



# Full wwPDB EM Validation Report ⓘ

Nov 15, 2022 – 02:28 AM JST

PDB ID : 6JRR  
EMDB ID : EMD-9879  
Title : Structure of RyR2 (\*F/A/C/L-Ca<sup>2+</sup> dataset)  
Authors : Gong, D.S.; Chi, X.M.; Zhou, G.W.; Huang, G.X.Y.; Lei, J.L.; Yan, N.  
Deposited on : 2019-04-05  
Resolution : 3.90 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

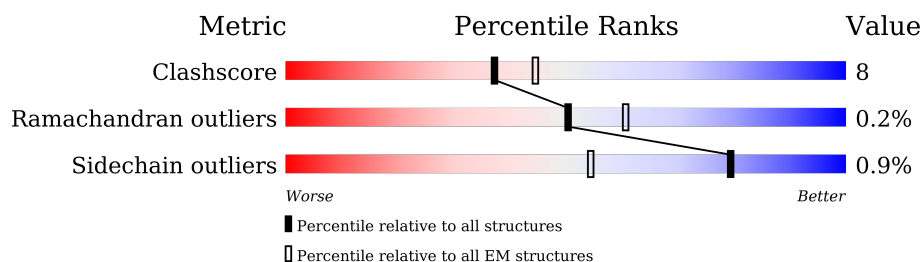
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.90 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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  $\geq 3$ , 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	4968	
1	C	4968	
1	E	4968	
1	G	4968	
2	B	108	
2	D	108	
2	F	108	
2	H	108	

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 109132 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 RyR2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	3460	Total	C	N	O	S	0	0
			26417	16833	4528	4900	156		
1	C	3460	Total	C	N	O	S	0	0
			26417	16833	4528	4900	156		
1	E	3460	Total	C	N	O	S	0	0
			26417	16833	4528	4900	156		
1	G	3460	Total	C	N	O	S	0	0
			26417	16833	4528	4900	156		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	107	Total	C	N	O	S	0	0
			819	516	144	155	4		
2	D	107	Total	C	N	O	S	0	0
			819	516	144	155	4		
2	F	107	Total	C	N	O	S	0	0
			819	516	144	155	4		
2	H	107	Total	C	N	O	S	0	0
			819	516	144	155	4		

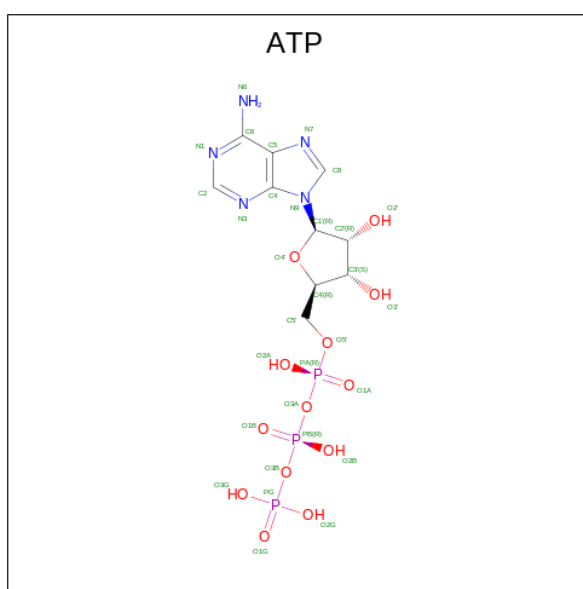
- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Zn	0
			1	1	
3	C	1	Total	Zn	0
			1	1	
3	E	1	Total	Zn	0
			1	1	
3	G	1	Total	Zn	0
			1	1	

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

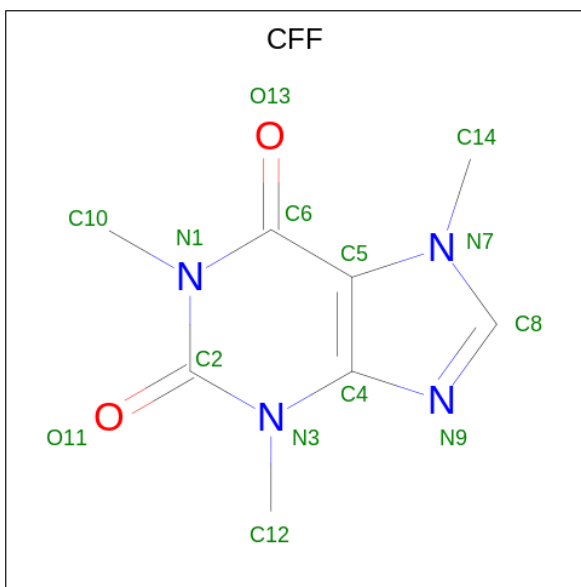
Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Ca	0
			1	1	
4	C	1	Total	Ca	0
			1	1	
4	E	1	Total	Ca	0
			1	1	
4	G	1	Total	Ca	0
			1	1	

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).



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

- Molecule 6 is CAFFEINE (three-letter code: CFF) (formula:  $C_8H_{10}N_4O_2$ ).

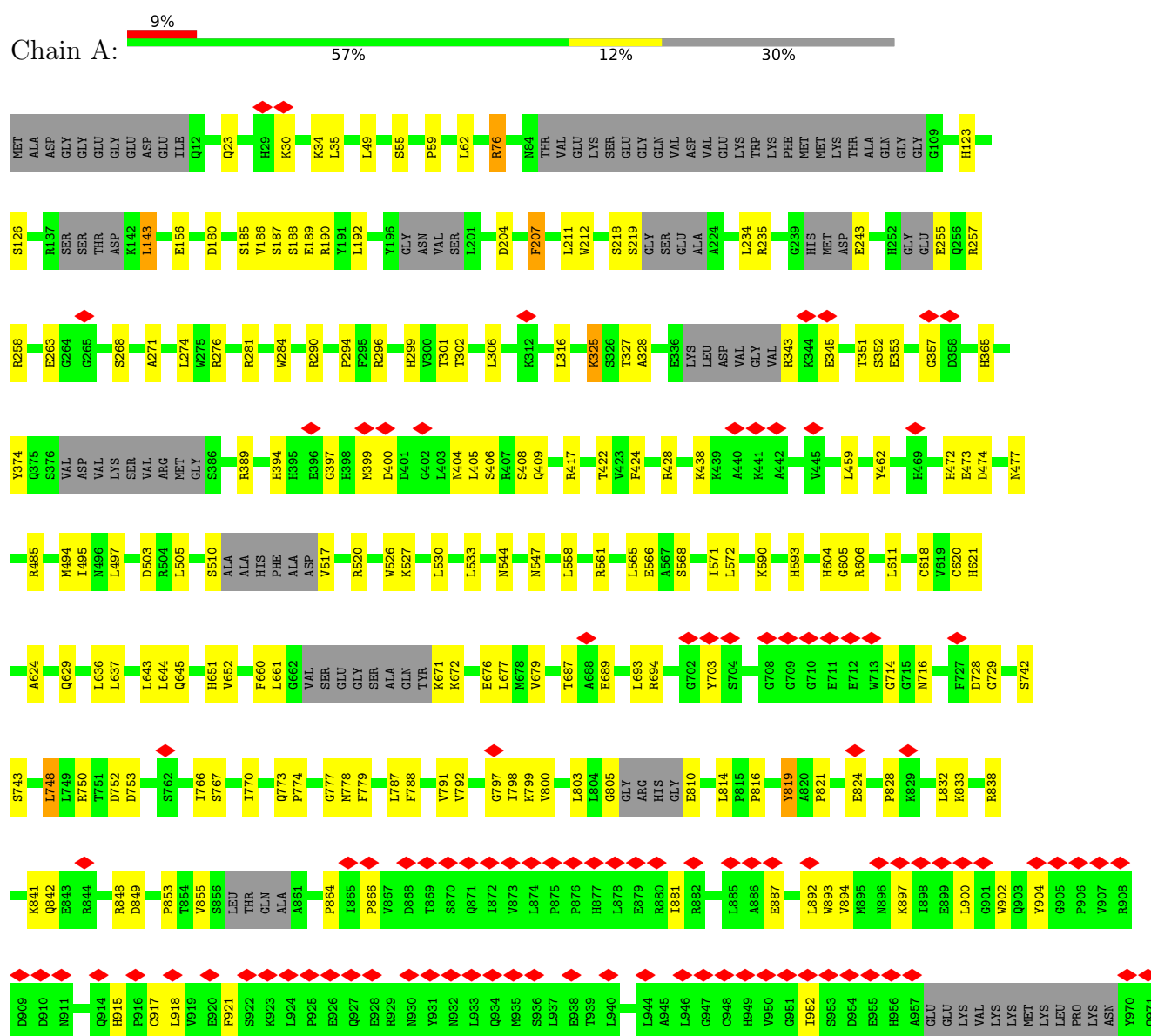


Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	N	O	0
			14	8	4	2	
6	C	1	Total	C	N	O	0
			14	8	4	2	
6	E	1	Total	C	N	O	0
			14	8	4	2	
6	G	1	Total	C	N	O	0
			14	8	4	2	

### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: RyR2







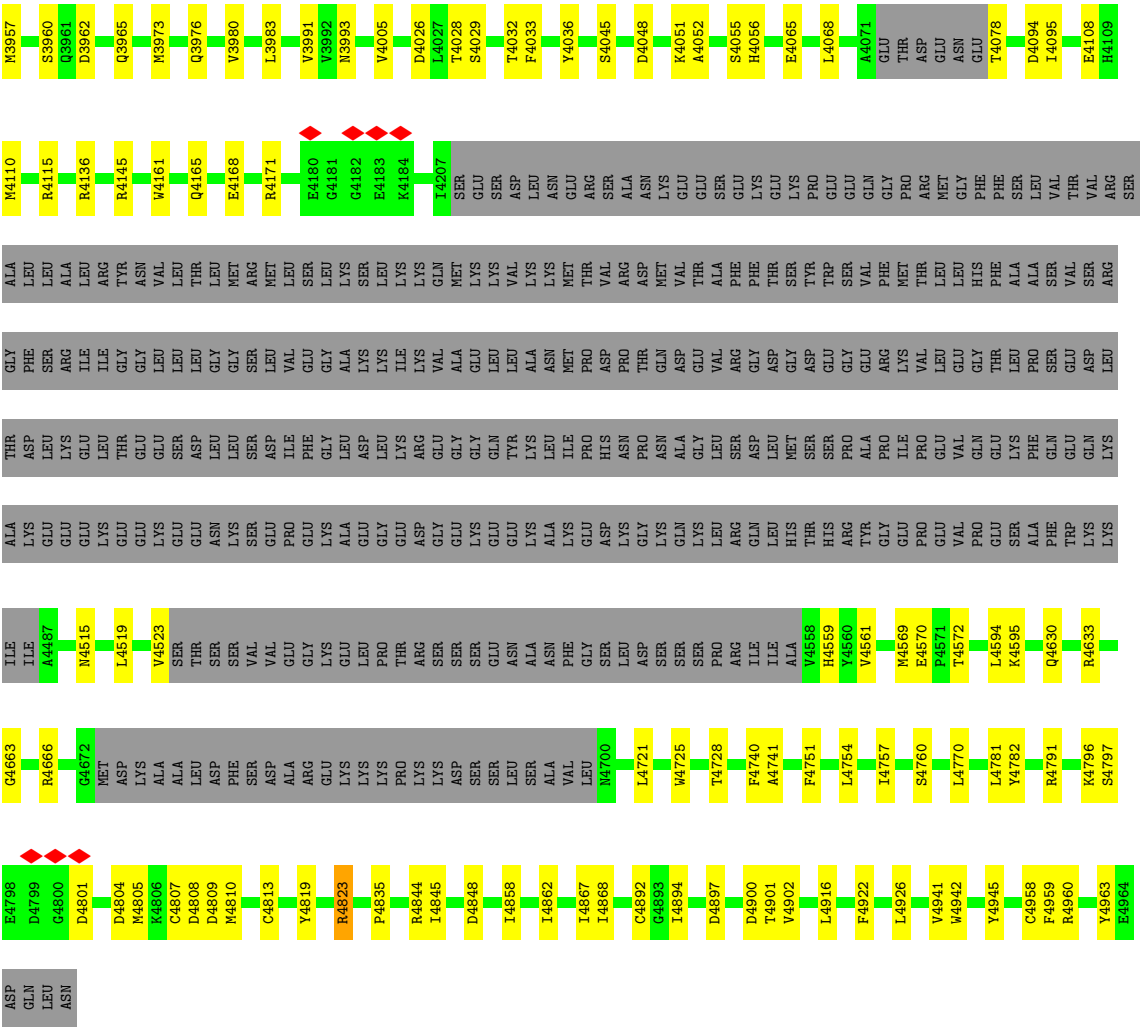




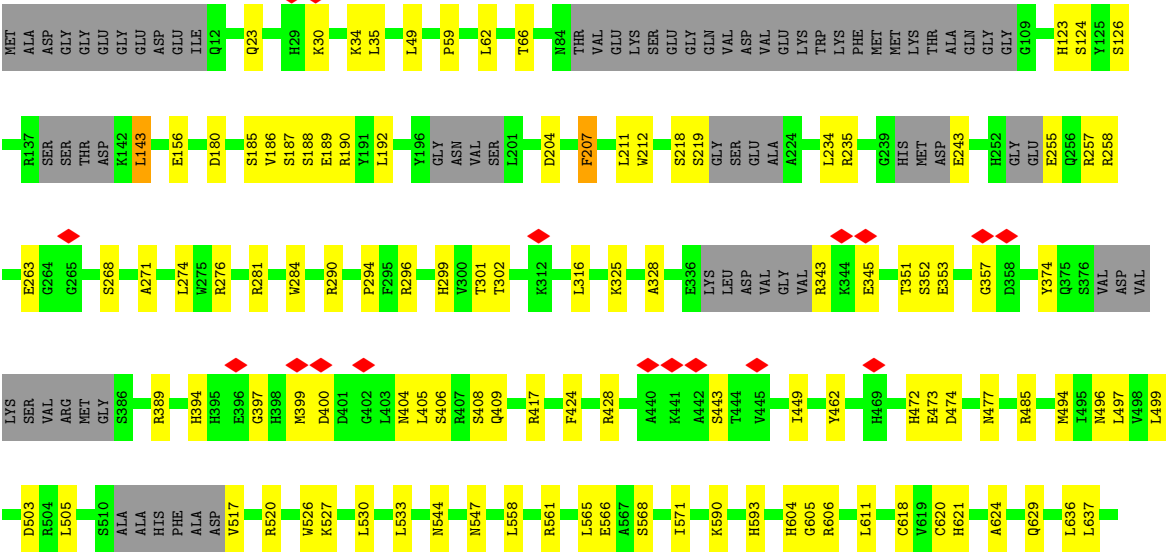




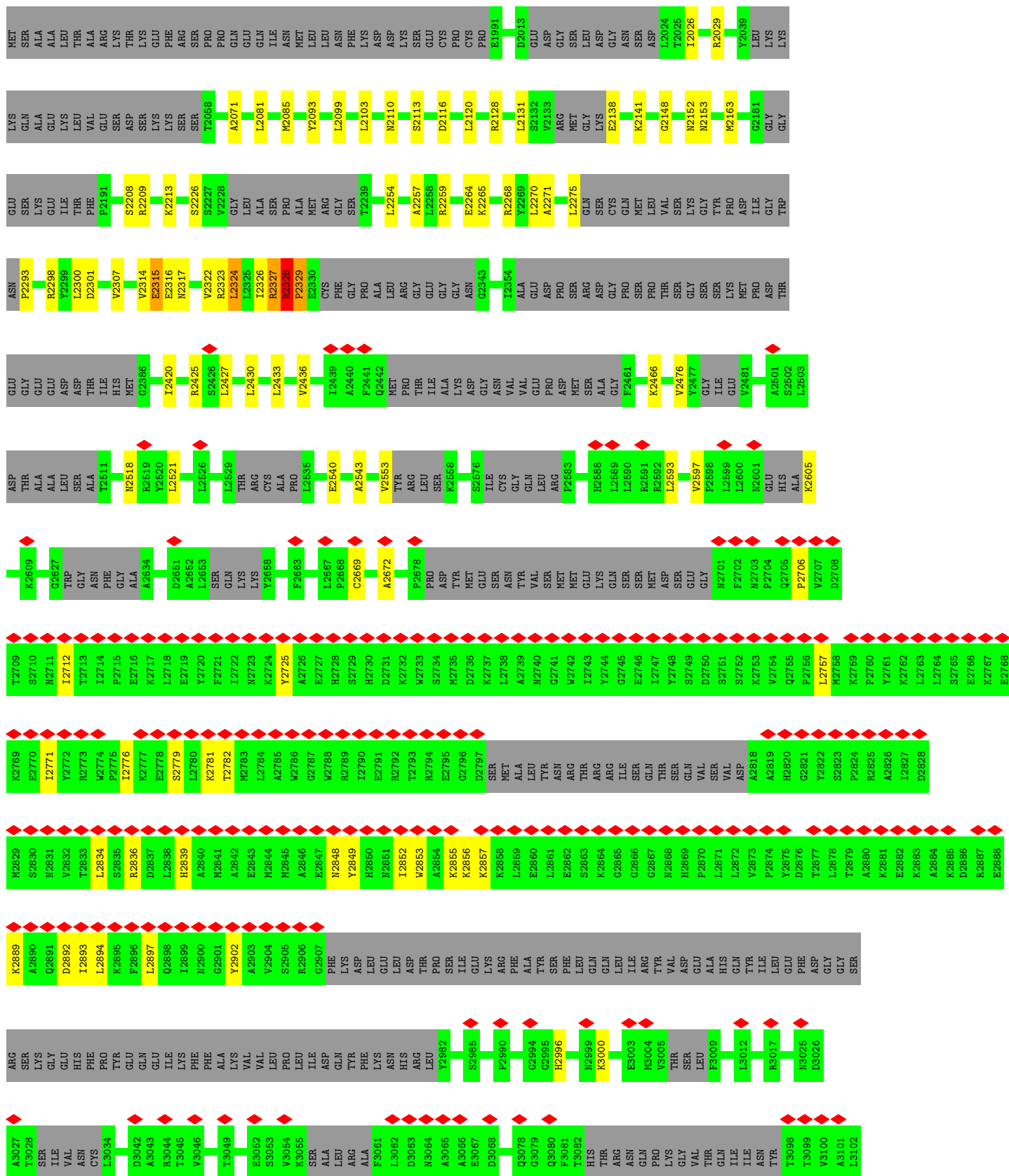




● Molecule 1: RyR2

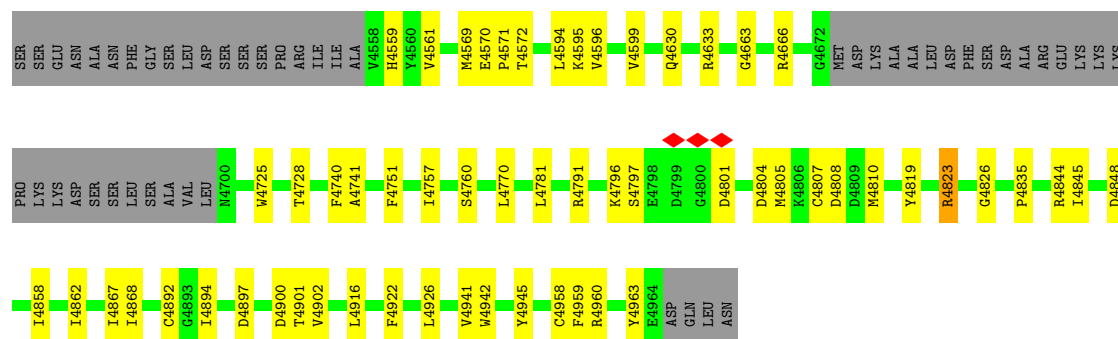




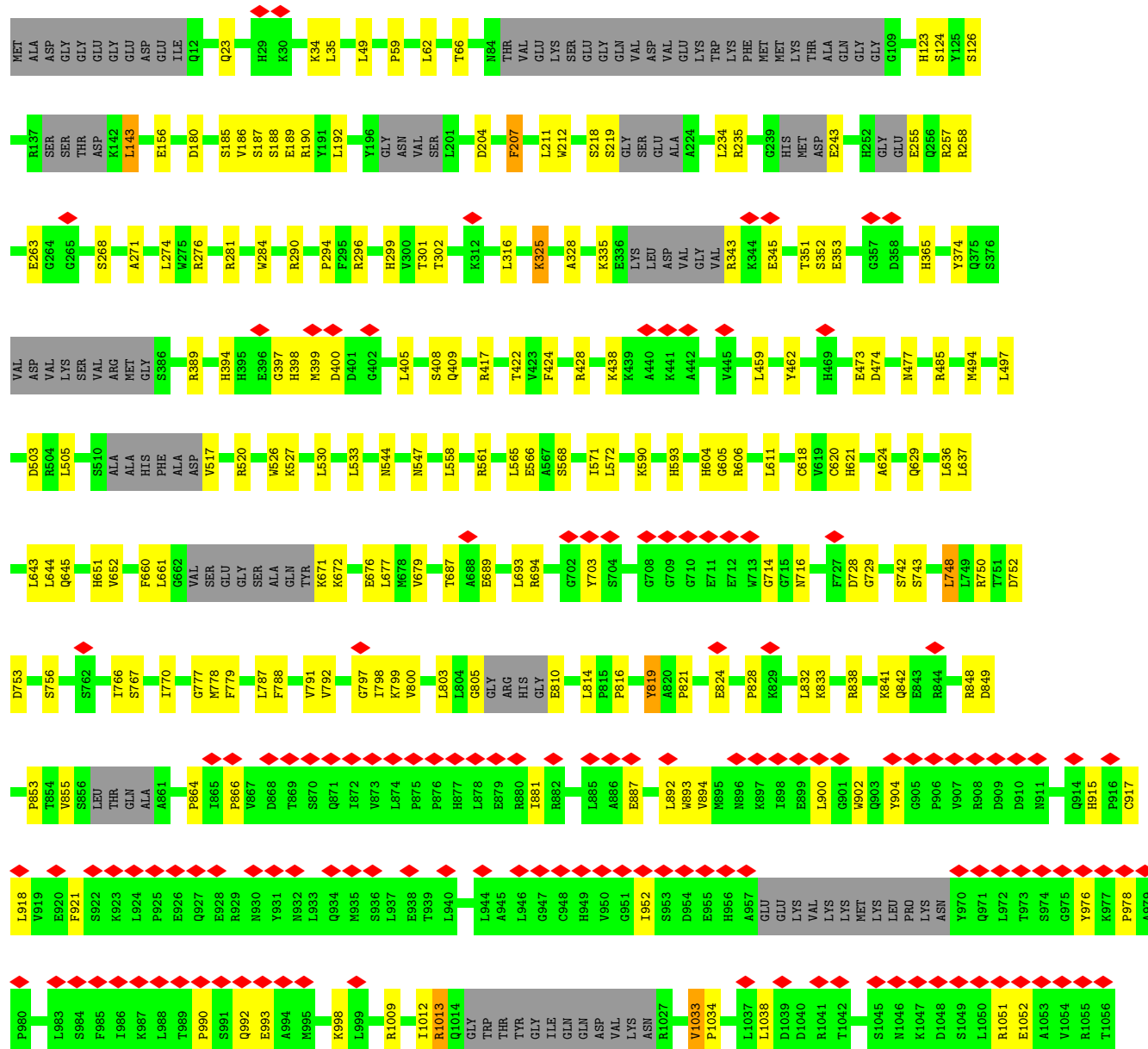






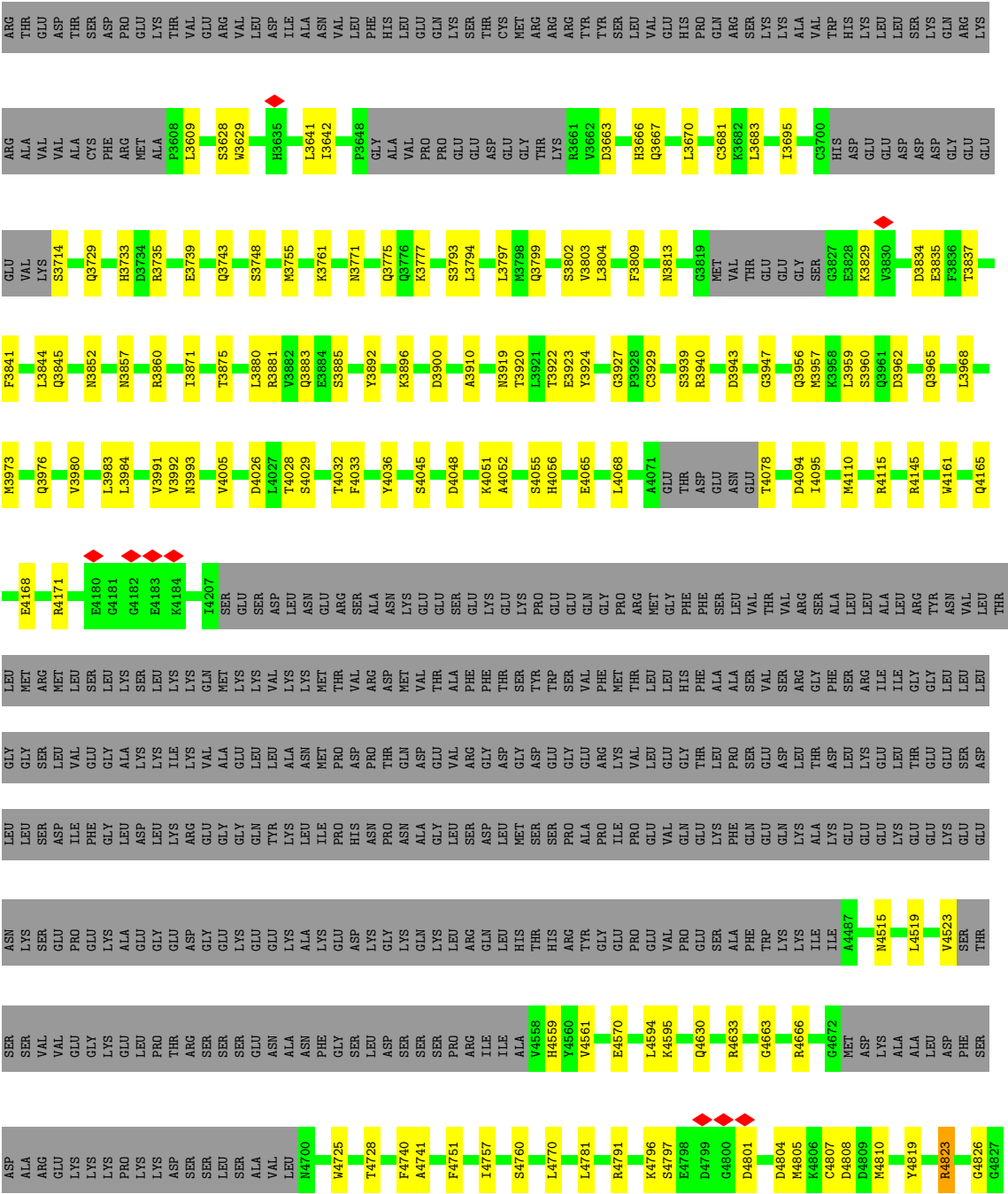


• Molecule 1: RyR2

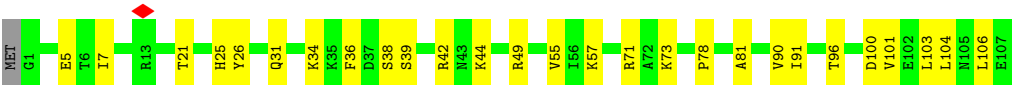


L1057	L1058	L1062	M1063	L1064	E1065	A1066	PRO	ASP	GLN	ASP	HIS	ALA	ALA	ALA	ARG	ALA	GLU	VAL	CYS	THR	GLY	GLY	R1084	R1089	R1100	W1101	F1103	E1104	F1105	E1106	A1110	G1111	S1118	C1122	Q1123	P1124	D1125	Q1126	E1127	R1133	R1144	E1150	W1156	G1163	M1165												
E1170	H1171	D1185	S1186	G1187	D1194	D1199	V1204	V1209	A1210	Q1211	R1214	K1219	D1220	S1221	S1222	T1223	L1224	F1227	T1228	I1229	Q1233	A1240	W1250	L1251	S1252	K1253	R1254	L1255	P1256	Q1257	F1258	H1265	E1266	H1267	I1273	D1274	GLY	THR	ILE	ASP	SER	PRO	CYS	LEU													
L1285	L1286	Q1287	M1300	F1301	Y1302	L1303	S1304	S1305	M1306	F1307	I1308	V1430	PHE	C1310	ALA	ASN	GLU	VAL	PHE	LYS	ASP	TYR	ALA	GLN	GLY	PRO	GLY	ILE	ARG	LEU	LYS	SER	GLN	LEU	PHE	ALA	SER	ASP	THR	LEU	GLU	MET	LYS	THR	VAL	LEU	ALA	HIS	GLY	HIS	LEU						
VAL	PRO	ASP	ARG	VAL	ASP	LYS	ASP	GLU	ASN	THR	LYS	PRO	GLU	ASN	ALA	ASN	HIS	LYS	ASP	TYR	ALA	ALA	GLN	GLY	LYS	PRO	ARG	LEU	LYS	ALA	ARG	THR	LYS	PRO	ASP	TYR	SER	THR	GLU	VAL	LEU	GLU	ASP	GLU	VAL	LEU	ALA	ALA	ASP	ARG							
ASP	ASP	TYR	TYR	LEU	MET	GLN	THR	T1425	Y1426	S1429	V1430	R1431	P1434	GLY	GLN	GLU	PRO	N1440	Y1443	G1444	W1445	T1446	D1454	L1459	ASP	ARG	VAL	ARG	THR	V1465	T1466	V1467	T1468	K1473	G1474	K1475	V1476	H1477	E1478	S1479	R1482	S1483	N1484	CYS	Y1486	M1487	A1490	GLY									
GLU	SER	MET	GLY	GLN	GLY	ASN	M1502	L1505	E1506	I1507	V1510	V1511	ASP	ALA	ALA	ASP	D1526	P1535	S1536	F1540	P1541	A1542	V1543	F1544	A1545	T1548	S1549	E1556	LEU	GLY	ARG	ILE	LYS	ASN	VAL	MET	PRO	SER	A1568	G1569	L1570	F1571	S1572	E1574													
H1575	V1579	P1580	R1585	Q1589	L1595	W1596	S1597	R1598	M1599	P1600	N1601	Q1602	F1603	R1610	I1611	S1612	E1613	R1614	W1617	L1618	V1619	Q1620	L1621	L1622	L1625	S1629	L1630	H1631	P1632	F1633	E1634	T1641	L1642	E1643	L1644	T1645	L1651	Y1655	L1658	R1659	L1660	L1667	G1668	N1669	S1678												
E1682	Y1687	N1691	S1712	S1713	Y1714	R1718	T1733	I1736	T1737	L1738	D1741	GLU	ASN	LYS	ASN	GLY	P1749	G1750	T1755	S1756	L1757	R1758	F1763	Y1769	E1781	F1782	D1785	T1792	D1808	P1809	V1810	G1811	F1816	K1840	H1841	I1842	L1843	Q1844	E1847																		
P1848	S1849	VAL	PHE	LYS	GLU	ALA	ALA	GLY	PRO	GLU	GLU	GLU	SER	ASP	THR	LEU	GLU	LYS	GLU	GLU	PRO	CYS	ALA	ALA	SER	GLN	ASP	GLN	ILE	ASN	LEU	ASN	PHE	LYS	ASP	GLY	PRO	CYS	PRO	LYS	GLU	G1893	K1904	L1911	A1925	S1930	D1931	D1932	D1939	R1942							
F1943	Q1950	A1951	L1952	ASN	MET	SER	ALA	ALA	LEU	THR	ALA	GLY	THR	PHE	ARG	SER	PRO	PRO	GLN	GLU	GLN	ILE	ASN	MET	LEU	ASN	PHE	LYS	ASP	SER	CYS	PRO	PRO	E1991	D2013	GLU	ASP	GLY	SER	LEU	ASP	GLY	ASN	ASP	L2024	T2025	L2026										
R2029	Y2039	LEU	LYS	LYS	LYS	GLN	ALA	GLU	LYS	LYS	VAL	GLU	SER	GLY	VAL	GLY	ASP	SER	THR	GLY	ALA	ALA	L2058	L2081	Y2093	N2110	S2113	D2116	L2120	R2128	L2131	S2132	V2133	ARG	GLN	CYS	GLY	LYS	E2138	K2141	G2148	N2152	M2153	M2163	G2181	GLY	GLY	GLU	GLY	SER							
LYS	GLU	ILE	THR	PHE	P2191	S2208	R2209	K2213	S2226	S2227	V2228	GLY	SER	LEU	ALA	SER	PRO	ALA	MET	ARG	GLY	SER	T2239	L2254	A2257	L2258	R2259	K2265	R2268	Y2269	L2270	L2275	GLN	SER	CYS	GLN	MET	LEU	VAL	SER	LYS	GLY	THR	SER	GLY	TYR	ASP	PRO	ASP	ASN	P2293	R2298					
Y2299	L2300	D2301	V2307	V2314	E2315	E2316	N2317	V2321	V2322	R2323	L2324	L2325	L2326	R2327	R2328	P2329	E2330	CYS	PHE	GLY	PRO	ALA	LEU	ARG	GLY	GLU	GLY	ASN	G2343	L2354	ALA	GLU	ASP	PRO	PRO	SER	ARG	ASP	GLY	PRO	ALA	GLY	THR	VAL	SER	LYS	GLY	TYR	ASP	PRO	MET	THR	ILE	GLU	V2481	A2501	S2502
G2386	L2397	R2402	R2425	S2426	L2427	L2430	L2433	V2436	L2439	A2440	F2441	Q2442	MET	PRO	THR	ILE	ALA	LYS	ASP	GLY	ASN	VAL	VAL	GLU	PRO	PRO	ASP	MET	SER	GLY	F2461	D2464	H2465	K2466	V2476	Y2477	GLY	ILE	THR	GLU	V2481	A2501	S2502														






