



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 07:16 PM UTC

PDB ID : 8W7M / pdb_00008w7m
EMDB ID : EMD-37343
Title : Yeast replisome in state V
Authors : Dang, S.; Zhai, Y.; Feng, J.; Yu, D.; Xu, Z.
Deposited on : 2023-08-30
Resolution : 4.12 Å(reported)
Based on initial model : 6SKL

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

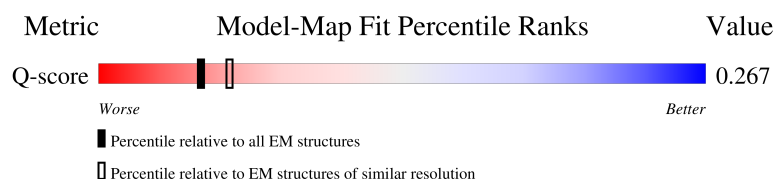
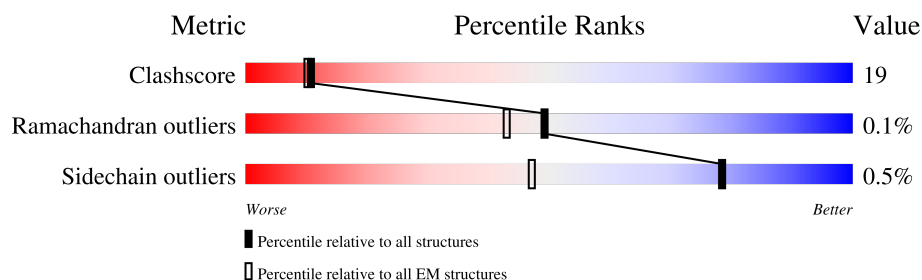
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance i

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

The reported resolution of this entry is 4.12 Å.

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



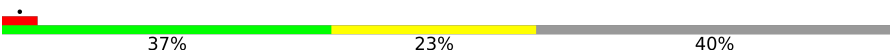
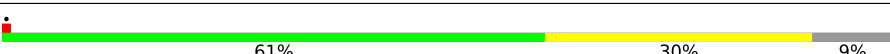
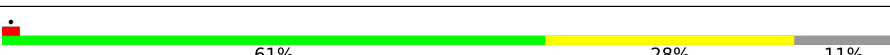
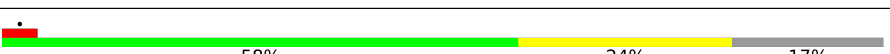
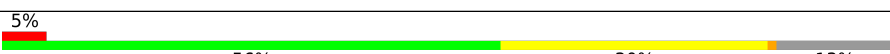
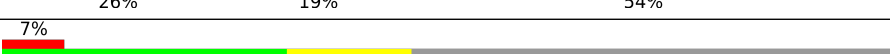
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	5662 (3.62 - 4.62)

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	2	868	6% 45% 28% 28%
2	3	971	38% 26% 36%
3	4	933	7% 39% 28% 33%
4	5	775	44% 25% 32%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	6	1017	
6	7	845	
7	A	208	
8	B	213	
9	C	194	
10	D	294	
11	E	650	
12	F	927	
12	G	927	
12	H	927	
13	I	71	
14	N	689	

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 51196 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called DNA replication licensing factor MCM2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	627	Total	C	N	O	S	0	0
			4955	3124	885	928	18		

- Molecule 2 is a protein called DNA replication licensing factor MCM3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	3	619	Total	C	N	O	S	0	0
			4835	3046	860	916	13		

- Molecule 3 is a protein called DNA replication licensing factor MCM4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	4	623	Total	C	N	O	S	0	0
			4947	3118	852	948	29		

- Molecule 4 is a protein called Minichromosome maintenance protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	5	529	Total	C	N	O	S	0	0
			4176	2644	714	796	22		

- Molecule 5 is a protein called DNA replication licensing factor MCM6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	6	613	Total	C	N	O	S	0	0
			4837	3051	839	923	24		

- Molecule 6 is a protein called DNA replication licensing factor MCM7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	7	657	Total	C	N	O	S	0	0
			5124	3238	888	970	28		

- Molecule 7 is a protein called DNA replication complex GINS protein PSF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A	196	Total	C	N	O	S	0	0
			1602	1006	276	311	9		

- Molecule 8 is a protein called DNA replication complex GINS protein PSF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	B	193	Total	C	N	O	S	0	0
			1617	1039	286	287	5		

- Molecule 9 is a protein called DNA replication complex GINS protein PSF3.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	C	172	Total	C	N	O	S	0	0
			1387	904	223	253	7		

- Molecule 10 is a protein called DNA replication complex GINS protein SLD5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	D	243	Total	C	N	O	S	0	0
			2004	1276	327	389	12		

- Molecule 11 is a protein called Cell division control protein 45.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	E	568	Total	C	N	O	S	0	0
			4591	2930	774	873	14		

- Molecule 12 is a protein called DNA polymerase alpha-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	F	424	Total	C	N	O	S	0	0
			3404	2188	564	637	15		
12	G	422	Total	C	N	O	S	0	0
			3380	2172	557	636	15		
12	H	425	Total	C	N	O	S	0	0
			3411	2193	565	638	15		

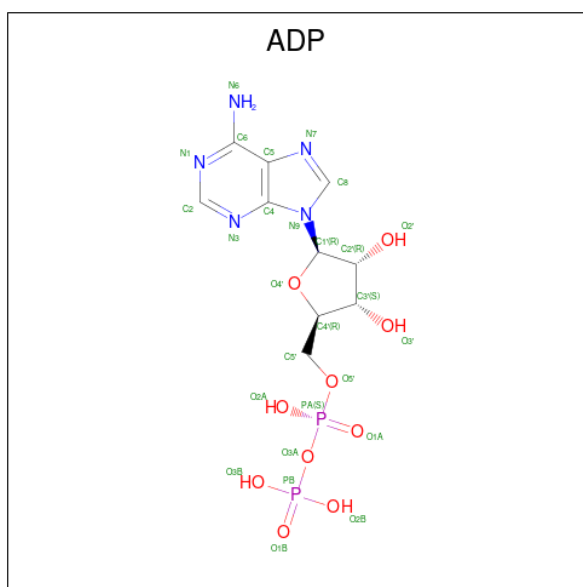
- Molecule 13 is a DNA chain called DNA (71-mer).

Mol	Chain	Residues	Atoms					AltConf	Trace
13	I	8	Total	C	N	O	P	0	0
			160	80	16	56	8		

- Molecule 14 is a protein called DNA polymerase epsilon subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	83	Total	C	N	O	S	0	0
			641	410	111	119	1		

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



Mol	Chain	Residues	Atoms					AltConf
15	2	1	Total	C	N	O	P	0
			27	10	5	10	2	
15	3	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
16	2	1	Total	Mg	0
			1	1	
16	3	1	Total	Mg	0
			1	1	

Continued on next page...

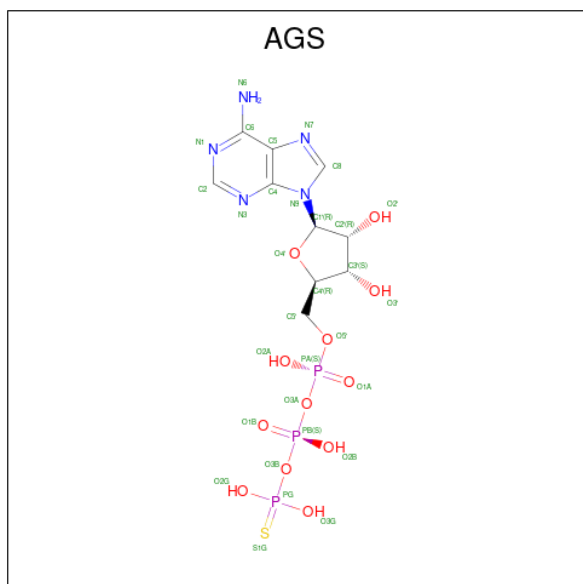
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
16	4	1	Total	Mg	0
			1	1	
16	7	1	Total	Mg	0
			1	1	

- Molecule 17 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
17	2	1	Total	Zn	0
			1	1	
17	4	1	Total	Zn	0
			1	1	
17	5	1	Total	Zn	0
			1	1	
17	6	1	Total	Zn	0
			1	1	
17	7	1	Total	Zn	0
			1	1	

- Molecule 18 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S) (labeled as "Ligand of Interest" by depositor).



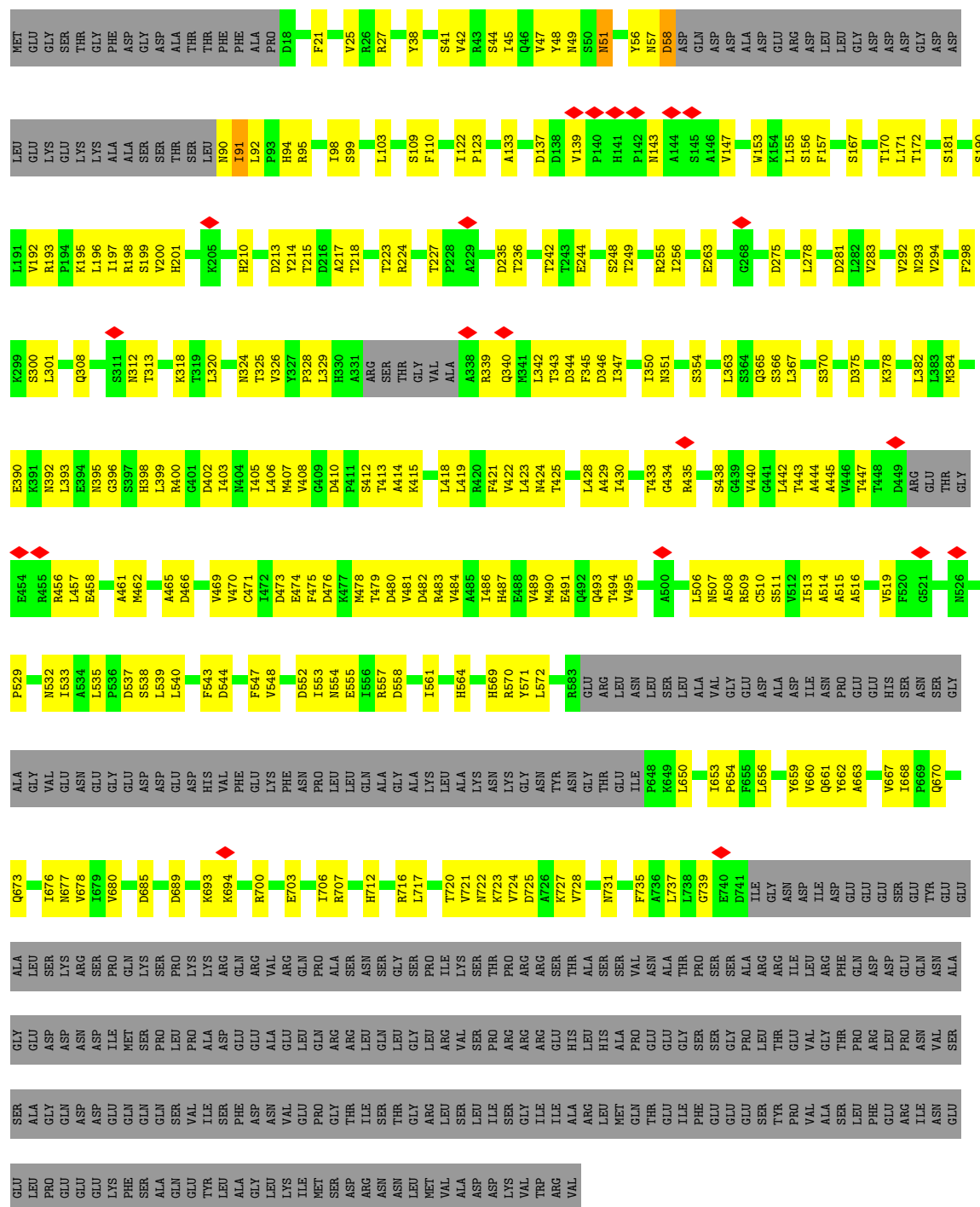
Continued from previous page...

Mol	Chain	Residues	Atoms						AltConf
			Total	C	N	O	P	S	
18	7	1	31	10	5	12	3	1	0

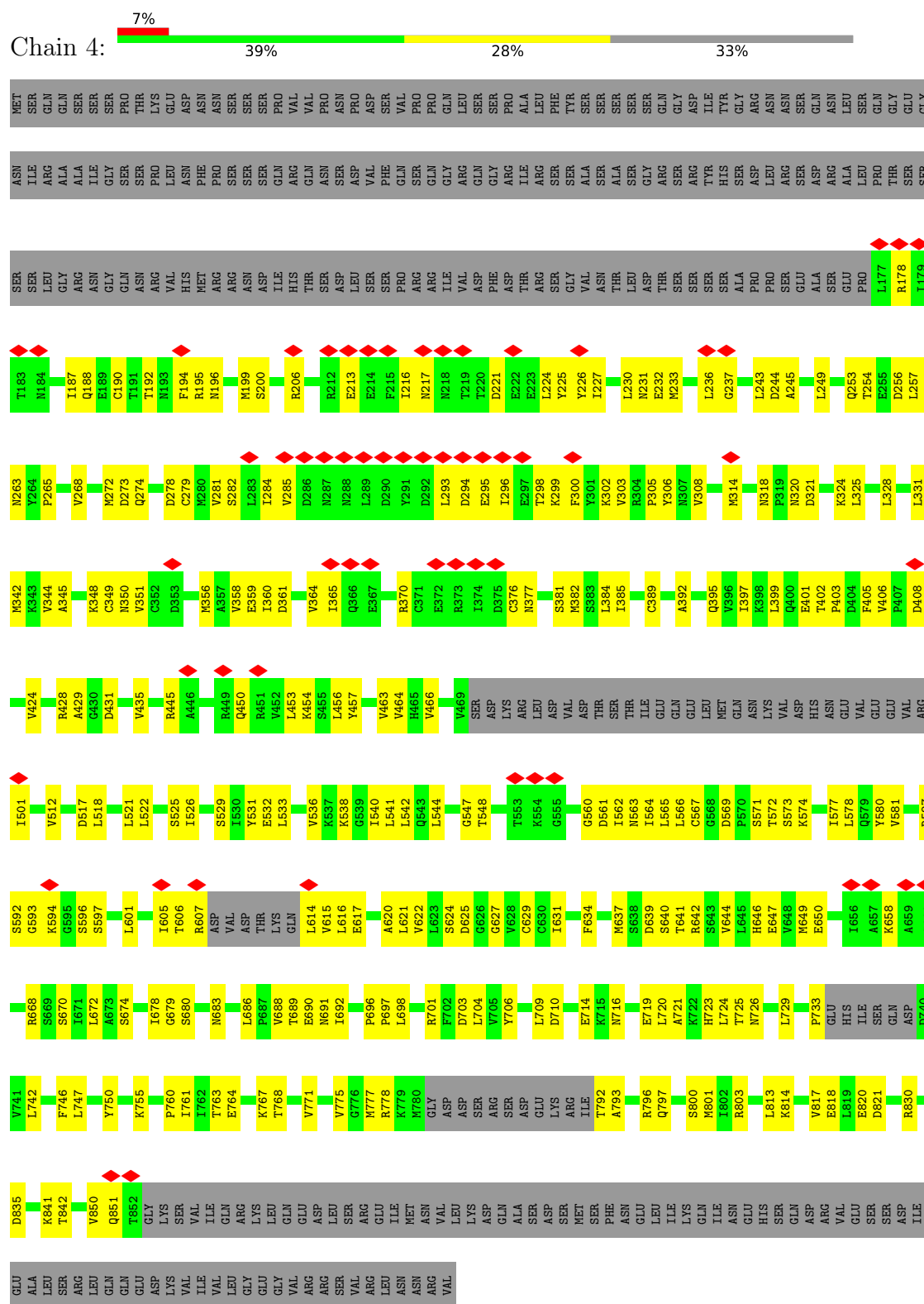


• Molecule 2: DNA replication licensing factor MCM3

Chain 3: 38% 26% 36%

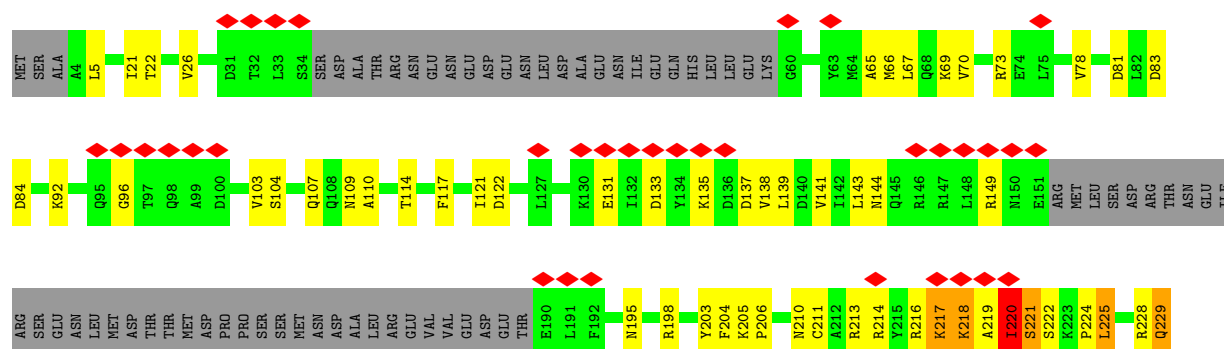
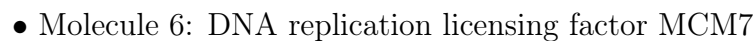


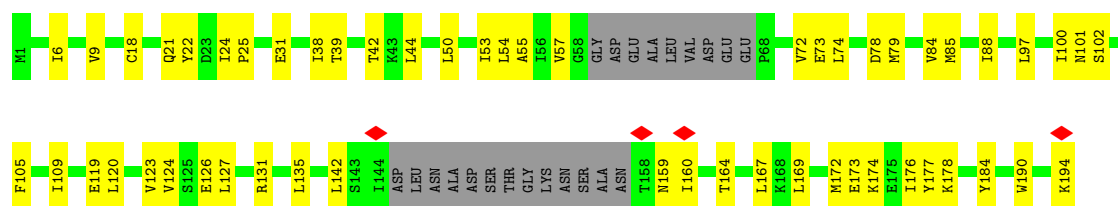
• Molecule 3: DNA replication licensing factor MCM4



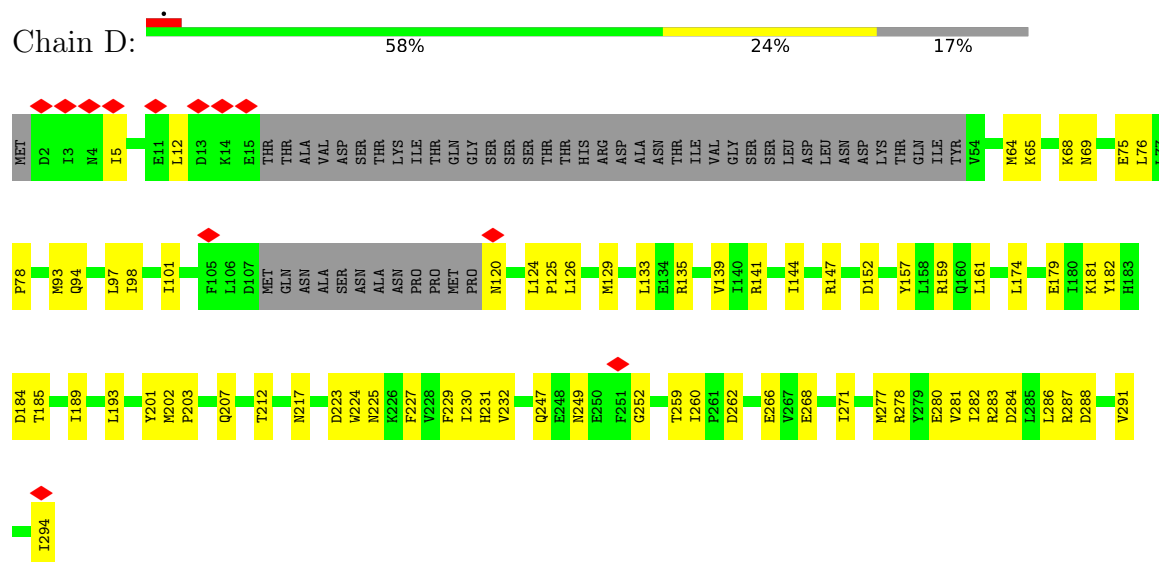
• Molecule 4: Minichromosome maintenance protein 5



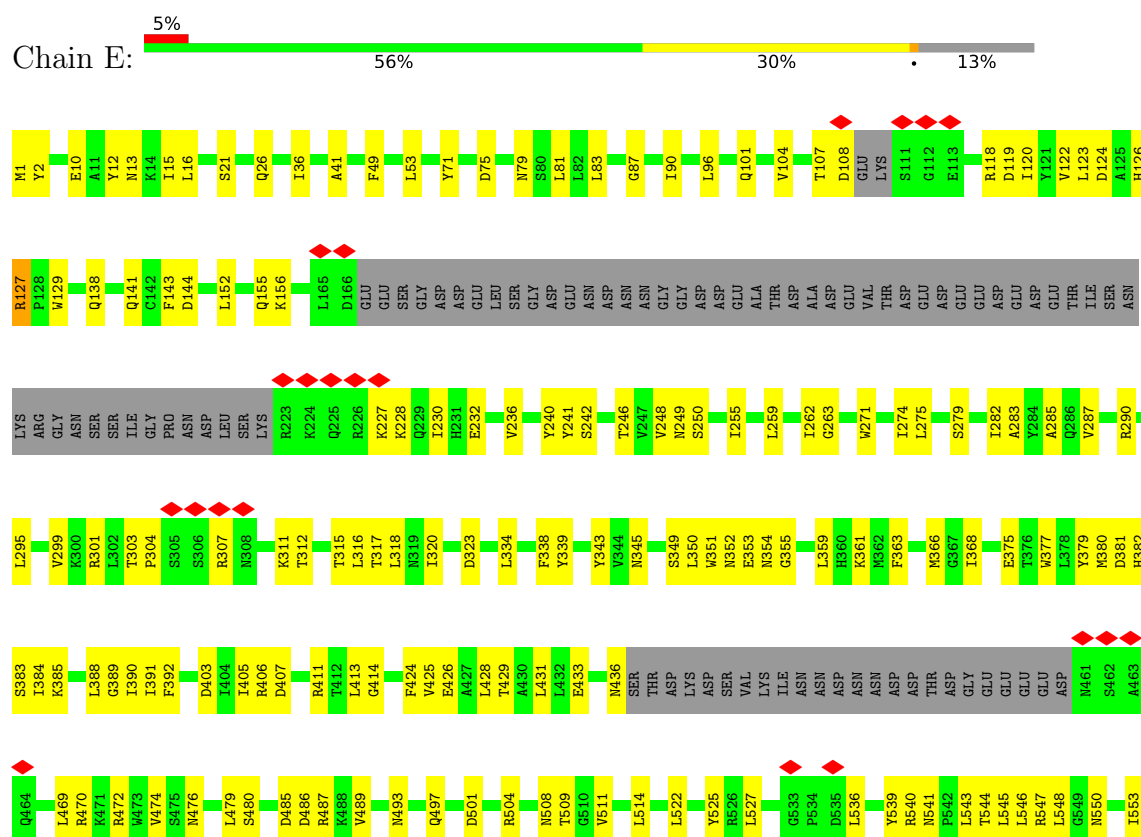


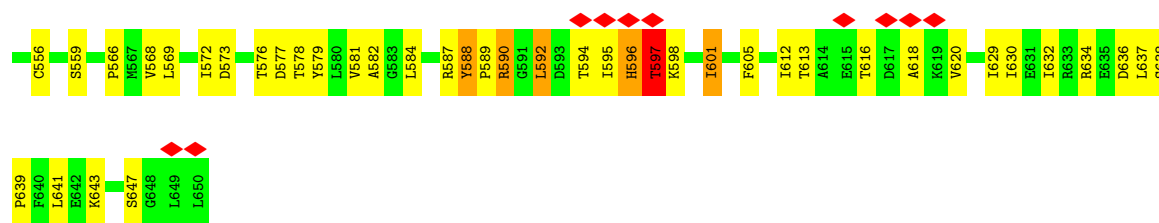


• Molecule 10: DNA replication complex GINS protein SLD5

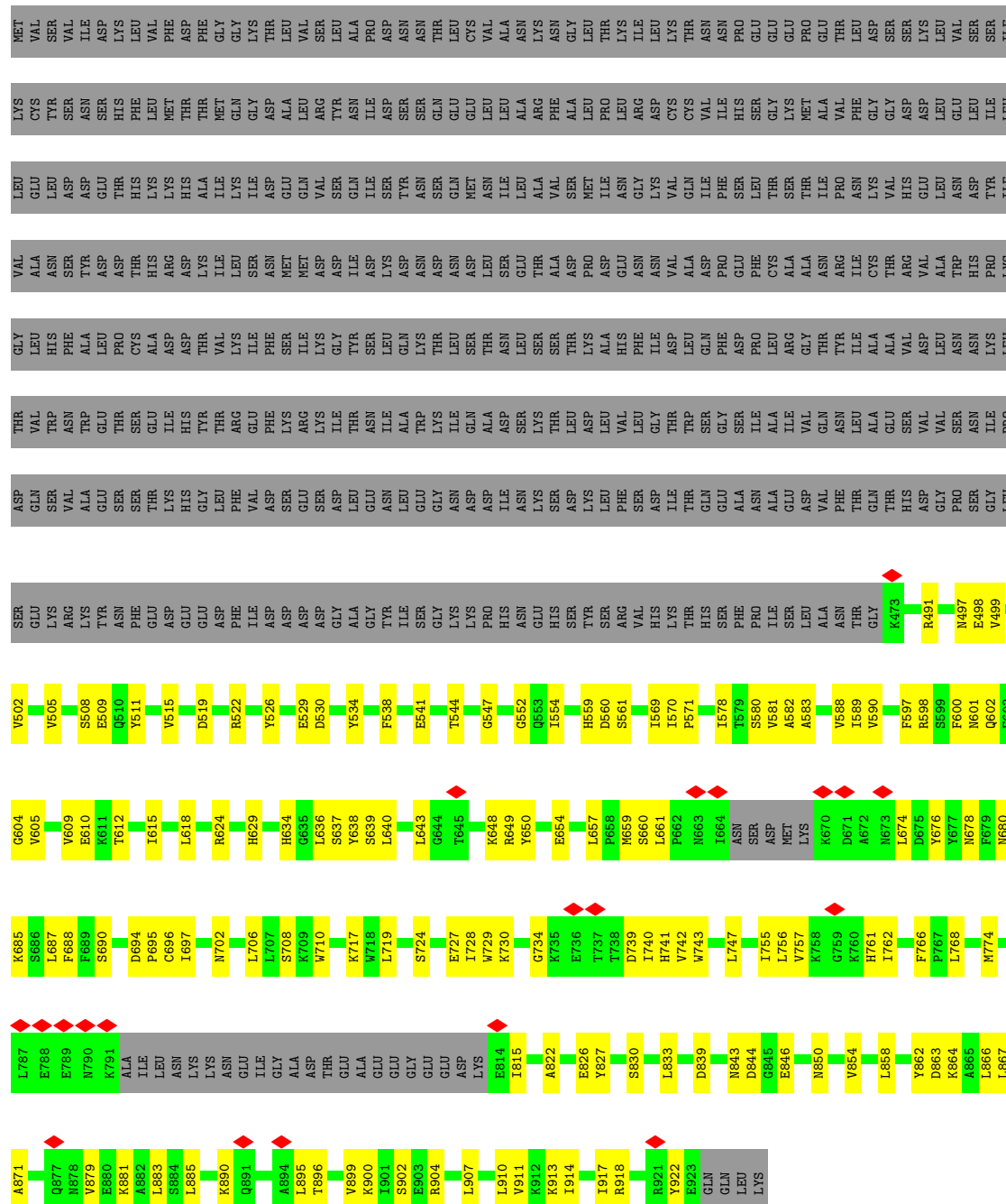
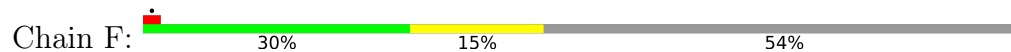


• Molecule 11: Cell division control protein 45

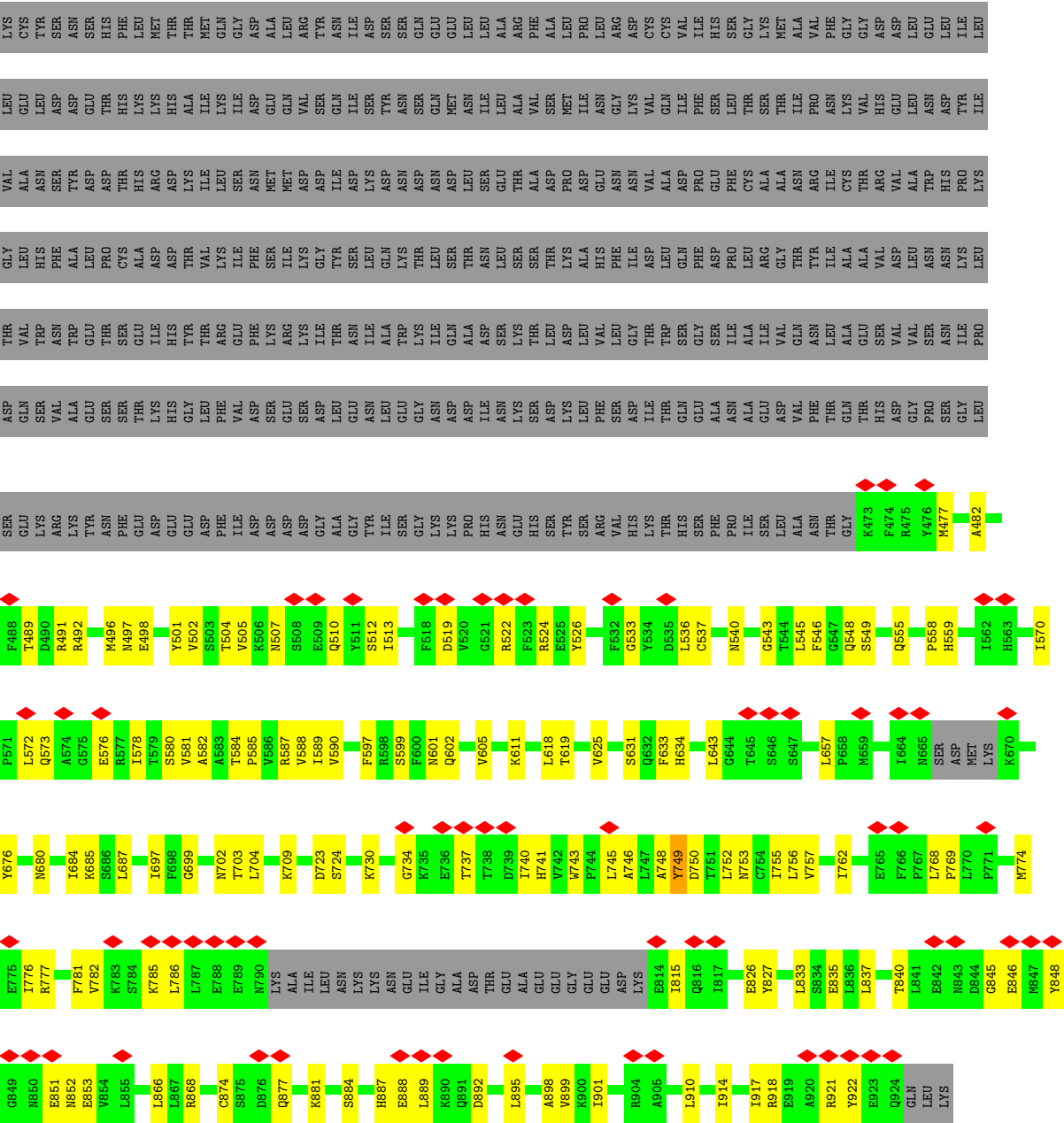




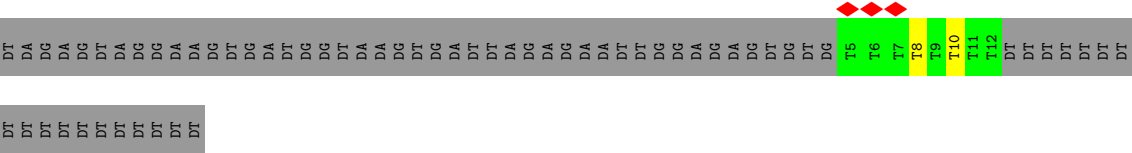
• Molecule 12: DNA polymerase alpha-binding protein



