



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 07:38 AM UTC

PDB ID : 9E8I / pdb_00009e8i
EMDB ID : EMD-47721
Title : Human proteasome in resting state conformation bound to TXNL1 in Forward conformation
Authors : Arkinson, C.; Gee, C.L.; Martin, A.
Deposited on : 2024-11-05
Resolution : 2.87 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

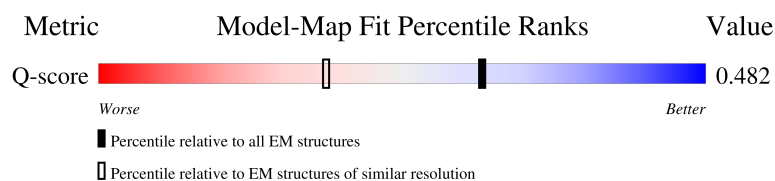
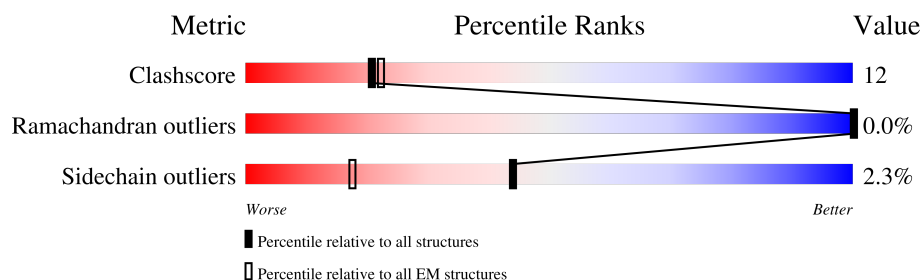
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.87 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.



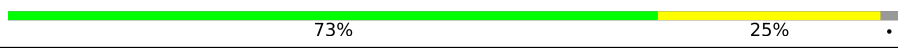
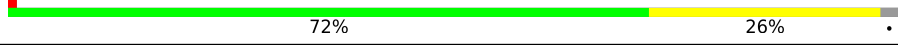
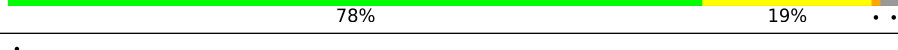
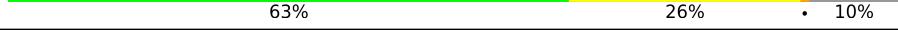
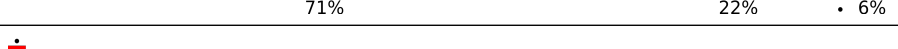
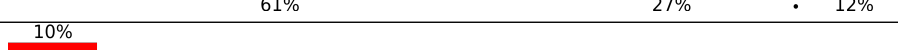
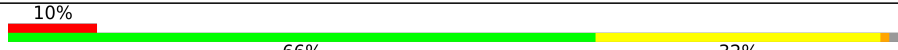
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12062 (2.37 - 3.37)

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

Mol	Chain	Length	Quality of chain
1	A	433	
2	B	440	
3	C	406	
4	D	418	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	E	389	
6	F	439	
7	G	246	
8	H	234	
9	I	261	
10	J	248	
11	K	241	
12	L	263	
13	M	255	
14	U	953	
15	V	534	
16	W	456	
17	X	422	
18	Y	389	
19	Z	324	
20	a	376	
21	b	377	
22	c	424	
23	d	350	
24	e	70	
25	f	908	
26	g	601	
27	u	289	

2 Entry composition

There are 31 unique types of molecules in this entry. The entry contains 71304 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 26S proteasome regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	395	Total	C	N	O	S	0	0
			3107	1956	547	586	18		

- Molecule 2 is a protein called 26S proteasome regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	405	Total	C	N	O	S	0	0
			3192	2012	546	619	15		

- Molecule 3 is a protein called 26S protease regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	366	Total	C	N	O	S	0	0
			2895	1824	518	536	17		

- Molecule 4 is a protein called 26S proteasome regulatory subunit 6B.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	380	Total	C	N	O	S	0	0
			3039	1923	524	579	13		

- Molecule 5 is a protein called 26S protease regulatory subunit 10B.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	354	Total	C	N	O	S	0	0
			2797	1761	495	525	16		

- Molecule 6 is a protein called 26S proteasome regulatory subunit 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	351	Total	C	N	O	S	0	0
			2743	1733	472	522	16		

- Molecule 7 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	242	Total	C	N	O	S	0	0
			1886	1197	315	361	13		

- Molecule 8 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	230	Total	C	N	O	S	0	0
			1793	1147	302	338	6		

- Molecule 9 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	236	Total	C	N	O	S	1	0
			1841	1161	316	354	10		

- Molecule 10 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	239	Total	C	N	O	S	0	0
			1887	1183	334	365	5		

- Molecule 11 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	234	Total	C	N	O	S	0	0
			1790	1125	295	359	11		

- Molecule 12 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	237	Total	C	N	O	S	0	0
			1864	1167	335	351	11		

- Molecule 13 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	240	Total	C	N	O	S	0	0
			1881	1193	321	356	11		

- Molecule 14 is a protein called 26S proteasome non-ATPase regulatory subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	U	838	Total	C	N	O	S	0	0
			6515	4135	1106	1230	44		

- Molecule 15 is a protein called 26S proteasome non-ATPase regulatory subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	V	470	Total	C	N	O	S	0	0
			3841	2438	685	704	14		

- Molecule 16 is a protein called 26S proteasome non-ATPase regulatory subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	W	438	Total	C	N	O	S	0	0
			3570	2261	609	677	23		

- Molecule 17 is a protein called 26S proteasome non-ATPase regulatory subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	X	419	Total	C	N	O	S	0	0
			3317	2105	564	636	12		

- Molecule 18 is a protein called 26S proteasome non-ATPase regulatory subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Y	386	Total	C	N	O	S	0	0
			3179	2025	542	595	17		

- Molecule 19 is a protein called 26S proteasome non-ATPase regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Z	286	Total	C	N	O	S	0	0
			2285	1461	392	427	5		

- Molecule 20 is a protein called 26S proteasome non-ATPase regulatory subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	a	373	Total	C	N	O	S	0	0
			2995	1911	510	559	15		

- Molecule 21 is a protein called 26S proteasome non-ATPase regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	b	189	Total	C	N	O	S	0	0
			1446	903	259	277	7		

- Molecule 22 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	c	290	Total	C	N	O	S	0	0
			2282	1447	392	424	19		

There are 114 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
c	311	LEU	-	expression tag	UNP O00487
c	312	ILE	-	expression tag	UNP O00487
c	313	ASN	-	expression tag	UNP O00487
c	314	HIS	-	expression tag	UNP O00487
c	315	HIS	-	expression tag	UNP O00487
c	316	HIS	-	expression tag	UNP O00487
c	317	HIS	-	expression tag	UNP O00487
c	318	HIS	-	expression tag	UNP O00487
c	319	HIS	-	expression tag	UNP O00487
c	320	ASP	-	expression tag	UNP O00487
c	321	TYR	-	expression tag	UNP O00487
c	322	ASP	-	expression tag	UNP O00487
c	323	ILE	-	expression tag	UNP O00487
c	324	PRO	-	expression tag	UNP O00487
c	325	THR	-	expression tag	UNP O00487
c	326	THR	-	expression tag	UNP O00487
c	327	ALA	-	expression tag	UNP O00487
c	328	SER	-	expression tag	UNP O00487
c	329	GLU	-	expression tag	UNP O00487
c	330	ASN	-	expression tag	UNP O00487
c	331	LEU	-	expression tag	UNP O00487
c	332	TYR	-	expression tag	UNP O00487
c	333	PHE	-	expression tag	UNP O00487
c	334	GLN	-	expression tag	UNP O00487
c	335	GLY	-	expression tag	UNP O00487
c	336	GLU	-	expression tag	UNP O00487
c	337	LEU	-	expression tag	UNP O00487
c	338	GLY	-	expression tag	UNP O00487
c	339	MET	-	expression tag	UNP O00487
c	340	ARG	-	expression tag	UNP O00487
c	341	GLY	-	expression tag	UNP O00487

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
c	342	SER	-	expression tag	UNP O00487
c	343	ALA	-	expression tag	UNP O00487
c	344	GLY	-	expression tag	UNP O00487
c	345	LYS	-	expression tag	UNP O00487
c	346	ALA	-	expression tag	UNP O00487
c	347	GLY	-	expression tag	UNP O00487
c	348	GLU	-	expression tag	UNP O00487
c	349	GLY	-	expression tag	UNP O00487
c	350	GLU	-	expression tag	UNP O00487
c	351	ILE	-	expression tag	UNP O00487
c	352	PRO	-	expression tag	UNP O00487
c	353	ALA	-	expression tag	UNP O00487
c	354	PRO	-	expression tag	UNP O00487
c	355	LEU	-	expression tag	UNP O00487
c	356	ALA	-	expression tag	UNP O00487
c	357	GLY	-	expression tag	UNP O00487
c	358	THR	-	expression tag	UNP O00487
c	359	VAL	-	expression tag	UNP O00487
c	360	SER	-	expression tag	UNP O00487
c	361	LYS	-	expression tag	UNP O00487
c	362	ILE	-	expression tag	UNP O00487
c	363	LEU	-	expression tag	UNP O00487
c	364	VAL	-	expression tag	UNP O00487
c	365	LYS	-	expression tag	UNP O00487
c	366	GLU	-	expression tag	UNP O00487
c	367	GLY	-	expression tag	UNP O00487
c	368	ASP	-	expression tag	UNP O00487
c	369	THR	-	expression tag	UNP O00487
c	370	VAL	-	expression tag	UNP O00487
c	371	LYS	-	expression tag	UNP O00487
c	372	ALA	-	expression tag	UNP O00487
c	373	GLY	-	expression tag	UNP O00487
c	374	GLN	-	expression tag	UNP O00487
c	375	THR	-	expression tag	UNP O00487
c	376	VAL	-	expression tag	UNP O00487
c	377	LEU	-	expression tag	UNP O00487
c	378	VAL	-	expression tag	UNP O00487
c	379	LEU	-	expression tag	UNP O00487
c	380	GLU	-	expression tag	UNP O00487
c	381	ALA	-	expression tag	UNP O00487
c	382	MET	-	expression tag	UNP O00487
c	383	LYS	-	expression tag	UNP O00487

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
c	384	MET	-	expression tag	UNP O00487
c	385	GLU	-	expression tag	UNP O00487
c	386	THR	-	expression tag	UNP O00487
c	387	GLU	-	expression tag	UNP O00487
c	388	ILE	-	expression tag	UNP O00487
c	389	ASN	-	expression tag	UNP O00487
c	390	ALA	-	expression tag	UNP O00487
c	391	PRO	-	expression tag	UNP O00487
c	392	THR	-	expression tag	UNP O00487
c	393	ASP	-	expression tag	UNP O00487
c	394	GLY	-	expression tag	UNP O00487
c	395	LYS	-	expression tag	UNP O00487
c	396	VAL	-	expression tag	UNP O00487
c	397	GLU	-	expression tag	UNP O00487
c	398	LYS	-	expression tag	UNP O00487
c	399	VAL	-	expression tag	UNP O00487
c	400	LEU	-	expression tag	UNP O00487
c	401	VAL	-	expression tag	UNP O00487
c	402	LYS	-	expression tag	UNP O00487
c	403	GLU	-	expression tag	UNP O00487
c	404	ARG	-	expression tag	UNP O00487
c	405	ASP	-	expression tag	UNP O00487
c	406	ALA	-	expression tag	UNP O00487
c	407	VAL	-	expression tag	UNP O00487
c	408	GLN	-	expression tag	UNP O00487
c	409	GLY	-	expression tag	UNP O00487
c	410	GLY	-	expression tag	UNP O00487
c	411	GLN	-	expression tag	UNP O00487
c	412	GLY	-	expression tag	UNP O00487
c	413	LEU	-	expression tag	UNP O00487
c	414	ILE	-	expression tag	UNP O00487
c	415	LYS	-	expression tag	UNP O00487
c	416	ILE	-	expression tag	UNP O00487
c	417	GLY	-	expression tag	UNP O00487
c	418	VAL	-	expression tag	UNP O00487
c	419	HIS	-	expression tag	UNP O00487
c	420	HIS	-	expression tag	UNP O00487
c	421	HIS	-	expression tag	UNP O00487
c	422	HIS	-	expression tag	UNP O00487
c	423	HIS	-	expression tag	UNP O00487
c	424	HIS	-	expression tag	UNP O00487

- Molecule 23 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	d	265	Total	C	N	O	S	0	0
			2166	1402	355	400	9		

- Molecule 24 is a protein called 26S proteasome complex subunit SEM1.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	e	50	Total	C	N	O	0	0
			425	260	65	100		

- Molecule 25 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	f	831	Total	C	N	O	S	0	0
			6433	4071	1089	1228	45		

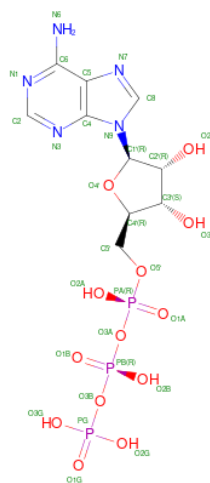
- Molecule 26 is a protein called Isoform 2 of NEDD8 ultimate buster 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	g	91	Total	C	N	O	S	0	0
			736	466	134	135	1		

- Molecule 27 is a protein called Thioredoxin-like protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	u	151	Total	C	N	O	S	0	0
			1210	767	192	243	8		

- Molecule 28 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).

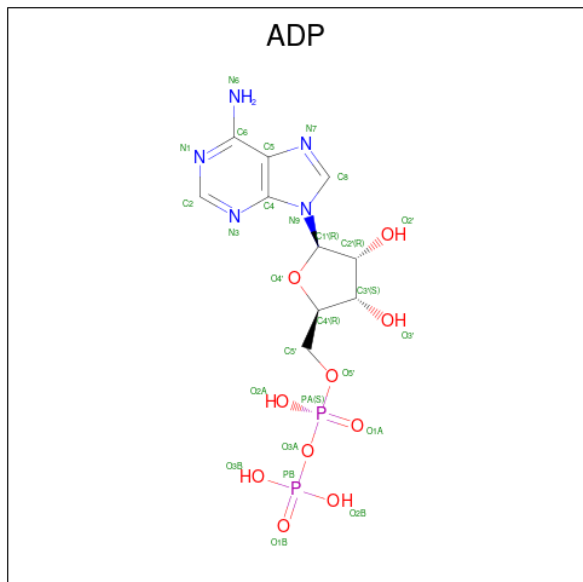


Mol	Chain	Residues	Atoms					AltConf
28	A	1	Total 31	C 10	N 5	O 13	P 3	0
28	B	1	Total 31	C 10	N 5	O 13	P 3	0
28	D	1	Total 31	C 10	N 5	O 13	P 3	0
28	E	1	Total 31	C 10	N 5	O 13	P 3	0
28	F	1	Total 31	C 10	N 5	O 13	P 3	0

- Molecule 29 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
29	A	1	Total Mg 1 1	0
29	B	1	Total Mg 1 1	0
29	C	1	Total Mg 1 1	0
29	D	1	Total Mg 1 1	0
29	E	1	Total Mg 1 1	0
29	F	1	Total Mg 1 1	0

- Molecule 30 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
30	C	1	Total	C	N	O	P	0
			27	10	5	10	2	

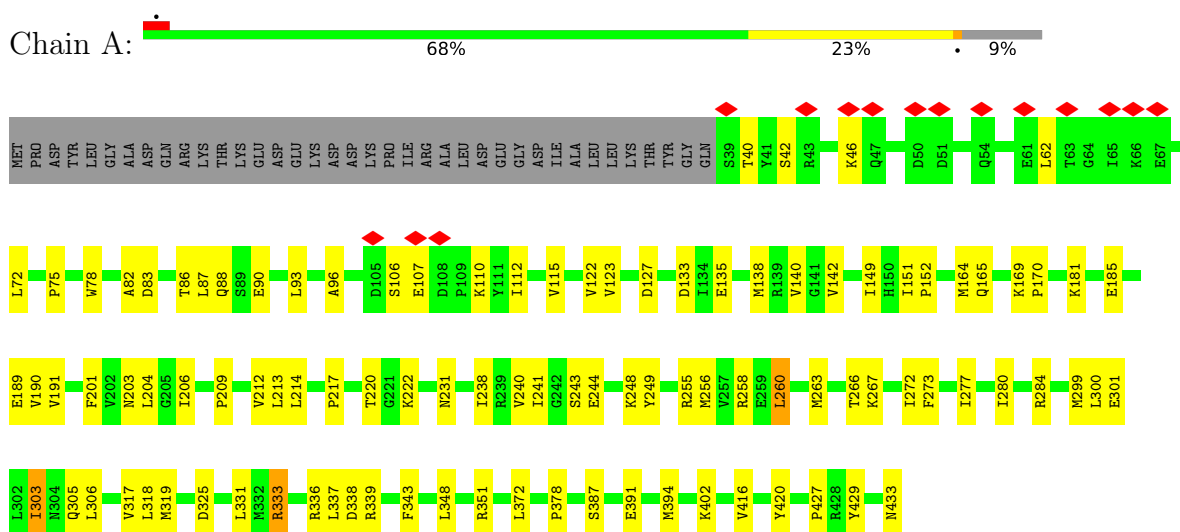
- Molecule 31 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
31	c	1	Total	Zn	0
			1	1	

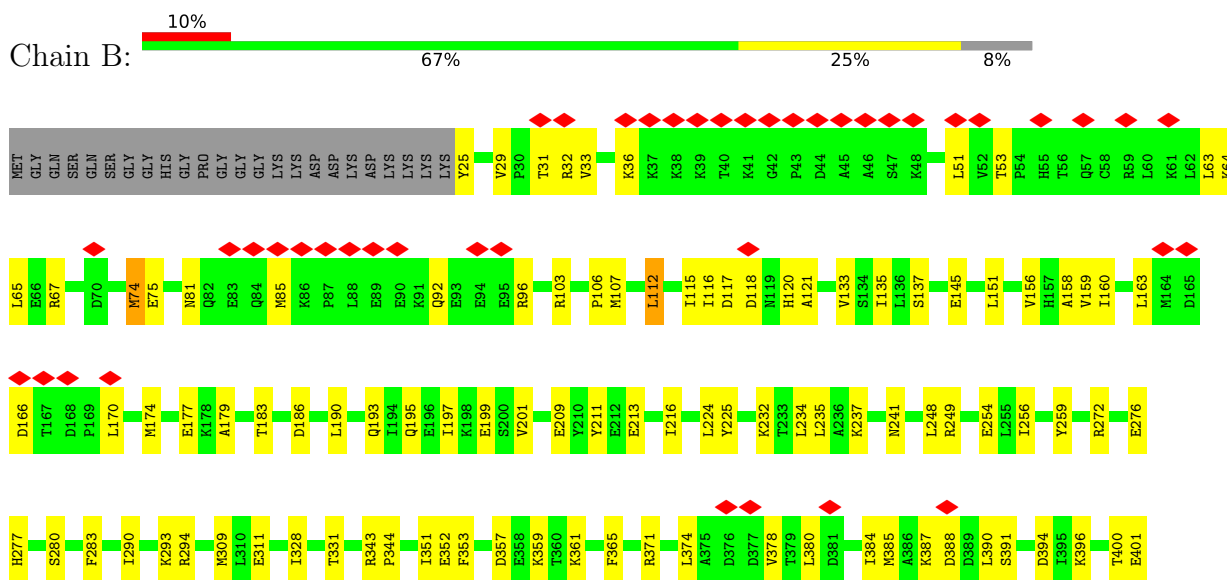
3 Residue-property plots

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: 26S proteasome regulatory subunit 7

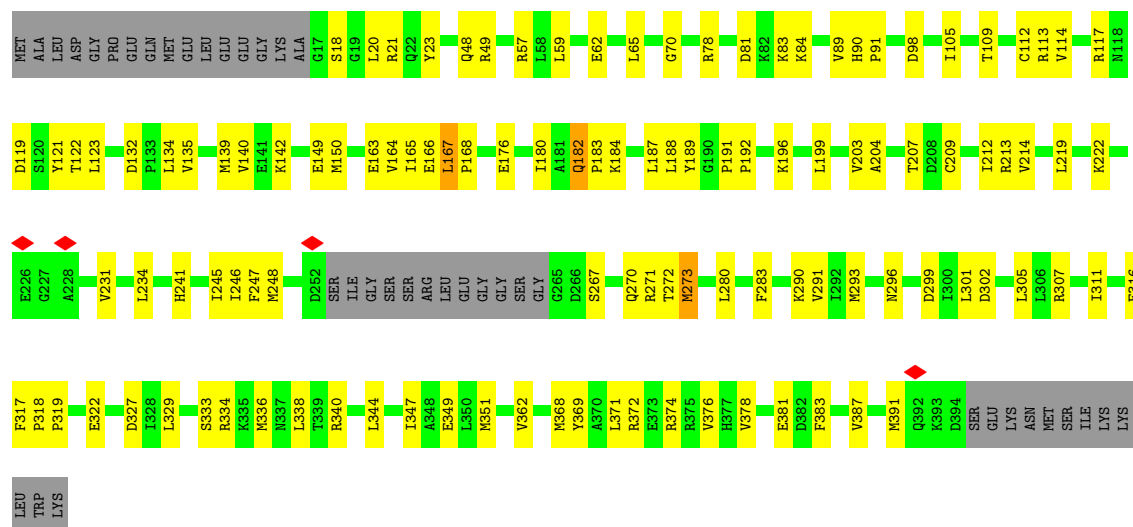


• Molecule 2: 26S proteasome regulatory subunit 4

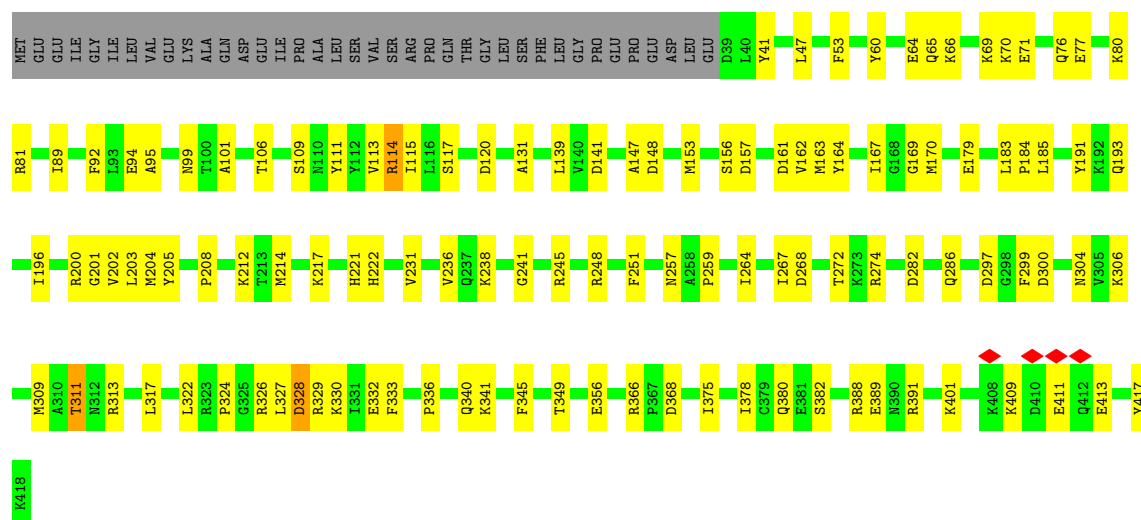




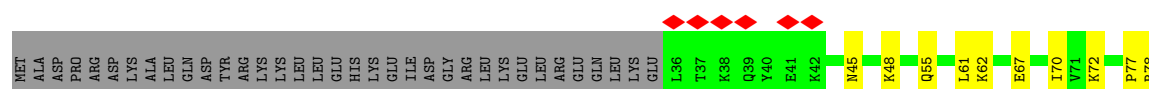
• Molecule 3: 26S protease regulatory subunit 8

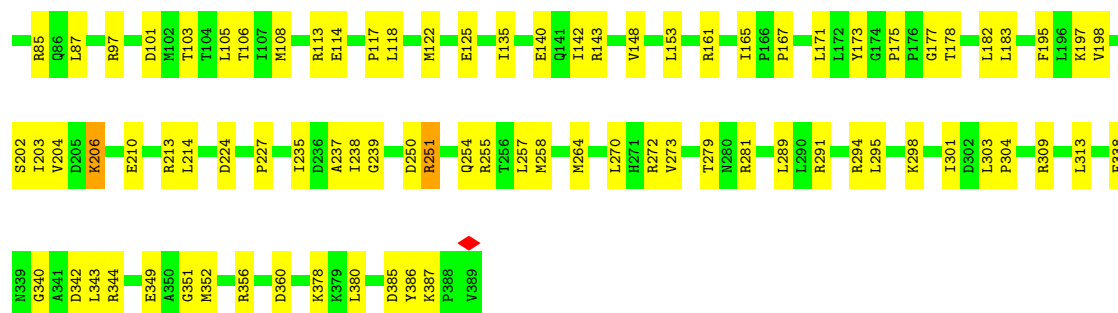


• Molecule 4: 26S proteasome regulatory subunit 6B

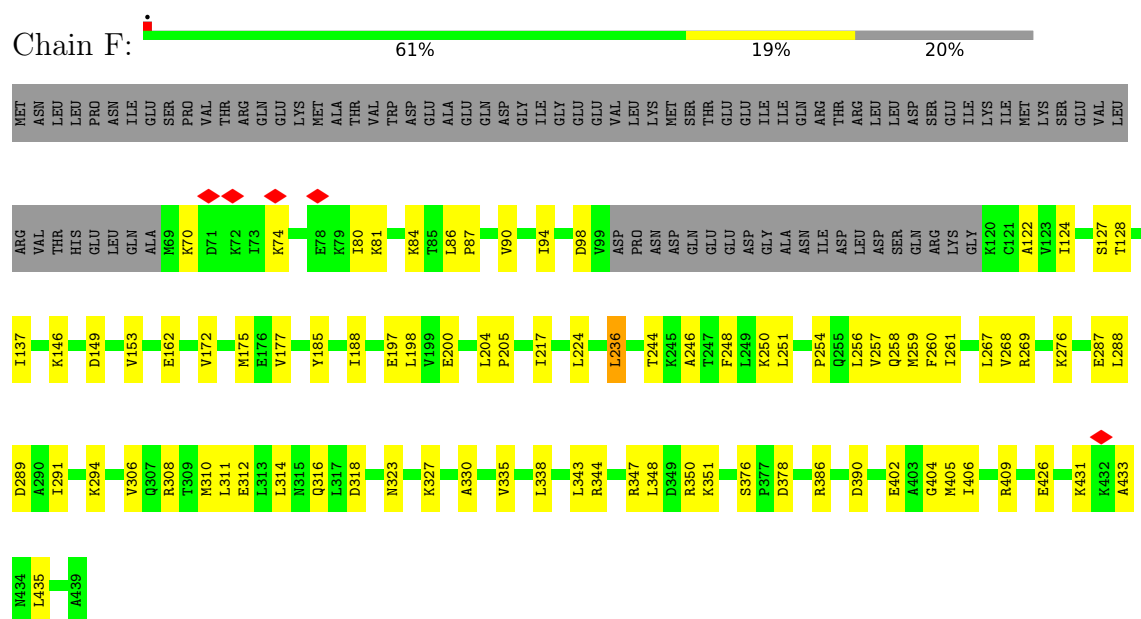


• Molecule 5: 26S protease regulatory subunit 10B

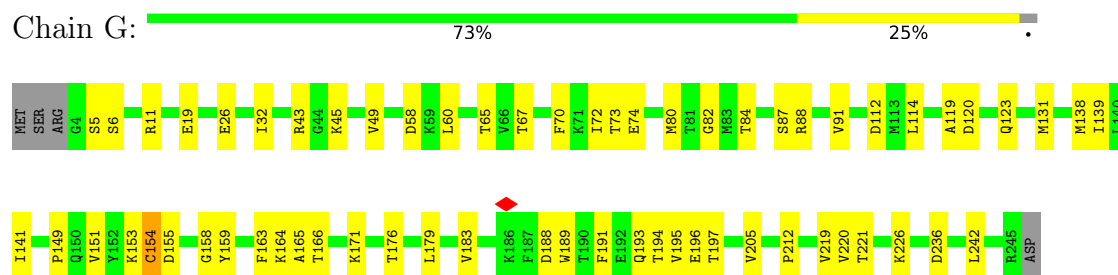




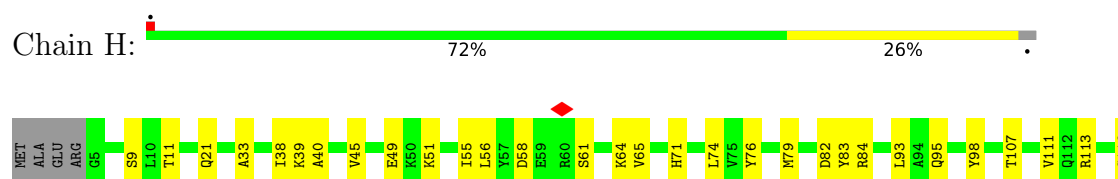
- Molecule 6: 26S proteasome regulatory subunit 6A



- Molecule 7: Proteasome subunit alpha type-6

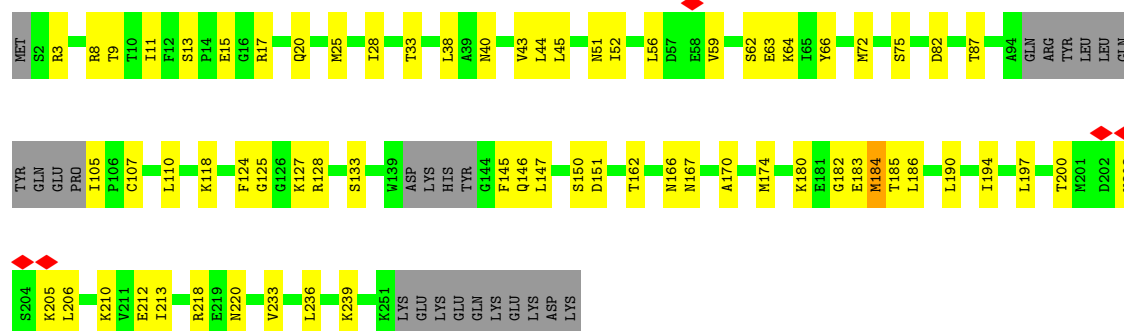


- Molecule 8: Proteasome subunit alpha type-2

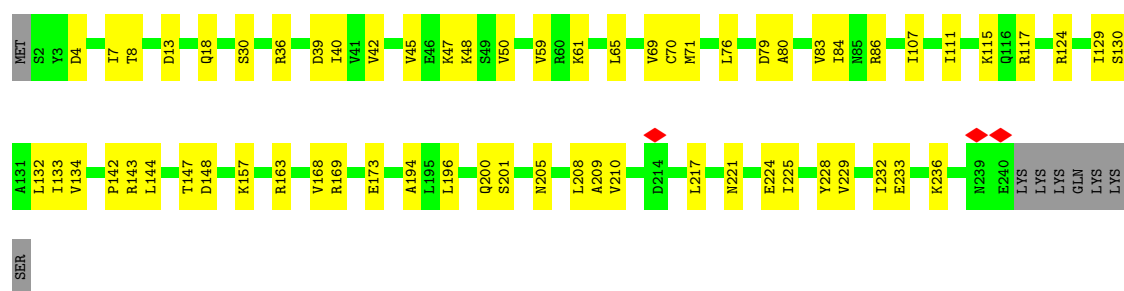




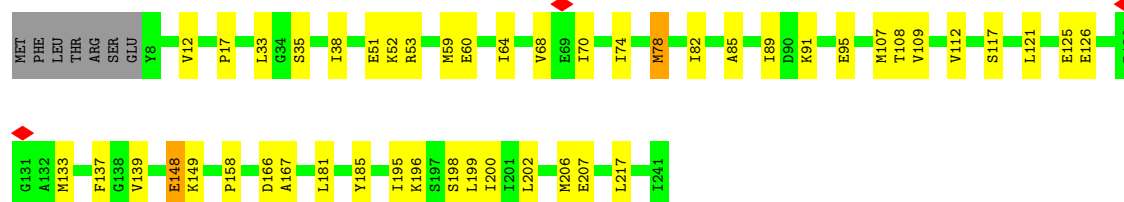
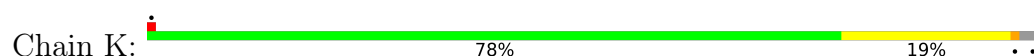
• Molecule 9: Proteasome subunit alpha type-4



• Molecule 10: Proteasome subunit alpha type-7

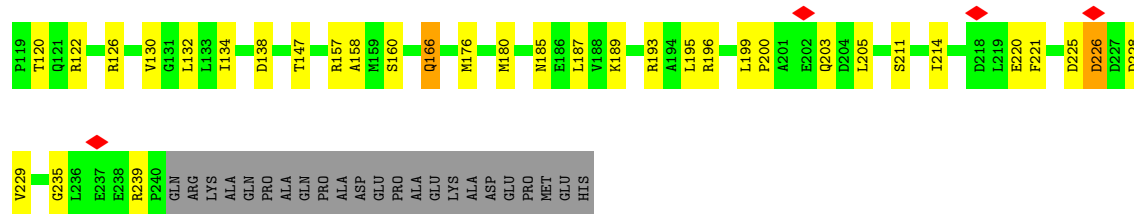


• Molecule 11: Proteasome subunit alpha type-5



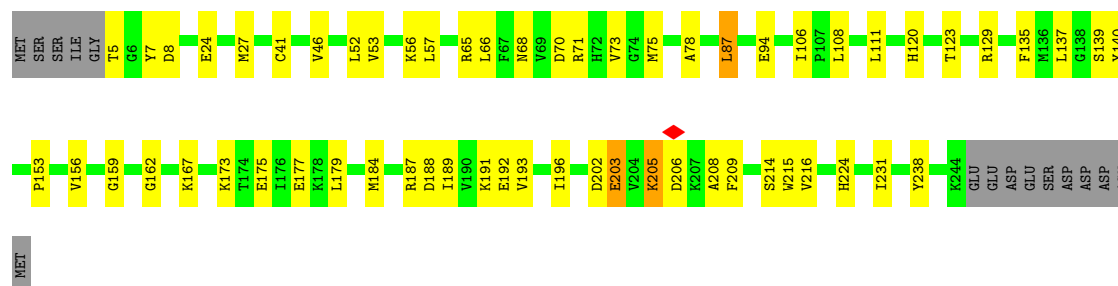
• Molecule 12: Proteasome subunit alpha type-1