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



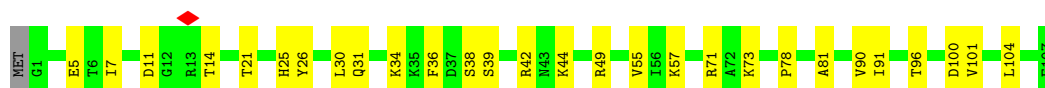
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain D:  75% 24%




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

Chain F:  73% 26%



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

Chain H:  75% 24%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	149212	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)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.141	Depositor
Minimum map value	-0.073	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.022	Depositor
Map size (Å)	436.4, 436.4, 436.4	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.091, 1.091, 1.091	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.47	0/26913	0.60	5/36395 (0.0%)
1	C	0.47	0/26913	0.60	5/36395 (0.0%)
1	E	0.47	0/26913	0.60	5/36395 (0.0%)
1	G	0.47	0/26913	0.60	5/36395 (0.0%)
2	B	0.41	0/835	0.58	0/1123
2	D	0.41	0/835	0.58	0/1123
2	F	0.41	0/835	0.58	0/1123
2	H	0.41	0/835	0.58	0/1123
All	All	0.47	0/110992	0.60	20/150072 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	15
1	C	0	15
1	E	0	15
1	G	0	15
All	All	0	60

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2430	LEU	CA-CB-CG	7.00	131.39	115.30
1	C	2430	LEU	CA-CB-CG	7.00	131.39	115.30
1	E	2430	LEU	CA-CB-CG	7.00	131.39	115.30
1	G	2430	LEU	CA-CB-CG	7.00	131.39	115.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	3681	CYS	CA-CB-SG	5.68	124.22	114.00
1	C	3681	CYS	CA-CB-SG	5.66	124.19	114.00
1	G	3681	CYS	CA-CB-SG	5.66	124.19	114.00
1	A	3681	CYS	CA-CB-SG	5.66	124.19	114.00
1	E	2757	LEU	CA-CB-CG	5.44	127.81	115.30
1	A	2757	LEU	CA-CB-CG	5.44	127.80	115.30
1	C	2757	LEU	CA-CB-CG	5.44	127.80	115.30
1	G	2757	LEU	CA-CB-CG	5.44	127.80	115.30
1	A	748	LEU	CA-CB-CG	5.10	127.03	115.30
1	C	748	LEU	CA-CB-CG	5.10	127.03	115.30
1	E	748	LEU	CA-CB-CG	5.10	127.03	115.30
1	G	748	LEU	CA-CB-CG	5.10	127.03	115.30
1	A	2300	LEU	CB-CG-CD2	-5.04	102.43	111.00
1	C	2300	LEU	CB-CG-CD2	-5.04	102.43	111.00
1	E	2300	LEU	CB-CG-CD2	-5.04	102.43	111.00
1	G	2300	LEU	CB-CG-CD2	-5.04	102.43	111.00

There are no chirality outliers.

All (60) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1127	GLU	Peptide
1	A	1545	ALA	Peptide
1	A	1570	LEU	Peptide
1	A	1579	VAL	Peptide
1	A	1750	GLY	Peptide
1	A	1808	ASP	Peptide
1	A	1809	PRO	Peptide
1	A	1847	GLU	Peptide
1	A	3802	SER	Peptide
1	A	729	GLY	Peptide
1	A	791	VAL	Peptide
1	A	814	LEU	Peptide
1	A	816	PRO	Peptide
1	A	819	TYR	Peptide
1	A	838	ARG	Peptide
1	C	1127	GLU	Peptide
1	C	1545	ALA	Peptide
1	C	1570	LEU	Peptide
1	C	1579	VAL	Peptide
1	C	1750	GLY	Peptide
1	C	1808	ASP	Peptide

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Group
1	C	1809	PRO	Peptide
1	C	1847	GLU	Peptide
1	C	3802	SER	Peptide
1	C	729	GLY	Peptide
1	C	791	VAL	Peptide
1	C	814	LEU	Peptide
1	C	816	PRO	Peptide
1	C	819	TYR	Peptide
1	C	838	ARG	Peptide
1	E	1127	GLU	Peptide
1	E	1545	ALA	Peptide
1	E	1570	LEU	Peptide
1	E	1579	VAL	Peptide
1	E	1750	GLY	Peptide
1	E	1808	ASP	Peptide
1	E	1809	PRO	Peptide
1	E	1847	GLU	Peptide
1	E	3802	SER	Peptide
1	E	729	GLY	Peptide
1	E	791	VAL	Peptide
1	E	814	LEU	Peptide
1	E	816	PRO	Peptide
1	E	819	TYR	Peptide
1	E	838	ARG	Peptide
1	G	1127	GLU	Peptide
1	G	1545	ALA	Peptide
1	G	1570	LEU	Peptide
1	G	1579	VAL	Peptide
1	G	1750	GLY	Peptide
1	G	1808	ASP	Peptide
1	G	1809	PRO	Peptide
1	G	1847	GLU	Peptide
1	G	3802	SER	Peptide
1	G	729	GLY	Peptide
1	G	791	VAL	Peptide
1	G	814	LEU	Peptide
1	G	816	PRO	Peptide
1	G	819	TYR	Peptide
1	G	838	ARG	Peptide

## 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	26417	0	24909	474	0
1	C	26417	0	24909	487	0
1	E	26417	0	24909	466	0
1	G	26417	0	24909	457	0
2	B	819	0	824	18	0
2	D	819	0	824	18	0
2	F	819	0	824	19	0
2	H	819	0	824	18	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
5	A	31	0	12	1	0
5	C	31	0	12	1	0
5	E	31	0	12	1	0
5	G	31	0	12	1	0
6	A	14	0	10	2	0
6	C	14	0	10	2	0
6	E	14	0	10	2	0
6	G	14	0	10	2	0
All	All	109132	0	103020	1741	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 8.

All (1741) 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:A:2427:LEU:HD13	1:G:143:LEU:CB	1.41	1.51
1:E:143:LEU:CB	1:G:2427:LEU:HD13	1.41	1.49
1:A:143:LEU:CB	1:C:2427:LEU:HD13	1.41	1.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:143:LEU:CB	1:E:2427:LEU:HD13	1.43	1.47
1:A:2427:LEU:CD1	1:G:143:LEU:HB3	1.48	1.42
1:A:143:LEU:HB3	1:C:2427:LEU:CD1	1.48	1.41
1:C:143:LEU:HB3	1:E:2427:LEU:CD1	1.50	1.39
1:E:143:LEU:HB3	1:G:2427:LEU:CD1	1.49	1.39
1:E:4845:ILE:HD12	1:G:4819:TYR:CD1	1.65	1.32
1:C:4845:ILE:HD12	1:E:4819:TYR:CD1	1.65	1.32
1:A:4819:TYR:CD1	1:G:4845:ILE:HD12	1.66	1.28
1:A:4845:ILE:HD12	1:C:4819:TYR:CD1	1.67	1.27
1:G:2327:ARG:O	1:G:2328:ARG:CG	1.83	1.27
1:C:4845:ILE:CD1	1:E:4819:TYR:CD1	2.20	1.25
1:A:2327:ARG:O	1:A:2328:ARG:CG	1.83	1.23
1:A:4819:TYR:O	1:A:4823:ARG:HD3	1.34	1.23
1:A:4819:TYR:CD1	1:G:4845:ILE:CD1	2.22	1.23
1:A:4845:ILE:CD1	1:C:4819:TYR:CD1	2.22	1.22
1:E:4845:ILE:CD1	1:G:4819:TYR:CD1	2.21	1.22
1:G:4819:TYR:O	1:G:4823:ARG:HD3	1.34	1.22
1:C:4819:TYR:O	1:C:4823:ARG:HD3	1.36	1.21
1:A:4862:ILE:HG22	1:C:4868:ILE:HD12	1.30	1.14
1:C:4862:ILE:HG22	1:E:4868:ILE:HD12	1.30	1.13
1:G:2327:ARG:O	1:G:2328:ARG:HG2	0.95	1.13
1:E:4862:ILE:HG22	1:G:4868:ILE:HD12	1.32	1.12
1:A:2327:ARG:O	1:A:2328:ARG:HG2	0.95	1.11
1:C:4845:ILE:HD13	1:E:4819:TYR:CE1	1.86	1.09
1:A:4819:TYR:CE1	1:G:4845:ILE:HD13	1.87	1.08
1:A:4868:ILE:HD12	1:G:4862:ILE:HG22	1.31	1.08
1:E:4845:ILE:HD13	1:G:4819:TYR:CE1	1.86	1.08
1:A:4845:ILE:HD13	1:C:4819:TYR:CE1	1.88	1.07
1:A:2427:LEU:HD13	1:G:143:LEU:CG	1.83	1.06
1:A:4858:ILE:HD12	1:C:4867:ILE:HG21	1.36	1.06
1:A:143:LEU:CG	1:C:2427:LEU:HD13	1.84	1.06
1:C:143:LEU:CG	1:E:2427:LEU:HD13	1.85	1.06
1:C:4858:ILE:HD12	1:E:4867:ILE:HG21	1.38	1.06
1:E:143:LEU:CG	1:G:2427:LEU:HD13	1.83	1.06
1:E:143:LEU:CD2	1:G:2427:LEU:HD13	1.87	1.05
1:A:4867:ILE:HG21	1:G:4858:ILE:HD12	1.36	1.04
1:A:2427:LEU:HD13	1:G:143:LEU:CD2	1.87	1.03
1:C:143:LEU:CD2	1:E:2427:LEU:HD13	1.88	1.03
1:A:143:LEU:CD2	1:C:2427:LEU:HD13	1.88	1.03
1:A:2427:LEU:CD1	1:G:143:LEU:HD22	1.89	1.03
1:E:4858:ILE:HD12	1:G:4867:ILE:HG21	1.36	1.02

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:143:LEU:HD22	1:E:2427:LEU:CD1	1.90	1.01
1:E:143:LEU:HD22	1:G:2427:LEU:CD1	1.89	1.00
1:A:143:LEU:HD22	1:C:2427:LEU:CD1	1.90	1.00
1:C:143:LEU:CB	1:E:2427:LEU:CD1	2.25	0.97
1:A:143:LEU:CB	1:C:2427:LEU:CD1	2.23	0.97
1:A:2427:LEU:CD1	1:G:143:LEU:CB	2.22	0.96
1:A:2427:LEU:HD13	1:G:143:LEU:HB3	0.99	0.96
1:A:143:LEU:HB3	1:C:2427:LEU:HD13	0.98	0.96
1:C:4862:ILE:CG2	1:E:4868:ILE:HD12	1.96	0.96
1:E:143:LEU:HB3	1:G:2427:LEU:HD13	1.00	0.95
1:C:143:LEU:HB3	1:E:2427:LEU:HD13	0.99	0.95
1:A:143:LEU:HD11	1:A:207:PHE:HD2	1.32	0.94
1:A:2427:LEU:CD1	1:G:143:LEU:CD2	2.45	0.94
1:A:143:LEU:CD2	1:C:2427:LEU:CD1	2.45	0.94
1:A:143:LEU:HD22	1:C:2427:LEU:CD2	1.98	0.94
1:A:4862:ILE:CG2	1:C:4868:ILE:HD12	1.96	0.94
1:C:76:ARG:HD3	1:E:3891:TRP:CD2	2.03	0.93
1:C:209:GLN:HE21	1:E:2327:ARG:HH11	1.13	0.93
1:E:143:LEU:CD2	1:G:2427:LEU:CD1	2.44	0.93
1:E:4862:ILE:CG2	1:G:4868:ILE:HD12	1.98	0.93
1:A:143:LEU:HB3	1:C:2427:LEU:HD12	1.51	0.92
1:C:76:ARG:HH21	1:C:76:ARG:HB3	1.33	0.92
1:C:143:LEU:CD2	1:E:2427:LEU:CD1	2.46	0.92
1:E:143:LEU:HD22	1:G:2427:LEU:CD2	1.99	0.92
1:A:76:ARG:HH21	1:A:76:ARG:HG3	1.34	0.92
1:C:143:LEU:HD22	1:E:2427:LEU:CD2	2.00	0.92
1:A:4868:ILE:HD12	1:G:4862:ILE:CG2	1.98	0.92
1:A:2427:LEU:CD2	1:G:143:LEU:HD22	1.99	0.91
1:G:4823:ARG:NH1	1:G:4823:ARG:HB2	1.86	0.90
1:A:2427:LEU:HD12	1:G:143:LEU:HB3	1.51	0.90
1:C:143:LEU:HB3	1:E:2427:LEU:HD12	1.53	0.90
1:C:4823:ARG:NH2	1:C:4823:ARG:HB2	1.87	0.90
1:E:143:LEU:HB3	1:G:2427:LEU:HD12	1.51	0.89
1:A:4819:TYR:CE1	1:G:4845:ILE:CD1	2.52	0.89
1:A:4823:ARG:NH2	1:A:4823:ARG:HB2	1.87	0.89
1:C:2323:ARG:HH21	1:C:2323:ARG:HG3	1.35	0.89
1:E:4845:ILE:CD1	1:G:4819:TYR:CE1	2.50	0.88
1:C:4862:ILE:CG2	1:E:4868:ILE:CD1	2.52	0.88
1:A:4845:ILE:CD1	1:C:4819:TYR:CE1	2.53	0.88
1:E:143:LEU:CB	1:G:2427:LEU:CD1	2.23	0.88
1:A:143:LEU:HD11	1:A:207:PHE:CD2	2.08	0.87

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4868:ILE:CD1	1:G:4862:ILE:CG2	2.53	0.86
1:A:4862:ILE:CG2	1:C:4868:ILE:CD1	2.52	0.86
1:A:4862:ILE:HD11	1:C:4757:ILE:HD12	1.58	0.86
1:G:4819:TYR:O	1:G:4823:ARG:CD	2.23	0.86
1:E:4862:ILE:HD11	1:G:4757:ILE:HD12	1.58	0.85
1:E:4862:ILE:CD1	1:G:4757:ILE:HD12	2.07	0.84
1:A:4757:ILE:HD12	1:G:4862:ILE:CD1	2.07	0.84
1:A:4862:ILE:CD1	1:C:4757:ILE:HD12	2.08	0.84
1:E:4862:ILE:CG2	1:G:4868:ILE:CD1	2.54	0.84
1:A:4819:TYR:O	1:A:4823:ARG:CD	2.24	0.84
1:A:4757:ILE:HD12	1:G:4862:ILE:HD11	1.58	0.84
1:C:209:GLN:HE21	1:E:2327:ARG:NH1	1.74	0.83
1:C:4862:ILE:HD11	1:E:4757:ILE:HD12	1.60	0.83
1:C:4845:ILE:CD1	1:E:4819:TYR:CE1	2.51	0.82
1:C:4862:ILE:CD1	1:E:4757:ILE:HD12	2.10	0.82
1:C:797:GLY:HA2	1:C:1621:CYS:O	1.82	0.79
1:A:797:GLY:HA2	1:A:1621:CYS:O	1.82	0.79
1:C:76:ARG:HH21	1:C:76:ARG:CB	1.94	0.79
1:E:797:GLY:HA2	1:E:1621:CYS:O	1.82	0.79
1:A:189:GLU:OE2	1:C:2323:ARG:CD	2.32	0.78
1:G:797:GLY:HA2	1:G:1621:CYS:O	1.82	0.78
1:C:2328:ARG:CB	1:C:2328:ARG:HH11	1.97	0.78
1:A:2427:LEU:HD13	1:G:143:LEU:HD22	1.59	0.76
1:A:143:LEU:HD22	1:C:2427:LEU:HD13	1.60	0.76
1:A:1219:LYS:H	1:A:1240:ALA:HB2	1.51	0.76
1:E:2328:ARG:HH11	1:E:2328:ARG:CB	1.99	0.76
1:C:4819:TYR:O	1:C:4823:ARG:CD	2.27	0.75
1:C:143:LEU:HD11	1:C:207:PHE:HD2	1.51	0.75
1:G:143:LEU:HD11	1:G:207:PHE:HD2	1.50	0.75
1:C:1219:LYS:H	1:C:1240:ALA:HB2	1.51	0.75
1:E:1219:LYS:H	1:E:1240:ALA:HB2	1.51	0.75
1:G:2327:ARG:C	1:G:2328:ARG:HG2	2.03	0.74
1:E:143:LEU:HD22	1:G:2427:LEU:HD22	1.70	0.74
1:G:1219:LYS:H	1:G:1240:ALA:HB2	1.51	0.74
1:C:4845:ILE:HD12	1:E:4819:TYR:CG	2.22	0.74
1:G:143:LEU:HD11	1:G:207:PHE:CD2	2.23	0.73
1:C:143:LEU:HD22	1:E:2427:LEU:HD22	1.69	0.73
1:C:143:LEU:HD11	1:C:207:PHE:CD2	2.23	0.73
1:A:143:LEU:HD22	1:C:2427:LEU:HD22	1.69	0.73
1:E:2328:ARG:HH11	1:E:2328:ARG:CA	2.02	0.73
1:A:189:GLU:OE2	1:C:2323:ARG:HD3	1.88	0.72

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2328:ARG:HH11	1:C:2328:ARG:CA	2.02	0.72
1:A:76:ARG:HG3	1:A:76:ARG:NH2	1.99	0.72
1:C:842:GLN:HE21	1:C:849:ASP:H	1.36	0.72
1:G:842:GLN:HE21	1:G:849:ASP:H	1.36	0.72
1:A:2427:LEU:HD22	1:G:143:LEU:HD22	1.70	0.72
1:C:76:ARG:CD	1:E:3891:TRP:CG	2.72	0.71
1:E:842:GLN:HE21	1:E:849:ASP:H	1.36	0.71
1:A:842:GLN:HE21	1:A:849:ASP:H	1.36	0.71
1:G:4823:ARG:HB2	1:G:4823:ARG:CZ	2.20	0.71
1:E:4845:ILE:HD12	1:G:4819:TYR:CG	2.24	0.71
1:C:2314:VAL:HG23	1:C:2317:ASN:HB2	1.73	0.71
1:A:728:ASP:HA	1:A:748:LEU:HA	1.72	0.70
1:E:4862:ILE:CD1	1:G:4757:ILE:CD1	2.70	0.70
1:C:728:ASP:HA	1:C:748:LEU:HA	1.72	0.70
1:G:728:ASP:HA	1:G:748:LEU:HA	1.72	0.70
1:C:4845:ILE:CD1	1:E:4819:TYR:CG	2.73	0.70
1:E:2314:VAL:HG23	1:E:2317:ASN:HB2	1.74	0.70
1:A:2327:ARG:C	1:A:2328:ARG:HG2	2.03	0.70
1:A:4757:ILE:CD1	1:G:4862:ILE:CD1	2.70	0.70
1:E:728:ASP:HA	1:E:748:LEU:HA	1.72	0.70
1:E:4845:ILE:CD1	1:G:4819:TYR:CG	2.75	0.69
1:C:4823:ARG:HB2	1:C:4823:ARG:CZ	2.21	0.69
1:A:4823:ARG:HB2	1:A:4823:ARG:CZ	2.20	0.69
1:A:4845:ILE:HD12	1:C:4819:TYR:CG	2.25	0.69
1:A:4862:ILE:CD1	1:C:4757:ILE:CD1	2.70	0.69
1:G:590:LYS:H	1:G:593:HIS:HD2	1.41	0.68
1:A:590:LYS:H	1:A:593:HIS:HD2	1.41	0.68
1:A:4845:ILE:CD1	1:C:4819:TYR:CG	2.76	0.68
1:C:2323:ARG:HG3	1:C:2323:ARG:NH2	2.05	0.68
1:A:4757:ILE:CD1	1:G:4862:ILE:HD12	2.24	0.68
1:A:4862:ILE:HD12	1:C:4757:ILE:CD1	2.24	0.68
1:E:4862:ILE:HD12	1:G:4757:ILE:CD1	2.24	0.68
1:E:1089:ARG:HH22	1:E:1600:PRO:HG3	1.59	0.68
1:A:2427:LEU:HD13	1:G:143:LEU:HB2	1.68	0.68
1:C:1089:ARG:HH22	1:C:1600:PRO:HG3	1.59	0.68
1:C:590:LYS:H	1:C:593:HIS:HD2	1.41	0.68
1:A:4819:TYR:CG	1:G:4845:ILE:HD12	2.24	0.67
1:E:660:PHE:HB3	1:E:787:LEU:HD22	1.77	0.67
1:A:1089:ARG:HH22	1:A:1600:PRO:HG3	1.59	0.67
1:C:4862:ILE:CD1	1:E:4757:ILE:CD1	2.72	0.67
1:G:1089:ARG:HH22	1:G:1600:PRO:HG3	1.59	0.67

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4819:TYR:CG	1:G:4845:ILE:CD1	2.76	0.67
1:G:660:PHE:HB3	1:G:787:LEU:HD22	1.77	0.67
1:E:590:LYS:H	1:E:593:HIS:HD2	1.41	0.66
1:C:143:LEU:HD22	1:E:2427:LEU:HD13	1.59	0.66
1:C:660:PHE:HB3	1:C:787:LEU:HD22	1.77	0.66
1:C:4862:ILE:HD12	1:E:4757:ILE:CD1	2.26	0.65
1:G:4796:LYS:NZ	1:G:4807:CYS:SG	2.68	0.65
1:C:1125:ASP:HA	1:C:1598:ARG:HB2	1.79	0.65
1:A:660:PHE:HB3	1:A:787:LEU:HD22	1.77	0.65
1:G:1125:ASP:HA	1:G:1598:ARG:HB2	1.79	0.65
1:C:4835:PRO:HG3	1:C:4844:ARG:HE	1.62	0.65
1:E:1125:ASP:HA	1:E:1598:ARG:HB2	1.78	0.65
1:A:189:GLU:OE2	1:C:2323:ARG:HD2	1.96	0.65
1:E:4823:ARG:NH2	1:E:4823:ARG:HB3	2.12	0.65
1:G:2314:VAL:HG23	1:G:2317:ASN:HB2	1.79	0.65
1:E:4835:PRO:HG3	1:E:4844:ARG:HE	1.62	0.65
1:A:1125:ASP:HA	1:A:1598:ARG:HB2	1.79	0.65
1:A:2314:VAL:HG23	1:A:2317:ASN:HB2	1.79	0.65
1:A:4796:LYS:NZ	1:A:4807:CYS:SG	2.68	0.64
1:C:207:PHE:CZ	1:E:2326:ILE:CB	2.80	0.64
1:E:4826:GLY:O	1:G:4823:ARG:NH2	2.31	0.64
1:G:4835:PRO:HG3	1:G:4844:ARG:HE	1.62	0.64
1:A:503:ASP:HA	1:A:561:ARG:HH22	1.63	0.64
1:C:4796:LYS:NZ	1:C:4807:CYS:SG	2.68	0.64
1:G:243:GLU:HA	1:G:263:GLU:O	1.98	0.64
1:A:2706:PRO:HB3	1:A:2855:LYS:HG3	1.80	0.64
1:C:503:ASP:HA	1:C:561:ARG:HH22	1.63	0.64
1:E:503:ASP:HA	1:E:561:ARG:HH22	1.63	0.64
1:A:2327:ARG:O	1:A:2328:ARG:CB	2.43	0.64
1:A:4823:ARG:NH1	1:G:4826:GLY:O	2.31	0.64
1:G:503:ASP:HA	1:G:561:ARG:HH22	1.63	0.64
1:E:243:GLU:HA	1:E:263:GLU:O	1.98	0.64
1:A:4835:PRO:HG3	1:A:4844:ARG:HE	1.62	0.63
1:C:1465:VAL:N	1:C:1483:SER:O	2.31	0.63
1:G:123:HIS:HD2	1:G:126:SER:H	1.47	0.63
1:G:1465:VAL:N	1:G:1483:SER:O	2.31	0.63
1:A:123:HIS:HD2	1:A:126:SER:H	1.47	0.63
1:C:1446:ILE:O	1:C:1540:PHE:HB2	1.98	0.63
1:E:2315:GLU:HA	1:E:2315:GLU:OE2	1.97	0.63
1:G:2706:PRO:HB3	1:G:2855:LYS:HG3	1.80	0.63
1:C:76:ARG:HD2	1:E:3891:TRP:CD1	2.34	0.63

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1446:ILE:O	1:E:1540:PHE:HB2	1.98	0.63
1:C:123:HIS:HD2	1:C:126:SER:H	1.47	0.63
1:C:374:TYR:HB2	1:C:389:ARG:HB3	1.81	0.63
1:E:123:HIS:HD2	1:E:126:SER:H	1.47	0.63
1:E:143:LEU:HB2	1:G:2427:LEU:HD13	1.68	0.63
1:E:374:TYR:HB2	1:E:389:ARG:HB3	1.81	0.63
1:A:4958:CYS:SG	1:A:4959:PHE:N	2.72	0.62
1:C:243:GLU:HA	1:C:263:GLU:O	1.98	0.62
1:G:374:TYR:HB2	1:G:389:ARG:HB3	1.81	0.62
1:G:4958:CYS:SG	1:G:4959:PHE:N	2.72	0.62
1:A:1465:VAL:N	1:A:1483:SER:O	2.31	0.62
1:E:1465:VAL:N	1:E:1483:SER:O	2.31	0.62
1:E:2706:PRO:HB3	1:E:2855:LYS:HG3	1.80	0.62
1:G:189:GLU:HG2	1:G:189:GLU:O	2.00	0.62
1:G:2327:ARG:O	1:G:2328:ARG:CB	2.43	0.62
1:A:243:GLU:HA	1:A:263:GLU:O	1.98	0.62
1:A:374:TYR:HB2	1:A:389:ARG:HB3	1.81	0.62
1:C:1265:HIS:HD2	1:C:1267:HIS:H	1.48	0.62
1:C:2706:PRO:HB3	1:C:2855:LYS:HG3	1.80	0.62
1:C:4958:CYS:SG	1:C:4959:PHE:N	2.72	0.62
1:G:1446:ILE:O	1:G:1540:PHE:HB2	1.98	0.62
1:A:143:LEU:HD22	1:C:2427:LEU:HD11	1.81	0.62
1:C:4791:ARG:HD2	1:C:4808:ASP:HB3	1.82	0.62
1:E:4958:CYS:SG	1:E:4959:PHE:N	2.72	0.62
1:C:462:TYR:O	1:C:485:ARG:NH1	2.33	0.62
1:E:4791:ARG:HD2	1:E:4808:ASP:HB3	1.82	0.62
1:A:4845:ILE:HD12	1:C:4819:TYR:HD1	1.57	0.62
1:E:189:GLU:O	1:E:189:GLU:HG2	2.00	0.62
1:G:1265:HIS:HD2	1:G:1267:HIS:H	1.48	0.62
1:C:189:GLU:O	1:C:189:GLU:HG2	2.00	0.62
1:E:143:LEU:HD22	1:G:2427:LEU:HD11	1.81	0.62
1:G:4791:ARG:HD2	1:G:4808:ASP:HB3	1.82	0.62
1:A:462:TYR:O	1:A:485:ARG:NH1	2.33	0.62
1:E:1265:HIS:HD2	1:E:1267:HIS:H	1.48	0.62
1:A:207:PHE:CZ	1:C:2326:ILE:CB	2.82	0.62
1:A:2427:LEU:HD11	1:G:143:LEU:CD2	2.30	0.62
1:A:1265:HIS:HD2	1:A:1267:HIS:H	1.48	0.61
1:A:1446:ILE:O	1:A:1540:PHE:HB2	1.98	0.61
1:A:2427:LEU:HD11	1:G:143:LEU:HD22	1.81	0.61
1:G:462:TYR:O	1:G:485:ARG:NH1	2.33	0.61
1:G:4145:ARG:NH2	1:G:4963:TYR:OH	2.33	0.61