• Molecule 12: DNA polymerase alpha-binding protein



• Molecule 13: DNA (71-mer)



• Molecule 14: DNA polymerase epsilon subunit B



PRO	GLY	SER	PHE	THR	ILE	LYS	ILE	MET	LEU	ASN	PRO	PHE	ASN	K61
GLY	SER	PHE	THR	ILE	THR	VAL	PHE	ILE	GLN	LEU	SER	SER	ASN	F62
THR	ILE	THR	THR	ASP	ASP	LYS	ARG	ASP	LEU	LEU	ASP	ASP	ASN	L63
HIS	ILE	THR	LEU	LEU	LEU	ILE	LEU	PRO	ASN	GLY	MET	HIS	LYS	E64
ASN	ASN	ASN	SER	SER	ASP	ASP	THR	ILE	ILE	HIS	PRO	LYS	PRO	Q65
ARG	ARG	GLY	GLY	GLY	ASP	PRO	PRO	ASN	HIS	VAL	ILE	MET	ILE	F66
ALA	GLY	GLY	PHE	PHE	THR	THR	THR	SER	LEU	LEU	ALA	GLN	ALA	A67
HIS	THR	HIS	LYS	LYS	THR	THR	THR	ILE	LEU	PHE	ILE	ASP	ALA	A68
TYR	ARG	TYR	ARG	ARG	GLY	GLY	GLY	ASN	ASN	PHE	ASN	SER	ASP	V69
MET	MET	SER	HIS	SER	GLY	ILE	THR	ASN	ASN	VAL	SER	SER	SER	W70
GLY	TYR	GLY	ARG	PRO	MET	PRO	MET	ASN	ASN	PRO	LEU	LEU	LEU	K71
VAL	VAL	VAL	GLY	GLY	VAL	GLN	VAL	PHE	PHE	THR	ASN	GLN	GLN	Q72
PRO	PRO	ASP	PHE	LEU	SER	ILE	SER	ILE	GLN	LYS	ASN	VAL	VAL	Q73
SER	SER	SER	GLY	THR	GLY	THR	THR	ARG	GLY	THR	ASN	GLN	SER	E74
LEU	LEU	LEU	PHE	THR	ALA	THR	THR	LEU	HIS	ARG	ASN	ASN	LEU	R75
LYS	ARG	ASN	ASN	SER	SER	SER	SER	ASP	TYR	GLN	GLY	SER	SER	G76
LYS	PRO	GLY	GLY	VAL	LYS	VAL	PRO	VAL	VAL	GLN	LEU	SER	SER	L77
THR	THR	ILE	SER	PRO	ASP	ASP	ASP	ASP	PRO	GLN	GLY	PRO	PRO	F78
ILE	ILE	GLU	GLU	VAL	LEU	LEU	LEU	LEU	GLY	SER	GLY	MET	ARG	I79
GLN	GLN	TRP	ASP	PHE	PHE	PHE	THR	VAL	CYS	SER	ILE	SER	ALA	D80
GLU	GLU	ASP	VAL	GLN	ALA	ALA	ILE	MET	ILE	GLN	GLN	PRO	PRO	Q81
LEU	LEU	LEU	THR	SER	SER	SER	MET	LEU	VAL	GLY	THR	THR	THR	S82
ASP	ASP	THR	THR	THR	THR	THR	THR	LEU	VAL	ILE	LEU	GLU	GLU	G83
HIS	HIS	PRO	GLY	ILE	HIS	VAL	SER	HIS	VAL	ASN	LYS	TYR	TYR	V84
LEU	LEU	LEU	ASN	ASN	LEU	ARG	ASN	LEU	GLY	GLY	ASN	ASP	ASP	K85
LYS	LYS	LYS	LYS	ILE	LYS	ILE	SER	GLY	ILE	ASN	LYS	GLY	TYR	E86
PRO	PRO	PRO	THR	SER	SER	SER	SER	LEU	THR	LEU	LYS	GLN	GLN	V87
ILE	ILE	ILE	LYS	THR	LYS	THR	VAL	THR	VAL	LEU	VAL	VAL	PRO	I88
THR	THR	THR	THR	THR	THR	THR	GLY	ASN	GLY	GLY	PHE	PHE	PHE	Q89
SER	SER	SER	THR	THR	ASN	GLN	HIS	ASN	LYS	ARG	MET	LYS	LYS	S35
MET	MET	MET	VAL	VAL	PHE	PHE	LYS	PHE	LYS	ALA	LEU	PRO	PRO	E90
VAL	VAL	VAL	VAL	VAL	ASN	ASN	VAL	VAL	PHE	GLN	GLY	SER	GLU	M91
LEU	LEU	LEU	PRO	PRO	ASN	ASN	ASN	ILE	VAL	ASN	ARG	SER	SER	K92
CYS	CYS	CYS	ASN	ASN	ILE	ASN	PHE	LEU	THR	LYS	LYS	LYS	LYS	E93
THR	THR	THR	THR	THR	THR	THR	THR	GLY	THR	TYR	TYR	ALA	ALA	R94
THR	THR	THR	THR	THR	THR	THR	ALA	ALA	MET	LEU	LEU	LEU	LEU	E95
SER	SER	SER	SER	SER	SER	SER	ALA	LEU	THR	THR	THR	ASP	TRP	L41
ALA	ALA	ALA	THR	THR	THR	THR	THR	PHE	PRO	GLY	ASN	TRP	LYS	A42
GLN	GLN	GLN	GLY	GLY	GLY	GLY	THR	PHE	PRO	LEU	GLU	ARG	GLU	E43
PHE	PHE	PHE	PRO	PRO	PRO	PRO	LEU	LEU	ASP	ARG	ASP	ASP	GLU	F44
ASP	ASP	ASP	THR	THR	THR	THR	SER	SER	GLY	VAL	TYR	TYR	SER	V45
LEU	LEU	LEU	ARG	ARG	ARG	ARG	SER	ASP	GLY	MET	PHE	PHE	HIS	G46
THR	THR	THR	ILE	ILE	ILE	ILE	PHE	ASN	ARG	ASN	LYS	VAL	GLU	T47
TYR	TYR	TYR	PRO	PRO	PRO	PRO	ASP	ILE	GLY	LYS	ILE	ILE	HIS	M48
ASN	ASN	ASN	GLN	GLN	GLN	GLN	ASN	MET	ILE	ASN	ASN	PRO	PRO	I49
CYS	CYS	CYS	VAL	VAL	VAL	VAL	THR	THR	GLY	ILE	ALA	ILE	GLN	Q50
LYS	LYS	LYS	VAL	VAL	VAL	VAL	THR	THR	THR	ASN	SER	GLN	HIS	A51
VAL	VAL	VAL	GLU	GLU	GLU	GLU	GLU	LEU	GLU	GLU	SER	GLN	GLU	N52
ILE	ILE	ILE	THR	THR	THR	THR	THR	ILE	THR	LEU	ASP	GLN	GLU	W53
ASN	ASN	ASN	THR	THR	THR	THR	ASN	SER	ILE	ASN	ASN	ASN	ASN	R54
														E55
														Q56
														G57
														A58
														T59
														I60
														GLU
														SNV

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	28871	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	53	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.261	Depositor
Minimum map value	-0.265	Depositor
Average map value	0.009	Depositor
Map value standard deviation	0.056	Depositor
Recommended contour level	0.45	Depositor
Map size (Å)	466.39996, 466.39996, 466.39996	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	2	0.15	0/5036	0.32	0/6796
2	3	0.21	0/4920	0.37	0/6675
3	4	0.14	0/5020	0.33	0/6785
4	5	0.18	0/4227	0.33	0/5701
5	6	0.15	0/4913	0.34	0/6631
6	7	0.27	0/5204	0.42	0/7039
7	A	0.16	0/1622	0.29	0/2183
8	B	0.18	0/1650	0.32	0/2231
9	C	0.16	0/1420	0.30	0/1918
10	D	0.17	0/2040	0.32	0/2755
11	E	0.22	0/4677	0.36	0/6335
12	F	0.14	0/3489	0.31	0/4724
12	G	0.14	0/3465	0.32	0/4696
12	H	0.14	0/3496	0.33	0/4735
13	I	0.20	0/175	0.53	0/268
14	N	0.32	0/654	0.53	0/883
All	All	0.18	0/52008	0.35	0/70355

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	4955	0	5000	187	0
2	3	4835	0	4881	202	0
3	4	4947	0	5020	208	0
4	5	4176	0	4261	173	0
5	6	4837	0	4830	185	0
6	7	5124	0	5175	169	0
7	A	1602	0	1604	51	0
8	B	1617	0	1674	57	0
9	C	1387	0	1405	41	0
10	D	2004	0	2001	62	0
11	E	4591	0	4567	153	0
12	F	3404	0	3352	114	0
12	G	3380	0	3310	153	0
12	H	3411	0	3355	104	0
13	I	160	0	97	2	0
14	N	641	0	622	151	0
15	2	27	0	12	8	0
15	3	27	0	12	6	0
16	2	1	0	0	0	0
16	3	1	0	0	0	0
16	4	1	0	0	0	0
16	7	1	0	0	0	0
17	2	1	0	0	0	0
17	4	1	0	0	0	0
17	5	1	0	0	0	0
17	6	1	0	0	0	0
17	7	1	0	0	0	0
18	4	31	0	12	6	0
18	7	31	0	12	7	0
All	All	51196	0	51202	1905	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 19.

All (1905) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:622:HIS:HB2	6:7:624:LYS:NZ	1.58	1.17
6:7:622:HIS:CB	6:7:624:LYS:NZ	2.08	1.17
14:N:25:LEU:HD13	14:N:63:LEU:HD12	1.42	1.01
11:E:589:PRO:HD2	11:E:592:LEU:HD12	1.44	1.00
6:7:622:HIS:CB	6:7:624:LYS:HZ3	1.73	0.99

