



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 06:20 AM UTC

PDB ID : 8DVE / pdb_00008dve
EMDB ID : EMD-27736
Title : RyR1 in presence of IpCa-T26E phosphomimetic and activating ligands
Authors : Haji-Ghassemi, O.; Van Petegm, F.
Deposited on : 2022-07-28
Resolution : 3.84 Å(reported)
Based on initial model : 6M2W

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:

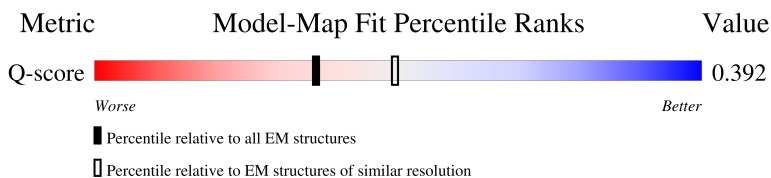
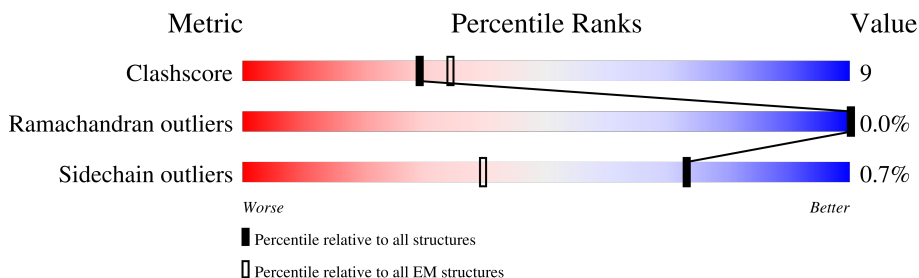
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.84 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.



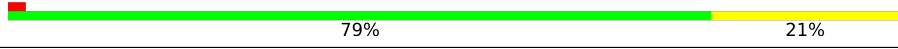
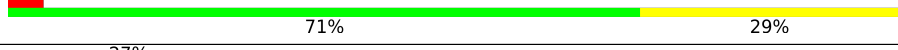
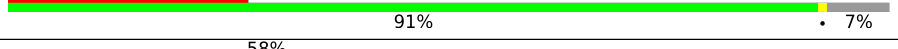
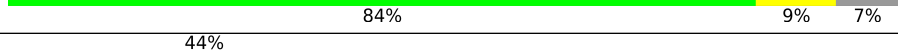
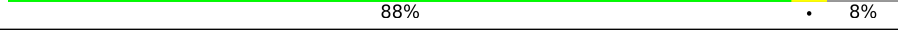
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	9033 (3.34 - 4.34)

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

Mol	Chain	Length	Quality of chain
1	A	5037	
1	D	5037	
1	G	5037	
1	J	5037	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	B	107	
2	E	107	
2	H	107	
2	K	107	
3	C	149	
3	F	149	
3	I	149	
3	L	149	

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 114229 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 Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	D	3942	Total	C	N	O	S	0	0
			26818	17244	4812	4614	148		
1	A	3943	Total	C	N	O	S	0	0
			27274	17556	4883	4676	159		
1	G	3944	Total	C	N	O	S	0	0
			27137	17456	4860	4662	159		
1	J	3943	Total	C	N	O	S	0	0
			26962	17331	4814	4668	149		

- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	107	Total	C	N	O	S	0	0
			743	475	132	133	3		
2	B	107	Total	C	N	O	S	0	0
			743	473	134	132	4		
2	H	107	Total	C	N	O	S	0	0
			745	474	134	134	3		
2	K	107	Total	C	N	O	S	0	0
			728	466	128	131	3		

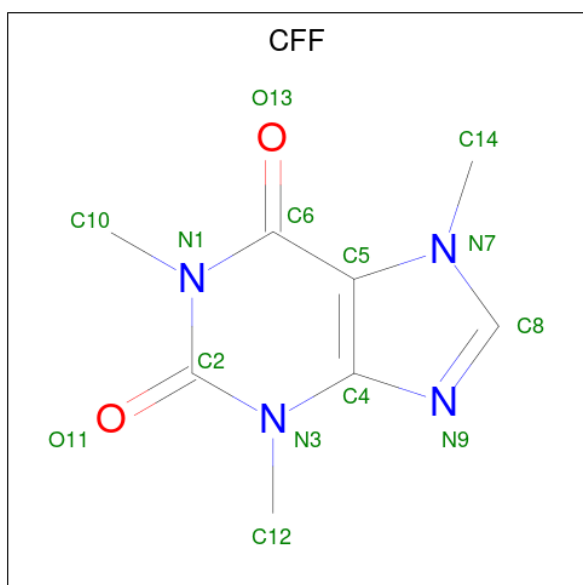
- Molecule 3 is a protein called Calmodulin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	F	138	Total	C	N	O	S	0	0
			715	437	138	139	1		
3	C	138	Total	C	N	O	S	0	0
			720	437	139	142	2		
3	I	138	Total	C	N	O	S	0	0
			730	447	140	142	1		
3	L	137	Total	C	N	O	S	0	0
			726	443	138	141	4		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	32	ALA	GLU	engineered mutation	UNP P0DP23
F	68	ALA	GLU	engineered mutation	UNP P0DP23
F	105	ALA	GLU	engineered mutation	UNP P0DP23
F	141	ALA	GLU	engineered mutation	UNP P0DP23
C	32	ALA	GLU	engineered mutation	UNP P0DP23
C	68	ALA	GLU	engineered mutation	UNP P0DP23
C	105	ALA	GLU	engineered mutation	UNP P0DP23
C	141	ALA	GLU	engineered mutation	UNP P0DP23
I	32	ALA	GLU	engineered mutation	UNP P0DP23
I	68	ALA	GLU	engineered mutation	UNP P0DP23
I	105	ALA	GLU	engineered mutation	UNP P0DP23
I	141	ALA	GLU	engineered mutation	UNP P0DP23
L	32	ALA	GLU	engineered mutation	UNP P0DP23
L	68	ALA	GLU	engineered mutation	UNP P0DP23
L	105	ALA	GLU	engineered mutation	UNP P0DP23
L	141	ALA	GLU	engineered mutation	UNP P0DP23

- Molecule 4 is CAFFEINE (CCD ID: CFF) (formula: $C_8H_{10}N_4O_2$).

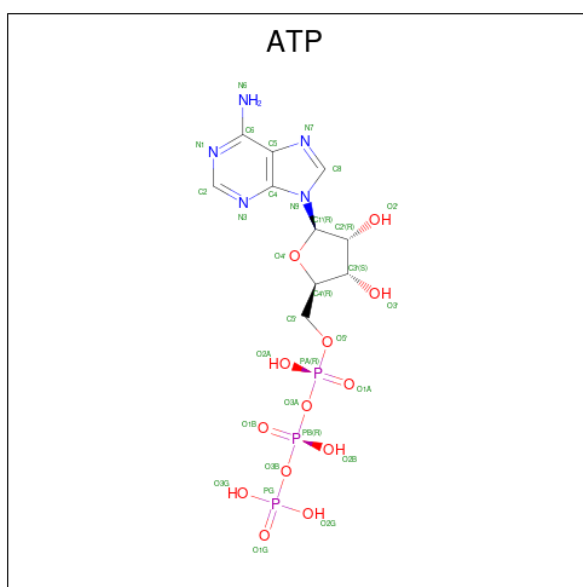


Mol	Chain	Residues	Atoms				AltConf
4	D	1	Total	C	N	O	0
			14	8	4	2	
4	A	1	Total	C	N	O	0
			14	8	4	2	
4	G	1	Total	C	N	O	0
			14	8	4	2	
4	J	1	Total	C	N	O	0
			14	8	4	2	

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
5	D	1	Total	Ca	0
			1	1	
5	A	1	Total	Ca	0
			1	1	
5	G	1	Total	Ca	0
			1	1	
5	J	1	Total	Ca	0
			1	1	

- Molecule 6 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



Mol	Chain	Residues	Atoms					AltConf
6	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
6	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
6	G	1	Total	C	N	O	P	0
			31	10	5	13	3	
6	J	1	Total	C	N	O	P	0
			31	10	5	13	3	

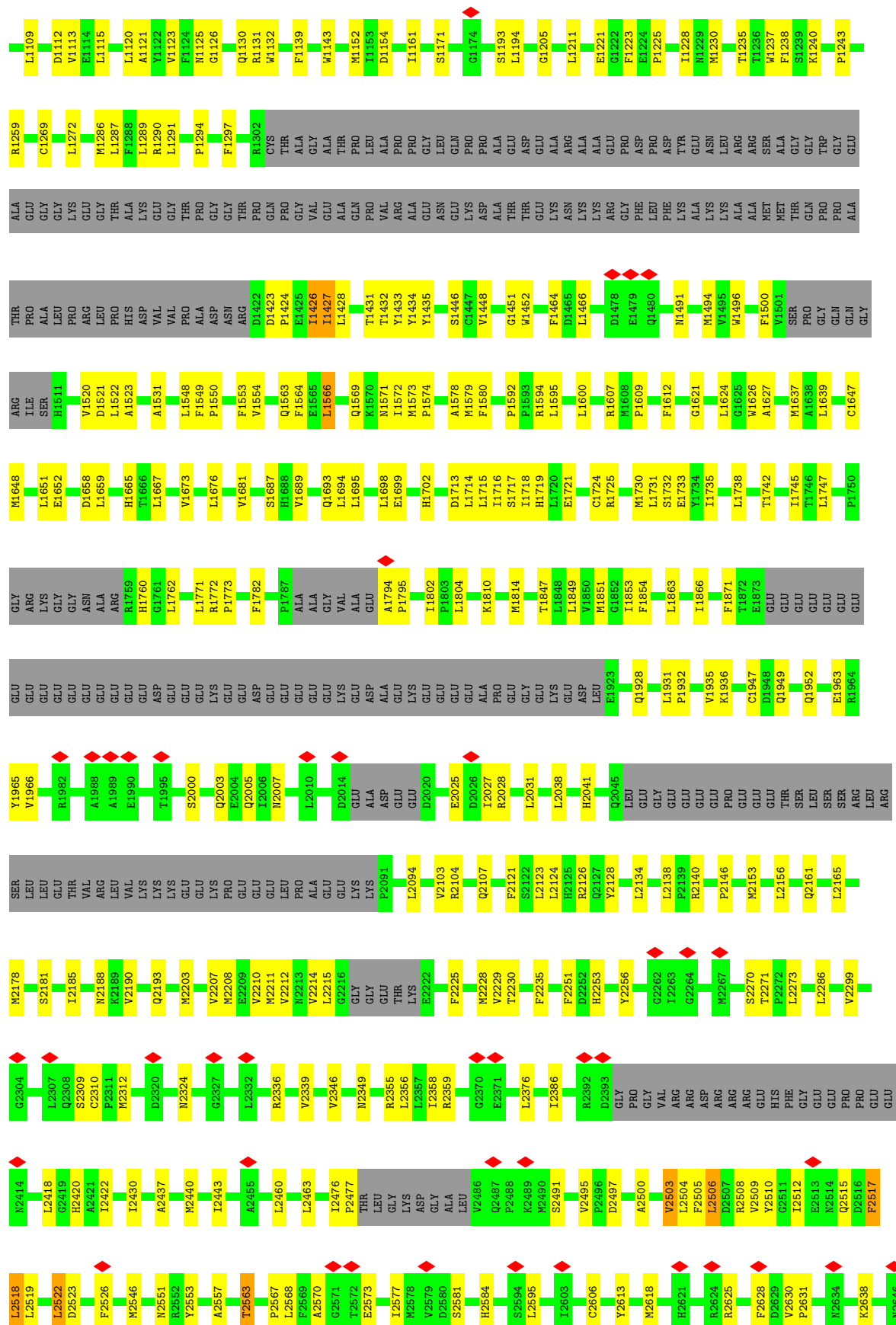
- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
7	D	1	Total	Zn	0
			1	1	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
7	A	1	Total 1	Zn 1	0
7	G	1	Total 1	Zn 1	0
7	J	1	Total 1	Zn 1	0

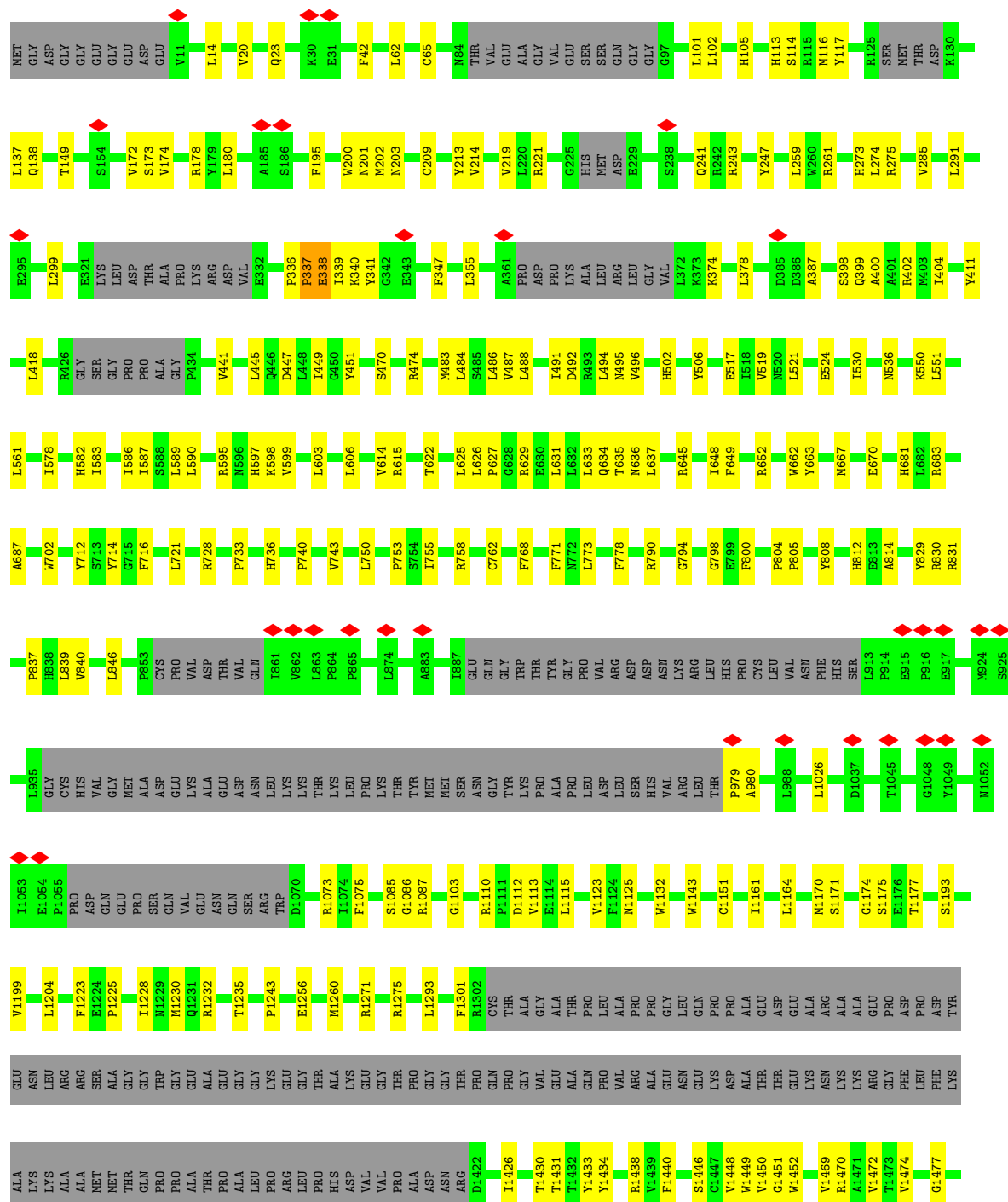






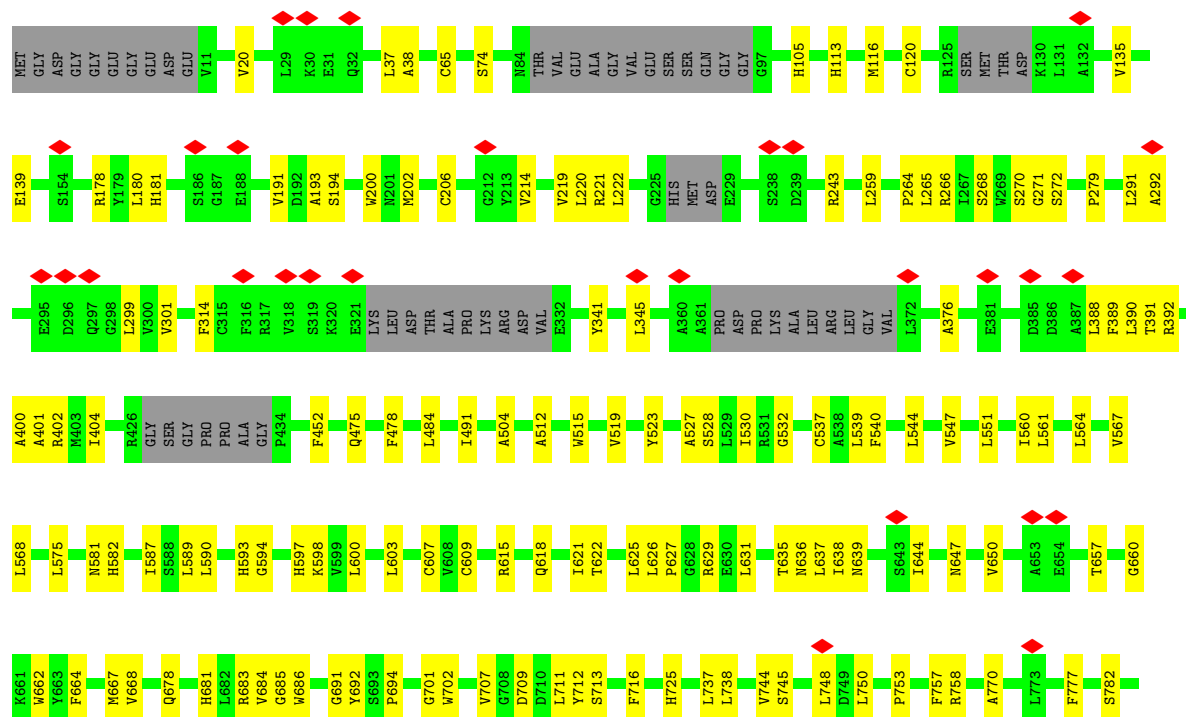


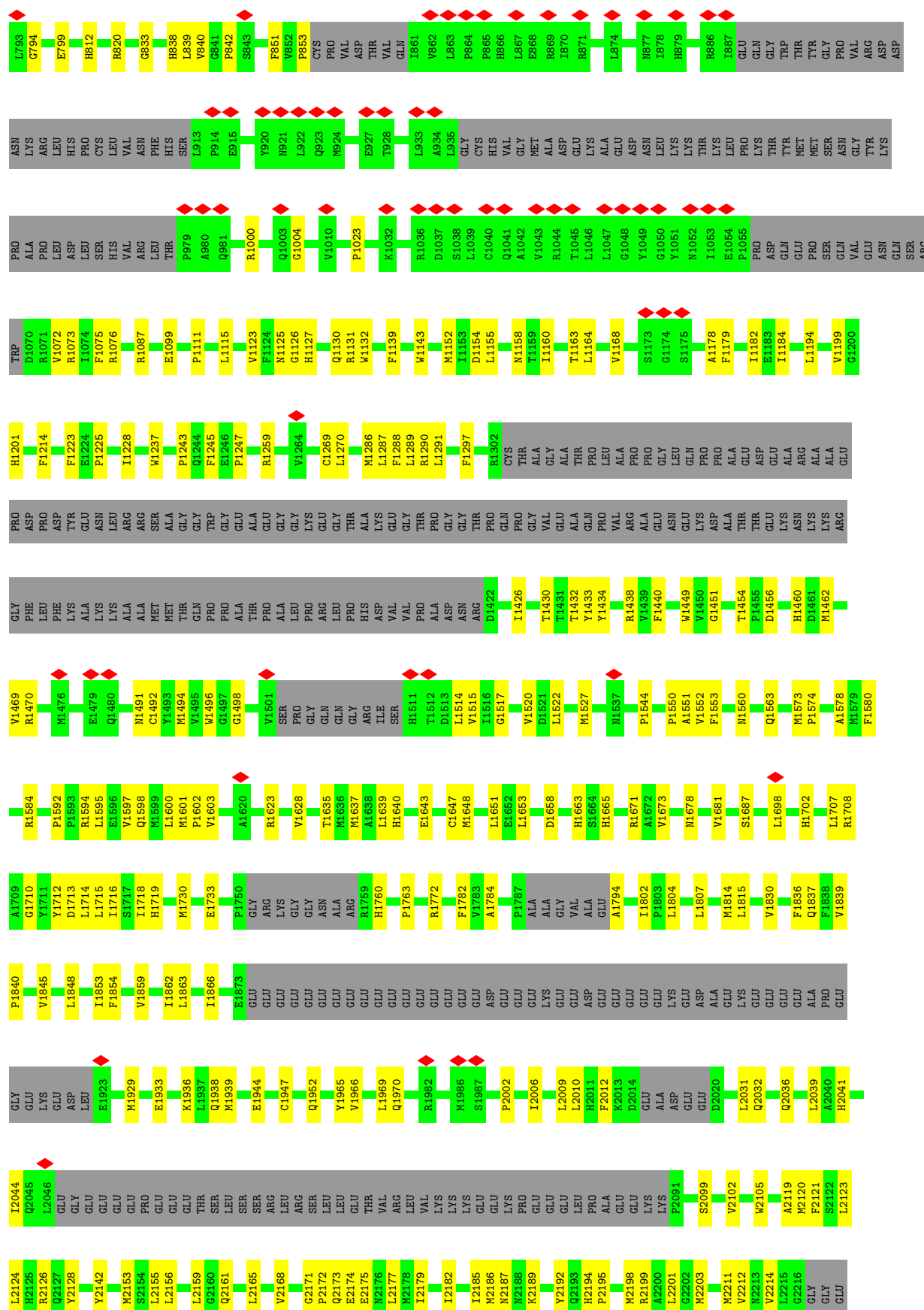
Molecule 1: Ryanodine receptor 1

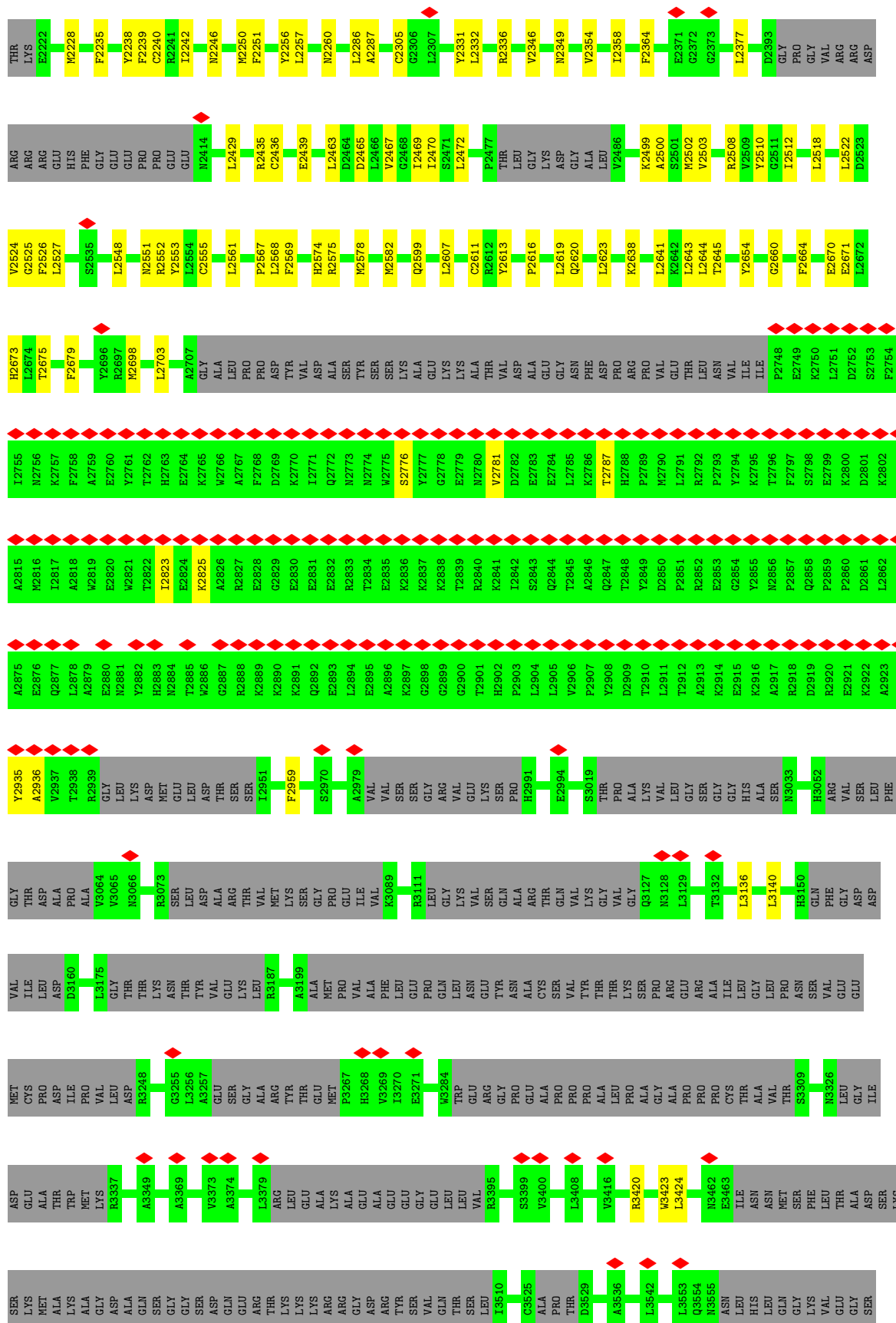










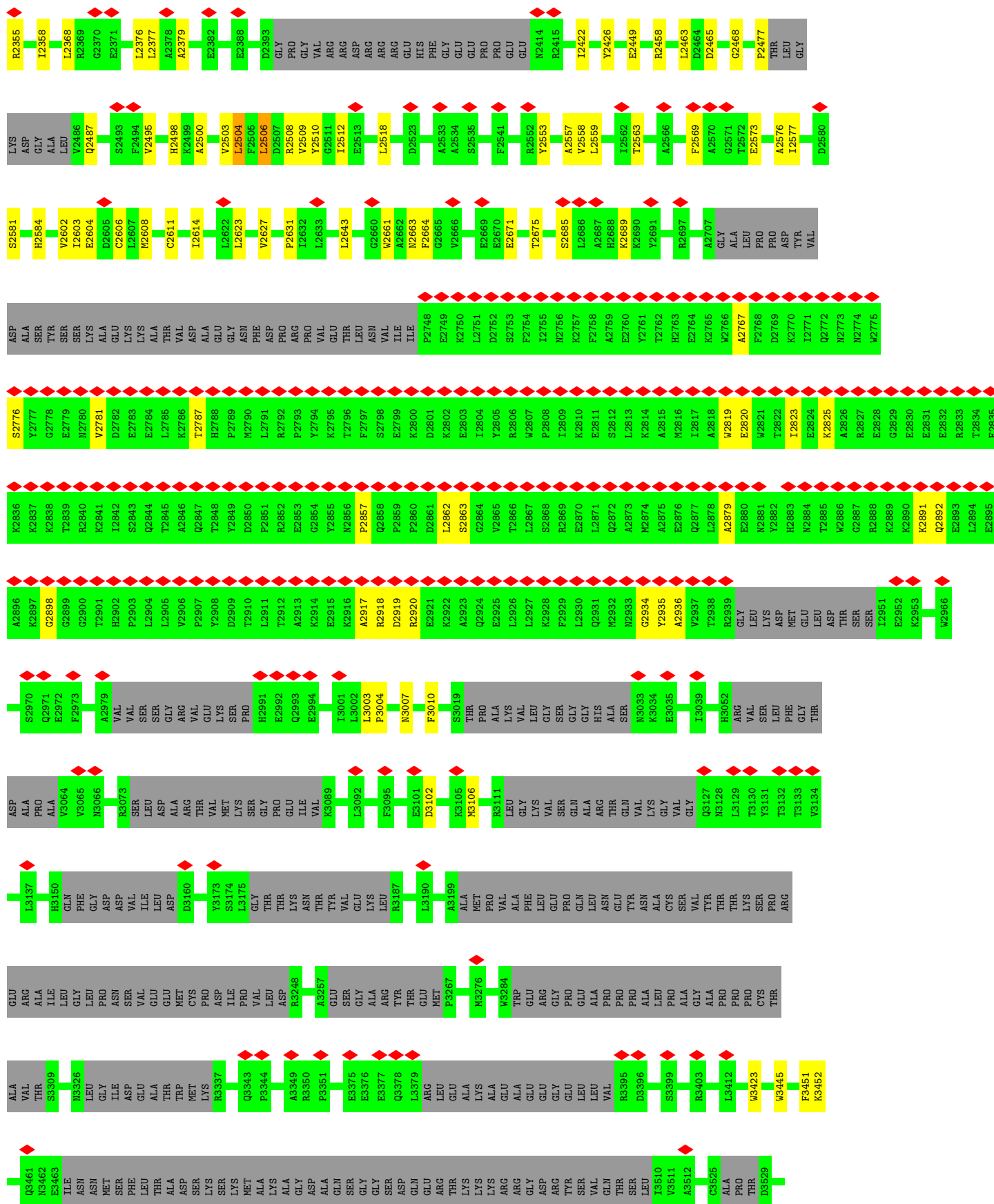




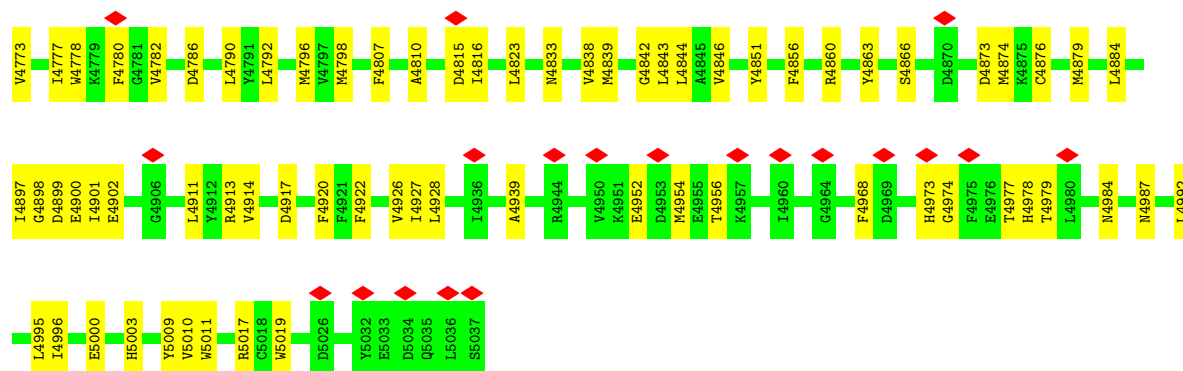
Chain J:







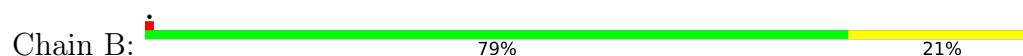




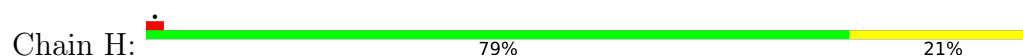
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B



- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B



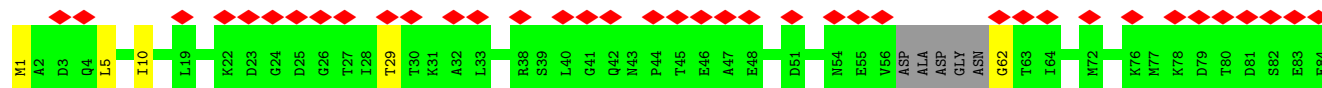
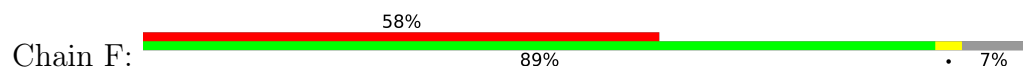
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

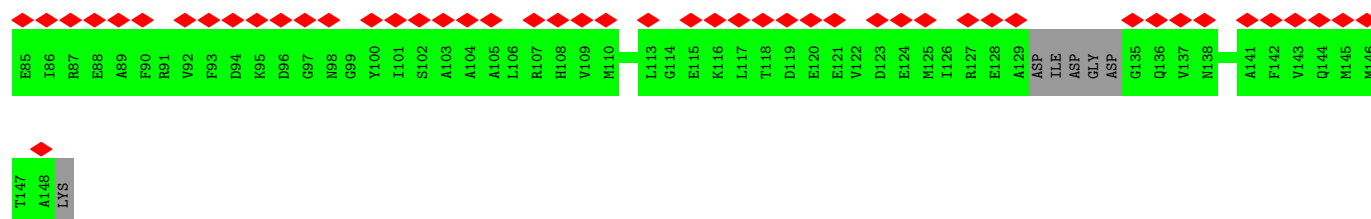


- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

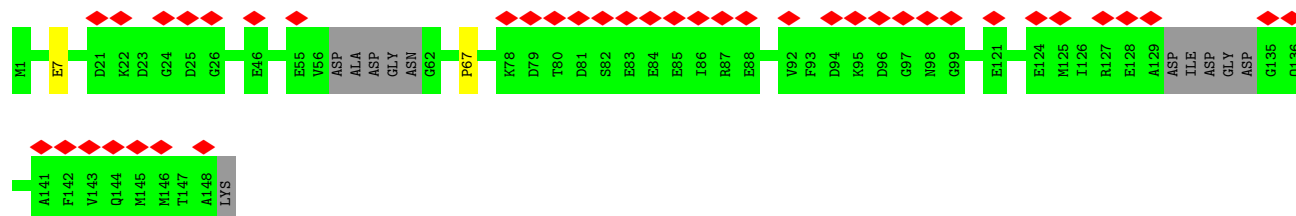


- Molecule 3: Calmodulin-1

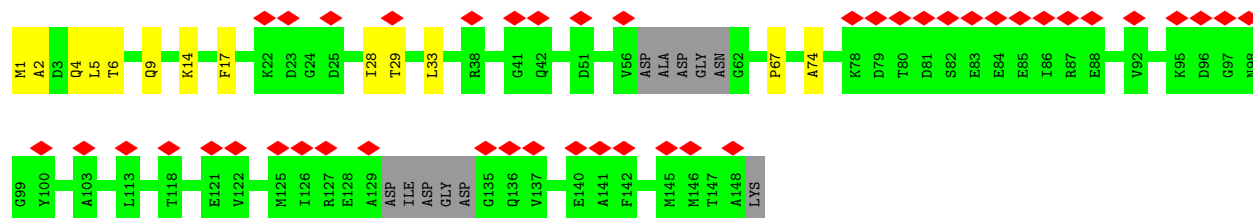
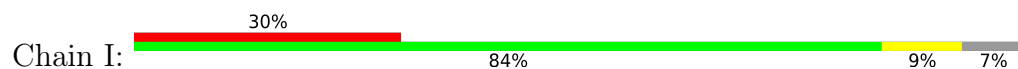




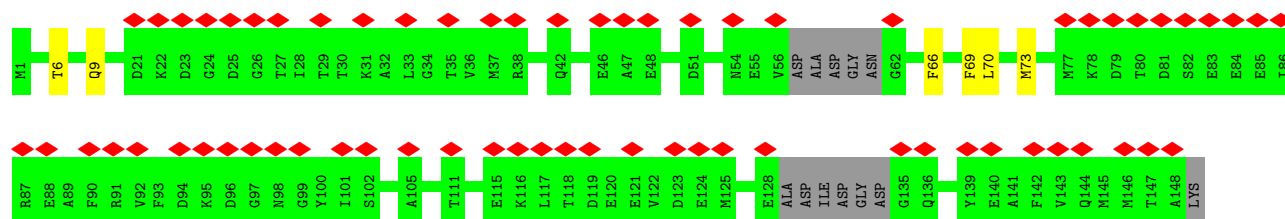
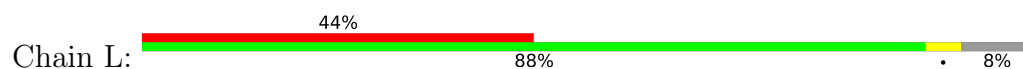
• Molecule 3: Calmodulin-1



• Molecule 3: Calmodulin-1



• Molecule 3: Calmodulin-1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	41834	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.366	Depositor
Minimum map value	-0.097	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.09	Depositor
Map size (Å)	481.28, 481.28, 481.28	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.94, 0.94, 0.94	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: CA, CFF, ZN, ATP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.16	0/27849	0.37	3/38070 (0.0%)
1	D	0.21	0/27383	0.41	3/37497 (0.0%)
1	G	0.18	2/27706 (0.0%)	0.37	1/37888 (0.0%)
1	J	0.18	0/27526	0.38	4/37679 (0.0%)
2	B	0.15	0/758	0.37	0/1032
2	E	0.26	0/758	0.45	0/1033
2	H	0.35	0/761	0.52	0/1036
2	K	0.10	0/744	0.31	0/1018
3	C	0.09	0/720	0.22	0/993
3	F	0.08	0/716	0.21	0/989
3	I	0.07	0/731	0.19	0/1007
3	L	0.08	0/727	0.21	0/1001
All	All	0.18	2/116379 (0.0%)	0.38	11/159243 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	3762	ARG	C-O	6.10	1.31	1.24
1	G	3766	GLN	C-O	5.62	1.30	1.24

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	338	GLU	N-CA-C	8.85	122.33	108.79
1	J	1675	ALA	CB-CA-C	-5.87	109.79	116.54
1	D	338	GLU	CB-CA-C	-5.82	109.88	116.63
1	G	2934	GLY	N-CA-C	-5.74	107.40	115.32
1	J	2934	GLY	N-CA-C	-5.74	107.41	115.32
1	A	2934	GLY	N-CA-C	-5.73	107.42	115.32
1	D	2898	GLY	N-CA-C	-5.51	108.04	115.21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	2917	ALA	CB-CA-C	-5.49	110.22	116.54
1	J	2917	ALA	CB-CA-C	-5.36	110.41	116.63
1	J	2898	GLY	N-CA-C	-5.19	108.52	114.69
1	A	340	LYS	N-CA-C	5.09	117.67	110.50

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	27274	0	23938	428	0
1	D	26818	0	23065	496	0
1	G	27137	0	23674	475	0
1	J	26962	0	23301	549	0
2	B	743	0	703	13	0
2	E	743	0	703	17	0
2	H	745	0	694	18	0
2	K	728	0	670	22	0
3	C	720	0	401	2	0
3	F	715	0	391	3	0
3	I	730	0	421	9	0
3	L	726	0	425	3	0
4	A	14	0	10	0	0
4	D	14	0	10	0	0
4	G	14	0	10	0	0
4	J	14	0	10	0	0
5	A	1	0	0	0	0
5	D	1	0	0	0	0
5	G	1	0	0	0	0
5	J	1	0	0	0	0
6	A	31	0	12	0	0
6	D	31	0	12	2	0
6	G	31	0	12	4	0
6	J	31	0	12	2	0
7	A	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	D	1	0	0	0	0
7	G	1	0	0	0	0
7	J	1	0	0	0	0
All	All	114229	0	98474	1978	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 9.