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4791:ARG:HD2	1:A:4808:ASP:HB3	1.82	0.61
1:G:143:LEU:HD12	1:G:143:LEU:O	2.01	0.61
1:C:143:LEU:HB2	1:E:2427:LEU:HD13	1.69	0.61
1:C:4145:ARG:NH2	1:C:4963:TYR:OH	2.33	0.61
1:E:143:LEU:HD12	1:E:143:LEU:O	2.01	0.61
1:E:4145:ARG:NH2	1:E:4963:TYR:OH	2.33	0.61
1:A:2315:GLU:OE2	1:A:2315:GLU:HA	2.00	0.61
1:E:207:PHE:CZ	1:G:2326:ILE:CB	2.84	0.61
1:E:4005:VAL:HG21	1:E:4115:ARG:HD2	1.83	0.61
1:G:3939:SER:OG	1:G:3940:ARG:N	2.34	0.61
1:A:4145:ARG:NH2	1:A:4963:TYR:OH	2.33	0.61
1:C:143:LEU:HD12	1:C:143:LEU:O	2.01	0.61
1:C:4005:VAL:HG21	1:C:4115:ARG:HD2	1.83	0.61
1:E:462:TYR:O	1:E:485:ARG:NH1	2.33	0.61
1:A:189:GLU:O	1:A:189:GLU:HG2	2.00	0.61
1:A:3939:SER:OG	1:A:3940:ARG:N	2.34	0.61
1:A:4826:GLY:O	1:C:4823:ARG:NH1	2.34	0.61
1:A:4868:ILE:CD1	1:G:4862:ILE:HG22	2.15	0.60
1:G:1443:VAL:HG12	1:G:1543:VAL:HG22	1.83	0.60
1:G:2315:GLU:HA	1:G:2315:GLU:OE2	2.00	0.60
1:A:143:LEU:O	1:A:143:LEU:HD12	2.01	0.60
1:A:4005:VAL:HG21	1:A:4115:ARG:HD2	1.83	0.60
1:A:4848:ASP:OD1	1:C:4823:ARG:NE	2.33	0.60
1:E:4165:GLN:HG2	1:E:4594:LEU:HD11	1.84	0.60
1:G:832:LEU:O	1:G:1614:ARG:NH1	2.35	0.60
1:E:1932:ASP:OD1	1:E:1932:ASP:N	2.35	0.60
1:G:1932:ASP:OD1	1:G:1932:ASP:N	2.35	0.60
1:A:4165:GLN:HG2	1:A:4594:LEU:HD11	1.84	0.60
1:C:4165:GLN:HG2	1:C:4594:LEU:HD11	1.84	0.60
1:E:2328:ARG:HH11	1:E:2328:ARG:HA	1.66	0.60
1:E:3939:SER:OG	1:E:3940:ARG:N	2.34	0.60
1:C:4791:ARG:HD2	1:C:4808:ASP:CB	2.32	0.60
1:E:4796:LYS:NZ	1:E:4807:CYS:SG	2.68	0.60
1:A:832:LEU:O	1:A:1614:ARG:NH1	2.35	0.60
1:G:2893:ILE:HG13	1:G:2894:LEU:HD12	1.84	0.60
1:C:832:LEU:O	1:C:1614:ARG:NH1	2.35	0.60
1:C:2893:ILE:HG13	1:C:2894:LEU:HD12	1.84	0.60
1:G:4165:GLN:HG2	1:G:4594:LEU:HD11	1.84	0.60
1:A:2893:ILE:HG13	1:A:2894:LEU:HD12	1.84	0.60
1:C:76:ARG:HD3	1:E:3891:TRP:CG	2.36	0.59
1:E:2893:ILE:HG13	1:E:2894:LEU:HD12	1.84	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:2138:GLU:O	1:G:2141:LYS:NZ	2.34	0.59
1:A:143:LEU:HB2	1:C:2427:LEU:HD13	1.68	0.59
1:E:1224:LEU:HD22	1:E:1227:PHE:HB2	1.84	0.59
1:E:4791:ARG:HD2	1:E:4808:ASP:CB	2.32	0.59
1:G:4005:VAL:HG21	1:G:4115:ARG:HD2	1.83	0.59
1:E:832:LEU:O	1:E:1614:ARG:NH1	2.35	0.59
1:G:3845:GLN:HG3	1:G:3923:GLU:HG3	1.85	0.59
1:A:1443:VAL:HG12	1:A:1543:VAL:HG22	1.83	0.59
1:C:235:ARG:NH1	1:C:268:SER:O	2.36	0.59
1:C:4515:ASN:ND2	1:C:4740:PHE:O	2.33	0.59
1:G:620:CYS:SG	1:G:621:HIS:N	2.74	0.59
1:G:235:ARG:NH1	1:G:268:SER:O	2.36	0.59
1:A:143:LEU:CD2	1:C:2427:LEU:HD11	2.30	0.59
1:C:620:CYS:SG	1:C:621:HIS:N	2.74	0.59
1:C:4897:ASP:OD1	1:C:4897:ASP:N	2.35	0.59
1:G:4791:ARG:HD2	1:G:4808:ASP:CB	2.32	0.59
1:A:620:CYS:SG	1:A:621:HIS:N	2.74	0.59
1:C:62:LEU:HB3	1:C:276:ARG:HH21	1.68	0.59
1:E:235:ARG:NH1	1:E:268:SER:O	2.36	0.59
1:E:258:ARG:NH1	1:E:316:LEU:O	2.36	0.59
1:C:1224:LEU:HD22	1:C:1227:PHE:HB2	1.84	0.59
1:G:258:ARG:NH1	1:G:316:LEU:O	2.36	0.59
1:A:235:ARG:NH1	1:A:268:SER:O	2.36	0.59
1:C:143:LEU:CD2	1:E:2427:LEU:HD11	2.33	0.59
1:E:1443:VAL:HG12	1:E:1543:VAL:HG22	1.83	0.59
1:A:3845:GLN:HG3	1:A:3923:GLU:HG3	1.85	0.58
1:E:143:LEU:CD2	1:G:2427:LEU:HD11	2.30	0.58
1:G:4515:ASN:ND2	1:G:4740:PHE:O	2.33	0.58
1:A:188:SER:OG	1:A:190:ARG:NH2	2.35	0.58
1:A:2540:GLU:O	1:A:2543:ALA:HB3	2.03	0.58
1:A:2427:LEU:CG	1:G:143:LEU:HD22	2.34	0.58
1:A:4791:ARG:HD2	1:A:4808:ASP:CB	2.32	0.58
1:C:2540:GLU:O	1:C:2543:ALA:HB3	2.03	0.58
1:E:62:LEU:HB3	1:E:276:ARG:HH21	1.68	0.58
1:E:2540:GLU:O	1:E:2543:ALA:HB3	2.03	0.58
1:A:805:GLY:HA2	1:A:810:GLU:HB2	1.85	0.58
1:C:2328:ARG:HH11	1:C:2328:ARG:CG	2.14	0.58
1:E:620:CYS:SG	1:E:621:HIS:N	2.74	0.58
1:G:1224:LEU:HD22	1:G:1227:PHE:HB2	1.84	0.58
1:C:1443:VAL:HG12	1:C:1543:VAL:HG22	1.83	0.58
1:C:1644:LEU:HD23	1:C:1651:LEU:HA	1.86	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2328:ARG:HH11	1:E:2328:ARG:CG	2.14	0.58
1:A:143:LEU:HD22	1:C:2427:LEU:CG	2.34	0.58
1:A:1224:LEU:HD22	1:A:1227:PHE:HB2	1.84	0.58
1:C:258:ARG:NH1	1:C:316:LEU:O	2.36	0.58
1:A:1304:LEU:HB2	1:A:1541:PRO:HG2	1.86	0.58
1:C:1102:TYR:HB2	1:C:1165:MET:HG2	1.86	0.58
1:G:1102:TYR:HB2	1:G:1165:MET:HG2	1.86	0.58
1:G:1304:LEU:HB2	1:G:1541:PRO:HG2	1.86	0.58
1:A:258:ARG:NH1	1:A:316:LEU:O	2.36	0.58
1:E:3845:GLN:HG3	1:E:3923:GLU:HG3	1.85	0.58
1:A:62:LEU:HB3	1:A:276:ARG:HH21	1.68	0.58
1:C:4862:ILE:HG23	1:E:4868:ILE:CD1	2.34	0.58
2:F:7:ILE:HB	2:F:71:ARG:HG3	1.86	0.58
1:G:62:LEU:HB3	1:G:276:ARG:HH21	1.68	0.58
1:G:2540:GLU:O	1:G:2543:ALA:HB3	2.03	0.58
1:A:778:MET:SD	1:A:1468:THR:OG1	2.62	0.58
1:A:1682:GLU:HG3	1:A:1782:PHE:HB2	1.85	0.58
2:B:7:ILE:HB	2:B:71:ARG:HG3	1.86	0.58
1:C:3939:SER:OG	1:C:3940:ARG:N	2.34	0.58
1:E:143:LEU:HD22	1:G:2427:LEU:CG	2.33	0.58
1:E:2897:LEU:HB3	1:E:2902:TYR:HB2	1.86	0.58
1:A:185:SER:HG	1:A:190:ARG:H	1.50	0.57
1:C:778:MET:SD	1:C:1468:THR:OG1	2.62	0.57
1:A:218:SER:OG	1:A:219:SER:N	2.37	0.57
1:E:1682:GLU:HG3	1:E:1782:PHE:HB2	1.85	0.57
1:G:2669:CYS:O	1:G:2672:ALA:HB3	2.04	0.57
2:H:90:VAL:HG23	2:H:91:ILE:HG12	1.86	0.57
1:A:2138:GLU:O	1:A:2141:LYS:NZ	2.34	0.57
1:A:2897:LEU:HB3	1:A:2902:TYR:HB2	1.86	0.57
1:C:1682:GLU:HG3	1:C:1782:PHE:HB2	1.85	0.57
1:E:778:MET:SD	1:E:1468:THR:OG1	2.62	0.57
1:E:1644:LEU:HD23	1:E:1651:LEU:HA	1.86	0.57
1:E:2138:GLU:O	1:E:2141:LYS:NZ	2.34	0.57
1:E:2669:CYS:O	1:E:2672:ALA:HB3	2.04	0.57
1:A:3775:GLN:OE1	1:A:3852:ASN:ND2	2.38	0.57
1:C:3845:GLN:HG3	1:C:3923:GLU:HG3	1.85	0.57
1:E:1102:TYR:HB2	1:E:1165:MET:HG2	1.86	0.57
1:G:218:SER:OG	1:G:219:SER:N	2.37	0.57
1:G:676:GLU:HB2	1:G:803:LEU:HB2	1.87	0.57
1:G:805:GLY:HA2	1:G:810:GLU:HB2	1.85	0.57
1:G:3775:GLN:OE1	1:G:3852:ASN:ND2	2.38	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1102:TYR:HB2	1:A:1165:MET:HG2	1.86	0.57
1:E:143:LEU:HD22	1:G:2427:LEU:HD13	1.58	0.57
1:E:143:LEU:HD11	1:E:207:PHE:CD2	2.40	0.57
1:E:805:GLY:HA2	1:E:810:GLU:HB2	1.85	0.57
1:C:766:ILE:HB	1:C:779:PHE:HB2	1.87	0.57
1:C:1104:GLU:HA	1:C:1163:GLY:HA2	1.87	0.57
1:C:2669:CYS:O	1:C:2672:ALA:HB3	2.04	0.57
2:D:90:VAL:HG23	2:D:91:ILE:HG12	1.86	0.57
1:G:778:MET:SD	1:G:1468:THR:OG1	2.62	0.57
1:A:1644:LEU:HD23	1:A:1651:LEU:HA	1.86	0.57
1:A:2669:CYS:O	1:A:2672:ALA:HB3	2.04	0.57
2:D:7:ILE:HB	2:D:71:ARG:HG3	1.86	0.57
1:E:3775:GLN:OE1	1:E:3852:ASN:ND2	2.38	0.57
1:G:1714:TYR:OH	1:G:1718:ARG:NH2	2.38	0.57
1:E:1104:GLU:HA	1:E:1163:GLY:HA2	1.87	0.57
1:G:1104:GLU:HA	1:G:1163:GLY:HA2	1.87	0.57
1:G:1736:ILE:HG22	1:G:1738:LEU:H	1.70	0.57
1:G:3667:GLN:HA	1:G:3670:LEU:HB2	1.87	0.57
1:A:766:ILE:HB	1:A:779:PHE:HB2	1.87	0.57
1:A:866:PRO:HG3	1:A:1009:ARG:HD2	1.86	0.57
1:A:1736:ILE:HG22	1:A:1738:LEU:H	1.70	0.57
1:E:4848:ASP:OD1	1:G:4823:ARG:NE	2.35	0.57
1:A:3667:GLN:HA	1:A:3670:LEU:HB2	1.87	0.57
1:A:4862:ILE:HG23	1:C:4868:ILE:CD1	2.34	0.57
1:C:676:GLU:HB2	1:C:803:LEU:HB2	1.87	0.57
1:C:1304:LEU:HB2	1:C:1541:PRO:HG2	1.86	0.57
1:C:2328:ARG:HH11	1:C:2328:ARG:HA	1.68	0.57
1:C:2897:LEU:HB3	1:C:2902:TYR:HB2	1.86	0.57
1:C:3775:GLN:OE1	1:C:3852:ASN:ND2	2.38	0.57
1:E:866:PRO:HG3	1:E:1009:ARG:HD2	1.86	0.57
1:E:1304:LEU:HB2	1:E:1541:PRO:HG2	1.86	0.57
2:H:7:ILE:HB	2:H:71:ARG:HG3	1.86	0.57
1:A:4897:ASP:OD1	1:A:4897:ASP:N	2.35	0.56
1:A:629:GLN:OE1	1:A:1669:ASN:ND2	2.38	0.56
1:C:866:PRO:HG3	1:C:1009:ARG:HD2	1.86	0.56
1:G:629:GLN:OE1	1:G:1669:ASN:ND2	2.38	0.56
1:G:1682:GLU:HG3	1:G:1782:PHE:HB2	1.85	0.56
1:A:1104:GLU:HA	1:A:1163:GLY:HA2	1.87	0.56
1:C:143:LEU:HD22	1:E:2427:LEU:HD11	1.83	0.56
1:E:748:LEU:HD23	1:E:750:ARG:HG3	1.86	0.56
1:E:766:ILE:HB	1:E:779:PHE:HB2	1.87	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1009:ARG:O	1:E:1013:ARG:NH2	2.39	0.56
1:G:1644:LEU:HD23	1:G:1651:LEU:HA	1.86	0.56
1:A:1009:ARG:O	1:A:1013:ARG:NH2	2.39	0.56
1:C:1111:GLY:H	1:C:1156:TRP:HZ2	1.54	0.56
1:E:3667:GLN:HA	1:E:3670:LEU:HB2	1.87	0.56
1:E:3729:GLN:O	1:E:3733:HIS:ND1	2.36	0.56
1:G:748:LEU:HD23	1:G:750:ARG:HG3	1.86	0.56
1:G:2897:LEU:HB3	1:G:2902:TYR:HB2	1.86	0.56
1:A:748:LEU:HD23	1:A:750:ARG:HG3	1.86	0.56
1:C:2138:GLU:O	1:C:2141:LYS:NZ	2.34	0.56
1:E:676:GLU:HB2	1:E:803:LEU:HB2	1.87	0.56
1:E:1678:SER:OG	2:F:36:PHE:O	2.24	0.56
1:G:766:ILE:HB	1:G:779:PHE:HB2	1.87	0.56
1:E:1736:ILE:HG22	1:E:1738:LEU:H	1.70	0.56
1:G:1111:GLY:H	1:G:1156:TRP:HZ2	1.54	0.56
1:G:1425:THR:N	1:G:1510:VAL:O	2.39	0.56
1:A:1678:SER:OG	2:B:36:PHE:O	2.24	0.56
1:A:4823:ARG:NE	1:G:4848:ASP:OD1	2.35	0.56
1:C:76:ARG:NE	1:E:3891:TRP:HB3	2.21	0.56
1:C:805:GLY:HA2	1:C:810:GLU:HB2	1.85	0.56
1:E:4862:ILE:HG23	1:G:4868:ILE:CD1	2.36	0.56
1:G:606:ARG:HH22	1:G:1632:ILE:HG23	1.70	0.56
1:G:866:PRO:HG3	1:G:1009:ARG:HD2	1.86	0.56
1:C:218:SER:OG	1:C:219:SER:N	2.37	0.56
1:C:1714:TYR:OH	1:C:1718:ARG:NH2	2.38	0.56
2:F:90:VAL:HG23	2:F:91:ILE:HG12	1.86	0.56
1:G:3729:GLN:O	1:G:3733:HIS:ND1	2.36	0.56
1:A:1111:GLY:H	1:A:1156:TRP:HZ2	1.54	0.56
2:B:90:VAL:HG23	2:B:91:ILE:HG12	1.86	0.56
1:E:218:SER:OG	1:E:219:SER:N	2.37	0.56
1:C:606:ARG:HH22	1:C:1632:ILE:HG23	1.70	0.56
1:C:3667:GLN:HA	1:C:3670:LEU:HB2	1.87	0.56
1:E:1429:SER:HA	1:E:1507:ILE:HG12	1.88	0.56
1:E:2436:VAL:O	1:E:2466:LYS:NZ	2.39	0.56
1:C:143:LEU:HD22	1:E:2427:LEU:CG	2.35	0.55
1:C:1009:ARG:O	1:C:1013:ARG:NH2	2.39	0.55
1:C:1429:SER:HA	1:C:1507:ILE:HG12	1.88	0.55
1:C:1736:ILE:HG22	1:C:1738:LEU:H	1.70	0.55
1:A:993:GLU:OE1	1:A:1051:ARG:NH1	2.39	0.55
1:E:188:SER:OG	1:E:190:ARG:NH2	2.35	0.55
1:E:629:GLN:OE1	1:E:1669:ASN:ND2	2.38	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1009:ARG:O	1:G:1013:ARG:NH2	2.39	0.55
1:G:4897:ASP:N	1:G:4897:ASP:OD1	2.35	0.55
1:A:2712:ILE:O	1:A:2781:LYS:NZ	2.40	0.55
1:A:1144:ARG:NH2	1:A:1150:GLU:OE1	2.40	0.55
2:B:78:PRO:HD3	2:B:96:THR:HG22	1.88	0.55
1:E:624:ALA:HB2	1:E:1667:LEU:HD12	1.88	0.55
1:A:676:GLU:HB2	1:A:803:LEU:HB2	1.87	0.55
1:A:3804:LEU:HD13	1:A:3910:ALA:HB2	1.89	0.55
1:C:624:ALA:HB2	1:C:1667:LEU:HD12	1.88	0.55
2:D:78:PRO:HD3	2:D:96:THR:HG22	1.88	0.55
1:E:606:ARG:HH22	1:E:1632:ILE:HG23	1.70	0.55
1:G:679:VAL:HA	1:G:800:VAL:HG12	1.89	0.55
1:A:624:ALA:HB2	1:A:1667:LEU:HD12	1.88	0.55
1:C:748:LEU:HD23	1:C:750:ARG:HG3	1.86	0.55
1:E:1425:THR:N	1:E:1510:VAL:O	2.39	0.55
1:G:4033:PHE:HA	1:G:4036:TYR:HB2	1.88	0.55
1:C:1220:ASP:O	1:C:1224:LEU:N	2.40	0.55
1:C:1425:THR:N	1:C:1510:VAL:O	2.39	0.55
1:A:679:VAL:HA	1:A:800:VAL:HG12	1.89	0.55
1:A:1220:ASP:O	1:A:1224:LEU:N	2.40	0.55
1:C:629:GLN:OE1	1:C:1669:ASN:ND2	2.38	0.55
1:E:993:GLU:OE1	1:E:1051:ARG:NH1	2.39	0.55
1:E:4900:ASP:O	1:E:4902:VAL:N	2.39	0.55
1:G:2712:ILE:O	1:G:2781:LYS:NZ	2.40	0.55
1:G:3804:LEU:HD13	1:G:3910:ALA:HB2	1.89	0.55
1:G:4900:ASP:O	1:G:4902:VAL:N	2.39	0.55
1:A:606:ARG:HH22	1:A:1632:ILE:HG23	1.70	0.55
1:A:1425:THR:N	1:A:1510:VAL:O	2.39	0.55
1:A:4033:PHE:HA	1:A:4036:TYR:HB2	1.88	0.55
1:C:1144:ARG:NH2	1:C:1150:GLU:OE1	2.40	0.55
1:A:1714:TYR:OH	1:A:1718:ARG:NH2	2.38	0.55
1:C:2436:VAL:O	1:C:2466:LYS:NZ	2.39	0.55
1:A:1429:SER:HA	1:A:1507:ILE:HG12	1.88	0.54
1:C:76:ARG:CD	1:E:3891:TRP:CD2	2.83	0.54
1:C:849:ASP:OD2	1:C:1214:ARG:NH2	2.40	0.54
1:C:4033:PHE:HA	1:C:4036:TYR:HB2	1.88	0.54
1:C:4823:ARG:CZ	1:C:4823:ARG:CB	2.85	0.54
1:E:1220:ASP:O	1:E:1224:LEU:N	2.40	0.54
1:E:2712:ILE:O	1:E:2781:LYS:NZ	2.40	0.54
1:G:624:ALA:HB2	1:G:1667:LEU:HD12	1.88	0.54
2:H:78:PRO:HD3	2:H:96:THR:HG22	1.88	0.54

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:849:ASP:OD2	1:A:1214:ARG:NH2	2.40	0.54
1:E:1111:GLY:H	1:E:1156:TRP:HZ2	1.54	0.54
1:E:2553:VAL:O	1:E:2605:LYS:N	2.41	0.54
1:C:4900:ASP:O	1:C:4902:VAL:N	2.39	0.54
1:C:4630:GLN:OE1	1:C:4633:ARG:NH2	2.41	0.54
1:E:1714:TYR:OH	1:E:1718:ARG:NH2	2.38	0.54
1:E:2328:ARG:HA	1:E:2328:ARG:NH1	2.22	0.54
1:E:4630:GLN:OE1	1:E:4633:ARG:NH2	2.41	0.54
1:A:848:ARG:HD2	1:A:1603:PHE:HE2	1.73	0.54
1:E:4033:PHE:HA	1:E:4036:TYR:HB2	1.88	0.54
1:G:1144:ARG:NH2	1:G:1150:GLU:OE1	2.40	0.54
1:G:1429:SER:HA	1:G:1507:ILE:HG12	1.88	0.54
1:G:3803:VAL:HG13	1:G:3885:SER:HB2	1.90	0.54
1:A:3919:ASN:O	1:A:3922:THR:OG1	2.24	0.54
1:E:1144:ARG:NH2	1:E:1150:GLU:OE1	2.40	0.54
1:E:3803:VAL:HG13	1:E:3885:SER:HB2	1.90	0.54
1:E:4515:ASN:ND2	1:E:4740:PHE:O	2.33	0.54
1:A:4515:ASN:ND2	1:A:4740:PHE:O	2.33	0.54
1:C:993:GLU:OE1	1:C:1051:ARG:NH1	2.39	0.54
1:C:2553:VAL:O	1:C:2605:LYS:N	2.41	0.54
1:G:993:GLU:OE1	1:G:1051:ARG:NH1	2.39	0.54
1:C:1678:SER:OG	2:D:36:PHE:O	2.24	0.54
2:F:78:PRO:HD3	2:F:96:THR:HG22	1.88	0.54
1:G:2307:VAL:HG11	1:G:2321:VAL:HG21	1.90	0.54
1:A:1256:PRO:HB3	1:A:1597:SER:HA	1.90	0.54
1:A:4823:ARG:CZ	1:A:4823:ARG:CB	2.85	0.54
1:C:679:VAL:HA	1:C:800:VAL:HG12	1.89	0.54
1:C:1305:SER:OG	1:C:1306:MET:N	2.41	0.54
1:C:2324:LEU:N	1:C:2324:LEU:HD23	2.22	0.54
1:C:2593:LEU:O	1:C:2597:VAL:N	2.41	0.54
1:E:679:VAL:HA	1:E:800:VAL:HG12	1.89	0.54
1:E:4897:ASP:N	1:E:4897:ASP:OD1	2.35	0.54
1:G:4823:ARG:CZ	1:G:4823:ARG:CB	2.85	0.54
1:A:2425:ARG:NH2	1:A:2476:VAL:O	2.42	0.53
1:C:1939:ASP:OD1	1:C:1939:ASP:N	2.40	0.53
1:G:1256:PRO:HB3	1:G:1597:SER:HA	1.90	0.53
1:A:2553:VAL:O	1:A:2605:LYS:N	2.41	0.53
1:C:2712:ILE:O	1:C:2781:LYS:NZ	2.40	0.53
1:C:3733:HIS:O	1:C:3777:LYS:NZ	2.41	0.53
1:E:4032:THR:OG1	1:E:4056:HIS:NE2	2.39	0.53
1:G:2425:ARG:NH2	1:G:2476:VAL:O	2.42	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:2593:LEU:O	1:G:2597:VAL:N	2.41	0.53
1:A:4797:SER:OG	1:A:4805:MET:N	2.40	0.53
1:C:753:ASP:HB2	1:C:770:ILE:HD11	1.90	0.53
1:G:2553:VAL:O	1:G:2605:LYS:N	2.41	0.53
1:G:4630:GLN:OE1	1:G:4633:ARG:NH2	2.41	0.53
1:A:2307:VAL:HG11	1:A:2321:VAL:HG21	1.90	0.53
1:A:2782:THR:OG1	1:A:2848:ASN:ND2	2.42	0.53
1:A:4804:ASP:N	1:A:4804:ASP:OD1	2.41	0.53
1:A:4900:ASP:O	1:A:4902:VAL:N	2.39	0.53
1:E:3804:LEU:HD13	1:E:3910:ALA:HB2	1.89	0.53
1:G:1220:ASP:O	1:G:1224:LEU:N	2.40	0.53
1:G:1305:SER:OG	1:G:1306:MET:N	2.41	0.53
1:E:849:ASP:OD2	1:E:1214:ARG:NH2	2.40	0.53
1:E:2425:ARG:NH2	1:E:2476:VAL:O	2.42	0.53
1:E:3733:HIS:O	1:E:3777:LYS:NZ	2.41	0.53
1:G:527:LYS:NZ	1:G:566:GLU:O	2.41	0.53
1:A:3803:VAL:HG13	1:A:3885:SER:HB2	1.90	0.53
1:C:1256:PRO:HB3	1:C:1597:SER:HA	1.90	0.53
1:C:2275:LEU:HB2	1:C:2293:PRO:HG3	1.91	0.53
1:C:3804:LEU:HD13	1:C:3910:ALA:HB2	1.89	0.53
1:C:4725:TRP:HA	1:C:4728:THR:HG22	1.91	0.53
1:G:2275:LEU:HB2	1:G:2293:PRO:HG3	1.91	0.53
1:G:3733:HIS:O	1:G:3777:LYS:NZ	2.41	0.53
1:A:4868:ILE:CD1	1:G:4862:ILE:HG23	2.35	0.53
1:A:4926:LEU:HD13	1:A:4942:TRP:HB2	1.91	0.53
1:C:742:SER:OG	1:C:743:SER:N	2.42	0.53
1:G:849:ASP:OD2	1:G:1214:ARG:NH2	2.40	0.53
1:A:752:ASP:OD1	1:A:752:ASP:N	2.41	0.53
1:A:4630:GLN:OE1	1:A:4633:ARG:NH2	2.41	0.53
2:B:26:TYR:N	2:B:39:SER:OG	2.41	0.53
1:C:2323:ARG:HH21	1:C:2323:ARG:CG	2.14	0.53
2:D:31:GLN:NE2	2:D:96:THR:OG1	2.42	0.53
1:E:848:ARG:HD2	1:E:1603:PHE:HE2	1.72	0.53
1:E:4725:TRP:HA	1:E:4728:THR:HG22	1.91	0.53
1:E:4797:SER:OG	1:E:4805:MET:N	2.40	0.53
1:A:2593:LEU:O	1:A:2597:VAL:N	2.41	0.53
2:B:31:GLN:NE2	2:B:96:THR:OG1	2.42	0.53
1:C:2425:ARG:NH2	1:C:2476:VAL:O	2.42	0.53
1:C:3803:VAL:HG13	1:C:3885:SER:HB2	1.90	0.53
1:E:1256:PRO:HB3	1:E:1597:SER:HA	1.90	0.53
1:E:1738:LEU:HG	1:E:1925:ALA:HB1	1.90	0.53

