



Full wwPDB EM Validation Report ⓘ

Mar 7, 2026 – 12:50 AM UTC

PDB ID : 7VBA / pdb_00007vba
EMDB ID : EMD-31876
Title : Structure of the pre state human RNA Polymerase I Elongation Complex
Authors : Zhao, D.; Liu, W.; Chen, K.; Yang, H.; Xu, Y.
Deposited on : 2021-08-31
Resolution : 2.89 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:

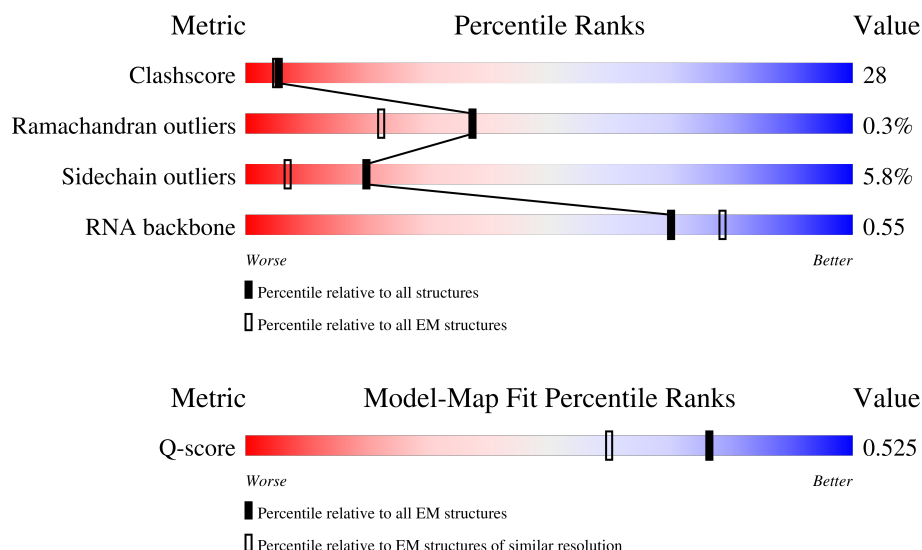
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.89 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



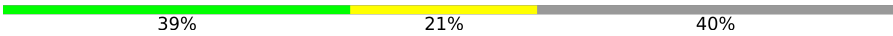
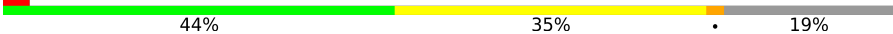
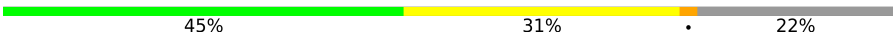
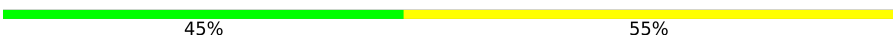
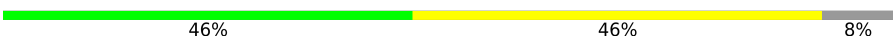
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	12148 (2.39 - 3.39)

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	1719	
2	B	1135	
3	C	346	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	E	210	
5	F	127	
6	H	150	
7	I	126	
8	J	67	
9	K	133	
10	L	58	
11	N	510	
12	G	338	
13	M	419	
14	R	8	
15	T	22	
16	U	13	

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 33093 atoms, of which 14 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called DNA-directed RNA polymerase I subunit RPA1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1473	Total	C	N	O	S	0	0
			11749	7474	2063	2134	78		

- Molecule 2 is a protein called DNA-directed RNA polymerase I subunit RPA2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1123	Total	C	N	O	S	0	0
			8912	5710	1517	1614	71		

- Molecule 3 is a protein called DNA-directed RNA polymerases I and III subunit RPAC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	337	Total	C	N	O	S	0	0
			2697	1701	480	505	11		

- Molecule 4 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	199	Total	C	N	O	S	0	0
			1641	1042	286	305	8		

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	76	Total	C	N	O	S	0	0
			610	392	103	110	5		

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	146	Total	C	N	O	S	0	0
			1176	744	192	235	5		

- Molecule 7 is a protein called DNA-directed RNA polymerase I subunit RPA12.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	60	Total	C	N	O	S	0	0
			447	277	76	89	5		

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	64	Total	C	N	O	S	0	0
			507	328	86	87	6		

- Molecule 9 is a protein called DNA-directed RNA polymerases I and III subunit RPAC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	108	Total	C	N	O	S	0	0
			863	535	156	165	7		

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	45	Total	C	N	O	S	0	0
			379	236	73	64	6		

- Molecule 11 is a protein called DNA-directed RNA polymerase I subunit RPA34.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	N	151	Total	C	N	O	S	0	0
			1105	698	198	204	5		

- Molecule 12 is a protein called DNA-directed RNA polymerase I subunit RPA43.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	G	157	Total	C	N	O	S	0	0
			1229	775	215	232	7		

- Molecule 13 is a protein called DNA-directed RNA polymerase I subunit RPA49.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	110	Total	C	N	O	S	0	0
			867	539	159	163	6		

- Molecule 14 is a RNA chain called RNA (5'-R(P*UP*GP*CP*UP*GP*AP*CP*U)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
14	R	8	Total	C	N	O	P	0	0
			168	75	27	58	8		

- Molecule 15 is a DNA chain called DNA (5'-D(P*GP*CP*CP*AP*GP*AP*GP*AP*CP*AP*GP*CP*GP*AP*GP*TP*CP*AP*GP*CP*AP*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
15	T	22	Total	C	N	O	P	0	0
			456	214	95	125	22		

- Molecule 16 is a DNA chain called DNA (5'-D(P*A*CP*TP*GP*TP*CP*CP*TP*CP*TP*GP*GP*C)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
16	U	12	Total	C	N	O	P	0	0
			238	115	38	74	11		

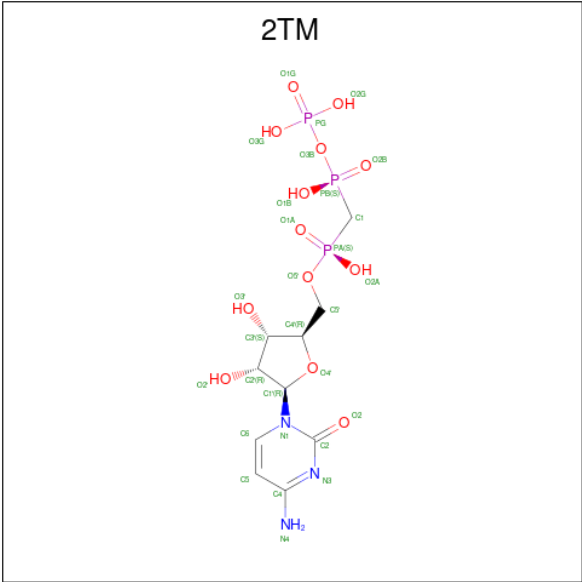
- Molecule 17 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
17	A	2	Total	Zn	0
			2	2	
17	B	1	Total	Zn	0
			1	1	
17	J	1	Total	Zn	0
			1	1	
17	L	1	Total	Zn	0
			1	1	

- Molecule 18 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

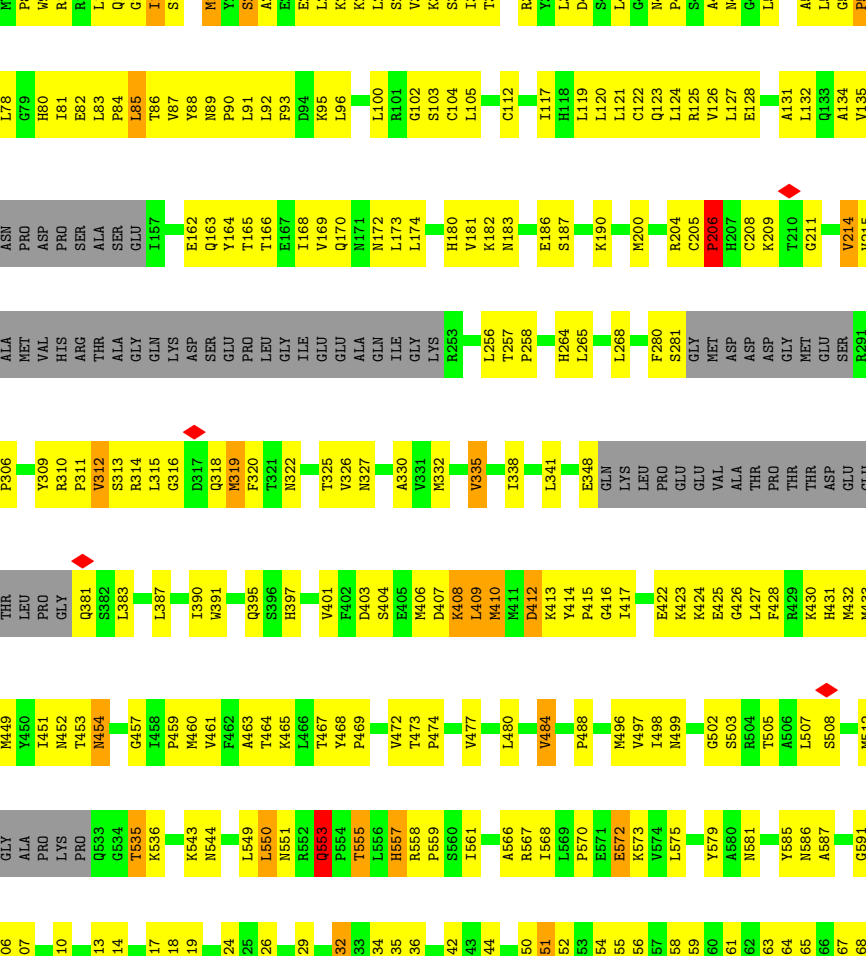
- Molecule 19 is 5'-O-[(S)-hydroxy{[(S)-hydroxy(phosphonooxy)phosphoryl]methyl}phosphoryl]cytidine (CCD ID: 2TM) (formula: C₁₀H₁₈N₃O₁₃P₃).



Mol	Chain	Residues	Atoms						AltConf
19	A	1	Total	C	H	N	O	P	0
			43	10	14	3	13	3	

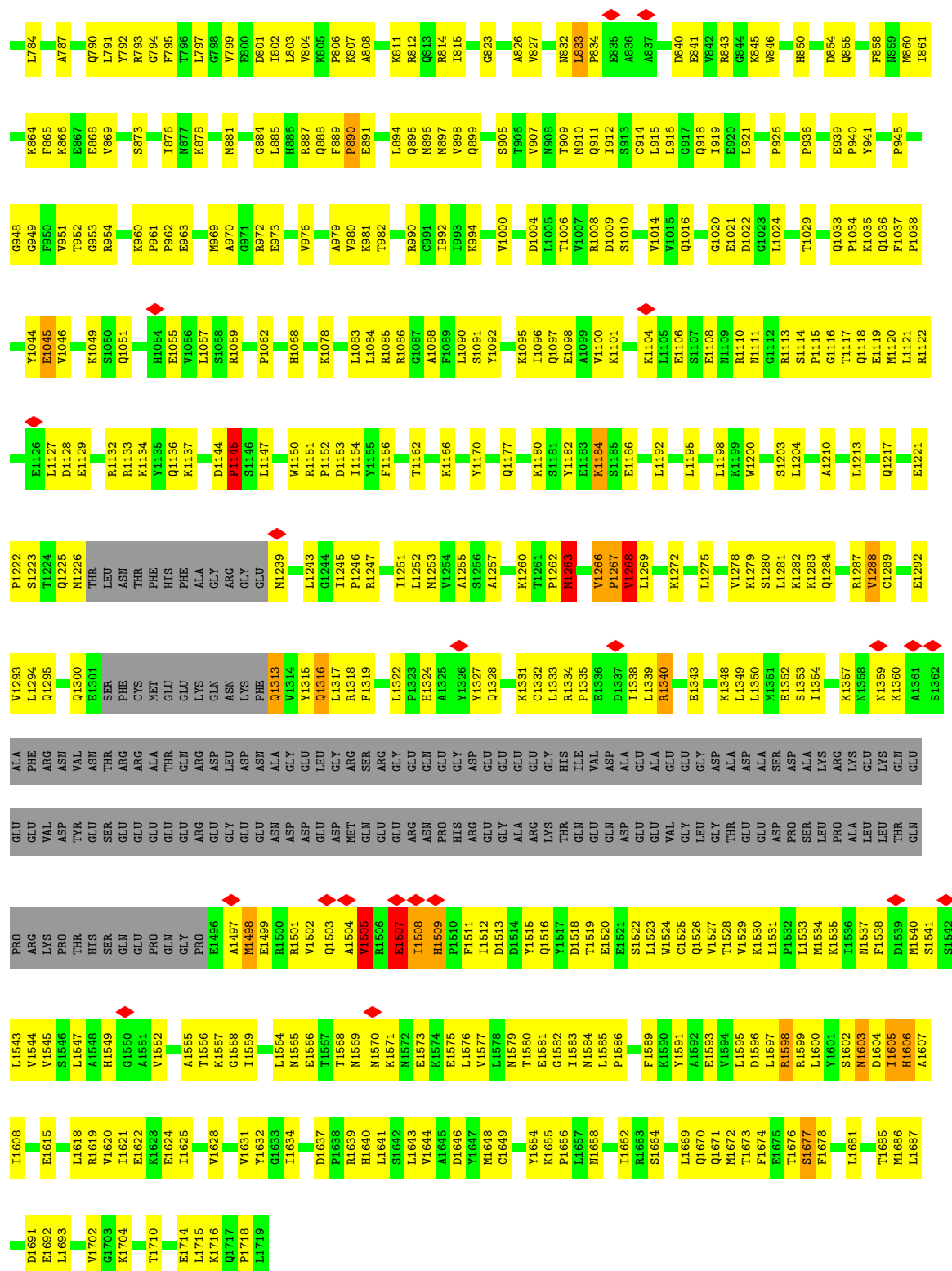
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Chain A: 



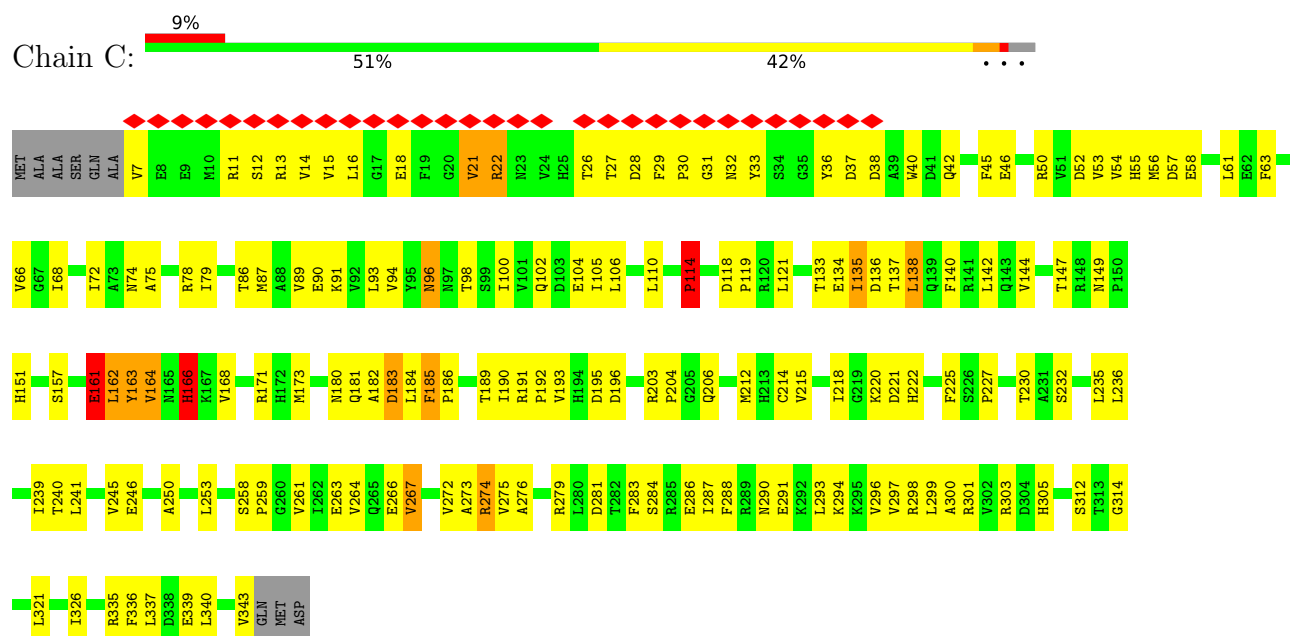
Chain A sequence (residues 1-67):

Residue	3-letter code	1-letter code
1	MET	M
2	LEU	L
3	ILE	I
4	LYS	K
5	W6	W
6	H7	H
7	P8	P
8	W9	W
9	R10	R
10	E11	E
11	L12	L
12	Q13	Q
13	G14	G
14	S15	S
15	M19	M
16	T20	T
17	S21	S
18	A22	A
19	E23	E
20	E24	E
21	L25	L
22	K26	K
23	K27	K
24	L28	L
25	S29	S
26	V30	V
27	K31	K
28	S32	S
29	I33	I
30	T34	T
31	R37	R
32	L38	L
33	D40	D
34	S41	S
35	L42	L
36	G43	G
37	N44	N
38	P45	P
39	S46	S
40	A47	A
41	N48	N
42	G49	G
43	L50	L
44	A54	A
45	L55	L
46	O56	O
47	P57	P
48	K61	K
49	C64	C
50	S65	S
51	T66	T
52	E67	E

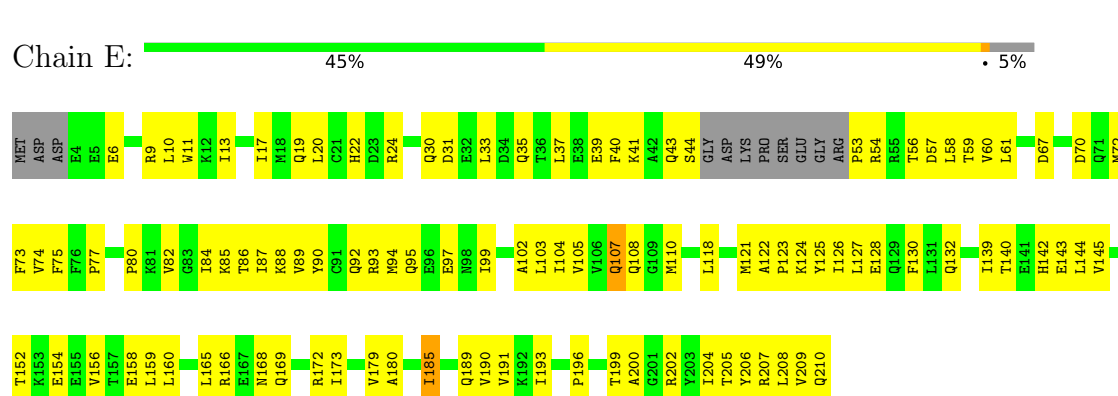


V1112	G1038	D946	S856	I785	L700	Q624	I542	A457	N365	M285	E217	C146	S74	MET
P1113	E1039	A947	R857	K786	L701	N625	D543	M461	V370	L286	E218	M147	F75	ASP
V1114	M1040	T948	T858	Q787	Y702	L626	G544	F462	N371	R287	H219	L148	T76	PRO
F1115	E1041		T859	G788	Y703	A627		F463	Q372	I288	H219	L149	I77	GLY
R1116	R1042			D789	Q704	L628	H547	I463		S220	A221	N150		S5
R1117	D1043			G789	R705	G629	S549	R464		M290	V222		I82	R6
L1123	A1044	M965	G862	S790	R706	K630	S549	Y465	K386	E291	M223	L156		U7
A1124	L1045	L966	K863	S791	S707	E631	S550	L466	K387	E292	M224		T86	R8
M1125	L1046	A969	K865	L792	D708	E632	S551		K388		N225	H159	V87	N9
N1127	T1050		K866	F793	N709	L633	E552	F469	L389	S295	H226	H160	P88	L10
I1128	S1051	N972	G868	G795	K710	M637	G553	C471	E390	Q297	L227	E161		P11
L1132	L1052			I796	L711	F638	Y554	V472	G391		L229	A163	T91	P14
D1133	L1054	L979	M871	K797	Y712	Q639	V561	H473	L393	L304	E230	E164	C93	S15
V1135	L1058	Y980	K882	D800	T716	M642	M562	R474	V394	C307	N231	E165	K94	H18
	F1059	S981	F883	R801	P717	N643	G564	G475	S395		G232	M166	E95	L19
	S1063	Q982	R882	R802	P720	E647	V565	T484	K397	L312	V234	G167	A96	T20
	M1060	S984	H887	V803	L721	E648	S666		I398	M235	M235	Y169	N97	D21
	G1061		G888	L804	V722	D649	D567	L489	A399	V314	L236	F170	V98	
S1063	R1064	E987	Q889	Q805	R723	E650	K568		F400	P315	N237	E102	I26	I26
R1064	L807	E988	K806	K806	D728	V651	D569	W494	K403	Y318	L247	R180	R11	T39
S1065	L807		L807	L570	Y729		L570	G495	A404	P319	P248	M181	G112	
A1067	R1067	V996	D809	A571	Y730	V655	A571	L496	Q405	N320	L249	L182	K113	H42
S1066	S1065	Y997	D810	P572	D731	T656	P572	L497	Q406	G105	G260	I183	L114	
A1067	H1068	Y998	G811	G573	M732	T657	G573	C498	T407	E321	E241	M184	T115	F46
H1069	Y999	Y999	L812	I574	D733	T658	I574	P499	K406	N320	K242	R185	A116	F46
	Q1000	R813	D576	A575	Q659	E650	A575	V500	T407	E322	E243	R186	D117	N47
L1076	L1001	T905	F814	S577	Y735	E660	S577	P503	V409	E325	L244	R187	I118	Y48
L1077	L1002	P736	L661		P736	L661			S410	F326	L247	P190	W120	A49
	R1003	I737	F662	K582	I737	F662	K582	E506	M411	L327	P248	K197	A121	V50
L1081	G908		P663	V583	I742	P663	V583	P507	D414	Q330	L249	K197	W120	G55
E1082	M909		L666	L584	Y742	L666	L584	C508	W415	I332	G260	I130	I130	V58
K1083	V910		L667	R585	A744	L667	R585	G509	M415	C331	F251	K131	A60	Q59
P1084			S668	P590	V745	S668	P590	M511	M417	I334	S258	Q132	I61	I61
PRO					V745			M512	M418	H335	F259	F133	P62	P62
PRO					I746			H513	I419	L336	S260	F133	P63	P63
SER								L514	F420	K337	D261	Q207	F64	F64
SER								L514	T421	S338	Y262	Y208	E95	E95
ALA								C518	M422	N339	I264	T206	P83	P83
MET								E519	G423	K342	F265	Q207	F66	F66
ARG								V520	I424	M345	Q266	Y208	E87	E87
M1093								V521	D425	L346	E267	K197	S126	S126
R1094								F524	L426	M346	L268	R201	I130	I130
K1095								V525	P429	L348	I269	R201	K131	A60
Y1096								V526	F430	C347	K270	Y205	Q132	P62
M1097								T527	E431	M349	D275	T206	F133	P62
								A528	F430	T350	D275	Q207	F133	P62
								S529	E432	R351	D275	Y208	E95	E95
								P531	L433	K352	S276	G209	F66	F66
								P531	F434	L353	F277	V210	A67	A67
								P616	A435	F354	L278	M140	F68	F68
								N536	T443	C361	R279	M212	K69	K69
								L537	G444	M362		H213	V141	V141
								V539	G444	G363		C214	K142	K142
									V623	D364		V282	S143	S143
												S283	V215	E71
												K144	R72	R72
												Q284	I73	I73

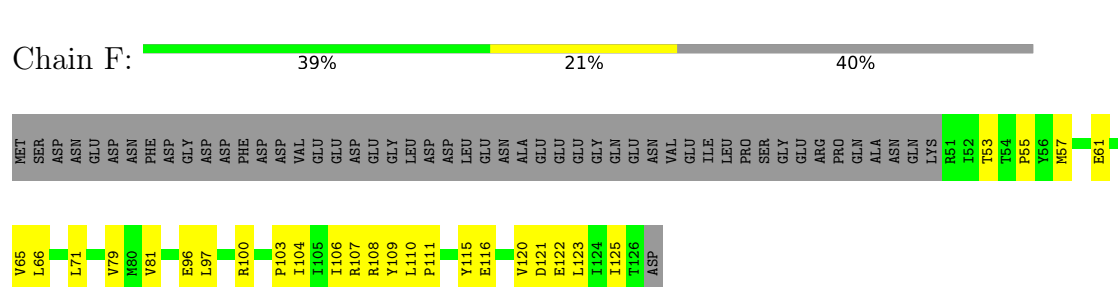
Chain C: 9% 51% 42% ...



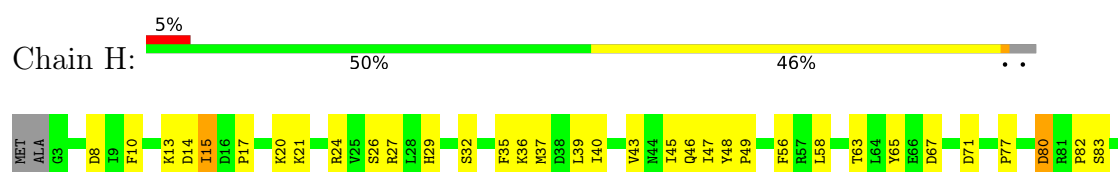
Chain E: 45% 49% 5%

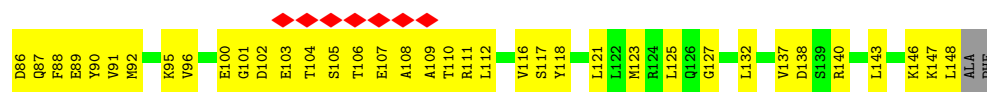


Chain F: 39% 21% 40%

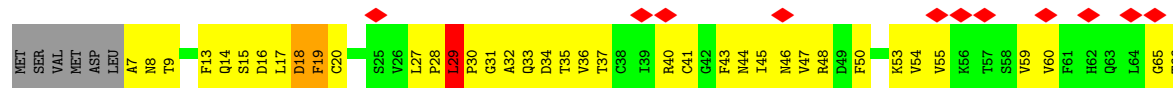


Chain H: 5% 50% 46% ..

