



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 05:08 AM UTC

PDB ID : 6QL6 / pdb_00006ql6
EMDB ID : EMD-4578
Title : Structure of Fatty acid synthase complex from *Saccharomyces cerevisiae* at 2.9 Angstrom
Authors : Singh, K.; Graf, B.; Linden, A.; Sautner, V.; Urlaub, H.; Tittmann, K.; Stark, H.; Chari, A.
Deposited on : 2019-01-31
Resolution : 2.90 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

A user guide is available at

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

The types of validation reports are described at

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

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

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

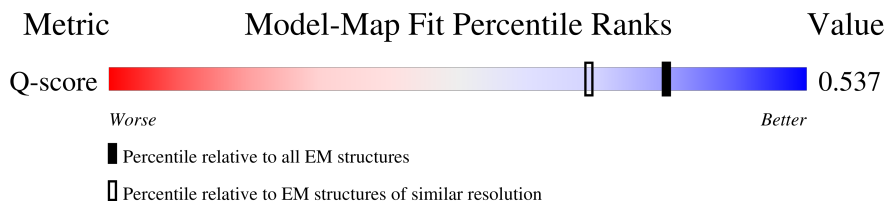
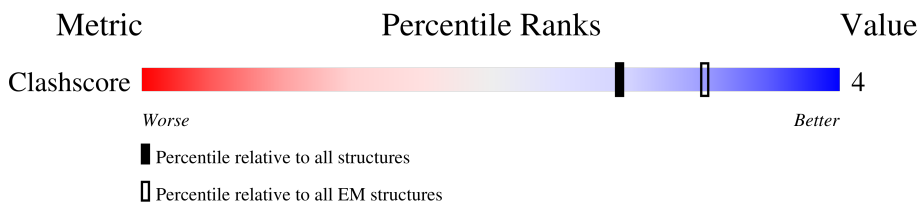
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

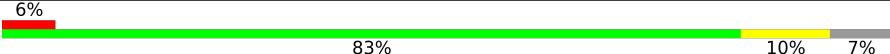
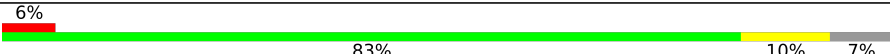
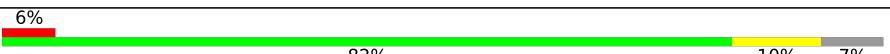
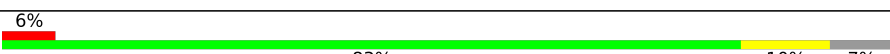
The reported resolution of this entry is 2.90 Å.

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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Q-score	-	25397	13054 (2.40 - 3.40)

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

Mol	Chain	Length	Quality of chain
1	A	1887	 6% 83% 10% 7%
1	B	1887	 6% 83% 10% 7%
1	C	1887	 6% 83% 10% 7%
1	D	1887	 6% 83% 10% 7%
1	E	1887	 6% 82% 10% 7%
1	F	1887	 6% 83% 10% 7%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	G	2040	 90%9%
2	H	2040	 90%9%
2	I	2040	 90%10%
2	J	2040	 90%10%
2	K	2040	 90%9%
2	L	2040	 90%9%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 178362 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.

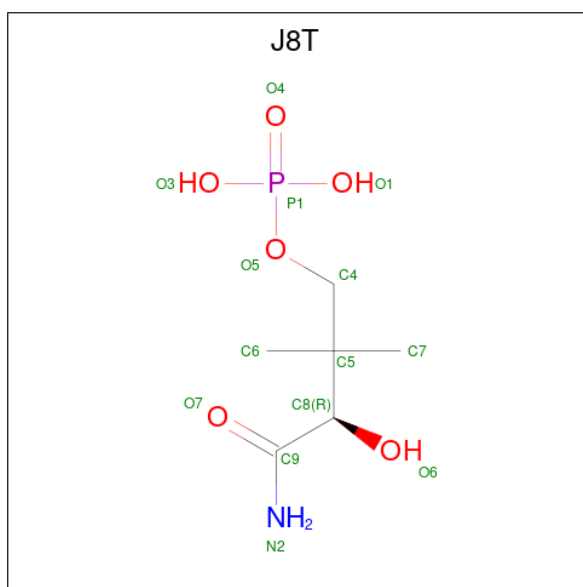
- Molecule 1 is a protein called Fatty acid synthase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1757	Total	C	N	O	S	0	0
			13665	8650	2305	2658	52		
1	B	1757	Total	C	N	O	S	0	0
			13665	8650	2305	2658	52		
1	C	1757	Total	C	N	O	S	0	0
			13665	8650	2305	2658	52		
1	D	1757	Total	C	N	O	S	0	0
			13665	8650	2305	2658	52		
1	E	1757	Total	C	N	O	S	0	0
			13665	8650	2305	2658	52		
1	F	1757	Total	C	N	O	S	0	0
			13665	8650	2305	2658	52		

- Molecule 2 is a protein called Fatty acid synthase subunit beta.

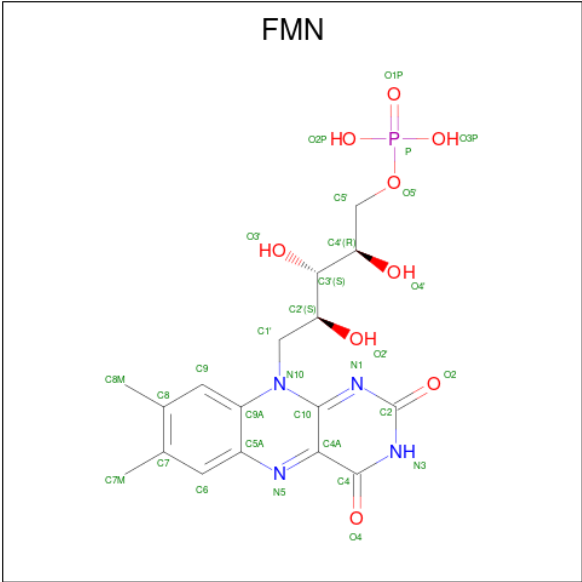
Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	2036	Total	C	N	O	S	0	0
			16018	10265	2663	3034	56		
2	H	2036	Total	C	N	O	S	0	0
			16018	10265	2663	3034	56		
2	I	2036	Total	C	N	O	S	0	0
			16018	10265	2663	3034	56		
2	J	2036	Total	C	N	O	S	0	0
			16018	10265	2663	3034	56		
2	K	2036	Total	C	N	O	S	0	0
			16018	10265	2663	3034	56		
2	L	2036	Total	C	N	O	S	0	0
			16018	10265	2663	3034	56		

- Molecule 3 is [(3 {R})-4-azanyl-2,2-dimethyl-3-oxidanyl-4-oxidanylidene-butyl] dihydrogen phosphate (CCD ID: J8T) (formula: C₆H₁₄NO₆P).

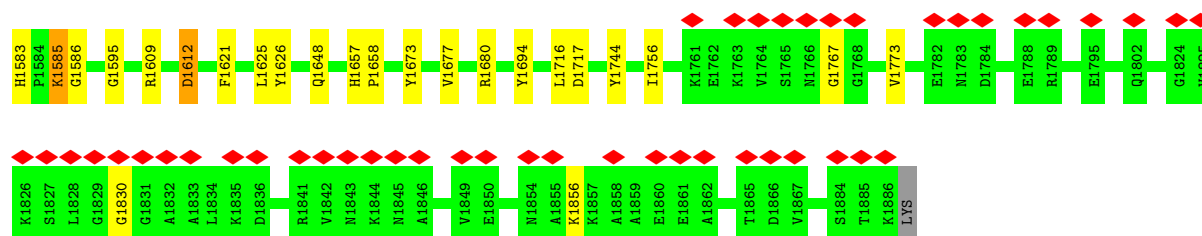


Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			13	6	1	5	1	
3	B	1	Total	C	N	O	P	0
			13	6	1	5	1	
3	C	1	Total	C	N	O	P	0
			13	6	1	5	1	
3	D	1	Total	C	N	O	P	0
			13	6	1	5	1	
3	E	1	Total	C	N	O	P	0
			13	6	1	5	1	
3	F	1	Total	C	N	O	P	0
			13	6	1	5	1	

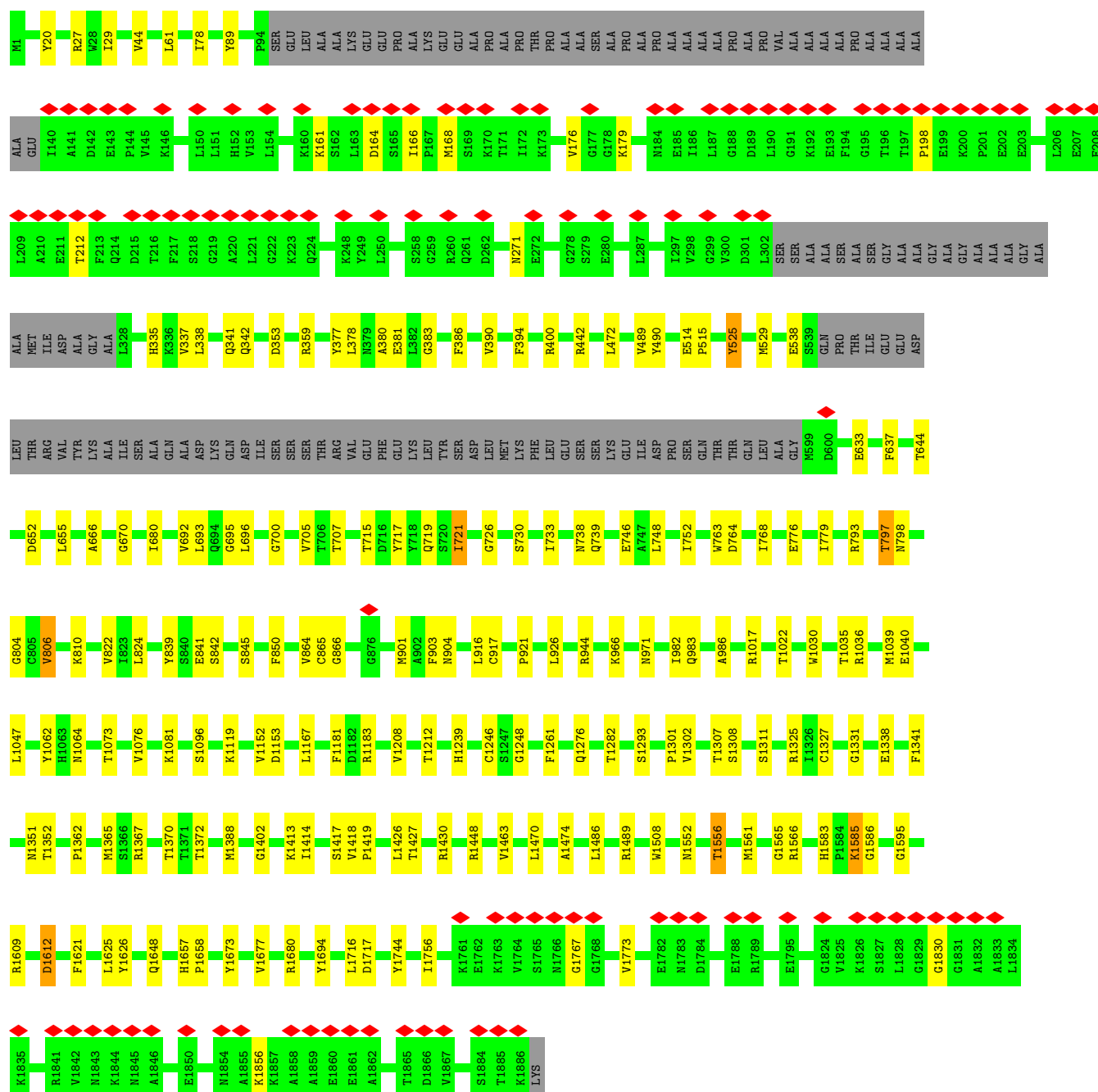
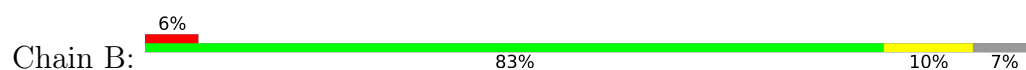
- Molecule 4 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



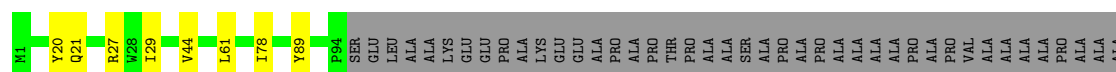
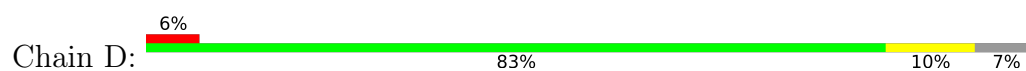
Mol	Chain	Residues	Atoms					AltConf
4	G	1	Total	C	N	O	P	0
			31	17	4	9	1	
4	H	1	Total	C	N	O	P	0
			31	17	4	9	1	
4	I	1	Total	C	N	O	P	0
			31	17	4	9	1	
4	J	1	Total	C	N	O	P	0
			31	17	4	9	1	
4	K	1	Total	C	N	O	P	0
			31	17	4	9	1	
4	L	1	Total	C	N	O	P	0
			31	17	4	9	1	

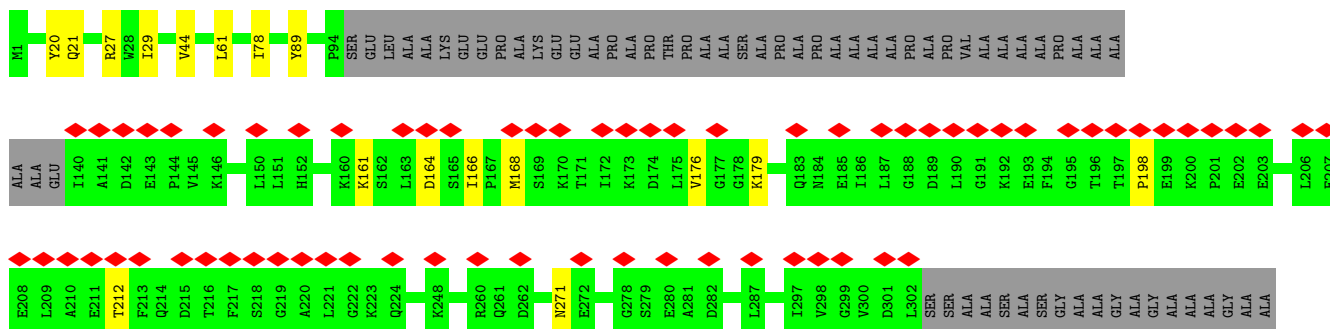
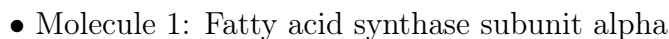


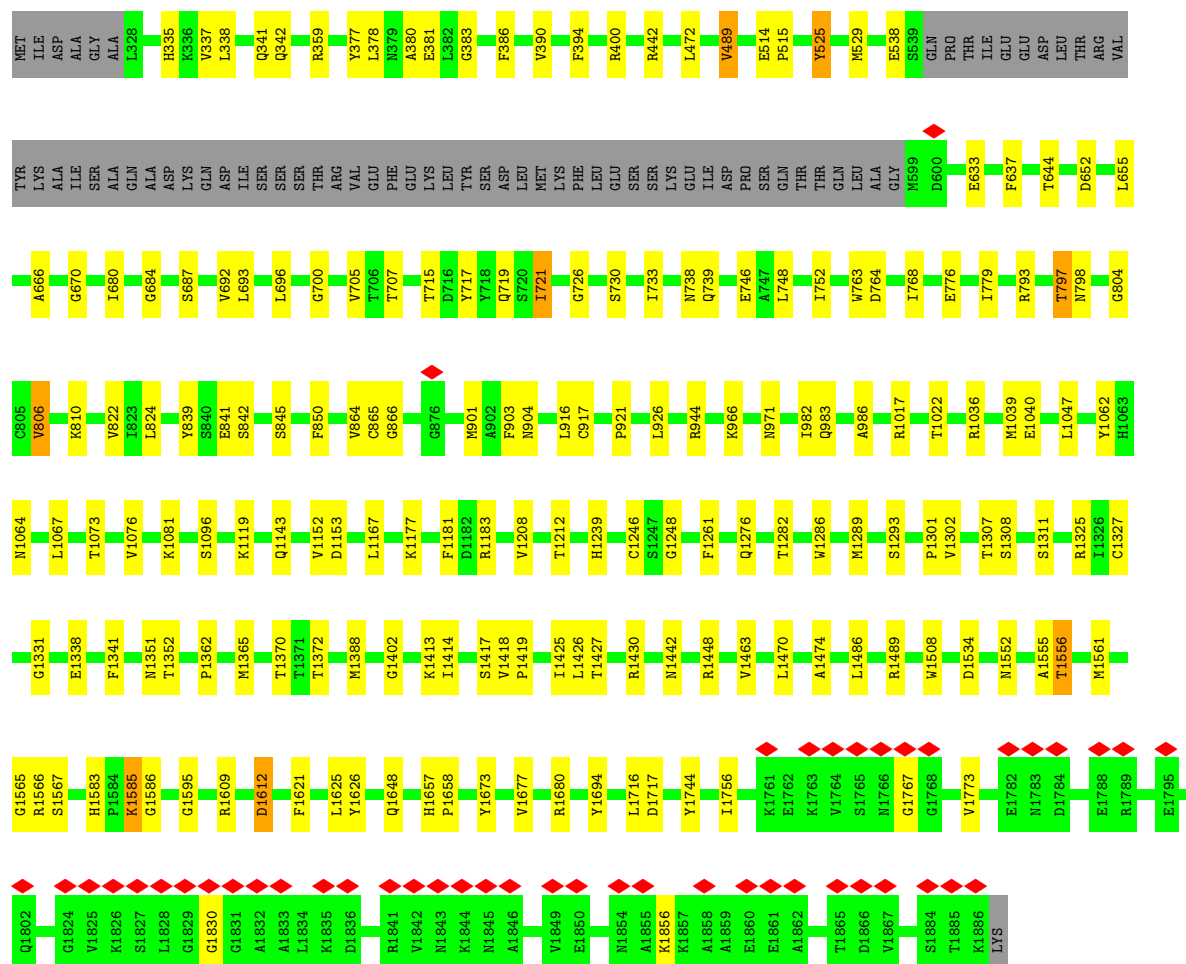
• Molecule 1: Fatty acid synthase subunit alpha



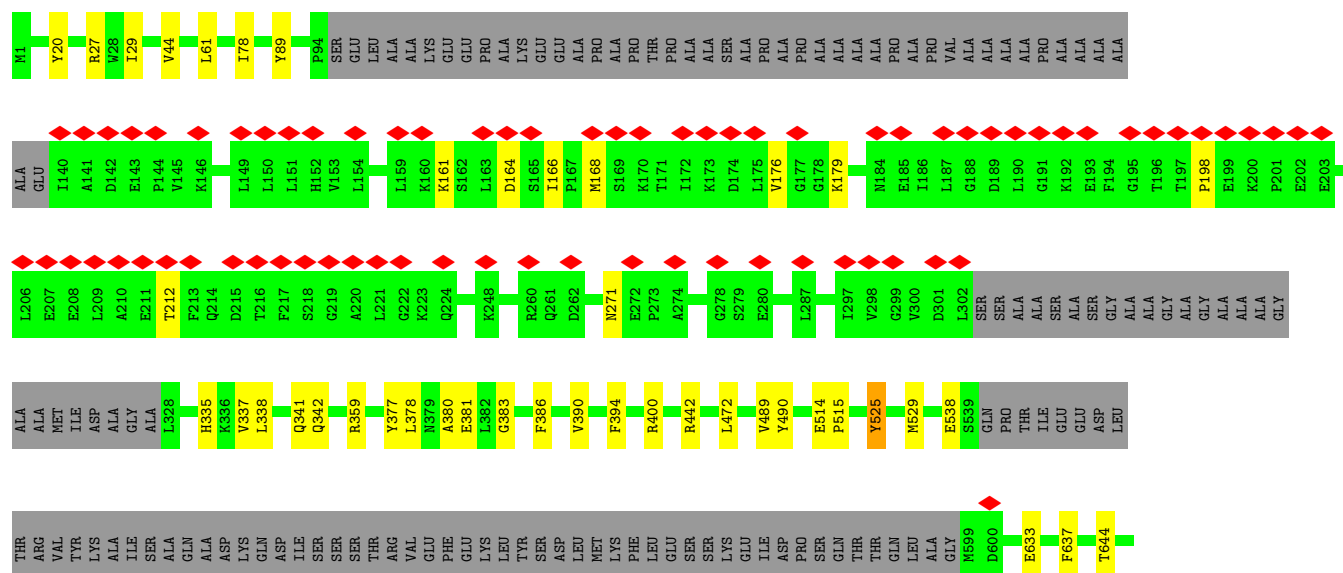
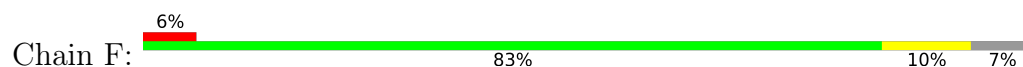
Chain C:

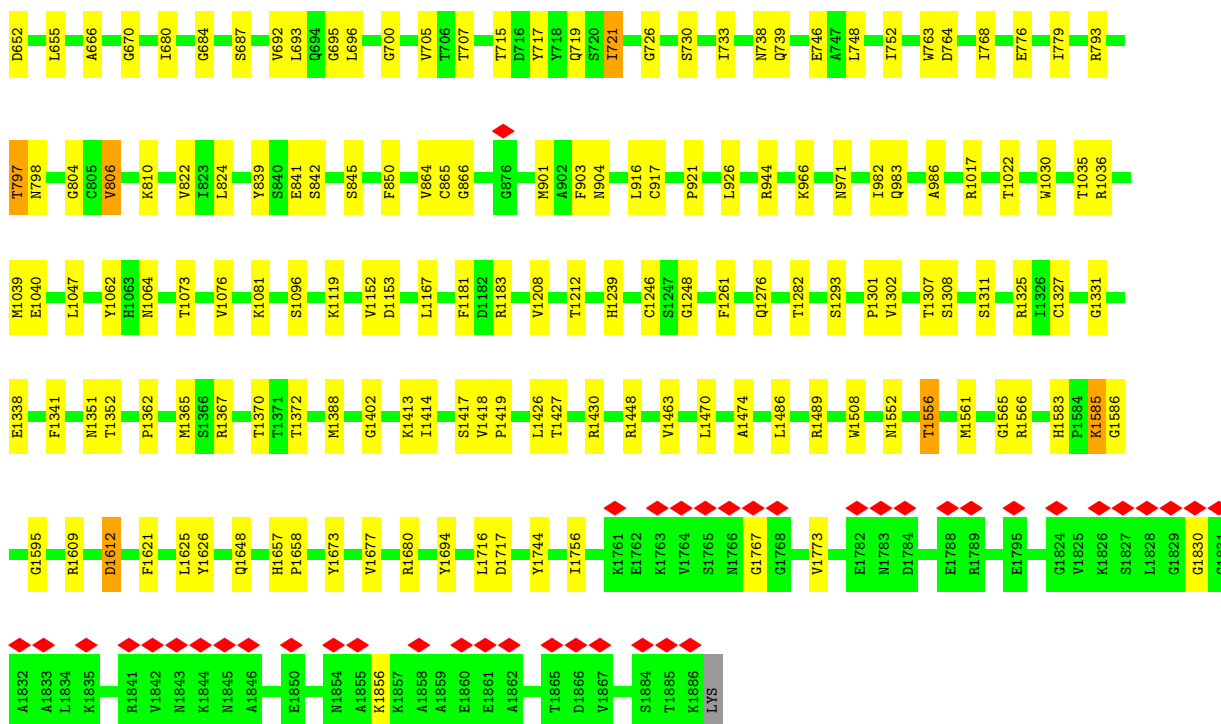






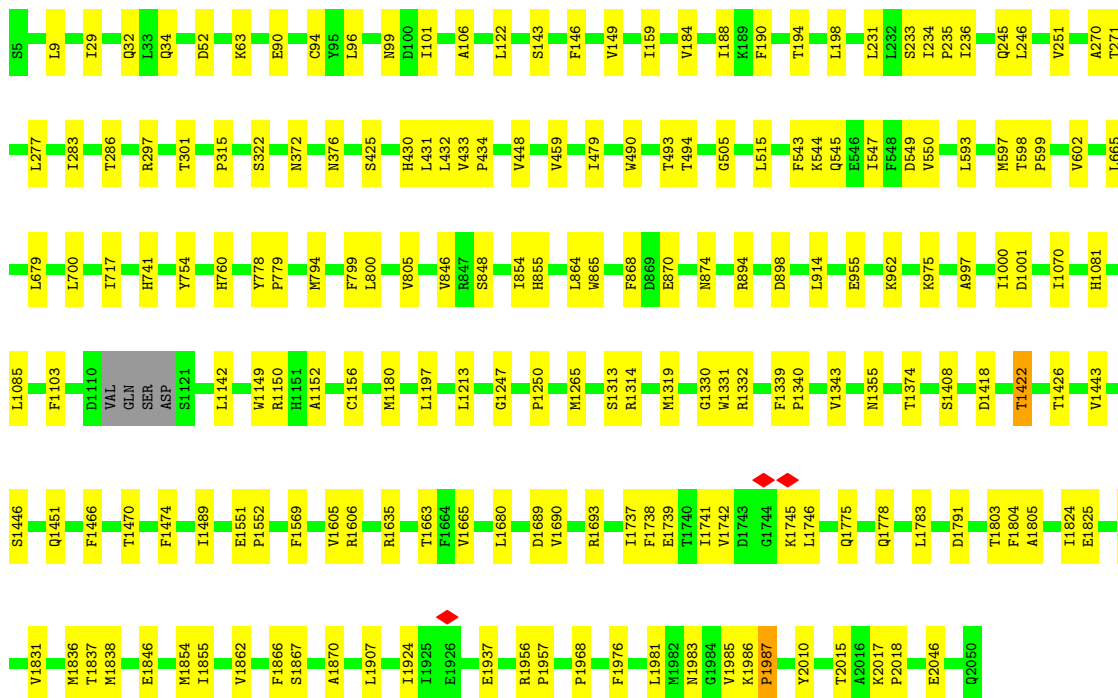
● Molecule 1: Fatty acid synthase subunit alpha





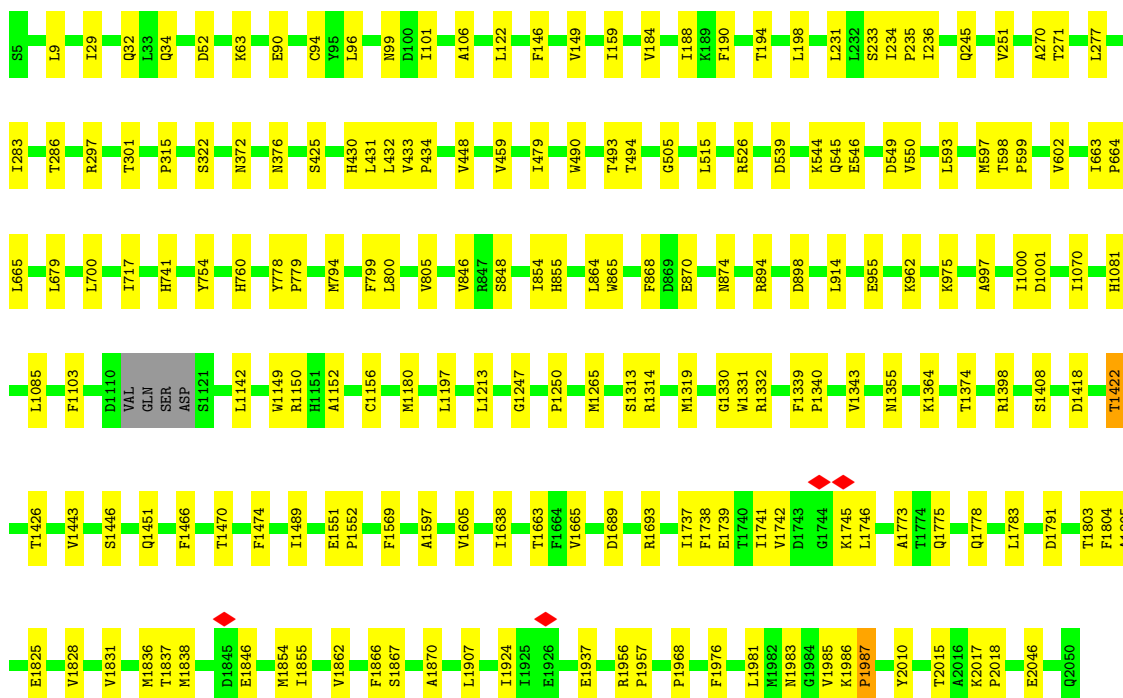
• Molecule 2: Fatty acid synthase subunit beta