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:3940:ARG:HG2	1:E:3943:ASP:HB2	1.91	0.53
1:E:4926:LEU:HD13	1:E:4942:TRP:HB2	1.91	0.53
1:G:753:ASP:HB2	1:G:770:ILE:HD11	1.90	0.53
1:G:2782:THR:OG1	1:G:2848:ASN:ND2	2.42	0.53
1:A:672:LYS:N	1:A:819:TYR:O	2.42	0.53
1:A:703:TYR:HA	1:A:1255:LEU:HD21	1.91	0.53
1:C:1738:LEU:HG	1:C:1925:ALA:HB1	1.90	0.53
1:C:1932:ASP:OD1	1:C:1932:ASP:N	2.35	0.53
1:C:2328:ARG:HA	1:C:2328:ARG:NH1	2.24	0.53
1:E:703:TYR:HA	1:E:1255:LEU:HD21	1.91	0.53
1:E:1305:SER:OG	1:E:1306:MET:N	2.41	0.53
1:E:2593:LEU:O	1:E:2597:VAL:N	2.41	0.53
1:E:4845:ILE:HD12	1:G:4819:TYR:HD1	1.55	0.53
1:G:1738:LEU:HG	1:G:1925:ALA:HB1	1.90	0.53
2:H:31:GLN:NE2	2:H:96:THR:OG1	2.42	0.53
1:A:742:SER:OG	1:A:743:SER:N	2.42	0.52
1:A:753:ASP:HB2	1:A:770:ILE:HD11	1.90	0.52
1:A:1738:LEU:HG	1:A:1925:ALA:HB1	1.90	0.52
1:A:2275:LEU:HB2	1:A:2293:PRO:HG3	1.91	0.52
1:A:3729:GLN:O	1:A:3733:HIS:ND1	2.36	0.52
1:A:3733:HIS:O	1:A:3777:LYS:NZ	2.41	0.52
1:C:848:ARG:HD2	1:C:1603:PHE:HE2	1.73	0.52
1:E:2275:LEU:HB2	1:E:2293:PRO:HG3	1.91	0.52
1:E:4065:GLU:HA	1:E:4068:LEU:HB2	1.92	0.52
1:A:1305:SER:OG	1:A:1306:MET:N	2.41	0.52
1:C:703:TYR:HA	1:C:1255:LEU:HD21	1.91	0.52
1:C:2782:THR:OG1	1:C:2848:ASN:ND2	2.42	0.52
1:C:4804:ASP:N	1:C:4804:ASP:OD1	2.41	0.52
1:E:527:LYS:NZ	1:E:566:GLU:O	2.41	0.52
1:E:672:LYS:N	1:E:819:TYR:O	2.42	0.52
1:E:1310:CYS:HB2	1:E:1536:SER:HA	1.91	0.52
1:E:2782:THR:OG1	1:E:2848:ASN:ND2	2.42	0.52
1:G:703:TYR:HA	1:G:1255:LEU:HD21	1.91	0.52
1:G:848:ARG:HD2	1:G:1603:PHE:HE2	1.73	0.52
1:G:4032:THR:OG1	1:G:4056:HIS:NE2	2.39	0.52
1:G:4926:LEU:HD13	1:G:4942:TRP:HB2	1.91	0.52
1:A:1310:CYS:HB2	1:A:1536:SER:HA	1.91	0.52
1:C:76:ARG:HD3	1:E:3891:TRP:CE2	2.44	0.52
1:C:204:ASP:OD1	1:C:204:ASP:N	2.43	0.52
1:C:1199:ASP:OD2	1:C:1199:ASP:N	2.37	0.52
1:E:143:LEU:HD11	1:E:207:PHE:HD2	1.73	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1426:TYR:HD2	1:A:1574:GLU:HB2	1.75	0.52
1:A:4065:GLU:HA	1:A:4068:LEU:HB2	1.92	0.52
1:C:3729:GLN:O	1:C:3733:HIS:ND1	2.36	0.52
1:E:752:ASP:N	1:E:752:ASP:OD1	2.41	0.52
1:E:2257:ALA:O	1:E:2259:ARG:NH1	2.43	0.52
2:F:31:GLN:NE2	2:F:96:THR:OG1	2.42	0.52
1:G:3940:ARG:HG2	1:G:3943:ASP:HB2	1.91	0.52
1:A:2436:VAL:O	1:A:2466:LYS:NZ	2.39	0.52
1:E:4804:ASP:OD1	1:E:4804:ASP:N	2.41	0.52
1:G:188:SER:OG	1:G:190:ARG:NH2	2.35	0.52
1:G:565:LEU:HD13	1:G:604:HIS:HE1	1.75	0.52
1:A:3683:LEU:HD22	1:A:3748:SER:HB3	1.92	0.52
1:A:3871:ILE:O	1:A:3875:THR:N	2.42	0.52
1:A:4032:THR:OG1	1:A:4056:HIS:NE2	2.39	0.52
1:C:2328:ARG:CG	1:C:2328:ARG:NH1	2.73	0.52
1:C:3940:ARG:HG2	1:C:3943:ASP:HB2	1.91	0.52
1:C:4823:ARG:HB2	1:C:4823:ARG:HH21	1.71	0.52
1:E:797:GLY:HA2	1:E:1622:LEU:HA	1.92	0.52
1:E:2328:ARG:CG	1:E:2328:ARG:NH1	2.73	0.52
1:G:2436:VAL:O	1:G:2466:LYS:NZ	2.39	0.52
1:C:565:LEU:HD13	1:C:604:HIS:HE1	1.75	0.52
1:C:752:ASP:OD1	1:C:752:ASP:N	2.41	0.52
1:C:3683:LEU:HD22	1:C:3748:SER:HB3	1.92	0.52
1:C:4926:LEU:HD13	1:C:4942:TRP:HB2	1.91	0.52
1:E:4052:ALA:O	1:E:4056:HIS:ND1	2.38	0.52
1:A:4725:TRP:HA	1:A:4728:THR:HG22	1.91	0.52
1:C:2257:ALA:O	1:C:2259:ARG:NH1	2.43	0.52
1:C:4844:ARG:NH2	1:E:4819:TYR:OH	2.43	0.52
1:E:1426:TYR:HD2	1:E:1574:GLU:HB2	1.75	0.52
1:G:3973:MET:HB3	1:G:4095:ILE:HG12	1.92	0.52
1:A:204:ASP:OD1	1:A:204:ASP:N	2.43	0.52
1:A:2257:ALA:O	1:A:2259:ARG:NH1	2.43	0.52
1:C:1310:CYS:HB2	1:C:1536:SER:HA	1.91	0.52
1:E:753:ASP:HB2	1:E:770:ILE:HD11	1.90	0.52
1:E:3683:LEU:HD22	1:E:3748:SER:HB3	1.92	0.52
1:G:742:SER:OG	1:G:743:SER:N	2.42	0.52
1:G:1426:TYR:HD2	1:G:1574:GLU:HB2	1.75	0.52
1:G:4725:TRP:HA	1:G:4728:THR:HG22	1.91	0.52
1:A:3973:MET:HB3	1:A:4095:ILE:HG12	1.92	0.52
1:E:833:LYS:HA	1:E:1614:ARG:HH12	1.75	0.52
1:E:3956:GLN:NE2	1:E:3973:MET:SD	2.83	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:4823:ARG:HB3	1:E:4823:ARG:HH21	1.74	0.52
2:F:26:TYR:N	2:F:39:SER:OG	2.41	0.52
1:G:4804:ASP:OD1	1:G:4804:ASP:N	2.41	0.52
1:A:3956:GLN:NE2	1:A:3973:MET:SD	2.83	0.51
1:C:185:SER:HG	1:C:190:ARG:H	1.56	0.51
1:C:188:SER:OG	1:C:190:ARG:NH2	2.35	0.51
1:C:797:GLY:HA2	1:C:1622:LEU:HA	1.92	0.51
1:C:1265:HIS:CD2	1:C:1267:HIS:H	2.28	0.51
1:C:1426:TYR:HD2	1:C:1574:GLU:HB2	1.75	0.51
1:E:742:SER:OG	1:E:743:SER:N	2.42	0.51
1:E:4823:ARG:NH2	1:E:4823:ARG:CB	2.73	0.51
1:E:4823:ARG:HB2	1:E:4823:ARG:CZ	2.40	0.51
1:G:204:ASP:N	1:G:204:ASP:OD1	2.43	0.51
1:G:1642:LEU:O	1:G:1645:THR:OG1	2.26	0.51
1:C:527:LYS:NZ	1:C:566:GLU:O	2.41	0.51
1:C:694:ARG:NH1	1:C:716:ASN:O	2.41	0.51
1:C:1904:LYS:HD2	1:C:2081:LEU:HD21	1.93	0.51
1:C:3956:GLN:NE2	1:C:3973:MET:SD	2.83	0.51
1:E:271:ALA:O	1:E:301:THR:OG1	2.25	0.51
1:E:565:LEU:HD13	1:E:604:HIS:HE1	1.75	0.51
1:E:4823:ARG:CB	1:E:4823:ARG:CZ	2.88	0.51
1:G:3956:GLN:NE2	1:G:3973:MET:SD	2.83	0.51
1:C:767:SER:HA	1:C:777:GLY:HA3	1.92	0.51
1:C:1431:ARG:HE	1:C:1505:LEU:HD21	1.76	0.51
1:C:1756:SER:OG	1:C:1757:LEU:N	2.44	0.51
1:C:1847:GLU:OE1	1:C:1849:SER:OG	2.29	0.51
2:D:26:TYR:N	2:D:39:SER:OG	2.41	0.51
1:G:833:LYS:HA	1:G:1614:ARG:HH12	1.75	0.51
1:G:2257:ALA:O	1:G:2259:ARG:NH1	2.43	0.51
1:A:343:ARG:NH2	1:A:345:GLU:O	2.44	0.51
1:A:661:LEU:O	1:A:788:PHE:N	2.43	0.51
1:A:3940:ARG:HG2	1:A:3943:ASP:HB2	1.91	0.51
1:C:661:LEU:O	1:C:788:PHE:N	2.43	0.51
1:E:1756:SER:OG	1:E:1757:LEU:N	2.44	0.51
1:E:1847:GLU:OE1	1:E:1849:SER:OG	2.28	0.51
1:G:1589:GLN:NE2	1:G:1634:GLU:OE1	2.43	0.51
1:C:904:TYR:HD1	1:C:918:LEU:HB2	1.76	0.51
1:C:3973:MET:HB3	1:C:4095:ILE:HG12	1.92	0.51
1:C:4065:GLU:HA	1:C:4068:LEU:HB2	1.92	0.51
1:E:694:ARG:NH1	1:E:716:ASN:O	2.41	0.51
1:E:1589:GLN:NE2	1:E:1634:GLU:OE1	2.43	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:185:SER:HG	1:G:190:ARG:H	1.57	0.51
1:A:693:LEU:HD22	1:A:798:ILE:HD13	1.93	0.51
1:A:904:TYR:HD1	1:A:918:LEU:HB2	1.76	0.51
1:C:209:GLN:NE2	1:E:2327:ARG:NH1	2.54	0.51
1:C:271:ALA:O	1:C:301:THR:OG1	2.25	0.51
1:C:693:LEU:HD22	1:C:798:ILE:HD13	1.93	0.51
1:C:833:LYS:HA	1:C:1614:ARG:HH12	1.75	0.51
1:C:887:GLU:HA	1:C:921:PHE:HB3	1.93	0.51
1:C:1589:GLN:NE2	1:C:1634:GLU:OE1	2.43	0.51
1:E:185:SER:HG	1:E:190:ARG:H	1.55	0.51
1:G:672:LYS:N	1:G:819:TYR:O	2.42	0.51
1:A:767:SER:HA	1:A:777:GLY:HA3	1.92	0.51
1:C:343:ARG:NH2	1:C:345:GLU:O	2.44	0.51
1:E:887:GLU:HA	1:E:921:PHE:HB3	1.93	0.51
1:E:3973:MET:HB3	1:E:4095:ILE:HG12	1.92	0.51
1:G:752:ASP:N	1:G:752:ASP:OD1	2.41	0.51
1:G:1310:CYS:HB2	1:G:1536:SER:HA	1.91	0.51
1:G:3683:LEU:HD22	1:G:3748:SER:HB3	1.92	0.51
1:A:143:LEU:HD22	1:C:2427:LEU:HD21	1.91	0.51
1:C:1718:ARG:HH12	1:C:1758:ARG:HD3	1.76	0.51
1:C:4094:ASP:N	1:C:4094:ASP:OD1	2.44	0.51
1:E:343:ARG:NH2	1:E:345:GLU:O	2.44	0.51
1:E:1431:ARG:HE	1:E:1505:LEU:HD21	1.76	0.51
1:G:887:GLU:HA	1:G:921:PHE:HB3	1.93	0.51
1:A:797:GLY:HA2	1:A:1622:LEU:HA	1.92	0.51
1:A:1589:GLN:NE2	1:A:1634:GLU:OE1	2.43	0.51
1:A:1756:SER:OG	1:A:1757:LEU:N	2.44	0.51
1:E:3683:LEU:HD23	1:E:3755:MET:HG2	1.93	0.51
1:A:1718:ARG:HH12	1:A:1758:ARG:HD3	1.76	0.51
1:E:767:SER:HA	1:E:777:GLY:HA3	1.92	0.51
1:E:2328:ARG:CA	1:E:2328:ARG:NH1	2.73	0.51
1:G:645:GLN:HE22	2:H:34:LYS:HB3	1.76	0.51
1:G:904:TYR:HD1	1:G:918:LEU:HB2	1.76	0.51
1:A:565:LEU:HD13	1:A:604:HIS:HE1	1.75	0.50
1:A:887:GLU:HA	1:A:921:PHE:HB3	1.93	0.50
1:A:1904:LYS:HD2	1:A:2081:LEU:HD21	1.93	0.50
1:C:645:GLN:HE22	2:D:34:LYS:HB3	1.76	0.50
1:C:2314:VAL:HG23	1:C:2314:VAL:O	2.11	0.50
1:E:645:GLN:HE22	2:F:34:LYS:HB3	1.76	0.50
1:E:1712:SER:OG	1:E:1712:SER:O	2.29	0.50
1:G:1718:ARG:HH12	1:G:1758:ARG:HD3	1.76	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1769:VAL:HG12	2:H:55:VAL:HG23	1.94	0.50
1:G:4065:GLU:HA	1:G:4068:LEU:HB2	1.92	0.50
1:A:645:GLN:HE22	2:B:34:LYS:HB3	1.76	0.50
1:A:694:ARG:NH1	1:A:716:ASN:O	2.41	0.50
1:A:4844:ARG:NH2	1:C:4819:TYR:OH	2.44	0.50
1:G:1763:PHE:HB3	1:G:1781:GLU:HB2	1.93	0.50
1:A:1769:VAL:HG12	2:B:55:VAL:HG23	1.94	0.50
1:A:4094:ASP:N	1:A:4094:ASP:OD1	2.44	0.50
1:E:473:GLU:O	1:E:477:ASN:ND2	2.45	0.50
1:E:1763:PHE:HB3	1:E:1781:GLU:HB2	1.94	0.50
1:E:4094:ASP:OD1	1:E:4094:ASP:N	2.44	0.50
1:G:1678:SER:OG	2:H:36:PHE:O	2.24	0.50
1:A:1431:ARG:HE	1:A:1505:LEU:HD21	1.76	0.50
1:A:4819:TYR:OH	1:G:4844:ARG:NH2	2.45	0.50
1:C:2433:LEU:HA	1:C:2436:VAL:HG12	1.93	0.50
1:E:4663:GLY:H	1:E:4666:ARG:HD3	1.77	0.50
1:G:473:GLU:O	1:G:477:ASN:ND2	2.45	0.50
1:G:797:GLY:HA2	1:G:1622:LEU:HA	1.92	0.50
1:G:1756:SER:OG	1:G:1757:LEU:N	2.44	0.50
1:A:833:LYS:HA	1:A:1614:ARG:HH12	1.75	0.50
1:A:1847:GLU:OE1	1:A:1849:SER:OG	2.29	0.50
1:A:2464:ASP:OD1	1:A:2464:ASP:N	2.44	0.50
1:E:1769:VAL:HG12	2:F:55:VAL:HG23	1.94	0.50
1:E:3729:GLN:OE1	1:E:3771:ASN:ND2	2.45	0.50
2:H:71:ARG:NH2	2:H:100:ASP:OD2	2.43	0.50
1:A:76:ARG:HG2	1:C:3891:TRP:CD2	2.47	0.50
1:A:527:LYS:NZ	1:A:566:GLU:O	2.41	0.50
1:C:473:GLU:O	1:C:477:ASN:ND2	2.45	0.50
1:C:3683:LEU:HD23	1:C:3755:MET:HG2	1.93	0.50
1:C:4032:THR:OG1	1:C:4056:HIS:NE2	2.39	0.50
1:E:693:LEU:HD22	1:E:798:ILE:HD13	1.93	0.50
1:E:904:TYR:HD1	1:E:918:LEU:HB2	1.76	0.50
1:E:1265:HIS:CD2	1:E:1267:HIS:H	2.28	0.50
1:E:2026:ILE:HA	1:E:2029:ARG:HH11	1.76	0.50
1:G:1847:GLU:OE1	1:G:1849:SER:OG	2.29	0.50
1:A:1939:ASP:O	1:A:1943:PHE:N	2.45	0.50
1:A:4858:ILE:HD12	1:C:4867:ILE:CG2	2.26	0.50
1:C:4845:ILE:HD12	1:E:4819:TYR:HD1	1.55	0.50
1:E:2433:LEU:HA	1:E:2436:VAL:HG12	1.93	0.50
1:G:343:ARG:NH2	1:G:345:GLU:O	2.44	0.50
1:G:767:SER:HA	1:G:777:GLY:HA3	1.92	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:4663:GLY:H	1:G:4666:ARG:HD3	1.77	0.50
1:A:473:GLU:O	1:A:477:ASN:ND2	2.45	0.50
1:C:1642:LEU:O	1:C:1645:THR:OG1	2.26	0.50
1:C:2849:TYR:HA	1:C:2852:ILE:HG22	1.94	0.50
1:C:4663:GLY:H	1:C:4666:ARG:HD3	1.77	0.50
1:E:1718:ARG:HH12	1:E:1758:ARG:HD3	1.76	0.50
1:E:2316:GLU:HG2	1:E:3811:ARG:NH2	2.27	0.50
1:E:4844:ARG:NH2	1:G:4819:TYR:OH	2.45	0.50
1:G:271:ALA:O	1:G:301:THR:OG1	2.25	0.50
1:G:1431:ARG:HE	1:G:1505:LEU:HD21	1.76	0.50
1:G:3919:ASN:O	1:G:3922:THR:OG1	2.24	0.50
1:A:1548:THR:OG1	1:A:1549:SER:N	2.45	0.50
1:A:2026:ILE:HA	1:A:2029:ARG:HH11	1.76	0.50
1:A:4770:LEU:O	1:C:4754:LEU:HD21	2.12	0.50
1:E:1939:ASP:O	1:E:1943:PHE:N	2.45	0.50
1:G:694:ARG:NH1	1:G:716:ASN:O	2.41	0.50
1:G:2026:ILE:HA	1:G:2029:ARG:HH11	1.76	0.50
1:G:3683:LEU:HD23	1:G:3755:MET:HG2	1.93	0.50
1:A:4028:THR:HA	1:A:4033:PHE:HD2	1.77	0.49
1:A:4823:ARG:HB2	1:A:4823:ARG:HH21	1.72	0.49
1:C:1769:VAL:HG12	2:D:55:VAL:HG23	1.94	0.49
1:C:2725:TYR:OH	1:C:2892:ASP:OD1	2.30	0.49
1:G:335:LYS:NZ	1:G:398:HIS:O	2.37	0.49
1:G:4028:THR:HA	1:G:4033:PHE:HD2	1.77	0.49
1:A:3800:SER:OG	1:A:3801:CYS:N	2.45	0.49
1:C:2328:ARG:CA	1:C:2328:ARG:NH1	2.73	0.49
1:C:3919:ASN:O	1:C:3922:THR:OG1	2.24	0.49
1:E:204:ASP:OD1	1:E:204:ASP:N	2.43	0.49
1:G:693:LEU:HD22	1:G:798:ILE:HD13	1.93	0.49
1:G:1904:LYS:HD2	1:G:2081:LEU:HD21	1.93	0.49
1:E:1904:LYS:HD2	1:E:2081:LEU:HD21	1.93	0.49
1:E:2725:TYR:OH	1:E:2892:ASP:OD1	2.30	0.49
1:G:2725:TYR:OH	1:G:2892:ASP:OD1	2.30	0.49
2:H:26:TYR:N	2:H:39:SER:OG	2.41	0.49
1:A:2433:LEU:HA	1:A:2436:VAL:HG12	1.94	0.49
1:C:992:GLN:HB3	1:C:1064:LEU:HD12	1.95	0.49
1:A:1763:PHE:HB3	1:A:1781:GLU:HB2	1.93	0.49
1:A:2849:TYR:HA	1:A:2852:ILE:HG22	1.94	0.49
1:C:2315:GLU:OE2	1:C:2315:GLU:HA	2.11	0.49
1:C:4028:THR:HA	1:C:4033:PHE:HD2	1.77	0.49
1:G:3871:ILE:O	1:G:3875:THR:N	2.42	0.49

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:4094:ASP:OD1	1:G:4094:ASP:N	2.44	0.49
1:A:156:GLU:HB3	1:A:186:VAL:HG12	1.95	0.49
1:A:671:LYS:N	1:A:819:TYR:O	2.46	0.49
1:A:1106:GLU:OE2	1:A:1214:ARG:NH1	2.46	0.49
1:A:2725:TYR:OH	1:A:2892:ASP:OD1	2.30	0.49
1:A:4663:GLY:H	1:A:4666:ARG:HD3	1.77	0.49
1:C:530:LEU:HA	1:C:533:LEU:HD12	1.95	0.49
1:C:2026:ILE:HA	1:C:2029:ARG:HH11	1.76	0.49
1:E:651:HIS:HD2	1:E:1625:LEU:HB3	1.78	0.49
2:F:71:ARG:NH2	2:F:100:ASP:OD2	2.43	0.49
1:A:530:LEU:HA	1:A:533:LEU:HD12	1.95	0.49
1:C:35:LEU:HB3	1:C:49:LEU:HD22	1.95	0.49
1:C:651:HIS:HD2	1:C:1625:LEU:HB3	1.78	0.49
1:C:1106:GLU:OE2	1:C:1214:ARG:NH1	2.46	0.49
1:C:1763:PHE:HB3	1:C:1781:GLU:HB2	1.93	0.49
1:C:1939:ASP:O	1:C:1943:PHE:N	2.45	0.49
1:C:4026:ASP:HA	1:C:4029:SER:HB3	1.94	0.49
1:E:992:GLN:HB3	1:E:1064:LEU:HD12	1.95	0.49
1:E:1106:GLU:OE2	1:E:1214:ARG:NH1	2.46	0.49
1:E:1548:THR:OG1	1:E:1549:SER:N	2.45	0.49
1:G:156:GLU:HB3	1:G:186:VAL:HG12	1.95	0.49
1:G:1548:THR:OG1	1:G:1549:SER:N	2.45	0.49
1:A:1642:LEU:O	1:A:1645:THR:OG1	2.26	0.49
1:A:3729:GLN:OE1	1:A:3771:ASN:ND2	2.45	0.49
1:C:3729:GLN:OE1	1:C:3771:ASN:ND2	2.45	0.49
1:E:3919:ASN:O	1:E:3922:THR:OG1	2.24	0.49
1:G:651:HIS:HD2	1:G:1625:LEU:HB3	1.78	0.49
1:C:3871:ILE:O	1:C:3875:THR:N	2.42	0.49
1:C:4797:SER:OG	1:C:4805:MET:N	2.40	0.49
1:C:4858:ILE:HD12	1:E:4867:ILE:CG2	2.27	0.49
1:E:530:LEU:HA	1:E:533:LEU:HD12	1.95	0.49
1:E:1209:VAL:N	1:E:1211:GLN:OE1	2.46	0.49
1:E:4028:THR:HA	1:E:4033:PHE:HD2	1.77	0.49
1:G:2433:LEU:HA	1:G:2436:VAL:HG12	1.94	0.49
1:G:4797:SER:OG	1:G:4805:MET:N	2.40	0.49
1:A:1253:LYS:NZ	1:A:1257:GLN:OE1	2.46	0.49
1:A:3683:LEU:HD23	1:A:3755:MET:HG2	1.93	0.49
1:A:4754:LEU:HD21	1:G:4770:LEU:O	2.13	0.49
1:C:4848:ASP:OD1	1:E:4823:ARG:CZ	2.61	0.49
1:E:671:LYS:N	1:E:819:TYR:O	2.46	0.49
1:E:2849:TYR:HA	1:E:2852:ILE:HG22	1.94	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:4026:ASP:HA	1:E:4029:SER:HB3	1.94	0.49
1:A:1209:VAL:N	1:A:1211:GLN:OE1	2.46	0.48
1:E:2314:VAL:HG23	1:E:2314:VAL:O	2.12	0.48
1:G:1265:HIS:CD2	1:G:1267:HIS:H	2.28	0.48
1:G:4026:ASP:HA	1:G:4029:SER:HB3	1.94	0.48
1:A:35:LEU:HB3	1:A:49:LEU:HD22	1.95	0.48
1:A:651:HIS:HD2	1:A:1625:LEU:HB3	1.78	0.48
1:E:1199:ASP:OD2	1:E:1199:ASP:N	2.37	0.48
1:G:1106:GLU:OE2	1:G:1214:ARG:NH1	2.46	0.48
1:G:1712:SER:O	1:G:1712:SER:OG	2.29	0.48
1:A:1199:ASP:OD2	1:A:1199:ASP:N	2.37	0.48
1:A:4026:ASP:HA	1:A:4029:SER:HB3	1.94	0.48
1:C:671:LYS:N	1:C:819:TYR:O	2.46	0.48
1:C:2328:ARG:CB	1:C:2329:PRO:CD	2.91	0.48
1:C:1209:VAL:N	1:C:1211:GLN:OE1	2.46	0.48
1:C:3800:SER:OG	1:C:3801:CYS:N	2.45	0.48
1:A:892:LEU:HD13	1:A:1052:GLU:HG3	1.95	0.48
1:C:517:VAL:HG23	1:C:520:ARG:HE	1.79	0.48
1:C:1712:SER:O	1:C:1712:SER:OG	2.29	0.48
1:E:35:LEU:HB3	1:E:49:LEU:HD22	1.95	0.48
1:G:1209:VAL:N	1:G:1211:GLN:OE1	2.46	0.48
1:G:3729:GLN:OE1	1:G:3771:ASN:ND2	2.45	0.48
1:A:4052:ALA:O	1:A:4056:HIS:ND1	2.38	0.48
1:C:156:GLU:HB3	1:C:186:VAL:HG12	1.95	0.48
1:E:3871:ILE:O	1:E:3875:THR:N	2.42	0.48
1:G:517:VAL:HG23	1:G:520:ARG:HE	1.79	0.48
1:G:671:LYS:N	1:G:819:TYR:O	2.46	0.48
1:G:3761:LYS:NZ	1:G:3835:GLU:OE2	2.42	0.48
1:A:517:VAL:HG23	1:A:520:ARG:HE	1.79	0.48
1:A:881:ILE:HD11	1:A:952:ILE:HD13	1.95	0.48
1:A:1932:ASP:OD1	1:A:1932:ASP:N	2.35	0.48
1:C:797:GLY:CA	1:C:1621:CYS:O	2.59	0.48
1:C:4051:LYS:O	1:C:4055:SER:N	2.46	0.48
1:C:4757:ILE:O	1:C:4760:SER:OG	2.32	0.48
1:G:1253:LYS:NZ	1:G:1257:GLN:OE1	2.46	0.48
1:G:2213:LYS:HA	1:G:2254:LEU:HD21	1.95	0.48
1:G:3892:TYR:O	1:G:3896:LYS:NZ	2.40	0.48
1:A:1265:HIS:CD2	1:A:1267:HIS:H	2.28	0.48
1:C:892:LEU:HD13	1:C:1052:GLU:HG3	1.94	0.48
1:C:2213:LYS:HA	1:C:2254:LEU:HD21	1.95	0.48
1:E:821:PRO:HG2	1:E:824:GLU:HG2	1.96	0.48