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:62:PHE:HE2	14:N:85:LYS:HA	1.29	0.97
8:B:20:VAL:HG21	8:B:121:VAL:HG11	1.47	0.97
2:3:466:ASP:OD2	2:3:509:ARG:NH1	1.99	0.95
6:7:622:HIS:HB2	6:7:624:LYS:HZ3	1.19	0.95
6:7:633:VAL:HG12	6:7:637:LYS:HE3	1.49	0.93
6:7:214:ARG:HB2	6:7:218:LYS:HB2	1.50	0.93
6:7:622:HIS:HB3	6:7:624:LYS:NZ	1.82	0.92
1:2:669:LEU:HD22	1:2:673:ILE:HG21	1.49	0.92
12:G:907:LEU:HD23	12:G:910:LEU:HD12	1.52	0.91
1:2:309:LEU:O	1:2:310:ARG:NH1	2.05	0.90
12:G:481:PRO:O	12:G:495:THR:OG1	1.90	0.90
12:G:892:ASP:OD2	12:G:918:ARG:NH2	2.04	0.90
12:G:484:THR:O	12:G:492:ARG:NH1	2.05	0.90
14:N:23:ARG:HA	14:N:27:ARG:HB2	1.52	0.89
12:H:709:LYS:NZ	12:H:835:GLU:OE2	2.06	0.88
6:7:622:HIS:HB3	6:7:624:LYS:HZ1	1.34	0.87
2:3:489:VAL:HG22	2:3:495:VAL:HG22	1.54	0.87
11:E:303:THR:O	12:F:491:ARG:NH1	2.08	0.87
7:A:48:ARG:NH1	10:D:201:TYR:O	2.07	0.86
1:2:310:ARG:NH2	5:6:387:GLU:OE1	2.08	0.86
6:7:344:SER:OG	6:7:347:ASP:OD2	1.92	0.86
5:6:702:THR:O	5:6:705:ILE:HG22	1.75	0.86
3:4:594:LYS:NZ	6:7:532:SER:O	2.08	0.86
8:B:196:HIS:O	8:B:199:SER:OG	1.93	0.86
14:N:40:ALA:O	14:N:43:GLU:HG3	1.76	0.86
2:3:193:ARG:NH2	6:7:360:TYR:OH	2.09	0.85
5:6:277:ARG:NH2	5:6:373:MET:O	2.10	0.85
3:4:763:THR:OG1	3:4:817:VAL:O	1.94	0.85
8:B:12:SER:OG	8:B:15:GLU:OE1	1.93	0.85
9:C:21:GLN:NE2	9:C:73:GLU:OE2	2.10	0.85
3:4:587:ARG:NH1	3:4:625:ASP:O	2.10	0.84
14:N:62:PHE:HA	14:N:88:ILE:HG13	1.58	0.84
3:4:258:TYR:OH	3:4:308:VAL:O	1.96	0.84
12:G:484:THR:HG23	12:G:496:MET:HE1	1.60	0.84
12:H:737:THR:HG21	12:H:740:ILE:HD12	1.59	0.83
5:6:633:ASN:N	5:6:675:ARG:O	2.11	0.83
12:G:544:THR:OG1	12:G:559:HIS:NE2	2.11	0.83
6:7:530:ASP:OD2	6:7:532:SER:OG	1.96	0.83
10:D:259:THR:OG1	10:D:266:GLU:OE1	1.96	0.82
2:3:400:ARG:NH1	2:3:490:MET:SD	2.51	0.82
12:F:676:TYR:O	12:F:680:ASN:N	2.13	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:56:TYR:H	6:7:216:ARG:HA	1.43	0.82
4:5:141:SER:O	11:E:379:TYR:OH	1.97	0.82
9:C:119:GLU:OE1	9:C:119:GLU:N	2.13	0.81
1:2:353:GLN:NE2	1:2:357:GLU:O	2.14	0.81
2:3:242:THR:OG1	2:3:244:GLU:OE2	1.99	0.81
6:7:656:VAL:HG13	6:7:713:VAL:HG21	1.60	0.81
4:5:350:THR:OG1	4:5:353:GLU:OE1	1.99	0.80
6:7:670:ASP:OD1	6:7:673:ARG:NH2	2.14	0.80
12:F:541:GLU:OE1	12:F:541:GLU:N	2.13	0.80
14:N:32:SER:HB3	14:N:74:GLU:H	1.46	0.80
4:5:184:ARG:N	4:5:240:PRO:O	2.13	0.80
2:3:569:HIS:O	4:5:398:LYS:NZ	2.16	0.79
14:N:72:GLN:NE2	14:N:80:ASP:OD2	2.15	0.79
4:5:258:LEU:HB2	4:5:276:MET:HE1	1.63	0.79
1:2:500:SER:OG	1:2:756:SER:OG	1.99	0.79
11:E:312:THR:O	11:E:315:THR:OG1	1.98	0.79
12:G:776:ILE:O	12:G:777:ARG:NH1	2.16	0.79
14:N:13:GLN:OE1	14:N:15:PRO:HG2	1.84	0.78
14:N:14:PRO:HB3	14:N:38:LEU:HG	1.63	0.78
1:2:763:LEU:O	1:2:767:ILE:HD12	1.83	0.78
1:2:236:GLU:OE2	11:E:361:LYS:NZ	2.17	0.78
14:N:15:PRO:HB3	14:N:18:ARG:HH21	1.48	0.78
3:4:206:ARG:NH1	3:4:244:ASP:OD2	2.17	0.78
14:N:62:PHE:CE2	14:N:85:LYS:HA	2.17	0.78
2:3:663:ALA:O	2:3:667:VAL:HG12	1.84	0.78
6:7:214:ARG:HB3	6:7:217:LYS:HB2	1.66	0.78
6:7:622:HIS:CB	6:7:624:LYS:HZ1	1.84	0.78
3:4:714:GLU:OE1	3:4:714:GLU:N	2.16	0.78
4:5:23:ASP:OD1	4:5:24:ASN:N	2.17	0.77
5:6:547:ILE:HD11	5:6:584:PHE:CE2	2.19	0.77
2:3:300:SER:HG	4:5:245:HIS:HD1	1.29	0.77
12:H:680:ASN:ND2	12:H:684:ILE:O	2.18	0.77
3:4:320:ASN:O	3:4:324:LYS:NZ	2.17	0.77
2:3:415:LYS:NZ	15:3:1001:ADP:O2B	2.16	0.77
6:7:465:ALA:N	18:7:902:AGS:O1B	2.16	0.77
14:N:17:LEU:HB2	14:N:20:LEU:HD11	1.65	0.77
4:5:182:MET:HB2	4:5:244:ILE:HD11	1.67	0.76
1:2:701:ASP:OD2	1:2:705:ARG:NH2	2.18	0.76
1:2:783:MET:HE2	4:5:573:ILE:HG23	1.68	0.76
15:2:901:ADP:O3'	5:6:801:GLU:OE2	2.03	0.76
6:7:529:MET:O	6:7:534:ARG:NH2	2.18	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:E:489:VAL:O	11:E:493:ASN:ND2	2.19	0.76
5:6:757:TYR:O	5:6:760:THR:OG1	2.03	0.76
6:7:233:ASP:O	6:7:237:GLN:NE2	2.19	0.76
5:6:570:ASN:OD1	5:6:678:ILE:N	2.19	0.75
5:6:279:ILE:O	5:6:280:ARG:NH1	2.19	0.75
5:6:408:THR:OG1	5:6:409:GLN:OE1	2.03	0.75
5:6:685:VAL:HG23	5:6:699:LEU:HA	1.68	0.75
4:5:483:ASP:HB3	4:5:525:PRO:HG2	1.69	0.75
5:6:769:ALA:HB1	5:6:824:ILE:HD11	1.68	0.75
12:G:492:ARG:NH1	12:G:493:TYR:O	2.20	0.75
4:5:544:THR:HG22	4:5:547:LEU:HD13	1.69	0.75
14:N:83:GLY:HA2	14:N:86:GLU:CD	2.12	0.75
2:3:490:MET:O	2:3:493:GLN:NE2	2.20	0.74
3:4:532:GLU:OE1	3:4:716:ASN:ND2	2.20	0.74
12:H:587:ARG:NH1	12:H:599:SER:OG	2.21	0.74
3:4:428:ARG:NH1	3:4:429:ALA:O	2.20	0.74
12:F:582:ALA:HB3	12:F:589:ILE:HB	1.70	0.74
3:4:572:THR:O	3:4:573:SER:OG	2.03	0.74
14:N:45:VAL:HG13	14:N:52:ASN:ND2	2.02	0.74
2:3:308:GLN:NE2	4:5:207:LEU:O	2.21	0.74
3:4:382:MET:HE2	3:4:382:MET:N	2.02	0.74
4:5:552:MET:HE3	4:5:659:ILE:HD11	1.69	0.73
2:3:495:VAL:HG23	2:3:508:ALA:HB2	1.68	0.73
3:4:563:ASN:N	3:4:703:ASP:OD2	2.22	0.73
3:4:571:SER:O	18:4:1001:AGS:H8	1.88	0.73
2:3:491:GLU:OE1	18:7:902:AGS:O2A	2.05	0.73
12:H:702:ASN:O	12:H:724:SER:N	2.20	0.73
8:B:72:VAL:HG12	8:B:75:ILE:HD12	1.70	0.73
5:6:634:GLY:O	5:6:676:THR:OG1	2.06	0.73
3:4:284:ILE:HD11	3:4:293:LEU:HD13	1.70	0.73
14:N:57:PRO:O	14:N:60:ILE:HG22	1.88	0.73
14:N:34:LYS:HB3	14:N:76:GLY:O	1.88	0.73
15:3:1001:ADP:H1'	4:5:650:ILE:HG21	1.71	0.73
7:A:12:GLU:OE1	7:A:15:ARG:NH1	2.22	0.72
14:N:13:GLN:HG3	14:N:16:LEU:HB2	1.71	0.72
12:F:624:ARG:NH2	12:F:844:ASP:OD2	2.22	0.72
14:N:66:PHE:HD2	14:N:84:VAL:HG21	1.55	0.72
3:4:314:MET:N	3:4:401:GLU:OE2	2.23	0.72
1:2:824:ARG:NH2	1:2:833:ASP:OD2	2.22	0.72
14:N:40:ALA:HB2	14:N:78:PHE:CD1	2.24	0.72
2:3:489:VAL:HG13	2:3:508:ALA:HB1	1.70	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:E:12:TYR:CZ	11:E:16:LEU:HD11	2.25	0.72
14:N:54:ARG:O	14:N:57:PRO:HD2	1.89	0.72
2:3:300:SER:OG	4:5:245:HIS:ND1	2.19	0.72
3:4:284:ILE:HD13	3:4:296:ILE:HD12	1.72	0.72
3:4:577:ILE:O	3:4:581:VAL:HG23	1.90	0.72
4:5:663:LEU:HA	4:5:666:LEU:HD12	1.69	0.72
6:7:110:ALA:O	6:7:114:THR:HG23	1.89	0.72
14:N:54:ARG:NH1	14:N:54:ARG:HA	2.05	0.72
6:7:198:ARG:O	6:7:306:LYS:NZ	2.23	0.71
11:E:556:CYS:O	11:E:559:SER:OG	2.08	0.71
8:B:105:GLU:OE2	8:B:113:SER:N	2.23	0.71
11:E:299:VAL:O	11:E:303:THR:OG1	2.08	0.71
2:3:390:GLU:OE1	2:3:392:ASN:ND2	2.23	0.71
14:N:52:ASN:ND2	14:N:55:GLN:OE1	2.23	0.71
3:4:775:VAL:HG21	5:6:725:THR:HG22	1.72	0.71
12:F:530:ASP:OD2	12:F:534:TYR:N	2.22	0.71
12:H:781:PHE:HB3	12:H:786:LEU:HD11	1.71	0.71
1:2:331:PHE:HD2	4:5:323:ILE:HD11	1.56	0.71
3:4:342:MET:HG2	5:6:437:VAL:HG11	1.73	0.71
11:E:312:THR:OG1	11:E:315:THR:HG23	1.91	0.71
14:N:17:LEU:O	14:N:20:LEU:HG	1.91	0.71
1:2:527:VAL:HG22	1:2:532:SER:N	2.06	0.70
14:N:82:SER:HA	14:N:85:LYS:HE2	1.72	0.70
3:4:709:LEU:HD12	3:4:850:VAL:HG11	1.71	0.70
12:G:684:ILE:HG12	12:G:697:ILE:HD11	1.72	0.70
2:3:354:SER:HB3	2:3:717:LEU:HD12	1.74	0.70
10:D:94:GLN:OE1	10:D:97:LEU:HD11	1.91	0.70
14:N:26:SER:O	14:N:30:GLY:HA2	1.92	0.70
12:G:601:ASN:OD1	12:G:604:GLY:N	2.25	0.70
12:H:507:ASN:ND2	12:H:512:SER:OG	2.25	0.69
1:2:335:LYS:N	1:2:381:VAL:O	2.24	0.69
14:N:41:LEU:O	14:N:45:VAL:HG23	1.92	0.69
14:N:43:GLU:O	14:N:47:THR:HG23	1.92	0.69
2:3:689:ASP:O	2:3:693:LYS:NZ	2.26	0.69
3:4:650:GLU:OE1	3:4:796:ARG:NE	2.25	0.69
2:3:419:LEU:HD11	2:3:515:ALA:HB2	1.75	0.69
4:5:370:LEU:O	4:5:374:ILE:HD12	1.93	0.69
11:E:596:HIS:C	11:E:598:LYS:H	1.99	0.69
2:3:197:ILE:HD11	2:3:249:THR:HG22	1.72	0.69
11:E:573:ASP:O	11:E:577:ASP:N	2.25	0.69
12:F:634:HIS:NE2	12:H:657:LEU:O	2.26	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:D:202:MET:O	10:D:207:GLN:NE2	2.26	0.69
12:F:895:LEU:HD21	12:F:917:ILE:HG22	1.74	0.69
12:F:910:LEU:O	12:F:914:ILE:HD12	1.92	0.69
2:3:423:LEU:HD12	2:3:429:ALA:HB3	1.75	0.69
3:4:336:THR:O	3:4:395:GLN:NE2	2.26	0.69
5:6:612:VAL:HG22	5:6:623:ILE:CD1	2.23	0.69
14:N:18:ARG:HG2	14:N:19:PRO:HD3	1.75	0.69
11:E:596:HIS:O	11:E:598:LYS:N	2.24	0.69
6:7:114:THR:HG22	6:7:204:PHE:HE2	1.58	0.68
8:B:164:ASN:OD1	8:B:165:GLU:N	2.26	0.68
11:E:592:LEU:CD2	11:E:594:THR:HG23	2.22	0.68
1:2:307:ARG:NH2	1:2:402:LEU:O	2.25	0.68
6:7:83:ASP:OD1	6:7:84:ASP:N	2.27	0.68
7:A:137:LEU:HD13	10:D:185:THR:HG21	1.75	0.68
11:E:126:HIS:O	11:E:248:VAL:HG13	1.93	0.68
12:F:498:GLU:OE2	12:F:499:VAL:HG23	1.94	0.68
14:N:44:PHE:O	14:N:47:THR:OG1	2.05	0.68
1:2:219:THR:HG22	1:2:225:SER:HA	1.74	0.68
12:H:581:VAL:HG12	12:H:590:VAL:HG13	1.74	0.68
12:F:629:HIS:O	12:F:637:SER:OG	2.04	0.68
1:2:280:GLU:OE2	1:2:285:ASP:N	2.26	0.68
1:2:705:ARG:O	1:2:751:LYS:NZ	2.26	0.68
2:3:312:ASN:OD1	2:3:313:THR:N	2.26	0.68
12:G:722:LEU:HD21	12:G:776:ILE:HA	1.75	0.68
4:5:393:MET:HA	4:5:603:ILE:HD11	1.75	0.68
7:A:198:ARG:NE	14:N:26:SER:HB3	2.09	0.68
3:4:592:SER:O	3:4:596:SER:OG	2.05	0.68
11:E:323:ASP:N	11:E:406:ARG:O	2.25	0.68
12:G:626:PHE:CE2	12:G:687:LEU:HD11	2.28	0.68
12:H:546:PHE:O	12:H:555:GLN:N	2.26	0.68
2:3:571:TYR:O	4:5:398:LYS:NZ	2.23	0.68
11:E:316:LEU:HD12	11:E:413:LEU:HD13	1.76	0.68
14:N:66:PHE:CZ	14:N:72:GLN:HG3	2.29	0.68
12:F:582:ALA:HB2	12:F:618:LEU:HB3	1.74	0.68
11:E:353:GLU:OE2	11:E:354:ASN:ND2	2.26	0.68
12:H:504:THR:HG22	12:H:513:ILE:HG23	1.76	0.68
1:2:617:ARG:HH12	1:2:669:LEU:HD23	1.58	0.67
12:F:846:GLU:OE1	12:F:846:GLU:N	2.27	0.67
12:G:836:LEU:O	12:G:840:THR:HG23	1.93	0.67
7:A:124:SER:OG	7:A:126:GLN:OE1	2.12	0.67
11:E:41:ALA:HB1	11:E:255:ILE:HD12	1.75	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:65:GLN:HB2	14:N:88:ILE:HD11	1.75	0.67
14:N:66:PHE:HZ	14:N:72:GLN:HG3	1.58	0.67
3:4:686:LEU:O	3:4:691:ASN:ND2	2.28	0.67
6:7:633:VAL:HG23	6:7:638:MET:SD	2.35	0.67
12:F:601:ASN:OD1	12:F:604:GLY:N	2.27	0.67
12:H:746:ALA:O	12:H:753:ASN:N	2.27	0.67
12:H:776:ILE:O	12:H:777:ARG:NE	2.26	0.67
14:N:51:ALA:HB1	14:N:53:TRP:HE3	1.59	0.67
14:N:83:GLY:HA2	14:N:86:GLU:OE2	1.93	0.67
5:6:671:THR:C	5:6:672:LEU:HD12	2.19	0.67
14:N:20:LEU:HA	14:N:23:ARG:HG2	1.74	0.67
14:N:37:GLY:HA3	14:N:76:GLY:C	2.20	0.67
12:G:882:ALA:HB3	12:G:910:LEU:HD11	1.75	0.67
6:7:287:GLU:O	6:7:291:GLN:N	2.26	0.67
11:E:377:TRP:O	11:E:385:LYS:NZ	2.28	0.67
11:E:539:TYR:CZ	11:E:548:LEU:HD22	2.30	0.67
1:2:539:VAL:HG13	1:2:679:ILE:HG23	1.77	0.67
2:3:363:LEU:O	2:3:366:SER:OG	2.11	0.67
2:3:435:ARG:HB3	4:5:491:VAL:HG21	1.77	0.67
8:B:14:GLU:OE1	8:B:14:GLU:N	2.28	0.67
11:E:249:ASN:OD1	11:E:250:SER:N	2.28	0.67
14:N:36:ASP:C	14:N:78:PHE:HB2	2.20	0.67
12:F:685:LYS:NZ	12:F:702:ASN:OD1	2.17	0.66
2:3:48:TYR:CD1	2:3:92:LEU:HG	2.30	0.66
14:N:60:ILE:O	14:N:64:GLU:HG2	1.95	0.66
2:3:438:SER:O	2:3:442:LEU:N	2.27	0.66
5:6:142:PHE:HA	5:6:145:ILE:HD12	1.77	0.66
12:H:502:VAL:HG21	12:H:537:CYS:SG	2.36	0.66
12:H:745:LEU:HD11	12:H:755:ILE:HG13	1.77	0.66
14:N:81:GLN:O	14:N:85:LYS:HG3	1.95	0.66
3:4:561:ASP:O	3:4:803:ARG:NH1	2.28	0.66
5:6:545:LYS:HD2	5:6:830:LEU:HD21	1.77	0.66
6:7:476:ILE:O	6:7:639:ARG:NE	2.28	0.66
11:E:388:LEU:HA	11:E:391:ILE:HD12	1.76	0.66
2:3:294:VAL:HG22	2:3:326:VAL:HG13	1.78	0.66
12:G:734:GLY:HA2	12:G:815:ILE:HD11	1.78	0.66
11:E:493:ASN:O	11:E:497:GLN:NE2	2.29	0.66
12:H:676:TYR:O	12:H:680:ASN:N	2.25	0.66
14:N:65:GLN:HG3	14:N:70:TRP:HZ3	1.61	0.66
7:A:177:GLU:HA	14:N:19:PRO:HA	1.77	0.66
12:F:571:PRO:HA	12:H:782:VAL:HG12	1.78	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:223:THR:O	2:3:224:ARG:NE	2.29	0.65
3:4:647:GLU:OE1	3:4:647:GLU:N	2.26	0.65
5:6:764:ILE:N	5:6:817:ASP:O	2.29	0.65
9:C:105:PHE:O	9:C:109:ILE:HD12	1.96	0.65
11:E:546:LEU:O	11:E:550:ASN:ND2	2.29	0.65
12:H:587:ARG:NH2	12:H:625:VAL:HG21	2.11	0.65
14:N:82:SER:HA	14:N:85:LYS:CE	2.26	0.65
2:3:716:ARG:NH2	2:3:720:THR:O	2.30	0.65
4:5:665:LYS:O	4:5:668:LEU:HD23	1.97	0.65
5:6:699:LEU:HD11	5:6:701:MET:HE3	1.78	0.65
6:7:534:ARG:O	6:7:538:HIS:ND1	2.30	0.65
4:5:377:SER:O	4:5:564:ARG:NH2	2.29	0.65
12:G:737:THR:HG21	12:G:740:ILE:HD12	1.79	0.65
2:3:700:ARG:NH2	18:7:902:AGS:O2B	2.30	0.65
3:4:284:ILE:HD13	3:4:296:ILE:CD1	2.27	0.65
5:6:767:LYS:HA	5:6:770:ARG:HE	1.62	0.65
12:H:874:CYS:O	12:H:877:GLN:NE2	2.29	0.65
2:3:410:ASP:O	2:3:413:THR:OG1	2.04	0.65
5:6:600:GLY:N	5:6:639:ASP:O	2.28	0.65
10:D:157:TYR:CZ	10:D:161:LEU:HD11	2.31	0.65
12:F:730:LYS:HA	12:F:815:ILE:HD12	1.78	0.65
1:2:534:ARG:NH1	1:2:536:ASP:O	2.30	0.65
2:3:418:LEU:O	2:3:422:VAL:HG23	1.97	0.65
4:5:385:LYS:O	4:5:389:VAL:HG23	1.96	0.65
5:6:585:LEU:HD11	5:6:681:ALA:CB	2.25	0.65
11:E:425:VAL:O	11:E:429:THR:HG23	1.97	0.65
1:2:842:VAL:O	1:2:846:VAL:HG23	1.97	0.65
14:N:51:ALA:HB1	14:N:53:TRP:CE3	2.32	0.65
14:N:80:ASP:OD1	14:N:81:GLN:N	2.30	0.65
1:2:310:ARG:N	1:2:313:ASN:OD1	2.30	0.64
12:F:918:ARG:NH2	12:F:922:TYR:OH	2.31	0.64
2:3:414:ALA:HB2	15:3:1001:ADP:H2'	1.79	0.64
2:3:402:ASP:O	2:3:707:ARG:NH1	2.29	0.64
14:N:15:PRO:HA	14:N:18:ARG:HB3	1.79	0.64
12:H:587:ARG:NE	12:H:643:LEU:HD21	2.13	0.64
14:N:72:GLN:NE2	14:N:75:ARG:HA	2.13	0.64
3:4:625:ASP:OD1	3:4:668:ARG:N	2.30	0.64
12:G:515:VAL:HG22	12:G:526:TYR:O	1.96	0.64
3:4:536:VAL:HG22	3:4:706:TYR:CD2	2.33	0.64
1:2:488:SER:HB2	1:2:825:LEU:HD12	1.80	0.64
7:A:177:GLU:O	14:N:18:ARG:HG3	1.97	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:639:ASP:OD1	3:4:640:SER:N	2.31	0.64
6:7:496:ALA:O	6:7:509:GLU:N	2.28	0.64
11:E:411:ARG:NH2	11:E:486:ASP:OD2	2.30	0.64
2:3:244:GLU:OE1	6:7:109:ASN:ND2	2.31	0.64
8:B:58:LYS:O	8:B:62:ASN:ND2	2.30	0.64
12:G:840:THR:O	12:G:844:ASP:N	2.31	0.64
5:6:308:SER:OG	5:6:351:SER:N	2.30	0.63
5:6:728:ALA:O	5:6:732:VAL:HG23	1.98	0.63
7:A:94:THR:HG23	7:A:130:TYR:CE2	2.33	0.63
14:N:35:SER:O	14:N:38:LEU:HB3	1.97	0.63
1:2:539:VAL:HG22	1:2:679:ILE:HG22	1.78	0.63
2:3:685:ASP:O	2:3:689:ASP:N	2.31	0.63
4:5:573:ILE:O	4:5:577:THR:HG22	1.98	0.63
14:N:40:ALA:HB1	14:N:85:LYS:HZ1	1.62	0.63
3:4:259:HIS:O	3:4:263:ASN:ND2	2.31	0.63
4:5:282:LEU:HD22	4:5:333:ILE:CD1	2.28	0.63
5:6:184:GLY:O	5:6:188:VAL:HG23	1.99	0.63
5:6:541:GLU:OE1	5:6:541:GLU:N	2.31	0.63
6:7:138:VAL:HG21	6:7:303:ARG:HD3	1.80	0.63
11:E:10:GLU:OE1	11:E:10:GLU:N	2.31	0.63
12:G:895:LEU:HD13	12:G:918:ARG:HA	1.80	0.63
14:N:25:LEU:HD13	14:N:63:LEU:CD1	2.23	0.63
1:2:217:GLU:O	1:2:219:THR:HG23	1.97	0.63
12:G:711:ARG:NH2	12:G:844:ASP:OD2	2.32	0.63
3:4:578:LEU:HD11	3:4:674:SER:HB2	1.79	0.63
6:7:78:VAL:O	6:7:203:TYR:N	2.31	0.63
15:2:901:ADP:HI'	5:6:797:VAL:CG1	2.29	0.63
2:3:557:ARG:O	2:3:561:ILE:HD12	1.99	0.63
4:5:101:ILE:O	8:B:154:ILE:HD11	1.98	0.63
12:G:903:GLU:OE2	12:G:911:VAL:HG21	1.99	0.63
6:7:225:LEU:O	6:7:241:VAL:HG23	1.99	0.63
7:A:93:ARG:NE	7:A:127:GLU:OE2	2.32	0.63
11:E:579:TYR:CG	11:E:637:LEU:HD22	2.33	0.63
12:F:680:ASN:ND2	12:F:684:ILE:O	2.31	0.63
1:2:659:SER:OG	1:2:684:ARG:NH1	2.31	0.63
5:6:796:THR:N	5:6:799:GLN:OE1	2.32	0.63
6:7:643:ALA:O	6:7:647:THR:HG23	1.99	0.63
11:E:274:ILE:HG13	11:E:295:LEU:HD12	1.81	0.63
14:N:37:GLY:O	14:N:41:LEU:HG	1.99	0.63
11:E:592:LEU:HD22	11:E:597:THR:HG21	1.80	0.62
12:F:695:PRO:O	12:F:706:LEU:HD12	1.98	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:2:901:ADP:O2B	5:6:798:ARG:NH2	2.32	0.62
6:7:103:VAL:HG22	6:7:214:ARG:HH21	1.63	0.62
12:F:727:GLU:N	12:F:727:GLU:OE1	2.33	0.62
12:G:683:GLY:O	12:G:700:SER:N	2.31	0.62
2:3:445:ALA:O	2:3:458:GLU:N	2.32	0.62
3:4:178:ARG:O	3:4:187:ILE:N	2.31	0.62
5:6:543:VAL:HG12	5:6:584:PHE:CE2	2.34	0.62
12:F:756:LEU:HD11	12:F:774:MET:HE1	1.81	0.62
14:N:14:PRO:CB	14:N:38:LEU:HG	2.29	0.62
1:2:260:LEU:HD12	1:2:264:PRO:HA	1.81	0.62
7:A:130:TYR:CD1	10:D:189:ILE:HG22	2.35	0.62
10:D:5:ILE:HD13	12:F:871:ALA:HB2	1.81	0.62
14:N:58:ALA:O	14:N:62:PHE:HD1	1.82	0.62
5:6:656:MET:SD	5:6:657:GLU:N	2.73	0.62
6:7:633:VAL:HG12	6:7:637:LYS:CE	2.28	0.62
12:F:879:VAL:CG2	12:F:907:LEU:HD22	2.29	0.62
3:4:256:ASP:OD1	3:4:257:LEU:N	2.33	0.62
3:4:606:THR:N	3:4:615:VAL:O	2.28	0.62
14:N:32:SER:O	14:N:75:ARG:N	2.28	0.62
3:4:541:LEU:HA	3:4:544:LEU:HD12	1.82	0.62
6:7:519:GLY:O	6:7:561:THR:OG1	2.18	0.62
6:7:654:GLU:N	6:7:654:GLU:OE1	2.33	0.62
7:A:154:SER:O	10:D:141:ARG:NH2	2.33	0.62
12:G:907:LEU:HD23	12:G:910:LEU:CD1	2.27	0.62
14:N:14:PRO:O	14:N:38:LEU:HD11	1.99	0.62
1:2:439:ASN:O	1:2:443:GLY:N	2.33	0.61
1:2:707:HIS:O	1:2:710:ASN:ND2	2.31	0.61
2:3:197:ILE:HD11	2:3:249:THR:CG2	2.30	0.61
7:A:26:ASP:OD2	7:A:103:ASN:ND2	2.32	0.61
12:H:582:ALA:HB3	12:H:589:ILE:HB	1.82	0.61
12:H:768:LEU:HD23	12:H:769:PRO:O	2.00	0.61
14:N:83:GLY:HA2	14:N:86:GLU:OE1	2.00	0.61
5:6:721:GLU:O	5:6:725:THR:HG23	1.98	0.61
11:E:577:ASP:OD1	11:E:634:ARG:NE	2.31	0.61
1:2:515:VAL:O	1:2:519:LEU:HD23	2.00	0.61
2:3:483:ARG:O	2:3:487:HIS:ND1	2.33	0.61
7:A:54:LEU:HD11	7:A:68:ALA:HA	1.83	0.61
12:G:744:PRO:CB	12:G:752:LEU:HD11	2.29	0.61
7:A:173:GLU:O	14:N:34:LYS:HD2	2.00	0.61
14:N:34:LYS:HG3	14:N:35:SER:N	2.15	0.61
5:6:516:LEU:HA	5:6:519:MET:SD	2.41	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:114:THR:HG22	6:7:204:PHE:CE2	2.35	0.61
4:5:415:LEU:O	4:5:556:VAL:N	2.33	0.61
11:E:41:ALA:HB1	11:E:255:ILE:CD1	2.30	0.61
12:G:749:TYR:HE1	12:G:837:LEU:HD11	1.65	0.61
15:2:901:ADP:H1'	5:6:797:VAL:HG11	1.82	0.61
2:3:435:ARG:HG2	4:5:491:VAL:HG11	1.81	0.61
3:4:254:THR:HG23	3:4:257:LEU:HD23	1.83	0.61
3:4:348:LYS:CB	3:4:385:ILE:HD11	2.30	0.61
3:4:561:ASP:OD1	3:4:562:ILE:N	2.34	0.61
7:A:40:ILE:O	7:A:44:VAL:HG23	2.00	0.61
12:G:746:ALA:O	12:G:752:LEU:HD12	1.99	0.61
14:N:24:VAL:HG12	14:N:25:LEU:HD22	1.83	0.61
5:6:143:MET:O	5:6:147:ASP:N	2.31	0.61
6:7:137:ASP:O	6:7:141:VAL:HG23	2.01	0.61
8:B:20:VAL:HG21	8:B:121:VAL:CG1	2.26	0.61
14:N:14:PRO:N	14:N:15:PRO:HD2	2.15	0.61
14:N:33:ILE:HA	14:N:76:GLY:H	1.66	0.61
1:2:673:ILE:HG22	1:2:677:PHE:HE2	1.66	0.61
10:D:277:MET:HA	10:D:277:MET:HE3	1.83	0.61
11:E:2:TYR:OH	11:E:138:GLN:O	2.15	0.61
12:H:582:ALA:HB2	12:H:618:LEU:HB3	1.83	0.61
1:2:617:ARG:NH1	1:2:669:LEU:HD23	2.16	0.60
5:6:383:GLY:O	5:6:386:VAL:HG22	2.00	0.60
12:H:684:ILE:HG21	12:H:687:LEU:HD11	1.83	0.60
2:3:656:LEU:O	2:3:660:VAL:HG23	2.01	0.60
3:4:188:GLN:O	3:4:192:THR:HG23	2.01	0.60
2:3:483:ARG:HA	2:3:486:ILE:HD12	1.81	0.60
2:3:569:HIS:ND1	4:5:657:ILE:HG21	2.16	0.60
3:4:457:TYR:CE2	6:7:255:VAL:HG13	2.36	0.60
10:D:179:GLU:OE1	10:D:179:GLU:N	2.32	0.60
12:G:658:PRO:O	12:H:611:LYS:NZ	2.33	0.60
14:N:45:VAL:HA	14:N:55:GLN:HE22	1.65	0.60
3:4:273:ASP:OD1	3:4:303:VAL:HG12	2.01	0.60
4:5:563:GLU:HA	4:5:566:ILE:HD12	1.84	0.60
5:6:149:ASN:OD1	5:6:150:THR:N	2.34	0.60
12:H:570:ILE:CD1	12:H:590:VAL:HG11	2.32	0.60
5:6:340:ASN:ND2	5:6:342:ALA:O	2.34	0.60
9:C:31:GLU:HG2	9:C:44:LEU:HD11	1.83	0.60
12:F:690:SER:N	12:F:694:ASP:O	2.35	0.60
12:H:840:THR:O	12:H:845:GLY:N	2.34	0.60
12:H:899:VAL:HG23	12:H:914:ILE:HG21	1.81	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:411:LEU:O	1:2:415:VAL:HG13	2.02	0.60
9:C:164:THR:HA	9:C:167:LEU:HD12	1.81	0.60
11:E:543:LEU:HA	11:E:546:LEU:HD12	1.84	0.60
2:3:392:ASN:OD1	2:3:398:HIS:ND1	2.34	0.60
3:4:295:GLU:O	3:4:299:LYS:N	2.34	0.60
3:4:578:LEU:HD11	3:4:674:SER:CB	2.32	0.60
4:5:136:GLN:OE1	4:5:281:TYR:N	2.35	0.60
4:5:58:ASN:OD1	4:5:60:SER:OG	2.20	0.60
5:6:185:LEU:O	5:6:189:VAL:HG23	2.01	0.60
4:5:70:GLY:O	11:E:311:LYS:NZ	2.34	0.60
2:3:366:SER:HA	2:3:650:LEU:HD22	1.84	0.60
2:3:678:VAL:HG21	2:3:723:LYS:HG3	1.83	0.60
3:4:345:ALA:O	3:4:358:VAL:N	2.35	0.60
3:4:569:ASP:OD2	3:4:710:ASP:N	2.33	0.60
10:D:247:GLN:OE1	10:D:247:GLN:N	2.35	0.60
1:2:526:ASN:OD1	1:2:527:VAL:N	2.35	0.59
5:6:198:ASN:OD1	5:6:199:THR:N	2.34	0.59
12:F:687:LEU:CD1	12:F:697:ILE:HG22	2.32	0.59
12:F:741:HIS:HB3	12:F:762:ILE:HG23	1.84	0.59
14:N:32:SER:CB	14:N:74:GLU:H	2.12	0.59
4:5:330:ILE:HG21	4:5:333:ILE:HD11	1.84	0.59
12:F:601:ASN:OD1	12:F:605:VAL:N	2.36	0.59
12:H:740:ILE:HG23	12:H:756:LEU:HD21	1.84	0.59
5:6:625:ALA:HB1	5:6:629:MET:HB2	1.82	0.59
1:2:334:LEU:HD23	1:2:337:VAL:HG12	1.85	0.59
1:2:541:LEU:N	1:2:648:ALA:O	2.34	0.59
2:3:495:VAL:HG23	2:3:508:ALA:CB	2.32	0.59
5:6:144:LYS:CA	5:6:196:LEU:HD11	2.31	0.59
6:7:195:ASN:O	6:7:306:LYS:NZ	2.19	0.59
1:2:237:MET:N	1:2:237:MET:HE2	2.16	0.59
3:4:233:MET:O	3:4:237:GLY:N	2.34	0.59
4:5:235:ASN:OD1	4:5:237:GLY:N	2.35	0.59
14:N:40:ALA:HB1	14:N:85:LYS:NZ	2.17	0.59
3:4:190:CYS:SG	3:4:257:LEU:HD13	2.42	0.59
3:4:571:SER:HA	18:4:1001:AGS:H5'2	1.84	0.59
4:5:412:VAL:O	4:5:521:ALA:N	2.34	0.59
12:G:850:ASN:O	12:G:854:VAL:HG23	2.03	0.59
11:E:304:PRO:O	11:E:307:ARG:NH1	2.36	0.59
12:G:751:THR:HG22	12:G:773:GLU:HG2	1.84	0.59
14:N:88:ILE:HA	14:N:91:MET:HE2	1.85	0.59
1:2:236:GLU:C	1:2:237:MET:HE2	2.27	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:3:1001:ADP:H1'	4:5:650:ILE:CG2	2.33	0.59
4:5:594:ILE:HD12	4:5:599:MET:SD	2.43	0.59
10:D:262:ASP:OD2	10:D:278:ARG:NH1	2.36	0.59
10:D:268:GLU:OE1	10:D:268:GLU:N	2.35	0.59
12:G:676:TYR:O	12:G:680:ASN:N	2.30	0.59
14:N:31:LEU:HD12	14:N:63:LEU:HG	1.85	0.59
3:4:572:THR:O	3:4:572:THR:HG22	2.03	0.59
12:G:841:LEU:HD21	12:G:851:GLU:HB2	1.85	0.59
1:2:340:ASN:N	1:2:374:ARG:O	2.35	0.59
3:4:348:LYS:HB3	3:4:385:ILE:HD11	1.84	0.59
3:4:381:SER:C	3:4:382:MET:HE2	2.28	0.59
14:N:82:SER:HA	14:N:85:LYS:NZ	2.18	0.59
4:5:684:PHE:O	4:5:688:THR:HG23	2.03	0.58
4:5:282:LEU:HD22	4:5:333:ILE:HD12	1.84	0.58
5:6:124:VAL:O	5:6:135:VAL:HG13	2.02	0.58
12:G:494:LEU:HD12	12:G:502:VAL:HG11	1.86	0.58
2:3:535:LEU:HB2	2:3:540:LEU:HD21	1.85	0.58
3:4:199:MET:HB3	3:4:227:ILE:HD11	1.85	0.58
11:E:587:ARG:HA	11:E:601:ILE:HD11	1.84	0.58
12:F:734:GLY:HA2	12:F:815:ILE:HD11	1.85	0.58
12:H:533:GLY:O	12:H:548:GLN:NE2	2.36	0.58
2:3:533:ILE:HG21	2:3:540:LEU:HD11	1.84	0.58
5:6:613:VAL:O	5:6:622:THR:N	2.31	0.58
6:7:635:PRO:HA	6:7:638:MET:HE2	1.85	0.58
12:G:475:ARG:NH2	12:G:477:MET:SD	2.76	0.58
12:H:826:GLU:OE1	12:H:868:ARG:NH2	2.36	0.58
12:H:846:GLU:OE2	12:H:852:ASN:ND2	2.36	0.58
5:6:615:ASP:N	5:6:620:ASP:O	2.36	0.58
12:G:676:TYR:CD2	12:G:762:ILE:HD11	2.37	0.58
12:G:833:LEU:O	12:G:837:LEU:HD12	2.03	0.58
12:H:741:HIS:O	12:H:757:VAL:N	2.36	0.58
3:4:581:VAL:HG21	3:4:672:LEU:CD2	2.33	0.58
14:N:15:PRO:HB3	14:N:18:ARG:NH2	2.16	0.58
4:5:414:LEU:HD23	4:5:554:PHE:HB2	1.85	0.58
4:5:477:VAL:CG1	4:5:519:VAL:HG22	2.33	0.58
5:6:308:SER:O	5:6:347:ASN:N	2.36	0.58
11:E:388:LEU:HD12	11:E:389:GLY:N	2.18	0.58
11:E:589:PRO:HB2	11:E:592:LEU:HB2	1.86	0.58
12:H:549:SER:OG	12:H:578:ILE:N	2.37	0.58
14:N:66:PHE:HA	14:N:70:TRP:HE3	1.68	0.58
4:5:686:ALA:HA	4:5:689:MET:HE2	1.86	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:F:687:LEU:HD11	12:F:697:ILE:HG22	1.86	0.58
14:N:66:PHE:HA	14:N:70:TRP:CE3	2.39	0.58
14:N:82:SER:HA	14:N:85:LYS:HZ3	1.69	0.58
1:2:361:ILE:HD11	1:2:373:PHE:CG	2.38	0.58
2:3:443:THR:HG22	2:3:489:VAL:HG21	1.86	0.58
8:B:193:ARG:NH2	10:D:223:ASP:OD2	2.37	0.58
12:F:729:TRP:NE1	12:F:734:GLY:O	2.37	0.58
12:G:749:TYR:CE1	12:G:837:LEU:HD11	2.39	0.58
2:3:462:MET:HG3	2:3:489:VAL:HG11	1.85	0.58
5:6:550:GLN:NE2	5:6:569:ILE:O	2.37	0.58
10:D:224:TRP:O	10:D:280:GLU:N	2.37	0.58
2:3:195:LYS:NZ	2:3:218:THR:OG1	2.37	0.57
5:6:625:ALA:HB1	5:6:629:MET:CB	2.34	0.57
8:B:152:ARG:O	8:B:156:VAL:HG23	2.04	0.57
12:F:602:GLN:OE1	12:F:602:GLN:N	2.33	0.57
12:G:591:GLY:HA3	12:G:618:LEU:HD11	1.86	0.57
12:G:825:GLU:OE1	12:G:829:ARG:NH1	2.36	0.57
1:2:359:ILE:HG22	1:2:361:ILE:HG23	1.86	0.57
1:2:813:ILE:HG13	1:2:841:VAL:HG21	1.86	0.57
5:6:543:VAL:HG22	5:6:713:PHE:CD1	2.39	0.57
9:C:101:ASN:OD1	9:C:102:SER:N	2.36	0.57
12:G:737:THR:CG2	12:G:740:ILE:HD12	2.34	0.57
2:3:217:ALA:HB1	2:3:301:LEU:HD21	1.87	0.57
12:F:864:LYS:HA	12:F:867:LEU:HD12	1.85	0.57
4:5:413:LEU:HA	4:5:521:ALA:HB3	1.86	0.57
7:A:168:LEU:N	7:A:204:TYR:O	2.37	0.57
9:C:159:ASN:OD1	9:C:160:ILE:N	2.37	0.57
10:D:249:ASN:O	10:D:252:GLY:N	2.35	0.57
1:2:707:HIS:NE2	5:6:763:PRO:O	2.38	0.57
3:4:349:CYS:SG	3:4:382:MET:HE1	2.44	0.57
5:6:771:SER:O	5:6:774:VAL:HG22	2.04	0.57
7:A:57:GLN:O	7:A:61:GLY:N	2.37	0.57
6:7:225:LEU:HB3	6:7:229:GLN:HB3	1.85	0.57
2:3:706:ILE:HD13	6:7:620:HIS:CE1	2.39	0.57
4:5:92:THR:O	4:5:95:THR:OG1	2.20	0.57
6:7:634:GLU:CD	6:7:637:LYS:HB2	2.30	0.57
14:N:13:GLN:CG	14:N:16:LEU:HB2	2.34	0.57
14:N:58:ALA:HA	14:N:61:LYS:HE2	1.87	0.57
3:4:797:GLN:O	3:4:800:SER:OG	2.19	0.57
10:D:230:ILE:HD11	10:D:277:MET:HG2	1.86	0.57
12:G:685:LYS:NZ	12:G:702:ASN:OD1	2.29	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:257:LEU:HD11	3:4:268:VAL:HG13	1.85	0.57
4:5:258:LEU:CB	4:5:276:MET:HE1	2.35	0.57
5:6:270:LEU:HD12	5:6:289:SER:HB3	1.86	0.57
5:6:579:THR:O	5:6:580:SER:OG	2.16	0.57
12:F:544:THR:HG23	12:F:559:HIS:NE2	2.19	0.57
12:G:587:ARG:HD2	12:G:643:LEU:HD22	1.86	0.57
12:H:892:ASP:HA	12:H:895:LEU:HD12	1.86	0.57
3:4:573:SER:HB3	18:4:1001:AGS:H2'	1.86	0.57
4:5:412:VAL:HG22	4:5:552:MET:HB2	1.86	0.57
5:6:144:LYS:N	5:6:196:LEU:HD11	2.20	0.57
6:7:149:ARG:NH2	6:7:265:CYS:O	2.37	0.57
8:B:16:ILE:HG23	8:B:175:LEU:HD22	1.87	0.57
9:C:39:THR:O	9:C:42:THR:OG1	2.18	0.57
3:4:261:LEU:HB2	3:4:268:VAL:HG11	1.87	0.56
8:B:126:LEU:O	8:B:130:ALA:N	2.38	0.56
11:E:122:VAL:N	11:E:141:GLN:O	2.37	0.56
12:F:827:TYR:CE1	12:F:866:LEU:HD21	2.39	0.56
12:H:545:LEU:HD22	12:H:588:VAL:HG13	1.85	0.56
1:2:704:VAL:O	1:2:710:ASN:ND2	2.36	0.56
4:5:360:LEU:O	4:5:366:LEU:HD22	2.05	0.56
12:F:756:LEU:HD11	12:F:774:MET:CE	2.35	0.56
1:2:402:LEU:HD21	5:6:625:ALA:HB2	1.87	0.56
2:3:344:ASP:OD1	2:3:345:PHE:N	2.38	0.56
2:3:408:VAL:CG1	2:3:548:VAL:HG22	2.35	0.56
4:5:415:LEU:N	4:5:554:PHE:O	2.38	0.56
6:7:615:HIS:O	6:7:619:VAL:HG23	2.06	0.56
12:G:555:GLN:OE1	12:G:567:THR:OG1	2.22	0.56
12:G:744:PRO:HB3	12:G:752:LEU:HD11	1.86	0.56
14:N:36:ASP:OD1	14:N:37:GLY:N	2.37	0.56
14:N:66:PHE:HE1	14:N:72:GLN:H	1.53	0.56
14:N:82:SER:CA	14:N:85:LYS:HZ3	2.18	0.56
2:3:370:SER:O	2:3:564:HIS:NE2	2.39	0.56
2:3:653:ILE:HG22	2:3:654:PRO:HD3	1.87	0.56
2:3:712:HIS:ND1	2:3:725:ASP:OD1	2.38	0.56
4:5:483:ASP:OD2	4:5:525:PRO:HB2	2.05	0.56
11:E:120:ILE:O	11:E:141:GLN:N	2.36	0.56
14:N:82:SER:O	14:N:86:GLU:OE1	2.22	0.56
5:6:367:GLU:C	5:6:368:ILE:HD12	2.30	0.56
7:A:173:GLU:OE2	14:N:35:SER:HB2	2.05	0.56
11:E:596:HIS:C	11:E:597:THR:HG23	2.29	0.56
12:G:863:ASP:O	12:G:867:LEU:HD23	2.06	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:166:ILE:O	4:5:289:GLY:N	2.36	0.56
5:6:771:SER:O	5:6:775:GLU:OE1	2.23	0.56
11:E:155:GLN:N	11:E:155:GLN:OE1	2.37	0.56
11:E:485:ASP:OD1	11:E:486:ASP:N	2.38	0.56
12:G:482:ALA:O	12:G:496:MET:HE2	2.05	0.56
14:N:23:ARG:HB3	14:N:27:ARG:NH1	2.19	0.56
3:4:841:LYS:O	3:4:842:THR:OG1	2.19	0.56
5:6:104:ASP:OD1	5:6:106:VAL:HG13	2.06	0.56
5:6:816:VAL:HG12	5:6:818:GLU:H	1.70	0.56
6:7:607:ASP:OD2	6:7:608:ASP:N	2.39	0.56
12:F:694:ASP:OD1	12:F:710:TRP:NE1	2.35	0.56
12:H:746:ALA:O	12:H:752:LEU:HD12	2.06	0.56
2:3:38:TYR:OH	2:3:99:SER:N	2.36	0.56
5:6:434:ASN:OD1	5:6:435:SER:N	2.39	0.56
5:6:629:MET:HE3	5:6:661:ILE:HD12	1.87	0.56
5:6:804:ILE:O	5:6:807:SER:OG	2.21	0.56
2:3:48:TYR:CE1	2:3:92:LEU:HG	2.41	0.56
3:4:237:GLY:O	3:4:299:LYS:NZ	2.31	0.56
4:5:178:TYR:HD1	4:5:193:THR:HG22	1.71	0.56
12:F:694:ASP:CB	12:F:706:LEU:HD11	2.36	0.56
1:2:354:ASP:O	1:2:355:SER:OG	2.17	0.56
4:5:596:ILE:HA	4:5:599:MET:HE2	1.88	0.56
6:7:211:CYS:HB2	6:7:213:ARG:HG2	1.88	0.56
11:E:79:ASN:O	11:E:119:ASP:N	2.39	0.56
12:H:833:LEU:O	12:H:837:LEU:HD23	2.05	0.56
14:N:40:ALA:HB2	14:N:78:PHE:HD1	1.71	0.56
2:3:470:VAL:N	2:3:511:SER:O	2.39	0.55
3:4:345:ALA:N	3:4:358:VAL:O	2.38	0.55
3:4:538:LYS:O	3:4:542:LEU:HD23	2.07	0.55
5:6:134:LYS:O	5:6:137:ARG:N	2.38	0.55
5:6:526:TYR:O	5:6:530:VAL:HG23	2.07	0.55
12:H:755:ILE:CD1	12:H:768:LEU:HD21	2.36	0.55
2:3:676:ILE:HD12	6:7:621:MET:HE2	1.87	0.55
3:4:724:LEU:HD21	6:7:690:LEU:HD21	1.87	0.55
7:A:32:TYR:CE2	7:A:37:ILE:HD13	2.42	0.55
9:C:172:MET:SD	9:C:173:GLU:N	2.80	0.55
11:E:129:TRP:N	11:E:240:TYR:OH	2.40	0.55
11:E:366:MET:SD	11:E:391:ILE:HG22	2.46	0.55
12:G:756:LEU:HD11	12:G:774:MET:HE2	1.88	0.55
1:2:411:LEU:C	1:2:415:VAL:HG13	2.31	0.55
11:E:13:ASN:HA	11:E:16:LEU:HD12	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:F:502:VAL:HG22	12:F:515:VAL:HA	1.87	0.55
6:7:464:VAL:HG23	6:7:466:LYS:HG3	1.86	0.55
10:D:181:LYS:O	10:D:185:THR:HG22	2.06	0.55
12:F:560:ASP:OD1	12:F:561:SER:N	2.40	0.55
12:F:728:ILE:HD12	12:F:740:ILE:HG21	1.88	0.55
12:G:701:ASP:OD2	12:G:703:THR:OG1	2.24	0.55
14:N:89:GLN:OE1	14:N:92:LYS:HG2	2.05	0.55
3:4:644:VAL:HG23	5:6:601:LYS:HE2	1.88	0.55
12:G:497:ASN:C	12:G:745:LEU:HD23	2.32	0.55
1:2:580:VAL:CG2	1:2:591:LEU:HD12	2.37	0.55
2:3:21:PHE:O	2:3:25:VAL:HG23	2.07	0.55
11:E:589:PRO:CD	11:E:592:LEU:HD12	2.29	0.55
12:G:680:ASN:ND2	12:G:684:ILE:O	2.35	0.55
1:2:539:VAL:HG22	1:2:679:ILE:CG2	2.36	0.55
4:5:212:LEU:O	4:5:213:SER:OG	2.15	0.55
8:B:66:MET:HA	8:B:66:MET:HE3	1.88	0.55
14:N:54:ARG:C	14:N:57:PRO:HD2	2.31	0.55
1:2:520:PHE:O	1:2:822:LYS:NZ	2.39	0.55
2:3:570:ARG:HG3	4:5:614:LEU:HD11	1.89	0.55
4:5:358:LEU:O	4:5:361:SER:OG	2.16	0.55
3:4:658:LYS:NZ	13:I:8:DT:OP2	2.40	0.55
12:F:694:ASP:HB2	12:F:706:LEU:HD11	1.88	0.55
2:3:444:ALA:HB1	2:3:457:LEU:HD11	1.89	0.55
6:7:456:VAL:HG22	6:7:596:ILE:HB	1.88	0.55
