASP:N	2.51	0.44
34:o:1020:LEU:HD22	34:o:1076:PHE:HB3	2.00	0.44
20:l:113:VAL:O	20:l:113:VAL:HG22	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:369:VAL:HG13	3:2:370:ASP:N	2.32	0.43
15:F:6:LYS:HE2	15:F:8:LYS:HG3	2.00	0.43
23:Q:18:ILE:HD11	23:Q:46:TRP:CH2	2.54	0.43
25:S:72:ASN:ND2	26:T:198:ASN:H	2.16	0.43
27:U:152:PHE:CZ	40:u:95:VAL:HG12	2.50	0.43
28:V:229:ASP:HA	28:V:232:LYS:HE2	1.99	0.43
33:m:87:VAL:HG13	33:m:97:PHE:HE1	1.83	0.43
34:o:531:ASN:HD21	34:o:1392:TYR:HE2	1.65	0.43
34:o:808:PRO:HB2	35:p:675:LEU:HD12	1.99	0.43
38:s:82:VAL:HB	38:s:110:MET:HG2	2.00	0.43
40:u:87:ALA:HB2	40:u:101:ILE:HG12	1.99	0.43
43:x:7:CYS:HB2	43:x:48:MET:HG3	2.00	0.43
45:z:43:ILE:O	45:z:44:MET:HE2	2.18	0.43
8:7:354:PRO:HB2	8:7:355:PRO:HD3	2.00	0.43
12:B:766:LEU:HA	12:B:807:THR:HG21	2.00	0.43
13:D:1080:TYR:OH	14:E:606:ASP:OD2	2.30	0.43
14:E:377:LEU:HD21	14:E:422:PRO:HG2	2.00	0.43
18:I:23:LEU:HD22	18:I:28:ILE:HD12	2.00	0.43
24:R:74:LEU:CD2	35:p:823:PHE:HB2	2.49	0.43
34:o:48:GLU:HB3	34:o:53:LYS:HA	2.00	0.43
34:o:952:LEU:HD21	34:o:1006:PRO:HB2	2.00	0.43
35:p:419:ALA:O	35:p:423:ILE:HG12	2.17	0.43
35:p:810:PHE:HZ	35:p:812:ARG:HE	1.64	0.43
36:q:44:ILE:HD11	36:q:178:PRO:HB3	2.00	0.43
45:z:17:TYR:HB3	45:z:44:MET:HB3	1.99	0.43
14:e:268:HIS:O	14:e:268:HIS:CG	2.70	0.43
1:0:68:VAL:HG11	8:7:338:GLU:HG2	2.00	0.43
1:0:116:ASP:OD1	1:0:117:ASN:N	2.51	0.43
11:A:1165:LEU:HD22	11:A:1165:LEU:HA	1.87	0.43
12:B:328:ASN:HA	17:H:227:LEU:HD21	2.00	0.43
15:F:283:MET:HE1	15:F:308:VAL:HG12	2.00	0.43
21:O:48:LEU:HG	23:Q:366:ILE:HD11	2.00	0.43
22:P:298:PRO:HB2	22:P:300:ILE:HG12	1.99	0.43
27:U:136:PHE:C	27:U:137:THR:HG1	2.19	0.43
28:V:78:LEU:O	28:V:82:VAL:HG23	2.18	0.43
29:X:-32:DC:H6	29:X:-32:DC:H5'	1.83	0.43
30:Y:27:DT:C6	30:Y:28:DT:H72	2.53	0.43
31:c:24:ASP:CB	19:j:192:LYS:HD2	2.48	0.43
34:o:216:LEU:HD12	34:o:216:LEU:HA	1.87	0.43
35:p:1115:GLN:HB3	35:p:1148:LEU:HD11	2.00	0.43
40:u:18:PHE:HA	40:u:22:LEU:HD13	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:y:82:SER:HB3	44:y:85:GLU:HG3	1.99	0.43
8:7:67:VAL:HG23	8:7:67:VAL:O	2.19	0.43
14:E:613:ALA:HB3	14:E:616:HIS:HD2	1.83	0.43
15:F:50:ILE:O	15:F:54:ALA:N	2.47	0.43
19:J:124:GLU:O	19:J:125:ASP:HB3	2.16	0.43
19:J:192:LYS:N	19:J:192:LYS:CE	2.66	0.43
20:L:113:VAL:C	20:L:115:ASP:N	2.75	0.43
32:k:179:MET:HB3	32:k:180:PRO:HD2	2.01	0.43
35:p:260:LEU:HD22	35:p:347:MET:SD	2.59	0.43
35:p:810:PHE:HB2	35:p:927:ARG:HE	1.81	0.43
18:i:16:ALA:HB2	18:i:40:LEU:HD11	2.00	0.43
18:i:45:ARG:HG3	19:j:212:LYS:HB3	2.01	0.43
3:2:69:ARG:H	3:2:69:ARG:HG3	1.71	0.43
7:6:133:THR:HG23	7:6:134:SER:N	2.33	0.43
12:B:492:MET:HE3	12:B:492:MET:HB2	1.85	0.43
13:D:891:ILE:HG21	20:L:111:LEU:HB2	2.00	0.43
13:D:958:LYS:HD2	13:D:958:LYS:HA	1.62	0.43
13:D:963:ARG:O	13:D:965:ILE:N	2.52	0.43
13:D:998:GLN:CG	13:D:1002:ARG:HH12	2.31	0.43
14:E:466:PHE:HB2	14:E:796:ALA:HA	2.00	0.43
15:F:370:TRP:CZ3	15:F:420:ALA:HA	2.53	0.43
18:I:21:GLN:HE22	18:I:24:LYS:HE2	1.84	0.43
25:S:77:GLU:OE2	25:S:81:ARG:NH2	2.51	0.43
28:V:184:ALA:O	28:V:189:ILE:HG23	2.19	0.43
29:X:-28:DA:H2'	29:X:-27:DA:C8	2.53	0.43
30:Y:-33:DC:H2''	30:Y:-32:DA:C8	2.53	0.43
34:o:1262:MET:HB3	34:o:1265:ASP:CB	2.48	0.43
34:o:1478:GLU:HA	34:o:1481:LYS:HE2	2.00	0.43
35:p:794:VAL:HG22	35:p:967:ILE:HG22	2.00	0.43
35:p:1060:HIS:HE1	35:p:1081:ASP:HA	1.83	0.43
40:u:30:LEU:HD22	40:u:70:VAL:HG11	2.00	0.43
15:f:11:ASN:OD1	15:f:48:LYS:NZ	2.51	0.43
14:E:351:GLN:HG2	14:E:355:MET:HE2	2.01	0.43
15:F:138:ILE:HB	17:H:159:TYR:HB3	2.00	0.43
30:Y:2:DA:N1	30:Y:3:DA:N6	2.66	0.43
34:o:1158:LEU:HD21	34:o:1336:LEU:HD22	1.99	0.43
40:u:91:GLN:HB3	40:u:98:PHE:HB2	1.99	0.43
15:f:105:TYR:O	19:j:217:PHE:N	2.51	0.43
2:1:303:ILE:HG22	2:1:307:PHE:CE2	2.54	0.43
3:2:206:ARG:CB	8:7:589:GLU:O	2.63	0.43
7:6:184:VAL:HG13	7:6:185:ILE:N	2.33	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:639:LEU:O	11:A:639:LEU:CD1	2.67	0.43
11:A:1052:ARG:O	11:A:1052:ARG:CG	2.67	0.43
16:G:181:TRP:O	16:G:181:TRP:CD2	2.72	0.43
32:k:182:LEU:HD23	32:k:182:LEU:HA	1.85	0.43
34:o:244:ARG:HH11	34:o:245:PRO:HD2	1.83	0.43
34:o:542:LEU:O	34:o:545:VAL:HG12	2.18	0.43
35:p:1060:HIS:CE1	35:p:1081:ASP:HA	2.54	0.43
3:2:89:GLU:OE2	3:2:132:LYS:NZ	2.42	0.43
5:4:426:ARG:NH2	5:4:434:GLU:OE1	2.52	0.43
7:6:532:LEU:HD23	7:6:532:LEU:O	2.19	0.43
8:7:168:VAL:O	8:7:168:VAL:HG13	2.19	0.43
9:N:6:CSX:HB2	9:N:7:ASN:H	1.42	0.43
14:E:327:ASN:HD22	14:E:327:ASN:N	2.07	0.43
14:E:518:LYS:C	14:E:520:SER:H	2.26	0.43
25:S:169:LYS:HE3	35:p:310:VAL:CG2	2.49	0.43
31:c:21:LEU:HD11	31:c:23:TRP:CD1	2.54	0.43
31:c:66:VAL:HG21	19:j:151:ILE:HG23	2.01	0.43
35:p:274:ARG:HG2	35:p:279:VAL:HA	2.01	0.43
37:r:91:LYS:H	37:r:122:PHE:HZ	1.67	0.43
38:s:61:LEU:HB2	38:s:73:PHE:CE2	2.54	0.43
43:x:47:ARG:CZ	43:x:48:MET:HE3	2.48	0.43
1:0:6:CYS:SG	1:0:8:ARG:HB3	2.59	0.43
7:6:193:VAL:HG11	7:6:283:ARG:CD	2.49	0.43
7:6:532:LEU:CD2	7:6:716:VAL:HG13	2.49	0.43
8:7:109:LEU:HD11	8:7:199:ILE:HD11	2.01	0.43
11:A:727:THR:HG23	11:A:727:THR:O	2.19	0.43
15:F:402:ARG:O	15:F:406:VAL:HG13	2.19	0.43
27:U:56:ARG:HH11	27:U:60:ARG:HH11	1.59	0.43
27:U:139:LEU:N	40:u:160:ILE:CD1	2.82	0.43
31:c:101:VAL:HG22	15:f:127:LEU:HA	2.00	0.43
34:o:120:ASP:O	34:o:126:ILE:HG13	2.19	0.43
34:o:279:LYS:HE2	34:o:316:THR:HB	2.01	0.43
34:o:527:THR:HB	34:o:534:VAL:HG22	2.01	0.43
34:o:663:ASP:OD1	34:o:666:ARG:NH1	2.46	0.43
34:o:1163:HIS:CE1	34:o:1297:THR:HG23	2.54	0.43
35:p:718:GLN:HG2	35:p:720:PRO:HD2	2.00	0.43
35:p:803:ARG:HH21	36:q:177:ASN:HD22	1.65	0.43
35:p:837:CYS:SG	35:p:889:LYS:HD3	2.58	0.43
36:q:193:ARG:HG2	36:q:220:TYR:HD1	1.84	0.43
36:q:263:LEU:HB2	44:y:19:ILE:HD12	2.01	0.43
14:e:667:GLY:O	14:e:692:ARG:NH2	2.52	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:353:LEU:HD22	15:f:273:GLN:HE22	1.84	0.43
11:A:925:ASP:N	11:A:925:ASP:OD1	2.52	0.43
12:B:882:HIS:CE1	17:H:216:ALA:HB1	2.54	0.43
19:J:148:ASP:HA	19:J:149:PRO:HD2	1.80	0.43
25:S:53:ASN:HB2	25:S:91:PHE:CZ	2.54	0.43
30:Y:4:DG:H2"	30:Y:5:DA:H8	1.83	0.43
33:m:91:ARG:HG2	33:m:92:LYS:N	2.34	0.43
34:o:459:ASN:HD21	35:p:1090:GLU:HG3	1.84	0.43
34:o:867:SER:HB3	34:o:1414:ILE:HG23	2.00	0.43
43:x:67:LYS:HG2	45:z:23:HIS:HB2	2.00	0.43
15:f:55:LEU:HD13	18:i:28:ILE:HG12	2.01	0.43
1:0:23:VAL:HG12	1:0:59:ARG:HB2	2.01	0.42
1:0:64:GLU:OE1	8:7:345:ARG:NH2	2.52	0.42
7:6:408:SER:HB3	7:6:413:LEU:HD11	2.01	0.42
12:B:603:LYS:H	12:B:603:LYS:HG2	1.64	0.42
15:F:401:GLU:C	15:F:401:GLU:CD	2.87	0.42
27:U:44:LYS:HB2	27:U:47:ASP:OD1	2.19	0.42
31:c:124:ILE:HD11	15:f:133:ALA:HB1	2.00	0.42
34:o:532:ARG:NH1	34:o:647:THR:O	2.52	0.42
34:o:1416:ARG:HB3	34:o:1433:GLU:OE1	2.19	0.42
35:p:214:LYS:HD3	35:p:214:LYS:H	1.85	0.42
45:z:16:ILE:HG22	45:z:25:GLU:HB3	2.00	0.42
15:f:26:MET:HE3	15:f:26:MET:HB3	1.77	0.42
2:1:496:ASN:HB3	2:1:536:LEU:HD11	2.01	0.42
3:2:112:LYS:N	3:2:142:GLU:O	2.41	0.42
4:3:175:MET:HE3	4:3:179:ASN:ND2	2.35	0.42
5:4:433:PHE:CE2	6:5:38:ILE:HG12	2.54	0.42
8:7:49:THR:HG23	8:7:50:VAL:N	2.34	0.42
8:7:111:SER:N	8:7:211:TYR:OH	2.52	0.42
48:Z:2500:W0F:O31	35:p:942:LYS:HE2	2.19	0.42
12:B:831:GLU:OE1	12:B:835:ARG:NH2	2.52	0.42
14:E:476:VAL:HB	14:E:782:HIS:HB2	2.00	0.42
15:F:233:GLY:HA2	15:F:239:ARG:HE	1.82	0.42
17:H:38:GLN:HG2	17:H:62:THR:HG21	2.01	0.42
17:H:178:LYS:HD3	17:H:178:LYS:HA	1.82	0.42
20:L:83:MET:HE3	20:L:83:MET:HB3	1.61	0.42
35:p:955:PRO:O	35:p:963:PRO:HD2	2.18	0.42
36:q:9:VAL:HG11	44:y:105:PHE:HD1	1.84	0.42
36:q:60:HIS:CE1	36:q:63:PHE:HB2	2.54	0.42
42:w:106:ASP:OD1	42:w:106:ASP:N	2.51	0.42
15:f:223:TYR:CD2	15:f:255:MET:HE1	2.52	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:6:409:THR:O	7:6:413:LEU:HD13	2.19	0.42
8:7:56:ILE:HG21	8:7:70:LEU:HD22	2.01	0.42
8:7:249:VAL:HG21	8:7:403:PHE:HB2	2.00	0.42
27:U:73:LYS:HD3	27:U:73:LYS:HA	1.70	0.42
27:U:74:CYS:SG	27:U:92:TYR:HA	2.60	0.42
27:U:188:TYR:O	27:U:191:LEU:HG	2.20	0.42
28:V:165:GLY:HA2	28:V:169:GLU:OE1	2.18	0.42
34:o:459:ASN:OD1	34:o:460:ARG:N	2.52	0.42
36:q:71:ILE:HD11	36:q:150:ILE:HG12	2.01	0.42
40:u:30:LEU:O	40:u:34:VAL:HG22	2.18	0.42
15:f:432:ALA:HB1	15:f:462:GLN:CB	2.49	0.42
4:3:53:ARG:HG3	5:4:46:ARG:CZ	2.50	0.42
5:4:70:ALA:HB1	5:4:74:TRP:CZ2	2.54	0.42
17:H:154:PRO:HB2	17:H:155:ASP:H	1.46	0.42
24:R:251:ILE:H	24:R:251:ILE:HD12	1.85	0.42
25:S:51:LEU:O	25:S:54:LYS:HG3	2.18	0.42
25:S:58:GLN:C	25:S:60:GLU:N	2.74	0.42
27:U:188:TYR:O	27:U:192:ARG:HG2	2.20	0.42
28:V:228:MET:O	28:V:232:LYS:HG3	2.20	0.42
30:Y:15:DA:C2'	30:Y:16:DA:C8	3.03	0.42
34:o:850:THR:O	34:o:853:LYS:HG2	2.19	0.42
34:o:1005:HIS:CD2	34:o:1007:ILE:HG22	2.52	0.42
34:o:1130:ILE:HD13	34:o:1411:LEU:HD22	2.01	0.42
35:p:550:MET:HG3	35:p:567:ILE:HD12	2.00	0.42
35:p:1091:ARG:O	35:p:1095:ILE:HG13	2.18	0.42
37:r:24:LYS:HA	37:r:27:GLU:CD	2.44	0.42
40:u:22:LEU:O	40:u:26:VAL:HG23	2.19	0.42
3:2:174:LEU:CD2	3:2:203:ALA:HB2	2.42	0.42
7:6:535:THR:HG23	7:6:627:SER:HB2	2.02	0.42
11:A:357:GLU:HB3	11:A:358:ASP:H	1.60	0.42
11:A:931:PRO:O	11:A:935:THR:OG1	2.25	0.42
12:B:487:LYS:O	12:B:487:LYS:CG	2.67	0.42
30:Y:-9:DT:H2''	30:Y:-8:DG:O5'	2.19	0.42
34:o:211:GLU:HB2	34:o:214:ILE:HG12	2.01	0.42
34:o:1040:LEU:HD12	34:o:1040:LEU:HA	1.92	0.42
37:r:17:ALA:HB1	37:r:95:PHE:CZ	2.54	0.42
40:u:117:MET:HA	40:u:130:THR:HA	2.01	0.42
45:z:36:CYS:HB3	45:z:39:CYS:SG	2.59	0.42
14:e:225:ILE:HD12	14:e:236:LEU:HB3	2.02	0.42
14:e:447:THR:O	14:e:450:ARG:HB2	2.19	0.42
15:f:317:LEU:HG	15:f:330:ARG:HE	1.83	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:524:HIS:NE2	2:1:528:MET:SD	2.93	0.42
5:4:433:PHE:CD2	6:5:38:ILE:HG12	2.53	0.42
5:4:442:VAL:HG21	6:5:44:PHE:CE2	2.54	0.42
5:4:456:LYS:HA	5:4:456:LYS:HD2	1.50	0.42
8:7:661:ALA:HA	8:7:664:VAL:HG12	2.02	0.42
11:A:468:PHE:CE1	15:F:221:GLN:HG3	2.54	0.42
11:A:468:PHE:HE1	15:F:221:GLN:HG3	1.85	0.42
12:B:594:SER:OG	12:B:595:LYS:N	2.52	0.42
15:F:410:PRO:O	15:F:411:VAL:C	2.63	0.42
20:L:62:LYS:HD2	20:L:62:LYS:HA	1.87	0.42
24:R:74:LEU:HD21	35:p:823:PHE:H	1.85	0.42
24:R:101:TYR:O	24:R:102:GLN:HG3	2.20	0.42
24:R:178:LYS:HE3	26:T:157:ALA:HB2	2.01	0.42
26:T:159:HIS:O	26:T:163:ILE:HG23	2.20	0.42
27:U:16:ARG:HA	27:U:16:ARG:HD2	1.94	0.42
27:U:44:LYS:HA	27:U:44:LYS:HD3	1.85	0.42
32:k:130:PRO:HD3	33:m:35:GLU:HG2	2.01	0.42
34:o:531:ASN:HB3	34:o:898:GLY:O	2.19	0.42
34:o:1144:LEU:HG	34:o:1353:ASP:HA	2.02	0.42
34:o:1162:GLU:O	34:o:1300:GLY:HA3	2.19	0.42
34:o:1286:ARG:NH2	42:w:54:TYR:HB2	2.35	0.42
35:p:89:GLU:HG3	35:p:127:ASP:HB2	2.00	0.42
35:p:1135:TYR:H	35:p:1143:LYS:HZ3	1.67	0.42
36:q:33:SER:O	36:q:37:VAL:HG23	2.19	0.42
1:0:85:ARG:NH2	1:0:139:LYS:HB3	2.34	0.42
5:4:380:THR:O	5:4:380:THR:HG23	2.18	0.42
5:4:415:GLN:HB2	5:4:439:ARG:HH21	1.85	0.42
7:6:559:ILE:HG22	7:6:561:PHE:CE1	2.55	0.42
14:E:790:LEU:HD13	17:H:146:ILE:HG12	2.00	0.42
15:F:324:ASP:CG	15:F:327:TRP:HD1	2.28	0.42
25:S:76:ARG:NH2	25:S:77:GLU:OE1	2.52	0.42
27:U:154:CYS:HB3	27:U:157:CYS:O	2.19	0.42
34:o:429:LEU:HA	34:o:433:PRO:HG3	2.02	0.42
34:o:1202:PHE:HB3	34:o:1263:ASN:HD22	1.85	0.42
35:p:676:ALA:HA	35:p:682:LEU:HD22	2.00	0.42
36:q:193:ARG:NH2	36:q:218:ALA:O	2.44	0.42
13:d:871:THR:O	20:l:62:LYS:NZ	2.42	0.42
14:e:504:LEU:HD22	14:e:575:PHE:HZ	1.84	0.42
2:1:374:LEU:HD12	2:1:374:LEU:C	2.45	0.42
2:1:503:THR:OG1	2:1:533:TYR:OH	2.01	0.42
7:6:412:MET:HA	7:6:415:HIS:CD2	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:7:557:ILE:HG22	8:7:561:ILE:HD12	2.01	0.42
11:A:819:LYS:HE2	11:A:819:LYS:HB2	1.94	0.42
12:B:216:SER:OG	12:B:217:ASN:N	2.52	0.42
15:F:329:LEU:HA	15:F:332:PHE:HB3	2.01	0.42
32:k:179:MET:HB3	32:k:180:PRO:CD	2.50	0.42
34:o:1417:HIS:O	34:o:1421:ARG:HG2	2.20	0.42
35:p:27:TRP:CD1	35:p:762:ARG:HH21	2.37	0.42
35:p:81:PRO:HA	35:p:82:PRO:HD3	1.93	0.42
15:f:104:LEU:HD22	19:j:216:TYR:HB2	2.02	0.42
1:0:8:ARG:HG3	27:U:173:ALA:N	2.34	0.42
4:3:257:CYS:HB2	4:3:258:HIS:CD2	2.54	0.42
5:4:261:PHE:CZ	5:4:265:LEU:HD21	2.54	0.42
11:A:464:TRP:CD1	11:A:464:TRP:C	2.96	0.42
12:B:367:GLU:OE2	12:B:371:LYS:NZ	2.40	0.42
12:B:562:GLY:O	12:B:581:ILE:HG12	2.19	0.42
13:D:998:GLN:HB2	13:D:1002:ARG:NH2	2.35	0.42
13:D:998:GLN:HA	13:D:1001:GLN:HB2	2.01	0.42
25:S:161:GLU:O	25:S:165:GLU:HG2	2.20	0.42
28:V:145:VAL:C	28:V:146:ARG:HD2	2.45	0.42
28:V:231:GLU:OE1	28:V:231:GLU:HA	2.18	0.42
34:o:214:ILE:H	34:o:214:ILE:HG13	1.43	0.42
35:p:177:CYS:SG	35:p:738:THR:OG1	2.58	0.42
35:p:285:LEU:HB3	35:p:292:PHE:CE1	2.55	0.42
35:p:725:GLN:HA	35:p:728:MET:HE2	2.01	0.42
36:q:69:GLY:HA3	45:z:57:ALA:HB1	2.01	0.42
14:e:332:ILE:HA	14:e:336:HIS:HD2	1.84	0.42
4:3:42:MET:HE3	4:3:108:ASN:HA	2.02	0.42
4:3:253:ALA:O	4:3:262:ILE:N	2.42	0.42
5:4:403:PHE:HA	6:5:8:VAL:HG13	2.01	0.42
8:7:114:ASN:C	8:7:114:ASN:ND2	2.78	0.42
8:7:272:ARG:HA	8:7:275:GLU:HG2	2.02	0.42
11:A:472:ASN:ND2	15:f:299:LYS:O	2.53	0.42
15:F:397:GLN:H	15:F:397:GLN:HG3	1.60	0.42
20:L:120:LEU:O	20:L:125:ASN:N	2.52	0.42
20:L:120:LEU:HD23	20:L:128:ILE:HG12	2.01	0.42
27:U:14:LEU:HD12	27:U:194:THR:HA	2.02	0.42
27:U:76:MET:HG3	27:U:89:HIS:C	2.45	0.42
28:V:109:LEU:HD23	28:V:109:LEU:H	1.84	0.42
29:X:-32:DC:H2'	29:X:-31:DT:H71	2.01	0.42
30:Y:0:DT:H2'	30:Y:1:DG:O4'	2.20	0.42
34:o:389:THR:HG21	34:o:417:LYS:HB2	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:o:712:ASP:HB3	34:o:744:ILE:HD13	2.01	0.42
34:o:992:LYS:HA	34:o:992:LYS:HD3	1.85	0.42
34:o:1374:VAL:HG11	34:o:1411:LEU:HD21	2.01	0.42
35:p:59:VAL:HG21	35:p:91:ILE:HD12	2.01	0.42
36:q:4:ALA:HB2	44:y:93:ASP:HB3	2.02	0.42
37:r:41:LEU:HD22	37:r:61:PHE:CE1	2.55	0.42
38:s:139:ILE:H	38:s:139:ILE:HG12	1.68	0.42
39:t:88:ASP:O	39:t:92:ILE:HG13	2.20	0.42
41:v:37:MET:HE2	41:v:37:MET:HB3	1.85	0.42
42:w:38:ALA:HB2	42:w:45:GLN:HG2	2.02	0.42
1:0:85:ARG:NH1	1:0:140:LEU:N	2.69	0.41
8:7:323:ILE:O	8:7:378:ARG:NH1	2.53	0.41
13:D:963:ARG:HA	13:D:966:LEU:H	1.84	0.41
15:F:233:GLY:CA	15:F:239:ARG:HE	2.33	0.41
25:S:44:GLN:HE21	25:S:44:GLN:HB3	1.66	0.41
31:c:94:HIS:CD2	15:f:122:LEU:HD22	2.55	0.41
34:o:114:CYS:SG	34:o:184:CYS:HB3	2.59	0.41
34:o:920:PHE:CE1	34:o:1053:ARG:HD2	2.55	0.41
34:o:1471:PHE:CZ	39:t:61:GLU:HA	2.55	0.41
35:p:264:LYS:HE2	35:p:264:LYS:HB3	1.88	0.41
35:p:751:LEU:HD12	35:p:808:SER:HB3	2.01	0.41
42:w:81:THR:HG23	42:w:96:PHE:CE1	2.55	0.41
42:w:114:CYS:HB2	42:w:123:TRP:HZ3	1.84	0.41
3:2:174:LEU:HD23	8:7:533:ASP:OD2	2.20	0.41
8:7:354:PRO:HA	8:7:416:ILE:HD12	2.03	0.41
8:7:462:SER:OG	8:7:463:PRO:CD	2.66	0.41
21:O:11:LEU:HD23	21:O:44:ILE:HD12	2.02	0.41
34:o:129:ILE:HD13	34:o:129:ILE:HA	1.96	0.41
34:o:544:ALA:HB2	34:o:680:LEU:HD13	2.02	0.41
34:o:779:ILE:O	34:o:783:GLN:HG3	2.20	0.41
35:p:300:MET:O	35:p:303:PRO:HD2	2.20	0.41
35:p:674:MET:HE2	35:p:690:CYS:SG	2.60	0.41
40:u:79:PRO:HG3	40:u:104:MET:SD	2.60	0.41
15:f:428:LEU:HD13	15:f:458:LEU:CB	2.49	0.41
1:0:8:ARG:CZ	1:0:37:LEU:HD13	2.51	0.41
4:3:175:MET:HE3	4:3:179:ASN:CG	2.45	0.41
5:4:237:LEU:HD21	5:4:261:PHE:HZ	1.86	0.41
11:A:463:PRO:HD2	15:F:218:VAL:HG22	2.02	0.41
11:A:464:TRP:CD1	11:A:464:TRP:O	2.73	0.41
11:A:639:LEU:O	11:A:639:LEU:HD13	2.20	0.41
15:F:231:CYS:HB3	15:F:285:MET:HE2	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:F:249:ASP:HB3	15:F:252:LEU:HB2	2.03	0.41
25:S:166:ARG:O	25:S:169:LYS:HG2	2.19	0.41
27:U:139:LEU:HA	40:u:160:ILE:CG1	2.28	0.41
28:V:166:ILE:HG22	28:V:167:LEU:H	1.86	0.41
28:V:229:ASP:HA	28:V:232:LYS:HG3	2.02	0.41
33:m:93:ASP:OD1	33:m:93:ASP:C	2.64	0.41
34:o:379:GLY:HA2	34:o:475:ARG:O	2.21	0.41
34:o:457:ILE:HG13	34:o:515:ILE:HD13	2.02	0.41
34:o:514:GLU:CD	35:p:1101:GLN:HB2	2.45	0.41
34:o:533:PRO:HD3	34:o:654:HIS:CD2	2.56	0.41
34:o:837:PHE:HB2	35:p:506:TRP:HZ3	1.85	0.41
34:o:1189:ASP:HA	34:o:1192:TRP:CZ2	2.56	0.41
35:p:19:PRO:C	35:p:21:LEU:H	2.28	0.41
35:p:95:LYS:HE3	35:p:162:LEU:HD23	2.01	0.41
44:y:45:ILE:HG13	44:y:45:ILE:H	1.62	0.41
14:e:703:MET:HE2	14:e:703:MET:HB3	1.83	0.41
15:f:402:ARG:HH22	15:f:403:ILE:HD12	1.85	0.41
4:3:98:ASP:O	5:4:125:GLY:CA	2.66	0.41
8:7:383:LEU:HD21	8:7:388:ILE:HD11	2.02	0.41
12:B:713:TRP:NE1	12:B:716:PRO:O	2.50	0.41
13:D:962:GLU:C	13:D:965:ILE:HG22	2.45	0.41
24:R:84:ILE:O	24:R:104:ARG:NH1	2.53	0.41
25:S:73:ARG:NH2	26:T:229:HIS:HB2	2.35	0.41
26:T:140:ARG:NH2	35:p:89:GLU:HB2	2.35	0.41
27:U:172:ASP:O	27:U:173:ALA:C	2.64	0.41
34:o:1416:ARG:O	34:o:1420:ASN:HB2	2.21	0.41
35:p:23:GLN:O	35:p:27:TRP:HD1	2.02	0.41
35:p:677:MET:CE	35:p:700:PRO:HB3	2.49	0.41
14:e:513:LEU:CD2	14:e:527:ILE:HG23	2.48	0.41
1:0:55:LYS:O	1:0:57:ASN:N	2.54	0.41
5:4:96:TRP:HB3	5:4:110:LEU:HD23	2.02	0.41
5:4:359:ILE:HG22	5:4:360:THR:N	2.35	0.41
5:4:400:ARG:NE	5:4:400:ARG:HA	2.35	0.41
7:6:128:SER:O	7:6:334:ARG:NH2	2.51	0.41
7:6:173:ASN:N	7:6:434:GLU:OE2	2.49	0.41
7:6:193:VAL:HG11	7:6:283:ARG:HD3	2.01	0.41
7:6:364:LEU:HD23	7:6:410:TYR:CD1	2.56	0.41
11:A:352:MET:HE3	11:A:352:MET:HB3	1.81	0.41
12:B:176:HIS:HE1	12:B:310:ASP:H	1.68	0.41
13:D:1002:ARG:HB2	26:T:182:HIS:HD2	1.78	0.41
13:D:1002:ARG:NE	26:T:182:HIS:CD2	2.86	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:L:110:THR:HG23	20:L:112:GLU:HG3	2.02	0.41
22:P:288:PHE:CD1	22:P:289:PRO:HD2	2.55	0.41
25:S:164:TRP:HZ2	35:p:268:PRO:HG2	1.85	0.41
27:U:172:ASP:OD1	27:U:172:ASP:N	2.51	0.41
33:m:70:HIS:HA	33:m:73:MET:HE3	2.02	0.41
34:o:233:CYS:SG	34:o:238:MET:HB2	2.60	0.41
35:p:528:LEU:HD23	35:p:528:LEU:HA	1.82	0.41
38:s:55:ARG:HE	38:s:76:PHE:HB3	1.86	0.41
15:f:83:LEU:HD11	18:i:42:PHE:HB2	2.03	0.41
3:2:186:ILE:HG12	3:2:211:LEU:HD12	2.03	0.41
4:3:192:ASP:OD1	4:3:213:LEU:N	2.45	0.41
11:A:337:ARG:HD3	11:A:338:VAL:H	1.85	0.41
11:A:413:ASP:O	11:A:414:ILE:C	2.63	0.41
12:B:639:LYS:NZ	12:B:641:GLU:OE2	2.42	0.41
12:B:984:PRO:HG2	12:B:987:LEU:HD22	2.02	0.41
13:D:998:GLN:HE22	26:T:186:MET:HA	1.82	0.41
14:E:476:VAL:HG11	14:E:794:ALA:HB3	2.02	0.41
26:T:123:ASN:OD1	26:T:123:ASN:N	2.53	0.41
27:U:194:THR:O	27:U:195:GLU:HG3	2.21	0.41
34:o:420:ILE:HB	34:o:445:LYS:HB2	2.03	0.41
34:o:621:ILE:HG12	41:v:115:TYR:HE2	1.84	0.41
14:e:481:ASP:OD1	14:e:481:ASP:N	2.52	0.41
19:j:173:HIS:HA	19:j:176:MET:HE3	2.02	0.41
1:0:8:ARG:NH1	1:0:9:CYS:SG	2.94	0.41
1:0:85:ARG:CZ	1:0:140:LEU:HG	2.38	0.41
4:3:255:CYS:HB2	4:3:276:CYS:N	2.36	0.41
5:4:146:PRO:HA	5:4:149:ASP:OD2	2.21	0.41
12:B:371:LYS:HA	12:B:371:LYS:HD3	1.87	0.41
12:B:417:ILE:HD13	12:B:417:ILE:HA	1.94	0.41
12:B:496:MET:HE3	12:B:496:MET:HB2	1.83	0.41
15:F:258:ARG:HA	15:F:258:ARG:HD2	1.83	0.41
15:F:312:ILE:HG13	15:F:334:ALA:HB1	2.00	0.41
15:F:388:ILE:HA	15:F:392:ILE:HG12	2.03	0.41
24:R:48:VAL:HG23	35:p:1069:ILE:HG12	2.03	0.41
26:T:31:TRP:CD1	26:T:62:LEU:HD21	2.56	0.41
34:o:189:PRO:HB3	34:o:202:TRP:CD2	2.56	0.41
34:o:488:VAL:O	34:o:491:PRO:HD2	2.21	0.41
35:p:474:THR:OG1	35:p:732:ALA:O	2.39	0.41
3:2:333:GLU:O	3:2:333:GLU:HG2	2.21	0.41
8:7:618:VAL:HG11	8:7:664:VAL:HA	2.03	0.41
11:A:592:SER:OG	11:A:695:GLY:O	2.31	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:731:LEU:HD23	11:A:731:LEU:HA	1.92	0.41
13:D:960:GLU:OE1	13:D:960:GLU:N	2.53	0.41
14:E:521:ASP:OD1	14:E:521:ASP:N	2.52	0.41
15:F:396:LEU:HA	15:F:399:GLU:OE1	2.20	0.41
22:P:169:VAL:HG22	22:P:222:THR:HG22	2.02	0.41
26:T:9:LEU:O	26:T:13:LYS:HG2	2.20	0.41
27:U:139:LEU:HG	40:u:159:ALA:CA	2.49	0.41
34:o:1471:PHE:CE2	39:t:64:ARG:HD3	2.56	0.41
35:p:818:GLU:HG3	35:p:827:GLU:O	2.21	0.41
35:p:1106:ARG:HD3	35:p:1106:ARG:HA	1.89	0.41
37:r:18:SER:HB2	37:r:116:PRO:HD2	2.03	0.41
37:r:31:THR:HG21	37:r:95:PHE:HA	2.03	0.41
45:z:43:ILE:C	45:z:44:MET:HE2	2.46	0.41
13:d:1064:ILE:HD13	13:d:1064:ILE:HA	1.94	0.41
15:f:216:LEU:HD21	15:f:254:GLN:O	2.21	0.41
15:f:320:ARG:HH11	15:f:320:ARG:HB2	1.83	0.41
1:0:13:LYS:HD3	1:0:13:LYS:N	2.35	0.41
1:0:84:LYS:CB	1:0:136:ASN:HD21	2.33	0.41
2:1:422:LEU:HD21	4:3:224:LEU:HB3	2.02	0.41
3:2:115:GLU:N	3:2:115:GLU:OE1	2.54	0.41
3:2:379:LEU:O	3:2:379:LEU:HD23	2.21	0.41
4:3:217:VAL:O	4:3:217:VAL:HG23	2.20	0.41
4:3:229:TRP:CZ3	5:4:58:ARG:CD	3.03	0.41
5:4:384:PRO:HB2	5:4:387:ILE:HG12	2.03	0.41
7:6:474:ASP:OD1	7:6:474:ASP:N	2.54	0.41
8:7:145:GLN:HG2	8:7:150:THR:HG22	2.03	0.41
11:A:335:LYS:HE2	11:A:495:LEU:HB2	2.03	0.41
12:B:55:PRO:HB3	12:B:60:LEU:HD22	2.03	0.41
12:B:77:ILE:HG12	12:B:146:ILE:HG23	2.03	0.41
12:B:203:LYS:HZ3	12:B:235:HIS:HB3	1.85	0.41
12:B:298:ARG:HH11	12:B:298:ARG:HD3	1.68	0.41
12:B:544:LEU:HD22	12:B:625:LEU:HD22	2.03	0.41
13:D:995:GLU:OE2	26:T:193:LYS:HD2	2.21	0.41
14:E:236:LEU:HD21	14:E:317:LEU:HB2	2.03	0.41
14:E:508:LYS:HB3	14:E:512:ASP:HB2	2.02	0.41
14:E:775:THR:CG2	14:E:778:THR:HB	2.51	0.41
15:F:114:LEU:HB2	17:H:52:SER:N	2.35	0.41
15:F:277:ALA:O	15:F:278:LEU:C	2.64	0.41
15:F:370:TRP:CH2	15:F:402:ARG:HB3	2.56	0.41
25:S:110:PHE:CE2	25:S:148:PRO:HB3	2.55	0.41
26:T:32:ALA:HA	26:T:35:SER:HB2	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:U:104:LYS:HE3	27:U:191:LEU:HB2	2.01	0.41
28:V:146:ARG:NE	28:V:173:GLU:O	2.54	0.41
28:V:187:ASP:HB2	28:V:189:ILE:HG22	2.02	0.41
34:o:225:PHE:HB3	34:o:245:PRO:HB2	2.03	0.41
34:o:893:GLU:OE1	38:s:197:SER:OG	2.29	0.41
34:o:970:PHE:HE2	34:o:1040:LEU:HD21	1.86	0.41
34:o:1262:MET:HB3	34:o:1265:ASP:HB3	2.01	0.41
34:o:1276:VAL:HB	34:o:1278:LYS:HD3	2.02	0.41
35:p:719:SER:OG	35:p:720:PRO:HD3	2.20	0.41
35:p:744:MET:HE3	35:p:744:MET:HB3	1.83	0.41
38:s:193:ILE:HB	38:s:205:THR:OG1	2.20	0.41
15:f:254:GLN:O	15:f:254:GLN:HG3	2.21	0.41
8:7:195:ALA:O	8:7:199:ILE:HG12	2.21	0.41
11:A:604:PRO:O	11:A:889:TYR:OH	2.34	0.41
12:B:295:LEU:HD13	12:B:477:LEU:HD11	2.03	0.41
12:B:464:ILE:HG12	12:B:513:LYS:HE2	2.02	0.41
12:B:881:GLY:HA3	17:H:218:PRO:HB3	2.03	0.41
13:D:963:ARG:C	13:D:966:LEU:H	2.29	0.41
14:E:265:GLU:OE1	14:E:265:GLU:HA	2.20	0.41
15:F:312:ILE:HG22	15:F:313:VAL:CG1	2.50	0.41
15:F:374:TYR:CE1	15:F:422:HIS:HB3	2.56	0.41
23:Q:19:GLU:O	23:Q:22:ILE:HG12	2.21	0.41
27:U:110:MET:HE1	28:V:219:LEU:HB3	2.03	0.41
28:V:90:GLN:HE22	28:V:176:PRO:HG3	1.84	0.41
28:V:189:ILE:HB	28:V:204:ASN:HB2	2.03	0.41
34:o:47:THR:HB	34:o:50:GLY:O	2.21	0.41
42:w:78:LEU:HD23	42:w:78:LEU:HA	1.90	0.41
14:e:246:HIS:CD2	14:e:246:HIS:C	2.98	0.41
14:e:378:LYS:HZ3	14:e:378:LYS:HG2	1.61	0.41
1:0:55:LYS:CE	40:u:166:ASP:OD2	2.69	0.40
4:3:46:ASN:OD1	5:4:123:LEU:HD23	2.20	0.40
5:4:229:ASP:OD1	5:4:229:ASP:N	2.54	0.40
8:7:28:LEU:HD22	8:7:55:LEU:CD2	2.51	0.40
12:B:887:ARG:NH2	12:B:917:ASP:OD2	2.49	0.40
12:B:957:MET:O	12:B:968:ARG:NH1	2.53	0.40
12:B:987:LEU:HG	12:B:988:PRO:HD2	2.03	0.40
15:F:324:ASP:CA	15:F:327:TRP:HB3	2.44	0.40
15:F:433:PRO:C	15:F:435:LEU:N	2.78	0.40
22:P:165:LEU:HD13	22:P:168:ILE:HD11	2.03	0.40
24:R:121:ILE:HD13	24:R:138:THR:HG22	2.03	0.40
27:U:19:LYS:HA	27:U:22:ILE:HB	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:U:192:ARG:O	27:U:195:GLU:HB3	2.21	0.40
28:V:166:ILE:HG22	28:V:167:LEU:N	2.36	0.40
29:X:25:DG:H2"	29:X:26:DC:C6	2.57	0.40
32:k:142:THR:OG1	32:k:143:GLY:N	2.55	0.40
33:m:52:GLU:OE1	33:m:52:GLU:N	2.40	0.40
34:o:76:GLY:HA2	34:o:80:GLU:HB3	2.02	0.40
34:o:552:ASP:OD1	41:v:22:PHE:HB3	2.20	0.40
34:o:1180:ASN:O	34:o:1183:SER:OG	2.26	0.40
34:o:1348:SER:CA	38:s:137:ILE:HD11	2.51	0.40
34:o:1474:LEU:HB2	39:t:105:ILE:HG13	2.03	0.40
35:p:110:PRO:HG2	35:p:163:LEU:HD11	2.03	0.40
35:p:712:PRO:HG2	35:p:939:HIS:CE1	2.56	0.40
36:q:78:ILE:HG12	36:q:82:LEU:HG	2.03	0.40
40:u:91:GLN:HG2	40:u:92:VAL:N	2.36	0.40
1:0:108:ASN:OD1	1:0:112:ASN:HB3	2.22	0.40
2:1:303:ILE:HG22	2:1:307:PHE:HE2	1.87	0.40
2:1:411:MET:HG2	2:1:411:MET:O	2.22	0.40
6:5:32:LYS:HE3	12:B:539:ARG:NH2	2.36	0.40
8:7:12:PHE:CE2	8:7:14:TYR:HB2	2.56	0.40
8:7:225:LEU:O	8:7:227:ARG:NH1	2.53	0.40
14:E:651:VAL:HG21	14:E:686:THR:HG21	2.01	0.40
15:F:329:LEU:HA	15:F:332:PHE:CB	2.52	0.40
15:F:396:LEU:HA	15:F:399:GLU:CD	2.46	0.40
24:R:125:ALA:HB1	24:R:130:LEU:HB2	2.03	0.40
26:T:175:ARG:HD2	26:T:207:LYS:HA	2.02	0.40
29:X:-18:DG:C2	29:X:-17:DG:C5	3.08	0.40
34:o:155:GLU:HB2	34:o:181:HIS:CD2	2.57	0.40
34:o:256:PRO:HA	34:o:257:PRO:HD3	1.97	0.40
34:o:384:ILE:HG12	35:p:1061:SER:HB3	2.03	0.40
34:o:1180:ASN:HB2	34:o:1183:SER:HB3	2.03	0.40
35:p:158:SER:O	35:p:164:ASN:HB2	2.21	0.40
3:2:318:LEU:HD12	4:3:272:LEU:CD2	2.51	0.40
4:3:242:ILE:HD13	5:4:73:LEU:O	2.21	0.40
5:4:62:LEU:O	5:4:115:ARG:NH2	2.54	0.40
5:4:352:GLN:HE22	5:4:398:ARG:NH1	2.20	0.40
7:6:340:LEU:CD2	7:6:491:ALA:HB2	2.51	0.40
8:7:72:TYR:HB3	8:7:206:VAL:HG12	2.04	0.40
8:7:101:LYS:C	8:7:102:LEU:HD12	2.46	0.40
11:A:1068:ARG:HD2	11:A:1068:ARG:C	2.46	0.40
12:B:62:ARG:H	12:B:62:ARG:HG2	1.58	0.40
12:B:219:ASP:OD1	12:B:219:ASP:N	2.52	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:F:350:ASN:O	15:F:354:ARG:HB2	2.22	0.40
17:H:201:GLN:HG3	17:H:215:ALA:HA	2.04	0.40
26:T:140:ARG:HD3	35:p:60:GLU:OE2	2.22	0.40
26:T:154:LYS:HE3	26:T:154:LYS:HB2	1.94	0.40
31:c:105:ASN:OD1	31:c:105:ASN:N	2.55	0.40
33:m:77:ARG:CZ	33:m:77:ARG:HB3	2.51	0.40
34:o:381:PRO:HG2	34:o:384:ILE:HB	2.02	0.40
1:O:1:MET:HG3	8:7:345:ARG:NH1	2.37	0.40
2:1:219:GLU:O	2:1:223:ARG:HG2	2.21	0.40
8:7:604:VAL:O	8:7:608:ILE:HG22	2.22	0.40
11:A:511:LEU:N	11:A:511:LEU:HD13	2.36	0.40
11:A:725:CYS:SG	11:A:734:LEU:HD12	2.61	0.40
13:D:1001:GLN:HG2	21:O:1:MET:HB3	2.03	0.40
14:E:668:HIS:NE2	14:E:686:THR:OG1	2.42	0.40
34:o:576:GLN:O	34:o:590:GLN:NE2	2.53	0.40
37:r:48:ASN:HD21	37:r:56:GLU:HA	1.86	0.40
38:s:7:THR:HG21	38:s:41:LYS:HG2	2.02	0.40
38:s:72:MET:HG3	38:s:101:ARG:HD2	2.03	0.40
41:v:37:MET:HE1	41:v:132:LEU:HD21	2.03	0.40
41:v:88:PHE:CG	41:v:144:LEU:HB3	2.57	0.40
15:f:446:ASP:O	15:f:450:ALA:N	2.54	0.40
3:2:174:LEU:HD23	8:7:533:ASP:CG	2.47	0.40
3:2:227:HIS:CE1	3:2:231:LEU:HD11	2.57	0.40
4:3:237:GLN:HG3	5:4:51:LEU:HD22	1.93	0.40
5:4:223:ALA:HA	5:4:226:ARG:HG2	2.02	0.40
5:4:448:HIS:CD2	5:4:452:LYS:HE3	2.56	0.40
11:A:411:GLU:H	11:A:411:GLU:HG3	1.64	0.40
12:B:835:ARG:HE	12:B:835:ARG:HB2	1.73	0.40
13:D:933:ARG:CZ	19:J:114:THR:HG21	2.51	0.40
14:E:239:LEU:HB3	14:E:307:LEU:HD21	2.03	0.40
15:F:274:ASN:HB2	15:F:317:LEU:N	2.31	0.40
24:R:94:ASP:H	24:R:98:ASN:H	1.70	0.40
25:S:89:LYS:HE2	25:S:89:LYS:HB2	1.75	0.40
28:V:121:THR:O	28:V:124:LEU:HB3	2.22	0.40
28:V:133:ILE:HG22	28:V:134:ASP:N	2.36	0.40
35:p:185:PHE:HB3	35:p:187:ILE:HD13	2.03	0.40
15:f:217:SER:H	15:f:220:GLN:HE21	1.70	0.40
15:f:284:ARG:HH21	15:f:284:ARG:HD2	1.76	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	169/309 (55%)	156 (92%)	13 (8%)	0	100	100
2	1	253/548 (46%)	243 (96%)	10 (4%)	0	100	100
3	2	325/395 (82%)	312 (96%)	13 (4%)	0	100	100
4	3	259/308 (84%)	253 (98%)	6 (2%)	0	100	100
5	4	384/462 (83%)	365 (95%)	19 (5%)	0	100	100
6	5	52/71 (73%)	48 (92%)	2 (4%)	2 (4%)	2	19
7	6	601/782 (77%)	573 (95%)	27 (4%)	1 (0%)	43	77
8	7	710/760 (93%)	683 (96%)	27 (4%)	0	100	100
9	N	4/8 (50%)	3 (75%)	1 (25%)	0	100	100
11	A	543/1872 (29%)	519 (96%)	23 (4%)	1 (0%)	43	77
12	B	959/1199 (80%)	911 (95%)	48 (5%)	0	100	100
13	D	158/1085 (15%)	153 (97%)	5 (3%)	0	100	100
13	d	154/1085 (14%)	150 (97%)	4 (3%)	0	100	100
14	E	541/800 (68%)	518 (96%)	22 (4%)	1 (0%)	43	77
14	e	531/800 (66%)	482 (91%)	48 (9%)	1 (0%)	43	77
15	F	408/677 (60%)	392 (96%)	15 (4%)	1 (0%)	43	77
15	f	399/677 (59%)	380 (95%)	19 (5%)	0	100	100
16	G	138/349 (40%)	135 (98%)	3 (2%)	0	100	100
17	H	207/310 (67%)	189 (91%)	13 (6%)	5 (2%)	4	26
18	I	118/264 (45%)	115 (98%)	3 (2%)	0	100	100
18	i	119/264 (45%)	115 (97%)	4 (3%)	0	100	100
19	J	86/218 (39%)	82 (95%)	4 (5%)	0	100	100
19	j	91/218 (42%)	85 (93%)	4 (4%)	2 (2%)	5	28
20	L	74/161 (46%)	72 (97%)	2 (3%)	0	100	100
20	l	105/161 (65%)	100 (95%)	5 (5%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	O	97/109 (89%)	95 (98%)	2 (2%)	0	100	100
22	P	177/339 (52%)	175 (99%)	2 (1%)	0	100	100
23	Q	109/376 (29%)	102 (94%)	7 (6%)	0	100	100
24	R	278/316 (88%)	261 (94%)	15 (5%)	2 (1%)	18	55
25	S	174/517 (34%)	161 (92%)	12 (7%)	1 (1%)	21	59
26	T	218/249 (88%)	211 (97%)	7 (3%)	0	100	100
27	U	180/439 (41%)	153 (85%)	26 (14%)	1 (1%)	21	59
28	V	163/291 (56%)	140 (86%)	23 (14%)	0	100	100
31	c	125/929 (14%)	116 (93%)	9 (7%)	0	100	100
32	k	96/211 (46%)	91 (95%)	5 (5%)	0	100	100
33	m	85/124 (68%)	82 (96%)	3 (4%)	0	100	100
34	o	1448/1970 (74%)	1399 (97%)	45 (3%)	4 (0%)	36	72
35	p	1145/1174 (98%)	1109 (97%)	36 (3%)	0	100	100
36	q	253/275 (92%)	246 (97%)	7 (3%)	0	100	100
37	r	126/142 (89%)	126 (100%)	0	0	100	100
38	s	207/210 (99%)	203 (98%)	4 (2%)	0	100	100
39	t	80/127 (63%)	79 (99%)	1 (1%)	0	100	100
40	u	169/172 (98%)	167 (99%)	2 (1%)	0	100	100
41	v	146/150 (97%)	142 (97%)	4 (3%)	0	100	100
42	w	112/125 (90%)	108 (96%)	4 (4%)	0	100	100
43	x	65/67 (97%)	62 (95%)	3 (5%)	0	100	100
44	y	113/117 (97%)	110 (97%)	3 (3%)	0	100	100
45	z	42/58 (72%)	40 (95%)	2 (5%)	0	100	100
All	All	12996/22270 (58%)	12412 (96%)	562 (4%)	22 (0%)	44	77