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:915:HIS:CE1	1:E:917:CYS:HB2	2.49	0.48
1:E:1426:TYR:HB3	1:E:1571:PHE:HA	1.96	0.48
1:G:35:LEU:HB3	1:G:49:LEU:HD22	1.95	0.48
1:G:2849:TYR:HA	1:G:2852:ILE:HG22	1.94	0.48
1:C:672:LYS:N	1:C:819:TYR:O	2.42	0.48
1:C:1426:TYR:HB3	1:C:1571:PHE:HA	1.96	0.48
1:E:1253:LYS:NZ	1:E:1257:GLN:OE1	2.46	0.48
1:E:3663:ASP:OD2	1:E:3735:ARG:NH2	2.47	0.48
1:G:881:ILE:HD11	1:G:952:ILE:HD13	1.95	0.48
1:A:271:ALA:O	1:A:301:THR:OG1	2.25	0.48
1:A:394:HIS:CD2	1:A:397:GLY:H	2.32	0.48
1:A:821:PRO:HG2	1:A:824:GLU:HG2	1.96	0.48
1:A:992:GLN:HB3	1:A:1064:LEU:HD12	1.95	0.48
1:A:1426:TYR:HB3	1:A:1571:PHE:HA	1.96	0.48
1:A:3663:ASP:OD2	1:A:3735:ARG:NH2	2.47	0.48
1:C:1253:LYS:NZ	1:C:1257:GLN:OE1	2.46	0.48
1:G:1521:THR:HA	1:G:1526:ASP:HA	1.96	0.48
1:G:3663:ASP:OD2	1:G:3735:ARG:NH2	2.47	0.48
1:E:156:GLU:HB3	1:E:186:VAL:HG12	1.95	0.47
1:E:1303:ARG:HH21	1:E:1595:LEU:HB2	1.79	0.47
1:E:1642:LEU:O	1:E:1645:THR:OG1	2.26	0.47
1:G:992:GLN:HB3	1:G:1064:LEU:HD12	1.95	0.47
1:G:1303:ARG:HH21	1:G:1595:LEU:HB2	1.79	0.47
1:G:1426:TYR:HB3	1:G:1571:PHE:HA	1.96	0.47
1:A:1521:THR:HA	1:A:1526:ASP:HA	1.96	0.47
2:B:71:ARG:NH2	2:B:100:ASP:OD2	2.43	0.47
1:E:517:VAL:HG23	1:E:520:ARG:HE	1.79	0.47
1:E:2213:LYS:HA	1:E:2254:LEU:HD21	1.95	0.47
1:E:4781:LEU:CD1	1:G:4741:ALA:O	2.62	0.47
1:G:530:LEU:HA	1:G:533:LEU:HD12	1.95	0.47
1:A:1930:SER:O	1:A:1930:SER:OG	2.31	0.47
1:A:1942:ARG:NH1	1:A:3609:LEU:H	2.13	0.47
1:A:3799:GLN:O	1:A:3881:ARG:NH2	2.48	0.47
1:A:4741:ALA:O	1:G:4781:LEU:CD1	2.62	0.47
1:A:4770:LEU:HB3	1:C:4754:LEU:CD1	2.44	0.47
1:C:1303:ARG:HH21	1:C:1595:LEU:HB2	1.79	0.47
1:C:3663:ASP:OD2	1:C:3735:ARG:NH2	2.47	0.47
1:C:3799:GLN:O	1:C:3881:ARG:NH2	2.48	0.47
1:G:23:GLN:HE21	1:G:34:LYS:HB3	1.80	0.47
1:C:3900:ASP:OD1	1:C:3900:ASP:N	2.47	0.47
1:G:394:HIS:CD2	1:G:397:GLY:H	2.32	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:4045:SER:HA	1:G:4078:THR:HG22	1.96	0.47
1:A:1303:ARG:HH21	1:A:1595:LEU:HB2	1.79	0.47
1:C:915:HIS:CE1	1:C:917:CYS:HB2	2.49	0.47
1:C:1942:ARG:NH1	1:C:3609:LEU:H	2.13	0.47
1:E:1118:SER:HB2	1:E:1204:VAL:HG11	1.96	0.47
1:E:1655:TYR:OH	1:E:1659:ARG:NH2	2.48	0.47
1:E:3642:ILE:HD11	1:E:3695:ILE:HG22	1.96	0.47
1:G:1118:SER:HB2	1:G:1204:VAL:HG11	1.96	0.47
1:G:1930:SER:O	1:G:1930:SER:OG	2.31	0.47
1:C:1611:ILE:HG13	1:C:1620:GLN:HB3	1.97	0.47
1:E:1521:THR:HA	1:E:1526:ASP:HA	1.96	0.47
1:E:1611:ILE:HG13	1:E:1620:GLN:HB3	1.97	0.47
1:G:1655:TYR:OH	1:G:1659:ARG:NH2	2.48	0.47
1:G:1942:ARG:NH1	1:G:3609:LEU:H	2.13	0.47
1:A:1171:HIS:O	1:A:1194:ASP:N	2.45	0.47
1:A:2213:LYS:HA	1:A:2254:LEU:HD21	1.95	0.47
1:A:3642:ILE:HD11	1:A:3695:ILE:HG22	1.96	0.47
1:A:4051:LYS:O	1:A:4055:SER:N	2.46	0.47
1:C:881:ILE:HD11	1:C:952:ILE:HD13	1.95	0.47
2:D:71:ARG:NH2	2:D:100:ASP:OD2	2.43	0.47
1:E:568:SER:HA	1:E:571:ILE:HD12	1.97	0.47
1:E:892:LEU:HD13	1:E:1052:GLU:HG3	1.94	0.47
1:G:892:LEU:HD13	1:G:1052:GLU:HG3	1.95	0.47
1:G:1629:SER:OG	1:G:1630:LEU:N	2.48	0.47
1:G:2116:ASP:OD1	1:G:2116:ASP:N	2.46	0.47
1:A:1655:TYR:OH	1:A:1659:ARG:NH2	2.48	0.47
1:A:4922:PHE:HE2	1:A:4941:VAL:HG11	1.80	0.47
1:C:1430:VAL:HG11	1:C:1443:VAL:HG11	1.97	0.47
1:C:1548:THR:OG1	1:C:1549:SER:N	2.45	0.47
1:C:1629:SER:OG	1:C:1630:LEU:N	2.48	0.47
1:E:1733:THR:HA	1:E:1755:THR:HG21	1.97	0.47
1:G:687:THR:OG1	1:G:689:GLU:O	2.33	0.47
1:G:3799:GLN:O	1:G:3881:ARG:NH2	2.48	0.47
1:A:1118:SER:HB2	1:A:1204:VAL:HG11	1.96	0.47
1:A:3900:ASP:OD1	1:A:3900:ASP:N	2.47	0.47
1:A:4171:ARG:NE	5:A:6002:ATP:O2G	2.41	0.47
2:B:25:HIS:HD2	2:B:104:LEU:HD11	1.80	0.47
1:C:23:GLN:HE21	1:C:34:LYS:HB3	1.80	0.47
1:C:299:HIS:HD2	1:C:302:THR:H	1.63	0.47
1:C:394:HIS:CD2	1:C:397:GLY:H	2.32	0.47
1:C:821:PRO:HG2	1:C:824:GLU:HG2	1.96	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4922:PHE:HE2	1:C:4941:VAL:HG11	1.80	0.47
1:E:1942:ARG:NH1	1:E:3609:LEU:H	2.13	0.47
1:E:4791:ARG:HH22	1:G:4559:HIS:HE1	1.63	0.47
1:G:661:LEU:O	1:G:788:PHE:N	2.43	0.47
1:G:915:HIS:CE1	1:G:917:CYS:HB2	2.49	0.47
1:G:2996:HIS:O	1:G:3000:LYS:CB	2.63	0.47
1:G:4051:LYS:O	1:G:4055:SER:N	2.46	0.47
1:A:23:GLN:HE21	1:A:34:LYS:HB3	1.80	0.47
1:A:915:HIS:CE1	1:A:917:CYS:HB2	2.49	0.47
1:A:1611:ILE:HG13	1:A:1620:GLN:HB3	1.97	0.47
1:A:2427:LEU:HD21	1:G:143:LEU:HD22	1.91	0.47
1:A:3875:THR:HG21	1:A:3924:TYR:HE2	1.80	0.47
1:C:1221:VAL:HA	1:C:1224:LEU:HB2	1.97	0.47
1:C:2323:ARG:NH2	1:C:2323:ARG:CG	2.73	0.47
1:E:3799:GLN:O	1:E:3881:ARG:NH2	2.48	0.47
1:E:3875:THR:HG21	1:E:3924:TYR:HE2	1.80	0.47
1:E:4810:MET:HB3	1:G:4519:LEU:O	2.15	0.47
1:G:568:SER:HA	1:G:571:ILE:HD12	1.97	0.47
2:H:25:HIS:HD2	2:H:104:LEU:HD11	1.80	0.47
1:A:2324:LEU:N	1:A:2324:LEU:HD23	2.30	0.46
1:A:4045:SER:HA	1:A:4078:THR:HG22	1.96	0.46
1:A:4781:LEU:CD1	1:C:4741:ALA:O	2.63	0.46
1:C:894:VAL:HG13	1:C:918:LEU:HD22	1.97	0.46
1:C:1521:THR:HA	1:C:1526:ASP:HA	1.96	0.46
1:C:2307:VAL:HG12	1:C:2317:ASN:HB3	1.98	0.46
1:C:3980:VAL:HA	1:C:3983:LEU:HG	1.97	0.46
1:E:881:ILE:HD11	1:E:952:ILE:HD13	1.95	0.46
1:E:2996:HIS:O	1:E:3000:LYS:CB	2.63	0.46
2:F:25:HIS:HD2	2:F:104:LEU:HD11	1.80	0.46
1:G:1733:THR:HA	1:G:1755:THR:HG21	1.97	0.46
1:G:1939:ASP:O	1:G:1943:PHE:N	2.45	0.46
1:C:1655:TYR:OH	1:C:1659:ARG:NH2	2.48	0.46
1:C:3875:THR:HG21	1:C:3924:TYR:HE2	1.80	0.46
1:C:4045:SER:HA	1:C:4078:THR:HG22	1.96	0.46
1:E:894:VAL:HG13	1:E:918:LEU:HD22	1.97	0.46
1:E:3980:VAL:HA	1:E:3983:LEU:HG	1.97	0.46
1:E:4045:SER:HA	1:E:4078:THR:HG22	1.96	0.46
1:G:1199:ASP:OD2	1:G:1199:ASP:N	2.37	0.46
1:G:1221:VAL:HA	1:G:1224:LEU:HB2	1.97	0.46
1:G:1611:ILE:HG13	1:G:1620:GLN:HB3	1.97	0.46
1:A:1221:VAL:HA	1:A:1224:LEU:HB2	1.97	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2226:SER:O	1:A:2226:SER:OG	2.33	0.46
1:C:2996:HIS:O	1:C:3000:LYS:CB	2.63	0.46
1:E:394:HIS:CD2	1:E:397:GLY:H	2.32	0.46
1:E:687:THR:OG1	1:E:689:GLU:O	2.33	0.46
1:G:4757:ILE:O	1:G:4760:SER:OG	2.32	0.46
1:A:3927:GLY:O	1:A:3929:CYS:N	2.48	0.46
1:C:3642:ILE:HD11	1:C:3695:ILE:HG22	1.96	0.46
1:E:797:GLY:CA	1:E:1621:CYS:O	2.59	0.46
1:G:821:PRO:HG2	1:G:824:GLU:HG2	1.96	0.46
1:G:1440:ASN:N	1:G:1440:ASN:OD1	2.49	0.46
1:G:2324:LEU:HD23	1:G:2324:LEU:N	2.30	0.46
1:A:299:HIS:HD2	1:A:302:THR:H	1.63	0.46
1:A:687:THR:OG1	1:A:689:GLU:O	2.33	0.46
1:A:2996:HIS:O	1:A:3000:LYS:CB	2.63	0.46
1:C:394:HIS:HD2	1:C:397:GLY:H	1.64	0.46
1:C:1118:SER:HB2	1:C:1204:VAL:HG11	1.96	0.46
1:E:605:GLY:HA2	1:E:1589:GLN:HE21	1.81	0.46
1:E:1430:VAL:HG11	1:E:1443:VAL:HG11	1.97	0.46
1:E:4757:ILE:O	1:E:4760:SER:OG	2.32	0.46
1:G:894:VAL:HG13	1:G:918:LEU:HD22	1.97	0.46
1:G:4922:PHE:HE2	1:G:4941:VAL:HG11	1.80	0.46
1:A:4559:HIS:HE1	1:G:4791:ARG:HH22	1.63	0.46
1:E:23:GLN:HE21	1:E:34:LYS:HB3	1.80	0.46
1:E:299:HIS:HD2	1:E:302:THR:H	1.63	0.46
1:E:2110:ASN:OD1	1:E:2113:SER:OG	2.34	0.46
1:E:4922:PHE:HE2	1:E:4941:VAL:HG11	1.80	0.46
1:G:3927:GLY:O	1:G:3929:CYS:N	2.48	0.46
1:A:2116:ASP:N	1:A:2116:ASP:OD1	2.46	0.46
1:C:255:GLU:HB2	1:C:257:ARG:H	1.81	0.46
1:E:394:HIS:HD2	1:E:397:GLY:H	1.64	0.46
1:E:3900:ASP:N	1:E:3900:ASP:OD1	2.47	0.46
1:G:255:GLU:HB2	1:G:257:ARG:H	1.81	0.46
1:G:394:HIS:HD2	1:G:397:GLY:H	1.64	0.46
1:G:3875:THR:HG21	1:G:3924:TYR:HE2	1.80	0.46
1:A:1629:SER:OG	1:A:1630:LEU:N	2.48	0.46
1:A:4757:ILE:O	1:A:4760:SER:OG	2.32	0.46
1:A:4770:LEU:HB3	1:C:4754:LEU:HD13	1.97	0.46
1:C:4168:GLU:OE1	1:C:4595:LYS:NZ	2.46	0.46
1:G:299:HIS:HD2	1:G:302:THR:H	1.63	0.46
1:A:1430:VAL:HG11	1:A:1443:VAL:HG11	1.97	0.46
1:C:568:SER:HA	1:C:571:ILE:HD12	1.97	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2110:ASN:OD1	1:C:2110:ASN:N	2.49	0.46
2:D:25:HIS:HD2	2:D:104:LEU:HD11	1.80	0.46
1:E:1221:VAL:HA	1:E:1224:LEU:HB2	1.97	0.46
1:E:1629:SER:OG	1:E:1630:LEU:N	2.48	0.46
1:E:2116:ASP:N	1:E:2116:ASP:OD1	2.46	0.46
1:G:605:GLY:HA2	1:G:1589:GLN:HE21	1.81	0.46
1:G:3642:ILE:HD11	1:G:3695:ILE:HG22	1.96	0.46
1:A:394:HIS:HD2	1:A:397:GLY:H	1.64	0.46
1:A:894:VAL:HG13	1:A:918:LEU:HD22	1.97	0.46
1:A:3892:TYR:O	1:A:3896:LYS:NZ	2.40	0.46
1:A:4801:ASP:OD1	1:A:4801:ASP:N	2.49	0.46
1:C:3794:LEU:HD23	1:C:3794:LEU:HA	1.82	0.46
1:E:1033:VAL:HG23	1:E:1038:LEU:HD12	1.98	0.46
1:G:636:LEU:HD21	1:G:643:LEU:HD11	1.98	0.46
1:G:1430:VAL:HG11	1:G:1443:VAL:HG11	1.97	0.46
1:A:568:SER:HA	1:A:571:ILE:HD12	1.97	0.45
1:A:605:GLY:HA2	1:A:1589:GLN:HE21	1.81	0.45
1:A:1733:THR:HA	1:A:1755:THR:HG21	1.97	0.45
1:C:1440:ASN:OD1	1:C:1440:ASN:N	2.49	0.45
1:E:1440:ASN:N	1:E:1440:ASN:OD1	2.49	0.45
1:G:2464:ASP:N	1:G:2464:ASP:OD1	2.44	0.45
1:A:255:GLU:HB2	1:A:257:ARG:H	1.81	0.45
1:A:3793:SER:O	1:A:3797:LEU:N	2.45	0.45
1:C:687:THR:OG1	1:C:689:GLU:O	2.33	0.45
1:C:1220:ASP:HB3	1:C:1223:THR:HB	1.97	0.45
1:C:1221:VAL:HA	1:C:1224:LEU:HD12	1.99	0.45
1:C:1733:THR:HA	1:C:1755:THR:HG21	1.97	0.45
1:E:1221:VAL:HA	1:E:1224:LEU:HD12	1.99	0.45
1:E:2324:LEU:N	1:E:2324:LEU:HD23	2.31	0.45
1:E:4858:ILE:HD12	1:G:4867:ILE:CG2	2.26	0.45
1:G:797:GLY:CA	1:G:1621:CYS:O	2.59	0.45
1:G:1033:VAL:HG23	1:G:1038:LEU:HD12	1.98	0.45
1:A:1100:ARG:HH12	1:A:1170:GLU:H	1.65	0.45
1:A:3794:LEU:HD23	1:A:3794:LEU:HA	1.82	0.45
1:C:1764:SER:OG	1:C:1779:SER:O	2.33	0.45
1:C:4171:ARG:NE	5:C:6002:ATP:O2G	2.41	0.45
1:E:294:PRO:HB2	1:E:328:ALA:HB1	1.99	0.45
1:E:636:LEU:HD21	1:E:643:LEU:HD11	1.99	0.45
1:G:1124:PRO:HB2	1:G:1252:SER:HB2	1.98	0.45
1:G:4823:ARG:HB2	1:G:4823:ARG:HH11	1.71	0.45
1:A:294:PRO:HB2	1:A:328:ALA:HB1	1.99	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2265:LYS:HA	1:A:2268:ARG:HB2	1.98	0.45
1:A:2326:ILE:CB	1:G:207:PHE:CZ	2.99	0.45
1:A:4819:TYR:HD1	1:G:4845:ILE:HD12	1.56	0.45
1:C:2464:ASP:N	1:C:2464:ASP:OD1	2.44	0.45
1:E:1220:ASP:HB3	1:E:1223:THR:HB	1.98	0.45
1:E:4801:ASP:OD1	1:E:4801:ASP:N	2.49	0.45
1:G:2776:ILE:O	1:G:2779:SER:HB3	2.16	0.45
1:G:3980:VAL:HA	1:G:3983:LEU:HG	1.97	0.45
1:A:1614:ARG:HH11	1:A:1617:TRP:HE1	1.64	0.45
1:A:4519:LEU:O	1:G:4810:MET:HB3	2.17	0.45
1:C:572:LEU:HD12	1:C:572:LEU:HA	1.84	0.45
1:C:1033:VAL:HG23	1:C:1038:LEU:HD12	1.98	0.45
1:C:1124:PRO:HB2	1:C:1252:SER:HB2	1.98	0.45
1:C:4052:ALA:O	1:C:4056:HIS:ND1	2.38	0.45
1:G:1220:ASP:HB3	1:G:1223:THR:HB	1.97	0.45
1:G:2110:ASN:OD1	1:G:2110:ASN:N	2.49	0.45
1:G:2771:ILE:H	1:G:2771:ILE:HG13	1.63	0.45
1:A:1124:PRO:HB2	1:A:1252:SER:HB2	1.98	0.45
1:A:2314:VAL:HG23	1:A:2314:VAL:O	2.17	0.45
1:C:294:PRO:HB2	1:C:328:ALA:HB1	1.99	0.45
1:C:605:GLY:HA2	1:C:1589:GLN:HE21	1.81	0.45
1:C:4801:ASP:OD1	1:C:4801:ASP:N	2.49	0.45
1:A:1033:VAL:HG23	1:A:1038:LEU:HD12	1.98	0.45
1:A:1220:ASP:HB3	1:A:1223:THR:HB	1.97	0.45
1:A:1221:VAL:HA	1:A:1224:LEU:HD12	1.99	0.45
1:A:2776:ILE:O	1:A:2779:SER:HB3	2.16	0.45
1:C:35:LEU:HD12	1:C:49:LEU:HB3	1.99	0.45
1:C:4862:ILE:HG23	1:E:4868:ILE:HD11	1.99	0.45
1:E:2776:ILE:O	1:E:2779:SER:HB3	2.16	0.45
1:E:4051:LYS:O	1:E:4055:SER:N	2.46	0.45
1:G:294:PRO:HB2	1:G:328:ALA:HB1	1.99	0.45
1:G:1100:ARG:HH12	1:G:1170:GLU:H	1.65	0.45
1:G:1171:HIS:O	1:G:1194:ASP:N	2.45	0.45
1:G:2141:LYS:HE2	1:G:2141:LYS:HB2	1.80	0.45
1:G:2208:SER:OG	1:G:2209:ARG:N	2.50	0.45
1:A:3980:VAL:HA	1:A:3983:LEU:HG	1.97	0.45
1:C:443:SER:O	1:C:443:SER:OG	2.35	0.45
1:C:1171:HIS:O	1:C:1194:ASP:N	2.45	0.45
1:C:2093:TYR:HD2	1:C:3641:LEU:HD22	1.82	0.45
1:C:3927:GLY:O	1:C:3929:CYS:N	2.48	0.45
2:D:26:TYR:HB2	2:D:101:VAL:HG12	1.99	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1210:ALA:N	1:G:1211:GLN:OE1	2.50	0.45
1:G:3957:MET:O	1:G:3960:SER:OG	2.33	0.45
1:A:4770:LEU:HD13	1:C:4751:PHE:HD1	1.82	0.45
1:A:4791:ARG:HH22	1:C:4559:HIS:HE1	1.64	0.45
1:A:4867:ILE:CG2	1:G:4858:ILE:HD12	2.26	0.45
1:C:894:VAL:HG22	1:C:918:LEU:HA	1.99	0.45
1:C:1614:ARG:NH1	1:C:1617:TRP:HE1	2.15	0.45
1:E:661:LEU:O	1:E:788:PHE:N	2.43	0.45
1:E:767:SER:OG	1:E:777:GLY:O	2.35	0.45
1:E:1614:ARG:NH1	1:E:1617:TRP:HE1	2.15	0.45
1:E:2208:SER:OG	1:E:2209:ARG:N	2.50	0.45
1:E:3809:PHE:O	1:E:3813:ASN:N	2.50	0.45
1:G:2265:LYS:HA	1:G:2268:ARG:HB2	1.98	0.45
1:G:4801:ASP:OD1	1:G:4801:ASP:N	2.49	0.45
1:A:767:SER:OG	1:A:777:GLY:O	2.35	0.45
1:A:1210:ALA:N	1:A:1211:GLN:OE1	2.50	0.45
1:E:2265:LYS:HA	1:E:2268:ARG:HB2	1.98	0.45
1:E:4569:MET:O	1:E:4572:THR:OG1	2.31	0.45
1:G:998:LYS:HB3	1:G:998:LYS:HE3	1.82	0.45
1:A:494:MET:HA	1:A:497:LEU:HB2	2.00	0.44
1:A:1718:ARG:NH1	1:A:1758:ARG:HD3	2.33	0.44
1:A:2110:ASN:OD1	1:A:2110:ASN:N	2.49	0.44
1:A:2208:SER:OG	1:A:2209:ARG:N	2.50	0.44
1:C:2776:ILE:O	1:C:2779:SER:HB3	2.16	0.44
1:E:1718:ARG:NH1	1:E:1758:ARG:HD3	2.33	0.44
1:E:2110:ASN:OD1	1:E:2110:ASN:N	2.49	0.44
1:G:2314:VAL:HG23	1:G:2314:VAL:O	2.17	0.44
1:A:35:LEU:HD12	1:A:49:LEU:HB3	1.99	0.44
1:A:306:LEU:O	1:A:327:THR:OG1	2.27	0.44
1:C:1602:GLN:HB2	1:C:1643:GLU:HG2	1.99	0.44
1:C:2208:SER:OG	1:C:2209:ARG:N	2.50	0.44
1:C:4781:LEU:CD1	1:E:4741:ALA:O	2.65	0.44
1:E:1124:PRO:HB2	1:E:1252:SER:HB2	1.98	0.44
1:E:1210:ALA:N	1:E:1211:GLN:OE1	2.50	0.44
1:E:2093:TYR:HD2	1:E:3641:LEU:HD22	1.82	0.44
1:E:3957:MET:O	1:E:3960:SER:OG	2.33	0.44
1:G:1221:VAL:HA	1:G:1224:LEU:HD12	1.99	0.44
1:G:1718:ARG:NH1	1:G:1758:ARG:HD3	2.33	0.44
1:G:1849:SER:OG	1:G:1849:SER:O	2.35	0.44
1:A:636:LEU:HD21	1:A:643:LEU:HD11	1.99	0.44
2:B:78:PRO:HA	2:B:81:ALA:HB3	2.00	0.44

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:290:ARG:HA	1:C:353:GLU:HG2	1.99	0.44
1:C:544:ASN:HB2	1:C:547:ASN:HD22	1.83	0.44
1:C:1718:ARG:NH1	1:C:1758:ARG:HD3	2.33	0.44
1:C:1930:SER:O	1:C:1930:SER:OG	2.31	0.44
1:C:2141:LYS:HE2	1:C:2141:LYS:HB2	1.80	0.44
2:D:78:PRO:HA	2:D:81:ALA:HB3	2.00	0.44
1:E:1614:ARG:HH11	1:E:1617:TRP:HE1	1.64	0.44
1:E:2264:GLU:HG2	1:E:2324:LEU:CD1	2.47	0.44
1:E:3927:GLY:O	1:E:3929:CYS:N	2.48	0.44
2:F:57:LYS:HD2	2:F:57:LYS:HA	1.69	0.44
1:G:290:ARG:HA	1:G:353:GLU:HG2	1.99	0.44
2:H:78:PRO:HA	2:H:81:ALA:HB3	2.00	0.44
1:A:1614:ARG:HA	1:A:1614:ARG:HD3	1.86	0.44
1:A:4168:GLU:OE1	1:A:4595:LYS:NZ	2.46	0.44
1:C:408:SER:OG	1:C:409:GLN:N	2.50	0.44
1:C:1210:ALA:N	1:C:1211:GLN:OE1	2.50	0.44
1:C:2110:ASN:OD1	1:C:2113:SER:OG	2.34	0.44
1:C:2265:LYS:HA	1:C:2268:ARG:HB2	1.98	0.44
1:C:2771:ILE:H	1:C:2771:ILE:HG13	1.63	0.44
2:F:26:TYR:HB2	2:F:101:VAL:HG12	1.99	0.44
2:F:78:PRO:HA	2:F:81:ALA:HB3	2.00	0.44
1:A:2110:ASN:OD1	1:A:2113:SER:OG	2.34	0.44
2:B:21:THR:HG22	2:B:49:ARG:HE	1.83	0.44
1:C:3761:LYS:NZ	1:C:3835:GLU:OE2	2.42	0.44
2:D:21:THR:HG22	2:D:49:ARG:HE	1.83	0.44
1:E:1939:ASP:OD1	1:E:1939:ASP:N	2.40	0.44
1:E:2307:VAL:HG12	1:E:2317:ASN:HB3	1.99	0.44
1:E:4168:GLU:OE1	1:E:4595:LYS:NZ	2.46	0.44
1:G:676:GLU:OE1	1:G:756:SER:OG	2.33	0.44
1:A:243:GLU:OE2	1:A:389:ARG:NH2	2.51	0.44
1:A:1440:ASN:OD1	1:A:1440:ASN:N	2.49	0.44
1:A:1811:GLY:HA3	1:A:1816:PHE:HB2	2.00	0.44
1:A:2093:TYR:HD2	1:A:3641:LEU:HD22	1.82	0.44
1:C:494:MET:HA	1:C:497:LEU:HB2	2.00	0.44
1:C:3809:PHE:O	1:C:3813:ASN:N	2.50	0.44
1:E:35:LEU:HD12	1:E:49:LEU:HB3	1.99	0.44
1:E:243:GLU:OE2	1:E:389:ARG:NH2	2.51	0.44
1:E:255:GLU:HB2	1:E:257:ARG:H	1.81	0.44
1:E:544:ASN:HB2	1:E:547:ASN:HD22	1.83	0.44
1:E:1930:SER:O	1:E:1930:SER:OG	2.31	0.44
1:G:408:SER:OG	1:G:409:GLN:N	2.50	0.44