14:N:70:TRP:CE3	14:N:84:VAL:HG22	2.41	0.55
2:3:462:MET:HE1	2:3:470:VAL:HG11	1.87	0.54
3:4:245:ALA:HB1	3:4:258:TYR:CE1	2.42	0.54
4:5:47:ARG:NH2	8:B:147:ASP:OD1	2.38	0.54
5:6:189:VAL:O	5:6:193:ALA:N	2.39	0.54
5:6:547:ILE:HD11	5:6:584:PHE:CZ	2.41	0.54
11:E:359:LEU:HD11	11:E:363:PHE:CE2	2.42	0.54
12:G:895:LEU:HD11	12:G:921:ARG:CZ	2.37	0.54
1:2:276:MET:HE1	1:2:293:ILE:N	2.21	0.54
1:2:324:VAL:HG23	1:2:420:PRO:HA	1.87	0.54
6:7:541:MET:HE2	6:7:593:ARG:HB3	1.89	0.54
7:A:1:MET:HE2	7:A:1:MET:HA	1.89	0.54
12:H:584:THR:OG1	12:H:587:ARG:O	2.12	0.54
12:H:587:ARG:HH21	12:H:625:VAL:HG21	1.72	0.54
14:N:26:SER:HA	14:N:31:LEU:N	2.23	0.54
14:N:26:SER:OG	14:N:31:LEU:O	2.16	0.54
4:5:39:ARG:O	4:5:40:LEU:HD23	2.08	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:407:ARG:NH1	4:5:409:ASP:O	2.40	0.54
8:B:82:GLN:CD	11:E:53:LEU:HD11	2.33	0.54
11:E:246:THR:HG23	11:E:246:THR:O	2.08	0.54
12:F:757:VAL:HG11	12:F:761:HIS:O	2.08	0.54
12:G:503:SER:O	12:G:514:THR:N	2.40	0.54
12:G:553:GLN:HE21	12:G:567:THR:HG21	1.73	0.54
14:N:32:SER:HB3	14:N:73:GLN:HB3	1.89	0.54
1:2:458:ARG:NH1	1:2:459:ARG:O	2.40	0.54
2:3:49:ASN:HA	2:3:91:ILE:HD12	1.88	0.54
3:4:500:GLN:NE2	3:4:501:ILE:O	2.40	0.54
5:6:368:ILE:O	5:6:368:ILE:HG22	2.07	0.54
2:3:343:THR:O	2:3:347:ILE:HD12	2.07	0.54
2:3:462:MET:CG	2:3:489:VAL:HG11	2.37	0.54
7:A:51:THR:HG23	7:A:75:THR:HG21	1.89	0.54
7:A:167:VAL:O	7:A:167:VAL:HG23	2.07	0.54
12:F:649:ARG:NH1	12:F:650:TYR:O	2.41	0.54
1:2:386:GLN:O	1:2:410:LEU:N	2.37	0.54
2:3:133:ALA:O	2:3:137:ASP:N	2.38	0.54
2:3:481:VAL:O	2:3:484:VAL:HG22	2.07	0.54
1:2:244:VAL:O	1:2:298:SER:N	2.40	0.54
5:6:502:GLU:HA	5:6:505:LEU:HD12	1.89	0.54
7:A:10:VAL:HG11	9:C:9:VAL:HG11	1.90	0.54
11:E:413:LEU:HD12	11:E:414:GLY:N	2.23	0.54
1:2:271:PHE:CD2	1:2:295:VAL:HG11	2.43	0.54
3:4:408:ASP:OD2	6:7:560:ARG:NH2	2.40	0.54
3:4:721:ALA:O	3:4:725:THR:HG23	2.08	0.54
6:7:670:ASP:O	6:7:674:GLU:N	2.39	0.54
12:F:734:GLY:CA	12:F:815:ILE:HD11	2.37	0.54
2:3:171:LEU:HD21	2:3:298:PHE:CE1	2.42	0.54
7:A:33:HIS:O	7:A:37:ILE:HD12	2.08	0.54
11:E:120:ILE:N	11:E:141:GLN:OE1	2.41	0.54
1:2:693:GLU:O	1:2:697:THR:HG23	2.08	0.54
3:4:775:VAL:CG2	5:6:725:THR:HG22	2.38	0.54
10:D:152:ASP:OD1	10:D:182:TYR:OH	2.16	0.54
14:N:20:LEU:HA	14:N:23:ARG:CG	2.38	0.54
1:2:813:ILE:CG1	1:2:841:VAL:HG21	2.39	0.53
2:3:554:ASN:O	2:3:557:ARG:N	2.42	0.53
2:3:724:VAL:O	2:3:728:VAL:HG23	2.08	0.53
4:5:164:GLY:HA3	4:5:258:LEU:HD11	1.90	0.53
11:E:596:HIS:C	11:E:598:LYS:N	2.60	0.53
12:G:515:VAL:O	12:G:515:VAL:HG23	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:G:586:VAL:HG21	12:G:623:TYR:HD1	1.72	0.53
14:N:13:GLN:HG3	14:N:16:LEU:CB	2.36	0.53
2:3:430:ILE:HB	2:3:470:VAL:HG13	1.90	0.53
3:4:445:ARG:HA	3:4:453:LEU:HD23	1.89	0.53
12:F:839:ASP:O	12:F:843:ASN:ND2	2.41	0.53
12:G:754:CYS:O	12:G:772:SER:N	2.41	0.53
14:N:45:VAL:HG13	14:N:52:ASN:CG	2.33	0.53
12:G:514:THR:HG23	12:G:527:HIS:CD2	2.43	0.53
12:G:753:ASN:ND2	12:G:773:GLU:OE2	2.42	0.53
14:N:15:PRO:O	14:N:18:ARG:HG2	2.08	0.53
1:2:386:GLN:OE1	1:2:416:ASP:N	2.41	0.53
3:4:274:GLN:NE2	3:4:278:ASP:OD1	2.40	0.53
11:E:232:GLU:O	11:E:236:VAL:HG23	2.08	0.53
11:E:579:TYR:CD2	11:E:637:LEU:HD22	2.44	0.53
12:F:511:TYR:O	12:F:530:ASP:N	2.37	0.53
12:F:902:SER:OG	12:F:911:VAL:HG22	2.09	0.53
3:4:624:SER:O	3:4:627:GLY:N	2.42	0.53
3:4:771:VAL:O	3:4:775:VAL:HG23	2.08	0.53
12:G:909:SER:OG	12:G:913:LYS:NZ	2.42	0.53
14:N:23:ARG:HB3	14:N:27:ARG:HH12	1.71	0.53
1:2:778:LEU:HB3	1:2:783:MET:SD	2.49	0.53
3:4:547:GLY:N	3:4:560:GLY:O	2.38	0.53
3:4:850:VAL:HG12	3:4:851:GLN:HG2	1.89	0.53
5:6:275:ARG:NH1	5:6:367:GLU:O	2.42	0.53
6:7:249:SER:O	6:7:311:GLN:NE2	2.42	0.53
3:4:272:MET:HE2	3:4:303:VAL:HG11	1.91	0.53
3:4:345:ALA:HB1	3:4:384:LEU:CD1	2.39	0.53
3:4:587:ARG:NH2	3:4:622:VAL:O	2.42	0.53
6:7:248:VAL:HG22	6:7:313:CYS:SG	2.48	0.53
6:7:463:GLY:N	18:7:902:AGS:O2B	2.36	0.53
9:C:120:LEU:O	9:C:124:VAL:HG23	2.07	0.53
11:E:618:ALA:HB1	11:E:636:ASP:HB3	1.91	0.53
2:3:343:THR:O	2:3:346:ASP:N	2.42	0.53
1:2:576:LEU:HD23	1:2:595:ALA:HB3	1.89	0.53
4:5:297:ILE:CD1	4:5:331:LEU:HD11	2.39	0.53
12:F:580:SER:C	12:F:618:LEU:HD12	2.34	0.53
12:F:743:TRP:HZ3	12:F:762:ILE:HG22	1.74	0.53
9:C:31:GLU:CG	9:C:44:LEU:HD11	2.40	0.52
1:2:426:VAL:HG22	1:2:456:ILE:HG13	1.91	0.52
5:6:803:MET:CE	5:6:831:LEU:HD12	2.39	0.52
12:F:717:LYS:HG3	12:F:719:LEU:HD21	1.90	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:H:755:ILE:HD11	12:H:768:LEU:HD21	1.91	0.52
1:2:520:PHE:CE1	1:2:767:ILE:HG13	2.44	0.52
2:3:412:SER:O	15:3:1001:ADP:H8	1.91	0.52
5:6:144:LYS:HA	5:6:196:LEU:HD11	1.89	0.52
5:6:287:LEU:C	5:6:288:LEU:HD12	2.34	0.52
6:7:22:THR:O	6:7:26:VAL:HG22	2.09	0.52
3:4:548:THR:HG21	3:4:760:PRO:O	2.10	0.52
1:2:564:VAL:HG11	1:2:595:ALA:HB1	1.92	0.52
3:4:243:LEU:O	3:4:306:TYR:N	2.37	0.52
3:4:349:CYS:SG	3:4:351:VAL:HG12	2.50	0.52
4:5:207:LEU:HD11	4:5:241:TYR:HB3	1.90	0.52
5:6:358:LYS:HA	5:6:380:ILE:HD13	1.90	0.52
9:C:135:LEU:HD21	9:C:177:TYR:HA	1.90	0.52
12:H:519:ASP:OD2	12:H:522:ARG:NE	2.43	0.52
14:N:38:LEU:HA	14:N:41:LEU:HD12	1.92	0.52
1:2:827:GLU:OE1	1:2:827:GLU:N	2.43	0.52
4:5:38:PHE:CZ	4:5:40:LEU:HD21	2.44	0.52
6:7:518:ASN:N	6:7:560:ARG:O	2.29	0.52
11:E:579:TYR:N	11:E:632:ILE:O	2.41	0.52
12:H:501:TYR:CG	12:H:768:LEU:HD13	2.45	0.52
14:N:17:LEU:HB2	14:N:20:LEU:CD1	2.39	0.52
2:3:200:VAL:N	2:3:248:SER:OG	2.43	0.52
3:4:217:ASN:N	3:4:221:ASP:OD2	2.43	0.52
3:4:361:ASP:O	3:4:364:VAL:HG12	2.10	0.52
11:E:49:PHE:O	11:E:53:LEU:N	2.43	0.52
11:E:127:ARG:O	11:E:129:TRP:N	2.43	0.52
1:2:244:VAL:HG21	1:2:295:VAL:HG13	1.91	0.52
1:2:849:GLN:HB3	1:2:853:VAL:HG22	1.91	0.52
2:3:424:ASN:OD1	2:3:425:THR:N	2.43	0.52
5:6:821:PRO:HA	5:6:824:ILE:HD12	1.91	0.52
8:B:16:ILE:O	8:B:20:VAL:HG23	2.10	0.52
12:H:477:MET:HA	12:H:477:MET:HE3	1.91	0.52
4:5:434:PRO:C	4:5:435:ILE:HD12	2.35	0.52
6:7:276:ARG:NH2	6:7:359:PRO:O	2.42	0.52
6:7:622:HIS:HB2	6:7:624:LYS:HZ2	1.67	0.52
12:F:864:LYS:HB3	12:F:868:ARG:NH1	2.25	0.52
4:5:606:CYS:SG	4:5:668:LEU:HD21	2.49	0.52
4:5:656:ILE:HA	4:5:659:ILE:HD12	1.92	0.52
5:6:557:LYS:HG3	5:6:565:LEU:HD12	1.91	0.52
12:G:580:SER:O	12:G:618:LEU:HD12	2.09	0.52
3:4:332:VAL:HG13	3:4:397:ILE:CG2	2.39	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:334:GLN:NE2	4:5:335:SER:O	2.42	0.51
5:6:548:LEU:O	5:6:552:LEU:HD13	2.10	0.51
11:E:259:LEU:O	11:E:263:GLY:N	2.43	0.51
1:2:439:ASN:ND2	1:2:444:PHE:O	2.42	0.51
5:6:324:SER:OG	5:6:325:PHE:N	2.42	0.51
5:6:409:GLN:OE1	5:6:409:GLN:N	2.42	0.51
11:E:541:ASN:OD1	11:E:544:THR:N	2.37	0.51
12:F:743:TRP:CZ3	12:F:762:ILE:HG22	2.45	0.51
1:2:249:LEU:HD22	1:2:257:ALA:HB2	1.91	0.51
2:3:479:THR:OG1	2:3:482:ASP:OD2	2.28	0.51
2:3:673:GLN:OE1	2:3:677:ASN:ND2	2.41	0.51
6:7:530:ASP:OD2	6:7:532:SER:N	2.43	0.51
11:E:71:TYR:CD2	11:E:96:LEU:HD13	2.45	0.51
11:E:527:LEU:HD21	11:E:641:LEU:HD13	1.91	0.51
1:2:393:ALA:O	1:2:397:VAL:HG23	2.10	0.51
4:5:437:VAL:HG21	4:5:472:ALA:HB2	1.91	0.51
4:5:521:ALA:HB2	4:5:550:PHE:CE1	2.44	0.51
5:6:105:ASP:OD1	5:6:108:GLY:N	2.41	0.51
12:G:484:THR:HG23	12:G:496:MET:CE	2.34	0.51
12:G:747:LEU:HD11	12:G:749:TYR:O	2.10	0.51
12:H:536:LEU:HB3	12:H:581:VAL:HG22	1.93	0.51
12:H:730:LYS:HA	12:H:815:ILE:HG12	1.92	0.51
1:2:777:LYS:N	1:2:827:GLU:O	2.43	0.51
3:4:631:ILE:HG23	3:4:631:ILE:O	2.11	0.51
6:7:260:TYR:CB	6:7:298:LEU:HD22	2.40	0.51
6:7:581:LEU:HD21	6:7:681:PHE:C	2.36	0.51
7:A:90:GLN:O	7:A:90:GLN:NE2	2.43	0.51
12:F:743:TRP:N	12:F:755:ILE:O	2.35	0.51
12:H:734:GLY:N	12:H:815:ILE:HD11	2.26	0.51
4:5:669:SER:OG	4:5:671:ILE:O	2.28	0.51
6:7:627:ASP:O	6:7:628:LEU:HG	2.10	0.51
7:A:1:MET:N	7:A:4:ASP:OD2	2.36	0.51
7:A:198:ARG:HH12	14:N:32:SER:HB2	1.75	0.51
10:D:212:THR:HG23	10:D:217:ASN:CG	2.36	0.51
11:E:588:TYR:CD2	11:E:597:THR:HA	2.46	0.51
12:H:887:HIS:CE1	12:H:917:ILE:HD11	2.44	0.51
2:3:481:VAL:HG12	6:7:486:LYS:NZ	2.25	0.51
3:4:261:LEU:HD12	3:4:265:PRO:HA	1.93	0.51
8:B:17:GLN:O	8:B:21:GLU:OE1	2.28	0.51
11:E:596:HIS:O	11:E:597:THR:HG23	2.11	0.51
12:G:837:LEU:HB2	12:G:855:LEU:HD21	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:322:GLY:C	1:2:390:LEU:HD11	2.35	0.51
2:3:324:ASN:OD1	2:3:325:THR:N	2.43	0.51
3:4:767:LYS:HB2	5:6:732:VAL:HG11	1.93	0.51
6:7:516:ALA:O	6:7:561:THR:OG1	2.29	0.51
8:B:33:THR:HG21	8:B:50:TRP:CH2	2.46	0.51
9:C:78:ASP:OD1	9:C:79:MET:N	2.44	0.51
11:E:406:ARG:HH22	11:E:590:ARG:HG2	1.76	0.51
12:G:778:MET:N	12:G:825:GLU:OE2	2.38	0.51
14:N:80:ASP:O	14:N:84:VAL:HG23	2.11	0.51
3:4:445:ARG:NH1	3:4:450:GLN:O	2.44	0.51
5:6:156:GLN:NE2	5:6:269:ASN:O	2.39	0.51
8:B:115:LEU:HD13	8:B:119:TRP:CD2	2.46	0.51
10:D:135:ARG:O	10:D:139:VAL:HG23	2.10	0.51
11:E:392:PHE:HB3	11:E:405:ILE:HD11	1.93	0.51
11:E:536:LEU:HD21	11:E:572:ILE:O	2.11	0.51
12:H:587:ARG:HE	12:H:643:LEU:HD21	1.76	0.51
12:H:853:GLU:OE1	12:H:853:GLU:N	2.40	0.51
14:N:20:LEU:HD12	14:N:21:ALA:N	2.25	0.51
1:2:546:GLY:HA2	15:2:901:ADP:H5'1	1.93	0.51
3:4:454:LYS:HA	6:7:277:THR:HG22	1.91	0.51
8:B:175:LEU:C	8:B:175:LEU:HD23	2.35	0.51
12:G:541:GLU:OE1	12:G:541:GLU:N	2.40	0.51
12:G:546:PHE:N	12:G:555:GLN:O	2.44	0.51
1:2:186:LEU:HD22	1:2:203:VAL:HG13	1.93	0.50
1:2:520:PHE:CD1	1:2:823:MET:HG2	2.47	0.50
1:2:658:ASN:ND2	1:2:660:THR:OG1	2.43	0.50
2:3:435:ARG:CG	4:5:491:VAL:HG11	2.41	0.50
4:5:20:ASN:O	4:5:23:ASP:N	2.44	0.50
6:7:656:VAL:CG1	6:7:713:VAL:HG21	2.35	0.50
11:E:75:ASP:O	11:E:118:ARG:NH2	2.43	0.50
12:G:672:ALA:HB1	12:G:761:HIS:HA	1.92	0.50
14:N:18:ARG:CG	14:N:19:PRO:HD3	2.39	0.50
1:2:556:VAL:O	1:2:560:ALA:N	2.44	0.50
2:3:406:LEU:HB3	2:3:543:PHE:CZ	2.46	0.50
5:6:356:TRP:HE1	5:6:380:ILE:HD12	1.77	0.50
6:7:397:VAL:HG13	6:7:640:GLU:CG	2.42	0.50
6:7:479:ARG:NH2	6:7:517:ASP:O	2.38	0.50
11:E:123:LEU:HD21	11:E:143:PHE:CD2	2.46	0.50
12:F:589:ILE:HD11	12:F:643:LEU:HD11	1.93	0.50
14:N:14:PRO:CD	14:N:15:PRO:HD2	2.40	0.50
3:4:254:THR:HG22	3:4:254:THR:O	2.10	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:463:TYR:OH	4:5:465:GLU:HB3	2.11	0.50
5:6:756:LYS:O	5:6:760:THR:HG23	2.11	0.50
12:F:708:SER:N	12:F:717:LYS:O	2.44	0.50
2:3:196:LEU:HD21	2:3:214:TYR:CZ	2.47	0.50
3:4:284:ILE:HG21	3:4:296:ILE:CD1	2.42	0.50
4:5:169:THR:HG22	4:5:256:LEU:HD22	1.94	0.50
12:F:629:HIS:N	12:F:637:SER:O	2.44	0.50
1:2:542:LEU:HD22	1:2:663:LEU:HD11	1.93	0.50
2:3:375:ASP:OD2	2:3:375:ASP:N	2.42	0.50
4:5:366:LEU:O	4:5:370:LEU:HD23	2.12	0.50
11:E:87:GLY:HA2	11:E:90:ILE:HG22	1.93	0.50
12:G:730:LYS:HA	12:G:815:ILE:HD12	1.93	0.50
1:2:847:ASP:OD1	1:2:848:ALA:N	2.45	0.50
2:3:98:ILE:HD11	2:3:157:PHE:HE1	1.75	0.50
2:3:215:THR:N	2:3:227:THR:OG1	2.42	0.50
3:4:797:GLN:C	3:4:801:MET:HE3	2.37	0.50
6:7:532:SER:O	6:7:535:THR:OG1	2.25	0.50
10:D:231:HIS:HB3	10:D:294:ILE:HD11	1.93	0.50
12:F:597:PHE:N	12:F:610:GLU:O	2.45	0.50
12:G:770:LEU:HD23	12:G:771:PRO:N	2.26	0.50
2:3:363:LEU:HB2	2:3:382:LEU:HD11	1.94	0.50
3:4:733:PRO:HG2	6:7:444:VAL:HG13	1.94	0.50
6:7:122:ASP:OD2	6:7:198:ARG:NH2	2.45	0.50
12:F:914:ILE:O	12:F:918:ARG:HG2	2.12	0.50
12:G:910:LEU:O	12:G:914:ILE:HD12	2.11	0.50
4:5:320:GLY:O	4:5:323:ILE:HG22	2.12	0.50
5:6:705:ILE:HG13	5:6:709:PHE:CZ	2.46	0.50
6:7:652:MET:HE1	6:7:657:ASN:OD1	2.12	0.50
11:E:1:MET:N	11:E:144:ASP:OD2	2.43	0.50
11:E:345:ASN:O	11:E:349:SER:N	2.45	0.50
12:H:536:LEU:HD11	12:H:578:ILE:O	2.12	0.50
14:N:60:ILE:HG13	14:N:64:GLU:OE2	2.11	0.50
1:2:559:THR:O	1:2:559:THR:HG22	2.11	0.50
2:3:495:VAL:O	2:3:506:LEU:N	2.37	0.50
2:3:535:LEU:HD22	2:3:539:LEU:HD23	1.93	0.50
4:5:297:ILE:HD11	4:5:331:LEU:HD11	1.94	0.50
6:7:240:THR:OG1	6:7:352:THR:HG22	2.12	0.50
6:7:385:LYS:H	6:7:385:LYS:HZ3	1.60	0.50
1:2:673:ILE:HG22	1:2:677:PHE:CE2	2.45	0.49
2:3:366:SER:CA	2:3:650:LEU:HD22	2.42	0.49
2:3:529:PRO:O	2:3:533:ILE:N	2.45	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:137:LEU:CD1	10:D:185:THR:HG21	2.43	0.49
11:E:522:LEU:HD22	11:E:525:TYR:CE2	2.47	0.49
12:F:762:ILE:H	12:F:762:ILE:HD12	1.77	0.49
1:2:784:ASP:O	1:2:787:SER:OG	2.24	0.49
1:2:810:LEU:HA	1:2:813:ILE:HD12	1.94	0.49
12:F:552:GLY:C	12:F:569:ILE:HG23	2.37	0.49
12:F:863:ASP:OD2	12:F:890:LYS:N	2.44	0.49
12:G:741:HIS:CD2	12:G:762:ILE:HG22	2.47	0.49
12:H:631:SER:OG	12:H:634:HIS:N	2.43	0.49
1:2:353:GLN:OE1	1:2:383:ARG:NH2	2.46	0.49
4:5:594:ILE:O	4:5:599:MET:HE1	2.12	0.49
4:5:614:LEU:HA	4:5:672:ALA:HB3	1.94	0.49
6:7:590:LEU:HD11	6:7:594:PHE:CE2	2.47	0.49
14:N:54:ARG:HA	14:N:54:ARG:CZ	2.42	0.49
5:6:313:MET:HE2	5:6:340:ASN:HB2	1.94	0.49
12:G:601:ASN:N	12:G:605:VAL:O	2.44	0.49
12:G:833:LEU:HB3	12:G:858:LEU:HD21	1.95	0.49
1:2:414:LEU:O	1:2:417:VAL:HG23	2.12	0.49
1:2:551:GLN:NE2	15:2:901:ADP:O3'	2.46	0.49
2:3:313:THR:O	4:5:175:ARG:NH2	2.43	0.49
4:5:466:GLY:HA3	4:5:470:VAL:HG21	1.94	0.49
4:5:625:ASN:HD22	4:5:681:ILE:HG21	1.78	0.49
6:7:107:GLN:NE2	6:7:221:SER:HB3	2.27	0.49
8:B:19:ILE:HD12	10:D:68:LYS:HD2	1.95	0.49
8:B:124:ARG:NH2	9:C:190:TRP:O	2.46	0.49
14:N:77:LEU:HB3	14:N:80:ASP:OD1	2.11	0.49
1:2:270:ILE:O	1:2:274:VAL:HG23	2.13	0.49
2:3:481:VAL:HG12	6:7:486:LYS:HZ3	1.78	0.49
6:7:225:LEU:HD13	6:7:229:GLN:HB3	1.95	0.49
6:7:444:VAL:HG12	6:7:446:ASP:H	1.77	0.49
6:7:463:GLY:C	18:7:902:AGS:H5'2	2.38	0.49
8:B:113:SER:O	8:B:152:ARG:NH2	2.45	0.49
10:D:284:ASP:O	10:D:288:ASP:N	2.43	0.49
12:G:597:PHE:N	12:G:610:GLU:O	2.45	0.49
2:3:58:ASP:HB2	6:7:219:ALA:O	2.12	0.49
2:3:419:LEU:HD11	2:3:515:ALA:CB	2.42	0.49
6:7:139:LEU:O	6:7:143:LEU:HB2	2.12	0.49
10:D:98:ILE:HD11	10:D:129:MET:HB3	1.94	0.49
11:E:21:SER:OG	11:E:26:GLN:NE2	2.44	0.49
11:E:381:ASP:OD2	11:E:383:SER:OG	2.22	0.49
12:G:629:HIS:O	12:G:637:SER:N	2.45	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:14:PRO:HG3	14:N:39:SER:HA	1.94	0.49
1:2:356:ASN:OD1	1:2:433:ASN:ND2	2.45	0.49
1:2:418:SER:OG	1:2:422:GLU:OE1	2.26	0.49
3:4:634:PHE:N	3:4:674:SER:O	2.42	0.49
12:H:895:LEU:HD11	12:H:921:ARG:CZ	2.43	0.49
14:N:13:GLN:N	14:N:14:PRO:HD3	2.27	0.49
14:N:81:GLN:HE22	14:N:85:LYS:HD3	1.77	0.49
2:3:384:MET:HE2	2:3:513:ILE:CD1	2.42	0.49
2:3:552:ASP:OD1	2:3:553:ILE:N	2.45	0.49
3:4:420:TYR:C	3:4:424:VAL:HG23	2.38	0.49
3:4:526:ILE:HD12	3:4:540:ILE:HD11	1.95	0.49
3:4:593:GLY:HA3	3:4:637:MET:HB2	1.95	0.49
4:5:165:ILE:N	4:5:258:LEU:HD11	2.28	0.49
5:6:298:SER:O	5:6:357:GLN:NE2	2.46	0.49
5:6:361:ILE:HG21	5:6:397:PHE:HE2	1.78	0.49
12:G:711:ARG:HH22	12:G:840:THR:HG22	1.77	0.49
12:H:570:ILE:HD12	12:H:590:VAL:HG11	1.95	0.49
14:N:62:PHE:CE1	14:N:88:ILE:HG21	2.48	0.49
3:4:605:ILE:CG2	3:4:614:LEU:HD11	2.43	0.49
8:B:102:ILE:HG13	8:B:148:LEU:HD21	1.94	0.49
12:F:638:TYR:HB3	12:F:657:LEU:HD12	1.94	0.49
14:N:14:PRO:HD2	14:N:15:PRO:HD2	1.93	0.49
1:2:244:VAL:N	1:2:296:ARG:O	2.43	0.48
1:2:331:PHE:CD2	4:5:323:ILE:HD11	2.43	0.48
5:6:128:ASP:O	5:6:129:THR:HG22	2.13	0.48
11:E:12:TYR:CE2	11:E:16:LEU:HD11	2.47	0.48
11:E:343:TYR:OH	11:E:403:ASP:OD2	2.30	0.48
12:G:545:LEU:HD12	12:G:546:PHE:H	1.78	0.48
12:G:757:VAL:HG21	12:G:764:PRO:HA	1.95	0.48
1:2:197:TRP:O	1:2:203:VAL:HG11	2.13	0.48
3:4:341:ASP:O	3:4:392:ALA:N	2.30	0.48
5:6:141:GLU:OE2	5:6:145:ILE:HD11	2.13	0.48
5:6:410:LEU:HD12	5:6:443:LEU:HD21	1.94	0.48
8:B:178:ILE:HG23	10:D:229:PHE:CD2	2.47	0.48
11:E:152:LEU:O	11:E:156:LYS:N	2.39	0.48
11:E:352:ASN:OD1	11:E:355:GLY:N	2.42	0.48
12:G:823:ALA:HB2	12:G:868:ARG:HE	1.77	0.48
12:H:741:HIS:CD2	12:H:762:ILE:HG22	2.48	0.48
1:2:785:LYS:O	1:2:789:VAL:HG23	2.13	0.48
15:2:901:ADP:O2A	5:6:798:ARG:NH2	2.46	0.48
5:6:519:MET:HB2	5:6:525:ILE:HD13	1.94	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:260:TYR:HB3	6:7:298:LEU:HD22	1.95	0.48
6:7:556:THR:C	6:7:557:LEU:HD22	2.38	0.48
12:G:484:THR:HG22	12:G:763:TRP:HB2	1.95	0.48
12:G:676:TYR:CG	12:G:762:ILE:HD11	2.48	0.48
12:G:706:LEU:HD23	12:G:707:LEU:N	2.28	0.48
12:G:910:LEU:O	12:G:911:VAL:C	2.57	0.48
14:N:15:PRO:HA	14:N:18:ARG:HE	1.77	0.48
14:N:20:LEU:O	14:N:24:VAL:HG23	2.13	0.48
14:N:70:TRP:CZ3	14:N:84:VAL:HG22	2.48	0.48
1:2:306:LEU:HD23	1:2:320:VAL:HG11	1.94	0.48
2:3:553:ILE:HG23	4:5:630:ARG:HG2	1.95	0.48
3:4:356:MET:N	3:4:356:MET:SD	2.85	0.48
5:6:585:LEU:HD11	5:6:681:ALA:HB3	1.94	0.48
5:6:628:LEU:O	5:6:632:ASP:N	2.46	0.48
8:B:48:THR:HG23	10:D:120:ASN:O	2.13	0.48
9:C:135:LEU:HD12	9:C:169:LEU:HD11	1.94	0.48
11:E:351:TRP:HA	11:E:511:VAL:HG12	1.96	0.48
11:E:375:GLU:HB2	11:E:380:MET:HE1	1.94	0.48
12:G:866:LEU:HD13	12:G:889:LEU:HD23	1.96	0.48
14:N:14:PRO:CG	14:N:39:SER:HA	2.44	0.48
1:2:261:ALA:O	1:2:316:SER:OG	2.27	0.48
1:2:821:ALA:N	1:2:833:ASP:OD1	2.46	0.48
6:7:626:PRO:O	6:7:628:LEU:HD23	2.14	0.48
11:E:612:ILE:O	11:E:616:THR:HG22	2.13	0.48
12:F:588:VAL:N	12:F:600:PHE:O	2.41	0.48
11:E:228:LYS:O	11:E:232:GLU:OE1	2.32	0.48
5:6:363:GLU:OE2	5:6:368:ILE:N	2.45	0.48
5:6:603:SER:HB2	5:6:608:LEU:HD11	1.95	0.48
5:6:627:ALA:HA	5:6:630:LEU:HD12	1.95	0.48
6:7:195:ASN:HA	6:7:198:ARG:HD2	1.96	0.48
11:E:613:THR:OG1	11:E:620:VAL:HG21	2.14	0.48
14:N:63:LEU:C	14:N:63:LEU:HD23	2.38	0.48
14:N:92:LYS:O	14:N:95:GLU:HG3	2.13	0.48
2:3:342:LEU:HB3	2:3:347:ILE:HD11	1.95	0.48
3:4:662:ILE:HG23	3:4:662:ILE:O	2.14	0.48
4:5:413:LEU:O	4:5:554:PHE:N	2.46	0.48
5:6:199:THR:O	5:6:261:ARG:NH2	2.47	0.48
5:6:552:LEU:O	5:6:812:ARG:NH1	2.46	0.48
5:6:764:ILE:O	5:6:819:ILE:N	2.43	0.48
9:C:53:ILE:O	9:C:57:VAL:HG22	2.14	0.48
11:E:227:LYS:HA	11:E:230:ILE:HG22	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:238:ASN:O	1:2:290:HIS:NE2	2.47	0.48
1:2:850:LYS:O	1:2:854:ARG:HB3	2.14	0.48
2:3:393:LEU:HD23	6:7:623:ASN:CG	2.39	0.48
4:5:393:MET:CE	4:5:666:LEU:HD23	2.44	0.48
5:6:576:ASP:O	5:6:579:THR:HG23	2.14	0.48
10:D:159:ARG:NH2	10:D:184:ASP:OD1	2.45	0.48
11:E:486:ASP:O	11:E:489:VAL:HG13	2.14	0.48
12:G:514:THR:HG23	12:G:527:HIS:NE2	2.29	0.48
12:G:737:THR:O	12:G:737:THR:HG23	2.14	0.48
1:2:570:GLY:O	5:6:665:LYS:NZ	2.47	0.48
2:3:223:THR:N	4:5:246:GLU:OE2	2.46	0.48
3:4:244:ASP:C	3:4:244:ASP:OD1	2.57	0.48
3:4:686:LEU:HD23	3:4:690:GLU:HG2	1.95	0.48
5:6:653:HIS:HA	5:6:705:ILE:HD13	1.95	0.48
8:B:124:ARG:NH2	9:C:194:LYS:O	2.47	0.48
9:C:22:TYR:HB2	9:C:24:ILE:HD11	1.96	0.48
12:G:489:THR:HG22	12:G:490:ASP:N	2.29	0.48
12:H:881:LYS:O	12:H:884:SER:OG	2.31	0.48
2:3:339:ARG:NE	2:3:340:GLN:O	2.47	0.47
2:3:537:ASP:OD1	2:3:538:SER:N	2.47	0.47
3:4:364:VAL:HG23	5:6:438:THR:HG23	1.96	0.47
3:4:370:ARG:NE	3:4:377:ASN:O	2.47	0.47
5:6:584:PHE:O	5:6:588:VAL:HG23	2.14	0.47
5:6:705:ILE:HG13	5:6:709:PHE:CE1	2.49	0.47
5:6:736:MET:HG3	5:6:737:LYS:HD2	1.96	0.47
6:7:73:ARG:NH1	6:7:133:ASP:HB2	2.29	0.47
6:7:383:GLN:HB3	6:7:385:LYS:HZ3	1.79	0.47
11:E:581:VAL:N	11:E:630:ILE:O	2.47	0.47
12:G:535:ASP:OD1	12:G:536:LEU:N	2.47	0.47
3:4:243:LEU:CD2	3:4:272:MET:HE1	2.45	0.47
4:5:572:VAL:HG13	4:5:576:HIS:CE1	2.50	0.47
6:7:313:CYS:O	6:7:333:ILE:N	2.45	0.47
11:E:576:THR:HG22	11:E:578:THR:HG23	1.96	0.47
12:F:661:LEU:HD12	12:G:633:PHE:CZ	2.49	0.47
12:G:696:CYS:SG	12:G:704:LEU:HD11	2.54	0.47
12:G:761:HIS:ND1	12:G:765:GLU:OE2	2.41	0.47
12:H:601:ASN:OD1	12:H:605:VAL:HB	2.13	0.47
12:H:899:VAL:HG23	12:H:914:ILE:CG2	2.44	0.47
1:2:540:LEU:C	1:2:541:LEU:HD22	2.39	0.47
3:4:294:ASP:O	3:4:298:THR:N	2.43	0.47
6:7:265:CYS:HB3	6:7:289:CYS:SG	2.53	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:F:643:LEU:HD22	12:F:648:LYS:CD	2.45	0.47
14:N:70:TRP:CH2	14:N:84:VAL:HA	2.49	0.47
1:2:669:LEU:HB2	1:2:674:LEU:HD21	1.95	0.47
2:3:367:LEU:O	2:3:378:LYS:NZ	2.24	0.47
4:5:614:LEU:HD12	4:5:614:LEU:O	2.15	0.47
8:B:196:HIS:CE1	8:B:200:LEU:HD11	2.49	0.47
11:E:596:HIS:CE1	11:E:597:THR:HG22	2.48	0.47
12:H:524:ARG:NH1	12:H:526:TYR:HB3	2.29	0.47
1:2:704:VAL:HG21	5:6:770:ARG:HH11	1.79	0.47
3:4:227:ILE:O	3:4:231:ASN:ND2	2.48	0.47
3:4:308:VAL:HG11	3:4:325:LEU:HB3	1.97	0.47
12:F:636:LEU:HD21	12:F:661:LEU:HD11	1.97	0.47
1:2:709:GLU:O	1:2:710:ASN:C	2.57	0.47
2:3:486:ILE:O	2:3:487:HIS:C	2.57	0.47
3:4:345:ALA:HB1	3:4:384:LEU:HD11	1.96	0.47
5:6:156:GLN:C	5:6:160:MET:HE3	2.40	0.47
10:D:282:ILE:O	10:D:283:ARG:C	2.57	0.47
12:F:598:ARG:HG2	12:F:609:VAL:HG22	1.95	0.47
12:F:833:LEU:HB2	12:F:858:LEU:HD21	1.96	0.47
12:G:826:GLU:OE1	12:G:868:ARG:NH2	2.47	0.47
1:2:187:SER:HA	1:2:255:ILE:HD11	1.97	0.47
2:3:365:GLN:O	2:3:378:LYS:NZ	2.47	0.47
2:3:721:VAL:HG12	2:3:722:ASN:N	2.29	0.47
4:5:165:ILE:O	4:5:258:LEU:HD12	2.14	0.47
4:5:211:CYS:O	4:5:241:TYR:OH	2.11	0.47
5:6:360:ARG:NH1	5:6:378:ASP:OD1	2.47	0.47
6:7:219:ALA:C	6:7:220:ILE:HG13	2.40	0.47
6:7:228:ARG:NH2	6:7:329:ARG:HG3	2.30	0.47
6:7:437:VAL:HG11	6:7:702:LEU:CD2	2.44	0.47
6:7:700:ALA:O	6:7:704:LEU:N	2.48	0.47
10:D:78:PRO:HA	10:D:174:LEU:HD12	1.97	0.47
10:D:212:THR:O	10:D:212:THR:HG22	2.15	0.47
10:D:282:ILE:CG2	10:D:291:VAL:HG21	2.45	0.47
12:G:510:GLN:NE2	12:G:529:GLU:HB3	2.30	0.47
12:G:728:ILE:HD12	12:G:740:ILE:HG21	1.97	0.47
12:H:510:GLN:OE1	12:H:510:GLN:N	2.48	0.47
14:N:66:PHE:HZ	14:N:72:GLN:HE21	1.62	0.47
1:2:219:THR:HG22	1:2:225:SER:CA	2.42	0.47
4:5:494:HIS:ND1	4:5:549:ARG:HG3	2.30	0.47
5:6:308:SER:OG	5:6:347:ASN:O	2.33	0.47
7:A:177:GLU:O	14:N:19:PRO:HG3	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:D:12:LEU:CD2	12:F:867:LEU:HD13	2.44	0.47
11:E:282:ILE:HG23	11:E:283:ALA:N	2.30	0.47
11:E:285:ALA:HB2	11:E:590:ARG:NH2	2.30	0.47
2:3:442:LEU:O	2:3:461:ALA:N	2.48	0.47
3:4:457:TYR:HE2	6:7:255:VAL:HG13	1.80	0.47
5:6:154:ASP:OD1	5:6:156:GLN:N	2.42	0.47
6:7:525:GLU:O	6:7:528:LYS:N	2.48	0.47
6:7:622:HIS:N	6:7:622:HIS:CD2	2.82	0.47
9:C:18:CYS:SG	9:C:74:LEU:HD13	2.55	0.47
12:H:587:ARG:HE	12:H:643:LEU:HD11	1.79	0.47
12:H:898:ALA:HA	12:H:901:ILE:HD12	1.96	0.47
2:3:494:THR:CA	2:3:508:ALA:HB3	2.45	0.47
3:4:376:CYS:O	3:4:377:ASN:OD1	2.32	0.47
3:4:529:SER:O	3:4:723:HIS:NE2	2.48	0.47
4:5:274:LEU:HD23	4:5:275:THR:N	2.30	0.47
11:E:536:LEU:HD21	11:E:572:ILE:HG23	1.97	0.47
11:E:568:VAL:C	11:E:569:LEU:HD22	2.41	0.47
12:G:513:ILE:HD12	12:G:530:ASP:HB2	1.96	0.47
1:2:388:VAL:N	1:2:407:GLU:OE2	2.49	0.46
1:2:482:ARG:HB3	1:2:486:LYS:HZ3	1.80	0.46
2:3:143:ASN:O	2:3:147:VAL:HG23	2.15	0.46
2:3:198:ARG:NE	2:3:213:ASP:OD1	2.40	0.46
10:D:97:LEU:O	10:D:101:ILE:HG12	2.15	0.46
10:D:202:MET:SD	10:D:203:PRO:HD2	2.55	0.46
1:2:606:ILE:HG22	1:2:647:ILE:O	2.15	0.46
2:3:263:GLU:OE1	2:3:263:GLU:N	2.40	0.46
2:3:365:GLN:HA	2:3:378:LYS:HZ1	1.79	0.46
3:4:213:GLU:HA	3:4:216:ILE:HG23	1.97	0.46
6:7:67:LEU:HD22	6:7:121:ILE:HG23	1.95	0.46
11:E:426:GLU:OE2	11:E:547:ARG:NH1	2.39	0.46
11:E:501:ASP:O	11:E:504:ARG:HG2	2.15	0.46
11:E:546:LEU:HD11	11:E:629:ILE:HD11	1.96	0.46
12:G:482:ALA:O	12:G:496:MET:N	2.49	0.46
12:G:749:TYR:CG	12:G:750:ASP:N	2.82	0.46
1:2:260:LEU:N	1:2:267:MET:SD	2.89	0.46
1:2:603:VAL:HG13	1:2:647:ILE:HG12	1.97	0.46
2:3:192:VAL:HG13	2:3:283:VAL:HG11	1.96	0.46
3:4:281:VAL:HG22	3:4:293:LEU:CD1	2.45	0.46
4:5:162:LEU:C	4:5:162:LEU:HD12	2.40	0.46
6:7:315:ILE:CG2	6:7:333:ILE:HD11	2.45	0.46
12:G:687:LEU:HD12	12:G:697:ILE:HB	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:H:741:HIS:N	12:H:757:VAL:O	2.37	0.46
14:N:34:LYS:HG3	14:N:35:SER:H	1.80	0.46
1:2:794:ARG:NH1	1:2:805:ILE:O	2.48	0.46
1:2:811:GLU:HA	1:2:814:LEU:HD12	1.96	0.46
3:4:349:CYS:CB	3:4:382:MET:HE1	2.45	0.46
3:4:601:LEU:O	3:4:620:ALA:N	2.48	0.46
5:6:156:GLN:O	5:6:160:MET:HE3	2.15	0.46
5:6:639:ASP:OD1	5:6:640:GLU:HG2	2.14	0.46
6:7:437:VAL:HG21	6:7:702:LEU:CD2	2.46	0.46
12:G:515:VAL:HG21	12:G:526:TYR:CE1	2.51	0.46
12:H:918:ARG:O	12:H:922:TYR:CD1	2.68	0.46
1:2:341:CYS:O	1:2:345:GLY:HA3	2.16	0.46
2:3:217:ALA:HB1	2:3:301:LEU:CD2	2.45	0.46
3:4:634:PHE:HZ	3:4:698:LEU:HD21	1.79	0.46
3:4:764:GLU:O	3:4:768:THR:HG23	2.16	0.46
4:5:649:THR:OG1	4:5:650:ILE:N	2.47	0.46
6:7:502:VAL:O	6:7:503:THR:HG22	2.15	0.46
11:E:81:LEU:HD12	11:E:120:ILE:HG12	1.97	0.46
12:G:485:PRO:HB3	12:G:679:PHE:HB2	1.97	0.46
12:H:580:SER:C	12:H:618:LEU:HD12	2.41	0.46
1:2:344:CYS:SG	1:2:345:GLY:N	2.88	0.46
4:5:623:SER:O	4:5:627:VAL:HG22	2.15	0.46
5:6:115:PHE:CE2	5:6:119:LEU:HD11	2.51	0.46
6:7:224:PRO:HG2	6:7:242:ARG:NH2	2.30	0.46
11:E:339:TYR:CD1	11:E:350:LEU:HD21	2.50	0.46
11:E:612:ILE:HD12	11:E:643:LYS:HB3	1.98	0.46
12:G:517:PHE:O	12:G:520:VAL:HG23	2.16	0.46
12:H:585:PRO:O	12:H:602:GLN:NE2	2.48	0.46
12:H:743:TRP:N	12:H:755:ILE:O	2.38	0.46
14:N:34:LYS:HG2	14:N:36:ASP:OD1	2.16	0.46
2:3:45:ILE:HA	2:3:92:LEU:HD12	1.96	0.46
2:3:167:SER:N	2:3:170:THR:OG1	2.47	0.46
4:5:164:GLY:C	4:5:258:LEU:HD11	2.40	0.46
8:B:166:SER:OG	8:B:167:HIS:N	2.49	0.46
10:D:101:ILE:CG2	10:D:126:LEU:HD11	2.45	0.46
2:3:256:ILE:HD13	2:3:278:LEU:HD11	1.98	0.46
2:3:570:ARG:CG	4:5:614:LEU:HD11	2.45	0.46
3:4:597:SER:O	3:4:601:LEU:N	2.45	0.46
6:7:494:THR:HA	6:7:513:LEU:HD12	1.97	0.46
12:F:491:ARG:HB3	12:F:505:VAL:HG13	1.98	0.46
12:G:566:TRP:NE1	12:G:602:GLN:O	2.48	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:17:LEU:HD11	14:N:38:LEU:HD12	1.96	0.46
14:N:78:PHE:O	14:N:82:SER:OG	2.33	0.46
3:4:226:TYR:O	3:4:230:LEU:HD13	2.15	0.46
3:4:403:PRO:HA	3:4:406:VAL:HG22	1.97	0.46
3:4:629:CYS:N	3:4:670:SER:O	2.47	0.46
4:5:412:VAL:HG13	4:5:552:MET:HB2	1.98	0.46
6:7:354:ILE:O	6:7:376:LEU:HD12	2.16	0.46
12:H:489:THR:HG22	12:H:491:ARG:H	1.81	0.46
1:2:691:ALA:O	1:2:695:LEU:HD23	2.16	0.46
2:3:103:LEU:HD11	2:3:110:PHE:CD2	2.51	0.46
3:4:305:PRO:HG2	3:4:464:VAL:HG21	1.98	0.46
5:6:766:THR:O	5:6:770:ARG:N	2.39	0.46
6:7:633:VAL:CG1	6:7:637:LYS:HE3	2.34	0.46
7:A:137:LEU:HD21	10:D:182:TYR:CD1	2.50	0.46
9:C:39:THR:C	9:C:42:THR:HG1	2.21	0.46
10:D:260:ILE:HG22	10:D:281:VAL:HG21	1.98	0.46
12:G:567:THR:HG22	12:G:568:LYS:N	2.31	0.46
1:2:306:LEU:HD12	1:2:392:GLU:HG3	1.98	0.45
2:3:476:ASP:N	2:3:476:ASP:OD1	2.49	0.45
4:5:323:ILE:O	4:5:324:ARG:NE	2.49	0.45
5:6:143:MET:HG3	5:6:196:LEU:HD13	1.98	0.45
9:C:119:GLU:O	9:C:123:VAL:HG23	2.15	0.45
11:E:262:ILE:O	11:E:262:ILE:HG22	2.17	0.45
12:G:708:SER:N	12:G:717:LYS:O	2.49	0.45
12:G:781:PHE:HB3	12:G:786:LEU:HD11	1.97	0.45
12:H:581:VAL:HG23	12:H:581:VAL:O	2.16	0.45
1:2:237:MET:HE2	1:2:237:MET:CA	2.45	0.45
1:2:340:ASN:O	1:2:374:ARG:N	2.48	0.45
1:2:474:PHE:CD1	1:2:474:PHE:C	2.95	0.45
2:3:48:TYR:HA	2:3:51:ASN:OD1	2.16	0.45
3:4:435:VAL:HG12	3:4:466:VAL:HG22	1.98	0.45
3:4:574:LYS:N	18:4:1001:AGS:O2B	2.40	0.45
3:4:817:VAL:HG12	3:4:818:GLU:N	2.31	0.45
4:5:360:LEU:C	4:5:366:LEU:HD22	2.41	0.45
4:5:634:LEU:C	4:5:634:LEU:HD23	2.41	0.45
5:6:632:ASP:N	5:6:632:ASP:OD1	2.49	0.45
7:A:67:VAL:HG22	9:C:25:PRO:HD2	1.98	0.45
11:E:83:LEU:HD12	11:E:83:LEU:N	2.31	0.45
12:F:879:VAL:HG23	12:F:907:LEU:HD22	1.97	0.45
12:G:536:LEU:CD1	12:G:578:ILE:HG22	2.47	0.45
12:G:711:ARG:NH2	12:G:840:THR:HG22	2.31	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:G:741:HIS:NE2	12:G:762:ILE:HG22	2.32	0.45
12:H:685:LYS:NZ	12:H:699:GLY:O	2.45	0.45
14:N:62:PHE:CE2	14:N:88:ILE:HB	2.51	0.45
1:2:246:TYR:CZ	1:2:257:ALA:HB1	2.51	0.45
1:2:482:ARG:HB3	1:2:486:LYS:NZ	2.32	0.45
1:2:756:SER:OG	1:2:758:ILE:O	2.28	0.45
2:3:668:ILE:HG22	2:3:670:GLN:HE22	1.79	0.45
4:5:552:MET:CE	4:5:659:ILE:HD11	2.42	0.45
5:6:771:SER:O	5:6:772:TYR:C	2.59	0.45
6:7:131:GLU:CD	6:7:135:LYS:HE3	2.41	0.45
12:F:640:LEU:HD21	12:F:710:TRP:CE3	2.51	0.45
12:F:850:ASN:O	12:F:854:VAL:HG23	2.15	0.45
12:G:496:MET:O	12:G:497:ASN:ND2	2.49	0.45
12:G:741:HIS:O	12:G:757:VAL:N	2.44	0.45
14:N:79:ILE:O	14:N:82:SER:HB2	2.16	0.45
1:2:273:LEU:O	1:2:276:MET:HB2	2.16	0.45
2:3:301:LEU:N	2:3:318:LYS:O	2.39	0.45
2:3:393:LEU:HG	2:3:399:LEU:HD11	1.98	0.45
2:3:428:LEU:HD21	2:3:465:ALA:HA	1.99	0.45
3:4:402:THR:HG23	3:4:405:PHE:H	1.81	0.45
3:4:726:ASN:HA	3:4:729:LEU:HD12	1.98	0.45
4:5:164:GLY:CA	4:5:258:LEU:HD11	2.46	0.45
4:5:389:VAL:HG12	4:5:666:LEU:HD21	1.98	0.45
5:6:448:LEU:HD23	5:6:450:TYR:OH	2.15	0.45
5:6:514:ASN:O	5:6:518:GLU:HG2	2.16	0.45
7:A:123:LEU:O	7:A:128:GLN:NE2	2.48	0.45
12:G:752:LEU:N	12:G:774:MET:O	2.48	0.45
1:2:306:LEU:HD12	1:2:404:ARG:O	2.17	0.45
2:3:395:ASN:OD1	2:3:396:GLY:N	2.49	0.45
2:3:489:VAL:CG1	2:3:508:ALA:HB1	2.45	0.45
4:5:278:CYS:HB3	4:5:330:ILE:HD12	1.98	0.45
4:5:616:PRO:O	4:5:620:GLU:OE1	2.35	0.45
5:6:794:ARG:NH2	5:6:835:ILE:O	2.49	0.45
10:D:65:LYS:O	10:D:69:ASN:ND2	2.49	0.45
10:D:223:ASP:OD1	10:D:225:ASN:N	2.50	0.45
11:E:301:ARG:O	12:F:491:ARG:NH2	2.46	0.45
12:H:892:ASP:OD1	12:H:895:LEU:HD12	2.17	0.45
1:2:783:MET:CE	4:5:573:ILE:HG23	2.43	0.45
2:3:294:VAL:HG13	2:3:326:VAL:HG22	1.99	0.45
2:3:405:ILE:O	2:3:513:ILE:HA	2.17	0.45
2:3:430:ILE:HG21	2:3:461:ALA:HB1	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:703:GLU:HA	2:3:706:ILE:HD12	1.99	0.45
5:6:766:THR:H	5:6:769:ALA:HB3	1.81	0.45
6:7:428:VAL:O	6:7:432:LEU:HD13	2.16	0.45
7:A:175:GLN:HB3	14:N:33:ILE:HG13	1.98	0.45
9:C:135:LEU:C	9:C:135:LEU:HD23	2.42	0.45
12:F:502:VAL:HG22	12:F:515:VAL:HG13	1.99	0.45