Chain G: 90% 9%



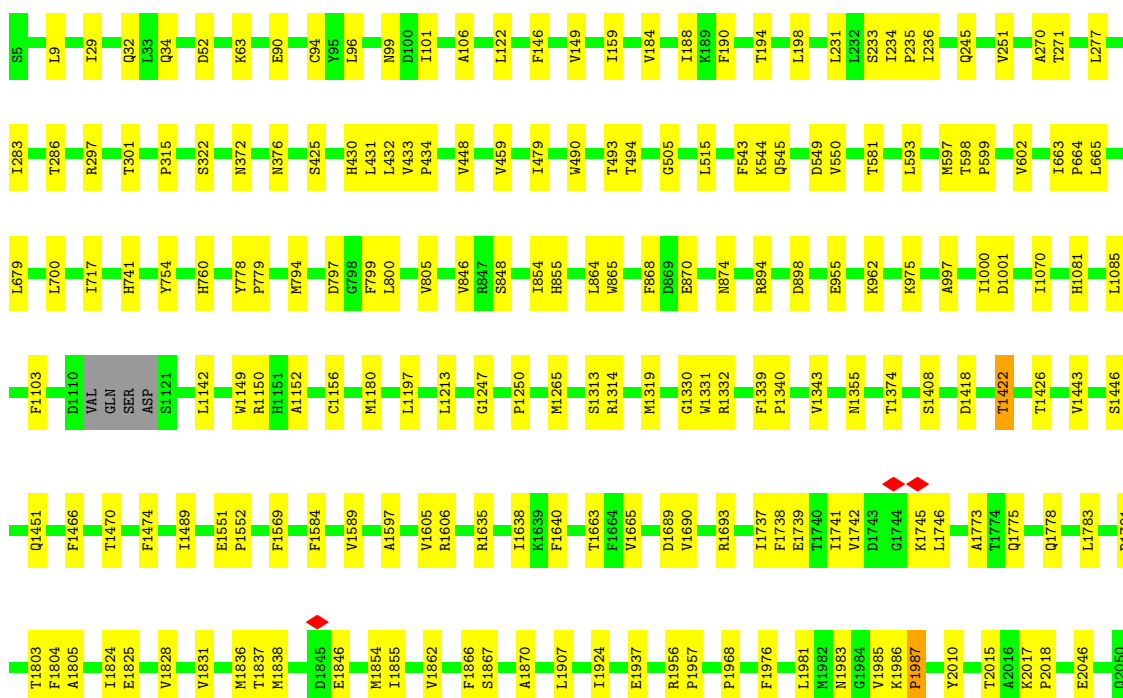
• Molecule 2: Fatty acid synthase subunit beta

Chain H: 90% 9%



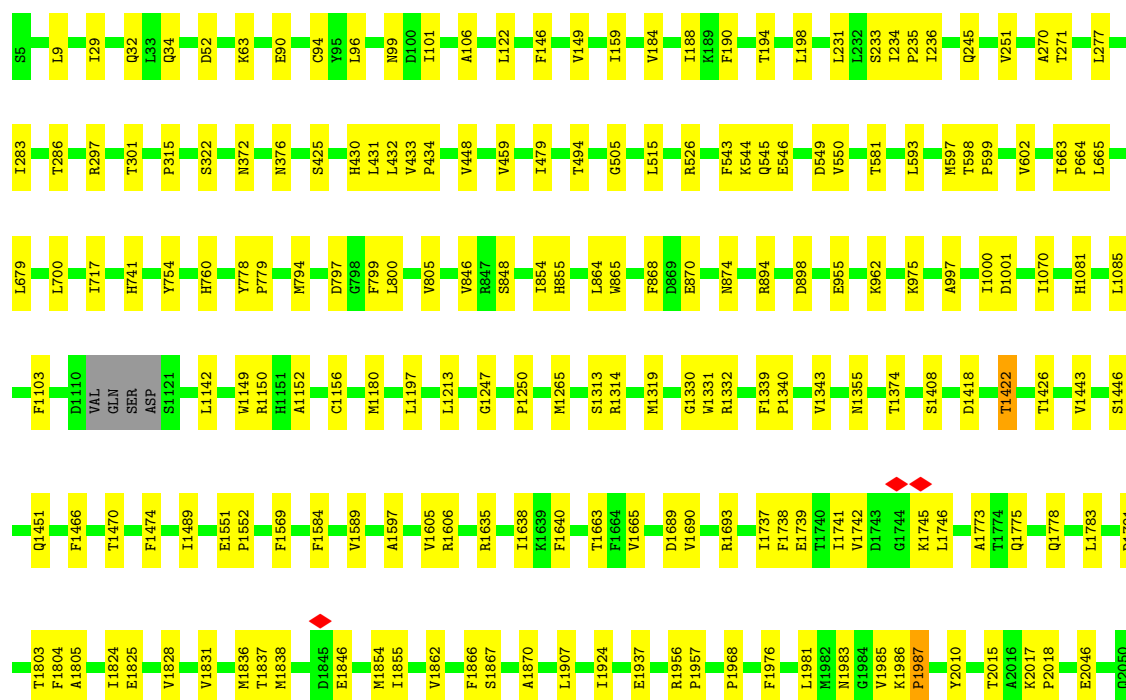
• Molecule 2: Fatty acid synthase subunit beta

Chain I: 90% 10%



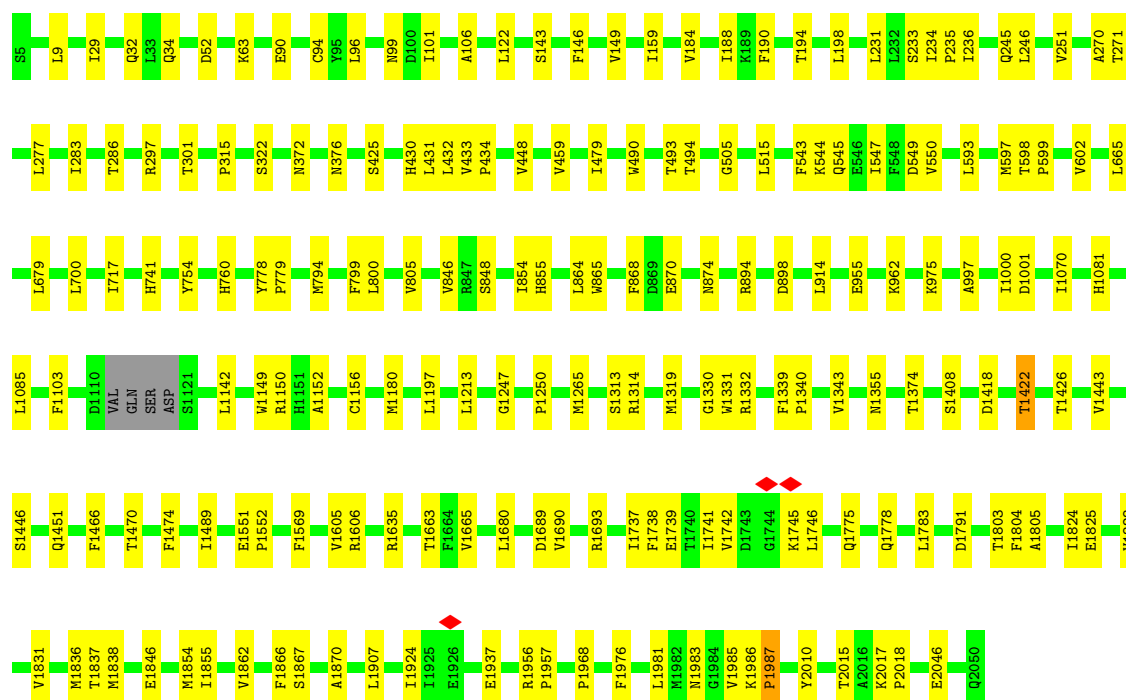
• Molecule 2: Fatty acid synthase subunit beta

Chain J: 90% 10%



• Molecule 2: Fatty acid synthase subunit beta

Chain K: 90% 9%



• Molecule 2: Fatty acid synthase subunit beta

Chain L: 90% 9%

V1828	V1831	M1836	T1837	M1838	D1845	E1846	M1854	I1855	V1862	F1866	S1867	A1870	M1884	A1906	L1907	I1924	I1925	E1926	E1937	R1956	P1957	P1968	F1976	L1981	M1982	N1983	G1984	V1985	K1986	P1987	Y2010	T2015	A2016	K2017	P2018	E2046	Q2050	
V1443	S1446	Q1451	F1466	T1470	F1474	I1489	E1551	P1552	F1569	A1597	V1605	I1638	T1663	F1664	V1665	D1689	R1693	I1737	F1738	E1739	T1740	I1741	V1742	D1743	G1744	K1745	L1746	A1773	T1774	Q1775	Q1778	L1783	D1791	T1803	F1804	A1805	E1825	
H1081	L1085	D1110	VAL	GLN	SER	ASP	S1121	L1142	W1149	R1150	H1151	A1152	C1156	M1180	L1197	L1213	P1250	M1265	S1313	R1314	M1319	G1330	W1331	R1332	F1339	P1340	V1343	N1355	K1364	T1374	R1398	S1408	D1418	T1422	T1426			
P664	L665	L679	L700	I717	H741	Y754	H760	Y778	P779	M794	F799	L800	V805	V846	R847	S848	I854	H855	L864	W865	F868	D869	E870	N874	R894	D898	L914	E955	K962	K975	A997	I1000	D1001	I1070				
S5	L9	I29	Q32	L33	Q34	D52	K63	E90	C94	Y95	L96	N99	D100	V433	I101	A106	L122	F146	V149	I159	V184	I188	K189	F190	T194	L198	L231	L232	S233	I234	P235	I236	Q245	L246	V251	A270	T271	L277

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D3	Depositor
Number of particles used	144526	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 ($e^-/\text{\AA}^2$)	62	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	132000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.106	Depositor
Minimum map value	-0.043	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	339.19998, 339.19998, 339.19998	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: J8T, FMN

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	1.12	2/13918 (0.0%)	1.60	54/18809 (0.3%)
1	B	1.12	2/13918 (0.0%)	1.60	52/18809 (0.3%)
1	C	1.12	2/13918 (0.0%)	1.60	57/18809 (0.3%)
1	D	1.12	2/13918 (0.0%)	1.60	52/18809 (0.3%)
1	E	1.12	2/13918 (0.0%)	1.60	55/18809 (0.3%)
1	F	1.12	2/13918 (0.0%)	1.60	54/18809 (0.3%)
2	G	1.03	0/16383	1.50	16/22229 (0.1%)
2	H	1.03	0/16383	1.50	16/22229 (0.1%)
2	I	1.03	0/16383	1.50	16/22229 (0.1%)
2	J	1.03	0/16383	1.50	16/22229 (0.1%)
2	K	1.03	0/16383	1.50	16/22229 (0.1%)
2	L	1.03	0/16383	1.50	16/22229 (0.1%)
All	All	1.07	12/181806 (0.0%)	1.55	420/246228 (0.2%)

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	1
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	1
2	G	0	3
2	H	0	3
2	I	0	3
2	J	0	3
2	K	0	3

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
2	L	0	3
All	All	0	24

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	693	LEU	C-O	-5.49	1.17	1.24
1	C	693	LEU	C-O	-5.43	1.17	1.24
1	A	693	LEU	C-O	-5.41	1.17	1.24
1	F	693	LEU	C-O	-5.39	1.17	1.24
1	B	693	LEU	C-O	-5.39	1.17	1.24
1	E	693	LEU	C-O	-5.37	1.17	1.24
1	C	752	ILE	C-O	-5.33	1.18	1.24
1	A	752	ILE	C-O	-5.27	1.18	1.24
1	D	752	ILE	C-O	-5.27	1.18	1.24
1	E	752	ILE	C-O	-5.24	1.18	1.24
1	B	752	ILE	C-O	-5.17	1.18	1.24
1	F	752	ILE	C-O	-5.17	1.18	1.24

All (420) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	692	VAL	N-CA-C	-8.82	103.25	111.45
1	A	692	VAL	N-CA-C	-8.81	103.25	111.45
1	C	692	VAL	N-CA-C	-8.81	103.26	111.45
1	D	692	VAL	N-CA-C	-8.77	103.30	111.45
1	B	692	VAL	N-CA-C	-8.74	103.32	111.45
1	E	692	VAL	N-CA-C	-8.72	103.34	111.45
1	A	1017	ARG	CB-CA-C	7.61	123.22	110.44
1	C	1017	ARG	CB-CA-C	7.60	123.21	110.44
1	B	1017	ARG	CB-CA-C	7.58	123.17	110.44
1	F	1017	ARG	CB-CA-C	7.58	123.18	110.44
1	D	1017	ARG	CB-CA-C	7.57	123.16	110.44
1	E	1017	ARG	CB-CA-C	7.53	123.08	110.44
2	G	494	THR	CB-CA-C	7.09	121.00	111.14
2	J	494	THR	CB-CA-C	7.09	121.00	111.14
2	L	494	THR	CB-CA-C	7.09	121.00	111.14
2	H	494	THR	CB-CA-C	7.09	120.99	111.14
2	K	494	THR	CB-CA-C	7.08	120.98	111.14
2	I	494	THR	CB-CA-C	7.07	120.97	111.14
1	E	1612	ASP	CA-CB-CG	6.91	119.50	112.60
1	A	1612	ASP	CA-CB-CG	6.89	119.49	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1612	ASP	CA-CB-CG	6.89	119.49	112.60
1	F	1612	ASP	CA-CB-CG	6.88	119.47	112.60
1	B	1612	ASP	CA-CB-CG	6.87	119.47	112.60
1	C	1612	ASP	CA-CB-CG	6.86	119.46	112.60
1	A	1585	LYS	CB-CA-C	6.34	123.04	110.42
2	I	799	PHE	CA-CB-CG	-6.33	107.47	113.80
1	C	1585	LYS	CB-CA-C	6.32	123.00	110.42
2	L	799	PHE	CA-CB-CG	-6.32	107.48	113.80
2	H	799	PHE	CA-CB-CG	-6.30	107.50	113.80
2	K	799	PHE	CA-CB-CG	-6.30	107.50	113.80
2	G	799	PHE	CA-CB-CG	-6.29	107.51	113.80
2	J	799	PHE	CA-CB-CG	-6.29	107.52	113.80
1	E	1585	LYS	CB-CA-C	6.26	122.88	110.42
1	B	1585	LYS	CB-CA-C	6.24	122.85	110.42
1	F	1585	LYS	CB-CA-C	6.24	122.83	110.42
1	D	1585	LYS	CB-CA-C	6.16	122.69	110.42
1	D	1830	GLY	CA-C-N	6.16	126.59	120.31
1	D	1830	GLY	C-N-CA	6.16	126.59	120.31
1	C	693	LEU	CA-C-O	-6.15	114.32	120.90
1	A	693	LEU	CA-C-O	-6.11	114.36	120.90
1	F	1830	GLY	CA-C-N	6.11	126.54	120.31
1	F	1830	GLY	C-N-CA	6.11	126.54	120.31
1	F	693	LEU	CA-C-O	-6.10	114.37	120.90
1	C	1830	GLY	CA-C-N	6.09	126.53	120.31
1	C	1830	GLY	C-N-CA	6.09	126.53	120.31
1	E	693	LEU	CA-C-O	-6.08	114.39	120.90
1	B	693	LEU	CA-C-O	-6.08	114.39	120.90
1	D	693	LEU	CA-C-O	-6.08	114.39	120.90
1	E	1830	GLY	CA-C-N	6.08	126.52	120.31
1	E	1830	GLY	C-N-CA	6.08	126.52	120.31
1	A	1556	THR	N-CA-CB	6.06	119.24	110.20
1	B	806	VAL	N-CA-CB	6.06	119.67	110.58
1	C	806	VAL	N-CA-CB	6.05	119.66	110.58
1	A	806	VAL	N-CA-CB	6.05	119.65	110.58
1	F	806	VAL	N-CA-CB	6.05	119.65	110.58
1	E	1556	THR	N-CA-CB	6.05	119.21	110.20
1	A	1830	GLY	CA-C-N	6.04	126.47	120.31
1	A	1830	GLY	C-N-CA	6.04	126.47	120.31
1	D	1556	THR	N-CA-CB	6.04	119.20	110.20
1	B	1830	GLY	CA-C-N	6.04	126.47	120.31
1	B	1830	GLY	C-N-CA	6.04	126.47	120.31
1	B	1556	THR	N-CA-CB	6.03	119.19	110.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	806	VAL	N-CA-CB	6.03	119.63	110.58
1	F	1556	THR	N-CA-CB	6.03	119.19	110.20
1	E	806	VAL	N-CA-CB	6.02	119.61	110.58
1	C	1556	THR	N-CA-CB	6.01	119.15	110.20
1	C	29	ILE	N-CA-C	-6.00	104.78	110.42
1	E	29	ILE	N-CA-C	-5.99	104.79	110.42
1	B	29	ILE	N-CA-C	-5.98	104.80	110.42
1	D	1325	ARG	N-CA-C	-5.98	106.12	113.41
1	D	29	ILE	N-CA-C	-5.97	104.80	110.42
1	A	29	ILE	N-CA-C	-5.97	104.81	110.42
1	B	1325	ARG	N-CA-C	-5.97	106.13	113.41
1	E	1325	ARG	N-CA-C	-5.96	106.14	113.41
1	E	806	VAL	CA-C-O	-5.96	114.54	120.85
1	C	806	VAL	CA-C-O	-5.96	114.54	120.85
1	C	1325	ARG	N-CA-C	-5.96	106.15	113.41
1	D	806	VAL	CA-C-O	-5.95	114.55	120.85
1	A	1325	ARG	N-CA-C	-5.94	106.16	113.41
1	E	1301	PRO	N-CA-C	5.94	120.60	111.57
1	B	1301	PRO	N-CA-C	5.93	120.59	111.57
1	C	1301	PRO	N-CA-C	5.93	120.59	111.57
1	F	1325	ARG	N-CA-C	-5.92	106.19	113.41
1	A	806	VAL	CA-C-O	-5.91	114.59	120.85
1	D	1301	PRO	N-CA-C	5.91	120.55	111.57
1	A	1301	PRO	N-CA-C	5.91	120.55	111.57
1	F	1680	ARG	CG-CD-NE	-5.91	99.01	112.00
1	B	806	VAL	CA-C-O	-5.90	114.60	120.85
1	F	1301	PRO	N-CA-C	5.90	120.53	111.57
1	F	806	VAL	CA-C-O	-5.89	114.61	120.85
1	E	1680	ARG	CG-CD-NE	-5.89	99.05	112.00
1	F	29	ILE	N-CA-C	-5.89	104.89	110.42
1	A	1680	ARG	CG-CD-NE	-5.88	99.06	112.00
1	D	383	GLY	CA-C-O	-5.88	118.17	122.23
1	D	1680	ARG	CG-CD-NE	-5.88	99.06	112.00
1	C	1680	ARG	CG-CD-NE	-5.88	99.07	112.00
1	C	383	GLY	CA-C-O	-5.87	118.18	122.23
1	B	1680	ARG	CG-CD-NE	-5.85	99.12	112.00
1	D	27	ARG	N-CA-CB	-5.84	103.63	110.35
1	E	27	ARG	N-CA-CB	-5.84	103.64	110.35
1	E	383	GLY	CA-C-O	-5.84	118.20	122.23
1	A	383	GLY	CA-C-O	-5.83	118.20	122.23
1	B	383	GLY	CA-C-O	-5.83	118.21	122.23
1	F	27	ARG	N-CA-CB	-5.82	103.65	110.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	383	GLY	CA-C-O	-5.82	118.22	122.23
1	A	27	ARG	N-CA-CB	-5.79	103.69	110.35
1	C	27	ARG	N-CA-CB	-5.77	103.71	110.35
1	E	841	GLU	CB-CG-CD	5.70	122.28	112.60
1	D	746	GLU	CA-C-N	5.68	128.16	120.38
1	D	746	GLU	C-N-CA	5.68	128.16	120.38
1	A	841	GLU	CB-CG-CD	5.68	122.25	112.60
1	B	27	ARG	N-CA-CB	-5.68	103.82	110.35
1	B	841	GLU	CB-CG-CD	5.67	122.23	112.60
1	C	841	GLU	CB-CG-CD	5.66	122.22	112.60
1	D	841	GLU	CB-CG-CD	5.66	122.22	112.60
2	H	1422	THR	CB-CA-C	5.66	121.21	109.38
2	J	1422	THR	CB-CA-C	5.66	121.20	109.38
1	F	841	GLU	CB-CG-CD	5.65	122.21	112.60
2	I	432	LEU	CA-C-N	5.65	123.80	120.24
2	I	432	LEU	C-N-CA	5.65	123.80	120.24
2	K	432	LEU	CA-C-N	5.64	123.79	120.24
2	K	432	LEU	C-N-CA	5.64	123.79	120.24
2	L	1422	THR	CB-CA-C	5.64	121.17	109.38
2	J	432	LEU	CA-C-N	5.64	123.79	120.24
2	J	432	LEU	C-N-CA	5.64	123.79	120.24
2	I	1422	THR	CB-CA-C	5.64	121.16	109.38
2	K	1422	THR	CB-CA-C	5.63	121.16	109.38
2	L	432	LEU	CA-C-N	5.63	123.79	120.24
2	L	432	LEU	C-N-CA	5.63	123.79	120.24
1	A	746	GLU	CA-C-N	5.63	128.09	120.38
1	A	746	GLU	C-N-CA	5.63	128.09	120.38
1	E	746	GLU	CA-C-N	5.63	128.09	120.38
1	E	746	GLU	C-N-CA	5.63	128.09	120.38
2	G	1422	THR	CB-CA-C	5.62	121.12	109.38
1	C	525	TYR	CA-C-O	-5.62	114.56	120.63
1	C	746	GLU	CA-C-N	5.62	128.08	120.38
1	C	746	GLU	C-N-CA	5.62	128.08	120.38
1	B	746	GLU	CA-C-N	5.61	128.06	120.38
1	B	746	GLU	C-N-CA	5.61	128.06	120.38
1	F	746	GLU	CA-C-N	5.61	128.06	120.38
1	F	746	GLU	C-N-CA	5.61	128.06	120.38
2	G	432	LEU	CA-C-N	5.60	123.77	120.24
2	G	432	LEU	C-N-CA	5.60	123.77	120.24
1	B	525	TYR	CA-C-O	-5.58	114.60	120.63
1	E	525	TYR	CA-C-O	-5.58	114.61	120.63
2	H	432	LEU	CA-C-N	5.57	123.75	120.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	432	LEU	C-N-CA	5.57	123.75	120.24
1	D	525	TYR	CA-C-O	-5.57	114.62	120.63
1	F	525	TYR	CA-C-O	-5.56	114.62	120.63
1	D	271	ASN	CA-C-N	5.54	128.09	120.39
1	D	271	ASN	C-N-CA	5.54	128.09	120.39
1	D	27	ARG	CB-CA-C	5.54	119.33	111.74
1	A	525	TYR	CA-C-O	-5.54	114.65	120.63
1	E	27	ARG	CB-CA-C	5.52	119.30	111.74
1	A	271	ASN	CA-C-N	5.51	128.06	120.39
1	A	271	ASN	C-N-CA	5.51	128.06	120.39
1	A	27	ARG	CB-CA-C	5.51	119.29	111.74
1	E	271	ASN	CA-C-N	5.49	128.02	120.39
1	E	271	ASN	C-N-CA	5.49	128.02	120.39
1	C	271	ASN	CA-C-N	5.49	128.02	120.39
1	C	271	ASN	C-N-CA	5.49	128.02	120.39
1	F	271	ASN	CA-C-N	5.49	128.02	120.39
1	F	271	ASN	C-N-CA	5.49	128.02	120.39
1	C	27	ARG	CB-CA-C	5.48	119.25	111.74
1	F	27	ARG	CB-CA-C	5.48	119.25	111.74
1	B	271	ASN	CA-C-N	5.47	128.00	120.39
1	B	271	ASN	C-N-CA	5.47	128.00	120.39
1	F	721	ILE	N-CA-C	-5.47	105.51	110.82
1	A	721	ILE	N-CA-C	-5.47	105.52	110.82
1	B	27	ARG	CB-CA-C	5.47	119.23	111.74
1	E	721	ILE	N-CA-C	-5.46	105.52	110.82
1	B	721	ILE	N-CA-C	-5.45	105.53	110.82
1	C	721	ILE	N-CA-C	-5.45	105.54	110.82
1	D	721	ILE	N-CA-C	-5.45	105.54	110.82
1	C	1595	GLY	CA-C-N	5.44	128.01	120.29
1	C	1595	GLY	C-N-CA	5.44	128.01	120.29
1	B	1595	GLY	CA-C-N	5.43	128.00	120.29
1	B	1595	GLY	C-N-CA	5.43	128.00	120.29
2	J	549	ASP	CA-C-N	5.43	127.97	121.84
2	J	549	ASP	C-N-CA	5.43	127.97	121.84
1	D	1595	GLY	CA-C-N	5.43	128.00	120.29
1	D	1595	GLY	C-N-CA	5.43	128.00	120.29
2	L	549	ASP	CA-C-N	5.42	127.96	121.84
2	L	549	ASP	C-N-CA	5.42	127.96	121.84
1	F	1595	GLY	CA-C-N	5.40	127.96	120.29
1	F	1595	GLY	C-N-CA	5.40	127.96	120.29
2	H	549	ASP	CA-C-N	5.40	127.94	121.84
2	H	549	ASP	C-N-CA	5.40	127.94	121.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	549	ASP	CA-C-N	5.40	127.94	121.84
2	K	549	ASP	C-N-CA	5.40	127.94	121.84
1	A	1595	GLY	CA-C-N	5.39	127.95	120.29
1	A	1595	GLY	C-N-CA	5.39	127.95	120.29
1	E	1595	GLY	CA-C-N	5.39	127.95	120.29
1	E	1595	GLY	C-N-CA	5.39	127.95	120.29
1	A	696	LEU	O-C-N	5.39	127.64	122.03
1	C	903	PHE	CA-C-O	-5.39	114.88	120.92
2	I	549	ASP	CA-C-N	5.39	127.93	121.84
2	I	549	ASP	C-N-CA	5.39	127.93	121.84
2	G	549	ASP	CA-C-N	5.38	127.92	121.84
2	G	549	ASP	C-N-CA	5.38	127.92	121.84
1	A	903	PHE	CA-C-O	-5.37	114.90	120.92
1	C	696	LEU	O-C-N	5.37	127.61	122.03
2	J	251	VAL	N-CA-CB	5.36	116.46	110.51
1	B	1325	ARG	CB-CA-C	5.35	118.61	109.24
1	D	1325	ARG	CB-CA-C	5.35	118.61	109.24
1	E	903	PHE	CA-C-O	-5.35	114.93	120.92
1	E	1325	ARG	CB-CA-C	5.35	118.61	109.24
1	B	1856	LYS	CA-C-N	5.35	127.39	120.44
1	B	1856	LYS	C-N-CA	5.35	127.39	120.44
1	F	1856	LYS	CA-C-N	5.35	127.39	120.44
1	F	1856	LYS	C-N-CA	5.35	127.39	120.44
1	B	903	PHE	CA-C-O	-5.34	114.93	120.92
1	C	1856	LYS	CA-C-N	5.34	127.39	120.44
1	C	1856	LYS	C-N-CA	5.34	127.39	120.44
1	A	1856	LYS	CA-C-N	5.34	127.39	120.44
1	A	1856	LYS	C-N-CA	5.34	127.39	120.44
1	A	1325	ARG	CB-CA-C	5.34	118.58	109.24
2	H	251	VAL	N-CA-CB	5.33	116.43	110.51
1	D	903	PHE	CA-C-O	-5.33	114.95	120.92
1	E	696	LEU	O-C-N	5.33	127.58	122.03
1	E	1856	LYS	CA-C-N	5.33	127.37	120.44
1	E	1856	LYS	C-N-CA	5.33	127.37	120.44
2	K	251	VAL	N-CA-CB	5.33	116.43	110.51
1	F	696	LEU	O-C-N	5.33	127.58	122.03
1	D	1856	LYS	CA-C-N	5.33	127.37	120.44
1	D	1856	LYS	C-N-CA	5.33	127.37	120.44
1	F	797	THR	N-CA-CB	5.33	117.95	110.12
1	F	1325	ARG	CB-CA-C	5.33	118.56	109.24
2	I	251	VAL	N-CA-CB	5.33	116.42	110.51
1	D	696	LEU	O-C-N	5.32	127.56	122.03