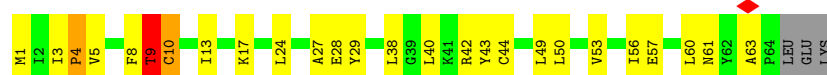




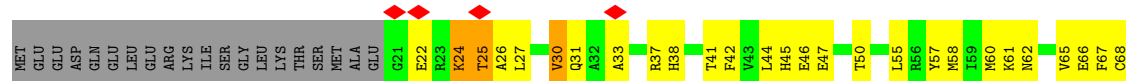
• Molecule 7: DNA-directed RNA polymerase I subunit RPA12



• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC5



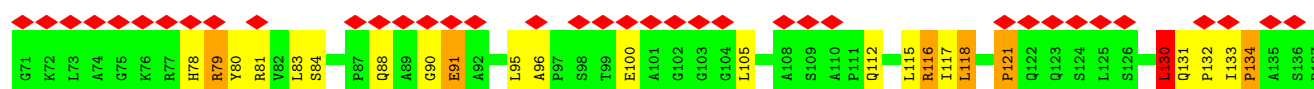
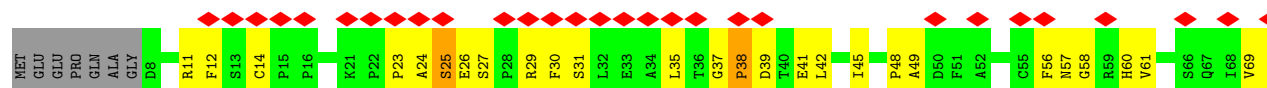
• Molecule 9: DNA-directed RNA polymerases I and III subunit RPAC2

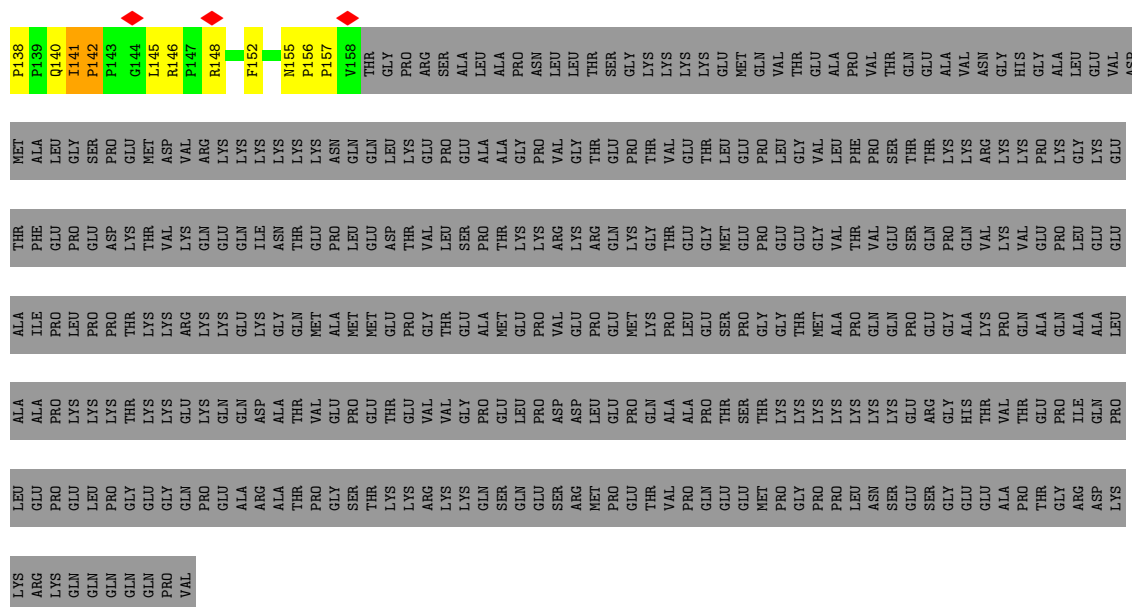


• Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC4

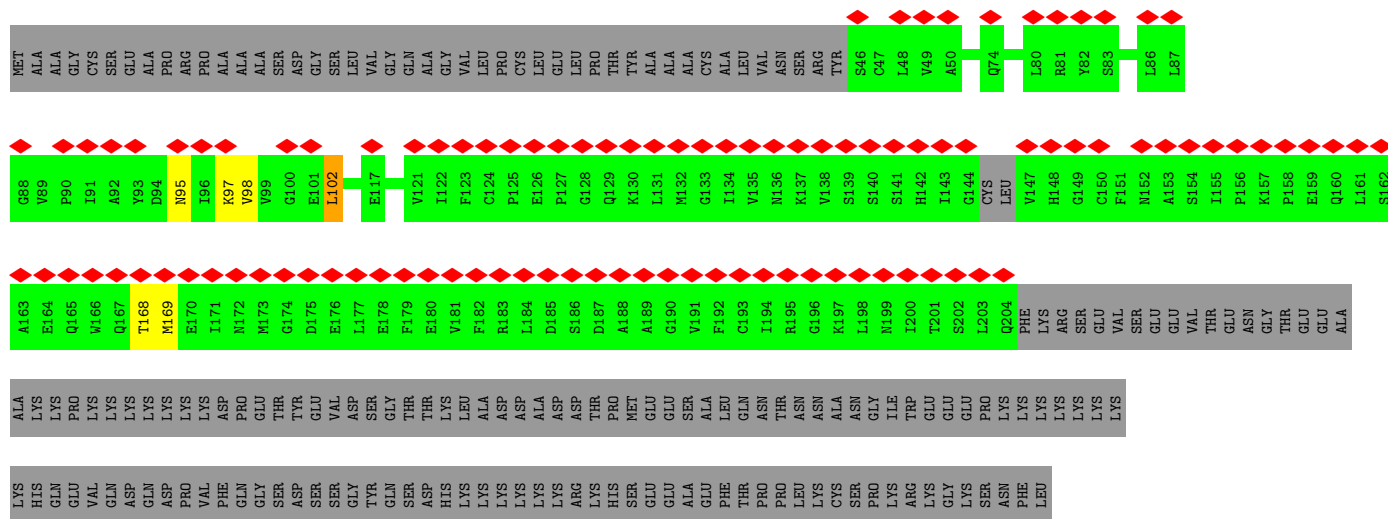
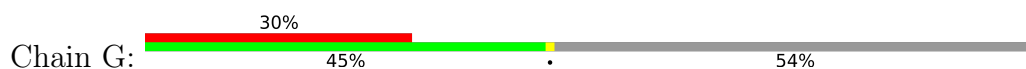


• Molecule 11: DNA-directed RNA polymerase I subunit RPA34

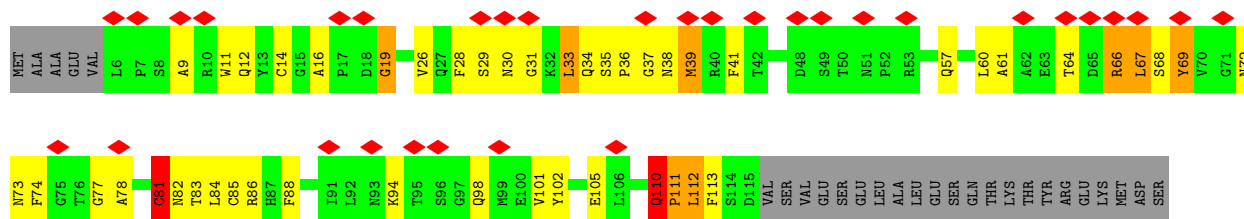


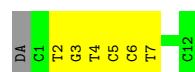


• Molecule 12: DNA-directed RNA polymerase I subunit RPA43



• Molecule 13: DNA-directed RNA polymerase I subunit RPA49





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	382890	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	5.648	Depositor
Minimum map value	-3.264	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.151	Depositor
Recommended contour level	0.351	Depositor
Map size ($\text{\AA}$)	337.28, 337.28, 337.28	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.054, 1.054, 1.054	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN, 2TM

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	0.65	9/11988 (0.1%)	0.98	55/16184 (0.3%)
2	B	0.71	6/9127 (0.1%)	1.09	66/12350 (0.5%)
3	C	0.74	2/2751 (0.1%)	1.19	29/3729 (0.8%)
4	E	0.35	0/1669	0.58	1/2254 (0.0%)
5	F	0.29	0/620	0.46	0/839
6	H	0.47	0/1197	0.84	3/1614 (0.2%)
7	I	0.52	0/454	0.88	1/615 (0.2%)
8	J	0.70	1/516 (0.2%)	1.02	4/696 (0.6%)
9	K	0.39	0/878	0.82	1/1182 (0.1%)
10	L	0.35	0/385	0.66	0/511
11	N	1.10	9/1140 (0.8%)	1.43	22/1560 (1.4%)
12	G	0.38	0/1252	0.64	1/1691 (0.1%)
13	M	1.03	4/884 (0.5%)	1.29	13/1192 (1.1%)
14	R	0.20	0/186	0.35	0/287
15	T	0.24	0/514	0.36	0/791
16	U	0.23	0/264	0.49	0/405
All	All	0.66	31/33825 (0.1%)	1.00	196/45900 (0.4%)

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	M	66	ARG	C-N	-8.99	1.22	1.33
2	B	590	PRO	C-O	-8.23	1.18	1.25
13	M	61	ALA	C-N	-7.76	1.23	1.33
11	N	155	ASN	C-N	7.54	1.42	1.33
11	N	100	GLU	C-N	-7.52	1.24	1.33
1	A	1498	MET	C-O	7.14	1.32	1.24
11	N	57	ASN	C-N	6.99	1.44	1.33
1	A	1503	GLN	C-O	-6.51	1.16	1.24
2	B	143	SER	CA-CB	-6.46	1.44	1.53
2	B	682	SER	CA-CB	-6.43	1.44	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	N	58	GLY	C-N	-6.31	1.24	1.33
13	M	57	GLN	C-N	-6.05	1.25	1.33
11	N	69	VAL	C-N	-6.00	1.25	1.33
13	M	39	MET	C-N	-5.97	1.25	1.33
1	A	629	GLY	C-O	-5.93	1.17	1.24
11	N	38	PRO	N-CD	5.83	1.55	1.47
1	A	581	ASN	C-O	-5.81	1.16	1.24
1	A	632	GLN	C-O	-5.81	1.19	1.24
2	B	283	SER	CA-CB	-5.78	1.44	1.53
2	B	507	PRO	C-O	-5.72	1.18	1.23
8	J	10	CYS	C-O	-5.71	1.17	1.24
11	N	14	CYS	C-N	-5.60	1.28	1.33
1	A	674	SER	CA-CB	-5.42	1.44	1.53
1	A	447	PRO	C-O	-5.31	1.18	1.23
11	N	91	GLU	C-N	-5.31	1.26	1.33
1	A	673	PRO	C-O	-5.25	1.17	1.23
1	A	57	PRO	C-O	-5.11	1.18	1.23
11	N	90	GLY	C-N	-5.10	1.26	1.33
3	C	114	PRO	C-O	-5.05	1.18	1.23
3	C	284	SER	CA-CB	-5.04	1.46	1.54
2	B	683	PRO	C-O	-5.02	1.17	1.24

All (196) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	164	VAL	N-CA-C	-16.03	98.66	112.12
1	A	1507	GLU	N-CA-C	-10.97	99.33	111.07
9	K	25	THR	N-CA-C	-10.17	100.87	113.18
2	B	19	LEU	N-CA-C	-9.84	97.54	110.53
2	B	159	HIS	N-CA-C	-9.44	95.31	110.32
1	A	1598	ARG	N-CA-C	-9.19	95.37	110.17
11	N	121	PRO	CA-N-CD	-8.98	99.43	112.00
11	N	155	ASN	CA-C-N	8.85	129.50	120.38
11	N	155	ASN	C-N-CA	8.85	129.50	120.38
2	B	1009	LYS	CB-CA-C	-8.82	98.88	111.85
3	C	163	TYR	CB-CA-C	-8.58	100.17	111.42
1	A	1606	HIS	N-CA-C	-8.51	103.41	113.88
2	B	734	ASN	N-CA-C	-8.34	102.14	111.82
1	A	1505	VAL	CA-C-O	-8.17	112.45	120.95
3	C	166	HIS	CA-CB-CG	8.05	121.85	113.80
2	B	791	SER	N-CA-C	-7.94	103.67	112.72
1	A	634	HIS	N-CA-C	-7.87	103.70	113.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	191	ARG	CB-CA-C	-7.80	99.92	110.22
8	J	27	ALA	N-CA-C	-7.60	99.78	110.50
1	A	57	PRO	CB-CA-C	-7.60	104.48	111.40
3	C	191	ARG	N-CA-CB	-7.58	103.14	111.10
2	B	291	GLU	N-CA-C	-7.57	104.02	113.18
13	M	111	PRO	N-CA-C	7.55	123.21	111.21
1	A	313	SER	CA-C-O	-7.48	115.51	119.77
2	B	662	PHE	CA-CB-CG	7.39	121.19	113.80
11	N	155	ASN	CA-C-O	-7.36	110.08	120.16
1	A	1268	VAL	N-CA-C	7.30	119.16	112.29
2	B	288	ILE	CA-C-N	-7.30	111.82	122.69
2	B	288	ILE	C-N-CA	-7.30	111.82	122.69
1	A	313	SER	O-C-N	7.20	126.16	120.83
2	B	730	TYR	CB-CA-C	-7.15	99.29	111.31
2	B	736	PRO	CB-CA-C	7.15	122.02	111.22
2	B	544	GLY	N-CA-C	7.10	120.78	110.63
2	B	791	SER	CA-C-N	-7.06	112.83	122.86
2	B	791	SER	C-N-CA	-7.06	112.83	122.86
8	J	4	PRO	CB-CA-C	7.04	120.53	111.46
13	M	14	CYS	N-CA-C	-6.99	103.59	111.07
1	A	412	ASP	N-CA-C	-6.97	104.72	113.23
2	B	34	ALA	N-CA-C	-6.97	104.40	113.12
3	C	163	TYR	CA-C-N	-6.97	115.45	122.77
3	C	163	TYR	C-N-CA	-6.97	115.45	122.77
2	B	839	MET	CA-C-O	-6.95	113.42	122.45
3	C	284	SER	N-CA-C	-6.93	105.75	114.56
1	A	469	PRO	CB-CA-C	-6.87	100.23	111.56
1	A	680	PRO	N-CA-CB	-6.86	97.09	103.27
11	N	138	PRO	N-CA-C	6.85	119.06	110.70
2	B	732	MET	N-CA-C	-6.83	104.07	112.88
3	C	183	ASP	N-CA-C	-6.83	101.72	110.53
1	A	1676	THR	CB-CA-C	6.83	121.58	111.89
11	N	25	SER	N-CA-C	-6.77	105.02	113.28
13	M	19	GLY	N-CA-C	-6.73	106.52	115.40
11	N	134	PRO	N-CA-C	6.70	121.75	111.57
3	C	114	PRO	N-CA-CB	-6.66	97.83	103.36
1	A	1182	TYR	CB-CA-C	6.59	121.69	110.56
13	M	110	GLN	CA-C-N	6.58	126.55	119.78
13	M	110	GLN	C-N-CA	6.58	126.55	119.78
2	B	75	PHE	CA-CB-CG	-6.53	107.27	113.80
6	H	77	PRO	N-CA-C	-6.52	106.20	114.35
3	C	22	ARG	N-CA-C	6.49	118.43	111.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	553	GLN	N-CA-C	6.47	122.50	113.57
1	A	678	PRO	N-CA-C	-6.45	103.33	113.78
3	C	258	SER	N-CA-C	-6.45	101.45	109.64
2	B	339	ASN	N-CA-C	-6.44	105.58	113.50
2	B	443	THR	CB-CA-C	-6.40	98.66	109.72
6	H	87	GLN	N-CA-C	-6.36	105.62	113.19
4	E	180	ALA	N-CA-C	-6.36	105.66	113.41
2	B	547	HIS	CB-CA-C	6.35	119.63	110.04
2	B	730	TYR	CA-C-O	-6.33	114.00	120.84
1	A	1267	PRO	CB-CA-C	6.31	119.26	111.12
3	C	225	PHE	CA-CB-CG	6.30	120.10	113.80
2	B	106	ARG	N-CA-C	-6.29	102.42	110.53
1	A	447	PRO	CB-CA-C	-6.27	102.87	111.21
2	B	590	PRO	N-CA-CB	-6.26	99.69	103.19
2	B	32	LYS	N-CA-C	6.24	118.08	111.28
11	N	78	HIS	CA-C-N	-6.22	114.22	122.99
11	N	78	HIS	C-N-CA	-6.22	114.22	122.99
3	C	166	HIS	CB-CA-C	6.20	121.40	110.85
1	A	1177	GLN	N-CA-C	-6.19	106.36	114.04
1	A	55	LEU	N-CA-C	-6.19	105.59	113.02
2	B	794	PHE	CB-CA-C	6.16	120.19	109.65
2	B	279	ARG	N-CA-C	-6.16	104.57	111.28
2	B	216	ARG	CB-CA-C	-6.14	100.12	110.19
2	B	351	ARG	N-CA-C	-6.13	104.66	111.71
3	C	259	PRO	N-CA-C	6.12	122.86	113.75
2	B	585	ARG	CB-CA-C	6.09	120.38	111.73
2	B	265	PHE	CA-CB-CG	6.08	119.88	113.80
2	B	147	ASN	CB-CA-C	6.04	120.88	110.01
2	B	500	VAL	N-CA-C	6.01	116.79	110.72
2	B	603	LYS	CB-CA-C	5.98	120.28	109.45
12	G	168	THR	N-CA-C	5.97	117.46	111.07
1	A	1503	GLN	CA-C-O	-5.93	114.59	120.82
8	J	8	PHE	CA-CB-CG	5.92	119.72	113.80
13	M	110	GLN	CB-CA-C	-5.90	100.29	109.55
13	M	77	GLY	CA-C-N	-5.89	112.70	120.95
13	M	77	GLY	C-N-CA	-5.89	112.70	120.95
2	B	824	PRO	N-CA-CB	-5.88	98.07	103.31
1	A	1049	LYS	CB-CA-C	-5.87	101.67	110.88
6	H	15	ILE	CA-C-O	-5.85	114.45	120.71
3	C	96	ASN	CA-C-N	-5.82	112.75	121.72
3	C	96	ASN	C-N-CA	-5.82	112.75	121.72
11	N	141	ILE	N-CA-C	5.81	114.65	108.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	88	TYR	CA-C-O	-5.81	114.65	121.16
3	C	180	ASN	N-CA-C	-5.80	106.06	113.02
2	B	731	ASP	CB-CA-C	5.73	118.02	110.06
2	B	266	GLN	CB-CA-C	5.71	121.19	110.63
2	B	826	TYR	CB-CA-C	5.71	122.36	111.17
2	B	464	ARG	N-CA-C	-5.70	103.83	112.04
2	B	32	LYS	CA-C-O	-5.70	114.51	120.55
2	B	318	TYR	CB-CA-C	-5.70	100.59	109.08
1	A	890	PRO	N-CA-C	-5.68	105.63	113.53
3	C	164	VAL	CB-CA-C	5.67	116.47	110.91
1	A	678	PRO	CB-CA-C	5.65	122.74	113.20
3	C	183	ASP	CA-C-O	-5.64	115.45	121.94
3	C	161	GLU	CA-C-O	-5.64	115.03	121.68
2	B	859	THR	CB-CA-C	5.63	120.33	110.64
11	N	26	GLU	N-CA-C	-5.63	106.18	113.16
1	A	1263	MET	CA-C-O	-5.62	115.43	121.45
1	A	90	PRO	N-CA-C	5.62	121.14	113.84
2	B	287	ARG	CB-CA-C	-5.62	100.86	110.24
1	A	832	ASN	CB-CA-C	5.61	119.99	111.80
2	B	609	GLY	CA-C-O	-5.60	116.26	122.14
1	A	293	ASN	N-CA-C	-5.59	103.12	110.39
2	B	461	ASN	N-CA-C	-5.57	100.66	108.96
3	C	52	ASP	CA-C-O	-5.55	114.71	120.70
2	B	594	GLU	CB-CA-C	-5.54	102.00	111.31
3	C	162	LEU	N-CA-C	-5.54	105.15	112.24
3	C	118	ASP	CA-CB-CG	5.53	118.13	112.60
1	A	1059	ARG	N-CA-C	-5.53	106.42	112.72
11	N	130	LEU	N-CA-CB	-5.50	102.04	110.01
1	A	718	LYS	CA-C-O	-5.49	114.45	120.43
2	B	19	LEU	CA-C-O	-5.45	115.54	121.87
13	M	69	TYR	CA-C-N	-5.45	115.42	122.99
13	M	69	TYR	C-N-CA	-5.45	115.42	122.99
3	C	192	PRO	CB-CA-C	5.44	118.11	110.98
1	A	54	ALA	N-CA-C	-5.41	107.04	113.97
3	C	185	PHE	CB-CA-C	5.41	116.37	110.15
2	B	259	PHE	CA-CB-CG	5.41	119.21	113.80
2	B	279	ARG	CB-CA-C	5.41	119.76	110.79
1	A	1257	ALA	N-CA-C	-5.40	106.54	113.23
13	M	111	PRO	CB-CA-C	-5.39	104.33	111.23
1	A	1145	PRO	N-CA-CB	-5.39	98.79	103.32
2	B	754	GLU	CA-C-O	-5.39	115.35	121.65
2	B	262	TYR	CB-CA-C	-5.38	101.70	110.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	351	ARG	CB-CA-C	5.36	120.54	110.63
1	A	452	ASN	CA-CB-CG	5.35	117.95	112.60
3	C	164	VAL	N-CA-CB	5.35	119.23	111.90
11	N	79	ARG	CB-CA-C	5.34	119.48	109.71
2	B	342	LYS	CB-CA-C	5.33	119.64	110.79
2	B	792	LEU	N-CA-CB	-5.32	102.76	110.84
1	A	452	ASN	CB-CA-C	5.31	119.31	109.54
1	A	1319	PHE	CB-CA-C	5.27	119.82	110.85
11	N	37	GLY	CA-C-N	5.27	124.94	119.56
11	N	37	GLY	C-N-CA	5.27	124.94	119.56
1	A	575	LEU	CA-C-O	-5.26	115.07	120.54
2	B	106	ARG	CA-C-N	-5.26	114.97	123.23
2	B	106	ARG	C-N-CA	-5.26	114.97	123.23
8	J	9	THR	CB-CA-C	5.24	119.07	110.95
7	I	29	LEU	N-CA-C	-5.23	103.13	109.57
11	N	23	PRO	CB-CA-C	-5.22	103.34	111.22
1	A	770	GLY	CA-C-O	-5.21	117.19	122.56
1	A	309	TYR	N-CA-C	-5.21	106.32	113.30
13	M	82	ASN	CB-CA-C	5.21	120.67	110.67
2	B	793	VAL	N-CA-C	-5.20	98.53	109.34
2	B	107	ARG	CB-CA-C	5.19	120.24	111.41
2	B	679	HIS	CA-CB-CG	5.19	118.99	113.80
1	A	682	TRP	CA-C-O	-5.15	114.62	121.46
1	A	840	ASP	CA-C-N	-5.14	112.50	120.31
1	A	840	ASP	C-N-CA	-5.14	112.50	120.31
3	C	57	ASP	CB-CA-C	-5.13	101.73	113.33
2	B	335	HIS	CA-CB-CG	5.13	118.93	113.80
3	C	283	PHE	CB-CA-C	5.12	119.33	110.77
1	A	1598	ARG	CA-C-O	-5.12	115.24	121.28
11	N	23	PRO	CA-C-N	-5.12	115.96	122.77
11	N	23	PRO	C-N-CA	-5.12	115.96	122.77
1	A	572	GLU	CA-C-O	-5.12	115.95	121.38
1	A	651	GLU	N-CA-CB	-5.12	102.42	110.30
1	A	451	ILE	N-CA-C	-5.12	100.52	108.86
1	A	67	CYS	CA-C-N	-5.11	113.51	121.18
1	A	67	CYS	C-N-CA	-5.11	113.51	121.18
11	N	142	PRO	N-CA-C	-5.10	104.48	110.70
2	B	143	SER	CA-C-O	-5.09	114.39	120.65
2	B	249	LEU	N-CA-C	-5.09	103.81	110.53
1	A	21	SER	CA-C-O	-5.09	115.16	120.55
1	A	557	HIS	CA-CB-CG	5.08	118.88	113.80
11	N	130	LEU	N-CA-C	5.08	116.50	111.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	335	VAL	N-CA-C	-5.07	105.44	110.62
11	N	140	GLN	N-CA-C	5.07	116.51	108.96
1	A	206	PRO	CB-CA-C	-5.07	103.20	111.56
1	A	573	LYS	N-CA-C	-5.06	104.89	112.54
1	A	1340	ARG	N-CA-C	-5.04	105.91	111.71
2	B	426	LEU	O-C-N	-5.02	115.75	122.43
13	M	81	CYS	CB-CA-C	-5.02	101.34	110.63
2	B	499	PRO	CA-C-N	5.02	127.55	120.42
2	B	499	PRO	C-N-CA	5.02	127.55	120.42
2	B	503	PRO	CB-CA-C	5.00	117.63	111.23
11	N	152	PHE	CA-CB-CG	5.00	118.80	113.80

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	11749	0	11888	755	0
2	B	8912	0	8896	573	0
3	C	2697	0	2676	152	0
4	E	1641	0	1671	114	0
5	F	610	0	642	22	0
6	H	1176	0	1137	62	0
7	I	447	0	429	57	0
8	J	507	0	523	26	0
9	K	863	0	850	67	0
10	L	379	0	387	26	0
11	N	1105	0	1098	51	0
12	G	1229	0	1212	0	0
13	M	867	0	844	66	0
14	R	168	0	85	3	0
15	T	456	0	244	19	0
16	U	238	0	138	6	0
17	A	2	0	0	0	0
17	B	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	J	1	0	0	0	0
17	L	1	0	0	0	0
18	A	1	0	0	0	0
19	A	29	14	14	0	0
All	All	33079	14	32734	1761	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 28.

All (1761) 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)
11:N:142:PRO:CG	11:N:145:LEU:HD21	1.50	1.42
11:N:142:PRO:HG2	11:N:145:LEU:CD2	1.54	1.35
7:I:16:ASP:O	13:M:67:LEU:CD2	1.76	1.33
1:A:408:LYS:NZ	1:A:409:LEU:HD22	1.46	1.29
1:A:407:ASP:OD2	1:A:410:MET:HG3	1.40	1.18
7:I:16:ASP:O	13:M:67:LEU:HD22	1.04	1.18
1:A:408:LYS:HZ3	1:A:409:LEU:CD2	1.56	1.17
1:A:408:LYS:NZ	1:A:409:LEU:CD2	2.06	1.15
2:B:792:LEU:HB2	2:B:865:LYS:HD3	1.24	1.15
13:M:67:LEU:HD21	13:M:69:TYR:CZ	1.83	1.13
2:B:785:ILE:HG21	2:B:792:LEU:HD21	1.27	1.12
1:A:316:GLY:HA2	15:T:10:DA:H2''	1.28	1.09
1:A:521:GLN:HA	1:A:524:THR:HB	1.36	1.07
2:B:14:PRO:HD3	2:B:946:ASP:HB3	1.36	1.05
3:C:267:VAL:HG12	3:C:272:VAL:CG1	1.86	1.05
1:A:312:VAL:HG21	1:A:320:PHE:HB3	1.34	1.05
2:B:73:ILE:HB	2:B:75:PHE:CZ	1.91	1.04
3:C:291:GLU:HA	3:C:294:LYS:HE3	1.36	1.04
3:C:267:VAL:HG12	3:C:272:VAL:HG12	1.36	1.02
8:J:1:MET:HE3	8:J:56:ILE:HD13	1.37	1.02
1:A:754:TYR:CE1	1:A:781:LEU:HD13	1.95	1.01
13:M:67:LEU:HD21	13:M:69:TYR:OH	1.59	1.00
1:A:881:MET:HG3	1:A:910:MET:HG2	1.39	1.00
1:A:408:LYS:HZ3	1:A:409:LEU:HD22	0.96	0.98
1:A:132:LEU:HG	4:E:210:GLN:HE22	1.27	0.98
7:I:16:ASP:OD1	13:M:67:LEU:HD23	1.62	0.97
2:B:568:LYS:HE2	2:B:600:MET:HE3	1.47	0.97
2:B:785:ILE:CG2	2:B:792:LEU:HD21	1.95	0.96
1:A:969:MET:HG3	2:B:489:LEU:HD22	1.47	0.95