1:2:425:GLU:O	1:2:457:LYS:N	2.49	0.45
2:3:727:LYS:O	2:3:731:ASN:ND2	2.39	0.45
3:4:199:MET:HE1	3:4:279:CYS:SG	2.57	0.45
3:4:342:MET:HE1	3:4:389:CYS:HB3	1.98	0.45
5:6:702:THR:HG23	5:6:705:ILE:HG22	1.99	0.45
6:7:402:MET:HA	6:7:405:ILE:HD12	1.98	0.45
7:A:25:GLN:NE2	7:A:27:VAL:HG22	2.31	0.45
7:A:176:THR:HG22	7:A:177:GLU:N	2.32	0.45
12:F:570:ILE:HD13	12:F:590:VAL:HG11	1.99	0.45
12:F:629:HIS:O	12:F:637:SER:N	2.48	0.45
12:F:881:LYS:O	12:F:885:LEU:HD13	2.17	0.45
12:G:722:LEU:HD12	12:G:752:LEU:HD22	1.99	0.45
1:2:861:PHE:O	1:2:865:THR:HG22	2.17	0.45
2:3:38:TYR:O	2:3:42:VAL:HG23	2.16	0.45
2:3:235:ASP:OD1	2:3:236:THR:N	2.49	0.45
3:4:200:SER:H	3:4:224:LEU:HD13	1.81	0.45
3:4:314:MET:HB2	3:4:328:LEU:HD11	1.99	0.45
3:4:331:LEU:C	3:4:399:LEU:HD12	2.42	0.45
3:4:342:MET:HG3	3:4:360:ILE:HG13	1.99	0.45
4:5:207:LEU:HD21	4:5:241:TYR:O	2.16	0.45
8:B:104:TYR:OH	8:B:111:ARG:NH2	2.45	0.45
11:E:541:ASN:OD1	11:E:543:LEU:N	2.50	0.45
12:G:570:ILE:CD1	12:G:590:VAL:HG11	2.47	0.45
1:2:826:SER:OG	1:2:828:PHE:O	2.35	0.45
2:3:543:PHE:CG	2:3:544:ASP:N	2.83	0.45
3:4:522:LEU:HD22	3:4:747:LEU:CD1	2.47	0.45
3:4:531:TYR:OH	3:4:719:GLU:OE1	2.35	0.45
4:5:45:ILE:HG13	4:5:46:TYR:N	2.32	0.45
4:5:616:PRO:O	4:5:619:ALA:HB3	2.16	0.45
5:6:105:ASP:O	5:6:108:GLY:N	2.50	0.45
5:6:525:ILE:HG13	5:6:529:LEU:HD11	1.98	0.45
5:6:642:ASP:N	5:6:642:ASP:OD1	2.49	0.45
6:7:463:GLY:O	18:7:902:AGS:H5'2	2.17	0.45
6:7:579:SER:O	6:7:583:ASN:ND2	2.50	0.45
7:A:37:ILE:HD12	7:A:37:ILE:H	1.82	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:E:589:PRO:O	11:E:592:LEU:HB2	2.16	0.45
12:F:538:PHE:HB2	12:F:581:VAL:HG23	1.99	0.45
12:H:504:THR:CG2	12:H:513:ILE:HG23	2.45	0.45
12:H:703:THR:HA	12:H:723:ASP:HA	1.99	0.45
14:N:16:LEU:O	14:N:19:PRO:HD2	2.17	0.45
1:2:249:LEU:CD2	1:2:257:ALA:HB2	2.46	0.45
6:7:260:TYR:HD2	6:7:298:LEU:HD13	1.82	0.45
8:B:189:MET:HB3	10:D:227:PHE:CD2	2.52	0.45
10:D:64:MET:HE1	10:D:65:LYS:HE2	1.98	0.45
12:H:899:VAL:HG21	12:H:918:ARG:HH22	1.81	0.45
1:2:660:THR:HG22	1:2:851:VAL:HG11	2.00	0.44
1:2:812:SER:OG	1:2:815:ARG:NH2	2.50	0.44
2:3:475:PHE:HB2	2:3:514:ALA:HB1	1.99	0.44
3:4:634:PHE:CZ	3:4:698:LEU:HD21	2.52	0.44
3:4:637:MET:HE1	3:4:642:ARG:HG3	1.99	0.44
3:4:820:GLU:OE1	3:4:820:GLU:N	2.45	0.44
10:D:93:MET:SD	10:D:94:GLN:N	2.89	0.44
12:F:610:GLU:OE1	12:F:610:GLU:N	2.50	0.44
12:G:516:SER:OG	12:G:525:GLU:OE2	2.27	0.44
1:2:572:SER:O	1:2:576:LEU:N	2.46	0.44
2:3:413:THR:O	2:3:413:THR:HG22	2.17	0.44
2:3:462:MET:CE	2:3:470:VAL:HG11	2.46	0.44
3:4:194:PHE:CE1	3:4:272:MET:HE3	2.53	0.44
3:4:232:GLU:O	3:4:236:LEU:HD23	2.16	0.44
4:5:182:MET:O	4:5:241:TYR:HA	2.17	0.44
4:5:395:GLY:N	4:5:408:GLY:O	2.51	0.44
8:B:173:LEU:HD23	8:B:178:ILE:CG1	2.47	0.44
10:D:260:ILE:HG13	10:D:260:ILE:O	2.17	0.44
11:E:643:LYS:O	11:E:647:SER:N	2.50	0.44
12:G:570:ILE:HD12	12:G:590:VAL:HG11	1.98	0.44
2:3:408:VAL:HG12	2:3:548:VAL:HG22	1.98	0.44
3:4:512:VAL:HG21	3:4:746:PHE:CE2	2.52	0.44
3:4:814:LYS:NZ	3:4:821:ASP:OD2	2.50	0.44
5:6:153:ILE:HD12	5:6:265:ILE:HG23	1.98	0.44
5:6:270:LEU:HD12	5:6:289:SER:CB	2.46	0.44
5:6:608:LEU:O	5:6:627:ALA:N	2.51	0.44
5:6:803:MET:HE1	5:6:828:TYR:HA	1.99	0.44
6:7:398:GLU:O	6:7:401:VAL:HG22	2.17	0.44
6:7:482:TYR:OH	6:7:524:ASP:OD2	2.15	0.44
9:C:39:THR:OG1	9:C:42:THR:OG1	2.23	0.44
11:E:126:HIS:O	11:E:127:ARG:CB	2.65	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:E:436:ASN:O	11:E:472:ARG:NH2	2.51	0.44
12:G:704:LEU:CD2	12:G:721:ILE:HD11	2.47	0.44
12:G:841:LEU:HD23	12:G:845:GLY:C	2.42	0.44
12:H:748:ALA:O	12:H:750:ASP:N	2.50	0.44
1:2:540:LEU:HD23	1:2:542:LEU:H	1.81	0.44
1:2:549:LYS:NZ	15:2:901:ADP:O3B	2.39	0.44
2:3:201:HIS:O	2:3:210:HIS:N	2.48	0.44
3:4:544:LEU:O	3:4:755:LYS:NZ	2.48	0.44
6:7:624:LYS:HG2	6:7:625:GLN:O	2.18	0.44
8:B:50:TRP:O	10:D:129:MET:HE2	2.18	0.44
9:C:142:LEU:HD11	9:C:184:TYR:HB3	1.99	0.44
11:E:553:ILE:HD11	11:E:584:LEU:HB3	2.00	0.44
12:G:744:PRO:HB3	12:G:752:LEU:HD21	2.00	0.44
12:G:866:LEU:HD12	12:G:890:LYS:HZ1	1.82	0.44
14:N:77:LEU:C	14:N:79:ILE:H	2.25	0.44
4:5:570:ASN:HA	4:5:573:ILE:HD12	2.00	0.44
6:7:206:PRO:HG3	6:7:352:THR:HG21	2.00	0.44
6:7:258:ILE:O	6:7:271:GLN:N	2.51	0.44
7:A:137:LEU:O	7:A:141:LEU:HD23	2.17	0.44
8:B:27:ILE:HD11	8:B:71:VAL:CG2	2.47	0.44
12:F:688:PHE:O	12:F:696:CYS:N	2.49	0.44
12:H:737:THR:HG23	12:H:737:THR:O	2.17	0.44
1:2:580:VAL:HA	1:2:591:LEU:HA	1.99	0.44
2:3:421:PHE:O	2:3:425:THR:HG22	2.17	0.44
3:4:580:TYR:OH	6:7:448:MET:HB2	2.18	0.44
3:4:750:TYR:CZ	3:4:813:LEU:HD21	2.52	0.44
4:5:59:TYR:N	4:5:281:TYR:OH	2.43	0.44
6:7:230:ILE:O	6:7:231:LYS:HD3	2.18	0.44
6:7:624:LYS:HB3	6:7:624:LYS:HE3	1.42	0.44
9:C:6:ILE:H	9:C:6:ILE:HD12	1.82	0.44
11:E:638:SER:OG	11:E:639:PRO:HD3	2.17	0.44
12:G:690:SER:N	12:G:694:ASP:O	2.51	0.44
12:G:692:TYR:CB	12:G:840:THR:HG21	2.47	0.44
14:N:14:PRO:N	14:N:15:PRO:CD	2.81	0.44
1:2:341:CYS:HB3	1:2:345:GLY:CA	2.48	0.44
1:2:632:SER:HB3	1:2:637:VAL:HG22	1.98	0.44
1:2:853:VAL:O	1:2:854:ARG:C	2.61	0.44
2:3:98:ILE:N	2:3:156:SER:O	2.50	0.44
2:3:103:LEU:HD11	2:3:110:PHE:HD2	1.83	0.44
2:3:694:LYS:HG2	2:3:737:LEU:O	2.17	0.44
3:4:195:ARG:NH1	3:4:279:CYS:SG	2.91	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:605:ILE:HG23	3:4:614:LEU:HD11	1.99	0.44
3:4:649:MET:HE2	3:4:701:ARG:HB3	2.00	0.44
4:5:437:VAL:HG21	4:5:472:ALA:CB	2.48	0.44
5:6:811:ALA:O	5:6:815:CYS:N	2.50	0.44
8:B:173:LEU:HD23	8:B:178:ILE:HG13	1.98	0.44
11:E:596:HIS:C	11:E:597:THR:CG2	2.90	0.44
12:G:577:ARG:O	12:G:593:SER:N	2.49	0.44
2:3:466:ASP:O	2:3:510:CYS:N	2.51	0.44
3:4:428:ARG:HG3	3:4:431:ASP:OD1	2.18	0.44
4:5:210:SER:OG	4:5:212:LEU:HD21	2.17	0.44
6:7:220:ILE:O	6:7:221:SER:C	2.61	0.44
6:7:398:GLU:O	6:7:402:MET:SD	2.76	0.44
7:A:130:TYR:CB	10:D:193:LEU:HD22	2.48	0.44
12:G:618:LEU:HD23	12:G:627:SER:HB3	1.98	0.44
12:H:782:VAL:HG23	12:H:785:LYS:HB2	1.98	0.44
14:N:36:ASP:O	14:N:39:SER:OG	2.25	0.44
14:N:70:TRP:CD2	14:N:84:VAL:HG22	2.52	0.44
3:4:364:VAL:HG22	3:4:365:ILE:N	2.33	0.44
4:5:393:MET:HE3	4:5:666:LEU:HD23	2.00	0.44
4:5:426:LEU:HG	4:5:520:LEU:HD23	2.00	0.44
6:7:483:THR:HG22	6:7:484:THR:N	2.33	0.44
6:7:599:LEU:HD11	6:7:601:LEU:HD21	1.99	0.44
8:B:23:GLU:O	8:B:73:LEU:N	2.46	0.44
11:E:287:VAL:HG22	11:E:290:ARG:HH21	1.82	0.44
12:G:866:LEU:HD11	12:G:888:GLU:HB3	2.00	0.44
12:H:774:MET:N	12:H:774:MET:SD	2.90	0.44
14:N:40:ALA:C	14:N:43:GLU:HG3	2.41	0.44
2:3:41:SER:O	2:3:44:SER:OG	2.28	0.43
2:3:466:ASP:OD1	2:3:507:ASN:C	2.61	0.43
3:4:764:GLU:HA	3:4:767:LYS:HG2	2.00	0.43
4:5:276:MET:HG3	4:5:328:ILE:HB	2.00	0.43
5:6:703:ALA:N	5:6:704:PRO:HD2	2.33	0.43
12:F:538:PHE:CD1	12:F:583:ALA:HB3	2.53	0.43
12:G:501:TYR:N	12:G:516:SER:O	2.51	0.43
12:G:672:ALA:HB2	12:G:760:LYS:HG2	1.98	0.43
12:G:685:LYS:N	12:G:698:PHE:O	2.50	0.43
14:N:17:LEU:CB	14:N:20:LEU:HD21	2.48	0.43
1:2:624:MET:HE2	1:2:673:ILE:HD13	1.99	0.43
3:4:196:ASN:OD1	3:4:253:GLN:NE2	2.45	0.43
3:4:644:VAL:HG23	5:6:601:LYS:CE	2.48	0.43
3:4:777:MET:HB3	3:4:793:ALA:HB2	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:614:LEU:HD13	4:5:619:ALA:HB2	2.01	0.43
5:6:402:ILE:O	5:6:453:SER:N	2.46	0.43
6:7:122:ASP:OD2	6:7:198:ARG:NE	2.51	0.43
6:7:535:THR:O	6:7:538:HIS:HB2	2.18	0.43
7:A:150:ASP:OD1	7:A:152:SER:OG	2.24	0.43
9:C:79:MET:O	9:C:84:VAL:HG11	2.18	0.43
12:F:529:GLU:OE1	12:F:529:GLU:N	2.39	0.43
12:G:740:ILE:HG23	12:G:756:LEU:HD22	1.99	0.43
12:H:497:ASN:OD1	12:H:498:GLU:N	2.51	0.43
12:H:573:GLN:OE1	12:H:576:GLU:OE1	2.36	0.43
1:2:485:ARG:NH2	1:2:488:SER:OG	2.51	0.43
3:4:282:SER:HA	3:4:285:VAL:HG22	2.00	0.43
3:4:658:LYS:N	3:4:661:ILE:O	2.52	0.43
3:4:683:ASN:N	3:4:691:ASN:OD1	2.48	0.43
3:4:764:GLU:O	3:4:767:LYS:HG2	2.19	0.43
4:5:497:MET:HE1	4:5:549:ARG:O	2.17	0.43
4:5:497:MET:O	4:5:500:GLN:NE2	2.51	0.43
5:6:591:PHE:O	5:6:591:PHE:CG	2.72	0.43
5:6:769:ALA:CB	5:6:824:ILE:HD11	2.43	0.43
5:6:803:MET:HE2	5:6:831:LEU:HD12	2.01	0.43
12:H:848:TYR:N	12:H:851:GLU:OE1	2.45	0.43
12:H:889:LEU:O	12:H:921:ARG:NH1	2.51	0.43
2:3:554:ASN:O	2:3:555:GLU:C	2.62	0.43
3:4:320:ASN:OD1	3:4:321:ASP:N	2.51	0.43
3:4:606:THR:OG1	3:4:607:ARG:N	2.51	0.43
5:6:659:GLN:O	5:6:673:ASN:O	2.36	0.43
6:7:491:VAL:O	6:7:495:ALA:N	2.51	0.43
7:A:130:TYR:CG	10:D:193:LEU:HD22	2.52	0.43
8:B:115:LEU:HD13	8:B:119:TRP:CE2	2.52	0.43
11:E:390:ILE:H	11:E:390:ILE:HD12	1.82	0.43
11:E:431:LEU:HD23	11:E:480:SER:HA	2.01	0.43
12:H:491:ARG:N	12:H:505:VAL:HG23	2.33	0.43
14:N:37:GLY:HA3	14:N:76:GLY:O	2.18	0.43
2:3:181:SER:OG	2:3:294:VAL:O	2.35	0.43
2:3:653:ILE:N	2:3:654:PRO:CD	2.82	0.43
4:5:185:ASN:HB2	4:5:236:CYS:SG	2.59	0.43
5:6:563:ILE:H	5:6:563:ILE:HD12	1.83	0.43
6:7:493:LEU:HD12	6:7:512:ALA:HB3	2.00	0.43
6:7:652:MET:CE	6:7:657:ASN:OD1	2.66	0.43
6:7:692:ILE:HD11	6:7:720:VAL:HG21	1.99	0.43
10:D:75:GLU:OE1	10:D:283:ARG:NH1	2.51	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:G:580:SER:C	12:G:618:LEU:HD12	2.43	0.43
12:G:584:THR:OG1	12:G:587:ARG:O	2.23	0.43
1:2:757:PRO:HG2	1:2:758:ILE:HD12	2.01	0.43
4:5:361:SER:HB3	4:5:668:LEU:HD12	2.00	0.43
5:6:259:THR:HG21	5:6:352:ARG:HD3	2.00	0.43
6:7:454:ILE:HA	6:7:595:ASP:OD2	2.19	0.43
11:E:476:ASN:HA	11:E:479:LEU:HD12	2.00	0.43
11:E:566:PRO:HB3	11:E:605:PHE:CZ	2.54	0.43
12:F:739:ASP:OD1	12:F:740:ILE:N	2.52	0.43
12:H:749:TYR:CG	12:H:750:ASP:N	2.86	0.43
2:3:199:SER:O	2:3:200:VAL:C	2.62	0.43
5:6:598:THR:O	5:6:639:ASP:N	2.44	0.43
7:A:191:VAL:HG12	7:A:192:ARG:N	2.34	0.43
9:C:126:GLU:O	9:C:127:LEU:C	2.62	0.43
12:H:489:THR:HG22	12:H:491:ARG:N	2.34	0.43
1:2:211:LEU:HD22	1:2:271:PHE:CD1	2.53	0.43
1:2:658:ASN:O	1:2:666:ASN:ND2	2.48	0.43
2:3:281:ASP:OD1	2:3:281:ASP:N	2.52	0.43
2:3:469:VAL:HG22	2:3:470:VAL:N	2.34	0.43
6:7:248:VAL:HG13	6:7:313:CYS:SG	2.58	0.43
7:A:120:THR:O	7:A:128:GLN:NE2	2.52	0.43
8:B:189:MET:HE2	8:B:192:LEU:HD12	2.00	0.43
10:D:76:LEU:HD11	10:D:147:ARG:CZ	2.49	0.43
12:G:867:LEU:HD12	12:G:901:ILE:HD12	2.00	0.43
12:H:545:LEU:CD2	12:H:588:VAL:HG13	2.47	0.43
12:H:910:LEU:HD23	12:H:914:ILE:HD11	1.99	0.43
14:N:29:TYR:HD1	14:N:31:LEU:HG	1.84	0.43
14:N:65:GLN:HG3	14:N:70:TRP:CZ3	2.49	0.43
2:3:95:ARG:NH1	2:3:155:LEU:O	2.52	0.43
2:3:406:LEU:N	2:3:543:PHE:HZ	2.17	0.43
3:4:521:LEU:HD21	3:4:742:LEU:CD1	2.48	0.43
3:4:573:SER:H	18:4:1001:AGS:H5'1	1.84	0.43
3:4:679:GLY:O	3:4:680:SER:C	2.61	0.43
4:5:25:THR:HA	4:5:28:ILE:HD12	2.01	0.43
6:7:92:LYS:O	6:7:96:GLY:N	2.49	0.43
6:7:283:GLU:O	6:7:298:LEU:HD12	2.19	0.43
8:B:119:TRP:CE2	8:B:120:LEU:HG	2.54	0.43
9:C:85:MET:HA	9:C:88:ILE:HD12	2.01	0.43
11:E:304:PRO:O	11:E:307:ARG:NH2	2.50	0.43
12:F:830:SER:HA	12:F:858:LEU:HD11	2.00	0.43
12:G:600:PHE:HA	12:G:606:PRO:HA	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:H:786:LEU:HB3	12:H:815:ILE:HG21	2.01	0.43
1:2:237:MET:HE2	1:2:237:MET:HA	2.01	0.43
1:2:321:THR:HG22	1:2:322:GLY:N	2.34	0.43
1:2:748:GLN:HA	1:2:751:LYS:HB2	2.01	0.43
2:3:351:ASN:O	2:3:354:SER:OG	2.30	0.43
4:5:77:LYS:HG2	11:E:382:HIS:ND1	2.34	0.43
4:5:404:MET:HE1	4:5:406:LEU:HD12	2.01	0.43
6:7:66:MET:O	6:7:70:VAL:HG23	2.19	0.43
9:C:55:ALA:HB2	9:C:74:LEU:HD23	2.00	0.43
11:E:241:TYR:O	11:E:242:SER:OG	2.32	0.43
11:E:596:HIS:CG	11:E:597:THR:N	2.86	0.43
12:F:570:ILE:HD11	12:F:578:ILE:HG12	2.01	0.43
12:G:484:THR:HG1	12:G:493:TYR:H	1.67	0.43
2:3:680:VAL:HG13	6:7:613:ALA:HB3	2.01	0.42
4:5:95:THR:HG22	4:5:135:PHE:HD1	1.84	0.42
4:5:370:LEU:O	4:5:373:SER:N	2.43	0.42
4:5:493:ILE:H	4:5:493:ILE:HD12	1.84	0.42
5:6:137:ARG:HA	5:6:140:ILE:HD12	2.01	0.42
5:6:367:GLU:HG2	5:6:368:ILE:HD12	2.01	0.42
5:6:657:GLU:O	5:6:659:GLN:NE2	2.52	0.42
5:6:701:MET:SD	5:6:705:ILE:CG2	3.07	0.42
5:6:765:LEU:HG	5:6:770:ARG:HD3	2.00	0.42
8:B:21:GLU:HB3	8:B:74:TRP:HB3	2.00	0.42
11:E:12:TYR:HA	11:E:15:ILE:HD12	2.01	0.42
11:E:101:GLN:O	11:E:104:VAL:HG12	2.18	0.42
11:E:589:PRO:O	11:E:590:ARG:C	2.62	0.42
12:H:884:SER:O	12:H:888:GLU:OE1	2.37	0.42
14:N:93:GLU:O	14:N:94:ARG:C	2.62	0.42
1:2:527:VAL:O	1:2:527:VAL:HG23	2.18	0.42
1:2:579:SER:O	1:2:592:GLU:N	2.46	0.42
2:3:48:TYR:CD1	2:3:48:TYR:C	2.98	0.42
2:3:223:THR:OG1	4:5:246:GLU:OE1	2.30	0.42
2:3:403:ILE:HD11	2:3:707:ARG:HB3	2.00	0.42
2:3:572:LEU:HD21	4:5:613:ARG:CD	2.49	0.42
3:4:567:CYS:SG	3:4:692:ILE:HG22	2.59	0.42
4:5:474:GLY:N	4:5:516:ARG:O	2.52	0.42
4:5:497:MET:SD	4:5:498:GLU:N	2.92	0.42
4:5:652:GLN:O	4:5:656:ILE:HD12	2.19	0.42
5:6:720:ASN:C	5:6:720:ASN:OD1	2.62	0.42
7:A:198:ARG:CZ	14:N:26:SER:HB3	2.49	0.42
8:B:151:ILE:HA	8:B:154:ILE:HD12	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:F:742:VAL:HG23	12:F:742:VAL:O	2.18	0.42
12:G:497:ASN:O	12:G:745:LEU:HD23	2.18	0.42
12:H:572:LEU:HD21	12:H:578:ILE:HD11	2.01	0.42
14:N:29:TYR:CG	14:N:29:TYR:O	2.73	0.42
2:3:255:ARG:NH2	2:3:275:ASP:OD2	2.52	0.42
2:3:350:ILE:HG23	2:3:659:TYR:CD2	2.54	0.42
3:4:254:THR:O	3:4:254:THR:CG2	2.67	0.42
3:4:642:ARG:O	3:4:646:HIS:CD2	2.73	0.42
4:5:138:ILE:C	4:5:139:LEU:HD12	2.44	0.42
11:E:41:ALA:CB	11:E:255:ILE:HD12	2.44	0.42
12:F:833:LEU:CB	12:F:858:LEU:HD21	2.49	0.42
12:G:538:PHE:O	12:G:545:LEU:N	2.45	0.42
1:2:245:ASN:ND2	1:2:299:ASP:OD2	2.52	0.42
1:2:289:ILE:HG22	1:2:290:HIS:CD2	2.54	0.42
1:2:566:ALA:O	1:2:606:ILE:HD12	2.19	0.42
1:2:660:THR:O	1:2:661:LEU:HB2	2.18	0.42
2:3:433:THR:HG22	2:3:473:ASP:HB3	2.01	0.42
2:3:473:ASP:OD1	2:3:474:GLU:N	2.53	0.42
3:4:532:GLU:HG2	3:4:533:LEU:H	1.83	0.42
3:4:571:SER:C	18:4:1001:AGS:H5'1	2.44	0.42
3:4:581:VAL:HG21	3:4:672:LEU:HD22	2.00	0.42
3:4:601:LEU:HD11	3:4:621:LEU:HD21	2.00	0.42
4:5:632:GLN:NE2	4:5:636:ASN:OD1	2.52	0.42
5:6:363:GLU:N	5:6:375:ARG:O	2.50	0.42
12:F:674:LEU:O	12:F:678:ASN:N	2.39	0.42
12:G:854:VAL:O	12:G:858:LEU:HD13	2.19	0.42
12:G:882:ALA:CB	12:G:910:LEU:HD11	2.48	0.42
12:G:889:LEU:HD13	12:G:894:ALA:C	2.44	0.42
12:H:587:ARG:CD	12:H:643:LEU:HD11	2.49	0.42
12:H:782:VAL:HG23	12:H:782:VAL:O	2.19	0.42
1:2:604:CYS:N	1:2:645:SER:O	2.52	0.42
1:2:783:MET:HE2	4:5:573:ILE:CG2	2.46	0.42
3:4:615:VAL:HG12	3:4:616:LEU:N	2.32	0.42
3:4:792:THR:HG22	3:4:793:ALA:N	2.35	0.42
5:6:571:ILE:HG12	5:6:711:LEU:HD12	2.02	0.42
6:7:414:LEU:HD23	6:7:633:VAL:HG21	2.00	0.42
8:B:51:GLN:O	10:D:129:MET:HE1	2.20	0.42
1:2:292:GLU:CG	1:2:293:ILE:N	2.83	0.42
1:2:319:ARG:HE	1:2:425:GLU:CD	2.28	0.42
3:4:258:TYR:CZ	3:4:262:LEU:HD11	2.55	0.42
3:4:350:ASN:N	3:4:381:SER:OG	2.47	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:778:ARG:O	3:4:778:ARG:NH1	2.52	0.42
3:4:830:ARG:NE	3:4:835:ASP:OD2	2.50	0.42
5:6:823:PHE:N	5:6:823:PHE:CD1	2.87	0.42
6:7:311:GLN:HB2	6:7:340:VAL:HG13	2.02	0.42
7:A:29:LEU:O	7:A:122:ASN:ND2	2.48	0.42
11:E:271:TRP:CZ2	11:E:275:LEU:HD21	2.54	0.42
11:E:345:ASN:OD1	11:E:350:LEU:N	2.52	0.42
1:2:417:VAL:HG11	1:2:456:ILE:HG21	2.02	0.42
2:3:190:SER:OG	2:3:255:ARG:O	2.29	0.42
2:3:293:ASN:HB2	2:3:329:LEU:HD11	2.00	0.42
2:3:447:THR:O	2:3:456:ARG:N	2.53	0.42
3:4:308:VAL:HG21	3:4:325:LEU:HB2	2.01	0.42
3:4:525:SER:OG	3:4:742:LEU:N	2.52	0.42
4:5:473:ASP:OD1	4:5:474:GLY:N	2.52	0.42
5:6:116:GLU:HB2	5:6:188:VAL:HG22	2.01	0.42
5:6:585:LEU:HD23	5:6:679:LEU:HD23	2.02	0.42
5:6:645:ASP:OD1	5:6:647:SER:N	2.53	0.42
6:7:214:ARG:HG3	6:7:218:LYS:NZ	2.35	0.42
8:B:16:ILE:HD12	8:B:175:LEU:HD21	2.01	0.42
11:E:316:LEU:HD23	11:E:317:THR:N	2.34	0.42
12:F:879:VAL:HG22	12:F:907:LEU:HD13	2.02	0.42
12:G:748:ALA:HB2	12:G:753:ASN:OD1	2.20	0.42
3:4:224:LEU:O	3:4:225:TYR:C	2.63	0.42
3:4:564:ILE:HG23	3:4:704:LEU:HB2	2.02	0.42
4:5:105:SER:C	4:5:106:ARG:HG2	2.45	0.42
4:5:599:MET:O	4:5:603:ILE:HG22	2.20	0.42
4:5:657:ILE:HG22	4:5:661:GLU:OE2	2.19	0.42
5:6:820:THR:HG22	5:6:822:SER:H	1.85	0.42
8:B:11:PHE:O	8:B:179:ASN:ND2	2.44	0.42
8:B:57:ASP:OD1	8:B:61:ASN:ND2	2.53	0.42
12:F:508:SER:O	12:F:509:GLU:HB2	2.20	0.42
2:3:301:LEU:CD1	2:3:320:LEU:HD12	2.50	0.42
3:4:199:MET:O	3:4:200:SER:CB	2.68	0.42
3:4:284:ILE:HD11	3:4:293:LEU:CD1	2.47	0.42
4:5:27:ILE:O	4:5:30:SER:OG	2.31	0.42
4:5:274:LEU:HD23	4:5:275:THR:O	2.19	0.42
5:6:379:VAL:HG12	5:6:380:ILE:N	2.34	0.42
5:6:438:THR:OG1	5:6:439:GLY:N	2.53	0.42
5:6:598:THR:HG21	5:6:608:LEU:HD21	2.02	0.42
6:7:398:GLU:HB3	6:7:402:MET:HE1	2.01	0.42
6:7:527:ASP:OD1	6:7:528:LYS:N	2.53	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:D:76:LEU:HG	10:D:174:LEU:HD11	2.02	0.42
11:E:107:THR:HG23	11:E:108:ASP:N	2.35	0.42
12:F:497:ASN:OD1	12:F:497:ASN:C	2.63	0.42
12:F:598:ARG:HG3	12:F:609:VAL:HG13	2.01	0.42
12:F:612:THR:OG1	12:F:615:ILE:HD11	2.20	0.42
12:G:910:LEU:HD22	12:G:914:ILE:HD11	2.01	0.42
14:N:40:ALA:HB3	14:N:81:GLN:OE1	2.20	0.42
1:2:215:LEU:HD12	1:2:274:VAL:HG12	2.01	0.42
1:2:255:ILE:HG23	1:2:256:LEU:N	2.35	0.42
1:2:359:ILE:CG2	1:2:361:ILE:HG23	2.49	0.42
3:4:463:VAL:HG23	3:4:463:VAL:O	2.19	0.42
4:5:75:ILE:H	4:5:75:ILE:HD12	1.85	0.42
5:6:326:LYS:HD3	5:6:410:LEU:HD23	2.01	0.42
5:6:734:LEU:O	5:6:738:ARG:HA	2.20	0.42
8:B:121:VAL:HG23	9:C:190:TRP:CH2	2.55	0.42
11:E:368:ILE:HG23	11:E:368:ILE:O	2.19	0.42
12:F:498:GLU:OE1	12:F:498:GLU:N	2.48	0.42
12:F:547:GLY:HA3	12:F:554:ILE:HD12	2.02	0.42
12:H:743:TRP:O	12:H:755:ILE:N	2.53	0.42
14:N:62:PHE:CD1	14:N:88:ILE:HG21	2.53	0.42
2:3:292:VAL:HG23	2:3:328:PRO:HA	2.01	0.41
3:4:318:ASN:OD1	3:4:320:ASN:OD1	2.38	0.41
3:4:830:ARG:NH2	3:4:835:ASP:OD2	2.52	0.41
4:5:383:ASP:OD1	4:5:682:ARG:NH1	2.53	0.41
5:6:629:MET:SD	5:6:672:LEU:HD22	2.59	0.41
18:7:902:AGS:O1A	18:7:902:AGS:H3'	2.20	0.41
11:E:509:THR:HG21	11:E:539:TYR:OH	2.19	0.41
12:F:519:ASP:OD1	12:F:522:ARG:N	2.39	0.41
12:F:822:ALA:O	12:F:826:GLU:OE1	2.38	0.41
12:F:900:LYS:O	12:F:904:ARG:HD3	2.20	0.41
14:N:26:SER:HA	14:N:30:GLY:C	2.44	0.41
1:2:517:CYS:HA	1:2:819:SER:OG	2.20	0.41
3:4:565:LEU:HD23	3:4:566:LEU:N	2.35	0.41
3:4:696:PRO:N	3:4:697:PRO:CD	2.83	0.41
4:5:181:ILE:HA	4:5:242:ILE:O	2.19	0.41
6:7:464:VAL:HG22	6:7:466:LYS:NZ	2.35	0.41
8:B:50:TRP:O	10:D:129:MET:CE	2.69	0.41
11:E:36:ILE:HG21	11:E:279:SER:HB3	2.02	0.41
11:E:470:ARG:O	11:E:474:VAL:HG23	2.20	0.41
12:F:643:LEU:HD22	12:F:648:LYS:HD3	2.02	0.41
12:F:910:LEU:O	12:F:914:ILE:CD1	2.66	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:339:PHE:HB2	1:2:348:LEU:HD12	2.01	0.41
1:2:658:ASN:CG	1:2:660:THR:HG1	2.28	0.41
2:3:347:ILE:HG23	2:3:662:TYR:CE1	2.55	0.41
3:4:344:VAL:HG22	3:4:359:GLU:HG3	2.02	0.41
4:5:632:GLN:O	4:5:635:ILE:HG22	2.19	0.41
6:7:65:ALA:HB1	6:7:69:LYS:NZ	2.34	0.41
6:7:103:VAL:HG13	6:7:104:SER:N	2.35	0.41
7:A:146:LEU:HD21	10:D:144:ILE:HG13	2.03	0.41
11:E:248:VAL:HG23	11:E:249:ASN:N	2.35	0.41
12:G:486:PHE:HA	12:G:492:ARG:HB3	2.00	0.41
12:H:482:ALA:HB1	12:H:496:MET:HB2	2.02	0.41
14:N:29:TYR:CD1	14:N:31:LEU:HG	2.55	0.41
14:N:45:VAL:CA	14:N:55:GLN:HE22	2.33	0.41
2:3:122:ILE:N	2:3:123:PRO:HD2	2.35	0.41
2:3:414:ALA:CB	15:3:1001:ADP:H2'	2.49	0.41
3:4:194:PHE:CZ	3:4:272:MET:HE3	2.55	0.41
4:5:323:ILE:O	4:5:323:ILE:HG23	2.21	0.41
4:5:521:ALA:HB2	4:5:550:PHE:CZ	2.56	0.41
5:6:137:ARG:NH2	5:6:192:TYR:OH	2.54	0.41
6:7:81:ASP:HA	6:7:205:LYS:HB3	2.03	0.41
6:7:219:ALA:O	6:7:220:ILE:HG23	2.20	0.41
8:B:16:ILE:HG23	8:B:175:LEU:CD2	2.49	0.41
8:B:193:ARG:O	8:B:197:THR:HG23	2.21	0.41
11:E:382:HIS:CG	11:E:383:SER:N	2.88	0.41
11:E:508:ASN:O	11:E:511:VAL:HG22	2.20	0.41
12:F:896:THR:O	12:F:899:VAL:HG12	2.20	0.41
12:G:661:LEU:HD22	12:H:633:PHE:CG	2.55	0.41
12:G:918:ARG:O	12:G:922:TYR:CD1	2.73	0.41
12:H:540:ASN:O	12:H:559:HIS:NE2	2.53	0.41
14:N:13:GLN:HG3	14:N:13:GLN:O	2.19	0.41
4:5:685:GLN:HB3	4:5:689:MET:HE1	2.01	0.41
5:6:632:ASP:HA	5:6:676:THR:HB	2.03	0.41
6:7:276:ARG:HG3	6:7:277:THR:HG23	2.02	0.41
6:7:441:ASP:O	6:7:649:ARG:NH2	2.49	0.41
6:7:497:VAL:N	13:I:10:DT:OP1	2.43	0.41
6:7:714:GLU:HA	6:7:717:LEU:HD12	2.01	0.41
8:B:121:VAL:HG23	9:C:190:TRP:CZ2	2.56	0.41
10:D:5:ILE:HD13	12:F:871:ALA:CB	2.49	0.41
10:D:232:VAL:HG11	10:D:271:ILE:HD13	2.02	0.41
11:E:334:LEU:HD11	11:E:338:PHE:HE1	1.86	0.41
11:E:368:ILE:HD13	11:E:384:ILE:HD12	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:E:406:ARG:HH12	11:E:590:ARG:NH1	2.18	0.41
11:E:545:LEU:HD23	11:E:582:ALA:HB2	2.02	0.41
12:F:515:VAL:HG21	12:F:526:TYR:CZ	2.56	0.41
12:F:883:LEU:HD13	12:F:913:LYS:HB3	2.02	0.41
12:G:752:LEU:O	12:G:773:GLU:HA	2.20	0.41
1:2:426:VAL:HG12	1:2:427:THR:N	2.35	0.41
1:2:574:VAL:HG13	1:2:578:ALA:O	2.21	0.41
2:3:471:CYS:HA	2:3:513:ILE:O	2.20	0.41
3:4:249:LEU:HD21	3:4:258:TYR:CD2	2.55	0.41
4:5:413:LEU:N	4:5:552:MET:O	2.50	0.41
6:7:107:GLN:O	6:7:237:GLN:HA	2.21	0.41
6:7:254:ALA:O	6:7:308:SER:N	2.39	0.41
7:A:175:GLN:HE21	14:N:18:ARG:HD3	1.85	0.41
8:B:21:GLU:HA	8:B:73:LEU:HB3	2.01	0.41
8:B:31:ILE:HG22	8:B:32:THR:N	2.34	0.41
10:D:124:LEU:N	10:D:125:PRO:HD2	2.36	0.41
12:H:619:THR:O	12:H:619:THR:HG23	2.20	0.41
12:H:704:LEU:HD22	12:H:752:LEU:HD13	2.02	0.41
14:N:54:ARG:HA	14:N:54:ARG:HH11	1.82	0.41
1:2:339:PHE:CB	1:2:348:LEU:HD12	2.50	0.41
1:2:397:VAL:HG21	1:2:403:PRO:HG3	2.01	0.41
1:2:865:THR:HG23	1:2:866:LEU:N	2.36	0.41
2:3:192:VAL:HG12	2:3:193:ARG:N	2.36	0.41
2:3:661:GLN:HG3	2:3:662:TYR:N	2.36	0.41
3:4:258:TYR:O	3:4:262:LEU:HD13	2.21	0.41
3:4:637:MET:CE	3:4:642:ARG:HG3	2.51	0.41
3:4:637:MET:SD	3:4:641:THR:HB	2.61	0.41
4:5:596:ILE:HG23	4:5:597:GLU:N	2.36	0.41
5:6:115:PHE:CZ	5:6:119:LEU:HD11	2.56	0.41
5:6:289:SER:HA	5:6:398:THR:HA	2.02	0.41
5:6:291:SER:OG	5:6:462:ILE:HD11	2.21	0.41
6:7:360:TYR:HB2	6:7:365:ALA:HB2	2.02	0.41
6:7:652:MET:HE2	6:7:656:VAL:HB	2.01	0.41
7:A:184:ILE:O	7:A:185:LYS:C	2.63	0.41
8:B:87:ILE:N	8:B:133:ASP:OD2	2.50	0.41
9:C:50:LEU:HD11	9:C:54:LEU:HD21	2.02	0.41
10:D:64:MET:SD	10:D:68:LYS:HD2	2.60	0.41
10:D:286:LEU:HD12	10:D:287:ARG:N	2.36	0.41
12:F:639:SER:OG	12:F:654:GLU:N	2.52	0.41
12:G:546:PHE:O	12:G:555:GLN:N	2.49	0.41
12:G:704:LEU:HB3	12:G:722:LEU:HB2	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:H:589:ILE:HG23	12:H:597:PHE:CZ	2.55	0.41
1:2:816:ILE:HG23	1:2:837:ALA:CB	2.51	0.41
2:3:440:VAL:O	2:3:444:ALA:N	2.54	0.41
2:3:480:ASP:OD1	2:3:483:ARG:NH2	2.53	0.41
3:4:456:LEU:H	3:4:456:LEU:HD23	1.86	0.41
4:5:183:CYS:SG	4:5:240:PRO:HB2	2.61	0.41
5:6:381:LEU:HD13	5:6:385:SER:O	2.21	0.41
11:E:433:GLU:HG2	11:E:543:LEU:HB2	2.02	0.41
12:F:694:ASP:HB3	12:F:706:LEU:HD11	2.02	0.41
12:G:541:GLU:O	12:G:559:HIS:ND1	2.53	0.41
14:N:24:VAL:C	14:N:25:LEU:HD22	2.46	0.41
1:2:323:VAL:HG13	1:2:422:GLU:C	2.46	0.41
1:2:326:ARG:O	1:2:388:VAL:HG13	2.20	0.41
1:2:342:LEU:N	1:2:372:PRO:O	2.52	0.41
1:2:483:GLU:OE2	1:2:487:ILE:HG21	2.20	0.41
1:2:523:VAL:HG23	1:2:776:PRO:HD2	2.03	0.41
1:2:626:GLN:O	1:2:628:SER:N	2.49	0.41
2:3:94:HIS:HB3	2:3:153:TRP:HA	2.03	0.41
2:3:139:VAL:HG22	2:3:139:VAL:O	2.20	0.41
2:3:236:THR:HG23	6:7:5:LEU:HD22	2.03	0.41
2:3:476:ASP:HB3	2:3:516:ALA:HB1	2.03	0.41
3:4:243:LEU:O	3:4:305:PRO:HA	2.21	0.41
3:4:517:ASP:O	3:4:518:LEU:C	2.63	0.41
3:4:678:ILE:HG23	3:4:679:GLY:N	2.36	0.41
3:4:688:VAL:HG13	3:4:689:THR:N	2.35	0.41
4:5:397:LYS:HD3	4:5:399:ILE:HD11	2.03	0.41
4:5:469:MET:N	4:5:469:MET:SD	2.94	0.41
4:5:469:MET:SD	4:5:470:VAL:HG23	2.61	0.41
4:5:479:ILE:HB	4:5:482:PHE:CE1	2.56	0.41
4:5:614:LEU:CD1	4:5:619:ALA:HB2	2.51	0.41
4:5:629:ILE:HG21	4:5:648:ILE:HG13	2.02	0.41
4:5:689:MET:O	4:5:692:ALA:HB3	2.21	0.41
5:6:543:VAL:HG12	5:6:584:PHE:HE2	1.83	0.41
5:6:585:LEU:HD11	5:6:681:ALA:HB2	2.01	0.41
6:7:21:ILE:HG23	6:7:117:PHE:CE1	2.56	0.41
7:A:173:GLU:OE1	14:N:34:LYS:HD2	2.21	0.41
10:D:94:GLN:CG	10:D:133:LEU:HD21	2.51	0.41
11:E:351:TRP:CG	11:E:514:LEU:HD12	2.55	0.41
11:E:592:LEU:HD22	11:E:594:THR:HG23	2.01	0.41
12:G:872:SER:O	12:G:875:SER:OG	2.31	0.41
12:H:492:ARG:N	12:H:504:THR:O	2.50	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:37:GLY:N	14:N:76:GLY:O	2.52	0.41
1:2:280:GLU:OE1	1:2:286:TYR:N	2.54	0.41
2:3:462:MET:HB3	2:3:489:VAL:HG11	2.02	0.41
3:4:606:THR:HG21	3:4:617:GLU:HG2	2.01	0.41
3:4:761:ILE:C	3:4:817:VAL:HG23	2.45	0.41
3:4:797:GLN:O	3:4:801:MET:HE3	2.20	0.41
4:5:434:PRO:HA	4:5:600:LYS:HE3	2.03	0.41
4:5:474:GLY:O	4:5:517:THR:OG1	2.38	0.41
5:6:113:GLU:HA	5:6:116:GLU:HG2	2.02	0.41
5:6:118:PHE:O	5:6:122:PHE:HB2	2.21	0.41
5:6:155:TYR:HB2	5:6:270:LEU:HD23	2.03	0.41
5:6:705:ILE:HD12	5:6:708:ARG:CG	2.50	0.41
6:7:631:THR:HA	6:7:632:PRO:HD3	1.94	0.41
7:A:171:ALA:HB3	7:A:183:LEU:HD12	2.03	0.41
11:E:271:TRP:CE3	11:E:318:LEU:HD11	2.56	0.41
11:E:282:ILE:HA	11:E:590:ARG:NH2	2.36	0.41
11:E:320:ILE:HG22	11:E:407:ASP:OD2	2.20	0.41
12:F:913:LYS:O	12:F:917:ILE:HG12	2.21	0.41
12:H:697:ILE:O	12:H:704:LEU:HD12	2.21	0.41
14:N:20:LEU:HA	14:N:23:ARG:HH11	1.85	0.41
1:2:249:LEU:O	1:2:252:SER:O	2.39	0.40
2:3:172:THR:HG23	4:5:252:ASP:OD2	2.21	0.40
2:3:519:VAL:HG23	2:3:532:ASN:C	2.46	0.40
4:5:39:ARG:C	4:5:40:LEU:HD23	2.46	0.40
4:5:282:LEU:HD22	4:5:333:ILE:HD13	2.03	0.40
5:6:158:LEU:HD22	5:6:167:ALA:HA	2.02	0.40
5:6:705:ILE:HD12	5:6:708:ARG:HD2	2.03	0.40
6:7:318:LEU:O	6:7:322:VAL:HG23	2.21	0.40
8:B:166:SER:HG	8:B:167:HIS:CE1	2.39	0.40
11:E:122:VAL:HG12	11:E:124:ASP:H	1.86	0.40
12:F:659:MET:SD	12:F:660:SER:N	2.93	0.40
12:G:704:LEU:HD23	12:G:721:ILE:HD11	2.02	0.40
12:G:891:GLN:CD	12:G:894:ALA:HB2	2.46	0.40
12:H:827:TYR:CE1	12:H:866:LEU:HG	2.56	0.40
14:N:91:MET:HE2	14:N:91:MET:HB2	1.93	0.40
1:2:494:ILE:HD12	1:2:823:MET:HB2	2.03	0.40
1:2:547:THR:OG1	1:2:683:VAL:HG11	2.21	0.40
1:2:842:VAL:HG11	1:2:865:THR:HB	2.02	0.40
4:5:681:ILE:HG13	4:5:682:ARG:N	2.36	0.40
5:6:157:HIS:O	5:6:160:MET:HG2	2.21	0.40
6:7:397:VAL:HG13	6:7:640:GLU:HG3	2.04	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:C:24:ILE:O	9:C:38:ILE:N	2.54	0.40
11:E:424:PHE:CE2	11:E:428:LEU:HD11	2.55	0.40
12:F:827:TYR:CE1	12:F:862:TYR:CE2	3.10	0.40
12:G:626:PHE:HE2	12:G:687:LEU:HD11	1.84	0.40
12:G:631:SER:HB3	12:G:634:HIS:HB2	2.03	0.40
12:G:850:ASN:O	12:G:850:ASN:OD1	2.40	0.40
12:H:543:GLY:HA3	12:H:558:PRO:HA	2.03	0.40
14:N:26:SER:OG	14:N:32:SER:HA	2.21	0.40
1:2:240:GLU:HG3	1:2:292:GLU:O	2.20	0.40
1:2:484:PHE:HA	1:2:487:ILE:HG12	2.04	0.40
1:2:567:THR:O	1:2:571:ALA:N	2.54	0.40
2:3:27:ARG:NH2	2:3:109:SER:OG	2.53	0.40
2:3:554:ASN:O	2:3:558:ASP:N	2.41	0.40
3:4:720:LEU:HD23	3:4:720:LEU:C	2.46	0.40
4:5:212:LEU:C	4:5:213:SER:HG	2.20	0.40
4:5:256:LEU:O	4:5:276:MET:N	2.47	0.40
4:5:613:ARG:O	4:5:672:ALA:N	2.47	0.40
5:6:557:LYS:O	5:6:565:LEU:N	2.43	0.40
8:B:184:PHE:HA	9:C:176:ILE:HD11	2.04	0.40
9:C:72:VAL:HG12	9:C:73:GLU:N	2.36	0.40
9:C:127:LEU:HD11	9:C:131:ARG:HD2	2.03	0.40
11:E:469:LEU:HD22	11:E:540:ARG:HD3	2.03	0.40
12:F:766:PHE:O	12:F:768:LEU:N	2.54	0.40
12:G:601:ASN:HB3	12:G:607:PHE:CE1	2.56	0.40
1:2:281:LEU:HD12	1:2:282:HIS:N	2.37	0.40
1:2:851:VAL:O	1:2:855:ARG:NH2	2.54	0.40
2:3:407:MET:HA	2:3:547:PHE:O	2.21	0.40
2:3:434:GLY:O	2:3:478:MET:SD	2.79	0.40
2:3:653:ILE:CG2	2:3:654:PRO:HD3	2.51	0.40
2:3:735:PHE:HA	2:3:739:GLY:O	2.22	0.40
3:4:199:MET:O	3:4:200:SER:OG	2.37	0.40
3:4:300:PHE:O	3:4:302:LYS:NZ	2.48	0.40
5:6:317:ILE:HD12	5:6:350:ARG:CZ	2.51	0.40
5:6:589:VAL:HG13	5:6:590:GLY:N	2.37	0.40
5:6:755:ILE:O	5:6:759:ARG:HG2	2.21	0.40
6:7:370:LEU:O	6:7:372:THR:HG23	2.22	0.40
6:7:540:VAL:HG12	6:7:546:ILE:HG12	2.03	0.40
6:7:597:LEU:HD23	6:7:597:LEU:C	2.46	0.40
9:C:18:CYS:O	9:C:44:LEU:N	2.50	0.40
9:C:97:LEU:O	9:C:100:ILE:HG22	2.22	0.40
9:C:174:LYS:O	9:C:178:LYS:HG2	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:E:318:LEU:HD23	11:E:318:LEU:C	2.47	0.40
11:E:485:ASP:OD2	11:E:487:ARG:NE	2.54	0.40
12:F:696:CYS:SG	12:F:747:LEU:HD23	2.61	0.40
12:F:702:ASN:HB3	12:F:724:SER:OG	2.22	0.40
1:2:278:ALA:O	1:2:281:LEU:HG	2.21	0.40
1:2:820:PHE:HA	1:2:823:MET:CE	2.50	0.40
2:3:44:SER:HA	2:3:47:VAL:HG22	2.03	0.40
2:3:413:THR:O	2:3:414:ALA:HB3	2.20	0.40
2:3:462:MET:CB	2:3:489:VAL:HG11	2.52	0.40
5:6:529:LEU:HD23	5:6:751:LEU:CD1	2.52	0.40
6:7:437:VAL:O	6:7:646:LYS:NZ	2.52	0.40
7:A:136:ASP:O	7:A:139:THR:HG22	2.21	0.40
7:A:174:ILE:CD1	14:N:74:GLU:HB3	2.52	0.40
10:D:282:ILE:O	10:D:282:ILE:HG22	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	2	613/868 (71%)	581 (95%)	32 (5%)	0	100	100
2	3	609/971 (63%)	579 (95%)	30 (5%)	0	100	100
3	4	613/933 (66%)	583 (95%)	30 (5%)	0	100	100
4	5	503/775 (65%)	484 (96%)	19 (4%)	0	100	100
5	6	599/1017 (59%)	567 (95%)	32 (5%)	0	100	100
6	7	649/845 (77%)	626 (96%)	21 (3%)	2 (0%)	36	70
7	A	192/208 (92%)	191 (100%)	1 (0%)	0	100	100
8	B	189/213 (89%)	180 (95%)	9 (5%)	0	100	100
9	C	166/194 (86%)	161 (97%)	5 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	D	237/294 (81%)	228 (96%)	9 (4%)	0	100	100
11	E	560/650 (86%)	529 (94%)	28 (5%)	3 (0%)	24	61
12	F	418/927 (45%)	407 (97%)	11 (3%)	0	100	100
12	G	416/927 (45%)	398 (96%)	18 (4%)	0	100	100
12	H	419/927 (45%)	399 (95%)	19 (4%)	1 (0%)	43	76
14	N	81/689 (12%)	71 (88%)	10 (12%)	0	100	100
All	All	6264/10438 (60%)	5984 (96%)	274 (4%)	6 (0%)	49	81