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:494:MET:HA	1:G:497:LEU:HB2	1.99	0.44
1:G:894:VAL:HG22	1:G:918:LEU:HA	1.99	0.44
1:G:1614:ARG:NH1	1:G:1617:TRP:HE1	2.15	0.44
1:G:1614:ARG:HH11	1:G:1617:TRP:HE1	1.64	0.44
1:G:2857:LYS:HZ3	1:G:2869:HIS:HB3	1.83	0.44
1:G:4052:ALA:O	1:G:4056:HIS:ND1	2.38	0.44
1:A:4751:PHE:HD1	1:G:4770:LEU:HD13	1.82	0.44
1:C:636:LEU:HD21	1:C:643:LEU:HD11	1.99	0.44
1:E:1811:GLY:HA3	1:E:1816:PHE:HB2	2.00	0.44
1:E:3962:ASP:HB2	1:E:3965:GLN:HE22	1.83	0.44
1:G:544:ASN:HB2	1:G:547:ASN:HD22	1.83	0.44
1:G:1602:GLN:HB2	1:G:1643:GLU:HG2	1.99	0.44
1:G:2110:ASN:OD1	1:G:2113:SER:OG	2.34	0.44
1:G:2148:GLY:O	1:G:2152:ASN:ND2	2.51	0.44
1:C:76:ARG:HD2	1:E:3891:TRP:CG	2.45	0.44
1:C:243:GLU:OE2	1:C:389:ARG:NH2	2.51	0.44
1:C:1614:ARG:HH11	1:C:1617:TRP:HE1	1.64	0.44
1:E:2141:LYS:HE2	1:E:2141:LYS:HB2	1.80	0.44
1:E:4045:SER:OG	1:E:4048:ASP:N	2.48	0.44
1:G:234:LEU:HD13	1:G:405:LEU:HD22	2.00	0.44
1:G:611:LEU:HD22	1:G:1660:LEU:HD22	1.99	0.44
1:G:3900:ASP:N	1:G:3900:ASP:OD1	2.47	0.44
2:H:21:THR:HG22	2:H:49:ARG:HE	1.83	0.44
1:A:290:ARG:HA	1:A:353:GLU:HG2	1.99	0.44
1:A:408:SER:OG	1:A:409:GLN:N	2.50	0.44
1:A:1009:ARG:HA	1:A:1012:ILE:HG12	2.00	0.44
1:A:4569:MET:O	1:A:4572:THR:OG1	2.31	0.44
2:B:57:LYS:HD2	2:B:57:LYS:HA	1.69	0.44
1:C:1687:TYR:OH	1:C:1691:ASN:ND2	2.51	0.44
1:C:2148:GLY:O	1:C:2152:ASN:ND2	2.51	0.44
1:C:4045:SER:OG	1:C:4048:ASP:N	2.48	0.44
1:C:4945:TYR:OH	6:C:6003:CFF:H81	2.18	0.44
2:F:21:THR:HG22	2:F:49:ARG:HE	1.83	0.44
1:G:767:SER:OG	1:G:777:GLY:O	2.35	0.44
1:A:652:VAL:HG21	1:A:714:GLY:HA3	2.00	0.43
1:A:4810:MET:HB3	1:C:4519:LEU:O	2.18	0.43
1:C:652:VAL:HG21	1:C:714:GLY:HA3	2.00	0.43
1:C:1572:LYS:HD2	1:C:1585:ARG:H	1.83	0.43
1:C:3892:TYR:O	1:C:3896:LYS:NZ	2.40	0.43
1:E:1687:TYR:OH	1:E:1691:ASN:ND2	2.51	0.43
1:E:2148:GLY:O	1:E:2152:ASN:ND2	2.51	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:35:LEU:HD12	1:G:49:LEU:HB3	1.99	0.43
1:A:1572:LYS:HD2	1:A:1585:ARG:H	1.83	0.43
1:A:1614:ARG:NH1	1:A:1617:TRP:HE1	2.15	0.43
1:A:2120:LEU:HD13	1:A:2153:ASN:HD22	1.83	0.43
2:B:26:TYR:HB2	2:B:101:VAL:HG12	1.99	0.43
1:C:1009:ARG:HA	1:C:1012:ILE:HG12	2.00	0.43
1:C:1100:ARG:HH12	1:C:1170:GLU:H	1.65	0.43
1:C:1811:GLY:HA3	1:C:1816:PHE:HB2	2.00	0.43
1:E:234:LEU:HD13	1:E:405:LEU:HD22	2.00	0.43
1:E:443:SER:O	1:E:443:SER:OG	2.35	0.43
1:E:652:VAL:HG21	1:E:714:GLY:HA3	2.00	0.43
1:E:2103:LEU:HD23	1:E:2103:LEU:HA	1.81	0.43
1:G:652:VAL:HG21	1:G:714:GLY:HA3	2.00	0.43
1:G:1687:TYR:OH	1:G:1691:ASN:ND2	2.51	0.43
1:G:1811:GLY:HA3	1:G:1816:PHE:HB2	2.00	0.43
1:G:2093:TYR:HD2	1:G:3641:LEU:HD22	1.82	0.43
1:G:2226:SER:O	1:G:2226:SER:OG	2.33	0.43
1:G:3809:PHE:O	1:G:3813:ASN:N	2.50	0.43
1:A:544:ASN:HB2	1:A:547:ASN:HD22	1.83	0.43
1:A:611:LEU:HD22	1:A:1660:LEU:HD22	1.99	0.43
1:A:2771:ILE:H	1:A:2771:ILE:HG13	1.63	0.43
1:E:494:MET:HA	1:E:497:LEU:HB2	2.00	0.43
1:E:894:VAL:HG22	1:E:918:LEU:HA	1.99	0.43
1:E:1100:ARG:HH12	1:E:1170:GLU:H	1.65	0.43
1:E:1602:GLN:HB2	1:E:1643:GLU:HG2	1.99	0.43
1:E:4945:TYR:OH	6:E:6003:CFF:H81	2.18	0.43
1:G:3962:ASP:HB2	1:G:3965:GLN:HE22	1.83	0.43
1:A:406:SER:O	1:A:406:SER:OG	2.35	0.43
1:A:797:GLY:CA	1:A:1621:CYS:O	2.59	0.43
1:A:894:VAL:HG22	1:A:918:LEU:HA	1.99	0.43
1:A:1823:LYS:HB2	1:A:1823:LYS:HE3	1.88	0.43
1:A:2088:LEU:HD12	1:A:2088:LEU:HA	1.84	0.43
1:C:2298:ARG:O	1:C:2301:ASP:HB3	2.19	0.43
1:E:1009:ARG:HA	1:E:1012:ILE:HG12	2.00	0.43
1:G:243:GLU:OE2	1:G:389:ARG:NH2	2.51	0.43
1:G:1009:ARG:HA	1:G:1012:ILE:HG12	2.00	0.43
1:G:3794:LEU:HD23	1:G:3794:LEU:HA	1.82	0.43
1:A:4862:ILE:HG23	1:C:4868:ILE:HD11	1.99	0.43
1:C:399:MET:SD	1:C:399:MET:N	2.92	0.43
1:C:2876:ASP:OD1	1:C:2876:ASP:N	2.47	0.43
1:C:4810:MET:HB3	1:E:4519:LEU:O	2.18	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:57:LYS:HD2	2:D:57:LYS:HA	1.69	0.43
1:E:30:LYS:HD3	1:E:30:LYS:HA	1.69	0.43
1:E:408:SER:OG	1:E:409:GLN:N	2.50	0.43
1:G:976:TYR:CZ	1:G:978:PRO:HB3	2.53	0.43
1:G:2120:LEU:HD13	1:G:2153:ASN:HD22	1.83	0.43
2:H:26:TYR:HB2	2:H:101:VAL:HG12	1.99	0.43
1:A:1228:THR:OG1	1:A:1229:ILE:N	2.52	0.43
1:A:4523:VAL:CG1	1:G:4808:ASP:HB2	2.49	0.43
1:C:611:LEU:HD22	1:C:1660:LEU:HD22	1.99	0.43
1:C:976:TYR:CZ	1:C:978:PRO:HB3	2.53	0.43
1:E:2270:LEU:HA	1:E:2270:LEU:HD23	1.81	0.43
1:G:1228:THR:OG1	1:G:1229:ILE:N	2.52	0.43
1:G:1572:LYS:HD2	1:G:1585:ARG:H	1.83	0.43
1:G:1610:ARG:HE	1:G:1610:ARG:HB3	1.64	0.43
1:G:2298:ARG:O	1:G:2301:ASP:HB3	2.19	0.43
1:G:3984:LEU:HD23	1:G:3984:LEU:HA	1.87	0.43
1:G:4945:TYR:OH	6:G:6003:CFF:H81	2.18	0.43
1:A:399:MET:SD	1:A:399:MET:N	2.92	0.43
1:A:1687:TYR:OH	1:A:1691:ASN:ND2	2.51	0.43
1:A:2298:ARG:O	1:A:2301:ASP:HB3	2.19	0.43
1:A:2323:ARG:HD2	1:G:189:GLU:OE2	2.18	0.43
1:C:180:ASP:HB3	1:C:211:LEU:HD12	2.01	0.43
1:C:374:TYR:HE1	1:C:400:ASP:HB2	1.84	0.43
1:C:3962:ASP:HB2	1:C:3965:GLN:HE22	1.83	0.43
1:E:66:THR:OG1	1:E:124:SER:OG	2.25	0.43
1:E:611:LEU:HD22	1:E:1660:LEU:HD22	1.99	0.43
1:E:1228:THR:OG1	1:E:1229:ILE:N	2.52	0.43
1:E:1572:LYS:HD2	1:E:1585:ARG:H	1.83	0.43
1:E:4892:CYS:HB3	1:E:4894:ILE:HG12	2.01	0.43
1:G:1211:GLN:OE1	1:G:1211:GLN:N	2.52	0.43
1:G:1630:LEU:HD22	1:G:1641:ILE:HG13	2.01	0.43
1:A:897:LYS:HE3	1:A:897:LYS:HB3	1.92	0.43
1:A:976:TYR:CZ	1:A:978:PRO:HB3	2.53	0.43
1:A:1211:GLN:OE1	1:A:1211:GLN:N	2.52	0.43
1:A:4754:LEU:HD21	1:G:4770:LEU:C	2.39	0.43
1:C:1211:GLN:OE1	1:C:1211:GLN:N	2.52	0.43
1:C:1840:LYS:O	1:C:1844:GLN:NE2	2.52	0.43
1:C:4892:CYS:HB3	1:C:4894:ILE:HG12	2.01	0.43
1:E:374:TYR:HE1	1:E:400:ASP:HB2	1.84	0.43
1:E:3892:TYR:O	1:E:3896:LYS:NZ	2.40	0.43
1:G:374:TYR:HE1	1:G:400:ASP:HB2	1.84	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:572:LEU:HD12	1:G:572:LEU:HA	1.84	0.43
1:G:2397:ILE:HD13	1:G:2397:ILE:HA	1.90	0.43
1:G:4171:ARG:NE	5:G:6002:ATP:O2G	2.41	0.43
1:A:1602:GLN:HB2	1:A:1643:GLU:HG2	1.99	0.43
1:A:4868:ILE:HD11	1:G:4862:ILE:HG23	2.00	0.43
2:B:42:ARG:HG3	2:B:44:LYS:HB2	2.01	0.43
1:C:156:GLU:HB2	1:C:187:SER:HB3	2.01	0.43
1:C:644:LEU:HB3	1:C:1630:LEU:HD12	2.01	0.43
1:C:4791:ARG:HH22	1:E:4559:HIS:HE1	1.66	0.43
1:E:3829:LYS:HB3	1:E:3829:LYS:HE3	1.86	0.43
2:F:38:SER:OG	2:F:39:SER:N	2.52	0.43
1:A:374:TYR:HE1	1:A:400:ASP:HB2	1.84	0.43
1:A:4744:LEU:HD23	1:A:4744:LEU:HA	1.78	0.43
1:C:900:LEU:HD23	1:C:902:TRP:HE1	1.84	0.43
1:C:2267:VAL:HG21	1:C:2324:LEU:HB3	2.00	0.43
1:E:290:ARG:HA	1:E:353:GLU:HG2	1.99	0.43
1:E:4770:LEU:HD13	1:G:4751:PHE:HD1	1.83	0.43
1:A:59:PRO:HB3	1:A:296:ARG:CZ	2.49	0.42
1:A:180:ASP:HB3	1:A:211:LEU:HD12	2.01	0.42
1:A:1526:ASP:OD1	1:A:1526:ASP:N	2.52	0.42
1:A:2148:GLY:O	1:A:2152:ASN:ND2	2.51	0.42
1:A:3962:ASP:HB2	1:A:3965:GLN:HE22	1.83	0.42
1:A:4945:TYR:OH	6:A:6003:CFF:H81	2.18	0.42
1:C:2120:LEU:HD13	1:C:2153:ASN:HD22	1.83	0.42
1:E:399:MET:SD	1:E:399:MET:N	2.92	0.42
1:E:2298:ARG:O	1:E:2301:ASP:HB3	2.19	0.42
1:E:4858:ILE:CD1	1:G:4867:ILE:HG21	2.27	0.42
1:A:572:LEU:HD12	1:A:572:LEU:HA	1.84	0.42
1:A:864:PRO:HG3	1:A:1034:PRO:HB3	2.01	0.42
1:A:1445:TRP:H	1:A:1487:MET:HG2	1.84	0.42
1:A:2270:LEU:HD23	1:A:2270:LEU:HA	1.81	0.42
1:C:767:SER:OG	1:C:777:GLY:O	2.35	0.42
1:C:2271:ALA:HB2	1:C:2328:ARG:HD3	2.01	0.42
2:D:11:ASP:OD1	2:D:11:ASP:N	2.52	0.42
1:E:474:ASP:HA	1:E:477:ASN:HD22	1.84	0.42
1:E:976:TYR:CZ	1:E:978:PRO:HB3	2.53	0.42
1:E:1211:GLN:OE1	1:E:1211:GLN:N	2.52	0.42
1:E:2271:ALA:HB2	1:E:2328:ARG:HD3	2.01	0.42
1:E:3857:ASN:OD1	1:E:3860:ARG:NH1	2.52	0.42
1:E:4808:ASP:HB2	1:G:4523:VAL:CG1	2.50	0.42
1:G:3880:LEU:HD21	1:G:3940:ARG:HD2	2.01	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:42:ARG:HG3	2:H:44:LYS:HB2	2.01	0.42
1:A:1840:LYS:O	1:A:1844:GLN:NE2	2.52	0.42
1:A:4770:LEU:C	1:C:4754:LEU:HD11	2.39	0.42
1:C:234:LEU:HD13	1:C:405:LEU:HD22	2.00	0.42
1:C:998:LYS:HB3	1:C:998:LYS:HE3	1.82	0.42
1:C:4823:ARG:H	1:C:4823:ARG:HG3	1.55	0.42
1:E:900:LEU:HD23	1:E:902:TRP:HE1	1.84	0.42
1:E:1250:TRP:HE1	1:E:1602:GLN:HG3	1.84	0.42
1:E:2226:SER:O	1:E:2226:SER:OG	2.33	0.42
1:E:4894:ILE:HD13	1:E:4894:ILE:HA	1.94	0.42
1:G:3857:ASN:OD1	1:G:3860:ARG:NH1	2.52	0.42
2:H:38:SER:OG	2:H:39:SER:N	2.52	0.42
1:A:156:GLU:HB2	1:A:187:SER:HB3	2.01	0.42
1:A:1630:LEU:HD22	1:A:1641:ILE:HG13	2.01	0.42
1:A:4589:ILE:HD13	1:A:4589:ILE:HA	1.92	0.42
1:C:1228:THR:OG1	1:C:1229:ILE:N	2.52	0.42
1:C:3880:LEU:HD21	1:C:3940:ARG:HD2	2.01	0.42
1:E:1823:LYS:HB2	1:E:1823:LYS:HE3	1.88	0.42
1:E:1828:LEU:HD12	1:E:1828:LEU:HA	1.87	0.42
1:E:1840:LYS:O	1:E:1844:GLN:NE2	2.52	0.42
2:F:30:LEU:HD23	2:F:30:LEU:HA	1.90	0.42
1:G:192:LEU:O	1:G:212:TRP:NE1	2.47	0.42
1:G:399:MET:SD	1:G:399:MET:N	2.92	0.42
1:G:4045:SER:OG	1:G:4048:ASP:N	2.48	0.42
1:A:3880:LEU:HD21	1:A:3940:ARG:HD2	2.01	0.42
1:A:4892:CYS:HB3	1:A:4894:ILE:HG12	2.01	0.42
1:C:1526:ASP:N	1:C:1526:ASP:OD1	2.52	0.42
1:C:3957:MET:O	1:C:3960:SER:OG	2.33	0.42
1:E:143:LEU:HD22	1:G:2427:LEU:HD21	1.92	0.42
1:E:189:GLU:OE2	1:G:2323:ARG:HD2	2.19	0.42
1:E:406:SER:O	1:E:406:SER:OG	2.35	0.42
1:E:449:ILE:HD13	1:E:449:ILE:HA	1.88	0.42
1:E:1556:GLU:O	1:E:1572:LYS:NZ	2.44	0.42
1:G:1250:TRP:NE1	1:G:1643:GLU:OE2	2.53	0.42
1:G:3844:LEU:HA	1:G:3844:LEU:HD23	1.84	0.42
2:H:5:GLU:HB3	2:H:73:LYS:HB3	2.02	0.42
1:A:234:LEU:HD13	1:A:405:LEU:HD22	2.00	0.42
1:A:677:LEU:HD11	1:A:792:VAL:HG21	2.02	0.42
1:A:3609:LEU:HD12	1:A:3609:LEU:HA	1.86	0.42
1:C:59:PRO:HB3	1:C:296:ARG:CZ	2.49	0.42
1:C:864:PRO:HG3	1:C:1034:PRO:HB3	2.01	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1250:TRP:HE1	1:C:1602:GLN:HG3	1.84	0.42
1:C:2030:LEU:HD23	1:C:2030:LEU:HA	1.90	0.42
1:E:59:PRO:HB3	1:E:296:ARG:CZ	2.50	0.42
1:E:351:THR:OG1	1:E:352:SER:N	2.53	0.42
1:E:1445:TRP:H	1:E:1487:MET:HG2	1.84	0.42
1:E:1526:ASP:N	1:E:1526:ASP:OD1	2.52	0.42
1:E:1610:ARG:HE	1:E:1610:ARG:HB3	1.64	0.42
1:E:3609:LEU:HD12	1:E:3609:LEU:HA	1.86	0.42
1:G:1556:GLU:O	1:G:1572:LYS:NZ	2.44	0.42
1:A:900:LEU:HD23	1:A:902:TRP:HE1	1.84	0.42
1:A:2518:ASN:HA	1:A:2521:LEU:HD12	2.02	0.42
1:A:4808:ASP:HB2	1:C:4523:VAL:HG11	2.02	0.42
1:C:351:THR:OG1	1:C:352:SER:N	2.53	0.42
1:C:1785:ASP:OD1	1:C:1785:ASP:N	2.53	0.42
1:C:1792:ILE:HG12	1:C:1842:ILE:HD11	2.01	0.42
1:C:3793:SER:O	1:C:3797:LEU:N	2.45	0.42
1:C:4770:LEU:HD13	1:E:4751:PHE:HD1	1.85	0.42
1:E:156:GLU:HB2	1:E:187:SER:HB3	2.01	0.42
1:E:357:GLY:O	1:E:404:ASN:ND2	2.46	0.42
1:E:505:LEU:HD23	1:E:505:LEU:HA	1.83	0.42
1:E:677:LEU:HD11	1:E:792:VAL:HG21	2.02	0.42
1:E:4862:ILE:HG23	1:G:4868:ILE:HD11	2.01	0.42
1:G:59:PRO:HB3	1:G:296:ARG:CZ	2.49	0.42
1:G:1658:LEU:HD23	1:G:1658:LEU:HA	1.80	0.42
1:G:1840:LYS:O	1:G:1844:GLN:NE2	2.52	0.42
1:G:2163:MET:SD	1:G:2163:MET:N	2.93	0.42
1:G:3834:ASP:O	1:G:3837:THR:OG1	2.33	0.42
1:A:1250:TRP:NE1	1:A:1643:GLU:OE2	2.53	0.42
1:A:1258:PHE:HA	1:A:1595:LEU:HA	2.02	0.42
1:A:2163:MET:SD	1:A:2163:MET:N	2.93	0.42
2:B:38:SER:OG	2:B:39:SER:N	2.52	0.42
1:C:1445:TRP:H	1:C:1487:MET:HG2	1.84	0.42
2:D:42:ARG:HG3	2:D:44:LYS:HB2	2.01	0.42
1:E:1258:PHE:HA	1:E:1595:LEU:HA	2.02	0.42
1:G:156:GLU:HB2	1:G:187:SER:HB3	2.01	0.42
1:G:180:ASP:HB3	1:G:211:LEU:HD12	2.01	0.42
1:G:1445:TRP:H	1:G:1487:MET:HG2	1.84	0.42
1:G:1785:ASP:OD1	1:G:1785:ASP:N	2.53	0.42
1:G:2518:ASN:HA	1:G:2521:LEU:HD12	2.02	0.42
1:G:3991:VAL:HG12	1:G:4145:ARG:NH2	2.35	0.42
1:A:325:LYS:O	1:A:365:HIS:NE2	2.53	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:GLY:O	1:A:404:ASN:ND2	2.46	0.42
1:A:472:HIS:O	1:A:472:HIS:ND1	2.53	0.42
1:A:644:LEU:HB3	1:A:1630:LEU:HD12	2.01	0.42
1:A:1273:ILE:HD11	1:A:1287:GLN:HB2	2.02	0.42
1:C:274:LEU:HD23	1:C:274:LEU:HA	1.90	0.42
1:C:1258:PHE:HA	1:C:1595:LEU:HA	2.02	0.42
2:D:38:SER:OG	2:D:39:SER:N	2.52	0.42
1:E:274:LEU:HD23	1:E:274:LEU:HA	1.90	0.42
1:E:1273:ILE:HD11	1:E:1287:GLN:HB2	2.02	0.42
1:E:2071:ALA:HB2	1:E:2085:MET:HE1	2.02	0.42
1:E:2120:LEU:HD13	1:E:2153:ASN:HD22	1.83	0.42
1:E:2771:ILE:H	1:E:2771:ILE:HG13	1.63	0.42
1:G:474:ASP:HA	1:G:477:ASN:HD22	1.84	0.42
1:G:1250:TRP:HE1	1:G:1602:GLN:HG3	1.84	0.42
1:G:1792:ILE:HG12	1:G:1842:ILE:HD11	2.01	0.42
1:A:1764:SER:OG	1:A:1779:SER:O	2.33	0.42
1:C:2316:GLU:HG2	1:C:3811:ARG:NH2	2.35	0.42
1:C:3630:ILE:HD13	1:C:3630:ILE:HA	1.93	0.42
1:E:1630:LEU:HD22	1:E:1641:ILE:HG13	2.01	0.42
1:G:1258:PHE:HA	1:G:1595:LEU:HA	2.02	0.42
1:G:1273:ILE:HD11	1:G:1287:GLN:HB2	2.02	0.42
1:G:1308:ILE:HG12	1:G:1575:HIS:HD1	1.85	0.42
1:G:1911:LEU:HD23	1:G:1911:LEU:HA	1.92	0.42
1:A:3991:VAL:HG12	1:A:4145:ARG:NH2	2.35	0.41
1:A:4867:ILE:HG21	1:G:4858:ILE:CD1	2.27	0.41
2:B:5:GLU:HB3	2:B:73:LYS:HB3	2.02	0.41
1:C:1273:ILE:HD11	1:C:1287:GLN:HB2	2.02	0.41
1:C:2103:LEU:HD23	1:C:2103:LEU:HA	1.81	0.41
1:C:3920:THR:O	1:C:3920:THR:OG1	2.38	0.41
1:E:180:ASP:HB3	1:E:211:LEU:HD12	2.01	0.41
1:E:799:LYS:HA	1:E:1619:VAL:O	2.20	0.41
1:E:1171:HIS:O	1:E:1194:ASP:N	2.45	0.41
1:E:1250:TRP:NE1	1:E:1643:GLU:OE2	2.53	0.41
1:E:4849:ILE:HD12	1:E:4849:ILE:HA	1.92	0.41
1:G:66:THR:OG1	1:G:124:SER:OG	2.25	0.41
1:G:438:LYS:HA	1:G:438:LYS:HD3	1.88	0.41
1:G:677:LEU:HD11	1:G:792:VAL:HG21	2.02	0.41
1:G:900:LEU:HD23	1:G:902:TRP:HE1	1.84	0.41
1:G:1526:ASP:N	1:G:1526:ASP:OD1	2.52	0.41
1:G:2402:ARG:HA	1:G:2402:ARG:HD3	1.86	0.41
1:G:4892:CYS:HB3	1:G:4894:ILE:HG12	2.01	0.41

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1250:TRP:HE1	1:A:1602:GLN:HG3	1.84	0.41
1:A:1300:MET:HB3	1:A:1302:TYR:CZ	2.55	0.41
1:A:1792:ILE:HG12	1:A:1842:ILE:HD11	2.01	0.41
1:A:1828:LEU:HD12	1:A:1828:LEU:HA	1.87	0.41
1:C:76:ARG:CB	1:C:76:ARG:NH2	2.73	0.41
1:C:676:GLU:OE1	1:C:756:SER:OG	2.33	0.41
1:C:1300:MET:HB3	1:C:1302:TYR:CZ	2.54	0.41
1:C:1849:SER:OG	1:C:1849:SER:O	2.35	0.41
1:E:2328:ARG:CB	1:E:2329:PRO:CD	2.97	0.41
1:G:325:LYS:O	1:G:365:HIS:NE2	2.53	0.41
1:G:351:THR:OG1	1:G:352:SER:N	2.53	0.41
1:G:864:PRO:HG3	1:G:1034:PRO:HB3	2.01	0.41
1:G:2270:LEU:HA	1:G:2270:LEU:HD23	1.81	0.41
1:A:438:LYS:HD3	1:A:438:LYS:HA	1.87	0.41
1:A:1689:ILE:HD11	1:A:1706:LEU:HD22	2.02	0.41
1:A:3841:PHE:HB3	1:A:3920:THR:HG21	2.02	0.41
1:C:1570:LEU:HD23	1:C:1570:LEU:HA	1.95	0.41
1:C:1689:ILE:HD11	1:C:1706:LEU:HD22	2.02	0.41
1:C:2116:ASP:OD1	1:C:2116:ASP:N	2.46	0.41
1:E:1300:MET:HB3	1:E:1302:TYR:CZ	2.55	0.41
1:E:2099:LEU:HD12	1:E:2099:LEU:HA	1.92	0.41
1:E:3880:LEU:HD21	1:E:3940:ARG:HD2	2.01	0.41
1:E:3991:VAL:HG12	1:E:4145:ARG:NH2	2.35	0.41
1:E:4819:TYR:O	1:E:4823:ARG:NE	2.53	0.41
1:G:1300:MET:HB3	1:G:1302:TYR:CZ	2.55	0.41
1:A:2073:GLU:H	1:A:2073:GLU:HG2	1.66	0.41
1:A:4523:VAL:HG11	1:G:4808:ASP:HB2	2.02	0.41
1:C:677:LEU:HD11	1:C:792:VAL:HG21	2.02	0.41
1:C:2128:ARG:O	1:C:2131:LEU:HB2	2.20	0.41
1:C:2270:LEU:HA	1:C:2270:LEU:HD23	1.81	0.41
1:E:281:ARG:NH2	1:E:284:TRP:O	2.54	0.41
1:E:1785:ASP:N	1:E:1785:ASP:OD1	2.53	0.41
1:E:1792:ILE:HG12	1:E:1842:ILE:HD11	2.01	0.41
2:F:42:ARG:HG3	2:F:44:LYS:HB2	2.01	0.41
1:G:281:ARG:NH2	1:G:284:TRP:O	2.54	0.41
1:G:1842:ILE:HD13	1:G:1842:ILE:HA	1.91	0.41
1:G:3920:THR:O	1:G:3920:THR:OG1	2.38	0.41
1:A:505:LEU:HD22	1:A:526:TRP:CD1	2.56	0.41
1:A:1942:ARG:HH12	1:A:3609:LEU:H	1.69	0.41
1:A:4808:ASP:HB2	1:C:4523:VAL:CG1	2.50	0.41
1:C:474:ASP:HA	1:C:477:ASN:HD22	1.85	0.41

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2141:LYS:H	1:C:2141:LYS:HG3	1.74	0.41
1:E:505:LEU:HD22	1:E:526:TRP:CD1	2.56	0.41
1:E:3628:SER:OG	1:E:3629:TRP:N	2.54	0.41
1:G:644:LEU:HB3	1:G:1630:LEU:HD12	2.01	0.41
1:G:3663:ASP:HB2	1:G:3666:HIS:HB2	2.02	0.41
1:G:3841:PHE:HB3	1:G:3920:THR:HG21	2.02	0.41
1:G:4168:GLU:OE1	1:G:4595:LYS:NZ	2.46	0.41
2:H:11:ASP:OD2	2:H:14:THR:OG1	2.35	0.41
1:A:1685:LEU:HD23	1:A:1685:LEU:HA	1.93	0.41
1:A:1712:SER:O	1:A:1712:SER:OG	2.29	0.41
1:A:2834:LEU:HD13	1:A:2839:HIS:HB3	2.03	0.41
1:C:505:LEU:HD22	1:C:526:TRP:CD1	2.56	0.41
1:C:1250:TRP:NE1	1:C:1643:GLU:OE2	2.53	0.41
1:C:1731:GLU:O	1:C:1735:SER:OG	2.37	0.41
1:C:1906:GLN:HE21	1:C:1906:GLN:HB3	1.67	0.41
1:C:2071:ALA:HB2	1:C:2085:MET:HE1	2.02	0.41
1:C:2518:ASN:HA	1:C:2521:LEU:HD12	2.02	0.41
1:E:192:LEU:O	1:E:212:TRP:NE1	2.47	0.41
1:E:2779:SER:HB2	1:E:2889:LYS:HZ3	1.85	0.41
1:E:2834:LEU:HD13	1:E:2839:HIS:HB3	2.03	0.41
1:E:3663:ASP:HB2	1:E:3666:HIS:HB2	2.02	0.41
1:G:618:CYS:HB2	1:G:629:GLN:HG2	2.02	0.41
1:G:1614:ARG:HA	1:G:1614:ARG:HD3	1.86	0.41
2:H:11:ASP:OD1	2:H:11:ASP:N	2.52	0.41
1:A:274:LEU:HD23	1:A:274:LEU:HA	1.90	0.41
1:A:558:LEU:HD23	1:A:558:LEU:HA	1.87	0.41
1:A:1757:LEU:HA	1:A:1757:LEU:HD12	1.89	0.41
1:A:2071:ALA:HB2	1:A:2085:MET:HE1	2.03	0.41
1:A:3663:ASP:HB2	1:A:3666:HIS:HB2	2.02	0.41
1:A:4809:ASP:O	1:A:4813:CYS:N	2.49	0.41
1:C:1122:CYS:HA	1:C:1133:ARG:HD3	2.03	0.41
1:C:1630:LEU:HD22	1:C:1641:ILE:HG13	2.01	0.41
1:C:3993:ASN:HD22	1:C:4110:MET:HG3	1.86	0.41
1:C:4561:VAL:HG11	1:C:4570:GLU:HB3	2.03	0.41
1:E:644:LEU:HB3	1:E:1630:LEU:HD12	2.01	0.41
1:E:1122:CYS:HA	1:E:1133:ARG:HD3	2.03	0.41
1:E:2853:TRP:HA	1:E:2856:LYS:HB2	2.03	0.41
1:E:3844:LEU:HD23	1:E:3844:LEU:HA	1.84	0.41
1:E:3993:ASN:HD22	1:E:4110:MET:HG3	1.86	0.41
1:G:799:LYS:HA	1:G:1619:VAL:O	2.20	0.41
1:G:4945:TYR:HE2	6:G:6003:CFF:H141	1.86	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:LEU:HD13	1:A:35:LEU:HA	1.96	0.41
1:A:618:CYS:HB2	1:A:629:GLN:HG2	2.02	0.41
1:A:2128:ARG:O	1:A:2131:LEU:HB2	2.20	0.41
1:A:4945:TYR:HE2	6:A:6003:CFF:H141	1.86	0.41
1:C:2163:MET:SD	1:C:2163:MET:N	2.93	0.41
1:E:2518:ASN:HA	1:E:2521:LEU:HD12	2.02	0.41
2:F:5:GLU:HB3	2:F:73:LYS:HB3	2.02	0.41
1:G:505:LEU:HD22	1:G:526:TRP:CD1	2.56	0.41
1:G:1942:ARG:HH12	1:G:3609:LEU:H	1.69	0.41
1:G:3739:GLU:O	1:G:3743:GLN:N	2.53	0.41
1:A:55:SER:O	1:A:296:ARG:NH2	2.45	0.41
1:A:351:THR:OG1	1:A:352:SER:N	2.53	0.41
1:A:424:PHE:HB3	1:A:428:ARG:HH21	1.86	0.41
1:A:1939:ASP:OD1	1:A:1939:ASP:N	2.40	0.41
1:A:3739:GLU:O	1:A:3743:GLN:N	2.53	0.41
1:A:3883:GLN:HE21	1:A:3947:GLY:HA3	1.86	0.41
1:A:4103:LEU:HD23	1:A:4103:LEU:HA	1.94	0.41
1:C:424:PHE:HB3	1:C:428:ARG:HH21	1.86	0.41
1:C:424:PHE:HB3	1:C:428:ARG:NH2	2.36	0.41
1:C:618:CYS:HB2	1:C:629:GLN:HG2	2.02	0.41
1:C:1610:ARG:HE	1:C:1610:ARG:HB3	1.64	0.41
1:C:1614:ARG:HD3	1:C:1614:ARG:HA	1.86	0.41
1:C:1658:LEU:HD23	1:C:1658:LEU:HA	1.80	0.41
1:C:2099:LEU:HD12	1:C:2099:LEU:HA	1.92	0.41
1:C:2264:GLU:HG2	1:C:2324:LEU:CD1	2.51	0.41
1:C:3844:LEU:HD23	1:C:3844:LEU:HA	1.84	0.41
1:C:3991:VAL:HG12	1:C:4145:ARG:NH2	2.35	0.41
1:C:4108:GLU:OE1	1:C:4136:ARG:NH2	2.54	0.41
1:E:424:PHE:HB3	1:E:428:ARG:NH2	2.36	0.41
1:E:472:HIS:O	1:E:472:HIS:ND1	2.53	0.41
1:E:558:LEU:HD22	1:E:571:ILE:HG23	2.03	0.41
1:E:864:PRO:HG3	1:E:1034:PRO:HB3	2.01	0.41
1:E:2163:MET:SD	1:E:2163:MET:N	2.93	0.41
1:E:3739:GLU:O	1:E:3743:GLN:N	2.53	0.41
1:G:422:THR:HG21	1:G:459:LEU:HD11	2.03	0.41
1:G:2128:ARG:O	1:G:2131:LEU:HB2	2.20	0.41
1:G:2328:ARG:HA	1:G:2328:ARG:HD3	1.91	0.41
1:G:2834:LEU:HD13	1:G:2839:HIS:HB3	2.03	0.41
1:G:3829:LYS:HE3	1:G:3829:LYS:HB3	1.86	0.41
1:G:3883:GLN:HE21	1:G:3947:GLY:HA3	1.86	0.41
1:G:4561:VAL:HG11	1:G:4570:GLU:HB3	2.03	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:4791:ARG:HD2	1:G:4808:ASP:HB2	2.03	0.41
1:A:510:SER:HA	1:A:520:ARG:NH2	2.36	0.41
1:A:773:GLN:HA	1:A:774:PRO:HD3	1.94	0.41
1:A:799:LYS:HA	1:A:1619:VAL:O	2.20	0.41
1:A:2210:GLN:H	1:A:2210:GLN:HG2	1.74	0.41
1:A:4770:LEU:HD13	1:C:4751:PHE:CD1	2.56	0.41
1:C:3841:PHE:HB3	1:C:3920:THR:HG21	2.02	0.41
2:D:5:GLU:HB3	2:D:73:LYS:HB3	2.02	0.41
1:E:618:CYS:HB2	1:E:629:GLN:HG2	2.02	0.41
1:E:3841:PHE:HB3	1:E:3920:THR:HG21	2.02	0.41
1:E:4171:ARG:NE	5:E:6002:ATP:O2G	2.41	0.41
1:E:4561:VAL:HG11	1:E:4570:GLU:HB3	2.03	0.41
1:G:3991:VAL:HG23	1:G:3992:VAL:H	1.87	0.41
1:A:235:ARG:HE	1:A:274:LEU:HD21	1.86	0.40
1:A:424:PHE:HB3	1:A:428:ARG:NH2	2.36	0.40
1:A:474:ASP:HA	1:A:477:ASN:HD22	1.85	0.40
1:A:1122:CYS:HA	1:A:1133:ARG:HD3	2.03	0.40
1:A:2103:LEU:HD23	1:A:2103:LEU:HA	1.81	0.40
1:A:3809:PHE:O	1:A:3813:ASN:N	2.50	0.40
1:C:143:LEU:HD22	1:E:2427:LEU:HD21	1.93	0.40
1:C:799:LYS:HA	1:C:1619:VAL:O	2.20	0.40
1:C:1719:LEU:HA	1:C:1719:LEU:HD23	1.87	0.40
1:C:4569:MET:O	1:C:4572:THR:OG1	2.31	0.40
1:C:4845:ILE:HD13	1:C:4845:ILE:HA	1.90	0.40
1:E:1942:ARG:HH12	1:E:3609:LEU:H	1.69	0.40
1:E:2327:ARG:HA	1:E:2327:ARG:HD2	1.60	0.40
1:E:3991:VAL:HG23	1:E:3992:VAL:H	1.87	0.40
1:E:4570:GLU:HG3	1:E:4571:PRO:HD3	2.03	0.40
1:E:4945:TYR:HE2	6:E:6003:CFF:H141	1.86	0.40
1:G:235:ARG:HE	1:G:274:LEU:HD21	1.86	0.40
1:G:2853:TRP:HA	1:G:2856:LYS:HB2	2.03	0.40
1:G:3628:SER:OG	1:G:3629:TRP:N	2.54	0.40
1:G:3793:SER:O	1:G:3797:LEU:N	2.45	0.40
1:A:30:LYS:HA	1:A:30:LYS:HD3	1.69	0.40
1:C:325:LYS:O	1:C:365:HIS:NE2	2.53	0.40
1:C:496:ASN:HA	1:C:499:LEU:HD12	2.04	0.40
1:C:3628:SER:OG	1:C:3629:TRP:N	2.54	0.40
1:C:4721:LEU:HD23	1:C:4721:LEU:HA	1.87	0.40
1:C:4782:TYR:HD1	1:C:4782:TYR:HA	1.78	0.40
1:E:496:ASN:HA	1:E:499:LEU:HD12	2.04	0.40
1:E:544:ASN:HB3	1:E:547:ASN:H	1.86	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:3883:GLN:HE21	1:E:3947:GLY:HA3	1.86	0.40
1:E:4791:ARG:HH22	1:G:4559:HIS:CE1	2.39	0.40
1:A:558:LEU:HD22	1:A:571:ILE:HG23	2.03	0.40
1:A:4823:ARG:H	1:A:4823:ARG:HG3	1.55	0.40
1:C:281:ARG:NH2	1:C:284:TRP:O	2.54	0.40
1:C:558:LEU:HD22	1:C:571:ILE:HG23	2.03	0.40
1:C:876:PRO:HA	1:C:879:GLU:HB3	2.04	0.40
1:C:1482:ARG:HD2	1:C:1531:TYR:HA	2.03	0.40
1:C:2402:ARG:HA	1:C:2402:ARG:HD3	1.86	0.40
1:C:3921:LEU:HA	1:C:3921:LEU:HD23	1.88	0.40
1:C:4809:ASP:O	1:C:4813:CYS:N	2.49	0.40
1:C:4945:TYR:HE2	6:C:6003:CFF:H141	1.86	0.40
1:E:876:PRO:HA	1:E:879:GLU:HB3	2.04	0.40
1:E:1102:TYR:HA	1:E:1164:CYS:O	2.22	0.40
1:E:2128:ARG:O	1:E:2131:LEU:HB2	2.20	0.40
1:E:2141:LYS:H	1:E:2141:LYS:HG3	1.74	0.40
1:G:544:ASN:HB3	1:G:547:ASN:H	1.86	0.40
1:G:1122:CYS:HA	1:G:1133:ARG:HD3	2.03	0.40
1:G:4845:ILE:HD13	1:G:4845:ILE:HA	1.90	0.40
1:A:281:ARG:NH2	1:A:284:TRP:O	2.54	0.40
1:A:422:THR:HG21	1:A:459:LEU:HD11	2.03	0.40
1:A:495:ILE:H	1:A:495:ILE:HG13	1.55	0.40
1:A:1102:TYR:HA	1:A:1164:CYS:O	2.22	0.40
1:A:1308:ILE:HG12	1:A:1575:HIS:HD1	1.85	0.40
1:A:3628:SER:OG	1:A:3629:TRP:N	2.54	0.40
2:B:103:LEU:HD11	2:B:106:LEU:HD21	2.03	0.40
1:C:510:SER:HA	1:C:520:ARG:NH2	2.36	0.40
1:C:2088:LEU:HA	1:C:2088:LEU:HD12	1.84	0.40
1:C:3714:SER:O	1:C:3714:SER:OG	2.34	0.40
1:C:3857:ASN:OD1	1:C:3860:ARG:NH1	2.52	0.40
1:E:424:PHE:HB3	1:E:428:ARG:HH21	1.86	0.40
1:E:1849:SER:OG	1:E:1849:SER:O	2.35	0.40
1:E:2322:VAL:HG11	1:E:2420:ILE:HG22	2.02	0.40
1:E:4596:VAL:HA	1:E:4599:VAL:HG12	2.04	0.40
1:E:4791:ARG:HD2	1:E:4808:ASP:HB2	2.03	0.40
1:G:424:PHE:HB3	1:G:428:ARG:NH2	2.36	0.40
1:G:558:LEU:HD22	1:G:571:ILE:HG23	2.03	0.40
1:G:3959:LEU:HD13	1:G:3968:LEU:HD22	2.04	0.40
1:G:4828:ILE:HD12	1:G:4828:ILE:HA	1.86	0.40
1:A:192:LEU:O	1:A:212:TRP:NE1	2.47	0.40
1:A:1591:LEU:HD23	1:A:1591:LEU:HA	1.92	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1658:LEU:HD23	1:A:1658:LEU:HA	1.80	0.40
1:A:1785:ASP:N	1:A:1785:ASP:OD1	2.53	0.40
1:A:2853:TRP:HA	1:A:2856:LYS:HB2	2.03	0.40
1:A:3957:MET:O	1:A:3960:SER:OG	2.33	0.40
1:A:3993:ASN:HD22	1:A:4110:MET:HG3	1.86	0.40
1:A:4561:VAL:HG11	1:A:4570:GLU:HB3	2.03	0.40
1:A:4888:LYS:HB3	1:A:4888:LYS:HE2	1.93	0.40
1:A:4911:LEU:HA	1:A:4915:ASN:HD22	1.87	0.40
1:C:192:LEU:O	1:C:212:TRP:NE1	2.47	0.40
1:C:472:HIS:ND1	1:C:472:HIS:O	2.53	0.40
1:C:1842:ILE:HD13	1:C:1842:ILE:HA	1.91	0.40
1:C:2834:LEU:HD13	1:C:2839:HIS:HB3	2.03	0.40
2:F:11:ASP:OD2	2:F:14:THR:OG1	2.35	0.40
1:G:424:PHE:HB3	1:G:428:ARG:HH21	1.86	0.40
1:G:3714:SER:O	1:G:3714:SER:OG	2.35	0.40
1:G:3993:ASN:HD22	1:G:4110:MET:HG3	1.86	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	3336/4968 (67%)	2981 (89%)	347 (10%)	8 (0%)	47	79
1	C	3336/4968 (67%)	2982 (89%)	345 (10%)	9 (0%)	41	75
1	E	3336/4968 (67%)	2980 (89%)	347 (10%)	9 (0%)	41	75
1	G	3336/4968 (67%)	2980 (89%)	348 (10%)	8 (0%)	47	79
2	B	105/108 (97%)	100 (95%)	5 (5%)	0	100	100
2	D	105/108 (97%)	100 (95%)	5 (5%)	0	100	100
2	F	105/108 (97%)	100 (95%)	5 (5%)	0	100	100