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1282:LYS:HE3	1:A:1564:LEU:HD13	1.49	0.94
2:B:709:ASN:ND2	15:T:7:DG:H5"	1.80	0.94
4:E:110:MET:HE1	4:E:118:LEU:HD11	1.49	0.94
4:E:72:MET:HE2	4:E:103:LEU:HB2	1.49	0.93
1:A:1512:ILE:HG21	1:A:1515:TYR:HE1	1.28	0.93
2:B:10:LEU:HD12	2:B:11:PRO:HD2	1.48	0.93
11:N:35:LEU:HD22	11:N:42:LEU:HD21	1.50	0.93
13:M:12:GLN:OE1	13:M:98:GLN:NE2	2.01	0.93
2:B:88:PRO:HD2	2:B:92:ILE:HD12	1.51	0.92
1:A:1145:PRO:HD2	4:E:204:ILE:HD11	1.52	0.92
2:B:396:ILE:HG22	2:B:422:MET:HB2	1.48	0.92
1:A:1090:LEU:HD22	4:E:30:GLN:HG2	1.51	0.91
1:A:939:GLU:HG2	1:A:940:PRO:HD2	1.48	0.91
6:H:104:THR:HG22	6:H:107:GLU:HB3	1.54	0.90
1:A:122:CYS:HB3	1:A:165:THR:HG21	1.53	0.90
2:B:600:MET:HB3	2:B:608:PRO:HB3	1.54	0.90
13:M:67:LEU:HD21	13:M:69:TYR:CE1	2.05	0.90
3:C:54:VAL:HG21	3:C:279:ARG:NH2	1.87	0.89
11:N:146:ARG:HH12	11:N:148:ARG:HH22	1.17	0.89
1:A:316:GLY:CA	15:T:10:DA:H2"	2.03	0.88
1:A:1313:GLN:HE22	1:A:1535:LYS:HB2	1.37	0.88
1:A:754:TYR:HE1	1:A:781:LEU:HD13	1.32	0.88
1:A:869:VAL:HG21	1:A:918:GLN:HE21	1.39	0.88
1:A:1580:THR:HG22	1:A:1582:GLY:H	1.35	0.88
2:B:73:ILE:HB	2:B:75:PHE:HZ	1.39	0.88
5:F:79:VAL:HG12	5:F:81:VAL:HG12	1.53	0.88
2:B:792:LEU:HB2	2:B:865:LYS:CD	2.04	0.88
1:A:407:ASP:OD2	1:A:410:MET:CG	2.22	0.87
2:B:408:SER:HA	2:B:411:MET:HB2	1.56	0.87
2:B:403:LYS:HB2	2:B:418:ARG:HH12	1.40	0.86
7:I:40:ARG:HD2	7:I:43:PHE:HA	1.55	0.86
2:B:216:ARG:HB2	2:B:334:ILE:HG22	1.54	0.86
2:B:392:TRP:HE1	2:B:423:GLY:HA2	1.39	0.85
13:M:28:PHE:CE1	13:M:33:LEU:HD11	2.11	0.85
2:B:68:PHE:HA	2:B:405:GLN:HE22	1.42	0.84
4:E:94:MET:HG2	4:E:99:ILE:HD11	1.58	0.84
2:B:117:ASP:HB3	2:B:131:LYS:HE2	1.57	0.84
13:M:33:LEU:HD22	13:M:39:MET:HE1	1.58	0.84
2:B:178:VAL:HB	2:B:457:ALA:HB2	1.60	0.84
2:B:648:GLU:HG3	11:N:130:LEU:HD22	1.59	0.84
4:E:85:LYS:O	4:E:89:VAL:HG13	1.78	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:713:GLY:O	6:H:20:LYS:HE3	1.78	0.83
1:A:860:MET:HE2	1:A:864:LYS:HE3	1.60	0.83
2:B:781:LEU:HD22	2:B:792:LEU:HB3	1.60	0.83
1:A:555:THR:HG21	2:B:1041:GLU:HG3	1.61	0.83
2:B:1068:HIS:HB3	2:B:1109:THR:HA	1.61	0.83
1:A:1334:ARG:HG3	1:A:1335:PRO:HD2	1.59	0.83
1:A:912:ILE:HD11	2:B:924:MET:HG2	1.61	0.83
1:A:1619:ARG:HH22	4:E:196:PRO:HD2	1.44	0.82
2:B:400:PHE:HA	2:B:418:ARG:CZ	2.10	0.82
2:B:796:ILE:HD11	2:B:807:LEU:HB2	1.60	0.82
2:B:792:LEU:HD12	2:B:865:LYS:HD2	1.61	0.82
3:C:91:LYS:HE2	10:L:54:VAL:HG11	1.62	0.82
1:A:312:VAL:CG2	1:A:320:PHE:HB3	2.10	0.81
2:B:14:PRO:CD	2:B:946:ASP:HB3	2.10	0.81
2:B:260:SER:HB3	7:I:18:ASP:HB2	1.61	0.81
1:A:1097:GLN:O	1:A:1101:LYS:HG2	1.81	0.81
2:B:631:GLU:HG3	2:B:631:GLU:O	1.80	0.81
1:A:1153:ASP:OD1	1:A:1154:ILE:N	2.12	0.81
2:B:708:ASP:O	2:B:776:SER:HB3	1.80	0.81
3:C:104:GLU:HG2	3:C:105:ILE:HD12	1.61	0.81
2:B:940:LEU:HD12	8:J:43:TYR:HB3	1.63	0.81
2:B:758:ILE:HB	2:B:914:LEU:HB2	1.62	0.80
9:K:22:GLU:HG3	9:K:25:THR:H	1.44	0.80
2:B:73:ILE:CB	2:B:75:PHE:CZ	2.65	0.80
8:J:40:LEU:HD11	8:J:49:LEU:HD12	1.64	0.80
1:A:1354:ILE:O	1:A:1357:LYS:HG2	1.81	0.80
1:A:1531:LEU:HB3	1:A:1535:LYS:HE2	1.64	0.80
1:A:417:ILE:HB	2:B:1126:MET:HE3	1.62	0.80
2:B:567:ASP:OD1	2:B:568:LYS:N	2.15	0.79
1:A:658:TYR:HB2	9:K:67:PHE:HZ	1.47	0.79
2:B:700:LEU:HD11	2:B:706:ARG:HG3	1.63	0.79
2:B:536:ASN:HA	11:N:48:PRO:HG3	1.64	0.79
2:B:783:GLU:OE1	2:B:783:GLU:N	2.15	0.79
2:B:396:ILE:HA	2:B:422:MET:HG3	1.62	0.79
1:A:1512:ILE:HG21	1:A:1515:TYR:CE1	2.15	0.79
3:C:102:GLN:HB2	3:C:105:ILE:HD13	1.65	0.79
2:B:1036:ARG:NH1	15:T:3:DG:OP1	2.16	0.79
1:A:404:SER:HB2	1:A:415:PRO:HA	1.65	0.78
3:C:163:TYR:HD1	3:C:166:HIS:HB3	1.49	0.78
2:B:856:SER:HB3	10:L:42:ARG:HB3	1.64	0.78
1:A:659:ARG:HH22	1:A:790:GLN:NE2	1.81	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:33:TYR:HB3	3:C:36:TYR:HB3	1.63	0.78
1:A:310:ARG:HE	1:A:325:THR:HG22	1.48	0.78
3:C:267:VAL:CG1	3:C:272:VAL:CG1	2.62	0.78
1:A:8:PRO:HG3	2:B:1066:VAL:HG13	1.65	0.78
2:B:92:ILE:HD11	2:B:859:THR:HA	1.66	0.78
1:A:914:CYS:H	1:A:954:ARG:HD3	1.48	0.78
1:A:403:ASP:HB3	1:A:406:MET:HE2	1.66	0.77
2:B:758:ILE:CD1	2:B:895:ARG:HB2	2.13	0.77
4:E:86:THR:O	4:E:89:VAL:HG22	1.84	0.77
4:E:168:ASN:O	4:E:169:GLN:HB3	1.84	0.77
1:A:425:GLU:HG3	1:A:426:GLY:H	1.48	0.77
1:A:1288:VAL:HG21	1:A:1333:LEU:HD22	1.67	0.77
1:A:1350:LEU:O	1:A:1354:ILE:HG12	1.83	0.77
1:A:1531:LEU:HB3	1:A:1535:LYS:CE	2.15	0.77
9:K:90:LEU:HD23	9:K:90:LEU:H	1.50	0.76
1:A:122:CYS:CB	1:A:165:THR:HG21	2.16	0.76
1:A:408:LYS:HZ2	1:A:409:LEU:HD22	1.48	0.76
1:A:465:LYS:HZ2	2:B:1014:THR:HG22	1.50	0.76
2:B:75:PHE:CD2	2:B:397:LYS:HE3	2.21	0.76
1:A:430:LYS:HE3	1:A:431:HIS:HE1	1.51	0.76
3:C:147:THR:H	3:C:164:VAL:HG22	1.50	0.76
2:B:68:PHE:HA	2:B:405:GLN:NE2	1.99	0.76
2:B:916:ASN:OD1	2:B:917:PRO:HD2	1.86	0.76
5:F:81:VAL:HB	5:F:96:GLU:HG2	1.66	0.76
15:T:-6:DA:H2'	15:T:-5:DG:C8	2.20	0.76
13:M:67:LEU:HD12	13:M:68:SER:O	1.86	0.75
2:B:73:ILE:CB	2:B:75:PHE:HZ	1.99	0.75
1:A:939:GLU:HG2	1:A:940:PRO:CD	2.17	0.75
1:A:1515:TYR:O	1:A:1516:GLN:HG2	1.85	0.75
3:C:186:PRO:HG2	3:C:189:THR:OG1	1.86	0.75
1:A:667:ARG:NH1	9:K:66:GLU:OE2	2.20	0.75
1:A:668:VAL:H	9:K:85:GLN:HE22	1.32	0.75
4:E:110:MET:CE	4:E:118:LEU:HD11	2.16	0.75
11:N:88:GLN:O	11:N:91:GLU:HG3	1.86	0.75
1:A:793:ARG:HG3	1:A:794:GLY:N	2.02	0.74
1:A:31:LYS:NZ	1:A:48:ASN:OD1	2.21	0.74
1:A:125:ARG:O	1:A:128:GLU:HG2	1.88	0.74
2:B:88:PRO:HD2	2:B:92:ILE:CD1	2.17	0.74
2:B:170:PHE:O	2:B:176:GLU:HA	1.87	0.74
6:H:37:MET:HE3	6:H:127:GLY:HA3	1.70	0.74
1:A:1225:GLN:O	1:A:1226:MET:HB2	1.87	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1003:ARG:HD2	2:B:1003:ARG:O	1.87	0.74
1:A:312:VAL:HG23	1:A:320:PHE:HA	1.70	0.74
3:C:53:VAL:C	11:N:157:PRO:HD3	2.13	0.73
2:B:743:VAL:HG21	2:B:999:TYR:HE2	1.53	0.73
3:C:27:THR:HA	3:C:32:ASN:ND2	2.03	0.73
1:A:749:LEU:HB3	1:A:754:TYR:HE2	1.53	0.73
1:A:797:LEU:HD12	1:A:897:MET:HE1	1.69	0.73
1:A:1545:VAL:HG21	7:I:53:LYS:HE3	1.69	0.73
2:B:1060:ASN:OD1	2:B:1064:ARG:NH1	2.20	0.73
1:A:134:ALA:O	1:A:138:LEU:HD23	1.89	0.73
1:A:1289:CYS:HA	1:A:1552:VAL:HA	1.71	0.73
1:A:1295:GLN:O	7:I:59:VAL:HG12	1.89	0.73
1:A:1615:GLU:HG3	4:E:193:ILE:HD13	1.71	0.73
2:B:141:VAL:O	2:B:146:CYS:SG	2.46	0.73
3:C:54:VAL:HG21	3:C:279:ARG:HH22	1.51	0.73
1:A:1334:ARG:CG	1:A:1335:PRO:HD2	2.19	0.73
1:A:911:GLN:HA	1:A:915:LEU:O	1.89	0.72
3:C:267:VAL:HG12	3:C:272:VAL:HG11	1.68	0.72
9:K:30:VAL:HG23	9:K:41:THR:HB	1.70	0.72
1:A:1349:LEU:HD21	1:A:1547:LEU:HD11	1.72	0.72
2:B:73:ILE:HB	2:B:75:PHE:CE2	2.24	0.72
2:B:181:MET:HE1	2:B:514:LEU:HD11	1.72	0.72
2:B:396:ILE:HA	2:B:422:MET:CG	2.19	0.72
2:B:536:ASN:HA	11:N:48:PRO:CG	2.20	0.72
1:A:1593:GLU:OE1	1:A:1593:GLU:N	2.21	0.72
2:B:64:PHE:HE2	2:B:397:LYS:HB2	1.54	0.72
8:J:57:GLU:O	8:J:61:ASN:ND2	2.21	0.72
1:A:1328:GLN:NE2	1:A:1333:LEU:O	2.22	0.72
2:B:403:LYS:HB3	2:B:418:ARG:HH22	1.52	0.72
1:A:1335:PRO:O	1:A:1338:ILE:HG22	1.90	0.72
2:B:92:ILE:HG22	2:B:93:CYS:H	1.53	0.72
3:C:53:VAL:O	11:N:157:PRO:HD3	1.90	0.72
4:E:61:LEU:HD13	4:E:73:PHE:HD1	1.55	0.72
1:A:104:CYS:SG	1:A:211:GLY:HA3	2.30	0.71
2:B:193:MET:SD	2:B:195:ARG:NH2	2.63	0.71
1:A:650:ARG:HG2	1:A:654:MET:HE2	1.72	0.71
1:A:713:GLY:O	6:H:20:LYS:CE	2.37	0.71
2:B:73:ILE:CG2	2:B:75:PHE:CZ	2.74	0.71
4:E:13:ILE:O	4:E:17:ILE:HG13	1.91	0.71
1:A:850:HIS:O	1:A:855:GLN:NE2	2.24	0.71
3:C:287:ILE:HD11	3:C:299:LEU:HD22	1.71	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:104:THR:CG2	6:H:107:GLU:HB3	2.21	0.71
1:A:749:LEU:HD23	1:A:754:TYR:OH	1.90	0.70
1:A:1545:VAL:HG21	7:I:53:LYS:CE	2.21	0.70
1:A:430:LYS:HE3	1:A:431:HIS:CE1	2.25	0.70
2:B:140:MET:CE	2:B:168:GLY:HA2	2.21	0.70
2:B:691:MET:HE3	2:B:884:ALA:HB1	1.73	0.70
1:A:1619:ARG:NH2	4:E:196:PRO:HD2	2.06	0.70
2:B:576:ASP:OD1	2:B:577:SER:N	2.25	0.70
2:B:622:PRO:HB3	2:B:631:GLU:OE2	1.91	0.70
1:A:1686:MET:HG3	1:A:1687:LEU:HD12	1.74	0.70
2:B:46:PHE:O	2:B:50:VAL:HG22	1.92	0.70
2:B:717:PRO:HB2	2:B:736:PRO:HB2	1.74	0.70
1:A:512:MET:SD	1:A:515:ARG:NH2	2.65	0.70
6:H:104:THR:HB	6:H:109:ALA:HB2	1.74	0.70
1:A:138:LEU:HD11	1:A:165:THR:HG23	1.72	0.70
4:E:190:VAL:HG22	4:E:208:LEU:HD12	1.73	0.70
6:H:96:VAL:HG22	6:H:116:VAL:HG22	1.73	0.70
1:A:686:GLN:O	1:A:690:THR:HG22	1.92	0.70
4:E:54:ARG:HD2	4:E:57:ASP:HB3	1.72	0.70
1:A:793:ARG:HG3	1:A:794:GLY:H	1.57	0.70
2:B:58:VAL:HA	2:B:61:ILE:HG13	1.71	0.70
3:C:184:LEU:HD23	3:C:185:PHE:CE2	2.27	0.70
1:A:19:MET:HE1	1:A:91:LEU:HD11	1.72	0.69
1:A:1145:PRO:HD2	4:E:204:ILE:CD1	2.21	0.69
1:A:1097:GLN:HA	1:A:1100:VAL:HG22	1.75	0.69
2:B:394:VAL:O	2:B:398:ILE:HG12	1.91	0.69
4:E:159:LEU:HD23	4:E:160:LEU:HD23	1.74	0.69
6:H:101:GLY:HA2	6:H:112:LEU:HD23	1.74	0.69
1:A:312:VAL:HG23	1:A:320:PHE:CA	2.22	0.69
2:B:781:LEU:HD23	2:B:781:LEU:O	1.92	0.69
3:C:267:VAL:CG1	3:C:272:VAL:HG11	2.22	0.69
4:E:92:GLN:O	4:E:95:GLN:HG2	1.92	0.69
4:E:93:ARG:NH1	4:E:97:GLU:OE2	2.26	0.69
7:I:16:ASP:OD2	13:M:66:ARG:HB2	1.93	0.69
1:A:87:VAL:HB	1:A:395:GLN:HE22	1.58	0.69
1:A:258:PRO:HD2	1:A:391:TRP:CZ3	2.27	0.69
7:I:8:ASN:ND2	13:M:34:GLN:HG2	2.07	0.69
2:B:392:TRP:O	2:B:396:ILE:HG23	1.93	0.69
1:A:654:MET:HE1	9:K:60:MET:HE1	1.73	0.69
1:A:745:LEU:HD22	6:H:117:SER:OG	1.93	0.69
2:B:651:VAL:HG13	2:B:656:THR:HG21	1.75	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:691:LEU:HD22	1:A:784:LEU:HD22	1.74	0.68
1:A:1024:LEU:HA	1:A:1203:SER:O	1.92	0.68
1:A:1702:VAL:HG23	1:A:1704:LYS:HG3	1.76	0.68
1:A:910:MET:O	1:A:911:GLN:HB3	1.94	0.68
1:A:1516:GLN:HG3	1:A:1526:GLN:HG3	1.76	0.68
2:B:400:PHE:CD1	2:B:418:ARG:HG2	2.29	0.68
7:I:16:ASP:OD2	13:M:66:ARG:HD2	1.94	0.68
1:A:44:ASN:HB2	1:A:45:PRO:HD2	1.74	0.68
1:A:1262:PRO:HA	1:A:1603:ASN:HD21	1.58	0.68
2:B:392:TRP:NE1	2:B:423:GLY:HA2	2.09	0.68
3:C:291:GLU:CA	3:C:294:LYS:HE3	2.21	0.68
1:A:140:ARG:HH11	1:A:144:ARG:HH12	1.42	0.68
1:A:754:TYR:HE1	1:A:781:LEU:CD1	2.05	0.68
1:A:806:PRO:O	1:A:807:LYS:HB3	1.93	0.68
11:N:70:LYS:HG2	11:N:79:ARG:HG2	1.74	0.68
1:A:843:ARG:NH1	1:A:939:GLU:OE2	2.27	0.68
1:A:1534:MET:C	1:A:1535:LYS:HD2	2.19	0.68
7:I:18:ASP:HB3	13:M:111:PRO:HG2	1.75	0.68
1:A:860:MET:CE	1:A:864:LYS:HE3	2.24	0.67
2:B:75:PHE:CE1	2:B:120:TRP:HB2	2.29	0.67
2:B:568:LYS:HG3	2:B:600:MET:HE2	1.75	0.67
1:A:338:ILE:HG12	1:A:390:ILE:HD12	1.77	0.67
1:A:1014:VAL:CG2	4:E:165:LEU:HD21	2.23	0.67
2:B:690:GLN:OE1	2:B:694:GLN:NE2	2.27	0.67
3:C:16:LEU:HD12	3:C:21:VAL:HG23	1.77	0.67
1:A:13:GLN:O	2:B:1133:ASP:HB2	1.94	0.67
1:A:654:MET:CE	9:K:60:MET:HE1	2.24	0.67
1:A:1512:ILE:HD13	1:A:1529:VAL:HG22	1.77	0.67
1:A:1515:TYR:CD1	1:A:1527:VAL:HG23	2.30	0.67
1:A:1566:GLU:HA	1:A:1576:LEU:HD13	1.75	0.67
3:C:138:LEU:HD12	3:C:181:GLN:HE22	1.57	0.67
3:C:235:LEU:HB2	3:C:301:ARG:HD3	1.76	0.67
1:A:166:THR:HA	1:A:169:VAL:HG22	1.77	0.67
7:I:17:LEU:HD11	7:I:37:THR:OG1	1.94	0.67
8:J:3:ILE:HD12	8:J:4:PRO:HD2	1.75	0.67
11:N:48:PRO:HD3	11:N:117:ILE:O	1.95	0.67
1:A:434:GLY:HA3	2:B:1036:ARG:NH2	2.10	0.66
1:A:465:LYS:NZ	2:B:1014:THR:HG22	2.10	0.66
1:A:916:LEU:HB2	1:A:953:GLY:O	1.96	0.66
1:A:979:ALA:O	1:A:982:THR:HG22	1.95	0.66
7:I:16:ASP:O	13:M:67:LEU:HD23	1.87	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:430:LYS:HG2	1:A:431:HIS:ND1	2.11	0.66
3:C:245:VAL:CG2	3:C:273:ALA:HB3	2.26	0.66
4:E:127:LEU:O	4:E:128:GLU:HG3	1.95	0.66
2:B:1066:VAL:O	2:B:1066:VAL:HG12	1.96	0.66
5:F:79:VAL:CG1	5:F:81:VAL:HG12	2.25	0.66
1:A:690:THR:O	1:A:694:ASN:ND2	2.27	0.66
2:B:187:ARG:HD2	2:B:615:THR:HB	1.77	0.66
6:H:48:TYR:OH	6:H:147:LYS:HG3	1.96	0.66
9:K:42:PHE:CE1	9:K:84:ILE:HD12	2.31	0.66
1:A:603:LEU:O	1:A:603:LEU:HD23	1.96	0.66
2:B:709:ASN:HD21	15:T:7:DG:H5"	1.61	0.66
2:B:806:LYS:HG2	2:B:824:PRO:HD2	1.78	0.66
4:E:77:PRO:HD2	4:E:105:VAL:O	1.96	0.66
2:B:403:LYS:HE2	2:B:418:ARG:NH2	2.11	0.65
2:B:757:MET:HE3	2:B:759:VAL:CG2	2.26	0.65
3:C:53:VAL:HG21	9:K:118:ILE:HD13	1.76	0.65
7:I:33:GLN:HG3	7:I:34:ASP:OD1	1.96	0.65
2:B:566:VAL:HG21	2:B:574:ILE:HD12	1.78	0.65
4:E:94:MET:SD	4:E:102:ALA:HB2	2.37	0.65
1:A:1566:GLU:HA	1:A:1576:LEU:CD1	2.26	0.65
2:B:233:THR:HG23	2:B:285:MET:HG2	1.78	0.65
4:E:84:ILE:O	4:E:88:LYS:HG2	1.95	0.65
1:A:642:THR:O	1:A:685:LYS:HE2	1.96	0.65
1:A:1034:PRO:HD3	1:A:1166:LYS:HD3	1.78	0.65
1:A:1104:LYS:HB2	1:A:1116:GLY:HA2	1.78	0.65
1:A:812:ARG:HD2	1:A:914:CYS:HA	1.78	0.65
2:B:194:ILE:HG23	2:B:207:GLN:OE1	1.97	0.65
6:H:102:ASP:OD2	6:H:111:ARG:HB2	1.96	0.65
2:B:1042:ARG:NH1	2:B:1043:ASP:OD1	2.30	0.65
11:N:112:GLN:OE1	11:N:112:GLN:N	2.30	0.65
1:A:12:LEU:HD21	2:B:1132:LEU:HD13	1.78	0.65
1:A:1104:LYS:CB	1:A:1116:GLY:HA2	2.27	0.65
3:C:11:ARG:O	3:C:303:ARG:HD3	1.97	0.65
1:A:1006:THR:HG21	1:A:1008:ARG:HE	1.62	0.65
1:A:1096:ILE:O	1:A:1100:VAL:HG13	1.97	0.65
8:J:1:MET:HE3	8:J:56:ILE:CD1	2.22	0.65
1:A:807:LYS:HG3	1:A:807:LYS:O	1.97	0.65
2:B:709:ASN:HD22	15:T:7:DG:H5"	1.61	0.65
2:B:785:ILE:HG21	2:B:792:LEU:CD2	2.17	0.65
2:B:936:LYS:HG2	2:B:966:LEU:HD21	1.79	0.65
7:I:14:GLN:NE2	7:I:32:ALA:HB3	2.11	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:346:LEU:O	2:B:350:THR:HG23	1.97	0.65
3:C:274:ARG:HB3	3:C:274:ARG:HH11	1.61	0.65
1:A:132:LEU:CG	4:E:210:GLN:HE22	2.08	0.64
1:A:1349:LEU:CD2	1:A:1547:LEU:HD11	2.26	0.64
4:E:110:MET:SD	4:E:118:LEU:HD11	2.37	0.64
11:N:142:PRO:HG2	11:N:145:LEU:CG	2.27	0.64
2:B:1028:GLY:O	2:B:1033:GLY:HA3	1.97	0.64
1:A:1334:ARG:CD	1:A:1335:PRO:HD2	2.27	0.64
4:E:20:LEU:HD11	4:E:24:ARG:HE	1.61	0.64
10:L:21:GLU:OE1	10:L:21:GLU:N	2.31	0.64
2:B:842:LYS:O	2:B:844:LYS:HE2	1.97	0.64
2:B:909:MET:HG2	8:J:42:ARG:HD3	1.80	0.64
1:A:1133:ARG:HG2	1:A:1133:ARG:O	1.97	0.64
4:E:90:TYR:OH	4:E:104:ILE:HD13	1.97	0.64
2:B:73:ILE:CG2	2:B:75:PHE:HZ	2.09	0.64
2:B:229:LEU:HD11	2:B:235:MET:HE3	1.78	0.64
1:A:137:GLU:HG2	1:A:164:TYR:OH	1.97	0.64
1:A:173:LEU:O	1:A:174:LEU:HB3	1.96	0.64
1:A:658:TYR:HB2	9:K:67:PHE:CZ	2.31	0.64
1:A:1119:GLU:OE1	1:A:1122:ARG:NH1	2.22	0.64
1:A:1318:ARG:HD2	1:A:1524:TRP:HE3	1.63	0.64
3:C:7:VAL:N	6:H:49:PRO:HD2	2.13	0.64
10:L:34:ILE:O	10:L:34:ILE:HG22	1.98	0.64
1:A:1516:GLN:HG3	1:A:1526:GLN:H	1.62	0.63
1:A:607:GLU:OE2	1:A:1710:THR:HG21	1.98	0.63
1:A:1313:GLN:HG2	1:A:1537:ASN:HD21	1.63	0.63
2:B:400:PHE:HD1	2:B:418:ARG:HG2	1.61	0.63
2:B:1013:ARG:NH2	2:B:1017:ALA:O	2.30	0.63
4:E:9:ARG:HD2	4:E:132:GLN:HE21	1.64	0.63
13:M:33:LEU:HD13	13:M:36:PRO:HB3	1.80	0.63
1:A:316:GLY:HA2	15:T:10:DA:C2'	2.17	0.63
1:A:939:GLU:CG	1:A:940:PRO:HD2	2.26	0.63
2:B:190:PRO:HB3	2:B:349:MET:HG2	1.79	0.63
1:A:221:SER:OG	1:A:395:GLN:HG3	1.99	0.63
1:A:430:LYS:HG2	1:A:431:HIS:CE1	2.34	0.63
1:A:749:LEU:HD23	1:A:754:TYR:CZ	2.32	0.63
2:B:75:PHE:CD1	2:B:120:TRP:HB2	2.34	0.63
2:B:538:GLY:O	11:N:116:ARG:NH2	2.31	0.63
2:B:566:VAL:CG2	2:B:574:ILE:HD12	2.28	0.63
4:E:185:ILE:HD12	4:E:191:VAL:HG11	1.80	0.63
1:A:414:TYR:HB3	1:A:415:PRO:HD2	1.81	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:823:GLY:HA2	1:A:865:PHE:HE1	1.64	0.63
1:A:1322:LEU:HD13	7:I:60:VAL:HB	1.81	0.63
2:B:1067:ALA:HB1	2:B:1076:LEU:HD11	1.81	0.63
3:C:15:VAL:HA	3:C:300:ALA:HB2	1.81	0.63
1:A:1022:ASP:HB3	4:E:200:ALA:HB2	1.81	0.63
1:A:1293:VAL:O	1:A:1294:LEU:HG	1.99	0.63
1:A:85:LEU:HD22	1:A:391:TRP:HE1	1.63	0.63
1:A:460:MET:HG3	1:A:570:PRO:HA	1.81	0.63
4:E:59:THR:HG23	4:E:74:VAL:O	1.99	0.63
2:B:171:ILE:HG23	2:B:174:GLY:HA2	1.81	0.62
2:B:791:SER:HB3	2:B:792:LEU:HD23	1.81	0.62
13:M:33:LEU:CD1	13:M:36:PRO:HB3	2.29	0.62
1:A:21:SER:HB3	1:A:24:GLU:HG2	1.81	0.62
6:H:39:LEU:HD13	6:H:125:LEU:HD13	1.80	0.62
1:A:408:LYS:HZ3	1:A:409:LEU:HD21	1.59	0.62
2:B:216:ARG:HB2	2:B:334:ILE:CG2	2.26	0.62
11:N:146:ARG:HH12	11:N:148:ARG:NH2	1.92	0.62
2:B:146:CYS:SG	2:B:147:ASN:N	2.73	0.62
2:B:743:VAL:HG22	2:B:913:ILE:HB	1.81	0.62
2:B:936:LYS:HE3	2:B:966:LEU:CD2	2.29	0.62
9:K:55:LEU:HD21	9:K:96:PHE:CE1	2.34	0.62
1:A:122:CYS:SG	1:A:165:THR:HG21	2.40	0.62
1:A:1681:LEU:HD21	2:B:1123:LEU:HD21	1.81	0.62
2:B:113:LYS:HG3	2:B:133:PHE:HE1	1.65	0.62
2:B:570:LEU:HD11	11:N:83:LEU:HD11	1.80	0.62
2:B:965:MET:HE1	11:N:142:PRO:HD3	1.81	0.62
11:N:142:PRO:HG2	11:N:145:LEU:HD21	0.70	0.62
1:A:607:GLU:HB3	2:B:1050:THR:HG22	1.82	0.62
1:A:677:LYS:O	1:A:678:PRO:C	2.42	0.62
1:A:1223:SER:HB2	1:A:1245:ILE:CD1	2.29	0.62
1:A:1338:ILE:HG23	1:A:1339:LEU:HD12	1.81	0.62
2:B:146:CYS:O	2:B:149:ARG:HG2	1.99	0.62
6:H:39:LEU:CD1	6:H:125:LEU:HD13	2.28	0.62
15:T:-7:DG:H2'	15:T:-6:DA:H1'	1.81	0.62
1:A:846:TRP:HE1	1:A:858:PHE:HE1	1.48	0.62
2:B:742:ILE:HD13	2:B:996:VAL:HG22	1.81	0.62
2:B:647:PHE:O	2:B:650:GLU:HB2	1.99	0.62
2:B:936:LYS:HE3	2:B:966:LEU:HD22	1.80	0.62
1:A:127:LEU:HD21	1:A:135:VAL:CG2	2.30	0.62
1:A:1335:PRO:HA	1:A:1338:ILE:HG22	1.82	0.62
1:A:1583:ILE:HD11	1:A:1607:ALA:CB	2.30	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:695:THR:HG21	2:B:737:ILE:HG12	1.81	0.62
2:B:791:SER:HA	2:B:830:ASN:HA	1.81	0.62
13:M:67:LEU:CD2	13:M:69:TYR:CE1	2.81	0.62
1:A:223:LEU:O	1:A:256:LEU:HB2	2.00	0.61
1:A:225:ILE:HG23	1:A:256:LEU:CD1	2.30	0.61
1:A:423:LYS:HG3	1:A:424:LYS:H	1.63	0.61
1:A:1004:ASP:OD1	1:A:1006:THR:HG22	2.01	0.61
2:B:583:VAL:HG13	2:B:630:LYS:HB3	1.81	0.61
9:K:25:THR:HB	9:K:46:GLU:OE1	2.00	0.61
2:B:237:ASN:HD21	2:B:244:LEU:HD22	1.65	0.61
10:L:16:ILE:HG23	10:L:25:GLU:HB3	1.81	0.61
3:C:241:LEU:HD23	3:C:297:VAL:HG22	1.80	0.61
3:C:326:ILE:HG21	9:K:111:LEU:HB2	1.82	0.61
1:A:790:GLN:NE2	2:B:983:ILE:HD13	2.15	0.61
1:A:1024:LEU:HD12	1:A:1204:LEU:HD12	1.81	0.61
1:A:1569:ASN:O	1:A:1573:GLU:HA	2.00	0.61
2:B:791:SER:HA	2:B:830:ASN:OD1	2.00	0.61
3:C:33:TYR:CB	3:C:36:TYR:HB3	2.29	0.61
4:E:173:ILE:HG23	4:E:209:VAL:HA	1.81	0.61
1:A:408:LYS:NZ	1:A:409:LEU:HD21	2.12	0.61
1:A:137:GLU:OE1	1:A:140:ARG:NH2	2.34	0.61
1:A:1498:MET:HA	1:A:1501:ARG:HH12	1.65	0.61
1:A:1670:GLN:O	1:A:1671:GLN:HB3	2.00	0.61
2:B:752:ASP:O	2:B:916:ASN:HB2	2.00	0.61
1:A:1282:LYS:CE	1:A:1564:LEU:HD13	2.27	0.61
2:B:92:ILE:HG22	2:B:93:CYS:N	2.16	0.61
11:N:61:VAL:HG11	13:M:11:TRP:CE3	2.35	0.61
1:A:549:LEU:HD11	2:B:1053:LEU:HD13	1.81	0.61
1:A:970:ALA:O	1:A:973:GLU:HG2	2.00	0.61
1:A:1289:CYS:N	1:A:1292:GLU:OE2	2.31	0.61
2:B:680:ASN:HD21	2:B:887:HIS:HD2	1.46	0.61
3:C:12:SER:O	3:C:303:ARG:N	2.34	0.61
4:E:126:ILE:O	4:E:126:ILE:HG13	1.99	0.61
1:A:812:ARG:HG3	1:A:876:ILE:HG23	1.82	0.61
1:A:895:GLN:O	1:A:896:MET:HB3	2.01	0.61
1:A:664:LYS:N	1:A:664:LYS:HD2	2.16	0.60
2:B:312:LEU:HD21	2:B:327:LEU:HD12	1.82	0.60
3:C:18:GLU:HB2	3:C:288:PHE:CD2	2.36	0.60
3:C:264:VAL:HG13	3:C:264:VAL:O	2.00	0.60
6:H:63:THR:HA	6:H:71:ASP:OD1	2.01	0.60
2:B:691:MET:HE3	2:B:884:ALA:CB	2.31	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:30:PRO:CG	9:K:61:LYS:HA	2.31	0.60
1:A:37:ARG:HH11	1:A:40:ASP:HA	1.67	0.60
1:A:919:ILE:HG12	1:A:949:GLY:O	2.01	0.60
1:A:926:PRO:HD2	1:A:948:GLY:O	2.01	0.60
4:E:37:LEU:O	4:E:41:LYS:HG2	2.01	0.60
2:B:703:TYR:HE1	2:B:711:LEU:HD22	1.67	0.60
8:J:40:LEU:CD1	8:J:49:LEU:HD12	2.31	0.60
1:A:132:LEU:HG	4:E:210:GLN:NE2	2.10	0.60
9:K:22:GLU:HG2	9:K:25:THR:OG1	2.02	0.60
9:K:83:ARG:HH11	9:K:85:GLN:HE21	1.48	0.60
1:A:468:TYR:CE2	1:A:605:ARG:HD2	2.37	0.60
1:A:1037:PHE:N	1:A:1038:PRO:HD2	2.16	0.60
1:A:1170:TYR:HE2	1:A:1192:LEU:HD21	1.67	0.60
1:A:1541:SER:HA	1:A:1544:VAL:HG22	1.83	0.60
2:B:185:PRO:O	2:B:372:GLN:HA	2.01	0.60
3:C:337:LEU:HD12	9:K:104:MET:CE	2.32	0.60
2:B:201:ARG:HB2	2:B:205:TYR:HD2	1.67	0.60
3:C:337:LEU:HD12	9:K:104:MET:HE1	1.84	0.60
1:A:1523:LEU:HD12	1:A:1524:TRP:N	2.17	0.60
3:C:245:VAL:HG21	3:C:253:LEU:CD2	2.32	0.60
2:B:498:CYS:HB2	2:B:668:SER:HB2	1.84	0.59
2:B:758:ILE:HD13	2:B:895:ARG:HB2	1.84	0.59
2:B:1067:ALA:HB2	2:B:1117:ARG:NE	2.16	0.59