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	5	48	GLU
14	E	523	VAL
17	H	156	PRO
25	S	87	VAL
34	o	1103	THR
34	o	1274	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
14	e	522	ASP
19	j	124	GLU
11	A	502	LEU
15	F	411	VAL
17	H	154	PRO
19	j	177	LYS
6	5	39	ASP
17	H	136	ALA
17	H	139	ASN
24	R	90	ALA
24	R	99	SER
7	6	416	THR
34	o	1433	GLU
17	H	158	THR
27	U	137	THR
34	o	184	CYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	164/283 (58%)	158 (96%)	6 (4%)	30	51
2	1	241/484 (50%)	241 (100%)	0	100	100
3	2	295/352 (84%)	294 (100%)	1 (0%)	86	85
4	3	234/272 (86%)	232 (99%)	2 (1%)	70	78
5	4	346/399 (87%)	339 (98%)	7 (2%)	48	66
6	5	48/64 (75%)	47 (98%)	1 (2%)	47	65
7	6	536/688 (78%)	535 (100%)	1 (0%)	87	86
8	7	624/664 (94%)	624 (100%)	0	100	100
9	N	2/2 (100%)	2 (100%)	0	100	100
11	A	496/1665 (30%)	452 (91%)	44 (9%)	9	28
12	B	876/1083 (81%)	862 (98%)	14 (2%)	55	69