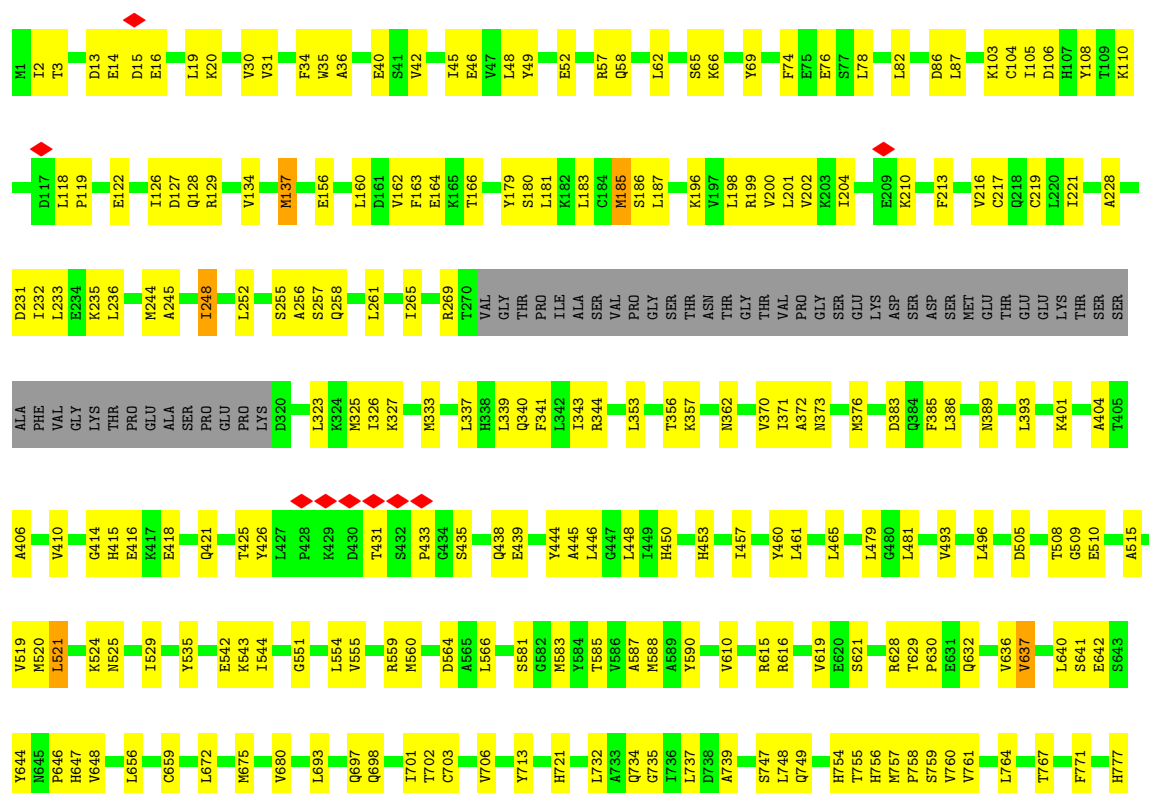
• Molecule 13: Proteasome subunit alpha type-3

Chain M: 71% 22% 6%



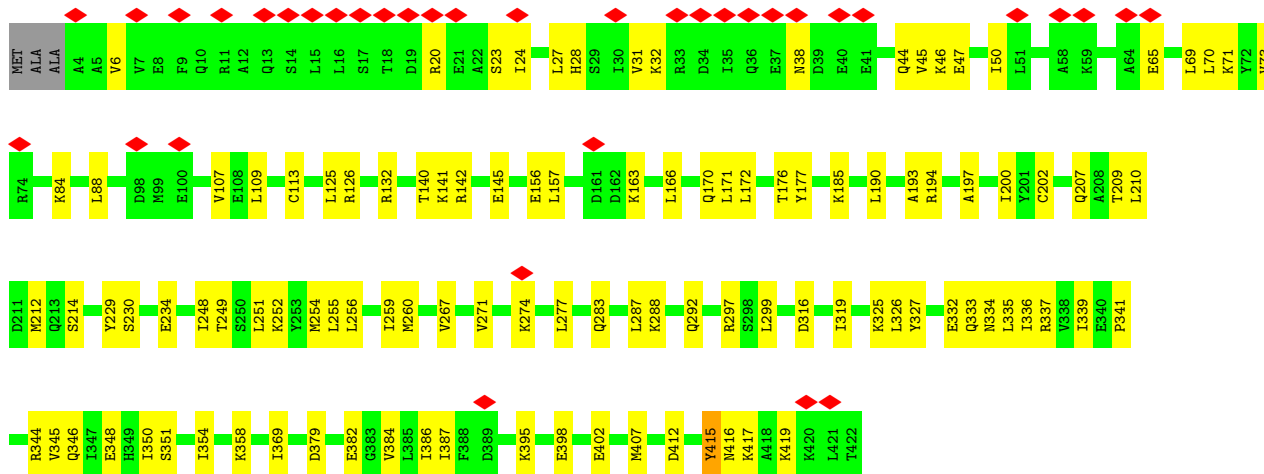
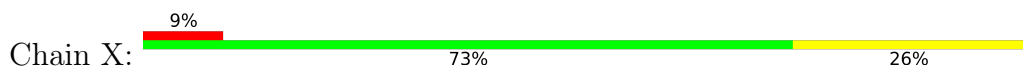
• Molecule 14: 26S proteasome non-ATPase regulatory subunit 1

Chain U: 61% 27% 12%

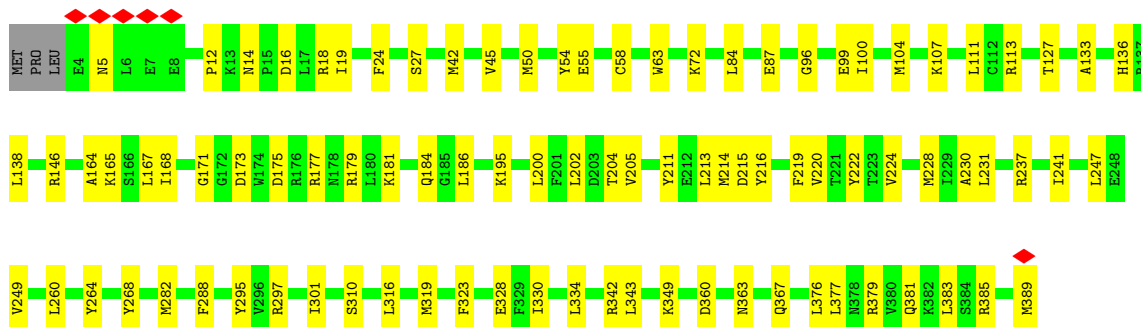
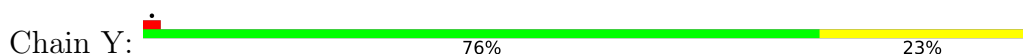




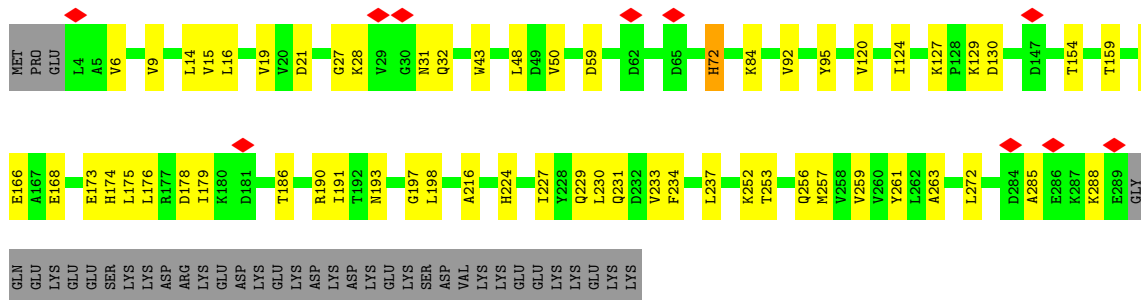
- Molecule 17: 26S proteasome non-ATPase regulatory subunit 11



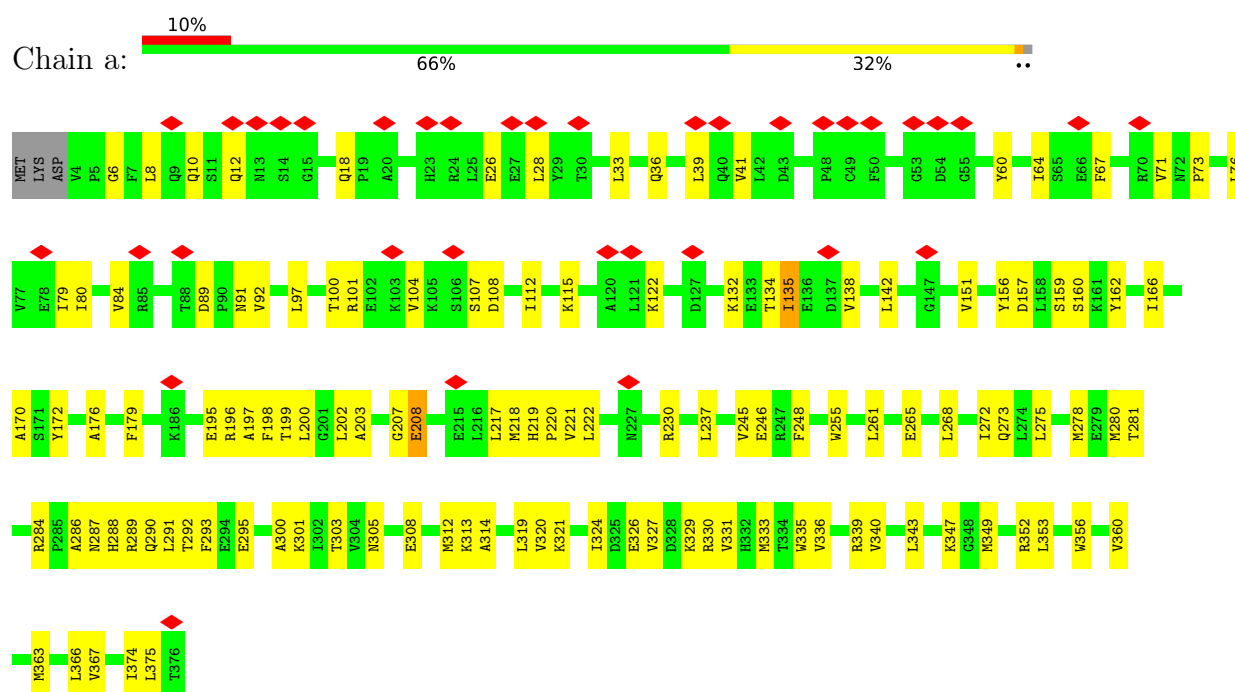
- Molecule 18: 26S proteasome non-ATPase regulatory subunit 6



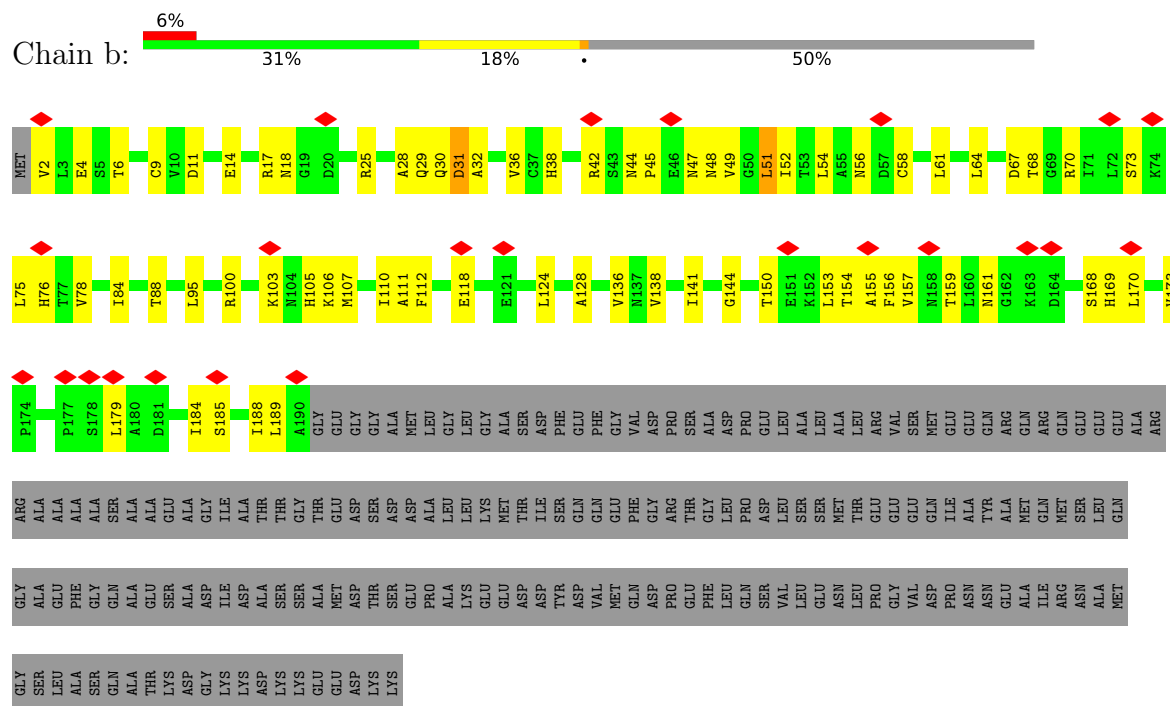
- Molecule 19: 26S proteasome non-ATPase regulatory subunit 7



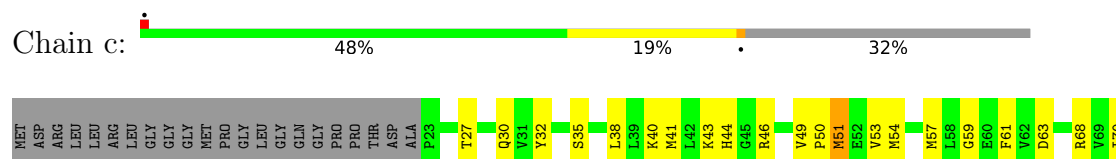
- Molecule 20: 26S proteasome non-ATPase regulatory subunit 13



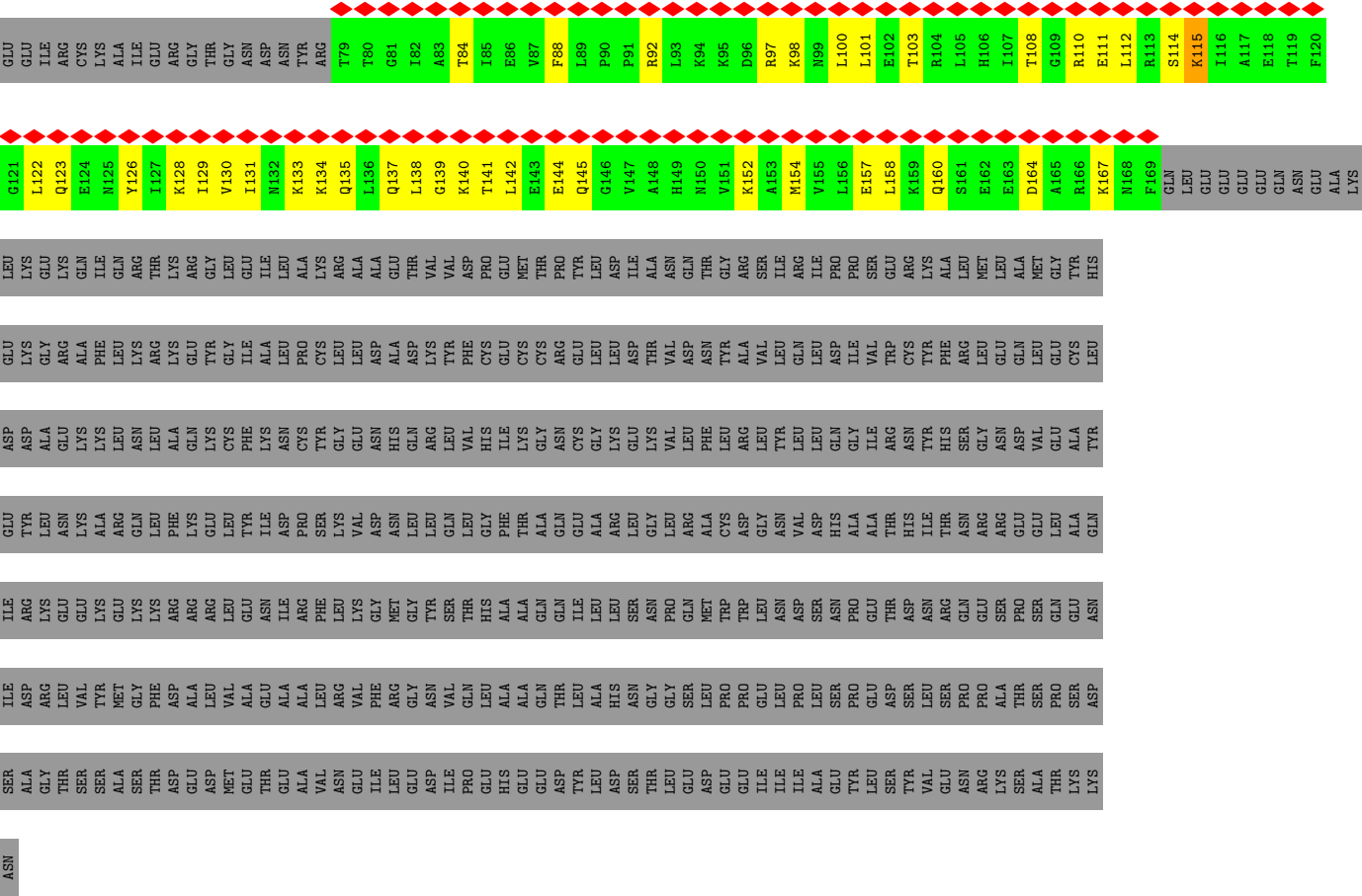
- Molecule 21: 26S proteasome non-ATPase regulatory subunit 4



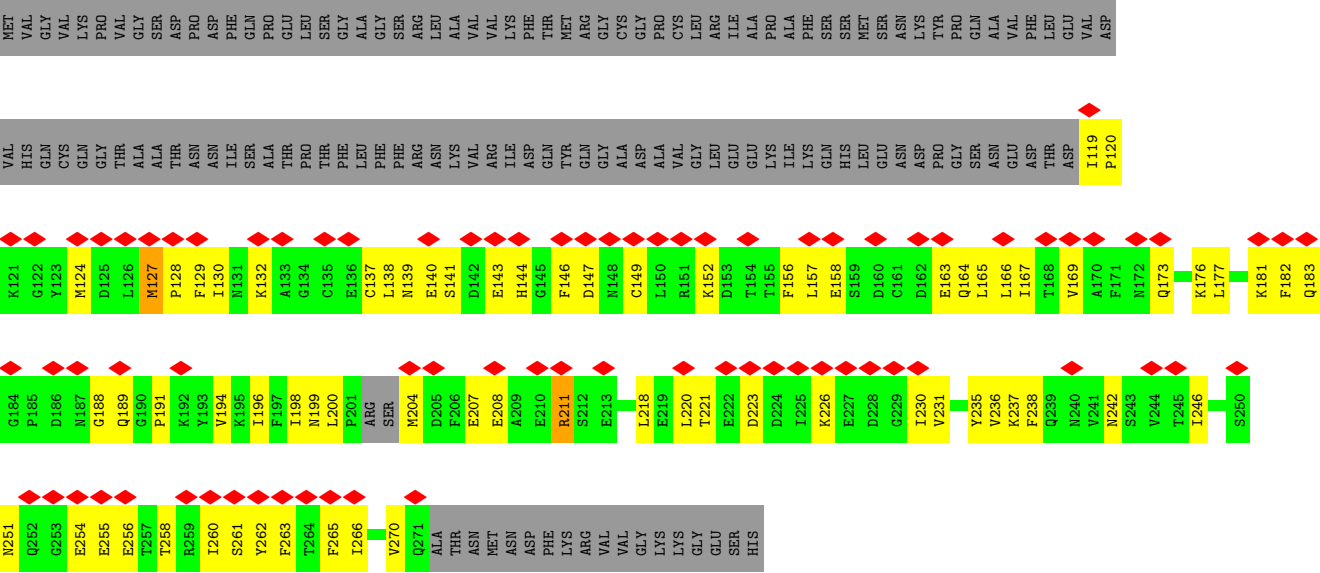
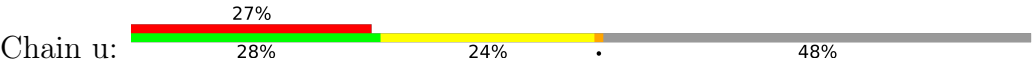
- Molecule 22: 26S proteasome non-ATPase regulatory subunit 14







● Molecule 27: Thioredoxin-like protein 1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	62431	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1700	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.025	Depositor
Minimum map value	-0.387	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.038	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	356.32, 356.32, 356.32	wwPDB
Map dimensions	340, 340, 340	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.048, 1.048, 1.048	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.14	0/3159	0.29	0/4265
2	B	0.13	0/3241	0.30	0/4372
3	C	0.14	0/2933	0.29	0/3946
4	D	0.15	0/3089	0.28	0/4168
5	E	0.14	0/2842	0.27	0/3832
6	F	0.14	0/2781	0.30	0/3748
7	G	0.13	0/1920	0.27	0/2595
8	H	0.14	0/1832	0.28	0/2481
9	I	0.13	0/1867	0.29	0/2509
10	J	0.14	0/1913	0.29	0/2581
11	K	0.14	0/1818	0.28	0/2455
12	L	0.13	0/1899	0.31	0/2567
13	M	0.13	0/1916	0.30	0/2580
14	U	0.15	0/6630	0.33	0/8977
15	V	0.12	0/3913	0.30	0/5277
16	W	0.12	0/3618	0.30	0/4868
17	X	0.13	0/3363	0.29	0/4534
18	Y	0.12	0/3237	0.26	0/4360
19	Z	0.14	0/2328	0.30	0/3156
20	a	0.13	0/3053	0.32	0/4133
21	b	0.14	0/1466	0.35	0/1986
22	c	0.14	0/2325	0.27	0/3143
23	d	0.14	0/2212	0.36	0/2988
24	e	0.13	0/437	0.31	0/595
25	f	0.13	0/6542	0.37	0/8856
26	g	0.14	0/743	0.41	0/994
27	u	0.15	0/1234	0.44	0/1668
All	All	0.14	0/72311	0.31	0/97634

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3107	0	3159	83	0
2	B	3192	0	3277	74	0
3	C	2895	0	3007	90	0
4	D	3039	0	3075	89	0
5	E	2797	0	2856	73	0
6	F	2743	0	2820	65	0
7	G	1886	0	1891	40	0
8	H	1793	0	1787	40	0
9	I	1841	0	1872	45	0
10	J	1887	0	1905	41	0
11	K	1790	0	1773	32	0
12	L	1864	0	1852	47	0
13	M	1881	0	1868	40	0
14	U	6515	0	6547	175	0
15	V	3841	0	3889	102	0
16	W	3570	0	3685	83	0
17	X	3317	0	3413	78	0
18	Y	3179	0	3174	61	0
19	Z	2285	0	2320	56	0
20	a	2995	0	3012	100	0
21	b	1446	0	1490	45	0
22	c	2282	0	2306	75	0
23	d	2166	0	2196	60	0
24	e	425	0	328	11	0
25	f	6433	0	6458	238	0
26	g	736	0	784	39	0
27	u	1210	0	1161	49	0
28	A	31	0	12	0	0
28	B	31	0	12	3	0
28	D	31	0	12	4	0
28	E	31	0	12	2	0
28	F	31	0	12	1	0
29	A	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	B	1	0	0	0	0
29	C	1	0	0	0	0
29	D	1	0	0	0	0
29	E	1	0	0	0	0
29	F	1	0	0	0	0
30	C	27	0	12	1	0
31	c	1	0	0	0	0
All	All	71304	0	71977	1725	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 12.