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	251	VAL	N-CA-CB	5.31	116.41	110.51
1	C	1325	ARG	CB-CA-C	5.31	118.54	109.24
1	F	903	PHE	CA-C-O	-5.30	114.98	120.92
1	B	696	LEU	O-C-N	5.29	127.53	122.03
2	G	251	VAL	N-CA-CB	5.29	116.38	110.51
1	C	797	THR	N-CA-CB	5.29	117.89	110.12
1	D	797	THR	N-CA-CB	5.29	117.89	110.12
1	A	797	THR	N-CA-CB	5.28	117.89	110.12
1	B	797	THR	N-CA-CB	5.28	117.89	110.12
1	C	1621	PHE	CA-C-N	5.27	128.07	120.38
1	C	1621	PHE	C-N-CA	5.27	128.07	120.38
1	E	797	THR	N-CA-CB	5.26	117.86	110.12
1	F	1621	PHE	CA-C-N	5.25	128.05	120.38
1	F	1621	PHE	C-N-CA	5.25	128.05	120.38
1	D	1621	PHE	CA-C-N	5.25	128.05	120.38
1	D	1621	PHE	C-N-CA	5.25	128.05	120.38
1	A	804	GLY	CA-C-N	5.24	127.62	120.54
1	A	804	GLY	C-N-CA	5.24	127.62	120.54
2	K	1937	GLU	CA-C-N	5.24	125.76	119.94
2	K	1937	GLU	C-N-CA	5.24	125.76	119.94
1	F	707	THR	CB-CA-C	5.24	119.38	109.37
2	L	1987	PRO	CA-C-N	5.24	127.72	120.29
2	L	1987	PRO	C-N-CA	5.24	127.72	120.29
2	I	1937	GLU	CA-C-N	5.23	125.74	119.94
2	I	1937	GLU	C-N-CA	5.23	125.74	119.94
2	J	1937	GLU	CA-C-N	5.23	125.74	119.94
2	J	1937	GLU	C-N-CA	5.23	125.74	119.94
1	A	1621	PHE	CA-C-N	5.23	128.01	120.38
1	A	1621	PHE	C-N-CA	5.23	128.01	120.38
1	E	1621	PHE	CA-C-N	5.23	128.01	120.38
1	E	1621	PHE	C-N-CA	5.23	128.01	120.38
1	B	1621	PHE	CA-C-N	5.22	128.01	120.38
1	B	1621	PHE	C-N-CA	5.22	128.01	120.38
2	L	1937	GLU	CA-C-N	5.22	125.74	119.94
2	L	1937	GLU	C-N-CA	5.22	125.74	119.94
1	D	804	GLY	CA-C-N	5.22	127.59	120.54
1	D	804	GLY	C-N-CA	5.22	127.59	120.54
1	E	707	THR	CB-CA-C	5.22	119.35	109.37
2	G	1937	GLU	CA-C-N	5.22	125.73	119.94
2	G	1937	GLU	C-N-CA	5.22	125.73	119.94
2	H	1987	PRO	CA-C-N	5.22	127.70	120.29
2	H	1987	PRO	C-N-CA	5.22	127.70	120.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	1987	PRO	CA-C-N	5.22	127.70	120.29
2	J	1987	PRO	C-N-CA	5.22	127.70	120.29
2	G	1987	PRO	CA-C-N	5.21	127.69	120.29
2	G	1987	PRO	C-N-CA	5.21	127.69	120.29
2	H	1937	GLU	CA-C-N	5.21	125.72	119.94
2	H	1937	GLU	C-N-CA	5.21	125.72	119.94
1	F	804	GLY	CA-C-N	5.21	127.57	120.54
1	F	804	GLY	C-N-CA	5.21	127.57	120.54
1	D	1744	TYR	CA-C-N	5.20	126.54	121.65
1	D	1744	TYR	C-N-CA	5.20	126.54	121.65
2	K	1987	PRO	CA-C-N	5.20	127.67	120.29
2	K	1987	PRO	C-N-CA	5.20	127.67	120.29
1	C	804	GLY	CA-C-N	5.20	127.56	120.54
1	C	804	GLY	C-N-CA	5.20	127.56	120.54
1	E	1744	TYR	CA-C-N	5.20	126.53	121.65
1	E	1744	TYR	C-N-CA	5.20	126.53	121.65
2	I	1987	PRO	CA-C-N	5.19	127.66	120.29
2	I	1987	PRO	C-N-CA	5.19	127.66	120.29
1	C	1744	TYR	CA-C-N	5.18	126.52	121.65
1	C	1744	TYR	C-N-CA	5.18	126.52	121.65
1	E	804	GLY	CA-C-N	5.18	127.54	120.54
1	E	804	GLY	C-N-CA	5.18	127.54	120.54
1	A	707	THR	CB-CA-C	5.18	119.27	109.37
1	B	804	GLY	CA-C-N	5.17	127.52	120.54
1	B	804	GLY	C-N-CA	5.17	127.52	120.54
1	C	707	THR	CB-CA-C	5.17	119.25	109.37
1	A	1744	TYR	CA-C-N	5.17	126.51	121.65
1	A	1744	TYR	C-N-CA	5.17	126.51	121.65
2	J	322	SER	CA-C-N	5.16	127.07	120.56
2	J	322	SER	C-N-CA	5.16	127.07	120.56
1	B	1744	TYR	CA-C-N	5.16	126.50	121.65
1	B	1744	TYR	C-N-CA	5.16	126.50	121.65
1	D	707	THR	CB-CA-C	5.15	119.21	109.37
1	D	644	THR	CB-CA-C	5.15	116.27	108.86
1	C	738	ASN	CA-C-O	-5.14	114.96	120.46
1	F	1744	TYR	CA-C-N	5.13	126.48	121.65
1	F	1744	TYR	C-N-CA	5.13	126.48	121.65
2	I	322	SER	CA-C-N	5.13	127.03	120.56
2	I	322	SER	C-N-CA	5.13	127.03	120.56
1	B	707	THR	CB-CA-C	5.13	119.17	109.37
2	L	322	SER	CA-C-N	5.13	127.02	120.56
2	L	322	SER	C-N-CA	5.13	127.02	120.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	738	ASN	CA-C-O	-5.12	114.98	120.46
1	C	644	THR	CB-CA-C	5.12	116.23	108.86
1	A	644	THR	CB-CA-C	5.12	116.23	108.86
1	B	644	THR	CB-CA-C	5.11	116.22	108.86
1	F	489	VAL	N-CA-CB	-5.11	103.30	111.58
1	D	738	ASN	CA-C-O	-5.11	114.99	120.46
2	H	322	SER	CA-C-N	5.11	127.00	120.56
2	H	322	SER	C-N-CA	5.11	127.00	120.56
1	F	644	THR	CB-CA-C	5.11	116.21	108.86
1	B	489	VAL	N-CA-CB	-5.10	103.31	111.58
1	B	738	ASN	CA-C-O	-5.10	115.00	120.46
2	K	1418	ASP	CA-CB-CG	5.10	117.70	112.60
2	K	322	SER	CA-C-N	5.10	126.99	120.56
2	K	322	SER	C-N-CA	5.10	126.99	120.56
2	G	322	SER	CA-C-N	5.10	126.98	120.56
2	G	322	SER	C-N-CA	5.10	126.98	120.56
1	E	644	THR	CB-CA-C	5.10	116.20	108.86
1	A	489	VAL	N-CA-CB	-5.09	103.33	111.58
1	B	1767	GLY	CA-C-N	5.09	125.50	120.31
1	B	1767	GLY	C-N-CA	5.09	125.50	120.31
1	E	489	VAL	N-CA-CB	-5.08	103.34	111.58
1	B	944	ARG	CA-C-N	5.08	127.40	120.54
1	B	944	ARG	C-N-CA	5.08	127.40	120.54
1	B	1096	SER	CA-C-N	5.08	126.97	120.56
1	B	1096	SER	C-N-CA	5.08	126.97	120.56
1	D	489	VAL	N-CA-CB	-5.08	103.34	111.58
1	A	944	ARG	CA-C-N	5.08	127.40	120.54
1	A	944	ARG	C-N-CA	5.08	127.40	120.54
1	F	738	ASN	CA-C-O	-5.08	115.02	120.46
1	E	738	ASN	CA-C-O	-5.08	115.03	120.46
1	C	1474	ALA	CA-C-N	5.08	127.04	120.44
1	C	1474	ALA	C-N-CA	5.08	127.04	120.44
1	A	1096	SER	CA-C-N	5.08	126.96	120.56
1	A	1096	SER	C-N-CA	5.08	126.96	120.56
2	L	1418	ASP	CA-CB-CG	5.07	117.67	112.60
2	H	1924	ILE	CA-C-O	-5.07	116.00	121.27
1	C	489	VAL	N-CA-CB	-5.07	103.37	111.58
1	D	944	ARG	CA-C-N	5.07	127.38	120.54
1	D	944	ARG	C-N-CA	5.07	127.38	120.54
1	C	944	ARG	CA-C-N	5.06	127.38	120.54
1	C	944	ARG	C-N-CA	5.06	127.38	120.54
1	F	164	ASP	CA-C-N	5.06	127.77	120.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	164	ASP	C-N-CA	5.06	127.77	120.38
1	A	1474	ALA	CA-C-N	5.05	127.01	120.44
1	A	1474	ALA	C-N-CA	5.05	127.01	120.44
1	A	1680	ARG	CB-CA-C	-5.05	102.09	110.68
1	C	1680	ARG	CB-CA-C	-5.05	102.10	110.68
1	E	1680	ARG	CB-CA-C	-5.05	102.09	110.68
1	C	1017	ARG	N-CA-CB	-5.05	102.89	111.27
1	D	1096	SER	CA-C-N	5.05	126.92	120.56
1	D	1096	SER	C-N-CA	5.05	126.92	120.56
1	E	1474	ALA	CA-C-N	5.05	127.00	120.44
1	E	1474	ALA	C-N-CA	5.05	127.00	120.44
2	J	1418	ASP	CA-CB-CG	5.05	117.65	112.60
1	C	164	ASP	CA-C-N	5.04	127.75	120.38
1	C	164	ASP	C-N-CA	5.04	127.75	120.38
1	E	1767	GLY	CA-C-N	5.04	125.46	120.31
1	E	1767	GLY	C-N-CA	5.04	125.46	120.31
2	G	1418	ASP	CA-CB-CG	5.04	117.64	112.60
1	F	1096	SER	CA-C-N	5.04	126.91	120.56
1	F	1096	SER	C-N-CA	5.04	126.91	120.56
1	D	1555	ALA	CA-C-O	-5.04	115.21	120.55
1	D	1474	ALA	CA-C-N	5.04	126.98	120.44
1	D	1474	ALA	C-N-CA	5.04	126.98	120.44
1	E	1017	ARG	N-CA-CB	-5.04	102.91	111.27
1	E	1096	SER	CA-C-N	5.04	126.91	120.56
1	E	1096	SER	C-N-CA	5.04	126.91	120.56
2	K	1924	ILE	CA-C-O	-5.04	116.03	121.27
1	D	886	GLU	CA-C-N	5.03	125.43	119.94
1	D	886	GLU	C-N-CA	5.03	125.43	119.94
1	F	944	ARG	CA-C-N	5.03	127.34	120.54
1	F	944	ARG	C-N-CA	5.03	127.34	120.54
1	F	1474	ALA	CA-C-N	5.03	126.98	120.44
1	F	1474	ALA	C-N-CA	5.03	126.98	120.44
1	A	164	ASP	CA-C-N	5.03	127.72	120.38
1	A	164	ASP	C-N-CA	5.03	127.72	120.38
2	H	1418	ASP	CA-CB-CG	5.03	117.63	112.60
2	L	1924	ILE	CA-C-O	-5.03	116.04	121.27
1	A	1767	GLY	CA-C-N	5.03	125.44	120.31
1	A	1767	GLY	C-N-CA	5.03	125.44	120.31
1	E	944	ARG	CA-C-N	5.02	127.32	120.54
1	E	944	ARG	C-N-CA	5.02	127.32	120.54
1	C	1096	SER	CA-C-N	5.02	126.89	120.56
1	C	1096	SER	C-N-CA	5.02	126.89	120.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1680	ARG	CB-CA-C	-5.02	102.14	110.68
1	F	1767	GLY	CA-C-N	5.02	125.43	120.31
1	F	1767	GLY	C-N-CA	5.02	125.43	120.31
2	G	1924	ILE	CA-C-O	-5.02	116.05	121.27
2	I	1924	ILE	CA-C-O	-5.02	116.05	121.27
2	J	1924	ILE	CA-C-O	-5.02	116.05	121.27
1	E	1555	ALA	CA-C-O	-5.02	115.23	120.55
1	F	1680	ARG	CB-CA-C	-5.02	102.15	110.68
1	C	1555	ALA	CA-C-O	-5.01	115.23	120.55
2	I	1418	ASP	CA-CB-CG	5.01	117.61	112.60
1	C	886	GLU	CA-C-N	5.01	125.40	119.94
1	C	886	GLU	C-N-CA	5.01	125.40	119.94
1	F	1017	ARG	N-CA-CB	-5.01	102.95	111.27
1	B	1474	ALA	CA-C-N	5.01	126.95	120.44
1	B	1474	ALA	C-N-CA	5.01	126.95	120.44
1	E	164	ASP	CA-C-N	5.01	127.69	120.38
1	E	164	ASP	C-N-CA	5.01	127.69	120.38
1	A	1017	ARG	N-CA-CB	-5.01	102.96	111.27
1	B	164	ASP	CA-C-N	5.01	127.69	120.38
1	B	164	ASP	C-N-CA	5.01	127.69	120.38
1	C	1767	GLY	CA-C-N	5.00	125.41	120.31
1	C	1767	GLY	C-N-CA	5.00	125.41	120.31

There are no chirality outliers.

All (24) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1565	GLY	Peptide
1	B	1565	GLY	Peptide
1	C	1565	GLY	Peptide
1	D	1565	GLY	Peptide
1	E	1565	GLY	Peptide
1	F	1565	GLY	Peptide
2	G	1605	VAL	Peptide
2	G	2046	GLU	Peptide
2	G	975	LYS	Peptide
2	H	1605	VAL	Peptide
2	H	2046	GLU	Peptide
2	H	975	LYS	Peptide
2	I	1605	VAL	Peptide
2	I	2046	GLU	Peptide
2	I	975	LYS	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
2	J	1605	VAL	Peptide
2	J	2046	GLU	Peptide
2	J	975	LYS	Peptide
2	K	1605	VAL	Peptide
2	K	2046	GLU	Peptide
2	K	975	LYS	Peptide
2	L	1605	VAL	Peptide
2	L	2046	GLU	Peptide
2	L	975	LYS	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	13665	0	13647	112	0
1	B	13665	0	13647	109	0
1	C	13665	0	13647	109	0
1	D	13665	0	13647	109	0
1	E	13665	0	13647	112	0
1	F	13665	0	13647	109	0
2	G	16018	0	15993	121	0
2	H	16018	0	15993	123	0
2	I	16018	0	15993	123	0
2	J	16018	0	15993	123	0
2	K	16018	0	15993	121	0
2	L	16018	0	15993	124	0
3	A	13	0	0	1	0
3	B	13	0	0	1	0
3	C	13	0	0	1	0
3	D	13	0	0	1	0
3	E	13	0	0	1	0
3	F	13	0	0	1	0
4	G	31	0	19	1	0
4	H	31	0	19	1	0
4	I	31	0	19	1	0
4	J	31	0	19	1	0
4	K	31	0	19	1	0
4	L	31	0	19	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	178362	0	177954	1309	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 4.