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	D	147/815 (18%)	136 (92%)	11 (8%)	12	33
13	d	146/815 (18%)	144 (99%)	2 (1%)	59	72
14	E	480/657 (73%)	467 (97%)	13 (3%)	39	60
14	e	475/657 (72%)	463 (98%)	12 (2%)	42	62
15	F	328/574 (57%)	307 (94%)	21 (6%)	16	37
15	f	322/574 (56%)	312 (97%)	10 (3%)	35	56
16	G	132/322 (41%)	124 (94%)	8 (6%)	17	38
17	H	181/270 (67%)	175 (97%)	6 (3%)	33	55
18	I	106/235 (45%)	106 (100%)	0	100	100
18	i	107/235 (46%)	107 (100%)	0	100	100
19	J	79/154 (51%)	72 (91%)	7 (9%)	9	28
19	j	83/154 (54%)	82 (99%)	1 (1%)	63	74
20	L	71/141 (50%)	66 (93%)	5 (7%)	14	36
20	l	98/141 (70%)	97 (99%)	1 (1%)	68	77
21	O	90/98 (92%)	90 (100%)	0	100	100
22	P	154/293 (53%)	154 (100%)	0	100	100
23	Q	105/324 (32%)	105 (100%)	0	100	100
24	R	238/268 (89%)	234 (98%)	4 (2%)	53	68
25	S	154/448 (34%)	134 (87%)	20 (13%)	4	16
26	T	196/218 (90%)	193 (98%)	3 (2%)	57	71
27	U	167/373 (45%)	166 (99%)	1 (1%)	78	82
28	V	150/261 (58%)	149 (99%)	1 (1%)	76	80
31	c	113/833 (14%)	111 (98%)	2 (2%)	51	67
32	k	87/182 (48%)	87 (100%)	0	100	100
33	m	80/106 (76%)	71 (89%)	9 (11%)	5	19
34	o	1280/1749 (73%)	1261 (98%)	19 (2%)	57	71
35	p	1004/1027 (98%)	987 (98%)	17 (2%)	53	68
36	q	234/252 (93%)	227 (97%)	7 (3%)	36	57
37	r	118/126 (94%)	118 (100%)	0	100	100
38	s	191/192 (100%)	188 (98%)	3 (2%)	55	69
39	t	71/111 (64%)	71 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	u	152/153 (99%)	150 (99%)	2 (1%)	61	73
41	v	129/131 (98%)	128 (99%)	1 (1%)	73	79
42	w	103/112 (92%)	98 (95%)	5 (5%)	22	43
43	x	56/56 (100%)	53 (95%)	3 (5%)	20	41
44	y	104/106 (98%)	101 (97%)	3 (3%)	37	57
45	z	41/55 (74%)	40 (98%)	1 (2%)	43	63
All	All	11634/19174 (61%)	11360 (98%)	274 (2%)	43	63