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	7	220	ILE
11	E	127	ARG
11	E	597	THR
12	H	749	TYR
11	E	596	HIS
6	7	632	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	2	544/770 (71%)	544 (100%)	0	100	100
2	3	534/835 (64%)	529 (99%)	5 (1%)	70	76
3	4	561/848 (66%)	561 (100%)	0	100	100
4	5	478/688 (70%)	478 (100%)	0	100	100
5	6	531/886 (60%)	531 (100%)	0	100	100
6	7	566/753 (75%)	549 (97%)	17 (3%)	36	57
7	A	181/193 (94%)	181 (100%)	0	100	100
8	B	183/198 (92%)	183 (100%)	0	100	100
9	C	155/173 (90%)	155 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	D	234/279 (84%)	234 (100%)	0	100	100
11	E	509/586 (87%)	503 (99%)	6 (1%)	63	73
12	F	375/825 (46%)	375 (100%)	0	100	100
12	G	372/825 (45%)	372 (100%)	0	100	100
12	H	375/825 (46%)	375 (100%)	0	100	100
14	N	63/629 (10%)	60 (95%)	3 (5%)	23	46
All	All	5661/9313 (61%)	5630 (100%)	31 (0%)	78	82

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	3	51	ASN
2	3	57	ASN
2	3	58	ASP
2	3	90	ASN
2	3	91	ILE
6	7	144	ASN
6	7	210	ASN
6	7	217	LYS
6	7	218	LYS
6	7	220	ILE
6	7	221	SER
6	7	222	SER
6	7	225	LEU
6	7	229	GLN
6	7	385	LYS
6	7	386	LYS
6	7	622	HIS
6	7	623	ASN
6	7	624	LYS
6	7	628	LEU
6	7	633	VAL
6	7	634	GLU
11	E	588	TYR
11	E	590	ARG
11	E	592	LEU
11	E	595	ILE
11	E	597	THR
11	E	601	ILE
14	N	77	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
14	N	92	LYS
14	N	93	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
1	2	641	GLN
2	3	46	GLN
2	3	51	ASN
2	3	351	ASN
2	3	517	ASN
2	3	526	ASN
2	3	691	ASN
3	4	263	ASN
3	4	386	HIS
3	4	576	GLN
3	4	651	GLN
4	5	49	GLN
4	5	514	ASN
4	5	632	GLN
6	7	19	ASN
6	7	76	ASN
6	7	112	HIS
6	7	237	GLN
6	7	264	GLN
6	7	293	GLN
6	7	332	ASN
6	7	379	GLN
6	7	543	GLN
6	7	622	HIS
6	7	662	GLN
7	A	58	GLN
7	A	206	GLN
8	B	47	HIS
9	C	103	HIS
9	C	130	GLN
9	C	138	HIS
10	D	89	ASN
10	D	186	HIS
10	D	249	ASN
11	E	55	GLN
11	E	130	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	E	138	GLN
11	E	229	GLN
11	E	269	ASN
11	E	354	ASN
11	E	402	GLN
11	E	461	ASN
11	E	497	GLN
12	F	527	HIS
12	F	622	ASN
12	F	843	ASN
12	G	510	GLN
12	G	540	ASN
12	G	553	GLN
12	G	634	HIS
12	G	673	ASN
12	G	915	ASN
12	H	852	ASN
12	H	877	GLN
14	N	72	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 13 ligands modelled in this entry, 9 are monoatomic - leaving 4 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	$\# Z > 2$
15	ADP	3	1001	16	28,29,29	1.38	4 (14%)	43,45,45	1.85	9 (20%)
15	ADP	2	901	16	28,29,29	1.40	4 (14%)	43,45,45	1.86	10 (23%)
18	AGS	7	902	16	32,33,33	0.61	1 (3%)	45,52,52	0.73	1 (2%)
18	AGS	4	1001	16	32,33,33	0.64	1 (3%)	45,52,52	0.74	1 (2%)