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	105/108 (97%)	100 (95%)	5 (5%)	0	100	100
All	All	13764/20304 (68%)	12323 (90%)	1407 (10%)	34 (0%)	50	79

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2328	ARG
1	A	4901	THR
1	C	2328	ARG
1	C	4901	THR
1	E	2328	ARG
1	E	4901	THR
1	G	2328	ARG
1	G	4901	THR
1	C	2329	PRO
1	E	2329	PRO
1	A	1580	PRO
1	C	1580	PRO
1	E	1580	PRO
1	G	1580	PRO
1	A	853	PRO
1	A	4916	LEU
1	C	853	PRO
1	C	4916	LEU
1	E	853	PRO
1	E	4916	LEU
1	G	853	PRO
1	G	4916	LEU
1	A	1848	PRO
1	C	1848	PRO
1	E	1848	PRO
1	G	1848	PRO
1	A	1535	PRO
1	C	1535	PRO
1	E	1535	PRO
1	G	1535	PRO
1	A	828	PRO
1	C	828	PRO
1	E	828	PRO
1	G	828	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	2650/4355 (61%)	2627 (99%)	23 (1%)	78	87
1	C	2650/4355 (61%)	2625 (99%)	25 (1%)	78	87
1	E	2648/4355 (61%)	2623 (99%)	25 (1%)	78	87
1	G	2650/4355 (61%)	2628 (99%)	22 (1%)	81	89
2	B	88/89 (99%)	88 (100%)	0	100	100
2	D	88/89 (99%)	88 (100%)	0	100	100
2	F	88/89 (99%)	88 (100%)	0	100	100
2	H	88/89 (99%)	88 (100%)	0	100	100
All	All	10950/17776 (62%)	10855 (99%)	95 (1%)	79	87

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	76	ARG
1	A	143	LEU
1	A	207	PHE
1	A	325	LYS
1	A	417	ARG
1	A	637	LEU
1	A	841	LYS
1	A	855	VAL
1	A	893	TRP
1	A	990	PRO
1	A	1013	ARG
1	A	1033	VAL
1	A	1466	THR
1	A	1610	ARG
1	A	1782	PHE
1	A	2315	GLU
1	A	2324	LEU
1	A	2836	ARG
1	A	2857	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	3976	GLN
1	A	4161	TRP
1	A	4823	ARG
1	A	4960	ARG
1	C	76	ARG
1	C	143	LEU
1	C	207	PHE
1	C	325	LYS
1	C	417	ARG
1	C	637	LEU
1	C	841	LYS
1	C	855	VAL
1	C	893	TRP
1	C	990	PRO
1	C	1013	ARG
1	C	1033	VAL
1	C	1466	THR
1	C	1610	ARG
1	C	1782	PHE
1	C	2323	ARG
1	C	2324	LEU
1	C	2327	ARG
1	C	2328	ARG
1	C	2836	ARG
1	C	2857	LYS
1	C	3976	GLN
1	C	4161	TRP
1	C	4823	ARG
1	C	4960	ARG
1	E	143	LEU
1	E	207	PHE
1	E	325	LYS
1	E	417	ARG
1	E	637	LEU
1	E	841	LYS
1	E	855	VAL
1	E	893	TRP
1	E	990	PRO
1	E	1013	ARG
1	E	1033	VAL
1	E	1466	THR
1	E	1610	ARG

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	E	1782	PHE
1	E	2315	GLU
1	E	2323	ARG
1	E	2324	LEU
1	E	2327	ARG
1	E	2328	ARG
1	E	2836	ARG
1	E	2857	LYS
1	E	3976	GLN
1	E	4161	TRP
1	E	4823	ARG
1	E	4960	ARG
1	G	143	LEU
1	G	207	PHE
1	G	325	LYS
1	G	417	ARG
1	G	637	LEU
1	G	841	LYS
1	G	855	VAL
1	G	893	TRP
1	G	990	PRO
1	G	1013	ARG
1	G	1033	VAL
1	G	1466	THR
1	G	1610	ARG
1	G	1782	PHE
1	G	2315	GLU
1	G	2324	LEU
1	G	2836	ARG
1	G	2857	LYS
1	G	3976	GLN
1	G	4161	TRP
1	G	4823	ARG
1	G	4960	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (149) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	123	HIS
1	A	394	HIS
1	A	477	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	490	GLN
1	A	550	GLN
1	A	593	HIS
1	A	604	HIS
1	A	651	HIS
1	A	890	HIS
1	A	914	GLN
1	A	915	HIS
1	A	1005	ASN
1	A	1149	ASN
1	A	1265	HIS
1	A	1440	ASN
1	A	1589	GLN
1	A	1691	ASN
1	A	1836	ASN
1	A	1906	GLN
1	A	1918	GLN
1	A	2152	ASN
1	A	2317	ASN
1	A	2820	HIS
1	A	2848	ASN
1	A	3611	ASN
1	A	3635	HIS
1	A	3852	ASN
1	A	3993	ASN
1	A	4494	ASN
1	A	4559	HIS
1	A	4880	GLN
1	A	4904	HIS
1	A	4915	ASN
1	A	4934	HIS
2	B	25	HIS
2	B	31	GLN
1	C	23	GLN
1	C	123	HIS
1	C	209	GLN
1	C	394	HIS
1	C	477	ASN
1	C	490	GLN
1	C	550	GLN
1	C	593	HIS
1	C	604	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	651	HIS
1	C	890	HIS
1	C	914	GLN
1	C	915	HIS
1	C	1005	ASN
1	C	1149	ASN
1	C	1265	HIS
1	C	1440	ASN
1	C	1589	GLN
1	C	1691	ASN
1	C	1836	ASN
1	C	1906	GLN
1	C	1918	GLN
1	C	2152	ASN
1	C	2317	ASN
1	C	2820	HIS
1	C	2848	ASN
1	C	3611	ASN
1	C	3635	HIS
1	C	3852	ASN
1	C	3993	ASN
1	C	4494	ASN
1	C	4559	HIS
1	C	4880	GLN
1	C	4904	HIS
1	C	4915	ASN
1	C	4934	HIS
2	D	25	HIS
2	D	31	GLN
1	E	23	GLN
1	E	123	HIS
1	E	394	HIS
1	E	477	ASN
1	E	490	GLN
1	E	544	ASN
1	E	550	GLN
1	E	593	HIS
1	E	604	HIS
1	E	651	HIS
1	E	890	HIS
1	E	914	GLN
1	E	915	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	E	1005	ASN
1	E	1149	ASN
1	E	1265	HIS
1	E	1589	GLN
1	E	1691	ASN
1	E	1836	ASN
1	E	1906	GLN
1	E	1918	GLN
1	E	2152	ASN
1	E	2317	ASN
1	E	2319	ASN
1	E	2820	HIS
1	E	2848	ASN
1	E	3611	ASN
1	E	3635	HIS
1	E	3852	ASN
1	E	3993	ASN
1	E	4494	ASN
1	E	4559	HIS
1	E	4880	GLN
1	E	4904	HIS
1	E	4915	ASN
1	E	4934	HIS
2	F	25	HIS
2	F	31	GLN
1	G	23	GLN
1	G	123	HIS
1	G	394	HIS
1	G	477	ASN
1	G	490	GLN
1	G	544	ASN
1	G	550	GLN
1	G	593	HIS
1	G	604	HIS
1	G	651	HIS
1	G	890	HIS
1	G	914	GLN
1	G	915	HIS
1	G	1005	ASN
1	G	1149	ASN
1	G	1265	HIS
1	G	1691	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	G	1836	ASN
1	G	1906	GLN
1	G	1918	GLN
1	G	2152	ASN
1	G	2317	ASN
1	G	2820	HIS
1	G	2848	ASN
1	G	3611	ASN
1	G	3852	ASN
1	G	3993	ASN
1	G	4490	GLN
1	G	4494	ASN
1	G	4559	HIS
1	G	4880	GLN
1	G	4904	HIS
1	G	4915	ASN
1	G	4934	HIS
2	H	25	HIS
2	H	31	GLN

### 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 monosaccharides 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	$\# Z  > 2$
6	CFF	E	6003	-	8,15,15	2.91	4 (50%)	8,23,23	1.32	1 (12%)
6	CFF	G	6003	-	8,15,15	2.93	4 (50%)	8,23,23	1.30	1 (12%)
6	CFF	A	6003	-	8,15,15	2.93	4 (50%)	8,23,23	1.30	1 (12%)
5	ATP	E	6002	-	26,33,33	0.91	1 (3%)	31,52,52	1.66	6 (19%)
5	ATP	G	6002	-	26,33,33	0.91	1 (3%)	31,52,52	1.66	6 (19%)
5	ATP	A	6002	-	26,33,33	0.91	1 (3%)	31,52,52	1.66	6 (19%)
6	CFF	C	6003	-	8,15,15	2.93	4 (50%)	8,23,23	1.30	1 (12%)
5	ATP	C	6002	-	26,33,33	0.91	1 (3%)	31,52,52	1.66	6 (19%)

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
6	CFF	E	6003	-	-	-	0/2/2/2
6	CFF	G	6003	-	-	-	0/2/2/2
6	CFF	A	6003	-	-	-	0/2/2/2
5	ATP	E	6002	-	-	4/18/38/38	0/3/3/3
5	ATP	G	6002	-	-	4/18/38/38	0/3/3/3
5	ATP	A	6002	-	-	4/18/38/38	0/3/3/3
6	CFF	C	6003	-	-	-	0/2/2/2
5	ATP	C	6002	-	-	4/18/38/38	0/3/3/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	6003	CFF	C5-C4	-5.46	1.32	1.39
6	C	6003	CFF	C5-C4	-5.46	1.32	1.39
6	G	6003	CFF	C5-C4	-5.46	1.32	1.39
6	E	6003	CFF	C5-C4	-5.39	1.32	1.39
6	A	6003	CFF	C6-N1	-4.45	1.31	1.38
6	C	6003	CFF	C6-N1	-4.45	1.31	1.38
6	G	6003	CFF	C6-N1	-4.45	1.31	1.38
6	E	6003	CFF	C6-N1	-4.44	1.31	1.38
6	A	6003	CFF	C5-C6	-2.78	1.36	1.41
6	C	6003	CFF	C5-C6	-2.78	1.36	1.41

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	6003	CFF	C5-C6	-2.78	1.36	1.41
6	G	6003	CFF	C5-C6	-2.78	1.36	1.41
6	A	6003	CFF	O13-C6	-2.57	1.18	1.24
6	C	6003	CFF	O13-C6	-2.57	1.18	1.24
6	E	6003	CFF	O13-C6	-2.57	1.18	1.24
6	G	6003	CFF	O13-C6	-2.57	1.18	1.24
5	A	6002	ATP	C5-N7	-2.16	1.31	1.39
5	C	6002	ATP	C5-N7	-2.16	1.31	1.39
5	E	6002	ATP	C5-N7	-2.16	1.31	1.39
5	G	6002	ATP	C5-N7	-2.16	1.31	1.39

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	6002	ATP	PA-O3A-PB	-4.88	116.07	132.83
5	A	6002	ATP	PA-O3A-PB	-4.87	116.11	132.83
5	C	6002	ATP	PA-O3A-PB	-4.87	116.11	132.83
5	G	6002	ATP	PA-O3A-PB	-4.86	116.15	132.83
5	A	6002	ATP	N3-C2-N1	-3.63	123.01	128.68
5	G	6002	ATP	N3-C2-N1	-3.63	123.01	128.68
5	C	6002	ATP	N3-C2-N1	-3.62	123.02	128.68
5	E	6002	ATP	N3-C2-N1	-3.61	123.04	128.68
6	A	6003	CFF	C14-N7-C8	-2.86	111.67	125.43
6	G	6003	CFF	C14-N7-C8	-2.86	111.67	125.43
6	C	6003	CFF	C14-N7-C8	-2.85	111.70	125.43
5	E	6002	ATP	N6-C6-N1	2.85	124.49	118.57
6	E	6003	CFF	C14-N7-C8	-2.85	111.73	125.43
5	A	6002	ATP	N6-C6-N1	2.83	124.45	118.57
5	C	6002	ATP	N6-C6-N1	2.83	124.45	118.57
5	G	6002	ATP	N6-C6-N1	2.83	124.45	118.57
5	G	6002	ATP	PB-O3B-PG	-2.76	123.35	132.83
5	A	6002	ATP	PB-O3B-PG	-2.75	123.38	132.83
5	C	6002	ATP	PB-O3B-PG	-2.75	123.38	132.83
5	E	6002	ATP	PB-O3B-PG	-2.75	123.38	132.83
5	C	6002	ATP	C3'-C2'-C1'	2.65	104.97	100.98
5	A	6002	ATP	C3'-C2'-C1'	2.64	104.95	100.98
5	E	6002	ATP	C3'-C2'-C1'	2.64	104.95	100.98
5	G	6002	ATP	C3'-C2'-C1'	2.64	104.95	100.98
5	E	6002	ATP	C5-C6-N6	-2.01	117.29	120.35
5	A	6002	ATP	C5-C6-N6	-2.01	117.30	120.35
5	C	6002	ATP	C5-C6-N6	-2.01	117.30	120.35
5	G	6002	ATP	C5-C6-N6	-2.01	117.30	120.35

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	6002	ATP	C3'-C4'-C5'-O5'
5	C	6002	ATP	C3'-C4'-C5'-O5'
5	E	6002	ATP	C3'-C4'-C5'-O5'
5	G	6002	ATP	C3'-C4'-C5'-O5'
5	A	6002	ATP	O4'-C4'-C5'-O5'
5	C	6002	ATP	O4'-C4'-C5'-O5'
5	E	6002	ATP	O4'-C4'-C5'-O5'
5	G	6002	ATP	O4'-C4'-C5'-O5'
5	A	6002	ATP	PA-O3A-PB-O1B
5	C	6002	ATP	PA-O3A-PB-O1B
5	E	6002	ATP	PA-O3A-PB-O1B
5	G	6002	ATP	PA-O3A-PB-O1B
5	A	6002	ATP	C4'-C5'-O5'-PA
5	C	6002	ATP	C4'-C5'-O5'-PA
5	E	6002	ATP	C4'-C5'-O5'-PA
5	G	6002	ATP	C4'-C5'-O5'-PA

There are no ring outliers.

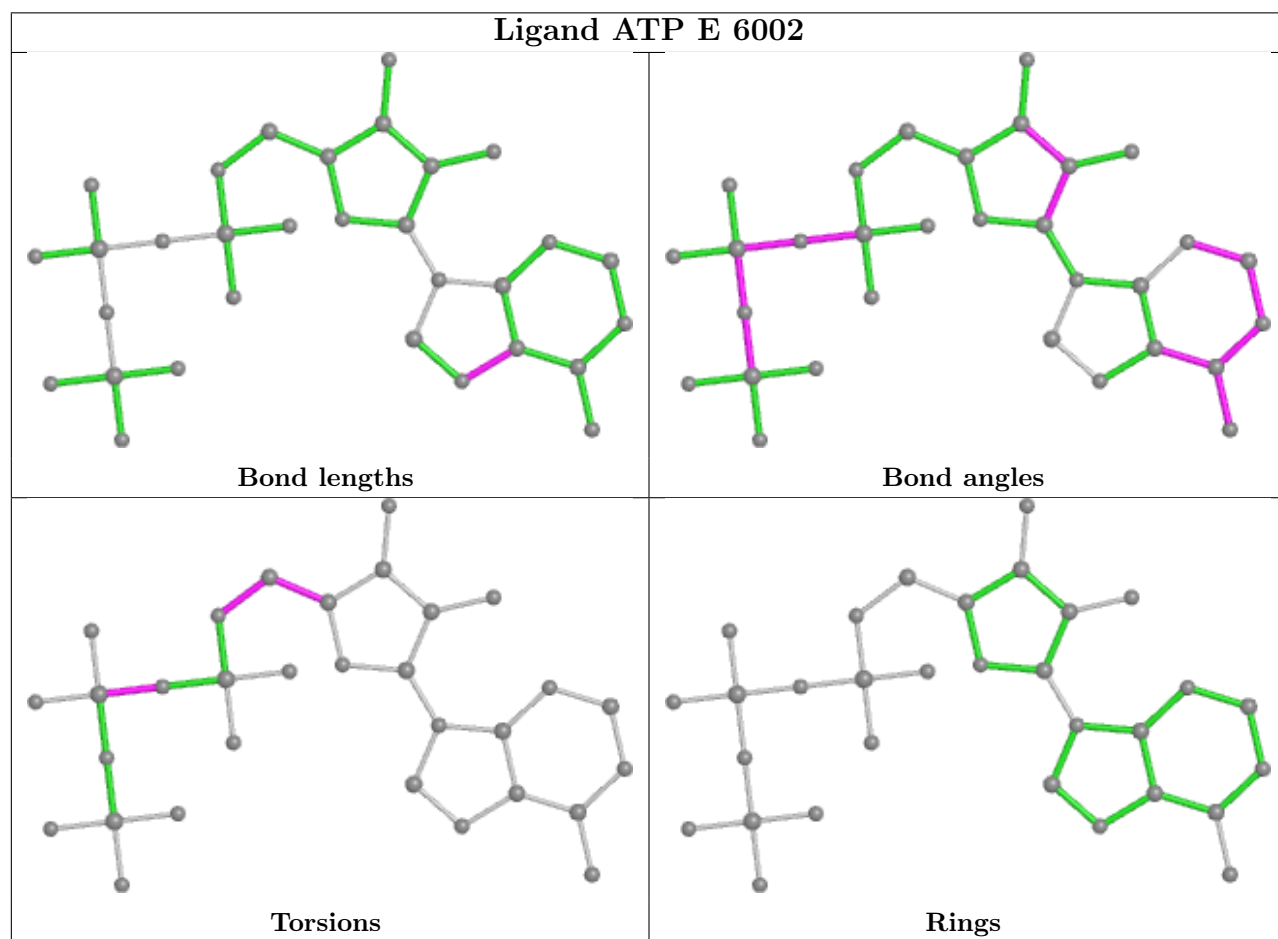
8 monomers are involved in 12 short contacts:

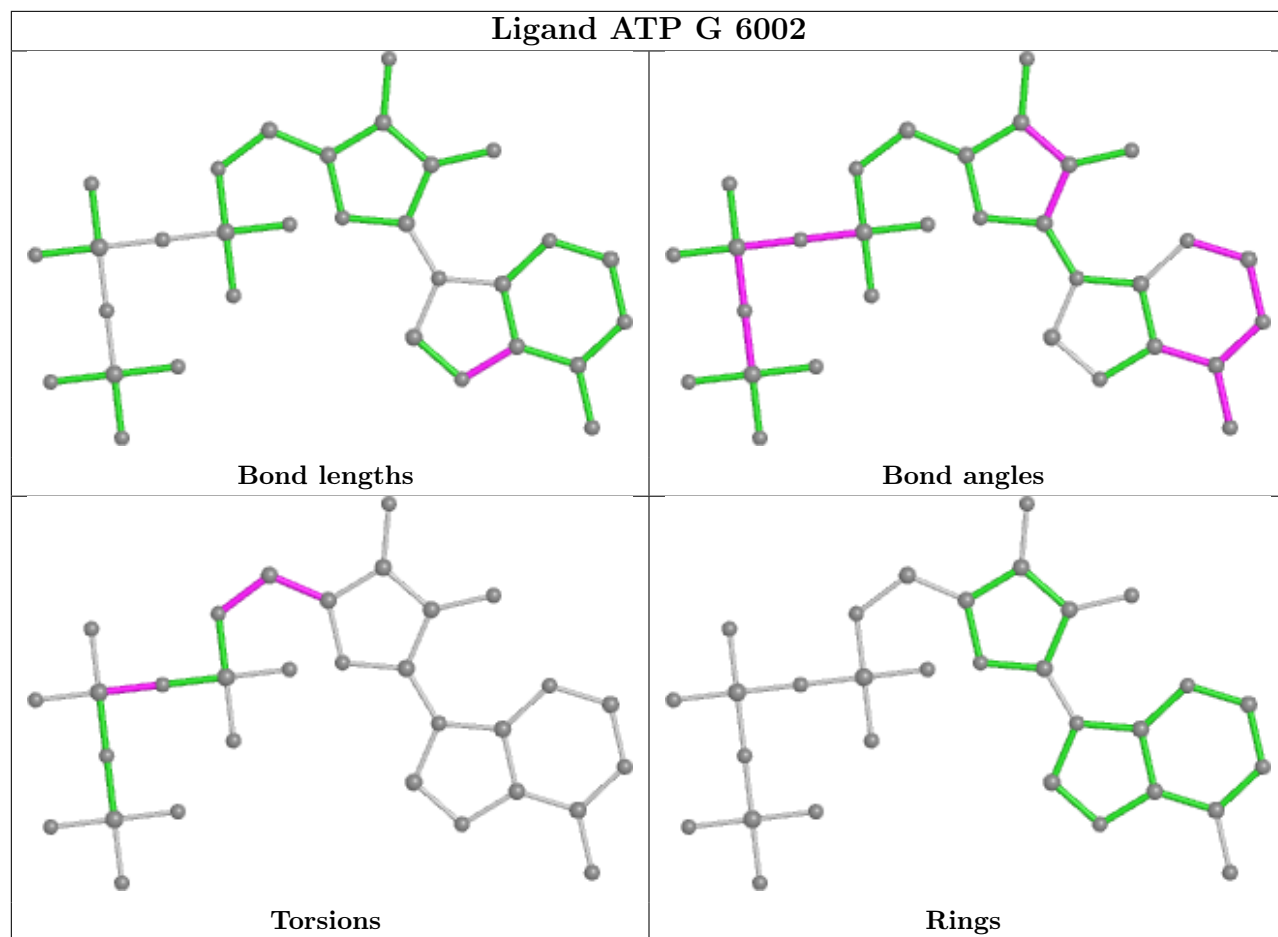
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	E	6003	CFF	2	0
6	G	6003	CFF	2	0
6	A	6003	CFF	2	0
5	E	6002	ATP	1	0
5	G	6002	ATP	1	0
5	A	6002	ATP	1	0
6	C	6003	CFF	2	0
5	C	6002	ATP	1	0

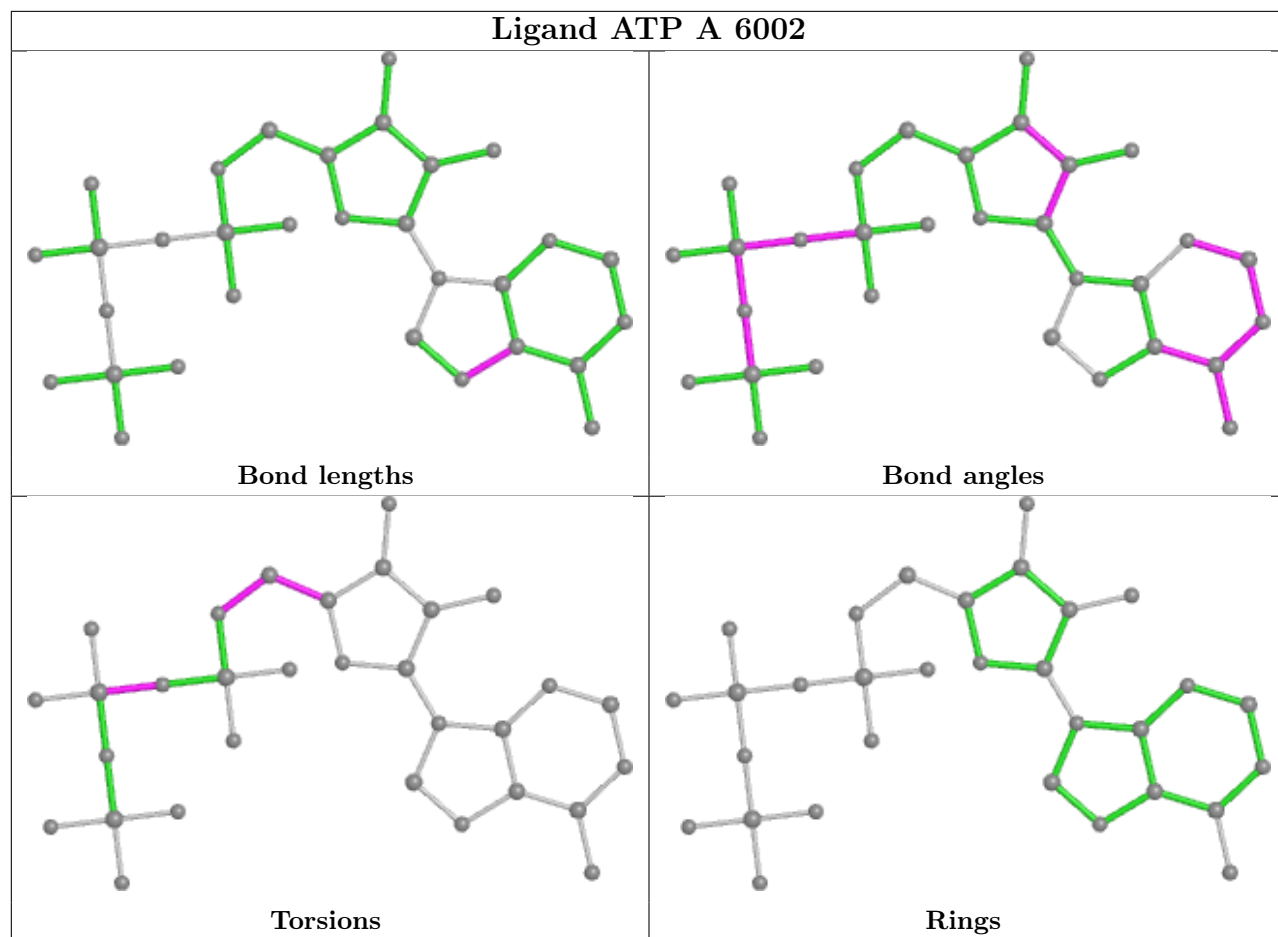
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

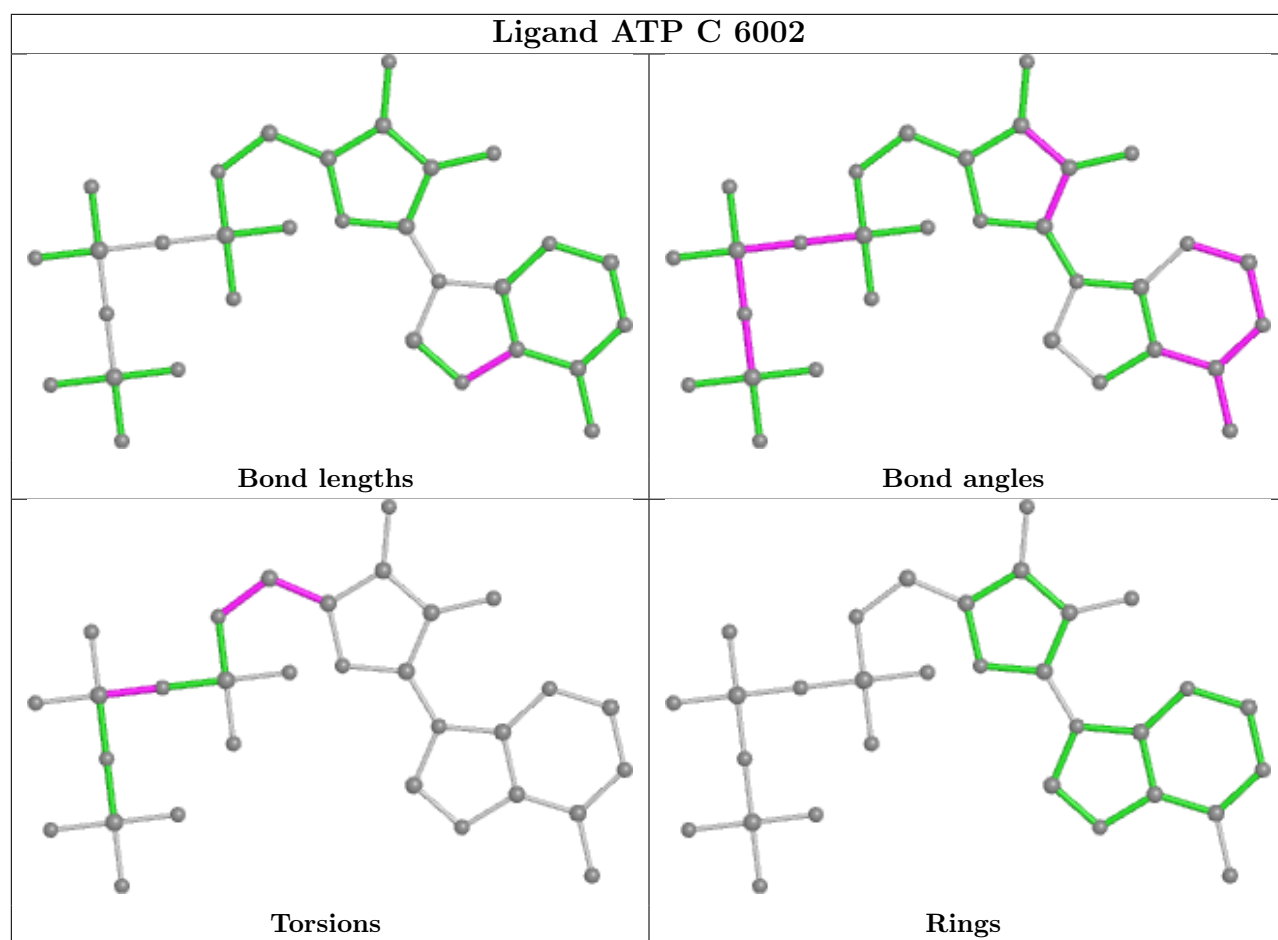


The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









## 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.

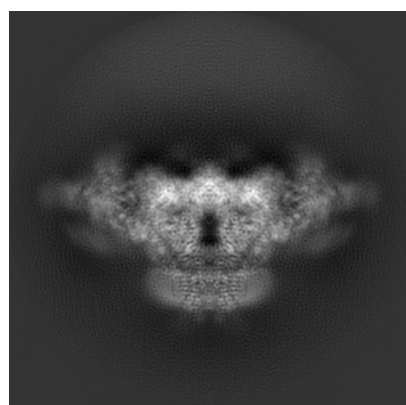
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9879. These allow visual inspection of the internal detail of the map and identification of artifacts.