All (274) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	8	ARG
1	0	11	THR
1	0	28	HIS
1	0	29	THR
1	0	127	LYS
1	0	128	GLU
3	2	69	ARG
4	3	257	CYS
4	3	258	HIS
5	4	398	ARG
5	4	400	ARG
5	4	401	LEU
5	4	404	THR
5	4	407	VAL
5	4	413	LEU
5	4	456	LYS
6	5	38	ILE
7	6	266	GLN
11	A	337	ARG
11	A	338	VAL
11	A	348	LEU
11	A	353	LEU
11	A	395	ASP
11	A	397	LEU
11	A	400	GLU
11	A	401	ASN
11	A	403	LEU
11	A	404	MET
11	A	408	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	A	415	ILE
11	A	416	TRP
11	A	419	GLU
11	A	470	ILE
11	A	475	LEU
11	A	481	GLU
11	A	483	ASN
11	A	491	MET
11	A	499	VAL
11	A	500	LEU
11	A	501	THR
11	A	502	LEU
11	A	505	ASN
11	A	511	LEU
11	A	639	LEU
11	A	661	GLU
11	A	667	THR
11	A	711	ASP
11	A	727	THR
11	A	730	PHE
11	A	819	LYS
11	A	821	ARG
11	A	828	GLU
11	A	925	ASP
11	A	943	LYS
11	A	970	ASN
11	A	1052	ARG
11	A	1058	HIS
11	A	1062	TYR
11	A	1068	ARG
11	A	1073	GLN
11	A	1165	LEU
11	A	1203	GLU
12	B	21	GLU
12	B	71	ARG
12	B	140	GLU
12	B	184	ASN
12	B	262	MET
12	B	266	THR
12	B	293	GLU
12	B	559	LYS
12	B	603	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	B	640	VAL
12	B	746	SER
12	B	771	VAL
12	B	818	THR
12	B	987	LEU
13	D	948	GLU
13	D	952	GLN
13	D	953	ILE
13	D	957	ARG
13	D	958	LYS
13	D	960	GLU
13	D	964	GLU
13	D	965	ILE
13	D	966	LEU
13	D	1006	LEU
13	D	1009	LEU
14	E	258	ASN
14	E	274	TYR
14	E	278	ASP
14	E	280	ARG
14	E	326	ASN
14	E	327	ASN
14	E	519	GLU
14	E	521	ASP
14	E	522	ASP
14	E	527	ILE
14	E	761	LEU
14	E	774	MET
14	E	775	THR
15	F	83	LEU
15	F	91	PHE
15	F	94	PHE
15	F	219	GLU
15	F	261	THR
15	F	269	VAL
15	F	271	VAL
15	F	280	ILE
15	F	295	LEU
15	F	301	VAL
15	F	312	ILE
15	F	317	LEU
15	F	326	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
15	F	340	ILE
15	F	348	THR
15	F	354	ARG
15	F	368	THR
15	F	397	GLN
15	F	406	VAL
15	F	415	ILE
15	F	427	LEU
16	G	41	ASP
16	G	129	LYS
16	G	131	ILE
16	G	143	VAL
16	G	153	LYS
16	G	181	TRP
16	G	182	GLU
16	G	183	ILE
17	H	27	ASP
17	H	36	THR
17	H	135	THR
17	H	157	HIS
17	H	161	LYS
17	H	162	THR
19	J	116	LEU
19	J	123	LEU
19	J	156	SER
19	J	164	SER
19	J	174	CYS
19	J	177	LYS
19	J	192	LYS
20	L	79	ASP
20	L	104	ARG
20	L	108	SER
20	L	113	VAL
20	L	114	LYS
24	R	48	VAL
24	R	95	GLU
24	R	104	ARG
24	R	277	ILE
25	S	59	GLU
25	S	60	GLU
25	S	61	GLU
25	S	70	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
25	S	72	ASN
25	S	74	LYS
25	S	75	LEU
25	S	76	ARG
25	S	82	LYS
25	S	83	LYS
25	S	86	ILE
25	S	88	LEU
25	S	89	LYS
25	S	90	GLU
25	S	151	ARG
25	S	155	LEU
25	S	156	THR
25	S	163	GLU
25	S	167	ARG
25	S	171	LEU
26	T	145	LEU
26	T	148	VAL
26	T	171	GLU
27	U	145	PHE
28	V	189	ILE
31	c	24	ASP
31	c	106	VAL
33	m	31	LEU
33	m	55	ASP
33	m	58	GLU
33	m	77	ARG
33	m	83	VAL
33	m	84	GLU
33	m	90	ILE
33	m	91	ARG
33	m	110	LEU
34	o	97	VAL
34	o	110	VAL
34	o	119	VAL
34	o	184	CYS
34	o	211	GLU
34	o	214	ILE
34	o	308	LYS
34	o	476	ILE
34	o	488	VAL
34	o	499	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	o	549	THR
34	o	585	LEU
34	o	621	ILE
34	o	934	LEU
34	o	996	ILE
34	o	1103	THR
34	o	1336	LEU
34	o	1385	VAL
34	o	1458	ILE
35	p	90	GLN
35	p	192	LYS
35	p	214	LYS
35	p	215	TYR
35	p	222	ARG
35	p	235	ILE
35	p	305	LEU
35	p	351	VAL
35	p	388	TYR
35	p	438	ARG
35	p	457	LYS
35	p	466	VAL
35	p	598	VAL
35	p	750	VAL
35	p	888	THR
35	p	1022	LEU
35	p	1043	ILE
36	q	58	VAL
36	q	61	ASP
36	q	82	LEU
36	q	93	PHE
36	q	100	GLU
36	q	259	LEU
36	q	266	GLU
38	s	58	LEU
38	s	71	GLN
38	s	139	ILE
40	u	50	THR
40	u	152	VAL
41	v	141	VAL
42	w	42	CYS
42	w	55	VAL
42	w	80	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
42	w	81	THR
42	w	115	THR
43	x	7	CYS
43	x	13	ILE
43	x	14	VAL
44	y	27	VAL
44	y	42	LEU
44	y	45	ILE
45	z	19	CYS
13	d	950	LEU
13	d	951	ASP
14	e	243	LEU
14	e	258	ASN
14	e	268	HIS
14	e	270	ASP
14	e	277	ASP
14	e	282	LEU
14	e	436	ASP
14	e	438	LEU
14	e	512	ASP
14	e	516	ILE
14	e	546	VAL
14	e	579	VAL
15	f	215	GLU
15	f	253	TYR
15	f	261	THR
15	f	272	VAL
15	f	322	ASP
15	f	323	VAL
15	f	326	HIS
15	f	356	THR
15	f	366	GLU
15	f	421	ASP
19	j	114	THR
20	l	114	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (217) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	24	ASN
1	0	45	ASN
1	0	136	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	1	420	GLN
2	1	537	HIS
3	2	140	HIS
3	2	227	HIS
3	2	293	GLN
3	2	317	HIS
4	3	9	ASN
4	3	48	HIS
4	3	240	GLN
5	4	211	GLN
5	4	218	GLN
5	4	352	GLN
5	4	390	GLN
5	4	411	GLN
5	4	424	HIS
5	4	458	GLN
5	4	460	HIS
6	5	42	HIS
7	6	281	GLN
7	6	415	HIS
7	6	498	ASN
7	6	598	HIS
7	6	629	HIS
7	6	709	GLN
8	7	645	GLN
11	A	401	ASN
11	A	472	ASN
11	A	489	GLN
11	A	590	GLN
11	A	630	GLN
11	A	702	ASN
11	A	755	HIS
11	A	802	HIS
11	A	896	GLN
11	A	1073	GLN
12	B	30	HIS
12	B	36	ASN
12	B	39	ASN
12	B	137	HIS
12	B	176	HIS
12	B	183	GLN
12	B	235	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	B	348	GLN
12	B	439	HIS
12	B	450	GLN
12	B	509	ASN
12	B	577	HIS
12	B	644	GLN
12	B	652	GLN
12	B	750	GLN
12	B	813	ASN
12	B	864	ASN
12	B	882	HIS
12	B	908	GLN
12	B	912	ASN
12	B	963	HIS
13	D	875	GLN
13	D	908	GLN
13	D	912	ASN
13	D	925	ASN
13	D	936	GLN
13	D	956	GLN
13	D	998	GLN
14	E	254	ASN
14	E	255	GLN
14	E	256	HIS
14	E	258	ASN
14	E	268	HIS
14	E	327	ASN
14	E	351	GLN
14	E	616	HIS
14	E	640	ASN
14	E	673	HIS
14	E	733	ASN
14	E	758	HIS
14	E	800	GLN
15	F	37	GLN
15	F	59	HIS
15	F	79	ASN
15	F	89	GLN
15	F	119	ASN
15	F	221	GLN
15	F	270	ASN
15	F	273	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
15	F	275	ASN
15	F	326	HIS
15	F	430	HIS
16	G	10	HIS
16	G	48	HIS
16	G	142	ASN
17	H	24	ASN
17	H	142	HIS
17	H	145	HIS
18	I	21	GLN
18	I	38	GLN
18	I	98	GLN
19	J	210	ASN
20	L	117	GLN
21	O	35	GLN
21	O	54	ASN
22	P	229	GLN
22	P	278	GLN
24	R	98	ASN
24	R	103	ASN
24	R	116	ASN
25	S	44	GLN
25	S	72	ASN
25	S	96	GLN
25	S	152	HIS
25	S	178	GLN
26	T	64	ASN
26	T	152	ASN
26	T	182	HIS
26	T	195	GLN
27	U	109	HIS
27	U	142	ASN
27	U	181	ASN
27	U	183	GLN
28	V	83	ASN
28	V	90	GLN
28	V	117	GLN
28	V	157	GLN
31	c	19	GLN
31	c	27	GLN
31	c	50	HIS
32	k	186	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	k	199	GLN
32	k	202	ASN
32	k	205	HIS
33	m	107	ASN
34	o	96	HIS
34	o	181	HIS
34	o	273	GLN
34	o	403	GLN
34	o	412	GLN
34	o	439	HIS
34	o	449	HIS
34	o	493	ASN
34	o	504	HIS
34	o	531	ASN
34	o	539	GLN
34	o	599	HIS
34	o	620	HIS
34	o	703	GLN
34	o	721	HIS
34	o	735	GLN
34	o	764	ASN
34	o	780	ASN
34	o	783	GLN
34	o	791	GLN
34	o	861	GLN
34	o	904	GLN
34	o	1032	GLN
34	o	1105	ASN
34	o	1163	HIS
34	o	1263	ASN
34	o	1384	HIS
34	o	1410	HIS
35	p	72	GLN
35	p	90	GLN
35	p	145	GLN
35	p	245	GLN
35	p	319	ASN
35	p	461	GLN
35	p	481	HIS
35	p	525	ASN
35	p	631	GLN
35	p	699	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	p	716	HIS
35	p	725	GLN
35	p	755	GLN
35	p	913	GLN
35	p	986	GLN
35	p	1025	ASN
35	p	1097	HIS
36	q	190	ASN
36	q	260	GLN
36	q	265	HIS
37	r	48	ASN
37	r	66	ASN
37	r	76	ASN
37	r	129	GLN
38	s	64	HIS
38	s	71	GLN
38	s	210	GLN
41	v	44	ASN
41	v	131	ASN
42	w	41	ASN
42	w	50	ASN
44	y	22	ASN
44	y	36	ASN
44	y	49	GLN
44	y	69	HIS
45	z	26	ASN
13	d	912	ASN
13	d	943	GLN
14	e	246	HIS
14	e	320	HIS
14	e	336	HIS
14	e	368	ASN
14	e	424	GLN
14	e	640	ASN
15	f	30	GLN
15	f	119	ASN
15	f	134	HIS
15	f	273	GLN
15	f	325	ASN
18	i	38	GLN
19	j	172	GLN
19	j	173	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
20	1	73	ASN
20	1	86	GLN
20	1	105	HIS
20	1	119	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	Z	0/2	-	-