All (1725) 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)
25:f:827:PRO:HB2	25:f:829:MET:HE3	1.49	0.92
17:X:50:ILE:HD11	17:X:73:VAL:HG11	1.58	0.83
2:B:117:ASP:OD2	2:B:118:ASP:N	2.11	0.82
27:u:143:GLU:HG3	27:u:144:HIS:HD2	1.43	0.82
17:X:252:LYS:HD2	17:X:283:GLN:HE21	1.44	0.82
16:W:440:ASN:ND2	22:c:226:MET:SD	2.52	0.82
20:a:292:THR:HG22	20:a:330:ARG:HH12	1.45	0.80
19:Z:21:ASP:OD1	22:c:104:ARG:NH2	2.14	0.79
9:I:167:ASN:HB2	9:I:200:THR:HG23	1.65	0.79
12:L:50:LYS:HD2	12:L:211:SER:HB3	1.65	0.78
3:C:270:GLN:HG3	3:C:293:MET:HE1	1.67	0.77
5:E:67:GLU:OE1	22:c:46:ARG:NH2	2.18	0.76
18:Y:16:ASP:HB3	18:Y:19:ILE:HD12	1.66	0.76
14:U:641:SER:HB2	14:U:675:MET:HE2	1.67	0.76
3:C:134:LEU:HD11	3:C:212:ILE:HG12	1.68	0.75
19:Z:216:ALA:HB1	20:a:347:LYS:HE3	1.68	0.75
25:f:94:LYS:HG2	25:f:95:PRO:HD3	1.68	0.75
14:U:164:GLU:HG3	14:U:204:ILE:HD11	1.67	0.75
14:U:13:ASP:OD1	23:d:166:ARG:NH1	2.20	0.74
3:C:168:PRO:HB3	3:C:182:GLN:HG2	1.67	0.74
22:c:310:LYS:HG2	22:c:312:ILE:HG22	1.69	0.74
20:a:360:VAL:HG22	22:c:308:VAL:HG13	1.68	0.74
25:f:822:VAL:HA	25:f:825:MET:HG3	1.70	0.74
7:G:158:GLY:O	8:H:84:ARG:NH2	2.22	0.73
25:f:320:ILE:HD11	25:f:837:LEU:HD11	1.70	0.73
25:f:198:HIS:O	25:f:199:ASN:ND2	2.21	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:107:MET:HG2	2:B:160:ILE:HD11	1.70	0.73
2:B:272:ARG:NH1	2:B:276:GLU:OE2	2.22	0.73
22:c:38:LEU:HA	22:c:41:MET:HE2	1.71	0.73
27:u:199:ASN:HD21	27:u:242:ASN:HB2	1.54	0.72
25:f:560:LEU:HD22	25:f:801:VAL:HG11	1.70	0.72
12:L:47:VAL:HG12	12:L:195:LEU:HD22	1.71	0.72
16:W:435:LEU:HD11	19:Z:237:LEU:HD23	1.71	0.72
27:u:251:ASN:ND2	27:u:255:GLU:OE2	2.20	0.71
1:A:170:PRO:O	1:A:231:ASN:ND2	2.21	0.71
15:V:304:GLU:OE1	15:V:304:GLU:N	2.22	0.71
16:W:143:ALA:HA	16:W:169:LEU:HD21	1.72	0.71
12:L:45:VAL:HG12	12:L:214:ILE:HG23	1.72	0.71
3:C:57:ARG:HB3	15:V:505:LEU:HD21	1.73	0.71
7:G:141:ILE:HG22	7:G:151:VAL:HG22	1.72	0.71
20:a:321:LYS:HB2	20:a:335:TRP:HB3	1.71	0.71
21:b:9:CYS:HB2	21:b:111:ALA:HA	1.74	0.70
3:C:333:SER:HB2	3:C:338:LEU:HD11	1.72	0.70
3:C:368:MET:HE2	4:D:196:ILE:HG21	1.73	0.70
18:Y:319:MET:HE1	18:Y:334:LEU:HD11	1.73	0.70
27:u:149:CYS:HB2	27:u:157:LEU:HB2	1.73	0.70
5:E:239:GLY:HA2	5:E:257:LEU:HD13	1.71	0.70
7:G:139:ILE:HG12	7:G:153:LYS:HG3	1.73	0.70
21:b:38:HIS:HB3	21:b:42:ARG:HH12	1.56	0.70
15:V:367:VAL:HA	15:V:402:VAL:HG22	1.74	0.70
25:f:459:CYS:HB3	26:g:152:LYS:HD2	1.74	0.70
11:K:70:ILE:HD11	11:K:89:ILE:HD12	1.73	0.70
15:V:421:ASP:OD2	18:Y:349:LYS:NZ	2.25	0.70
21:b:58:CYS:SG	21:b:88:THR:OG1	2.47	0.70
14:U:797:MET:HE1	14:U:881:PRO:HG3	1.74	0.70
21:b:51:LEU:HD11	21:b:75:LEU:HD13	1.74	0.69
25:f:417:ILE:HD12	25:f:418:LEU:HG	1.74	0.69
15:V:219:GLU:HA	15:V:224:LEU:HD21	1.73	0.69
23:d:94:MET:HE1	23:d:122:VAL:HG21	1.74	0.69
4:D:153:MET:SD	4:D:257:ASN:ND2	2.64	0.69
14:U:505:ASP:HB3	14:U:508:THR:HG22	1.74	0.69
25:f:208:LEU:HG	25:f:214:VAL:HA	1.74	0.69
3:C:164:VAL:HG13	3:C:183:PRO:HB2	1.75	0.69
14:U:431:THR:HG22	14:U:433:PRO:HD2	1.75	0.69
27:u:163:GLU:HB2	27:u:258:THR:HG23	1.73	0.69
9:I:218:ARG:HH11	9:I:218:ARG:HG3	1.56	0.69
17:X:107:VAL:HG21	17:X:142:ARG:HH12	1.57	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:u:189:GLN:HA	27:u:251:ASN:HD22	1.57	0.69
3:C:20:LEU:HD11	14:U:137:MET:HG3	1.74	0.68
13:M:66:LEU:HD13	13:M:214:SER:HB3	1.75	0.68
9:I:62:SER:OG	9:I:212:GLU:OE2	2.08	0.68
16:W:271:VAL:HG22	16:W:306:LEU:HD22	1.75	0.68
18:Y:99:GLU:N	18:Y:99:GLU:OE2	2.25	0.68
21:b:14:GLU:OE1	21:b:17:ARG:NH2	2.26	0.68
28:E:501:ATP:O1G	6:F:347:ARG:NH2	2.27	0.68
14:U:74:PHE:HB3	14:U:103:LYS:HG2	1.75	0.68
25:f:295:ALA:HB1	25:f:321:MET:HB3	1.76	0.68
12:L:72:ILE:HG21	12:L:88:MET:HE1	1.76	0.67
16:W:375:MET:HE3	16:W:411:GLY:HA2	1.74	0.67
21:b:4:GLU:HA	21:b:106:LYS:H	1.58	0.67
1:A:402:LYS:NZ	2:B:213:GLU:OE1	2.25	0.67
25:f:459:CYS:SG	26:g:154:MET:HE3	2.34	0.67
20:a:18:GLN:OE1	20:a:18:GLN:N	2.28	0.67
25:f:348:ILE:HG13	25:f:381:VAL:HG21	1.77	0.67
25:f:842:VAL:H	25:f:870:THR:HG23	1.59	0.67
10:J:209:ALA:HB1	10:J:217:LEU:HD11	1.77	0.67
16:W:24:VAL:HG22	16:W:28:LEU:HG	1.77	0.67
25:f:441:LYS:HB3	25:f:477:MET:HE1	1.77	0.67
2:B:371:ARG:HH12	3:C:176:GLU:HG2	1.60	0.67
26:g:128:LYS:HE2	26:g:158:LEU:HD21	1.77	0.67
15:V:440:LYS:HD3	15:V:443:ARG:HH21	1.60	0.66
20:a:135:ILE:HD11	20:a:159:SER:HA	1.77	0.66
25:f:275:MET:HE2	25:f:275:MET:HA	1.77	0.66
5:E:264:MET:HE3	5:E:294:ARG:HB3	1.77	0.66
9:I:118:LYS:NZ	9:I:150:SER:OG	2.28	0.66
25:f:690:VAL:HG13	25:f:691:PRO:HD3	1.78	0.66
18:Y:215:ASP:OD1	18:Y:216:TYR:N	2.27	0.66
19:Z:14:LEU:HD11	22:c:40:LYS:HG2	1.77	0.66
11:K:167:ALA:HB3	12:L:56:LEU:HD13	1.76	0.66
25:f:610:GLN:O	25:f:614:HIS:ND1	2.26	0.66
1:A:90:GLU:OE1	2:B:120:HIS:NE2	2.28	0.65
13:M:24:GLU:HA	13:M:27:MET:HG3	1.76	0.65
27:u:188:GLY:O	27:u:251:ASN:ND2	2.29	0.65
25:f:692:LEU:HD12	25:f:800:LEU:HD12	1.78	0.65
6:F:251:LEU:HD21	6:F:256:LEU:HD11	1.77	0.65
6:F:433:ALA:HB1	6:F:435:LEU:HD13	1.79	0.65
4:D:208:PRO:HB2	5:E:291:ARG:HD3	1.78	0.65
3:C:372:ARG:NE	4:D:179:GLU:OE2	2.24	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:201:SER:OG	10:J:205:ASN:OD1	2.14	0.65
2:B:31:THR:OG1	2:B:118:ASP:OD2	2.15	0.65
16:W:108:CYS:HB3	16:W:128:LEU:HD11	1.78	0.65
16:W:385:SER:HB3	16:W:388:GLU:HG3	1.78	0.65
22:c:49:VAL:HG22	22:c:116:PRO:HB3	1.78	0.64
23:d:145:ARG:NH2	23:d:183:PRO:O	2.31	0.64
25:f:208:LEU:HA	25:f:211:ILE:HG12	1.78	0.64
25:f:242:GLU:HG3	25:f:243:PRO:HA	1.79	0.64
27:u:120:PRO:HD2	27:u:266:ILE:HG21	1.78	0.64
7:G:155:ASP:OD1	7:G:159:TYR:N	2.31	0.64
1:A:333:ARG:HH12	28:F:501:ATP:H5'1	1.63	0.64
8:H:39:LYS:HE3	8:H:143:ARG:HH12	1.62	0.64
25:f:208:LEU:HD11	25:f:217:LEU:HB2	1.78	0.64
13:M:167:LYS:NZ	13:M:206:ASP:OD2	2.25	0.63
18:Y:237:ARG:NH1	18:Y:264:TYR:OH	2.28	0.63
20:a:8:LEU:HD21	20:a:26:GLU:HG2	1.79	0.63
12:L:189:LYS:HE2	12:L:235:GLY:HA3	1.80	0.63
16:W:125:ILE:HD13	16:W:145:LEU:HD23	1.80	0.63
24:e:42:ASN:ND2	24:e:44:ASP:OD2	2.30	0.63
21:b:188:ILE:HG22	21:b:189:LEU:HD12	1.80	0.63
14:U:444:TYR:CD1	14:U:479:LEU:HB3	2.33	0.63
27:u:260:ILE:HG22	27:u:261:SER:H	1.62	0.63
4:D:341:LYS:NZ	4:D:368:ASP:O	2.29	0.63
17:X:346:GLN:HB3	17:X:348:GLU:HG2	1.81	0.63
26:g:108:THR:HG21	26:g:110:ARG:HH21	1.63	0.63
4:D:89:ILE:O	4:D:106:THR:OG1	2.15	0.63
6:F:376:SER:OG	6:F:378:ASP:OD1	2.15	0.63
22:c:27:THR:HB	22:c:182:GLY:HA3	1.81	0.63
25:f:288:VAL:HA	25:f:291:GLN:HG3	1.80	0.63
23:d:280:GLU:OE1	23:d:281:LYS:HG2	1.99	0.63
25:f:71:TYR:HB3	25:f:72:ARG:HH21	1.64	0.63
25:f:478:ARG:HG2	25:f:482:ILE:HD11	1.81	0.63
1:A:255:ARG:HG2	1:A:255:ARG:HH11	1.63	0.63
25:f:240:VAL:HG11	25:f:248:LEU:HD12	1.80	0.63
25:f:266:LEU:HD13	25:f:294:MET:HB3	1.80	0.63
1:A:241:ILE:HB	1:A:244:GLU:HG3	1.80	0.62
2:B:75:GLU:OE2	25:f:677:HIS:NE2	2.27	0.62
3:C:219:LEU:HD12	4:D:286:GLN:HG3	1.80	0.62
4:D:120:ASP:OD1	22:c:282:ARG:NH1	2.31	0.62
23:d:147:ILE:H	23:d:147:ILE:HD12	1.64	0.62
14:U:119:PRO:HG2	14:U:122:GLU:HB2	1.81	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:U:610:VAL:HG12	19:Z:178:ASP:HB2	1.79	0.62
18:Y:237:ARG:HA	18:Y:241:ILE:HB	1.80	0.62
7:G:49:VAL:HG22	7:G:219:VAL:HG12	1.80	0.62
14:U:885:MET:HB2	14:U:888:GLN:HG3	1.79	0.62
16:W:409:LEU:HD21	17:X:384:VAL:HG11	1.81	0.62
21:b:157:VAL:HG21	21:b:170:LEU:HB2	1.80	0.62
25:f:662:MET:HE1	25:f:696:LEU:HD22	1.81	0.62
1:A:112:ILE:HG12	1:A:122:VAL:HG22	1.80	0.62
25:f:288:VAL:HG21	25:f:313:GLU:HG3	1.80	0.62
11:K:85:ALA:HB2	11:K:139:VAL:HG21	1.80	0.62
3:C:196:LYS:N	30:C:501:ADP:O1B	2.31	0.62
12:L:103:LEU:HD12	12:L:104:PRO:HD2	1.82	0.62
14:U:16:GLU:HB3	14:U:19:LEU:HD12	1.82	0.62
16:W:374:THR:HG22	16:W:376:LYS:H	1.64	0.62
23:d:319:ALA:HB1	23:d:322:GLN:HE22	1.65	0.62
25:f:720:GLU:HG3	25:f:807:ARG:NH2	2.15	0.62
4:D:282:ASP:OD2	5:E:251:ARG:NH2	2.29	0.62
17:X:297:ARG:HG2	17:X:333:GLN:HB3	1.80	0.62
26:g:110:ARG:HG3	26:g:138:LEU:HB3	1.81	0.62
14:U:894:MET:SD	14:U:902:PRO:HD3	2.40	0.62
17:X:44:GLN:O	17:X:44:GLN:NE2	2.32	0.62
25:f:560:LEU:HA	25:f:594:LEU:HD11	1.82	0.62
1:A:165:GLN:NE2	1:A:263:MET:SD	2.72	0.62
14:U:40:GLU:OE1	15:V:269:LYS:NZ	2.23	0.62
16:W:256:ILE:HG23	16:W:262:LYS:HB3	1.82	0.62
5:E:122:MET:HG2	5:E:198:VAL:HB	1.82	0.61
14:U:811:PHE:HB3	14:U:885:MET:HG3	1.81	0.61
19:Z:19:VAL:HG21	19:Z:124:ILE:HD12	1.81	0.61
2:B:179:ALA:HB1	2:B:241:ASN:HA	1.83	0.61
20:a:60:TYR:HA	20:a:64:ILE:HG12	1.82	0.61
25:f:485:LEU:HD12	25:f:501:LEU:HD13	1.82	0.61
6:F:197:GLU:HG3	6:F:350:ARG:HE	1.66	0.61
26:g:140:LYS:HE3	26:g:144:GLU:HG3	1.82	0.61
6:F:390:ASP:OD2	12:L:18:ARG:NH2	2.33	0.61
15:V:146:GLN:HB3	15:V:148:ARG:HE	1.65	0.61
25:f:482:ILE:HG21	25:f:518:THR:HA	1.82	0.61
4:D:184:PRO:HB2	4:D:306:LYS:HE3	1.81	0.61
6:F:122:ALA:HB2	6:F:137:ILE:HD13	1.83	0.61
14:U:535:TYR:HE1	14:U:544:ILE:HG21	1.65	0.61
25:f:296:PHE:CD1	25:f:320:ILE:HG23	2.35	0.61
1:A:213:LEU:HB2	1:A:337:LEU:HD13	1.83	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:U:385:PHE:O	14:U:389:ASN:ND2	2.30	0.61
14:U:386:LEU:HD22	14:U:393:LEU:HD13	1.83	0.61
20:a:176:ALA:HB3	20:a:200:LEU:HD23	1.83	0.61
27:u:183:GLN:HB2	27:u:261:SER:HB2	1.83	0.61
1:A:391:GLU:HA	1:A:394:MET:HB2	1.83	0.61
14:U:835:ILE:HB	25:f:607:LEU:HD21	1.82	0.61
1:A:351:ARG:NH1	1:A:378:PRO:O	2.33	0.60
25:f:466:LEU:HB2	25:f:485:LEU:HD21	1.83	0.60
14:U:446:LEU:HG	14:U:450:HIS:HE1	1.66	0.60
14:U:542:GLU:OE1	22:c:32:TYR:OH	2.15	0.60
3:C:246:ILE:HB	3:C:291:VAL:HG22	1.84	0.60
20:a:112:ILE:HG21	20:a:142:LEU:HD13	1.83	0.60
27:u:143:GLU:HG3	27:u:144:HIS:CD2	2.32	0.60
17:X:252:LYS:HD2	17:X:283:GLN:NE2	2.14	0.60
23:d:108:ASN:HB3	23:d:111:LYS:HE3	1.83	0.60
25:f:106:LEU:HD23	25:f:109:ILE:HD13	1.83	0.60
6:F:318:ASP:O	6:F:347:ARG:NH1	2.35	0.60
15:V:320:THR:O	15:V:325:LYS:NZ	2.35	0.60
4:D:417:TYR:OH	7:G:26:GLU:OE1	2.19	0.60
14:U:228:ALA:O	14:U:232:ILE:HG22	2.01	0.60
14:U:878:LEU:HD23	14:U:882:ALA:HB1	1.84	0.60
18:Y:42:MET:HE2	18:Y:42:MET:HA	1.84	0.60
21:b:107:MET:HE2	21:b:107:MET:HA	1.84	0.60
28:B:501:ATP:O3G	3:C:307:ARG:NH1	2.32	0.60
15:V:109:ASN:HA	15:V:174:PHE:HE1	1.65	0.60
15:V:367:VAL:HG21	15:V:398:LEU:HD13	1.82	0.60
25:f:769:THR:HG23	25:f:770:HIS:CD2	2.37	0.60
18:Y:360:ASP:OD1	18:Y:360:ASP:N	2.35	0.60
20:a:290:GLN:HB3	20:a:330:ARG:HD3	1.82	0.60
6:F:224:LEU:HB2	6:F:348:LEU:HD13	1.83	0.60
20:a:280:MET:HE2	20:a:291:LEU:HD13	1.83	0.59
14:U:370:VAL:HG11	14:U:404:ALA:HA	1.84	0.59
26:g:88:PHE:H	26:g:154:MET:HA	1.66	0.59
15:V:463:MET:HA	15:V:463:MET:HE2	1.83	0.59
17:X:339:ILE:HD12	17:X:387:ILE:HD11	1.85	0.59
27:u:157:LEU:HB3	27:u:260:ILE:HD12	1.82	0.59
10:J:157:LYS:NZ	11:K:60:GLU:OE2	2.35	0.59
21:b:9:CYS:N	21:b:110:ILE:O	2.23	0.59
25:f:682:GLY:HA3	25:f:686:LEU:HD12	1.84	0.59
15:V:289:LEU:HD13	15:V:311:ASN:HB3	1.83	0.59
22:c:233:ASP:HB3	22:c:236:GLU:HG3	1.85	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:g:101:LEU:HD11	26:g:115:LYS:HZ1	1.68	0.59
27:u:157:LEU:HD22	27:u:165:LEU:HD11	1.85	0.59
4:D:53:PHE:HZ	14:U:636:VAL:HB	1.67	0.59
15:V:216:ARG:NH1	24:e:20:GLU:OE2	2.36	0.59
16:W:375:MET:HE1	16:W:408:ARG:HA	1.84	0.59
17:X:177:TYR:CE2	17:X:185:LYS:HD3	2.38	0.59
19:Z:257:MET:HE1	23:d:342:TYR:HE2	1.66	0.59
21:b:75:LEU:HD12	21:b:78:VAL:HG21	1.84	0.59
25:f:463:LEU:N	25:f:489:TYR:OH	2.35	0.59
1:A:243:SER:OG	2:B:311:GLU:OE2	2.21	0.59
1:A:319:MET:HG3	1:A:337:LEU:HD21	1.84	0.59
1:A:189:GLU:OE2	1:A:339:ARG:NH2	2.36	0.59
3:C:89:VAL:HG12	3:C:91:PRO:HD2	1.85	0.59
7:G:120:ASP:OD1	8:H:84:ARG:NH1	2.35	0.59
15:V:161:PRO:HA	15:V:164:GLU:HG2	1.85	0.59
6:F:318:ASP:OD1	6:F:344:ARG:NH2	2.36	0.59
2:B:256:ILE:O	3:C:271:ARG:NH2	2.29	0.59
5:E:153:LEU:HD13	5:E:227:PRO:HB2	1.85	0.59
25:f:374:SER:HB2	25:f:398:TRP:HH2	1.68	0.59
3:C:18:SER:HB3	3:C:21:ARG:HB3	1.85	0.58
5:E:356:ARG:NH1	6:F:200:GLU:OE2	2.36	0.58
14:U:791:LEU:HD13	14:U:795:LEU:HD13	1.84	0.58
3:C:207:THR:OG1	3:C:209:CYS:SG	2.56	0.58
4:D:272:THR:HG21	5:E:251:ARG:HD2	1.84	0.58
9:I:13:SER:HB3	9:I:17:ARG:HG2	1.83	0.58
14:U:810:THR:HG23	14:U:811:PHE:CD1	2.38	0.58
15:V:435:GLU:OE2	23:d:279:TYR:OH	2.17	0.58
19:Z:27:GLY:O	19:Z:32:GLN:NE2	2.36	0.58
23:d:141:LEU:HB3	23:d:182:LEU:HD21	1.85	0.58
25:f:127:SER:HB3	25:f:142:TYR:HB2	1.84	0.58
27:u:207:GLU:HB2	27:u:211:ARG:HH21	1.68	0.58
14:U:202:VAL:HG23	14:U:216:VAL:HG13	1.84	0.58
25:f:679:LEU:HD13	25:f:713:PHE:CE2	2.38	0.58
14:U:747:SER:OG	14:U:749:GLN:O	2.22	0.58
20:a:28:LEU:HD22	20:a:33:LEU:HD12	1.84	0.58
6:F:172:VAL:HA	6:F:175:MET:HE3	1.85	0.58
6:F:200:GLU:OE2	6:F:350:ARG:NH2	2.37	0.58
14:U:832:VAL:HG13	14:U:836:THR:HG21	1.84	0.58
15:V:330:LYS:HZ2	15:V:356:SER:HB2	1.69	0.58
21:b:6:THR:HG23	21:b:49:VAL:HG23	1.86	0.58
22:c:163:ILE:HG23	22:c:174:PRO:HB3	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:g:126:TYR:C	26:g:158:LEU:HB2	2.29	0.58
18:Y:84:LEU:HD13	18:Y:107:LYS:HA	1.84	0.58
7:G:70:PHE:HZ	7:G:88:ARG:HE	1.52	0.57
8:H:203:MET:HE3	8:H:208:ILE:HG21	1.85	0.57
16:W:312:MET:HA	16:W:312:MET:HE3	1.85	0.57
6:F:244:THR:HG22	6:F:246:ALA:H	1.69	0.57
7:G:141:ILE:HD12	7:G:220:VAL:HG22	1.86	0.57
14:U:587:ALA:HB2	14:U:621:SER:HB3	1.86	0.57
22:c:50:PRO:HA	22:c:116:PRO:HG2	1.86	0.57
25:f:659:LEU:HD21	25:f:797:LEU:HD11	1.86	0.57
25:f:456:ARG:HH12	25:f:492:SER:HA	1.68	0.57
1:A:214:LEU:HD22	1:A:343:PHE:HE1	1.69	0.57
8:H:9:SER:HB2	9:I:127:LYS:HA	1.86	0.57
14:U:529:ILE:HD12	14:U:566:LEU:HD22	1.85	0.57
21:b:155:ALA:O	21:b:159:THR:OG1	2.16	0.57
23:d:116:LEU:HD11	23:d:151:GLY:HA2	1.86	0.57
25:f:505:MET:HB3	25:f:518:THR:HG21	1.85	0.57
20:a:303:THR:HG22	20:a:305:ASN:H	1.68	0.57
17:X:417:LYS:NZ	22:c:262:GLU:OE2	2.37	0.57
14:U:36:ALA:HB1	15:V:269:LYS:HB3	1.87	0.57
14:U:105:ILE:HD11	14:U:137:MET:HG2	1.87	0.57
14:U:588:MET:HE3	14:U:764:LEU:HD22	1.85	0.57
21:b:153:LEU:HB3	21:b:170:LEU:HD11	1.86	0.57
5:E:171:LEU:HB2	5:E:295:LEU:HD13	1.85	0.57
23:d:344:ARG:HB3	23:d:348:MET:HE2	1.87	0.57
8:H:93:LEU:HD13	8:H:113:ARG:HB3	1.85	0.57
19:Z:224:HIS:NE2	20:a:340:VAL:HG13	2.20	0.57
24:e:59:GLU:HG2	24:e:62:LYS:HE2	1.87	0.57
27:u:146:PHE:HE2	27:u:167:ILE:HG23	1.68	0.57
10:J:168:VAL:HG13	10:J:194:ALA:HB1	1.87	0.56
11:K:196:LYS:O	11:K:200:ILE:HD12	2.05	0.56
17:X:382:GLU:N	17:X:382:GLU:OE2	2.37	0.56
25:f:611:GLN:O	25:f:615:ILE:HG13	2.04	0.56
25:f:861:THR:OG1	25:f:881:GLU:OE2	2.22	0.56
26:g:112:LEU:HD22	26:g:142:LEU:HD11	1.87	0.56
2:B:67:ARG:NH2	25:f:604:GLY:O	2.38	0.56
3:C:381:GLU:OE2	17:X:194:ARG:NH1	2.36	0.56
17:X:412:ASP:OD1	18:Y:379:ARG:NH2	2.24	0.56
20:a:363:MET:HE1	22:c:307:VAL:HB	1.86	0.56
25:f:250:ARG:NH2	25:f:274:ASP:OD2	2.36	0.56
25:f:683:GLU:N	25:f:683:GLU:OE2	2.38	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:409:LYS:NZ	4:D:413:GLU:OE2	2.38	0.56
5:E:272:ARG:HG2	5:E:272:ARG:HH11	1.70	0.56
6:F:200:GLU:HA	6:F:204:LEU:HB2	1.87	0.56
17:X:259:ILE:HG22	17:X:326:LEU:HD21	1.87	0.56
21:b:100:ARG:NH1	21:b:105:HIS:O	2.38	0.56
27:u:166:LEU:HD21	27:u:204:MET:HB3	1.88	0.56
6:F:311:LEU:HD23	6:F:314:LEU:HD12	1.86	0.56
13:M:46:VAL:HG22	13:M:215:TRP:HB3	1.86	0.56
14:U:198:LEU:HD22	14:U:219:CYS:HB3	1.86	0.56
14:U:269:ARG:HH21	14:U:326:ILE:HD13	1.69	0.56
16:W:41:GLN:H	16:W:41:GLN:CD	2.12	0.56
14:U:764:LEU:O	14:U:767:THR:OG1	2.22	0.56
16:W:63:THR:HA	16:W:66:ILE:HD12	1.88	0.56
17:X:142:ARG:NE	17:X:145:GLU:OE1	2.35	0.56
17:X:252:LYS:NZ	17:X:316:ASP:OD2	2.36	0.56
20:a:197:ALA:HB1	20:a:222:LEU:HD23	1.87	0.56
25:f:159:VAL:HA	25:f:162:LEU:HB3	1.87	0.56
25:f:679:LEU:HD13	25:f:713:PHE:HE2	1.71	0.56
5:E:108:MET:HE1	22:c:50:PRO:CG	2.36	0.56
12:L:176:MET:HE1	13:M:56:LYS:HB3	1.88	0.56
13:M:52:LEU:HA	13:M:209:PHE:HA	1.86	0.56
14:U:431:THR:O	14:U:435:SER:OG	2.15	0.56
15:V:168:GLN:HG2	15:V:191:LEU:HD22	1.87	0.56
1:A:212:VAL:HG22	1:A:339:ARG:HB2	1.87	0.56
13:M:68:ASN:OD1	13:M:224:HIS:ND1	2.29	0.56
14:U:2:ILE:HG13	14:U:2:ILE:O	2.06	0.56
17:X:194:ARG:HA	17:X:210:LEU:HD21	1.87	0.56
17:X:274:LYS:HA	17:X:277:LEU:HD12	1.87	0.56
25:f:829:MET:HA	25:f:829:MET:HE2	1.86	0.56
4:D:147:ALA:HA	5:E:62:LYS:HD2	1.87	0.56
14:U:406:ALA:HA	14:U:445:ALA:HB2	1.87	0.56
21:b:54:LEU:HB3	21:b:84:ILE:HD12	1.87	0.56
22:c:44:HIS:CE1	22:c:53:VAL:HB	2.40	0.56
9:I:33:THR:HG21	9:I:200:THR:HG21	1.88	0.56
14:U:3:THR:N	23:d:177:ASP:OD1	2.22	0.56
14:U:108:TYR:CE1	14:U:134:VAL:HG11	2.41	0.56
20:a:84:VAL:HG21	20:a:97:LEU:HD11	1.87	0.56
25:f:441:LYS:HE2	25:f:469:TYR:HE2	1.70	0.56
25:f:870:THR:O	25:f:872:VAL:N	2.39	0.56
1:A:266:THR:O	25:f:355:ASN:ND2	2.38	0.56
2:B:151:LEU:HD21	2:B:163:LEU:HB2	1.88	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:V:482:PHE:HZ	18:Y:381:GLN:HG3	1.71	0.56
25:f:369:ARG:HG2	25:f:369:ARG:HH11	1.71	0.56
14:U:460:TYR:HD1	14:U:461:LEU:HD22	1.71	0.55
15:V:287:ARG:NH1	24:e:21:GLU:OE1	2.39	0.55
17:X:256:LEU:HD22	17:X:319:ILE:HG12	1.88	0.55
26:g:84:THR:HG23	26:g:100:LEU:HD21	1.87	0.55
17:X:299:LEU:HD21	17:X:327:TYR:HE1	1.71	0.55
12:L:22:ILE:HD11	12:L:120:THR:HB	1.87	0.55
14:U:628:ARG:NH2	14:U:755:THR:OG1	2.39	0.55
15:V:372:LEU:HD21	15:V:403:ILE:HG13	1.87	0.55
3:C:113:ARG:NH2	4:D:94:GLU:OE1	2.40	0.55
9:I:107:CYS:HB2	9:I:146:GLN:NE2	2.21	0.55
9:I:124:PHE:HB3	10:J:124:ARG:HG3	1.89	0.55
15:V:161:PRO:HG2	15:V:200:ARG:HH11	1.70	0.55
21:b:11:ASP:O	21:b:29:GLN:NE2	2.32	0.55
22:c:61:PHE:HB3	22:c:139:ARG:NH2	2.21	0.55
25:f:80:ARG:HH12	25:f:84:SER:HB2	1.72	0.55
1:A:303:ILE:HG23	1:A:336:ARG:CZ	2.36	0.55
4:D:389:GLU:OE1	4:D:391:ARG:NH1	2.33	0.55
5:E:173:TYR:HE2	5:E:298:LYS:HB3	1.72	0.55
2:B:209:GLU:O	2:B:213:GLU:HG3	2.07	0.55
12:L:80:ASP:OD2	12:L:126:ARG:NH1	2.36	0.55
12:L:180:MET:HA	12:L:180:MET:HE3	1.87	0.55
13:M:179:LEU:HD21	13:M:192:GLU:HB3	1.89	0.55
14:U:42:VAL:O	14:U:46:GLU:HG2	2.07	0.55
15:V:195:ILE:H	15:V:195:ILE:HD12	1.71	0.55
18:Y:202:LEU:HD11	18:Y:231:LEU:HD11	1.88	0.55
20:a:97:LEU:HA	20:a:100:THR:HB	1.87	0.55
3:C:347:ILE:HG12	3:C:383:PHE:HB3	1.89	0.55
11:K:33:LEU:O	11:K:53:ARG:NH2	2.39	0.55
12:L:185:ASN:OD1	12:L:189:LYS:NZ	2.39	0.55
5:E:135:ILE:HG12	5:E:182:LEU:HD23	1.88	0.55
18:Y:184:GLN:HB3	18:Y:200:LEU:HD13	1.87	0.55
15:V:95:LEU:O	15:V:99:ARG:N	2.39	0.55
17:X:163:LYS:HB2	17:X:200:ILE:HD13	1.89	0.55
17:X:271:VAL:HG21	17:X:288:LYS:HD3	1.89	0.55
14:U:697:GLN:O	14:U:885:MET:HE1	2.07	0.55
15:V:68:ASP:OD1	15:V:109:ASN:ND2	2.24	0.55
22:c:63:ASP:O	22:c:139:ARG:NH2	2.40	0.55
25:f:257:ARG:NH1	25:f:280:ASP:OD2	2.25	0.55
25:f:450:ILE:HG23	25:f:822:VAL:HG11	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:272:THR:HG22	4:D:274:ARG:H	1.71	0.54
5:E:386:TYR:OH	6:F:294:LYS:NZ	2.39	0.54
10:J:111:ILE:HD12	10:J:133:ILE:HD11	1.88	0.54
15:V:355:ARG:NH2	24:e:28:ALA:O	2.40	0.54
17:X:255:LEU:O	17:X:259:ILE:HG12	2.07	0.54
27:u:119:ILE:HD12	27:u:124:MET:HA	1.89	0.54
1:A:204:LEU:HB3	1:A:206:ILE:HG12	1.89	0.54
7:G:45:LYS:HB3	7:G:188:ASP:HB3	1.88	0.54
7:G:72:ILE:HG21	7:G:114:LEU:HD21	1.89	0.54
17:X:170:GLN:HB2	17:X:193:ALA:HB2	1.89	0.54
19:Z:6:VAL:HG22	19:Z:43:TRP:CH2	2.42	0.54
20:a:255:TRP:HH2	20:a:265:GLU:HG3	1.72	0.54
21:b:30:GLN:OE1	21:b:76:HIS:ND1	2.40	0.54
1:A:301:GLU:OE2	1:A:305:GLN:NE2	2.35	0.54
2:B:103:ARG:HB3	2:B:160:ILE:HD12	1.89	0.54
2:B:183:THR:OG1	2:B:186:ASP:OD2	2.25	0.54
14:U:160:LEU:HA	14:U:163:PHE:HB3	1.89	0.54
14:U:444:TYR:HD1	14:U:479:LEU:HB3	1.72	0.54
17:X:31:VAL:O	17:X:46:LYS:NZ	2.40	0.54
25:f:335:ARG:HE	25:f:340:MET:HG2	1.73	0.54
3:C:20:LEU:HB3	3:C:23:TYR:HB3	1.90	0.54
5:E:175:PRO:HG2	5:E:303:LEU:HG	1.89	0.54
5:E:203:ILE:HD11	5:E:238:ILE:HD13	1.88	0.54
11:K:133:MET:HA	11:K:133:MET:HE3	1.89	0.54
25:f:293:GLN:O	25:f:297:MET:HG3	2.07	0.54
2:B:53:THR:O	2:B:64:LYS:NZ	2.30	0.54
3:C:90:HIS:HB3	3:C:91:PRO:HD3	1.89	0.54
4:D:101:ALA:HB2	4:D:115:ILE:HD11	1.90	0.54
5:E:117:PRO:HG3	6:F:94:ILE:HA	1.90	0.54
16:W:81:ASP:OD2	16:W:123:ARG:NH1	2.39	0.54
16:W:122:LEU:HD21	16:W:152:ILE:HG21	1.89	0.54
25:f:319:GLU:OE1	26:g:97:ARG:NH2	2.36	0.54
25:f:597:VAL:HG12	25:f:659:LEU:HD23	1.89	0.54
3:C:376:VAL:HG13	4:D:193:GLN:HB3	1.90	0.54
14:U:376:MET:HA	14:U:739:ALA:HA	1.90	0.54
2:B:290:ILE:HG21	2:B:309:MET:HE1	1.89	0.54
4:D:204:MET:HE3	4:D:333:PHE:CZ	2.43	0.54
8:H:160:ALA:HB1	8:H:174:LEU:HD22	1.90	0.54
15:V:330:LYS:NZ	15:V:356:SER:HB2	2.23	0.54
23:d:241:TYR:HB3	23:d:271:ILE:HD11	1.90	0.54
26:g:140:LYS:O	26:g:145:GLN:NE2	2.32	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:VAL:HG21	1:A:260:LEU:HD11	1.88	0.54
4:D:268:ASP:HB2	5:E:258:MET:HE1	1.90	0.54
9:I:52:ILE:HG21	9:I:210:LYS:HG2	1.89	0.54
2:B:135:ILE:HA	2:B:159:VAL:HB	1.90	0.54
5:E:206:LYS:HA	6:F:261:ILE:HG13	1.90	0.54
4:D:214:MET:HA	4:D:217:LYS:HG3	1.89	0.53
14:U:509:GLY:HA3	14:U:544:ILE:HG12	1.89	0.53
18:Y:186:LEU:HD22	18:Y:213:LEU:HD13	1.90	0.53
21:b:141:ILE:HG13	21:b:141:ILE:O	2.07	0.53
25:f:688:ARG:HG2	25:f:720:GLU:HB2	1.90	0.53
26:g:164:ASP:HA	26:g:167:LYS:HE3	1.89	0.53
27:u:177:LEU:HD22	27:u:265:PHE:HB3	1.89	0.53
15:V:303:SER:HA	15:V:339:LEU:HD11	1.90	0.53
1:A:429:TYR:O	1:A:433:ASN:ND2	2.33	0.53
3:C:270:GLN:HE21	3:C:302:ASP:H	1.56	0.53
7:G:80:MET:SD	7:G:138:MET:HG3	2.48	0.53
16:W:66:ILE:O	16:W:70:VAL:HG13	2.08	0.53
23:d:215:LEU:HD22	23:d:226:ILE:HG13	1.90	0.53
4:D:238:LYS:HB2	4:D:238:LYS:HZ3	1.73	0.53
4:D:356:GLU:OE1	4:D:356:GLU:N	2.42	0.53
7:G:58:ASP:N	7:G:58:ASP:OD1	2.42	0.53
14:U:421:GLN:NE2	14:U:425:THR:OG1	2.41	0.53
15:V:371:ASN:HB3	15:V:374:LYS:HD2	1.91	0.53
16:W:107:GLN:O	16:W:110:THR:OG1	2.25	0.53
5:E:161:ARG:HH21	16:W:174:TYR:HA	1.73	0.53
6:F:338:LEU:HD12	6:F:343:LEU:HD21	1.89	0.53
8:H:79:MET:H	8:H:132:VAL:HG12	1.74	0.53
10:J:39:ASP:N	10:J:39:ASP:OD1	2.41	0.53
17:X:70:LEU:HD21	17:X:113:CYS:SG	2.49	0.53
3:C:351:MET:HA	3:C:391:MET:HE2	1.90	0.53
6:F:256:LEU:HD12	6:F:291:ILE:HD13	1.90	0.53
10:J:134:VAL:HG12	10:J:144:LEU:HD13	1.91	0.53
14:U:221:ILE:HD11	14:U:252:LEU:HD13	1.91	0.53
21:b:28:ALA:HB1	21:b:179:LEU:HD22	1.91	0.53
4:D:380:GLN:NE2	5:E:165:ILE:O	2.25	0.53
10:J:148:ASP:OD1	10:J:148:ASP:N	2.40	0.53
3:C:270:GLN:NE2	3:C:301:LEU:HA	2.23	0.53
5:E:313:LEU:HD13	5:E:343:LEU:HD22	1.91	0.53
12:L:49:LEU:HB2	12:L:195:LEU:HD21	1.91	0.53
18:Y:138:LEU:HD13	18:Y:167:LEU:HB2	1.90	0.53
19:Z:6:VAL:HG22	19:Z:43:TRP:HH2	1.74	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:d:313:ASN:HB2	23:d:315:TYR:HD2	1.73	0.53
3:C:109:THR:OG1	3:C:112:CYS:SG	2.66	0.53
5:E:385:ASP:OD1	5:E:387:LYS:NZ	2.42	0.53
22:c:113:HIS:HE2	22:c:115:HIS:CD2	2.24	0.53
23:d:143:LEU:HG	23:d:147:ILE:HD11	1.91	0.53
2:B:357:ASP:OD2	10:J:200:GLN:NE2	2.43	0.52
5:E:178:THR:HB	5:E:301:ILE:HG22	1.91	0.52
6:F:224:LEU:HD23	6:F:351:LYS:HG2	1.91	0.52
15:V:77:GLU:OE2	15:V:81:GLN:NE2	2.42	0.52
15:V:131:LEU:HD12	15:V:171:VAL:HG21	1.91	0.52
18:Y:12:PRO:O	18:Y:146:ARG:NH1	2.41	0.52
25:f:430:ASP:HA	25:f:433:LEU:HB2	1.89	0.52
8:H:135:LEU:HD22	8:H:146:LEU:HD11	1.92	0.52
9:I:28:ILE:HG12	9:I:133:SER:HB2	1.90	0.52
23:d:204:ARG:NH2	23:d:207:GLU:OE1	2.42	0.52
25:f:140:LEU:HD21	25:f:184:LEU:HD21	1.90	0.52
25:f:350:LYS:HB3	25:f:353:LEU:HD23	1.91	0.52
4:D:162:VAL:HG11	4:D:214:MET:HG3	1.90	0.52
7:G:49:VAL:HG21	7:G:195:VAL:HG22	1.90	0.52
8:H:51:LYS:NZ	8:H:200:GLU:O	2.42	0.52
9:I:203:VAL:HG11	9:I:210:LYS:HZ1	1.75	0.52
25:f:72:ARG:HH22	25:f:75:LEU:HD12	1.75	0.52
25:f:333:LEU:HD22	25:f:829:MET:SD	2.49	0.52
3:C:142:LYS:NZ	4:D:297:ASP:OD1	2.36	0.52
9:I:44:LEU:HD22	9:I:190:LEU:HD12	1.91	0.52
14:U:788:VAL:HG13	14:U:912:ILE:HD12	1.92	0.52
22:c:296:ILE:HG23	23:d:339:VAL:HG13	1.92	0.52
1:A:189:GLU:OE2	6:F:409:ARG:NH2	2.42	0.52
4:D:185:LEU:HD22	4:D:259:PRO:HB3	1.90	0.52
11:K:38:ILE:HD12	11:K:202:LEU:HG	1.91	0.52
18:Y:282:MET:HB3	18:Y:288:PHE:HB3	1.91	0.52
23:d:135:LYS:NZ	23:d:136:LEU:O	2.39	0.52
1:A:255:ARG:HG2	1:A:255:ARG:NH1	2.22	0.52
4:D:163:MET:HE3	4:D:221:HIS:CE1	2.44	0.52
6:F:175:MET:HB2	6:F:250:LYS:O	2.10	0.52
10:J:132:LEU:HD22	10:J:144:LEU:HD11	1.90	0.52
14:U:31:VAL:HG11	14:U:66:LYS:HD2	1.91	0.52
17:X:229:TYR:CE2	17:X:254:MET:HG2	2.44	0.52
25:f:285:CYS:O	25:f:291:GLN:NE2	2.43	0.52
3:C:65:LEU:HD23	4:D:114:ARG:NH1	2.25	0.52
5:E:140:GLU:OE2	5:E:143:ARG:NH2	2.43	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:W:214:PHE:HB3	16:W:223:LYS:HD2	1.91	0.52
18:Y:24:PHE:O	18:Y:27:SER:OG	2.26	0.52
19:Z:186:THR:O	19:Z:190:ARG:HG2	2.09	0.52
25:f:159:VAL:O	25:f:163:ALA:N	2.29	0.52
4:D:214:MET:HE1	28:D:501:ATP:C4	2.45	0.52
8:H:11:THR:HG23	8:H:21:GLN:HB3	1.90	0.52
13:M:65:ARG:HH21	13:M:78:ALA:HA	1.74	0.52
15:V:269:LYS:O	15:V:273:LYS:HG2	2.09	0.52
17:X:344:ARG:HD3	17:X:386:ILE:HG23	1.92	0.52
18:Y:282:MET:HE1	18:Y:295:TYR:HB3	1.91	0.52
20:a:112:ILE:HG23	20:a:138:VAL:HG23	1.91	0.52
23:d:232:LEU:HD11	23:d:244:VAL:HG13	1.92	0.52
25:f:512:MET:HE1	25:f:545:LYS:HD2	1.91	0.52
25:f:689:ALA:HA	25:f:692:LEU:HD23	1.91	0.52
25:f:869:THR:HG23	25:f:871:PRO:HD2	1.92	0.52
3:C:166:GLU:OE2	3:C:207:THR:HG22	2.10	0.52
4:D:184:PRO:HG3	4:D:191:TYR:CZ	2.45	0.52
11:K:107:MET:HG2	11:K:112:VAL:HG23	1.91	0.52
12:L:138:ASP:OD1	12:L:138:ASP:N	2.40	0.52
14:U:333:MET:O	14:U:337:LEU:HD22	2.10	0.52
14:U:341:PHE:CE1	14:U:787:CYS:HB3	2.45	0.52
14:U:416:GLU:OE1	14:U:450:HIS:HD2	1.91	0.52
15:V:399:ARG:NH1	23:d:238:GLU:OE1	2.42	0.52
17:X:190:LEU:HD21	17:X:214:SER:HA	1.92	0.52
18:Y:214:MET:HE1	18:Y:222:TYR:CD2	2.45	0.52
22:c:267:PRO:HA	22:c:270:LEU:HG	1.91	0.52
23:d:111:LYS:HE2	23:d:111:LYS:H	1.75	0.52
23:d:178:TYR:HB2	23:d:182:LEU:HD23	1.91	0.52
25:f:463:LEU:HD13	25:f:497:VAL:HG22	1.92	0.52
26:g:108:THR:HG21	26:g:110:ARG:HE	1.75	0.52
5:E:349:GLU:OE2	6:F:350:ARG:NH1	2.43	0.52
11:K:68:VAL:HG21	11:K:89:ILE:HG13	1.92	0.52
14:U:15:ASP:OD1	14:U:15:ASP:N	2.35	0.52
14:U:646:PRO:HB3	14:U:680:VAL:HG21	1.92	0.52
15:V:223:LYS:O	15:V:261:TYR:OH	2.27	0.52
25:f:694:LEU:HD22	25:f:706:ILE:HG22	1.91	0.52
4:D:201:GLY:HA3	4:D:327:LEU:HD23	1.92	0.51
4:D:378:ILE:O	4:D:382:SER:OG	2.23	0.51
10:J:47:LYS:HE3	10:J:50:VAL:HG22	1.92	0.51
17:X:202:CYS:HB2	17:X:207:GLN:HG2	1.92	0.51
25:f:71:TYR:HB3	25:f:72:ARG:NH2	2.25	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Y:328:GLU:H	18:Y:328:GLU:CD	2.18	0.51
19:Z:231:GLN:NE2	20:a:339:ARG:O	2.43	0.51
20:a:132:LYS:NZ	20:a:162:TYR:OH	2.26	0.51
22:c:57:MET:HA	22:c:72:VAL:HG12	1.90	0.51
23:d:301:ASP:OD1	23:d:301:ASP:N	2.42	0.51
25:f:211:ILE:HG13	25:f:213:GLN:HB2	1.92	0.51
2:B:343:ARG:NH1	2:B:344:PRO:O	2.37	0.51
16:W:363:ILE:HG12	16:W:378:MET:HE2	1.92	0.51
17:X:248:ILE:HG13	17:X:249:THR:N	2.25	0.51
25:f:337:LEU:O	25:f:339:ILE:HG23	2.10	0.51
1:A:165:GLN:HA	1:A:238:ILE:HA	1.91	0.51
1:A:256:MET:O	1:A:260:LEU:HB2	2.10	0.51
15:V:171:VAL:O	15:V:175:MET:HG2	2.11	0.51
20:a:134:THR:O	20:a:138:VAL:HG12	2.09	0.51
25:f:390:LEU:HD21	25:f:398:TRP:CE2	2.45	0.51
27:u:139:ASN:ND2	27:u:164:GLN:O	2.44	0.51
28:D:501:ATP:O1G	5:E:294:ARG:NH1	2.41	0.51
13:M:5:THR:HG23	13:M:7:TYR:H	1.75	0.51
14:U:163:PHE:HE1	14:U:180:SER:HG	1.58	0.51
25:f:829:MET:HB3	25:f:896:GLY:HA2	1.91	0.51
4:D:179:GLU:O	4:D:191:TYR:OH	2.26	0.51
17:X:132:ARG:HG2	17:X:132:ARG:HH11	1.75	0.51
21:b:56:ASN:N	21:b:56:ASN:OD1	2.43	0.51
23:d:156:ILE:HG22	23:d:258:PHE:HD1	1.76	0.51
25:f:585:GLU:HG2	25:f:588:ARG:HE	1.76	0.51
25:f:740:ARG:O	25:f:744:MET:HG3	2.11	0.51
2:B:29:VAL:HG21	25:f:750:GLN:HB3	1.92	0.51
7:G:123:GLN:NE2	8:H:82:ASP:OD1	2.35	0.51
7:G:196:GLU:HG2	7:G:242:LEU:HG	1.92	0.51
10:J:48:LYS:HG2	10:J:163:ARG:NH2	2.25	0.51
12:L:105:VAL:O	12:L:109:VAL:HG23	2.10	0.51
15:V:360:TYR:OH	15:V:391:THR:OG1	2.25	0.51
16:W:187:LEU:HD13	16:W:225:LYS:HG2	1.93	0.51
27:u:182:PHE:CD2	27:u:191:PRO:HG3	2.46	0.51
9:I:11:ILE:HG22	10:J:7:ILE:HG23	1.92	0.51
14:U:236:LEU:HD21	14:U:244:MET:HG2	1.92	0.51
14:U:415:HIS:NE2	14:U:418:GLU:OE1	2.35	0.51
18:Y:107:LYS:HZ2	18:Y:111:LEU:HD11	1.76	0.51
22:c:307:VAL:HA	22:c:310:LYS:HE3	1.93	0.51
25:f:384:ALA:HB2	25:f:419:LEU:HB3	1.92	0.51
26:g:123:GLN:OE1	26:g:126:TYR:N	2.43	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:288:LEU:HD22	6:F:330:ALA:HB1	1.91	0.51
14:U:210:LYS:H	14:U:210:LYS:HE2	1.76	0.51
16:W:86:ASN:O	16:W:90:LEU:HD12	2.11	0.51
16:W:194:LEU:HD12	16:W:229:LEU:HG	1.93	0.51
16:W:283:GLN:O	16:W:287:VAL:HG23	2.11	0.51
25:f:459:CYS:O	25:f:461:PRO:HD3	2.10	0.51
25:f:581:GLU:OE2	25:f:588:ARG:NH1	2.43	0.51
16:W:147:LYS:HE2	16:W:188:GLU:HG3	1.93	0.51
19:Z:31:ASN:N	19:Z:31:ASN:OD1	2.42	0.51
27:u:137:CYS:HB2	27:u:146:PHE:HD2	1.74	0.51
3:C:371:LEU:O	3:C:374:ARG:NH1	2.40	0.50
14:U:465:LEU:HB3	14:U:496:LEU:HD21	1.92	0.50
14:U:521:LEU:HD11	14:U:761:VAL:HG21	1.93	0.50
21:b:150:THR:O	21:b:154:THR:OG1	2.27	0.50
23:d:263:LEU:O	23:d:266:THR:OG1	2.26	0.50
25:f:140:LEU:HD13	25:f:166:VAL:HG12	1.93	0.50
25:f:151:LEU:HD21	25:f:187:LEU:HD22	1.93	0.50
25:f:520:LEU:O	25:f:524:MET:HG3	2.11	0.50
26:g:103:THR:HB	26:g:115:LYS:HE3	1.93	0.50
3:C:117:ARG:HG3	3:C:122:THR:HB	1.93	0.50
4:D:203:LEU:HB2	4:D:327:LEU:HD13	1.93	0.50
13:M:108:LEU:HD11	13:M:137:LEU:HB3	1.94	0.50
14:U:69:TYR:HE2	15:V:240:LEU:HD11	1.76	0.50
20:a:12:GLN:HE21	20:a:26:GLU:HG3	1.75	0.50
25:f:870:THR:OG1	25:f:871:PRO:HD3	2.10	0.50
27:u:176:LYS:HE2	27:u:270:VAL:HA	1.92	0.50
1:A:325:ASP:OD2	1:A:325:ASP:N	2.45	0.50
5:E:106:THR:OG1	22:c:50:PRO:HG3	2.11	0.50
14:U:756:HIS:CE1	14:U:758:PRO:HG2	2.46	0.50
16:W:69:ALA:O	16:W:73:MET:HG2	2.11	0.50
27:u:194:VAL:HG13	27:u:246:ILE:HG23	1.94	0.50
1:A:123:VAL:HG12	6:F:87:PRO:HB3	1.93	0.50
12:L:109:VAL:HG22	12:L:134:ILE:HD12	1.93	0.50
19:Z:15:VAL:HG21	19:Z:50:VAL:HG12	1.93	0.50
21:b:36:VAL:HG21	21:b:110:ILE:HG12	1.93	0.50
22:c:54:MET:HE2	22:c:75:MET:HG3	1.93	0.50
25:f:72:ARG:NH1	25:f:117:GLU:O	2.44	0.50
4:D:41:TYR:OH	14:U:156:GLU:OE1	2.24	0.50
9:I:3:ARG:HG2	9:I:8:ARG:HH22	1.76	0.50
10:J:228:TYR:O	10:J:232:ILE:HD12	2.12	0.50
17:X:299:LEU:H	17:X:334:ASN:HD22	1.60	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:70:GLY:HA3	4:D:113:VAL:HG12	1.93	0.50
5:E:45:ASN:HA	5:E:48:LYS:HD3	1.94	0.50
10:J:4:ASP:OD2	11:K:126:GLU:HA	2.11	0.50
12:L:71:GLY:HA3	12:L:221:PHE:CZ	2.47	0.50
15:V:320:THR:OG1	15:V:321:ALA:N	2.45	0.50
20:a:41:VAL:HG12	20:a:79:ILE:HD12	1.94	0.50
25:f:208:LEU:HD21	25:f:217:LEU:HD22	1.94	0.50
4:D:214:MET:HE1	28:D:501:ATP:N9	2.27	0.50
5:E:108:MET:HE1	22:c:50:PRO:HG3	1.94	0.50
10:J:115:LYS:NZ	10:J:147:THR:OG1	2.35	0.50
14:U:560:MET:HA	14:U:560:MET:HE3	1.93	0.50
15:V:161:PRO:HG2	15:V:200:ARG:NH1	2.27	0.50
15:V:231:LEU:HD23	15:V:250:LEU:HD23	1.93	0.50
15:V:235:LEU:HA	15:V:250:LEU:HD13	1.93	0.50
16:W:99:GLN:OE1	16:W:99:GLN:N	2.33	0.50
23:d:259:PHE:HA	23:d:262:ILE:HD12	1.94	0.50
3:C:212:ILE:HG21	3:C:234:LEU:HD11	1.92	0.50
4:D:202:VAL:HG22	4:D:329:ARG:HB3	1.93	0.50
4:D:236:VAL:HG21	5:E:255:ARG:HD3	1.93	0.50
7:G:43:ARG:HG3	7:G:149:PRO:HB2	1.94	0.50
12:L:200:PRO:O	12:L:239:ARG:NH2	2.35	0.50
22:c:245:VAL:HA	22:c:248:MET:HE3	1.92	0.50
2:B:166:ASP:HB2	3:C:78:ARG:NH1	2.27	0.50
8:H:145:TYR:HE1	9:I:59:VAL:HG21	1.77	0.50
9:I:203:VAL:HG12	9:I:205:LYS:H	1.77	0.50
14:U:213:PHE:CD2	14:U:232:ILE:HD11	2.47	0.50
14:U:401:LYS:HE3	14:U:438:GLN:HG3	1.94	0.50
20:a:12:GLN:NE2	20:a:26:GLU:HG3	2.26	0.50
23:d:301:ASP:HA	23:d:304:LYS:HE2	1.93	0.50
25:f:322:SER:HB2	25:f:456:ARG:O	2.11	0.50
27:u:182:PHE:HD2	27:u:191:PRO:HG3	1.77	0.50
1:A:82:ALA:O	1:A:86:THR:HG23	2.12	0.49
4:D:99:ASN:OD1	4:D:99:ASN:N	2.45	0.49
14:U:233:LEU:HD21	14:U:325:MET:SD	2.52	0.49
14:U:446:LEU:O	14:U:450:HIS:ND1	2.45	0.49
15:V:104:THR:O	15:V:108:LEU:HD23	2.12	0.49
15:V:363:LEU:HB2	15:V:378:VAL:HG11	1.94	0.49
19:Z:227:ILE:O	19:Z:231:GLN:HG3	2.11	0.49
25:f:348:ILE:HD12	25:f:770:HIS:ND1	2.26	0.49
3:C:214:VAL:HB	3:C:248:MET:HG2	1.93	0.49
5:E:113:ARG:NH1	5:E:224:ASP:OD2	2.45	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:40:ALA:HB2	8:H:187:ALA:HB2	1.94	0.49
11:K:91:LYS:O	11:K:95:GLU:N	2.29	0.49
12:L:81:ALA:HB2	12:L:130:VAL:HG21	1.94	0.49
14:U:213:PHE:HD2	14:U:232:ILE:HD11	1.75	0.49
16:W:93:ARG:HB2	16:W:96:GLN:HG2	1.95	0.49
19:Z:9:VAL:HG21	19:Z:120:VAL:HG11	1.94	0.49
25:f:418:LEU:HD13	25:f:425:GLY:HA2	1.94	0.49
25:f:814:SER:HA	25:f:816:TYR:CZ	2.47	0.49
27:u:130:ILE:HG21	27:u:169:VAL:HG13	1.94	0.49
27:u:138:LEU:HD22	27:u:166:LEU:HD23	1.94	0.49
15:V:365:GLN:O	15:V:369:THR:HG23	2.12	0.49
26:g:108:THR:HG23	26:g:110:ARG:H	1.77	0.49
2:B:106:PRO:HG3	3:C:121:TYR:CD1	2.47	0.49
10:J:42:VAL:HG13	10:J:210:VAL:HG12	1.95	0.49
11:K:166:ASP:HB3	11:K:185:TYR:CZ	2.47	0.49
15:V:264:TYR:OH	15:V:294:ARG:NH1	2.45	0.49
18:Y:195:LYS:HA	18:Y:230:ALA:HB1	1.93	0.49
25:f:437:GLU:OE2	25:f:438:ASP:N	2.45	0.49
2:B:407:LEU:HD21	3:C:167:LEU:HD23	1.94	0.49
3:C:163:GLU:HA	3:C:167:LEU:HD22	1.94	0.49
3:C:270:GLN:HG2	3:C:305:LEU:HD12	1.94	0.49
13:M:184:MET:HG3	13:M:189:ILE:HD13	1.94	0.49
15:V:469:THR:OG1	15:V:470:ARG:N	2.41	0.49
15:V:512:ARG:HG3	15:V:516:GLN:HE21	1.77	0.49
17:X:335:LEU:O	17:X:339:ILE:HG12	2.13	0.49
19:Z:127:LYS:HD3	19:Z:127:LYS:N	2.26	0.49
25:f:659:LEU:HD22	25:f:797:LEU:HD21	1.95	0.49
3:C:273:MET:HG3	3:C:293:MET:SD	2.52	0.49
5:E:270:LEU:HG	5:E:273:VAL:HB	1.94	0.49
12:L:157:ARG:HG2	12:L:157:ARG:HH11	1.78	0.49
12:L:203:GLN:O	12:L:239:ARG:NH2	2.45	0.49
14:U:616:ARG:HB2	14:U:647:HIS:HB3	1.94	0.49
15:V:371:ASN:ND2	15:V:373:ALA:H	2.10	0.49
22:c:121:TRP:HZ3	22:c:123:SER:HB3	1.78	0.49
23:d:282:ILE:HG22	23:d:318:PHE:HE1	1.78	0.49
25:f:725:SER:O	25:f:729:MET:HG3	2.13	0.49
2:B:158:ALA:O	2:B:160:ILE:HG23	2.11	0.49
23:d:251:ILE:HD12	23:d:251:ILE:O	2.13	0.49
27:u:144:HIS:HB3	27:u:156:PHE:O	2.13	0.49
4:D:92:PHE:HZ	4:D:95:ALA:HB2	1.78	0.49
9:I:72:MET:SD	9:I:107:CYS:HA	2.52	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:U:899:ARG:NH2	14:U:916:ASP:OD2	2.46	0.49
16:W:331:GLY:HA3	16:W:337:ALA:HB2	1.94	0.49
25:f:106:LEU:HA	25:f:109:ILE:HD12	1.94	0.49
25:f:494:ARG:HG2	25:f:497:VAL:H	1.77	0.49
25:f:654:VAL:HG22	25:f:678:LEU:HD13	1.95	0.49
1:A:181:LYS:O	1:A:185:GLU:HG3	2.13	0.49
9:I:147:LEU:HD21	9:I:162:THR:HG22	1.94	0.49
14:U:416:GLU:OE2	14:U:453:HIS:ND1	2.45	0.49
25:f:319:GLU:OE1	25:f:324:VAL:HG21	2.12	0.49
26:g:130:VAL:HB	26:g:154:MET:SD	2.53	0.49
8:H:203:MET:HA	8:H:207:ASN:HD21	1.78	0.49
10:J:80:ALA:O	10:J:84:ILE:HG13	2.13	0.49
10:J:169:ARG:O	10:J:173:GLU:HG3	2.13	0.49
14:U:554:LEU:HD22	14:U:761:VAL:HG22	1.94	0.49
15:V:228:ARG:HD3	15:V:257:ASN:OD1	2.13	0.49
17:X:20:ARG:O	17:X:24:ILE:HG12	2.13	0.49
17:X:197:ALA:HB1	17:X:202:CYS:SG	2.53	0.49
21:b:25:ARG:NH1	21:b:144:GLY:HA2	2.28	0.49
22:c:278:GLN:HG3	22:c:283:HIS:CD2	2.48	0.49
25:f:82:ILE:HD13	25:f:128:VAL:HG21	1.93	0.49
25:f:373:ALA:HB2	25:f:760:PHE:HD1	1.78	0.49
1:A:300:LEU:HD22	6:F:287:GLU:HB3	1.95	0.48
14:U:78:LEU:O	14:U:82:LEU:HD12	2.13	0.48
16:W:260:SER:HA	16:W:263:TRP:NE1	2.28	0.48
1:A:140:VAL:HB	1:A:149:ILE:HG23	1.96	0.48
10:J:40:ILE:HD11	10:J:210:VAL:HB	1.95	0.48
12:L:132:LEU:HB2	12:L:147:THR:HB	1.96	0.48
14:U:371:ILE:HB	14:U:732:LEU:HD21	1.95	0.48
14:U:789:ILE:HB	14:U:911:ILE:HA	1.95	0.48
18:Y:45:VAL:HG11	18:Y:54:TYR:HD2	1.79	0.48
21:b:48:ASN:HB3	21:b:64:LEU:HB3	1.95	0.48
25:f:466:LEU:HD12	25:f:485:LEU:HD23	1.95	0.48
3:C:351:MET:SD	3:C:362:VAL:HG21	2.54	0.48
4:D:164:TYR:H	4:D:222:HIS:CE1	2.31	0.48
4:D:238:LYS:HB2	4:D:238:LYS:NZ	2.27	0.48
13:M:206:ASP:OD1	13:M:206:ASP:N	2.47	0.48
14:U:756:HIS:HB3	14:U:759:SER:HB2	1.94	0.48
1:A:206:ILE:HD12	6:F:404:GLY:HA3	1.95	0.48
4:D:245:ARG:O	4:D:248:ARG:HG2	2.14	0.48
5:E:237:ALA:HB1	6:F:308:ARG:HG2	1.96	0.48
7:G:171:LYS:HB3	7:G:205:VAL:HG11	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:105:ILE:HD13	9:I:110:LEU:HD13	1.95	0.48
25:f:72:ARG:NH2	25:f:118:ASN:HA	2.28	0.48
25:f:296:PHE:CE1	25:f:320:ILE:HG23	2.48	0.48
17:X:407:MET:HE1	22:c:255:TYR:HD2	1.78	0.48
18:Y:385:ARG:HG3	18:Y:389:MET:HE2	1.95	0.48
25:f:491:GLY:N	25:f:524:MET:O	2.28	0.48
1:A:217:PRO:HD2	1:A:220:THR:HG21	1.95	0.48
3:C:48:GLN:HB3	4:D:65:GLN:NE2	2.28	0.48
4:D:264:ILE:HD12	4:D:309:MET:HE2	1.94	0.48
5:E:304:PRO:HB2	5:E:309:ARG:HG2	1.96	0.48
9:I:51:ASN:HB3	9:I:56:LEU:HD13	1.94	0.48
10:J:86:ARG:HH22	10:J:117:ARG:HH22	1.60	0.48
16:W:21:SER:OG	16:W:22:ALA:N	2.45	0.48
17:X:171:LEU:HD21	17:X:210:LEU:HD12	1.96	0.48
25:f:449:GLY:HA2	25:f:488:ALA:HB2	1.95	0.48
26:g:92:ARG:HH12	26:g:157:GLU:HG2	1.77	0.48
26:g:110:ARG:NH1	26:g:139:GLY:HA2	2.29	0.48
12:L:7:ASP:HB2	12:L:24:TYR:CE2	2.48	0.48
16:W:370:TYR:OH	20:a:308:GLU:OE1	2.29	0.48
23:d:344:ARG:O	23:d:348:MET:HB3	2.13	0.48
25:f:473:ASN:OD1	25:f:473:ASN:N	2.42	0.48
25:f:796:LEU:O	25:f:800:LEU:HD22	2.13	0.48
25:f:840:LEU:HD21	25:f:887:PHE:CE2	2.49	0.48
15:V:426:LEU:HB2	15:V:428:LEU:HG	1.95	0.48
20:a:80:ILE:O	20:a:84:VAL:HG23	2.12	0.48
26:g:92:ARG:NH1	26:g:157:GLU:HG2	2.29	0.48
27:u:152:LYS:HD3	27:u:262:TYR:CD1	2.48	0.48
27:u:198:ILE:HD11	27:u:238:PHE:CD1	2.49	0.48
3:C:187:LEU:HB2	3:C:311:ILE:HD13	1.96	0.48
3:C:336:MET:HE3	3:C:378:VAL:HG21	1.95	0.48
4:D:341:LYS:HG2	4:D:375:ILE:HD11	1.95	0.48
15:V:429:ASP:OD2	15:V:429:ASP:N	2.47	0.48
20:a:217:LEU:HD21	20:a:237:LEU:HB3	1.96	0.48
8:H:188:ILE:HD11	8:H:212:ILE:HG21	1.96	0.48
10:J:225:ILE:O	10:J:229:VAL:HG23	2.14	0.48
14:U:333:MET:SD	14:U:795:LEU:HD12	2.54	0.48
17:X:395:LYS:HB2	22:c:242:GLU:OE1	2.14	0.48
19:Z:16:LEU:HD22	22:c:216:MET:HE3	1.95	0.48
23:d:146:ASP:O	23:d:150:ILE:HD12	2.14	0.48
25:f:249:LEU:HD12	25:f:272:LEU:HD12	1.95	0.48
25:f:267:ARG:HE	25:f:783:SER:HB3	1.79	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:f:562:LEU:HD11	25:f:576:ILE:HG21	1.94	0.48
27:u:230:ILE:HD12	27:u:230:ILE:O	2.14	0.48
1:A:190:VAL:HG11	1:A:212:VAL:HG23	1.96	0.47
1:A:190:VAL:HG21	1:A:339:ARG:HG3	1.95	0.47
4:D:336:PRO:HB3	4:D:340:GLN:HB3	1.95	0.47
20:a:8:LEU:HD11	20:a:26:GLU:HB2	1.95	0.47
20:a:195:GLU:O	20:a:199:THR:HG22	2.14	0.47
20:a:197:ALA:HB2	20:a:221:VAL:HG22	1.96	0.47
25:f:335:ARG:HG2	25:f:335:ARG:HH11	1.79	0.47
12:L:157:ARG:HD2	12:L:176:MET:SD	2.54	0.47
14:U:217:CYS:O	14:U:221:ILE:HG13	2.14	0.47
14:U:701:ILE:HG13	14:U:810:THR:HA	1.96	0.47
21:b:184:ILE:HD12	21:b:185:SER:N	2.28	0.47
22:c:302:ALA:O	22:c:306:THR:HG23	2.15	0.47
23:d:104:ARG:HG3	23:d:106:SER:H	1.78	0.47
2:B:232:LYS:N	28:B:501:ATP:O2B	2.35	0.47
3:C:369:TYR:HA	3:C:372:ARG:HG3	1.96	0.47
18:Y:342:ARG:NH1	18:Y:342:ARG:HB3	2.29	0.47
19:Z:193:ASN:ND2	22:c:223:LYS:HE3	2.29	0.47
25:f:88:SER:HB2	25:f:91:SER:HB2	1.94	0.47
2:B:241:ASN:C	2:B:241:ASN:HD22	2.20	0.47
6:F:98:ASP:OD1	6:F:98:ASP:N	2.48	0.47
6:F:276:LYS:HG3	6:F:323:ASN:HD21	1.80	0.47
9:I:197:LEU:HB3	9:I:206:LEU:HD11	1.96	0.47
15:V:122:THR:HG21	15:V:150:ARG:HB2	1.96	0.47
20:a:112:ILE:HB	20:a:151:VAL:HG21	1.97	0.47
2:B:193:GLN:HG3	2:B:351:ILE:HG22	1.97	0.47
8:H:58:ASP:HB3	8:H:61:SER:HB3	1.96	0.47
14:U:269:ARG:HH11	14:U:269:ARG:HG3	1.78	0.47
16:W:378:MET:HE1	16:W:393:LEU:HD13	1.95	0.47
16:W:397:VAL:HG11	17:X:341:PRO:HA	1.97	0.47
20:a:273:GLN:HG2	20:a:300:ALA:HB1	1.97	0.47
20:a:366:LEU:HD21	23:d:337:LYS:HZ3	1.78	0.47
25:f:53:GLN:HA	25:f:56:LEU:HG	1.96	0.47
25:f:293:GLN:HE22	25:f:898:VAL:HA	1.80	0.47
25:f:463:LEU:O	25:f:467:SER:OG	2.18	0.47
5:E:272:ARG:HG2	5:E:272:ARG:NH1	2.29	0.47
11:K:149:LYS:HB3	11:K:149:LYS:HE3	1.62	0.47
14:U:748:LEU:HD23	14:U:760:VAL:HG22	1.95	0.47
15:V:345:ARG:NE	24:e:46:ASP:OD2	2.29	0.47
16:W:47:LEU:HD23	16:W:47:LEU:HA	1.77	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Y:220:VAL:HG21	18:Y:249:VAL:HG21	1.97	0.47
18:Y:316:LEU:HD22	18:Y:330:ILE:HG23	1.97	0.47
25:f:213:GLN:HA	25:f:213:GLN:OE1	2.13	0.47
2:B:174:MET:HB3	2:B:248:LEU:HB3	1.95	0.47
2:B:199:GLU:O	2:B:211:TYR:OH	2.32	0.47
2:B:225:TYR:CE2	2:B:352:GLU:HG3	2.50	0.47
2:B:401:GLU:OE2	2:B:425:ASN:ND2	2.45	0.47
3:C:135:VAL:O	3:C:139:MET:HG3	2.14	0.47
3:C:299:ASP:OD1	3:C:299:ASP:N	2.40	0.47
8:H:71:HIS:CD2	8:H:140:ASN:HD21	2.33	0.47
8:H:168:VAL:O	8:H:172:THR:HG23	2.15	0.47
11:K:12:VAL:HG22	11:K:125:GLU:HG3	1.96	0.47
11:K:59:MET:HE3	11:K:64:ILE:HD11	1.97	0.47
12:L:226:ASP:OD1	12:L:226:ASP:N	2.47	0.47
14:U:833:LEU:HD12	25:f:607:LEU:HD13	1.96	0.47
15:V:109:ASN:H	15:V:112:VAL:HB	1.80	0.47
16:W:259:GLU:OE2	16:W:261:GLU:HB3	2.15	0.47
17:X:230:SER:O	17:X:234:GLU:HG3	2.15	0.47
19:Z:191:ILE:HD12	20:a:374:ILE:HD11	1.96	0.47
20:a:275:LEU:HD23	20:a:278:MET:HE2	1.96	0.47
24:e:61:GLU:OE1	24:e:61:GLU:N	2.47	0.47
25:f:217:LEU:HG	25:f:221:ILE:HD11	1.96	0.47
2:B:63:LEU:HD13	25:f:239:TYR:HB2	1.97	0.47
2:B:235:LEU:HD23	2:B:353:PHE:HZ	1.80	0.47
2:B:361:LYS:HB3	2:B:384:ILE:HD13	1.96	0.47
3:C:188:LEU:HB3	3:C:317:PHE:CE1	2.50	0.47
4:D:164:TYR:H	4:D:222:HIS:HE1	1.61	0.47
14:U:62:LEU:O	14:U:65:SER:OG	2.27	0.47