All (1978) 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)
1:D:4577:LEU:HD12	1:D:4580:TYR:HE2	1.12	1.10
1:D:4577:LEU:HD12	1:D:4580:TYR:CE2	1.96	1.00
1:J:4017:LEU:HD12	1:J:4139:ILE:HG21	1.50	0.92
2:H:10:GLY:HA3	2:H:70:GLN:HB2	1.53	0.91
1:D:4577:LEU:CD1	1:D:4580:TYR:HE2	1.85	0.90
1:J:4654:ALA:HB1	1:J:4796:MET:HE1	1.55	0.89
1:A:2179:ILE:HD11	1:A:2228:MET:HA	1.54	0.88
1:D:636:ASN:HB3	1:D:702:TRP:HZ2	1.42	0.85
1:D:3676:ASP:HA	1:D:3679:LYS:HZ2	1.41	0.85
2:E:39:SER:HA	2:E:42:ARG:NH2	1.91	0.85
1:D:2121:PHE:HB3	1:D:3725:TYR:HE2	1.41	0.84
1:D:2573:GLU:HA	1:D:2618:MET:HE1	1.60	0.83
1:G:1712:TYR:HD2	1:G:1840:PRO:HB2	1.43	0.83
1:J:49:LEU:HD11	1:J:191:VAL:HG23	1.61	0.83
1:G:1143:TRP:HB3	1:G:1164:LEU:HD11	1.62	0.82
1:J:103:TYR:CD2	1:J:152:PRO:HB3	2.14	0.82
1:A:1698:LEU:HD11	1:A:1814:MET:HE1	1.61	0.82
1:D:1115:LEU:HD21	1:D:1193:SER:HB2	1.61	0.82
1:D:1131:ARG:HB3	1:D:1139:PHE:HE1	1.44	0.82
1:J:2503:VAL:HG21	1:J:2558:VAL:HG12	1.61	0.82
1:A:1440:PHE:HD2	1:A:1560:ASN:HB3	1.45	0.81
1:G:2575:ARG:HH21	1:G:2578:MET:HE3	1.44	0.81
1:G:3768:SER:HA	1:G:3771:HIS:CE1	2.16	0.81
1:A:1849:LEU:HD12	1:A:1942:LEU:HD11	1.64	0.80
1:D:2512:ILE:HA	1:D:2517:PHE:HE2	1.45	0.80
1:D:1205:GLY:HA2	1:D:1211:LEU:HD11	1.63	0.80
1:G:3886:ARG:HD2	1:G:3889:GLN:HE21	1.48	0.79
1:D:1651:LEU:HD23	1:D:1702:HIS:HB2	1.64	0.78
1:A:1698:LEU:HA	1:A:1712:TYR:HE1	1.49	0.78
1:J:668:VAL:HG21	1:J:738:LEU:HD21	1.66	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:1293:LEU:HB2	1:J:1579:MET:HE3	1.66	0.78
1:J:1743:ARG:HA	1:J:1964:ARG:HH12	1.48	0.77
1:G:3990:VAL:HG23	1:G:4051:SER:HB3	1.66	0.77
1:D:1698:LEU:HB3	1:D:1814:MET:HE1	1.66	0.76
1:G:2670:GLU:HA	1:G:2673:HIS:CE1	2.20	0.76
1:J:594:GLY:HA2	1:J:1594:ARG:HD2	1.68	0.75
1:J:3969:ILE:HG12	1:J:4030:LEU:HA	1.68	0.75
1:J:63:ALA:HB2	1:J:261:ARG:HH12	1.52	0.74
1:J:2377:LEU:HD21	1:J:2465:ASP:HA	1.68	0.74
1:D:1694:LEU:HB3	1:D:1715:LEU:HD12	1.70	0.74
1:G:2512:ILE:HG21	1:G:2518:LEU:HD12	1.70	0.74
1:A:3817:LEU:HB2	1:A:3899:PHE:HE1	1.53	0.74
1:D:551:LEU:HA	1:D:560:ILE:HG21	1.70	0.73
1:J:2310:CYS:HB2	1:J:2324:ASN:HD22	1.53	0.73
1:J:716:PHE:HD2	1:J:718:GLY:H	1.35	0.73
1:G:2121:PHE:HB3	1:G:3725:TYR:HE2	1.52	0.73
1:G:833:GLY:HA3	1:G:838:HIS:CD2	2.23	0.73
1:J:1289:LEU:HD23	1:J:1597:VAL:HB	1.69	0.73
1:J:2355:ARG:NH1	1:J:2449:GLU:OE2	2.22	0.73
2:H:82:TYR:HB3	2:H:86:GLY:HA2	1.71	0.73
1:G:3817:LEU:HB2	1:G:3899:PHE:HE1	1.51	0.73
1:A:728:ARG:NH2	1:A:1489:CYS:SG	2.62	0.72
1:J:1161:ILE:HG13	1:J:1177:THR:HA	1.71	0.72
1:G:3768:SER:HA	1:G:3771:HIS:ND1	2.04	0.72
1:J:682:LEU:HD21	1:J:787:VAL:HG11	1.70	0.72
1:G:1163:THR:HG22	1:G:1168:VAL:HA	1.70	0.72
1:J:4901:ILE:HG21	1:J:4913:ARG:HE	1.55	0.72
1:J:2239:PHE:O	1:J:2246:ASN:ND2	2.23	0.72
1:D:2563:THR:HG23	1:D:2606:CYS:HA	1.71	0.72
1:D:1731:LEU:HD12	1:D:1772:ARG:HH12	1.54	0.72
1:A:411:TYR:HB3	1:A:486:LEU:HD21	1.71	0.72
1:A:1235:THR:HG22	1:A:1610:ASN:HD21	1.53	0.72
1:J:1731:LEU:HG	1:J:1772:ARG:HH22	1.53	0.72
1:D:580:GLU:HA	1:D:620:LEU:HD21	1.72	0.71
1:D:1291:LEU:HD13	1:D:1550:PRO:HB2	1.70	0.71
1:D:1448:VAL:HG22	1:D:1554:VAL:HG23	1.73	0.71
1:G:2781:VAL:HA	1:G:2787:THR:O	1.90	0.71
1:J:708:GLY:HA3	1:J:722:TRP:HB3	1.70	0.71
1:G:4839:MET:HB3	1:J:4823:LEU:HD11	1.71	0.71
1:A:530:ILE:HG22	1:A:536:ASN:HB3	1.72	0.71
1:A:2214:VAL:HG11	1:A:2228:MET:HE1	1.70	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1143:TRP:HB3	1:A:1164:LEU:HD11	1.71	0.71
1:J:1448:VAL:HG22	1:J:1554:VAL:HG23	1.72	0.71
1:D:4215:ARG:NH2	6:D:5103:ATP:O1B	2.23	0.71
1:A:2781:VAL:HA	1:A:2787:THR:O	1.90	0.71
1:A:4911:LEU:HA	1:A:4914:VAL:HG12	1.72	0.71
1:D:4732:PHE:HD2	1:D:4737:ILE:HD11	1.56	0.71
1:G:1969:LEU:HD21	1:G:2009:LEU:HD13	1.73	0.71
1:D:636:ASN:HB3	1:D:702:TRP:CZ2	2.24	0.71
1:G:222:LEU:HD12	1:G:388:LEU:HD13	1.73	0.71
1:G:1601:MET:HE3	1:G:1602:PRO:HD2	1.72	0.71
1:A:3969:ILE:HD11	1:A:3980:LEU:HD12	1.70	0.70
1:G:2377:LEU:HA	1:G:2469:ILE:HD11	1.71	0.70
1:D:1115:LEU:HD13	1:D:1123:VAL:HG11	1.73	0.70
1:D:4913:ARG:NH1	1:A:4888:TYR:OH	2.24	0.70
1:A:219:VAL:HG21	1:A:398:SER:HB3	1.71	0.70
1:D:716:PHE:HD2	1:D:718:GLY:H	1.39	0.70
1:A:1673:VAL:HG12	1:A:1681:VAL:HG11	1.73	0.70
1:J:4027:LEU:HG	1:J:4044:MET:HE1	1.73	0.70
1:J:2781:VAL:HA	1:J:2787:THR:O	1.90	0.70
1:G:1430:THR:HG22	1:G:1432:THR:H	1.56	0.70
2:E:78:PRO:HD3	2:E:96:THR:HG22	1.72	0.70
1:A:1161:ILE:HG22	1:A:1177:THR:HA	1.74	0.70
1:D:2271:THR:HG22	1:D:2273:LEU:H	1.56	0.70
1:A:2509:VAL:HG23	1:A:2510:TYR:HD1	1.57	0.69
1:A:2575:ARG:HG3	1:A:2578:MET:HB3	1.74	0.69
1:D:3673:MET:HE2	1:D:3728:ILE:HG12	1.72	0.69
1:D:2214:VAL:HG11	1:D:2228:MET:HE1	1.75	0.69
1:G:1225:PRO:HG2	1:G:1228:ILE:HB	1.74	0.69
1:A:4913:ARG:NH1	1:A:4917:ASP:OD2	2.26	0.69
1:J:2879:ALA:HB2	1:J:2920:ARG:HA	1.74	0.69
1:J:4677:LEU:HD22	1:J:4711:PHE:CZ	2.27	0.69
1:D:2625:ARG:CB	1:D:2904:LEU:H	2.06	0.69
1:A:14:LEU:HD23	1:A:101:LEU:HD22	1.75	0.69
1:A:2551:ASN:HD21	1:A:2595:LEU:HG	1.57	0.68
1:A:2512:ILE:HD12	1:A:2518:LEU:HD12	1.75	0.68
1:J:2044:ILE:HG13	1:J:3667:HIS:HD2	1.56	0.68
1:D:1269:CYS:SG	1:D:1563:GLN:NE2	2.66	0.68
1:J:720:HIS:HE1	1:J:722:TRP:HE1	1.38	0.68
1:A:3977:GLN:NE2	1:A:4030:LEU:O	2.26	0.68
1:D:1851:MET:HB3	1:D:1853:ILE:HG13	1.76	0.68
1:D:2376:LEU:HD11	1:D:2430:ILE:HD11	1.76	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:220:LEU:HD23	1:G:390:LEU:HB3	1.75	0.68
1:A:2518:LEU:HD13	1:A:2568:LEU:HD23	1.75	0.67
1:D:4577:LEU:CD1	1:D:4580:TYR:CE2	2.69	0.67
1:G:341:TYR:OH	1:G:392:ARG:N	2.26	0.67
1:D:2522:LEU:HA	1:D:2526:PHE:HB2	1.77	0.67
1:A:3970:GLN:HE22	1:A:5004:THR:HG22	1.59	0.67
1:D:113:HIS:NE2	1:D:402:ARG:HB3	2.10	0.67
1:D:4578:LEU:HD12	1:J:4879:MET:HB3	1.75	0.67
1:J:1863:LEU:HD11	1:J:1871:PHE:HD2	1.59	0.67
1:J:4001:MET:HE1	1:J:4061:PHE:HB2	1.77	0.67
1:J:794:GLY:HA3	1:J:812:HIS:HB3	1.76	0.67
1:G:701:GLY:HA3	1:G:725:HIS:NE2	2.10	0.67
1:J:1125:ASN:N	1:J:1130:GLN:O	2.28	0.67
1:J:636:ASN:OD1	1:J:1693:GLN:NE2	2.28	0.67
1:G:1698:LEU:HA	1:G:1712:TYR:HE1	1.60	0.67
1:J:451:TYR:CE2	1:J:474:ARG:HD3	2.30	0.67
1:D:3726:ALA:HA	1:D:3729:MET:HE3	1.76	0.66
1:G:1440:PHE:HD2	1:G:1560:ASN:HB3	1.60	0.66
1:G:4989:MET:HE1	1:G:4993:MET:HE2	1.76	0.66
1:J:647:ASN:ND2	1:J:820:ARG:O	2.28	0.66
1:D:3969:ILE:HD11	1:D:3980:LEU:HD22	1.75	0.66
1:A:2124:LEU:HD21	1:A:3677:LEU:HD11	1.77	0.66
1:A:635:THR:HB	1:A:1693:GLN:HE22	1.60	0.66
1:J:150:MET:HE1	1:J:163:VAL:HG21	1.75	0.66
1:J:551:LEU:HD21	1:J:589:LEU:HB2	1.77	0.66
1:D:670:GLU:HA	1:D:740:PRO:HB3	1.77	0.66
2:B:71:ARG:HG2	2:B:102:GLU:HB3	1.76	0.66
1:G:180:LEU:O	1:G:200:TRP:NE1	2.27	0.66
1:J:716:PHE:HZ	1:J:744:VAL:HG21	1.59	0.66
1:D:438:ILE:HG23	1:D:518:ILE:HD11	1.77	0.66
1:D:1747:LEU:HD21	1:D:2041:HIS:HB2	1.78	0.66
1:A:3673:MET:CE	1:A:3728:ILE:HG12	2.25	0.66
1:J:3989:VAL:HG23	1:J:4023:MET:HE2	1.78	0.65
1:G:833:GLY:HA3	1:G:838:HIS:HD2	1.60	0.65
1:G:3901:ASN:OD1	1:G:3904:ARG:NH2	2.26	0.65
1:A:4737:ILE:HG23	1:A:4741:LEU:HD23	1.78	0.65
1:J:2661:TRP:CD1	1:J:2664:PHE:HD1	2.14	0.65
1:A:4879:MET:HG3	1:G:4578:LEU:HA	1.77	0.65
1:G:1594:ARG:NH2	1:G:1643:GLU:OE2	2.29	0.65
1:G:1578:ALA:HA	1:G:1584:ARG:HH12	1.62	0.65
2:K:30:LEU:HD23	2:K:32:ASN:H	1.61	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4816:ILE:HG12	1:D:4823:LEU:HG	1.79	0.64
1:J:171:LEU:HB2	1:J:180:LEU:HD23	1.79	0.64
2:E:25:HIS:CD2	2:E:45:PRO:HA	2.32	0.64
1:G:2155:LEU:HD21	1:G:2198:MET:HE1	1.79	0.64
1:J:102:LEU:HB2	1:J:105:HIS:HE1	1.61	0.64
1:J:758:ARG:HG2	1:J:763:PRO:HA	1.79	0.64
1:J:103:TYR:CE1	1:J:163:VAL:HG13	2.32	0.64
1:J:3778:MET:HG2	1:J:3782:MET:HE2	1.78	0.64
1:J:4085:ARG:HE	1:J:4087:LEU:HD12	1.61	0.64
1:A:3904:ARG:O	1:A:3914:ASN:ND2	2.31	0.64
1:G:1160:ILE:HD11	1:G:1182:ILE:HD13	1.77	0.64
1:G:1639:LEU:HD11	1:G:1653:LEU:HD11	1.80	0.64
1:G:4798:MET:HB3	1:G:4812:HIS:NE2	2.12	0.64
1:J:683:ARG:HH21	1:J:708:GLY:H	1.45	0.64
1:D:2358:ILE:HD11	1:D:2460:LEU:HD11	1.79	0.64
1:D:4578:LEU:O	1:J:4879:MET:HB2	1.97	0.64
1:D:2584:HIS:HA	1:D:2903:PRO:CB	2.28	0.64
1:A:1110:ARG:NH2	1:A:1112:ASP:OD2	2.31	0.64
1:J:4208:PRO:HA	1:J:4211:LYS:HB2	1.78	0.64
1:D:4960:ILE:HD11	1:D:4985:LEU:HA	1.79	0.64
1:A:595:ARG:NH1	1:A:631:LEU:O	2.31	0.64
1:G:3813:GLN:HB3	1:G:3899:PHE:CE2	2.32	0.64
1:J:4673:ARG:HD2	1:J:4782:VAL:HG21	1.79	0.64
1:D:4892:ARG:NH1	1:J:4917:ASP:OD2	2.31	0.63
1:G:618:GLN:O	1:G:621:ILE:HG22	1.98	0.63
1:J:638:ILE:HG22	1:J:678:GLN:HE22	1.63	0.63
1:G:3733:CYS:SG	1:G:3803:SER:HB3	2.38	0.63
1:J:579:GLN:H	1:J:582:HIS:HD2	1.43	0.63
1:J:2293:GLN:OE1	1:J:2293:GLN:N	2.30	0.63
1:D:794:GLY:HA2	1:D:812:HIS:HB3	1.78	0.63
1:G:4067:LYS:NZ	1:G:4169:SER:OG	2.31	0.63
1:D:3892:CYS:SG	1:D:3900:GLN:NE2	2.72	0.63
1:G:2469:ILE:HA	1:G:2472:LEU:HD23	1.79	0.63
1:J:103:TYR:CG	1:J:152:PRO:HB3	2.32	0.63
1:D:2000:SER:O	1:D:2005:GLN:NE2	2.23	0.63
1:D:3676:ASP:HA	1:D:3679:LYS:NZ	2.13	0.63
1:D:221:ARG:N	1:D:391:THR:O	2.30	0.63
1:D:4204:GLN:NE2	1:D:4245:MET:O	2.31	0.63
1:A:2470:ILE:HG22	1:A:2525:GLY:HA3	1.81	0.63
1:J:1293:LEU:HD11	1:J:1594:ARG:HG2	1.79	0.63
1:D:232:THR:HG21	1:D:252:VAL:HG11	1.80	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:627:PRO:HD3	2:E:89:GLY:HA2	1.79	0.63
1:A:3673:MET:HE3	1:A:3728:ILE:HG21	1.81	0.63
1:D:648:ILE:HD11	1:D:814:ALA:HB3	1.81	0.63
1:A:4909:TYR:HA	1:A:4912:TYR:HD2	1.64	0.63
2:K:25:HIS:NE2	2:K:102:GLU:OE1	2.32	0.63
1:D:4800:LEU:HA	1:D:4803:HIS:HD2	1.64	0.62
1:D:3886:ARG:HD2	1:D:3889:GLN:HE21	1.64	0.62
1:G:3817:LEU:HB2	1:G:3899:PHE:CE1	2.31	0.62
1:G:4961:CYS:HB3	1:G:5023:PRO:HB2	1.80	0.62
1:J:2661:TRP:HD1	1:J:2664:PHE:H	1.47	0.62
1:A:2592:GLY:HA3	1:A:2595:LEU:HD13	1.82	0.62
1:J:2158:CYS:HG	1:J:2181:SER:HG	1.45	0.62
1:J:2604:GLU:O	1:J:2608:MET:HE3	1.98	0.62
1:J:1150:GLY:N	1:J:1163:THR:O	2.31	0.62
1:D:1139:PHE:HB2	1:D:1171:SER:HA	1.80	0.62
1:A:2495:VAL:HG12	1:A:2497:ASP:H	1.64	0.62
1:G:4238:CYS:O	1:G:4242:ILE:HG12	1.99	0.62
1:G:664:PHE:HE1	1:G:686:TRP:HE1	1.45	0.62
1:G:4992:LEU:O	1:G:4996:ILE:HG12	1.99	0.62
1:J:359:TYR:HA	1:J:376:ALA:HA	1.82	0.62
1:J:2158:CYS:SG	1:J:2181:SER:OG	2.53	0.62
1:J:4705:VAL:HG22	1:J:4711:PHE:HD1	1.65	0.62
1:D:341:TYR:OH	1:D:392:ARG:N	2.24	0.62
1:A:2476:ILE:HB	1:A:2536:LEU:HD11	1.81	0.62
1:G:4068:LEU:HD13	1:G:4111:LEU:HD11	1.82	0.62
1:A:1115:LEU:HD13	1:A:1193:SER:HB2	1.82	0.62
1:J:1237:TRP:HH2	1:J:1652:GLU:HG3	1.65	0.62
1:A:3648:ARG:NH2	3:C:7:GLU:OE2	2.33	0.62
1:J:4060:LYS:O	1:J:4064:MET:HG3	1.99	0.62
1:D:4582:VAL:HB	1:J:4856:PHE:HZ	1.63	0.61
1:J:4003:LEU:HD21	1:J:4012:LEU:HD22	1.82	0.61
1:D:1966:VAL:HG21	1:D:3650:CYS:HA	1.80	0.61
1:A:794:GLY:HA3	1:A:812:HIS:HB3	1.82	0.61
1:G:650:VAL:O	1:G:777:PHE:N	2.33	0.61
1:G:1454:THR:HG23	1:G:1456:ASP:H	1.64	0.61
1:G:1573:MET:SD	1:G:1574:PRO:HD2	2.39	0.61
1:J:670:GLU:HA	1:J:740:PRO:HB3	1.82	0.61
1:A:1573:MET:SD	1:A:1574:PRO:HD2	2.40	0.61
1:J:1668:ARG:HE	1:J:1671:ARG:NH2	1.97	0.61
1:D:1714:LEU:O	1:D:1718:ILE:HG12	2.01	0.61
1:A:1780:PRO:HG2	2:B:42:ARG:HD3	1.81	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:3724:ALA:O	1:J:3728:ILE:HG13	2.00	0.61
1:D:3847:PHE:O	1:D:3851:ASN:ND2	2.33	0.61
1:A:1431:THR:HG21	1:A:1523:ALA:HB3	1.82	0.61
1:J:2323:TRP:HH2	1:J:2422:ILE:HG13	1.65	0.61
1:D:1673:VAL:HG12	1:D:1681:VAL:HG11	1.83	0.61
1:J:1732:SER:HB2	1:J:2140:ARG:HH11	1.65	0.61
2:K:29:MET:HA	2:K:35:LYS:HA	1.82	0.61
1:A:839:LEU:HB3	1:A:1075:PHE:HE2	1.65	0.61
1:G:2619:LEU:HD23	1:G:2623:LEU:HB2	1.82	0.61
1:J:418:LEU:HA	1:J:421:PHE:CE1	2.34	0.61
1:G:2574:HIS:CD2	1:G:2575:ARG:HG2	2.35	0.61
1:G:4654:ALA:C	1:G:4796:MET:HE1	2.25	0.61
1:J:2495:VAL:HB	1:J:2498:HIS:CG	2.36	0.60
1:G:3977:GLN:NE2	1:G:4030:LEU:O	2.34	0.60
1:J:2518:LEU:HD21	1:J:2569:PHE:CE1	2.35	0.60
1:A:2271:THR:HG23	1:A:2274:ASP:H	1.65	0.60
1:J:284:HIS:ND1	1:J:287:THR:OG1	2.33	0.60
1:J:551:LEU:HA	1:J:560:ILE:HG21	1.82	0.60
1:D:21:VAL:HB	1:D:205:ILE:HD11	1.83	0.60
1:D:2776:SER:O	1:D:2787:THR:HA	2.02	0.60
1:J:1928:GLN:HA	1:J:2104:ARG:HH22	1.66	0.60
1:J:4899:ASP:OD1	1:J:4900:GLU:N	2.34	0.60
1:A:3837:GLN:OE1	1:A:3837:GLN:HA	2.00	0.60
2:B:78:PRO:HD3	2:B:96:THR:HG22	1.83	0.60
1:J:223:PHE:HD1	1:J:230:CYS:HB3	1.66	0.60
1:D:157:ARG:HH21	1:D:164:ARG:HG3	1.65	0.60
1:D:1431:THR:HG21	1:D:1523:ALA:HB3	1.84	0.60
1:G:292:ALA:HA	1:G:314:PHE:HZ	1.66	0.60
1:G:4817:ALA:HA	1:G:4823:LEU:HB3	1.83	0.60
1:J:587:ILE:HG12	1:J:625:LEU:HD12	1.83	0.60
1:J:1594:ARG:NH2	1:J:1643:GLU:OE2	2.32	0.60
1:D:4991:PHE:HE2	1:D:5010:VAL:HG11	1.67	0.60
1:D:755:ILE:HG13	1:D:771:PHE:CE2	2.37	0.60
1:A:4895:GLY:O	1:G:4892:ARG:NH1	2.35	0.60
1:G:1470:ARG:HB2	1:G:1491:ASN:HD21	1.67	0.60
2:H:71:ARG:HB3	2:H:102:GLU:HG3	1.82	0.60
1:J:4979:THR:HG21	6:J:5103:ATP:H2'	1.84	0.60
1:D:2778:GLY:O	1:D:2789:PRO:HA	2.01	0.60
1:D:2994:GLU:HA	1:D:2997:PHE:CE1	2.36	0.60
1:A:1115:LEU:HD21	1:A:1123:VAL:HG11	1.84	0.60
1:A:1639:LEU:HD11	1:A:1653:LEU:HD11	1.84	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4222:VAL:HG21	1:A:4954:MET:HE3	1.84	0.60
1:G:345:LEU:HD23	1:G:389:PHE:HB3	1.82	0.60
1:J:111:HIS:CD2	1:J:113:HIS:HB3	2.37	0.60
1:J:2767:ALA:HB3	1:J:2857:PRO:CB	2.32	0.60
1:D:107:ILE:HD13	1:D:150:MET:HE2	1.83	0.60
1:D:1427:ILE:HD11	1:D:1571:ASN:HA	1.83	0.60
1:D:4339:VAL:HA	1:J:4839:MET:HE1	1.84	0.60
1:J:1742:THR:HG23	1:J:1769:THR:HG21	1.83	0.60
1:D:2821:TRP:HA	1:D:2938:THR:C	2.27	0.59
1:A:830:ARG:HE	1:A:837:PRO:HB3	1.67	0.59
1:D:4927:ILE:HG13	1:A:4936:ILE:HG21	1.84	0.59
1:A:495:ASN:HD22	1:A:550:LYS:HD3	1.67	0.59
1:A:1434:TYR:HB3	1:A:1519:LEU:HD23	1.82	0.59
1:G:4576:ILE:HD11	1:G:4639:MET:HG3	1.84	0.59
1:J:619:ASP:OD1	1:J:620:LEU:N	2.35	0.59
1:D:3845:ASN:OD1	1:D:3846:ALA:N	2.34	0.59
1:D:2211:MET:HE3	1:D:2215:LEU:HD12	1.85	0.59
1:G:2165:LEU:HD22	1:G:2177:LEU:HD23	1.84	0.59
1:G:4856:PHE:O	1:G:4860:ARG:NH1	2.34	0.59
1:G:1440:PHE:CD2	1:G:1560:ASN:HB3	2.36	0.59
1:J:2581:SER:HA	1:J:2584:HIS:CE1	2.37	0.59
1:J:3007:ASN:HA	1:J:3010:PHE:CE2	2.38	0.59
1:D:4581:LYS:HB2	1:D:4632:LEU:HD23	1.85	0.59
1:D:4839:MET:HE3	1:A:4820:VAL:HG11	1.84	0.59
1:A:1440:PHE:CD2	1:A:1560:ASN:HB3	2.34	0.59
1:J:3977:GLN:NE2	1:J:4030:LEU:O	2.36	0.59
1:J:4992:LEU:O	1:J:4996:ILE:HG12	2.03	0.59
1:D:220:LEU:HA	1:D:392:ARG:HA	1.83	0.59
1:G:1733:GLU:HG2	1:G:2201:LEU:HD12	1.85	0.59
1:D:548:VAL:HG11	1:D:582:HIS:HD2	1.68	0.59
1:J:3829:PHE:HE2	1:J:3902:TYR:HE2	1.49	0.59
1:D:1810:LYS:HG2	1:D:1814:MET:HE3	1.85	0.59
1:D:2781:VAL:HA	1:D:2787:THR:O	2.01	0.59
1:D:4820:VAL:HB	1:D:4823:LEU:HD23	1.85	0.59
1:A:195:PHE:CZ	1:G:2358:ILE:HD11	2.38	0.59
1:A:4680:LYS:HD2	1:A:4686:LEU:HD22	1.85	0.59
1:J:102:LEU:HB2	1:J:105:HIS:CE1	2.37	0.59
1:J:495:ASN:OD1	1:J:553:ARG:NH1	2.35	0.59
1:J:1936:LYS:HB2	1:J:2116:LEU:HD11	1.84	0.59
1:J:2503:VAL:O	1:J:2506:LEU:HG	2.03	0.59
1:J:4816:ILE:HG22	1:J:4823:LEU:HD22	1.85	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:692:TYR:O	1:D:827:LYS:NZ	2.35	0.59
1:D:1259:ARG:NH2	1:D:1595:LEU:O	2.34	0.59
1:A:1438:ARG:HD3	1:A:1563:GLN:HE21	1.68	0.59
1:G:4562:LEU:HD21	1:G:4656:LEU:HB3	1.85	0.59
1:J:590:LEU:HB2	1:J:599:VAL:HG11	1.85	0.59
1:D:1109:LEU:HA	1:D:1120:LEU:HD13	1.85	0.58
1:D:4138:ASP:O	1:D:4142:ASN:ND2	2.32	0.58
2:E:62:GLY:HA3	2:E:74:LEU:HD11	1.85	0.58
1:J:1804:LEU:HD11	1:J:1853:ILE:HG13	1.84	0.58
1:J:2032:GLN:O	1:J:2036:GLN:HG2	2.03	0.58
1:J:2500:ALA:O	1:J:2503:VAL:HG12	2.02	0.58
1:A:1714:LEU:O	1:A:1718:ILE:HG12	2.03	0.58
1:G:622:THR:HA	1:G:626:LEU:HD13	1.85	0.58
1:J:3842:LEU:O	1:J:3929:SER:OG	2.20	0.58
1:G:2518:LEU:HD22	1:G:2569:PHE:HE1	1.67	0.58
1:J:755:ILE:HB	1:J:768:PHE:HB2	1.86	0.58
1:G:794:GLY:HA3	1:G:812:HIS:HB3	1.84	0.58
1:G:1713:ASP:HA	1:G:1716:ILE:HG22	1.85	0.58
1:G:3965:LEU:HA	1:G:3968:TYR:HD2	1.69	0.58
1:J:2044:ILE:HG13	1:J:3667:HIS:CD2	2.37	0.58
1:D:1433:TYR:CZ	1:D:1578:ALA:HB2	2.38	0.58
1:A:1230:MET:HE3	1:A:1827:ARG:HH21	1.69	0.58
2:H:8:SER:HB2	2:H:71:ARG:HG2	1.86	0.58
2:H:21:THR:HA	2:H:49:ARG:HA	1.86	0.58
1:J:415:ILE:HD11	1:J:490:CYS:SG	2.44	0.58
1:J:2296:GLU:HA	1:J:2299:VAL:HG22	1.85	0.58
1:D:1573:MET:SD	1:D:1574:PRO:HD2	2.43	0.58
1:D:2476:ILE:HD12	1:D:2477:PRO:HD2	1.85	0.58
1:A:1477:GLY:HA2	1:A:1484:HIS:H	1.69	0.58
1:A:1747:LEU:HD21	1:A:2041:HIS:HB2	1.85	0.58
1:G:2155:LEU:HD12	1:G:2185:ILE:HD11	1.83	0.58
2:B:31:GLN:NE2	2:B:96:THR:OG1	2.28	0.58
1:G:1804:LEU:HD11	1:G:1853:ILE:HG13	1.86	0.58
1:G:4799:SER:HB2	1:G:4812:HIS:HE1	1.69	0.58
1:D:221:ARG:NH1	1:D:253:CYS:O	2.36	0.58
1:D:660:GLY:HA2	1:D:750:LEU:HB2	1.84	0.58
1:D:4027:LEU:HD13	1:D:4044:MET:HE1	1.84	0.58
1:G:637:LEU:HA	1:G:1637:MET:HA	1.86	0.58
1:G:1698:LEU:HA	1:G:1712:TYR:CE1	2.38	0.58
1:G:2121:PHE:HB3	1:G:3725:TYR:CE2	2.37	0.58
1:G:4576:ILE:HD11	1:G:4639:MET:CG	2.34	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:799:GLU:H	1:J:1623:ARG:HA	1.67	0.58
1:D:451:TYR:O	1:D:474:ARG:NH2	2.37	0.58
1:D:839:LEU:HD13	1:D:1075:PHE:HD2	1.68	0.58
1:J:632:LEU:HD23	1:J:1666:THR:HG23	1.86	0.58
1:D:1434:TYR:HB2	1:D:1572:ILE:HG21	1.85	0.57
1:A:670:GLU:HA	1:A:740:PRO:HB3	1.86	0.57
1:G:716:PHE:HE1	1:G:757:PHE:CD1	2.22	0.57
1:G:1269:CYS:SG	1:G:1563:GLN:HB2	2.44	0.57
1:D:4817:ALA:HA	1:D:4823:LEU:HB3	1.86	0.57
1:G:206:CYS:HB2	1:G:271:GLY:HA3	1.86	0.57
1:D:530:ILE:HG22	1:D:536:ASN:HB3	1.86	0.57
1:A:275:ARG:HB3	1:A:336:PRO:HG3	1.85	0.57
1:G:2607:LEU:HD21	1:G:2643:LEU:HD22	1.86	0.57
1:D:716:PHE:HE1	1:D:757:PHE:CD1	2.22	0.57
1:G:4241:THR:HG22	1:G:4245:MET:HE2	1.86	0.57
2:H:87:HIS:HD2	2:H:88:PRO:HD2	1.68	0.57
1:D:4016:LEU:O	1:D:4019:LEU:HG	2.05	0.57
2:E:39:SER:HA	2:E:42:ARG:HH21	1.66	0.57
1:A:4045:VAL:O	1:A:4049:VAL:HG23	2.05	0.57
1:G:4708:THR:OG1	1:G:4772:ASP:OD2	2.22	0.57
1:J:1743:ARG:O	1:J:1964:ARG:NH2	2.35	0.57
1:A:1301:PHE:HE2	1:A:1544:PRO:HA	1.70	0.57
1:A:2159:LEU:HD13	1:A:2203:MET:HG2	1.85	0.57
1:G:219:VAL:HG12	1:G:259:LEU:HD12	1.86	0.57
1:D:233:ILE:O	1:D:257:ARG:NH1	2.38	0.57
1:D:1733:GLU:N	1:D:1733:GLU:OE2	2.36	0.57
1:D:2477:PRO:HG3	1:D:2546:MET:HG3	1.86	0.57
1:J:2503:VAL:HG11	1:J:2557:ALA:HB1	1.86	0.57
1:D:3658:LYS:HA	1:D:3662:ILE:HD13	1.85	0.57
1:D:4895:GLY:O	1:A:4892:ARG:NH1	2.38	0.57
1:J:1437:VAL:HG21	1:J:1552:VAL:HG21	1.87	0.57
1:D:830:ARG:HH21	1:D:1612:PHE:HB2	1.69	0.57
1:D:2822:THR:O	1:D:2937:VAL:HA	2.04	0.57
1:G:515:TRP:O	1:G:519:VAL:HG23	2.04	0.57
1:G:4029:SER:O	1:G:4032:GLU:HG3	2.05	0.57
1:J:2879:ALA:CB	1:J:2920:ARG:HA	2.35	0.57
1:A:470:SER:OG	1:A:474:ARG:NH1	2.38	0.57
1:A:4580:TYR:OH	1:A:4806:ASN:ND2	2.34	0.57
1:G:452:PHE:HZ	1:G:478:PHE:HD2	1.53	0.57
1:G:551:LEU:HD21	1:G:589:LEU:HD22	1.86	0.57
1:G:842:PRO:HD3	1:G:1073:ARG:HG2	1.85	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:2039:LEU:HD22	1:G:2044:ILE:HG13	1.87	0.57
1:J:1862:ILE:O	1:J:1866:ILE:HG12	2.05	0.57
1:G:2364:PHE:HD1	1:G:2429:LEU:HD21	1.69	0.56
1:J:1477:GLY:HA2	1:J:1483:VAL:HA	1.86	0.56
1:J:1863:LEU:HD11	1:J:1871:PHE:CD2	2.39	0.56
1:D:1112:ASP:OD1	1:D:1113:VAL:N	2.38	0.56
1:D:3680:ALA:O	1:D:3681:GLY:C	2.48	0.56
1:A:603:LEU:HD23	1:A:606:LEU:HD12	1.87	0.56
1:J:1109:LEU:HA	1:J:1120:LEU:HD13	1.87	0.56
1:D:468:LEU:O	1:D:472:ARG:HG2	2.04	0.56
1:D:637:LEU:HA	1:D:1637:MET:HA	1.87	0.56
1:D:1687:SER:OG	2:E:36:PHE:O	2.21	0.56
1:D:4097:MET:HG2	1:D:4108:ILE:HG12	1.87	0.56
1:D:4569:LEU:HD23	1:D:4650:HIS:HA	1.86	0.56
1:A:583:ILE:O	1:A:587:ILE:HG12	2.05	0.56
1:G:3722:TYR:CE1	1:G:3782:MET:HE1	2.40	0.56
1:G:3927:GLN:HB2	1:G:3992:PHE:CZ	2.40	0.56
1:J:1747:LEU:HD21	1:J:2041:HIS:HB2	1.87	0.56
1:J:2118:ARG:HD2	1:J:3721:LEU:HD22	1.86	0.56
1:D:291:LEU:HD23	1:D:301:VAL:HG12	1.87	0.56
1:G:1802:ILE:HG21	1:G:1807:LEU:HD11	1.87	0.56
1:J:1649:ASP:HB2	1:J:1652:GLU:HB2	1.85	0.56
2:K:90:VAL:HG23	2:K:91:ILE:HG12	1.87	0.56
1:D:4226:GLY:O	1:D:4230:LYS:N	2.38	0.56
1:G:686:TRP:HZ3	1:G:748:LEU:HD22	1.70	0.56
1:D:1932:PRO:O	1:D:1936:LYS:HG2	2.06	0.56
1:A:4242:ILE:HG13	1:A:4989:MET:HE3	1.86	0.56
1:G:1130:GLN:HG3	1:G:1132:TRP:HE1	1.71	0.56
1:G:3775:ALA:O	1:G:3778:MET:HG3	2.06	0.56
1:J:1255:TYR:HE1	1:J:1274:HIS:HD2	1.52	0.56
1:J:2152:THR:HG22	1:J:2190:VAL:HG11	1.88	0.56
1:D:2178:MET:SD	1:D:2210:VAL:HG11	2.46	0.56
1:D:2299:VAL:HG21	1:D:2356:LEU:HB3	1.87	0.56
1:A:1449:TRP:HB2	1:A:1553:PHE:HB2	1.88	0.56
1:G:840:VAL:HG22	1:G:1199:VAL:HG22	1.88	0.56
1:J:213:TYR:HB3	1:J:337:PRO:HG3	1.88	0.56
1:D:3904:ARG:HG2	1:D:3905:THR:HG23	1.88	0.56
1:A:2128:TYR:CD2	1:A:3673:MET:HG2	2.40	0.56
1:G:2349:ASN:OD1	1:G:3849:ARG:NH2	2.39	0.56
1:D:1426:ILE:HG23	1:D:1427:ILE:HD13	1.88	0.56
1:A:615:ARG:NH2	1:A:1676:LEU:O	2.38	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3001:ILE:HG22	1:A:3005:LEU:HD23	1.87	0.56
1:G:1714:LEU:O	1:G:1718:ILE:HG12	2.06	0.56
1:J:2661:TRP:CD1	1:J:2664:PHE:CD1	2.93	0.56
1:A:2515:GLN:NE2	1:A:2568:LEU:O	2.39	0.55
1:A:4687:TYR:OH	1:A:4699:GLY:O	2.20	0.55
1:A:733:PRO:HG2	1:A:762:CYS:HB3	1.89	0.55
1:A:1446:SER:O	1:A:1496:TRP:NE1	2.30	0.55
1:G:701:GLY:O	1:G:1640:HIS:HD2	1.89	0.55
1:G:839:LEU:HB3	1:G:1075:PHE:HE2	1.71	0.55
1:G:2522:LEU:HA	1:G:2526:PHE:HD2	1.70	0.55
1:G:4151:SER:HB2	1:G:4164:LEU:HD11	1.86	0.55
1:J:2238:TYR:HA	1:J:2241:ARG:HG2	1.87	0.55
1:D:195:PHE:CE1	1:A:2358:ILE:HD11	2.40	0.55
1:J:1830:VAL:N	1:J:1837:GLN:OE1	2.38	0.55
1:J:2107:GLN:NE2	1:J:3681:GLY:H	2.04	0.55
1:D:59:PRO:HB3	1:D:281:ARG:HH11	1.72	0.55
1:D:830:ARG:NH2	1:D:1612:PHE:HB2	2.21	0.55
1:D:4666:VAL:HG21	1:D:4783:ILE:HG12	1.89	0.55
2:E:71:ARG:HG2	2:E:102:GLU:HB3	1.88	0.55
1:J:564:LEU:HA	1:J:567:VAL:HG12	1.88	0.55
2:K:68:LEU:HD12	2:K:106:LEU:HD23	1.88	0.55
1:J:2012:PHE:CG	1:J:2028:ARG:HG2	2.42	0.55
1:J:3927:GLN:HE21	1:J:3991:GLY:HA3	1.71	0.55
1:J:4863:TYR:HD2	1:J:4876:CYS:HB2	1.72	0.55
1:J:4974:GLY:O	1:J:4977:THR:OG1	2.22	0.55
1:D:1446:SER:O	1:D:1496:TRP:NE1	2.31	0.55
1:A:2377:LEU:HA	1:A:2469:ILE:HD11	1.88	0.55
1:G:291:LEU:HA	1:G:301:VAL:HA	1.88	0.55
1:G:1297:PHE:HD2	1:G:1522:LEU:HA	1.72	0.55
1:G:3813:GLN:HB3	1:G:3899:PHE:HE2	1.72	0.55
1:J:1449:TRP:HB2	1:J:1553:PHE:HB2	1.88	0.55
1:D:1871:PHE:HZ	1:D:2094:LEU:HD13	1.72	0.55
1:J:421:PHE:CE2	1:J:507:ALA:HB2	2.42	0.55
1:J:498:THR:O	1:J:553:ARG:NH2	2.40	0.55
1:D:491:ILE:HD11	1:D:519:VAL:HG23	1.88	0.55
1:D:551:LEU:HD21	1:D:589:LEU:HD22	1.88	0.55
1:D:1947:CYS:SG	1:D:2126:ARG:HD2	2.47	0.55
1:D:4837:LEU:HD22	1:D:4936:ILE:HD11	1.88	0.55
1:J:4954:MET:SD	6:J:5103:ATP:H1'	2.46	0.55
1:G:2142:TYR:HE1	1:G:3651:ASN:HD22	1.55	0.54
1:J:4677:LEU:HD22	1:J:4711:PHE:HZ	1.68	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3916:ILE:O	1:D:3919:THR:OG1	2.22	0.54
1:D:4577:LEU:O	1:J:4879:MET:HG3	2.07	0.54
1:A:633:LEU:HD21	1:A:1659:LEU:HD12	1.88	0.54
1:G:523:TYR:CZ	1:G:560:ILE:HD11	2.41	0.54
1:G:4655:PHE:N	1:G:4796:MET:HE1	2.22	0.54
1:J:4773:VAL:O	1:J:4777:ILE:HD12	2.07	0.54
1:D:2188:ASN:OD1	1:D:2190:VAL:HG12	2.08	0.54
1:D:2823:ILE:HA	1:D:2936:ALA:O	2.07	0.54
1:A:1947:CYS:HB2	1:A:2127:GLN:HE22	1.73	0.54
1:J:579:GLN:H	1:J:582:HIS:CD2	2.23	0.54
1:J:663:TYR:HB2	1:J:808:TYR:HB3	1.89	0.54
1:J:2272:PRO:HA	1:J:2275:VAL:HG12	1.88	0.54
1:J:3889:GLN:HG3	1:J:3967:GLU:HG3	1.88	0.54
1:D:606:LEU:HD22	1:D:621:ILE:HD11	1.89	0.54
1:A:1733:GLU:OE1	1:A:1733:GLU:N	2.41	0.54
1:A:4992:LEU:O	1:A:4996:ILE:HG12	2.06	0.54
1:G:2099:SER:HB3	1:G:2128:TYR:HE1	1.71	0.54
1:G:4721:LYS:HD3	1:G:4741:LEU:HD12	1.89	0.54
1:D:206:CYS:HB2	1:D:271:GLY:HA3	1.89	0.54
1:D:633:LEU:HD23	1:D:1639:LEU:HD13	1.88	0.54
1:A:736:HIS:HB2	2:B:9:PRO:HD3	1.89	0.54
1:A:1260:MET:SD	1:A:1271:ARG:NH1	2.80	0.54
1:G:2679:PHE:HE2	1:G:2959:PHE:HE1	1.54	0.54
1:J:4692:PRO:HG2	1:J:4703:ARG:HH21	1.73	0.54
1:D:3673:MET:CE	1:D:3728:ILE:HG12	2.38	0.54
1:D:4992:LEU:O	1:D:4996:ILE:HG12	2.08	0.54
1:A:202:MET:HG3	1:A:202:MET:O	2.06	0.54
1:J:400:ALA:O	1:J:404:ILE:HG12	2.07	0.54
1:D:2121:PHE:HB3	1:D:3725:TYR:CE2	2.33	0.54
1:D:4673:ARG:HD2	1:D:4782:VAL:HG21	1.90	0.54
1:A:2102:VAL:HG13	1:A:2120:MET:HG2	1.88	0.54
1:G:527:ALA:HA	1:G:530:ILE:HG22	1.90	0.54
1:G:638:ILE:HG13	1:G:678:GLN:OE1	2.08	0.54
1:J:2096:GLU:O	1:J:2100:HIS:ND1	2.41	0.54
1:D:2121:PHE:CZ	1:D:3701:LEU:HB2	2.42	0.54
1:D:3963:ASN:O	1:D:3966:THR:OG1	2.24	0.54
1:G:587:ILE:HD12	1:G:625:LEU:HD13	1.89	0.54
1:J:4952:GLU:O	1:J:4956:THR:HG23	2.07	0.54
1:A:4822:THR:O	1:A:4826:ILE:HG12	2.07	0.54
1:G:4027:LEU:HD22	1:G:4044:MET:HE1	1.88	0.54
1:J:2012:PHE:HZ	1:J:2031:LEU:HD13	1.72	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:2114:PRO:HG3	1:J:3707:ARG:HH22	1.72	0.54
2:E:4:ILE:HB	2:E:72:ALA:HB1	1.90	0.54
1:A:3844:LEU:HD21	1:A:3936:TYR:HB2	1.88	0.54
2:B:16:PRO:HG2	2:B:63:ALA:O	2.07	0.54
1:G:636:ASN:OD1	2:H:35:LYS:NZ	2.37	0.54
1:J:180:LEU:O	1:J:200:TRP:NE1	2.36	0.54
1:J:1454:THR:HG23	1:J:1456:ASP:H	1.73	0.54
1:J:1712:TYR:OH	1:J:1814:MET:SD	2.66	0.54
1:D:2386:ILE:HG21	1:D:2418:LEU:HD22	1.89	0.53
1:A:113:HIS:NE2	1:A:399:GLN:HA	2.22	0.53
1:G:2332:LEU:HD11	1:G:2429:LEU:HA	1.89	0.53
1:D:400:ALA:O	1:D:404:ILE:HG12	2.08	0.53
2:H:78:PRO:HD3	2:H:96:THR:HG22	1.90	0.53
1:J:1470:ARG:O	1:J:1490:SER:OG	2.25	0.53
1:A:2505:PHE:O	1:A:2509:VAL:HG22	2.07	0.53
1:G:1794:ALA:O	1:G:2173:GLN:NE2	2.41	0.53
1:J:3445:TRP:HZ3	1:J:3452:LYS:HA	1.73	0.53
1:D:415:ILE:HD11	1:D:493:ARG:HD2	1.90	0.53
1:D:1286:MET:HE3	1:D:1287:LEU:H	1.73	0.53
1:D:1452:TRP:CE3	1:D:1548:LEU:HB3	2.43	0.53
1:D:2938:THR:O	1:D:2939:ARG:C	2.52	0.53
1:D:4629:TYR:OH	1:J:4860:ARG:NH2	2.42	0.53
1:A:116:MET:HB2	1:A:137:LEU:HD12	1.90	0.53
1:A:4572:ALA:O	1:A:4576:ILE:HG12	2.08	0.53
1:J:355:LEU:HB2	1:J:378:LEU:HD23	1.91	0.53
1:J:1131:ARG:NH1	1:J:1178:ALA:O	2.42	0.53
1:J:2559:LEU:HD23	1:J:2602:VAL:HG12	1.91	0.53
1:D:3723:MET:HE3	1:D:3796:SER:HB2	1.89	0.53
1:D:4055:VAL:HA	1:D:4058:ILE:HG22	1.90	0.53
1:A:62:LEU:HD12	1:A:65:CYS:HB2	1.90	0.53
1:A:561:LEU:HD21	1:A:598:LYS:HB3	1.91	0.53
1:G:3420:ARG:HA	1:G:3423:TRP:HB3	1.89	0.53
1:J:243:ARG:HA	1:J:301:VAL:HB	1.90	0.53
1:J:2661:TRP:CD1	1:J:2663:ASN:H	2.27	0.53
1:A:418:LEU:HD11	1:A:494:LEU:HG	1.89	0.53
1:A:3673:MET:HE1	1:A:3728:ILE:HG12	1.90	0.53
1:G:644:ILE:HD11	1:G:1628:VAL:HG11	1.90	0.53
1:G:3842:LEU:O	1:G:3929:SER:OG	2.21	0.53
1:G:4215:ARG:NH2	6:G:5103:ATP:O2G	2.39	0.53
1:G:4879:MET:HG3	1:J:4578:LEU:HD12	1.89	0.53
1:J:150:MET:HB2	1:J:169:LEU:HD21	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:4911:LEU:HA	1:J:4914:VAL:HG12	1.91	0.53
1:D:4204:GLN:HE21	1:D:4248:ALA:HB3	1.73	0.53
1:A:1293:LEU:HD11	1:A:1594:ARG:HG2	1.91	0.53
1:G:2010:LEU:HD21	1:G:3653:PHE:CE1	2.43	0.53
1:D:2355:ARG:O	1:D:2359:ARG:HG2	2.09	0.53
1:G:684:VAL:HG21	1:G:744:VAL:HG21	1.90	0.53
1:G:1715:LEU:HD12	1:G:1719:HIS:HD2	1.74	0.53
1:G:2124:LEU:HD11	1:G:2128:TYR:CZ	2.44	0.53
1:G:3927:GLN:HE21	1:G:3991:GLY:HA3	1.73	0.53
1:D:1087:ARG:NE	1:D:1154:ASP:OD1	2.42	0.53
1:D:2025:GLU:HA	1:D:2028:ARG:HG2	1.91	0.53
1:D:3970:GLN:HE22	1:D:5004:THR:HG22	1.73	0.53
1:A:2555:CYS:SG	1:A:2599:GLN:HA	2.49	0.53
1:A:3927:GLN:HB2	1:A:3992:PHE:CZ	2.44	0.53
1:A:4818:MET:O	1:A:4824:ARG:NH2	2.42	0.53
1:G:2214:VAL:HG11	1:G:2228:MET:HE1	1.91	0.53
1:J:4583:SER:HB2	1:J:4630:TYR:HE2	1.72	0.53
1:D:657:THR:HB	1:D:1006:SER:HA	1.91	0.53
1:A:2518:LEU:HD21	1:A:2569:PHE:HE1	1.74	0.53
1:G:484:LEU:HD23	1:G:539:LEU:HD22	1.91	0.53
1:J:2500:ALA:N	1:J:2553:TYR:HE1	2.06	0.53
1:D:209:CYS:SG	1:D:273:HIS:NE2	2.77	0.52
1:D:2134:LEU:O	1:D:2138:LEU:HG	2.09	0.52
1:A:2000:SER:O	1:A:2005:GLN:NE2	2.38	0.52
1:A:2142:TYR:CD2	1:A:2197:LEU:HD13	2.44	0.52
1:G:629:ARG:NH1	2:H:90:VAL:O	2.41	0.52
1:G:2638:LYS:HD2	1:G:2698:MET:HG3	1.91	0.52
1:J:1965:TYR:CZ	1:J:2031:LEU:HB2	2.44	0.52
1:A:4813:LEU:O	1:A:4816:ILE:HG22	2.09	0.52
1:G:113:HIS:NE2	1:G:402:ARG:HB3	2.24	0.52
1:G:1947:CYS:SG	1:G:2126:ARG:NH2	2.82	0.52
1:G:2192:TYR:HD1	1:G:2242:ILE:HD13	1.74	0.52
1:G:2567:PRO:HA	1:G:2613:TYR:HD2	1.75	0.52
2:H:10:GLY:HA3	2:H:70:GLN:CB	2.33	0.52
1:G:1289:LEU:HD23	1:G:1597:VAL:HG21	1.92	0.52
1:G:2257:LEU:HA	1:G:2260:ASN:HD22	1.74	0.52
1:G:2641:LEU:O	1:G:2645:THR:HG23	2.08	0.52
1:G:3890:LEU:HA	1:G:3893:GLU:HB2	1.92	0.52
1:J:4777:ILE:HA	1:J:4780:PHE:CE2	2.43	0.52
1:G:3733:CYS:SG	1:G:3734:HIS:N	2.82	0.52
2:H:70:GLN:NE2	2:H:71:ARG:O	2.41	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:133:PHE:O	1:J:193:ALA:N	2.32	0.52
1:D:4843:LEU:HB2	1:A:4823:LEU:HD21	1.90	0.52
1:A:831:ARG:HE	1:A:840:VAL:HG21	1.73	0.52
1:G:1115:LEU:HD13	1:G:1123:VAL:HG11	1.90	0.52
1:D:3813:GLN:HB3	1:D:3899:PHE:CE2	2.45	0.52
1:D:4235:VAL:HG21	1:D:5019:TRP:NE1	2.24	0.52
1:G:707:VAL:HG13	1:G:782:SER:HB2	1.91	0.52
1:G:1291:LEU:HD23	1:G:1550:PRO:HB2	1.90	0.52
1:G:2332:LEU:HD21	1:G:2429:LEU:N	2.24	0.52
1:D:4180:ARG:HG2	1:D:4192:ARG:HH21	1.74	0.52
1:G:181:HIS:HB3	1:G:194:SER:HB3	1.92	0.52
1:G:4034:ASN:HD21	1:G:4041:ALA:HB2	1.74	0.52
1:J:1492:CYS:SG	1:J:1494:MET:HE2	2.49	0.52
1:J:4577:LEU:HD11	1:J:4807:PHE:CD1	2.45	0.52
1:D:2573:GLU:CA	1:D:2618:MET:HE1	2.36	0.52
1:D:3539:ARG:O	1:D:3543:LYS:N	2.43	0.52
1:A:622:THR:HG21	1:A:1681:VAL:HG22	1.91	0.52
1:A:629:ARG:HB3	1:A:634:GLN:OE1	2.10	0.52
1:G:2171:GLY:H	1:G:2174:GLU:HB2	1.74	0.52
1:G:2551:ASN:OD1	1:G:2552:ARG:N	2.43	0.52
1:J:597:HIS:HB2	1:J:1665:HIS:ND1	2.25	0.52
1:J:2323:TRP:CH2	1:J:2422:ILE:HG13	2.44	0.52
1:J:4712:PRO:HB2	1:J:4718:LYS:HA	1.92	0.52
2:K:25:HIS:ND1	2:K:25:HIS:O	2.42	0.52
1:G:3680:ALA:O	1:G:3681:GLY:C	2.53	0.52
1:G:4799:SER:HB2	1:G:4812:HIS:CE1	2.45	0.52
1:J:650:VAL:HG12	1:J:750:LEU:HD11	1.92	0.52
1:J:688:LEU:HD22	1:J:712:TYR:HD2	1.75	0.52
1:D:2894:LEU:O	1:D:2899:GLY:N	2.43	0.52
1:A:2004:GLU:O	1:A:2008:MET:HE3	2.10	0.52
1:G:2287:ALA:O	1:G:2349:ASN:ND2	2.38	0.52
1:J:103:TYR:CE2	1:J:152:PRO:HB3	2.45	0.52
1:J:1475:THR:HG22	1:J:1486:SER:HA	1.92	0.52
1:J:2103:VAL:O	1:J:2107:GLN:HG3	2.10	0.52
1:D:1452:TRP:HE3	1:D:1548:LEU:HB3	1.75	0.51
1:D:1699:GLU:HA	1:D:1814:MET:HE2	1.92	0.51
1:A:830:ARG:NE	1:A:837:PRO:HB3	2.25	0.51
1:A:1944:GLU:HB2	1:A:2123:LEU:HD21	1.92	0.51
1:A:3959:LYS:HG3	1:A:4022:ASP:OD2	2.10	0.51
1:A:4115:SER:HB2	1:A:4123:ILE:HG23	1.92	0.51
1:G:745:SER:N	1:G:758:ARG:O	2.42	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:1130:GLN:HG2	1:J:1138:PRO:HA	1.91	0.51
1:J:2504:LEU:HD11	1:J:2508:ARG:HH12	1.75	0.51
1:D:4580:TYR:OH	1:D:4643:LEU:HD21	2.10	0.51
1:A:1232:ARG:NH2	1:A:1828:ASP:O	2.41	0.51
1:A:4206:GLU:O	1:A:4211:LYS:NZ	2.43	0.51
1:G:1155:LEU:HD12	1:G:1184:ILE:HG22	1.91	0.51
1:G:2128:TYR:HD2	1:G:3673:MET:SD	2.33	0.51
1:G:2189:LYS:HB3	3:I:14:LYS:HG2	1.91	0.51
1:D:1732:SER:O	1:D:2140:ARG:NE	2.42	0.51
1:D:4031:LEU:O	1:D:4034:ASN:ND2	2.43	0.51
1:D:4060:LYS:O	1:D:4064:MET:HG2	2.11	0.51
1:A:578:ILE:HG23	1:A:582:HIS:HB2	1.92	0.51
1:A:1849:LEU:HB3	1:A:1945:TYR:CE2	2.46	0.51
1:A:2522:LEU:HD21	1:A:2582:MET:HE1	1.93	0.51
1:J:1965:TYR:CE1	1:J:2031:LEU:HB2	2.45	0.51
1:J:2012:PHE:CZ	1:J:2031:LEU:HD13	2.45	0.51
1:J:2095:GLN:OE1	1:J:2127:GLN:NE2	2.43	0.51
1:J:3994:HIS:CD2	1:J:3998:HIS:CD2	2.99	0.51
1:D:537:CYS:SG	1:D:571:SER:HB2	2.50	0.51
1:D:791:PHE:N	1:D:1626:TRP:O	2.41	0.51
1:D:4570:ALA:O	1:D:4573:ILE:HG22	2.10	0.51
1:A:840:VAL:HG22	1:A:1199:VAL:HG22	1.93	0.51
1:G:2251:PHE:CD2	1:G:2286:LEU:HD22	2.45	0.51
1:G:3420:ARG:O	1:G:3424:LEU:HG	2.10	0.51
1:J:1607:ARG:NH2	1:J:1610:ASN:OD1	2.43	0.51
1:D:1297:PHE:HA	1:D:1522:LEU:HD22	1.92	0.51
1:A:113:HIS:NE2	1:A:402:ARG:HB3	2.26	0.51
1:A:451:TYR:CE2	1:A:474:ARG:HD2	2.46	0.51
1:A:3844:LEU:HD13	1:A:3933:PHE:HA	1.92	0.51
2:B:56:ILE:HD11	2:B:81:ALA:HA	1.91	0.51
1:G:711:LEU:HD22	1:G:1491:ASN:HD22	1.74	0.51
1:G:1772:ARG:NH2	1:G:1952:GLN:OE1	2.43	0.51
1:G:4805:ASN:HD21	1:G:4807:PHE:HB2	1.76	0.51
1:J:2559:LEU:HD21	1:J:2603:ILE:HA	1.92	0.51
1:D:1130:GLN:HG3	1:D:1132:TRP:HE1	1.75	0.51
1:D:2515:GLN:HA	1:D:2518:LEU:HD23	1.92	0.51
1:D:3816:MET:SD	1:D:3891:LEU:HD11	2.49	0.51
1:G:2186:MET:HE1	1:G:2235:PHE:HA	1.92	0.51
1:J:42:PHE:CE1	1:J:116:MET:HE3	2.45	0.51
1:D:59:PRO:HB3	1:D:281:ARG:NH1	2.26	0.51
1:D:4820:VAL:HG11	1:J:4839:MET:HE3	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:SER:HB2	1:A:178:ARG:H	1.76	0.51
1:A:1698:LEU:HA	1:A:1712:TYR:CE1	2.38	0.51
1:G:1243:PRO:HB2	1:G:1600:LEU:HD11	1.91	0.51
1:G:1438:ARG:HB3	1:G:1563:GLN:HE21	1.75	0.51
1:G:2238:TYR:CE2	3:I:67:PRO:HB2	2.46	0.51
1:J:35:LEU:HD21	1:J:182:LEU:HD21	1.92	0.51
1:J:468:LEU:O	1:J:472:ARG:HG2	2.10	0.51
3:L:69:PHE:O	3:L:73:MET:HG3	2.10	0.51
1:D:421:PHE:HE1	1:D:436:LEU:HD21	1.75	0.51
1:D:1730:MET:HA	1:D:1730:MET:HE3	1.92	0.51
1:A:3992:PHE:HB3	1:A:3996:PHE:CE2	2.46	0.51
1:G:1936:LYS:HZ1	1:G:2105:TRP:CG	2.29	0.51
3:I:1:MET:O	3:I:4:GLN:NE2	2.44	0.51
1:J:290:TYR:HD1	1:J:304:ALA:HA	1.74	0.51
1:A:2155:LEU:HB2	1:A:2188:ASN:ND2	2.26	0.51
1:A:2469:ILE:HG21	1:A:2502:MET:HE3	1.91	0.51
1:J:42:PHE:HE1	1:J:116:MET:HE3	1.75	0.51
1:J:753:PRO:HB2	1:J:770:ALA:H	1.76	0.51
1:A:1683:HIS:HD2	1:A:1800:PRO:HG3	1.74	0.51
1:A:4839:MET:HB3	1:G:4823:LEU:HD21	1.93	0.51
1:J:719:LEU:HD11	2:K:7:ILE:HA	1.93	0.51
1:D:257:ARG:O	1:D:284:HIS:NE2	2.43	0.50
1:G:799:GLU:N	1:G:1623:ARG:O	2.39	0.50
1:G:1126:GLY:HA3	1:G:1143:TRP:NE1	2.26	0.50
1:J:1115:LEU:HD21	1:J:1123:VAL:HG11	1.93	0.50
1:J:2186:MET:HE1	1:J:2238:TYR:HD2	1.76	0.50
1:J:4145:VAL:HG13	1:J:4194:TYR:HD2	1.76	0.50
1:D:14:LEU:HD21	1:D:204:PRO:HB3	1.93	0.50
1:D:1695:LEU:HD12	1:D:1810:LYS:HE3	1.92	0.50
1:D:3722:TYR:CZ	1:D:3782:MET:SD	3.04	0.50
1:A:4001:MET:HE3	1:A:4057:MET:HG3	1.92	0.50
1:G:627:PRO:HD3	2:H:89:GLY:HA2	1.93	0.50
1:D:3836:MET:HE1	1:D:3919:THR:HG22	1.93	0.50
1:A:551:LEU:HD21	1:A:589:LEU:HD22	1.91	0.50
1:A:1621:GLY:HA3	1:A:1624:LEU:HB2	1.92	0.50
1:A:2627:VAL:HG11	1:A:2674:LEU:HD12	1.94	0.50
1:A:3844:LEU:HD21	1:A:3936:TYR:CG	2.46	0.50
1:G:692:TYR:CZ	1:G:694:PRO:HG3	2.46	0.50
1:G:4927:ILE:HG22	1:G:4928:LEU:HD22	1.93	0.50
1:J:217:GLY:HA2	1:J:261:ARG:HD3	1.93	0.50
1:J:1440:PHE:HD2	1:J:1560:ASN:HB3	1.77	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:568:LEU:HD21	1:D:578:ILE:HD11	1.92	0.50
1:D:1928:GLN:HA	1:D:2104:ARG:HH22	1.76	0.50
1:D:2515:GLN:HB2	1:D:2568:LEU:CD1	2.42	0.50
2:E:74:LEU:HB2	2:E:99:PHE:HB2	1.93	0.50
1:A:3442:PHE:O	1:A:3445:TRP:HB3	2.11	0.50
1:G:838:HIS:ND1	1:G:1201:HIS:HB2	2.26	0.50
1:G:4839:MET:HB3	1:J:4823:LEU:CD1	2.39	0.50
1:J:1713:ASP:HA	1:J:1716:ILE:HG22	1.93	0.50
1:J:4069:LYS:HA	1:J:4072:VAL:HG12	1.93	0.50
1:D:2103:VAL:HG12	1:D:2107:GLN:NE2	2.26	0.50
1:A:794:GLY:O	1:A:798:GLY:N	2.36	0.50
1:A:4072:VAL:HG21	1:A:4129:ALA:HB2	1.93	0.50
1:G:1658:ASP:N	1:G:1658:ASP:OD1	2.45	0.50
1:G:2195:PRO:HB2	1:G:2246:ASN:HD21	1.76	0.50
1:G:3844:LEU:HD11	1:G:3936:TYR:CD2	2.46	0.50
1:J:276:TRP:CZ2	1:J:339:ILE:HG13	2.47	0.50
1:J:640:TYR:CZ	1:J:1636:MET:HG2	2.46	0.50
1:J:1601:MET:HE3	1:J:1602:PRO:HD2	1.94	0.50
1:D:2251:PHE:CD2	1:D:2286:LEU:HD22	2.46	0.50
1:A:1125:ASN:HB2	1:A:1132:TRP:HD1	1.76	0.50
1:A:4241:THR:O	1:A:4245:MET:HG3	2.11	0.50
1:A:4928:LEU:HD23	1:A:4931:ILE:HD12	1.94	0.50
1:G:1839:VAL:HG13	1:G:1938:GLN:HE21	1.76	0.50
1:J:202:MET:N	1:J:202:MET:SD	2.85	0.50
1:J:2825:LYS:HA	1:J:2935:TYR:HA	1.94	0.50
1:D:667:MET:HA	1:D:743:VAL:HA	1.94	0.50
1:D:4574:ASN:HD21	1:D:4810:ALA:HA	1.77	0.50
1:A:1087:ARG:HB3	1:A:1223:PHE:CD2	2.47	0.50
1:A:4241:THR:HG22	1:A:4989:MET:HE1	1.94	0.50
1:A:4677:LEU:HD22	1:A:4702:ASP:HB3	1.94	0.50
1:G:2465:ASP:O	1:G:2469:ILE:HG12	2.11	0.50
1:G:4666:VAL:HG13	1:G:4783:ILE:HD11	1.93	0.50
1:G:4849:TYR:HA	1:G:4852:THR:HG22	1.94	0.50
1:G:4955:GLU:OE2	6:G:5103:ATP:O2'	2.30	0.50
1:J:4786:ASP:O	1:J:4790:LEU:HD23	2.12	0.50
2:K:8:SER:HB2	2:K:71:ARG:HB2	1.94	0.50
1:D:2638:LYS:NZ	1:D:2695:LEU:HA	2.27	0.50
1:A:2470:ILE:HG21	1:A:2526:PHE:HE1	1.75	0.50
1:G:1259:ARG:NH2	1:G:1595:LEU:O	2.45	0.50
1:G:1862:ILE:O	1:G:1866:ILE:HG12	2.12	0.50
1:G:2102:VAL:HG13	1:G:2120:MET:HG2	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:4574:ASN:HD21	1:J:4810:ALA:HA	1.77	0.50
1:D:1760:HIS:CE1	1:D:2041:HIS:HA	2.47	0.50
1:D:4104:THR:O	1:D:4108:ILE:HG13	2.12	0.50
1:D:4580:TYR:OH	1:D:4643:LEU:CD2	2.60	0.50
1:A:4218:ILE:HG23	1:A:4954:MET:HE1	1.93	0.50
1:A:4643:LEU:HD11	1:A:4806:ASN:HD21	1.76	0.50
1:G:4000:MET:HE1	1:G:4058:ILE:HG13	1.93	0.50
1:J:417:GLY:O	1:J:420:SER:OG	2.21	0.50
1:J:1298:HIS:CD2	1:J:1522:LEU:HB3	2.46	0.50
1:J:4856:PHE:CD2	1:J:4879:MET:HE1	2.47	0.50
1:D:594:GLY:HA2	1:D:1594:ARG:HD2	1.93	0.49
1:A:273:HIS:CG	1:A:337:PRO:O	2.65	0.49
1:A:625:LEU:HD12	1:A:626:LEU:N	2.27	0.49
1:A:4013:LEU:HD12	1:A:4016:LEU:HD23	1.94	0.49
1:G:2242:ILE:HD12	3:I:2:ALA:HB3	1.94	0.49
1:J:686:TRP:NE1	1:J:746:CYS:SG	2.85	0.49
1:J:2458:ARG:HG2	1:J:2510:TYR:CE1	2.47	0.49
1:J:3805:LEU:HG	1:J:3890:LEU:HB3	1.93	0.49
1:D:1735:ILE:HD11	1:D:2156:LEU:HD11	1.94	0.49
1:A:1452:TRP:HE1	1:A:1518:CYS:HB3	1.76	0.49
1:A:1698:LEU:CA	1:A:1712:TYR:HE1	2.22	0.49
1:G:1451:GLY:HA3	1:G:1494:MET:HA	1.93	0.49
1:G:1678:ASN:HB3	1:G:1681:VAL:HB	1.93	0.49
1:J:4567:LEU:HD21	1:J:4816:ILE:HD11	1.93	0.49
1:J:4667:PRO:HA	1:J:4670:ILE:HG22	1.94	0.49
1:D:1698:LEU:HD11	1:D:1715:LEU:HD13	1.94	0.49
1:D:1719:HIS:CD2	1:D:1802:ILE:HD12	2.47	0.49
1:D:2551:ASN:HD21	1:D:2595:LEU:HD23	1.78	0.49
1:D:3955:MET:HE2	1:D:4019:LEU:HD23	1.95	0.49
1:A:597:HIS:HB2	1:A:1665:HIS:ND1	2.26	0.49
1:A:4145:VAL:HG13	1:A:4194:TYR:HD2	1.77	0.49
1:G:2212:VAL:HG22	1:G:2256:TYR:OH	2.13	0.49
1:J:2503:VAL:HA	1:J:2506:LEU:HD21	1.94	0.49
1:J:3965:LEU:HA	1:J:3968:TYR:HD2	1.75	0.49
1:J:3966:THR:O	1:J:3970:GLN:HG3	2.12	0.49
1:D:3788:GLY:HA2	1:D:3835:LEU:HG	1.95	0.49
1:D:4999:ASP:N	1:D:5002:GLU:OE2	2.44	0.49
1:A:800:PHE:HD2	1:A:804:PRO:HG3	1.78	0.49
1:G:709:ASP:HA	1:G:725:HIS:HA	1.94	0.49
1:G:1087:ARG:HB2	1:G:1223:PHE:CD1	2.47	0.49
1:G:4859:PHE:HE2	1:G:4913:ARG:HB2	1.76	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:2148:SER:O	1:J:2152:THR:HG23	2.12	0.49
1:J:2463:LEU:HD13	1:J:2510:TYR:CD2	2.47	0.49
1:A:291:LEU:HD21	1:A:299:LEU:HD11	1.93	0.49
1:A:1474:VAL:N	1:A:1487:LEU:O	2.31	0.49
1:A:2172:PRO:O	1:A:2175:GLU:HG3	2.11	0.49
1:G:266:ARG:HD2	1:G:268:SER:O	2.12	0.49
1:G:1288:PHE:HB3	1:G:1553:PHE:HE1	1.77	0.49
1:G:2825:LYS:HA	1:G:2935:TYR:HA	1.94	0.49
1:J:347:PHE:HE1	1:J:387:ALA:HA	1.77	0.49
1:J:1248:VAL:HG23	1:J:1599:MET:HE1	1.94	0.49
1:D:1230:MET:HA	1:D:1230:MET:HE3	1.94	0.49
1:D:3770:LEU:HD12	1:D:3804:ILE:HD11	1.94	0.49
1:D:4218:ILE:HA	1:D:4221:VAL:HG12	1.94	0.49
1:A:1448:VAL:HG22	1:A:1554:VAL:HG23	1.93	0.49
1:A:2825:LYS:HA	1:A:2935:TYR:HA	1.94	0.49
1:G:667:MET:HE3	1:G:668:VAL:H	1.77	0.49
1:G:4059:LEU:HD13	1:G:4167:ALA:HB2	1.94	0.49
1:J:534:ARG:HH21	1:J:572:PRO:HD2	1.76	0.49
1:J:4679:ARG:NH2	1:J:4715:TYR:OH	2.45	0.49
1:A:2238:TYR:CE1	3:C:67:PRO:HB2	2.48	0.49
1:G:2182:ILE:O	1:G:2185:ILE:HG22	2.13	0.49
1:G:4183:ILE:O	1:G:4190:ILE:HG13	2.13	0.49
1:J:103:TYR:HD1	1:J:150:MET:HE2	1.78	0.49
1:D:195:PHE:CZ	1:A:2358:ILE:HD11	2.48	0.49
1:D:2631:PRO:HB3	1:D:2681:GLY:HA2	1.95	0.49
1:A:648:ILE:HG23	1:A:814:ALA:HB3	1.94	0.49
1:A:1594:ARG:NH2	1:A:1643:GLU:OE2	2.41	0.49
1:G:2354:VAL:HG23	1:G:2436:CYS:SG	2.53	0.49
1:J:637:LEU:HA	1:J:1637:MET:HA	1.95	0.49
1:J:1073:ARG:HG2	1:J:1075:PHE:HE1	1.78	0.49
1:J:1842:LEU:HA	1:J:1845:VAL:HG12	1.95	0.49
1:D:2153:MET:HE3	1:D:2153:MET:HA	1.94	0.49
1:D:2567:PRO:HA	1:D:2613:TYR:CG	2.47	0.49
1:A:491:ILE:HD11	1:A:519:VAL:HG23	1.94	0.49
1:A:1694:LEU:HD22	1:A:1715:LEU:HB2	1.94	0.49
1:G:1580:PHE:HE2	1:G:1592:PRO:HG2	1.78	0.49
1:G:4573:ILE:HA	1:G:4576:ILE:HG22	1.95	0.49
1:J:1773:PRO:HA	1:J:2153:MET:HE1	1.95	0.49
1:J:2040:ALA:HA	1:J:2045:GLN:HA	1.95	0.49
1:D:3829:PHE:HB3	1:D:3913:ILE:HD11	1.95	0.49
1:G:4991:PHE:HE1	1:G:5010:VAL:HG11	1.78	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1424:PRO:O	1:D:1428:LEU:HD23	2.13	0.48
1:D:3875:MET:HE2	1:D:3875:MET:HA	1.95	0.48
1:D:3935:TRP:HB3	1:J:76:ARG:HB3	1.95	0.48
1:D:4892:ARG:HH12	1:J:4898:GLY:HA3	1.77	0.48
1:A:2240:CYS:SG	1:A:2250:MET:HG2	2.53	0.48
1:G:475:GLN:NE2	1:G:528:SER:O	2.45	0.48
1:J:273:HIS:HB3	1:J:337:PRO:HB3	1.94	0.48
1:J:4856:PHE:CG	1:J:4879:MET:HE1	2.48	0.48
1:D:461:HIS:CD2	1:D:3707:ARG:HG3	2.48	0.48
1:D:523:TYR:CZ	1:D:560:ILE:HD11	2.48	0.48
1:D:2654:TYR:HA	1:D:2660:GLY:HA2	1.94	0.48
1:D:2875:ALA:HB1	1:D:2923:ALA:C	2.38	0.48
1:A:829:TYR:HB3	1:A:1073:ARG:HH11	1.78	0.48
1:A:3817:LEU:HB2	1:A:3899:PHE:CE1	2.42	0.48
1:G:214:VAL:HG22	1:G:341:TYR:HD2	1.78	0.48
3:I:6:THR:HG23	3:I:9:GLN:H	1.77	0.48
1:D:162:LYS:HE3	1:A:3984:ARG:HD3	1.95	0.48
1:D:4654:ALA:O	1:D:4658:ILE:HG12	2.12	0.48
1:D:4821:LYS:O	1:D:4825:THR:HG23	2.13	0.48
1:A:484:LEU:O	1:A:488:LEU:HG	2.13	0.48
1:G:3966:THR:O	1:G:3970:GLN:N	2.41	0.48
1:J:1252:HIS:O	1:J:1275:ARG:NE	2.46	0.48
1:J:1958:LEU:HD12	1:J:2038:LEU:HD11	1.95	0.48
1:J:4567:LEU:HD12	1:J:4815:ASP:HB3	1.95	0.48
2:K:21:THR:HA	2:K:49:ARG:HA	1.94	0.48
1:D:4863:TYR:HD2	1:D:4876:CYS:HB2	1.78	0.48
1:J:686:TRP:NE1	1:J:748:LEU:HB2	2.28	0.48
1:J:4235:VAL:HG21	1:J:5019:TRP:NE1	2.29	0.48
1:D:4036:VAL:HB	1:D:5032:TYR:CD1	2.48	0.48
1:A:1639:LEU:O	1:A:1647:CYS:HA	2.14	0.48
1:G:839:LEU:HB3	1:G:1075:PHE:CE2	2.49	0.48
1:G:1286:MET:HB2	1:G:1462:MET:HE3	1.96	0.48
1:G:3679:LYS:O	1:G:3680:ALA:HB3	2.12	0.48
1:G:3889:GLN:HG3	1:G:3890:LEU:HD12	1.94	0.48
1:G:4863:TYR:HH	1:G:4886:HIS:HE2	1.60	0.48
1:J:4577:LEU:HD12	1:J:4580:TYR:CE2	2.48	0.48
1:D:441:VAL:O	1:D:445:LEU:HD23	2.13	0.48
1:D:636:ASN:OD1	1:D:637:LEU:N	2.46	0.48
1:D:1963:GLU:HA	1:D:3650:CYS:SG	2.54	0.48
1:D:2959:PHE:HE2	1:D:3009:TYR:CE1	2.32	0.48
1:A:149:THR:OG1	1:A:172:VAL:O	2.31	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4170:ILE:HG23	1:A:4171:LEU:HD12	1.96	0.48
1:D:1621:GLY:HA3	1:D:1624:LEU:HB2	1.95	0.48
1:A:2310:CYS:N	1:A:2324:ASN:HB3	2.28	0.48
1:A:3650:CYS:O	1:A:3654:LEU:HG	2.13	0.48
1:J:1154:ASP:O	1:J:1158:ASN:N	2.47	0.48
1:J:1727:ARG:O	1:J:1731:LEU:HB2	2.13	0.48
1:J:4995:LEU:HD21	1:J:5010:VAL:HG13	1.96	0.48
1:D:1294:PRO:HB3	1:D:1549:PHE:CZ	2.49	0.48
1:A:3648:ARG:HG2	1:A:3652:MET:HE1	1.96	0.48
1:G:1152:MET:HB3	1:G:1223:PHE:CE1	2.49	0.48
1:G:1426:ILE:O	1:G:1430:THR:OG1	2.20	0.48
1:G:1730:MET:HE1	1:G:2156:LEU:HD22	1.95	0.48
1:J:1566:LEU:HD12	1:J:1575:LEU:HB3	1.95	0.48
1:J:1970:GLN:HG2	1:J:3642:TYR:HA	1.96	0.48
1:D:3981:ALA:O	1:D:3986:TRP:NE1	2.41	0.48
1:A:221:ARG:HH21	1:A:259:LEU:HD21	1.79	0.48
1:A:4218:ILE:HG23	1:A:4954:MET:CE	2.44	0.48
1:A:4844:LEU:HD21	1:A:4891:VAL:HG21	1.96	0.48
1:G:400:ALA:HB1	1:G:478:PHE:CE1	2.49	0.48
1:G:1673:VAL:HG12	1:G:1681:VAL:HG11	1.95	0.48
1:G:2153:MET:HA	1:G:2153:MET:HE3	1.96	0.48
1:G:2527:LEU:HD21	1:G:2582:MET:HB2	1.95	0.48
1:G:3709:ALA:HB2	1:G:3782:MET:HG2	1.95	0.48
1:G:4568:PHE:HD2	1:G:4569:LEU:HD12	1.79	0.48
1:J:2298:VAL:HG21	1:J:2334:PHE:CE2	2.48	0.48
1:D:101:LEU:HD13	1:D:150:MET:HE1	1.95	0.48
1:D:839:LEU:HB3	1:D:1075:PHE:HE2	1.79	0.48
1:D:2500:ALA:HB2	1:D:2553:TYR:HD1	1.78	0.48
1:A:23:GLN:OE1	1:A:203:ASN:ND2	2.46	0.48
1:A:2349:ASN:OD1	1:A:3849:ARG:NH2	2.35	0.48
1:A:4839:MET:HA	1:A:4839:MET:HE3	1.96	0.48
1:G:597:HIS:HB2	1:G:1665:HIS:ND1	2.28	0.48
1:G:1708:ARG:NH1	1:G:1836:PHE:O	2.47	0.48
1:G:2502:MET:HA	1:G:2502:MET:HE3	1.96	0.48
1:J:2171:GLY:N	1:J:2174:GLU:OE2	2.47	0.48
1:J:2284:ASN:ND2	1:J:2342:ASN:HD22	2.12	0.48
1:D:3934:TYR:CZ	1:D:3998:HIS:HB3	2.49	0.47
1:A:102:LEU:HB2	1:A:105:HIS:CD2	2.49	0.47
1:A:712:TYR:HE1	1:A:1470:ARG:HE	1.62	0.47
1:A:4843:LEU:HB2	1:G:4823:LEU:HD11	1.96	0.47
1:G:2467:VAL:HA	1:G:2470:ILE:HD12	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:3781:GLN:NE2	1:G:3819:TYR:OH	2.34	0.47
1:J:1245:PHE:CE2	1:J:1290:ARG:HD3	2.49	0.47
1:J:1451:GLY:HA3	1:J:1494:MET:HA	1.94	0.47
1:J:1685:LEU:HD21	1:J:1714:LEU:HD11	1.96	0.47
1:J:1930:LYS:O	1:J:1931:LEU:HD23	2.13	0.47
1:J:2573:GLU:HA	1:J:2576:ALA:HB2	1.96	0.47
1:D:213:TYR:HE2	1:D:337:PRO:HB2	1.79	0.47
1:D:1432:THR:HA	1:D:1520:VAL:O	2.13	0.47
1:D:2185:ILE:HD13	1:D:2203:MET:CE	2.44	0.47
1:A:1433:TYR:CD1	1:A:1573:MET:HB3	2.49	0.47
1:G:647:ASN:ND2	1:G:820:ARG:O	2.44	0.47
1:G:1944:GLU:HA	1:G:2123:LEU:HD11	1.97	0.47
1:G:2670:GLU:HA	1:G:2673:HIS:ND1	2.29	0.47
1:G:3903:LEU:HD22	1:G:3915:ILE:HG21	1.94	0.47
1:J:530:ILE:HG22	1:J:536:ASN:HB3	1.96	0.47
1:J:671:VAL:HG23	1:J:787:VAL:HG22	1.95	0.47
1:J:2611:CYS:CB	1:J:2643:LEU:HD11	2.44	0.47
1:J:2776:SER:O	1:J:2787:THR:HA	2.15	0.47
1:J:4680:LYS:O	1:J:4685:GLY:N	2.47	0.47
1:D:590:LEU:HD22	1:D:631:LEU:HD23	1.97	0.47
1:D:1579:MET:HG2	1:D:1595:LEU:HD11	1.97	0.47
1:A:1617:THR:HA	1:A:1628:VAL:HG12	1.97	0.47
1:A:2776:SER:O	1:A:2787:THR:HA	2.14	0.47
1:A:3842:LEU:O	1:A:3929:SER:HB3	2.15	0.47
1:G:650:VAL:HG11	1:G:662:TRP:CD1	2.48	0.47
1:G:1639:LEU:O	1:G:1647:CYS:HA	2.14	0.47
1:G:3784:SER:HA	1:G:3828:PHE:HA	1.96	0.47
1:G:3986:TRP:HA	1:G:3989:VAL:HG12	1.96	0.47
1:J:1732:SER:HB2	1:J:2140:ARG:NH1	2.29	0.47
1:D:674:PHE:CE1	1:D:679:ALA:HA	2.49	0.47
1:A:839:LEU:HD13	1:A:1075:PHE:HD2	1.79	0.47
1:G:120:CYS:HA	1:G:135:VAL:HA	1.95	0.47
1:G:1131:ARG:NH1	1:G:1178:ALA:O	2.46	0.47
1:G:1287:LEU:HD13	1:G:1289:LEU:CD1	2.44	0.47
1:G:1469:VAL:HG13	1:G:1492:CYS:HB3	1.96	0.47
1:G:1830:VAL:HB	1:G:1837:GLN:HG2	1.95	0.47
1:G:2161:GLN:HE21	1:G:2177:LEU:HD21	1.78	0.47
1:J:3829:PHE:HE2	1:J:3902:TYR:CE2	2.31	0.47
2:K:66:MET:HA	2:K:66:MET:HE2	1.96	0.47
1:D:587:ILE:HG12	1:D:625:LEU:HD12	1.95	0.47
1:D:2124:LEU:HD21	1:D:3677:LEU:HD11	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4661:TYR:HE1	1:D:4665:LYS:HD2	1.80	0.47
1:D:4802:GLY:HA2	1:D:4808:PHE:HB2	1.96	0.47
1:D:4904:PRO:HG3	1:D:4913:ARG:HD3	1.97	0.47
1:G:530:ILE:HD11	1:G:537:CYS:HA	1.97	0.47
1:G:1123:VAL:HG23	1:G:1132:TRP:HB2	1.96	0.47
1:G:2239:PHE:O	1:G:2242:ILE:HG22	2.14	0.47
1:G:4680:LYS:HD2	1:G:4686:LEU:HD22	1.97	0.47
1:J:523:TYR:CZ	1:J:560:ILE:HD11	2.49	0.47
1:J:707:VAL:O	1:J:713:SER:HB2	2.13	0.47
1:J:1105:ALA:HA	1:J:1121:ALA:HA	1.95	0.47
1:J:1288:PHE:HB3	1:J:1553:PHE:CE1	2.50	0.47
1:J:1291:LEU:HD12	1:J:1550:PRO:HG2	1.96	0.47
1:J:1933:GLU:HA	1:J:1936:LYS:HD2	1.97	0.47
1:J:2623:LEU:O	1:J:2627:VAL:HG23	2.14	0.47
1:J:3821:LYS:HE2	1:J:3902:TYR:HE1	1.80	0.47
1:J:4866:SER:HB3	1:J:4873:ASP:H	1.79	0.47
1:D:3779:VAL:HG13	1:D:3797:THR:HG22	1.95	0.47
1:D:3966:THR:HG22	1:D:4026:MET:HA	1.96	0.47
1:D:4000:MET:HE1	1:D:4058:ILE:HD12	1.95	0.47
1:D:4087:LEU:HB3	1:D:4122:MET:HA	1.97	0.47
1:D:4192:ARG:HG3	1:D:5028:PHE:CD1	2.50	0.47
1:D:4548:ARG:O	1:D:4552:LEU:HD23	2.14	0.47
1:D:4927:ILE:O	1:D:4931:ILE:HG13	2.15	0.47
1:A:213:TYR:CG	1:A:338:GLU:CB	2.98	0.47
1:G:2776:SER:O	1:G:2787:THR:HA	2.15	0.47
1:J:2238:TYR:O	1:J:2242:ILE:HG12	2.14	0.47
1:J:3821:LYS:HE2	1:J:3902:TYR:CE1	2.49	0.47
1:D:4028:LEU:O	1:D:4031:LEU:HG	2.15	0.47
1:A:614:VAL:HG12	1:A:2169:GLN:HG3	1.97	0.47
1:A:1802:ILE:HG13	1:A:1803:PRO:HD2	1.96	0.47
1:A:3812:VAL:HG12	1:A:3816:MET:HE3	1.96	0.47
1:A:4230:LYS:HE3	1:A:4231:MET:HE3	1.96	0.47
2:B:62:GLY:O	2:B:66:MET:HG2	2.14	0.47
1:G:299:LEU:HD22	1:G:376:ALA:HB3	1.97	0.47
1:G:589:LEU:HD12	1:G:593:HIS:ND1	2.29	0.47
1:G:1580:PHE:CE2	1:G:1592:PRO:HG2	2.50	0.47
1:G:2199:ARG:NH1	1:G:2246:ASN:OD1	2.47	0.47
1:G:2256:TYR:O	1:G:2260:ASN:ND2	2.48	0.47
1:G:3995:VAL:O	1:G:3999:MET:HG2	2.14	0.47
1:G:5017:ARG:CZ	1:G:5019:TRP:HH2	2.27	0.47
1:J:103:TYR:CD1	1:J:163:VAL:HG22	2.50	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:277:GLY:HA2	1:J:315:CYS:HB2	1.96	0.47
1:J:504:ALA:HB2	1:J:512:ALA:HB2	1.97	0.47
1:J:3768:SER:HA	1:J:3771:HIS:CE1	2.50	0.47
1:J:3962:PHE:HZ	1:J:3992:PHE:CE2	2.32	0.47
1:D:4850:LEU:O	1:D:4853:VAL:HG12	2.14	0.47
1:D:5019:TRP:HD1	1:D:5022:PHE:HE2	1.62	0.47
1:A:2238:TYR:O	1:A:2242:ILE:HG12	2.14	0.47
1:A:3965:LEU:HA	1:A:3968:TYR:HD2	1.78	0.47
1:G:753:PRO:HB2	1:G:770:ALA:H	1.80	0.47
1:G:1269:CYS:SG	1:G:1270:LEU:N	2.87	0.47
1:J:212:GLY:HA2	1:J:341:TYR:CD2	2.49	0.47
1:D:444:SER:O	1:D:448:LEU:HD23	2.15	0.47
1:D:4692:PRO:HB3	1:D:4703:ARG:HH12	1.80	0.47
1:A:492:ASP:O	1:A:496:VAL:HG23	2.15	0.47
1:A:1769:THR:HG22	1:A:1769:THR:O	2.15	0.47
1:A:2346:VAL:HG23	1:A:2349:ASN:HB2	1.97	0.47
1:G:3722:TYR:CD2	1:G:3793:MET:SD	3.08	0.47
1:J:619:ASP:HA	1:J:622:THR:HG22	1.96	0.47
1:J:1561:VAL:HG12	1:J:1562:ILE:H	1.80	0.47
1:D:1289:LEU:HD23	1:D:1564:PHE:CZ	2.50	0.47
1:D:3695:PRO:HB2	1:D:3699:HIS:HB3	1.97	0.47
1:A:1719:HIS:CD2	1:A:1802:ILE:HD13	2.50	0.47
1:A:3999:MET:HE3	1:A:4003:LEU:HG	1.97	0.47
1:G:4961:CYS:SG	1:G:4983:HIS:HE1	2.17	0.47
1:D:1225:PRO:HD2	1:D:1228:ILE:HD13	1.97	0.46
1:D:1609:PRO:HD2	1:D:1612:PHE:CZ	2.50	0.46
1:D:1717:SER:HA	1:D:1721:GLU:HB2	1.96	0.46
1:D:2951:ILE:O	1:D:2955:PHE:N	2.44	0.46
3:F:29:THR:HA	3:F:62:GLY:HA2	1.97	0.46
1:A:716:PHE:HB3	1:A:721:LEU:HG	1.96	0.46
1:A:2196:ASN:OD1	1:A:2199:ARG:NH2	2.44	0.46
1:G:1671:ARG:HH22	1:G:1710:GLY:HA2	1.80	0.46
1:G:2142:TYR:OH	1:G:2194:HIS:ND1	2.46	0.46
1:G:3658:LYS:HG3	1:G:3662:ILE:HD11	1.97	0.46
1:G:3813:GLN:O	1:G:3899:PHE:HZ	1.97	0.46
1:G:4184:MET:HB3	1:G:5021:PHE:HA	1.97	0.46
1:J:1717:SER:HA	1:J:1721:GLU:HB2	1.97	0.46
1:J:3853:ALA:HA	1:J:3856:LEU:HD23	1.96	0.46
1:J:3904:ARG:HG2	1:J:3905:THR:HG22	1.96	0.46
1:J:4673:ARG:HD3	1:J:4778:TRP:CZ2	2.49	0.46
1:D:2567:PRO:HA	1:D:2613:TYR:CB	2.46	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4708:THR:HB	1:D:4774:LYS:HD2	1.97	0.46
1:D:4888:TYR:CD1	1:J:4914:VAL:HG23	2.50	0.46
1:J:2102:VAL:HG13	1:J:2120:MET:CG	2.45	0.46
1:J:4968:PHE:CE2	1:J:4978:HIS:HB2	2.50	0.46
2:K:23:VAL:HG12	2:K:104:LEU:HB3	1.97	0.46
1:A:687:ALA:HB3	1:A:778:PHE:CE1	2.50	0.46
1:A:2465:ASP:O	1:A:2469:ILE:HG12	2.15	0.46
1:G:214:VAL:HG22	1:G:341:TYR:CD2	2.49	0.46
1:G:1651:LEU:HD23	1:G:1702:HIS:HB2	1.96	0.46
1:G:2499:LYS:O	1:G:2503:VAL:HG12	2.15	0.46
1:G:4108:ILE:O	1:G:4112:LEU:HG	2.15	0.46
1:J:38:ALA:HB1	1:J:64:ILE:HG22	1.96	0.46
1:J:261:ARG:HH21	1:J:283:ARG:HD3	1.80	0.46
1:J:592:LYS:HB3	1:J:1592:PRO:HB3	1.97	0.46
1:J:1246:GLU:O	1:J:1598:GLN:HB2	2.14	0.46
1:J:2250:MET:HE2	1:J:2250:MET:HA	1.98	0.46
1:J:4658:ILE:CD1	1:J:4792:LEU:HB3	2.45	0.46
1:D:664:PHE:HB2	1:D:793:LEU:HA	1.98	0.46
1:D:2193:GLN:HG2	3:F:10:ILE:HG21	1.97	0.46
1:D:2506:LEU:HD13	1:D:2510:TYR:HD2	1.81	0.46
1:D:2518:LEU:O	1:D:2522:LEU:HB3	2.15	0.46
2:E:39:SER:CA	2:E:42:ARG:NH2	2.70	0.46
1:A:149:THR:HG23	1:A:174:VAL:HG22	1.97	0.46
1:A:663:TYR:HB2	1:A:808:TYR:HB3	1.97	0.46
1:A:755:ILE:HB	1:A:768:PHE:HB2	1.96	0.46
1:A:4167:ALA:O	1:A:4171:LEU:HD13	2.14	0.46
1:A:4843:LEU:HD13	1:G:4823:LEU:HD12	1.98	0.46
1:G:711:LEU:HD13	1:G:1491:ASN:HB3	1.97	0.46
1:G:1247:PRO:HA	1:G:1598:GLN:HG2	1.97	0.46
1:G:2159:LEU:HD12	1:G:2203:MET:HE3	1.98	0.46
1:G:4904:PRO:HG3	1:G:4913:ARG:HG2	1.97	0.46
1:G:4973:HIS:ND1	1:G:4973:HIS:O	2.48	0.46
1:J:2024:PRO:C	1:J:2028:ARG:HH21	2.24	0.46
1:J:2182:ILE:O	1:J:2185:ILE:HG22	2.16	0.46
1:D:2638:LYS:HZ1	1:D:2695:LEU:HA	1.79	0.46
1:D:4687:TYR:HE2	1:D:4703:ARG:HA	1.81	0.46
1:D:4876:CYS:HA	1:D:4882:CYS:HB2	1.97	0.46
1:A:1731:LEU:HD23	1:A:1772:ARG:HH12	1.80	0.46
1:A:3890:LEU:HA	1:A:3893:GLU:HB2	1.97	0.46
1:G:4159:ARG:HD3	1:G:4159:ARG:H	1.81	0.46
1:G:4217:PHE:CE1	1:G:4221:VAL:HG21	2.51	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2212:VAL:HG22	1:D:2256:TYR:CZ	2.51	0.46
1:D:3872:GLU:O	1:D:3876:ALA:HB2	2.16	0.46
1:A:241:GLN:O	1:A:243:ARG:NH1	2.49	0.46
1:A:662:TRP:CH2	1:A:814:ALA:HB2	2.49	0.46
1:A:2328:GLY:O	1:A:2332:LEU:HD23	2.15	0.46
1:A:4851:TYR:HD2	1:A:4920:PHE:HD2	1.63	0.46
1:G:607:CYS:SG	1:G:618:GLN:HG3	2.55	0.46
1:G:4704:LEU:O	1:G:4774:LYS:HE2	2.16	0.46
1:J:1124:PHE:HA	1:J:1131:ARG:HA	1.96	0.46
1:J:1673:VAL:HG12	1:J:1681:VAL:HG21	1.97	0.46
1:D:561:LEU:HD11	1:D:599:VAL:HG22	1.98	0.46
1:D:1272:LEU:HD13	1:D:1289:LEU:HD21	1.98	0.46
1:D:1747:LEU:HD11	1:D:2038:LEU:HA	1.98	0.46
1:D:4688:ILE:HG13	1:D:4689:THR:N	2.30	0.46
1:A:1578:ALA:O	1:A:1584:ARG:NH1	2.49	0.46
1:A:2103:VAL:O	1:A:2107:GLN:HG3	2.16	0.46
1:A:3951:PHE:HD2	1:A:4012:LEU:HD11	1.80	0.46
1:A:4994:TYR:OH	1:A:4998:LYS:NZ	2.34	0.46
1:J:1669:LEU:O	1:J:1673:VAL:HG23	2.16	0.46
1:J:1815:LEU:HD23	1:J:1862:ILE:HD11	1.96	0.46
1:J:2379:ALA:HB1	1:J:2426:TYR:HE2	1.81	0.46
1:J:4863:TYR:HD2	1:J:4876:CYS:CB	2.27	0.46
1:D:4235:VAL:HG21	1:D:5019:TRP:CD1	2.51	0.46
1:A:1494:MET:HE1	1:A:1553:PHE:CZ	2.51	0.46
1:A:2035:HIS:O	1:A:2039:LEU:HD23	2.16	0.46
1:A:4049:VAL:HG21	1:A:4159:ARG:HD2	1.98	0.46
1:G:3679:LYS:HA	1:G:3679:LYS:HD2	1.58	0.46
1:A:114:SER:OG	1:A:116:MET:HG3	2.14	0.46
1:A:652:ARG:NE	1:A:750:LEU:O	2.47	0.46
1:A:1256:GLU:CB	1:A:1275:ARG:HE	2.29	0.46
1:A:2174:GLU:H	1:A:2174:GLU:CD	2.22	0.46
1:A:2641:LEU:HD21	1:A:2699:ALA:HA	1.98	0.46
1:A:3102:ASP:O	1:A:3106:MET:HG2	2.14	0.46
1:G:544:LEU:HA	1:G:547:VAL:HG12	1.98	0.46
1:G:603:LEU:HB3	1:G:621:ILE:HD11	1.96	0.46
1:G:707:VAL:O	1:G:713:SER:HB2	2.16	0.46
1:G:1496:TRP:CD1	1:G:1498:GLY:H	2.34	0.46
1:G:3943:ILE:HD11	1:G:4002:LYS:NZ	2.29	0.46
1:J:1494:MET:HE1	1:J:1553:PHE:CD2	2.51	0.46
2:K:40:ARG:O	2:K:43:ASN:ND2	2.49	0.46
1:D:414:PHE:CD1	1:D:436:LEU:HD12	2.51	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:714:TYR:OH	1:A:1472:VAL:HB	2.16	0.46
1:A:4927:ILE:HD12	1:G:4936:ILE:HG21	1.98	0.46
1:G:1970:GLN:HG3	1:G:3642:TYR:HA	1.97	0.46
1:G:2463:LEU:HB2	1:G:2510:TYR:CE2	2.51	0.46
1:J:408:ALA:O	1:J:412:ASN:ND2	2.49	0.46
1:J:1473:THR:HA	1:J:1488:LYS:HA	1.97	0.46
1:J:2351:ASN:HB3	1:J:2355:ARG:HH22	1.81	0.46
1:J:2563:THR:HG23	1:J:2606:CYS:HA	1.98	0.46
1:J:3820:LEU:HD21	1:J:3902:TYR:CE2	2.51	0.46
1:D:2336:ARG:HA	1:D:2339:VAL:HG12	1.97	0.45
1:D:3736:GLU:HA	1:D:3766:GLN:HE22	1.80	0.45
1:D:4039:MET:O	1:D:4043:GLN:HG2	2.16	0.45
1:D:4819:GLY:O	1:D:4824:ARG:NH2	2.49	0.45
1:A:634:GLN:HE21	1:A:702:TRP:HH2	1.64	0.45
1:A:2175:GLU:O	1:A:2179:ILE:HG12	2.15	0.45
1:A:2554:LEU:HA	1:A:2558:VAL:HG12	1.99	0.45
1:A:3886:ARG:HD2	1:A:3889:GLN:HE21	1.81	0.45
1:A:4335:LEU:O	1:A:4339:VAL:HG23	2.16	0.45
1:A:4567:LEU:HD11	1:A:4571:PHE:CZ	2.51	0.45
1:A:4679:ARG:HD3	1:A:5017:ARG:CZ	2.46	0.45
1:G:615:ARG:NH2	1:G:2168:VAL:HG11	2.31	0.45
1:G:2620:GLN:HA	1:G:2623:LEU:HB3	1.98	0.45
1:J:206:CYS:SG	1:J:207:SER:N	2.89	0.45
1:J:665:GLU:HA	1:J:745:SER:HA	1.97	0.45
1:J:2182:ILE:HA	1:J:2185:ILE:HG22	1.98	0.45
1:J:3102:ASP:O	1:J:3106:MET:HG2	2.15	0.45
1:J:4798:MET:HE2	1:J:4798:MET:HA	1.98	0.45
1:A:180:LEU:HB3	1:A:200:TRP:NE1	2.31	0.45
1:A:551:LEU:HD21	1:A:589:LEU:HB2	1.98	0.45
1:A:1490:SER:HB2	1:A:1493:TYR:CE1	2.52	0.45
1:G:2119:ALA:O	1:G:2123:LEU:HD23	2.16	0.45
1:G:4655:PHE:HA	1:G:4796:MET:HE1	1.98	0.45
1:J:273:HIS:ND1	1:J:335:GLY:O	2.49	0.45
1:J:545:ASP:HA	1:J:548:VAL:HG12	1.97	0.45
1:J:1236:THR:O	1:J:1608:MET:HG3	2.16	0.45
1:J:2021:CYS:SG	1:J:2028:ARG:HD3	2.56	0.45
1:J:2495:VAL:HG12	1:J:2498:HIS:H	1.81	0.45
1:D:575:LEU:HD11	1:D:606:LEU:HA	1.98	0.45
1:D:2628:PHE:CD2	1:D:2906:VAL:CB	3.00	0.45
1:A:180:LEU:HB3	1:A:200:TRP:HE1	1.82	0.45
1:A:4160:LEU:HD12	1:A:4163:PHE:HD2	1.81	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4743:MET:HA	1:A:4743:MET:HE2	1.97	0.45
1:G:221:ARG:N	1:G:391:THR:O	2.48	0.45
1:G:3886:ARG:HD2	1:G:3889:GLN:NE2	2.25	0.45
1:J:1295:VAL:HG21	1:J:1575:LEU:HD11	1.98	0.45
1:J:1639:LEU:HD11	1:J:1653:LEU:HD11	1.98	0.45
1:D:1238:PHE:CE2	1:D:1240:LYS:HG3	2.52	0.45
2:E:21:THR:HA	2:E:49:ARG:HA	1.98	0.45
1:A:1170:MET:HE3	1:A:1174:GLY:HA2	1.98	0.45
2:B:55:VAL:HG11	2:B:59:PHE:HD2	1.82	0.45
1:G:1520:VAL:HG23	1:G:1527:MET:HG2	1.98	0.45
1:J:219:VAL:HG21	1:J:398:SER:HB3	1.97	0.45
1:J:572:PRO:HB3	1:J:609:CYS:SG	2.57	0.45
1:J:716:PHE:CZ	1:J:744:VAL:HG21	2.46	0.45
1:J:2500:ALA:CA	1:J:2553:TYR:HE1	2.29	0.45
1:J:3906:GLN:CD	1:J:3906:GLN:N	2.74	0.45
1:J:4984:ASN:OD1	1:J:4987:ASN:N	2.41	0.45
1:D:247:TYR:HB2	1:D:374:LYS:HG3	1.98	0.45
1:D:1100:MET:HG2	1:D:1194:LEU:HA	1.97	0.45
1:D:1152:MET:HB3	1:D:1161:ILE:O	2.17	0.45
1:D:2463:LEU:HD13	1:D:2510:TYR:CD2	2.50	0.45
1:D:3962:PHE:O	1:D:3966:THR:HG23	2.17	0.45
1:D:3965:LEU:HA	1:D:3968:TYR:CD2	2.51	0.45
1:D:4879:MET:HB3	1:A:4578:LEU:O	2.17	0.45
1:D:4927:ILE:HG23	1:D:4928:LEU:N	2.32	0.45
2:E:4:ILE:HG13	2:E:4:ILE:O	2.17	0.45
1:A:1125:ASN:HB2	1:A:1132:TRP:CD1	2.52	0.45
1:A:2204:HIS:HB2	1:A:2250:MET:HE1	1.97	0.45
1:A:2616:PRO:HD2	1:A:2664:PHE:CD2	2.52	0.45
1:A:4180:ARG:HG2	1:A:4194:TYR:CE1	2.51	0.45
1:G:594:GLY:H	1:G:1594:ARG:HB2	1.81	0.45
1:G:2002:PRO:O	1:G:2006:ILE:HG12	2.16	0.45
1:G:2336:ARG:HG3	1:G:2435:ARG:HD2	1.97	0.45
1:J:1088:TRP:HE3	1:J:1226:PHE:HA	1.80	0.45
1:J:2102:VAL:HG11	1:J:2124:LEU:HB2	1.98	0.45
2:K:66:MET:SD	2:K:70:GLN:HB3	2.57	0.45
1:D:2128:TYR:CD2	1:D:3673:MET:HG2	2.52	0.45
1:D:3801:GLY:O	1:D:3805:LEU:HB2	2.17	0.45
1:D:4961:CYS:HB3	1:D:4983:HIS:ND1	2.32	0.45
1:A:1469:VAL:HG13	1:A:1492:CYS:HB3	1.98	0.45
1:A:2118:ARG:HD2	1:A:3721:LEU:HD22	1.99	0.45
1:A:2212:VAL:HG21	1:A:2256:TYR:CE2	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2340:PHE:CZ	1:A:2343:GLY:HA2	2.51	0.45
1:A:3966:THR:O	1:A:3970:GLN:HG2	2.16	0.45
1:A:4090:LYS:HG3	1:A:4112:LEU:HD22	1.99	0.45
1:G:1000:ARG:O	1:G:1004:GLY:N	2.49	0.45
1:J:615:ARG:HD3	1:J:1678:ASN:ND2	2.32	0.45
2:K:91:ILE:HD12	2:K:97:LEU:HD22	1.98	0.45
1:A:790:ARG:HA	1:A:1627:ALA:HA	1.97	0.45
1:A:1225:PRO:HG2	1:A:1228:ILE:HB	1.99	0.45
1:A:1667:LEU:HD22	1:A:1714:LEU:HD13	1.99	0.45
1:A:2354:VAL:HG23	1:A:2436:CYS:SG	2.57	0.45
2:B:23:VAL:HG12	2:B:47:LYS:HG2	1.98	0.45
1:G:1125:ASN:HD21	1:G:1127:HIS:CE1	2.35	0.45
1:G:1243:PRO:HG3	1:G:1460:HIS:HB2	1.98	0.45
1:G:3766:GLN:HG2	1:G:3769:ARG:HH21	1.81	0.45
1:G:3900:GLN:HB3	1:G:3976:ASN:ND2	2.32	0.45
1:J:152:PRO:HB2	1:J:157:ARG:CB	2.47	0.45
1:J:720:HIS:CE1	1:J:722:TRP:HE1	2.26	0.45
1:J:1426:ILE:O	1:J:1430:THR:N	2.50	0.45
1:J:3923:LEU:HD21	1:J:3962:PHE:CZ	2.52	0.45
1:J:4670:ILE:HD11	1:J:4778:TRP:CZ3	2.52	0.45
1:D:1667:LEU:HD22	1:D:1714:LEU:HD22	1.99	0.45
1:D:2503:VAL:HG11	1:D:2557:ALA:HB1	1.98	0.45
1:D:3725:TYR:HD1	1:D:3725:TYR:HA	1.70	0.45
1:D:4582:VAL:HB	1:J:4856:PHE:CZ	2.49	0.45
1:A:1713:ASP:HA	1:A:1716:ILE:HG22	1.98	0.45
1:G:635:THR:HG22	1:G:1639:LEU:HD23	1.98	0.45
1:G:686:TRP:HE3	1:G:777:PHE:HB3	1.81	0.45
1:G:1434:TYR:HE1	1:G:1517:GLY:HA3	1.81	0.45
1:G:1663:HIS:HD2	1:G:1707:LEU:HD22	1.81	0.45
1:G:1708:ARG:HH21	1:G:1814:MET:HE2	1.82	0.45
1:G:3980:LEU:HD11	1:G:3985:LEU:HD22	1.99	0.45
1:J:1723:ALA:HB1	1:J:1775:HIS:CE1	2.52	0.45
1:J:2001:PRO:O	1:J:2005:GLN:HG3	2.16	0.45
1:J:2003:GLN:HA	1:J:3652:MET:HE1	1.97	0.45
1:J:2495:VAL:HB	1:J:2498:HIS:HB2	1.98	0.45
1:J:3986:TRP:HA	1:J:3989:VAL:HG12	1.99	0.45
1:D:636:ASN:HD21	2:E:35:LYS:NZ	2.15	0.45
1:D:3640:PRO:HG2	1:D:3643:ASN:HB2	1.98	0.45
1:D:4031:LEU:HD13	1:D:4149:ASN:ND2	2.32	0.45
1:D:4055:VAL:O	1:D:4058:ILE:HG22	2.16	0.45
1:D:4154:VAL:O	1:D:4154:VAL:HG13	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:TYR:O	1:A:138:GLN:N	2.45	0.45
1:A:4198:SER:HB2	1:A:4201:ASN:ND2	2.32	0.45
1:G:590:LEU:HD22	1:G:631:LEU:HD23	1.99	0.45
1:G:1663:HIS:HD2	1:G:1707:LEU:CD2	2.30	0.45
1:G:1944:GLU:CA	1:G:2123:LEU:HD11	2.47	0.45
1:G:4671:PHE:HB2	1:G:4714:ASN:HB3	1.98	0.45
1:G:4852:THR:HG21	1:G:4883:TYR:HD1	1.82	0.45
1:J:35:LEU:HD13	1:J:49:LEU:HD23	1.99	0.45
1:J:3777:GLU:O	1:J:3781:GLN:HG2	2.16	0.45
1:J:4631:PHE:CE2	1:J:4639:MET:HG3	2.52	0.45
1:J:4863:TYR:CE1	1:J:4901:ILE:HG12	2.52	0.45
1:D:707:VAL:O	1:D:713:SER:HB2	2.17	0.45
1:D:1432:THR:HA	1:D:1521:ASP:HA	1.99	0.45
1:D:2504:LEU:HD22	1:D:2508:ARG:HG3	1.99	0.45
1:A:2112:GLN:OE1	1:A:2112:GLN:N	2.50	0.45
1:G:1297:PHE:HB2	1:G:1544:PRO:O	2.17	0.45
1:G:2555:CYS:SG	1:G:2599:GLN:HG2	2.57	0.45
1:G:4045:VAL:HG22	1:G:4160:LEU:HD21	1.98	0.45
1:J:150:MET:CE	1:J:163:VAL:HG21	2.45	0.45
1:J:753:PRO:HB3	1:J:771:PHE:CE2	2.52	0.45
1:J:1255:TYR:CE1	1:J:1274:HIS:HD2	2.32	0.45
1:J:1561:VAL:HG12	1:J:1562:ILE:N	2.32	0.45
1:D:284:HIS:HB3	1:D:287:THR:HG22	1.99	0.44
1:D:663:TYR:HB2	1:D:808:TYR:HB3	1.99	0.44
1:D:1205:GLY:HA2	1:D:1211:LEU:CD1	2.42	0.44
1:D:2495:VAL:HG12	1:D:2497:ASP:H	1.83	0.44
1:A:209:CYS:SG	1:A:273:HIS:NE2	2.89	0.44
1:A:247:TYR:HB2	1:A:374:LYS:HG3	1.98	0.44
1:A:495:ASN:HB3	1:A:550:LYS:HZ1	1.82	0.44
1:A:652:ARG:HD2	1:A:773:LEU:HD22	1.99	0.44
2:B:67:SER:OG	2:B:70:GLN:OE1	2.28	0.44
1:J:110:ARG:HA	1:J:117:TYR:HA	1.97	0.44
1:J:411:TYR:O	1:J:415:ILE:HG12	2.16	0.44
1:J:2346:VAL:HG23	1:J:2349:ASN:HB2	1.99	0.44
1:J:4183:ILE:HG12	1:J:4193:ILE:HD13	1.98	0.44
1:J:4995:LEU:HD23	1:J:5011:TRP:HE3	1.81	0.44
2:K:25:HIS:HB2	2:K:39:SER:HB2	1.97	0.44
1:D:698:GLY:O	1:D:703:GLY:HA2	2.17	0.44
1:D:3897:ASN:OD1	1:D:3898:ASP:N	2.50	0.44
1:A:2114:PRO:HB3	1:A:3707:ARG:HH21	1.82	0.44
1:A:3003:LEU:HB2	1:A:3004:PRO:HD3	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4675:LYS:HG3	1:A:4679:ARG:HE	1.82	0.44
1:G:266:ARG:HH21	1:G:272:SER:HB3	1.82	0.44
1:G:491:ILE:HG12	1:G:523:TYR:CE1	2.52	0.44
1:G:2500:ALA:HB2	1:G:2553:TYR:HD1	1.81	0.44
1:G:4154:VAL:O	1:G:4154:VAL:HG13	2.18	0.44
1:J:526:LEU:HD11	1:J:540:PHE:HZ	1.83	0.44
1:J:1469:VAL:HG13	1:J:1492:CYS:HB3	1.99	0.44
1:J:1641:ILE:HG22	1:J:1643:GLU:HG2	2.00	0.44
1:D:790:ARG:HA	1:D:1627:ALA:HA	1.98	0.44
1:D:1101:ARG:HH21	1:D:1125:ASN:HD22	1.65	0.44
1:D:1435:TYR:HE1	1:D:1452:TRP:CZ2	2.35	0.44
1:D:1676:LEU:HA	1:D:1725:ARG:HH12	1.81	0.44
1:D:2515:GLN:HB2	1:D:2568:LEU:HD11	2.00	0.44
1:D:4149:ASN:ND2	1:D:4153:HIS:HD2	2.14	0.44
1:A:20:VAL:HG21	1:A:202:MET:SD	2.58	0.44
1:A:355:LEU:HB2	1:A:378:LEU:HD23	1.99	0.44
1:A:445:LEU:HB3	1:A:521:LEU:HB3	1.99	0.44
1:A:1641:ILE:HG22	1:A:1643:GLU:HG2	1.99	0.44
1:A:2423:MET:HE1	1:A:2494:PHE:HA	1.99	0.44
1:G:243:ARG:HA	1:G:301:VAL:HG22	1.99	0.44
1:G:1601:MET:HE3	1:G:1601:MET:HA	1.98	0.44
1:G:2182:ILE:O	1:G:2186:MET:HG2	2.18	0.44
1:G:4548:ARG:HD2	1:G:4552:LEU:HD13	2.00	0.44
1:J:411:TYR:HB3	1:J:486:LEU:HD21	1.99	0.44
1:J:583:ILE:O	1:J:587:ILE:HG13	2.17	0.44
1:J:1271:ARG:HA	1:J:1563:GLN:HB2	1.99	0.44
1:J:1434:TYR:HB3	1:J:1572:ILE:HG21	1.98	0.44
1:J:4226:GLY:O	1:J:4230:LYS:HG3	2.18	0.44
1:J:4687:TYR:HB3	1:J:4740:LEU:HD21	1.98	0.44
1:D:1451:GLY:HA3	1:D:1494:MET:HA	1.98	0.44
1:D:2959:PHE:HE2	1:D:3009:TYR:CZ	2.35	0.44
1:D:4060:LYS:HD2	1:D:4060:LYS:HA	1.83	0.44
1:A:102:LEU:HB2	1:A:105:HIS:HD2	1.82	0.44
1:A:2359:ARG:NE	1:A:2359:ARG:HA	2.33	0.44
1:A:4017:LEU:HD22	1:A:4139:ILE:HG21	1.99	0.44
1:G:37:LEU:HD13	1:G:191:VAL:HG11	1.99	0.44
1:G:551:LEU:HA	1:G:560:ILE:HG21	1.99	0.44
1:G:2439:GLU:OE2	1:G:2508:ARG:NH2	2.50	0.44
1:G:3886:ARG:HG3	1:G:3890:LEU:HD13	1.99	0.44
1:G:4041:ALA:O	1:G:4045:VAL:HG23	2.17	0.44
1:G:4235:VAL:HG21	1:G:5019:TRP:NE1	2.33	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:231:LEU:C	1:J:260:TRP:HH2	2.26	0.44
1:J:2293:GLN:O	1:J:2296:GLU:HG3	2.17	0.44
1:J:3678:SER:HB2	1:J:3773:ARG:HH21	1.82	0.44
1:D:839:LEU:HD13	1:D:1075:PHE:CD2	2.52	0.44
1:D:2959:PHE:CE2	1:D:3009:TYR:CZ	3.05	0.44
1:A:2178:MET:O	1:A:2182:ILE:HG12	2.17	0.44
1:A:4323:THR:OG1	1:A:4324:ALA:N	2.50	0.44
1:A:4961:CYS:HB3	1:A:4983:HIS:CE1	2.52	0.44
1:G:20:VAL:HG21	1:G:202:MET:SD	2.57	0.44
1:G:4979:THR:HG21	6:G:5103:ATP:H3'	1.99	0.44
1:J:444:SER:O	1:J:448:LEU:HD23	2.18	0.44
1:J:1438:ARG:NH2	1:J:1513:ASP:OD2	2.50	0.44
1:J:1451:GLY:CA	1:J:1494:MET:HG2	2.48	0.44
1:J:3003:LEU:HB3	1:J:3004:PRO:HD3	1.99	0.44
1:D:4910:GLU:O	1:D:4914:VAL:HG23	2.18	0.44
1:D:4998:LYS:HD3	1:D:5002:GLU:HG2	2.00	0.44
1:A:3723:MET:HE2	1:A:3723:MET:HB3	1.75	0.44
1:G:2518:LEU:HD13	1:G:2568:LEU:HD23	1.99	0.44
1:G:2671:GLU:O	1:G:2675:THR:HG23	2.17	0.44
1:J:2280:VAL:O	1:J:2280:VAL:HG13	2.17	0.44
1:J:2500:ALA:HB2	1:J:2553:TYR:HD1	1.83	0.44
1:J:4562:LEU:HD12	1:J:4565:LEU:HD11	2.00	0.44
1:D:518:ILE:O	1:D:522:LEU:HD23	2.18	0.44
1:D:1126:GLY:HA3	1:D:1143:TRP:CZ3	2.52	0.44
1:D:3722:TYR:CD1	1:D:3782:MET:HE1	2.52	0.44
1:D:3955:MET:HB2	1:D:4019:LEU:HD23	2.00	0.44
1:D:4554:TYR:HA	1:D:4557:ARG:HH21	1.82	0.44
1:A:1450:VAL:HG22	1:A:1552:VAL:HG22	2.00	0.44
1:A:4054:ASN:O	1:A:4058:ILE:HG12	2.17	0.44
1:G:452:PHE:HZ	1:G:478:PHE:CD2	2.33	0.44
1:G:657:THR:HB	1:G:851:PHE:CE2	2.53	0.44
1:G:4096:ALA:O	1:G:4100:GLN:HG2	2.17	0.44
1:G:4180:ARG:HG2	1:G:4194:TYR:CE1	2.53	0.44
1:G:4555:LEU:HD13	1:G:4656:LEU:HG	1.99	0.44
1:G:4586:PRO:HB3	1:G:4628:VAL:HG11	1.99	0.44
1:G:4791:TYR:HD1	1:G:4792:LEU:HD23	1.82	0.44
3:I:29:THR:O	3:I:33:LEU:N	2.47	0.44
1:J:671:VAL:HG12	1:J:740:PRO:HD3	2.00	0.44
1:J:2294:ASP:O	1:J:2298:VAL:HG23	2.17	0.44
1:J:3445:TRP:HE3	1:J:3451:PHE:HD2	1.64	0.44
1:J:4667:PRO:O	1:J:4670:ILE:HG22	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:716:PHE:HD2	1:D:718:GLY:N	2.12	0.44
1:D:1931:LEU:HD22	1:D:1935:VAL:HG11	1.99	0.44
1:D:2420:HIS:CD2	1:D:2491:SER:HA	2.53	0.44
1:D:3135:ALA:O	1:D:3139:VAL:N	2.45	0.44
1:D:4979:THR:HG21	6:D:5103:ATP:H2'	1.99	0.44
1:A:441:VAL:O	1:A:445:LEU:HD23	2.18	0.44
1:A:667:MET:HA	1:A:743:VAL:HA	1.99	0.44
1:A:1085:SER:OG	1:A:1086:GLY:N	2.51	0.44
1:A:2159:LEU:HD22	1:A:2201:LEU:HD23	2.00	0.44
1:A:4823:LEU:O	1:A:4827:LEU:HD23	2.18	0.44
1:G:1245:PHE:CG	1:G:1290:ARG:HD3	2.52	0.44
1:G:1815:LEU:HD22	1:G:1845:VAL:HG21	2.00	0.44
1:G:4642:ALA:O	1:G:4646:LEU:HD23	2.18	0.44
1:G:4675:LYS:HD2	1:G:4679:ARG:HH21	1.83	0.44
1:J:1442:GLY:O	1:J:1557:THR:OG1	2.35	0.44
1:J:1814:MET:HE3	1:J:1814:MET:HB2	1.83	0.44
1:J:4185:GLY:HA3	1:J:5009:TYR:CE2	2.52	0.44
1:D:1580:PHE:CE1	1:D:1592:PRO:HG2	2.53	0.44
1:D:1849:LEU:HG	1:D:1854:PHE:HD2	1.81	0.44
1:A:2298:VAL:HG21	1:A:2334:PHE:CE2	2.53	0.44
1:G:1214:PHE:CE2	1:G:1225:PRO:HD3	2.53	0.44
1:G:2611:CYS:CB	1:G:2643:LEU:HD11	2.48	0.44
1:G:3722:TYR:HE1	1:G:3782:MET:HE1	1.83	0.44
1:G:4989:MET:CE	1:G:4993:MET:HE2	2.46	0.44
1:J:3423:TRP:O	1:J:3423:TRP:CG	2.71	0.44
2:K:71:ARG:HG2	2:K:102:GLU:HG3	1.99	0.44
1:D:1289:LEU:HD23	1:D:1564:PHE:CE2	2.52	0.43
1:D:1742:THR:O	1:D:1745:ILE:HG22	2.18	0.43
1:D:2522:LEU:HG	1:D:2523:ASP:N	2.33	0.43
1:D:2638:LYS:HE2	1:D:2695:LEU:HA	1.99	0.43
1:A:3673:MET:CE	1:A:3728:ILE:HG21	2.46	0.43
1:G:660:GLY:HA2	1:G:750:LEU:HD12	2.00	0.43
1:G:2211:MET:HA	1:G:2214:VAL:HG12	2.00	0.43
1:G:4201:ASN:HB3	1:G:4993:MET:HE1	1.99	0.43
1:J:1235:THR:HG21	1:J:1607:ARG:HH21	1.82	0.43
1:J:3445:TRP:CE3	1:J:3451:PHE:HD2	2.36	0.43
1:J:3658:LYS:HG3	1:J:3662:ILE:HD11	2.00	0.43
1:J:3889:GLN:O	1:J:3893:GLU:N	2.51	0.43
1:J:4562:LEU:HD21	1:J:4656:LEU:HB3	1.99	0.43
1:J:4926:VAL:HG13	1:J:4927:ILE:HG13	2.00	0.43
1:D:2225:PHE:O	1:D:2229:VAL:HG23	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2365:GLY:HA3	1:A:2426:TYR:HE1	1.82	0.43
1:A:4984:ASN:HB3	1:A:4987:ASN:HB2	2.00	0.43
1:G:561:LEU:HD21	1:G:598:LYS:HB2	2.00	0.43
1:G:581:ASN:OD1	1:G:582:HIS:N	2.51	0.43
1:G:2012:PHE:HB2	1:G:3661:TRP:HZ2	1.84	0.43
1:G:4181:ILE:HB	1:G:4988:TYR:CE1	2.53	0.43
1:J:1076:ARG:O	1:J:1237:TRP:N	2.32	0.43
1:J:1077:ALA:HA	1:J:1236:THR:HA	1.99	0.43
1:D:3536:ALA:HB1	1:D:3597:GLN:HA	2.00	0.43
1:A:214:VAL:HG22	1:A:341:TYR:CE1	2.53	0.43
1:A:582:HIS:O	1:A:586:ILE:HG13	2.18	0.43
1:A:1171:SER:OG	1:A:1175:SER:N	2.52	0.43
1:A:1619:ARG:HA	1:A:1626:TRP:HA	2.00	0.43
1:G:540:PHE:HD2	1:G:567:VAL:HG21	1.83	0.43
1:G:1158:ASN:ND2	1:G:1182:ILE:O	2.51	0.43
1:J:1074:ILE:CD1	1:J:1115:LEU:HD12	2.49	0.43
1:J:1556:PRO:HB3	1:J:1561:VAL:HG21	1.99	0.43
1:J:2293:GLN:HA	1:J:2296:GLU:HG3	1.99	0.43
1:J:4066:LEU:HD13	1:J:4170:ILE:HA	1.99	0.43
1:D:1427:ILE:CD1	1:D:1571:ASN:HA	2.47	0.43
1:D:1771:LEU:HD11	1:D:2153:MET:SD	2.59	0.43
1:A:2323:TRP:HH2	1:A:2422:ILE:HG13	1.82	0.43
1:A:3836:MET:HA	1:A:3839:CYS:SG	2.58	0.43
1:A:4235:VAL:HG11	1:A:5019:TRP:CZ2	2.54	0.43
1:G:3136:LEU:O	1:G:3140:LEU:N	2.39	0.43
1:G:3695:PRO:HB2	1:G:3699:HIS:HB3	2.01	0.43
2:H:10:GLY:CA	2:H:70:GLN:HB2	2.38	0.43
1:J:2240:CYS:HB2	1:J:2250:MET:HG2	1.99	0.43
1:J:2297:LYS:HG2	1:J:2301:TYR:CE2	2.54	0.43
1:J:2351:ASN:HB3	1:J:2355:ARG:NH2	2.32	0.43
1:J:4020:GLN:HG3	1:J:4139:ILE:CD1	2.49	0.43
1:D:445:LEU:HD11	1:D:522:LEU:HD13	2.00	0.43
1:D:711:LEU:HD12	1:D:1491:ASN:HB3	1.99	0.43
1:D:723:THR:O	1:D:726:VAL:HG12	2.17	0.43
1:D:850:ASP:O	1:D:1023:PRO:HG3	2.19	0.43
1:D:1651:LEU:HD12	1:D:1651:LEU:H	1.82	0.43
1:D:2346:VAL:HG23	1:D:2349:ASN:HB2	2.00	0.43
1:D:2669:GLU:HA	1:D:2672:LEU:HD12	2.01	0.43
1:D:2822:THR:C	1:D:2937:VAL:HA	2.43	0.43
1:A:275:ARG:HB3	1:A:336:PRO:CG	2.48	0.43
1:A:3980:LEU:HD23	1:A:3980:LEU:HA	1.78	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:16:THR:HG22	1:J:98:HIS:HA	1.99	0.43
1:J:1074:ILE:HD11	1:J:1115:LEU:HD12	2.01	0.43
1:J:4576:ILE:HG21	1:J:4643:LEU:HB2	1.99	0.43
1:D:495:ASN:OD1	1:D:553:ARG:NH1	2.52	0.43
1:D:2208:MET:HE1	1:D:2253:HIS:CG	2.54	0.43
1:D:4027:LEU:HD23	1:D:4027:LEU:HA	1.90	0.43
1:D:4149:ASN:HD21	1:D:4153:HIS:HD2	1.66	0.43
1:D:4874:MET:HE2	1:D:4874:MET:HA	2.01	0.43
1:A:590:LEU:HB2	1:A:599:VAL:HG11	2.00	0.43
1:A:2470:ILE:HG21	1:A:2526:PHE:CE1	2.53	0.43
1:A:4705:VAL:HB	1:A:4778:TRP:CG	2.54	0.43
1:G:2142:TYR:HE1	1:G:3651:ASN:ND2	2.17	0.43
1:J:626:LEU:HB3	1:J:1688:HIS:NE2	2.33	0.43
1:J:716:PHE:CD1	1:J:757:PHE:CD2	3.07	0.43
1:J:3716:LEU:HD21	1:J:3785:ALA:HB1	2.01	0.43
1:D:633:LEU:HD21	1:D:1659:LEU:HD12	1.99	0.43
1:D:647:ASN:OD1	1:D:822:ARG:N	2.44	0.43
1:D:1648:MET:HE2	1:D:1648:MET:HB3	1.96	0.43
1:D:3351:PRO:O	1:D:3353:LEU:N	2.51	0.43
1:D:4027:LEU:HD22	1:D:4044:MET:HE1	2.00	0.43
1:D:4044:MET:HE3	1:D:4146:LEU:HD11	2.00	0.43
1:D:4182:GLU:O	1:D:4183:ILE:HD13	2.19	0.43
1:D:4562:LEU:HG	1:D:4653:VAL:HG13	2.01	0.43
1:A:1989:ALA:O	1:A:1993:ARG:HG2	2.18	0.43
1:A:4687:TYR:CG	1:A:4706:LEU:HD11	2.53	0.43
1:G:3729:MET:HB3	1:G:3770:LEU:HD13	2.00	0.43
1:J:23:GLN:HE22	1:J:267:ILE:HD12	1.82	0.43
1:J:107:ILE:N	1:J:148:TRP:O	2.42	0.43
1:J:272:SER:HB2	1:J:334:MET:HA	2.01	0.43
1:J:625:LEU:HD21	1:J:632:LEU:HD11	2.00	0.43
1:J:1454:THR:OG1	1:J:1455:PRO:HD2	2.19	0.43
1:J:2671:GLU:O	1:J:2675:THR:HG23	2.19	0.43
1:J:2823:ILE:HA	1:J:2936:ALA:O	2.18	0.43
1:J:4842:GLY:O	1:J:4846:VAL:HG23	2.18	0.43
1:J:4973:HIS:O	1:J:4977:THR:HG23	2.18	0.43
1:D:688:LEU:HD13	1:D:712:TYR:O	2.19	0.43
1:D:1464:PHE:CE2	1:D:1553:PHE:HD2	2.37	0.43
1:D:1724:CYS:HB2	1:D:1851:MET:HE1	1.99	0.43
1:D:4849:TYR:O	1:D:4852:THR:HG22	2.19	0.43
1:D:5000:GLU:HA	1:D:5003:HIS:CD2	2.54	0.43
1:A:979:PRO:HB2	1:A:980:ALA:H	1.66	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2500:ALA:N	1:A:2553:TYR:HE1	2.16	0.43
1:A:2554:LEU:O	1:A:2559:LEU:HD23	2.18	0.43
1:G:475:GLN:OE1	1:G:532:GLY:HA3	2.19	0.43
1:G:1933:GLU:HA	1:G:1936:LYS:HD3	2.00	0.43
1:J:701:GLY:HA2	1:J:1645:ASN:OD1	2.18	0.43
1:J:1073:ARG:HG2	1:J:1075:PHE:CE1	2.53	0.43
1:J:1237:TRP:CH2	1:J:1652:GLU:HG3	2.47	0.43
1:J:3722:TYR:CE1	1:J:3726:ALA:HB2	2.53	0.43
1:J:4069:LYS:HA	1:J:4069:LYS:HD3	1.91	0.43
1:J:4190:ILE:H	1:J:4190:ILE:HD12	1.84	0.43
1:D:2161:GLN:HE21	1:D:2165:LEU:HG	1.84	0.43
1:D:4017:LEU:HD12	1:D:4139:ILE:HG21	2.01	0.43
1:A:634:GLN:NE2	1:A:702:TRP:HH2	2.17	0.43
1:A:1228:ILE:CG2	1:A:1827:ARG:HH12	2.31	0.43
1:A:2336:ARG:HD3	1:A:2435:ARG:HD2	2.00	0.43
1:A:2960:LEU:HD11	1:A:3017:PHE:HZ	1.83	0.43
1:A:4805:ASN:HB3	1:A:4808:PHE:HD2	1.83	0.43
1:G:737:LEU:HD23	1:G:738:LEU:N	2.33	0.43
1:G:1131:ARG:HD2	1:G:1179:PHE:CE1	2.53	0.43
1:G:1687:SER:HB3	1:G:1782:PHE:CE2	2.53	0.43
1:J:470:SER:OG	1:J:474:ARG:NH2	2.51	0.43
1:J:1115:LEU:HD23	1:J:1115:LEU:C	2.44	0.43
1:J:2500:ALA:HB2	1:J:2553:TYR:CD1	2.54	0.43
1:J:4066:LEU:HD11	1:J:4173:TYR:HB3	2.01	0.43
1:J:4777:ILE:HA	1:J:4780:PHE:CD2	2.53	0.43
1:D:830:ARG:HH21	1:D:1612:PHE:CB	2.31	0.43
1:D:1089:TYR:O	1:D:1225:PRO:HA	2.19	0.43
1:D:1965:TYR:CZ	1:D:2031:LEU:HB2	2.53	0.43
2:E:91:ILE:HD12	2:E:97:LEU:HD21	2.00	0.43
1:A:753:PRO:HB3	1:A:771:PHE:CZ	2.54	0.43
1:A:846:LEU:HD22	1:A:1026:LEU:HD21	2.01	0.43
1:A:1228:ILE:HG23	1:A:1827:ARG:HH12	1.84	0.43
1:A:1433:TYR:CD1	1:A:1578:ALA:HB2	2.53	0.43
1:G:1939:MET:HE3	1:G:1939:MET:HB3	1.76	0.43
1:G:2305:CYS:HG	1:G:2331:TYR:HE2	1.66	0.43
1:G:2522:LEU:HD11	1:G:2582:MET:HE1	2.01	0.43
1:G:4586:PRO:HA	1:G:4587:PRO:HD3	1.88	0.43
1:G:4844:LEU:HD12	1:G:4928:LEU:HB3	2.01	0.43
1:J:19:GLU:HA	1:J:68:THR:HA	2.01	0.43
1:J:213:TYR:HB3	1:J:273:HIS:CD2	2.53	0.43
1:J:791:PHE:N	1:J:1626:TRP:O	2.52	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:1684:ALA:HB1	2:K:89:GLY:HA3	2.01	0.43
1:J:4833:ASN:ND2	1:J:4939:ALA:HB2	2.33	0.43
1:J:4874:MET:HE2	1:J:4874:MET:HA	2.01	0.43
1:J:5017:ARG:CZ	1:J:5019:TRP:HH2	2.32	0.43
1:D:119:SER:OG	1:D:120:CYS:N	2.51	0.42
1:D:597:HIS:HB2	1:D:1665:HIS:ND1	2.33	0.42
1:D:1073:ARG:HB3	1:D:1075:PHE:CE1	2.54	0.42
1:D:1087:ARG:NH1	1:D:1221:GLU:O	2.52	0.42
1:D:1689:VAL:HA	1:D:1693:GLN:OE1	2.18	0.42
1:D:1713:ASP:O	1:D:1716:ILE:HG22	2.19	0.42
1:D:4581:LYS:HE2	1:D:4632:LEU:HB3	2.00	0.42
1:D:4701:TRP:CZ2	1:D:4781:GLY:HA3	2.54	0.42
1:D:4715:TYR:CE2	1:D:4717:ASP:HB2	2.54	0.42
1:A:1426:ILE:O	1:A:1430:THR:N	2.52	0.42
1:A:1849:LEU:CD2	1:A:1854:PHE:HD2	2.32	0.42
1:A:2123:LEU:O	1:A:2127:GLN:HG2	2.19	0.42
1:G:2548:LEU:O	1:G:2552:ARG:HG3	2.19	0.42
1:J:582:HIS:O	1:J:586:ILE:HG13	2.19	0.42
1:J:1931:LEU:HD12	1:J:1939:MET:HE1	2.00	0.42
1:J:2323:TRP:H	1:J:2323:TRP:CD1	2.37	0.42
1:J:2518:LEU:HD21	1:J:2569:PHE:HE1	1.79	0.42
1:J:2891:LYS:O	1:J:2892:GLN:C	2.60	0.42
1:J:4146:LEU:O	1:J:4150:LEU:HD23	2.19	0.42
1:J:4569:LEU:HD21	1:J:4649:LEU:HG	2.01	0.42
1:D:716:PHE:HE1	1:D:757:PHE:CG	2.36	0.42
1:D:1290:ARG:HD2	1:D:1291:LEU:O	2.20	0.42
1:D:2437:ALA:HB3	1:D:2508:ARG:HE	1.84	0.42
1:D:2879:ALA:HB2	1:D:2923:ALA:CB	2.49	0.42
1:A:637:LEU:HD23	1:A:1693:GLN:HA	2.01	0.42
1:A:1717:SER:HA	1:A:1721:GLU:HB2	2.01	0.42
1:A:2355:ARG:HA	1:A:2358:ILE:HG22	2.00	0.42
1:A:3701:LEU:HD11	1:A:3705:PHE:CZ	2.54	0.42
1:A:4154:VAL:O	1:A:4154:VAL:HG13	2.19	0.42
1:A:4683:PHE:HZ	1:A:5017:ARG:HG3	1.84	0.42
1:G:2102:VAL:HG13	1:G:2120:MET:CG	2.49	0.42
1:G:2240:CYS:SG	1:G:2250:MET:HG2	2.59	0.42
1:G:3886:ARG:HE	1:G:3890:LEU:HD11	1.85	0.42
1:G:3966:THR:O	1:G:3970:GLN:HG2	2.18	0.42
1:G:4655:PHE:CA	1:G:4796:MET:HE1	2.50	0.42
1:J:1727:ARG:HG3	1:J:1775:HIS:HE1	1.83	0.42
1:J:1936:LYS:HA	1:J:1939:MET:HE3	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:2918:ARG:O	1:J:2919:ASP:C	2.62	0.42
1:D:76:ARG:CZ	1:A:3844:LEU:HD23	2.49	0.42
1:D:2208:MET:HE1	1:D:2253:HIS:ND1	2.34	0.42
1:D:2821:TRP:HA	1:D:2939:ARG:N	2.34	0.42
1:D:4068:LEU:O	1:D:4072:VAL:HG23	2.20	0.42
1:D:4338:VAL:HG11	1:J:4838:VAL:HG11	2.01	0.42
2:E:56:ILE:HG23	2:E:59:PHE:H	1.83	0.42
1:A:517:GLU:O	1:A:521:LEU:HD13	2.19	0.42
1:A:1849:LEU:HD23	1:A:1854:PHE:HD2	1.85	0.42
1:A:2823:ILE:HA	1:A:2936:ALA:O	2.18	0.42
1:A:3007:ASN:HA	1:A:3010:PHE:CE1	2.54	0.42
1:A:4040:ILE:H	1:A:4040:ILE:HD12	1.83	0.42
1:G:1966:VAL:HG21	1:G:3649:ALA:HB1	2.02	0.42
1:J:345:LEU:HD23	1:J:387:ALA:HB1	2.00	0.42
1:J:3650:CYS:O	1:J:3654:LEU:HG	2.19	0.42
1:J:4851:TYR:HE2	1:J:4920:PHE:HA	1.84	0.42
3:L:66:PHE:O	3:L:70:LEU:HD23	2.19	0.42
1:D:535:ALA:O	1:D:539:LEU:HD23	2.20	0.42
1:D:1466:LEU:HD11	1:D:1496:TRP:HB2	2.02	0.42
1:D:2207:VAL:HG21	1:D:2235:PHE:CE2	2.54	0.42
1:D:2505:PHE:CE1	1:D:2509:VAL:HG21	2.54	0.42
1:D:3890:LEU:HA	1:D:3893:GLU:HB2	2.00	0.42
1:A:261:ARG:HB2	1:A:285:VAL:HG12	2.02	0.42
1:G:116:MET:SD	1:G:139:GLU:HA	2.59	0.42
1:G:575:LEU:HD22	1:G:609:CYS:SG	2.59	0.42
1:G:1072:VAL:HG23	1:G:1194:LEU:O	2.19	0.42
1:G:1099:GLU:HA	1:G:1127:HIS:ND1	2.34	0.42
1:G:2641:LEU:O	1:G:2644:LEU:HG	2.18	0.42
1:G:4180:ARG:HG2	1:G:4194:TYR:HE1	1.84	0.42
1:G:4184:MET:N	1:G:5021:PHE:O	2.48	0.42
1:J:839:LEU:HB3	1:J:1194:LEU:HD11	2.00	0.42
1:J:1259:ARG:NH1	1:J:1595:LEU:O	2.52	0.42
1:J:2335:LEU:O	1:J:2339:VAL:HG23	2.20	0.42
1:J:2918:ARG:C	1:J:2920:ARG:N	2.76	0.42
1:D:1235:THR:HG21	1:D:1607:ARG:HH21	1.85	0.42
1:D:3999:MET:HG3	1:D:4016:LEU:HD21	2.01	0.42
1:A:635:THR:CB	1:A:1693:GLN:HE22	2.29	0.42
1:A:645:ARG:HG3	1:A:778:PHE:CD1	2.54	0.42
1:A:3834:ALA:O	1:A:3838:THR:HG23	2.20	0.42
1:G:504:ALA:HB2	1:G:512:ALA:HB2	2.00	0.42
1:G:3955:MET:HE1	1:G:4016:LEU:HD13	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:2290:LEU:HD23	1:J:2291:GLN:O	2.19	0.42
1:J:4901:ILE:HG22	1:J:4902:GLU:O	2.19	0.42
1:D:14:LEU:HD23	1:D:14:LEU:HA	1.77	0.42
1:A:400:ALA:O	1:A:404:ILE:HG12	2.20	0.42
1:A:2273:LEU:HD23	1:A:2330:ARG:HB3	2.02	0.42
1:A:2453:ILE:HA	1:A:2456:ILE:HG22	2.02	0.42
1:A:3848:GLU:HA	1:A:3851:ASN:ND2	2.35	0.42
1:G:615:ARG:HD2	1:G:1678:ASN:HD21	1.84	0.42
1:G:4138:ASP:O	1:G:4142:ASN:ND2	2.44	0.42
1:G:4927:ILE:O	1:G:4931:ILE:HG13	2.18	0.42
1:J:2142:TYR:CD2	1:J:2197:LEU:HD12	2.54	0.42
1:J:2862:LEU:O	1:J:2863:SER:C	2.63	0.42
1:J:3829:PHE:CD2	1:J:3906:GLN:HG2	2.55	0.42
1:J:4218:ILE:HD12	1:J:4218:ILE:HA	1.95	0.42
1:D:110:ARG:HD3	1:D:115:ARG:HH21	1.84	0.42
1:D:283:ARG:HH21	1:D:288:GLY:HA2	1.84	0.42
1:D:1794:ALA:HA	1:D:1795:PRO:HD3	1.93	0.42
1:D:4104:THR:O	1:D:4108:ILE:N	2.50	0.42
1:A:1451:GLY:HA3	1:A:1494:MET:HA	2.01	0.42
1:A:2670:GLU:O	1:A:2674:LEU:HD23	2.20	0.42
1:A:4666:VAL:O	1:A:4670:ILE:HG12	2.20	0.42
1:G:638:ILE:HD12	1:G:702:TRP:CD1	2.54	0.42
1:G:716:PHE:HE1	1:G:757:PHE:CG	2.37	0.42
1:G:1130:GLN:HG3	1:G:1132:TRP:NE1	2.35	0.42
1:G:1936:LYS:HZ1	1:G:2105:TRP:CD1	2.37	0.42
1:G:2616:PRO:HG2	1:G:2664:PHE:CE2	2.55	0.42
1:G:2823:ILE:HA	1:G:2936:ALA:O	2.18	0.42
1:G:3798:LEU:O	1:G:3802:ILE:HG23	2.20	0.42
1:G:3889:GLN:O	1:G:3893:GLU:N	2.53	0.42
1:G:3943:ILE:HD11	1:G:4002:LYS:HZ1	1.84	0.42
1:J:1775:HIS:NE2	1:J:1851:MET:SD	2.92	0.42
1:D:1423:ASP:O	1:D:1427:ILE:HG12	2.20	0.42
1:D:3701:LEU:HD11	1:D:3705:PHE:CZ	2.55	0.42
1:A:3625:SER:OG	1:A:3626:LYS:N	2.53	0.42
1:A:4189:ARG:HA	1:A:5031:GLN:HE22	1.85	0.42
1:G:2670:GLU:HA	1:G:2673:HIS:HE1	1.80	0.42
1:G:4631:PHE:HZ	1:G:4639:MET:SD	2.42	0.42
1:J:3775:ALA:O	1:J:3779:VAL:HG23	2.20	0.42
1:J:4243:PHE:O	1:J:4247:ILE:HG13	2.20	0.42
1:J:4654:ALA:CB	1:J:4796:MET:HE1	2.35	0.42
1:D:4072:VAL:HA	1:D:4077:PHE:HD2	1.83	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1243:PRO:HB2	1:A:1600:LEU:HD11	2.02	0.42
1:A:2546:MET:HA	1:A:2546:MET:HE2	2.01	0.42
1:G:74:SER:HA	1:G:105:HIS:HD2	1.85	0.42
1:G:1763:PRO:HG2	1:G:1863:LEU:HD11	2.01	0.42
1:G:2698:MET:HE3	1:G:2698:MET:HB3	1.90	0.42
1:G:3965:LEU:O	1:G:3969:ILE:HG12	2.20	0.42
1:G:4805:ASN:ND2	1:G:4807:PHE:HB2	2.34	0.42
1:J:349:GLN:NE2	1:J:350:HIS:O	2.53	0.42
1:J:1844:LEU:O	1:J:1848:LEU:HD23	2.20	0.42
1:J:4668:LEU:CD2	1:J:4672:LYS:HE2	2.49	0.42
1:D:3768:SER:HA	1:D:3771:HIS:CE1	2.55	0.42
1:D:3768:SER:HA	1:D:3771:HIS:ND1	2.35	0.42
1:D:4214:LYS:HE2	1:D:4985:LEU:HD22	2.02	0.42
1:A:274:LEU:HB3	1:A:339:ILE:HD11	2.02	0.42
1:A:1103:GLY:HA2	1:A:1151:CYS:SG	2.59	0.42
1:A:2280:VAL:HG13	1:A:2280:VAL:O	2.20	0.42
1:A:4145:VAL:HG22	1:A:4178:LEU:HD13	2.02	0.42
1:A:4822:THR:O	1:A:4825:THR:OG1	2.28	0.42
1:G:1111:PRO:HG2	1:G:1603:VAL:HG13	2.02	0.42
1:G:1772:ARG:NH1	1:G:1952:GLN:HE22	2.18	0.42
1:G:1859:VAL:O	1:G:1863:LEU:HD23	2.20	0.42
1:G:4222:VAL:HG12	1:G:4950:VAL:HG22	2.02	0.42
1:J:119:SER:OG	1:J:120:CYS:N	2.53	0.42
1:J:548:VAL:HG11	1:J:582:HIS:ND1	2.35	0.42
1:J:3670:GLU:O	1:J:3674:ILE:HG12	2.20	0.42
1:J:3966:THR:O	1:J:3970:GLN:N	2.47	0.42
1:J:4686:LEU:HD11	1:J:4692:PRO:HA	2.02	0.42
1:D:530:ILE:HD11	1:D:563:VAL:HG13	2.01	0.41
1:D:714:TYR:HB3	1:D:768:PHE:CE2	2.55	0.41
1:D:2440:MET:HA	1:D:2443:ILE:HG22	2.01	0.41
1:A:681:HIS:CE1	1:A:683:ARG:HH21	2.37	0.41
1:A:2671:GLU:O	1:A:2675:THR:HG23	2.20	0.41
1:A:3675:ASP:O	1:A:3679:LYS:HG2	2.20	0.41
1:G:1648:MET:HE2	1:G:1648:MET:HB3	1.83	0.41
1:G:2179:ILE:HD11	1:G:2228:MET:HA	2.01	0.41
1:G:3756:LYS:HD2	1:G:3756:LYS:HA	1.89	0.41
1:G:4229:GLU:O	1:G:4233:LEU:HD23	2.20	0.41
1:J:112:ALA:HA	1:J:115:ARG:NH1	2.34	0.41
1:J:636:ASN:HB3	1:J:702:TRP:CZ3	2.54	0.41
1:J:1466:LEU:HD11	1:J:1496:TRP:HB2	2.01	0.41
1:J:1699:GLU:OE1	1:J:1699:GLU:N	2.53	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:2685:SER:O	1:J:2689:LYS:N	2.53	0.41
1:D:1087:ARG:HD3	1:D:1223:PHE:CE1	2.55	0.41
1:D:1863:LEU:HA	1:D:1866:ILE:HG22	2.02	0.41
1:D:2181:SER:O	1:D:2185:ILE:HG13	2.20	0.41
1:D:4204:GLN:HB3	1:D:4245:MET:HE2	2.02	0.41
1:A:645:ARG:HD2	1:A:649:PHE:HE1	1.84	0.41
1:A:4181:ILE:HD11	1:A:4193:ILE:HB	2.02	0.41
1:G:1076:ARG:O	1:G:1237:TRP:N	2.35	0.41
1:G:1126:GLY:HA3	1:G:1143:TRP:HE1	1.85	0.41
1:G:2470:ILE:HG22	1:G:2525:GLY:HA3	2.00	0.41
2:H:7:ILE:H	2:H:72:ALA:HA	1.84	0.41
1:J:178:ARG:NH1	1:J:193:ALA:O	2.46	0.41
1:J:461:HIS:CE1	1:J:3707:ARG:HG2	2.55	0.41
1:J:1152:MET:HE2	1:J:1152:MET:HA	2.03	0.41
1:J:1862:ILE:HD12	1:J:1865:MET:SD	2.60	0.41
1:J:2611:CYS:O	1:J:2614:ILE:HG22	2.21	0.41
1:D:1432:THR:HB	1:D:1572:ILE:HD12	2.02	0.41
1:D:1762:LEU:HD23	1:D:1762:LEU:HA	1.89	0.41
1:D:1810:LYS:CG	1:D:1814:MET:HE3	2.49	0.41
1:D:4658:ILE:HG13	1:D:4796:MET:SD	2.60	0.41
1:A:23:GLN:O	1:A:201:ASN:N	2.46	0.41
1:A:3776:ALA:O	1:A:3780:LEU:HD23	2.21	0.41
1:G:650:VAL:HG11	1:G:662:TRP:NE1	2.36	0.41
1:G:853:PRO:HB3	1:G:1023:PRO:HD3	2.01	0.41
1:G:1154:ASP:O	1:G:1158:ASN:N	2.53	0.41
1:G:2102:VAL:HG11	1:G:2124:LEU:HD22	2.02	0.41
1:J:1242:LEU:HD21	1:J:1458:HIS:CD2	2.55	0.41
1:J:1294:PRO:HB3	1:J:1549:PHE:CE1	2.55	0.41
1:J:1698:LEU:O	1:J:1708:ARG:NH1	2.40	0.41
1:J:2190:VAL:HA	1:J:2193:GLN:HB2	2.02	0.41
1:J:4013:LEU:O	1:J:4017:LEU:HD23	2.20	0.41
1:J:4844:LEU:HD12	1:J:4928:LEU:HB3	2.03	0.41
2:K:87:HIS:HD2	2:K:88:PRO:HD2	1.85	0.41
1:D:44:ASN:N	1:D:44:ASN:OD1	2.53	0.41
1:D:102:LEU:HB2	1:D:105:HIS:CE1	2.55	0.41
1:D:1965:TYR:OH	1:D:2027:ILE:O	2.30	0.41
1:D:2418:LEU:O	1:D:2422:ILE:HG12	2.21	0.41
1:D:3943:ILE:HD12	1:D:3943:ILE:HA	1.93	0.41
1:D:4888:TYR:OH	1:J:4913:ARG:NH1	2.53	0.41
1:A:663:TYR:OH	1:A:758:ARG:NH1	2.50	0.41
1:A:805:PRO:HB2	1:A:808:TYR:CD2	2.54	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1112:ASP:OD1	1:A:1113:VAL:N	2.53	0.41
1:A:1965:TYR:CE2	1:A:2031:LEU:HB2	2.56	0.41
1:A:2648:TYR:HD2	1:A:2706:ILE:HA	1.86	0.41
1:A:2960:LEU:HD11	1:A:3017:PHE:CZ	2.56	0.41
1:A:3768:SER:O	1:A:3772:THR:HG22	2.20	0.41
1:A:4851:TYR:HD2	1:A:4920:PHE:CD2	2.38	0.41
1:A:4914:VAL:HG23	1:G:4888:TYR:CD1	2.55	0.41
1:G:1290:ARG:HA	1:G:1551:ALA:HA	2.01	0.41
1:G:2172:PRO:O	1:G:2175:GLU:HG3	2.20	0.41
1:G:4085:ARG:HE	1:G:4085:ARG:HB2	1.67	0.41
2:H:16:PRO:HG2	2:H:64:ALA:HA	2.01	0.41
1:J:2172:PRO:O	1:J:2175:GLU:HG3	2.20	0.41
1:J:4863:TYR:HE1	1:J:4901:ILE:HG12	1.85	0.41
1:J:5000:GLU:HA	1:J:5003:HIS:CD2	2.55	0.41
1:D:1433:TYR:CE2	1:D:1578:ALA:HB2	2.55	0.41
1:D:1566:LEU:HD13	1:D:1566:LEU:HA	1.81	0.41
1:D:1658:ASP:N	1:D:1658:ASP:OD1	2.54	0.41
1:D:3805:LEU:HD21	1:D:3891:LEU:HD13	2.02	0.41
1:A:483:MET:O	1:A:487:VAL:HG23	2.20	0.41
1:A:2323:TRP:CH2	1:A:2422:ILE:HG13	2.54	0.41
1:A:2512:ILE:HG13	1:A:2512:ILE:O	2.21	0.41
1:A:4794:TRP:O	1:A:4798:MET:HG2	2.20	0.41
1:A:4922:PHE:HA	1:A:4926:VAL:HG12	2.01	0.41
1:G:839:LEU:HD13	1:G:1075:PHE:HD2	1.85	0.41
1:G:1760:HIS:CE1	1:G:2041:HIS:HA	2.55	0.41
1:G:2032:GLN:O	1:G:2036:GLN:HG2	2.19	0.41
1:G:2187:ASN:O	3:I:14:LYS:NZ	2.48	0.41
1:G:2512:ILE:HD12	1:G:2561:LEU:HD21	2.01	0.41
1:G:3817:LEU:HD11	1:G:3821:LYS:HE2	2.01	0.41
1:J:700:GLU:H	1:J:705:ASN:HD21	1.68	0.41
1:J:1426:ILE:O	1:J:1430:THR:OG1	2.29	0.41
1:J:2627:VAL:O	1:J:2631:PRO:HD3	2.20	0.41
1:D:682:LEU:HB3	1:D:738:LEU:HD12	2.02	0.41
1:D:1433:TYR:N	1:D:1520:VAL:O	2.42	0.41
1:D:1773:PRO:HA	1:D:2153:MET:HE1	2.03	0.41
1:D:4702:ASP:O	1:D:4705:VAL:HG12	2.20	0.41
1:A:1514:LEU:HD23	1:A:1514:LEU:H	1.85	0.41
1:A:2162:ILE:HD11	1:A:2178:MET:HE1	2.03	0.41
1:A:2203:MET:O	1:A:2207:VAL:HG23	2.21	0.41
1:A:3726:ALA:HA	1:A:3729:MET:HE3	2.02	0.41
1:G:1965:TYR:CE2	1:G:2031:LEU:HB2	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:4958:CYS:HA	6:G:5103:ATP:N7	2.36	0.41
2:H:10:GLY:O	2:H:11:ASP:C	2.62	0.41
1:J:287:THR:HB	1:J:289:ARG:HH11	1.85	0.41
1:J:337:PRO:O	1:J:339:ILE:HD12	2.21	0.41
1:J:1229:ASN:HB2	1:J:1827:ARG:NE	2.36	0.41
1:J:3875:MET:N	1:J:3875:MET:SD	2.93	0.41
1:J:3927:GLN:NE2	1:J:3991:GLY:HA3	2.33	0.41
1:J:4040:ILE:HD12	1:J:4040:ILE:H	1.86	0.41
1:J:4922:PHE:HA	1:J:4926:VAL:HG12	2.03	0.41
3:L:6:THR:HG23	3:L:9:GLN:H	1.84	0.41
1:D:1237:TRP:CH2	1:D:1652:GLU:HG3	2.54	0.41
1:D:2215:LEU:HD23	1:D:2215:LEU:HA	1.88	0.41
1:A:3916:ILE:HG13	1:A:3980:LEU:HD21	2.02	0.41
1:A:4031:LEU:HD23	1:A:4044:MET:HE1	2.01	0.41
1:G:2039:LEU:HD23	1:G:2039:LEU:HA	1.93	0.41
1:G:2467:VAL:HG22	1:G:2524:VAL:HG11	2.03	0.41
1:J:551:LEU:HD11	1:J:589:LEU:HD22	2.02	0.41
1:J:1095:VAL:O	1:J:1145:SER:OG	2.31	0.41
1:J:1112:ASP:OD1	1:J:1113:VAL:N	2.53	0.41
1:J:1454:THR:HG22	1:J:1491:ASN:O	2.19	0.41
1:J:2500:ALA:N	1:J:2553:TYR:CE1	2.87	0.41
2:K:7:ILE:H	2:K:72:ALA:HA	1.86	0.41
1:D:668:VAL:O	1:D:741:GLU:N	2.51	0.41
1:D:1804:LEU:HD21	1:D:1853:ILE:HD13	2.01	0.41
1:D:2570:ALA:HB2	1:D:2613:TYR:O	2.21	0.41
1:D:3723:MET:SD	1:D:3792:ALA:HB1	2.61	0.41
1:A:626:LEU:N	1:A:627:PRO:HD2	2.36	0.41
1:A:2346:VAL:HG21	1:A:2349:ASN:HD22	1.84	0.41
1:A:2463:LEU:HD21	1:A:2517:PHE:CE1	2.55	0.41
1:A:3731:LYS:O	1:A:3731:LYS:HG2	2.21	0.41
1:A:3768:SER:HA	1:A:3771:HIS:CE1	2.55	0.41
1:A:4701:TRP:CZ2	1:A:4781:GLY:HA3	2.56	0.41
2:B:38:SER:H	2:B:42:ARG:HH21	1.69	0.41
1:G:265:LEU:HD22	1:G:279:PRO:O	2.21	0.41
1:G:636:ASN:ND2	1:G:637:LEU:H	2.18	0.41
1:G:1449:TRP:O	1:G:1552:VAL:HG13	2.21	0.41
1:G:1514:LEU:H	1:G:1514:LEU:HD23	1.86	0.41
1:G:2654:TYR:HA	1:G:2660:GLY:HA2	2.02	0.41
2:H:56:ILE:HD13	2:H:81:ALA:HB1	2.02	0.41
1:J:2355:ARG:HA	1:J:2358:ILE:HG22	2.01	0.41
1:J:2512:ILE:HD12	1:J:2518:LEU:HD12	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:559:GLY:O	1:D:563:VAL:HG23	2.21	0.41
1:D:1500:PHE:CE2	1:D:1531:ALA:HB3	2.56	0.41
1:D:1569:GLN:CB	1:D:1572:ILE:HB	2.51	0.41
1:D:2309:SER:HA	1:D:2324:ASN:HB3	2.02	0.41
1:D:2638:LYS:CE	1:D:2695:LEU:HA	2.50	0.41
1:D:4823:LEU:HD11	1:J:4843:LEU:HB2	2.02	0.41
1:D:5019:TRP:CD1	1:D:5022:PHE:HE2	2.39	0.41
1:A:337:PRO:HB2	1:A:338:GLU:H	1.77	0.41
1:A:1204:LEU:HD23	1:A:1204:LEU:HA	1.96	0.41
1:A:1301:PHE:HB2	1:A:1523:ALA:O	2.21	0.41
1:A:2442:LEU:HD22	1:A:2447:LYS:HD2	2.03	0.41
1:A:2463:LEU:HB2	1:A:2510:TYR:CE2	2.56	0.41
1:G:401:ALA:O	1:G:404:ILE:HG22	2.21	0.41
1:G:564:LEU:O	1:G:568:LEU:HD23	2.21	0.41
1:G:615:ARG:HD2	1:G:1678:ASN:ND2	2.36	0.41
1:G:685:GLY:C	1:G:686:TRP:HD1	2.28	0.41
1:G:691:GLY:HA3	1:G:712:TYR:CG	2.56	0.41
1:G:3699:HIS:HB2	1:G:3773:ARG:HD2	2.02	0.41
1:G:3780:LEU:HB2	1:G:3816:MET:HE3	2.03	0.41
1:G:4020:GLN:HG3	1:G:4139:ILE:HD11	2.02	0.41
1:G:4914:VAL:HG11	1:J:4884:LEU:HD11	2.01	0.41
1:J:288:GLY:HA3	1:J:405:HIS:CE1	2.56	0.41
1:J:311:ALA:HA	1:J:350:HIS:NE2	2.36	0.41
1:J:484:LEU:HD12	1:J:485:SER:N	2.36	0.41
1:J:1514:LEU:HD23	1:J:1514:LEU:H	1.85	0.41
1:J:1783:VAL:O	2:K:56:ILE:HG23	2.21	0.41
1:J:2477:PRO:HB3	1:J:2487:GLN:HA	2.02	0.41
1:J:3927:GLN:HB2	1:J:3992:PHE:CE1	2.55	0.41
1:J:3986:TRP:O	1:J:3989:VAL:HG12	2.21	0.41
1:J:4093:PHE:CE2	1:J:4097:MET:HE1	2.56	0.41
1:J:4555:LEU:HD21	1:J:4656:LEU:HG	2.02	0.41
1:J:4639:MET:HA	1:J:4642:ALA:HB3	2.03	0.41
2:K:7:ILE:HD11	2:K:73:LYS:HB2	2.02	0.41
1:D:2230:THR:HB	1:D:2270:SER:HB2	2.03	0.41
1:A:1712:TYR:CD2	1:A:1840:PRO:HB2	2.56	0.41
1:A:2159:LEU:CD2	1:A:2201:LEU:HD23	2.50	0.41
1:G:1130:GLN:HA	1:G:1139:PHE:H	1.86	0.41
1:G:1515:VAL:O	1:G:1515:VAL:HG23	2.21	0.41
1:J:223:PHE:CD1	1:J:230:CYS:HB3	2.52	0.41
1:J:308:HIS:HB2	1:J:311:ALA:HB3	2.02	0.41
1:J:1851:MET:HE2	1:J:1851:MET:HB2	1.98	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:2368:LEU:HD21	1:J:2376:LEU:HD12	2.01	0.41
1:J:2377:LEU:HD11	1:J:2468:GLY:HA3	2.02	0.41
1:J:3851:ASN:OD1	1:J:3852:LYS:N	2.54	0.41
1:D:491:ILE:HG12	1:D:523:TYR:CE1	2.55	0.40
1:D:561:LEU:HD21	1:D:599:VAL:HG23	2.03	0.40
1:D:614:VAL:HG23	1:D:617:ASN:HB2	2.02	0.40
1:D:698:GLY:HA3	1:D:1647:CYS:O	2.21	0.40
1:D:3934:TYR:CD2	1:D:3995:VAL:HG23	2.56	0.40
1:D:4661:TYR:CE1	1:D:4665:LYS:HD2	2.56	0.40
3:F:1:MET:O	3:F:5:LEU:HG	2.20	0.40
1:A:2159:LEU:HA	1:A:2162:ILE:HG22	2.03	0.40
1:A:4879:MET:O	1:A:4883:TYR:HB2	2.21	0.40
1:G:178:ARG:HB2	1:G:193:ALA:HB1	2.04	0.40
1:G:681:HIS:NE2	1:G:683:ARG:HG3	2.35	0.40
1:G:725:HIS:O	1:G:725:HIS:CG	2.73	0.40
1:G:3701:LEU:HD11	1:G:3705:PHE:CZ	2.56	0.40
1:G:4088:ILE:HG22	1:G:4125:PHE:HD2	1.86	0.40
1:J:169:LEU:HB3	1:J:202:MET:HE1	2.04	0.40
1:J:2819:TRP:O	1:J:2820:GLU:CB	2.69	0.40
1:J:3829:PHE:CE2	1:J:3906:GLN:HG3	2.57	0.40
1:D:415:ILE:HD13	1:D:490:CYS:HA	2.03	0.40
1:D:662:TRP:CH2	1:D:814:ALA:HB2	2.56	0.40
1:D:1105:ALA:HA	1:D:1121:ALA:HA	2.02	0.40
1:D:1716:ILE:HD11	1:D:1847:THR:OG1	2.21	0.40
1:D:2003:GLN:O	1:D:2007:ASN:ND2	2.43	0.40
1:D:4579:PHE:O	1:D:4632:LEU:HG	2.21	0.40
1:D:4732:PHE:CD2	1:D:4737:ILE:HD11	2.46	0.40
1:A:2155:LEU:HB2	1:A:2188:ASN:HD22	1.85	0.40
1:A:3695:PRO:HB2	1:A:3699:HIS:HB3	2.02	0.40
1:A:4150:LEU:HD23	1:A:4150:LEU:HA	1.96	0.40
1:G:600:LEU:HD23	1:G:1665:HIS:HB3	2.02	0.40
1:G:839:LEU:HD13	1:G:1075:PHE:CD2	2.56	0.40
1:G:1848:LEU:HB3	1:G:1854:PHE:HE2	1.85	0.40
1:G:1929:MET:HE3	1:G:1929:MET:HB2	1.89	0.40
1:J:347:PHE:CE1	1:J:387:ALA:HA	2.56	0.40
1:J:1155:LEU:HD12	1:J:1184:ILE:HG23	2.02	0.40
1:J:4204:GLN:HB3	1:J:4245:MET:HE3	2.04	0.40
2:K:74:LEU:O	2:K:99:PHE:N	2.37	0.40
1:D:1243:PRO:HB2	1:D:1600:LEU:HD11	2.02	0.40
1:D:1949:GLN:OE1	1:D:1952:GLN:NE2	2.55	0.40
1:D:2630:VAL:N	1:D:2631:PRO:HD2	2.37	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4067:LYS:O	1:D:4071:ILE:HG12	2.20	0.40
1:D:4217:PHE:CZ	1:D:4234:PHE:HA	2.57	0.40
1:D:4651:THR:OG1	1:D:4803:HIS:NE2	2.43	0.40
1:A:42:PHE:HA	1:A:447:ASP:OD2	2.21	0.40
1:A:449:ILE:HD11	1:A:524:GLU:C	2.46	0.40
1:A:502:HIS:CE1	1:A:506:TYR:CE2	3.09	0.40
1:A:1449:TRP:N	1:A:1553:PHE:O	2.54	0.40
1:A:1929:MET:HE3	1:A:1929:MET:HB2	1.94	0.40
1:A:2299:VAL:HG21	1:A:2356:LEU:HD13	2.03	0.40
1:A:2773:ASN:O	1:A:2774:ASN:CB	2.70	0.40
1:A:3722:TYR:CZ	1:A:3782:MET:SD	3.14	0.40
1:A:4247:ILE:O	1:A:4251:ILE:HG12	2.21	0.40
2:B:83:GLY:C	2:B:85:THR:H	2.30	0.40
1:G:567:VAL:HG13	1:G:568:LEU:HD22	2.03	0.40
1:G:2679:PHE:CE1	1:G:2703:LEU:HA	2.56	0.40
1:G:4551:PHE:CD2	1:G:4552:LEU:HD12	2.56	0.40
1:J:172:VAL:HG22	1:J:179:TYR:CE2	2.56	0.40
1:J:596:ASN:HD21	1:J:599:VAL:HG23	1.86	0.40
1:J:771:PHE:HB3	1:J:1472:VAL:HG23	2.03	0.40
1:J:3962:PHE:CZ	1:J:3992:PHE:CE2	3.09	0.40
1:J:4049:VAL:HG21	1:J:4159:ARG:HD2	2.04	0.40
1:J:4716:TRP:CZ3	1:J:4717:ASP:HB2	2.57	0.40
1:D:692:TYR:CZ	1:D:694:PRO:HG3	2.57	0.40
1:D:979:PRO:HB2	1:D:980:ALA:H	1.66	0.40
1:D:1782:PHE:CE1	2:E:90:VAL:HG21	2.56	0.40
1:D:2310:CYS:SG	1:D:2312:MET:HB3	2.62	0.40
1:D:2773:ASN:O	1:D:2774:ASN:CB	2.70	0.40
1:D:4577:LEU:HD21	1:D:4807:PHE:HA	2.02	0.40
1:A:347:PHE:CZ	1:A:387:ALA:HB2	2.56	0.40
1:A:636:ASN:HB3	1:A:702:TRP:HE1	1.85	0.40
1:A:2182:ILE:HA	1:A:2185:ILE:HG22	2.02	0.40
1:A:2208:MET:HE1	1:A:2253:HIS:ND1	2.37	0.40
1:A:4648:LEU:HD22	1:A:4803:HIS:HE1	1.85	0.40
1:G:38:ALA:HB2	1:G:65:CYS:SG	2.61	0.40
1:G:1433:TYR:CE1	1:G:1578:ALA:HB2	2.56	0.40
1:G:2346:VAL:HG23	1:G:2349:ASN:HB2	2.04	0.40
3:I:5:LEU:HD11	3:I:74:ALA:HA	2.04	0.40
1:J:1124:PHE:CE1	1:J:1140:GLY:HA3	2.56	0.40
1:J:2236:LEU:HD23	1:J:2236:LEU:HA	1.94	0.40
1:J:3882:GLN:HG3	1:J:3960:GLN:HG3	2.04	0.40
1:J:4336:TRP:CH2	1:J:4568:PHE:HB2	2.56	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:4692:PRO:HG2	1:J:4703:ARG:NH2	2.36	0.40
1:D:61:ASP:HB3	1:D:283:ARG:HH12	1.87	0.40
1:D:1738:LEU:HB2	1:D:2146:PRO:HG3	2.03	0.40
1:D:4093:PHE:CZ	1:D:4097:MET:HE1	2.57	0.40
1:A:3892:CYS:SG	1:A:3903:LEU:HD12	2.61	0.40
1:A:4235:VAL:HG21	1:A:5019:TRP:CE2	2.57	0.40
1:G:264:PRO:HG2	1:G:270:SER:O	2.22	0.40
1:G:639:ASN:HA	1:G:1635:THR:HA	2.03	0.40
1:G:1707:LEU:HD23	1:G:1707:LEU:HA	1.80	0.40
1:G:1784:ALA:O	2:H:82:TYR:OH	2.37	0.40
1:G:3845:ASN:O	1:G:3849:ARG:HG3	2.22	0.40
1:G:4562:LEU:HG	1:G:4653:VAL:HG13	2.03	0.40
3:I:17:PHE:CE1	3:I:28:ILE:HD12	2.57	0.40
1:J:864:PRO:HA	1:J:865:PRO:HD3	1.98	0.40
1:J:1794:ALA:HA	1:J:1795:PRO:HD3	1.94	0.40
1:J:2577:ILE:HD12	1:J:2577:ILE:H	1.86	0.40
1:J:4020:GLN:HG3	1:J:4139:ILE:HD11	2.03	0.40
1:J:4060:LYS:HE3	1:J:4064:MET:HE3	2.02	0.40
1:J:4093:PHE:O	1:J:4097:MET:HE3	2.21	0.40
1:J:4658:ILE:HG13	1:J:4796:MET:SD	2.61	0.40
1:J:4897:ILE:O	1:J:4901:ILE:HG13	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	A	3853/5037 (76%)	3782 (98%)	68 (2%)	3 (0%)	48	80
1	D	3852/5037 (76%)	3792 (98%)	60 (2%)	0	100	100
1	G	3854/5037 (76%)	3797 (98%)	57 (2%)	0	100	100
1	J	3853/5037 (76%)	3778 (98%)	75 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	105/107 (98%)	102 (97%)	3 (3%)	0	100	100
2	E	105/107 (98%)	103 (98%)	2 (2%)	0	100	100
2	H	105/107 (98%)	100 (95%)	5 (5%)	0	100	100
2	K	105/107 (98%)	104 (99%)	1 (1%)	0	100	100
3	C	132/149 (89%)	131 (99%)	1 (1%)	0	100	100
3	F	132/149 (89%)	131 (99%)	1 (1%)	0	100	100
3	I	132/149 (89%)	131 (99%)	1 (1%)	0	100	100
3	L	131/149 (88%)	128 (98%)	3 (2%)	0	100	100
All	All	16359/21172 (77%)	16079 (98%)	277 (2%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	337	PRO
1	A	2859	PRO
1	A	2857	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	2211/4276 (52%)	2201 (100%)	10 (0%)	81	81
1	D	2042/4276 (48%)	2020 (99%)	22 (1%)	65	73
1	G	1596/4276 (37%)	1581 (99%)	15 (1%)	70	75
1	J	2139/4276 (50%)	2130 (100%)	9 (0%)	84	83
2	B	68/88 (77%)	68 (100%)	0	100	100
2	E	68/88 (77%)	68 (100%)	0	100	100
2	H	68/88 (77%)	68 (100%)	0	100	100
2	K	65/88 (74%)	65 (100%)	0	100	100
3	C	11/123 (9%)	11 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	F	9/123 (7%)	9 (100%)	0	100	100
3	I	13/123 (11%)	13 (100%)	0	100	100
3	L	15/123 (12%)	15 (100%)	0	100	100
All	All	8305/17948 (46%)	8249 (99%)	56 (1%)	73	78