All (1309) 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)
3:B:1901:J8T:O4	1:E:1417:SER:OG	1.97	0.82
3:C:1901:J8T:O4	1:D:1417:SER:OG	1.98	0.81
3:A:1901:J8T:O4	1:F:1417:SER:OG	1.98	0.79
2:K:894:ARG:NH1	2:K:898:ASP:OD2	2.16	0.78
2:G:894:ARG:NH1	2:G:898:ASP:OD2	2.16	0.78
2:H:1741:ILE:HG22	2:H:1983:ASN:HA	1.65	0.78
2:H:894:ARG:NH1	2:H:898:ASP:OD2	2.16	0.78
2:L:894:ARG:NH1	2:L:898:ASP:OD2	2.16	0.78
2:L:1741:ILE:HG22	2:L:1983:ASN:HA	1.64	0.78
1:B:1417:SER:OG	3:E:1901:J8T:O4	2.01	0.78
1:C:845:SER:OG	1:D:845:SER:OG	2.01	0.78
2:I:894:ARG:NH1	2:I:898:ASP:OD2	2.16	0.77
2:J:894:ARG:NH1	2:J:898:ASP:OD2	2.16	0.77
2:K:1741:ILE:HG22	2:K:1983:ASN:HA	1.64	0.77
2:J:1741:ILE:HG22	2:J:1983:ASN:HA	1.64	0.77
1:A:845:SER:OG	1:F:845:SER:OG	2.01	0.77
2:I:1741:ILE:HG22	2:I:1983:ASN:HA	1.64	0.77
2:G:1741:ILE:HG22	2:G:1983:ASN:HA	1.65	0.77
1:B:845:SER:OG	1:E:845:SER:OG	2.01	0.77
1:A:1417:SER:OG	3:F:1901:J8T:O4	2.01	0.74
1:B:901:MET:HE1	1:B:926:LEU:HB3	1.70	0.74
1:F:901:MET:HE1	1:F:926:LEU:HB3	1.70	0.74
1:D:901:MET:HE1	1:D:926:LEU:HB3	1.69	0.73
1:C:901:MET:HE1	1:C:926:LEU:HB3	1.69	0.73
1:A:901:MET:HE1	1:A:926:LEU:HB3	1.70	0.73
1:C:1417:SER:OG	3:D:1901:J8T:O4	2.01	0.73
1:E:901:MET:HE1	1:E:926:LEU:HB3	1.70	0.72
2:H:1739:GLU:O	2:H:1987:PRO:HD3	1.90	0.71
2:J:1739:GLU:O	2:J:1987:PRO:HD3	1.90	0.71
2:L:1739:GLU:O	2:L:1987:PRO:HD3	1.90	0.71
2:I:1739:GLU:O	2:I:1987:PRO:HD3	1.90	0.71
2:G:1739:GLU:O	2:G:1987:PRO:HD3	1.90	0.71
2:K:1739:GLU:O	2:K:1987:PRO:HD3	1.90	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1261:PHE:CE1	1:F:1338:GLU:HG3	2.29	0.68
1:B:1338:GLU:HG3	1:D:1261:PHE:CE1	2.29	0.68
1:B:1261:PHE:CE1	1:D:1338:GLU:HG3	2.29	0.68
1:C:1338:GLU:HG3	1:F:1261:PHE:CE1	2.29	0.68
1:A:1261:PHE:CE1	1:E:1338:GLU:HG3	2.29	0.67
1:A:1338:GLU:HG3	1:E:1261:PHE:CE1	2.29	0.67
2:H:1742:VAL:HG22	2:H:1983:ASN:HD22	1.62	0.65
2:L:1742:VAL:HG22	2:L:1983:ASN:HD22	1.62	0.65
1:A:1022:THR:HG21	1:A:1388:MET:HE3	1.79	0.65
1:E:1022:THR:HG21	1:E:1388:MET:HE3	1.80	0.64
2:G:1742:VAL:HG22	2:G:1983:ASN:HD22	1.62	0.64
2:K:1742:VAL:HG22	2:K:1983:ASN:HD22	1.62	0.64
2:K:870:GLU:O	2:K:874:ASN:ND2	2.31	0.64
2:I:1742:VAL:HG22	2:I:1983:ASN:HD22	1.62	0.63
2:J:1742:VAL:HG22	2:J:1983:ASN:HD22	1.62	0.63
2:G:870:GLU:O	2:G:874:ASN:ND2	2.31	0.63
1:F:1022:THR:HG21	1:F:1388:MET:HE3	1.79	0.63
2:L:870:GLU:O	2:L:874:ASN:ND2	2.31	0.63
1:B:1022:THR:HG21	1:B:1388:MET:HE3	1.79	0.63
1:C:1022:THR:HG21	1:C:1388:MET:HE3	1.79	0.63
2:H:870:GLU:O	2:H:874:ASN:ND2	2.31	0.63
1:D:1022:THR:HG21	1:D:1388:MET:HE3	1.79	0.63
2:J:870:GLU:O	2:J:874:ASN:ND2	2.31	0.63
2:I:870:GLU:O	2:I:874:ASN:ND2	2.31	0.62
1:A:901:MET:HE3	1:A:904:ASN:HD22	1.64	0.62
1:E:901:MET:HE3	1:E:904:ASN:HD22	1.64	0.62
1:F:901:MET:HE3	1:F:904:ASN:HD22	1.64	0.62
1:B:901:MET:HE3	1:B:904:ASN:HD22	1.64	0.62
1:D:901:MET:HE3	1:D:904:ASN:HD22	1.64	0.61
1:C:901:MET:HE3	1:C:904:ASN:HD22	1.64	0.61
2:I:2015:THR:O	2:I:2017:LYS:N	2.34	0.61
2:H:2015:THR:O	2:H:2017:LYS:N	2.34	0.61
2:J:2015:THR:O	2:J:2017:LYS:N	2.34	0.61
2:L:2015:THR:O	2:L:2017:LYS:N	2.34	0.61
1:B:1039:MET:O	1:B:1609:ARG:NH2	2.34	0.61
1:F:1039:MET:O	1:F:1609:ARG:NH2	2.34	0.61
2:K:1775:GLN:HG2	2:K:1836:MET:HE2	1.83	0.61
2:G:1775:GLN:HG2	2:G:1836:MET:HE2	1.83	0.61
2:H:245:GLN:HE21	2:H:505:GLY:HA2	1.66	0.61
2:I:1775:GLN:HG2	2:I:1836:MET:HE2	1.83	0.60
2:J:1314:ARG:NH2	2:L:315:PRO:O	2.34	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:245:GLN:HE21	2:L:505:GLY:HA2	1.66	0.60
2:G:315:PRO:O	2:H:1314:ARG:NH2	2.34	0.60
2:I:245:GLN:HE21	2:I:505:GLY:HA2	1.66	0.60
2:J:245:GLN:HE21	2:J:505:GLY:HA2	1.66	0.60
2:H:315:PRO:O	2:I:1314:ARG:NH2	2.34	0.60
2:J:1775:GLN:HG2	2:J:1836:MET:HE2	1.83	0.60
2:K:315:PRO:O	2:L:1314:ARG:NH2	2.35	0.60
2:J:315:PRO:O	2:K:1314:ARG:NH2	2.34	0.60
2:H:1265:MET:HE1	2:H:1569:PHE:CZ	2.37	0.60
1:A:717:TYR:CZ	1:A:721:ILE:HD11	2.37	0.60
2:G:1314:ARG:NH2	2:I:315:PRO:O	2.34	0.60
2:L:1265:MET:HE1	2:L:1569:PHE:CZ	2.37	0.60
2:G:1986:LYS:N	2:G:1987:PRO:HD2	2.17	0.60
1:D:1039:MET:O	1:D:1609:ARG:NH2	2.34	0.60
1:E:717:TYR:CZ	1:E:721:ILE:HD11	2.37	0.60
2:H:1775:GLN:HG2	2:H:1836:MET:HE2	1.83	0.60
2:K:1986:LYS:N	2:K:1987:PRO:HD2	2.17	0.60
2:H:1986:LYS:N	2:H:1987:PRO:HD2	2.17	0.59
2:G:245:GLN:HE21	2:G:505:GLY:HA2	1.66	0.59
1:C:1039:MET:O	1:C:1609:ARG:NH2	2.34	0.59
1:E:1039:MET:O	1:E:1609:ARG:NH2	2.34	0.59
1:A:1039:MET:O	1:A:1609:ARG:NH2	2.34	0.59
2:G:1265:MET:HE1	2:G:1569:PHE:CZ	2.37	0.59
1:C:717:TYR:CZ	1:C:721:ILE:HD11	2.37	0.59
1:D:717:TYR:CZ	1:D:721:ILE:HD11	2.37	0.59
2:K:1265:MET:HE1	2:K:1569:PHE:CZ	2.37	0.59
2:L:1775:GLN:HG2	2:L:1836:MET:HE2	1.83	0.59
2:L:1986:LYS:N	2:L:1987:PRO:HD2	2.17	0.59
2:K:245:GLN:HE21	2:K:505:GLY:HA2	1.66	0.59
2:J:1265:MET:HE1	2:J:1569:PHE:CZ	2.37	0.59
2:I:1265:MET:HE1	2:I:1569:PHE:CZ	2.37	0.59
2:I:1986:LYS:N	2:I:1987:PRO:HD2	2.17	0.59
2:L:231:LEU:HA	2:L:236:ILE:HD11	1.84	0.59
2:J:1986:LYS:N	2:J:1987:PRO:HD2	2.17	0.59
1:A:168:MET:SD	1:A:168:MET:N	2.75	0.59
1:E:168:MET:SD	1:E:168:MET:N	2.75	0.59
1:C:168:MET:SD	1:C:168:MET:N	2.75	0.59
1:D:168:MET:SD	1:D:168:MET:N	2.75	0.59
2:H:231:LEU:HA	2:H:236:ILE:HD11	1.84	0.59
2:K:2015:THR:O	2:K:2017:LYS:N	2.34	0.59
1:A:1276:GLN:O	1:A:1282:THR:HG21	2.03	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:717:TYR:CZ	1:B:721:ILE:HD11	2.37	0.58
2:G:2015:THR:O	2:G:2017:LYS:N	2.34	0.58
1:C:1276:GLN:O	1:C:1282:THR:HG21	2.03	0.58
1:D:1276:GLN:O	1:D:1282:THR:HG21	2.03	0.58
1:F:717:TYR:CZ	1:F:721:ILE:HD11	2.37	0.58
2:I:231:LEU:HA	2:I:236:ILE:HD11	1.84	0.58
2:J:231:LEU:HA	2:J:236:ILE:HD11	1.84	0.58
1:E:1276:GLN:O	1:E:1282:THR:HG21	2.03	0.58
1:F:1276:GLN:O	1:F:1282:THR:HG21	2.03	0.58
2:K:231:LEU:HA	2:K:236:ILE:HD11	1.84	0.58
2:G:231:LEU:HA	2:G:236:ILE:HD11	1.84	0.58
1:B:1276:GLN:O	1:B:1282:THR:HG21	2.03	0.58
2:G:1745:LYS:CE	2:G:1745:LYS:HA	2.34	0.58
1:E:89:TYR:OH	2:K:1791:ASP:OD2	2.17	0.58
2:K:1745:LYS:HA	2:K:1745:LYS:CE	2.34	0.58
2:H:1745:LYS:HA	2:H:1745:LYS:CE	2.34	0.58
2:L:1745:LYS:CE	2:L:1745:LYS:HA	2.34	0.58
2:I:1778:GLN:HB3	2:I:1831:VAL:HG13	1.86	0.57
2:J:1778:GLN:HB3	2:J:1831:VAL:HG13	1.86	0.57
1:A:161:LYS:HD2	1:A:166:ILE:HD11	1.85	0.57
1:E:1064:ASN:ND2	1:E:1073:THR:OG1	2.37	0.57
1:A:1064:ASN:ND2	1:A:1073:THR:OG1	2.37	0.57
2:I:1745:LYS:HA	2:I:1745:LYS:CE	2.34	0.57
2:J:1745:LYS:HA	2:J:1745:LYS:CE	2.34	0.57
2:H:234:ILE:N	2:H:235:PRO:CD	2.68	0.57
2:L:234:ILE:N	2:L:235:PRO:CD	2.68	0.57
2:G:1778:GLN:HB3	2:G:1831:VAL:HG13	1.86	0.57
1:C:1302:VAL:HG23	1:F:1302:VAL:HG23	1.86	0.57
1:E:161:LYS:HD2	1:E:166:ILE:HD11	1.86	0.57
2:H:1156:CYS:SG	2:H:1250:PRO:HD2	2.45	0.57
2:K:1778:GLN:HB3	2:K:1831:VAL:HG13	1.86	0.57
2:L:1156:CYS:SG	2:L:1250:PRO:HD2	2.45	0.57
1:A:1302:VAL:HG23	1:E:1302:VAL:HG23	1.86	0.57
1:B:1302:VAL:HG23	1:D:1302:VAL:HG23	1.86	0.57
1:F:161:LYS:HD2	1:F:166:ILE:HD11	1.85	0.57
2:G:1156:CYS:SG	2:G:1250:PRO:HD2	2.45	0.57
2:K:234:ILE:N	2:K:235:PRO:CD	2.68	0.57
2:G:234:ILE:N	2:G:235:PRO:CD	2.68	0.57
1:B:161:LYS:HD2	1:B:166:ILE:HD11	1.85	0.57
1:D:161:LYS:HD2	1:D:166:ILE:HD11	1.86	0.57
2:K:1156:CYS:SG	2:K:1250:PRO:HD2	2.45	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1064:ASN:ND2	1:C:1073:THR:OG1	2.37	0.56
1:D:1064:ASN:ND2	1:D:1073:THR:OG1	2.37	0.56
2:H:1778:GLN:HB3	2:H:1831:VAL:HG13	1.86	0.56
2:G:1689:ASP:O	2:G:1693:ARG:HB2	2.06	0.56
1:B:168:MET:SD	1:B:168:MET:N	2.75	0.56
1:C:161:LYS:HD2	1:C:166:ILE:HD11	1.86	0.56
1:F:1064:ASN:ND2	1:F:1073:THR:OG1	2.37	0.56
2:I:1866:PHE:CE1	2:I:1870:ALA:HB1	2.41	0.56
2:J:1156:CYS:SG	2:J:1250:PRO:HD2	2.45	0.56
2:J:1866:PHE:CE1	2:J:1870:ALA:HB1	2.41	0.56
2:L:1778:GLN:HB3	2:L:1831:VAL:HG13	1.86	0.56
1:B:1064:ASN:ND2	1:B:1073:THR:OG1	2.37	0.56
2:I:234:ILE:N	2:I:235:PRO:CD	2.68	0.56
2:I:1156:CYS:SG	2:I:1250:PRO:HD2	2.45	0.56
2:J:234:ILE:N	2:J:235:PRO:CD	2.68	0.56
2:K:1689:ASP:O	2:K:1693:ARG:HB2	2.06	0.56
1:F:168:MET:SD	1:F:168:MET:N	2.75	0.56
2:L:1451:GLN:N	2:L:1451:GLN:HE21	2.03	0.56
1:D:793:ARG:HA	1:D:797:THR:HG23	1.88	0.56
2:G:1866:PHE:CE1	2:G:1870:ALA:HB1	2.41	0.56
2:H:1451:GLN:HE21	2:H:1451:GLN:N	2.04	0.56
2:H:1689:ASP:O	2:H:1693:ARG:HB2	2.06	0.56
2:K:1866:PHE:CE1	2:K:1870:ALA:HB1	2.41	0.56
2:L:1689:ASP:O	2:L:1693:ARG:HB2	2.06	0.56
1:C:793:ARG:HA	1:C:797:THR:HG23	1.88	0.56
2:I:1689:ASP:O	2:I:1693:ARG:HB2	2.06	0.55
2:I:159:ILE:HA	2:I:271:THR:O	2.06	0.55
2:I:1451:GLN:HE21	2:I:1451:GLN:N	2.04	0.55
2:J:159:ILE:HA	2:J:271:THR:O	2.06	0.55
2:J:1451:GLN:N	2:J:1451:GLN:HE21	2.04	0.55
2:K:1451:GLN:HE21	2:K:1451:GLN:N	2.03	0.55
2:J:1689:ASP:O	2:J:1693:ARG:HB2	2.06	0.55
1:D:1362:PRO:HA	1:D:1365:MET:SD	2.47	0.55
2:G:159:ILE:HA	2:G:271:THR:O	2.06	0.55
2:G:1451:GLN:HE21	2:G:1451:GLN:N	2.03	0.55
1:C:1362:PRO:HA	1:C:1365:MET:SD	2.47	0.55
2:H:159:ILE:HA	2:H:271:THR:O	2.06	0.55
2:L:159:ILE:HA	2:L:271:THR:O	2.06	0.55
2:L:1866:PHE:CE1	2:L:1870:ALA:HB1	2.41	0.55
2:K:159:ILE:HA	2:K:271:THR:O	2.06	0.55
1:C:1402:GLY:HA2	1:C:1658:PRO:HD3	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1866:PHE:CE1	2:H:1870:ALA:HB1	2.41	0.55
2:K:52:ASP:O	2:K:63:LYS:NZ	2.40	0.55
2:G:52:ASP:O	2:G:63:LYS:NZ	2.40	0.55
1:B:1362:PRO:HA	1:B:1365:MET:SD	2.47	0.55
1:F:1362:PRO:HA	1:F:1365:MET:SD	2.47	0.55
1:D:1402:GLY:HA2	1:D:1658:PRO:HD3	1.88	0.55
2:J:52:ASP:O	2:J:63:LYS:NZ	2.40	0.55
2:I:52:ASP:O	2:I:63:LYS:NZ	2.40	0.54
2:I:1775:GLN:HG2	2:I:1836:MET:CE	2.37	0.54
1:F:793:ARG:HA	1:F:797:THR:HG23	1.88	0.54
1:F:1402:GLY:HA2	1:F:1658:PRO:HD3	1.88	0.54
1:B:793:ARG:HA	1:B:797:THR:HG23	1.88	0.54
2:J:1775:GLN:HG2	2:J:1836:MET:CE	2.37	0.54
2:G:1775:GLN:HG2	2:G:1836:MET:CE	2.37	0.54
1:E:793:ARG:HA	1:E:797:THR:HG23	1.88	0.54
2:K:1775:GLN:HG2	2:K:1836:MET:CE	2.37	0.54
1:B:1402:GLY:HA2	1:B:1658:PRO:HD3	1.88	0.54
1:E:1402:GLY:HA2	1:E:1658:PRO:HD3	1.88	0.54
1:A:1402:GLY:HA2	1:A:1658:PRO:HD3	1.88	0.54
1:A:793:ARG:HA	1:A:797:THR:HG23	1.88	0.54
1:B:1414:ILE:HG12	1:D:1293:SER:HB2	1.90	0.54
1:A:1362:PRO:HA	1:A:1365:MET:SD	2.47	0.54
2:H:52:ASP:O	2:H:63:LYS:NZ	2.40	0.54
2:L:52:ASP:O	2:L:63:LYS:NZ	2.40	0.54
1:C:1414:ILE:HG12	1:F:1293:SER:HB2	1.90	0.54
1:E:1362:PRO:HA	1:E:1365:MET:SD	2.47	0.54
1:D:966:LYS:CE	1:D:971:ASN:HD21	2.21	0.53
2:I:301:THR:HG21	2:I:448:VAL:HG21	1.90	0.53
2:J:301:THR:HG21	2:J:448:VAL:HG21	1.90	0.53
2:L:1775:GLN:HG2	2:L:1836:MET:CE	2.37	0.53
1:A:1414:ILE:HG12	1:E:1293:SER:HB2	1.90	0.53
1:B:1293:SER:HB2	1:D:1414:ILE:HG12	1.90	0.53
2:H:1775:GLN:HG2	2:H:1836:MET:CE	2.37	0.53
1:C:966:LYS:CE	1:C:971:ASN:HD21	2.22	0.53
2:H:1331:TRP:O	2:H:1332:ARG:C	2.52	0.53
2:L:1331:TRP:O	2:L:1332:ARG:C	2.52	0.53
1:F:966:LYS:CE	1:F:971:ASN:HD21	2.22	0.53
1:B:966:LYS:CE	1:B:971:ASN:HD21	2.22	0.53
1:C:1293:SER:HB2	1:F:1414:ILE:HG12	1.91	0.53
1:E:966:LYS:CE	1:E:971:ASN:HD21	2.21	0.53
1:F:1470:LEU:HD13	1:F:1489:ARG:HD2	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1293:SER:HB2	1:E:1414:ILE:HG12	1.91	0.53
2:G:1956:ARG:HB3	2:G:1957:PRO:HD3	1.91	0.53
2:L:1956:ARG:HB3	2:L:1957:PRO:HD3	1.91	0.53
1:A:966:LYS:CE	1:A:971:ASN:HD21	2.22	0.53
2:G:90:GLU:O	2:G:94:CYS:SG	2.65	0.53
1:B:1470:LEU:HD13	1:B:1489:ARG:HD2	1.91	0.53
2:I:1956:ARG:HB3	2:I:1957:PRO:HD3	1.91	0.53
1:B:986:ALA:HB2	1:B:1047:LEU:HD13	1.90	0.53
2:H:1956:ARG:HB3	2:H:1957:PRO:HD3	1.91	0.53
2:I:1330:GLY:HA2	2:I:1374:THR:HG21	1.91	0.53
2:J:1956:ARG:HB3	2:J:1957:PRO:HD3	1.91	0.53
2:G:1152:ALA:O	2:G:1156:CYS:HB2	2.09	0.52
2:H:301:THR:HG21	2:H:448:VAL:HG21	1.90	0.52
2:J:1330:GLY:HA2	2:J:1374:THR:HG21	1.91	0.52
2:K:301:THR:HG21	2:K:448:VAL:HG21	1.90	0.52
2:K:1152:ALA:O	2:K:1156:CYS:HB2	2.09	0.52
2:K:1956:ARG:HB3	2:K:1957:PRO:HD3	1.91	0.52
2:G:301:THR:HG21	2:G:448:VAL:HG21	1.90	0.52
1:F:986:ALA:HB2	1:F:1047:LEU:HD13	1.91	0.52
2:K:90:GLU:O	2:K:94:CYS:SG	2.65	0.52
2:L:301:THR:HG21	2:L:448:VAL:HG21	1.90	0.52
2:H:1152:ALA:O	2:H:1156:CYS:HB2	2.09	0.52
2:L:1152:ALA:O	2:L:1156:CYS:HB2	2.09	0.52
1:A:986:ALA:HB2	1:A:1047:LEU:HD13	1.91	0.52
1:A:1246:CYS:SG	1:A:1327:CYS:SG	3.05	0.52
1:D:1470:LEU:HD13	1:D:1489:ARG:HD2	1.91	0.52
2:J:283:ILE:O	2:J:286:THR:HG22	2.09	0.52
1:A:1657:HIS:CD2	1:A:1658:PRO:HD2	2.45	0.52
2:G:1330:GLY:HA2	2:G:1374:THR:HG21	1.91	0.52
1:C:1470:LEU:HD13	1:C:1489:ARG:HD2	1.91	0.52
1:D:1657:HIS:CD2	1:D:1658:PRO:HD2	2.45	0.52
1:E:986:ALA:HB2	1:E:1047:LEU:HD13	1.91	0.52
1:E:1246:CYS:SG	1:E:1327:CYS:SG	3.05	0.52
2:K:1330:GLY:HA2	2:K:1374:THR:HG21	1.92	0.52
1:C:986:ALA:HB2	1:C:1047:LEU:HD13	1.91	0.52
1:C:1657:HIS:CD2	1:C:1658:PRO:HD2	2.45	0.52
1:D:986:ALA:HB2	1:D:1047:LEU:HD13	1.91	0.52
1:E:1657:HIS:CD2	1:E:1658:PRO:HD2	2.45	0.52
2:I:283:ILE:O	2:I:286:THR:HG22	2.09	0.52
2:I:1152:ALA:O	2:I:1156:CYS:HB2	2.09	0.52
2:J:1152:ALA:O	2:J:1156:CYS:HB2	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:1331:TRP:O	2:J:1332:ARG:C	2.52	0.52
2:K:1331:TRP:O	2:K:1332:ARG:C	2.52	0.52
1:A:1036:ARG:NH1	1:A:1040:GLU:OE1	2.41	0.52
1:A:1470:LEU:HD13	1:A:1489:ARG:HD2	1.91	0.52
1:B:1583:HIS:CE1	1:B:1585:LYS:HA	2.45	0.52
1:C:1246:CYS:SG	1:C:1327:CYS:SG	3.05	0.52
1:D:1246:CYS:SG	1:D:1327:CYS:SG	3.05	0.52
1:E:1470:LEU:HD13	1:E:1489:ARG:HD2	1.91	0.52
1:F:1583:HIS:CE1	1:F:1585:LYS:HA	2.45	0.52
2:I:1331:TRP:O	2:I:1332:ARG:C	2.52	0.52
2:G:1331:TRP:O	2:G:1332:ARG:C	2.52	0.52
1:E:1036:ARG:NH1	1:E:1040:GLU:OE1	2.41	0.52
1:E:1583:HIS:CE1	1:E:1585:LYS:HA	2.45	0.52
2:H:283:ILE:O	2:H:286:THR:HG22	2.09	0.52
2:L:283:ILE:O	2:L:286:THR:HG22	2.09	0.52
1:B:1657:HIS:CD2	1:B:1658:PRO:HD2	2.45	0.51
1:F:1657:HIS:CD2	1:F:1658:PRO:HD2	2.45	0.51
2:I:864:LEU:HD11	2:I:868:PHE:CZ	2.45	0.51
2:J:864:LEU:HD11	2:J:868:PHE:CZ	2.46	0.51
1:A:1583:HIS:CE1	1:A:1585:LYS:HA	2.45	0.51
1:F:89:TYR:OH	2:L:1791:ASP:OD2	2.17	0.51
2:K:190:PHE:O	2:K:194:THR:OG1	2.28	0.51
1:B:89:TYR:OH	2:H:1791:ASP:OD2	2.18	0.51
2:H:864:LEU:HD11	2:H:868:PHE:CZ	2.46	0.51
2:H:1804:PHE:CZ	2:H:2010:TYR:HB2	2.46	0.51
2:L:864:LEU:HD11	2:L:868:PHE:CZ	2.46	0.51
1:A:1430:ARG:HG2	1:A:1430:ARG:O	2.11	0.51
2:G:190:PHE:O	2:G:194:THR:OG1	2.28	0.51
1:E:1430:ARG:O	1:E:1430:ARG:HG2	2.11	0.51
2:I:90:GLU:O	2:I:94:CYS:SG	2.65	0.51
2:L:1838:MET:HE3	2:L:1976:PHE:CD1	2.45	0.51
2:G:1804:PHE:CZ	2:G:2010:TYR:HB2	2.46	0.51
2:G:1838:MET:HE3	2:G:1976:PHE:CD1	2.46	0.51
2:H:1330:GLY:HA2	2:H:1374:THR:HG21	1.91	0.51
2:H:1838:MET:HE3	2:H:1976:PHE:CD1	2.45	0.51
2:I:1804:PHE:CZ	2:I:2010:TYR:HB2	2.46	0.51
2:J:1804:PHE:CZ	2:J:2010:TYR:HB2	2.46	0.51
2:K:1804:PHE:CZ	2:K:2010:TYR:HB2	2.46	0.51
2:L:1804:PHE:CZ	2:L:2010:TYR:HB2	2.46	0.51
2:G:283:ILE:O	2:G:286:THR:HG22	2.09	0.51
2:J:146:PHE:HA	2:J:149:VAL:HG12	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:283:ILE:O	2:K:286:THR:HG22	2.09	0.51
1:D:1583:HIS:CE1	1:D:1585:LYS:HA	2.44	0.51
2:I:146:PHE:HA	2:I:149:VAL:HG12	1.93	0.51
2:I:1838:MET:HE3	2:I:1976:PHE:CD1	2.46	0.51
2:K:1838:MET:HE3	2:K:1976:PHE:CD1	2.46	0.51
1:B:1030:TRP:O	1:B:1035:THR:OG1	2.27	0.51
1:B:1248:GLY:O	1:B:1331:GLY:HA2	2.11	0.51
1:F:1030:TRP:O	1:F:1035:THR:OG1	2.27	0.51
2:H:190:PHE:O	2:H:194:THR:OG1	2.28	0.51
2:J:90:GLU:O	2:J:94:CYS:SG	2.65	0.51
2:J:1838:MET:HE3	2:J:1976:PHE:CD1	2.45	0.51
2:L:1330:GLY:HA2	2:L:1374:THR:HG21	1.91	0.51
2:L:1665:VAL:HA	2:L:1805:ALA:O	2.11	0.51
1:A:1248:GLY:O	1:A:1331:GLY:HA2	2.11	0.51
2:G:864:LEU:HD11	2:G:868:PHE:CZ	2.46	0.51
1:F:1248:GLY:O	1:F:1331:GLY:HA2	2.11	0.51
2:H:1665:VAL:HA	2:H:1805:ALA:O	2.11	0.51
2:I:1665:VAL:HA	2:I:1805:ALA:O	2.11	0.51
2:J:1665:VAL:HA	2:J:1805:ALA:O	2.11	0.51
2:K:864:LEU:HD11	2:K:868:PHE:CZ	2.46	0.51
1:E:1248:GLY:O	1:E:1331:GLY:HA2	2.11	0.51
2:L:190:PHE:O	2:L:194:THR:OG1	2.28	0.51
2:H:1343:VAL:HG22	2:H:1343:VAL:O	2.11	0.50
2:J:1343:VAL:O	2:J:1343:VAL:HG22	2.11	0.50
2:G:9:LEU:HD21	2:G:34:GLN:HB2	1.93	0.50
1:C:1583:HIS:CE1	1:C:1585:LYS:HA	2.45	0.50
1:D:1248:GLY:O	1:D:1331:GLY:HA2	2.11	0.50
1:F:1036:ARG:NH1	1:F:1040:GLU:OE1	2.40	0.50
2:I:1343:VAL:HG22	2:I:1343:VAL:O	2.11	0.50
2:L:1343:VAL:O	2:L:1343:VAL:HG22	2.11	0.50
2:H:106:ALA:HB2	2:H:545:GLN:HG2	1.94	0.50
2:K:9:LEU:HD21	2:K:34:GLN:HB2	1.94	0.50
2:L:106:ALA:HB2	2:L:545:GLN:HG2	1.94	0.50
2:G:1737:ILE:HD12	2:G:1739:GLU:HG2	1.94	0.50
1:C:89:TYR:OH	2:I:1791:ASP:OD2	2.18	0.50
1:C:1248:GLY:O	1:C:1331:GLY:HA2	2.11	0.50
1:D:1430:ARG:O	1:D:1430:ARG:HG2	2.11	0.50
2:K:1343:VAL:HG22	2:K:1343:VAL:O	2.11	0.50
1:B:1036:ARG:NH1	1:B:1040:GLU:OE1	2.41	0.50
1:C:1430:ARG:O	1:C:1430:ARG:HG2	2.11	0.50
1:D:89:TYR:OH	2:J:1791:ASP:OD2	2.18	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1430:ARG:HG2	1:F:1430:ARG:O	2.11	0.50
2:K:1737:ILE:HD12	2:K:1739:GLU:HG2	1.94	0.50
2:L:9:LEU:HD21	2:L:34:GLN:HB2	1.94	0.50
2:G:1343:VAL:O	2:G:1343:VAL:HG22	2.11	0.50
2:G:1665:VAL:HA	2:G:1805:ALA:O	2.11	0.50
1:B:525:TYR:O	1:B:529:MET:HG2	2.12	0.50
1:B:1430:ARG:O	1:B:1430:ARG:HG2	2.11	0.50
2:H:9:LEU:HD21	2:H:34:GLN:HB2	1.94	0.50
2:G:146:PHE:HA	2:G:149:VAL:HG12	1.93	0.50
2:K:1665:VAL:HA	2:K:1805:ALA:O	2.11	0.50
2:L:1737:ILE:HD12	2:L:1739:GLU:HG2	1.94	0.50
1:A:525:TYR:O	1:A:529:MET:HG2	2.12	0.50
2:G:1738:PHE:CD1	2:G:1837:THR:HG23	2.47	0.50
1:F:525:TYR:O	1:F:529:MET:HG2	2.12	0.50
2:I:1355:ASN:ND2	2:I:1408:SER:OG	2.45	0.50
2:J:1355:ASN:ND2	2:J:1408:SER:OG	2.45	0.50
2:K:1738:PHE:CD1	2:K:1837:THR:HG23	2.47	0.50
1:C:764:ASP:OD1	1:C:810:LYS:NZ	2.45	0.49
1:D:764:ASP:OD1	1:D:810:LYS:NZ	2.45	0.49
1:E:525:TYR:O	1:E:529:MET:HG2	2.12	0.49
2:H:1737:ILE:HD12	2:H:1739:GLU:HG2	1.94	0.49
2:K:146:PHE:HA	2:K:149:VAL:HG12	1.93	0.49
2:G:106:ALA:HB2	2:G:545:GLN:HG2	1.94	0.49
1:D:198:PRO:HG3	1:D:212:THR:HG21	1.94	0.49
2:H:146:PHE:HA	2:H:149:VAL:HG12	1.93	0.49
2:H:297:ARG:O	2:H:301:THR:HG22	2.13	0.49
2:J:9:LEU:HD21	2:J:34:GLN:HB2	1.94	0.49
2:K:297:ARG:O	2:K:301:THR:HG22	2.13	0.49
2:L:146:PHE:HA	2:L:149:VAL:HG12	1.93	0.49
2:L:297:ARG:O	2:L:301:THR:HG22	2.12	0.49
1:A:764:ASP:OD1	1:A:810:LYS:NZ	2.45	0.49
2:G:297:ARG:O	2:G:301:THR:HG22	2.13	0.49
2:H:1738:PHE:CD1	2:H:1837:THR:HG23	2.47	0.49
2:I:1737:ILE:HD12	2:I:1739:GLU:HG2	1.94	0.49
2:J:1737:ILE:HD12	2:J:1739:GLU:HG2	1.94	0.49
2:K:106:ALA:HB2	2:K:545:GLN:HG2	1.94	0.49
1:C:198:PRO:HG3	1:C:212:THR:HG21	1.95	0.49
2:I:9:LEU:HD21	2:I:34:GLN:HB2	1.94	0.49
1:B:1064:ASN:HD22	1:B:1073:THR:HG1	1.60	0.49
1:E:764:ASP:OD1	1:E:810:LYS:NZ	2.45	0.49
2:L:1738:PHE:CD1	2:L:1837:THR:HG23	2.47	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:764:ASP:OD1	1:F:810:LYS:NZ	2.45	0.49
2:H:1355:ASN:ND2	2:H:1408:SER:OG	2.45	0.49
2:L:1355:ASN:ND2	2:L:1408:SER:OG	2.45	0.49
1:B:764:ASP:OD1	1:B:810:LYS:NZ	2.45	0.49
2:K:1355:ASN:ND2	2:K:1408:SER:OG	2.45	0.49
2:G:1355:ASN:ND2	2:G:1408:SER:OG	2.45	0.49
2:I:106:ALA:HB2	2:I:545:GLN:HG2	1.94	0.49
2:J:106:ALA:HB2	2:J:545:GLN:HG2	1.94	0.49
1:D:983:GLN:HE22	2:J:962:LYS:HD2	1.78	0.49
2:I:997:ALA:HA	2:I:1000:ILE:HD12	1.95	0.49
2:G:1739:GLU:HB2	2:G:1987:PRO:HB3	1.95	0.49
2:H:778:TYR:HB3	2:H:779:PRO:HD3	1.95	0.49
2:K:1180:MET:HE3	2:K:1197:LEU:HD11	1.95	0.49
2:K:1739:GLU:HB2	2:K:1987:PRO:HB3	1.95	0.49
2:L:778:TYR:HB3	2:L:779:PRO:HD3	1.95	0.49
2:G:1180:MET:HE3	2:G:1197:LEU:HD11	1.95	0.48
2:J:372:ASN:HB3	2:J:515:LEU:HD21	1.95	0.48
2:H:1775:GLN:CG	2:H:1836:MET:HE2	2.43	0.48
2:I:372:ASN:HB3	2:I:515:LEU:HD21	1.95	0.48
2:J:997:ALA:HA	2:J:1000:ILE:HD12	1.95	0.48
2:L:1775:GLN:CG	2:L:1836:MET:HE2	2.43	0.48
1:A:89:TYR:OH	2:G:1791:ASP:OD2	2.18	0.48
1:F:1064:ASN:HD22	1:F:1073:THR:HG1	1.60	0.48
2:J:778:TYR:HB3	2:J:779:PRO:HD3	1.95	0.48
2:J:1738:PHE:CD1	2:J:1837:THR:HG23	2.47	0.48
2:I:297:ARG:O	2:I:301:THR:HG22	2.12	0.48
2:I:778:TYR:HB3	2:I:779:PRO:HD3	1.95	0.48
2:I:1738:PHE:CD1	2:I:1837:THR:HG23	2.47	0.48
1:C:472:LEU:HD13	1:C:472:LEU:C	2.39	0.48
1:D:472:LEU:C	1:D:472:LEU:HD13	2.39	0.48
2:J:297:ARG:O	2:J:301:THR:HG22	2.13	0.48
2:L:597:MET:HA	4:L:2101:FMN:N5	2.28	0.48
1:F:198:PRO:HG3	1:F:212:THR:HG21	1.95	0.48
2:I:190:PHE:O	2:I:194:THR:OG1	2.28	0.48
2:J:190:PHE:O	2:J:194:THR:OG1	2.28	0.48
1:C:525:TYR:O	1:C:529:MET:HG2	2.12	0.48
1:C:983:GLN:HE22	2:I:962:LYS:HD2	1.78	0.48
1:E:198:PRO:HG3	1:E:212:THR:HG21	1.95	0.48
2:I:1775:GLN:CG	2:I:1836:MET:HE2	2.43	0.48
2:J:1775:GLN:CG	2:J:1836:MET:HE2	2.43	0.48
2:L:1180:MET:HE3	2:L:1197:LEU:HD11	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:PRO:HG3	1:A:212:THR:HG21	1.95	0.48
1:A:472:LEU:HD13	1:A:472:LEU:C	2.39	0.48
1:B:198:PRO:HG3	1:B:212:THR:HG21	1.95	0.48
1:C:381:GLU:HG3	1:D:390:VAL:HG13	1.96	0.48
1:D:525:TYR:O	1:D:529:MET:HG2	2.12	0.48
1:E:472:LEU:C	1:E:472:LEU:HD13	2.39	0.48
2:H:90:GLU:O	2:H:94:CYS:SG	2.65	0.48
2:H:1180:MET:HE3	2:H:1197:LEU:HD11	1.95	0.48
2:I:1739:GLU:HB2	2:I:1987:PRO:HB3	1.95	0.48
2:H:597:MET:HA	4:H:2101:FMN:N5	2.28	0.48
2:J:1739:GLU:HB2	2:J:1987:PRO:HB3	1.95	0.48
1:D:1036:ARG:NH1	1:D:1040:GLU:OE1	2.41	0.48
2:I:1180:MET:HE3	2:I:1197:LEU:HD11	1.95	0.48
2:J:1180:MET:HE3	2:J:1197:LEU:HD11	1.95	0.48
2:L:90:GLU:O	2:L:94:CYS:SG	2.65	0.48
2:G:997:ALA:HA	2:G:1000:ILE:HD12	1.95	0.47
1:B:1486:LEU:HG	1:B:1756:ILE:HD11	1.96	0.47
1:E:983:GLN:HE22	2:K:962:LYS:HD2	1.79	0.47
1:F:400:ARG:NH1	1:F:715:THR:HG21	2.29	0.47
2:H:997:ALA:HA	2:H:1000:ILE:HD12	1.95	0.47
2:H:1443:VAL:O	2:H:1446:SER:HB3	2.14	0.47
2:I:234:ILE:HG21	2:I:425:SER:HB3	1.96	0.47
2:J:234:ILE:HG21	2:J:425:SER:HB3	1.96	0.47
2:K:1775:GLN:CG	2:K:1836:MET:HE2	2.43	0.47
2:L:997:ALA:HA	2:L:1000:ILE:HD12	1.95	0.47
1:A:983:GLN:HE22	2:G:962:LYS:HD2	1.79	0.47
1:C:44:VAL:CG1	1:C:78:ILE:HG13	2.45	0.47
1:C:390:VAL:HG13	1:D:381:GLU:HG3	1.96	0.47
1:C:1036:ARG:NH1	1:C:1040:GLU:OE1	2.41	0.47
1:D:1119:LYS:HE2	1:D:1341:PHE:CD1	2.49	0.47
1:F:1352:THR:HG23	1:F:1365:MET:HE1	1.96	0.47
2:I:1443:VAL:O	2:I:1446:SER:HB3	2.14	0.47
2:J:1443:VAL:O	2:J:1446:SER:HB3	2.14	0.47
2:K:997:ALA:HA	2:K:1000:ILE:HD12	1.95	0.47
2:G:372:ASN:HB3	2:G:515:LEU:HD21	1.95	0.47
2:G:1775:GLN:CG	2:G:1836:MET:HE2	2.43	0.47
1:B:400:ARG:NH1	1:B:715:THR:HG21	2.29	0.47
1:B:1352:THR:HG23	1:B:1365:MET:HE1	1.96	0.47
1:D:44:VAL:CG1	1:D:78:ILE:HG13	2.45	0.47
1:F:472:LEU:HD13	1:F:472:LEU:C	2.39	0.47
2:H:848:SER:HB3	2:H:854:ILE:HD11	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:372:ASN:HB3	2:K:515:LEU:HD21	1.95	0.47
2:K:1443:VAL:O	2:K:1446:SER:HB3	2.14	0.47
2:L:848:SER:HB3	2:L:854:ILE:HD11	1.96	0.47
2:L:1443:VAL:O	2:L:1446:SER:HB3	2.14	0.47
1:A:1239:HIS:CE1	1:A:1717:ASP:O	2.68	0.47
2:G:1443:VAL:O	2:G:1446:SER:HB3	2.14	0.47
1:B:472:LEU:C	1:B:472:LEU:HD13	2.39	0.47
1:D:1352:THR:HG23	1:D:1365:MET:HE1	1.96	0.47
1:F:1486:LEU:HG	1:F:1756:ILE:HD11	1.96	0.47
2:J:848:SER:HB3	2:J:854:ILE:HD11	1.96	0.47
2:K:778:TYR:HB3	2:K:779:PRO:HD3	1.95	0.47
2:L:1739:GLU:HB2	2:L:1987:PRO:HB3	1.95	0.47
1:B:390:VAL:HG13	1:E:381:GLU:HG3	1.95	0.47
1:B:1119:LYS:HE2	1:B:1341:PHE:CD1	2.49	0.47
1:B:1239:HIS:CE1	1:B:1717:ASP:O	2.68	0.47
1:C:1119:LYS:HE2	1:C:1341:PHE:CD1	2.49	0.47
1:C:1352:THR:HG23	1:C:1365:MET:HE1	1.96	0.47
1:E:1239:HIS:CE1	1:E:1717:ASP:O	2.68	0.47
1:F:983:GLN:HE22	2:L:962:LYS:HD2	1.79	0.47
1:F:1239:HIS:CE1	1:F:1717:ASP:O	2.68	0.47
2:I:848:SER:HB3	2:I:854:ILE:HD11	1.96	0.47
2:K:848:SER:HB3	2:K:854:ILE:HD11	1.97	0.47
2:G:778:TYR:HB3	2:G:779:PRO:HD3	1.95	0.47
2:G:848:SER:HB3	2:G:854:ILE:HD11	1.97	0.47
2:G:1426:THR:HG23	2:G:1470:THR:HG23	1.97	0.47
1:B:44:VAL:CG1	1:B:78:ILE:HG13	2.45	0.47
1:E:655:LEU:HD22	1:E:916:LEU:HD11	1.97	0.47
1:F:44:VAL:CG1	1:F:78:ILE:HG13	2.45	0.47
1:F:1119:LYS:HE2	1:F:1341:PHE:CD1	2.49	0.47
2:H:1739:GLU:HB2	2:H:1987:PRO:HB3	1.95	0.47
2:K:1426:THR:HG23	2:K:1470:THR:HG23	1.97	0.47
1:A:390:VAL:HG13	1:F:381:GLU:HG3	1.96	0.47
1:A:400:ARG:NH1	1:A:715:THR:HG21	2.29	0.47
1:A:655:LEU:HD22	1:A:916:LEU:HD11	1.97	0.47
1:B:381:GLU:HG3	1:E:390:VAL:HG13	1.96	0.47
1:C:1486:LEU:HG	1:C:1756:ILE:HD11	1.96	0.47
1:D:983:GLN:HE22	2:J:962:LYS:CD	2.27	0.47
1:E:1119:LYS:HE2	1:E:1341:PHE:CD1	2.49	0.47
2:H:372:ASN:HB3	2:H:515:LEU:HD21	1.95	0.47
2:I:597:MET:HA	4:I:2101:FMN:N5	2.30	0.47
2:J:597:MET:HA	4:J:2101:FMN:N5	2.30	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:372:ASN:HB3	2:L:515:LEU:HD21	1.95	0.47
1:A:1119:LYS:HE2	1:A:1341:PHE:CD1	2.49	0.47
2:G:805:VAL:HG22	2:G:1070:ILE:HD13	1.97	0.47
1:D:1486:LEU:HG	1:D:1756:ILE:HD11	1.96	0.47
1:E:1486:LEU:HG	1:E:1756:ILE:HD11	1.96	0.47
2:I:1426:THR:HG23	2:I:1470:THR:HG23	1.97	0.47
2:K:805:VAL:HG22	2:K:1070:ILE:HD13	1.97	0.47
1:A:864:VAL:HG22	1:A:921:PRO:HB3	1.97	0.47
2:G:597:MET:HA	4:G:2101:FMN:N5	2.29	0.47
1:C:1427:THR:O	1:C:1430:ARG:HD2	2.15	0.47
1:E:44:VAL:CG1	1:E:78:ILE:HG13	2.45	0.47
1:E:400:ARG:NH1	1:E:715:THR:HG21	2.29	0.47
1:E:864:VAL:HG22	1:E:921:PRO:HB3	1.97	0.47
2:H:1854:MET:HA	2:H:1907:LEU:HD21	1.97	0.47
2:J:1426:THR:HG23	2:J:1470:THR:HG23	1.97	0.47
1:A:381:GLU:HG3	1:F:390:VAL:HG13	1.96	0.47
1:A:1352:THR:HG23	1:A:1365:MET:HE1	1.96	0.47
1:A:1486:LEU:HG	1:A:1756:ILE:HD11	1.96	0.47
1:B:1427:THR:O	1:B:1430:ARG:HD2	2.15	0.47
1:C:1239:HIS:CE1	1:C:1717:ASP:O	2.68	0.47
1:E:338:LEU:HD11	1:E:342:GLN:HE21	1.80	0.47
1:E:1352:THR:HG23	1:E:1365:MET:HE1	1.96	0.47
2:L:1854:MET:HA	2:L:1907:LEU:HD21	1.97	0.47
1:A:338:LEU:HD11	1:A:342:GLN:HE21	1.80	0.46
1:B:983:GLN:HE22	2:H:962:LYS:HD2	1.79	0.46
1:C:1418:VAL:N	1:C:1419:PRO:CD	2.78	0.46
1:D:1239:HIS:CE1	1:D:1717:ASP:O	2.68	0.46
1:D:1427:THR:O	1:D:1430:ARG:HD2	2.15	0.46
1:E:1427:THR:O	1:E:1430:ARG:HD2	2.15	0.46
1:F:1427:THR:O	1:F:1430:ARG:HD2	2.15	0.46
2:H:1663:THR:HA	2:H:1803:THR:O	2.16	0.46
2:K:597:MET:HA	4:K:2101:FMN:N5	2.29	0.46
2:L:1663:THR:HA	2:L:1803:THR:O	2.16	0.46
1:A:44:VAL:CG1	1:A:78:ILE:HG13	2.45	0.46
1:A:538:GLU:OE2	1:A:633:GLU:HA	2.16	0.46
2:G:234:ILE:HG21	2:G:425:SER:HB3	1.96	0.46
1:C:655:LEU:HD22	1:C:916:LEU:HD11	1.97	0.46
1:D:1418:VAL:N	1:D:1419:PRO:CD	2.78	0.46
1:E:538:GLU:OE2	1:E:633:GLU:HA	2.16	0.46
1:F:983:GLN:HE22	2:L:962:LYS:CD	2.28	0.46
2:J:1745:LYS:HA	2:J:1745:LYS:HE2	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1427:THR:O	1:A:1430:ARG:HD2	2.15	0.46
1:C:538:GLU:OE2	1:C:633:GLU:HA	2.16	0.46
1:C:983:GLN:HE22	2:I:962:LYS:CD	2.28	0.46
1:D:538:GLU:OE2	1:D:633:GLU:HA	2.16	0.46
1:D:655:LEU:HD22	1:D:916:LEU:HD11	1.97	0.46
2:H:233:SER:C	2:H:235:PRO:HD2	2.41	0.46
2:H:1745:LYS:HA	2:H:1745:LYS:HE2	1.97	0.46
2:I:233:SER:C	2:I:235:PRO:HD2	2.41	0.46
2:J:233:SER:C	2:J:235:PRO:HD2	2.41	0.46
2:L:234:ILE:HG21	2:L:425:SER:HB3	1.96	0.46
2:G:1854:MET:HA	2:G:1907:LEU:HD21	1.97	0.46
1:C:966:LYS:HE3	1:C:971:ASN:HD21	1.81	0.46
1:E:529:MET:HE3	1:E:637:PHE:HB2	1.97	0.46
1:F:733:ILE:HD13	1:F:763:TRP:CH2	2.50	0.46
1:F:1418:VAL:N	1:F:1419:PRO:CD	2.78	0.46
2:H:234:ILE:HG21	2:H:425:SER:HB3	1.96	0.46
2:I:1663:THR:HA	2:I:1803:THR:O	2.16	0.46
2:I:1745:LYS:HA	2:I:1745:LYS:HE2	1.98	0.46
2:J:1663:THR:HA	2:J:1803:THR:O	2.16	0.46
2:L:233:SER:C	2:L:235:PRO:HD2	2.41	0.46
1:A:529:MET:HE3	1:A:637:PHE:HB2	1.97	0.46
1:B:733:ILE:HD13	1:B:763:TRP:CH2	2.50	0.46
1:C:338:LEU:HD11	1:C:342:GLN:HE21	1.80	0.46
1:C:400:ARG:NH1	1:C:715:THR:HG21	2.29	0.46
1:D:400:ARG:NH1	1:D:715:THR:HG21	2.29	0.46
2:H:1426:THR:HG23	2:H:1470:THR:HG23	1.97	0.46
2:K:234:ILE:HG21	2:K:425:SER:HB3	1.96	0.46
1:A:733:ILE:HD13	1:A:763:TRP:CH2	2.50	0.46
1:A:1152:VAL:HG23	1:A:1167:LEU:HD12	1.98	0.46
1:A:1418:VAL:N	1:A:1419:PRO:CD	2.78	0.46
2:G:754:TYR:CD1	2:G:794:MET:HG2	2.51	0.46
1:B:1418:VAL:N	1:B:1419:PRO:CD	2.78	0.46
1:C:1030:TRP:O	1:C:1035:THR:OG1	2.27	0.46
1:C:1152:VAL:HG23	1:C:1167:LEU:HD12	1.98	0.46
1:D:864:VAL:HG22	1:D:921:PRO:HB3	1.97	0.46
1:D:1030:TRP:O	1:D:1035:THR:OG1	2.27	0.46
1:F:538:GLU:OE2	1:F:633:GLU:HA	2.15	0.46
2:J:1854:MET:HA	2:J:1907:LEU:HD21	1.97	0.46
2:K:1854:MET:HA	2:K:1907:LEU:HD21	1.97	0.46
2:L:754:TYR:CD1	2:L:794:MET:HG2	2.51	0.46
2:L:1426:THR:HG23	2:L:1470:THR:HG23	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:29:ILE:O	2:G:32:GLN:HB3	2.16	0.46
2:G:1081:HIS:O	2:G:1085:LEU:HB2	2.16	0.46
1:B:1152:VAL:HG23	1:B:1167:LEU:HD12	1.98	0.46
1:E:733:ILE:HD13	1:E:763:TRP:CH2	2.51	0.46
1:E:1152:VAL:HG23	1:E:1167:LEU:HD12	1.98	0.46
1:E:1418:VAL:N	1:E:1419:PRO:CD	2.78	0.46
1:F:1625:LEU:HD23	1:F:1626:TYR:N	2.31	0.46
2:H:754:TYR:CD1	2:H:794:MET:HG2	2.51	0.46
2:K:29:ILE:O	2:K:32:GLN:HB3	2.16	0.46
2:K:754:TYR:CD1	2:K:794:MET:HG2	2.51	0.46
2:K:1081:HIS:O	2:K:1085:LEU:HB2	2.16	0.46
2:L:29:ILE:O	2:L:32:GLN:HB3	2.16	0.46
2:L:1745:LYS:HA	2:L:1745:LYS:HE2	1.98	0.46
1:C:864:VAL:HG22	1:C:921:PRO:HB3	1.97	0.46
2:H:29:ILE:O	2:H:32:GLN:HB3	2.16	0.46
2:I:1339:PHE:N	2:I:1340:PRO:CD	2.79	0.46
2:I:1854:MET:HA	2:I:1907:LEU:HD21	1.97	0.46
2:L:1081:HIS:O	2:L:1085:LEU:HB2	2.16	0.46
2:G:233:SER:C	2:G:235:PRO:HD2	2.41	0.46
2:G:1339:PHE:N	2:G:1340:PRO:CD	2.79	0.46
1:B:1448:ARG:HD2	1:B:1508:TRP:O	2.16	0.46
1:B:1625:LEU:HD23	1:B:1626:TYR:N	2.31	0.46
1:C:1448:ARG:HD2	1:C:1508:TRP:O	2.16	0.46
1:D:338:LEU:HD11	1:D:342:GLN:HE21	1.80	0.46
1:D:1152:VAL:HG23	1:D:1167:LEU:HD12	1.98	0.46
1:F:655:LEU:HD22	1:F:916:LEU:HD11	1.98	0.46
1:F:1152:VAL:HG23	1:F:1167:LEU:HD12	1.98	0.46
2:H:1081:HIS:O	2:H:1085:LEU:HB2	2.16	0.46
2:I:805:VAL:HG22	2:I:1070:ILE:HD13	1.97	0.46
2:J:1339:PHE:N	2:J:1340:PRO:CD	2.79	0.46
2:K:1339:PHE:N	2:K:1340:PRO:CD	2.79	0.46
1:B:338:LEU:HD11	1:B:342:GLN:HE21	1.81	0.46
1:B:538:GLU:OE2	1:B:633:GLU:HA	2.16	0.46
1:F:865:CYS:HB2	1:F:917:CYS:SG	2.56	0.46
1:F:1448:ARG:HD2	1:F:1508:TRP:O	2.16	0.46
2:I:29:ILE:O	2:I:32:GLN:HB3	2.16	0.46
2:J:805:VAL:HG22	2:J:1070:ILE:HD13	1.97	0.46
2:K:233:SER:C	2:K:235:PRO:HD2	2.41	0.46
2:K:1663:THR:HA	2:K:1803:THR:O	2.16	0.46
1:B:865:CYS:HB2	1:B:917:CYS:SG	2.56	0.45
1:B:983:GLN:HE22	2:H:962:LYS:CD	2.29	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1302:VAL:CG2	1:D:1302:VAL:CG2	2.94	0.45
1:C:1625:LEU:HD23	1:C:1626:TYR:N	2.31	0.45
1:F:338:LEU:HD11	1:F:342:GLN:HE21	1.81	0.45
2:J:29:ILE:O	2:J:32:GLN:HB3	2.16	0.45
2:G:1663:THR:HA	2:G:1803:THR:O	2.16	0.45