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 ⓘ

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	CSX	N	6	9	3,6,7	1.09	0	1,6,8	2.18	1 (100%)
9	ILX	N	1	9	8,9,10	0.63	0	8,11,13	1.41	1 (12%)
9	HYP	N	8	9	7,8,9	0.83	0	5,10,12	2.37	2 (40%)
10	G2L	Z	2	30,10	23,26,30	1.21	3 (13%)	31,38,44	2.12	7 (22%)
9	TRX	N	2	9	15,16,17	1.05	1 (6%)	17,22,24	0.98	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	CSX	N	6	9	-	2/2/5/7	-
9	ILX	N	1	9	-	7/11/12/14	-
9	HYP	N	8	9	-	0/0/11/13	0/1/1/1
10	G2L	Z	2	30,10	-	2/9/27/31	0/3/3/3
9	TRX	N	2	9	-	2/5/6/8	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	Z	2	G2L	C5-C4	3.18	1.47	1.38
10	Z	2	G2L	C6-N1	-2.45	1.34	1.38
9	N	2	TRX	CD2-CE2	2.12	1.44	1.41
10	Z	2	G2L	C5-N7	-2.01	1.35	1.39

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	Z	2	G2L	C5-C4-N3	-6.21	118.50	128.39
10	Z	2	G2L	C2-N3-C4	5.04	120.98	112.30
10	Z	2	G2L	N9-C4-N3	4.56	135.06	125.95
9	N	8	HYP	CB-CG-CD	3.46	107.01	103.16
9	N	8	HYP	O-C-CA	-3.36	116.12	124.77
10	Z	2	G2L	C6-C5-N7	3.24	136.19	130.29
9	N	1	ILX	OD1-CD1-CG1	-3.04	104.77	111.16
10	Z	2	G2L	C3'-C2'-C1'	2.73	105.89	99.89
10	Z	2	G2L	C4-C5-N7	-2.61	106.53	110.67
9	N	6	CSX	CA-CB-SG	2.18	118.30	113.17
10	Z	2	G2L	O6-C6-C5	-2.11	120.97	126.53

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	N	1	ILX	C-CA-CB-CG2
9	N	1	ILX	OD1-CD1-CG1-CB
9	N	1	ILX	OD1-CD1-CG1-OG1
9	N	6	CSX	N-CA-CB-SG
9	N	6	CSX	C-CA-CB-SG
10	Z	2	G2L	C3'-C4'-C5'-O5'
9	N	2	TRX	CA-CB-CG-CD2
10	Z	2	G2L	O4'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	N	2	TRX	CA-CB-CG-CD1
9	N	1	ILX	C-CA-CB-CG1
9	N	1	ILX	N-CA-CB-CG2
9	N	1	ILX	CG2-CB-CG1-CD1
9	N	1	ILX	CG2-CB-CG1-OG1

There are no ring outliers.

5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	N	6	CSX	1	0
9	N	1	ILX	2	0
9	N	8	HYP	1	0
10	Z	2	G2L	5	0
9	N	2	TRX	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 18 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
48	W0F	Z	2500	-	34,35,35	4.05	14 (41%)	43,55,55	3.45	17 (39%)
47	SF4	7	1000	8	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	W0F	Z	2500	-	-	3/24/40/40	0/3/3/3
47	SF4	7	1000	8	-	-	0/6/5/5

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	Z	2500	W0F	P26-O29	13.76	1.74	1.59
48	Z	2500	W0F	C03-C04	-9.77	1.27	1.52
48	Z	2500	W0F	P22-O25	8.40	1.68	1.59
48	Z	2500	W0F	O05-C04	6.91	1.60	1.45
48	Z	2500	W0F	O05-C06	-6.02	1.28	1.42
48	Z	2500	W0F	C12-C13	5.61	1.47	1.38
48	Z	2500	W0F	P26-O25	5.35	1.65	1.59
48	Z	2500	W0F	C13-N09	-3.11	1.34	1.37
48	Z	2500	W0F	C07-C03	-2.99	1.46	1.53
48	Z	2500	W0F	C20-C04	2.55	1.59	1.51
48	Z	2500	W0F	C06-N09	2.34	1.54	1.47
48	Z	2500	W0F	P22-O21	2.16	1.67	1.59
48	Z	2500	W0F	C12-N11	-2.13	1.34	1.39
48	Z	2500	W0F	C17-N16	-2.08	1.34	1.38

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	Z	2500	W0F	O05-C06-N09	-14.57	75.35	108.36
48	Z	2500	W0F	C07-C06-N09	8.27	136.27	113.25
48	Z	2500	W0F	O05-C04-C03	-5.80	92.69	104.92
48	Z	2500	W0F	O27-P26-O25	-5.27	93.02	107.27
48	Z	2500	W0F	O05-C04-C20	4.94	125.15	109.33
48	Z	2500	W0F	O05-C06-C07	-4.15	97.74	106.62
48	Z	2500	W0F	O21-C20-C04	3.98	122.56	108.99
48	Z	2500	W0F	O32-P30-O29	3.91	117.73	104.64
48	Z	2500	W0F	O33-P30-O31	-3.37	97.71	110.83
48	Z	2500	W0F	C06-N09-C10	-3.24	117.54	126.73
48	Z	2500	W0F	O08-C07-C06	2.82	119.83	110.10
48	Z	2500	W0F	O33-P30-O29	2.66	113.57	104.64
48	Z	2500	W0F	O21-P22-O24	-2.29	99.88	108.94
48	Z	2500	W0F	O29-P26-O28	2.28	117.56	110.70
48	Z	2500	W0F	O27-P26-O29	2.16	113.10	107.27
48	Z	2500	W0F	C13-C12-N11	-2.07	106.57	109.26
48	Z	2500	W0F	C10-N09-C13	2.06	108.41	106.67

There are no chirality outliers.