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	1426	ILE
1	D	1427	ILE
1	D	1566	LEU
1	D	2123	LEU
1	D	2503	VAL
1	D	2506	LEU
1	D	2517	PHE
1	D	2518	LEU
1	D	2519	LEU
1	D	2522	LEU
1	D	2563	THR
1	D	2577	ILE
1	D	2581	SER
1	D	3679	LYS
1	D	3721	LEU
1	D	3723	MET
1	D	3728	ILE
1	D	4567	LEU
1	D	4569	LEU
1	D	4581	LYS
1	D	4672	LYS
1	D	4677	LEU
1	A	1693	GLN
1	A	1695	LEU
1	A	1698	LEU
1	A	3721	LEU
1	A	3725	TYR
1	A	3727	ASP
1	A	3728	ILE
1	A	3731	LYS
1	A	3841	VAL
1	A	3845	ASN
1	G	3673	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	3674	ILE
1	G	3679	LYS
1	G	3721	LEU
1	G	3723	MET
1	G	3727	ASP
1	G	3728	ILE
1	G	3763	LEU
1	G	3764	LEU
1	G	3768	SER
1	G	4790	LEU
1	G	4792	LEU
1	G	4796	MET
1	G	4800	LEU
1	G	4801	LEU
1	J	2504	LEU
1	J	2506	LEU
1	J	2509	VAL
1	J	3899	PHE
1	J	3903	LEU
1	J	3905	THR
1	J	3907	THR
1	J	3910	THR
1	J	3911	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (148) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	79	GLN
1	D	105	HIS
1	D	203	ASN
1	D	405	HIS
1	D	461	HIS
1	D	489	ASN
1	D	502	HIS
1	D	533	ASN
1	D	593	HIS
1	D	1125	ASN
1	D	1158	ASN
1	D	1231	GLN
1	D	1563	GLN
1	D	1586	ASN
1	D	1590	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	1640	HIS
1	D	1691	GLN
1	D	1696	HIS
1	D	1719	HIS
1	D	2092	GLN
1	D	2125	HIS
1	D	2161	GLN
1	D	2194	HIS
1	D	2487	GLN
1	D	3647	HIS
1	D	3761	GLN
1	D	3781	GLN
1	D	3851	ASN
1	D	3901	ASN
1	D	3909	ASN
1	D	3994	HIS
1	D	3998	HIS
1	D	4020	GLN
1	D	4149	ASN
1	D	4153	HIS
1	D	4204	GLN
1	D	4558	ASN
1	D	4574	ASN
1	D	4978	HIS
2	E	65	GLN
2	E	94	ASN
1	A	203	ASN
1	A	218	HIS
1	A	308	HIS
1	A	412	ASN
1	A	465	GLN
1	A	495	ASN
1	A	502	HIS
1	A	536	ASN
1	A	617	ASN
1	A	720	HIS
1	A	1165	ASN
1	A	1274	HIS
1	A	1299	GLN
1	A	1563	GLN
1	A	1590	GLN
1	A	1631	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1683	HIS
1	A	1693	GLN
1	A	1702	HIS
1	A	1719	HIS
1	A	1972	ASN
1	A	2107	GLN
1	A	2260	ASN
1	A	2284	ASN
1	A	2417	HIS
1	A	2551	ASN
1	A	3647	HIS
1	A	3889	GLN
1	A	3895	HIS
1	A	3900	GLN
1	A	3960	GLN
1	A	4054	ASN
1	A	4201	ASN
1	A	4558	ASN
1	A	4574	ASN
1	A	4650	HIS
1	A	4728	HIS
1	A	4806	ASN
1	A	5006	GLN
2	B	25	HIS
2	B	32	ASN
2	B	43	ASN
1	G	151	HIS
1	G	190	GLN
1	G	383	HIS
1	G	412	ASN
1	G	461	HIS
1	G	502	HIS
1	G	634	GLN
1	G	838	HIS
1	G	993	HIS
1	G	1127	HIS
1	G	1158	ASN
1	G	1491	ASN
1	G	1537	ASN
1	G	1563	GLN
1	G	2515	GLN
1	G	3651	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	3837	GLN
1	G	3882	GLN
1	G	3889	GLN
1	G	3895	HIS
1	G	3900	GLN
1	G	4009	GLN
1	G	4574	ASN
1	G	5006	GLN
2	H	87	HIS
1	J	23	GLN
1	J	151	HIS
1	J	308	HIS
1	J	349	GLN
1	J	383	HIS
1	J	399	GLN
1	J	412	ASN
1	J	576	ASN
1	J	618	GLN
1	J	634	GLN
1	J	678	GLN
1	J	705	ASN
1	J	720	HIS
1	J	797	HIS
1	J	1127	HIS
1	J	1158	ASN
1	J	1254	HIS
1	J	1274	HIS
1	J	1298	HIS
1	J	1598	GLN
1	J	1678	ASN
1	J	1702	HIS
1	J	1953	HIS
1	J	2107	GLN
1	J	2127	GLN
1	J	2260	ASN
1	J	2284	ASN
1	J	2584	HIS
1	J	2599	GLN
1	J	3013	HIS
1	J	3761	GLN
1	J	3781	GLN
1	J	3909	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	3994	HIS
1	J	3998	HIS
1	J	4020	GLN
1	J	4043	GLN
1	J	4209	GLN
1	J	4728	HIS
2	K	43	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 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	$\# Z > 2$
4	CFF	G	5101	-	15,15,15	0.61	0	23,23,23	0.49	0
4	CFF	J	5101	-	15,15,15	0.62	0	23,23,23	0.47	0
4	CFF	D	5101	-	15,15,15	0.62	0	23,23,23	0.47	0
6	ATP	D	5103	-	32,33,33	0.26	0	48,52,52	0.30	0
6	ATP	A	5103	-	32,33,33	0.26	0	48,52,52	0.31	0
6	ATP	G	5103	-	32,33,33	0.26	0	48,52,52	0.34	0
6	ATP	J	5103	-	32,33,33	0.27	0	48,52,52	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	CFF	A	5101	-	15,15,15	0.62	0	23,23,23	0.47	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CFF	G	5101	-	-	-	0/2/2/2
4	CFF	J	5101	-	-	-	0/2/2/2
4	CFF	D	5101	-	-	-	0/2/2/2
6	ATP	D	5103	-	-	9/22/38/38	0/3/3/3
6	ATP	A	5103	-	-	5/22/38/38	0/3/3/3
6	ATP	G	5103	-	-	7/22/38/38	0/3/3/3
6	ATP	J	5103	-	-	9/22/38/38	0/3/3/3
4	CFF	A	5101	-	-	-	0/2/2/2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	D	5103	ATP	PB-O3B-PG-O3G
6	D	5103	ATP	C5'-O5'-PA-O1A
6	D	5103	ATP	C5'-O5'-PA-O3A
6	G	5103	ATP	O4'-C4'-C5'-O5'
6	G	5103	ATP	O4'-C1'-N9-C8
6	G	5103	ATP	O4'-C1'-N9-C4
6	J	5103	ATP	PB-O3B-PG-O2G
6	J	5103	ATP	C5'-O5'-PA-O3A
6	G	5103	ATP	C3'-C4'-C5'-O5'
6	A	5103	ATP	O4'-C1'-N9-C4
6	J	5103	ATP	C3'-C4'-C5'-O5'
6	A	5103	ATP	O4'-C1'-N9-C8
6	D	5103	ATP	PB-O3B-PG-O1G
6	G	5103	ATP	C4'-C5'-O5'-PA
6	J	5103	ATP	PB-O3A-PA-O5'
6	J	5103	ATP	PB-O3B-PG-O3G
6	D	5103	ATP	C3'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