17:X:416:ASN:HA	17:X:419:LYS:HE3	1.97	0.47
25:f:233:LEU:HD21	25:f:252:ALA:HB2	1.96	0.47
25:f:612:LEU:HA	25:f:615:ILE:HD12	1.96	0.47
27:u:141:SER:HB3	27:u:158:GLU:HG3	1.96	0.47
1:A:248:LYS:HD3	2:B:259:TYR:HB3	1.97	0.47
4:D:167:ILE:HG21	4:D:170:MET:HE2	1.96	0.47
15:V:121:PHE:O	15:V:150:ARG:NH2	2.40	0.47
15:V:349:ARG:NH2	24:e:41:ASP:OD2	2.48	0.47
16:W:307:LYS:O	16:W:311:THR:HG23	2.15	0.47
18:Y:205:VAL:HA	18:Y:219:PHE:HE2	1.80	0.47
19:Z:178:ASP:OD1	19:Z:178:ASP:N	2.37	0.47
23:d:283:LEU:HB3	23:d:286:GLU:HB2	1.95	0.47
25:f:731:MET:HE1	25:f:796:LEU:HD22	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:62:LYS:HB3	12:L:62:LYS:HE3	1.65	0.47
14:U:520:MET:HE2	14:U:525:ASN:HD21	1.79	0.47
14:U:564:ASP:OD1	14:U:590:TYR:OH	2.32	0.47
17:X:166:LEU:O	17:X:170:GLN:HG3	2.15	0.47
19:Z:285:ALA:HA	19:Z:288:LYS:HE2	1.97	0.47
23:d:230:VAL:O	23:d:234:GLN:HG3	2.14	0.47
25:f:187:LEU:O	25:f:191:ILE:N	2.43	0.47
1:A:110:LYS:NZ	6:F:162:GLU:OE1	2.49	0.46
6:F:124:ILE:HD13	6:F:153:VAL:HG11	1.97	0.46
12:L:19:ILE:HD12	12:L:22:ILE:HD12	1.97	0.46
14:U:30:VAL:HB	14:U:34:PHE:HD2	1.80	0.46
14:U:431:THR:HB	14:U:435:SER:HB3	1.97	0.46
20:a:64:ILE:HA	20:a:67:PHE:CE2	2.51	0.46
20:a:198:PHE:CD1	20:a:230:ARG:HD2	2.50	0.46
22:c:63:ASP:N	22:c:63:ASP:OD2	2.48	0.46
22:c:113:HIS:NE2	22:c:115:HIS:CD2	2.82	0.46
22:c:157:ILE:HG23	22:c:205:ILE:HD12	1.97	0.46
23:d:143:LEU:O	23:d:147:ILE:HD12	2.15	0.46
25:f:82:ILE:HG21	25:f:128:VAL:HG21	1.96	0.46
25:f:321:MET:HE2	25:f:321:MET:O	2.15	0.46
25:f:452:ASN:O	25:f:452:ASN:ND2	2.44	0.46
6:F:177:VAL:HG12	6:F:248:PHE:HB3	1.97	0.46
14:U:637:VAL:HG11	14:U:656:LEU:HG	1.98	0.46
16:W:435:LEU:HD21	20:a:356:TRP:HH2	1.80	0.46
17:X:398:GLU:O	17:X:402:GLU:HG3	2.15	0.46
22:c:130:GLN:HG2	22:c:162:LEU:HG	1.96	0.46
2:B:384:ILE:HG22	2:B:385:MET:SD	2.56	0.46
5:E:67:GLU:OE2	5:E:85:ARG:NE	2.29	0.46
5:E:351:GLY:HA3	6:F:217:ILE:HD13	1.98	0.46
8:H:107:THR:O	8:H:111:VAL:HG23	2.15	0.46
8:H:219:ARG:NH2	8:H:225:GLU:OE1	2.29	0.46
9:I:38:LEU:HD12	9:I:43:VAL:HB	1.97	0.46
10:J:76:LEU:HB2	10:J:79:ASP:HB2	1.98	0.46
15:V:199:ASN:OD1	15:V:241:ARG:NE	2.48	0.46
16:W:105:VAL:HG12	16:W:141:GLU:HG2	1.97	0.46
16:W:226:TYR:CE1	16:W:230:MET:HE3	2.50	0.46
26:g:130:VAL:HG13	26:g:134:LYS:C	2.40	0.46
1:A:338:ASP:OD2	1:A:338:ASP:N	2.48	0.46
2:B:112:LEU:HD11	2:B:115:ILE:HG13	1.98	0.46
3:C:222:LYS:HB2	3:C:222:LYS:HE3	1.56	0.46
4:D:77:GLU:OE1	4:D:80:LYS:HE2	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:388:ARG:NH2	5:E:143:ARG:HH12	2.13	0.46
5:E:342:ASP:OD2	5:E:378:LYS:HD3	2.14	0.46
7:G:191:PHE:O	7:G:195:VAL:HG23	2.15	0.46
9:I:40:ASN:ND2	9:I:182:GLY:O	2.43	0.46
9:I:233:VAL:HA	9:I:236:LEU:HD12	1.97	0.46
12:L:94:ASP:O	12:L:98:VAL:HG23	2.15	0.46
15:V:483:CYS:SG	18:Y:377:LEU:HD21	2.55	0.46
20:a:324:ILE:HG23	20:a:331:VAL:HG22	1.98	0.46
25:f:887:PHE:HB3	25:f:900:LEU:HB3	1.97	0.46
5:E:125:GLU:HB3	5:E:197:LYS:HD2	1.96	0.46
7:G:84:THR:HB	13:M:156:VAL:HG22	1.96	0.46
14:U:86:ASP:N	14:U:86:ASP:OD1	2.49	0.46
15:V:285:TRP:HB3	15:V:315:LYS:HD3	1.96	0.46
16:W:268:LYS:NZ	16:W:336:PRO:O	2.41	0.46
17:X:348:GLU:HB3	17:X:358:LYS:NZ	2.30	0.46
19:Z:263:ALA:HB1	22:c:288:VAL:HG13	1.98	0.46
20:a:6:GLY:O	20:a:10:GLN:N	2.41	0.46
20:a:284:ARG:HE	20:a:291:LEU:HD22	1.79	0.46
23:d:251:ILE:HD13	23:d:253:ALA:O	2.16	0.46
25:f:441:LYS:HE2	25:f:469:TYR:CE2	2.50	0.46
1:A:83:ASP:OD2	2:B:137:SER:OG	2.27	0.46
15:V:71:THR:HG22	15:V:107:ARG:NH1	2.31	0.46
18:Y:297:ARG:O	18:Y:301:ILE:HG13	2.16	0.46
25:f:215:ASP:N	25:f:215:ASP:OD2	2.48	0.46
1:A:280:ILE:O	1:A:299:MET:HB2	2.16	0.46
12:L:49:LEU:HD11	12:L:199:LEU:HD21	1.97	0.46
14:U:616:ARG:HH22	14:U:771:PHE:HZ	1.63	0.46
22:c:104:ARG:HD2	22:c:106:GLU:HG3	1.97	0.46
25:f:57:GLU:OE2	25:f:102:HIS:NE2	2.48	0.46
27:u:129:PHE:HE2	27:u:173:GLN:HB2	1.80	0.46
10:J:143:ARG:HA	10:J:143:ARG:HD2	1.78	0.46
14:U:875:PHE:C	14:U:875:PHE:CD1	2.93	0.46
19:Z:198:LEU:HD11	22:c:304:LEU:HD13	1.97	0.46
20:a:366:LEU:HD21	23:d:337:LYS:NZ	2.31	0.46
3:C:59:LEU:HD21	4:D:76:GLN:HG3	1.97	0.46
5:E:118:LEU:HD13	5:E:214:LEU:HD21	1.98	0.46
6:F:128:THR:HG22	6:F:128:THR:O	2.16	0.46
16:W:59:ASP:O	16:W:63:THR:OG1	2.29	0.46
16:W:220:GLU:H	16:W:220:GLU:HG3	1.56	0.46
21:b:103:LYS:HA	21:b:103:LYS:HD3	1.84	0.46
25:f:301:HIS:HA	25:f:782:HIS:HE1	1.80	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:f:784:ASP:OD1	25:f:785:ARG:NH2	2.49	0.46
25:f:788:MET:SD	25:f:793:VAL:HG21	2.56	0.46
25:f:902:LYS:N	25:f:902:LYS:HD3	2.31	0.46
25:f:903:ASN:HB3	25:f:906:TYR:HB2	1.98	0.46
26:g:97:ARG:HB3	26:g:98:LYS:HE2	1.97	0.46
26:g:134:LYS:HD3	26:g:137:GLN:HE22	1.79	0.46
1:A:260:LEU:HD22	1:A:272:ILE:HD13	1.97	0.46
5:E:161:ARG:HG2	5:E:161:ARG:HH11	1.81	0.46
5:E:177:GLY:N	6:F:344:ARG:HD2	2.31	0.46
14:U:807:LYS:O	14:U:810:THR:HG22	2.16	0.46
15:V:117:VAL:HG21	15:V:135:LEU:HD21	1.98	0.46
15:V:395:ILE:O	15:V:398:LEU:HB2	2.16	0.46
17:X:84:LYS:HE2	17:X:84:LYS:HB2	1.77	0.46
19:Z:253:THR:O	19:Z:257:MET:HG2	2.16	0.46
20:a:89:ASP:HB3	20:a:92:VAL:HG22	1.97	0.46
22:c:146:ASP:HB3	22:c:156:VAL:HB	1.97	0.46
25:f:239:TYR:CE2	25:f:664:GLU:HG3	2.52	0.46
26:g:128:LYS:O	26:g:129:ILE:HD13	2.15	0.46
2:B:133:VAL:HB	2:B:158:ALA:HA	1.99	0.45
3:C:62:GLU:OE1	4:D:117:SER:OG	2.27	0.45
5:E:87:LEU:HD23	5:E:87:LEU:HA	1.84	0.45
14:U:82:LEU:HD23	14:U:129:ARG:HB2	1.98	0.45
15:V:224:LEU:HD12	15:V:257:ASN:ND2	2.32	0.45
20:a:36:GLN:HG3	21:b:18:ASN:HD21	1.81	0.45
20:a:100:THR:O	20:a:104:VAL:HG22	2.16	0.45
26:g:122:LEU:HD23	26:g:122:LEU:HA	1.80	0.45
3:C:132:ASP:OD1	3:C:241:HIS:NE2	2.49	0.45
3:C:231:VAL:HG11	3:C:272:THR:HG23	1.97	0.45
4:D:81:ARG:NH2	22:c:149:GLN:OE1	2.33	0.45
4:D:401:LYS:HE2	4:D:401:LYS:HB2	1.74	0.45
12:L:96:ARG:NH1	12:L:102:PRO:HA	2.31	0.45
16:W:112:VAL:HG13	16:W:121:LYS:HE3	1.97	0.45
16:W:263:TRP:CE3	16:W:295:LYS:HD3	2.51	0.45
17:X:47:GLU:O	17:X:50:ILE:HG22	2.16	0.45
20:a:367:VAL:HG13	23:d:340:ILE:HD11	1.99	0.45
27:u:221:THR:HG23	27:u:223:ASP:H	1.79	0.45
1:A:306:LEU:HD21	1:A:317:VAL:HG11	1.98	0.45
2:B:121:ALA:HB2	2:B:135:ILE:HD11	1.99	0.45
14:U:20:LYS:HE3	14:U:48:LEU:HD11	1.98	0.45
14:U:186:SER:HB3	14:U:187:LEU:HD22	1.97	0.45
14:U:640:LEU:HD22	14:U:648:VAL:HG11	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:W:366:MET:O	16:W:370:TYR:HB2	2.16	0.45
19:Z:14:LEU:HD22	22:c:43:LYS:HD3	1.99	0.45
20:a:286:ALA:HA	20:a:289:ARG:HG3	1.97	0.45
21:b:161:ASN:ND2	21:b:168:SER:O	2.50	0.45
3:C:316:GLU:HG2	3:C:318:PRO:HD3	1.98	0.45
4:D:169:GLY:O	4:D:340:GLN:HG3	2.16	0.45
10:J:69:VAL:HG11	10:J:107:ILE:HG21	1.98	0.45
12:L:39:LYS:HA	12:L:44:ALA:HA	1.98	0.45
15:V:124:ASN:HA	15:V:128:ARG:HD3	1.98	0.45
16:W:448:LYS:HE3	16:W:448:LYS:HB3	1.63	0.45
20:a:320:VAL:HB	20:a:333:MET:HE1	1.97	0.45
22:c:61:PHE:HB3	22:c:139:ARG:HH21	1.81	0.45
1:A:301:GLU:O	1:A:305:GLN:HG2	2.16	0.45
16:W:73:MET:HG2	16:W:73:MET:H	1.61	0.45
17:X:369:ILE:HG21	18:Y:310:SER:HA	1.98	0.45
2:B:422:SER:O	2:B:426:VAL:HG22	2.17	0.45
3:C:119:ASP:OD1	3:C:119:ASP:N	2.45	0.45
9:I:63:GLU:OE1	9:I:64:LYS:HG3	2.17	0.45
17:X:251:LEU:HA	17:X:254:MET:HE3	1.98	0.45
18:Y:133:ALA:HB3	18:Y:136:HIS:HB2	1.98	0.45
18:Y:164:ALA:O	18:Y:168:ILE:HG13	2.17	0.45
21:b:67:ASP:OD1	21:b:68:THR:N	2.50	0.45
25:f:83:ARG:HD3	25:f:86:THR:HB	1.97	0.45
25:f:600:TYR:CE1	25:f:608:LYS:HE3	2.52	0.45
3:C:340:ARG:NH1	18:Y:211:TYR:OH	2.29	0.45
9:I:82:ASP:CG	9:I:128:ARG:HH22	2.25	0.45
12:L:50:LYS:HB3	12:L:59:HIS:HB3	1.98	0.45
13:M:87:LEU:HD23	13:M:135:PHE:CE1	2.52	0.45
16:W:212:LYS:HB3	16:W:212:LYS:HE3	1.70	0.45
20:a:246:GLU:H	20:a:246:GLU:CD	2.25	0.45
21:b:44:ASN:OD1	21:b:45:PRO:HD2	2.16	0.45
21:b:107:MET:HG3	21:b:136:VAL:HG22	1.98	0.45
25:f:679:LEU:HD23	25:f:687:ARG:HG2	1.98	0.45
26:g:128:LYS:HE2	26:g:158:LEU:CD2	2.45	0.45
3:C:139:MET:O	4:D:326:ARG:NH2	2.46	0.45
4:D:212:LYS:NZ	28:D:501:ATP:O1B	2.44	0.45
7:G:32:ILE:HA	7:G:82:GLY:HA2	1.98	0.45
8:H:33:ALA:HB3	8:H:64:LYS:NZ	2.32	0.45
12:L:36:VAL:HG22	12:L:160:SER:HB2	1.97	0.45
14:U:261:LEU:O	14:U:265:ILE:HG12	2.15	0.45
14:U:372:ALA:O	14:U:376:MET:HG3	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:U:581:SER:O	14:U:585:THR:OG1	2.32	0.45
18:Y:175:ASP:O	18:Y:179:ARG:HG3	2.16	0.45
18:Y:363:ASN:O	18:Y:367:GLN:HG2	2.17	0.45
23:d:150:ILE:HD12	23:d:150:ILE:H	1.81	0.45
25:f:182:GLU:HB2	25:f:183:PRO:HD3	1.99	0.45
25:f:649:HIS:CD2	25:f:649:HIS:C	2.94	0.45
27:u:220:LEU:HD22	27:u:231:VAL:HG21	1.98	0.45
1:A:127:ASP:OD1	1:A:127:ASP:N	2.48	0.45
2:B:403:GLY:HA3	3:C:180:ILE:HG21	1.99	0.45
7:G:165:ALA:HB3	8:H:56:LEU:HD22	1.97	0.45
8:H:150:ASP:OD1	8:H:154:ALA:N	2.46	0.45
11:K:74:ILE:HD12	11:K:109:VAL:HG13	1.98	0.45
14:U:672:LEU:HA	14:U:675:MET:HG3	1.99	0.45
18:Y:165:LYS:HZ3	18:Y:165:LYS:HG3	1.34	0.45
19:Z:129:LYS:HA	19:Z:129:LYS:HD3	1.70	0.45
20:a:156:TYR:O	20:a:160:SER:OG	2.22	0.45
25:f:256:PHE:CE2	25:f:264:GLU:HB2	2.52	0.45
1:A:222:LYS:HB2	1:A:222:LYS:HE2	1.72	0.45
3:C:84:LYS:NZ	3:C:98:ASP:OD1	2.36	0.45
3:C:139:MET:HE3	3:C:139:MET:HB3	1.89	0.45
13:M:187:ARG:HH11	13:M:187:ARG:HG3	1.82	0.45
14:U:52:GLU:OE2	14:U:52:GLU:N	2.48	0.45
14:U:244:MET:HA	14:U:903:PHE:HE2	1.82	0.45
14:U:748:LEU:H	14:U:748:LEU:HD12	1.81	0.45
17:X:379:ASP:HB3	17:X:384:VAL:HG22	1.99	0.45
18:Y:224:VAL:O	18:Y:228:MET:HG3	2.17	0.45
18:Y:385:ARG:HE	18:Y:385:ARG:HB2	1.50	0.45
19:Z:19:VAL:HG22	19:Z:95:TYR:CZ	2.52	0.45
20:a:352:ARG:HG2	20:a:352:ARG:HH11	1.82	0.45
23:d:145:ARG:NH2	23:d:182:LEU:HB3	2.32	0.45
25:f:495:GLU:O	25:f:499:THR:OG1	2.24	0.45
25:f:765:ALA:O	25:f:769:THR:HG22	2.17	0.45
1:A:87:LEU:HD22	2:B:156:VAL:HG21	1.99	0.44
1:A:303:ILE:HG13	1:A:331:LEU:HD12	1.99	0.44
2:B:92:GLN:OE1	2:B:92:GLN:N	2.40	0.44
2:B:190:LEU:HB3	2:B:193:GLN:HB2	1.98	0.44
5:E:204:VAL:HG21	6:F:308:ARG:HD2	1.99	0.44
13:M:192:GLU:O	13:M:196:ILE:HG13	2.17	0.44
16:W:41:GLN:CD	16:W:41:GLN:N	2.75	0.44
17:X:351:SER:HA	17:X:354:ILE:HG22	1.99	0.44
19:Z:165:GLU:HG2	19:Z:166:GLU:H	1.82	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:a:33:LEU:HB3	20:a:36:GLN:HG3	1.99	0.44
22:c:248:MET:HG2	22:c:284:LEU:HD12	1.99	0.44
25:f:460:ASP:HB3	26:g:133:LYS:HG2	1.99	0.44
2:B:197:ILE:O	2:B:201:VAL:HG22	2.17	0.44
5:E:352:MET:HE1	6:F:200:GLU:HG3	1.99	0.44
7:G:6:SER:OG	7:G:11:ARG:NE	2.49	0.44
7:G:65:THR:HG21	13:M:159:GLY:HA3	1.99	0.44
13:M:27:MET:HE3	13:M:153:PRO:HD2	1.99	0.44
13:M:189:ILE:O	13:M:193:VAL:HG23	2.17	0.44
14:U:231:ASP:O	14:U:235:LYS:HG2	2.16	0.44
15:V:305:ALA:O	15:V:309:MET:HG3	2.18	0.44
20:a:308:GLU:O	20:a:312:MET:HG2	2.17	0.44
25:f:136:GLU:OE1	25:f:136:GLU:N	2.33	0.44
25:f:457:ASN:HD21	25:f:461:PRO:HD3	1.82	0.44
25:f:560:LEU:O	25:f:564:LEU:N	2.43	0.44
1:A:372:LEU:HD21	11:K:207:GLU:HG3	1.98	0.44
4:D:313:ARG:HA	4:D:313:ARG:HD2	1.73	0.44
11:K:35:SER:HB2	11:K:51:GLU:HG2	1.98	0.44
13:M:175:GLU:HB2	13:M:196:ILE:HG23	1.99	0.44
16:W:435:LEU:HD21	20:a:356:TRP:CH2	2.52	0.44
25:f:77:GLU:O	25:f:81:GLN:N	2.49	0.44
27:u:177:LEU:HD12	27:u:238:PHE:HD1	1.83	0.44
2:B:359:LYS:HB2	2:B:359:LYS:HE2	1.79	0.44
3:C:114:VAL:HG11	3:C:123:LEU:HD11	1.99	0.44
3:C:204:ALA:HB2	3:C:245:ILE:HD12	1.98	0.44
5:E:235:ILE:HG22	5:E:279:THR:HB	1.99	0.44
7:G:194:THR:HA	7:G:197:THR:HG22	1.98	0.44
9:I:220:ASN:CG	9:I:220:ASN:O	2.61	0.44
10:J:208:LEU:HD12	10:J:208:LEU:HA	1.75	0.44
15:V:68:ASP:O	15:V:71:THR:OG1	2.32	0.44
15:V:169:LEU:HD13	15:V:210:CYS:HA	1.99	0.44
15:V:309:MET:HE2	15:V:309:MET:HB3	1.93	0.44
16:W:105:VAL:HG22	16:W:128:LEU:HD22	1.99	0.44
17:X:255:LEU:HD22	17:X:267:VAL:HG13	1.98	0.44
19:Z:252:LYS:O	19:Z:256:GLN:HG3	2.18	0.44
25:f:119:LYS:O	25:f:119:LYS:HG2	2.18	0.44
25:f:663:GLY:HA2	25:f:781:TYR:OH	2.17	0.44
26:g:137:GLN:H	26:g:137:GLN:CD	2.23	0.44
5:E:206:LYS:HB2	6:F:260:PHE:HB3	1.99	0.44
9:I:15:GLU:HB2	9:I:17:ARG:HD2	1.99	0.44
9:I:45:LEU:HD13	9:I:75:SER:HB2	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:U:108:TYR:CE2	14:U:126:ILE:HG21	2.51	0.44
17:X:259:ILE:HD11	17:X:267:VAL:HG21	1.99	0.44
18:Y:5:ASN:N	18:Y:5:ASN:OD1	2.50	0.44
20:a:122:LYS:HE2	20:a:122:LYS:HB2	1.68	0.44
22:c:68:ARG:NH1	22:c:208:ARG:HH21	2.14	0.44
23:d:108:ASN:HB3	23:d:111:LYS:CE	2.45	0.44
25:f:129:LEU:O	25:f:132:THR:OG1	2.35	0.44
25:f:213:GLN:HB3	25:f:216:MET:HE2	1.99	0.44
25:f:305:LEU:HD12	25:f:305:LEU:HA	1.80	0.44
25:f:478:ARG:NH1	25:f:507:ASP:OD2	2.47	0.44
1:A:93:LEU:HD23	1:A:151:ILE:HG22	1.99	0.44
1:A:140:VAL:HG21	1:A:149:ILE:HG12	2.00	0.44
1:A:203:ASN:OD1	1:A:204:LEU:N	2.51	0.44
6:F:257:VAL:HG13	6:F:306:VAL:HG22	2.00	0.44
6:F:402:GLU:O	6:F:406:ILE:HG12	2.17	0.44
9:I:38:LEU:HD11	9:I:145:PHE:HB3	1.99	0.44
9:I:125:GLY:O	9:I:127:LYS:NZ	2.43	0.44
13:M:73:VAL:HG22	13:M:139:SER:HB2	1.99	0.44
14:U:789:ILE:HD13	14:U:881:PRO:HB3	1.99	0.44
15:V:338:LEU:HD23	15:V:398:LEU:HD23	1.98	0.44
16:W:17:GLU:OE1	16:W:17:GLU:N	2.51	0.44
1:A:42:SER:O	1:A:46:LYS:HG2	2.18	0.44
3:C:49:ARG:HE	4:D:64:GLU:CD	2.26	0.44
3:C:371:LEU:HD21	4:D:183:LEU:HD23	2.00	0.44
5:E:148:VAL:HG22	5:E:167:PRO:HB2	2.00	0.44
9:I:25:MET:HE2	9:I:151:ASP:HB3	1.99	0.44
9:I:145:PHE:CZ	9:I:218:ARG:HG2	2.52	0.44
13:M:70:ASP:OD1	13:M:71:ARG:N	2.48	0.44
13:M:120:HIS:O	13:M:123:THR:OG1	2.31	0.44
15:V:192:MET:HE3	15:V:214:HIS:HB2	2.00	0.44
17:X:70:LEU:HD23	17:X:109:LEU:HD12	2.00	0.44
17:X:126:ARG:NH1	17:X:156:GLU:OE2	2.50	0.44
22:c:70:ILE:HD13	22:c:70:ILE:HA	1.85	0.44
23:d:244:VAL:HG11	23:d:267:ILE:HG13	2.00	0.44
25:f:221:ILE:HG22	25:f:259:PHE:HE2	1.81	0.44
25:f:347:ASP:O	25:f:350:LYS:NZ	2.50	0.44
25:f:460:ASP:OD2	25:f:460:ASP:C	2.61	0.44
1:A:273:PHE:CD1	1:A:318:LEU:HD23	2.53	0.44
1:A:427:PRO:HG3	10:J:13:ASP:OD2	2.18	0.44
7:G:179:LEU:O	7:G:183:VAL:HG23	2.17	0.44
8:H:95:GLN:O	8:H:98:TYR:N	2.51	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:U:524:LYS:HD2	14:U:559:ARG:HD2	1.99	0.44
15:V:102:PRO:HG3	24:e:16:ASP:O	2.17	0.44
18:Y:319:MET:CE	18:Y:334:LEU:HD11	2.46	0.44
18:Y:328:GLU:OE1	18:Y:328:GLU:N	2.47	0.44
25:f:52:LEU:HB3	25:f:95:PRO:HG2	2.00	0.44
25:f:465:LEU:HA	26:g:135:GLN:NE2	2.33	0.44
25:f:505:MET:SD	25:f:537:THR:OG1	2.74	0.44
1:A:122:VAL:HG23	6:F:90:VAL:HG22	1.99	0.44
1:A:416:VAL:O	1:A:420:TYR:HB2	2.18	0.44
17:X:337:ARG:HG2	17:X:337:ARG:HH11	1.81	0.44
17:X:345:VAL:HG13	17:X:350:ILE:HD11	1.99	0.44
19:Z:84:LYS:HD3	22:c:91:PHE:HE2	1.83	0.44
20:a:160:SER:HB2	20:a:172:TYR:CE1	2.52	0.44
4:D:267:ILE:HG23	4:D:317:LEU:HD21	2.00	0.43
5:E:380:LEU:HD22	6:F:335:VAL:HG11	2.00	0.43
13:M:53:VAL:HG22	13:M:208:ALA:O	2.18	0.43
15:V:428:LEU:HD13	15:V:437:ILE:HD12	2.00	0.43
26:g:108:THR:HG21	26:g:110:ARG:NH2	2.32	0.43
1:A:75:PRO:HA	1:A:78:TRP:CG	2.53	0.43
2:B:396:LYS:O	2:B:400:THR:HG22	2.19	0.43
3:C:164:VAL:HG13	3:C:183:PRO:CB	2.47	0.43
10:J:130:SER:OG	10:J:147:THR:O	2.29	0.43
11:K:78:MET:HE2	11:K:82:ILE:HG23	1.99	0.43
12:L:193:ARG:HG2	12:L:196:ARG:NH2	2.32	0.43
12:L:199:LEU:HD11	12:L:205:LEU:HD23	2.00	0.43
14:U:376:MET:HG2	14:U:735:GLY:HA2	2.00	0.43
14:U:383:ASP:OD2	14:U:426:TYR:OH	2.18	0.43
14:U:444:TYR:OH	14:U:777:HIS:HB2	2.18	0.43
17:X:23:SER:O	17:X:27:LEU:HD12	2.17	0.43
17:X:157:LEU:HB2	17:X:166:LEU:HD13	2.00	0.43
18:Y:45:VAL:HA	18:Y:50:MET:HG3	2.00	0.43
18:Y:228:MET:SD	18:Y:260:LEU:HA	2.58	0.43
19:Z:252:LYS:HD3	19:Z:252:LYS:HA	1.68	0.43
25:f:216:MET:HE3	25:f:216:MET:HB2	1.79	0.43
1:A:277:ILE:HG12	1:A:319:MET:SD	2.58	0.43
4:D:148:ASP:OD1	5:E:78:ARG:HD3	2.18	0.43
16:W:313:GLU:OE1	20:a:313:LYS:HG2	2.17	0.43
16:W:428:TRP:O	16:W:432:LEU:HG	2.17	0.43
19:Z:72:HIS:ND1	19:Z:72:HIS:C	2.76	0.43
21:b:11:ASP:HB2	21:b:112:PHE:O	2.17	0.43
25:f:68:THR:HA	25:f:71:TYR:HD1	1.83	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:138:MET:HB3	7:G:154:CYS:HB3	2.01	0.43
9:I:185:THR:OG1	9:I:186:LEU:N	2.51	0.43
10:J:8:THR:HG23	10:J:18:GLN:HB2	2.00	0.43
10:J:80:ALA:HB2	10:J:129:ILE:HG21	1.99	0.43
15:V:424:GLN:O	15:V:427:GLN:NE2	2.50	0.43
20:a:196:ARG:HG2	20:a:196:ARG:NH1	2.33	0.43
20:a:314:ALA:HB1	20:a:320:VAL:HG22	2.00	0.43
22:c:223:LYS:HB2	22:c:223:LYS:HE2	1.50	0.43
23:d:260:ILE:O	23:d:264:LEU:HD13	2.18	0.43
25:f:472:HIS:CE1	25:f:474:SER:HB3	2.54	0.43
25:f:688:ARG:HA	25:f:721:VAL:HG22	1.99	0.43
1:A:164:MET:HE2	1:A:240:VAL:HG13	2.01	0.43
1:A:301:GLU:OE1	6:F:254:PRO:HB2	2.19	0.43
4:D:161:ASP:OD1	4:D:161:ASP:N	2.43	0.43
14:U:13:ASP:CG	23:d:166:ARG:HH12	2.22	0.43
14:U:210:LYS:HE2	14:U:210:LYS:N	2.34	0.43
14:U:356:THR:HG21	14:U:734:GLN:OE1	2.18	0.43
14:U:619:VAL:HG21	14:U:648:VAL:HG13	2.00	0.43
14:U:697:GLN:NE2	14:U:786:THR:OG1	2.42	0.43
15:V:218:TYR:HA	15:V:221:LEU:HB2	2.01	0.43
15:V:338:LEU:HD23	15:V:338:LEU:HA	1.89	0.43
16:W:368:LYS:HB2	16:W:368:LYS:NZ	2.34	0.43
25:f:521:ALA:O	25:f:525:ILE:HD12	2.19	0.43
25:f:665:GLU:O	25:f:669:GLU:HG3	2.18	0.43
25:f:832:THR:HB	25:f:900:LEU:HG	2.01	0.43
27:u:261:SER:O	27:u:263:PHE:N	2.51	0.43
1:A:299:MET:SD	1:A:303:ILE:HD12	2.59	0.43
3:C:189:TYR:CZ	3:C:316:GLU:HB2	2.53	0.43
3:C:329:LEU:HG	3:C:344:LEU:HD22	2.01	0.43
4:D:205:TYR:HA	4:D:311:THR:O	2.18	0.43
13:M:140:TYR:HB3	13:M:216:VAL:HG22	2.01	0.43
13:M:173:LYS:O	13:M:177:GLU:HG3	2.19	0.43
25:f:513:GLU:OE1	25:f:814:SER:OG	2.37	0.43
25:f:893:ILE:HG22	25:f:895:GLU:HG2	1.99	0.43
27:u:200:LEU:HD22	27:u:204:MET:HG2	2.01	0.43
3:C:49:ARG:N	4:D:65:GLN:HE21	2.16	0.43
6:F:312:GLU:O	6:F:316:GLN:HG2	2.19	0.43
7:G:119:ALA:HB1	7:G:158:GLY:O	2.18	0.43
8:H:38:ILE:HB	8:H:45:VAL:HG12	2.00	0.43
10:J:30:SER:OG	10:J:48:LYS:HG3	2.18	0.43
16:W:130:MET:HE2	16:W:130:MET:HB3	1.75	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:c:210:ASN:OD1	22:c:210:ASN:N	2.41	0.43
23:d:168:MET:HG2	23:d:195:ASN:HB2	1.99	0.43
23:d:260:ILE:HD13	23:d:260:ILE:HA	1.86	0.43
25:f:289:VAL:HA	25:f:292:LYS:NZ	2.34	0.43
25:f:770:HIS:CD2	25:f:770:HIS:N	2.85	0.43
1:A:75:PRO:HA	1:A:78:TRP:CD2	2.54	0.43
1:A:209:PRO:HB3	1:A:338:ASP:HB2	2.00	0.43
2:B:387:LYS:HB3	2:B:390:LEU:HD13	2.00	0.43
3:C:23:TYR:OH	14:U:106:ASP:OD1	2.24	0.43
5:E:175:PRO:HD2	5:E:178:THR:HG21	2.01	0.43
6:F:172:VAL:HG23	6:F:267:LEU:HD22	2.00	0.43
7:G:189:TRP:HB3	7:G:193:GLN:HB2	2.00	0.43
14:U:583:MET:N	14:U:583:MET:HE2	2.33	0.43
15:V:195:ILE:HG21	15:V:207:ALA:HB2	2.01	0.43
16:W:122:LEU:HD23	16:W:122:LEU:HA	1.87	0.43
19:Z:176:LEU:HD11	22:c:217:LEU:HB2	2.01	0.43
20:a:170:ALA:HB2	20:a:208:GLU:H	1.84	0.43
21:b:64:LEU:H	21:b:64:LEU:HG	1.61	0.43
1:A:75:PRO:HB2	25:f:680:ARG:HH21	1.83	0.43
2:B:96:ARG:HH11	2:B:96:ARG:HG3	1.84	0.43
8:H:76:TYR:HB3	8:H:83:TYR:CD1	2.54	0.43
10:J:36:ARG:HD2	10:J:142:PRO:O	2.18	0.43
11:K:148:GLU:H	11:K:148:GLU:HG3	1.57	0.43
14:U:344:ARG:HD2	14:U:881:PRO:HD2	2.00	0.43
15:V:100:MET:O	15:V:104:THR:HG23	2.18	0.43
17:X:172:LEU:O	17:X:176:THR:OG1	2.29	0.43
18:Y:268:TYR:HB3	18:Y:323:PHE:CE1	2.54	0.43
25:f:790:GLN:OE1	25:f:790:GLN:HA	2.18	0.43
1:A:201:PHE:CE2	6:F:405:MET:HE1	2.54	0.43
2:B:96:ARG:HG3	2:B:96:ARG:NH1	2.34	0.43
2:B:391:SER:OG	2:B:394:ASP:OD1	2.37	0.43
2:B:411:ARG:HH22	2:B:418:ASP:CG	2.27	0.43
4:D:251:PHE:HD1	4:D:299:PHE:CE2	2.36	0.43
4:D:322:LEU:HB3	4:D:330:LYS:HE3	2.01	0.43
14:U:196:LYS:O	14:U:200:VAL:HG12	2.18	0.43
14:U:323:LEU:O	14:U:327:LYS:HD3	2.19	0.43
15:V:212:TYR:HA	15:V:253:LEU:HD11	2.00	0.43
15:V:479:ARG:HB3	19:Z:261:TYR:CE1	2.54	0.43
16:W:30:GLU:O	16:W:34:LEU:HG	2.18	0.43
20:a:132:LYS:NZ	20:a:132:LYS:HB2	2.34	0.43
25:f:100:ARG:HG2	25:f:129:LEU:HD13	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:f:829:MET:O	25:f:896:GLY:N	2.48	0.43
25:f:832:THR:HA	25:f:898:VAL:O	2.19	0.43
1:A:138:MET:HE2	1:A:138:MET:HB3	1.82	0.42
3:C:322:GLU:CD	3:C:349:GLU:HG2	2.44	0.42
4:D:157:ASP:C	4:D:157:ASP:OD2	2.62	0.42
5:E:210:GLU:OE2	5:E:213:ARG:NH2	2.37	0.42
9:I:9:THR:HB	9:I:20:GLN:HG3	2.00	0.42
10:J:107:ILE:HD12	10:J:107:ILE:HA	1.89	0.42
12:L:158:ALA:O	13:M:57:LEU:HB3	2.19	0.42
14:U:481:LEU:HG	14:U:493:VAL:HG13	2.00	0.42
16:W:180:LYS:O	16:W:184:GLU:HG3	2.19	0.42
18:Y:58:CYS:HA	18:Y:63:TRP:HB2	2.01	0.42
20:a:245:VAL:HG12	20:a:272:ILE:HG12	2.01	0.42
23:d:108:ASN:O	23:d:112:CYS:N	2.49	0.42
23:d:218:LYS:O	23:d:222:THR:HG23	2.18	0.42
23:d:242:ASN:C	23:d:242:ASN:OD1	2.62	0.42
24:e:16:ASP:N	24:e:16:ASP:OD1	2.51	0.42
27:u:163:GLU:N	27:u:256:GLU:O	2.52	0.42
1:A:333:ARG:HH21	1:A:336:ARG:NH2	2.17	0.42
3:C:347:ILE:HG23	3:C:387:VAL:HG21	2.00	0.42
8:H:143:ARG:HH21	9:I:59:VAL:HB	1.83	0.42
14:U:357:LYS:HE2	14:U:357:LYS:HB3	1.78	0.42
14:U:357:LYS:NZ	14:U:389:ASN:OD1	2.52	0.42
14:U:510:GLU:OE1	14:U:543:LYS:NZ	2.47	0.42
15:V:268:GLU:HG3	15:V:299:GLN:NE2	2.34	0.42
21:b:9:CYS:HA	21:b:52:ILE:HG22	2.00	0.42
25:f:119:LYS:NZ	25:f:146:GLY:HA2	2.33	0.42
25:f:175:ASP:HA	25:f:178:LYS:HE2	2.01	0.42
25:f:185:LEU:O	25:f:188:VAL:HG22	2.19	0.42
25:f:905:ASN:HA	25:f:908:LEU:HD13	2.01	0.42
4:D:71:GLU:HG2	14:U:644:TYR:CE2	2.53	0.42
4:D:106:THR:HB	5:E:77:PRO:HB3	2.00	0.42
11:K:107:MET:HE3	11:K:112:VAL:HG22	2.02	0.42
13:M:214:SER:OG	13:M:224:HIS:NE2	2.47	0.42
14:U:524:LYS:HE3	14:U:524:LYS:HB2	1.90	0.42
14:U:551:GLY:O	14:U:555:VAL:HG23	2.20	0.42
14:U:615:ARG:O	14:U:619:VAL:HG23	2.19	0.42
14:U:698:GLN:HG3	14:U:702:THR:OG1	2.20	0.42
16:W:190:MET:HE2	16:W:229:LEU:HD23	2.01	0.42
16:W:438:LEU:HB3	19:Z:233:VAL:HG22	2.00	0.42
18:Y:168:ILE:HD13	18:Y:177:ARG:HA	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:Z:224:HIS:HE1	20:a:218:MET:SD	2.42	0.42
19:Z:272:LEU:HD23	19:Z:272:LEU:HA	1.88	0.42
20:a:97:LEU:O	20:a:101:ARG:N	2.39	0.42
25:f:597:VAL:HG11	25:f:656:GLY:HA2	2.01	0.42
26:g:112:LEU:HD12	26:g:115:LYS:HZ2	1.85	0.42
2:B:225:TYR:HA	2:B:331:THR:O	2.20	0.42
3:C:89:VAL:HG21	3:C:121:TYR:HE2	1.84	0.42
3:C:142:LYS:HE2	4:D:324:PRO:O	2.20	0.42
4:D:66:LYS:NZ	4:D:66:LYS:HB3	2.34	0.42
5:E:55:GLN:CD	5:E:108:MET:HG3	2.44	0.42
8:H:65:VAL:HG12	8:H:218:PHE:HZ	1.83	0.42
11:K:195:ILE:N	11:K:195:ILE:HD13	2.35	0.42
13:M:8:ASP:OD2	13:M:8:ASP:N	2.51	0.42
14:U:245:ALA:HA	14:U:248:ILE:HB	2.02	0.42
14:U:721:HIS:HB3	15:V:516:GLN:OE1	2.20	0.42
15:V:392:TYR:CZ	15:V:396:ILE:HD11	2.55	0.42
16:W:112:VAL:HG11	16:W:125:ILE:HD11	2.01	0.42
16:W:172:GLU:OE2	16:W:172:GLU:N	2.36	0.42
17:X:38:ASN:OD1	17:X:38:ASN:N	2.50	0.42
17:X:212:MET:HE2	17:X:212:MET:HB2	1.90	0.42
20:a:281:THR:HG22	20:a:291:LEU:HD11	2.01	0.42
21:b:70:ARG:HA	21:b:73:SER:HB3	2.02	0.42
23:d:240:SER:O	23:d:244:VAL:HG23	2.19	0.42
25:f:100:ARG:HB2	25:f:101:PRO:HD3	2.00	0.42
25:f:123:ALA:HB1	25:f:142:TYR:HB3	2.01	0.42
1:A:106:SER:OG	1:A:107:GLU:N	2.53	0.42
1:A:169:LYS:HB2	1:A:231:ASN:HA	2.00	0.42
2:B:234:LEU:HD22	28:B:501:ATP:H2'	2.01	0.42
6:F:198:LEU:HD22	6:F:236:LEU:HD22	2.00	0.42
8:H:176:LYS:HE3	8:H:176:LYS:HB3	1.80	0.42
8:H:184:LEU:O	8:H:188:ILE:HG13	2.19	0.42
10:J:45:VAL:HG11	10:J:61:LYS:HB2	2.01	0.42
14:U:199:ARG:HD3	14:U:199:ARG:HA	1.87	0.42
15:V:502:ASN:HA	15:V:505:LEU:HD13	2.01	0.42
16:W:412:ILE:HG23	20:a:327:VAL:HG21	2.02	0.42
16:W:414:ASN:OD1	16:W:416:GLN:HG2	2.18	0.42
17:X:140:THR:O	17:X:141:LYS:HB2	2.18	0.42
19:Z:130:ASP:OD1	19:Z:130:ASP:N	2.53	0.42
19:Z:175:LEU:HD13	22:c:35:SER:HB3	2.01	0.42
20:a:278:MET:SD	20:a:319:LEU:HB3	2.59	0.42
21:b:61:LEU:HD23	21:b:61:LEU:HA	1.94	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:c:282:ARG:O	22:c:286:GLU:HG3	2.20	0.42
25:f:610:GLN:HG2	25:f:614:HIS:CE1	2.55	0.42
2:B:374:LEU:HD12	2:B:378:VAL:HG11	2.00	0.42
3:C:109:THR:HG1	3:C:112:CYS:HG	1.60	0.42
3:C:192:PRO:HD3	3:C:296:ASN:OD1	2.19	0.42
6:F:74:LYS:HA	6:F:74:LYS:HD2	1.78	0.42
7:G:60:LEU:HB3	13:M:162:GLY:O	2.20	0.42
10:J:83:VAL:HG21	10:J:129:ILE:HD11	2.01	0.42
14:U:42:VAL:O	14:U:45:ILE:HG22	2.20	0.42
14:U:198:LEU:HA	14:U:201:LEU:HB2	2.02	0.42
14:U:339:LEU:HD22	14:U:414:GLY:O	2.19	0.42
15:V:466:ILE:HD13	15:V:466:ILE:HA	1.80	0.42
16:W:357:ARG:HA	16:W:357:ARG:HD3	1.88	0.42
18:Y:96:GLY:O	18:Y:100:ILE:HG13	2.20	0.42
19:Z:50:VAL:HG22	19:Z:92:VAL:HG21	2.00	0.42
20:a:132:LYS:HA	20:a:135:ILE:HG22	2.02	0.42
20:a:375:LEU:HD23	20:a:375:LEU:HA	1.82	0.42
21:b:32:ALA:O	21:b:36:VAL:HG12	2.20	0.42
25:f:163:ALA:O	25:f:166:VAL:HG22	2.20	0.42
25:f:429:ILE:H	25:f:429:ILE:HG13	1.65	0.42
25:f:764:LEU:HA	25:f:764:LEU:HD23	1.78	0.42
26:g:140:LYS:HE3	26:g:140:LYS:HB3	1.82	0.42
27:u:196:ILE:HG12	27:u:246:ILE:HG12	2.02	0.42
1:A:96:ALA:HB2	1:A:115:VAL:HG22	2.02	0.42
7:G:80:MET:HE2	7:G:87:SER:HA	2.02	0.42
11:K:17:PRO:HA	12:L:24:TYR:CD1	2.54	0.42
13:M:106:ILE:HG12	13:M:111:LEU:HB2	2.02	0.42
14:U:185:MET:HE3	14:U:185:MET:HB3	1.87	0.42
14:U:221:ILE:HD13	14:U:256:ALA:HB2	2.02	0.42
15:V:175:MET:HB2	15:V:184:ALA:HB2	2.01	0.42
17:X:88:LEU:HA	17:X:88:LEU:HD12	1.77	0.42
22:c:284:LEU:HD12	22:c:284:LEU:HA	1.83	0.42
25:f:378:ASN:CG	25:f:390:LEU:HD22	2.45	0.42
27:u:147:ASP:OD1	27:u:147:ASP:N	2.52	0.42
2:B:237:LYS:HG2	3:C:283:PHE:CZ	2.55	0.42
3:C:391:MET:HE3	3:C:391:MET:HB3	1.92	0.42
4:D:205:TYR:CE2	4:D:332:GLU:HG3	2.54	0.42
5:E:72:LYS:HB2	5:E:78:ARG:HG2	2.01	0.42
6:F:431:LYS:HE3	6:F:431:LYS:HB3	1.88	0.42
9:I:183:GLU:H	9:I:183:GLU:HG2	1.74	0.42
9:I:190:LEU:HD23	9:I:236:LEU:HD21	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:120:THR:O	13:M:129:ARG:NH2	2.44	0.42
14:U:181:LEU:O	14:U:185:MET:HG2	2.20	0.42
14:U:525:ASN:OD1	14:U:525:ASN:N	2.52	0.42
20:a:248:PHE:HB2	20:a:272:ILE:HD13	2.02	0.42
20:a:286:ALA:HB3	22:c:311:LEU:HD11	2.01	0.42
20:a:293:PHE:CD2	20:a:329:LYS:HE2	2.55	0.42
22:c:226:MET:HB2	22:c:226:MET:HE2	1.73	0.42
3:C:164:VAL:O	3:C:168:PRO:HG2	2.20	0.42
7:G:74:GLU:OE1	7:G:226:LYS:HD3	2.20	0.42
10:J:233:GLU:HG2	10:J:236:LYS:HZ1	1.85	0.42
14:U:713:TYR:HE2	14:U:737:LEU:HD22	1.84	0.42
15:V:263:LEU:HB3	15:V:266:GLN:HB2	2.02	0.42
16:W:316:ARG:HD2	16:W:383:ASP:OD1	2.20	0.42
17:X:337:ARG:HG2	17:X:337:ARG:NH1	2.35	0.42
19:Z:165:GLU:HB3	19:Z:168:GLU:HB2	2.01	0.42
20:a:343:LEU:HD12	20:a:343:LEU:HA	1.86	0.42
22:c:73:PHE:CD1	22:c:95:MET:HG2	2.55	0.42
25:f:478:ARG:O	25:f:482:ILE:HD12	2.20	0.42
25:f:713:PHE:N	25:f:713:PHE:CD1	2.88	0.42
1:A:152:PRO:HG2	2:B:25:TYR:CE2	2.55	0.42
6:F:185:TYR:HA	6:F:188:ILE:HD12	2.01	0.42
7:G:212:PRO:HG3	7:G:236:ASP:CG	2.45	0.42
9:I:194:ILE:HD11	9:I:213:ILE:HD11	2.02	0.42
10:J:65:LEU:CD1	10:J:71:MET:HG2	2.49	0.42
13:M:231:ILE:H	13:M:231:ILE:HG13	1.69	0.42
15:V:527:GLU:OE2	22:c:198:ARG:NH1	2.53	0.42
16:W:409:LEU:HD12	17:X:346:GLN:NE2	2.35	0.42
17:X:171:LEU:HD13	17:X:209:THR:HG22	2.00	0.42
20:a:39:LEU:H	20:a:39:LEU:HD22	1.85	0.42
25:f:541:THR:O	25:f:545:LYS:HG2	2.20	0.42
25:f:702:PRO:HD3	25:f:736:THR:HG21	2.01	0.42
1:A:133:ASP:OD2	2:B:25:TYR:HB3	2.19	0.41
2:B:371:ARG:NH1	3:C:176:GLU:HG2	2.32	0.41
6:F:256:LEU:HD13	6:F:268:VAL:HG22	2.01	0.41
11:K:196:LYS:HE2	11:K:196:LYS:HB3	1.93	0.41
16:W:160:LYS:HE2	16:W:160:LYS:HB3	1.94	0.41
17:X:332:GLU:O	17:X:336:ILE:HG12	2.20	0.41
19:Z:197:GLY:HA2	22:c:225:TRP:HB2	2.02	0.41
20:a:292:THR:OG1	20:a:295:GLU:HG3	2.20	0.41
21:b:112:PHE:CD1	21:b:141:ILE:HG12	2.55	0.41
23:d:102:TRP:CD2	23:d:150:ILE:HG23	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:f:316:ASP:N	25:f:316:ASP:OD1	2.50	0.41
1:A:249:TYR:HB3	6:F:259:MET:HG3	2.02	0.41
3:C:191:PRO:HG2	3:C:319:PRO:HD3	2.03	0.41
5:E:264:MET:HE3	5:E:294:ARG:HD3	2.02	0.41
5:E:304:PRO:HD2	5:E:338:PHE:O	2.20	0.41
7:G:70:PHE:CD2	7:G:91:VAL:HG21	2.55	0.41
11:K:117:SER:HB3	12:L:82:ARG:NH2	2.34	0.41
11:K:121:LEU:HD12	12:L:79:ALA:HB3	2.02	0.41
12:L:157:ARG:HG2	12:L:157:ARG:NH1	2.34	0.41
15:V:200:ARG:HH11	15:V:200:ARG:HG3	1.84	0.41
15:V:326:GLN:O	15:V:330:LYS:HG3	2.20	0.41
19:Z:234:PHE:HB3	20:a:352:ARG:HH21	1.84	0.41
20:a:71:VAL:HG13	20:a:76:LEU:HD12	2.02	0.41
22:c:44:HIS:CE1	22:c:74:ALA:HB1	2.54	0.41
25:f:489:TYR:O	25:f:525:ILE:HG13	2.20	0.41
25:f:564:LEU:HD21	25:f:794:ALA:HA	2.02	0.41
25:f:844:VAL:HG12	25:f:882:LEU:HD23	2.02	0.41
1:A:72:LEU:HD12	1:A:72:LEU:HA	1.79	0.41
2:B:170:LEU:HG	2:B:174:MET:HE3	2.00	0.41
2:B:277:HIS:O	2:B:280:SER:HB3	2.19	0.41
3:C:83:LYS:HE2	3:C:83:LYS:HB3	1.65	0.41
5:E:202:SER:HA	6:F:269:ARG:NH2	2.35	0.41
8:H:118:MET:HE2	8:H:118:MET:HB3	1.78	0.41
10:J:221:ASN:OD1	10:J:224:GLU:N	2.42	0.41
11:K:206:MET:HE3	11:K:206:MET:HB3	1.81	0.41
12:L:225:ASP:O	12:L:229:VAL:N	2.53	0.41
14:U:353:LEU:HD11	14:U:373:ASN:HA	2.02	0.41
16:W:426:ASN:ND2	22:c:233:ASP:OD1	2.53	0.41
17:X:65:GLU:O	17:X:69:LEU:HB2	2.20	0.41
18:Y:171:GLY:O	18:Y:173:ASP:N	2.50	0.41
19:Z:173:GLU:HG3	22:c:152:LYS:HD2	2.02	0.41
20:a:245:VAL:HG12	20:a:272:ILE:HG23	2.03	0.41
20:a:356:TRP:O	20:a:360:VAL:HG23	2.20	0.41
21:b:173:VAL:HG21	21:b:179:LEU:HB2	2.01	0.41
25:f:113:MET:HE2	25:f:118:ASN:HD22	1.85	0.41
25:f:206:ASP:OD1	25:f:232:TYR:OH	2.26	0.41
25:f:546:SER:H	25:f:549:GLU:HB2	1.85	0.41
27:u:149:CYS:O	27:u:262:TYR:HA	2.20	0.41
27:u:223:ASP:HA	27:u:226:LYS:HD2	2.02	0.41
1:A:169:LYS:HE2	1:A:169:LYS:HB3	1.85	0.41
5:E:250:ASP:O	5:E:254:GLN:HG3	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:264:MET:HE1	5:E:289:LEU:HD12	2.02	0.41
7:G:5:SER:OG	7:G:19:GLU:OE1	2.31	0.41
14:U:58:GLN:HB3	14:U:87:LEU:HD12	2.01	0.41
14:U:693:LEU:HD21	14:U:779:LEU:HD21	2.02	0.41
15:V:98:LEU:HD22	15:V:209:LYS:HG3	2.02	0.41
16:W:63:THR:O	16:W:67:LEU:HG	2.20	0.41
16:W:272:LEU:HD12	16:W:272:LEU:HA	1.85	0.41
17:X:71:LYS:HE2	17:X:71:LYS:HB3	1.88	0.41
18:Y:247:LEU:HD23	18:Y:247:LEU:HA	1.91	0.41
19:Z:31:ASN:HB3	27:u:208:GLU:CD	2.45	0.41
20:a:157:ASP:HB2	20:a:179:PHE:CE2	2.56	0.41
20:a:203:ALA:O	20:a:207:GLY:N	2.53	0.41
20:a:353:LEU:HD23	20:a:353:LEU:HA	1.85	0.41
21:b:31:ASP:OD1	21:b:31:ASP:N	2.52	0.41
22:c:122:LEU:HD22	22:c:126:ASP:HB3	2.02	0.41
1:A:284:ARG:HG3	1:A:299:MET:HE1	2.02	0.41
1:A:387:SER:O	1:A:391:GLU:HG2	2.20	0.41
5:E:281:ARG:HE	5:E:281:ARG:HB3	1.51	0.41
5:E:344:ARG:HE	5:E:344:ARG:HB3	1.78	0.41
6:F:146:LYS:O	6:F:149:ASP:HB2	2.21	0.41
6:F:402:GLU:CD	6:F:426:GLU:HG2	2.46	0.41
7:G:163:PHE:CG	7:G:166:THR:HB	2.56	0.41
8:H:205:GLU:HB2	8:H:223:PRO:O	2.21	0.41
10:J:70:CYS:SG	10:J:217:LEU:HD13	2.61	0.41
13:M:191:LYS:HB3	13:M:238:TYR:CD2	2.56	0.41
14:U:127:ASP:OD2	14:U:128:GLN:N	2.53	0.41
16:W:308:LEU:HD12	16:W:308:LEU:HA	1.88	0.41
16:W:324:TYR:HB3	16:W:328:LEU:HD13	2.03	0.41
17:X:415:TYR:CE2	18:Y:383:LEU:HB2	2.55	0.41
18:Y:14:ASN:HD21	18:Y:113:ARG:HE	1.67	0.41
21:b:128:ALA:HB2	21:b:156:PHE:CD1	2.55	0.41
22:c:30:GLN:HG2	22:c:204:THR:HG23	2.03	0.41
25:f:304:PHE:CD2	25:f:321:MET:HE1	2.56	0.41
25:f:590:PHE:CD2	25:f:590:PHE:C	2.99	0.41
25:f:699:VAL:HG13	25:f:779:CYS:HA	2.02	0.41
3:C:327:ASP:N	3:C:327:ASP:OD1	2.53	0.41
5:E:351:GLY:HA3	6:F:217:ILE:HG21	2.01	0.41
6:F:386:ARG:NH2	12:L:166:GLN:O	2.54	0.41
7:G:151:VAL:HB	7:G:163:PHE:O	2.21	0.41
7:G:176:THR:HG23	8:H:56:LEU:HD12	2.03	0.41
11:K:78:MET:HE3	11:K:85:ALA:HB3	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:184:MET:H	13:M:184:MET:HG2	1.74	0.41
13:M:202:ASP:HB3	13:M:205:LYS:HB3	2.01	0.41
14:U:14:GLU:OE1	14:U:14:GLU:N	2.53	0.41
14:U:255:SER:HB2	14:U:754:HIS:HB2	2.03	0.41
14:U:257:SER:O	14:U:261:LEU:HD12	2.21	0.41
14:U:559:ARG:HD3	14:U:559:ARG:HA	1.89	0.41
14:U:805:ASN:OD1	14:U:805:ASN:N	2.53	0.41
16:W:448:LYS:NZ	19:Z:154:THR:HB	2.35	0.41
17:X:287:LEU:HD11	17:X:319:ILE:HD13	2.03	0.41
18:Y:104:MET:HE3	18:Y:127:THR:HA	2.03	0.41
19:Z:43:TRP:CE2	19:Z:48:LEU:HD13	2.56	0.41
20:a:301:LYS:HA	20:a:301:LYS:HD3	1.91	0.41
21:b:118:GLU:CD	21:b:118:GLU:H	2.29	0.41
23:d:96:GLU:O	23:d:100:GLY:N	2.41	0.41
25:f:119:LYS:HD2	25:f:145:VAL:HG12	2.03	0.41
25:f:217:LEU:O	25:f:221:ILE:HG12	2.21	0.41
25:f:256:PHE:CE1	25:f:264:GLU:HG3	2.55	0.41
25:f:420:TRP:CH2	25:f:827:PRO:HD3	2.56	0.41
27:u:144:HIS:HB2	27:u:158:GLU:HG2	2.03	0.41
1:A:299:MET:HE3	1:A:299:MET:HB3	1.99	0.41
2:B:32:ARG:NH2	2:B:36:LYS:O	2.52	0.41
2:B:201:VAL:HG11	2:B:328:ILE:HD11	2.02	0.41
4:D:241:GLY:O	4:D:245:ARG:HB2	2.21	0.41
4:D:267:ILE:HG22	4:D:311:THR:HB	2.02	0.41
4:D:345:PHE:O	4:D:349:THR:OG1	2.27	0.41
14:U:446:LEU:HG	14:U:450:HIS:CE1	2.52	0.41
14:U:515:ALA:O	14:U:519:VAL:HG23	2.19	0.41
17:X:6:VAL:HG22	17:X:45:VAL:HG21	2.02	0.41
19:Z:259:VAL:CG1	22:c:291:LEU:HD13	2.51	0.41
20:a:115:LYS:HE2	20:a:115:LYS:HB3	1.93	0.41
22:c:76:PRO:HD3	22:c:91:PHE:CZ	2.56	0.41
25:f:546:SER:N	25:f:549:GLU:OE1	2.43	0.41
26:g:108:THR:HG23	26:g:110:ARG:N	2.35	0.41
26:g:111:GLU:O	26:g:114:SER:OG	2.37	0.41
2:B:249:ARG:HG3	2:B:283:PHE:HD2	1.85	0.41
2:B:388:ASP:OD1	2:B:388:ASP:N	2.53	0.41
9:I:33:THR:OG1	9:I:166:ASN:O	2.39	0.41
13:M:188:ASP:OD1	13:M:188:ASP:N	2.54	0.41
14:U:410:VAL:HG23	14:U:448:LEU:HD13	2.02	0.41
14:U:807:LYS:HB3	14:U:872:GLU:OE2	2.20	0.41
15:V:179:LYS:HG3	15:V:181:TYR:OH	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:V:318:GLN:HE21	15:V:318:GLN:HB3	1.57	0.41
20:a:73:PRO:HB2	20:a:107:SER:HB2	2.02	0.41
20:a:218:MET:HE2	20:a:218:MET:HB2	1.95	0.41
20:a:330:ARG:CZ	20:a:330:ARG:HB2	2.51	0.41
22:c:51:MET:H	22:c:51:MET:HG2	1.63	0.41
23:d:88:LEU:HD13	23:d:140:GLN:HG3	2.02	0.41
24:e:18:GLU:OE2	24:e:20:GLU:HB3	2.20	0.41
25:f:52:LEU:HG	25:f:95:PRO:HB2	2.03	0.41
25:f:339:ILE:HD12	25:f:773:LYS:HB2	2.02	0.41
25:f:600:TYR:O	25:f:660:ILE:HD12	2.21	0.41
26:g:134:LYS:HB3	26:g:134:LYS:HE3	1.76	0.41
27:u:246:ILE:HD12	27:u:263:PHE:CE1	2.56	0.41
1:A:258:ARG:NH1	1:A:301:GLU:OE1	2.54	0.41
2:B:51:LEU:HD13	2:B:51:LEU:HA	1.93	0.41
2:B:74:MET:HE1	25:f:609:VAL:HB	2.02	0.41
2:B:365:PHE:HB3	2:B:380:LEU:HD13	2.03	0.41
3:C:213:ARG:HD3	3:C:247:PHE:HD2	1.86	0.41
4:D:109:SER:HB2	4:D:111:TYR:CE2	2.56	0.41
4:D:183:LEU:HD12	4:D:183:LEU:HA	1.87	0.41
5:E:61:LEU:HB2	5:E:70:ILE:HG22	2.03	0.41
5:E:97:ARG:NH1	5:E:114:GLU:HB2	2.35	0.41
5:E:340:GLY:HA3	28:E:501:ATP:C8	2.56	0.41
6:F:276:LYS:HE3	6:F:276:LYS:HB3	1.81	0.41
7:G:164:LYS:HE2	8:H:55:ILE:O	2.21	0.41
8:H:116:SER:O	8:H:120:GLU:HG3	2.21	0.41
9:I:239:LYS:HE3	9:I:239:LYS:HB3	1.68	0.41
12:L:118:ILE:O	12:L:122:ARG:HG3	2.21	0.41
14:U:49:TYR:O	14:U:57:ARG:NH2	2.53	0.41
15:V:167:LEU:HD22	15:V:167:LEU:H	1.86	0.41
15:V:224:LEU:HB3	15:V:261:TYR:HE2	1.86	0.41
16:W:373:ILE:HA	20:a:326:GLU:HB3	2.03	0.41
17:X:28:HIS:O	17:X:32:LYS:HD2	2.21	0.41
19:Z:174:HIS:HA	22:c:153:GLY:HA2	2.02	0.41
19:Z:230:LEU:HB3	20:a:349:MET:SD	2.61	0.41
20:a:219:HIS:ND1	20:a:220:PRO:HD2	2.36	0.41
23:d:126:LEU:HB3	23:d:140:GLN:HG2	2.02	0.41
23:d:228:HIS:HB3	23:d:229:PRO:HD3	2.03	0.41
25:f:301:HIS:NE2	25:f:788:MET:O	2.52	0.41
25:f:391:LEU:HD12	25:f:391:LEU:HA	1.83	0.41
25:f:787:LEU:HD23	25:f:787:LEU:HA	1.97	0.41
25:f:832:THR:HG23	25:f:870:THR:HB	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:g:130:VAL:HB	26:g:154:MET:CE	2.50	0.41
27:u:127:MET:HB3	27:u:128:PRO:HD3	2.03	0.41
27:u:218:LEU:HD23	27:u:218:LEU:HA	1.90	0.41
2:B:81:ASN:O	2:B:85:MET:HG2	2.20	0.41
3:C:149:GLU:OE1	18:Y:133:ALA:HB1	2.21	0.41
9:I:66:TYR:CD2	9:I:87:THR:HG21	2.56	0.41
14:U:179:TYR:CZ	14:U:183:LEU:HD11	2.56	0.41
15:V:221:LEU:HD23	15:V:221:LEU:HA	1.89	0.41
15:V:516:GLN:O	15:V:520:GLU:HG2	2.20	0.41
17:X:407:MET:HB3	18:Y:376:LEU:HD21	2.03	0.41
19:Z:224:HIS:CE1	20:a:218:MET:HE1	2.56	0.41
20:a:352:ARG:HG2	20:a:352:ARG:NH1	2.36	0.41
22:c:41:MET:HE3	22:c:41:MET:HB2	1.83	0.41
22:c:118:PHE:O	22:c:121:TRP:NE1	2.51	0.41
25:f:75:LEU:HD23	25:f:75:LEU:HA	1.88	0.41
25:f:218:GLU:O	25:f:258:LYS:NZ	2.45	0.41
26:g:141:THR:O	26:g:144:GLU:HG2	2.21	0.41
27:u:262:TYR:O	27:u:262:TYR:CG	2.74	0.41
4:D:47:LEU:HD12	4:D:47:LEU:HA	1.88	0.40
5:E:101:ASP:O	5:E:105:LEU:HD23	2.21	0.40
8:H:159:LYS:HB2	8:H:159:LYS:HE2	1.91	0.40
11:K:137:PHE:O	11:K:158:PRO:HB3	2.22	0.40
12:L:18:ARG:NH2	12:L:23:GLU:OE1	2.54	0.40
14:U:118:LEU:HD12	14:U:118:LEU:HA	1.94	0.40
14:U:757:MET:HE3	14:U:757:MET:HB3	1.99	0.40
14:U:806:CYS:SG	14:U:810:THR:HG21	2.62	0.40
15:V:256:ARG:HB2	15:V:291:TYR:CZ	2.57	0.40
18:Y:181:LYS:HB2	18:Y:204:THR:HG21	2.03	0.40
19:Z:59:ASP:HB3	21:b:95:LEU:HD22	2.02	0.40
20:a:261:LEU:HD22	20:a:268:LEU:HD11	2.02	0.40
25:f:781:TYR:HB3	25:f:785:ARG:HA	2.03	0.40
4:D:131:ALA:HB3	4:D:141:ASP:HB3	2.03	0.40
6:F:84:LYS:HB3	6:F:84:LYS:HE3	1.92	0.40
14:U:353:LEU:HA	14:U:353:LEU:HD23	1.81	0.40
14:U:450:HIS:CE1	14:U:457:ILE:HG12	2.57	0.40
16:W:102:ALA:O	16:W:106:GLN:HG3	2.22	0.40
17:X:132:ARG:HG2	17:X:132:ARG:NH1	2.36	0.40
17:X:260:MET:HE1	17:X:325:LYS:HB3	2.02	0.40
21:b:107:MET:CB	21:b:136:VAL:HA	2.51	0.40
25:f:390:LEU:HD21	25:f:398:TRP:NE1	2.36	0.40
25:f:615:ILE:HG13	25:f:615:ILE:H	1.65	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:f:814:SER:HA	25:f:816:TYR:CE2	2.57	0.40
27:u:221:THR:HG23	27:u:223:ASP:N	2.36	0.40
3:C:81:ASP:OD1	3:C:81:ASP:N	2.52	0.40
3:C:105:ILE:HD12	3:C:105:ILE:HA	1.91	0.40
4:D:120:ASP:CG	22:c:282:ARG:HH12	2.25	0.40
4:D:200:ARG:NH2	4:D:300:ASP:O	2.54	0.40
4:D:328:ASP:OD1	4:D:328:ASP:N	2.49	0.40
5:E:142:ILE:HG12	5:E:183:LEU:HD11	2.02	0.40
6:F:205:PRO:HB2	6:F:327:LYS:NZ	2.37	0.40
8:H:39:LYS:HE3	8:H:143:ARG:NH1	2.33	0.40
11:K:38:ILE:HG23	11:K:181:LEU:HD11	2.04	0.40
13:M:203:GLU:H	13:M:203:GLU:CD	2.29	0.40
14:U:35:TRP:CD1	14:U:35:TRP:H	2.40	0.40
15:V:398:LEU:HD23	15:V:398:LEU:HA	1.86	0.40
16:W:128:LEU:HD23	16:W:128:LEU:HA	1.92	0.40
16:W:189:GLN:HB3	16:W:205:ILE:HD13	2.04	0.40
19:Z:231:GLN:HE22	20:a:339:ARG:N	2.19	0.40
20:a:108:ASP:O	20:a:112:ILE:HG12	2.20	0.40
25:f:738:ASN:HB3	25:f:741:LEU:HB3	2.03	0.40
25:f:783:SER:H	25:f:895:GLU:CD	2.30	0.40
2:B:224:LEU:HB3	2:B:353:PHE:CE1	2.57	0.40
2:B:413:LYS:HE2	2:B:413:LYS:HB2	1.80	0.40
3:C:199:LEU:O	3:C:203:VAL:HG23	2.21	0.40
3:C:334:ARG:H	3:C:334:ARG:HG2	1.64	0.40
6:F:258:GLN:OE1	6:F:258:GLN:HA	2.21	0.40
9:I:170:ALA:O	9:I:174:MET:HG3	2.21	0.40
9:I:180:LYS:O	9:I:184:MET:HG3	2.21	0.40
12:L:40:SER:HB3	12:L:187:LEU:HD13	2.02	0.40
14:U:162:VAL:O	14:U:166:THR:OG1	2.36	0.40
14:U:703:CYS:O	14:U:706:VAL:HG12	2.21	0.40
15:V:482:PHE:CE2	18:Y:377:LEU:HD22	2.57	0.40
18:Y:18:ARG:HA	18:Y:18:ARG:HD2	1.98	0.40
19:Z:231:GLN:HE22	20:a:339:ARG:H	1.69	0.40
20:a:287:ASN:HB2	20:a:288:HIS:CE1	2.56	0.40
25:f:189:LYS:HE2	25:f:189:LYS:HB2	1.84	0.40
25:f:890:VAL:HG23	25:f:899:ILE:O	2.21	0.40
1:A:110:LYS:HG2	6:F:86:LEU:HD11	2.04	0.40
1:A:142:VAL:HG12	1:A:149:ILE:HA	2.03	0.40
1:A:263:MET:HE2	1:A:263:MET:HB3	1.88	0.40
4:D:300:ASP:OD1	4:D:300:ASP:N	2.41	0.40
5:E:195:PHE:HB3	5:E:197:LYS:HE3	2.04	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:73:THR:HG22	7:G:74:GLU:N	2.36	0.40
8:H:49:GLU:HG3	8:H:199:PHE:CE2	2.57	0.40
8:H:74:LEU:CD2	8:H:136:ILE:HG13	2.52	0.40
10:J:59:VAL:O	10:J:59:VAL:HG23	2.22	0.40
11:K:199:LEU:HD21	11:K:217:LEU:HD21	2.03	0.40
13:M:75:MET:HE3	13:M:135:PHE:CG	2.57	0.40
14:U:110:LYS:NZ	14:U:110:LYS:HB2	2.37	0.40
14:U:269:ARG:HG3	14:U:269:ARG:NH1	2.36	0.40
14:U:339:LEU:O	14:U:343:ILE:HD12	2.22	0.40
14:U:630:PRO:HA	14:U:659:CYS:SG	2.61	0.40
15:V:300:LEU:HD11	23:d:205:VAL:HG22	2.03	0.40
15:V:512:ARG:O	15:V:516:GLN:HG2	2.20	0.40
18:Y:177:ARG:O	18:Y:181:LYS:HG3	2.22	0.40
22:c:59:GLY:HA3	22:c:68:ARG:O	2.21	0.40
23:d:286:GLU:HA	23:d:289:ARG:HH22	1.87	0.40
25:f:460:ASP:OD2	25:f:489:TYR:OH	2.40	0.40
25:f:829:MET:HE2	25:f:829:MET:CA	2.51	0.40
25:f:884:THR:OG1	25:f:885:GLU:N	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	393/433 (91%)	376 (96%)	17 (4%)	0	100	100
2	B	403/440 (92%)	390 (97%)	13 (3%)	0	100	100
3	C	362/406 (89%)	355 (98%)	7 (2%)	0	100	100
4	D	378/418 (90%)	371 (98%)	7 (2%)	0	100	100
5	E	352/389 (90%)	347 (99%)	5 (1%)	0	100	100
6	F	347/439 (79%)	338 (97%)	9 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	G	240/246 (98%)	234 (98%)	6 (2%)	0	100	100
8	H	228/234 (97%)	227 (100%)	1 (0%)	0	100	100
9	I	231/261 (88%)	226 (98%)	5 (2%)	0	100	100
10	J	237/248 (96%)	235 (99%)	2 (1%)	0	100	100
11	K	232/241 (96%)	226 (97%)	6 (3%)	0	100	100
12	L	235/263 (89%)	231 (98%)	4 (2%)	0	100	100
13	M	238/255 (93%)	233 (98%)	5 (2%)	0	100	100
14	U	830/953 (87%)	814 (98%)	16 (2%)	0	100	100
15	V	468/534 (88%)	462 (99%)	6 (1%)	0	100	100
16	W	436/456 (96%)	426 (98%)	10 (2%)	0	100	100
17	X	417/422 (99%)	405 (97%)	12 (3%)	0	100	100
18	Y	384/389 (99%)	383 (100%)	1 (0%)	0	100	100
19	Z	284/324 (88%)	276 (97%)	8 (3%)	0	100	100
20	a	371/376 (99%)	365 (98%)	6 (2%)	0	100	100
21	b	187/377 (50%)	178 (95%)	9 (5%)	0	100	100
22	c	288/424 (68%)	285 (99%)	3 (1%)	0	100	100
23	d	263/350 (75%)	245 (93%)	18 (7%)	0	100	100
24	e	48/70 (69%)	43 (90%)	5 (10%)	0	100	100
25	f	825/908 (91%)	801 (97%)	24 (3%)	0	100	100
26	g	89/601 (15%)	84 (94%)	4 (4%)	1 (1%)	11	33
27	u	147/289 (51%)	137 (93%)	10 (7%)	0	100	100
All	All	8913/10746 (83%)	8693 (98%)	219 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
26	g	160	GLN