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
15	ADP	3	1001	16	-	3/16/32/32	0/3/3/3
15	ADP	2	901	16	-	3/16/32/32	0/3/3/3
18	AGS	7	902	16	-	5/21/38/38	0/3/3/3
18	AGS	4	1001	16	-	8/21/38/38	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	2	901	ADP	C5-C4	4.66	1.47	1.39
15	3	1001	ADP	C5-C4	4.61	1.47	1.39
15	3	1001	ADP	C5-C6	2.77	1.48	1.41
15	2	901	ADP	C5-C6	2.76	1.48	1.41
15	2	901	ADP	C8-N7	2.40	1.36	1.31
15	3	1001	ADP	C8-N7	2.34	1.36	1.31
15	3	1001	ADP	C5-N7	-2.25	1.35	1.39
15	2	901	ADP	C5-N7	-2.22	1.35	1.39
18	7	902	AGS	PG-S1G	2.13	1.95	1.90
18	4	1001	AGS	PG-S1G	2.13	1.95	1.90

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	3	1001	ADP	C5-C4-N3	-5.93	118.56	126.72
15	2	901	ADP	C5-C4-N3	-5.70	118.86	126.72
15	3	1001	ADP	N3-C4-N9	4.52	134.85	127.17
15	2	901	ADP	N3-C4-N9	4.44	134.72	127.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	4	1001	AGS	PB-O3B-PG	-4.22	117.74	133.17
18	7	902	AGS	PB-O3B-PG	-4.20	117.80	133.17
15	2	901	ADP	C2-N3-C4	3.70	120.86	111.83
15	3	1001	ADP	C2-N3-C4	3.69	120.84	111.83
15	2	901	ADP	C4-C5-N7	-3.62	106.44	110.58
15	3	1001	ADP	C4-C5-N7	-3.62	106.44	110.58
15	2	901	ADP	N3-C2-N1	-3.26	123.64	128.58
15	3	1001	ADP	N3-C2-N1	-3.03	124.00	128.58
15	2	901	ADP	C4-N9-C8	2.75	108.63	105.74
15	2	901	ADP	C5-N7-C8	2.66	107.63	103.45
15	3	1001	ADP	C5-N7-C8	2.55	107.46	103.45
15	3	1001	ADP	C4-N9-C8	2.42	108.28	105.74
15	2	901	ADP	C6-C5-N7	2.29	136.50	132.09
15	3	1001	ADP	C3'-C2'-C1'	2.28	105.77	101.46
15	2	901	ADP	O4'-C1'-N9	2.17	112.25	108.09
15	2	901	ADP	N9-C8-N7	-2.15	110.89	113.94
15	3	1001	ADP	C6-C5-N7	2.13	136.20	132.09

There are no chirality outliers.

All (19) torsion outliers are listed below:

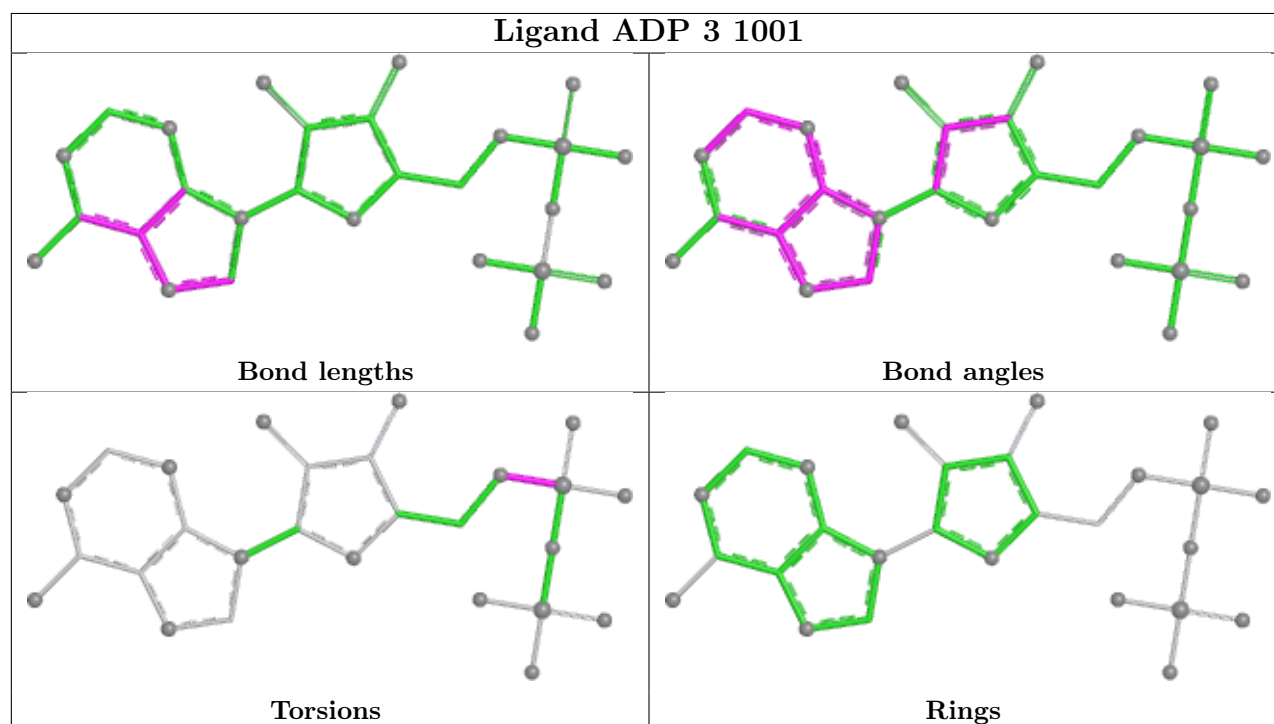
Mol	Chain	Res	Type	Atoms
15	2	901	ADP	C5'-O5'-PA-O1A
15	2	901	ADP	C5'-O5'-PA-O2A
15	2	901	ADP	C5'-O5'-PA-O3A
15	3	1001	ADP	C5'-O5'-PA-O1A
15	3	1001	ADP	C5'-O5'-PA-O2A
15	3	1001	ADP	C5'-O5'-PA-O3A
18	4	1001	AGS	PB-O3B-PG-O3G
18	4	1001	AGS	C5'-O5'-PA-O1A
18	4	1001	AGS	C5'-O5'-PA-O2A
18	7	902	AGS	C5'-O5'-PA-O1A
18	7	902	AGS	C5'-O5'-PA-O2A
18	7	902	AGS	C5'-O5'-PA-O3A
18	4	1001	AGS	O4'-C4'-C5'-O5'
18	4	1001	AGS	C3'-C4'-C5'-O5'
18	7	902	AGS	C4'-C5'-O5'-PA
18	7	902	AGS	PB-O3A-PA-O5'
18	4	1001	AGS	C5'-O5'-PA-O3A
18	4	1001	AGS	PB-O3B-PG-O2G
18	4	1001	AGS	PA-O3A-PB-O2B

There are no ring outliers.

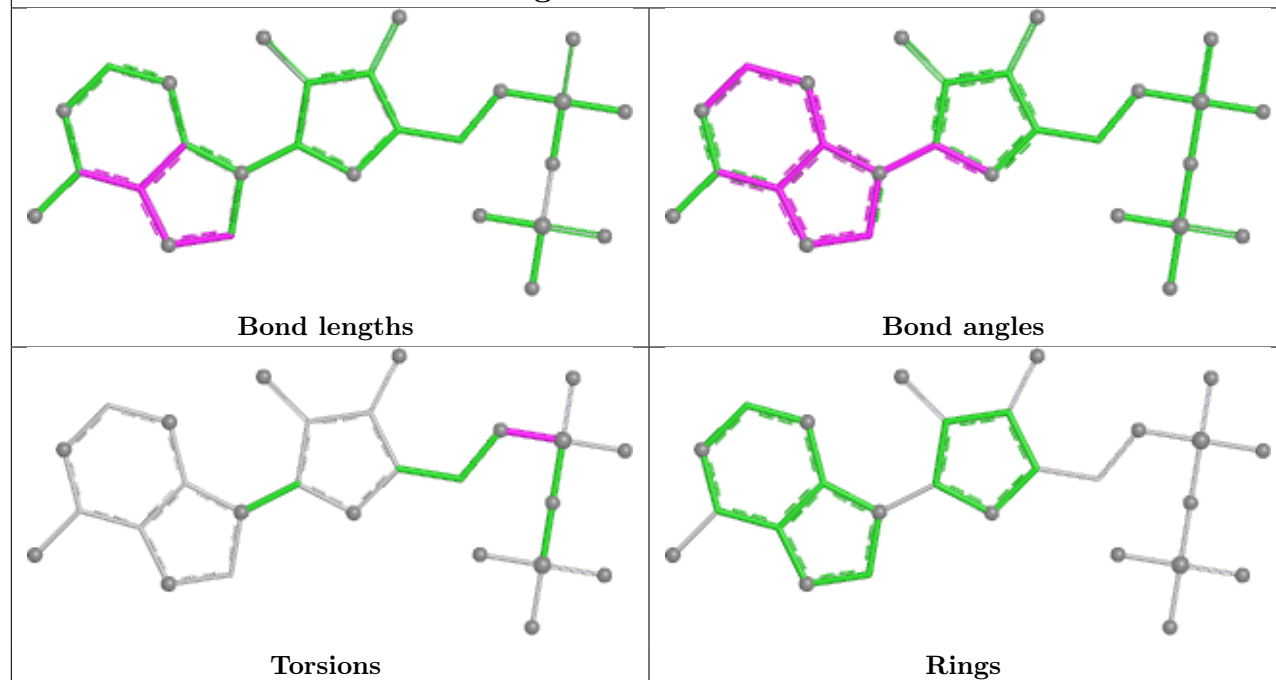
4 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	3	1001	ADP	6	0
15	2	901	ADP	8	0
18	7	902	AGS	7	0
18	4	1001	AGS	6	0

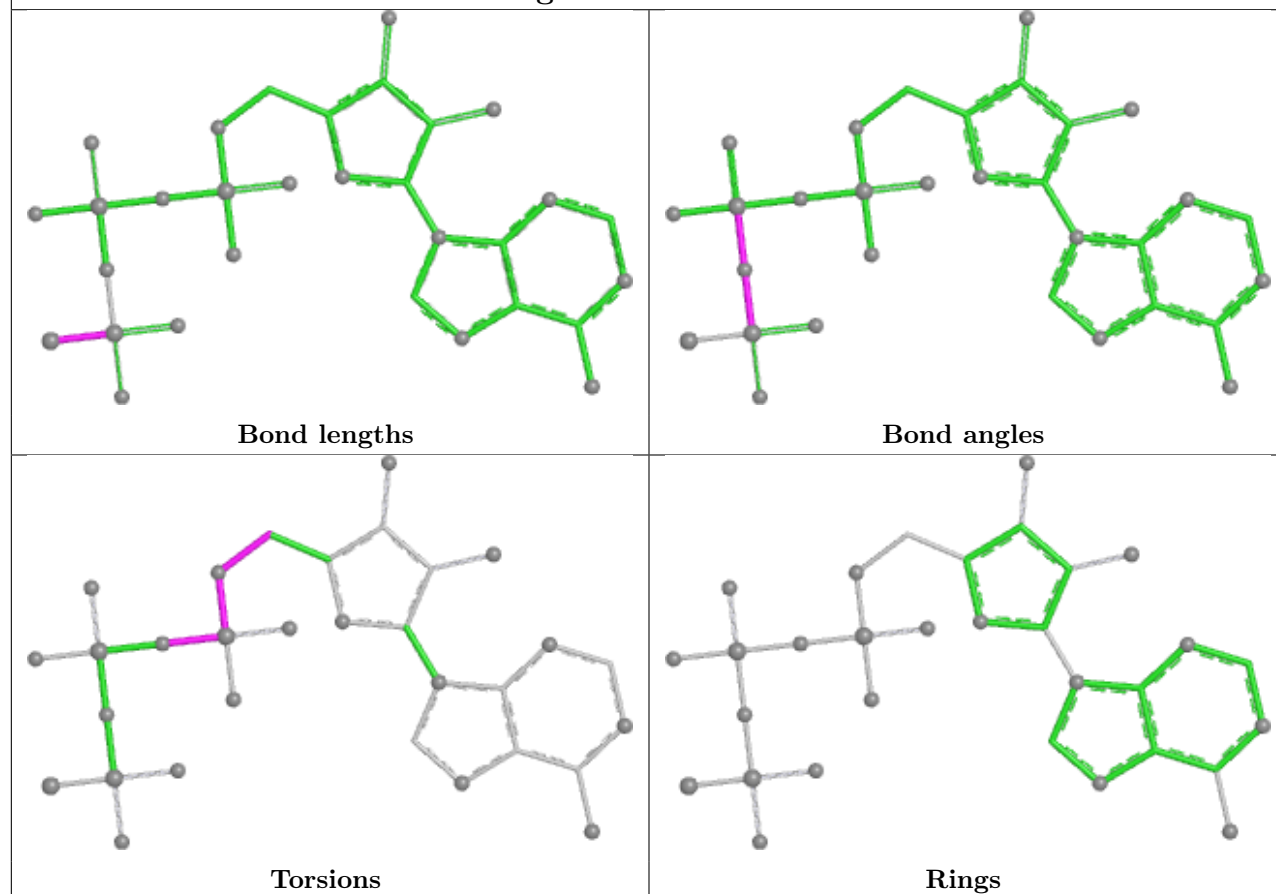
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

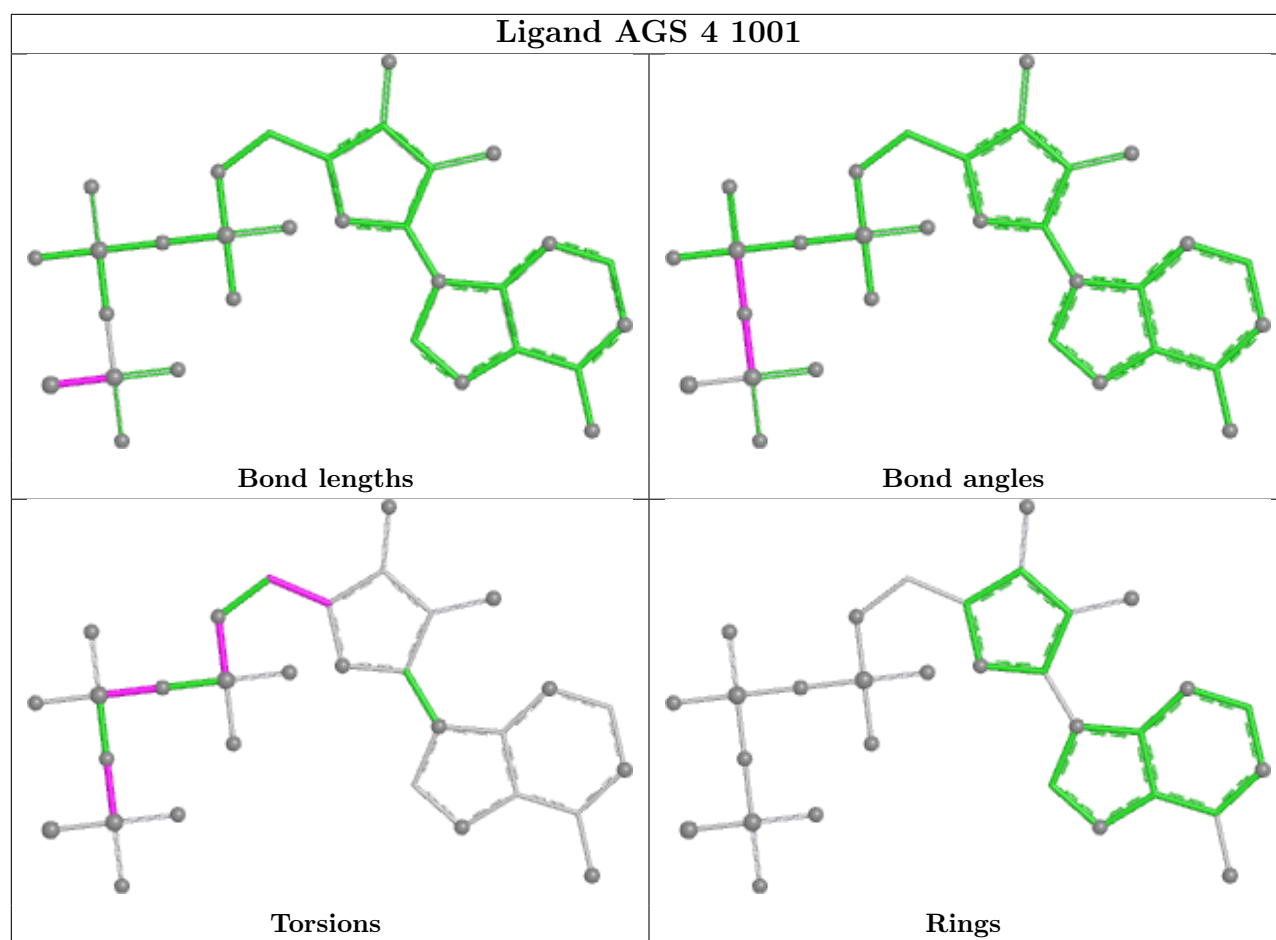


Ligand ADP 2 901



Ligand AGS 7 902





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

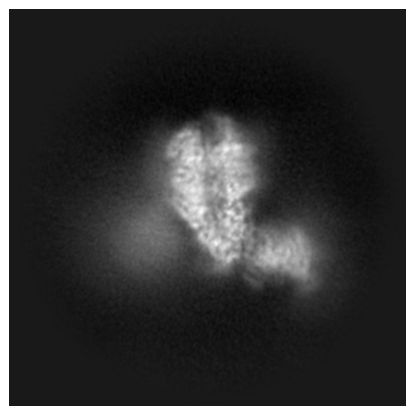
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37343. These allow visual inspection of the internal detail of the map and identification of artifacts.

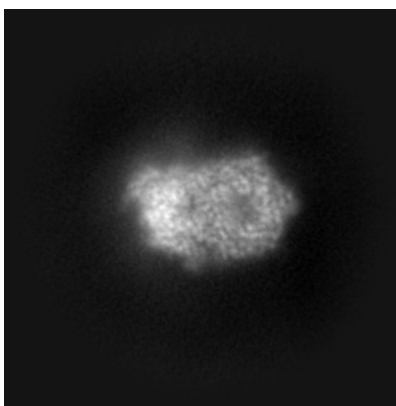
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

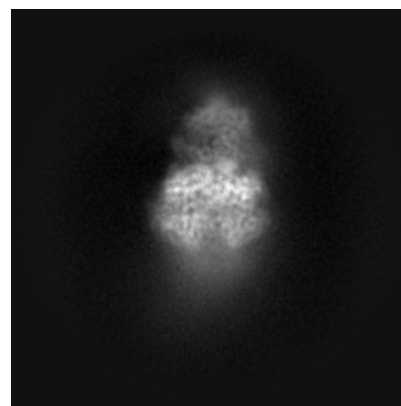
6.1.1 Primary map



X

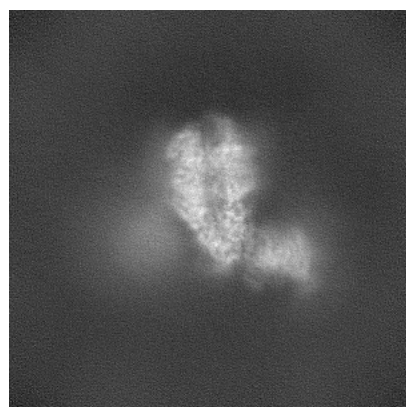


Y

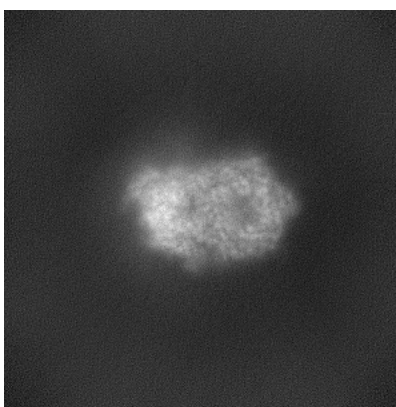


Z

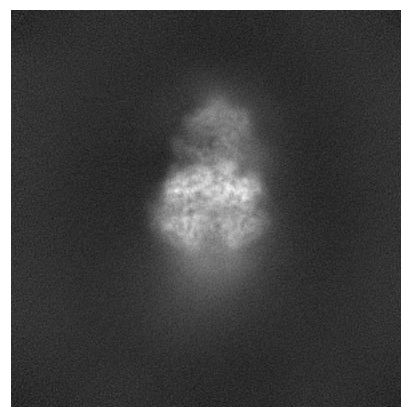
6.1.2 Raw map



X



Y

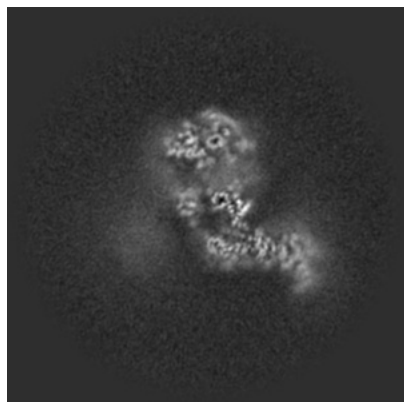


Z

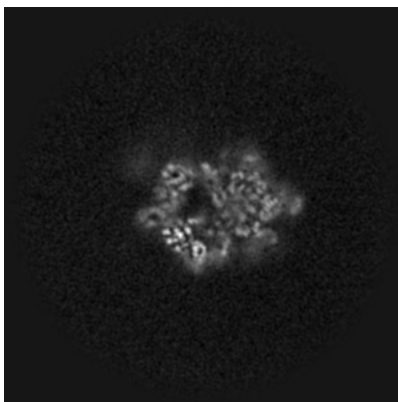
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

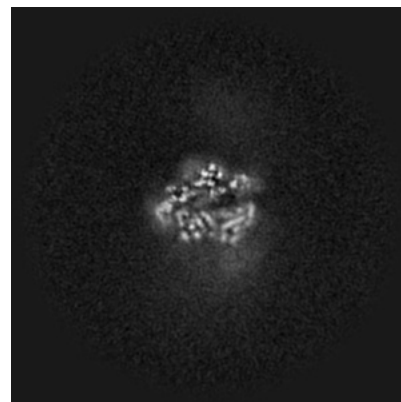
6.2.1 Primary map



X Index: 220

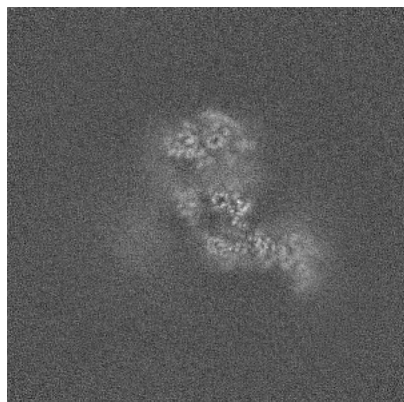


Y Index: 220

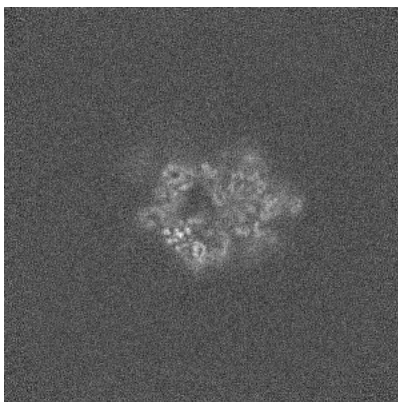


Z Index: 220

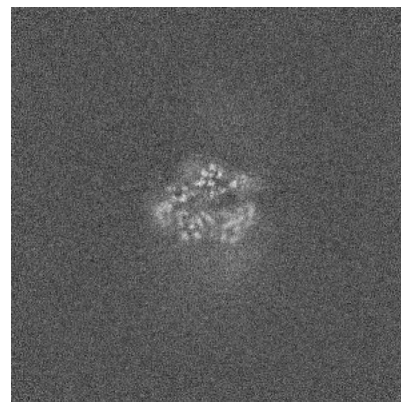
6.2.2 Raw map



X Index: 220



Y Index: 220

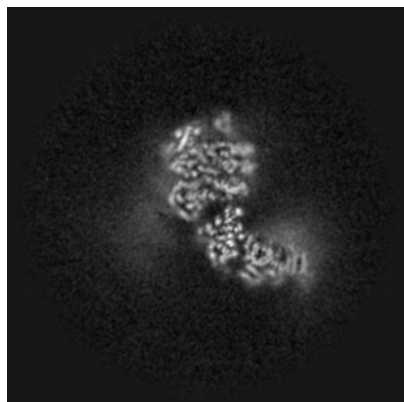


Z Index: 220

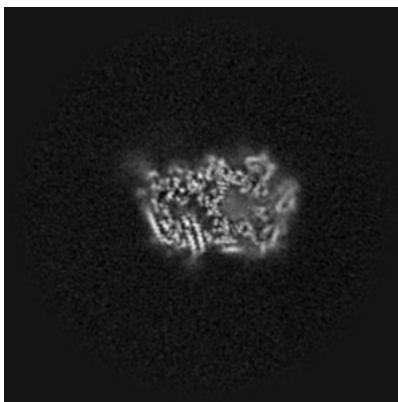
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

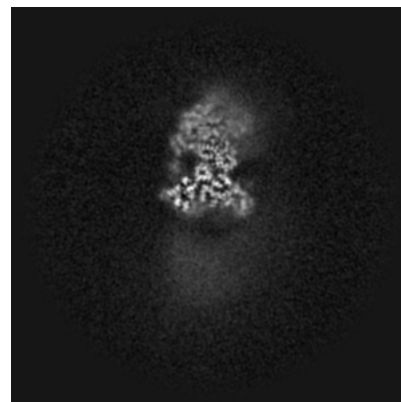
6.3.1 Primary map



X Index: 240

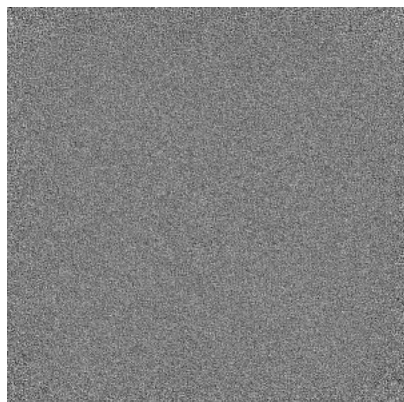


Y Index: 241

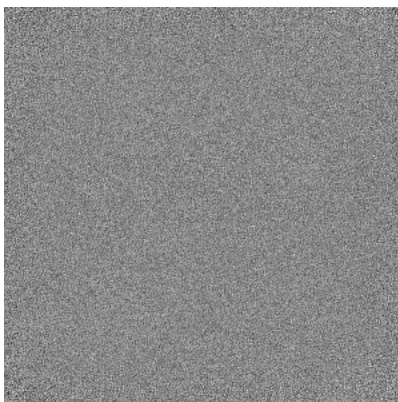


Z Index: 178

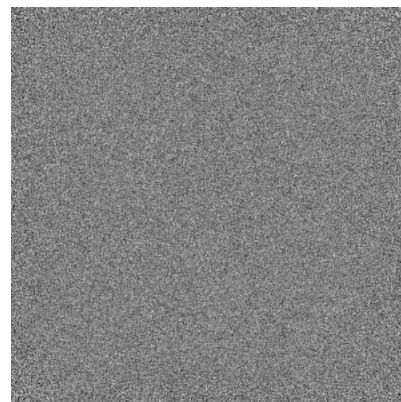
6.3.2 Raw map



X Index: 0



Y Index: 0

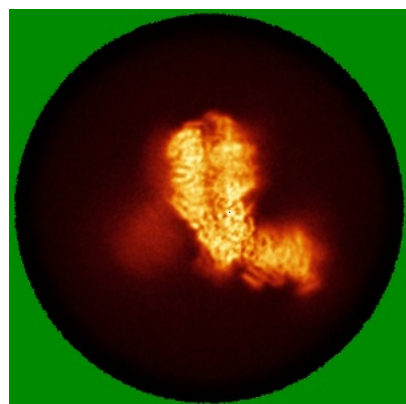


Z Index: 0

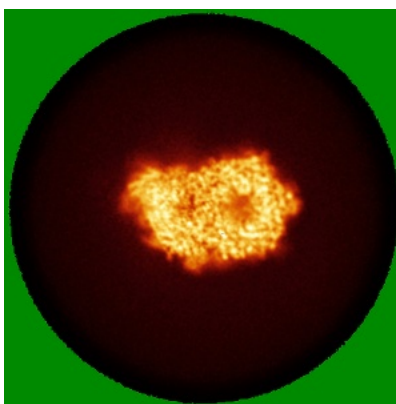
The images above show the largest variance slices of the map in three orthogonal directions.