2:B:1068:HIS:CB	2:B:1109:THR:HA	2.31	0.59
1:A:651:GLU:CD	3:C:29:PHE:HD2	2.09	0.59
1:A:951:VAL:HG22	1:A:963:GLU:OE1	2.01	0.59
2:B:235:MET:HE2	2:B:248:PRO:HA	1.85	0.59
2:B:526:TYR:CE2	2:B:528:ALA:HB3	2.37	0.59
2:B:403:LYS:HB2	2:B:418:ARG:NH1	2.14	0.59
6:H:14:ASP:HB2	6:H:29:HIS:HB2	1.85	0.59
1:A:866:LYS:HA	1:A:869:VAL:HG22	1.84	0.59
1:A:898:VAL:HG21	1:A:909:THR:HG21	1.83	0.59
1:A:1505:VAL:HG22	1:A:1509:HIS:CE1	2.38	0.59
7:I:36:VAL:O	7:I:36:VAL:HG12	2.02	0.59
1:A:1669:LEU:HB2	1:A:1691:ASP:OD2	2.03	0.59
2:B:75:PHE:CE2	2:B:397:LYS:HE3	2.37	0.59
2:B:1026:ILE:HG22	2:B:1033:GLY:HA2	1.84	0.59
1:A:404:SER:O	1:A:413:LYS:HD2	2.03	0.59
1:A:408:LYS:HZ1	1:A:409:LEU:CD2	2.15	0.59
1:A:1006:THR:HG23	1:A:1008:ARG:HG3	1.83	0.59
1:A:1565:ASN:HD22	1:A:1579:ASN:ND2	2.01	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:93:LEU:HD22	10:L:54:VAL:HG22	1.84	0.59
6:H:24:ARG:HG2	6:H:46:GLN:OE1	2.02	0.59
9:K:44:LEU:HD12	9:K:80:ILE:HD11	1.84	0.59
1:A:1088:ALA:O	1:A:1091:SER:OG	2.20	0.59
1:A:1117:THR:O	1:A:1121:LEU:HD23	2.03	0.59
2:B:39:THR:HG22	2:B:469:PHE:CG	2.38	0.59
2:B:229:LEU:HD21	2:B:235:MET:HB2	1.85	0.59
2:B:562:MET:HE2	2:B:564:GLY:HA2	1.83	0.59
2:B:1030:ASN:OD1	2:B:1031:VAL:N	2.35	0.59
9:K:66:GLU:HB3	9:K:87:ARG:HE	1.67	0.59
2:B:64:PHE:CE2	2:B:397:LYS:HB2	2.35	0.58
2:B:106:ARG:HG2	2:B:855:CYS:HB3	1.84	0.58
2:B:414:ASP:CB	2:B:417:MET:HE3	2.33	0.58
2:B:536:ASN:OD1	11:N:48:PRO:HB3	2.03	0.58
3:C:42:GLN:O	3:C:46:GLU:HG3	2.03	0.58
2:B:42:HIS:O	2:B:140:MET:HE1	2.03	0.58
3:C:290:ASN:ND2	3:C:293:LEU:HD12	2.18	0.58
6:H:100:GLU:HG3	6:H:100:GLU:O	2.02	0.58
1:A:122:CYS:HB3	1:A:165:THR:CG2	2.31	0.58
1:A:521:GLN:HA	1:A:524:THR:CB	2.23	0.58
1:A:603:LEU:HD22	2:B:1052:PHE:CD2	2.39	0.58
2:B:68:PHE:HB3	2:B:73:ILE:HD11	1.83	0.58
2:B:753:MET:HA	2:B:916:ASN:HD22	1.68	0.58
2:B:882:LYS:HD2	2:B:1002:LEU:HD23	1.85	0.58
1:A:39:LEU:HD12	1:A:39:LEU:O	2.03	0.58
2:B:239:ILE:HD11	2:B:242:LYS:HA	1.85	0.58
2:B:416:LEU:HA	2:B:419:ILE:HG12	1.85	0.58
4:E:60:VAL:HG22	4:E:74:VAL:HB	1.84	0.58
1:A:91:LEU:H	1:A:91:LEU:HD23	1.69	0.58
1:A:112:CYS:HB2	1:A:117:ILE:HD11	1.85	0.58
1:A:435:LYS:HD2	2:B:1058:LEU:O	2.03	0.58
1:A:1145:PRO:HG2	4:E:202:ARG:O	2.03	0.58
2:B:139:ILE:HG22	2:B:140:MET:O	2.02	0.58
3:C:30:PRO:HG2	9:K:60:MET:O	2.03	0.58
3:C:91:LYS:HE2	10:L:54:VAL:CG1	2.32	0.58
13:M:68:SER:O	13:M:111:PRO:HA	2.02	0.58
4:E:35:GLN:HA	4:E:39:GLU:OE2	2.03	0.58
13:M:11:TRP:CE2	13:M:101:VAL:HG21	2.39	0.58
15:T:6:DA:H2'	15:T:7:DG:C8	2.38	0.58
1:A:553:GLN:HG2	15:T:3:DG:C4'	2.33	0.58
1:A:1110:ARG:HB3	1:A:1118:GLN:HE22	1.69	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:549:SER:O	2:B:550:TYR:HB2	2.02	0.58
2:B:703:TYR:HE1	2:B:711:LEU:CD2	2.17	0.58
1:A:33:ILE:CD1	1:A:50:LEU:HD13	2.34	0.58
1:A:93:PHE:CZ	1:A:223:LEU:HD11	2.39	0.58
1:A:438:ASP:HB3	2:B:1014:THR:O	2.04	0.58
1:A:797:LEU:HD12	1:A:897:MET:CE	2.34	0.58
2:B:92:ILE:HD11	2:B:858:ASP:O	2.03	0.58
2:B:781:LEU:CD2	2:B:792:LEU:HB3	2.31	0.58
1:A:754:TYR:CD1	1:A:781:LEU:HD13	2.37	0.58
1:A:718:LYS:HG3	6:H:21:LYS:HB2	1.85	0.57
2:B:66:PHE:HZ	2:B:400:PHE:CD2	2.21	0.57
2:B:130:ILE:HG21	2:B:419:ILE:HD13	1.86	0.57
2:B:743:VAL:CG2	2:B:999:TYR:HE2	2.16	0.57
3:C:245:VAL:HG23	3:C:273:ALA:HB3	1.85	0.57
1:A:488:PRO:HG3	1:A:508:SER:HA	1.86	0.57
1:A:652:HIS:O	1:A:656:LEU:HB2	2.04	0.57
1:A:1519:THR:HG23	1:A:1520:GLU:CD	2.29	0.57
2:B:568:LYS:HE2	2:B:600:MET:CE	2.29	0.57
2:B:648:GLU:O	2:B:649:ASP:HB2	2.03	0.57
3:C:86:THR:CG2	3:C:227:PRO:HB3	2.34	0.57
6:H:103:GLU:OE1	6:H:103:GLU:N	2.29	0.57
13:M:72:ASN:ND2	13:M:74:PHE:O	2.37	0.57
1:A:1318:ARG:HA	1:A:1526:GLN:HA	1.86	0.57
2:B:162:GLU:C	2:B:164:GLU:H	2.11	0.57
2:B:524:PHE:CE2	2:B:616:PRO:HG3	2.39	0.57
3:C:245:VAL:CG1	3:C:296:VAL:HG11	2.35	0.57
1:A:84:PRO:HD3	1:A:335:VAL:HG22	1.85	0.57
1:A:1533:LEU:H	1:A:1535:LYS:HZ2	1.52	0.57
2:B:554:TYR:O	2:B:565:TRP:HA	2.05	0.57
4:E:73:PHE:HB2	4:E:99:ILE:CD1	2.34	0.57
1:A:137:GLU:HG2	1:A:164:TYR:CZ	2.39	0.57
2:B:392:TRP:HE1	2:B:423:GLY:CA	2.13	0.57
1:A:654:MET:O	1:A:655:GLU:HB3	2.05	0.57
1:A:739:ILE:HD13	1:A:761:LEU:HD13	1.87	0.57
1:A:873:SER:HB2	1:A:915:LEU:CD2	2.34	0.57
2:B:104:ARG:O	2:B:707:SER:OG	2.22	0.57
2:B:889:GLN:NE2	2:B:925:THR:OG1	2.36	0.57
4:E:122:ALA:HB1	4:E:123:PRO:HD2	1.85	0.57
6:H:147:LYS:O	6:H:148:LEU:HD23	2.04	0.57
1:A:76:GLY:HA3	1:A:306:PRO:HB3	1.86	0.57
1:A:651:GLU:HG3	9:K:60:MET:HE2	1.85	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:141:VAL:HG12	2:B:142:LYS:HG2	1.87	0.57
2:B:201:ARG:HB2	2:B:205:TYR:CD2	2.40	0.57
2:B:821:TYR:HB2	2:B:844:LYS:NZ	2.18	0.57
2:B:854:VAL:HG12	10:L:34:ILE:HG21	1.87	0.57
1:A:42:LEU:O	1:A:42:LEU:HD23	2.04	0.57
1:A:225:ILE:HG23	1:A:256:LEU:HG	1.85	0.57
2:B:186:ARG:HG3	2:B:187:ARG:H	1.69	0.57
11:N:70:LYS:HE2	11:N:79:ARG:CZ	2.34	0.57
1:A:1117:THR:HG22	1:A:1121:LEU:HD23	1.85	0.57
1:A:1585:LEU:HB2	1:A:1586:PRO:HD3	1.87	0.57
2:B:742:ILE:CD1	2:B:996:VAL:HG22	2.34	0.57
3:C:75:ALA:HA	9:K:50:THR:HG23	1.86	0.57
7:I:9:THR:CG2	7:I:15:SER:HA	2.34	0.57
9:K:25:THR:HB	9:K:46:GLU:CD	2.29	0.57
1:A:749:LEU:HD23	1:A:754:TYR:CE2	2.39	0.57
1:A:1110:ARG:HB3	1:A:1118:GLN:NE2	2.19	0.57
1:A:1585:LEU:HD12	1:A:1600:LEU:HD21	1.87	0.57
2:B:700:LEU:HD21	2:B:711:LEU:HD11	1.86	0.57
2:B:745:VAL:HG12	2:B:917:PRO:HB3	1.86	0.57
4:E:165:LEU:HD23	4:E:169:GLN:HE21	1.68	0.57
11:N:49:ALA:HA	13:M:86:ARG:HG3	1.87	0.57
1:A:1349:LEU:HA	1:A:1352:GLU:CD	2.30	0.56
2:B:600:MET:HB3	2:B:608:PRO:CB	2.32	0.56
3:C:98:THR:O	3:C:206:GLN:HG2	2.05	0.56
11:N:45:ILE:HB	13:M:88:PHE:HB2	1.87	0.56
1:A:430:LYS:HA	2:B:1036:ARG:HH21	1.70	0.56
1:A:1631:VAL:HG23	1:A:1632:TYR:CD2	2.39	0.56
2:B:527:THR:OG1	2:B:530:ILE:HD12	2.05	0.56
4:E:142:HIS:HB3	4:E:145:VAL:HG23	1.85	0.56
13:M:11:TRP:CZ2	13:M:101:VAL:HG21	2.40	0.56
1:A:507:LEU:CD2	1:A:518:VAL:HG11	2.35	0.56
1:A:674:SER:HB3	1:A:686:GLN:OE1	2.05	0.56
1:A:1618:LEU:HD11	1:A:1649:CYS:HB2	1.87	0.56
2:B:1028:GLY:H	2:B:1033:GLY:HA3	1.70	0.56
8:J:1:MET:CE	8:J:56:ILE:HD13	2.24	0.56
8:J:63:ALA:HB1	10:L:23:HIS:NE2	2.20	0.56
1:A:553:GLN:HG2	15:T:3:DG:H4'	1.86	0.56
1:A:1531:LEU:HB3	1:A:1535:LYS:CD	2.36	0.56
6:H:36:LYS:HA	6:H:36:LYS:HE3	1.87	0.56
1:A:438:ASP:OD1	2:B:1025:PRO:HG3	2.06	0.56
2:B:333:CYS:HB3	2:B:342:LYS:HG3	1.88	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:696:MET:HG3	2:B:712:TYR:HB3	1.87	0.56
7:I:13:PHE:CE1	7:I:20:CYS:HB3	2.41	0.56
2:B:781:LEU:HD23	2:B:792:LEU:HD22	1.85	0.56
4:E:80:PRO:O	4:E:108:GLN:HB2	2.05	0.56
1:A:225:ILE:HG23	1:A:256:LEU:HD11	1.88	0.56
1:A:1213:LEU:HD22	2:B:1046:LEU:CD1	2.35	0.56
1:A:1318:ARG:CD	1:A:1524:TRP:HE3	2.18	0.56
1:A:1497:ALA:O	1:A:1498:MET:C	2.47	0.56
2:B:530:ILE:HB	2:B:531:PRO:HD3	1.87	0.56
2:B:736:PRO:HG2	8:J:53:VAL:HG11	1.87	0.56
10:L:19:CYS:HB3	10:L:23:HIS:H	1.71	0.56
1:A:505:THR:HG23	1:A:505:THR:O	2.06	0.56
1:A:914:CYS:O	1:A:915:LEU:HB2	2.05	0.56
1:A:1083:LEU:HD12	1:A:1083:LEU:O	2.06	0.56
1:A:1502:VAL:O	1:A:1505:VAL:HG12	2.06	0.56
2:B:785:ILE:HD12	2:B:791:SER:HB2	1.88	0.56
1:A:827:VAL:HG22	1:A:861:ILE:CG2	2.36	0.56
1:A:1090:LEU:HD11	4:E:33:LEU:CD1	2.36	0.56
1:A:1239:MET:HG3	1:A:1239:MET:O	2.05	0.56
2:B:103:CYS:SG	2:B:171:ILE:HG21	2.45	0.56
1:A:8:PRO:O	1:A:9:TRP:HB3	2.05	0.56
1:A:921:LEU:HA	1:A:973:GLU:OE2	2.06	0.56
1:A:1637:ASP:OD2	1:A:1639:ARG:HD3	2.06	0.56
1:A:1583:ILE:HD12	1:A:1604:ASP:HB2	1.88	0.55
2:B:1059:PHE:CE2	2:B:1064:ARG:HD3	2.40	0.55
3:C:138:LEU:HD21	3:C:190:ILE:HD13	1.86	0.55
1:A:19:MET:HG2	1:A:296:VAL:CG1	2.37	0.55
1:A:397:HIS:NE2	1:A:410:MET:HE1	2.21	0.55
1:A:912:ILE:CD1	2:B:924:MET:HG2	2.35	0.55
1:A:961:PRO:HD2	1:A:962:PRO:HD2	1.89	0.55
1:A:1128:ASP:HB3	1:A:1133:ARG:HD3	1.88	0.55
1:A:1300:GLN:HE21	7:I:48:ARG:HH11	1.53	0.55
1:A:1685:THR:HG21	2:B:1128:ILE:HG12	1.86	0.55
1:A:619:LEU:HD22	1:A:624:GLY:O	2.06	0.55
1:A:881:MET:HE1	1:A:895:GLN:NE2	2.20	0.55
1:A:972:ARG:NH1	2:B:489:LEU:HD12	2.22	0.55
1:A:1213:LEU:O	1:A:1217:GLN:HG3	2.06	0.55
3:C:288:PHE:CZ	3:C:299:LEU:HD21	2.41	0.55
9:K:89:THR:HG23	9:K:90:LEU:N	2.20	0.55
1:A:1512:ILE:HD12	1:A:1527:VAL:HG21	1.86	0.55
16:U:4:DT:H2'	16:U:5:DC:C6	2.41	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:GLY:HA2	1:A:1691:ASP:O	2.06	0.55
1:A:123:GLN:O	1:A:127:LEU:HD23	2.06	0.55
2:B:61:ILE:HG22	2:B:61:ILE:O	2.06	0.55
2:B:1026:ILE:HG21	2:B:1031:VAL:CG1	2.37	0.55
2:B:1112:VAL:HG22	2:B:1113:PRO:HD2	1.88	0.55
3:C:28:ASP:O	3:C:29:PHE:HD1	1.89	0.55
1:A:459:PRO:HB2	1:A:572:GLU:O	2.06	0.55
1:A:799:VAL:O	1:A:803:LEU:HG	2.07	0.55
1:A:1605:ILE:HG21	1:A:1621:ILE:CG1	2.36	0.55
2:B:10:LEU:CD1	2:B:11:PRO:HD2	2.30	0.55
2:B:86:THR:HG23	2:B:96:ALA:O	2.05	0.55
2:B:399:ALA:O	2:B:418:ARG:NH1	2.39	0.55
2:B:965:MET:HE1	11:N:142:PRO:CD	2.36	0.55
1:A:711:ILE:N	1:A:750:ASP:OD2	2.35	0.55
1:A:1693:LEU:HD13	1:A:1702:VAL:HG21	1.88	0.55
1:A:1714:GLU:HG2	5:F:109:TYR:HE2	1.72	0.55
3:C:74:ASN:O	3:C:78:ARG:HG3	2.06	0.55
13:M:68:SER:HB2	13:M:112:LEU:CB	2.36	0.55
1:A:1293:VAL:HA	1:A:1322:LEU:HD12	1.87	0.55
2:B:399:ALA:HB2	2:B:422:MET:HE2	1.88	0.55
4:E:54:ARG:HD2	4:E:57:ASP:CB	2.35	0.55
6:H:104:THR:HB	6:H:109:ALA:CB	2.37	0.55
11:N:142:PRO:HG3	11:N:145:LEU:HD21	1.72	0.55
13:M:36:PRO:C	13:M:38:ASN:H	2.15	0.55
1:A:310:ARG:HB3	1:A:322:ASN:HD22	1.72	0.55
2:B:113:LYS:HG3	2:B:133:PHE:CE1	2.42	0.55
2:B:903:PRO:HB2	2:B:979:LEU:HD23	1.89	0.55
4:E:122:ALA:HB1	4:E:123:PRO:CD	2.37	0.55
15:T:-7:DG:H2'	15:T:-6:DA:C1'	2.36	0.55
1:A:661:LEU:HG	1:A:691:LEU:HD12	1.89	0.55
1:A:1034:PRO:O	1:A:1035:LYS:HB3	2.06	0.55
1:A:1221:GLU:HB3	1:A:1222:PRO:HD3	1.89	0.55
1:A:1516:GLN:CG	1:A:1526:GLN:HG3	2.36	0.55
1:A:1529:VAL:HG12	1:A:1530:LYS:N	2.22	0.55
2:B:568:LYS:HG3	2:B:600:MET:CE	2.37	0.55
4:E:152:THR:HG23	4:E:154:GLU:HG2	1.89	0.55
13:M:67:LEU:CD2	13:M:69:TYR:OH	2.45	0.55
1:A:606:ALA:O	1:A:610:VAL:HG23	2.06	0.54
2:B:319:PRO:HB2	2:B:321:GLU:HG2	1.89	0.54
2:B:651:VAL:HG13	2:B:656:THR:CG2	2.36	0.54
5:F:61:GLU:O	5:F:65:VAL:HG23	2.07	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:54:VAL:HG12	7:I:55:VAL:H	1.72	0.54
11:N:83:LEU:HD12	11:N:116:ARG:NH1	2.22	0.54
1:A:10:ARG:HD2	2:B:1108:ASP:HB3	1.87	0.54
1:A:220:ASN:O	1:A:221:SER:HB2	2.07	0.54
1:A:739:ILE:CD1	1:A:761:LEU:HD13	2.37	0.54
1:A:795:PHE:HE2	1:A:897:MET:HE2	1.72	0.54
1:A:1605:ILE:HG12	1:A:1620:VAL:HG12	1.89	0.54
2:B:66:PHE:HE1	2:B:75:PHE:CE2	2.24	0.54
3:C:183:ASP:O	3:C:184:LEU:HB3	2.06	0.54
6:H:110:THR:HG23	6:H:110:THR:O	2.06	0.54
7:I:55:VAL:HA	7:I:59:VAL:HG11	1.89	0.54
11:N:146:ARG:NH1	11:N:148:ARG:HH22	1.96	0.54
1:A:1108:GLU:N	1:A:1108:GLU:OE1	2.40	0.54
2:B:194:ILE:HG12	2:B:208:TYR:CD1	2.42	0.54
2:B:987:GLU:CD	3:C:301:ARG:HE	2.15	0.54
3:C:15:VAL:HG23	3:C:22:ARG:HB2	1.89	0.54
3:C:30:PRO:HA	3:C:38:ASP:H	1.72	0.54
3:C:267:VAL:CG1	3:C:272:VAL:HG12	2.24	0.54
1:A:312:VAL:CG2	1:A:320:PHE:CB	2.84	0.54
2:B:263:GLN:CD	13:M:29:SER:HB2	2.32	0.54
2:B:808:ASP:HB3	2:B:814:PHE:CE2	2.42	0.54
9:K:55:LEU:HD23	9:K:82:LEU:HD11	1.90	0.54
1:A:522:LEU:O	1:A:523:LEU:HB2	2.08	0.54
2:B:1069:VAL:HG21	2:B:1134:VAL:HG21	1.89	0.54
3:C:14:VAL:O	3:C:300:ALA:HB1	2.07	0.54
4:E:61:LEU:HD12	4:E:72:MET:O	2.07	0.54
9:K:86:THR:HG22	9:K:92:ALA:HB2	1.89	0.54
1:A:8:PRO:HG2	2:B:1111:SER:HB3	1.89	0.54
1:A:1068:HIS:CE1	1:A:1144:ASP:O	2.61	0.54
2:B:259:PHE:HA	13:M:110:GLN:HE22	1.73	0.54
6:H:90:TYR:OH	6:H:92:MET:HE3	2.08	0.54
13:M:67:LEU:HD21	13:M:69:TYR:HH	1.69	0.54
1:A:121:LEU:O	1:A:125:ARG:HG3	2.07	0.54
1:A:502:GLY:O	1:A:503:SER:OG	2.18	0.54
2:B:703:TYR:O	2:B:704:GLN:HB3	2.08	0.54
1:A:905:SER:OG	1:A:907:VAL:HG12	2.08	0.54
1:A:1044:TYR:HD1	1:A:1195:LEU:HD22	1.73	0.54
2:B:178:VAL:O	2:B:178:VAL:HG13	2.07	0.54
2:B:940:LEU:HD23	2:B:969:ALA:CB	2.37	0.54
3:C:239:ILE:HD13	3:C:261:VAL:HG11	1.90	0.54
7:I:48:ARG:HD3	7:I:50:PHE:CZ	2.43	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:N:11:ARG:O	11:N:12:PHE:C	2.49	0.54
3:C:13:ARG:HA	3:C:301:ARG:O	2.08	0.54
1:A:422:GLU:O	1:A:423:LYS:HB2	2.08	0.54
2:B:217:GLU:HB2	2:B:219:HIS:CE1	2.43	0.53
2:B:835:GLU:HG3	2:B:837:PHE:CZ	2.43	0.53
3:C:12:SER:O	3:C:303:ARG:HB2	2.08	0.53
1:A:404:SER:HB2	1:A:416:GLY:H	1.73	0.53
1:A:1170:TYR:CE2	1:A:1192:LEU:HD21	2.42	0.53
1:A:1300:GLN:NE2	7:I:48:ARG:HH11	2.06	0.53
1:A:1714:GLU:HB2	5:F:107:ARG:HB3	1.89	0.53
3:C:184:LEU:CD2	3:C:185:PHE:CE2	2.91	0.53
11:N:95:LEU:HD11	13:M:26:VAL:HG11	1.89	0.53
1:A:30:VAL:HB	1:A:66:THR:HG21	1.90	0.53
1:A:182:LYS:O	1:A:183:ASN:HB2	2.09	0.53
1:A:668:VAL:H	9:K:85:GLN:NE2	2.04	0.53
1:A:1357:LYS:HZ1	1:A:1538:PHE:HE1	1.55	0.53
5:F:125:ILE:HG13	5:F:125:ILE:O	2.07	0.53
6:H:8:ASP:HB3	6:H:10:PHE:CE1	2.44	0.53
9:K:58:MET:HG3	9:K:103:LEU:HB2	1.90	0.53
1:A:120:LEU:O	1:A:124:LEU:HD23	2.08	0.53
1:A:632:GLN:HE22	2:B:754:GLU:H	1.57	0.53
1:A:1324:HIS:HA	1:A:1327:TYR:CE1	2.43	0.53
1:A:1566:GLU:H	1:A:1566:GLU:CD	2.16	0.53
1:A:1718:PRO:HD2	5:F:103:PRO:O	2.08	0.53
2:B:695:THR:CG2	2:B:1000:GLN:HB3	2.39	0.53
4:E:13:ILE:HD11	4:E:132:GLN:HG3	1.91	0.53
5:F:57:MET:HE1	5:F:120:VAL:HG13	1.90	0.53
13:M:68:SER:HB2	13:M:112:LEU:HB3	1.90	0.53
1:A:1640:HIS:O	1:A:1644:VAL:HG23	2.07	0.53
3:C:340:LEU:HD23	9:K:97:GLN:HB2	1.90	0.53
7:I:34:ASP:C	7:I:35:THR:HG1	2.09	0.53
1:A:105:LEU:HD12	1:A:264:HIS:ND1	2.24	0.53
1:A:457:GLY:HA2	1:A:567:ARG:O	2.09	0.53
1:A:960:LYS:HB3	1:A:961:PRO:CD	2.39	0.53
1:A:1245:ILE:N	1:A:1246:PRO:HD2	2.24	0.53
2:B:514:LEU:HD22	2:B:518:CYS:SG	2.48	0.53
3:C:68:ILE:HD11	3:C:72:ILE:HG21	1.91	0.53
1:A:180:HIS:HB3	1:A:1692:GLU:OE2	2.08	0.53
1:A:280:PHE:O	1:A:281:SER:OG	2.17	0.53
2:B:270:LYS:HG3	2:B:550:TYR:CD2	2.44	0.53
2:B:656:THR:HG22	2:B:656:THR:O	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:173:ILE:CG2	4:E:209:VAL:HA	2.38	0.53
6:H:37:MET:HE1	6:H:132:LEU:HD21	1.89	0.53
7:I:40:ARG:CD	7:I:43:PHE:HA	2.36	0.53
1:A:1618:LEU:O	1:A:1622:GLU:HG3	2.09	0.53
2:B:75:PHE:CG	2:B:397:LYS:HE3	2.43	0.53
2:B:643:ASN:ND2	2:B:655:VAL:HG13	2.24	0.53
1:A:914:CYS:H	1:A:954:ARG:CD	2.20	0.53
1:A:1619:ARG:HH22	4:E:196:PRO:CD	2.20	0.53
2:B:69:LYS:HD3	2:B:407:THR:H	1.73	0.53
2:B:716:THR:O	2:B:716:THR:HG23	2.09	0.53
2:B:757:MET:HE3	2:B:759:VAL:HG23	1.90	0.53
2:B:862:GLY:O	10:L:33:PRO:HA	2.08	0.53
2:B:906:GLU:CD	3:C:301:ARG:HH22	2.17	0.53
3:C:18:GLU:OE1	3:C:18:GLU:HA	2.08	0.53
1:A:397:HIS:CE1	1:A:410:MET:HE1	2.44	0.53
1:A:1133:ARG:C	1:A:1134:LYS:HE2	2.33	0.53
2:B:396:ILE:HG13	2:B:397:LYS:N	2.22	0.53
2:B:1068:HIS:HB3	2:B:1109:THR:HG22	1.91	0.53
4:E:205:THR:HG22	4:E:206:TYR:H	1.74	0.53
15:T:-8:DA:H2"	15:T:-7:DG:H8	1.74	0.53
1:A:312:VAL:CG2	1:A:320:PHE:HA	2.39	0.52
1:A:618:TYR:CE2	1:A:626:PRO:HB3	2.44	0.52
2:B:48:TYR:CE1	2:B:52:GLU:HG2	2.44	0.52
3:C:66:VAL:HG22	3:C:305:HIS:CE1	2.44	0.52
4:E:20:LEU:HD12	4:E:20:LEU:O	2.08	0.52
6:H:29:HIS:CE1	6:H:40:ILE:HD12	2.45	0.52
7:I:44:ASN:OD1	7:I:45:ILE:N	2.37	0.52
1:A:15:ILE:HD13	2:B:1132:LEU:HB3	1.92	0.52
1:A:465:LYS:HD3	2:B:1012:VAL:HB	1.92	0.52
1:A:613:CYS:O	1:A:617:GLN:HG2	2.09	0.52
1:A:1518:ASP:HB3	1:A:1523:LEU:H	1.73	0.52
1:A:712:THR:HG22	1:A:714:LYS:H	1.73	0.52
2:B:808:ASP:HB3	2:B:814:PHE:CZ	2.44	0.52
3:C:339:GLU:HG2	9:K:26:ALA:CB	2.39	0.52
9:K:42:PHE:HE1	9:K:84:ILE:HD12	1.73	0.52
1:A:550:LEU:HD23	1:A:594:MET:SD	2.49	0.52
1:A:667:ARG:HH21	9:K:38:HIS:HB2	1.74	0.52
1:A:1589:PHE:HA	1:A:1597:LEU:HD13	1.91	0.52
1:A:1619:ARG:HH12	4:E:196:PRO:HG2	1.74	0.52
2:B:721:LEU:CD2	8:J:50:LEU:HD23	2.40	0.52
2:B:1067:ALA:HB2	2:B:1117:ARG:CZ	2.40	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:173:MET:HE3	3:C:212:MET:HE1	1.91	0.52
3:C:312:SER:HB3	3:C:321:LEU:CD1	2.39	0.52
1:A:85:LEU:CD2	1:A:391:TRP:HE1	2.23	0.52
2:B:178:VAL:O	2:B:179:ILE:C	2.53	0.52
2:B:1014:THR:HG23	2:B:1015:THR:H	1.73	0.52
7:I:54:VAL:HG12	7:I:55:VAL:N	2.23	0.52
1:A:873:SER:HB2	1:A:915:LEU:HD21	1.91	0.52
1:A:1518:ASP:OD2	1:A:1525:CYS:HB3	2.09	0.52
1:A:1624:GLU:O	1:A:1628:VAL:HG23	2.09	0.52
2:B:742:ILE:HD12	8:J:43:TYR:HE1	1.75	0.52
4:E:72:MET:HE1	4:E:103:LEU:HD12	1.91	0.52
8:J:53:VAL:HG13	8:J:53:VAL:O	2.09	0.52
1:A:682:TRP:N	1:A:682:TRP:CD1	2.76	0.52
1:A:1293:VAL:O	1:A:1293:VAL:HG13	2.09	0.52
1:A:1348:LYS:CE	1:A:1508:ILE:HB	2.40	0.52
1:A:1349:LEU:HG	1:A:1547:LEU:HD21	1.91	0.52
1:A:1512:ILE:HD12	1:A:1527:VAL:CG2	2.39	0.52
2:B:262:TYR:HD2	13:M:30:ASN:HA	1.74	0.52
2:B:411:MET:HE2	2:B:411:MET:N	2.24	0.52
16:U:5:DC:H2'	16:U:6:DC:C6	2.44	0.52
1:A:166:THR:O	1:A:170:GLN:HG2	2.09	0.52
1:A:1096:ILE:HA	1:A:1120:MET:CE	2.40	0.52
2:B:972:ASN:HA	3:C:286:GLU:OE2	2.10	0.52
2:B:1082:GLU:HG3	2:B:1095:LYS:O	2.08	0.52
9:K:124:GLN:O	9:K:128:ARG:HG2	2.09	0.52
2:B:169:TYR:CE1	2:B:176:GLU:HG2	2.44	0.52
7:I:9:THR:HG22	7:I:15:SER:HA	1.92	0.52
1:A:766:TYR:HD1	1:A:771:GLY:HA2	1.75	0.52
2:B:595:VAL:HA	2:B:612:LEU:HD23	1.91	0.52
2:B:943:LEU:HD11	11:N:142:PRO:HG3	1.90	0.52
1:A:1110:ARG:HD3	1:A:1110:ARG:C	2.35	0.51
1:A:1154:ILE:HG23	1:A:1154:ILE:O	2.10	0.51
5:F:121:ASP:OD1	5:F:122:GLU:N	2.43	0.51
2:B:224:MET:HE1	2:B:346:LEU:HD21	1.91	0.51
6:H:65:TYR:HB3	6:H:67:ASP:OD2	2.10	0.51
11:N:121:PRO:HD2	11:N:121:PRO:O	2.10	0.51
1:A:225:ILE:HG23	1:A:256:LEU:CG	2.40	0.51
1:A:1359:ASN:O	1:A:1360:LYS:HD2	2.10	0.51
1:A:312:VAL:CG2	1:A:320:PHE:CA	2.88	0.51
2:B:473:HIS:HD2	2:B:475:GLY:H	1.58	0.51
2:B:965:MET:HE2	11:N:141:ILE:HD13	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:221:ASP:OD2	10:L:58:ARG:NH2	2.40	0.51
6:H:137:VAL:O	6:H:138:ASP:HB2	2.09	0.51
7:I:43:PHE:CE1	7:I:46:ASN:HA	2.45	0.51
1:A:163:GLN:O	1:A:166:THR:HG22	2.11	0.51
1:A:215:VAL:HG22	1:A:225:ILE:HG22	1.92	0.51
1:A:732:MET:HE2	6:H:27:ARG:HH12	1.76	0.51
1:A:1134:LYS:HE2	1:A:1134:LYS:HA	1.92	0.51
1:A:1318:ARG:HH21	1:A:1526:GLN:HG2	1.75	0.51
1:A:1353:SER:OG	1:A:1543:LEU:HD11	2.11	0.51
2:B:77:ILE:HG12	2:B:118:ILE:HG22	1.91	0.51
2:B:212:MET:SD	2:B:345:MET:HE3	2.51	0.51
2:B:639:GLN:O	2:B:639:GLN:HG2	2.09	0.51
2:B:648:GLU:HG2	2:B:649:ASP:N	2.25	0.51
2:B:791:SER:C	2:B:792:LEU:HD23	2.36	0.51
3:C:15:VAL:HA	3:C:300:ALA:CB	2.40	0.51
13:M:36:PRO:C	13:M:38:ASN:N	2.67	0.51
2:B:194:ILE:HG12	2:B:208:TYR:CE1	2.45	0.51
2:B:624:GLN:NE2	2:B:629:GLY:HA2	2.26	0.51
3:C:335:ARG:NH2	9:K:25:THR:O	2.43	0.51
1:A:33:ILE:HD11	1:A:81:ILE:HG13	1.92	0.51
1:A:551:ASN:HD21	2:B:1041:GLU:HG2	1.74	0.51
1:A:961:PRO:CD	1:A:962:PRO:HD2	2.41	0.51
1:A:1068:HIS:HE1	1:A:1144:ASP:O	1.93	0.51
1:A:1279:LYS:O	1:A:1283:LYS:HD3	2.11	0.51
2:B:691:MET:CE	2:B:884:ALA:HB1	2.41	0.51
3:C:163:TYR:CD1	3:C:166:HIS:HB3	2.39	0.51
1:A:166:THR:HA	1:A:169:VAL:CG2	2.41	0.51
1:A:1583:ILE:HD11	1:A:1607:ALA:HB3	1.93	0.51
2:B:743:VAL:HG21	2:B:999:TYR:CE2	2.42	0.51
4:E:190:VAL:HG22	4:E:208:LEU:CD1	2.38	0.51
3:C:29:PHE:HB3	3:C:30:PRO:CD	2.41	0.51
9:K:86:THR:OG1	9:K:90:LEU:HD21	2.11	0.51
1:A:123:GLN:O	1:A:126:VAL:HG22	2.10	0.51
1:A:543:LYS:HG3	1:A:543:LYS:O	2.10	0.51
1:A:603:LEU:HD22	2:B:1052:PHE:CG	2.45	0.51
1:A:841:GLU:O	1:A:845:LYS:HG2	2.11	0.51
4:E:87:ILE:HG22	4:E:121:MET:HE1	1.93	0.51
1:A:1147:LEU:HD22	1:A:1152:PRO:HB3	1.93	0.50
2:B:785:ILE:HG12	2:B:786:LYS:O	2.11	0.50
2:B:920:PHE:N	2:B:921:PRO:HD2	2.26	0.50
1:A:163:GLN:HG3	1:A:164:TYR:N	2.26	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:428:PHE:O	1:A:432:MET:HB3	2.11	0.50
1:A:499:ASN:HD22	1:A:536:LYS:HD2	1.76	0.50
1:A:1300:GLN:HB2	1:A:1316:GLN:HG2	1.94	0.50
1:A:1625:ILE:HG21	1:A:1641:LEU:HD22	1.94	0.50
2:B:419:ILE:HG13	2:B:420:PHE:N	2.26	0.50
1:A:465:LYS:O	1:A:467:THR:HG23	2.12	0.50
1:A:480:LEU:O	1:A:484:VAL:HG12	2.11	0.50