All (3) torsion outliers are listed below:

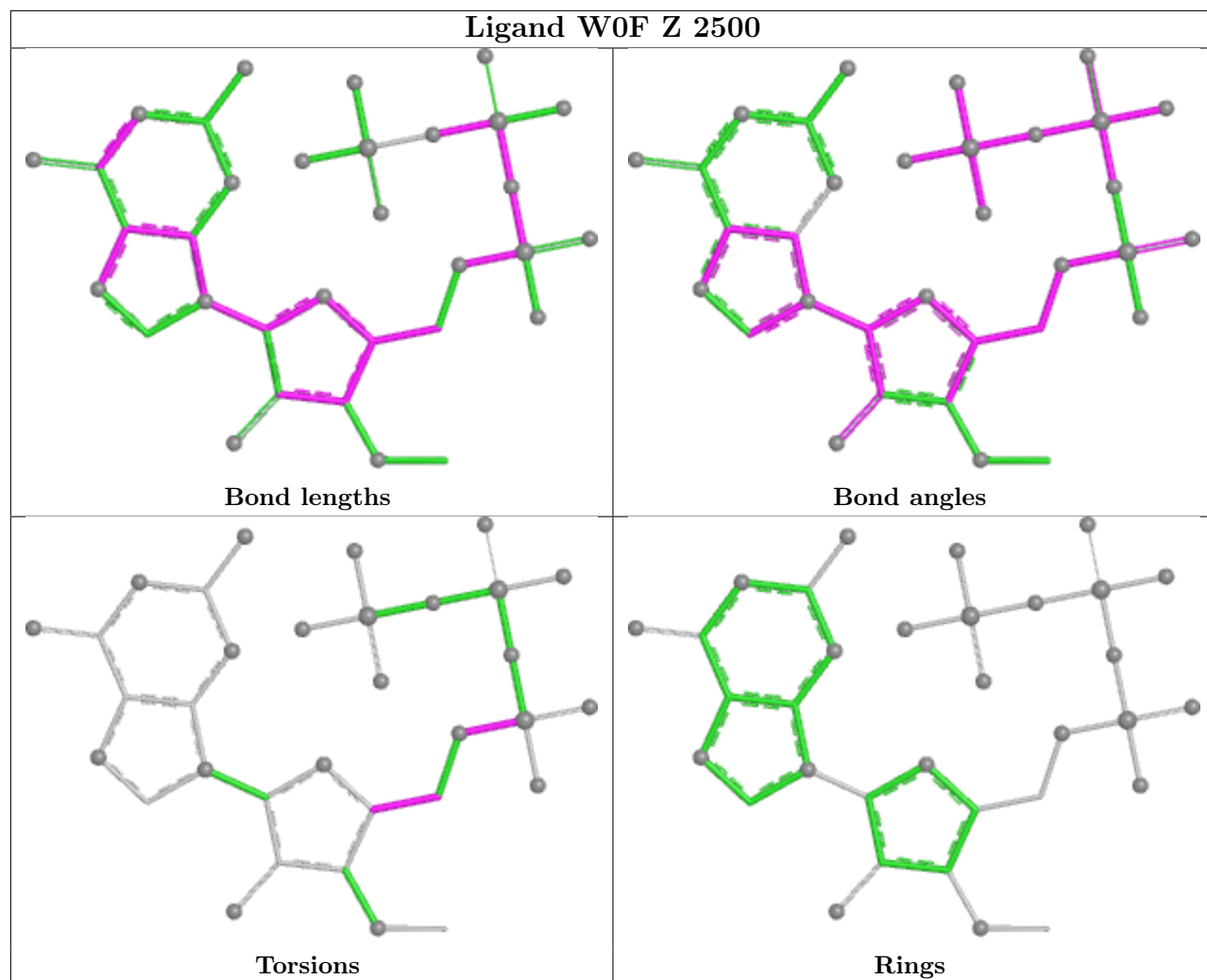
Mol	Chain	Res	Type	Atoms
48	Z	2500	W0F	C20-O21-P22-O24
48	Z	2500	W0F	C20-O21-P22-O25
48	Z	2500	W0F	C03-C04-C20-O21

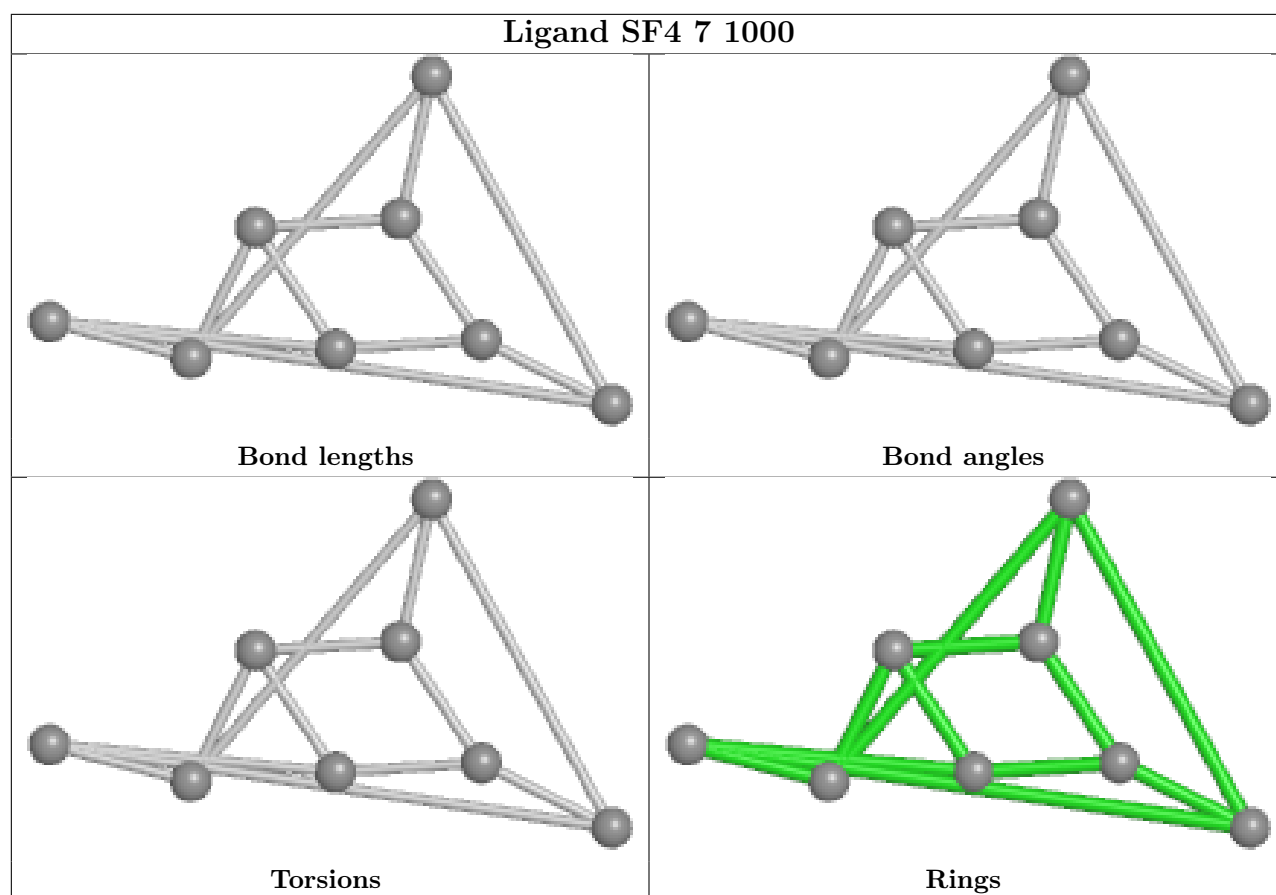
There are no ring outliers.

1 monomer is involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
48	Z	2500	W0F	9	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

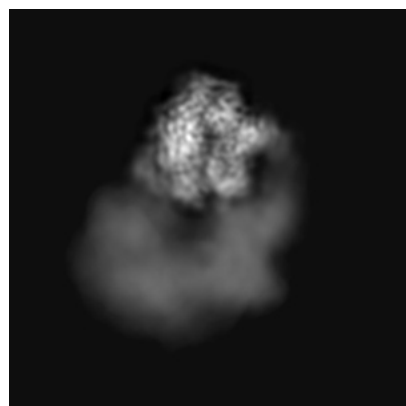
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37395. These allow visual inspection of the internal detail of the map and identification of artifacts.

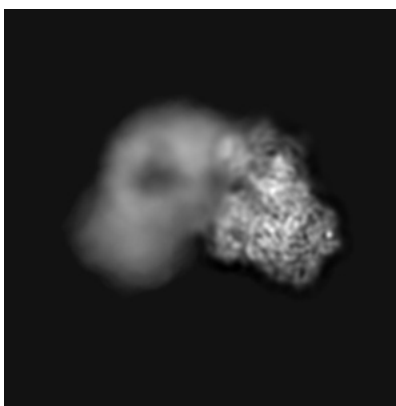
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

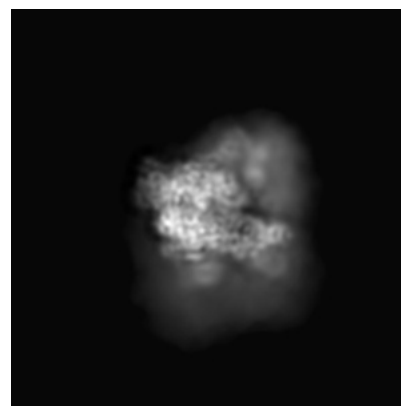
6.1.1 Primary map



X

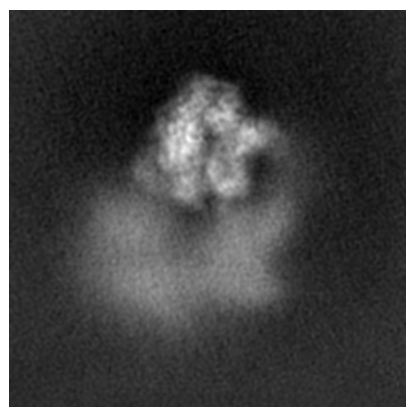


Y

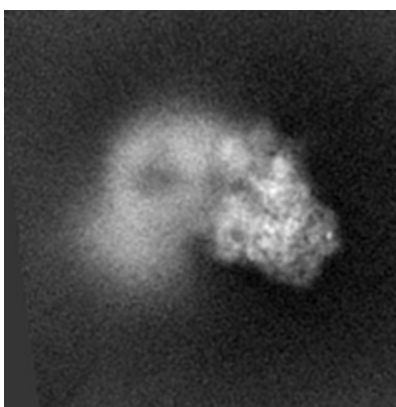


Z

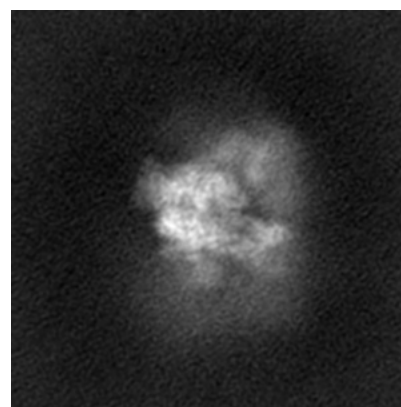
6.1.2 Raw map



X



Y

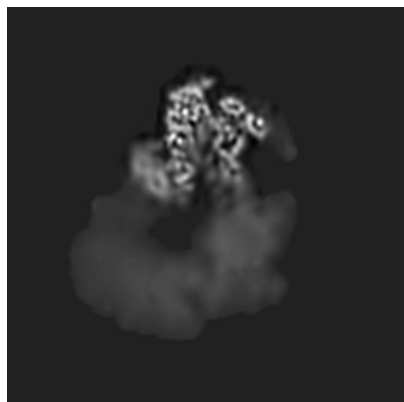


Z

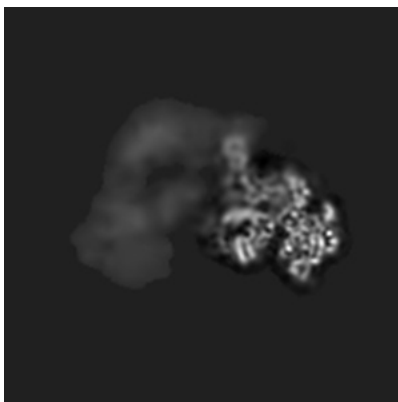
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

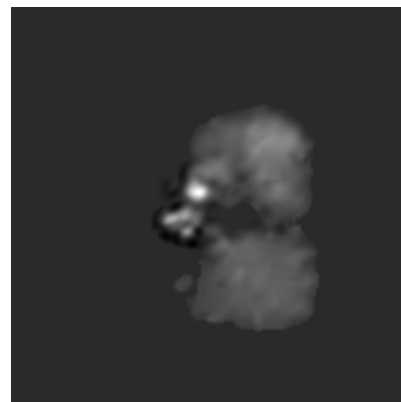
6.2.1 Primary map



X Index: 80

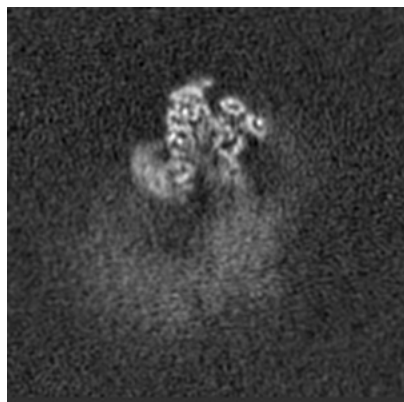


Y Index: 80

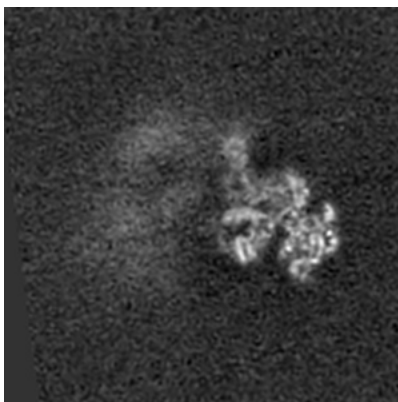


Z Index: 80

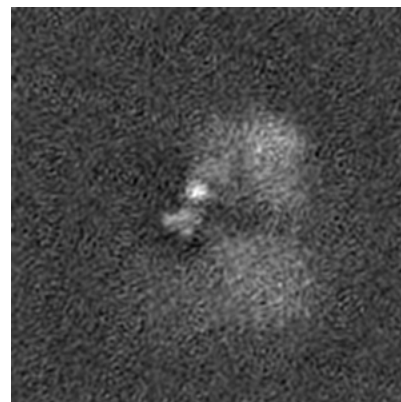
6.2.2 Raw map



X Index: 80



Y Index: 80

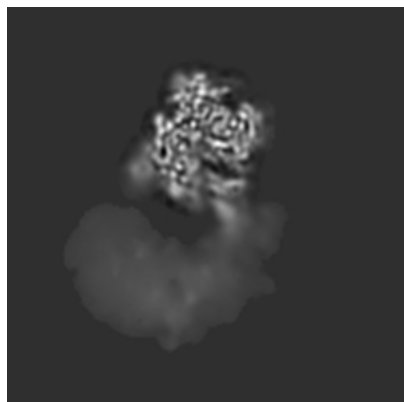


Z Index: 80

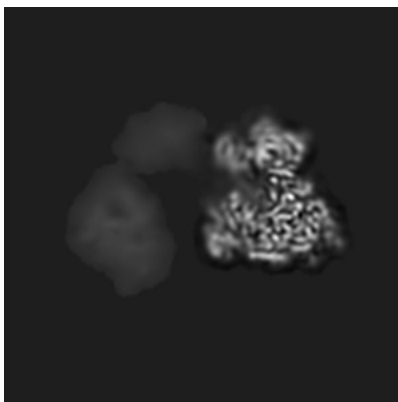
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 73