5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	340/372 (91%)	330 (97%)	10 (3%)	37	68
2	B	359/385 (93%)	345 (96%)	14 (4%)	28	60
3	C	320/352 (91%)	310 (97%)	10 (3%)	35	66
4	D	333/366 (91%)	321 (96%)	12 (4%)	31	63
5	E	309/341 (91%)	305 (99%)	4 (1%)	61	84
6	F	299/379 (79%)	292 (98%)	7 (2%)	44	74
7	G	206/210 (98%)	201 (98%)	5 (2%)	43	73
8	H	188/191 (98%)	187 (100%)	1 (0%)	81	93
9	I	197/221 (89%)	196 (100%)	1 (0%)	81	93
10	J	203/211 (96%)	202 (100%)	1 (0%)	81	93
11	K	196/203 (97%)	191 (97%)	5 (3%)	40	71
12	L	203/224 (91%)	196 (97%)	7 (3%)	32	64
13	M	198/212 (93%)	193 (98%)	5 (2%)	42	72
14	U	712/816 (87%)	695 (98%)	17 (2%)	43	73
15	V	415/460 (90%)	406 (98%)	9 (2%)	45	75
16	W	403/416 (97%)	395 (98%)	8 (2%)	48	76
17	X	361/362 (100%)	358 (99%)	3 (1%)	73	89
18	Y	341/344 (99%)	337 (99%)	4 (1%)	63	84
19	Z	258/295 (88%)	253 (98%)	5 (2%)	50	77
20	a	333/336 (99%)	327 (98%)	6 (2%)	51	78
21	b	166/312 (53%)	159 (96%)	7 (4%)	26	58
22	c	255/359 (71%)	249 (98%)	6 (2%)	43	73
23	d	235/294 (80%)	227 (97%)	8 (3%)	32	64
24	e	44/63 (70%)	41 (93%)	3 (7%)	14	39
25	f	701/763 (92%)	687 (98%)	14 (2%)	48	76
26	g	81/527 (15%)	79 (98%)	2 (2%)	42	72
27	u	138/253 (54%)	129 (94%)	9 (6%)	15	41
All	All	7794/9267 (84%)	7611 (98%)	183 (2%)	44	74