1:A:521:GLN:CA	1:A:524:THR:HB	2.25	0.50
1:A:1114:SER:OG	1:A:1115:PRO:HD2	2.10	0.50
2:B:87:VAL:HB	2:B:92:ILE:HD12	1.93	0.50
2:B:948:THR:O	2:B:951:ILE:HG12	2.11	0.50
5:F:104:ILE:O	5:F:120:VAL:HG23	2.10	0.50
1:A:87:VAL:HB	1:A:395:GLN:NE2	2.26	0.50
1:A:802:ILE:HG22	1:A:894:LEU:HD22	1.92	0.50
1:A:1086:ARG:CZ	1:A:1086:ARG:HB2	2.42	0.50
1:A:1151:ARG:HG3	1:A:1153:ASP:OD1	2.11	0.50
1:A:1632:TYR:HB2	1:A:1634:ILE:HD12	1.94	0.50
2:B:29:GLU:H	2:B:29:GLU:CD	2.20	0.50
2:B:102:GLU:O	2:B:103:CYS:SG	2.68	0.50
4:E:10:LEU:CD2	4:E:58:LEU:HD11	2.40	0.50
5:F:107:ARG:HD2	5:F:115:TYR:CG	2.46	0.50
1:A:440:ALA:HB1	2:B:1035:ILE:HD11	1.92	0.50
2:B:6:ARG:O	2:B:6:ARG:HD3	2.12	0.50
2:B:94:LYS:HG2	10:L:39:CYS:HA	1.91	0.50
2:B:172:ILE:HG12	2:B:434:PHE:HB3	1.93	0.50
2:B:552:GLU:O	2:B:568:LYS:HB2	2.11	0.50
2:B:657:THR:HG22	2:B:658:HIS:ND1	2.27	0.50
2:B:743:VAL:CG2	2:B:997:VAL:HG22	2.41	0.50
3:C:114:PRO:HG3	8:J:13:ILE:CD1	2.41	0.50
4:E:154:GLU:O	4:E:158:GLU:HG3	2.11	0.50
1:A:551:ASN:ND2	2:B:1041:GLU:HG2	2.26	0.50
2:B:417:MET:O	2:B:421:THR:OG1	2.30	0.50
3:C:15:VAL:HG12	3:C:298:ARG:HH21	1.77	0.50
3:C:93:LEU:HB3	10:L:52:LEU:HD11	1.94	0.50
1:A:1147:LEU:CD2	1:A:1152:PRO:HB3	2.42	0.50
2:B:187:ARG:HD2	2:B:615:THR:CB	2.40	0.50
2:B:659:GLN:HG3	2:B:660:GLU:N	2.23	0.50
2:B:695:THR:HG21	2:B:1000:GLN:HB3	1.94	0.50
1:A:601:SER:O	1:A:602:GLU:HB3	2.10	0.50
2:B:882:LYS:HD2	2:B:1002:LEU:CD2	2.41	0.50
1:A:257:THR:HB	1:A:391:TRP:HZ3	1.77	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:425:GLU:CG	1:A:426:GLY:H	2.24	0.50
1:A:1014:VAL:HG21	4:E:165:LEU:HD21	1.94	0.50
2:B:118:ILE:HD11	2:B:419:ILE:HG21	1.93	0.50
1:A:57:PRO:HD3	1:A:64:CYS:HB3	1.93	0.49
1:A:636:VAL:HG11	1:A:795:PHE:CZ	2.47	0.49
1:A:656:LEU:HD13	1:A:792:TYR:HE2	1.77	0.49
1:A:791:LEU:HD22	2:B:984:SER:HB3	1.94	0.49
1:A:1545:VAL:HG21	7:I:53:LYS:NZ	2.28	0.49
2:B:91:THR:HG22	2:B:91:THR:O	2.12	0.49
2:B:802:ARG:HB3	2:B:838:VAL:HG21	1.94	0.49
4:E:92:GLN:HA	4:E:95:GLN:CD	2.37	0.49
1:A:936:PRO:HG2	2:B:494:TRP:CD1	2.45	0.49
2:B:396:ILE:CG2	2:B:422:MET:HB2	2.33	0.49
2:B:615:THR:HB	2:B:616:PRO:HD2	1.94	0.49
2:B:781:LEU:O	2:B:792:LEU:HD22	2.13	0.49
8:J:10:CYS:SG	8:J:10:CYS:O	2.70	0.49
16:U:6:DC:H2"	16:U:7:DT:H71	1.92	0.49
1:A:322:ASN:HB3	1:A:325:THR:HG23	1.94	0.49
1:A:1504:ALA:O	1:A:1507:GLU:HB3	2.12	0.49
2:B:319:PRO:HG2	2:B:322:GLN:HB2	1.93	0.49
2:B:387:GLU:OE1	2:B:445:LEU:HD11	2.13	0.49
2:B:901:ASP:OD1	3:C:78:ARG:NH1	2.38	0.49
7:I:7:ALA:HB3	13:M:34:GLN:HG3	1.94	0.49
1:A:795:PHE:CE2	1:A:897:MET:HE2	2.47	0.49
1:A:1029:THR:O	1:A:1033:GLN:NE2	2.41	0.49
2:B:187:ARG:NH1	2:B:616:PRO:HD2	2.27	0.49
2:B:1126:MET:O	2:B:1127:ASN:HB2	2.12	0.49
3:C:26:THR:OG1	3:C:303:ARG:NE	2.45	0.49
7:I:60:VAL:O	7:I:60:VAL:HG12	2.10	0.49
13:M:74:PHE:N	13:M:78:ALA:HB2	2.27	0.49
1:A:137:GLU:OE1	1:A:137:GLU:HA	2.12	0.49
1:A:425:GLU:HG3	1:A:426:GLY:N	2.24	0.49
1:A:1022:ASP:HB3	4:E:200:ALA:CB	2.43	0.49
1:A:1662:ILE:HD13	1:A:1674:PHE:HD2	1.78	0.49
2:B:92:ILE:CD1	2:B:859:THR:HA	2.40	0.49
2:B:626:LEU:O	2:B:627:ALA:HB3	2.12	0.49
3:C:140:PHE:HE2	3:C:214:CYS:HG	1.60	0.49
2:B:315:PRO:O	2:B:318:TYR:HB2	2.12	0.49
2:B:497:LEU:HD23	2:B:512:ASN:CB	2.43	0.49
2:B:648:GLU:HG2	2:B:649:ASP:H	1.77	0.49
2:B:655:VAL:HG12	2:B:656:THR:H	1.76	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:752:ASP:HB3	2:B:758:ILE:HG12	1.95	0.49
3:C:29:PHE:HB3	3:C:30:PRO:HD2	1.95	0.49
7:I:14:GLN:HG2	7:I:17:LEU:HD12	1.95	0.49
1:A:19:MET:HG2	1:A:296:VAL:HG11	1.93	0.49
1:A:428:PHE:CE1	1:A:432:MET:HE3	2.48	0.49
1:A:1213:LEU:HD22	2:B:1046:LEU:HD11	1.95	0.49
2:B:583:VAL:CG1	2:B:630:LYS:HB3	2.43	0.49
3:C:14:VAL:C	3:C:300:ALA:HB1	2.38	0.49
3:C:110:LEU:HD13	3:C:212:MET:SD	2.53	0.49
3:C:340:LEU:O	3:C:343:VAL:HG22	2.12	0.49
6:H:39:LEU:HD11	6:H:123:MET:SD	2.52	0.49
7:I:17:LEU:HD22	7:I:35:THR:HB	1.95	0.49
7:I:19:PHE:CE2	7:I:34:ASP:HB2	2.48	0.49
1:A:497:VAL:O	1:A:505:THR:HG22	2.13	0.49
1:A:1222:PRO:O	1:A:1226:MET:N	2.44	0.49
1:A:1505:VAL:HG11	1:A:1515:TYR:CZ	2.48	0.49
2:B:426:LEU:HD23	2:B:426:LEU:O	2.13	0.49
3:C:90:GLU:HB2	3:C:215:VAL:HG22	1.94	0.49
1:A:990:ARG:O	1:A:994:LYS:HG2	2.13	0.49
2:B:539:VAL:HG22	2:B:566:VAL:HB	1.95	0.49
4:E:205:THR:HG22	4:E:206:TYR:N	2.27	0.49
8:J:3:ILE:HD11	8:J:49:LEU:HD23	1.95	0.49
9:K:31:GLN:OE1	9:K:37:ARG:HA	2.12	0.49
1:A:25:LEU:O	1:A:28:LEU:HB2	2.13	0.49
1:A:47:ALA:O	1:A:48:ASN:HB2	2.12	0.49
1:A:127:LEU:HD11	1:A:187:SER:OG	2.13	0.49
1:A:717:VAL:HG22	6:H:20:LYS:HG2	1.95	0.49
1:A:1281:LEU:HD21	1:A:1595:LEU:HD11	1.94	0.49
2:B:269:ILE:HD11	2:B:282:VAL:HG21	1.95	0.49
3:C:56:MET:HE2	9:K:121:TYR:CD2	2.47	0.49
7:I:31:GLY:HA3	7:I:36:VAL:HG13	1.95	0.49
11:N:30:PHE:HZ	13:M:102:TYR:CG	2.31	0.49
11:N:41:GLU:OE1	13:M:94:LYS:HD3	2.12	0.49
1:A:9:TRP:O	1:A:9:TRP:CG	2.66	0.48
1:A:222:LYS:C	1:A:223:LEU:HD12	2.38	0.48
1:A:812:ARG:HH11	1:A:914:CYS:C	2.21	0.48
1:A:1016:GLN:NE2	1:A:1646:ASP:OD2	2.46	0.48
1:A:144:ARG:CD	4:E:122:ALA:HB2	2.43	0.48
1:A:1024:LEU:HD23	1:A:1029:THR:HG22	1.95	0.48
4:E:189:GLN:O	4:E:209:VAL:HG23	2.13	0.48
1:A:915:LEU:HD12	1:A:952:THR:HA	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:926:ILE:O	2:B:930:ILE:HG13	2.13	0.48
4:E:123:PRO:HA	4:E:126:ILE:CG2	2.42	0.48
1:A:1255:ALA:HB3	1:A:1656:PRO:HB3	1.94	0.48
2:B:58:VAL:O	2:B:61:ILE:HB	2.13	0.48
4:E:80:PRO:HA	4:E:107:GLN:HG3	1.95	0.48
4:E:87:ILE:CG2	4:E:121:MET:HE1	2.43	0.48
7:I:30:PRO:O	7:I:31:GLY:C	2.57	0.48
7:I:47:VAL:HG23	7:I:47:VAL:O	2.14	0.48
1:A:162:GLU:HA	1:A:165:THR:OG1	2.13	0.48
1:A:654:MET:C	1:A:656:LEU:H	2.22	0.48
1:A:663:ASP:OD1	1:A:664:LYS:N	2.46	0.48
1:A:678:PRO:HB2	6:H:47:ILE:HG23	1.95	0.48
1:A:1558:GLY:O	1:A:1582:GLY:HA3	2.14	0.48
1:A:1702:VAL:CG2	1:A:1704:LYS:HG3	2.43	0.48
2:B:745:VAL:CG1	2:B:917:PRO:HB3	2.43	0.48
2:B:1069:VAL:CG2	2:B:1134:VAL:HG21	2.44	0.48
3:C:222:HIS:CD2	10:L:58:ARG:HD3	2.49	0.48
10:L:19:CYS:SG	10:L:20:GLY:N	2.86	0.48
1:A:668:VAL:N	9:K:85:GLN:HE22	2.05	0.48
2:B:909:MET:HE3	8:J:44:CYS:HB3	1.94	0.48
7:I:14:GLN:O	7:I:15:SER:HB3	2.12	0.48
1:A:1605:ILE:HG21	1:A:1621:ILE:HG12	1.96	0.48
2:B:166:MET:O	2:B:166:MET:HG2	2.14	0.48
2:B:251:PHE:CE1	2:B:290:MET:HE3	2.48	0.48
2:B:392:TRP:CE3	2:B:393:LEU:HD23	2.49	0.48
1:A:163:GLN:HG3	1:A:164:TYR:H	1.79	0.48
1:A:960:LYS:HB3	1:A:961:PRO:HD2	1.96	0.48
2:B:796:ILE:HD12	2:B:809:ASP:H	1.77	0.48
3:C:171:ARG:HG3	3:C:195:ASP:HB2	1.94	0.48
4:E:17:ILE:HD11	4:E:105:VAL:HG21	1.95	0.48
7:I:35:THR:HG21	13:M:113:PHE:CE1	2.49	0.48
13:M:26:VAL:HG12	13:M:60:LEU:CD2	2.44	0.48
1:A:34:THR:HA	1:A:332:MET:HE1	1.95	0.48
1:A:1223:SER:HB2	1:A:1245:ILE:HD11	1.94	0.48
1:A:1281:LEU:HD11	1:A:1591:TYR:CE2	2.48	0.48
2:B:286:LEU:O	2:B:290:MET:HB2	2.13	0.48
2:B:571:ALA:HB3	2:B:572:PRO:HD3	1.94	0.48
2:B:905:THR:CG2	2:B:909:MET:HB2	2.43	0.48
2:B:981:SER:HB2	2:B:988:LEU:HD21	1.96	0.48
4:E:67:ASP:CG	4:E:70:ASP:HB2	2.39	0.48
9:K:47:GLU:OE1	9:K:47:GLU:HA	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:T:-2:DA:H2''	15:T:-1:DG:C8	2.49	0.48
1:A:164:TYR:O	1:A:168:ILE:HG12	2.14	0.48
1:A:677:LYS:HB3	1:A:678:PRO:HD3	1.94	0.48
1:A:1122:ARG:O	1:A:1127:LEU:HD13	2.14	0.48
2:B:8:ARG:O	2:B:9:ASN:ND2	2.47	0.48
2:B:435:ALA:HB1	15:T:9:DA:H5''	1.94	0.48
2:B:681:GLN:HG3	2:B:683:PRO:HD2	1.96	0.48
3:C:250:ALA:HB1	3:C:273:ALA:HB2	1.96	0.48
1:A:683:THR:HG22	1:A:683:THR:O	2.12	0.47
1:A:753:HIS:O	1:A:754:TYR:HB2	2.14	0.47
2:B:162:GLU:C	2:B:164:GLU:N	2.72	0.47
2:B:178:VAL:O	2:B:178:VAL:HG22	2.14	0.47
5:F:66:LEU:HD21	5:F:97:LEU:HD22	1.96	0.47
2:B:498:CYS:CB	2:B:668:SER:HB2	2.43	0.47
2:B:746:ILE:HG22	2:B:914:LEU:HD22	1.95	0.47
2:B:785:ILE:HD12	2:B:791:SER:CB	2.43	0.47
3:C:162:LEU:HG	3:C:204:PRO:HD3	1.95	0.47
3:C:182:ALA:O	3:C:185:PHE:O	2.32	0.47
7:I:17:LEU:HD13	7:I:35:THR:O	2.15	0.47
1:A:89:ASN:HD21	1:A:92:LEU:HD12	1.78	0.47
1:A:423:LYS:HG3	1:A:424:LYS:N	2.27	0.47
1:A:1498:MET:HA	1:A:1501:ARG:NH1	2.29	0.47
1:A:1527:VAL:HG22	1:A:1528:THR:N	2.30	0.47
1:A:1681:LEU:HD21	2:B:1123:LEU:CD2	2.45	0.47
2:B:527:THR:HG23	2:B:527:THR:O	2.14	0.47
5:F:81:VAL:O	5:F:81:VAL:HG22	2.14	0.47
6:H:106:THR:O	6:H:106:THR:HG22	2.13	0.47
11:N:29:ARG:C	11:N:31:SER:H	2.22	0.47
1:A:71:PHE:O	1:A:72:SER:OG	2.21	0.47
1:A:591:GLY:O	14:R:-1:U:H4'	2.14	0.47
1:A:1084:LEU:HG	1:A:1084:LEU:O	2.14	0.47
2:B:122:VAL:O	2:B:123:ASN:HB2	2.14	0.47
2:B:179:ILE:HG12	2:B:454:CYS:HB2	1.96	0.47
3:C:30:PRO:HG2	9:K:61:LYS:HA	1.95	0.47
4:E:139:ILE:HG13	4:E:140:THR:N	2.28	0.47
6:H:13:LYS:HE2	6:H:13:LYS:HA	1.95	0.47
9:K:55:LEU:HD21	9:K:96:PHE:HE1	1.76	0.47
11:N:105:LEU:HB2	13:M:41:PHE:HB2	1.95	0.47
16:U:2:DT:H2''	16:U:3:DG:C8	2.50	0.47
1:A:100:LEU:HD21	1:A:265:LEU:HD22	1.96	0.47
1:A:936:PRO:HG2	2:B:494:TRP:CG	2.50	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1106:GLU:N	1:A:1106:GLU:OE2	2.48	0.47
1:A:1287:ARG:HG2	1:A:1555:ALA:HB1	1.96	0.47
1:A:1545:VAL:CG2	7:I:53:LYS:HE3	2.41	0.47
1:A:1669:LEU:O	1:A:1673:THR:HG23	2.15	0.47
1:A:1670:GLN:C	1:A:1672:MET:H	2.22	0.47
2:B:140:MET:HE3	2:B:168:GLY:C	2.40	0.47
2:B:141:VAL:O	2:B:146:CYS:CB	2.63	0.47
2:B:743:VAL:HG21	2:B:997:VAL:HG22	1.97	0.47
3:C:86:THR:HG21	3:C:227:PRO:HB3	1.96	0.47
3:C:245:VAL:HG21	3:C:253:LEU:HD23	1.97	0.47
3:C:337:LEU:HD21	9:K:100:LEU:HB2	1.97	0.47
1:A:845:LYS:HA	1:A:845:LYS:HE2	1.97	0.47
1:A:1332:CYS:O	1:A:1332:CYS:SG	2.73	0.47
3:C:33:TYR:HB3	3:C:36:TYR:CB	2.39	0.47
13:M:36:PRO:O	13:M:38:ASN:N	2.47	0.47
1:A:66:THR:O	2:B:1083:LYS:HE3	2.14	0.47
1:A:89:ASN:OD1	1:A:92:LEU:HB2	2.14	0.47
1:A:119:LEU:HB2	1:A:142:LEU:HD22	1.97	0.47
1:A:173:LEU:O	1:A:174:LEU:CB	2.63	0.47
1:A:181:VAL:HG11	4:E:166:ARG:HH21	1.79	0.47
1:A:257:THR:HB	1:A:391:TRP:CZ3	2.50	0.47
2:B:181:MET:SD	2:B:520:VAL:HG21	2.55	0.47
2:B:576:ASP:OD1	2:B:576:ASP:C	2.57	0.47
2:B:785:ILE:CG2	2:B:792:LEU:CD2	2.81	0.47
4:E:72:MET:CE	4:E:103:LEU:HD12	2.45	0.47
1:A:811:LYS:O	1:A:814:ARG:HG2	2.15	0.47
1:A:1247:ARG:HG2	1:A:1628:VAL:HG22	1.97	0.47
1:A:1253:MET:O	1:A:1658:ASN:HB3	2.14	0.47
2:B:278:LEU:HD11	2:B:354:PHE:HB3	1.95	0.47
2:B:790:SER:C	2:B:792:LEU:H	2.22	0.47
1:A:713:GLY:O	6:H:20:LYS:HE2	2.15	0.47
1:A:1318:ARG:HB2	1:A:1526:GLN:HB3	1.97	0.47
1:A:1580:THR:HG22	1:A:1581:GLU:N	2.29	0.47
2:B:1026:ILE:HG21	2:B:1031:VAL:HG12	1.96	0.47
3:C:31:GLY:HA2	3:C:37:ASP:OD1	2.15	0.47
3:C:299:LEU:HD23	3:C:299:LEU:H	1.79	0.47
4:E:53:PRO:HB2	4:E:54:ARG:CZ	2.45	0.47
9:K:62:ASN:O	9:K:65:VAL:HG22	2.15	0.47
1:A:181:VAL:HG11	4:E:166:ARG:NH2	2.30	0.47
1:A:512:MET:HG3	1:A:512:MET:O	2.15	0.47
1:A:558:ARG:HB3	1:A:559:PRO:HD3	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1518:ASP:CB	1:A:1522:SER:HA	2.44	0.47
2:B:60:ALA:O	2:B:61:ILE:C	2.58	0.47
2:B:332:ILE:HG13	2:B:332:ILE:O	2.14	0.47
2:B:337:LYS:HB2	2:B:337:LYS:HE2	1.66	0.47
2:B:742:ILE:HD12	8:J:43:TYR:CE1	2.50	0.47
3:C:240:THR:CG2	3:C:298:ARG:HB3	2.44	0.47
6:H:105:SER:O	6:H:106:THR:HB	2.14	0.47
7:I:55:VAL:HA	7:I:59:VAL:CG1	2.45	0.47
1:A:258:PRO:HD2	1:A:391:TRP:CE3	2.50	0.46
1:A:464:THR:HG22	1:A:464:THR:O	2.14	0.46
1:A:1085:ARG:NH2	4:E:19:GLN:HG2	2.30	0.46
1:A:1162:THR:HG21	4:E:199:THR:O	2.14	0.46
1:A:1354:ILE:HD12	1:A:1540:MET:CE	2.45	0.46
2:B:64:PHE:HE2	2:B:397:LYS:CB	2.25	0.46
2:B:626:LEU:HD13	2:B:659:GLN:HB3	1.97	0.46
3:C:147:THR:N	3:C:164:VAL:HG22	2.26	0.46
1:A:140:ARG:NH1	1:A:144:ARG:HH12	2.09	0.46
1:A:1565:ASN:HD22	1:A:1579:ASN:HD22	1.63	0.46
1:A:1575:GLU:O	1:A:1576:LEU:HD22	2.15	0.46
1:A:89:ASN:HB3	1:A:299:LEU:HG	1.97	0.46
1:A:889:PHE:O	1:A:890:PRO:C	2.56	0.46
1:A:972:ARG:HD3	2:B:489:LEU:HD12	1.97	0.46
3:C:15:VAL:HG12	3:C:298:ARG:NH2	2.30	0.46
3:C:27:THR:O	3:C:27:THR:HG22	2.14	0.46
4:E:159:LEU:HD11	4:E:206:TYR:CD2	2.50	0.46
5:F:71:LEU:HD12	5:F:71:LEU:O	2.15	0.46
13:M:67:LEU:CG	13:M:69:TYR:CE1	2.98	0.46
16:U:2:DT:H2"	16:U:3:DG:H5"	1.97	0.46
1:A:595:ASN:HD22	2:B:1035:ILE:HD12	1.79	0.46
1:A:1037:PHE:H	1:A:1038:PRO:HD2	1.78	0.46
2:B:141:VAL:HB	2:B:167:GLY:HA3	1.97	0.46
2:B:175:ILE:CG2	2:B:175:ILE:O	2.64	0.46
2:B:269:ILE:HD13	2:B:278:LEU:HD23	1.98	0.46
2:B:673:PHE:CZ	2:B:732:MET:HE3	2.50	0.46
2:B:910:VAL:O	8:J:9:THR:HG22	2.15	0.46
2:B:926:ILE:O	2:B:926:ILE:HG22	2.15	0.46
2:B:940:LEU:HD12	8:J:43:TYR:CB	2.41	0.46
2:B:1037:PHE:CD2	2:B:1058:LEU:HD21	2.51	0.46
2:B:1069:VAL:HG12	2:B:1076:LEU:HD13	1.97	0.46
11:N:24:ALA:HB3	11:N:27:SER:HB3	1.98	0.46
1:A:551:ASN:O	1:A:594:MET:HG3	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:665:VAL:CG1	9:K:33:ALA:HB2	2.45	0.46
1:A:869:VAL:HG21	1:A:918:GLN:NE2	2.20	0.46
1:A:1106:GLU:O	1:A:1106:GLU:HG2	2.14	0.46
2:B:66:PHE:CE1	2:B:75:PHE:CE2	3.02	0.46
2:B:410:SER:HB3	2:B:411:MET:HE2	1.97	0.46
2:B:722:VAL:HG21	2:B:934:ALA:CB	2.44	0.46
1:A:936:PRO:HG2	2:B:494:TRP:HB3	1.97	0.46
2:B:386:LYS:O	2:B:390:GLU:HG3	2.16	0.46
2:B:393:LEU:O	2:B:396:ILE:HG12	2.16	0.46
2:B:403:LYS:HB3	2:B:418:ARG:NH2	2.26	0.46
2:B:705:ASP:HA	2:B:853:LYS:HZ3	1.79	0.46
3:C:138:LEU:HD21	3:C:190:ILE:HG21	1.98	0.46
3:C:339:GLU:HG2	9:K:26:ALA:HB3	1.97	0.46
13:M:81:CYS:SG	13:M:85:CYS:SG	3.05	0.46
1:A:1669:LEU:HD23	1:A:1669:LEU:HA	1.81	0.46
2:B:39:THR:HG21	2:B:166:MET:HG2	1.98	0.46
2:B:632:GLU:HG2	2:B:633:LEU:N	2.31	0.46
2:B:808:ASP:O	2:B:809:ASP:HB2	2.15	0.46
2:B:821:TYR:HB2	2:B:844:LYS:HZ2	1.80	0.46
6:H:35:PHE:HB3	6:H:37:MET:HG3	1.96	0.46
6:H:86:ASP:C	6:H:88:PHE:H	2.23	0.46
1:A:221:SER:HA	1:A:395:GLN:HG2	1.98	0.46
1:A:497:VAL:HG13	1:A:505:THR:CG2	2.45	0.46
1:A:498:ILE:O	1:A:536:LYS:HA	2.16	0.46
1:A:1518:ASP:CG	1:A:1524:TRP:H	2.23	0.46
2:B:282:VAL:HA	2:B:285:MET:HE3	1.98	0.46
2:B:333:CYS:SG	2:B:345:MET:SD	3.13	0.46
3:C:173:MET:SD	3:C:212:MET:HE1	2.56	0.46
10:L:37:ARG:O	10:L:38:GLU:HB3	2.15	0.46
13:M:28:PHE:CZ	13:M:33:LEU:HD11	2.50	0.46
1:A:430:LYS:O	1:A:431:HIS:HB2	2.16	0.46
1:A:926:PRO:HB3	1:A:969:MET:HE1	1.98	0.46
1:A:1318:ARG:HD2	1:A:1524:TRP:CE3	2.48	0.46
2:B:39:THR:CG2	2:B:166:MET:HG2	2.45	0.46
2:B:269:ILE:HG22	2:B:273:GLU:HA	1.98	0.46
2:B:471:CYS:SG	2:B:511:MET:HG2	2.56	0.46
2:B:847:CYS:SG	2:B:871:MET:HG2	2.56	0.46
3:C:245:VAL:HG21	3:C:253:LEU:HD22	1.98	0.46
7:I:29:LEU:N	7:I:41:CYS:HA	2.30	0.46
9:K:90:LEU:HD12	9:K:95:PRO:HD3	1.98	0.46
1:A:881:MET:HE3	1:A:881:MET:HB3	1.63	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1533:LEU:H	1:A:1535:LYS:NZ	2.14	0.46
2:B:700:LEU:HD11	2:B:706:ARG:CG	2.39	0.46
2:B:707:SER:HB2	2:B:868:CYS:SG	2.56	0.46
2:B:722:VAL:HG21	2:B:934:ALA:HB3	1.98	0.46
3:C:61:LEU:HG	3:C:63:PHE:HD1	1.80	0.46
5:F:55:PRO:O	5:F:123:LEU:HD12	2.16	0.46
1:A:33:ILE:HD13	1:A:304:VAL:HG11	1.98	0.45
1:A:214:VAL:HG21	1:A:216:ARG:NH2	2.30	0.45
1:A:804:VAL:HG13	1:A:884:GLY:O	2.15	0.45
1:A:1090:LEU:HD21	4:E:33:LEU:HD12	1.99	0.45
1:A:1275:LEU:O	1:A:1278:VAL:HG12	2.15	0.45
1:A:1288:VAL:HB	1:A:1331:LYS:HE3	1.98	0.45
3:C:87:MET:HE3	3:C:87:MET:HB3	1.91	0.45
3:C:290:ASN:HD22	3:C:293:LEU:HB2	1.81	0.45
4:E:125:TYR:O	4:E:127:LEU:HD12	2.16	0.45
1:A:1000:VAL:HG12	1:A:1210:ALA:HA	1.96	0.45
1:A:1343:GLU:HG3	1:A:1505:VAL:CG2	2.46	0.45
2:B:905:THR:HG21	2:B:909:MET:HB2	1.98	0.45
6:H:37:MET:HE3	6:H:127:GLY:CA	2.45	0.45
9:K:83:ARG:HH11	9:K:85:GLN:NE2	2.11	0.45
11:N:38:PRO:O	13:M:94:LYS:NZ	2.47	0.45
1:A:897:MET:SD	2:B:921:PRO:HG3	2.56	0.45
2:B:183:ILE:HG13	2:B:472:VAL:HG12	1.98	0.45
2:B:496:PHE:C	2:B:497:LEU:HD12	2.41	0.45
11:N:81:ARG:HB3	11:N:118:LEU:HG	1.98	0.45
1:A:678:PRO:HB2	6:H:47:ILE:CG2	2.47	0.45
2:B:167:GLY:O	2:B:169:TYR:CD2	2.68	0.45
2:B:642:MET:HE3	2:B:658:HIS:ND1	2.31	0.45
2:B:667:LEU:HD12	2:B:667:LEU:HA	1.86	0.45
3:C:236:LEU:HD22	3:C:305:HIS:CD2	2.51	0.45
3:C:261:VAL:HG21	3:C:281:ASP:HB2	1.97	0.45
1:A:1511:PHE:HB3	1:A:1529:VAL:HG13	1.97	0.45
2:B:336:LEU:CD2	2:B:561:VAL:HG22	2.46	0.45
2:B:818:LYS:HG2	2:B:848:VAL:HG12	1.99	0.45
1:A:406:MET:HE2	1:A:406:MET:HB2	1.81	0.45
1:A:592:ASP:O	1:A:593:GLU:C	2.60	0.45
1:A:972:ARG:HH11	2:B:489:LEU:HD12	1.82	0.45
1:A:1184:LYS:HE3	1:A:1184:LYS:HB3	1.83	0.45
1:A:1348:LYS:NZ	1:A:1509:HIS:HB3	2.32	0.45
1:A:1512:ILE:HG22	1:A:1513:ASP:N	2.31	0.45
2:B:149:ARG:O	2:B:150:ASN:HB2	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:238:PHE:CE1	2:B:327:LEU:HD11	2.51	0.45
2:B:247:LEU:HD12	2:B:248:PRO:HD2	1.98	0.45
4:E:11:TRP:HB2	4:E:40:PHE:CD2	2.52	0.45
5:F:122:GLU:O	5:F:122:GLU:HG3	2.15	0.45
13:M:67:LEU:HD11	13:M:69:TYR:CE1	2.52	0.45
1:A:716:TRP:HZ2	1:A:748:VAL:HG11	1.80	0.45
2:B:75:PHE:CD2	2:B:75:PHE:N	2.82	0.45
2:B:800:ASP:HB3	2:B:803:VAL:HG22	1.99	0.45
3:C:193:VAL:HG11	3:C:314:GLY:HA3	1.99	0.45
6:H:63:THR:HG22	6:H:71:ASP:OD1	2.17	0.45
6:H:92:MET:HE2	6:H:121:LEU:HD12	1.99	0.45
1:A:314:ARG:HD2	1:A:319:MET:HE3	1.98	0.45
1:A:619:LEU:HD23	1:A:626:PRO:HA	1.99	0.45
1:A:1128:ASP:CB	1:A:1133:ARG:HD3	2.46	0.45
1:A:1531:LEU:CB	1:A:1535:LYS:HD3	2.47	0.45
2:B:140:MET:HE2	2:B:168:GLY:HA2	1.98	0.45
2:B:400:PHE:HA	2:B:418:ARG:NH1	2.30	0.45
2:B:797:LYS:HE2	2:B:797:LYS:HB3	1.82	0.45
3:C:236:LEU:HB2	3:C:305:HIS:HD2	1.82	0.45
9:K:22:GLU:HG2	9:K:25:THR:CB	2.46	0.45
1:A:138:LEU:HD11	1:A:165:THR:CG2	2.42	0.45
1:A:387:LEU:HD12	1:A:390:ILE:HD11	1.97	0.45
2:B:35:LEU:HD13	2:B:35:LEU:HA	1.86	0.45
2:B:336:LEU:HD22	2:B:561:VAL:HG22	1.99	0.45
2:B:810:ASP:OD2	10:L:17:TYR:OH	2.30	0.45
7:I:65:GLY:O	7:I:66:THR:C	2.59	0.45
13:M:16:ALA:HB3	13:M:19:GLY:HA2	1.98	0.45
1:A:105:LEU:HD12	1:A:264:HIS:CE1	2.52	0.45
1:A:1589:PHE:HA	1:A:1597:LEU:CD1	2.47	0.45
2:B:98:VAL:O	2:B:110:TYR:HE1	2.00	0.45
2:B:206:THR:OG1	2:B:228:TYR:O	2.34	0.45
2:B:689:CYS:O	2:B:693:LYS:HD3	2.17	0.45
2:B:698:PHE:HE2	2:B:701:LEU:HD23	1.80	0.45
2:B:721:LEU:HD21	8:J:50:LEU:HD23	1.97	0.45
2:B:792:LEU:CD1	2:B:865:LYS:HD2	2.41	0.45
2:B:853:LYS:HE2	10:L:45:TYR:HE2	1.82	0.45
4:E:13:ILE:CD1	4:E:132:GLN:HG3	2.47	0.45
4:E:87:ILE:HD11	4:E:110:MET:HE2	1.99	0.45
8:J:24:LEU:O	8:J:29:TYR:HB2	2.17	0.45
2:B:92:ILE:CG2	2:B:93:CYS:H	2.24	0.44
2:B:184:MET:HB3	2:B:185:PRO:HD2	1.98	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:205:TYR:CD1	2:B:229:LEU:HD22	2.52	0.44
2:B:284:GLN:O	2:B:288:ILE:HB	2.17	0.44
3:C:241:LEU:HD21	3:C:253:LEU:HD21	1.99	0.44
1:A:174:LEU:HG	1:A:174:LEU:O	2.17	0.44
1:A:854:ASP:O	1:A:855:GLN:HB2	2.17	0.44
2:B:730:TYR:O	2:B:731:ASP:C	2.57	0.44
2:B:760:ASN:OD1	2:B:761:LYS:N	2.50	0.44
4:E:168:ASN:HA	4:E:172:ARG:HH12	1.82	0.44
1:A:121:LEU:HD23	1:A:121:LEU:C	2.43	0.44
1:A:715:ALA:HB2	1:A:899:GLN:NE2	2.33	0.44
1:A:969:MET:CG	2:B:489:LEU:HD22	2.33	0.44
2:B:5:SER:O	2:B:6:ARG:HB3	2.17	0.44
2:B:758:ILE:HD12	2:B:895:ARG:HB2	1.95	0.44
5:F:53:THR:OG1	5:F:108:ARG:NH1	2.48	0.44
13:M:39:MET:HG2	13:M:64:THR:HG22	1.99	0.44
1:A:464:THR:O	1:A:464:THR:CG2	2.66	0.44
1:A:518:VAL:HG22	1:A:518:VAL:O	2.17	0.44
1:A:555:THR:HG23	2:B:1041:GLU:OE2	2.17	0.44
1:A:833:LEU:HD22	1:A:833:LEU:HA	1.85	0.44
1:A:1180:LYS:HD3	1:A:1180:LYS:HA	1.83	0.44
1:A:1655:LYS:HB3	1:A:1655:LYS:HE3	1.69	0.44
2:B:186:ARG:O	2:B:213:HIS:HB3	2.18	0.44
2:B:197:LYS:HG2	2:B:197:LYS:O	2.18	0.44
4:E:168:ASN:HA	4:E:172:ARG:HH22	1.83	0.44
13:M:11:TRP:CZ2	13:M:101:VAL:HG11	2.53	0.44
1:A:93:PHE:O	1:A:96:LEU:HB3	2.18	0.44
1:A:422:GLU:HG2	1:A:1677:SER:HB3	1.99	0.44
1:A:472:VAL:CG2	1:A:477:VAL:HG23	2.47	0.44
1:A:598:PHE:O	1:A:600:GLN:HG2	2.18	0.44
1:A:766:TYR:CD1	1:A:771:GLY:HA2	2.52	0.44
1:A:1628:VAL:O	1:A:1631:VAL:HG22	2.17	0.44
2:B:526:TYR:O	2:B:527:THR:HG22	2.17	0.44
4:E:87:ILE:HD11	4:E:110:MET:CE	2.48	0.44
7:I:40:ARG:O	7:I:40:ARG:HG3	2.16	0.44
13:M:69:TYR:HA	13:M:110:GLN:O	2.18	0.44
1:A:268:LEU:HD23	1:A:268:LEU:O	2.16	0.44
1:A:544:ASN:HA	1:A:566:ALA:O	2.17	0.44