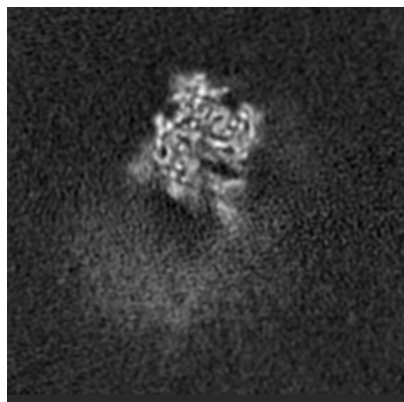


Y Index: 71

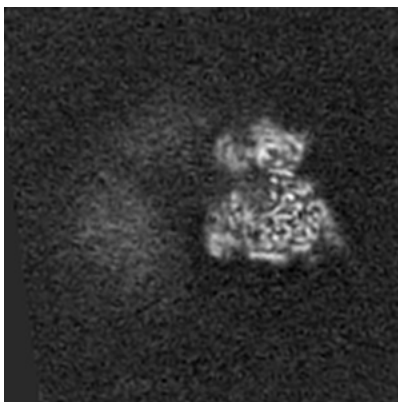


Z Index: 111

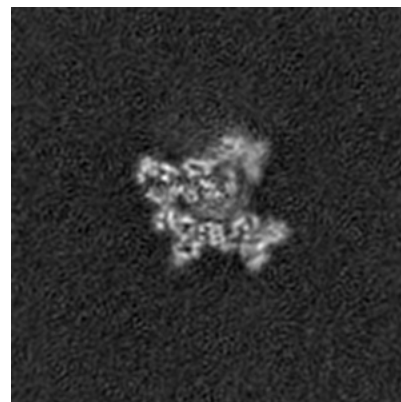
6.3.2 Raw map



X Index: 73



Y Index: 71

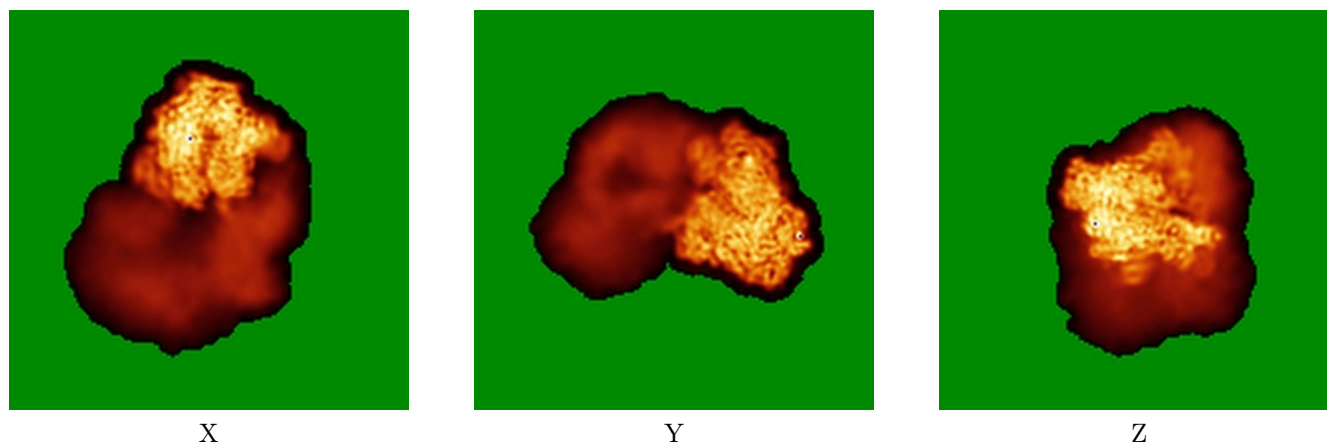


Z Index: 111

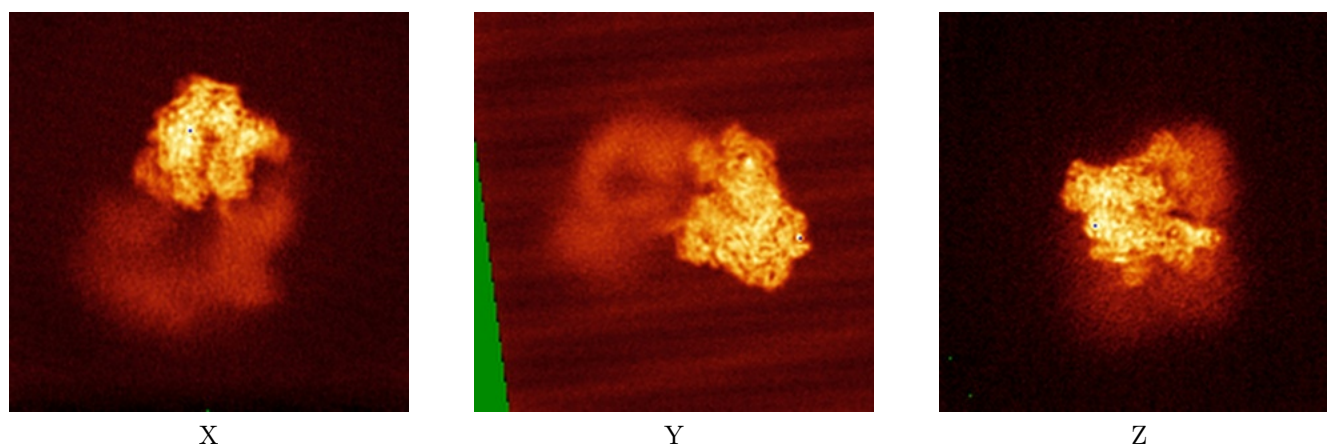
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

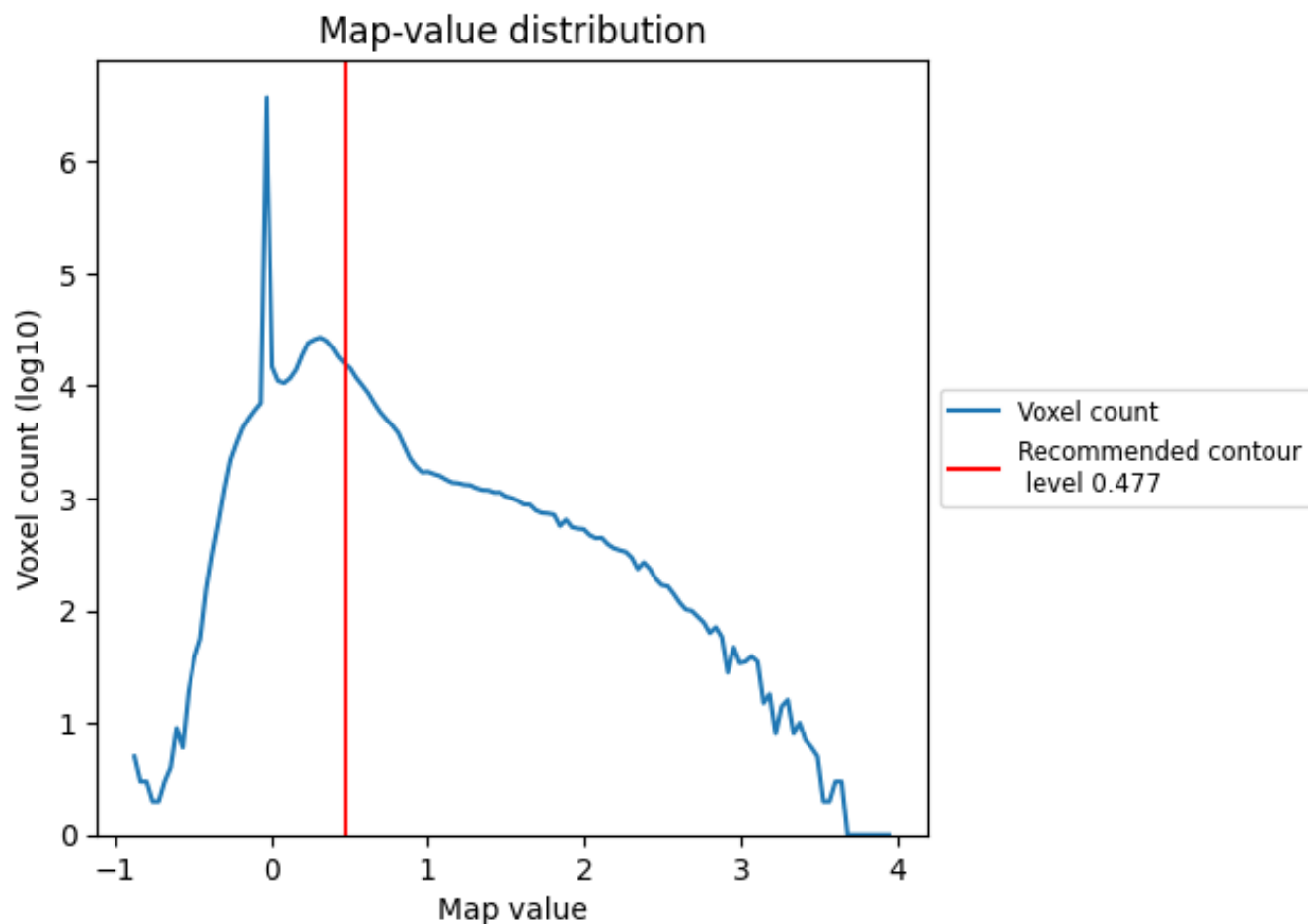
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

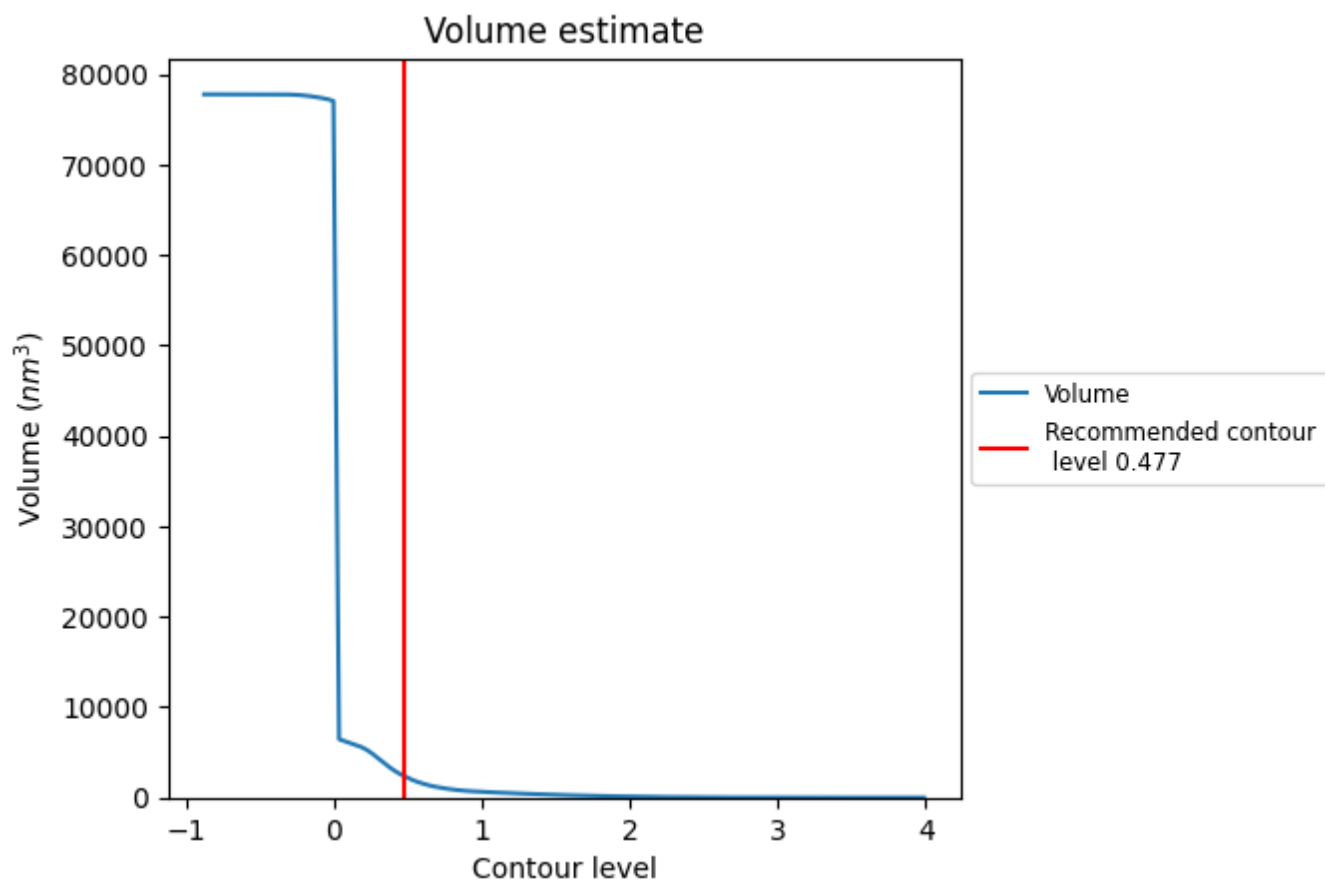
This section contains the results of statistical analysis of the map.

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.