1:B:1246:CYS:SG	1:B:1327:CYS:SG	3.05	0.45
1:C:1302:VAL:CG2	1:F:1302:VAL:CG2	2.94	0.45
1:D:865:CYS:HB2	1:D:917:CYS:SG	2.56	0.45
1:D:966:LYS:HE3	1:D:971:ASN:HD21	1.82	0.45
1:D:1448:ARG:HD2	1:D:1508:TRP:O	2.16	0.45
1:F:966:LYS:HE2	1:F:971:ASN:HD21	1.81	0.45
1:A:529:MET:HE3	1:A:637:PHE:CB	2.46	0.45
1:A:1302:VAL:CG2	1:E:1302:VAL:CG2	2.94	0.45
2:G:1745:LYS:HA	2:G:1745:LYS:HE2	1.98	0.45
1:B:864:VAL:HG22	1:B:921:PRO:HB3	1.97	0.45
1:C:865:CYS:HB2	1:C:917:CYS:SG	2.56	0.45
1:C:1307:THR:HG22	1:C:1586:GLY:HA2	1.99	0.45
1:D:684:GLY:O	1:D:687:SER:OG	2.31	0.45
1:D:966:LYS:HE2	1:D:971:ASN:HD21	1.81	0.45
1:D:1625:LEU:HD23	1:D:1626:TYR:N	2.31	0.45
1:E:865:CYS:HB2	1:E:917:CYS:SG	2.56	0.45
1:E:966:LYS:HE2	1:E:971:ASN:HD21	1.81	0.45
1:F:1246:CYS:SG	1:F:1327:CYS:SG	3.05	0.45
2:K:1745:LYS:HA	2:K:1745:LYS:HE2	1.97	0.45
2:L:1339:PHE:N	2:L:1340:PRO:CD	2.79	0.45
1:B:966:LYS:HE3	1:B:971:ASN:HD21	1.81	0.45
1:C:684:GLY:O	1:C:687:SER:OG	2.32	0.45
2:H:805:VAL:HG22	2:H:1070:ILE:HD13	1.97	0.45
2:I:184:VAL:HG12	2:I:188:ILE:HG12	1.99	0.45
2:K:184:VAL:HG12	2:K:188:ILE:HG12	1.99	0.45
1:A:865:CYS:HB2	1:A:917:CYS:SG	2.56	0.45
1:B:529:MET:HE3	1:B:637:PHE:CB	2.46	0.45
1:B:655:LEU:HD22	1:B:916:LEU:HD11	1.99	0.45
1:B:966:LYS:HE2	1:B:971:ASN:HD21	1.82	0.45
1:D:982:ILE:HD13	2:J:955:GLU:HB2	1.99	0.45
1:D:1307:THR:HG22	1:D:1586:GLY:HA2	1.99	0.45
1:E:1673:TYR:CZ	1:E:1677:VAL:HG21	2.52	0.45
1:F:529:MET:HE3	1:F:637:PHE:CB	2.46	0.45
1:F:864:VAL:HG22	1:F:921:PRO:HB3	1.97	0.45
2:H:1339:PHE:N	2:H:1340:PRO:CD	2.79	0.45
2:J:184:VAL:HG12	2:J:188:ILE:HG12	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:805:VAL:HG22	2:L:1070:ILE:HD13	1.97	0.45
2:G:194:THR:O	2:G:198:LEU:HD23	2.17	0.45
1:D:529:MET:HE3	1:D:637:PHE:HB2	1.97	0.45
1:E:529:MET:HE3	1:E:637:PHE:CB	2.46	0.45
1:E:966:LYS:HE3	1:E:971:ASN:HD21	1.81	0.45
1:E:1448:ARG:HD2	1:E:1508:TRP:O	2.16	0.45
1:E:1625:LEU:HD23	1:E:1626:TYR:N	2.31	0.45
1:F:684:GLY:O	1:F:687:SER:OG	2.31	0.45
2:I:754:TYR:CD1	2:I:794:MET:HG2	2.51	0.45
2:K:194:THR:O	2:K:198:LEU:HD23	2.17	0.45
1:A:966:LYS:HE2	1:A:971:ASN:HD21	1.82	0.45
1:A:1448:ARG:HD2	1:A:1508:TRP:O	2.16	0.45
2:G:184:VAL:HG12	2:G:188:ILE:HG12	1.99	0.45
1:B:529:MET:HE3	1:B:637:PHE:HB2	1.97	0.45
1:C:529:MET:HE3	1:C:637:PHE:HB2	1.97	0.45
1:D:733:ILE:HD13	1:D:763:TRP:CH2	2.50	0.45
1:F:966:LYS:HE3	1:F:971:ASN:HD21	1.81	0.45
1:A:966:LYS:HE3	1:A:971:ASN:HD21	1.81	0.45
1:A:1625:LEU:HD23	1:A:1626:TYR:N	2.31	0.45
1:A:1673:TYR:CZ	1:A:1677:VAL:HG21	2.52	0.45
1:B:1307:THR:HG22	1:B:1586:GLY:HA2	1.99	0.45
1:C:733:ILE:HD13	1:C:763:TRP:CH2	2.50	0.45
1:D:529:MET:HE3	1:D:637:PHE:CB	2.46	0.45
2:L:194:THR:O	2:L:198:LEU:HD23	2.17	0.45
2:G:96:LEU:HD11	2:G:101:ILE:HA	1.99	0.45
1:C:901:MET:CE	1:C:926:LEU:HB3	2.45	0.45
1:C:982:ILE:HD13	2:I:955:GLU:HB2	1.99	0.45
1:E:1307:THR:HG22	1:E:1586:GLY:HA2	1.99	0.45
1:F:529:MET:HE3	1:F:637:PHE:HB2	1.98	0.45
1:F:1307:THR:HG22	1:F:1586:GLY:HA2	1.99	0.45
1:F:1370:THR:HG22	1:F:1372:THR:H	1.82	0.45
2:H:194:THR:O	2:H:198:LEU:HD23	2.17	0.45
2:J:754:TYR:CD1	2:J:794:MET:HG2	2.51	0.45
2:K:96:LEU:HD11	2:K:101:ILE:HA	1.99	0.45
1:A:1307:THR:HG22	1:A:1586:GLY:HA2	1.99	0.45
1:B:901:MET:CE	1:B:926:LEU:HB3	2.45	0.45
1:B:1370:THR:HG22	1:B:1372:THR:H	1.82	0.45
1:C:529:MET:HE3	1:C:637:PHE:CB	2.46	0.45
1:C:966:LYS:HE2	1:C:971:ASN:HD21	1.82	0.45
1:D:901:MET:CE	1:D:926:LEU:HB3	2.45	0.45
1:F:901:MET:CE	1:F:926:LEU:HB3	2.45	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:430:HIS:CE1	2:H:431:LEU:HD13	2.52	0.45
2:I:1313:SER:HB2	2:I:1319:MET:HE3	1.99	0.45
2:I:1775:GLN:HG2	2:I:1836:MET:SD	2.58	0.45
2:I:1981:LEU:HD23	2:I:1981:LEU:H	1.82	0.45
2:J:1313:SER:HB2	2:J:1319:MET:HE3	1.99	0.45
2:K:1313:SER:HB2	2:K:1319:MET:HE3	1.99	0.45
1:A:176:VAL:HG11	1:A:179:LYS:O	2.17	0.44
2:G:1313:SER:HB2	2:G:1319:MET:HE3	1.99	0.44
2:G:1981:LEU:HD23	2:G:1981:LEU:H	1.82	0.44
1:B:1561:MET:O	1:B:1566:ARG:HB2	2.17	0.44
1:D:1561:MET:O	1:D:1566:ARG:HB2	2.17	0.44
1:D:1694:TYR:OH	2:J:1001:ASP:OD2	2.31	0.44
1:F:1673:TYR:CZ	1:F:1677:VAL:HG21	2.52	0.44
2:H:1981:LEU:H	2:H:1981:LEU:HD23	1.82	0.44
2:I:1866:PHE:CD1	2:I:1870:ALA:HB1	2.53	0.44
2:L:430:HIS:CE1	2:L:431:LEU:HD13	2.52	0.44
2:L:1981:LEU:HD23	2:L:1981:LEU:H	1.82	0.44
2:G:430:HIS:CE1	2:G:431:LEU:HD13	2.52	0.44
2:G:1985:VAL:C	2:G:1987:PRO:HD2	2.42	0.44
1:C:378:LEU:HD23	1:D:378:LEU:HD23	1.99	0.44
1:C:1561:MET:O	1:C:1566:ARG:HB2	2.17	0.44
1:C:1694:TYR:OH	2:I:1001:ASP:OD2	2.32	0.44
1:E:176:VAL:HG11	1:E:179:LYS:O	2.18	0.44
1:F:1561:MET:O	1:F:1566:ARG:HB2	2.17	0.44
2:I:430:HIS:CE1	2:I:431:LEU:HD13	2.52	0.44
2:I:1081:HIS:O	2:I:1085:LEU:HB2	2.16	0.44
2:I:1551:GLU:N	2:I:1552:PRO:CD	2.81	0.44
2:J:430:HIS:CE1	2:J:431:LEU:HD13	2.52	0.44
2:J:1775:GLN:HG2	2:J:1836:MET:SD	2.58	0.44
2:J:1866:PHE:CD1	2:J:1870:ALA:HB1	2.53	0.44
2:K:430:HIS:CE1	2:K:431:LEU:HD13	2.52	0.44
2:K:1142:LEU:O	2:K:1150:ARG:NE	2.51	0.44
2:K:1775:GLN:HG2	2:K:1836:MET:SD	2.58	0.44
1:A:378:LEU:HD23	1:F:378:LEU:HD23	1.98	0.44
2:G:1142:LEU:O	2:G:1150:ARG:NE	2.51	0.44
2:G:1775:GLN:HG2	2:G:1836:MET:SD	2.58	0.44
1:D:21:GLN:HE21	1:D:21:GLN:HB3	1.60	0.44
1:E:983:GLN:HE22	2:K:962:LYS:CD	2.29	0.44
2:I:376:ASN:C	2:I:376:ASN:HD22	2.26	0.44
2:J:376:ASN:C	2:J:376:ASN:HD22	2.26	0.44
2:J:1081:HIS:O	2:J:1085:LEU:HB2	2.16	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:1551:GLU:N	2:J:1552:PRO:CD	2.81	0.44
2:J:1981:LEU:H	2:J:1981:LEU:HD23	1.82	0.44
2:K:1981:LEU:HD23	2:K:1981:LEU:H	1.82	0.44
2:K:1985:VAL:C	2:K:1987:PRO:HD2	2.43	0.44
1:A:1351:ASN:C	1:A:1351:ASN:OD1	2.61	0.44
1:B:378:LEU:HD23	1:E:378:LEU:HD23	1.98	0.44
1:B:1673:TYR:CZ	1:B:1677:VAL:HG21	2.52	0.44
1:C:21:GLN:HE21	1:C:21:GLN:HB3	1.60	0.44
1:E:1351:ASN:OD1	1:E:1351:ASN:C	2.61	0.44
2:H:1313:SER:HB2	2:H:1319:MET:HE3	1.99	0.44
2:L:1551:GLU:N	2:L:1552:PRO:CD	2.81	0.44
1:A:768:ILE:HD11	1:A:806:VAL:HG11	2.00	0.44
2:G:1551:GLU:N	2:G:1552:PRO:CD	2.80	0.44
1:C:176:VAL:HG11	1:C:179:LYS:O	2.17	0.44
1:D:1370:THR:HG22	1:D:1372:THR:H	1.82	0.44
2:H:1551:GLU:N	2:H:1552:PRO:CD	2.81	0.44
2:J:1142:LEU:O	2:J:1150:ARG:NE	2.51	0.44
1:A:983:GLN:HE22	2:G:962:LYS:CD	2.30	0.44
1:A:1552:ASN:O	1:A:1556:THR:HG23	2.18	0.44
1:E:768:ILE:HD11	1:E:806:VAL:HG11	2.00	0.44
1:E:1552:ASN:O	1:E:1556:THR:HG23	2.18	0.44
2:H:122:LEU:C	2:H:122:LEU:HD23	2.43	0.44
2:I:194:THR:O	2:I:198:LEU:HD23	2.17	0.44
2:I:1142:LEU:O	2:I:1150:ARG:NE	2.51	0.44
2:K:1551:GLU:N	2:K:1552:PRO:CD	2.81	0.44
2:L:1313:SER:HB2	2:L:1319:MET:HE3	1.99	0.44
2:G:665:LEU:O	2:G:665:LEU:HD22	2.18	0.44
1:B:1552:ASN:O	1:B:1556:THR:HG23	2.18	0.44
1:C:1370:THR:HG22	1:C:1372:THR:H	1.82	0.44
2:H:1985:VAL:C	2:H:1987:PRO:HD2	2.42	0.44
2:I:1866:PHE:HE1	2:I:1870:ALA:HB1	1.82	0.44
2:J:593:LEU:O	2:J:800:LEU:HA	2.18	0.44
2:J:1866:PHE:HE1	2:J:1870:ALA:HB1	1.82	0.44
2:K:665:LEU:O	2:K:665:LEU:HD22	2.18	0.44
2:L:122:LEU:C	2:L:122:LEU:HD23	2.43	0.44
2:L:1866:PHE:CD1	2:L:1870:ALA:HB1	2.53	0.44
2:G:1866:PHE:CD1	2:G:1870:ALA:HB1	2.53	0.44
1:D:176:VAL:HG11	1:D:179:LYS:O	2.18	0.44
1:F:1351:ASN:C	1:F:1351:ASN:OD1	2.61	0.44
1:F:1552:ASN:O	1:F:1556:THR:HG23	2.18	0.44
2:H:1866:PHE:CD1	2:H:1870:ALA:HB1	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:593:LEU:O	2:I:800:LEU:HA	2.18	0.44
2:J:194:THR:O	2:J:198:LEU:HD23	2.17	0.44
2:L:1985:VAL:C	2:L:1987:PRO:HD2	2.43	0.44
1:A:337:VAL:HG12	1:A:341:GLN:HE21	1.83	0.44
2:G:1422:THR:HG22	2:G:1474:PHE:CD1	2.53	0.44
1:C:768:ILE:HD11	1:C:806:VAL:HG11	2.00	0.44
1:D:739:GLN:O	1:D:798:ASN:ND2	2.37	0.44
1:D:768:ILE:HD11	1:D:806:VAL:HG11	2.00	0.44
1:E:337:VAL:HG12	1:E:341:GLN:HE21	1.83	0.44
1:F:680:ILE:HG23	1:F:705:VAL:HG22	1.99	0.44
2:H:96:LEU:HD11	2:H:101:ILE:HA	1.99	0.44
2:H:99:ASN:HD21	2:H:550:VAL:H	1.66	0.44
2:H:184:VAL:HG12	2:H:188:ILE:HG12	1.99	0.44
2:H:665:LEU:HD22	2:H:665:LEU:O	2.18	0.44
2:I:122:LEU:C	2:I:122:LEU:HD23	2.43	0.44
2:I:679:LEU:HB3	2:I:700:LEU:HD13	2.00	0.44
2:J:122:LEU:HD23	2:J:122:LEU:C	2.43	0.44
2:K:1866:PHE:CD1	2:K:1870:ALA:HB1	2.53	0.44
2:L:96:LEU:HD11	2:L:101:ILE:HA	1.99	0.44
2:L:665:LEU:O	2:L:665:LEU:HD22	2.18	0.44
1:A:61:LEU:HD11	1:A:78:ILE:HD11	2.00	0.43
2:G:1783:LEU:HD21	2:G:1828:VAL:CG1	2.48	0.43
1:B:1351:ASN:OD1	1:B:1351:ASN:C	2.61	0.43
1:C:700:GLY:HA2	1:C:730:SER:HB3	2.01	0.43
1:C:1208:VAL:HG13	1:C:1212:THR:HB	2.00	0.43
1:D:700:GLY:HA2	1:D:730:SER:HB3	2.01	0.43
1:D:1208:VAL:HG13	1:D:1212:THR:HB	2.00	0.43
1:D:1673:TYR:CZ	1:D:1677:VAL:HG21	2.52	0.43
1:F:982:ILE:HD13	2:L:955:GLU:HB2	1.99	0.43
1:F:1694:TYR:OH	2:L:1001:ASP:OD2	2.31	0.43
2:J:679:LEU:HB3	2:J:700:LEU:HD13	2.00	0.43
2:K:376:ASN:C	2:K:376:ASN:HD22	2.26	0.43
1:A:20:TYR:CE1	2:G:1985:VAL:HG11	2.53	0.43
1:A:1561:MET:O	1:A:1566:ARG:HB2	2.17	0.43
1:B:680:ILE:HG23	1:B:705:VAL:HG22	1.99	0.43
1:B:982:ILE:HD13	2:H:955:GLU:HB2	1.99	0.43
1:B:1694:TYR:OH	2:H:1001:ASP:OD2	2.31	0.43
1:C:680:ILE:HG23	1:C:705:VAL:HG22	1.99	0.43
1:D:1552:ASN:O	1:D:1556:THR:HG23	2.18	0.43
1:F:700:GLY:HA2	1:F:730:SER:HB3	2.01	0.43
2:H:1142:LEU:O	2:H:1150:ARG:NE	2.51	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1775:GLN:HG2	2:H:1836:MET:SD	2.57	0.43
2:K:1422:THR:HG22	2:K:1474:PHE:CD1	2.53	0.43
2:K:1783:LEU:HD21	2:K:1828:VAL:CG1	2.49	0.43
2:L:99:ASN:HD21	2:L:550:VAL:H	1.66	0.43
2:L:184:VAL:HG12	2:L:188:ILE:HG12	1.99	0.43
2:L:1142:LEU:O	2:L:1150:ARG:NE	2.51	0.43
2:G:376:ASN:C	2:G:376:ASN:HD22	2.26	0.43
1:B:700:GLY:HA2	1:B:730:SER:HB3	2.01	0.43
1:C:1064:ASN:HD22	1:C:1073:THR:HG1	1.62	0.43
1:C:1351:ASN:OD1	1:C:1351:ASN:C	2.61	0.43
1:C:1673:TYR:CZ	1:C:1677:VAL:HG21	2.52	0.43
1:D:61:LEU:HD11	1:D:78:ILE:HD11	2.00	0.43
1:E:61:LEU:HD11	1:E:78:ILE:HD11	2.00	0.43
1:E:680:ILE:HG23	1:E:705:VAL:HG22	1.99	0.43
1:E:1153:ASP:OD2	1:F:359:ARG:NH1	2.51	0.43
1:E:1370:THR:HG22	1:E:1372:THR:H	1.82	0.43
2:I:1985:VAL:C	2:I:1987:PRO:HD2	2.42	0.43
1:A:680:ILE:HG23	1:A:705:VAL:HG22	2.00	0.43
1:A:1208:VAL:HG13	1:A:1212:THR:HB	2.00	0.43
2:G:99:ASN:HD21	2:G:550:VAL:H	1.66	0.43
2:G:1866:PHE:HE1	2:G:1870:ALA:HB1	1.82	0.43
1:C:61:LEU:HD11	1:C:78:ILE:HD11	2.00	0.43
1:C:394:PHE:CE1	1:C:748:LEU:HD23	2.53	0.43
1:C:739:GLN:O	1:C:798:ASN:ND2	2.37	0.43
1:C:1552:ASN:O	1:C:1556:THR:HG23	2.18	0.43
1:D:394:PHE:CE1	1:D:748:LEU:HD23	2.53	0.43
1:D:680:ILE:HG23	1:D:705:VAL:HG22	1.99	0.43
1:D:1351:ASN:OD1	1:D:1351:ASN:C	2.61	0.43
1:E:652:ASP:OD2	1:E:655:LEU:HG	2.19	0.43
1:E:1208:VAL:HG13	1:E:1212:THR:HB	2.00	0.43
2:J:1985:VAL:C	2:J:1987:PRO:HD2	2.43	0.43
2:K:1866:PHE:HE1	2:K:1870:ALA:HB1	1.82	0.43
2:L:1775:GLN:HG2	2:L:1836:MET:SD	2.57	0.43
1:A:652:ASP:OD2	1:A:655:LEU:HG	2.19	0.43
1:A:1370:THR:HG22	1:A:1372:THR:H	1.82	0.43
2:I:665:LEU:O	2:I:665:LEU:HD22	2.18	0.43
2:J:665:LEU:HD22	2:J:665:LEU:O	2.18	0.43
2:K:99:ASN:HD21	2:K:550:VAL:H	1.66	0.43
2:L:1783:LEU:HD21	2:L:1828:VAL:CG1	2.48	0.43
1:A:739:GLN:O	1:A:798:ASN:ND2	2.37	0.43
1:A:850:PHE:HZ	1:A:866:GLY:HA3	1.84	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:176:VAL:HG11	1:B:179:LYS:O	2.17	0.43
1:E:739:GLN:O	1:E:798:ASN:ND2	2.37	0.43
1:E:1561:MET:O	1:E:1566:ARG:HB2	2.17	0.43
2:H:1783:LEU:HD21	2:H:1828:VAL:CG1	2.48	0.43
2:I:96:LEU:HD11	2:I:101:ILE:HA	1.99	0.43
2:I:1783:LEU:HD21	2:I:1828:VAL:CG1	2.49	0.43
2:J:96:LEU:HD11	2:J:101:ILE:HA	1.99	0.43
2:J:1783:LEU:HD21	2:J:1828:VAL:CG1	2.49	0.43
2:K:679:LEU:HB3	2:K:700:LEU:HD13	2.00	0.43
2:L:376:ASN:C	2:L:376:ASN:HD22	2.26	0.43
1:E:850:PHE:HZ	1:E:866:GLY:HA3	1.84	0.43
2:H:101:ILE:HD11	2:H:122:LEU:CD2	2.48	0.43
1:A:700:GLY:HA2	1:A:730:SER:HB3	2.01	0.43
1:A:1153:ASP:OD2	1:B:359:ARG:NH1	2.52	0.43
1:A:1426:LEU:HD22	1:E:1716:LEU:HD21	2.00	0.43
2:G:679:LEU:HB3	2:G:700:LEU:HD13	2.00	0.43
1:D:386:PHE:O	1:D:390:VAL:HB	2.19	0.43
1:F:176:VAL:HG11	1:F:179:LYS:O	2.17	0.43
2:H:376:ASN:C	2:H:376:ASN:HD22	2.26	0.43
2:I:101:ILE:HD11	2:I:122:LEU:CD2	2.49	0.43
2:I:1422:THR:HG22	2:I:1474:PHE:CD1	2.53	0.43
2:J:101:ILE:HD11	2:J:122:LEU:CD2	2.49	0.43
2:J:1422:THR:HG22	2:J:1474:PHE:CD1	2.54	0.43
2:K:433:VAL:N	2:K:434:PRO:CD	2.82	0.43
2:L:101:ILE:HD11	2:L:122:LEU:CD2	2.49	0.43
1:A:982:ILE:HD13	2:G:955:GLU:HB2	2.00	0.43
2:G:433:VAL:N	2:G:434:PRO:CD	2.82	0.43
2:G:544:LYS:O	2:G:545:GLN:C	2.62	0.43
1:C:386:PHE:O	1:C:390:VAL:HB	2.19	0.43
1:E:700:GLY:HA2	1:E:730:SER:HB3	2.01	0.43
2:K:544:LYS:O	2:K:545:GLN:C	2.62	0.43
2:K:717:ILE:HG23	2:K:760:HIS:CE1	2.54	0.43
2:L:593:LEU:O	2:L:800:LEU:HA	2.18	0.43
1:A:394:PHE:CE1	1:A:748:LEU:HD23	2.54	0.43
1:A:1716:LEU:HD21	1:E:1426:LEU:HD22	2.00	0.43
2:G:717:ILE:HG23	2:G:760:HIS:CE1	2.54	0.43
1:B:394:PHE:CE1	1:B:748:LEU:HD23	2.53	0.43
1:B:768:ILE:HD11	1:B:806:VAL:HG11	2.00	0.43
1:F:335:HIS:O	1:F:338:LEU:HB3	2.19	0.43
1:F:394:PHE:CE1	1:F:748:LEU:HD23	2.54	0.43
1:F:850:PHE:HZ	1:F:866:GLY:HA3	1.84	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:593:LEU:O	2:H:800:LEU:HA	2.18	0.43
2:I:1867:SER:O	2:I:1870:ALA:HB3	2.19	0.43
2:G:1956:ARG:CB	2:G:1957:PRO:HD3	2.49	0.42
1:B:335:HIS:O	1:B:338:LEU:HB3	2.19	0.42
1:B:850:PHE:HZ	1:B:866:GLY:HA3	1.84	0.42
1:E:394:PHE:CE1	1:E:748:LEU:HD23	2.54	0.42
1:F:768:ILE:HD11	1:F:806:VAL:HG11	2.00	0.42
2:J:1867:SER:O	2:J:1870:ALA:HB3	2.19	0.42
2:K:1680:LEU:HD23	2:K:1680:LEU:HA	1.86	0.42
2:K:1956:ARG:CB	2:K:1957:PRO:HD3	2.49	0.42
2:L:914:LEU:HD13	2:L:914:LEU:HA	1.93	0.42
1:A:1413:LYS:O	1:A:1648:GLN:NE2	2.43	0.42
1:B:1716:LEU:HD21	1:D:1426:LEU:HD22	2.00	0.42
1:C:1426:LEU:HD22	1:F:1716:LEU:HD21	2.00	0.42
1:E:335:HIS:O	1:E:338:LEU:HB3	2.19	0.42
1:E:982:ILE:HD13	2:K:955:GLU:HB2	2.00	0.42
1:F:719:GLN:HG3	1:F:1612:ASP:HA	2.01	0.42
1:F:1208:VAL:HG13	1:F:1212:THR:HB	2.00	0.42
2:H:1364:LYS:O	2:H:1398:ARG:NH2	2.47	0.42
2:H:1867:SER:O	2:H:1870:ALA:HB3	2.19	0.42
2:J:1738:PHE:CE1	2:J:1837:THR:HG23	2.54	0.42
2:J:2017:LYS:O	2:J:2018:PRO:C	2.63	0.42
2:K:593:LEU:O	2:K:800:LEU:HA	2.18	0.42
2:L:1867:SER:O	2:L:1870:ALA:HB3	2.19	0.42
2:G:101:ILE:HD11	2:G:122:LEU:CD2	2.49	0.42
2:G:122:LEU:C	2:G:122:LEU:HD23	2.43	0.42
1:B:386:PHE:O	1:B:390:VAL:HB	2.19	0.42
1:B:719:GLN:HG3	1:B:1612:ASP:HA	2.01	0.42
1:B:1208:VAL:HG13	1:B:1212:THR:HB	2.00	0.42
1:D:335:HIS:O	1:D:338:LEU:HB3	2.19	0.42
1:F:386:PHE:O	1:F:390:VAL:HB	2.19	0.42
2:H:717:ILE:HG23	2:H:760:HIS:CE1	2.54	0.42
2:H:1738:PHE:CE1	2:H:1837:THR:HG23	2.54	0.42
2:I:2017:LYS:O	2:I:2018:PRO:C	2.63	0.42
2:K:101:ILE:HD11	2:K:122:LEU:CD2	2.49	0.42
2:L:717:ILE:HG23	2:L:760:HIS:CE1	2.54	0.42
1:A:335:HIS:O	1:A:338:LEU:HB3	2.19	0.42
1:A:386:PHE:O	1:A:390:VAL:HB	2.19	0.42
2:G:593:LEU:O	2:G:800:LEU:HA	2.18	0.42
2:G:1680:LEU:HD23	2:G:1680:LEU:HA	1.87	0.42
1:B:61:LEU:HD11	1:B:78:ILE:HD11	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1153:ASP:OD2	1:C:359:ARG:NH1	2.50	0.42
1:C:335:HIS:O	1:C:338:LEU:HB3	2.19	0.42
2:I:1738:PHE:CE1	2:I:1837:THR:HG23	2.54	0.42
1:A:1308:SER:O	1:A:1311:SER:HB3	2.20	0.42
2:G:598:THR:O	2:G:602:VAL:HB	2.19	0.42
1:B:337:VAL:HG12	1:B:341:GLN:HE21	1.84	0.42
1:C:337:VAL:HG12	1:C:341:GLN:HE21	1.84	0.42
1:D:337:VAL:HG12	1:D:341:GLN:HE21	1.84	0.42
1:E:386:PHE:O	1:E:390:VAL:HB	2.19	0.42
1:E:1308:SER:O	1:E:1311:SER:HB3	2.20	0.42
2:H:914:LEU:HD13	2:H:914:LEU:HA	1.92	0.42
2:I:270:ALA:O	2:I:459:VAL:HA	2.20	0.42
2:K:122:LEU:C	2:K:122:LEU:HD23	2.43	0.42
2:K:1149:TRP:CE2	2:K:1213:LEU:HD23	2.55	0.42
2:L:526:ARG:NH1	2:L:539:ASP:O	2.44	0.42
2:L:1364:LYS:O	2:L:1398:ARG:NH2	2.48	0.42
2:G:1149:TRP:CE2	2:G:1213:LEU:HD23	2.55	0.42
1:B:1463:VAL:HB	1:B:1773:VAL:HG21	2.01	0.42
1:D:1067:LEU:HD23	1:D:1067:LEU:HA	1.91	0.42
1:E:1413:LYS:O	1:E:1648:GLN:NE2	2.43	0.42
1:F:61:LEU:HD11	1:F:78:ILE:HD11	2.00	0.42
2:H:1846:GLU:CD	2:H:1846:GLU:H	2.28	0.42
2:I:99:ASN:HD21	2:I:550:VAL:H	1.66	0.42
2:I:277:LEU:CD1	2:I:479:ILE:HG12	2.50	0.42
2:J:270:ALA:O	2:J:459:VAL:HA	2.20	0.42
2:J:277:LEU:CD1	2:J:479:ILE:HG12	2.50	0.42
2:K:598:THR:O	2:K:602:VAL:HB	2.19	0.42
2:L:1422:THR:HG22	2:L:1474:PHE:CD1	2.54	0.42
2:L:1738:PHE:CE1	2:L:1837:THR:HG23	2.54	0.42
1:C:666:ALA:O	1:C:670:GLY:HA2	2.20	0.42
1:C:1716:LEU:HD21	1:F:1426:LEU:HD22	2.01	0.42
1:D:666:ALA:O	1:D:670:GLY:HA2	2.20	0.42
1:D:719:GLN:HG3	1:D:1612:ASP:HA	2.01	0.42
1:F:1076:VAL:HG13	1:F:1081:LYS:HA	2.02	0.42
1:F:1463:VAL:HB	1:F:1773:VAL:HG21	2.01	0.42
2:H:526:ARG:NH2	2:H:546:GLU:OE2	2.51	0.42
2:H:544:LYS:O	2:H:545:GLN:C	2.62	0.42
2:H:598:THR:O	2:H:602:VAL:HB	2.19	0.42
2:I:717:ILE:HG23	2:I:760:HIS:CE1	2.54	0.42
2:J:1746:LEU:C	2:J:1746:LEU:HD12	2.45	0.42
2:L:544:LYS:O	2:L:545:GLN:C	2.62	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:1846:GLU:CD	2:L:1846:GLU:H	2.28	0.42
1:A:359:ARG:NH1	1:C:1153:ASP:OD2	2.51	0.42
2:G:1746:LEU:HD12	2:G:1746:LEU:C	2.45	0.42
1:B:20:TYR:CE1	2:H:1985:VAL:HG11	2.55	0.42
1:B:666:ALA:O	1:B:670:GLY:HA2	2.20	0.42
1:B:1076:VAL:HG13	1:B:1081:LYS:HA	2.02	0.42
1:C:44:VAL:HG12	1:C:78:ILE:HG13	2.02	0.42
1:C:719:GLN:HG3	1:C:1612:ASP:HA	2.01	0.42
1:C:1067:LEU:HD23	1:C:1067:LEU:HA	1.91	0.42
1:D:850:PHE:HZ	1:D:866:GLY:HA3	1.84	0.42
1:E:44:VAL:HG12	1:E:78:ILE:HG13	2.02	0.42
1:F:337:VAL:HG12	1:F:341:GLN:HE21	1.84	0.42
1:F:666:ALA:O	1:F:670:GLY:HA2	2.20	0.42
2:H:526:ARG:NH1	2:H:539:ASP:O	2.44	0.42
2:I:598:THR:O	2:I:602:VAL:HB	2.19	0.42
2:J:99:ASN:HD21	2:J:550:VAL:H	1.66	0.42
2:J:1149:TRP:CE2	2:J:1213:LEU:HD23	2.55	0.42
2:L:526:ARG:NH2	2:L:546:GLU:OE2	2.51	0.42
2:L:598:THR:O	2:L:602:VAL:HB	2.19	0.42
1:A:1067:LEU:HD23	1:A:1067:LEU:HA	1.91	0.42
2:G:1867:SER:O	2:G:1870:ALA:HB3	2.19	0.42
1:B:1426:LEU:HD22	1:D:1716:LEU:HD21	2.01	0.42
1:C:20:TYR:CE1	2:I:1985:VAL:HG11	2.55	0.42
1:C:850:PHE:HZ	1:C:866:GLY:HA3	1.84	0.42
1:D:44:VAL:HG12	1:D:78:ILE:HG13	2.02	0.42
1:D:1308:SER:O	1:D:1311:SER:HB3	2.20	0.42
1:E:1067:LEU:HD23	1:E:1067:LEU:HA	1.91	0.42
1:E:1425:ILE:HD12	1:E:1425:ILE:HA	1.90	0.42
1:E:1463:VAL:HB	1:E:1773:VAL:HG21	2.01	0.42
1:F:652:ASP:OD2	1:F:655:LEU:HG	2.19	0.42
2:H:679:LEU:HB3	2:H:700:LEU:HD13	2.00	0.42
2:H:1422:THR:HG22	2:H:1474:PHE:CD1	2.54	0.42
2:H:1866:PHE:HE1	2:H:1870:ALA:HB1	1.82	0.42
2:H:1956:ARG:CB	2:H:1957:PRO:HD3	2.49	0.42
2:I:741:HIS:CD2	2:I:855:HIS:ND1	2.88	0.42
2:I:1149:TRP:CE2	2:I:1213:LEU:HD23	2.55	0.42
2:I:1746:LEU:HD12	2:I:1746:LEU:C	2.45	0.42
2:I:1862:VAL:HG11	2:I:1866:PHE:CD2	2.55	0.42
2:J:433:VAL:N	2:J:434:PRO:CD	2.82	0.42
2:J:717:ILE:HG23	2:J:760:HIS:CE1	2.54	0.42
2:K:1746:LEU:C	2:K:1746:LEU:HD12	2.45	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:679:LEU:HB3	2:L:700:LEU:HD13	2.00	0.42
2:L:1956:ARG:CB	2:L:1957:PRO:HD3	2.49	0.42
1:A:44:VAL:HG12	1:A:78:ILE:HG13	2.02	0.42
1:A:666:ALA:O	1:A:670:GLY:HA2	2.20	0.42
1:A:1425:ILE:HD12	1:A:1425:ILE:HA	1.90	0.42
1:B:739:GLN:O	1:B:798:ASN:ND2	2.37	0.42
1:C:1308:SER:O	1:C:1311:SER:HB3	2.20	0.42
1:E:20:TYR:CE1	2:K:1985:VAL:HG11	2.55	0.42
2:H:270:ALA:O	2:H:459:VAL:HA	2.20	0.42
2:H:1862:VAL:HG11	2:H:1866:PHE:CD2	2.55	0.42
2:I:433:VAL:N	2:I:434:PRO:CD	2.82	0.42
2:I:1956:ARG:CB	2:I:1957:PRO:HD3	2.49	0.42
2:J:598:THR:O	2:J:602:VAL:HB	2.19	0.42
2:J:741:HIS:CD2	2:J:855:HIS:ND1	2.88	0.42
2:J:1862:VAL:HG11	2:J:1866:PHE:CD2	2.55	0.42
2:J:1956:ARG:CB	2:J:1957:PRO:HD3	2.49	0.42
2:K:270:ALA:O	2:K:459:VAL:HA	2.20	0.42
2:K:1867:SER:O	2:K:1870:ALA:HB3	2.19	0.42
2:L:270:ALA:O	2:L:459:VAL:HA	2.20	0.42
1:A:21:GLN:HE21	1:A:21:GLN:HB3	1.60	0.41
1:A:1463:VAL:HB	1:A:1773:VAL:HG21	2.01	0.41
2:G:270:ALA:O	2:G:459:VAL:HA	2.20	0.41
1:B:652:ASP:OD2	1:B:655:LEU:HG	2.19	0.41
1:B:1308:SER:O	1:B:1311:SER:HB3	2.20	0.41
1:B:1367:ARG:HG3	1:B:1370:THR:HG21	2.02	0.41
1:B:1413:LYS:O	1:B:1648:GLN:NE2	2.43	0.41
1:E:21:GLN:HE21	1:E:21:GLN:HB3	1.60	0.41
1:E:666:ALA:O	1:E:670:GLY:HA2	2.20	0.41
1:F:739:GLN:O	1:F:798:ASN:ND2	2.37	0.41
1:F:1367:ARG:HG3	1:F:1370:THR:HG21	2.02	0.41
2:H:277:LEU:CD1	2:H:479:ILE:HG12	2.50	0.41
2:H:741:HIS:CD2	2:H:855:HIS:ND1	2.88	0.41
2:K:277:LEU:CD1	2:K:479:ILE:HG12	2.50	0.41
2:L:1862:VAL:HG11	2:L:1866:PHE:CD2	2.55	0.41
2:L:1866:PHE:HE1	2:L:1870:ALA:HB1	1.82	0.41
2:G:741:HIS:CD2	2:G:855:HIS:ND1	2.88	0.41
1:C:514:GLU:O	1:C:515:PRO:C	2.64	0.41
1:C:652:ASP:OD2	1:C:655:LEU:HG	2.19	0.41
1:D:514:GLU:O	1:D:515:PRO:C	2.63	0.41
1:D:652:ASP:OD2	1:D:655:LEU:HG	2.19	0.41
1:D:1076:VAL:HG13	1:D:1081:LYS:HA	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1308:SER:O	1:F:1311:SER:HB3	2.20	0.41
2:L:277:LEU:CD1	2:L:479:ILE:HG12	2.50	0.41
2:L:741:HIS:CD2	2:L:855:HIS:ND1	2.88	0.41
1:A:514:GLU:O	1:A:515:PRO:C	2.64	0.41
1:A:684:GLY:O	1:A:687:SER:OG	2.32	0.41
1:A:822:VAL:HG12	1:A:824:LEU:HD13	2.02	0.41
2:G:277:LEU:CD1	2:G:479:ILE:HG12	2.50	0.41
1:B:1181:PHE:CE2	1:B:1183:ARG:HB2	2.56	0.41
1:C:1181:PHE:CE2	1:C:1183:ARG:HB2	2.56	0.41
1:C:1463:VAL:HB	1:C:1773:VAL:HG21	2.01	0.41
1:D:359:ARG:NH1	1:F:1153:ASP:OD2	2.51	0.41
1:D:1153:ASP:OD2	1:E:359:ARG:NH1	2.51	0.41
1:D:1367:ARG:HG3	1:D:1370:THR:HG21	2.02	0.41
1:D:1463:VAL:HB	1:D:1773:VAL:HG21	2.01	0.41
1:E:514:GLU:O	1:E:515:PRO:C	2.64	0.41
1:E:684:GLY:O	1:E:687:SER:OG	2.32	0.41
1:F:1062:TYR:OH	1:F:1073:THR:HG23	2.21	0.41
2:H:433:VAL:N	2:H:434:PRO:CD	2.82	0.41
2:K:741:HIS:CD2	2:K:855:HIS:ND1	2.88	0.41
2:L:1597:ALA:HB1	2:L:1638:ILE:HD13	2.02	0.41
2:G:490:TRP:HA	2:G:493:THR:HG22	2.03	0.41
2:G:1738:PHE:CE1	2:G:1837:THR:HG23	2.54	0.41
1:B:1062:TYR:OH	1:B:1073:THR:HG23	2.21	0.41
1:C:1076:VAL:HG13	1:C:1081:LYS:HA	2.02	0.41
1:C:1367:ARG:HG3	1:C:1370:THR:HG21	2.02	0.41
1:D:61:LEU:CD1	1:D:78:ILE:HD11	2.51	0.41
1:D:1181:PHE:CE2	1:D:1183:ARG:HB2	2.56	0.41
1:E:822:VAL:HG12	1:E:824:LEU:HD13	2.02	0.41
1:E:1694:TYR:OH	2:K:1001:ASP:OD2	2.31	0.41
1:F:1181:PHE:CE2	1:F:1183:ARG:HB2	2.56	0.41
2:H:234:ILE:N	2:H:235:PRO:HD3	2.35	0.41
2:H:1597:ALA:HB1	2:H:1638:ILE:HD13	2.02	0.41
2:H:2017:LYS:O	2:H:2018:PRO:C	2.63	0.41
2:K:143:SER:OG	2:K:547:ILE:O	2.35	0.41
2:K:490:TRP:HA	2:K:493:THR:HG22	2.03	0.41
2:K:1862:VAL:HG11	2:K:1866:PHE:CD2	2.55	0.41
2:L:234:ILE:N	2:L:235:PRO:HD3	2.35	0.41
2:L:433:VAL:N	2:L:434:PRO:CD	2.82	0.41
2:L:2017:LYS:O	2:L:2018:PRO:C	2.62	0.41
2:G:1862:VAL:HG11	2:G:1866:PHE:CD2	2.55	0.41
1:B:514:GLU:O	1:B:515:PRO:C	2.63	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1286:TRP:CZ3	1:C:1289:MET:HE2	2.56	0.41
1:E:839:TYR:O	1:E:842:SER:HB2	2.20	0.41
1:F:514:GLU:O	1:F:515:PRO:C	2.64	0.41
2:H:846:VAL:HG13	2:H:865:TRP:NE1	2.36	0.41
2:I:1103:PHE:O	2:I:1247:GLY:HA3	2.21	0.41
2:J:544:LYS:O	2:J:545:GLN:C	2.62	0.41
2:L:846:VAL:HG13	2:L:865:TRP:NE1	2.36	0.41
1:A:719:GLN:HG3	1:A:1612:ASP:HA	2.01	0.41
1:A:839:TYR:O	1:A:842:SER:HB2	2.20	0.41
1:C:61:LEU:CD1	1:C:78:ILE:HD11	2.51	0.41
1:C:839:TYR:O	1:C:842:SER:HB2	2.20	0.41
1:D:1286:TRP:CZ3	1:D:1289:MET:HE2	2.56	0.41
1:F:1413:LYS:O	1:F:1648:GLN:NE2	2.43	0.41
2:H:1085:LEU:HD12	2:H:1085:LEU:HA	1.94	0.41
2:H:1149:TRP:CE2	2:H:1213:LEU:HD23	2.55	0.41
2:H:1976:PHE:HA	2:H:1981:LEU:HD21	2.03	0.41
2:I:544:LYS:O	2:I:545:GLN:C	2.62	0.41
2:I:1606:ARG:HG2	2:I:1635:ARG:HD3	2.03	0.41
2:J:1103:PHE:O	2:J:1247:GLY:HA3	2.21	0.41
2:J:1606:ARG:HG2	2:J:1635:ARG:HD3	2.03	0.41
2:J:1693:ARG:HD3	2:J:1825:GLU:OE2	2.21	0.41
2:K:1738:PHE:CE1	2:K:1837:THR:HG23	2.55	0.41
2:K:2017:LYS:O	2:K:2018:PRO:C	2.62	0.41
1:A:1694:TYR:OH	2:G:1001:ASP:OD2	2.31	0.41
2:G:1466:PHE:CD1	2:G:1489:ILE:HG12	2.56	0.41
2:G:1690:VAL:HG13	2:G:1824:ILE:HD12	2.03	0.41
1:D:442:ARG:HD3	1:D:726:GLY:O	2.21	0.41
1:D:839:TYR:O	1:D:842:SER:HB2	2.20	0.41
1:E:719:GLN:HG3	1:E:1612:ASP:HA	2.01	0.41
1:E:1062:TYR:OH	1:E:1073:THR:HG23	2.20	0.41
1:E:1442:ASN:HD22	1:E:1442:ASN:HA	1.79	0.41
1:F:44:VAL:HG12	1:F:78:ILE:HG13	2.02	0.41
2:H:1855:ILE:HG22	2:H:1968:PRO:HA	2.03	0.41
2:I:543:PHE:HB2	2:I:545:GLN:HE22	1.86	0.41
2:I:1693:ARG:HD3	2:I:1825:GLU:OE2	2.21	0.41
2:J:526:ARG:NH2	2:J:546:GLU:OE2	2.51	0.41
2:J:1597:ALA:HB1	2:J:1638:ILE:HD13	2.02	0.41
2:J:1976:PHE:HA	2:J:1981:LEU:HD21	2.03	0.41
2:K:914:LEU:HD13	2:K:914:LEU:HA	1.92	0.41
2:K:1466:PHE:CD1	2:K:1489:ILE:HG12	2.56	0.41
2:L:246:LEU:HD13	2:L:246:LEU:HA	1.96	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:1149:TRP:CE2	2:L:1213:LEU:HD23	2.55	0.41
2:L:1855:ILE:HG22	2:L:1968:PRO:HA	2.03	0.41
2:L:1976:PHE:HA	2:L:1981:LEU:HD21	2.03	0.41
2:G:599:PRO:O	2:G:602:VAL:HG12	2.21	0.41
2:G:1976:PHE:HA	2:G:1981:LEU:HD21	2.03	0.41
2:G:2017:LYS:O	2:G:2018:PRO:C	2.63	0.41
1:C:822:VAL:HG12	1:C:824:LEU:HD13	2.02	0.41
1:C:1062:TYR:OH	1:C:1073:THR:HG23	2.20	0.41
1:D:822:VAL:HG12	1:D:824:LEU:HD13	2.02	0.41
1:D:1062:TYR:OH	1:D:1073:THR:HG23	2.21	0.41
1:E:61:LEU:CD1	1:E:78:ILE:HD11	2.51	0.41
1:F:20:TYR:CE1	2:L:1985:VAL:HG11	2.56	0.41
1:F:61:LEU:CD1	1:F:78:ILE:HD11	2.51	0.41
2:H:1773:ALA:HB1	2:H:1775:GLN:NE2	2.36	0.41
2:I:663:ILE:HB	2:I:664:PRO:HD3	2.03	0.41
2:I:1597:ALA:HB1	2:I:1638:ILE:HD13	2.02	0.41
2:I:1690:VAL:HG13	2:I:1824:ILE:HD12	2.03	0.41
2:I:1976:PHE:HA	2:I:1981:LEU:HD21	2.03	0.41
2:J:543:PHE:HB2	2:J:545:GLN:HE22	1.86	0.41
2:K:234:ILE:N	2:K:235:PRO:HD3	2.35	0.41
2:K:599:PRO:O	2:K:602:VAL:HG12	2.21	0.41
2:K:1690:VAL:HG13	2:K:1824:ILE:HD12	2.03	0.41
2:K:1855:ILE:HG22	2:K:1968:PRO:HA	2.03	0.41
2:K:1976:PHE:HA	2:K:1981:LEU:HD21	2.03	0.41
2:L:1773:ALA:HB1	2:L:1775:GLN:NE2	2.36	0.41
1:A:61:LEU:CD1	1:A:78:ILE:HD11	2.51	0.41
1:A:1062:TYR:OH	1:A:1073:THR:HG23	2.21	0.41
1:A:1143:GLN:HB3	1:E:1177:LYS:HB2	2.03	0.41
1:A:1177:LYS:HB2	1:E:1143:GLN:HB3	2.03	0.41
1:A:1286:TRP:CZ3	1:A:1289:MET:HE2	2.56	0.41
2:G:234:ILE:N	2:G:235:PRO:HD3	2.35	0.41
2:G:543:PHE:HB2	2:G:545:GLN:HE22	1.86	0.41
2:G:1103:PHE:O	2:G:1247:GLY:HA3	2.21	0.41
1:B:44:VAL:HG12	1:B:78:ILE:HG13	2.02	0.41
1:C:442:ARG:HD3	1:C:726:GLY:O	2.21	0.41
1:D:20:TYR:CE1	2:J:1985:VAL:HG11	2.56	0.41
1:E:1076:VAL:HG13	1:E:1081:LYS:HA	2.01	0.41
1:E:1286:TRP:CZ3	1:E:1289:MET:HE2	2.56	0.41
2:H:1693:ARG:HD3	2:H:1825:GLU:OE2	2.21	0.41
2:I:1584:PHE:CD2	2:I:1584:PHE:C	2.99	0.41
2:I:1846:GLU:CD	2:I:1846:GLU:H	2.28	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:663:ILE:HB	2:J:664:PRO:HD3	2.03	0.41
2:J:1584:PHE:CD2	2:J:1584:PHE:C	2.99	0.41
2:J:1690:VAL:HG13	2:J:1824:ILE:HD12	2.03	0.41
2:J:1855:ILE:HG22	2:J:1968:PRO:HA	2.03	0.41
2:K:1103:PHE:O	2:K:1247:GLY:HA3	2.21	0.41
1:A:1076:VAL:HG13	1:A:1081:LYS:HA	2.02	0.41
2:G:1855:ILE:HG22	2:G:1968:PRO:HA	2.03	0.41
1:B:61:LEU:CD1	1:B:78:ILE:HD11	2.51	0.41
1:B:377:TYR:O	1:B:380:ALA:HB3	2.21	0.41
1:F:776:GLU:HB2	1:F:779:ILE:HD12	2.03	0.41
2:H:1746:LEU:C	2:H:1746:LEU:HD12	2.45	0.41
2:I:1589:VAL:HG11	2:I:1640:PHE:CE2	2.56	0.41
2:I:1855:ILE:HG22	2:I:1968:PRO:HA	2.03	0.41
2:J:1846:GLU:CD	2:J:1846:GLU:H	2.28	0.41
2:K:543:PHE:HB2	2:K:545:GLN:HE22	1.86	0.41
2:K:846:VAL:HG13	2:K:865:TRP:NE1	2.36	0.41
2:L:1085:LEU:HD12	2:L:1085:LEU:HA	1.94	0.41
2:L:1693:ARG:HD3	2:L:1825:GLU:OE2	2.21	0.41
2:L:1746:LEU:HD12	2:L:1746:LEU:C	2.45	0.41
2:G:246:LEU:HD13	2:G:246:LEU:HA	1.96	0.40
1:B:839:TYR:O	1:B:842:SER:HB2	2.20	0.40
1:B:1367:ARG:O	1:B:1370:THR:HB	2.21	0.40
1:F:442:ARG:HD3	1:F:726:GLY:O	2.21	0.40
2:H:846:VAL:HG13	2:H:865:TRP:CD1	2.56	0.40
2:I:581:THR:OG1	2:I:797:ASP:O	2.35	0.40
2:I:846:VAL:HG13	2:I:865:TRP:CD1	2.56	0.40
2:I:1466:PHE:CD1	2:I:1489:ILE:HG12	2.56	0.40
2:I:1773:ALA:HB1	2:I:1775:GLN:NE2	2.36	0.40
2:J:1466:PHE:CD1	2:J:1489:ILE:HG12	2.56	0.40
2:J:1589:VAL:HG11	2:J:1640:PHE:CE2	2.57	0.40
2:J:1773:ALA:HB1	2:J:1775:GLN:NE2	2.36	0.40
2:L:599:PRO:O	2:L:602:VAL:HG12	2.21	0.40
1:A:1534:ASP:OD1	1:A:1567:SER:OG	2.38	0.40
2:G:143:SER:OG	2:G:547:ILE:O	2.35	0.40
2:G:846:VAL:HG13	2:G:865:TRP:NE1	2.36	0.40
2:G:914:LEU:HD13	2:G:914:LEU:HA	1.92	0.40
1:B:353:ASP:OD2	1:B:359:ARG:NH2	2.49	0.40
1:B:442:ARG:HD3	1:B:726:GLY:O	2.21	0.40
1:C:891:MET:HE2	1:C:891:MET:HA	2.03	0.40
1:E:442:ARG:HD3	1:E:726:GLY:O	2.21	0.40
1:F:377:TYR:O	1:F:380:ALA:HB3	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:839:TYR:O	1:F:842:SER:HB2	2.20	0.40
2:H:599:PRO:O	2:H:602:VAL:HG12	2.21	0.40
2:K:1846:GLU:CD	2:K:1846:GLU:H	2.28	0.40
1:A:377:TYR:O	1:A:380:ALA:HB3	2.21	0.40
1:A:489:VAL:HG13	1:A:670:GLY:HA3	2.03	0.40
1:A:1181:PHE:CE2	1:A:1183:ARG:HB2	2.56	0.40
2:G:1693:ARG:HD3	2:G:1825:GLU:OE2	2.21	0.40
1:B:776:GLU:HB2	1:B:779:ILE:HD12	2.03	0.40
1:E:377:TYR:O	1:E:380:ALA:HB3	2.21	0.40
1:E:489:VAL:HG13	1:E:670:GLY:HA3	2.03	0.40
1:E:1534:ASP:OD1	1:E:1567:SER:OG	2.38	0.40
1:F:1367:ARG:O	1:F:1370:THR:HB	2.21	0.40
2:H:490:TRP:HA	2:H:493:THR:HG22	2.03	0.40
2:H:663:ILE:HB	2:H:664:PRO:HD3	2.03	0.40
2:H:1466:PHE:CD1	2:H:1489:ILE:HG12	2.56	0.40
2:I:599:PRO:O	2:I:602:VAL:HG12	2.21	0.40
2:J:581:THR:OG1	2:J:797:ASP:O	2.35	0.40
2:J:846:VAL:HG13	2:J:865:TRP:CD1	2.56	0.40
2:K:1693:ARG:HD3	2:K:1825:GLU:OE2	2.21	0.40
2:L:846:VAL:HG13	2:L:865:TRP:CD1	2.56	0.40
1:A:776:GLU:HB2	1:A:779:ILE:HD12	2.03	0.40
2:G:1606:ARG:HG2	2:G:1635:ARG:HD3	2.03	0.40
2:G:1846:GLU:CD	2:G:1846:GLU:H	2.28	0.40
1:B:490:TYR:CD1	1:B:695:GLY:HA2	2.57	0.40
1:D:891:MET:HE2	1:D:891:MET:HA	2.03	0.40
1:D:1367:ARG:O	1:D:1370:THR:HB	2.21	0.40
1:E:1181:PHE:CE2	1:E:1183:ARG:HB2	2.56	0.40
2:J:846:VAL:HG13	2:J:865:TRP:NE1	2.36	0.40
2:K:246:LEU:HD13	2:K:246:LEU:HA	1.96	0.40
2:L:490:TRP:HA	2:L:493:THR:HG22	2.03	0.40
2:L:663:ILE:HB	2:L:664:PRO:HD3	2.03	0.40
2:L:1466:PHE:CD1	2:L:1489:ILE:HG12	2.56	0.40
1:A:414:LEU:HD12	1:A:414:LEU:HA	1.94	0.40
1:A:442:ARG:HD3	1:A:726:GLY:O	2.21	0.40
1:B:822:VAL:HG12	1:B:824:LEU:HD13	2.03	0.40
1:C:1367:ARG:O	1:C:1370:THR:HB	2.21	0.40
1:D:776:GLU:HB2	1:D:779:ILE:HD12	2.03	0.40
1:E:776:GLU:HB2	1:E:779:ILE:HD12	2.03	0.40
1:F:490:TYR:CD1	1:F:695:GLY:HA2	2.57	0.40
1:F:822:VAL:HG12	1:F:824:LEU:HD13	2.02	0.40
2:H:1103:PHE:O	2:H:1247:GLY:HA3	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:490:TRP:HA	2:I:493:THR:HG22	2.03	0.40
2:I:846:VAL:HG13	2:I:865:TRP:NE1	2.36	0.40
2:J:599:PRO:O	2:J:602:VAL:HG12	2.21	0.40
2:K:1606:ARG:HG2	2:K:1635:ARG:HD3	2.03	0.40
2:L:1884:TRP:HB2	2:L:1906:ALA:HB2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