1:A:1113:ARG:O	1:A:1114:SER:HB2	2.17	0.44
2:B:55:GLY:O	2:B:59:GLN:HG2	2.18	0.44
6:H:56:PHE:HE1	6:H:58:LEU:HD12	1.83	0.44
1:A:716:TRP:CZ2	1:A:748:VAL:HG11	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:801:ASP:HB3	1:A:887:ARG:HD2	2.00	0.44
2:B:106:ARG:HG3	10:L:43:ILE:HD11	1.98	0.44
2:B:239:ILE:HB	2:B:244:LEU:HD23	1.99	0.44
2:B:525:VAL:HG21	2:B:590:PRO:HG3	2.00	0.44
2:B:647:PHE:CE1	2:B:663:PRO:HB3	2.53	0.44
2:B:651:VAL:HG22	2:B:656:THR:HG21	1.99	0.44
2:B:655:VAL:HG12	2:B:656:THR:N	2.32	0.44
2:B:781:LEU:HD22	2:B:792:LEU:CB	2.37	0.44
2:B:804:LEU:HG	2:B:805:GLN:OE1	2.18	0.44
6:H:40:ILE:O	6:H:123:MET:HA	2.17	0.44
1:A:865:PHE:CZ	1:A:945:PRO:HA	2.53	0.44
1:A:1530:LYS:C	1:A:1531:LEU:HD12	2.43	0.44
2:B:688:GLN:OE1	2:B:688:GLN:HA	2.18	0.44
2:B:767:GLY:HA2	2:B:770:HIS:CE1	2.53	0.44
2:B:828:TYR:CD1	2:B:828:TYR:N	2.86	0.44
3:C:30:PRO:HG3	9:K:61:LYS:HA	1.99	0.44
3:C:142:LEU:HD21	3:C:168:VAL:HG11	1.99	0.44
7:I:14:GLN:CG	7:I:17:LEU:HD12	2.47	0.44
1:A:1598:ARG:O	1:A:1599:ARG:HB2	2.17	0.44
2:B:92:ILE:HG21	10:L:42:ARG:NH1	2.32	0.44
2:B:1084:PRO:HD3	2:B:1094:ARG:NH2	2.33	0.44
11:N:30:PHE:O	11:N:96:ALA:HB1	2.18	0.44
11:N:84:SER:OG	11:N:115:LEU:CD2	2.66	0.44
15:T:-5:DG:H2"	15:T:-4:DA:H8	1.82	0.44
1:A:29:SER:HB3	1:A:80:HIS:HD2	1.81	0.43
1:A:860:MET:HE2	1:A:864:LYS:CE	2.38	0.43
1:A:1348:LYS:O	1:A:1352:GLU:HG3	2.18	0.43
2:B:18:HIS:HE1	2:B:723:ARG:HH22	1.66	0.43
2:B:109:THR:HA	2:B:171:ILE:O	2.18	0.43
2:B:116:ALA:H	2:B:134:LEU:HD23	1.83	0.43
2:B:811:GLY:O	2:B:812:LEU:HD23	2.18	0.43
4:E:122:ALA:O	4:E:124:LYS:N	2.50	0.43
10:L:15:MET:CA	10:L:15:MET:HE3	2.49	0.43
1:A:56:GLY:HA2	1:A:64:CYS:HB3	2.00	0.43
1:A:64:CYS:SG	1:A:67:CYS:O	2.75	0.43
1:A:100:LEU:HD21	1:A:265:LEU:CD2	2.48	0.43
1:A:459:PRO:HB2	1:A:572:GLU:C	2.43	0.43
1:A:472:VAL:O	1:A:535:THR:HG21	2.18	0.43
2:B:115:THR:HG22	2:B:133:PHE:HA	1.99	0.43
2:B:156:LEU:HG	2:B:161:GLU:HB2	2.00	0.43
2:B:743:VAL:HG21	2:B:997:VAL:CG2	2.47	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:782:SER:HA	2:B:792:LEU:HD13	2.00	0.43
2:B:1132:LEU:HD12	2:B:1132:LEU:O	2.18	0.43
3:C:75:ALA:O	3:C:79:ILE:HG12	2.18	0.43
1:A:40:ASP:HB2	1:A:44:ASN:O	2.18	0.43
1:A:186:GLU:HB2	1:A:1664:SER:HB2	2.00	0.43
1:A:218:GLU:HG2	1:A:219:HIS:H	1.82	0.43
1:A:976:VAL:O	1:A:980:VAL:HG13	2.18	0.43
1:A:1300:GLN:HE22	7:I:48:ARG:HD3	1.83	0.43
2:B:175:ILE:O	2:B:175:ILE:HG22	2.18	0.43
2:B:403:LYS:CB	2:B:418:ARG:HH12	2.20	0.43
3:C:149:ASN:OD1	3:C:161:GLU:HA	2.17	0.43
6:H:118:TYR:OH	6:H:143:LEU:HB2	2.18	0.43
11:N:39:ASP:HA	13:M:94:LYS:HE3	1.99	0.43
1:A:332:MET:HE2	1:A:332:MET:HB3	1.68	0.43
1:A:433:MET:HB3	2:B:1039:GLU:HG2	1.98	0.43
1:A:595:ASN:HB3	2:B:1035:ILE:HD12	2.00	0.43
2:B:143:SER:O	2:B:144:LYS:HB2	2.18	0.43
2:B:295:SER:HB3	7:I:34:ASP:OD2	2.19	0.43
4:E:82:VAL:HG13	4:E:86:THR:HB	1.99	0.43
9:K:65:VAL:HA	9:K:86:THR:HA	2.00	0.43
13:M:33:LEU:HD13	13:M:39:MET:SD	2.59	0.43
1:A:26:LYS:O	1:A:27:LYS:HB2	2.18	0.43
1:A:553:GLN:HG2	15:T:3:DG:O4'	2.18	0.43
1:A:745:LEU:HD21	6:H:95:LYS:HD3	2.00	0.43
1:A:1531:LEU:HB3	1:A:1535:LYS:HD3	1.99	0.43
2:B:63:PRO:HB3	2:B:76:THR:HG22	2.00	0.43
2:B:240:TYR:HB2	2:B:331:CYS:SG	2.58	0.43
2:B:918:HIS:C	2:B:921:PRO:HD2	2.43	0.43
4:E:43:GLN:O	4:E:44:SER:HB3	2.18	0.43
6:H:32:SER:HB3	6:H:37:MET:H	1.83	0.43
10:L:15:MET:HE3	10:L:15:MET:HA	2.00	0.43
10:L:37:ARG:C	10:L:39:CYS:H	2.25	0.43
1:A:186:GLU:HG2	1:A:190:LYS:HE3	2.01	0.43
1:A:718:LYS:HB3	1:A:718:LYS:HE2	1.82	0.43
1:A:812:ARG:HD2	1:A:914:CYS:CA	2.46	0.43
1:A:1095:LYS:O	1:A:1098:GLU:HB3	2.19	0.43
2:B:625:ASN:O	2:B:629:GLY:N	2.48	0.43
2:B:856:SER:CB	10:L:42:ARG:HB3	2.43	0.43
4:E:56:THR:O	4:E:56:THR:HG22	2.18	0.43
4:E:73:PHE:HB2	4:E:99:ILE:HD13	2.00	0.43
4:E:143:GLU:HG3	4:E:144:LEU:HG	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:459:PRO:O	1:A:461:VAL:N	2.52	0.43
1:A:472:VAL:HG12	1:A:536:LYS:O	2.19	0.43
1:A:743:GLU:CD	6:H:140:ARG:HH22	2.27	0.43
1:A:754:TYR:CE1	1:A:781:LEU:HD22	2.54	0.43
1:A:846:TRP:NE1	1:A:858:PHE:HE1	2.13	0.43
1:A:866:LYS:O	1:A:869:VAL:HG22	2.19	0.43
1:A:1006:THR:CG2	1:A:1008:ARG:HE	2.29	0.43
1:A:1114:SER:HB3	1:A:1117:THR:H	1.84	0.43
1:A:1583:ILE:CD1	1:A:1604:ASP:HB2	2.48	0.43
1:A:1631:VAL:HG23	1:A:1632:TYR:CE2	2.53	0.43
2:B:69:LYS:HE2	2:B:69:LYS:HB3	1.57	0.43
3:C:100:ILE:HG13	8:J:60:LEU:HD23	2.00	0.43
16:U:3:DG:H2'	16:U:4:DT:C6	2.53	0.43
1:A:205:CYS:HB3	1:A:208:CYS:O	2.19	0.43
1:A:811:LYS:O	1:A:815:ILE:HG13	2.18	0.43
1:A:1531:LEU:O	1:A:1535:LYS:HD3	2.19	0.43
2:B:18:HIS:O	2:B:21:ASP:HB2	2.19	0.43
2:B:32:LYS:O	2:B:33:ALA:HB3	2.19	0.43
2:B:388:LYS:HE3	2:B:429:PRO:HB3	2.01	0.43
2:B:432:TYR:HE1	15:T:10:DA:H5''	1.82	0.43
9:K:89:THR:HG23	9:K:90:LEU:H	1.81	0.43
1:A:30:VAL:CG1	1:A:66:THR:HG21	2.49	0.43
1:A:454:ASN:HA	1:A:614:THR:HG21	2.00	0.43
1:A:1134:LYS:HE2	1:A:1134:LYS:CA	2.49	0.43
1:A:1300:GLN:NE2	7:I:48:ARG:HD3	2.34	0.43
1:A:1566:GLU:O	1:A:1576:LEU:HD22	2.19	0.43
1:A:1639:ARG:HE	4:E:199:THR:HG21	1.83	0.43
2:B:172:ILE:O	2:B:173:ASN:HB2	2.17	0.43
2:B:248:PRO:HB2	2:B:251:PHE:HD2	1.82	0.43
3:C:246:GLU:HG2	3:C:272:VAL:HA	2.01	0.43
5:F:57:MET:HE2	5:F:106:ILE:HD11	2.00	0.43
1:A:131:ALA:HB2	1:A:172:ASN:HD22	1.83	0.43
1:A:404:SER:CB	1:A:415:PRO:HA	2.42	0.43
1:A:642:THR:HB	1:A:748:VAL:O	2.19	0.43
1:A:833:LEU:HD13	1:A:834:PRO:HD2	2.00	0.43
1:A:980:VAL:HG11	2:B:484:THR:HG21	2.01	0.43
1:A:1515:TYR:O	1:A:1526:GLN:NE2	2.52	0.43
1:A:1523:LEU:HD12	1:A:1524:TRP:HB2	2.01	0.43
2:B:258:SER:HB3	2:B:297:GLN:OE1	2.19	0.43
2:B:430:PHE:O	2:B:434:PHE:HD1	2.02	0.43
2:B:804:LEU:N	2:B:804:LEU:HD23	2.34	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:102:GLN:O	3:C:106:LEU:HB2	2.19	0.43
3:C:337:LEU:HD21	9:K:100:LEU:CB	2.49	0.43
4:E:179:VAL:O	4:E:179:VAL:HG12	2.18	0.43
1:A:217:LYS:HD2	1:A:218:GLU:O	2.19	0.42
1:A:431:HIS:O	2:B:1115:VAL:HG11	2.19	0.42
1:A:459:PRO:C	1:A:461:VAL:H	2.26	0.42
1:A:680:PRO:HG2	3:C:31:GLY:O	2.18	0.42
1:A:1129:GLU:OE1	1:A:1132:ARG:CB	2.67	0.42
1:A:1133:ARG:O	1:A:1133:ARG:CG	2.66	0.42
1:A:1251:ILE:O	1:A:1654:TYR:OH	2.30	0.42
1:A:1605:ILE:HG21	1:A:1621:ILE:HG13	1.98	0.42
2:B:214:CYS:O	2:B:221:ALA:HA	2.19	0.42
2:B:370:VAL:HG13	2:B:637:MET:HA	2.01	0.42
2:B:519:GLU:HG3	2:B:620:VAL:HG23	2.01	0.42
2:B:704:GLN:HG3	2:B:704:GLN:O	2.18	0.42
2:B:908:GLY:HA2	3:C:232:SER:OG	2.19	0.42
11:N:56:PHE:HZ	11:N:80:TYR:HB2	1.83	0.42
1:A:1062:PRO:HB3	1:A:1156:PHE:HD2	1.83	0.42
1:A:1111:ASN:ND2	4:E:61:LEU:HD23	2.34	0.42
1:A:1615:GLU:OE2	4:E:207:ARG:NE	2.46	0.42
2:B:863:LYS:O	2:B:865:LYS:HG2	2.19	0.42
2:B:920:PHE:N	2:B:921:PRO:CD	2.83	0.42
2:B:1003:ARG:O	2:B:1003:ARG:CD	2.64	0.42
3:C:30:PRO:HB3	3:C:38:ASP:O	2.19	0.42
6:H:107:GLU:HG3	6:H:108:ALA:N	2.34	0.42
11:N:61:VAL:HG21	13:M:11:TRP:HE3	1.84	0.42
11:N:142:PRO:CG	11:N:145:LEU:CD2	2.43	0.42
11:N:146:ARG:NH1	11:N:148:ARG:NH2	2.63	0.42
1:A:312:VAL:HG23	1:A:320:PHE:C	2.44	0.42
1:A:806:PRO:C	1:A:808:ALA:H	2.26	0.42
1:A:1009:ASP:OD1	1:A:1010:SER:N	2.47	0.42
1:A:1334:ARG:HG3	1:A:1335:PRO:CD	2.40	0.42
2:B:116:ALA:N	2:B:134:LEU:HD23	2.34	0.42
2:B:720:PRO:O	2:B:723:ARG:HD3	2.19	0.42
7:I:7:ALA:HA	7:I:15:SER:OG	2.19	0.42
1:A:127:LEU:HD21	1:A:135:VAL:HG21	1.98	0.42
1:A:408:LYS:HD3	1:A:408:LYS:H	1.85	0.42
1:A:427:LEU:HG	1:A:427:LEU:O	2.19	0.42
1:A:654:MET:HE3	9:K:60:MET:HE1	2.00	0.42
1:A:703:LEU:HD23	1:A:703:LEU:H	1.84	0.42
1:A:961:PRO:N	1:A:962:PRO:HD2	2.33	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:972:ARG:NH2	2:B:509:GLY:HA2	2.35	0.42
1:A:1150:TRP:O	1:A:1151:ARG:C	2.62	0.42
1:A:1715:LEU:HD23	1:A:1715:LEU:HA	1.85	0.42
2:B:73:ILE:HG22	2:B:75:PHE:CZ	2.51	0.42
2:B:269:ILE:HG22	2:B:269:ILE:O	2.19	0.42
2:B:290:MET:HA	2:B:290:MET:HE2	2.00	0.42
2:B:796:ILE:HD11	2:B:807:LEU:CB	2.41	0.42
5:F:53:THR:HG23	5:F:116:GLU:CD	2.45	0.42
13:M:83:THR:O	13:M:84:LEU:C	2.62	0.42
1:A:12:LEU:CD2	2:B:1132:LEU:HD13	2.49	0.42
1:A:225:ILE:CG2	1:A:256:LEU:HD11	2.49	0.42
1:A:496:MET:HB2	1:A:496:MET:HE3	1.73	0.42
1:A:636:VAL:HG11	1:A:795:PHE:CE1	2.54	0.42
1:A:659:ARG:HD3	1:A:787:ALA:HB1	2.01	0.42
2:B:210:VAL:HG21	2:B:349:MET:HB3	2.01	0.42
2:B:997:VAL:CG2	2:B:999:TYR:CE2	3.02	0.42
3:C:40:TRP:HZ2	9:K:106:VAL:CG2	2.33	0.42
1:A:463:ALA:CB	1:A:568:ILE:HD12	2.49	0.42
1:A:1045:GLU:H	1:A:1045:GLU:HG2	1.43	0.42
1:A:1092:TYR:CZ	1:A:1095:LYS:HD2	2.55	0.42
1:A:1243:LEU:O	1:A:1246:PRO:HG2	2.19	0.42
1:A:1335:PRO:C	1:A:1338:ILE:HG22	2.45	0.42
1:A:1618:LEU:HD11	1:A:1649:CYS:CB	2.49	0.42
2:B:194:ILE:HD12	2:B:363:GLU:HB2	2.01	0.42
2:B:746:ILE:CG2	2:B:914:LEU:HD22	2.50	0.42
4:E:122:ALA:C	4:E:124:LYS:N	2.77	0.42
1:A:78:LEU:HD12	1:A:306:PRO:HD3	2.01	0.42
1:A:121:LEU:HD23	1:A:125:ARG:HG3	2.01	0.42
1:A:711:ILE:HG13	1:A:750:ASP:OD2	2.19	0.42
1:A:1037:PHE:N	1:A:1038:PRO:CD	2.82	0.42
1:A:1086:ARG:HB2	1:A:1086:ARG:NH1	2.35	0.42
1:A:1268:VAL:O	1:A:1268:VAL:HG12	2.20	0.42
1:A:1535:LYS:HD2	1:A:1535:LYS:N	2.34	0.42
1:A:1648:MET:HE2	1:A:1654:TYR:CE1	2.55	0.42
2:B:210:VAL:HG23	2:B:349:MET:HE2	2.02	0.42
2:B:346:LEU:HD23	2:B:346:LEU:HA	1.93	0.42
2:B:489:LEU:O	2:B:489:LEU:HD23	2.20	0.42
2:B:1027:GLY:H	2:B:1033:GLY:HA2	1.83	0.42
3:C:50:ARG:HG3	3:C:66:VAL:HB	2.02	0.42
3:C:86:THR:HA	3:C:119:PRO:CG	2.49	0.42
3:C:138:LEU:HD12	3:C:138:LEU:HA	1.92	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:100:ARG:HE	5:F:100:ARG:HB3	1.72	0.42
6:H:105:SER:C	6:H:107:GLU:H	2.28	0.42
7:I:13:PHE:CD1	7:I:20:CYS:HB3	2.55	0.42
1:A:326:VAL:HG11	1:A:414:TYR:CE1	2.55	0.42
1:A:330:ALA:HB1	1:A:397:HIS:ND1	2.35	0.42
1:A:513:THR:HG23	1:A:514:GLN:N	2.34	0.42
1:A:705:LEU:CD1	1:A:761:LEU:HA	2.49	0.42
1:A:1016:GLN:OE1	1:A:1643:LEU:HD13	2.19	0.42
1:A:1200:TRP:CD1	1:A:1200:TRP:C	2.98	0.42
1:A:1559:ILE:HG23	1:A:1580:THR:HG23	2.01	0.42
1:A:1704:LYS:HE2	1:A:1704:LYS:HB3	1.74	0.42
2:B:162:GLU:HB2	2:B:165:GLU:HB3	2.01	0.42
2:B:844:LYS:HA	2:B:844:LYS:HD3	1.94	0.42
3:C:236:LEU:HB2	3:C:305:HIS:CD2	2.55	0.42
4:E:169:GLN:O	4:E:169:GLN:CG	2.67	0.42
1:A:397:HIS:CD2	1:A:410:MET:HE1	2.54	0.42
1:A:860:MET:HE2	1:A:864:LYS:HG3	2.01	0.42
1:A:939:GLU:HG2	1:A:940:PRO:N	2.34	0.42
1:A:1104:LYS:HD2	1:A:1104:LYS:O	2.20	0.42
1:A:1280:SER:O	1:A:1284:GLN:HB2	2.19	0.42
2:B:179:ILE:HD11	2:B:434:PHE:CE2	2.55	0.42
2:B:668:SER:O	2:B:672:ASN:ND2	2.53	0.42
2:B:1097:ASN:OD1	2:B:1104:SER:HB2	2.20	0.42
3:C:135:ILE:H	3:C:135:ILE:HG12	1.48	0.42
3:C:336:PHE:CZ	9:K:44:LEU:HB3	2.55	0.42
4:E:103:LEU:HD21	4:E:130:PHE:CD2	2.55	0.42
4:E:110:MET:SD	4:E:118:LEU:CD1	3.06	0.42
5:F:110:LEU:HB3	5:F:111:PRO:HD2	2.01	0.42
1:A:602:GLU:O	1:A:602:GLU:HG3	2.19	0.42
1:A:1268:VAL:HG23	1:A:1576:LEU:O	2.19	0.42
1:A:1716:LYS:HD3	1:A:1716:LYS:HA	1.87	0.42
2:B:167:GLY:O	2:B:169:TYR:HD2	2.02	0.42
2:B:521:VAL:O	2:B:616:PRO:O	2.38	0.42
2:B:1053:LEU:HD23	2:B:1053:LEU:HA	1.91	0.42
3:C:240:THR:O	3:C:240:THR:HG23	2.20	0.42
3:C:312:SER:HB3	3:C:321:LEU:HD11	2.01	0.42
7:I:43:PHE:HE1	7:I:46:ASN:HA	1.84	0.42
1:A:302:LEU:HD23	1:A:302:LEU:HA	1.82	0.41
1:A:613:CYS:SG	1:A:614:THR:N	2.93	0.41
1:A:1034:PRO:C	1:A:1036:GLN:H	2.28	0.41
1:A:1266:VAL:HG12	1:A:1596:ASP:O	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:75:PHE:CD1	2:B:120:TRP:CB	3.03	0.41
2:B:171:ILE:CG2	2:B:174:GLY:HA2	2.47	0.41
2:B:792:LEU:HD12	2:B:865:LYS:CD	2.40	0.41
4:E:85:LYS:HE2	4:E:85:LYS:HB3	1.87	0.41
9:K:45:HIS:O	9:K:46:GLU:HB2	2.19	0.41
1:A:754:TYR:HE1	1:A:781:LEU:HD22	1.85	0.41
1:A:896:MET:O	1:A:896:MET:CG	2.67	0.41
1:A:1568:THR:HG21	1:A:1577:VAL:HG11	2.01	0.41
2:B:626:LEU:C	2:B:628:LEU:H	2.29	0.41
4:E:6:GLU:O	4:E:10:LEU:HD13	2.19	0.41
4:E:73:PHE:HD2	4:E:75:PHE:CZ	2.38	0.41
1:A:543:LYS:O	1:A:543:LYS:CG	2.68	0.41
1:A:1137:LYS:HD2	1:A:1137:LYS:HA	1.89	0.41
1:A:1162:THR:O	1:A:1166:LYS:HG3	2.20	0.41
1:A:1570:ASN:OD1	1:A:1571:LYS:N	2.53	0.41
1:A:1672:MET:O	1:A:1677:SER:HB2	2.19	0.41
2:B:804:LEU:HD23	2:B:804:LEU:H	1.85	0.41
6:H:26:SER:HB3	6:H:45:ILE:HG21	2.02	0.41
14:R:-7:G:H2'	14:R:-6:C:C6	2.55	0.41
1:A:910:MET:C	1:A:912:ILE:H	2.28	0.41
1:A:912:ILE:CG1	2:B:924:MET:HG2	2.50	0.41
1:A:992:ILE:HD11	1:A:1252:LEU:HD13	2.01	0.41
1:A:1090:LEU:CD2	4:E:30:GLN:HG2	2.34	0.41
1:A:1247:ARG:HG2	1:A:1628:VAL:CG2	2.49	0.41
1:A:1324:HIS:HD2	1:A:1328:GLN:HG3	1.84	0.41
1:A:1504:ALA:O	1:A:1508:ILE:HG13	2.21	0.41
2:B:549:SER:C	2:B:551:SER:H	2.28	0.41
6:H:39:LEU:HD12	6:H:125:LEU:HD13	2.00	0.41
9:K:24:LYS:C	9:K:26:ALA:N	2.77	0.41
9:K:60:MET:SD	9:K:68:CYS:HB3	2.60	0.41
13:M:73:ASN:ND2	13:M:105:GLU:OE1	2.50	0.41
1:A:33:ILE:HD11	1:A:81:ILE:CG1	2.51	0.41
1:A:433:MET:CB	2:B:1039:GLU:HG2	2.51	0.41
1:A:661:LEU:HG	1:A:691:LEU:CD1	2.51	0.41
1:A:866:LYS:HA	1:A:869:VAL:CG2	2.49	0.41
1:A:1678:PHE:CE1	2:B:1126:MET:HE1	2.56	0.41
2:B:804:LEU:HG	2:B:805:GLN:N	2.36	0.41
3:C:230:THR:HG23	8:J:10:CYS:HB2	2.01	0.41
3:C:263:GLU:CB	3:C:276:ALA:HB2	2.50	0.41
3:C:312:SER:HB3	3:C:321:LEU:HD12	2.02	0.41
8:J:17:LYS:HE3	8:J:38:LEU:O	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:81:CYS:O	13:M:85:CYS:SG	2.69	0.41
1:A:215:VAL:HG22	1:A:225:ILE:CG2	2.50	0.41
1:A:327:ASN:HB3	1:A:401:VAL:HG22	2.02	0.41
1:A:737:VAL:HA	1:A:746:CYS:O	2.20	0.41
1:A:811:LYS:HA	1:A:814:ARG:HG2	2.03	0.41
1:A:1136:GLN:HE21	1:A:1136:GLN:HB3	1.63	0.41
1:A:1324:HIS:CD2	1:A:1328:GLN:HG3	2.56	0.41
1:A:1580:THR:CG2	1:A:1581:GLU:N	2.84	0.41
2:B:35:LEU:HD13	2:B:730:TYR:HD2	1.85	0.41
2:B:86:THR:HG22	2:B:87:VAL:N	2.35	0.41
2:B:104:ARG:NH2	2:B:169:TYR:OH	2.52	0.41
2:B:786:LYS:O	2:B:788:GLY:N	2.52	0.41
2:B:909:MET:HE2	2:B:909:MET:HB3	1.72	0.41
3:C:203:ARG:O	3:C:204:PRO:C	2.64	0.41
1:A:674:SER:HB2	6:H:118:TYR:O	2.20	0.41
1:A:850:HIS:HD2	1:A:941:TYR:OH	2.04	0.41
1:A:1268:VAL:HG13	1:A:1595:LEU:HD23	2.01	0.41
2:B:185:PRO:O	2:B:186:ARG:HB2	2.21	0.41
2:B:247:LEU:HD11	2:B:304:LEU:HD21	2.03	0.41
2:B:396:ILE:HA	2:B:422:MET:CB	2.51	0.41
2:B:566:VAL:HG23	2:B:574:ILE:HD12	2.02	0.41
2:B:1066:VAL:O	2:B:1066:VAL:CG1	2.67	0.41
13:M:67:LEU:CD1	13:M:68:SER:O	2.64	0.41
1:A:95:LYS:HA	1:A:95:LYS:HD3	1.74	0.41
1:A:445:ILE:HD11	1:A:587:ALA:HB1	2.03	0.41
1:A:1078:LYS:HB2	1:A:1078:LYS:HE3	1.82	0.41
1:A:1090:LEU:HD12	4:E:22:HIS:NE2	2.36	0.41
2:B:416:LEU:HD12	2:B:419:ILE:HD11	2.02	0.41
2:B:700:LEU:HA	2:B:735:TYR:HE1	1.85	0.41
2:B:821:TYR:HD2	2:B:844:LYS:HZ2	1.64	0.41
2:B:853:LYS:HG2	10:L:45:TYR:CE2	2.56	0.41
2:B:1065:SER:HB2	2:B:1117:ARG:NH2	2.36	0.41
2:B:1069:VAL:HG21	2:B:1134:VAL:CG2	2.50	0.41
3:C:218:ILE:HD12	3:C:220:LYS:HB3	2.03	0.41
3:C:245:VAL:O	3:C:246:GLU:HG3	2.21	0.41
1:A:26:LYS:HE3	1:A:301:PHE:CE2	2.55	0.41
1:A:61:LYS:HE3	1:A:61:LYS:HB2	1.86	0.41
1:A:85:LEU:HD22	1:A:391:TRP:NE1	2.33	0.41
1:A:441:ALA:HB2	2:B:1012:VAL:HG13	2.03	0.41
1:A:468:TYR:HB2	1:A:598:PHE:CE2	2.56	0.41
1:A:579:TYR:CE1	2:B:753:MET:HB2	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:644:ARG:HE	1:A:644:ARG:HB2	1.70	0.41
1:A:705:LEU:HD23	1:A:706:SER:N	2.36	0.41
1:A:981:LYS:HE3	1:A:981:LYS:HB3	1.90	0.41
1:A:1020:GLY:O	1:A:1021:GLU:HB2	2.20	0.41
1:A:1300:GLN:O	1:A:1315:TYR:HA	2.20	0.41
1:A:1602:SER:HB3	1:A:1608:ILE:HD11	2.02	0.41
2:B:215:VAL:HA	2:B:220:SER:O	2.20	0.41
2:B:364:ASP:OD1	2:B:606:LEU:HD22	2.21	0.41
2:B:408:SER:HA	2:B:411:MET:CB	2.38	0.41
2:B:820:GLN:O	2:B:823:ASP:HB2	2.21	0.41
2:B:1026:ILE:HG21	2:B:1031:VAL:HG11	2.02	0.41
3:C:89:VAL:HG22	3:C:214:CYS:SG	2.61	0.41
3:C:186:PRO:CG	3:C:189:THR:OG1	2.63	0.41
4:E:17:ILE:HG21	4:E:74:VAL:HG11	2.03	0.41
4:E:159:LEU:CD2	4:E:160:LEU:HD23	2.45	0.41
6:H:14:ASP:HB3	6:H:17:PRO:HG3	2.02	0.41
6:H:80:ASP:O	6:H:82:PRO:HD3	2.21	0.41
7:I:28:PRO:O	7:I:29:LEU:C	2.63	0.41
9:K:92:ALA:C	9:K:95:PRO:HD2	2.46	0.41
9:K:93:VAL:O	9:K:93:VAL:HG12	2.21	0.41
11:N:61:VAL:N	13:M:9:ALA:O	2.54	0.41
11:N:70:LYS:HE2	11:N:79:ARG:NH1	2.36	0.41
13:M:67:LEU:HD12	13:M:68:SER:N	2.36	0.41
13:M:68:SER:HB2	13:M:112:LEU:HB2	2.02	0.41
1:A:826:ALA:HB2	1:A:868:GLU:HG3	2.02	0.41
1:A:1267:PRO:HG2	1:A:1596:ASP:HB3	2.03	0.41
1:A:1583:ILE:HG23	1:A:1583:ILE:O	2.21	0.41
2:B:82:ILE:HD13	2:B:137:VAL:HG21	2.02	0.41
2:B:1019:ASP:O	2:B:1023:ASN:N	2.50	0.41
3:C:29:PHE:CE1	9:K:57:TYR:HE1	2.39	0.41
3:C:157:SER:O	3:C:161:GLU:HG3	2.21	0.41
6:H:125:LEU:HD12	6:H:125:LEU:HA	1.90	0.41
9:K:22:GLU:CG	9:K:25:THR:H	2.25	0.41
1:A:293:ASN:O	1:A:296:VAL:HG23	2.22	0.40
1:A:498:ILE:O	1:A:536:LYS:HG3	2.21	0.40
1:A:753:HIS:C	1:A:755:GLY:H	2.29	0.40
1:A:1289:CYS:SG	1:A:1549:HIS:O	2.80	0.40
1:A:1543:LEU:C	1:A:1543:LEU:HD23	2.46	0.40
1:A:1639:ARG:HE	4:E:199:THR:CG2	2.34	0.40
2:B:267:GLU:HA	2:B:270:LYS:HD3	2.02	0.40
2:B:1112:VAL:HG21	2:B:1116:PHE:CD2	2.56	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:29:LEU:H	7:I:41:CYS:HA	1.86	0.40
9:K:90:LEU:H	9:K:90:LEU:CD2	2.26	0.40
1:A:102:GLY:O	1:A:103:SER:OG	2.31	0.40
2:B:42:HIS:C	2:B:140:MET:HE1	2.47	0.40
2:B:146:CYS:O	2:B:149:ARG:NH1	2.47	0.40
2:B:333:CYS:SG	2:B:333:CYS:O	2.79	0.40
2:B:399:ALA:HB2	2:B:422:MET:SD	2.61	0.40
2:B:543:ASP:HB2	13:M:81:CYS:HB2	2.03	0.40
2:B:989:GLU:HG2	3:C:21:VAL:HG12	2.03	0.40
2:B:1026:ILE:HD12	2:B:1026:ILE:HA	1.97	0.40
3:C:40:TRP:HB2	9:K:61:LYS:HB3	2.02	0.40
4:E:10:LEU:HD21	4:E:58:LEU:HD11	2.02	0.40
4:E:169:GLN:O	4:E:169:GLN:HG2	2.21	0.40
6:H:143:LEU:O	6:H:143:LEU:HG	2.21	0.40
11:N:49:ALA:HB2	13:M:84:LEU:O	2.21	0.40
14:R:-6:C:H2'	14:R:-5:U:C6	2.57	0.40
1:A:677:LYS:HB3	6:H:91:VAL:H	1.86	0.40
1:A:714:LYS:HB3	1:A:714:LYS:HE3	1.84	0.40
1:A:1024:LEU:HB3	1:A:1029:THR:HG21	2.03	0.40
1:A:1281:LEU:CD2	1:A:1595:LEU:HD11	2.51	0.40
1:A:1357:LYS:NZ	1:A:1538:PHE:HE1	2.19	0.40
2:B:95:GLU:HA	2:B:95:GLU:OE1	2.21	0.40
2:B:648:GLU:C	2:B:650:GLU:H	2.28	0.40
2:B:1045:LEU:HD23	2:B:1054:LEU:HD13	2.04	0.40
3:C:45:PHE:CZ	9:K:106:VAL:HG13	2.56	0.40
4:E:156:VAL:O	4:E:160:LEU:HG	2.21	0.40
1:A:32:SER:HB2	1:A:80:HIS:CE1	2.57	0.40
1:A:305:PRO:HG3	2:B:1125:ALA:HB2	2.02	0.40
1:A:436:ARG:O	2:B:1062:SER:HB3	2.21	0.40
1:A:448:ASP:O	1:A:449:MET:CB	2.69	0.40
1:A:585:TYR:O	1:A:586:ASN:HB3	2.21	0.40
1:A:896:MET:O	1:A:896:MET:HG3	2.19	0.40
1:A:915:LEU:CD1	1:A:952:THR:HA	2.51	0.40
1:A:1497:ALA:C	1:A:1499:GLU:N	2.78	0.40
1:A:1557:LYS:O	1:A:1584:ASN:ND2	2.53	0.40
2:B:15:SER:O	2:B:723:ARG:NH2	2.55	0.40
2:B:46:PHE:CE1	2:B:50:VAL:HG11	2.56	0.40
2:B:410:SER:C	2:B:411:MET:HE2	2.46	0.40
2:B:1101:CYS:O	2:B:1101:CYS:SG	2.79	0.40
6:H:43:VAL:HG23	6:H:90:TYR:CE2	2.57	0.40
11:N:131:GLN:HB2	11:N:134:PRO:HB3	2.02	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:26:VAL:CG1	13:M:60:LEU:HD21	2.52	0.40
1:A:137:GLU:HG2	1:A:164:TYR:HH	1.86	0.40
1:A:473:THR:HB	1:A:474:PRO:CD	2.52	0.40
1:A:740:ARG:O	1:A:741:GLU:HB2	2.22	0.40
1:A:1034:PRO:O	1:A:1035:LYS:CB	2.69	0.40
1:A:1156:PHE:HE1	1:A:1198:LEU:CD2	2.35	0.40
1:A:1263:MET:HE2	1:A:1263:MET:HB2	1.97	0.40
2:B:166:MET:SD	2:B:166:MET:N	2.94	0.40
6:H:88:PHE:HA	6:H:146:LYS:HB2	2.03	0.40
13:M:28:PHE:HB2	13:M:31:GLY:O	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1455/1719 (85%)	1310 (90%)	138 (10%)	7 (0%)	24	54
2	B	1119/1135 (99%)	1019 (91%)	100 (9%)	0	100	100
3	C	335/346 (97%)	313 (93%)	22 (7%)	0	100	100
4	E	195/210 (93%)	185 (95%)	10 (5%)	0	100	100
5	F	74/127 (58%)	71 (96%)	3 (4%)	0	100	100
6	H	144/150 (96%)	130 (90%)	14 (10%)	0	100	100
7	I	58/126 (46%)	43 (74%)	13 (22%)	2 (3%)	3	12
8	J	62/67 (92%)	58 (94%)	4 (6%)	0	100	100
9	K	106/133 (80%)	96 (91%)	9 (8%)	1 (1%)	14	41
10	L	43/58 (74%)	37 (86%)	6 (14%)	0	100	100
11	N	149/510 (29%)	134 (90%)	13 (9%)	2 (1%)	9	32
12	G	153/338 (45%)	139 (91%)	13 (8%)	1 (1%)	18	48