All (183) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	THR
1	A	62	LEU
1	A	88	GLN
1	A	135	GLU
1	A	191	VAL
1	A	260	LEU
1	A	267	LYS
1	A	303	ILE
1	A	333	ARG
1	A	348	LEU
2	B	33	VAL
2	B	65	LEU
2	B	74	MET
2	B	112	LEU
2	B	116	ILE
2	B	145	GLU
2	B	177	GLU
2	B	195	GLN
2	B	216	ILE
2	B	254	GLU
2	B	293	LYS
2	B	294	ARG
2	B	408	ARG
2	B	424	GLU
3	C	140	VAL
3	C	150	MET
3	C	165	ILE
3	C	167	LEU
3	C	182	GLN
3	C	184	LYS
3	C	267	SER
3	C	273	MET
3	C	280	LEU
3	C	290	LYS
4	D	60	TYR
4	D	69	LYS
4	D	70	LYS
4	D	114	ARG
4	D	139	LEU
4	D	156	SER
4	D	231	VAL
4	D	304	ASN
4	D	311	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	D	328	ASP
4	D	366	ARG
4	D	411	GLU
5	E	103	THR
5	E	206	LYS
5	E	251	ARG
5	E	360	ASP
6	F	70	LYS
6	F	80	ILE
6	F	81	LYS
6	F	127	SER
6	F	236	LEU
6	F	289	ASP
6	F	310	MET
7	G	67	THR
7	G	112	ASP
7	G	131	MET
7	G	154	CYS
7	G	221	THR
8	H	132	VAL
9	I	184	MET
10	J	196	LEU
11	K	52	LYS
11	K	78	MET
11	K	108	THR
11	K	148	GLU
11	K	198	SER
12	L	4	ASN
12	L	35	THR
12	L	112	ILE
12	L	166	GLN
12	L	220	GLU
12	L	226	ASP
12	L	228	ASP
13	M	41	CYS
13	M	87	LEU
13	M	94	GLU
13	M	203	GLU
13	M	205	LYS
14	U	76	GLU
14	U	104	CYS
14	U	137	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
14	U	185	MET
14	U	248	ILE
14	U	258	GLN
14	U	340	GLN
14	U	362	ASN
14	U	439	GLU
14	U	521	LEU
14	U	629	THR
14	U	632	GLN
14	U	637	VAL
14	U	642	GLU
14	U	792	ASN
14	U	879	ASP
14	U	892	LEU
15	V	80	LYS
15	V	118	GLN
15	V	132	LEU
15	V	226	VAL
15	V	227	VAL
15	V	442	ILE
15	V	466	ILE
15	V	489	MET
15	V	507	SER
16	W	50	LEU
16	W	104	MET
16	W	212	LYS
16	W	220	GLU
16	W	272	LEU
16	W	299	ILE
16	W	322	GLU
16	W	425	LEU
17	X	125	LEU
17	X	292	GLN
17	X	415	TYR
18	Y	55	GLU
18	Y	72	LYS
18	Y	87	GLU
18	Y	343	LEU
19	Z	28	LYS
19	Z	72	HIS
19	Z	159	THR
19	Z	179	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
19	Z	229	GLN
20	a	91	ASN
20	a	135	ILE
20	a	166	ILE
20	a	202	LEU
20	a	208	GLU
20	a	336	VAL
21	b	2	VAL
21	b	31	ASP
21	b	47	ASN
21	b	51	LEU
21	b	124	LEU
21	b	138	VAL
21	b	169	HIS
22	c	51	MET
22	c	204	THR
22	c	210	ASN
22	c	223	LYS
22	c	226	MET
22	c	303	MET
23	d	119	LEU
23	d	142	ILE
23	d	190	GLN
23	d	246	LEU
23	d	268	ARG
23	d	294	ASN
23	d	299	MET
23	d	337	LYS
24	e	21	GLU
24	e	50	ASP
24	e	59	GLU
25	f	68	THR
25	f	109	ILE
25	f	113	MET
25	f	190	GLU
25	f	253	LEU
25	f	399	LEU
25	f	401	LYS
25	f	422	VAL
25	f	452	ASN
25	f	502	LEU
25	f	606	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
25	f	690	VAL
25	f	706	ILE
25	f	816	TYR
26	g	115	LYS
26	g	131	ILE
27	u	127	MET
27	u	132	LYS
27	u	140	GLU
27	u	181	LYS
27	u	211	ARG
27	u	235	TYR
27	u	236	VAL
27	u	237	LYS
27	u	254	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (74) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	GLN
1	A	183	GLN
2	B	82	GLN
2	B	241	ASN
2	B	257	GLN
2	B	366	GLN
3	C	64	GLN
3	C	221	GLN
3	C	343	ASN
4	D	65	GLN
4	D	221	HIS
4	D	222	HIS
4	D	278	GLN
5	E	55	GLN
5	E	194	ASN
5	E	262	ASN
6	F	130	GLN
6	F	321	GLN
8	H	88	HIS
8	H	179	ASN
8	H	189	HIS
9	I	166	ASN
9	I	167	ASN
10	J	146	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	J	154	HIS
11	K	41	GLN
11	K	155	HIS
11	K	164	GLN
11	K	221	GLN
12	L	146	GLN
14	U	398	ASN
14	U	421	GLN
14	U	450	HIS
14	U	604	HIS
14	U	611	ASN
14	U	707	ASN
15	V	124	ASN
15	V	299	GLN
15	V	311	ASN
15	V	365	GLN
15	V	517	GLN
16	W	228	ASN
16	W	264	GLN
16	W	414	ASN
16	W	416	GLN
17	X	48	GLN
17	X	127	GLN
17	X	144	GLN
17	X	283	GLN
17	X	405	GLN
18	Y	160	ASN
18	Y	184	GLN
18	Y	365	GLN
19	Z	193	ASN
19	Z	202	ASN
20	a	12	GLN
20	a	36	GLN
20	a	46	GLN
20	a	52	GLN
21	b	47	ASN
22	c	44	HIS
22	c	92	GLN
22	c	131	GLN
22	c	164	ASN
22	c	199	HIS
23	d	195	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
23	d	322	GLN
25	f	195	ASN
25	f	199	ASN
25	f	457	ASN
25	f	786	GLN
25	f	876	HIS
26	g	150	ASN
26	g	168	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 7 are monoatomic - leaving 6 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	$\# Z > 2$
28	ATP	E	501	29	32,33,33	0.36	0	48,52,52	0.38	0
30	ADP	C	501	-	28,29,29	1.38	4 (14%)	43,45,45	1.85	8 (18%)
28	ATP	B	501	29	32,33,33	0.31	0	48,52,52	0.34	0
28	ATP	A	501	29	32,33,33	0.38	0	48,52,52	0.32	0
28	ATP	F	501	29	32,33,33	0.37	0	48,52,52	0.34	0
28	ATP	D	501	29	32,33,33	0.37	0	48,52,52	0.43	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
28	ATP	E	501	29	-	7/22/38/38	0/3/3/3
30	ADP	C	501	-	-	4/16/32/32	0/3/3/3
28	ATP	B	501	29	-	4/22/38/38	0/3/3/3
28	ATP	A	501	29	-	2/22/38/38	0/3/3/3
28	ATP	F	501	29	-	4/22/38/38	0/3/3/3
28	ATP	D	501	29	-	5/22/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	C	501	ADP	C5-C4	4.52	1.47	1.39
30	C	501	ADP	C5-C6	2.51	1.48	1.41
30	C	501	ADP	C5-N7	-2.50	1.34	1.39
30	C	501	ADP	C8-N7	2.12	1.35	1.31