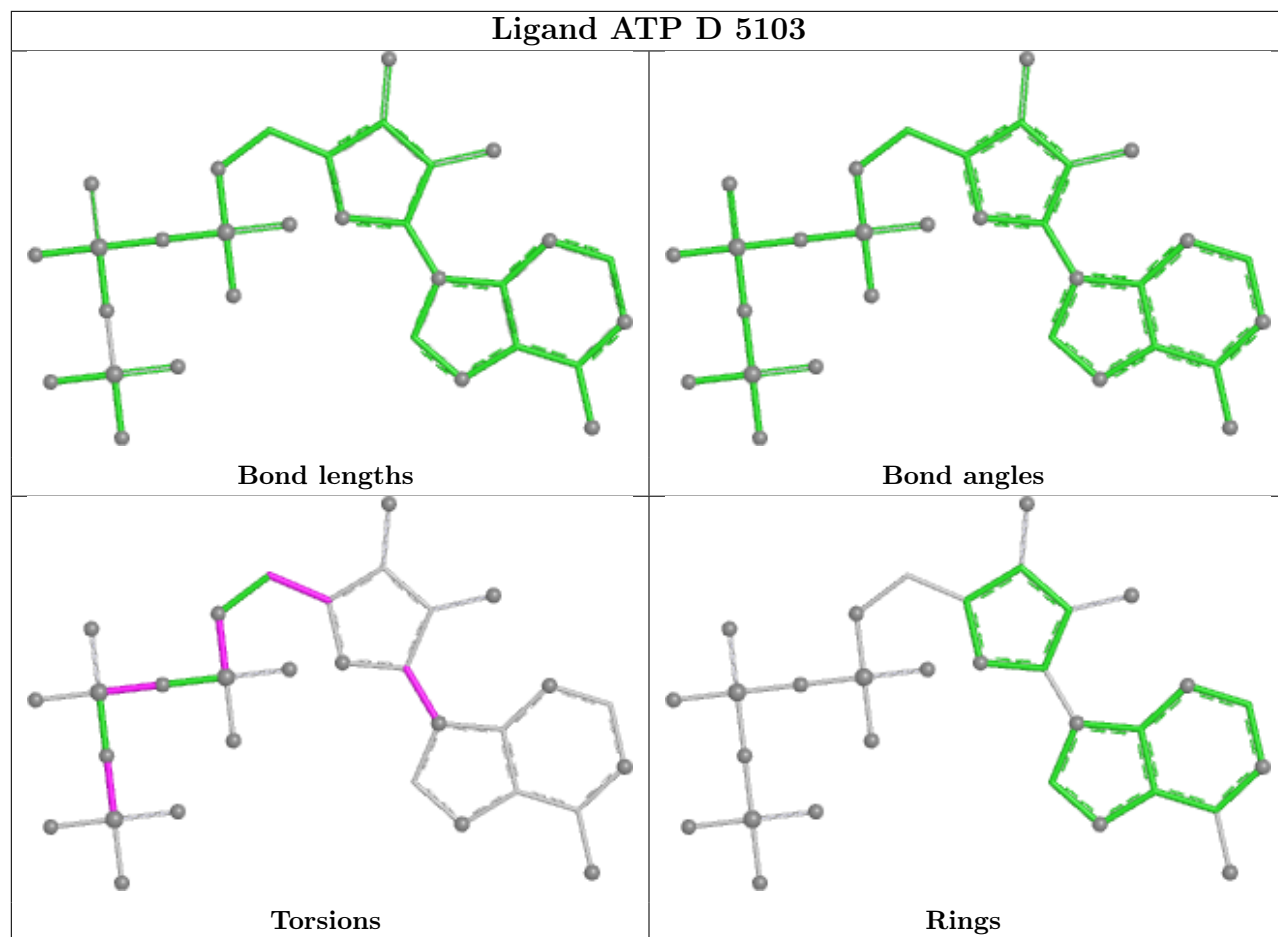
Mol	Chain	Res	Type	Atoms
6	G	5103	ATP	PG-O3B-PB-O2B
6	A	5103	ATP	C3'-C4'-C5'-O5'
6	A	5103	ATP	C5'-O5'-PA-O1A
6	J	5103	ATP	C5'-O5'-PA-O1A
6	D	5103	ATP	O4'-C1'-N9-C8
6	D	5103	ATP	O4'-C1'-N9-C4
6	D	5103	ATP	O4'-C4'-C5'-O5'
6	J	5103	ATP	O4'-C4'-C5'-O5'
6	D	5103	ATP	PA-O3A-PB-O2B
6	J	5103	ATP	PB-O3A-PA-O1A
6	A	5103	ATP	O4'-C4'-C5'-O5'
6	J	5103	ATP	PB-O3B-PG-O1G
6	G	5103	ATP	PG-O3B-PB-O1B