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	M	108/419 (26%)	106 (98%)	1 (1%)	1 (1%)	14	41
All	All	4001/5338 (75%)	3641 (91%)	346 (9%)	14 (0%)	37	65

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	214	VAL
1	A	1605	ILE
11	N	156	PRO
13	M	37	GLY
12	G	102	LEU
7	I	19	PHE
11	N	132	PRO
1	A	677	LYS
1	A	719	GLU
7	I	18	ASP
1	A	22	ALA
1	A	206	PRO
9	K	24	LYS
1	A	311	PRO

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	1295/1503 (86%)	1220 (94%)	75 (6%)	18	49
2	B	982/992 (99%)	907 (92%)	75 (8%)	12	36
3	C	296/302 (98%)	274 (93%)	22 (7%)	13	38
4	E	183/192 (95%)	180 (98%)	3 (2%)	55	83
5	F	66/111 (60%)	66 (100%)	0	100	100
6	H	129/131 (98%)	125 (97%)	4 (3%)	35	69
7	I	53/111 (48%)	51 (96%)	2 (4%)	29	64
8	J	53/56 (95%)	50 (94%)	3 (6%)	18	49

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	K	96/119 (81%)	94 (98%)	2 (2%)	47	77
10	L	42/55 (76%)	41 (98%)	1 (2%)	43	75
11	N	119/427 (28%)	113 (95%)	6 (5%)	22	53
12	G	135/288 (47%)	130 (96%)	5 (4%)	30	64
13	M	94/366 (26%)	88 (94%)	6 (6%)	16	44
All	All	3543/4653 (76%)	3339 (94%)	204 (6%)	20	49

All (204) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	ILE
1	A	16	SER
1	A	19	MET
1	A	65	SER
1	A	82	GLU
1	A	83	LEU
1	A	85	LEU
1	A	86	THR
1	A	200	MET
1	A	204	ARG
1	A	206	PRO
1	A	209	LYS
1	A	292	PHE
1	A	295	SER
1	A	296	VAL
1	A	303	VAL
1	A	304	VAL
1	A	312	VAL
1	A	315	LEU
1	A	318	GLN
1	A	319	MET
1	A	341	LEU
1	A	348	GLU
1	A	381	GLN
1	A	383	LEU
1	A	408	LYS
1	A	409	LEU
1	A	410	MET
1	A	412	ASP
1	A	453	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	454	ASN
1	A	484	VAL
1	A	535	THR
1	A	550	LEU
1	A	553	GLN
1	A	555	THR
1	A	557	HIS
1	A	561	ILE
1	A	635	MET
1	A	676	LEU
1	A	680	PRO
1	A	701	ILE
1	A	718	LYS
1	A	833	LEU
1	A	878	LYS
1	A	885	LEU
1	A	888	GLN
1	A	891	GLU
1	A	1045	GLU
1	A	1046	VAL
1	A	1051	GLN
1	A	1055	GLU
1	A	1057	LEU
1	A	1145	PRO
1	A	1184	LYS
1	A	1186	GLU
1	A	1260	LYS
1	A	1263	MET
1	A	1266	VAL
1	A	1268	VAL
1	A	1269	LEU
1	A	1272	LYS
1	A	1288	VAL
1	A	1313	GLN
1	A	1316	GLN
1	A	1317	LEU
1	A	1340	ARG
1	A	1505	VAL
1	A	1507	GLU
1	A	1508	ILE
1	A	1509	HIS
1	A	1556	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1603	ASN
1	A	1606	HIS
1	A	1677	SER
2	B	26	ILE
2	B	29	GLU
2	B	31	GLN
2	B	32	LYS
2	B	35	LEU
2	B	71	GLU
2	B	73	ILE
2	B	74	SER
2	B	76	THR
2	B	111	ARG
2	B	144	LYS
2	B	222	VAL
2	B	224	MET
2	B	226	LEU
2	B	229	LEU
2	B	231	ASN
2	B	235	MET
2	B	249	LEU
2	B	260	SER
2	B	267	GLU
2	B	273	GLU
2	B	274	ASP
2	B	276	SER
2	B	278	LEU
2	B	289	VAL
2	B	290	MET
2	B	292	GLU
2	B	307	CYS
2	B	314	VAL
2	B	318	TYR
2	B	321	GLU
2	B	325	GLU
2	B	327	LEU
2	B	330	GLN
2	B	332	ILE
2	B	334	ILE
2	B	337	LYS
2	B	338	SER
2	B	345	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	348	LEU
2	B	353	LEU
2	B	361	CYS
2	B	365	ASN
2	B	429	PRO
2	B	430	PHE
2	B	454	CYS
2	B	461	ASN
2	B	463	ILE
2	B	466	LEU
2	B	506	GLU
2	B	537	LEU
2	B	542	ILE
2	B	547	HIS
2	B	582	LYS
2	B	601	THR
2	B	659	GLN
2	B	666	LEU
2	B	667	LEU
2	B	678	ASP
2	B	680	ASN
2	B	728	ASP
2	B	755	ASP
2	B	792	LEU
2	B	793	VAL
2	B	797	LYS
2	B	828	TYR
2	B	859	THR
2	B	864	PHE
2	B	866	CYS
2	B	1011	GLN
2	B	1012	VAL
2	B	1015	THR
2	B	1077	LEU
2	B	1081	LEU
2	B	1106	THR
3	C	21	VAL
3	C	55	HIS
3	C	58	GLU
3	C	94	VAL
3	C	96	ASN
3	C	114	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	121	LEU
3	C	133	THR
3	C	134	GLU
3	C	135	ILE
3	C	136	ASP
3	C	137	THR
3	C	138	LEU
3	C	144	VAL
3	C	151	HIS
3	C	161	GLU
3	C	166	HIS
3	C	196	ASP
3	C	266	GLU
3	C	267	VAL
3	C	274	ARG
3	C	275	VAL
4	E	31	ASP
4	E	107	GLN
4	E	185	ILE
6	H	15	ILE
6	H	80	ASP
6	H	83	SER
6	H	89	GLU
7	I	27	LEU
7	I	29	LEU
8	J	5	VAL
8	J	9	THR
8	J	28	GLU
9	K	27	LEU
9	K	30	VAL
10	L	52	LEU
11	N	25	SER
11	N	60	HIS
11	N	116	ARG
11	N	118	LEU
11	N	130	LEU
11	N	133	ILE
12	G	95	ASN
12	G	97	LYS
12	G	98	VAL
12	G	102	LEU
12	G	169	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	M	33	LEU
13	M	35	SER
13	M	67	LEU
13	M	81	CYS
13	M	110	GLN
13	M	112	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (99) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	HIS
1	A	89	ASN
1	A	108	HIS
1	A	133	GLN
1	A	163	GLN
1	A	170	GLN
1	A	324	GLN
1	A	347	GLN
1	A	395	GLN
1	A	397	HIS
1	A	478	GLN
1	A	482	GLN
1	A	486	ASN
1	A	499	ASN
1	A	564	HIS
1	A	578	HIS
1	A	595	ASN
1	A	597	HIS
1	A	600	GLN
1	A	616	GLN
1	A	617	GLN
1	A	632	GLN
1	A	652	HIS
1	A	728	ASN
1	A	753	HIS
1	A	790	GLN
1	A	832	ASN
1	A	847	GLN
1	A	850	HIS
1	A	859	ASN
1	A	918	GLN
1	A	989	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1051	GLN
1	A	1068	HIS
1	A	1076	GLN
1	A	1094	GLN
1	A	1109	ASN
1	A	1111	ASN
1	A	1118	GLN
1	A	1136	GLN
1	A	1177	GLN
1	A	1295	GLN
1	A	1300	GLN
1	A	1313	GLN
1	A	1565	ASN
1	A	1579	ASN
1	A	1603	ASN
1	A	1683	GLN
1	A	1690	HIS
1	A	1717	GLN
2	B	9	ASN
2	B	18	HIS
2	B	30	GLN
2	B	31	GLN
2	B	36	GLN
2	B	97	ASN
2	B	147	ASN
2	B	150	ASN
2	B	219	HIS
2	B	223	ASN
2	B	237	ASN
2	B	313	ASN
2	B	371	ASN
2	B	473	HIS
2	B	501	HIS
2	B	523	GLN
2	B	547	HIS
2	B	672	ASN
2	B	690	GLN
2	B	694	GLN
2	B	709	ASN
2	B	846	ASN
2	B	887	HIS
2	B	889	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	1068	HIS
3	C	48	ASN
3	C	102	GLN
3	C	116	HIS
3	C	127	GLN
3	C	166	HIS
3	C	180	ASN
3	C	181	GLN
3	C	222	HIS
3	C	277	ASN
3	C	290	ASN
3	C	305	HIS
4	E	132	GLN
4	E	133	GLN
4	E	169	GLN
6	H	126	GLN
7	I	8	ASN
7	I	33	GLN
8	J	61	ASN
9	K	85	GLN
11	N	67	GLN
11	N	88	GLN
13	M	34	GLN
13	M	98	GLN
13	M	110	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
14	R	7/8 (87%)	1 (14%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
14	R	-5	U

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 6 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
19	2TM	A	2004	-	26,30,30	0.82	2 (7%)	39,47,47	0.70	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
19	2TM	A	2004	-	-	3/19/38/38	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	2004	2TM	PA-O2A	-2.46	1.50	1.56
19	A	2004	2TM	PB-O1B	-2.34	1.50	1.56

There are no bond angle outliers.

There are no chirality outliers.

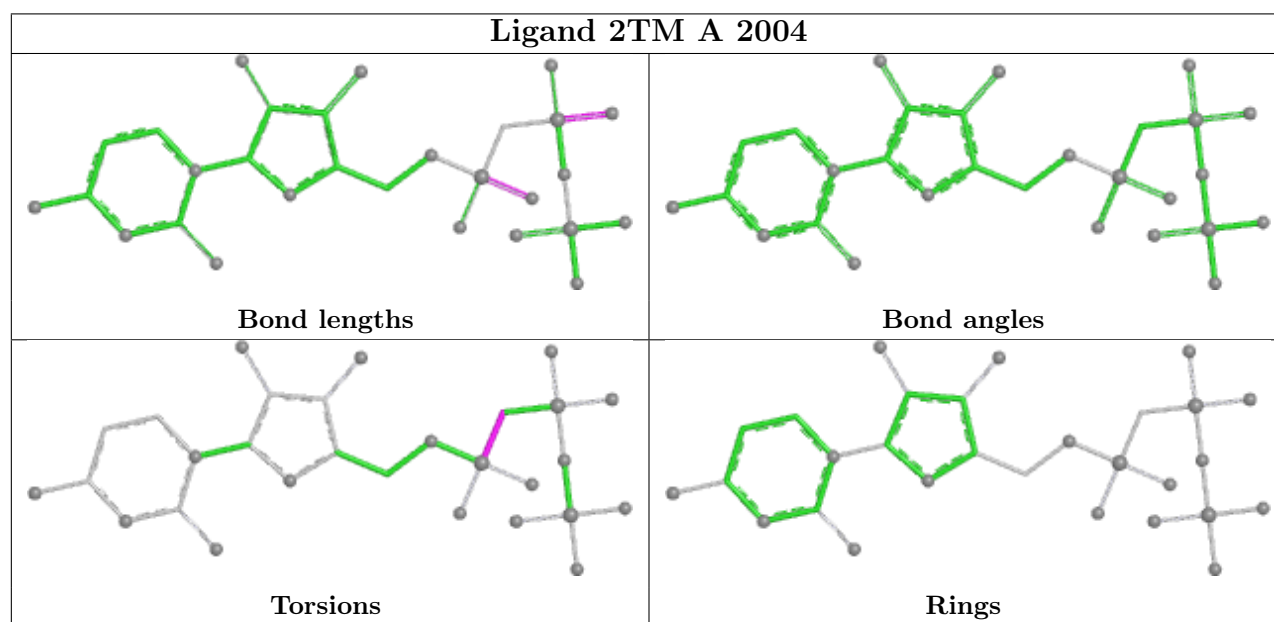
All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	A	2004	2TM	PB-C1-PA-O5'
19	A	2004	2TM	PB-C1-PA-O1A
19	A	2004	2TM	PB-C1-PA-O2A

There are no ring outliers.