12 ligands are modelled in this entry.

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
3	J8T	B	1901	1	7,12,13	1.04	0	11,17,20	1.22	1 (9%)
4	FMN	G	2101	-	33,33,33	1.55	7 (21%)	48,50,50	1.48	11 (22%)
4	FMN	H	2101	-	33,33,33	1.58	8 (24%)	48,50,50	1.46	10 (20%)
3	J8T	E	1901	1	7,12,13	1.03	0	11,17,20	1.23	1 (9%)
3	J8T	C	1901	1	7,12,13	1.03	0	11,17,20	1.22	1 (9%)
4	FMN	I	2101	-	33,33,33	1.57	8 (24%)	48,50,50	1.46	10 (20%)
4	FMN	K	2101	-	33,33,33	1.56	7 (21%)	48,50,50	1.49	11 (22%)
4	FMN	L	2101	-	33,33,33	1.57	7 (21%)	48,50,50	1.47	11 (22%)
4	FMN	J	2101	-	33,33,33	1.56	7 (21%)	48,50,50	1.47	11 (22%)
3	J8T	D	1901	1	7,12,13	1.03	0	11,17,20	1.24	1 (9%)
3	J8T	A	1901	1	7,12,13	1.03	0	11,17,20	1.23	1 (9%)
3	J8T	F	1901	1	7,12,13	1.04	0	11,17,20	1.23	1 (9%)