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

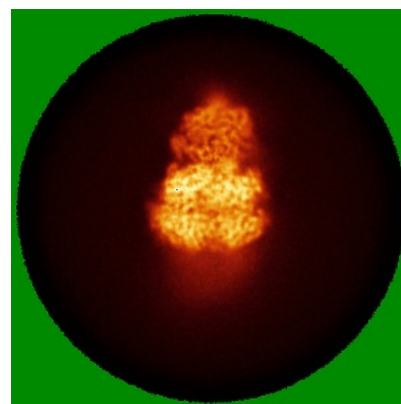
6.4.1 Primary map



X

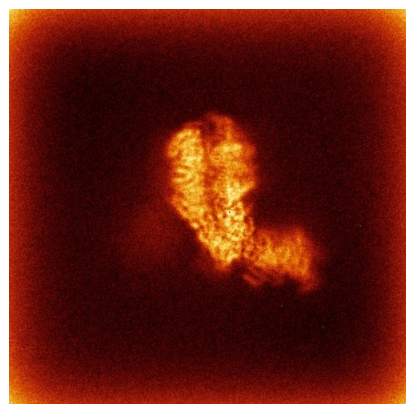


Y

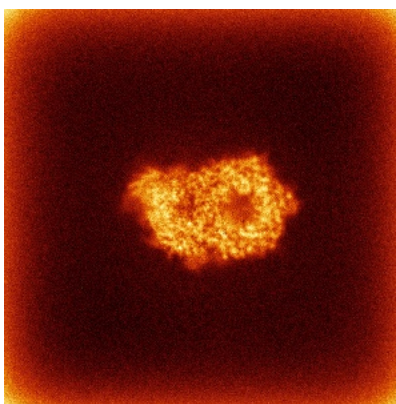


Z

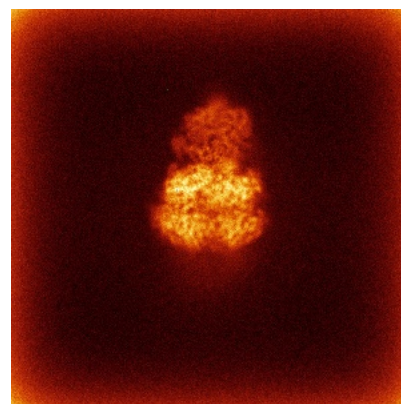
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

This section was not generated.

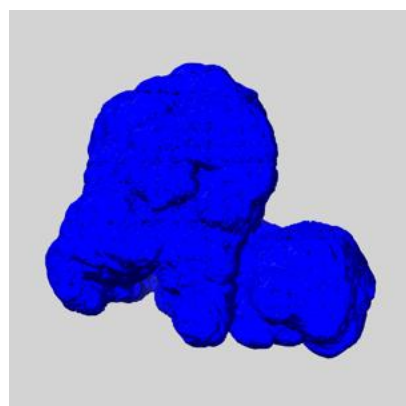
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

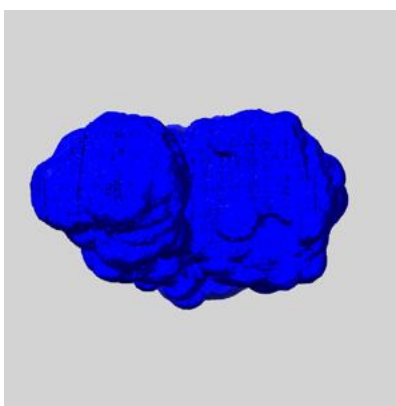
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

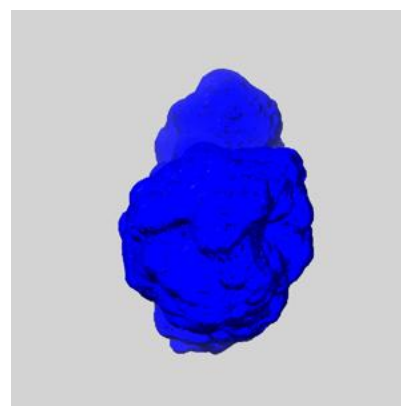
6.6.1 emd_37343_msk_1.map [i](#)



X



Y

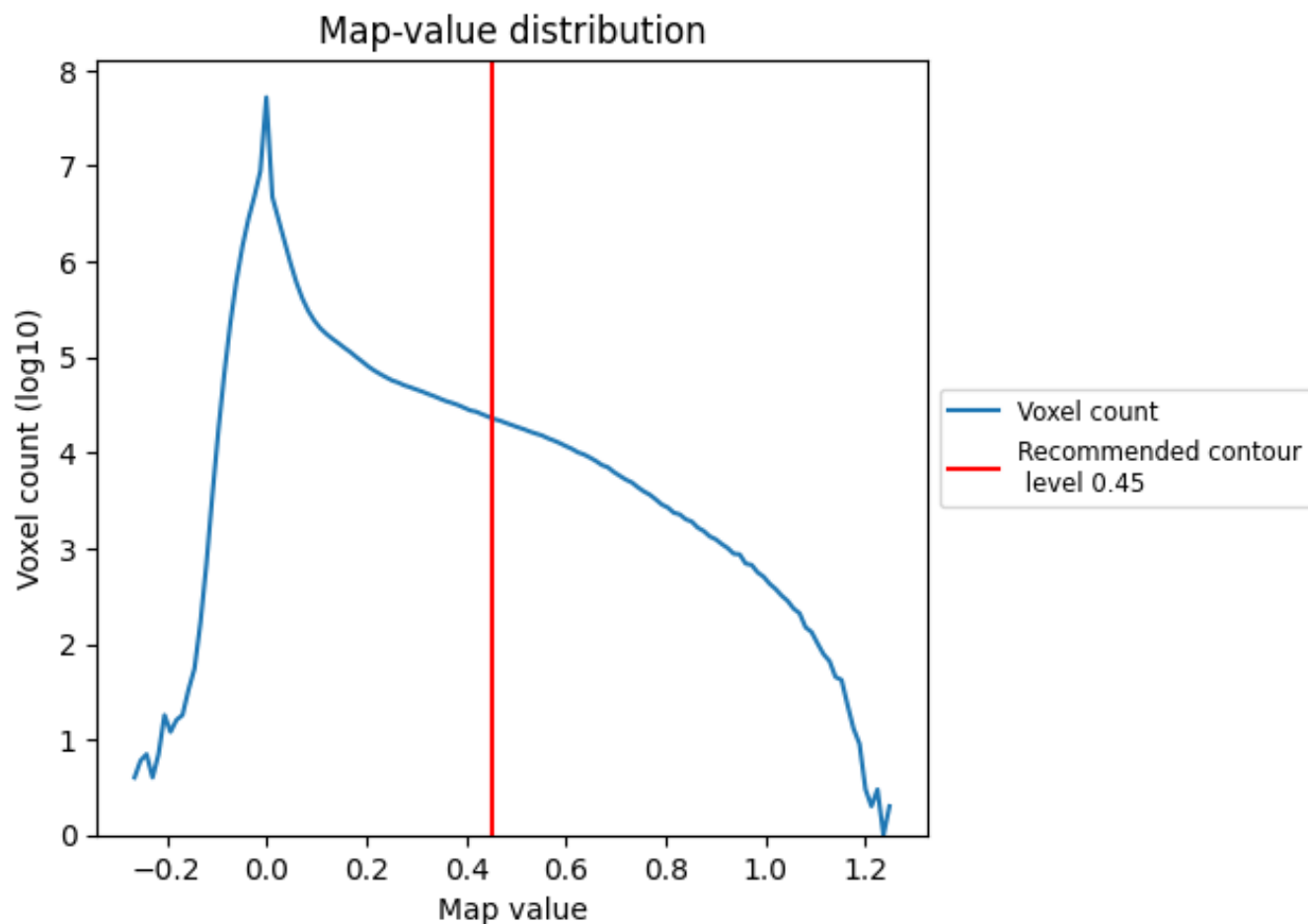


Z

7 Map analysis [i](#)

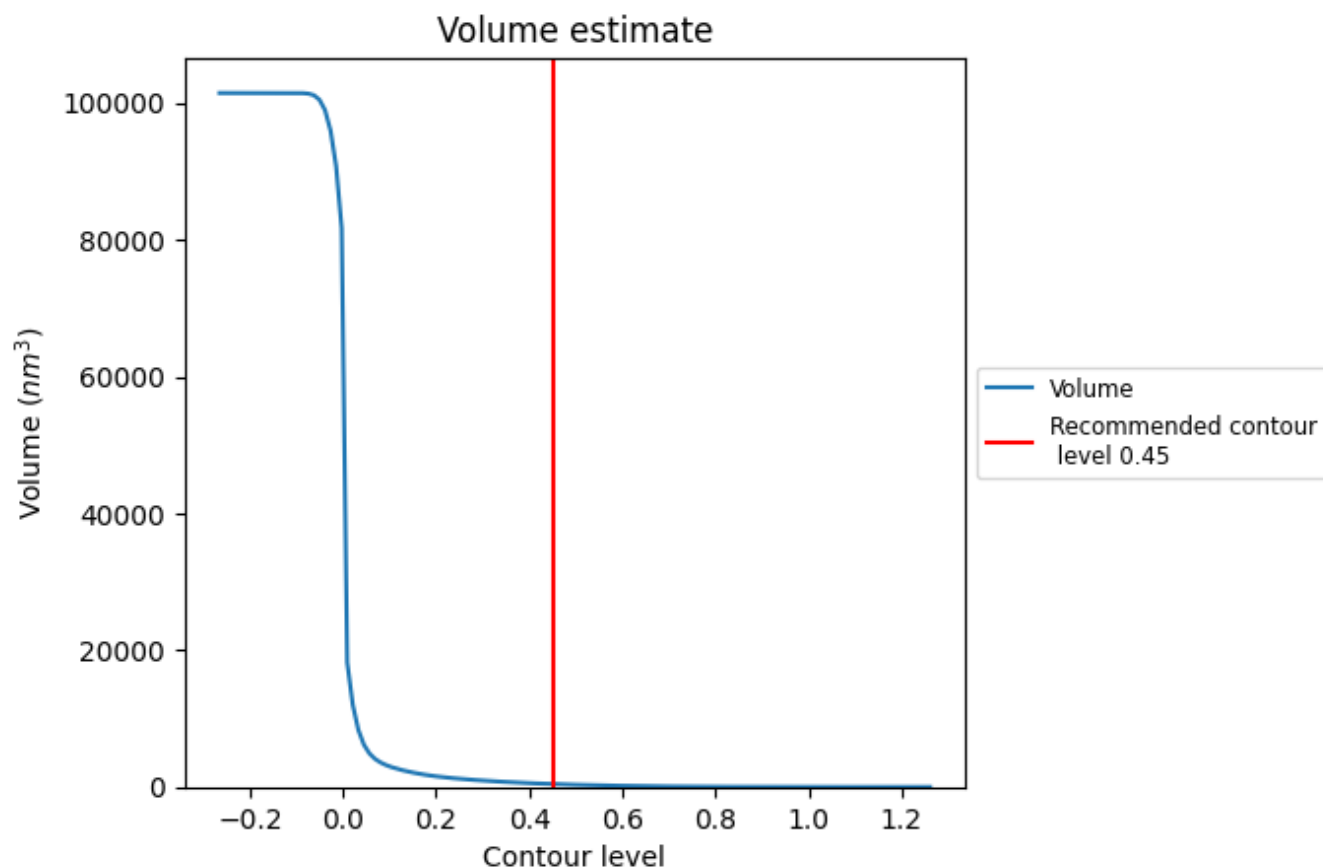
This section contains the results of statistical analysis of the map.

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.

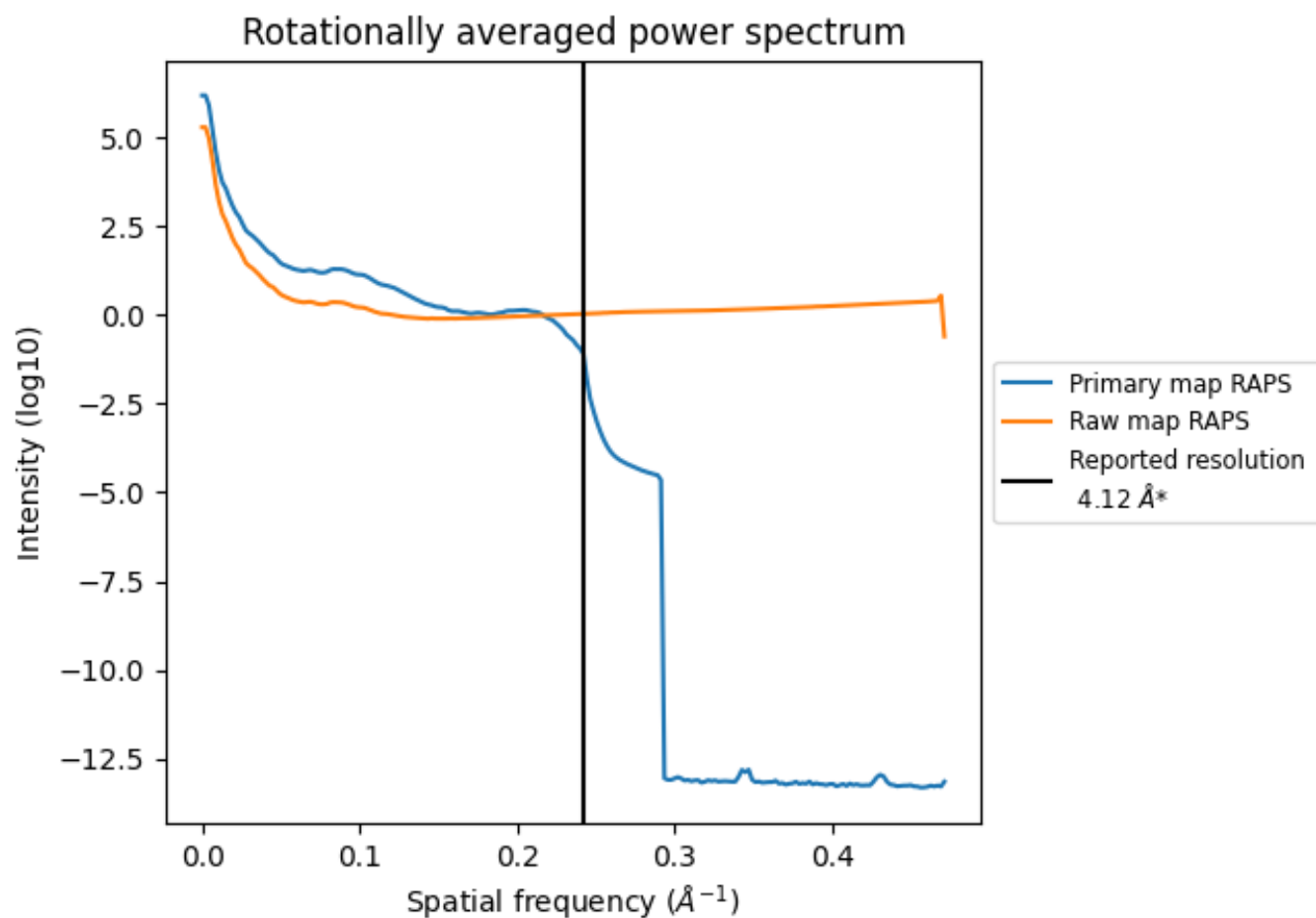
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 427 nm³; this corresponds to an approximate mass of 386 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 ⓘ

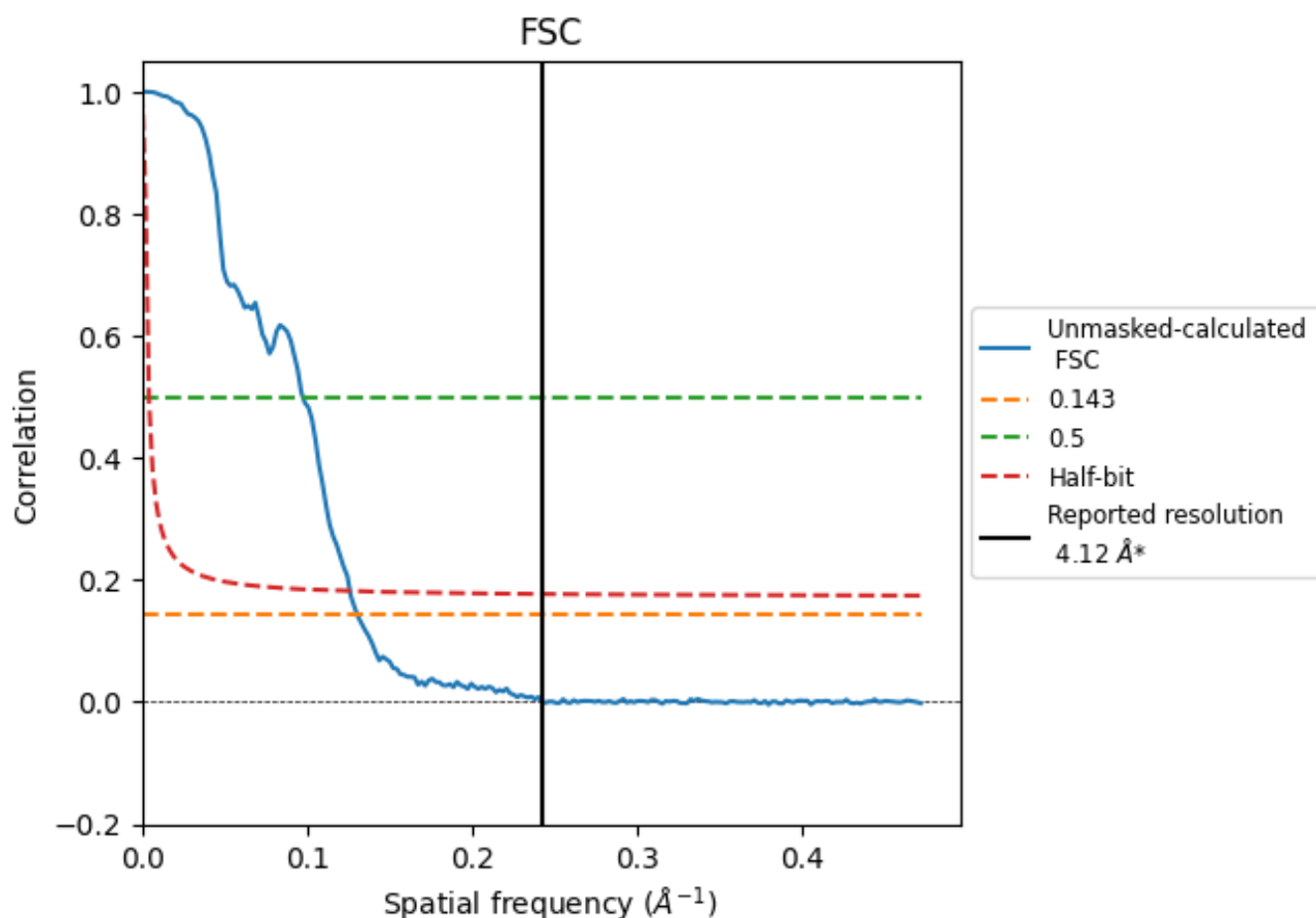


*Reported resolution corresponds to spatial frequency of 0.243 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.243 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

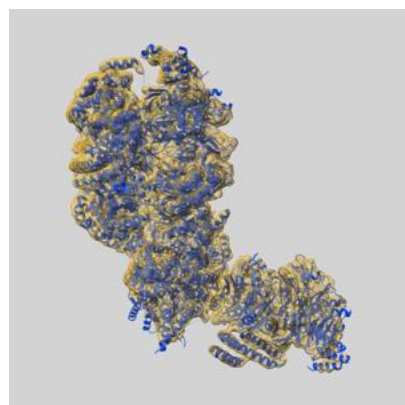
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.12	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.67	10.27	7.94

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.67 differs from the reported value 4.12 by more than 10 %

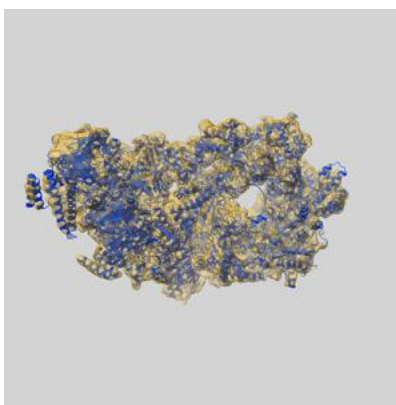
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-37343 and PDB model 8W7M. Per-residue inclusion information can be found in [section 3](#) on [page 9](#).

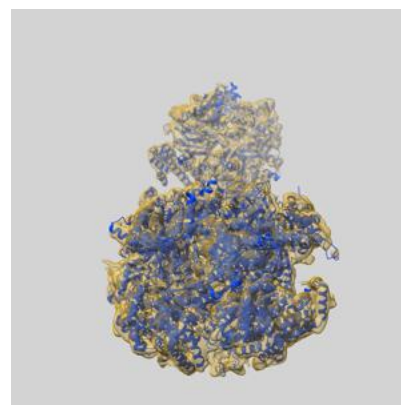
9.1 Map-model overlay [i](#)



X



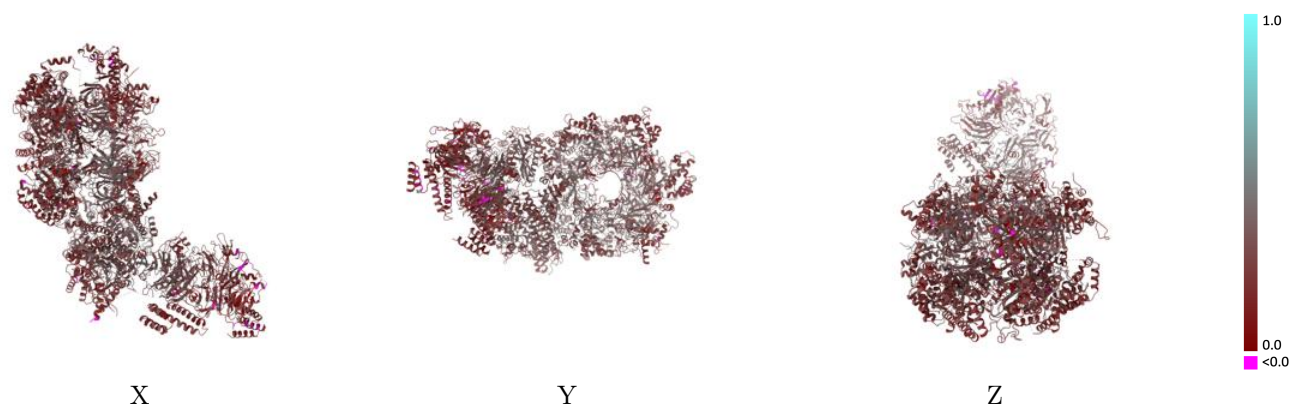
Y



Z

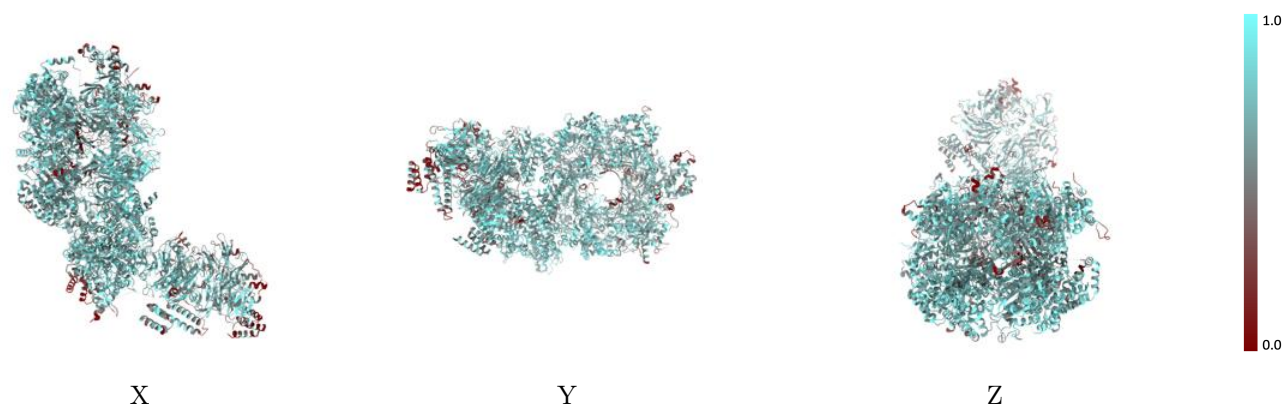
The images above show the 3D surface view of the map at the recommended contour level 0.45 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



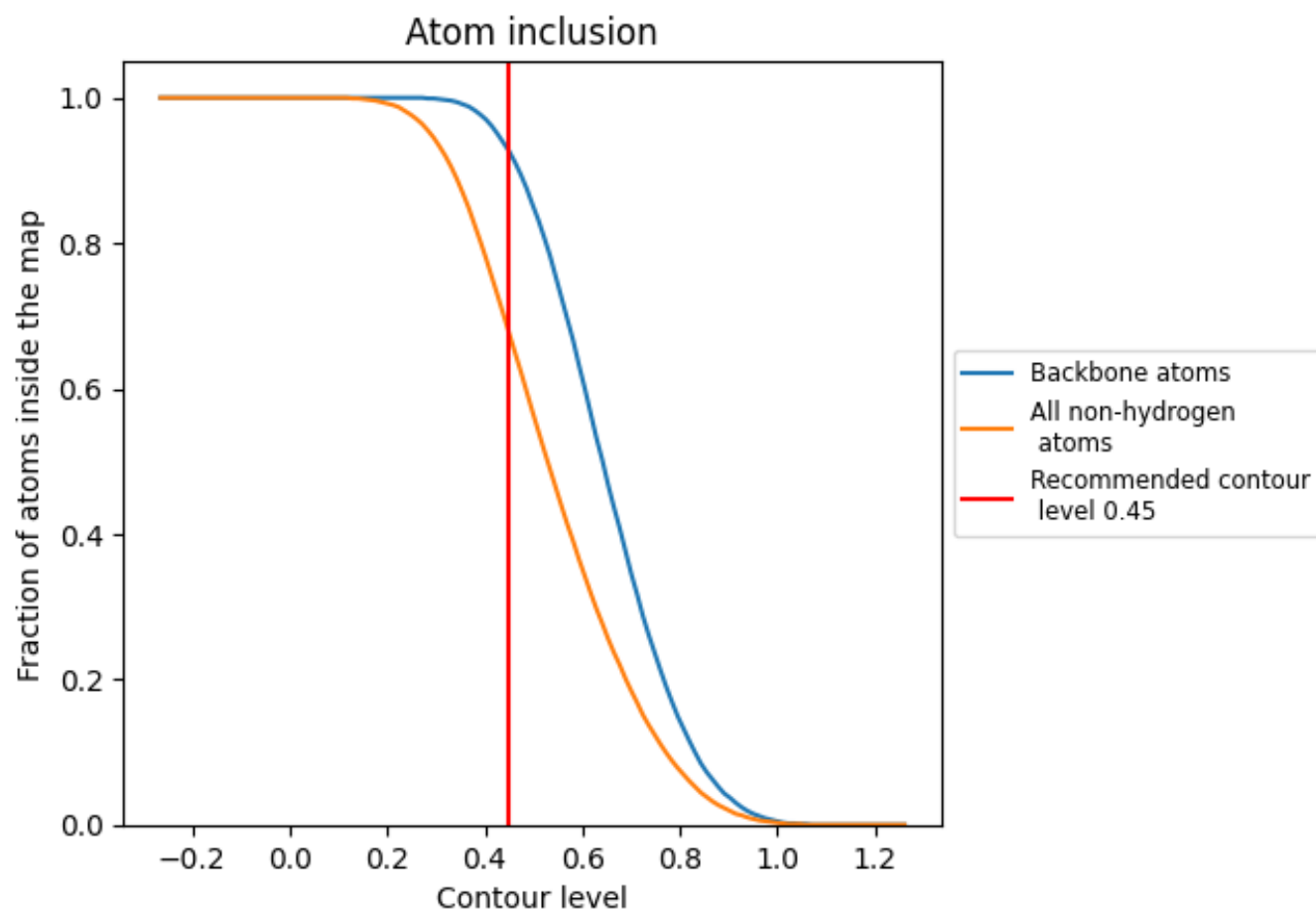
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.45).

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 68% 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 (0.45) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6760	 0.2670
2	 0.6790	 0.2610
3	 0.7350	 0.2910
4	 0.6630	 0.2440
5	 0.7140	 0.2920
6	 0.6790	 0.2490
7	 0.6590	 0.2580
A	 0.7130	 0.2750
B	 0.7520	 0.3310
C	 0.7550	 0.2980
D	 0.7450	 0.3110
E	 0.7050	 0.2900
F	 0.6880	 0.2980
G	 0.5560	 0.2050
H	 0.6160	 0.2210
I	 0.4560	 0.2750
N	 0.2230	 0.2120