No monomer is involved in short contacts.

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

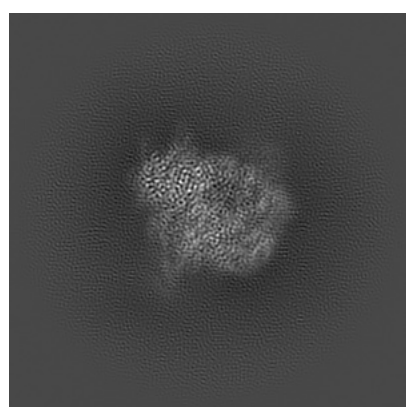
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31876. These allow visual inspection of the internal detail of the map and identification of artifacts.

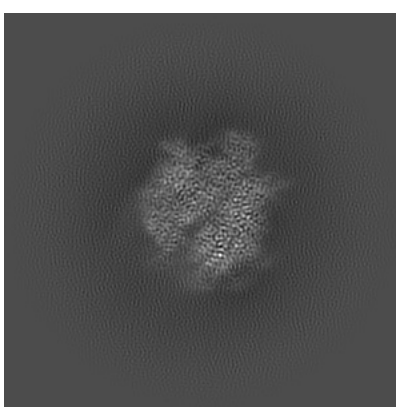
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

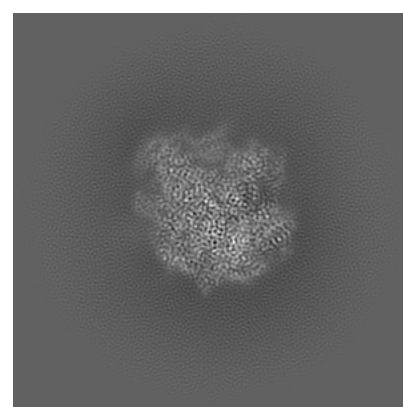
6.1.1 Primary map



X



Y

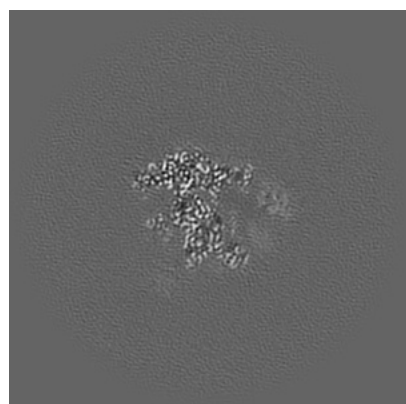


Z

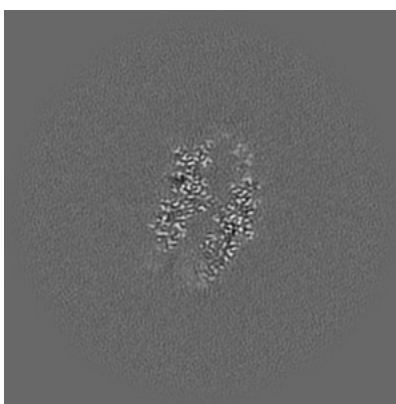
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

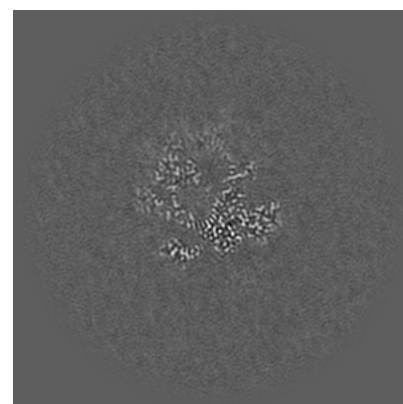
6.2.1 Primary map



X Index: 160



Y Index: 160

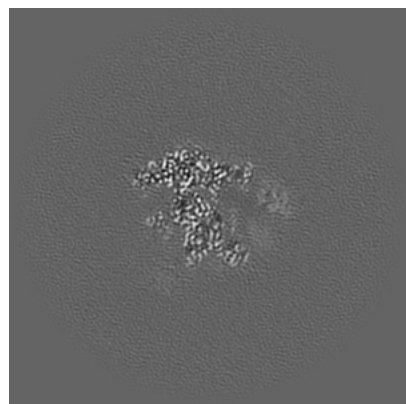


Z Index: 160

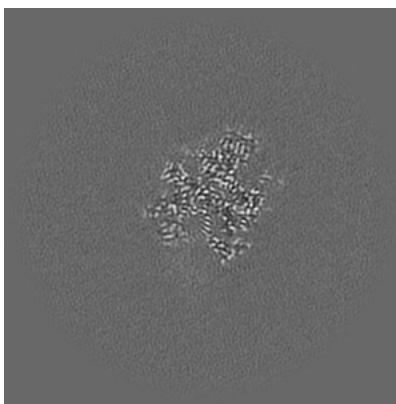
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

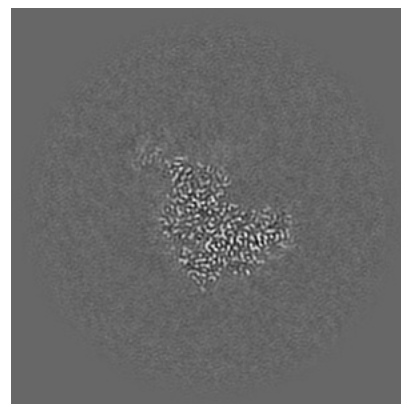
6.3.1 Primary map



X Index: 160



Y Index: 146

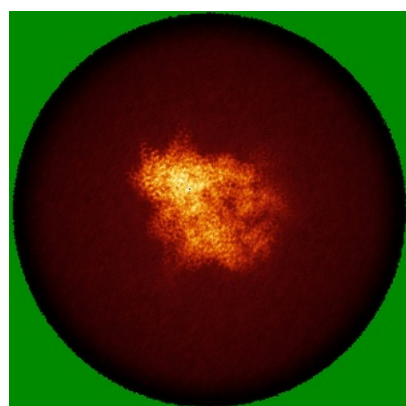


Z Index: 184

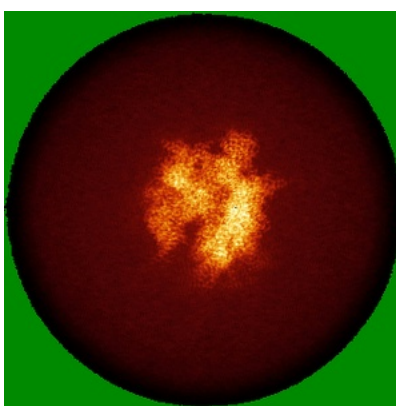
The images above show the largest variance slices of the map in three orthogonal directions.

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

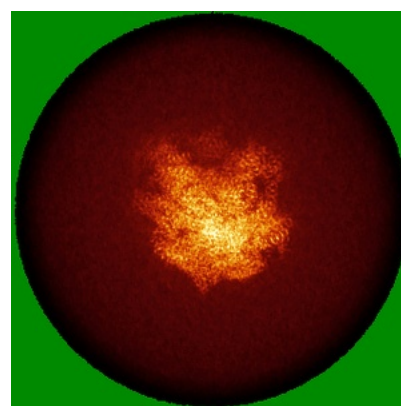
6.4.1 Primary map



X



Y

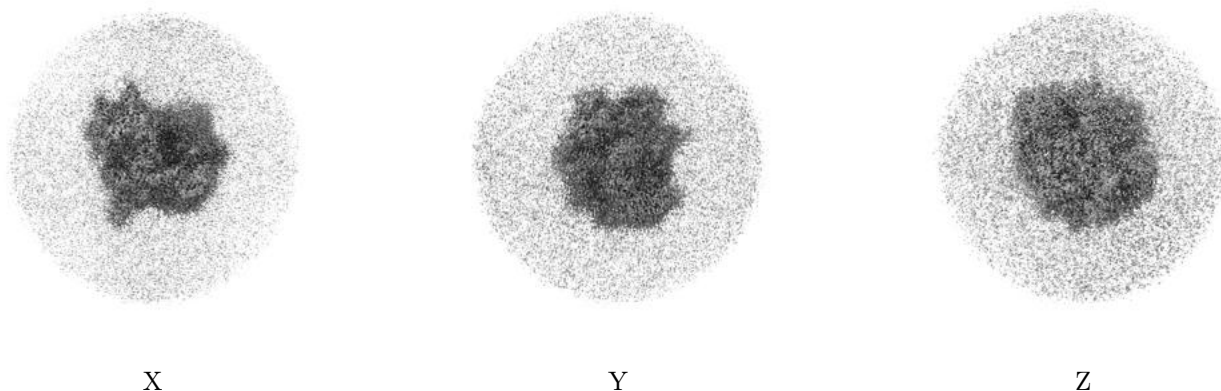


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.351. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

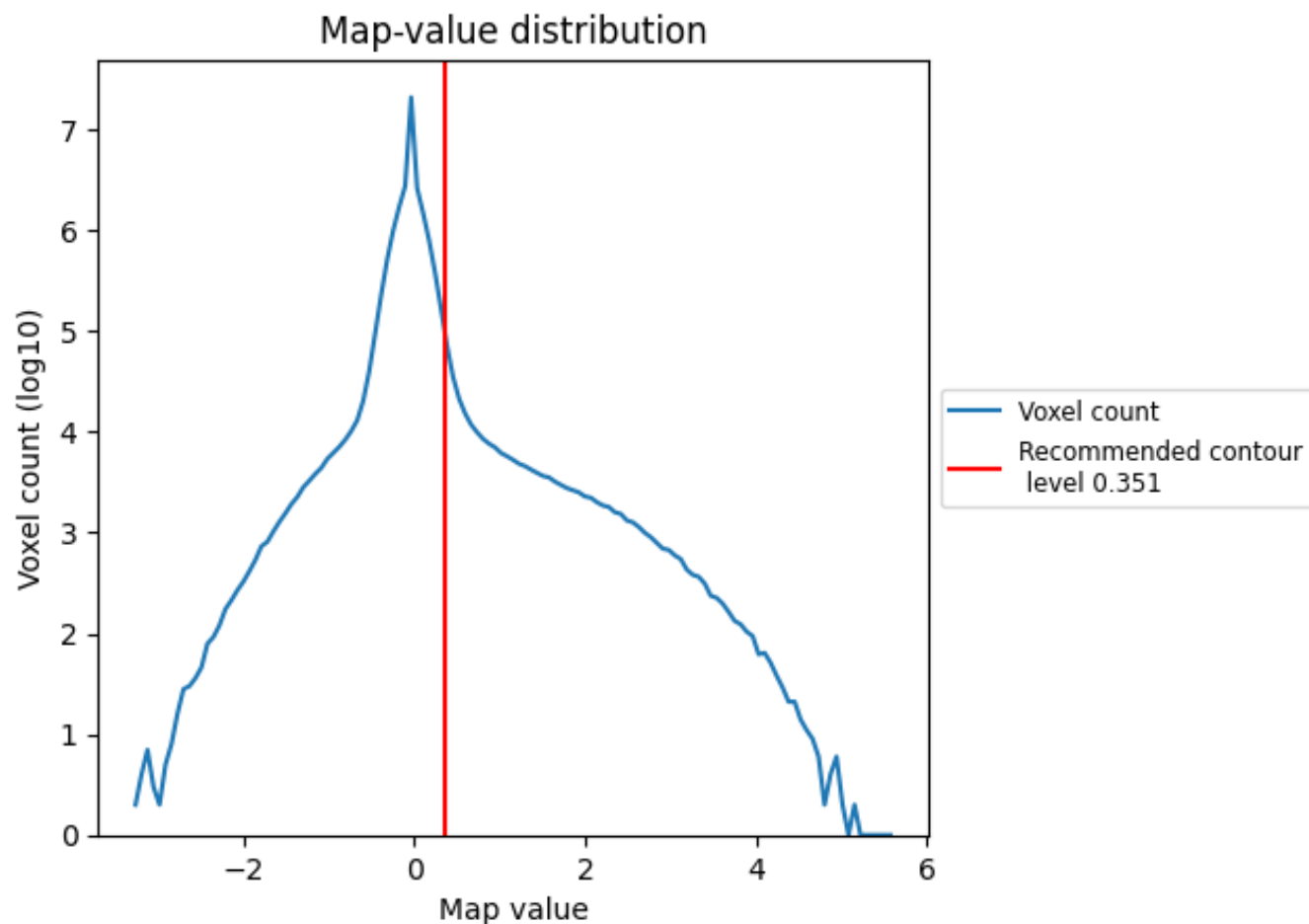
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

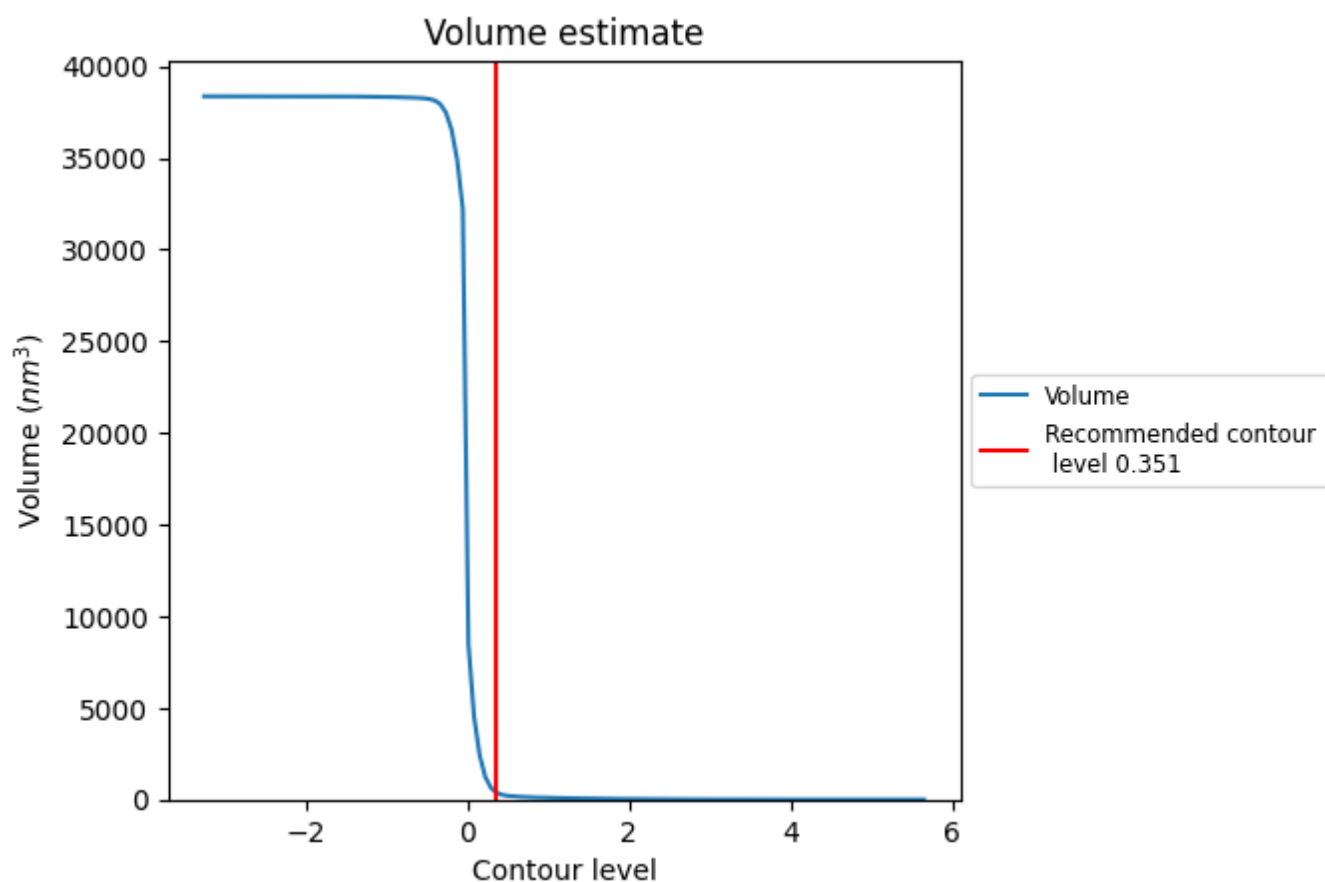
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

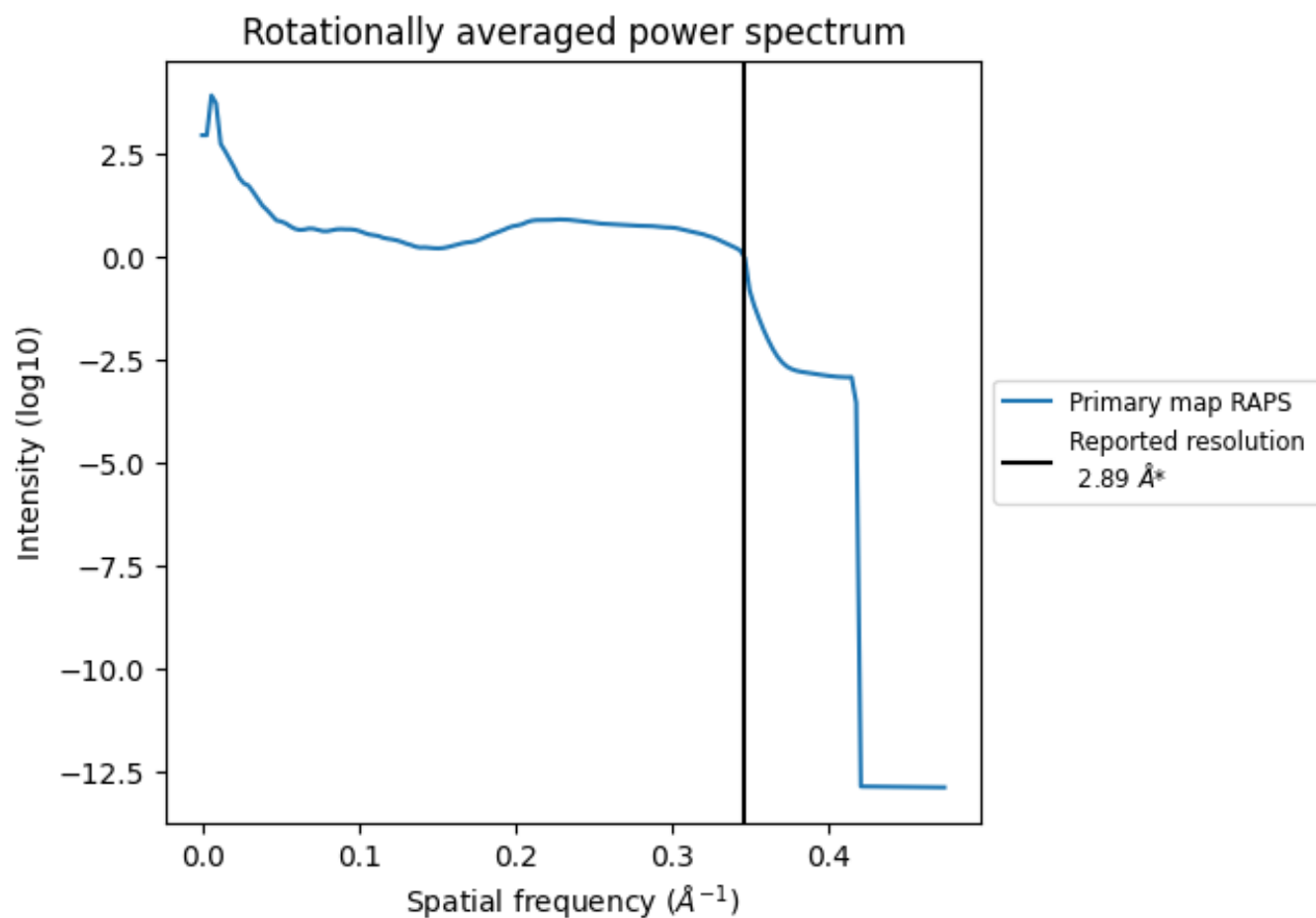
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 392 nm³; this corresponds to an approximate mass of 354 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 0.346 Å⁻¹

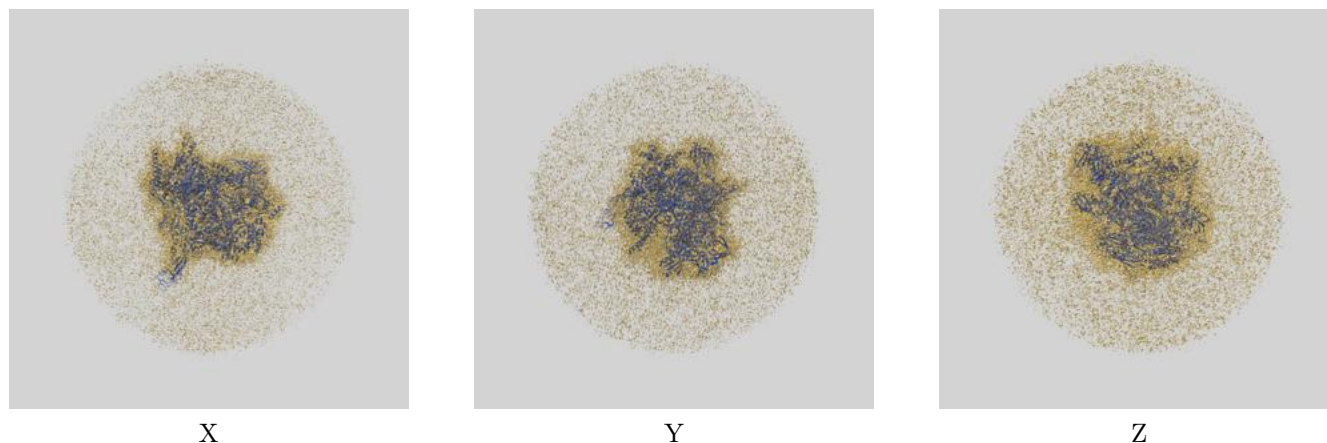
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

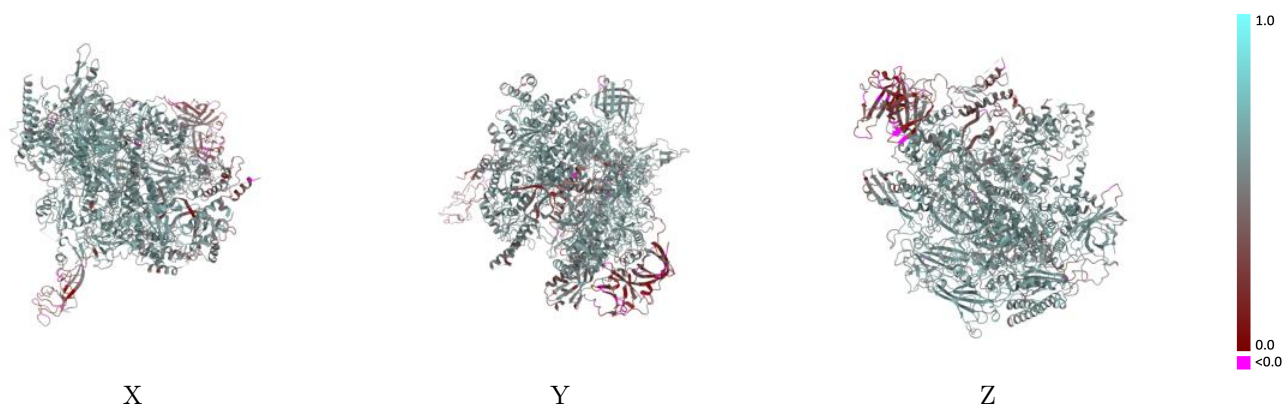
This section contains information regarding the fit between EMDB map EMD-31876 and PDB model 7VBA. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

9.1 Map-model overlay [i](#)



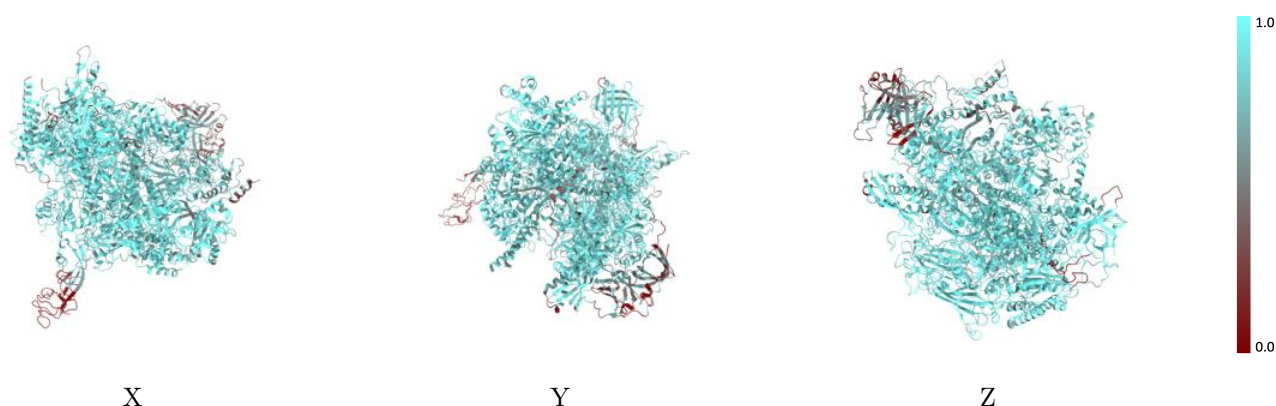
The images above show the 3D surface view of the map at the recommended contour level 0.351 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



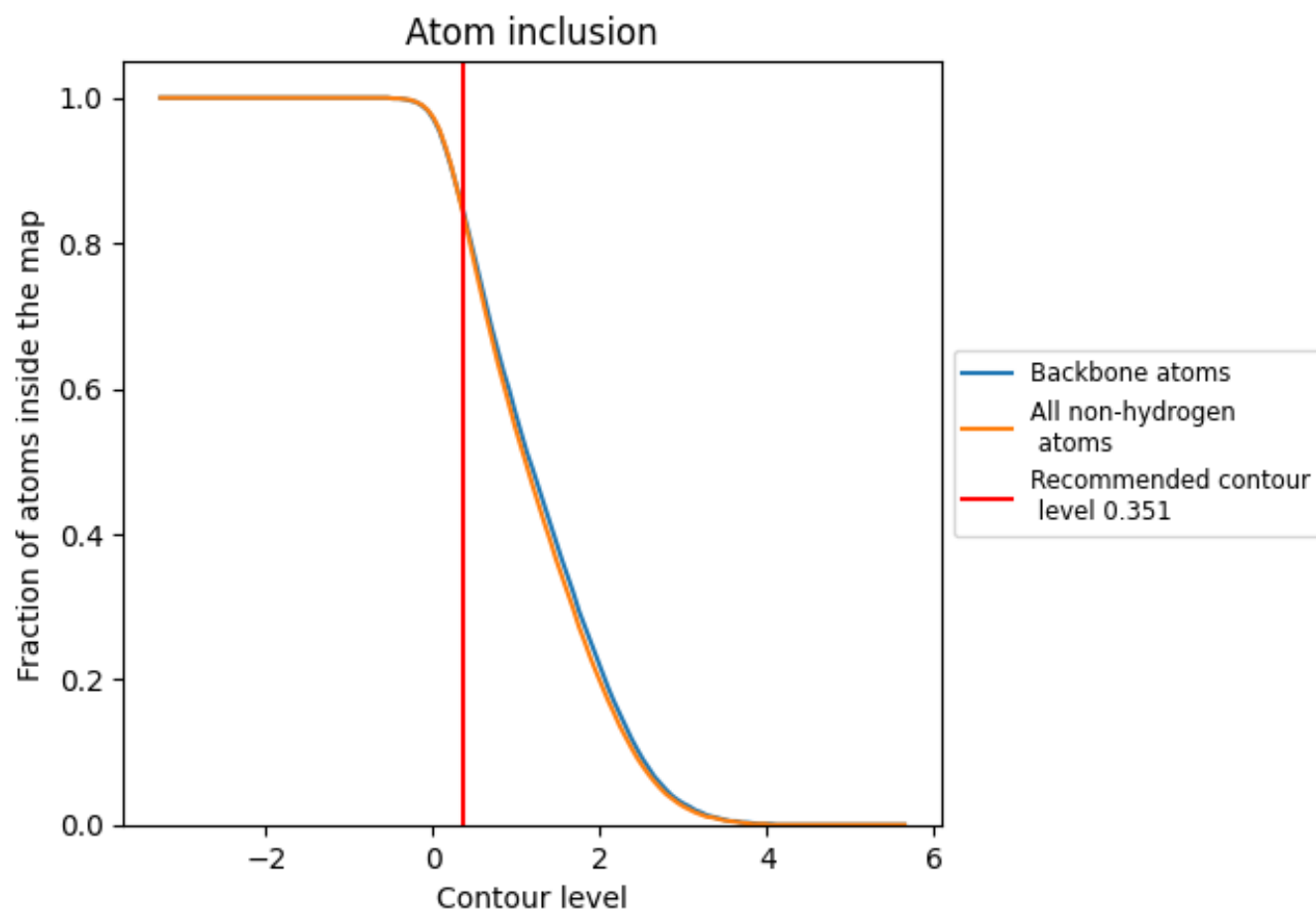
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.351).

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 85% 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 (0.351) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8460	 0.5250
A	 0.8910	 0.5470
B	 0.9240	 0.5720
C	 0.8410	 0.5430
E	 0.9060	 0.5570
F	 0.9360	 0.5820
G	 0.3230	 0.3130
H	 0.8740	 0.5410
I	 0.6300	 0.3680
J	 0.9500	 0.6030
K	 0.8840	 0.5490
L	 0.9150	 0.5540
M	 0.5340	 0.2580
N	 0.4430	 0.2390
R	 0.9170	 0.5640
T	 0.8600	 0.4980
U	 0.7560	 0.3880