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	C	501	ADP	C5-C4-N3	-5.94	118.54	126.72
30	C	501	ADP	N3-C4-N9	4.81	135.34	127.17
30	C	501	ADP	C2-N3-C4	3.64	120.73	111.83
30	C	501	ADP	C4-C5-N7	-3.30	106.81	110.58
30	C	501	ADP	N3-C2-N1	-3.14	123.83	128.58
30	C	501	ADP	C4-N9-C8	2.63	108.50	105.74
30	C	501	ADP	C3'-C2'-C1'	2.61	106.40	101.46
30	C	501	ADP	C5-N7-C8	2.47	107.34	103.45

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
28	B	501	ATP	PB-O3B-PG-O2G
28	B	501	ATP	C5'-O5'-PA-O1A
28	B	501	ATP	C5'-O5'-PA-O2A
28	B	501	ATP	C5'-O5'-PA-O3A
28	E	501	ATP	PB-O3B-PG-O2G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
28	E	501	ATP	C5'-O5'-PA-O2A
28	F	501	ATP	C5'-O5'-PA-O1A
28	F	501	ATP	C5'-O5'-PA-O3A
30	C	501	ADP	C5'-O5'-PA-O1A
30	C	501	ADP	C5'-O5'-PA-O2A
30	C	501	ADP	C5'-O5'-PA-O3A
28	D	501	ATP	O4'-C4'-C5'-O5'
28	D	501	ATP	C3'-C4'-C5'-O5'
28	F	501	ATP	O4'-C4'-C5'-O5'
28	F	501	ATP	C3'-C4'-C5'-O5'
28	A	501	ATP	O4'-C4'-C5'-O5'
28	D	501	ATP	C5'-O5'-PA-O1A
28	E	501	ATP	C5'-O5'-PA-O1A
28	E	501	ATP	O4'-C4'-C5'-O5'
28	E	501	ATP	PG-O3B-PB-O2B
28	D	501	ATP	PA-O3A-PB-O1B
28	E	501	ATP	PB-O3B-PG-O1G
30	C	501	ADP	O4'-C4'-C5'-O5'
28	A	501	ATP	C4'-C5'-O5'-PA
28	E	501	ATP	C3'-C4'-C5'-O5'
28	D	501	ATP	PA-O3A-PB-O2B

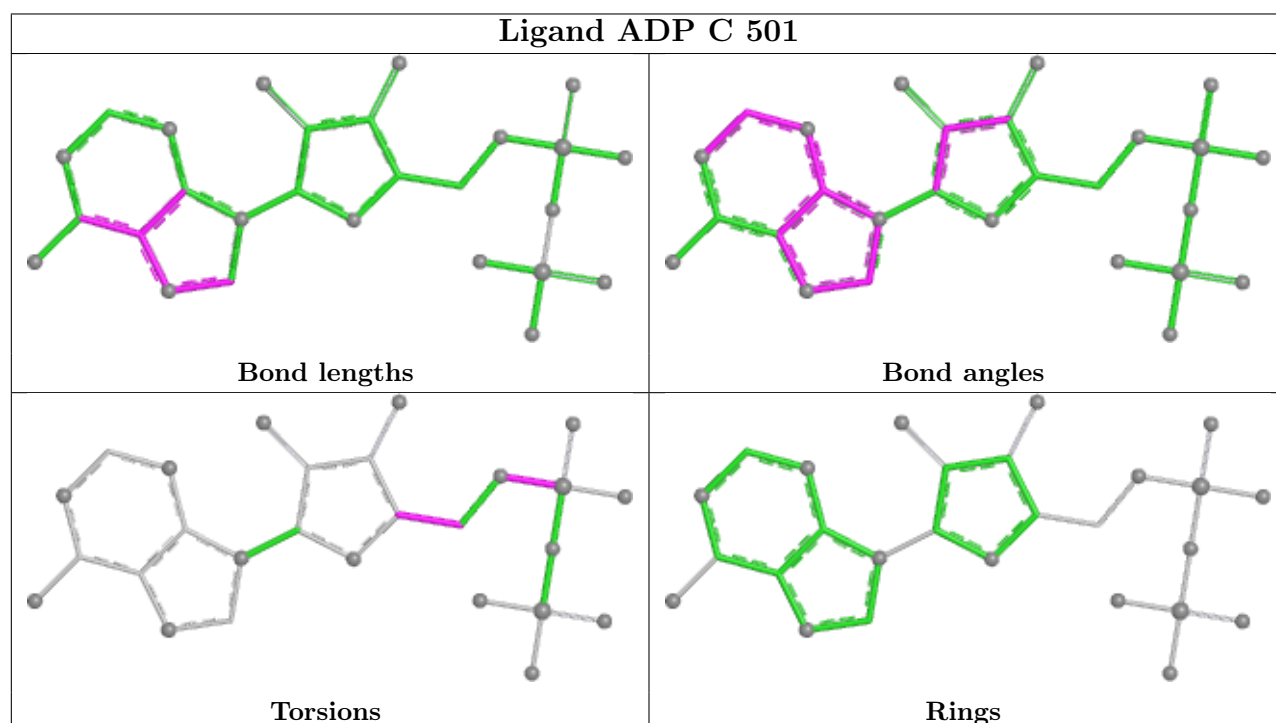
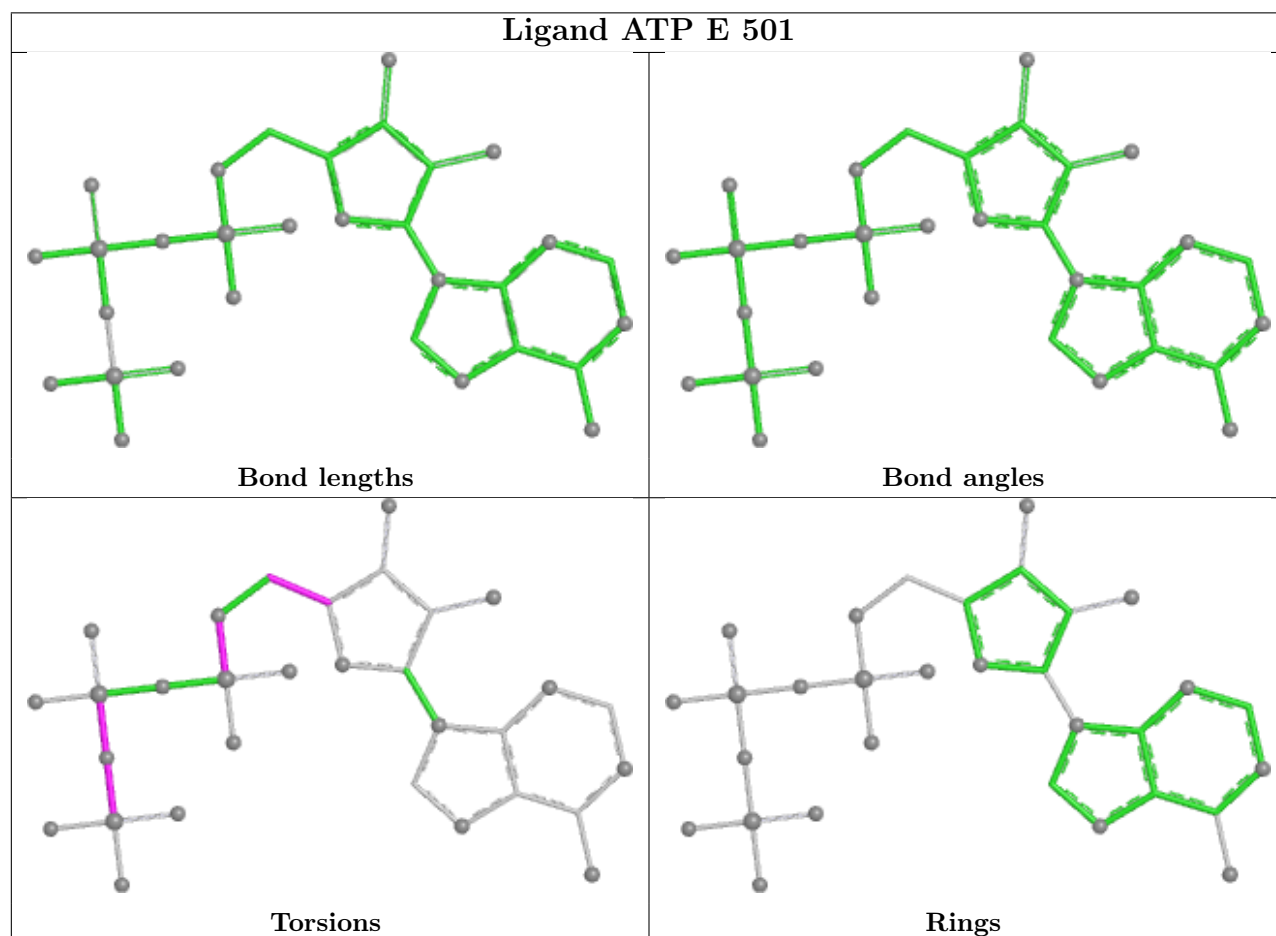
There are no ring outliers.

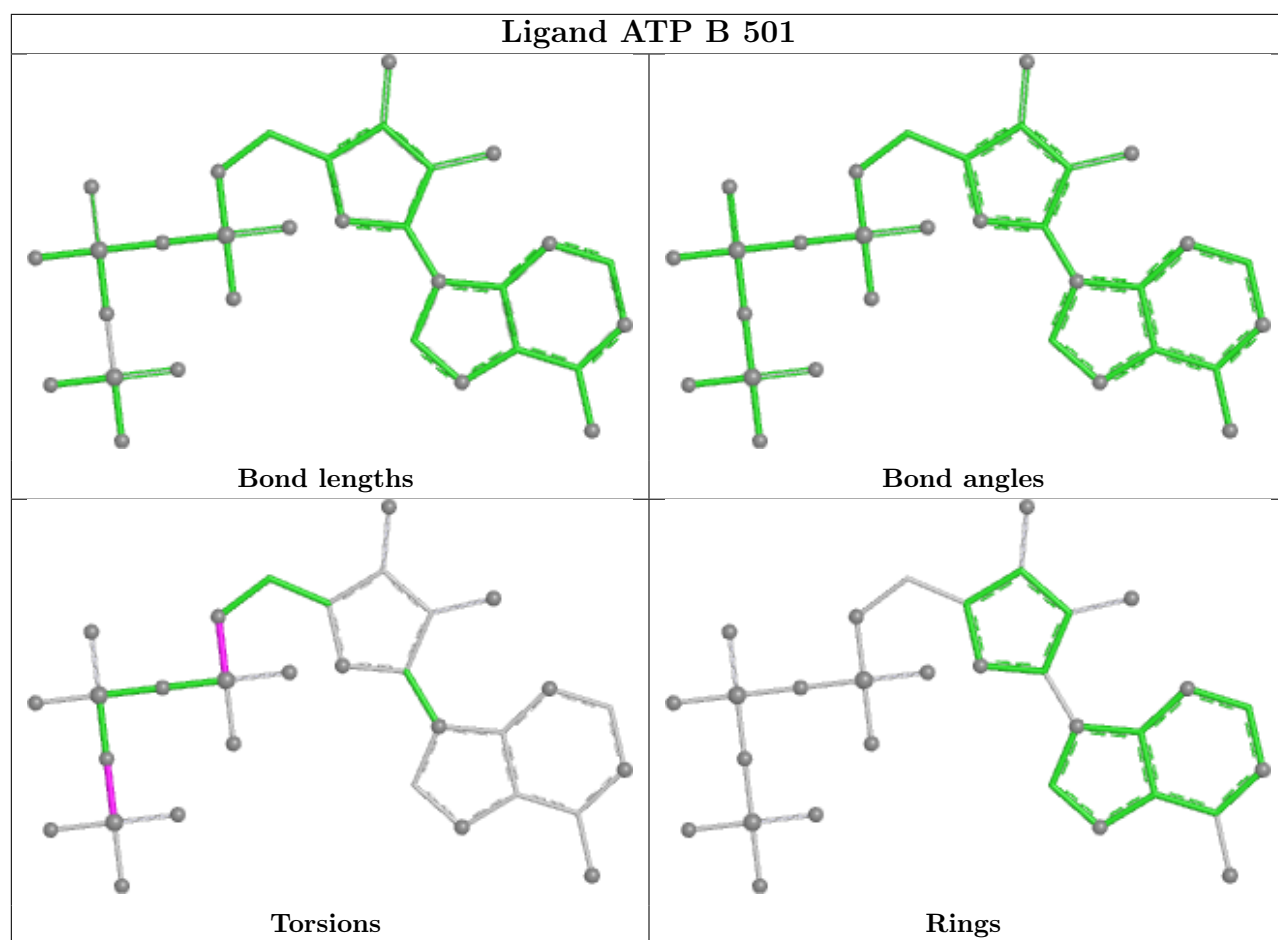
5 monomers are involved in 11 short contacts:

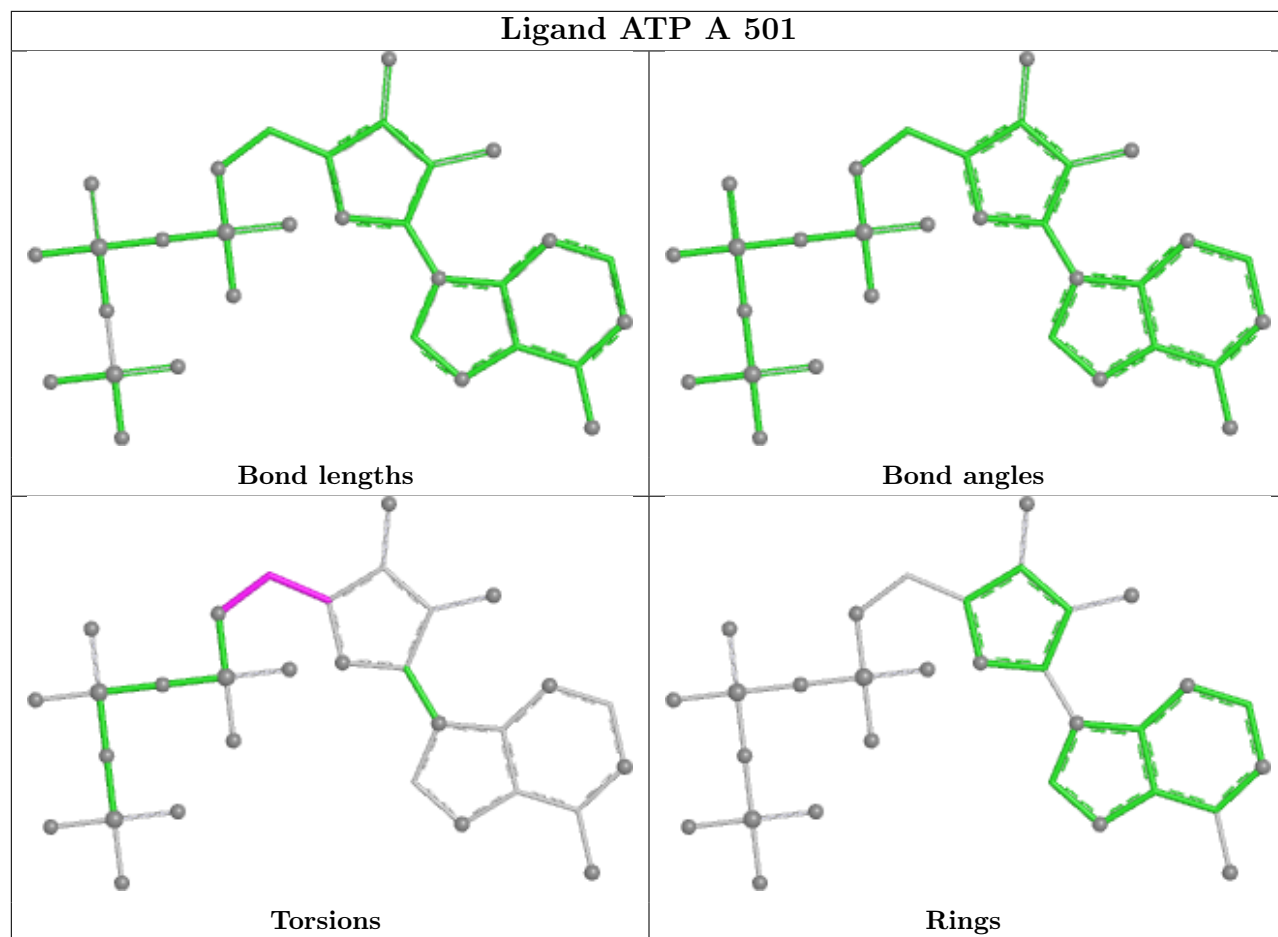
Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	E	501	ATP	2	0
30	C	501	ADP	1	0
28	B	501	ATP	3	0
28	F	501	ATP	1	0
28	D	501	ATP	4	0

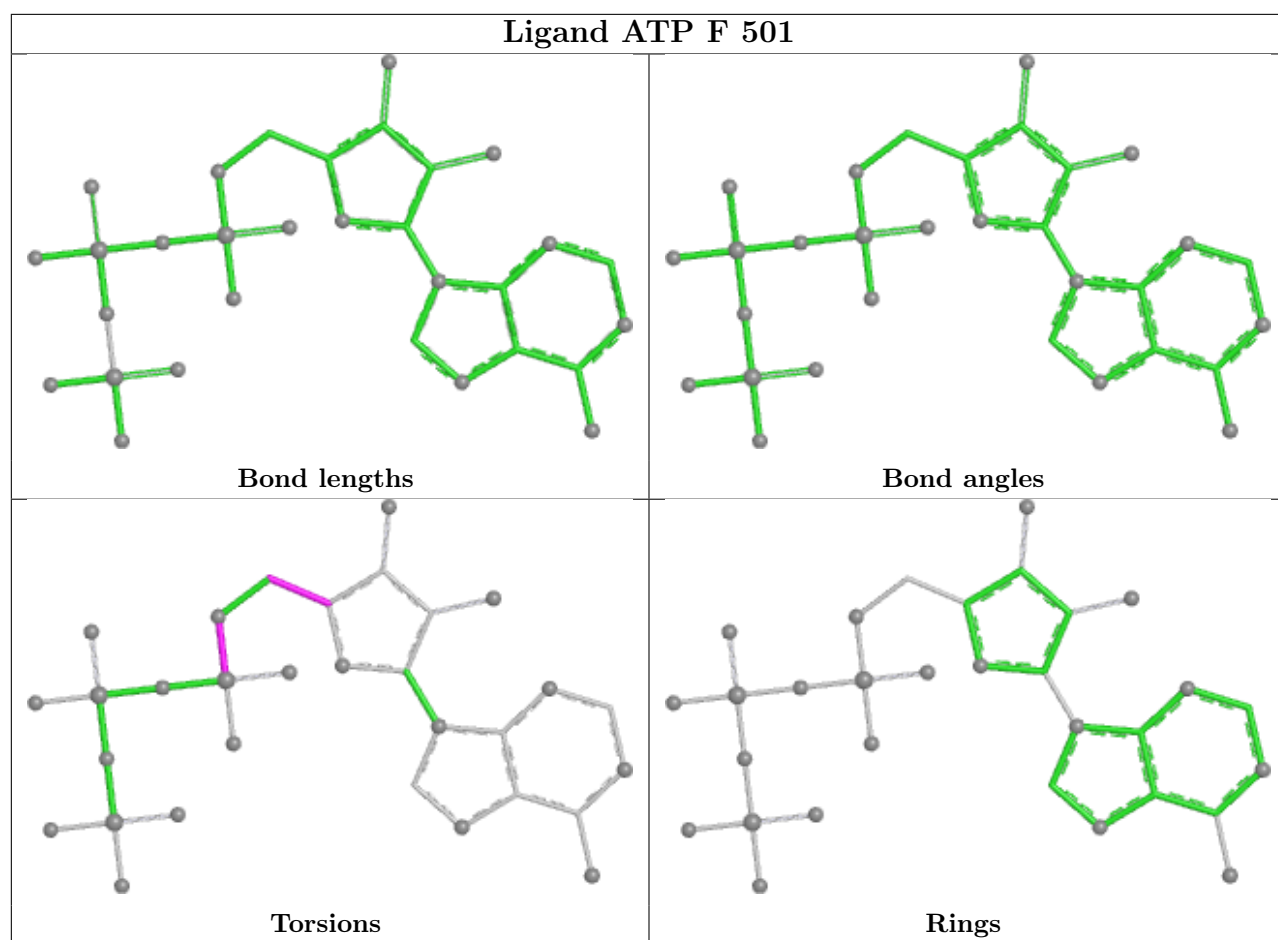
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

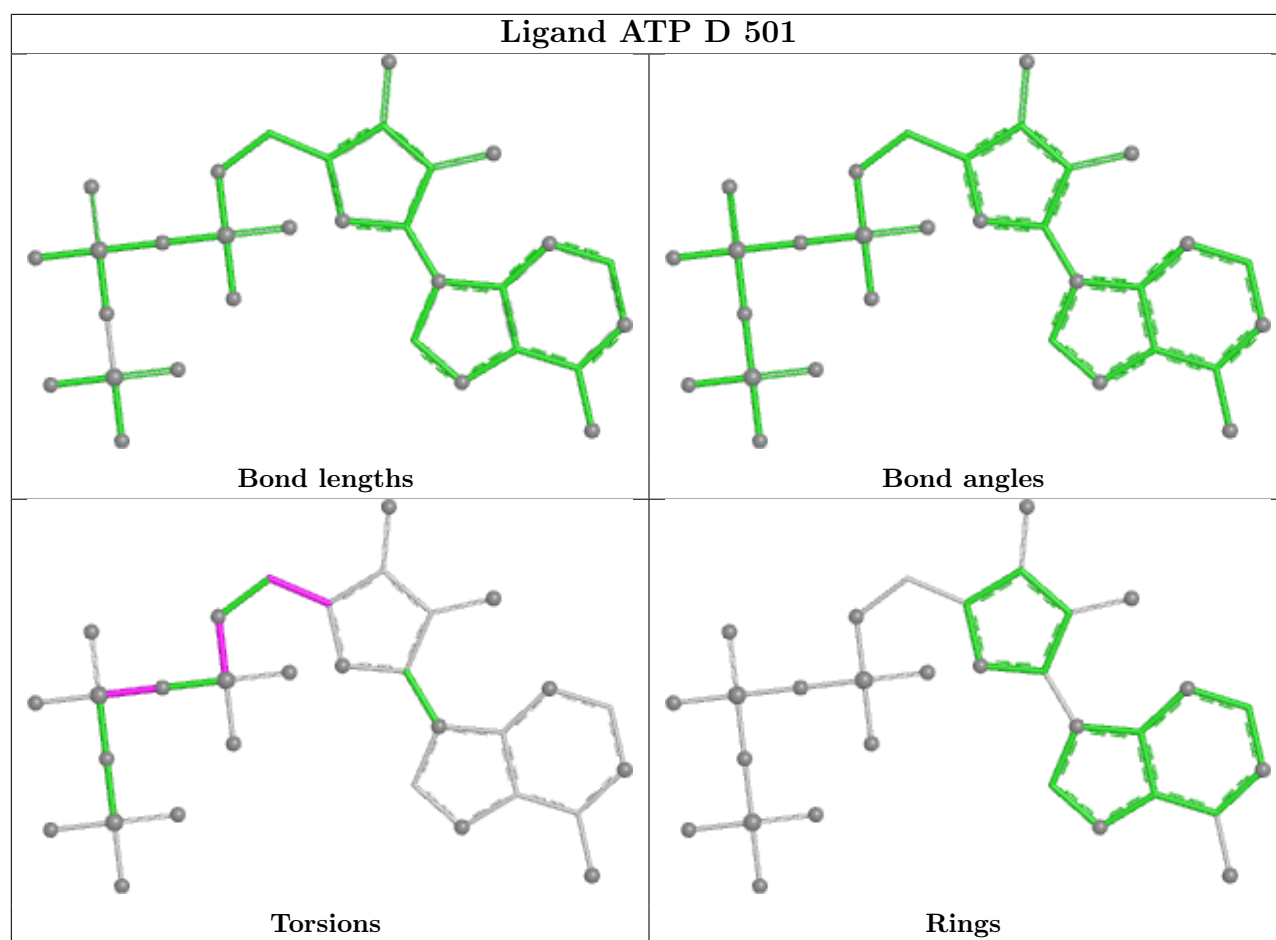
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











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.

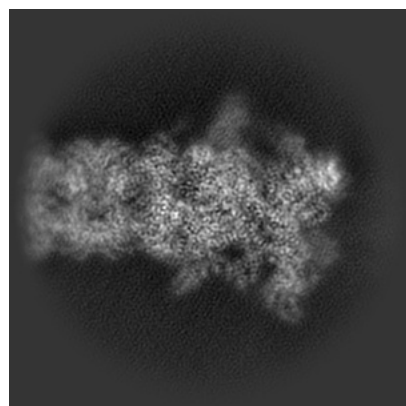
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-47721. These allow visual inspection of the internal detail of the map and identification of artifacts.