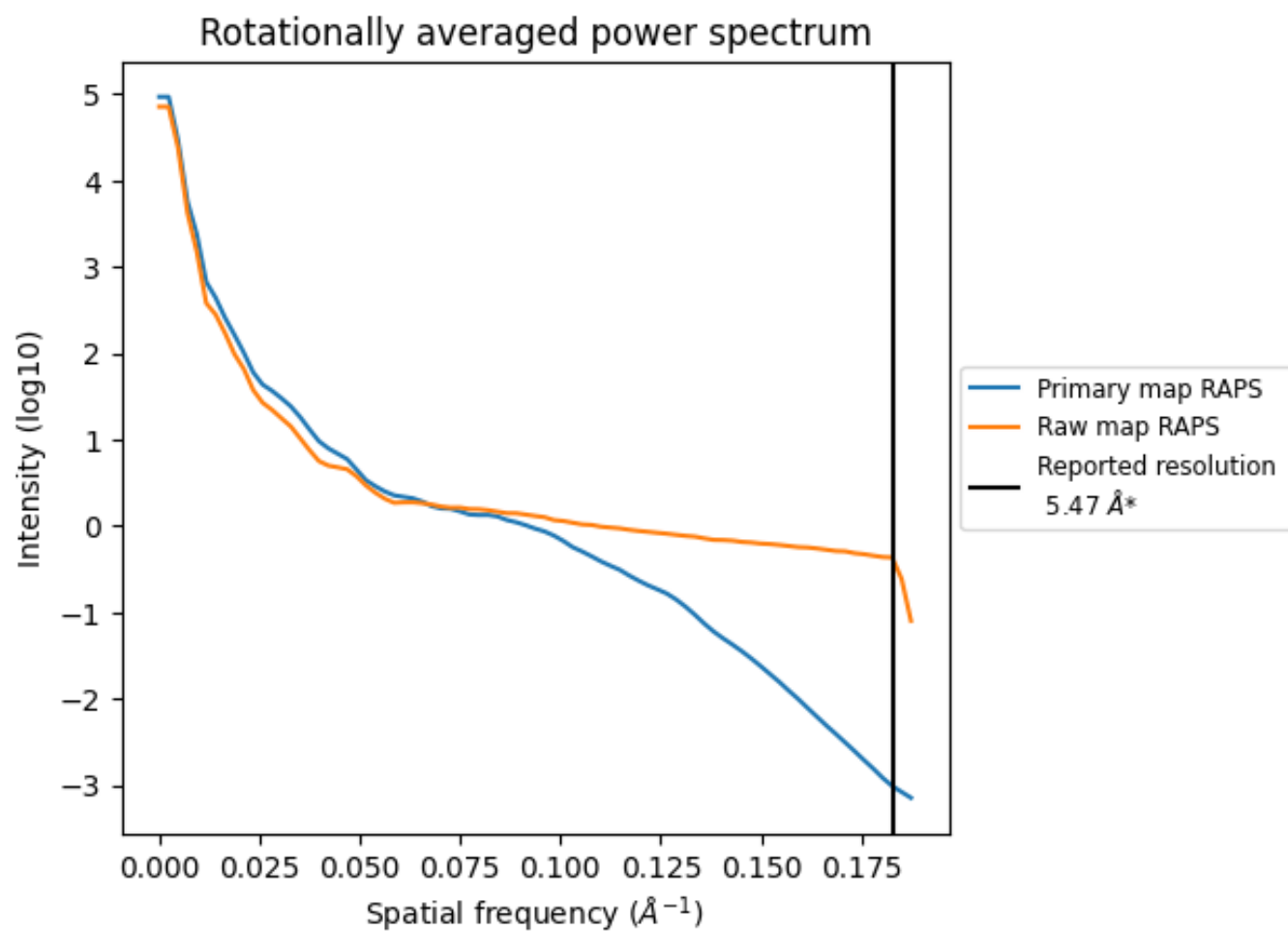
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2372 nm³; this corresponds to an approximate mass of 2142 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 [i](#)

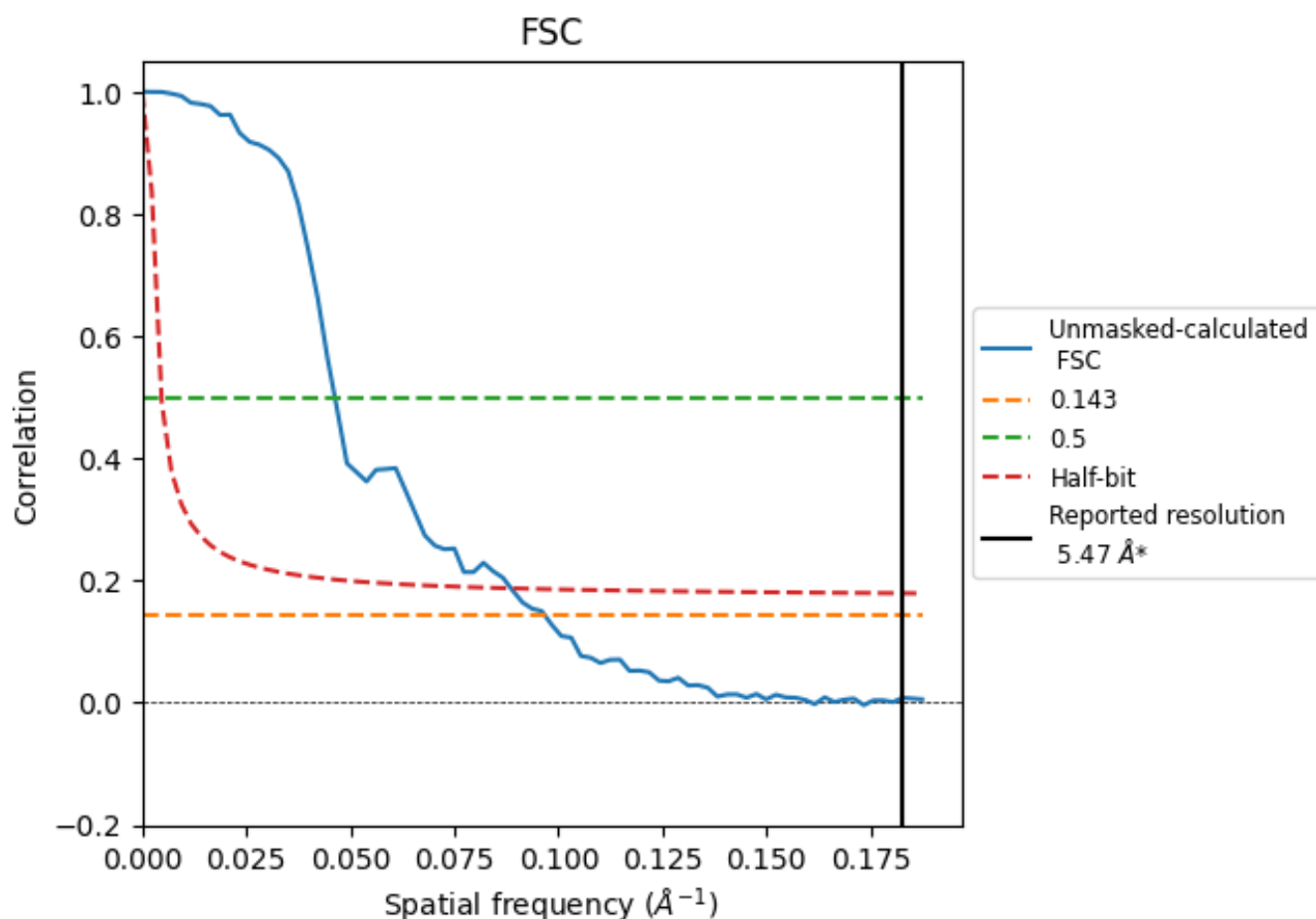


*Reported resolution corresponds to spatial frequency of 0.183 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.183 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

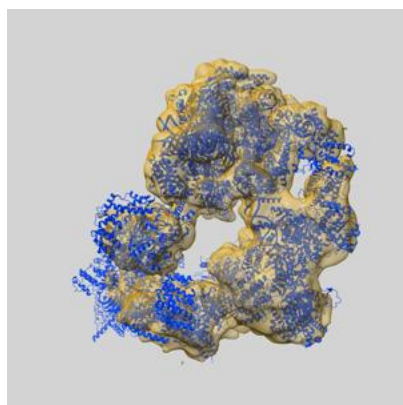
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.47	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	10.33	21.65	11.29

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 10.33 differs from the reported value 5.47 by more than 10 %

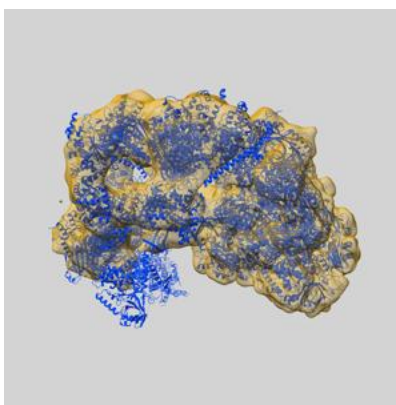
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-37395 and PDB model 8WAK. Per-residue inclusion information can be found in section [3](#) on page [15](#).

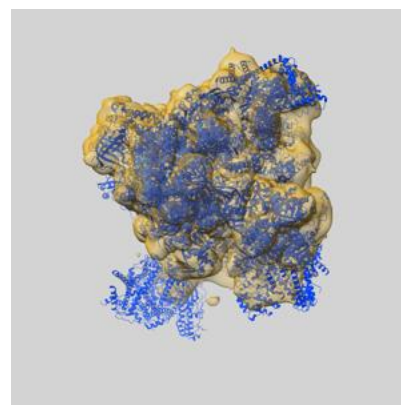
9.1 Map-model overlay [i](#)



X



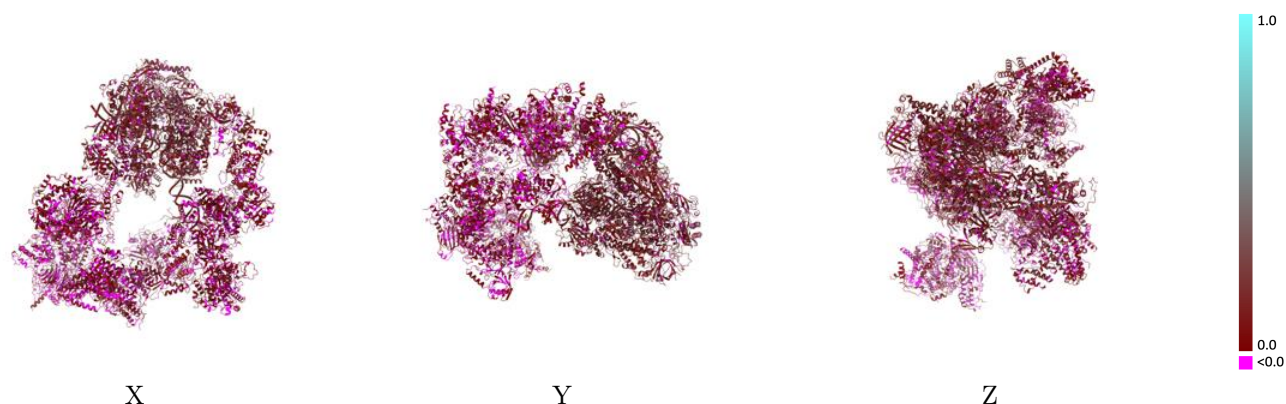
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.477 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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

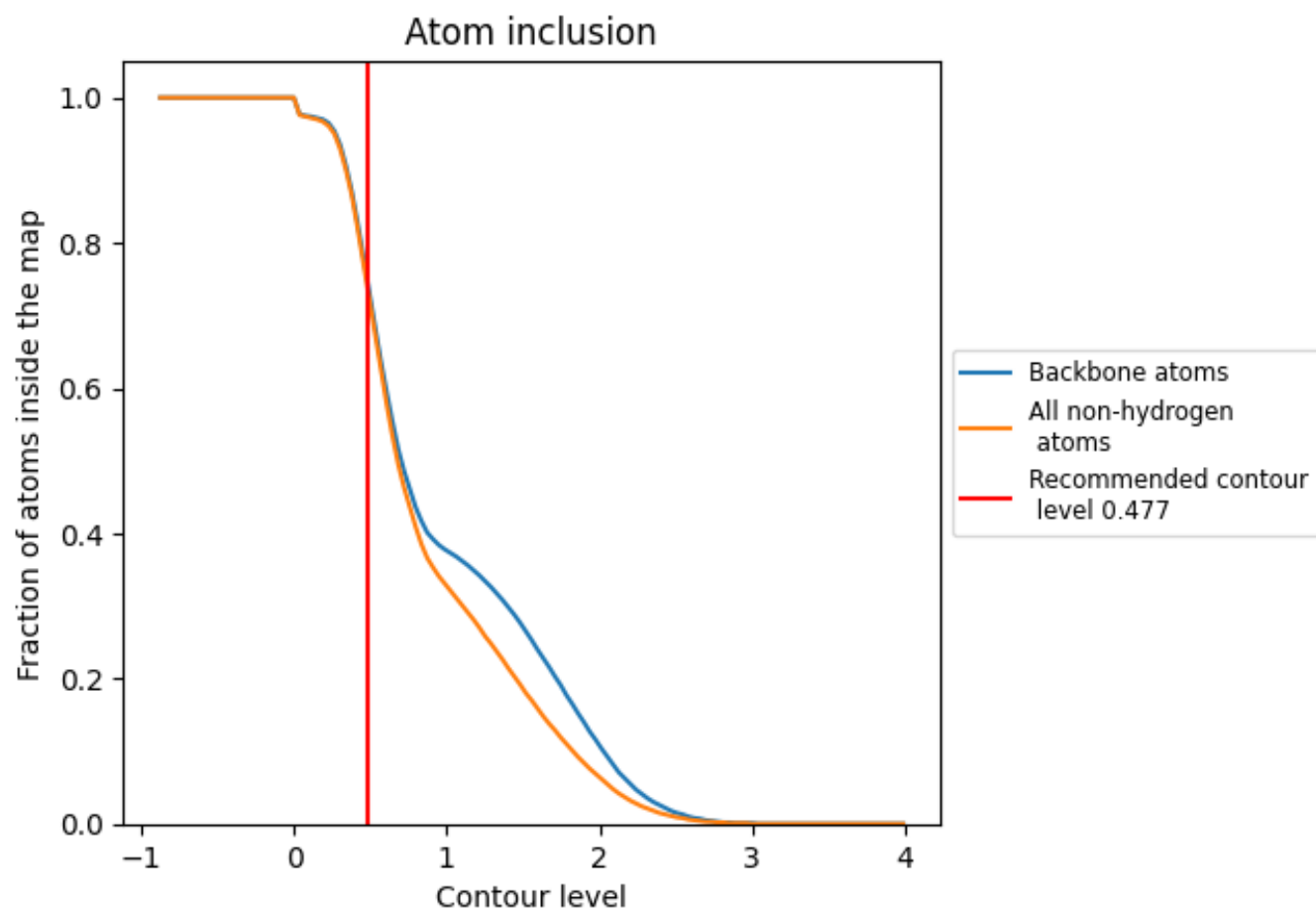


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 74% 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 (0.477) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7430	 0.0790
0	 0.1990	 0.0570
1	 0.8310	 0.0510
2	 0.9070	 0.0560
3	 0.8880	 0.0360
4	 0.7980	 0.0540
5	 0.5430	 0.0320
6	 0.7990	 0.0370
7	 0.8640	 0.0540
A	 0.1940	 0.0270
B	 0.8830	 0.0400
D	 0.3660	 0.0370
E	 0.7930	 0.0460
F	 0.3630	 0.0230
G	 0.0050	 -0.0180
H	 0.6150	 0.0330
I	 0.4590	 0.0240
J	 0.6000	 0.0310
L	 0.0590	 0.0510
N	 1.0000	 0.1710
O	 0.9530	 0.0810
P	 0.9990	 0.1320
Q	 0.9530	 0.0880
R	 0.9810	 0.1380
S	 0.9750	 0.1110
T	 0.9840	 0.1290
U	 0.9760	 0.1120
V	 0.9870	 0.1180
X	 0.9780	 0.1750
Y	 0.9250	 0.1430
Z	 0.7500	 0.0690
c	 0.1170	 0.0100
d	 0.0000	 0.0100
e	 0.1930	 0.0110
f	 0.6810	 0.0390



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
i	 0.1480	 0.0210
j	 0.0510	 0.0500
k	 0.0000	 0.0060
l	 0.0050	 0.0380
m	 0.0000	 -0.0220
o	 0.9740	 0.1470
p	 0.9640	 0.1360
q	 0.9810	 0.1440
r	 0.9900	 0.1420
s	 0.9820	 0.1560
t	 0.9880	 0.1560
u	 0.9940	 0.1270
v	 0.9870	 0.1500
w	 0.9800	 0.1240
x	 0.9540	 0.1250
y	 0.9830	 0.1450
z	 0.9920	 0.1700