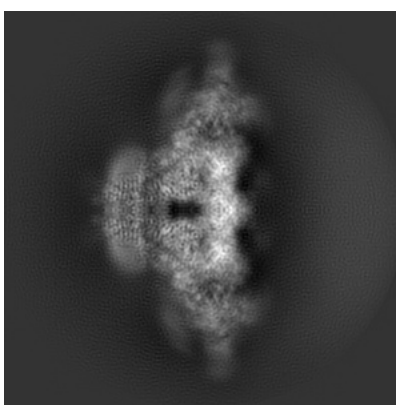
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

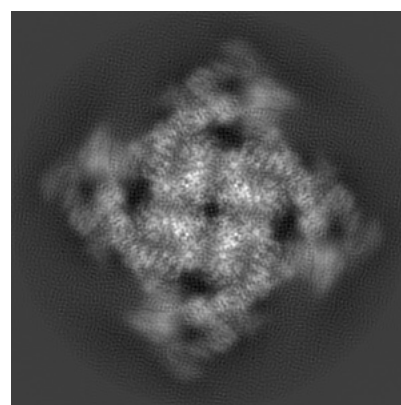
#### 6.1.1 Primary map



X



Y

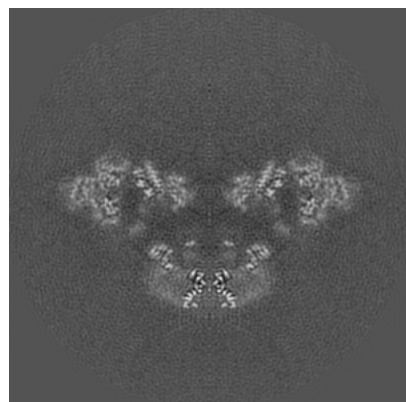


Z

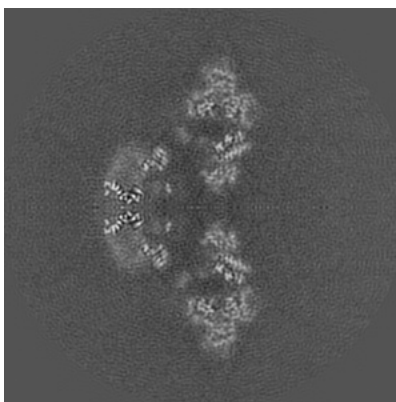
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

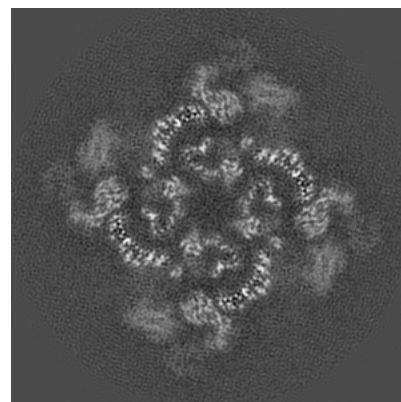
#### 6.2.1 Primary map



X Index: 200



Y Index: 200

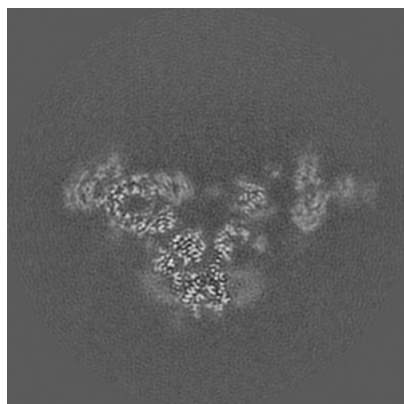


Z Index: 200

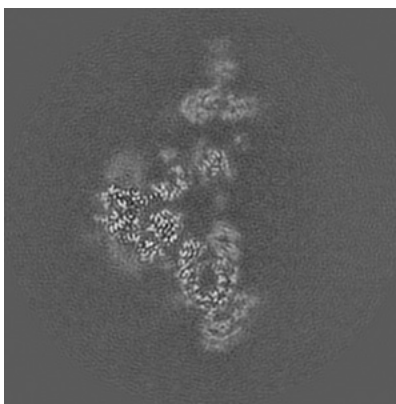
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

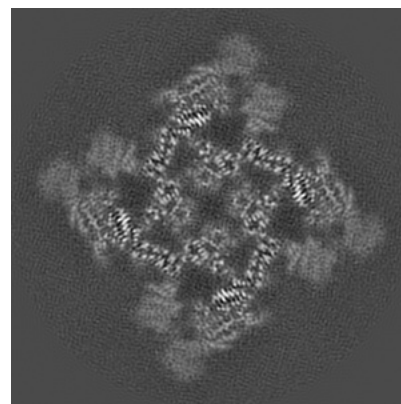
### 6.3.1 Primary map



X Index: 213



Y Index: 187

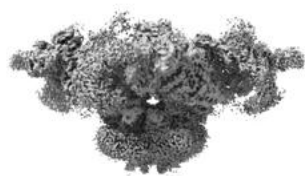


Z Index: 211

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

## 6.4 Orthogonal surface views [i](#)

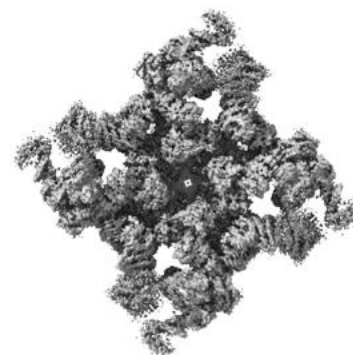
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.022. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

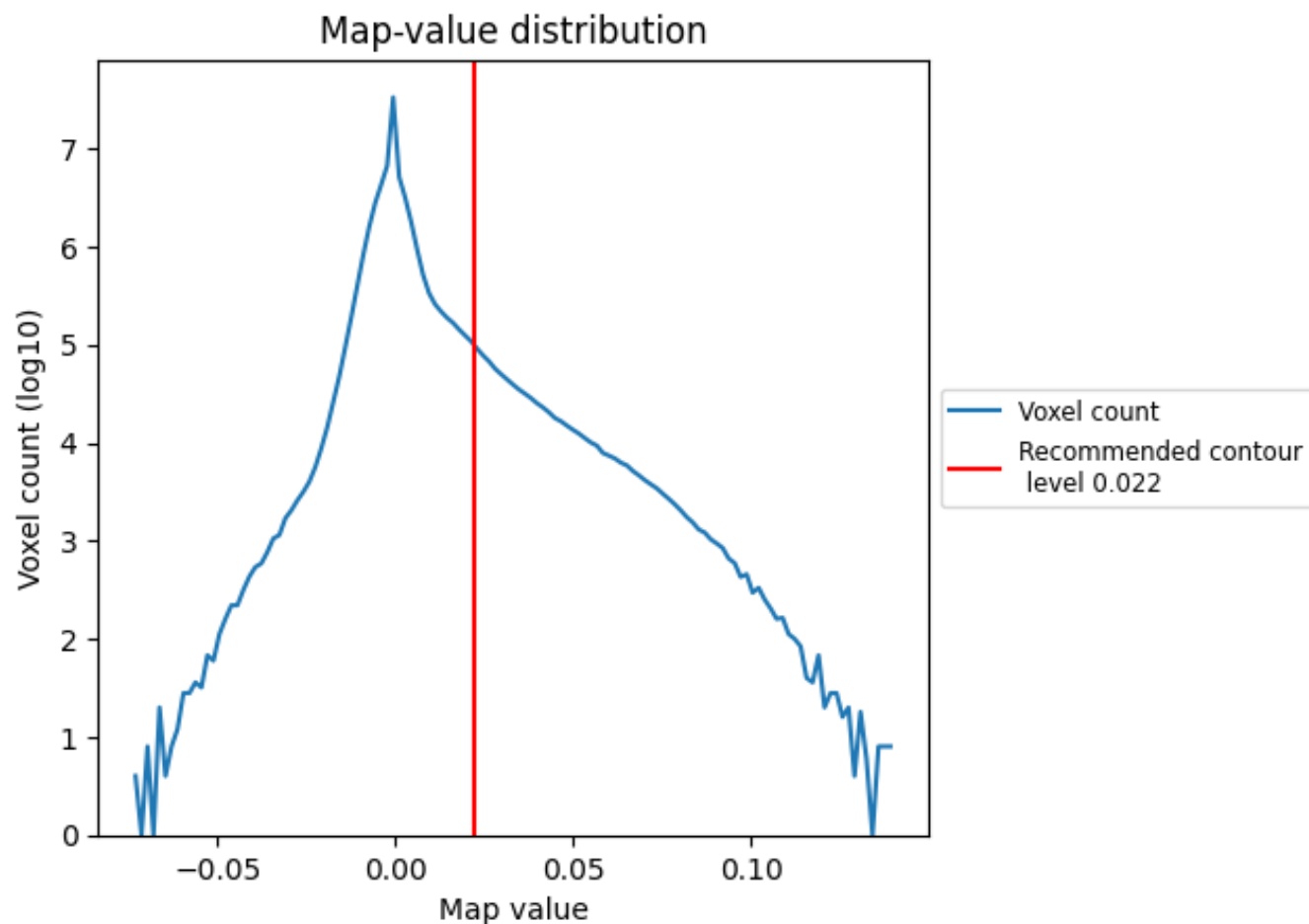
## 6.5 Mask visualisation

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.

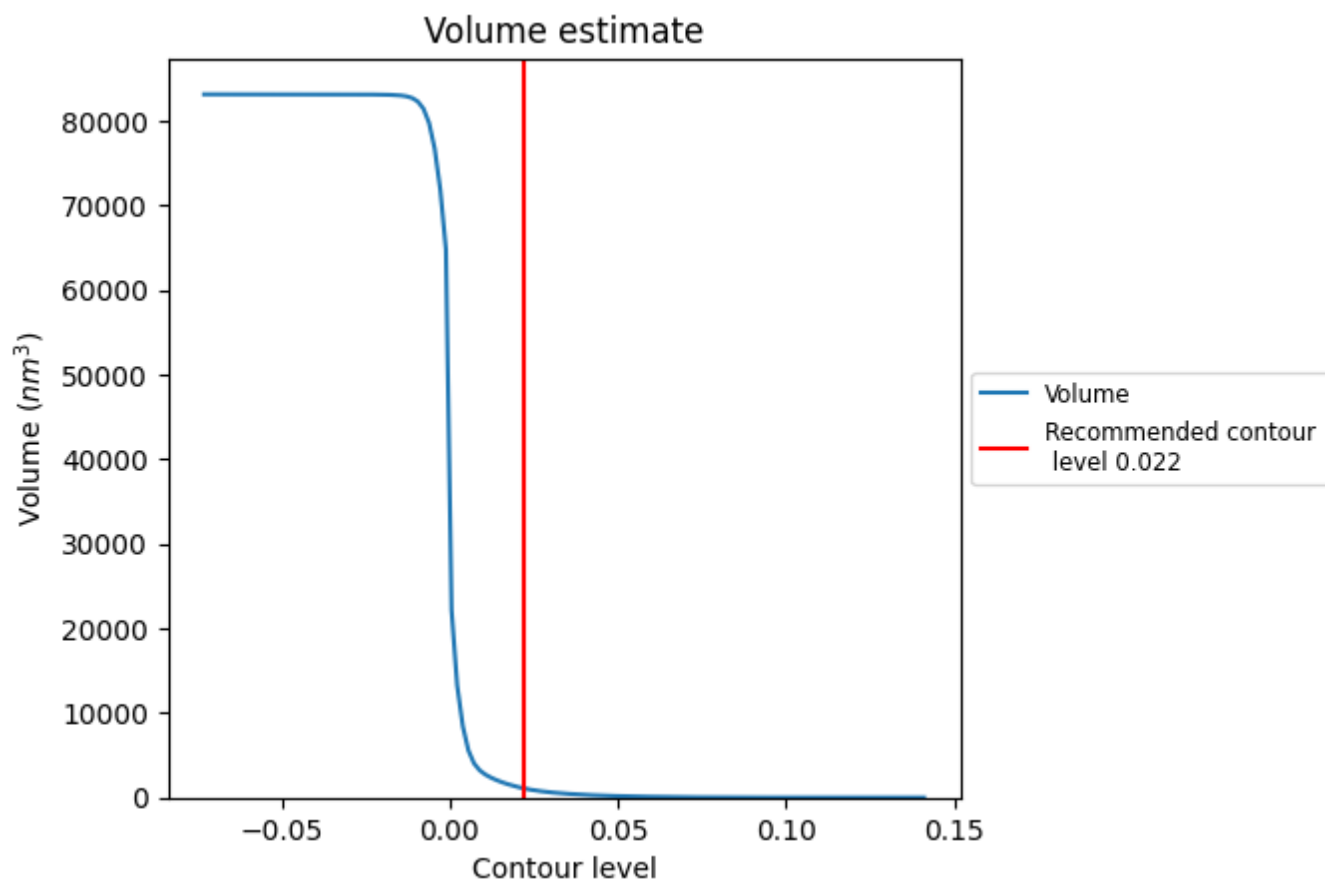
### 7.1 Map-value distribution [i](#)



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.



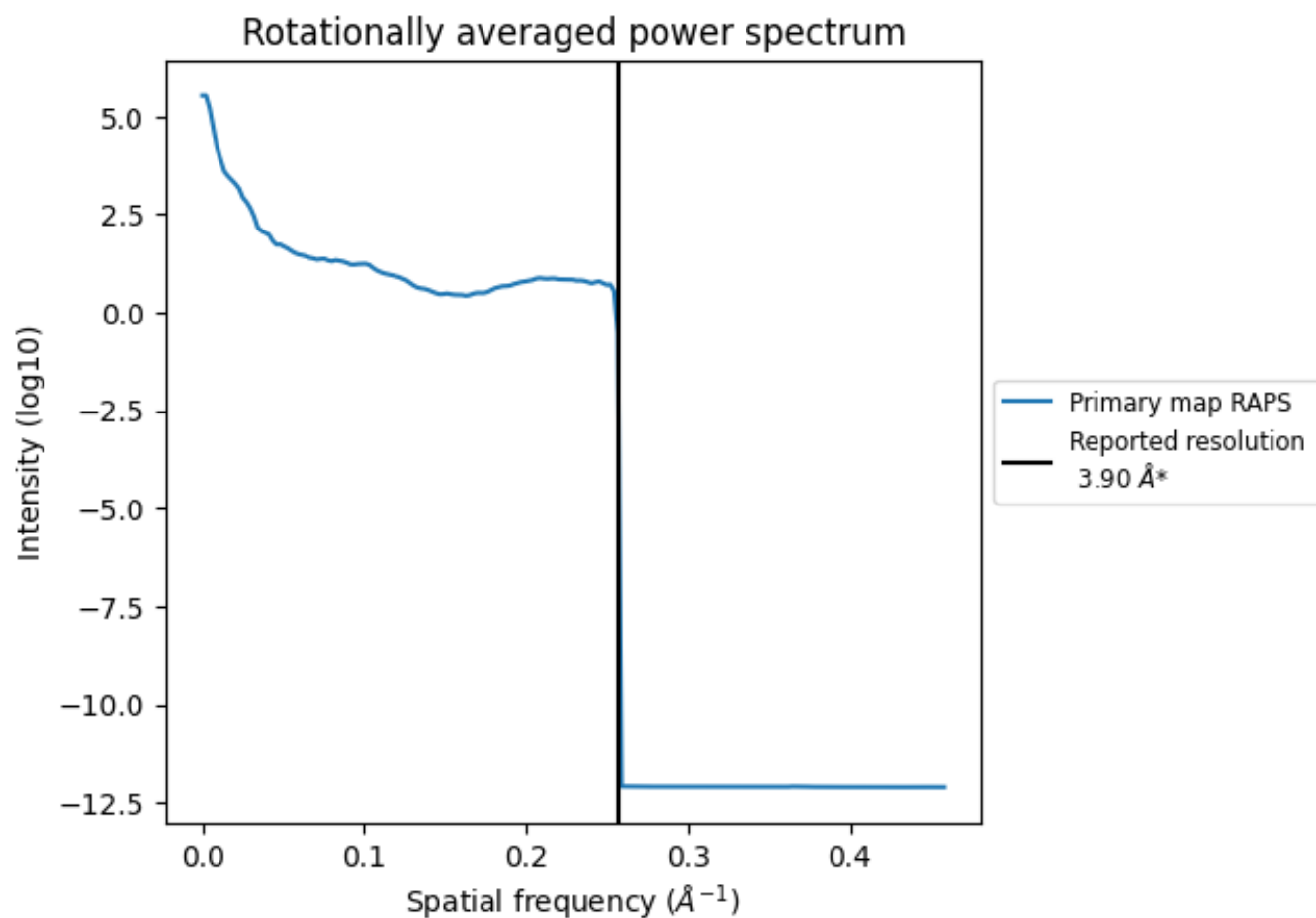
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1096 nm<sup>3</sup>; this corresponds to an approximate mass of 990 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 ⓘ

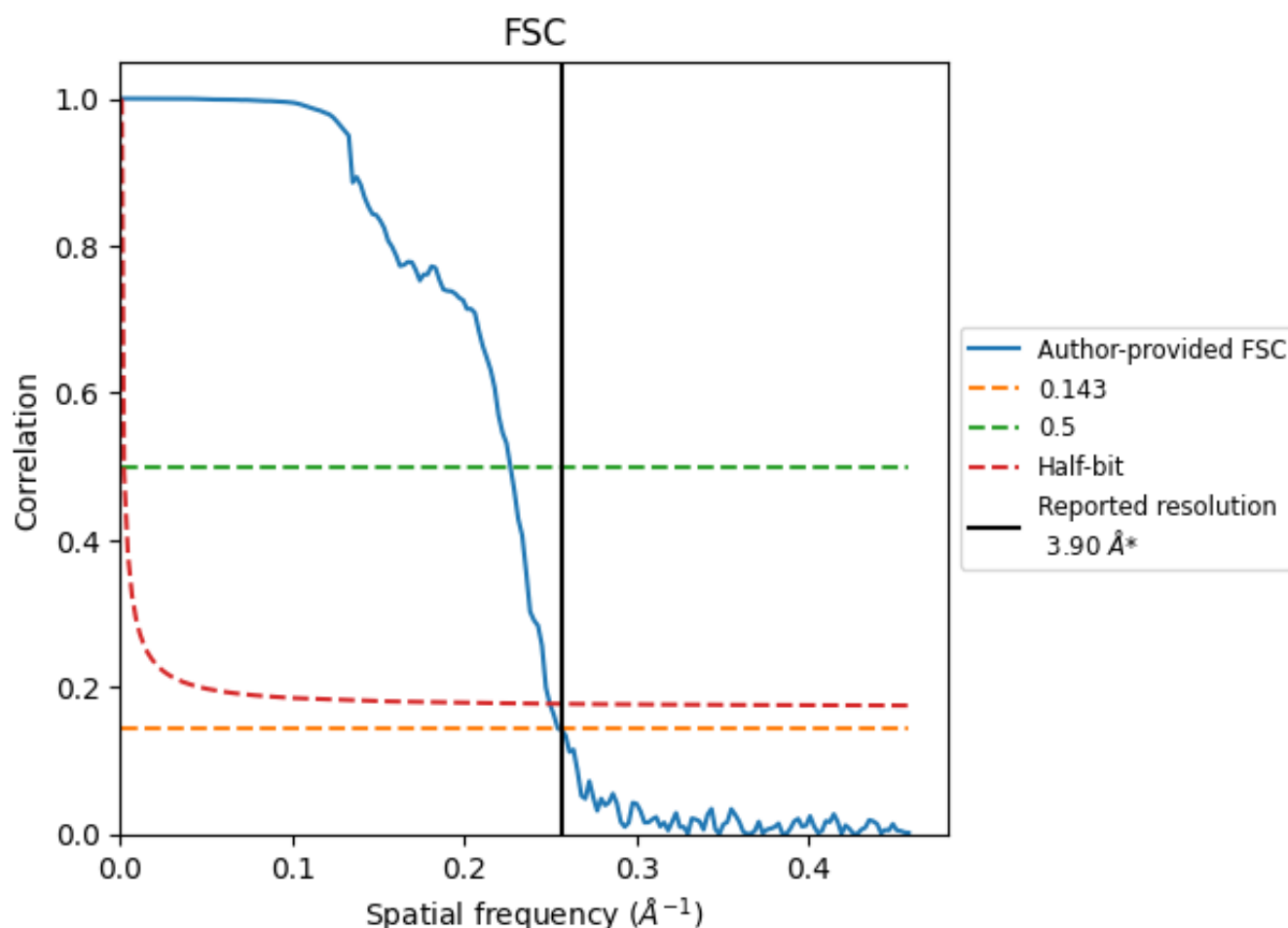


\*Reported resolution corresponds to spatial frequency of 0.256 Å<sup>-1</sup>

## 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 0.256 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

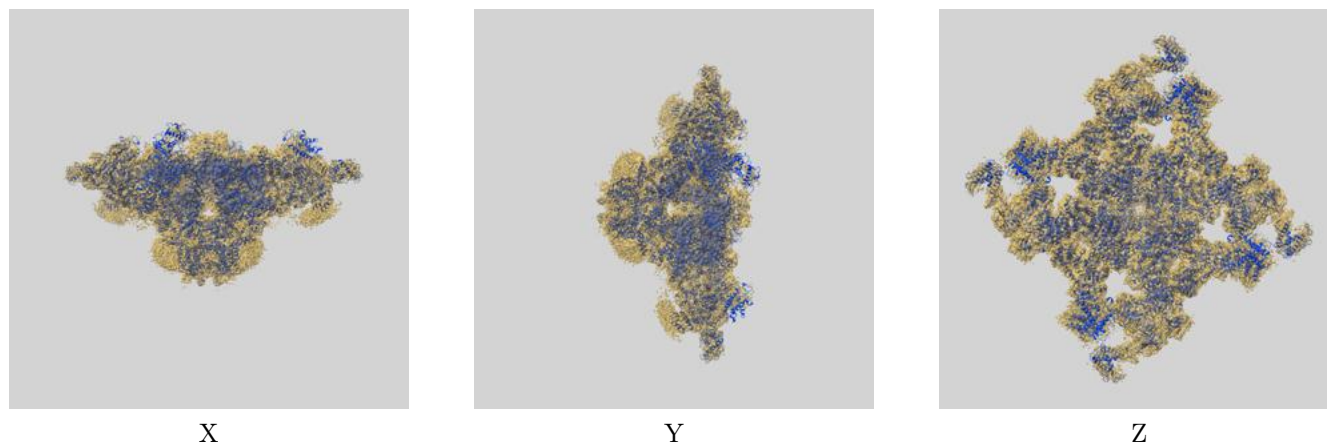
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	3.93	4.41	4.00
Unmasked-calculated*	-	-	-

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

## 9 Map-model fit [i](#)

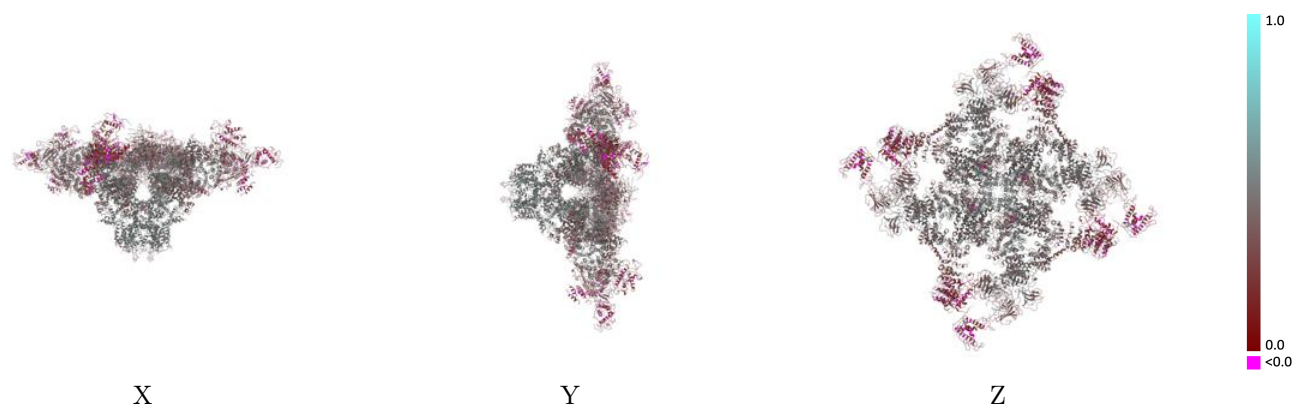
This section contains information regarding the fit between EMDB map EMD-9879 and PDB model 6JRR. Per-residue inclusion information can be found in section [3](#) on page [6](#).

### 9.1 Map-model overlay [i](#)



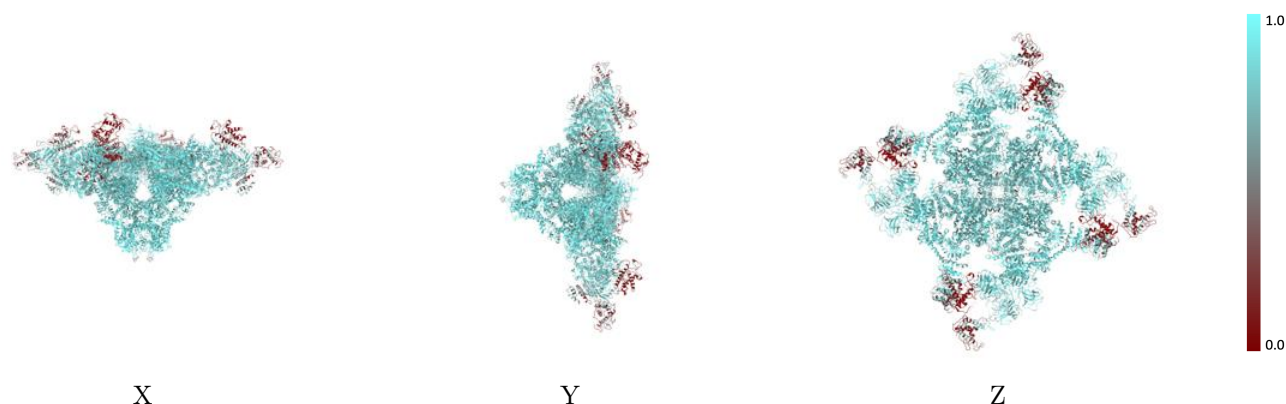
The images above show the 3D surface view of the map at the recommended contour level 0.022 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



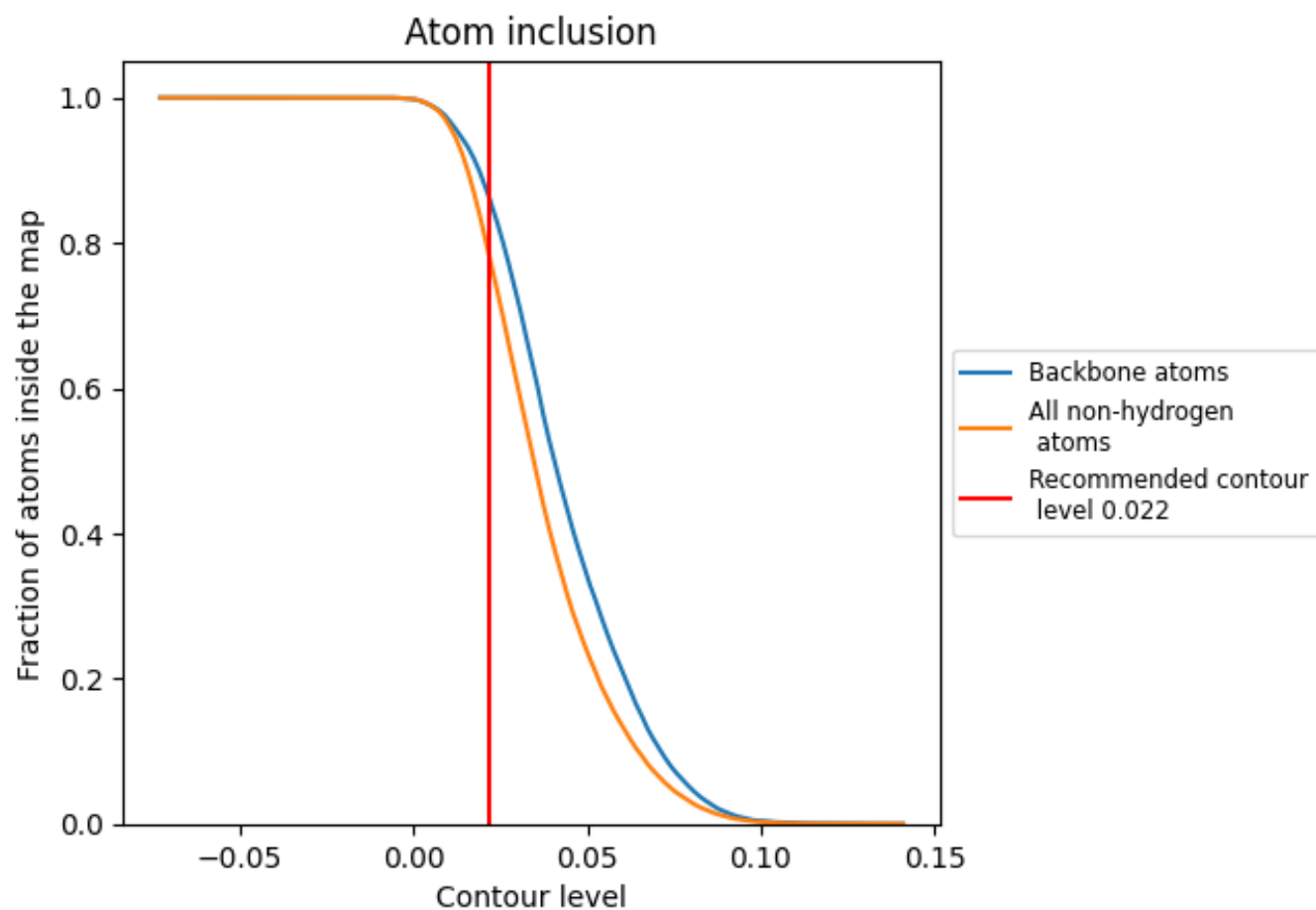
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.022).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 78% 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 (0.022) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.7780	<div><div></div></div> 0.3900
A	<div><div></div></div> 0.7770	<div><div></div></div> 0.3900
B	<div><div></div></div> 0.8141	<div><div></div></div> 0.4170
C	<div><div></div></div> 0.7767	<div><div></div></div> 0.3890
D	<div><div></div></div> 0.8154	<div><div></div></div> 0.4160
E	<div><div></div></div> 0.7768	<div><div></div></div> 0.3890
F	<div><div></div></div> 0.8178	<div><div></div></div> 0.4170
G	<div><div></div></div> 0.7770	<div><div></div></div> 0.3890
H	<div><div></div></div> 0.8154	<div><div></div></div> 0.4160

1.0

0.0

<0.0