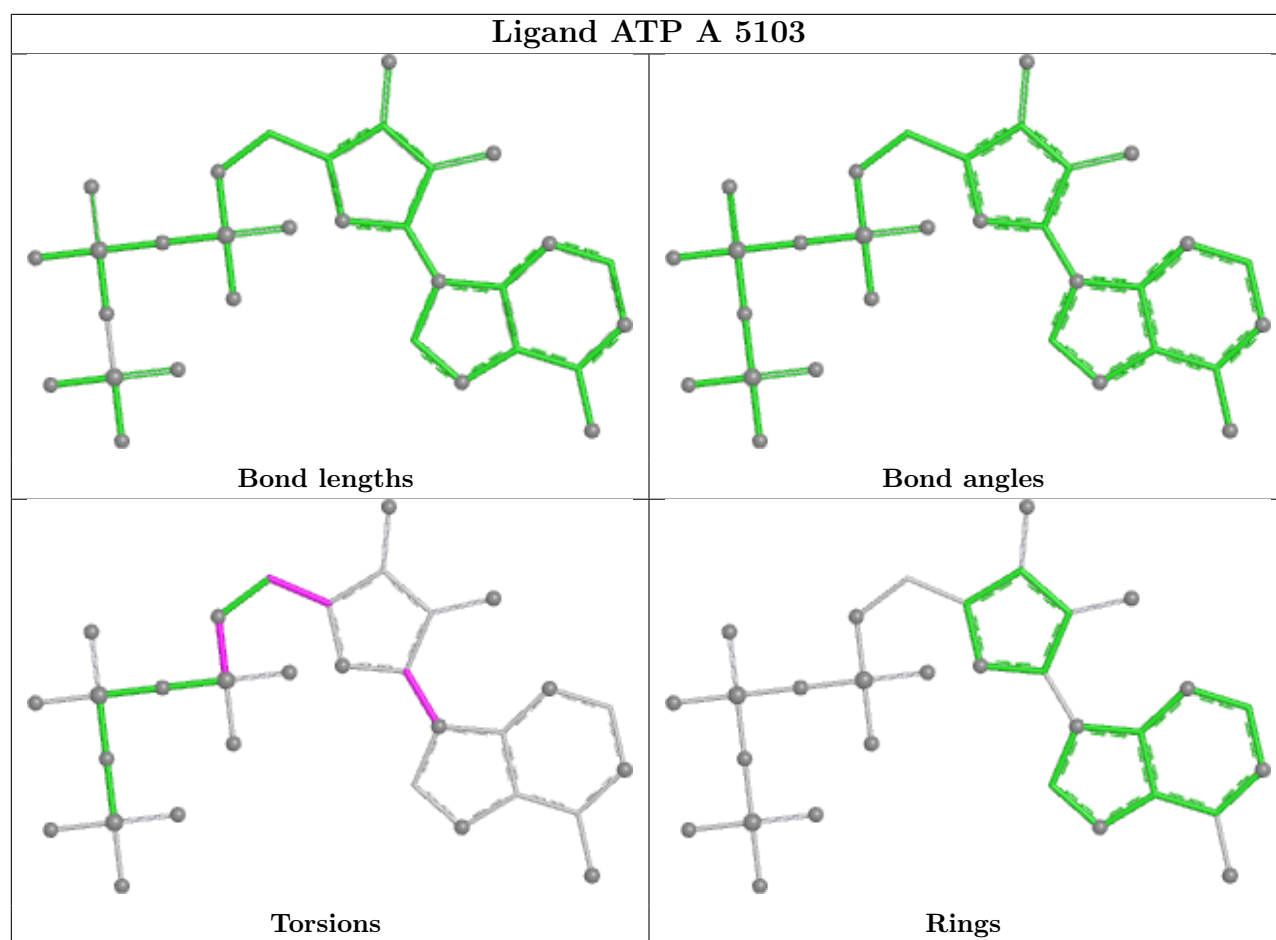
There are no ring outliers.