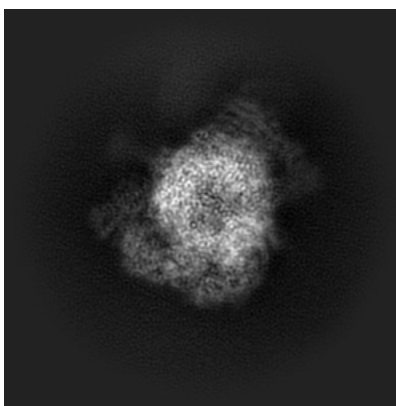
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

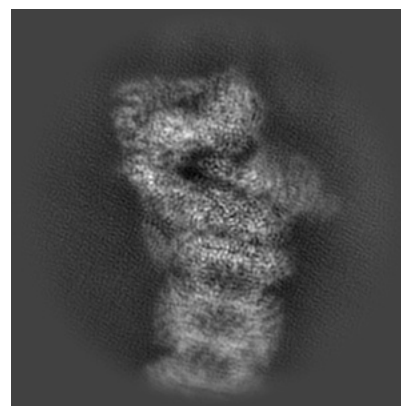
6.1.1 Primary map



X

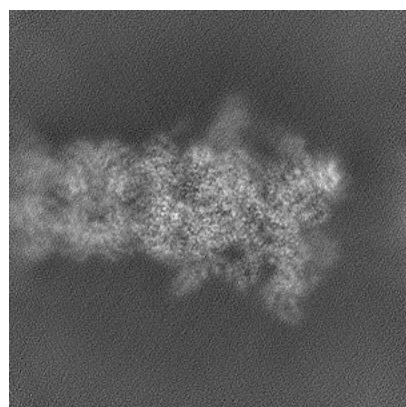


Y

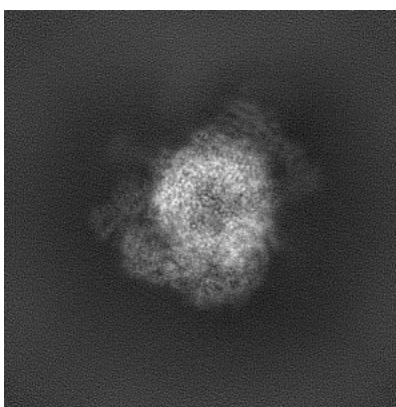


Z

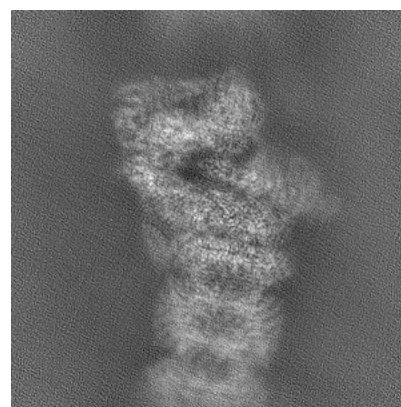
6.1.2 Raw map



X



Y

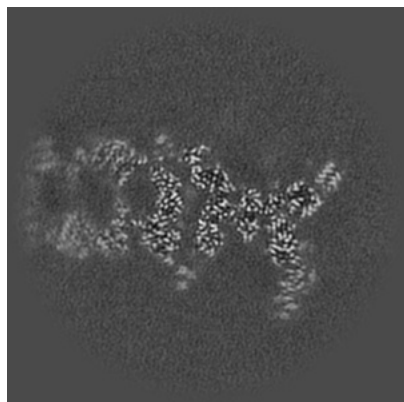


Z

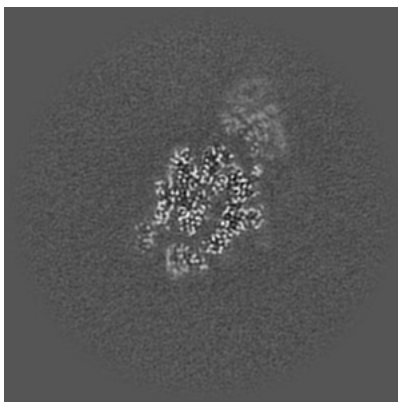
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

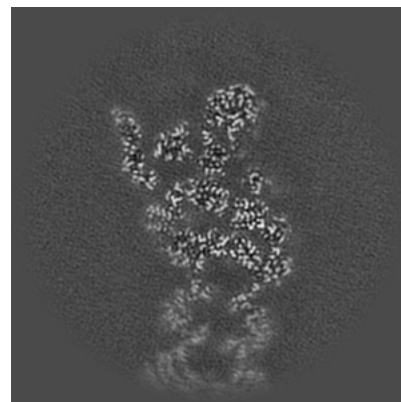
6.2.1 Primary map



X Index: 170

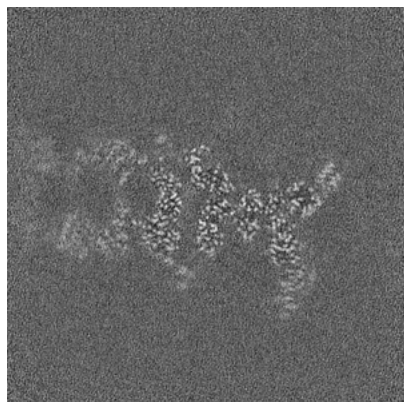


Y Index: 170

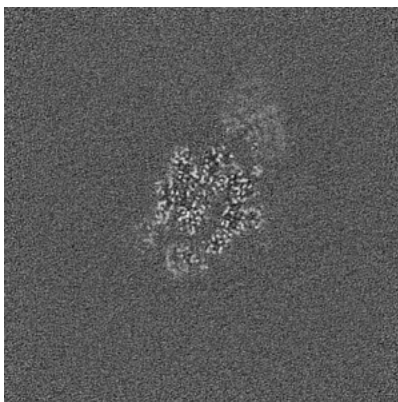


Z Index: 170

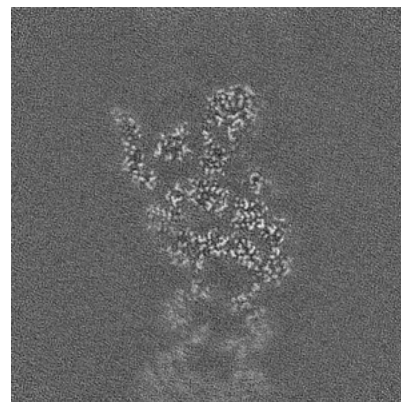
6.2.2 Raw map



X Index: 170



Y Index: 170

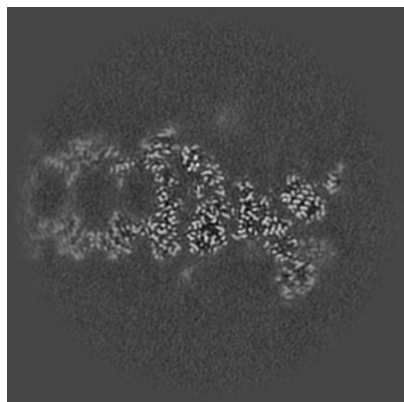


Z Index: 170

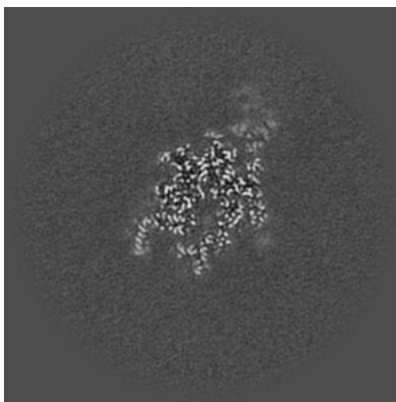
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

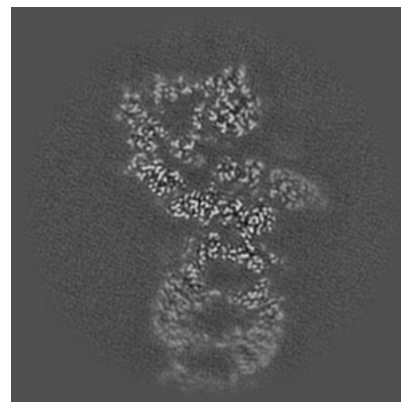
6.3.1 Primary map



X Index: 177

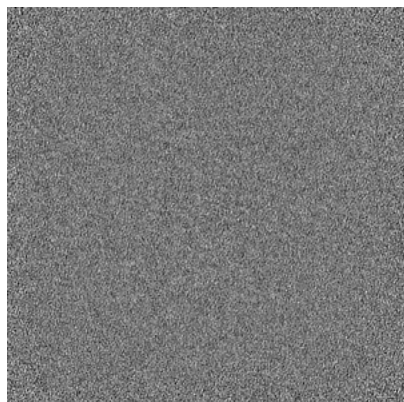


Y Index: 164

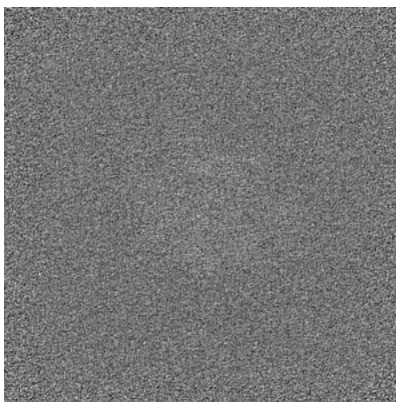


Z Index: 189

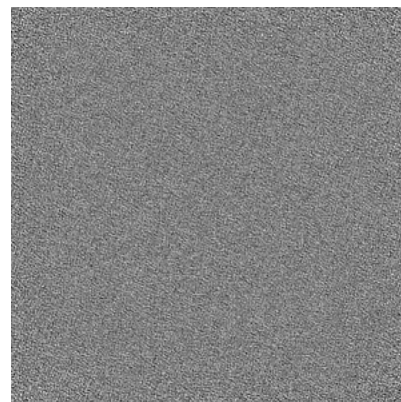
6.3.2 Raw map



X Index: 0



Y Index: 0

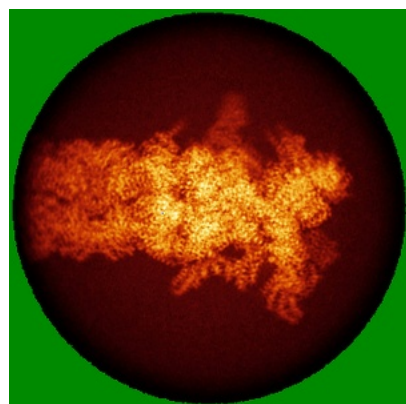


Z Index: 0

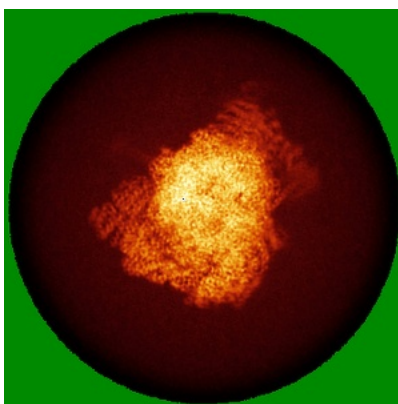
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

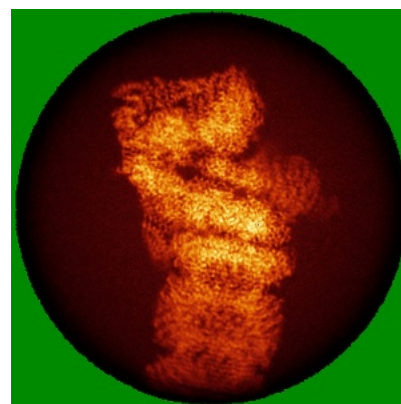
6.4.1 Primary map



X

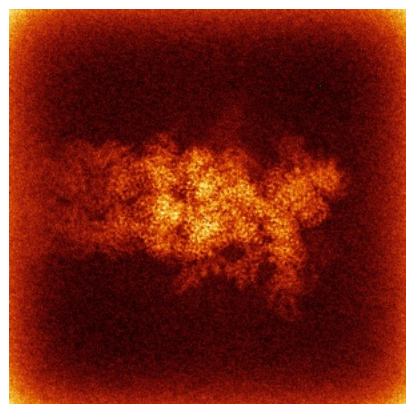


Y

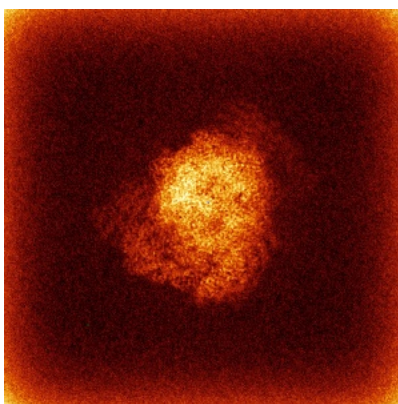


Z

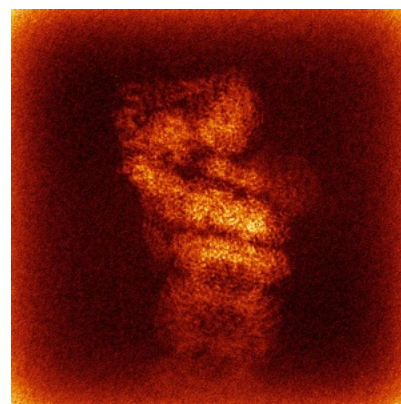
6.4.2 Raw map



X



Y

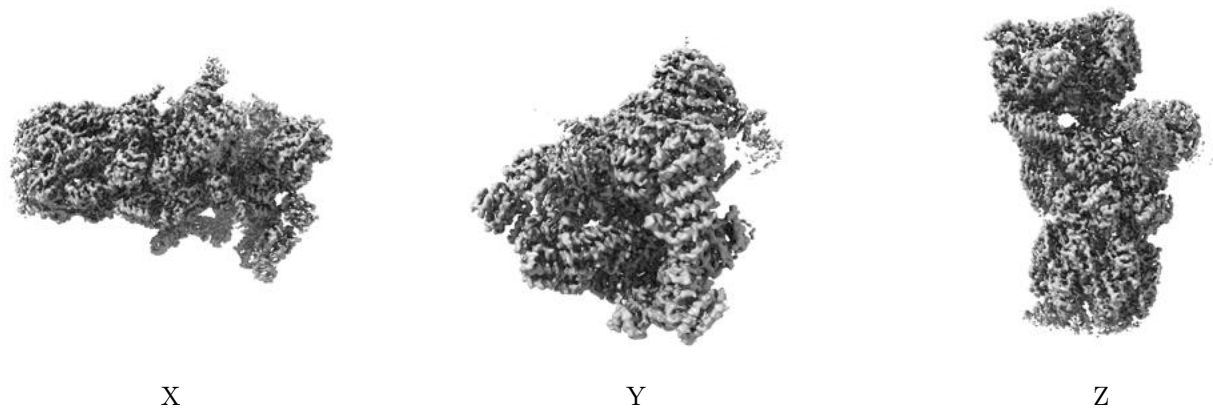


Z

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

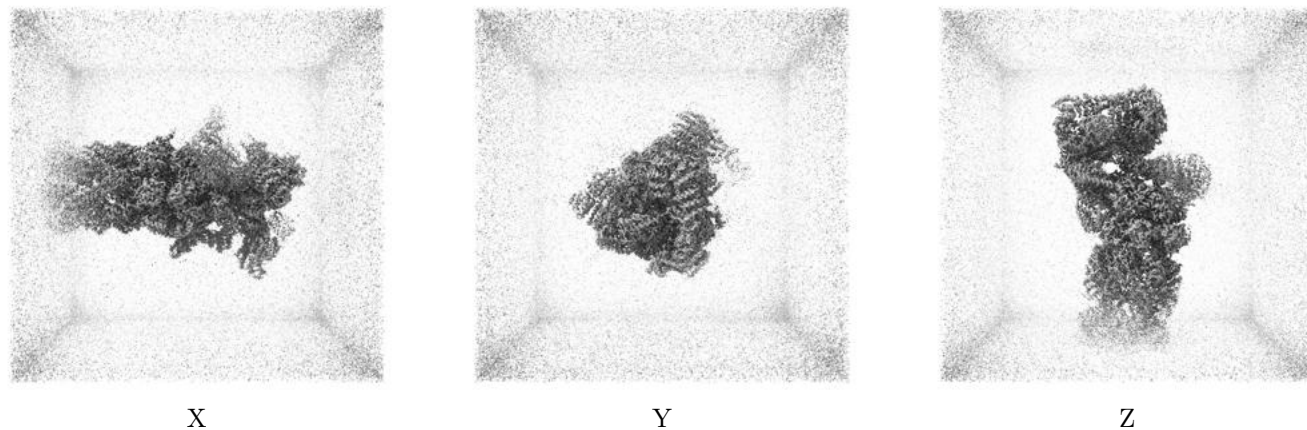
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

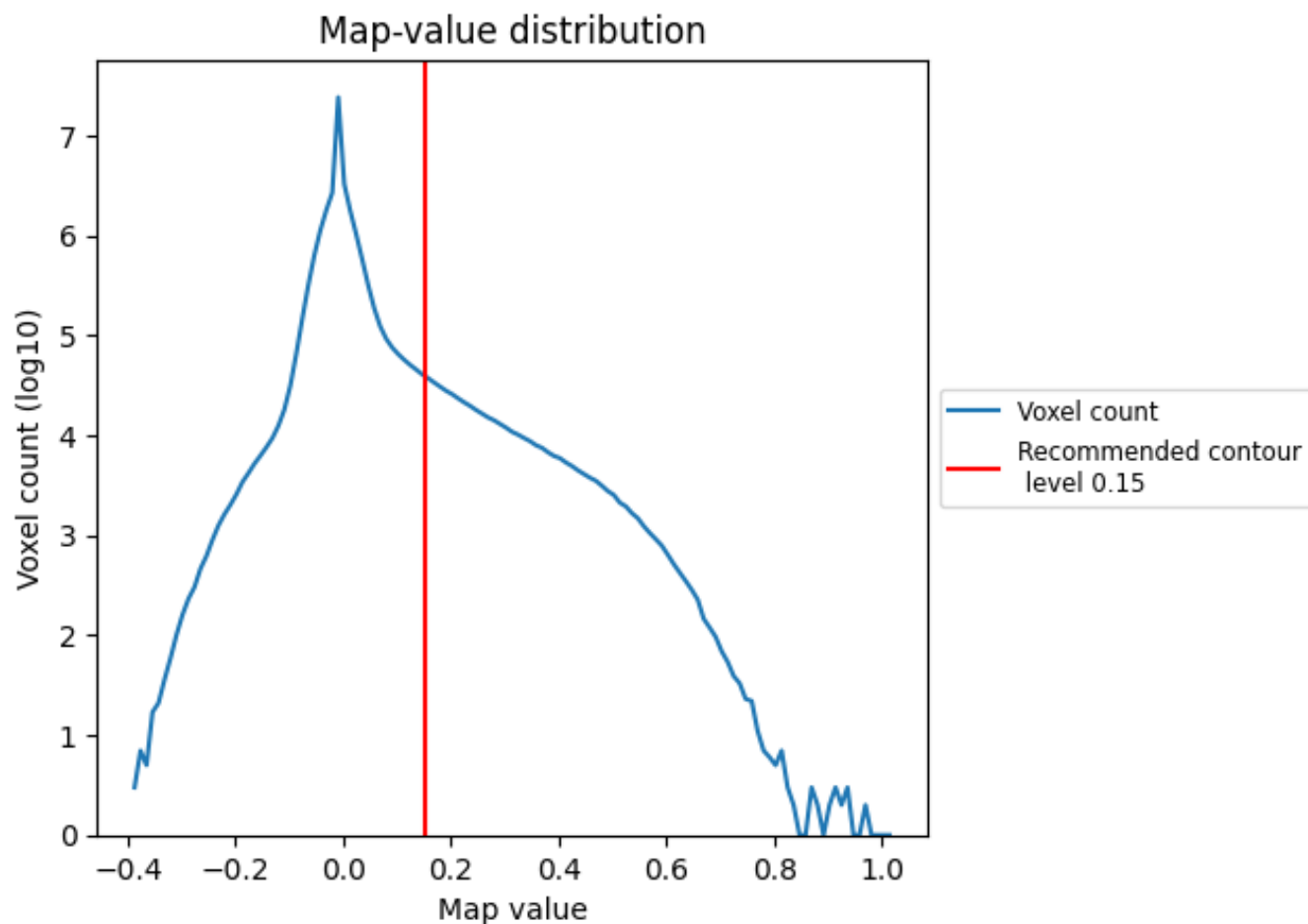
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

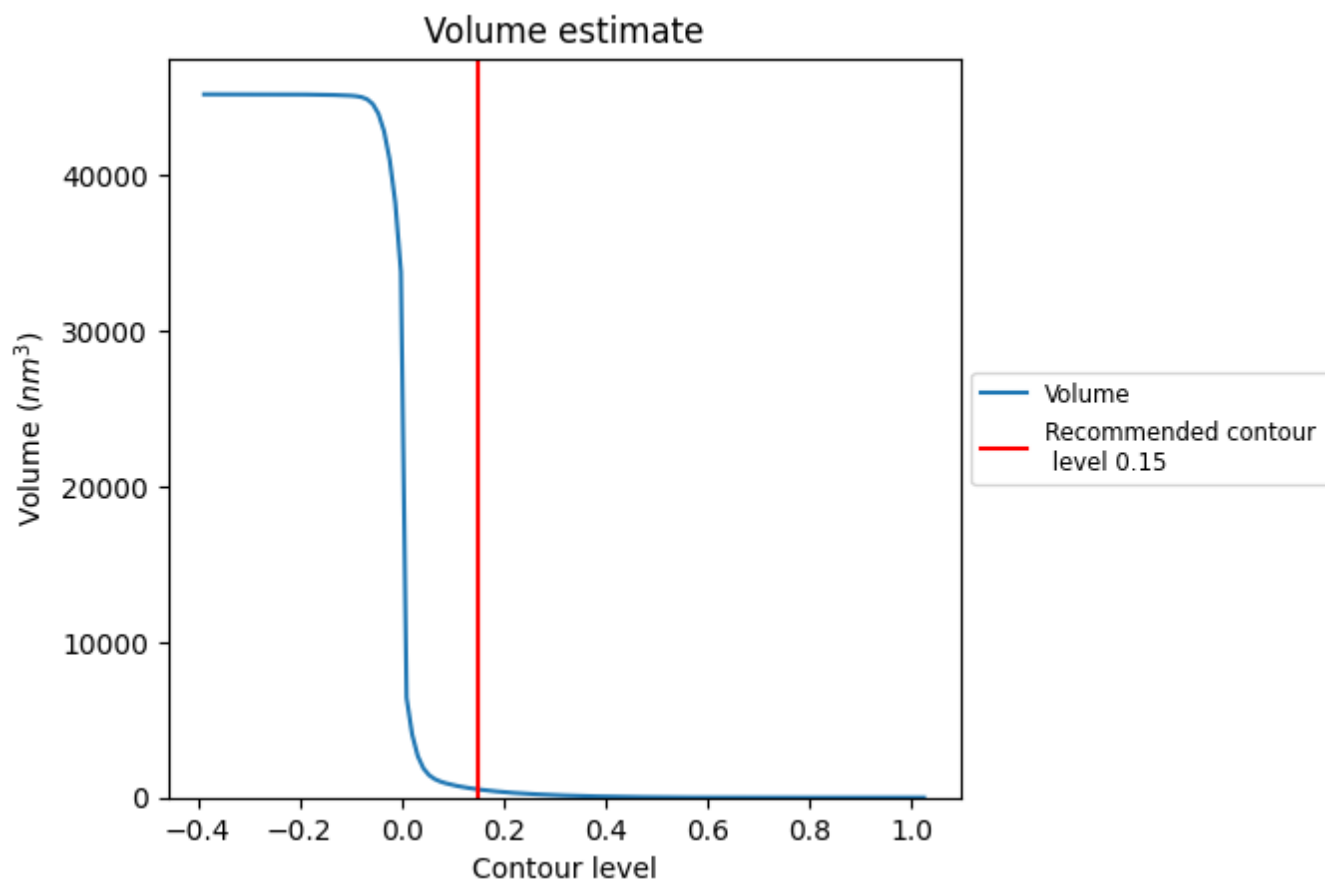
This section contains the results of statistical analysis of the map.

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.

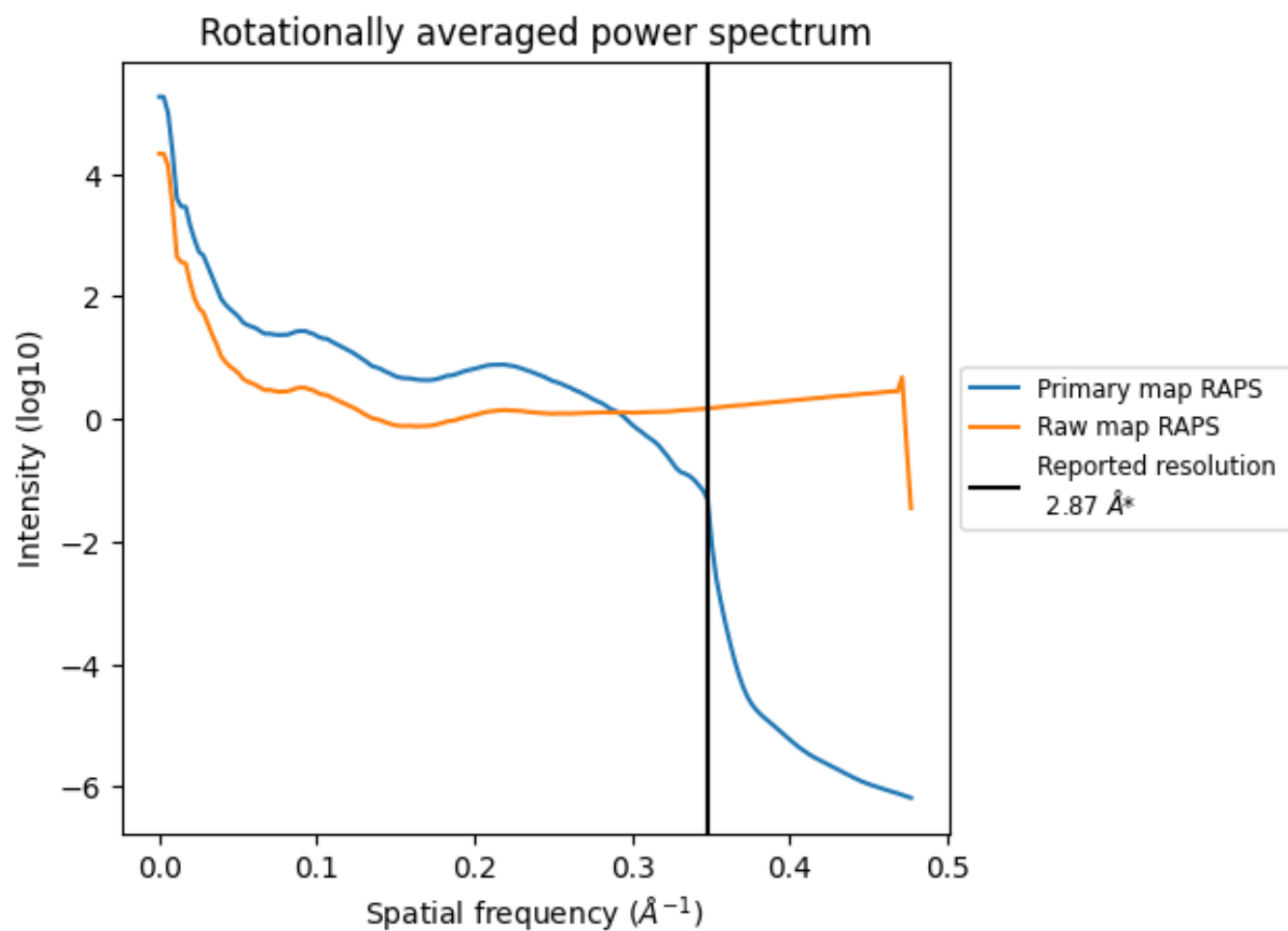
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 530 nm³; this corresponds to an approximate mass of 478 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

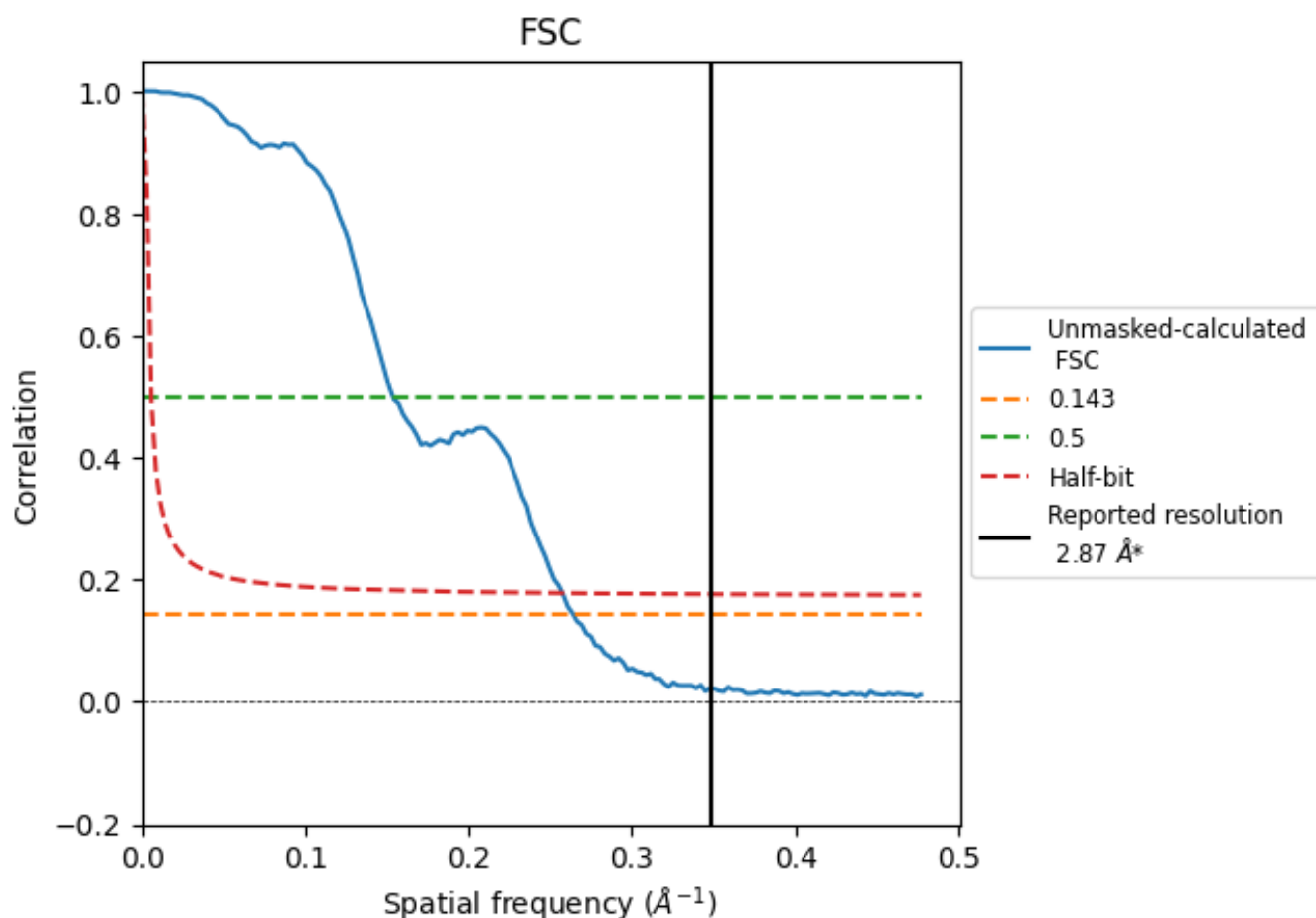


*Reported resolution corresponds to spatial frequency of 0.348 Å⁻¹

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 $0.348 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.87	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.78	6.51	3.88

*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 3.78 differs from the reported value 2.87 by more than 10 %

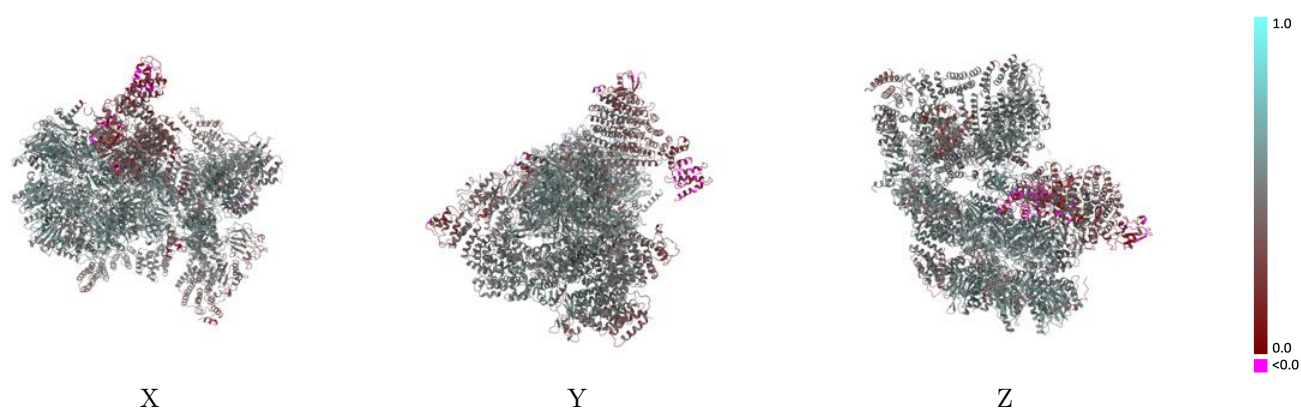
9 Map-model fit [i](#)

This section contains information regarding the fit between EMD map EMD-47721 and PDB model 9E8I. Per-residue inclusion information can be found in section 3 on page 13.

9.1 Map-model overlay [i](#)

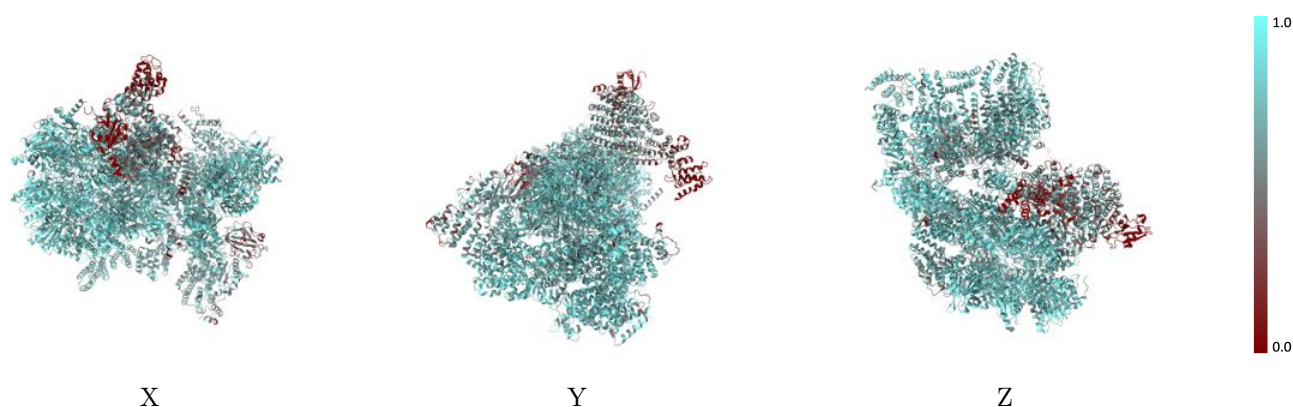
This section was not generated.

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



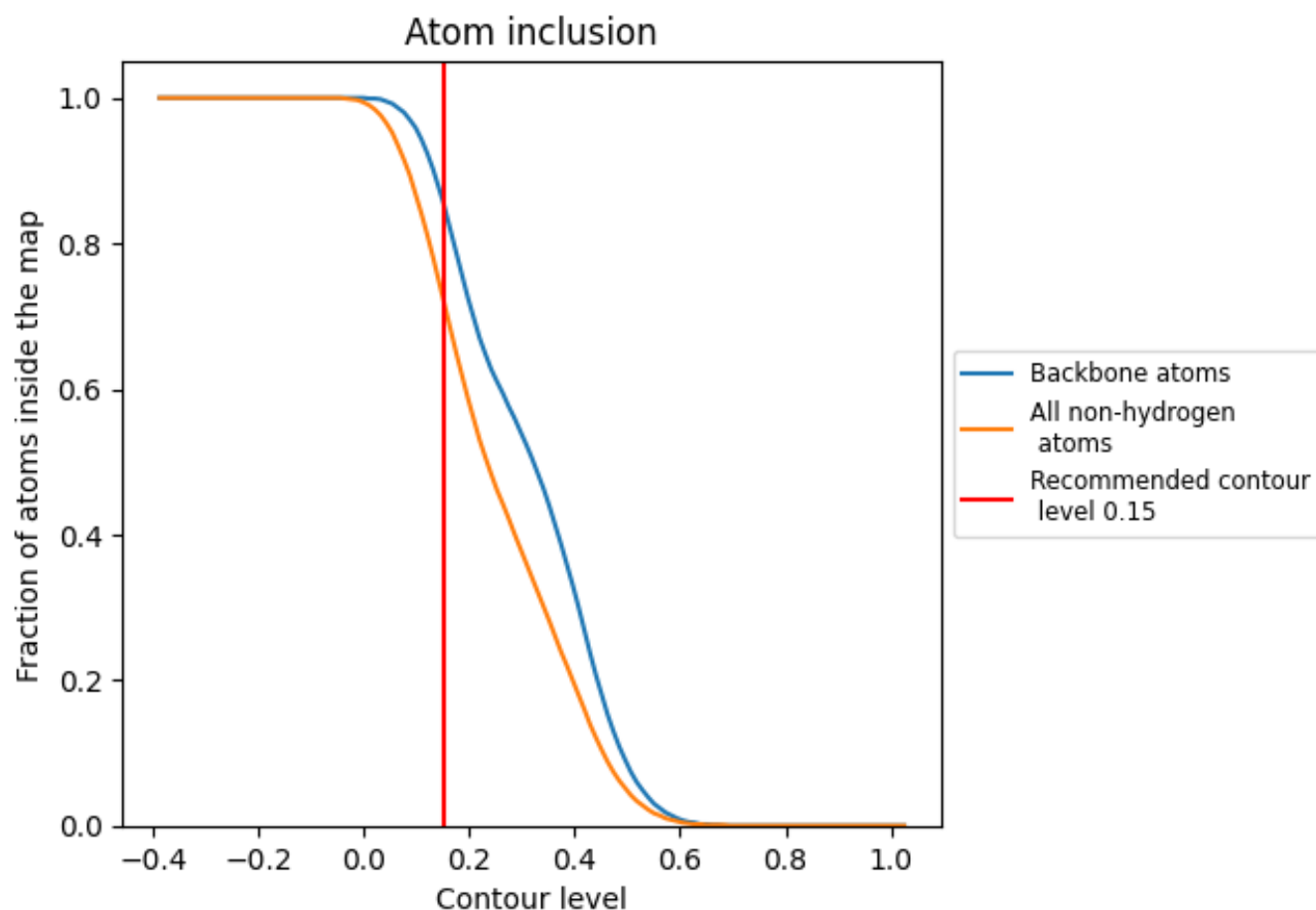
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.15).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 72% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7250	 0.4820
A	 0.7880	 0.5240
B	 0.7190	 0.5010
C	 0.8030	 0.5400
D	 0.8020	 0.5410
E	 0.8260	 0.5440
F	 0.8120	 0.5430
G	 0.8140	 0.5350
H	 0.8240	 0.5420
I	 0.7780	 0.5150
J	 0.7940	 0.5140
K	 0.7880	 0.5320
L	 0.8060	 0.5360
M	 0.8070	 0.5380
U	 0.7630	 0.4900
V	 0.7240	 0.4510
W	 0.7590	 0.4760
X	 0.6990	 0.4660
Y	 0.8280	 0.5220
Z	 0.7720	 0.5140
a	 0.7040	 0.4410
b	 0.6240	 0.4260
c	 0.7830	 0.5320
d	 0.7180	 0.4270
e	 0.6160	 0.3910
f	 0.4490	 0.3310
g	 0.0000	 0.1330
u	 0.4030	 0.4000