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
3	J8T	B	1901	1	-	5/13/16/17	-
4	FMN	G	2101	-	-	3/18/18/18	0/3/3/3
4	FMN	H	2101	-	-	2/18/18/18	0/3/3/3
3	J8T	E	1901	1	-	4/13/16/17	-
3	J8T	C	1901	1	-	4/13/16/17	-
4	FMN	I	2101	-	-	1/18/18/18	0/3/3/3
4	FMN	K	2101	-	-	2/18/18/18	0/3/3/3
4	FMN	L	2101	-	-	4/18/18/18	0/3/3/3
4	FMN	J	2101	-	-	1/18/18/18	0/3/3/3
3	J8T	D	1901	1	-	4/13/16/17	-
3	J8T	A	1901	1	-	4/13/16/17	-
3	J8T	F	1901	1	-	4/13/16/17	-

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	K	2101	FMN	C9A-C5A	3.61	1.47	1.41
4	H	2101	FMN	C9A-C5A	3.57	1.46	1.41
4	G	2101	FMN	C9A-C5A	3.57	1.46	1.41
4	L	2101	FMN	C9A-C5A	3.56	1.46	1.41
4	I	2101	FMN	C9A-C5A	3.50	1.46	1.41
4	J	2101	FMN	C9A-C5A	3.47	1.46	1.41
4	H	2101	FMN	C5A-N5	-3.45	1.33	1.39
4	L	2101	FMN	C5A-N5	-3.42	1.33	1.39
4	J	2101	FMN	C5A-N5	-3.42	1.33	1.39
4	I	2101	FMN	C5A-N5	-3.37	1.33	1.39
4	K	2101	FMN	C5A-N5	-3.36	1.33	1.39
4	G	2101	FMN	C5A-N5	-3.31	1.33	1.39
4	G	2101	FMN	C8-C7	2.79	1.47	1.40
4	K	2101	FMN	C8-C7	2.79	1.47	1.40
4	H	2101	FMN	C8-C7	2.76	1.47	1.40
4	I	2101	FMN	C6-C5A	-2.71	1.35	1.40
4	L	2101	FMN	C8-C7	2.70	1.47	1.40
4	I	2101	FMN	C8-C7	2.69	1.47	1.40
4	J	2101	FMN	C8-C7	2.67	1.47	1.40
4	L	2101	FMN	C6-C5A	-2.65	1.35	1.40
4	J	2101	FMN	C6-C5A	-2.64	1.36	1.40
4	G	2101	FMN	C6-C5A	-2.64	1.36	1.40
4	H	2101	FMN	C6-C5A	-2.62	1.36	1.40
4	H	2101	FMN	C4-N3	-2.61	1.34	1.38
4	K	2101	FMN	C6-C5A	-2.60	1.36	1.40
4	I	2101	FMN	C4-N3	-2.54	1.34	1.38
4	J	2101	FMN	C4-N3	-2.53	1.34	1.38
4	L	2101	FMN	C4-N3	-2.49	1.34	1.38
4	K	2101	FMN	C4-N3	-2.49	1.34	1.38
4	G	2101	FMN	C4-N3	-2.48	1.34	1.38
4	J	2101	FMN	C9-C8	-2.37	1.36	1.39
4	G	2101	FMN	C9-C8	-2.36	1.36	1.39
4	I	2101	FMN	C6-C7	-2.31	1.36	1.39
4	I	2101	FMN	C9-C8	-2.30	1.36	1.39
4	L	2101	FMN	C9-C8	-2.29	1.36	1.39
4	K	2101	FMN	C9-C8	-2.27	1.36	1.39
4	J	2101	FMN	C6-C7	-2.24	1.36	1.39
4	H	2101	FMN	C9-C8	-2.23	1.36	1.39
4	L	2101	FMN	C6-C7	-2.22	1.36	1.39
4	G	2101	FMN	C6-C7	-2.18	1.36	1.39
4	K	2101	FMN	C6-C7	-2.18	1.36	1.39
4	H	2101	FMN	C6-C7	-2.14	1.36	1.39
4	H	2101	FMN	C2-N3	-2.05	1.34	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	2101	FMN	C2-N3	-2.00	1.34	1.39

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	2101	FMN	O4'-C4'-C5'	-3.45	102.39	109.99
4	K	2101	FMN	O4'-C4'-C5'	-3.44	102.39	109.99
4	L	2101	FMN	O4'-C4'-C5'	-3.40	102.50	109.99
4	H	2101	FMN	O4'-C4'-C5'	-3.38	102.53	109.99
4	J	2101	FMN	O4'-C4'-C5'	-3.37	102.56	109.99
4	I	2101	FMN	O4'-C4'-C5'	-3.33	102.64	109.99
3	F	1901	J8T	C5-C8-C9	3.04	119.49	113.69
3	A	1901	J8T	C5-C8-C9	3.04	119.49	113.69
3	D	1901	J8T	C5-C8-C9	3.03	119.47	113.69
3	E	1901	J8T	C5-C8-C9	3.03	119.47	113.69
3	C	1901	J8T	C5-C8-C9	3.02	119.45	113.69
3	B	1901	J8T	C5-C8-C9	3.01	119.44	113.69
4	J	2101	FMN	C4-C4A-N5	2.90	122.22	118.21
4	I	2101	FMN	C4-C4A-N5	2.87	122.18	118.21
4	L	2101	FMN	C4-C4A-N5	2.85	122.14	118.21
4	K	2101	FMN	C4-C4A-N5	2.84	122.13	118.21
4	G	2101	FMN	C4-C4A-N5	2.83	122.12	118.21
4	H	2101	FMN	C4-C4A-N5	2.82	122.10	118.21
4	K	2101	FMN	O3P-P-O5'	-2.77	99.44	106.67
4	G	2101	FMN	O3P-P-O5'	-2.76	99.47	106.67
4	L	2101	FMN	O2-C2-N1	-2.74	117.26	121.80
4	G	2101	FMN	O2-C2-N1	-2.71	117.29	121.80
4	H	2101	FMN	C4A-C10-N1	-2.70	117.98	124.59
4	L	2101	FMN	O3P-P-O5'	-2.70	99.64	106.67
4	I	2101	FMN	O3P-P-O5'	-2.69	99.65	106.67
4	J	2101	FMN	O3P-P-O5'	-2.69	99.66	106.67
4	H	2101	FMN	O2-C2-N1	-2.69	117.34	121.80
4	J	2101	FMN	O2-C2-N1	-2.68	117.34	121.80
4	K	2101	FMN	O2-C2-N1	-2.68	117.35	121.80
4	H	2101	FMN	O3P-P-O5'	-2.68	99.69	106.67
4	I	2101	FMN	C4A-C10-N1	-2.68	118.03	124.59
4	J	2101	FMN	C4A-C10-N1	-2.66	118.08	124.59
4	L	2101	FMN	C4A-C10-N1	-2.65	118.10	124.59
4	K	2101	FMN	C4A-C10-N1	-2.64	118.13	124.59
4	I	2101	FMN	O2-C2-N1	-2.62	117.44	121.80
4	G	2101	FMN	C4A-C10-N1	-2.58	118.26	124.59
4	K	2101	FMN	O4-C4-C4A	-2.57	119.74	126.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	2101	FMN	O4-C4-C4A	-2.57	119.75	126.53
4	J	2101	FMN	O4-C4-C4A	-2.52	119.88	126.53
4	J	2101	FMN	C10-N1-C2	2.46	122.18	116.85
4	I	2101	FMN	O4-C4-C4A	-2.46	120.04	126.53
4	L	2101	FMN	O4-C4-C4A	-2.45	120.06	126.53
4	H	2101	FMN	O4-C4-C4A	-2.45	120.07	126.53
4	I	2101	FMN	C10-N1-C2	2.44	122.12	116.85
4	H	2101	FMN	C10-N1-C2	2.39	122.02	116.85
4	L	2101	FMN	C10-N1-C2	2.39	122.02	116.85
4	K	2101	FMN	C10-N1-C2	2.37	121.98	116.85
4	G	2101	FMN	C10-N1-C2	2.34	121.91	116.85
4	G	2101	FMN	C4'-C3'-C2'	-2.28	109.78	113.57
4	K	2101	FMN	C4'-C3'-C2'	-2.27	109.80	113.57
4	I	2101	FMN	C10-C4A-N5	-2.27	120.18	124.81
4	L	2101	FMN	C10-C4A-N5	-2.25	120.22	124.81
4	H	2101	FMN	C10-C4A-N5	-2.24	120.24	124.81
4	K	2101	FMN	C10-C4A-N5	-2.24	120.24	124.81
4	J	2101	FMN	C10-C4A-N5	-2.24	120.24	124.81
4	G	2101	FMN	C10-C4A-N5	-2.19	120.33	124.81
4	J	2101	FMN	C4'-C3'-C2'	-2.16	109.98	113.57
4	I	2101	FMN	C5A-N5-C4A	2.15	121.57	118.09
4	H	2101	FMN	C4-N3-C2	-2.13	121.85	125.64
4	K	2101	FMN	C5A-N5-C4A	2.12	121.52	118.09
4	K	2101	FMN	C4-N3-C2	-2.11	121.89	125.64
4	L	2101	FMN	C4-N3-C2	-2.11	121.90	125.64
4	G	2101	FMN	C5A-N5-C4A	2.10	121.48	118.09
4	G	2101	FMN	C4-N3-C2	-2.10	121.92	125.64
4	L	2101	FMN	C4'-C3'-C2'	-2.10	110.08	113.57
4	H	2101	FMN	C5A-N5-C4A	2.07	121.44	118.09
4	J	2101	FMN	C5A-N5-C4A	2.07	121.43	118.09
4	J	2101	FMN	C4-N3-C2	-2.04	122.02	125.64
4	L	2101	FMN	C5A-N5-C4A	2.04	121.39	118.09
4	I	2101	FMN	C4-N3-C2	-2.04	122.02	125.64

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1901	J8T	O6-C8-C9-O7
3	A	1901	J8T	O6-C8-C9-N2
3	B	1901	J8T	O6-C8-C9-O7
3	B	1901	J8T	O6-C8-C9-N2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	C	1901	J8T	O6-C8-C9-O7
3	C	1901	J8T	O6-C8-C9-N2
3	D	1901	J8T	O6-C8-C9-O7
3	D	1901	J8T	O6-C8-C9-N2
3	E	1901	J8T	O6-C8-C9-O7
3	E	1901	J8T	O6-C8-C9-N2
3	F	1901	J8T	O6-C8-C9-O7
3	F	1901	J8T	O6-C8-C9-N2
3	A	1901	J8T	O5-C4-C5-C6
3	A	1901	J8T	O5-C4-C5-C7
3	B	1901	J8T	O5-C4-C5-C6
3	B	1901	J8T	O5-C4-C5-C7
3	C	1901	J8T	O5-C4-C5-C6
3	C	1901	J8T	O5-C4-C5-C7
3	D	1901	J8T	O5-C4-C5-C6
3	D	1901	J8T	O5-C4-C5-C7
3	E	1901	J8T	O5-C4-C5-C6
3	E	1901	J8T	O5-C4-C5-C7
3	F	1901	J8T	O5-C4-C5-C6
3	F	1901	J8T	O5-C4-C5-C7
4	G	2101	FMN	C4'-C5'-O5'-P
4	H	2101	FMN	C4'-C5'-O5'-P
4	I	2101	FMN	C4'-C5'-O5'-P
4	J	2101	FMN	C4'-C5'-O5'-P
4	K	2101	FMN	C4'-C5'-O5'-P
4	L	2101	FMN	C4'-C5'-O5'-P
4	G	2101	FMN	C2'-C3'-C4'-C5'
4	L	2101	FMN	C2'-C3'-C4'-C5'
4	K	2101	FMN	C2'-C3'-C4'-C5'
4	L	2101	FMN	C1'-C2'-C3'-C4'
4	L	2101	FMN	O3'-C3'-C4'-C5'
4	G	2101	FMN	O3'-C3'-C4'-C5'
3	B	1901	J8T	C5-C8-C9-O7
4	H	2101	FMN	C2'-C3'-C4'-C5'

There are no ring outliers.

12 monomers are involved in 12 short contacts:

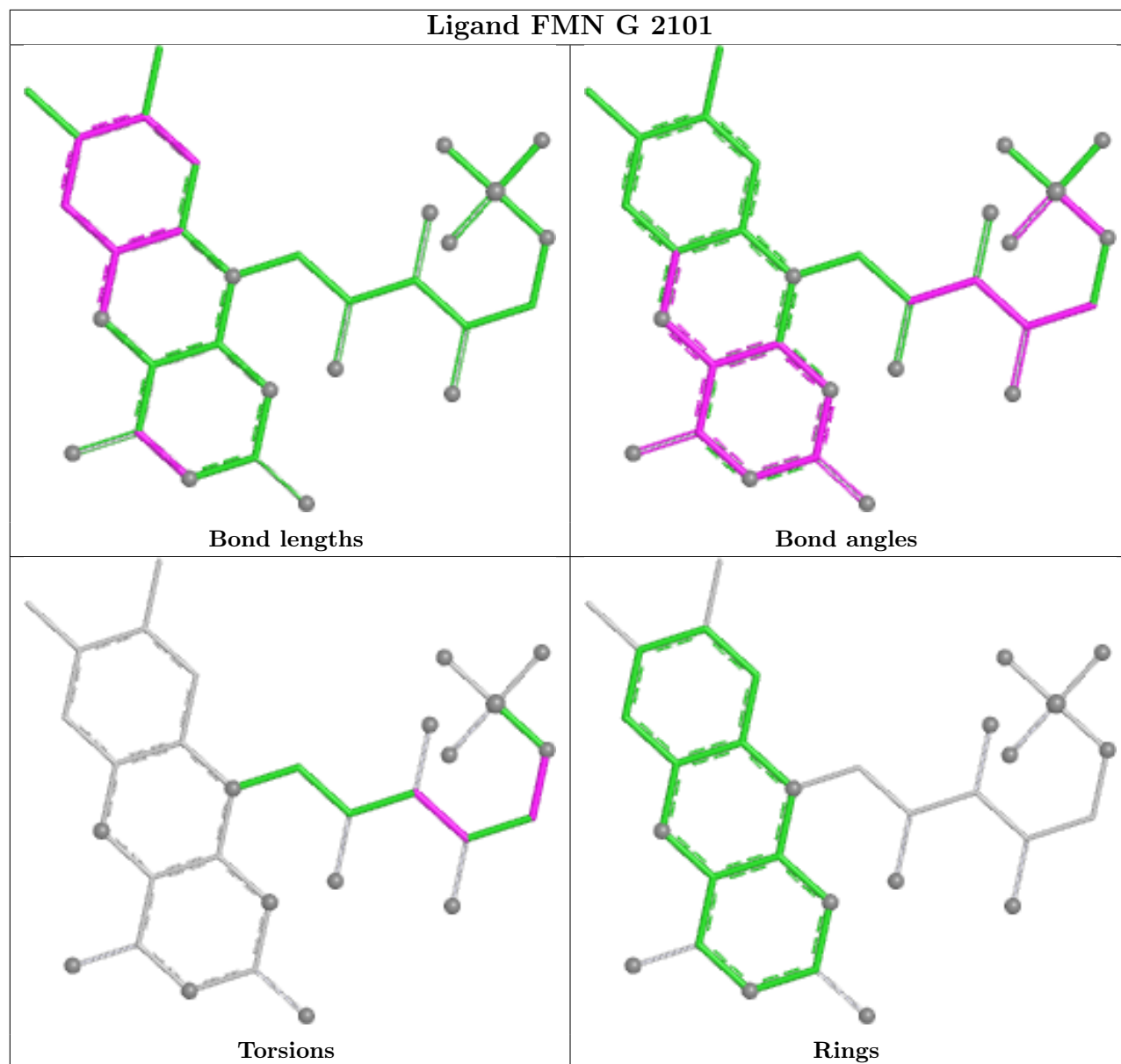
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1901	J8T	1	0
4	G	2101	FMN	1	0
4	H	2101	FMN	1	0

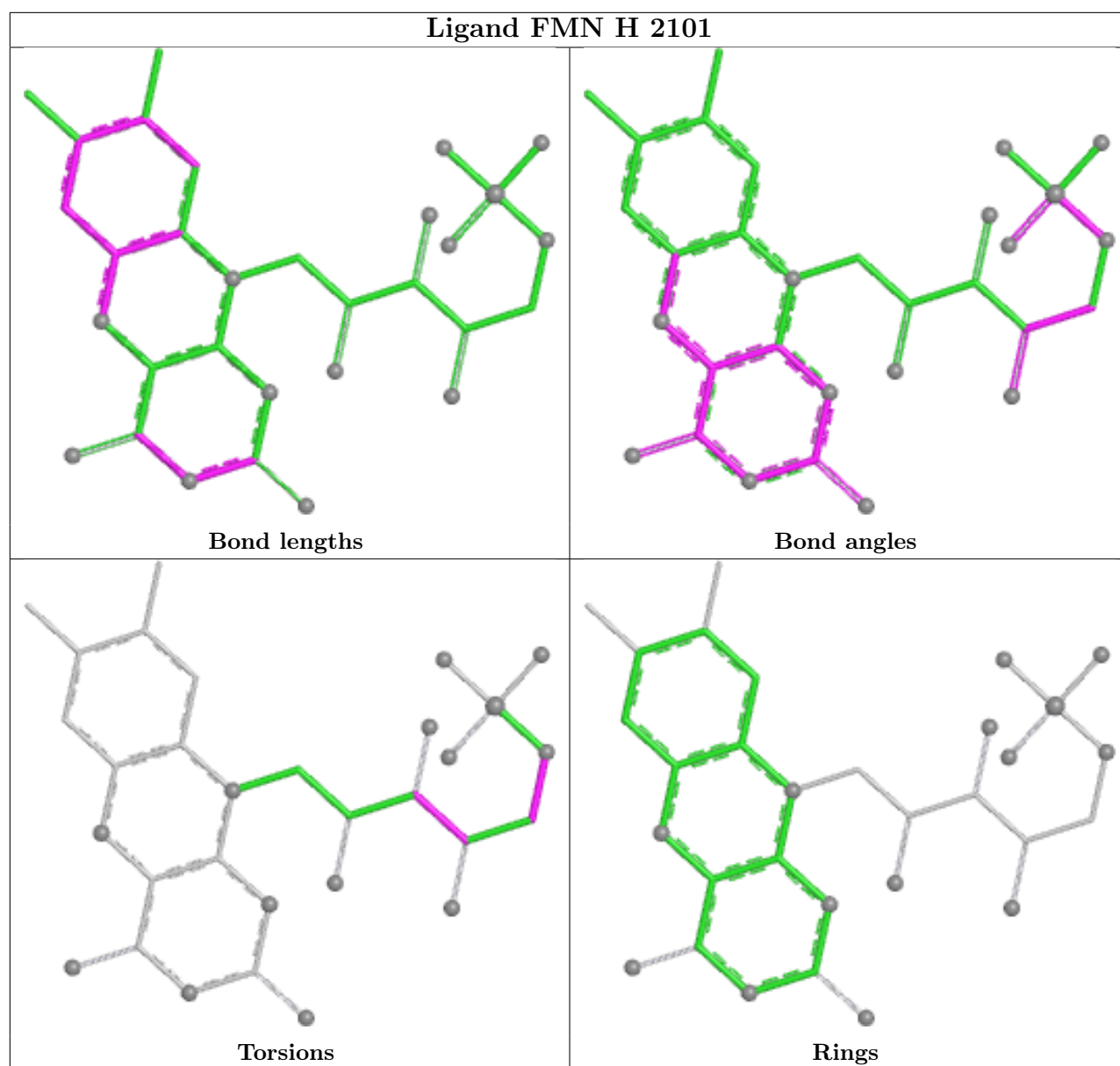
Continued on next page...

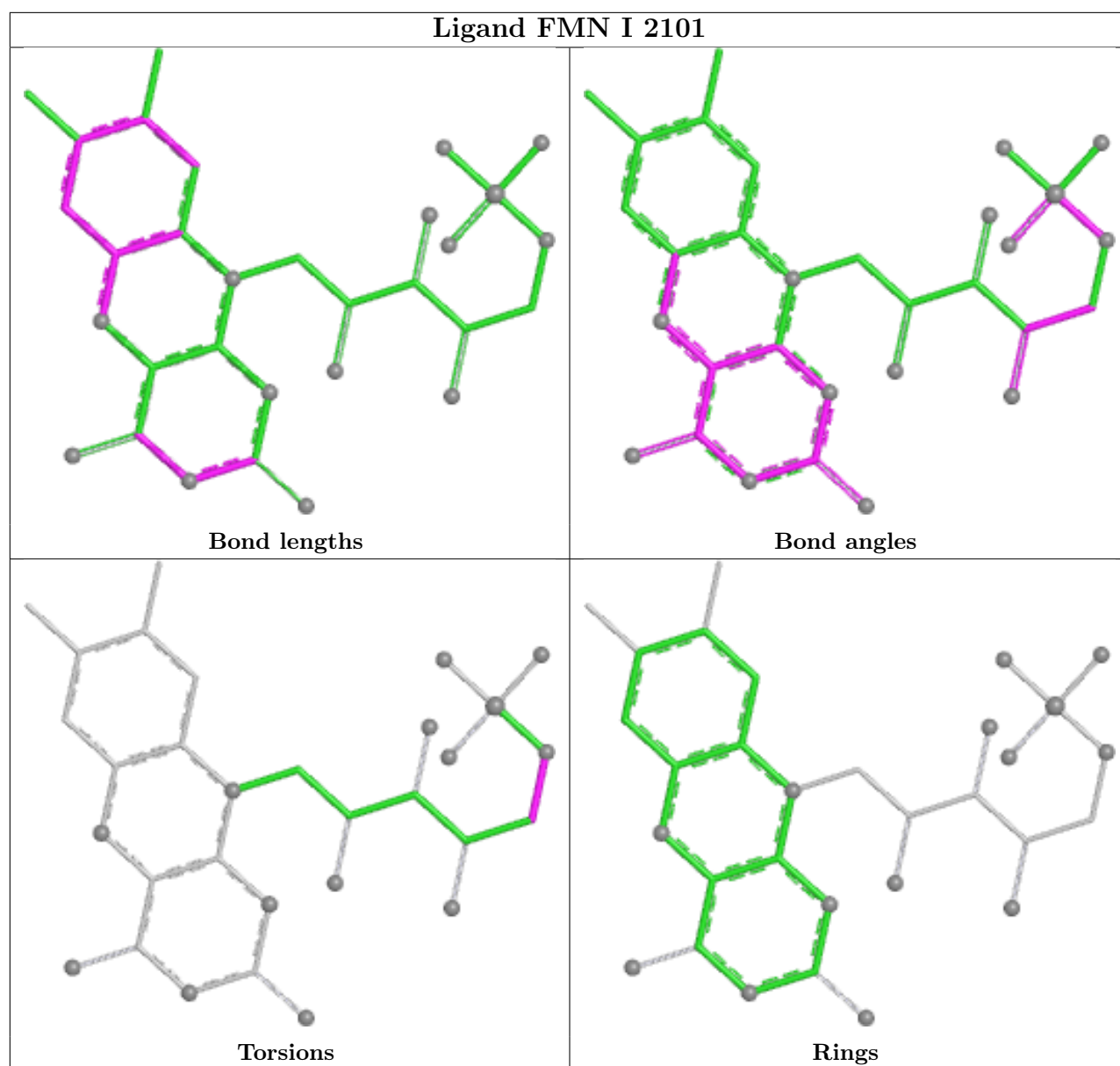
Continued from previous page...