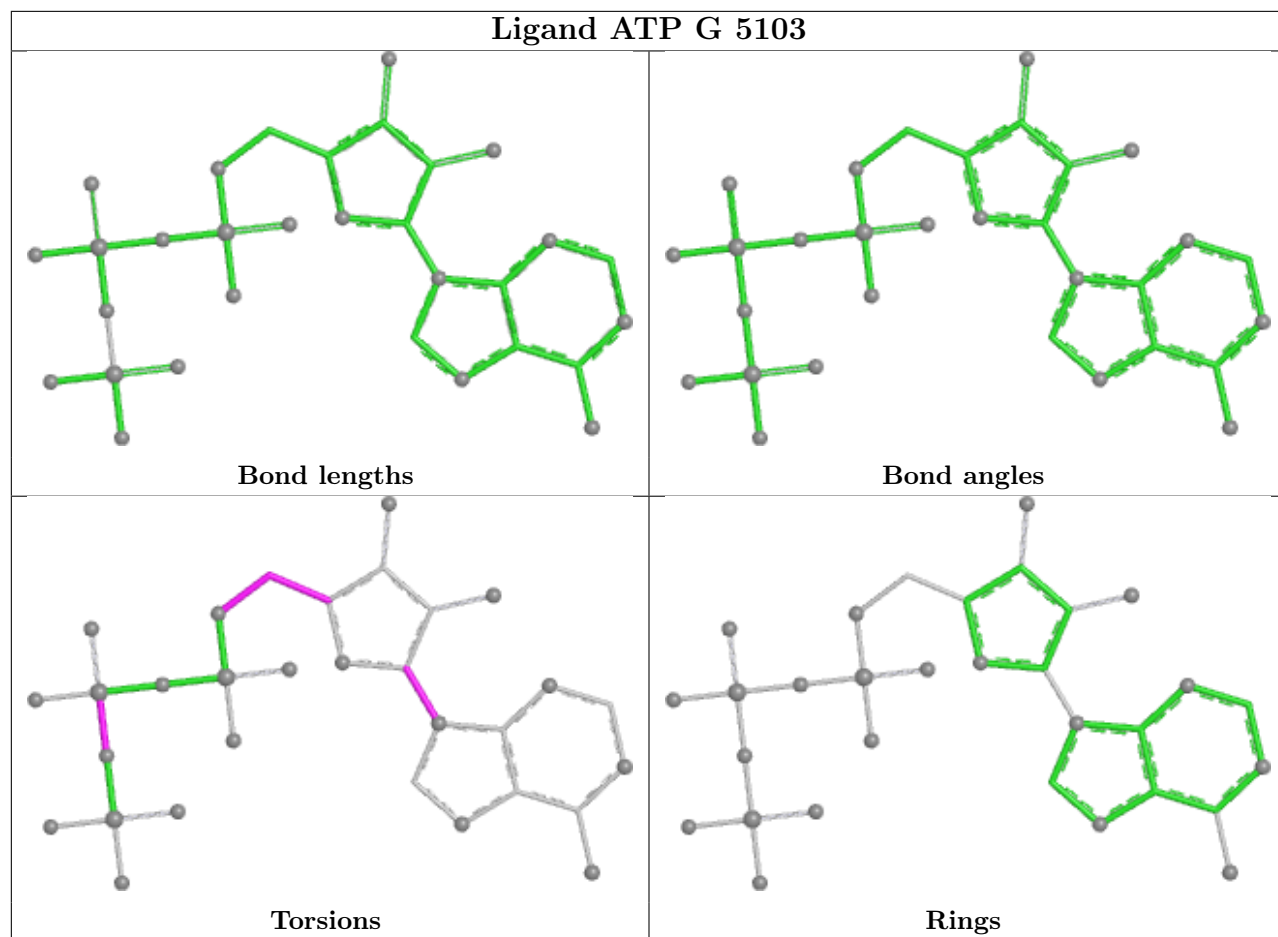
3 monomers are involved in 8 short contacts:

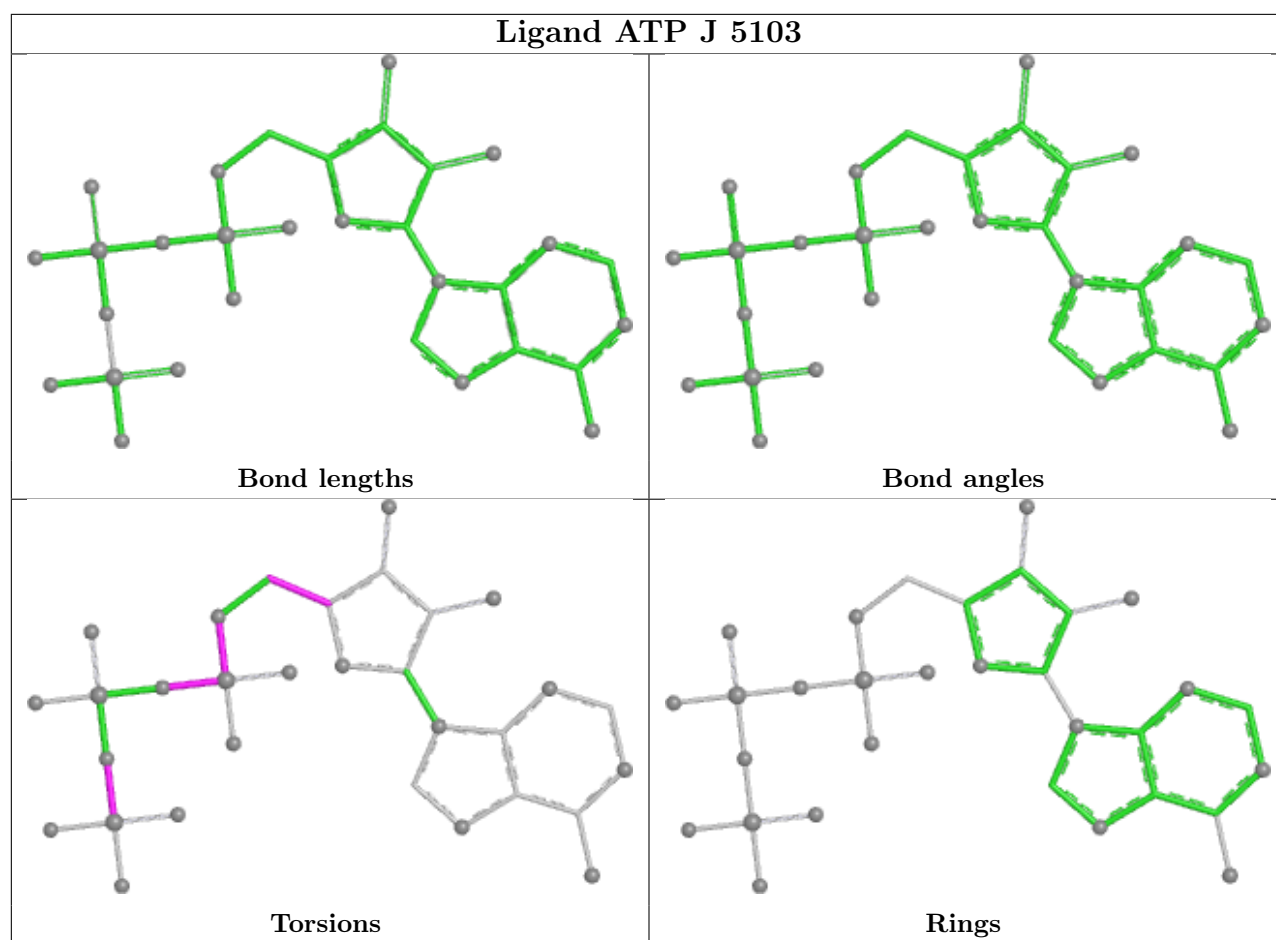
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	5103	ATP	2	0
6	G	5103	ATP	4	0
6	J	5103	ATP	2	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

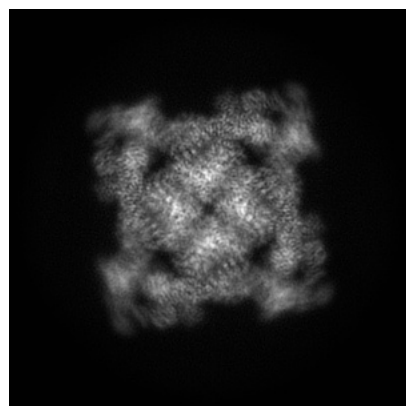
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-27736. These allow visual inspection of the internal detail of the map and identification of artifacts.

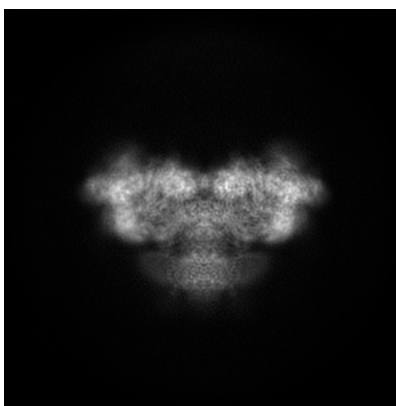
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

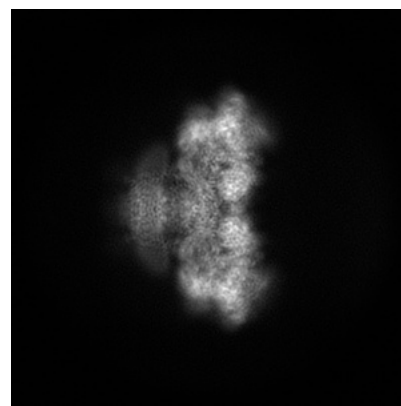
6.1.1 Primary map



X

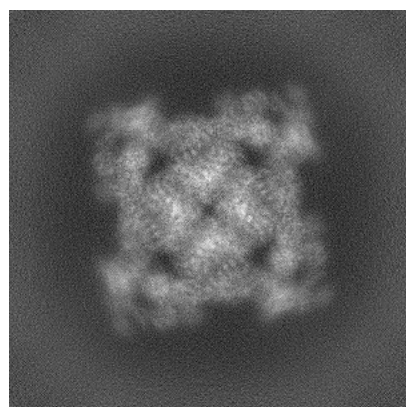


Y

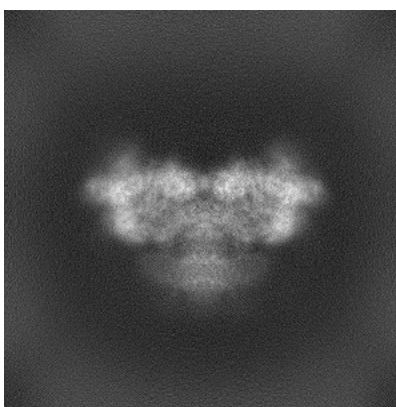


Z

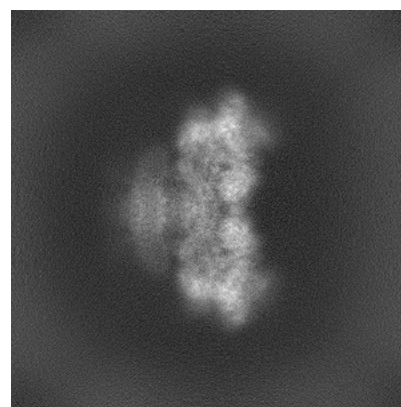
6.1.2 Raw map



X



Y

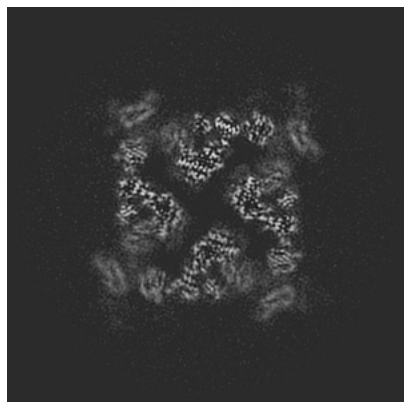


Z

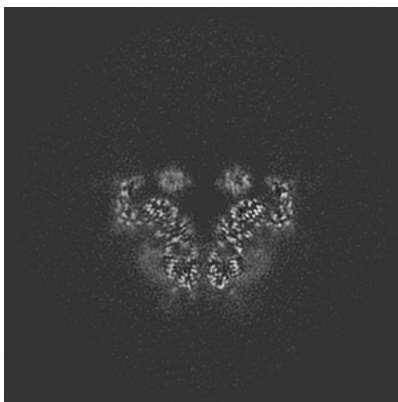
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

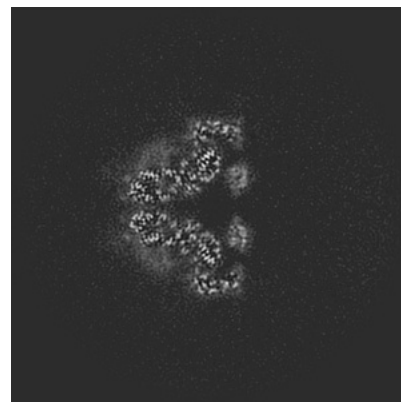
6.2.1 Primary map



X Index: 256

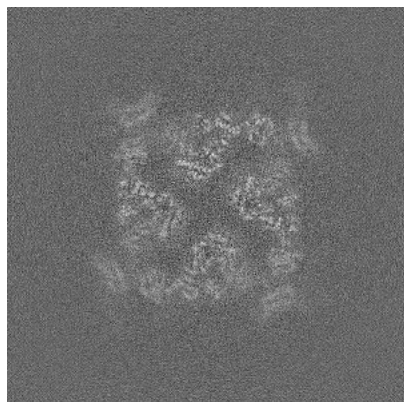


Y Index: 256

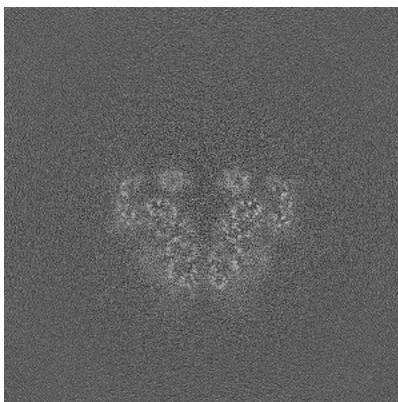


Z Index: 256

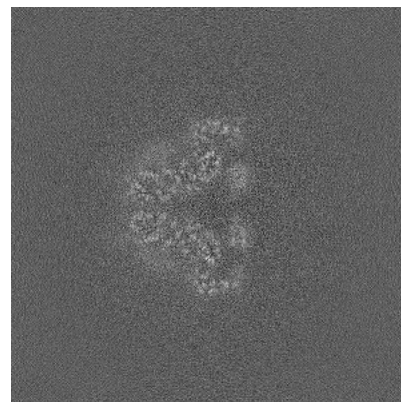
6.2.2 Raw map



X Index: 256



Y Index: 256

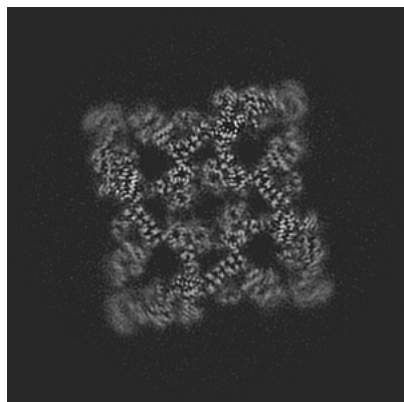


Z Index: 256

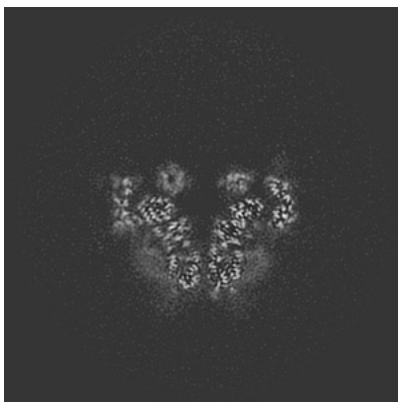
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

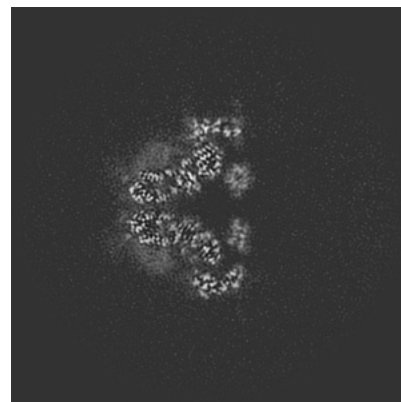
6.3.1 Primary map



X Index: 281

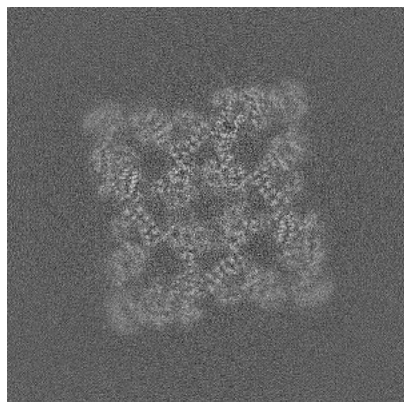


Y Index: 253

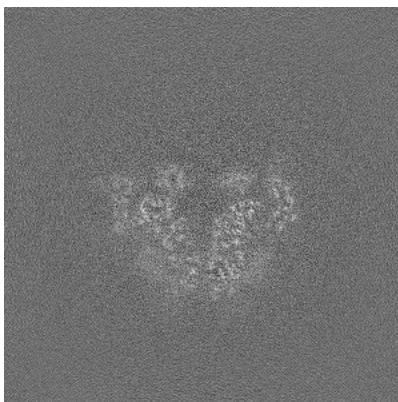


Z Index: 254

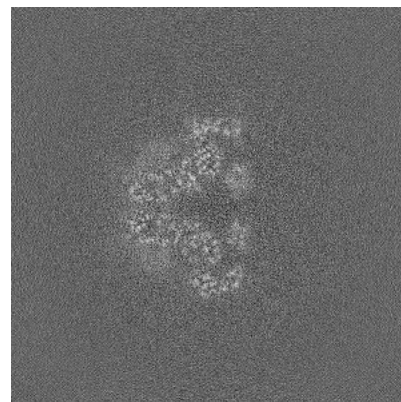
6.3.2 Raw map



X Index: 281



Y Index: 251

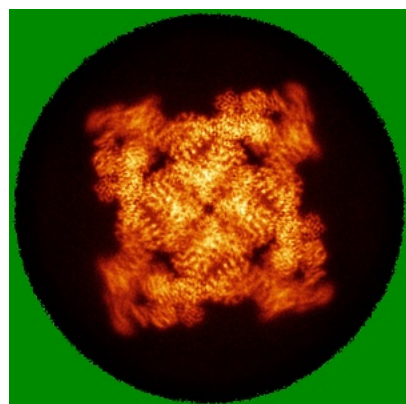


Z Index: 254

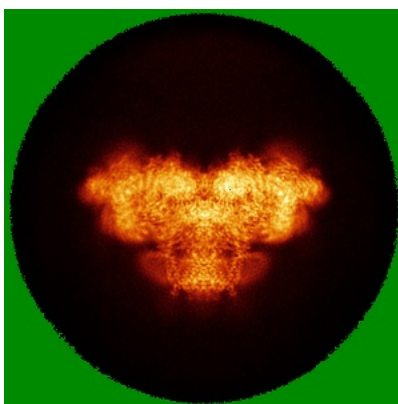
The images above show the largest variance slices of the map in three orthogonal directions.

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

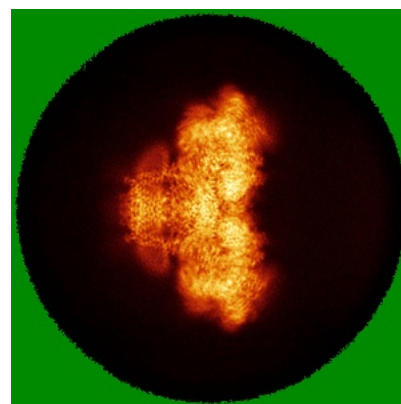
6.4.1 Primary map



X

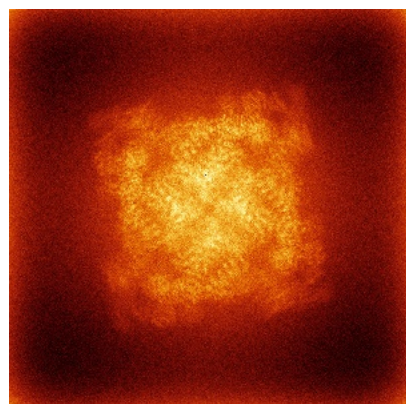


Y

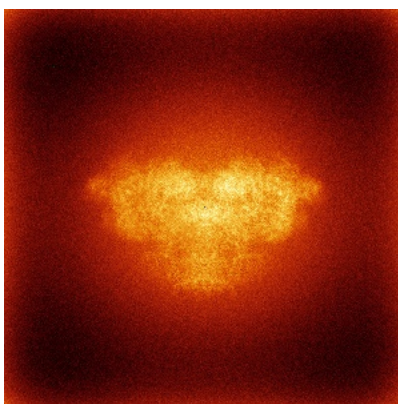


Z

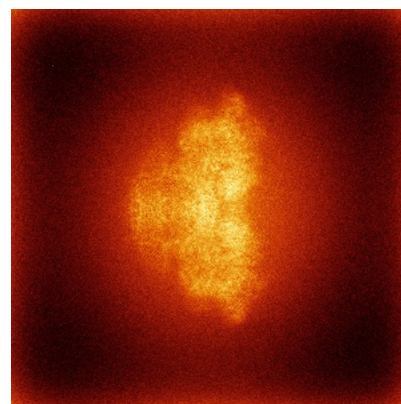
6.4.2 Raw map



X



Y

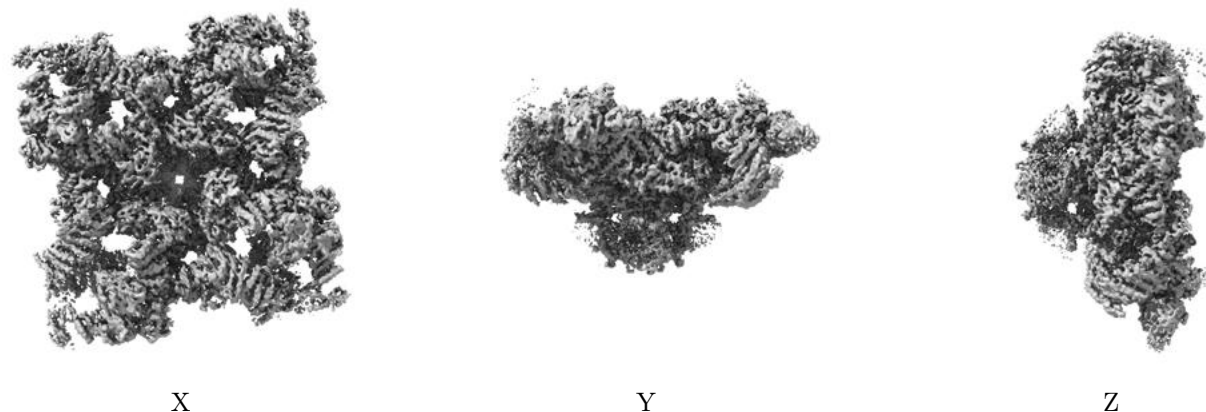


Z

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](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.09. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

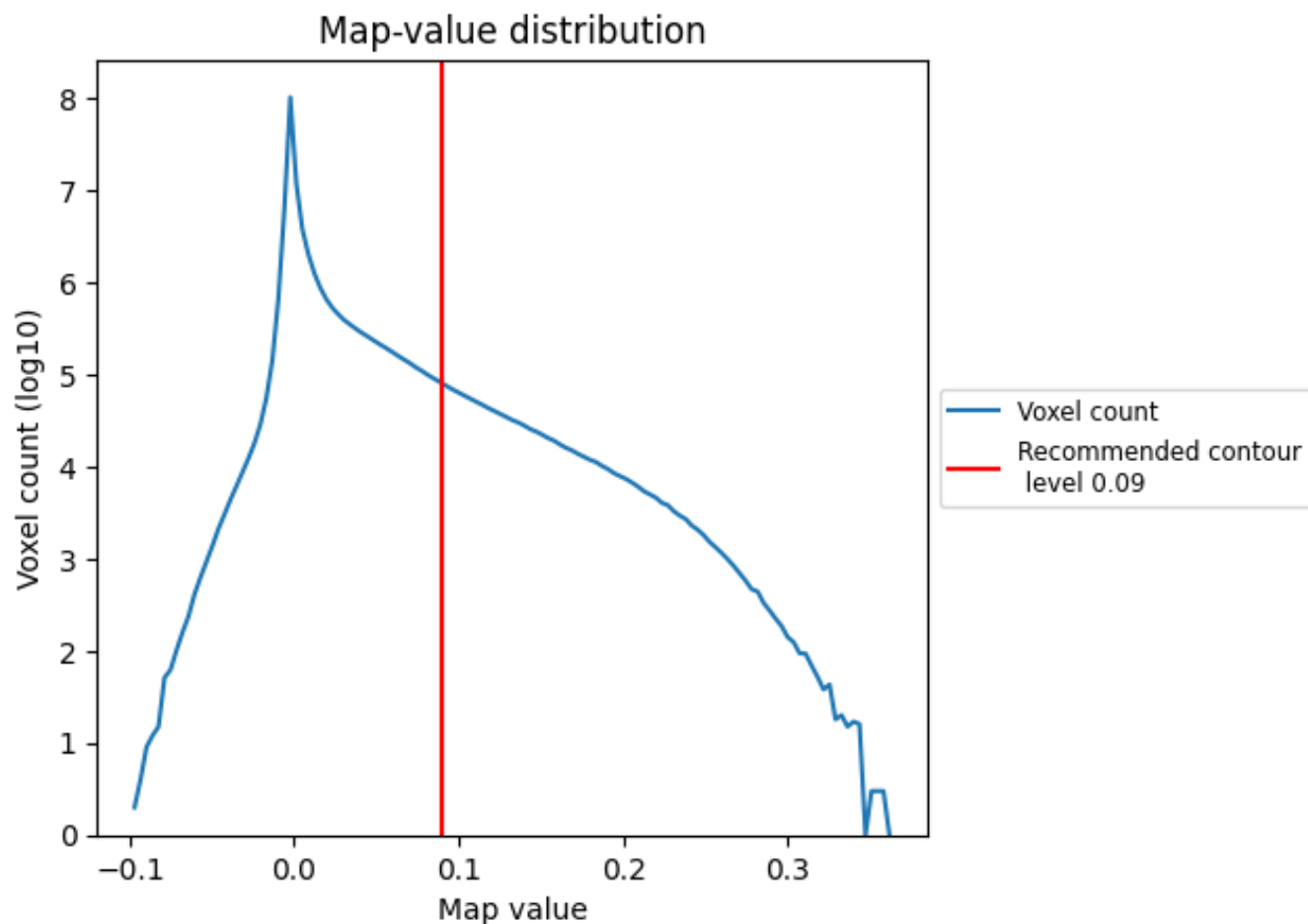
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

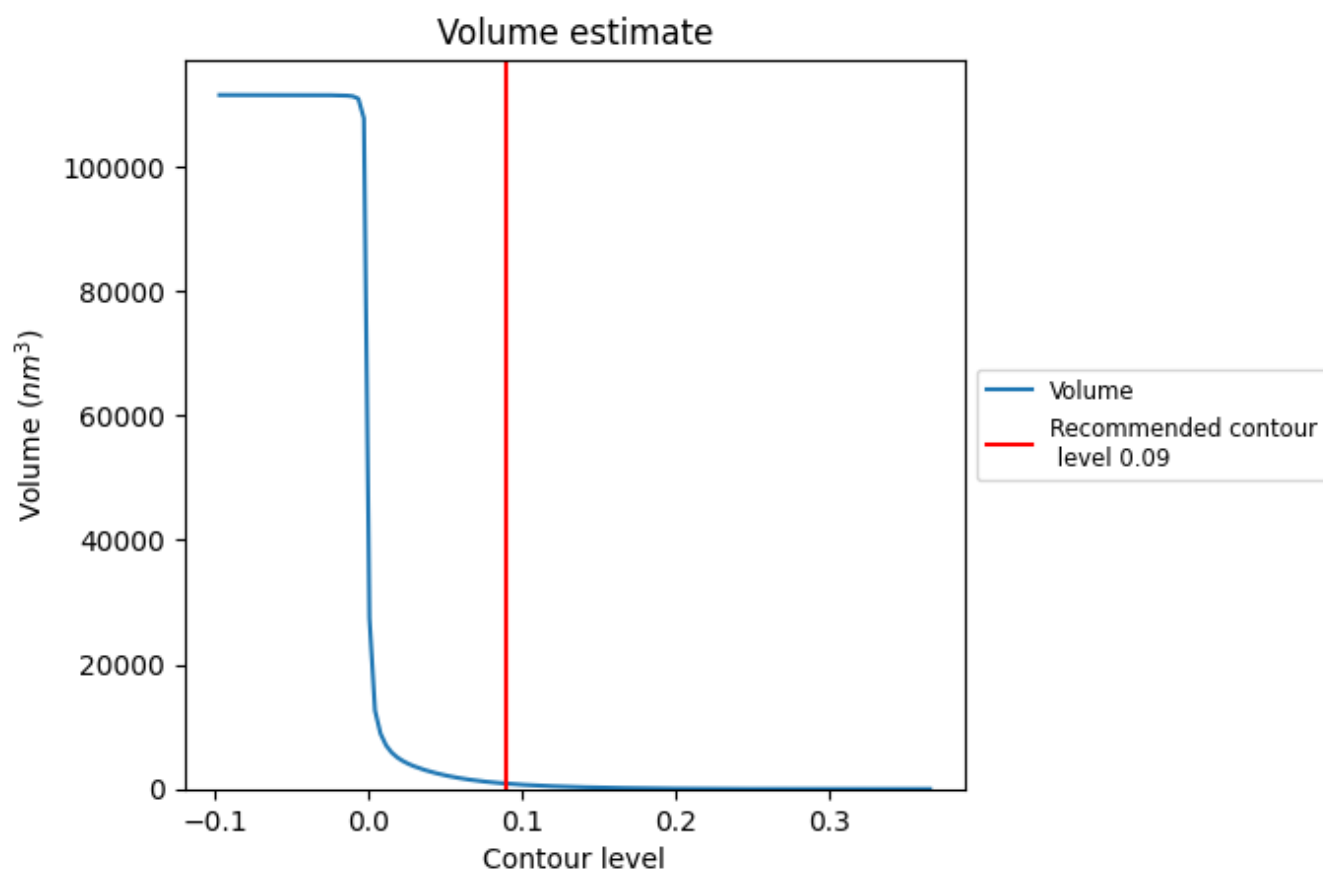
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

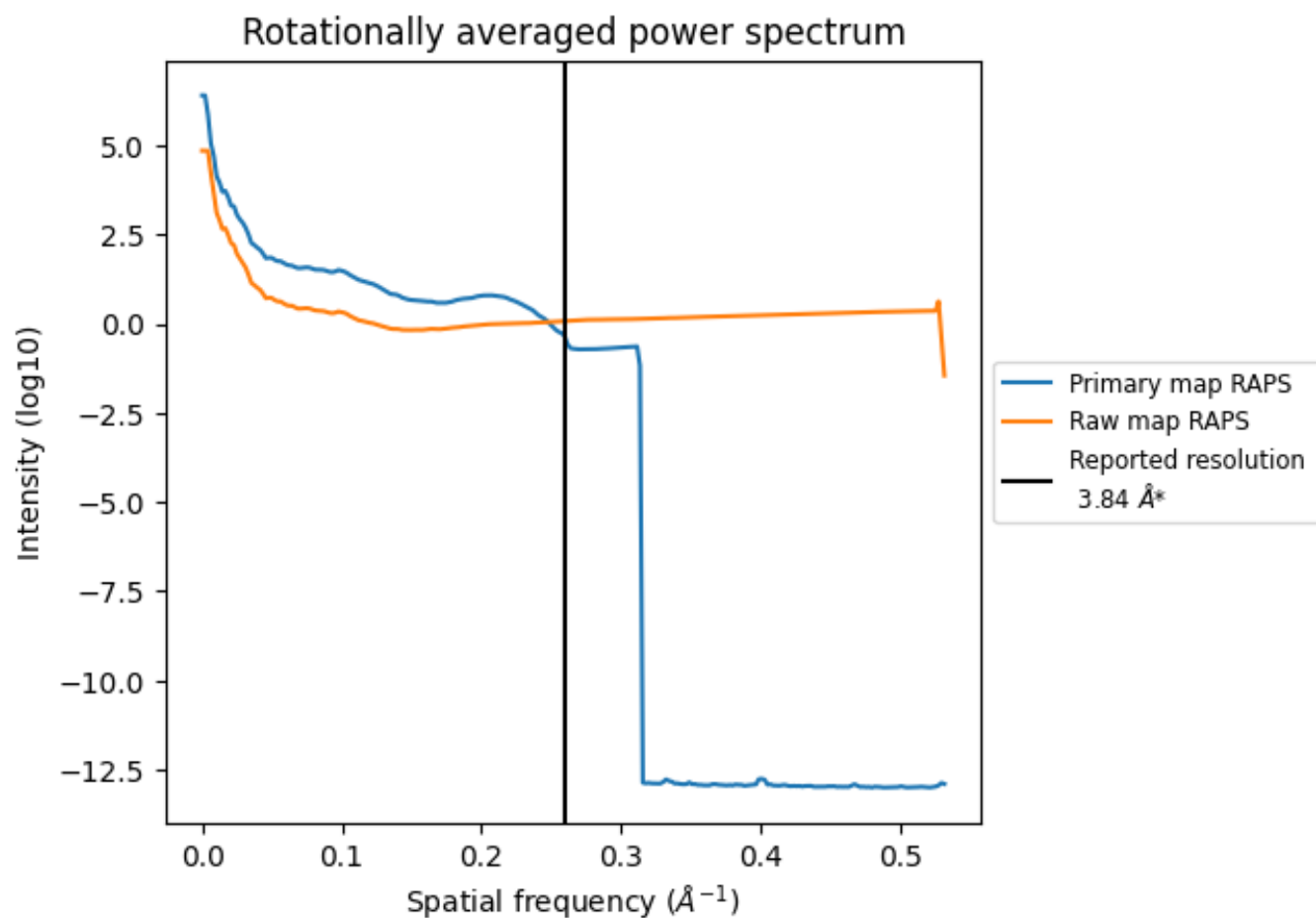
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 854 nm³; this corresponds to an approximate mass of 772 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 ⓘ

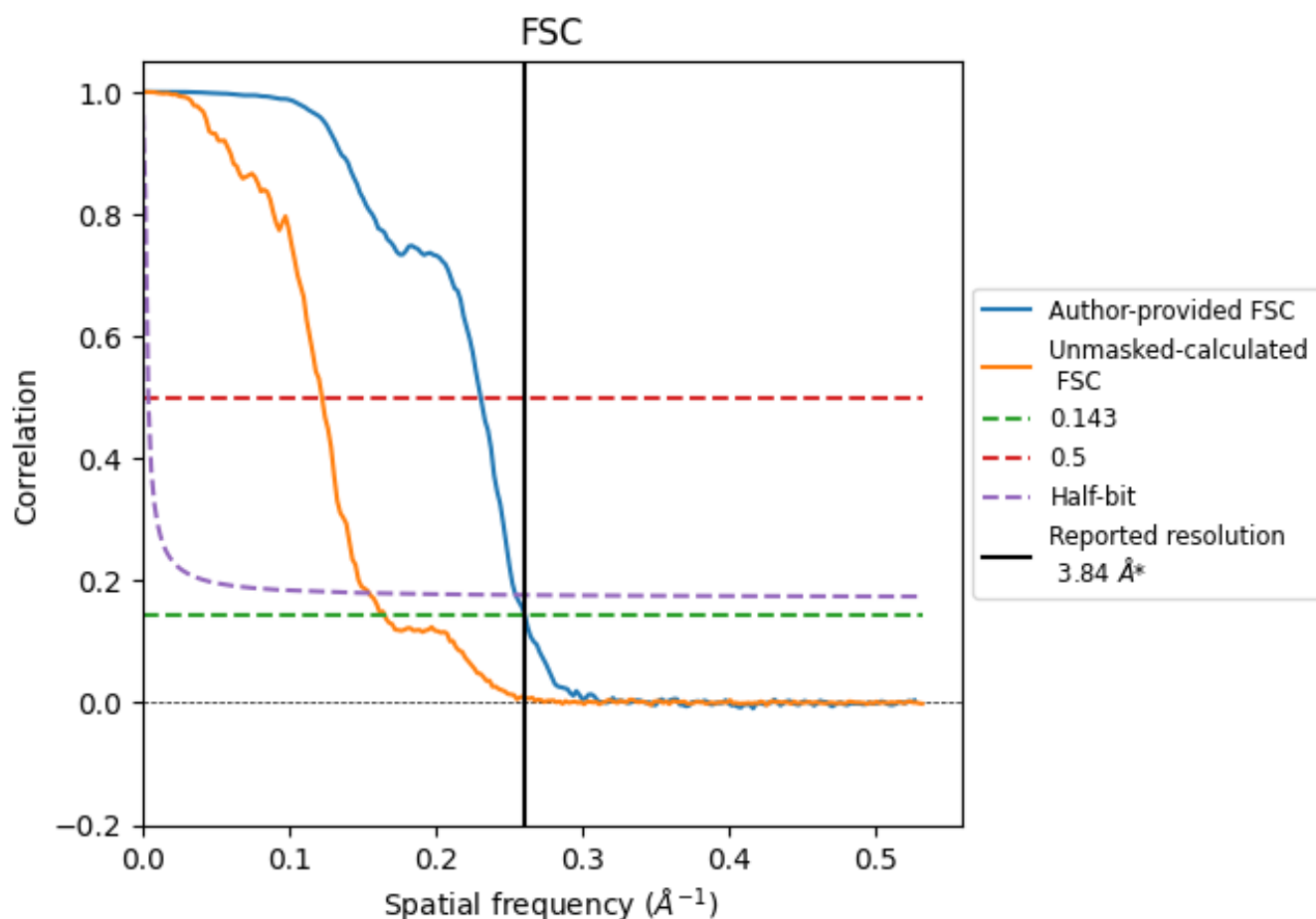


*Reported resolution corresponds to spatial frequency of 0.260 Å⁻¹

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 0.260 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

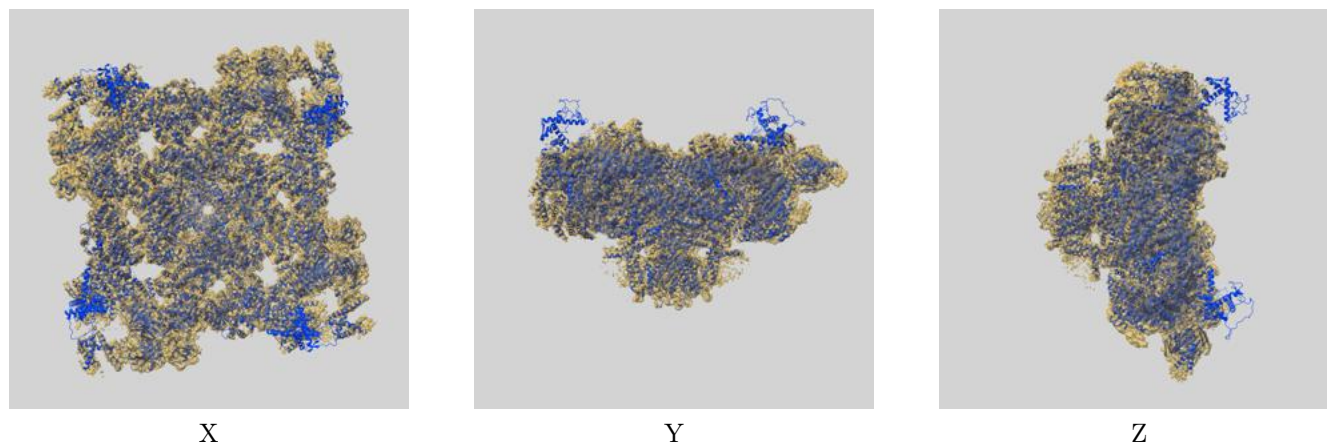
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.84	-	-
Author-provided FSC curve	3.83	4.33	3.93
Unmasked-calculated*	6.05	8.16	6.46

*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 6.05 differs from the reported value 3.84 by more than 10 %

9 Map-model fit [i](#)

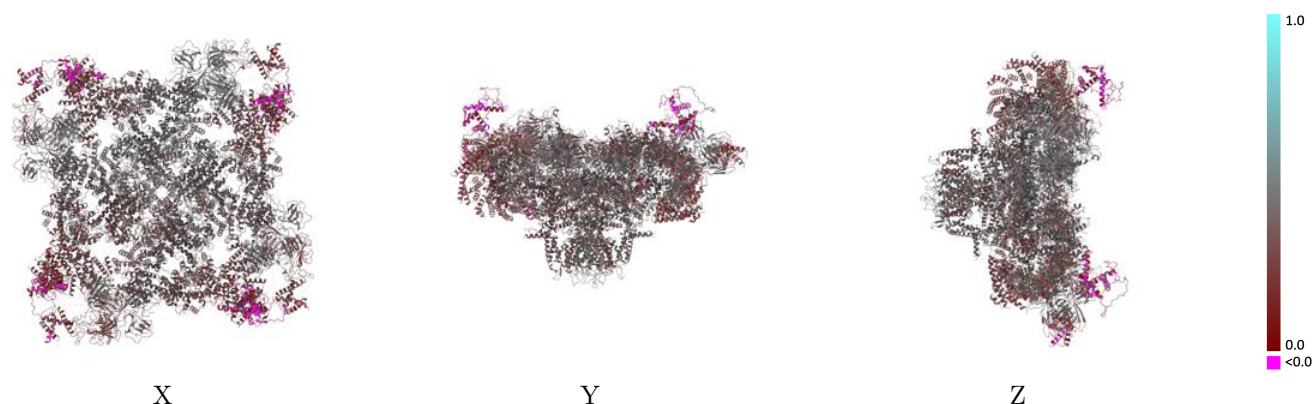
This section contains information regarding the fit between EMDB map EMD-27736 and PDB model 8DVE. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



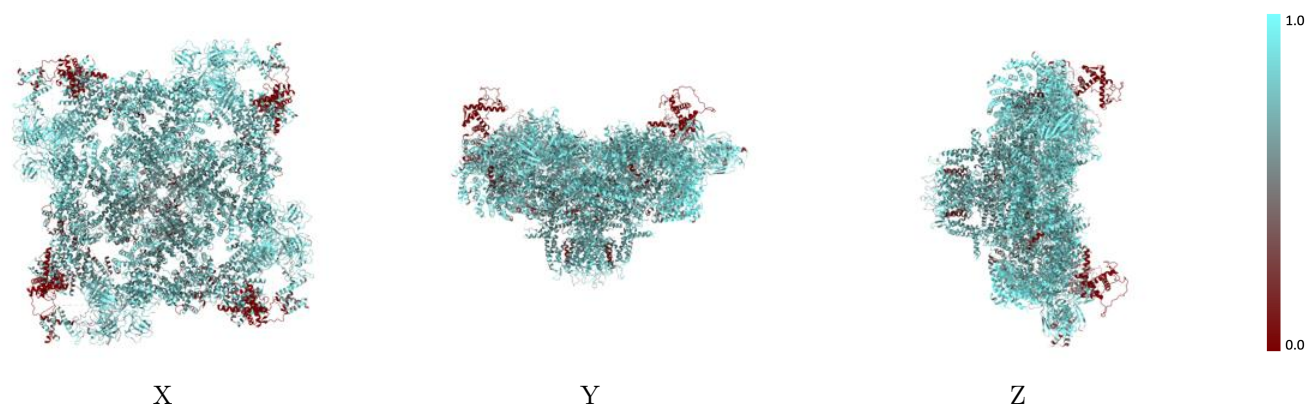
The images above show the 3D surface view of the map at the recommended contour level 0.09 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



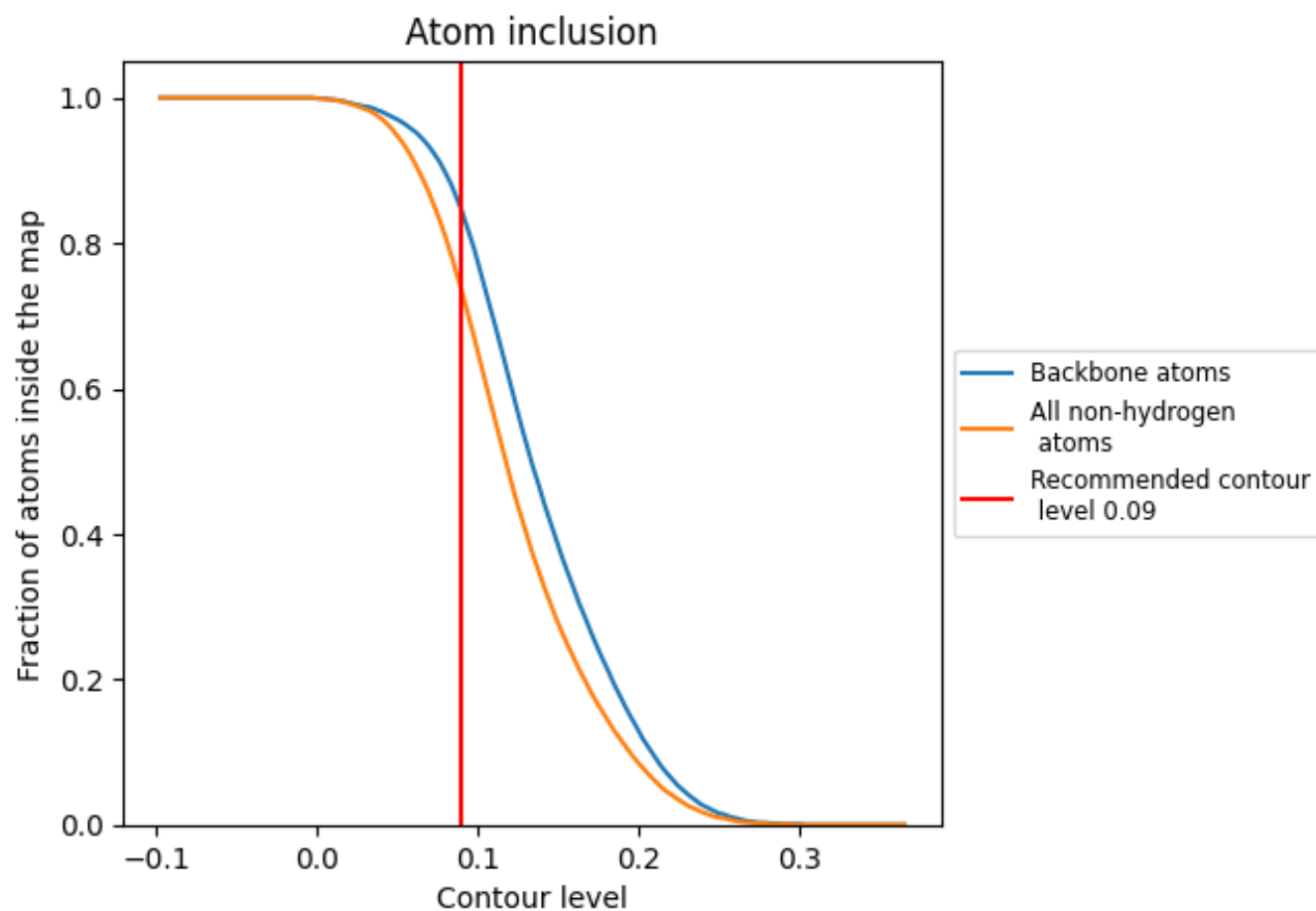
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.09).

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 74% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.09) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7350	0.3920
A	0.7850	0.4170
B	0.8400	0.4640
C	0.6260	0.3710
D	0.7290	0.3920
E	0.8030	0.4430
F	0.3730	0.3380
G	0.7510	0.3940
H	0.7880	0.4340
I	0.5750	0.3400
J	0.6930	0.3630
K	0.7510	0.4140
L	0.4590	0.3390