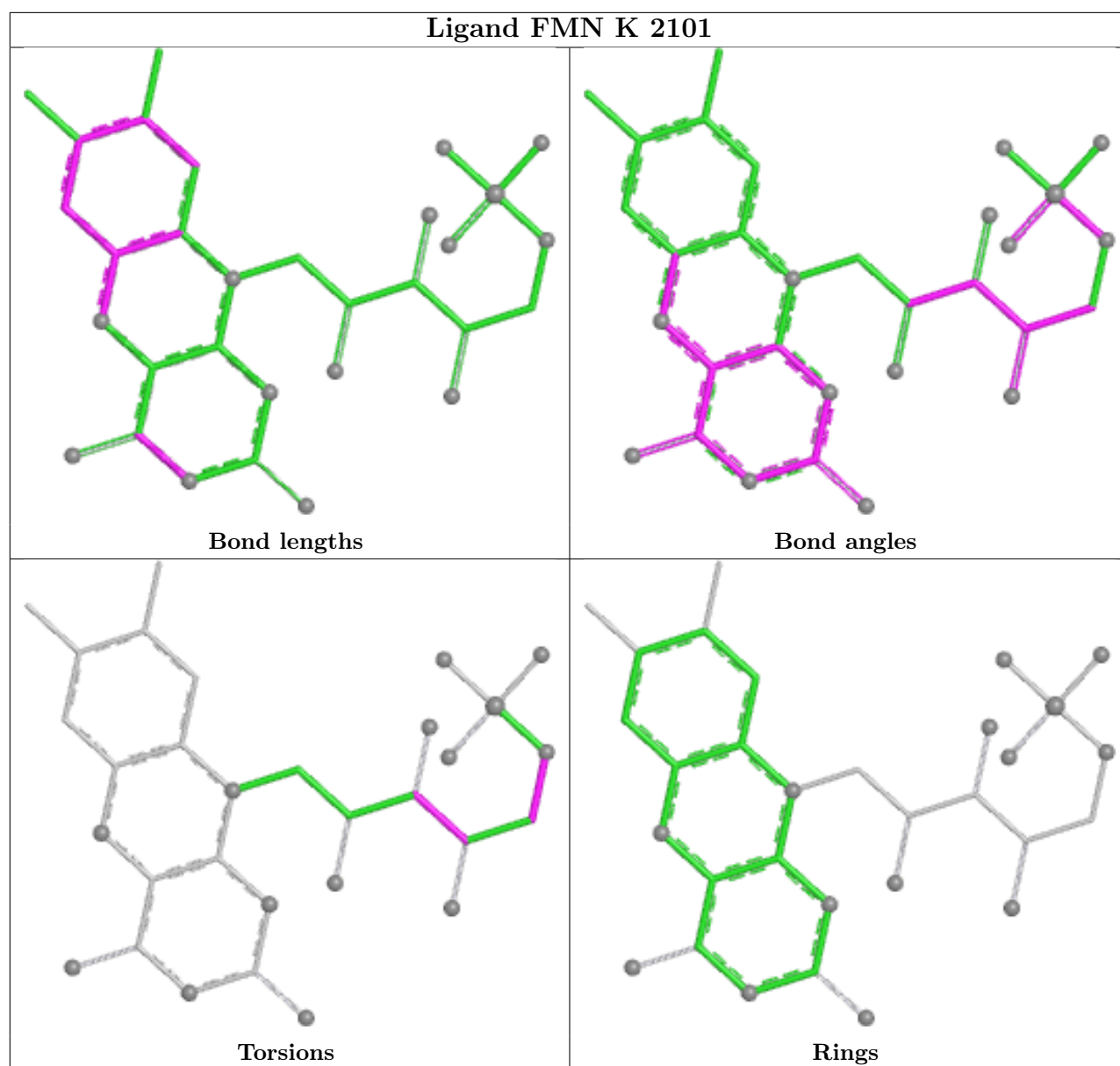
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	1901	J8T	1	0
3	C	1901	J8T	1	0
4	I	2101	FMN	1	0
4	K	2101	FMN	1	0
4	L	2101	FMN	1	0
4	J	2101	FMN	1	0
3	D	1901	J8T	1	0
3	A	1901	J8T	1	0
3	F	1901	J8T	1	0

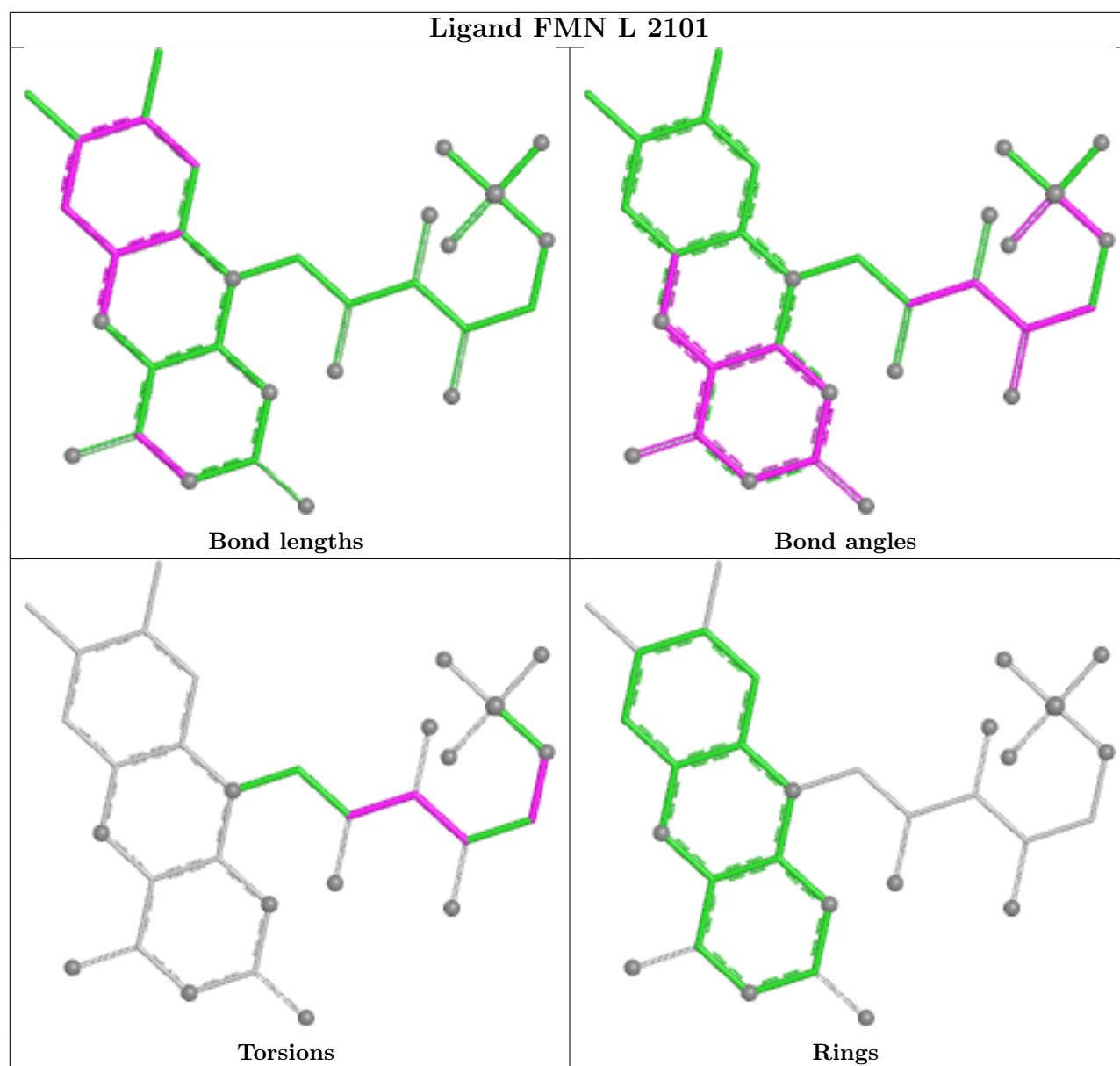
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

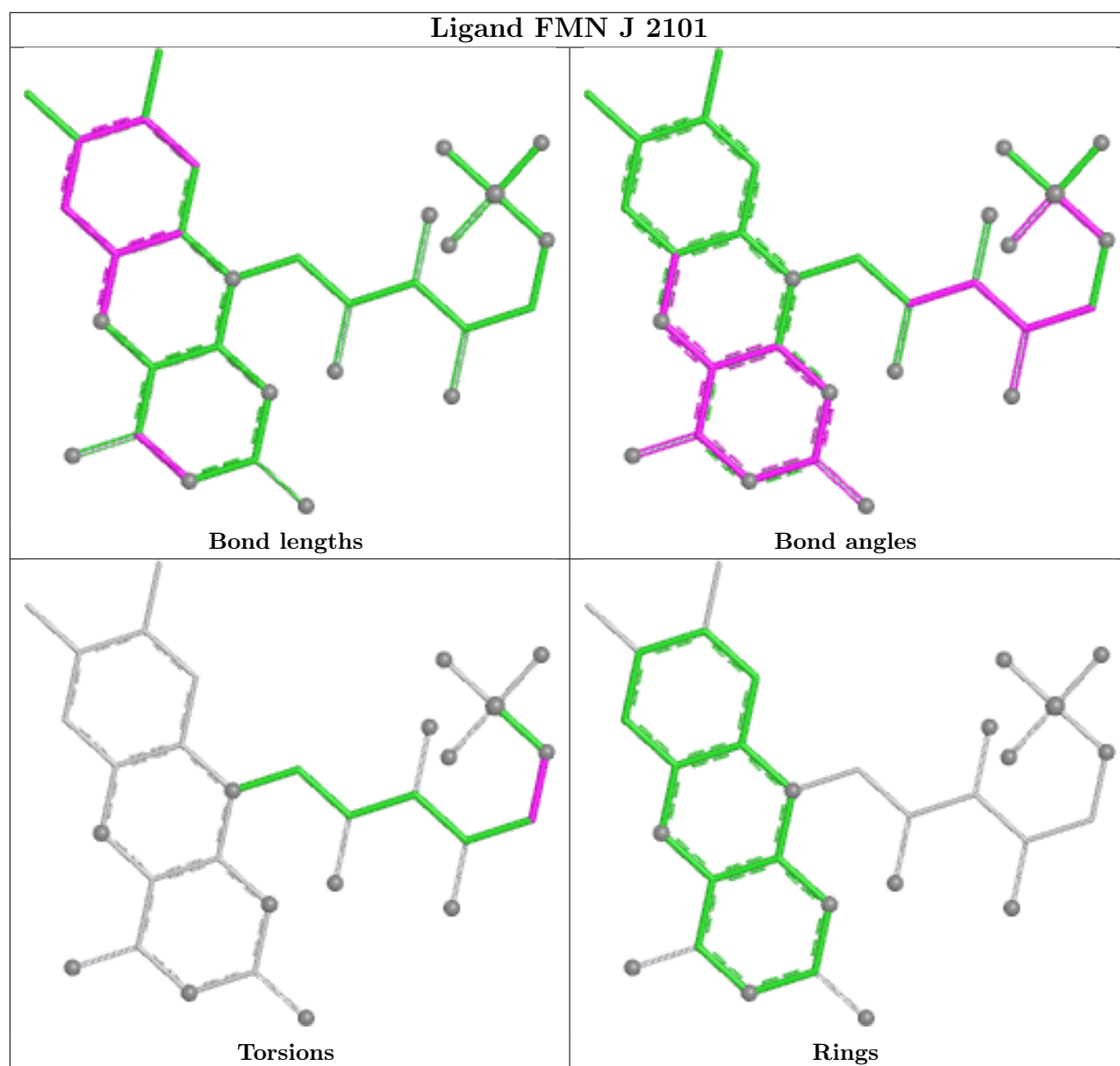












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

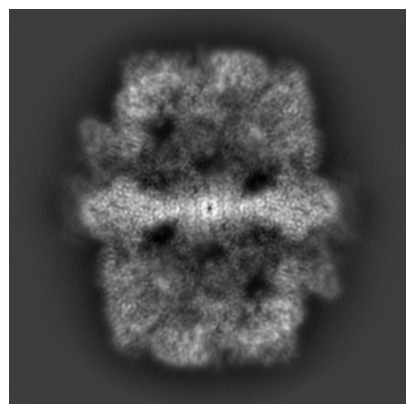
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4578. These allow visual inspection of the internal detail of the map and identification of artifacts.

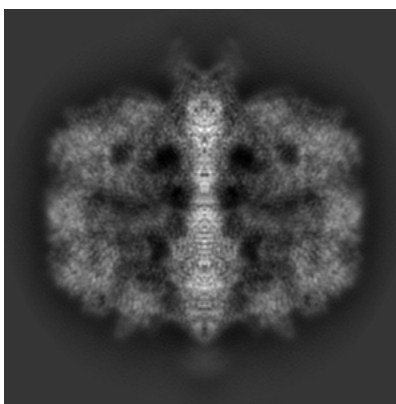
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

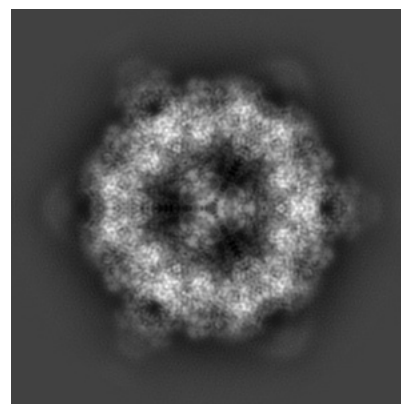
6.1.1 Primary map



X

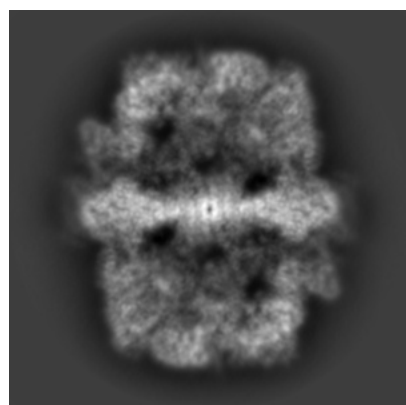


Y

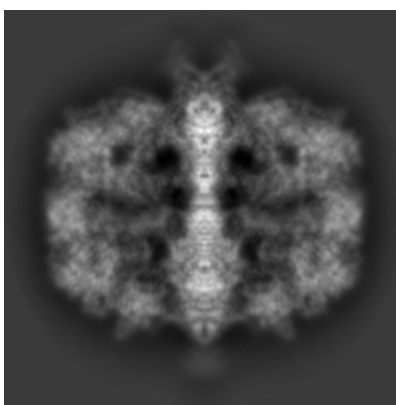


Z

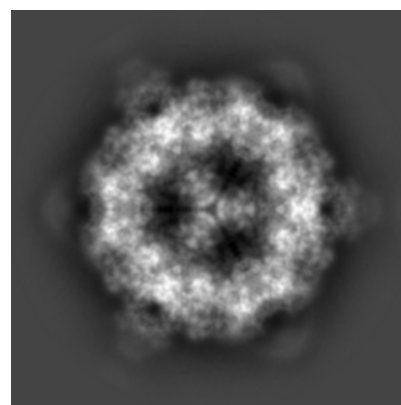
6.1.2 Raw map



X



Y

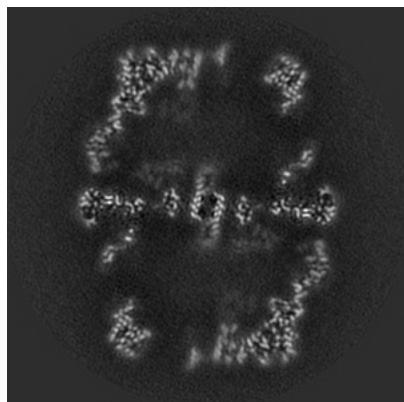


Z

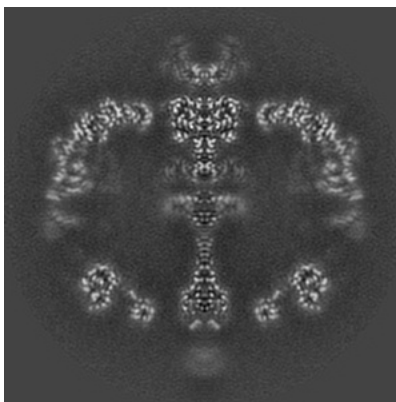
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

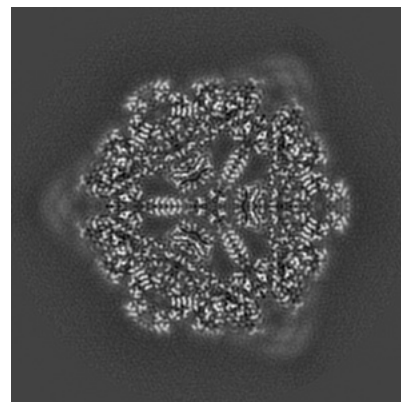
6.2.1 Primary map



X Index: 160

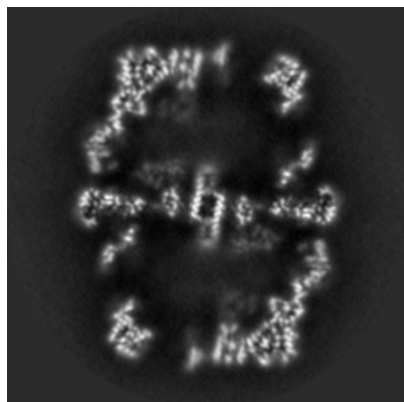


Y Index: 160

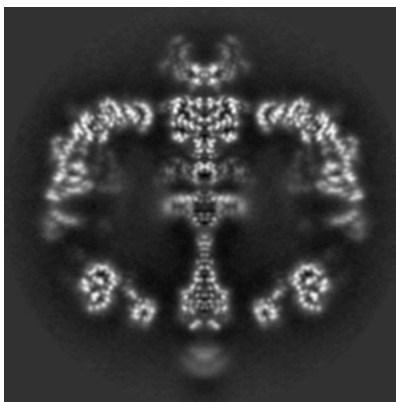


Z Index: 160

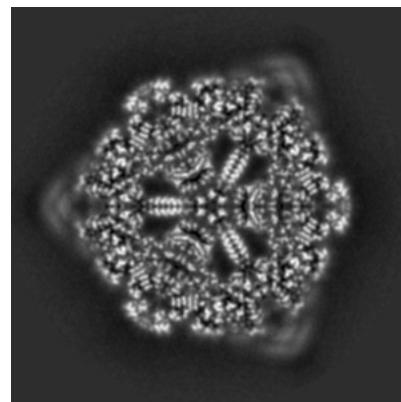
6.2.2 Raw map



X Index: 160



Y Index: 160

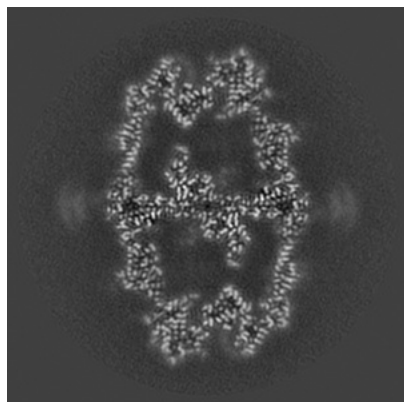


Z Index: 160

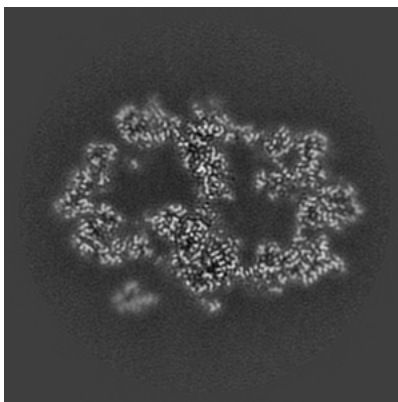
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

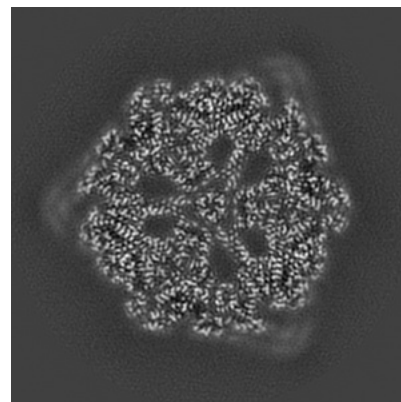
6.3.1 Primary map



X Index: 216

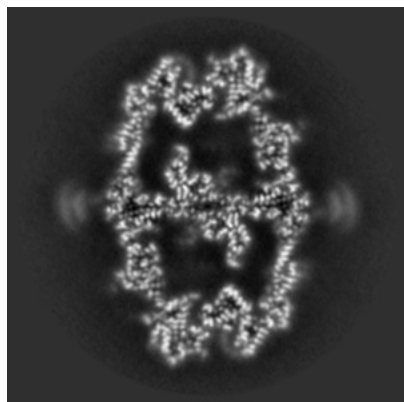


Y Index: 98

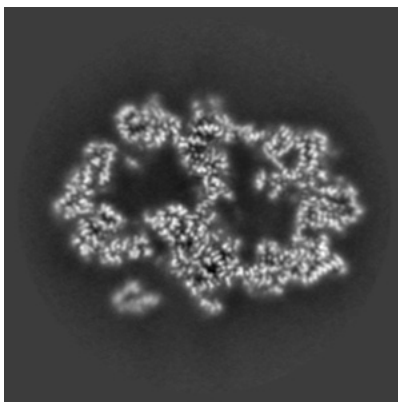


Z Index: 157

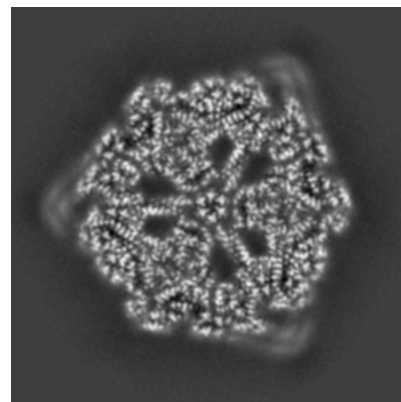
6.3.2 Raw map



X Index: 216



Y Index: 99

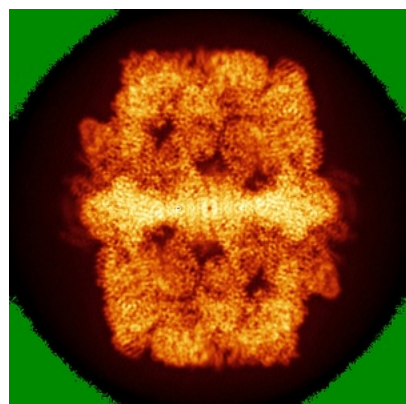


Z Index: 157

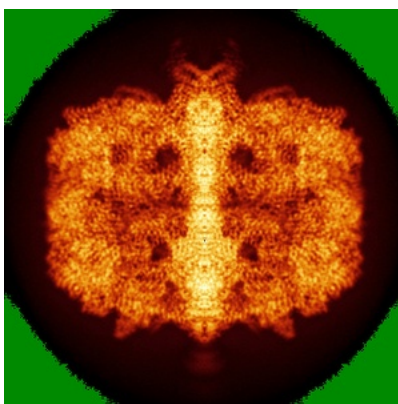
The images above show the largest variance slices of the map in three orthogonal directions.

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

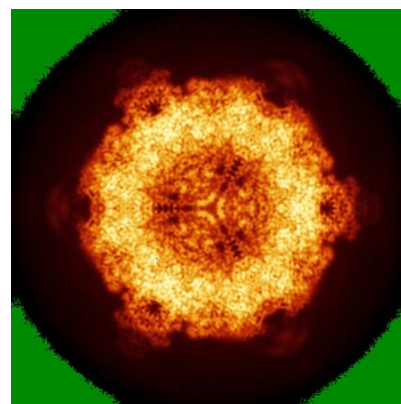
6.4.1 Primary map



X

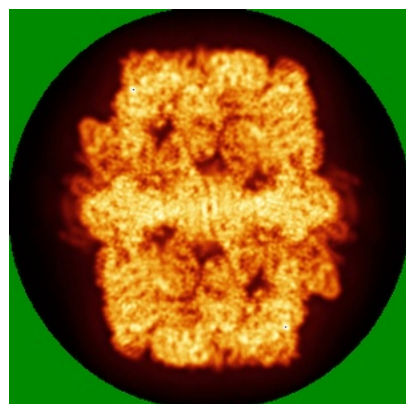


Y

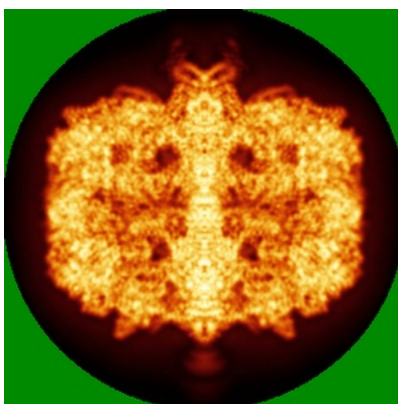


Z

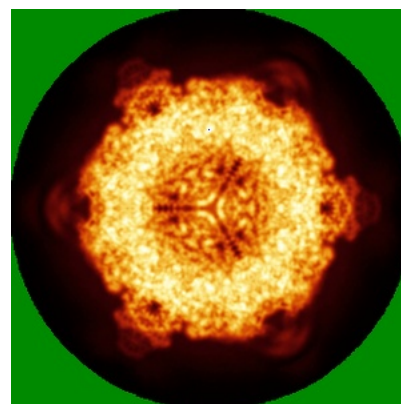
6.4.2 Raw map



X



Y

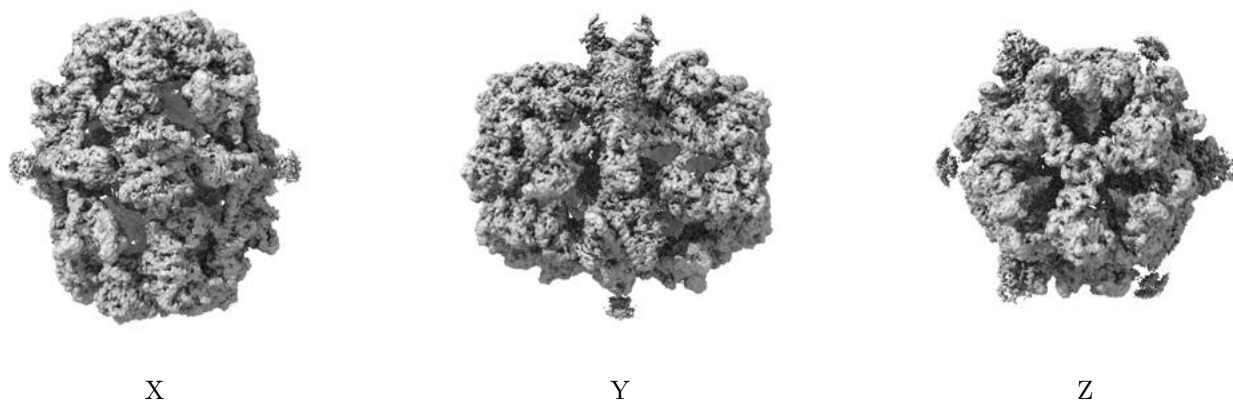


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

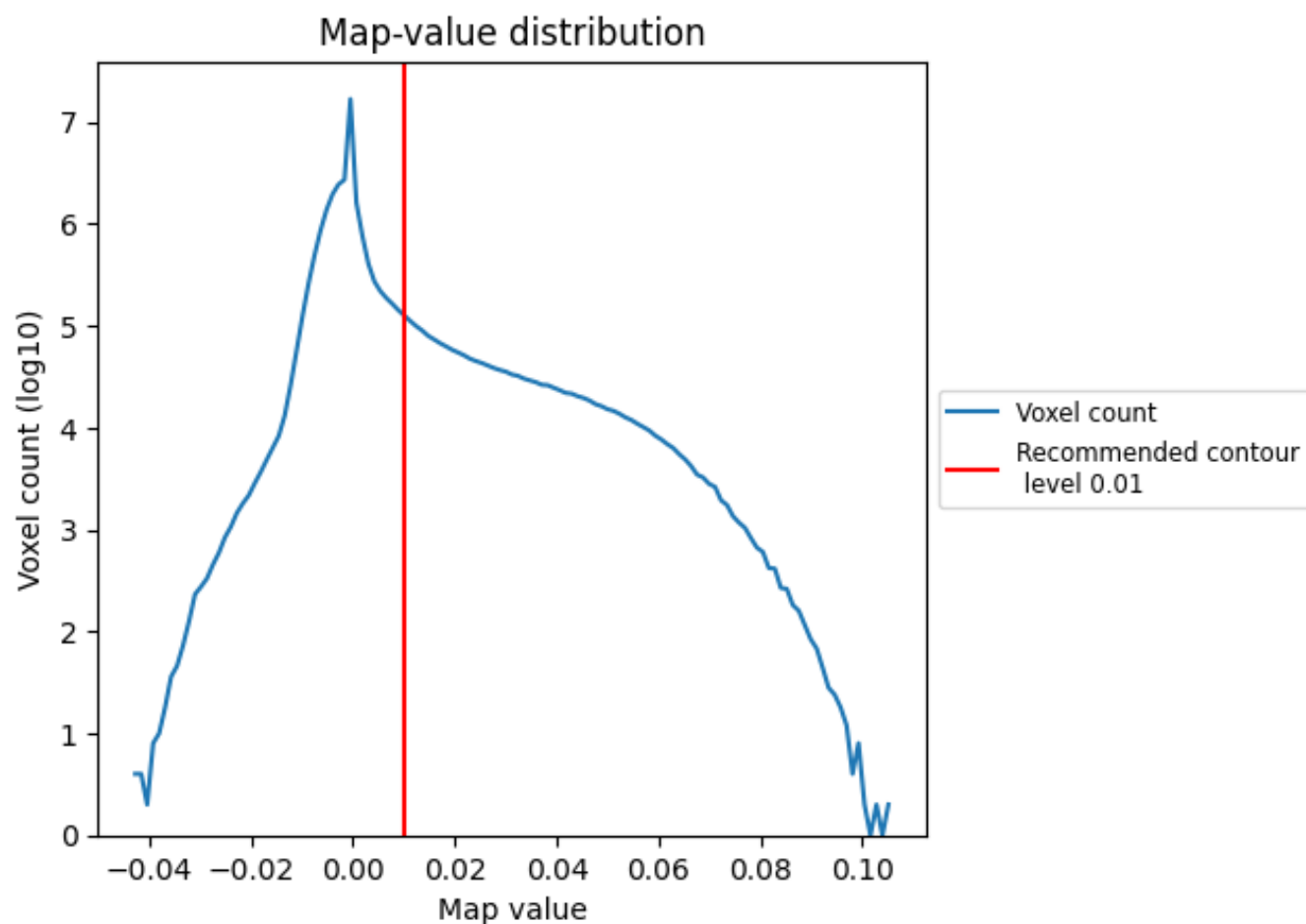
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

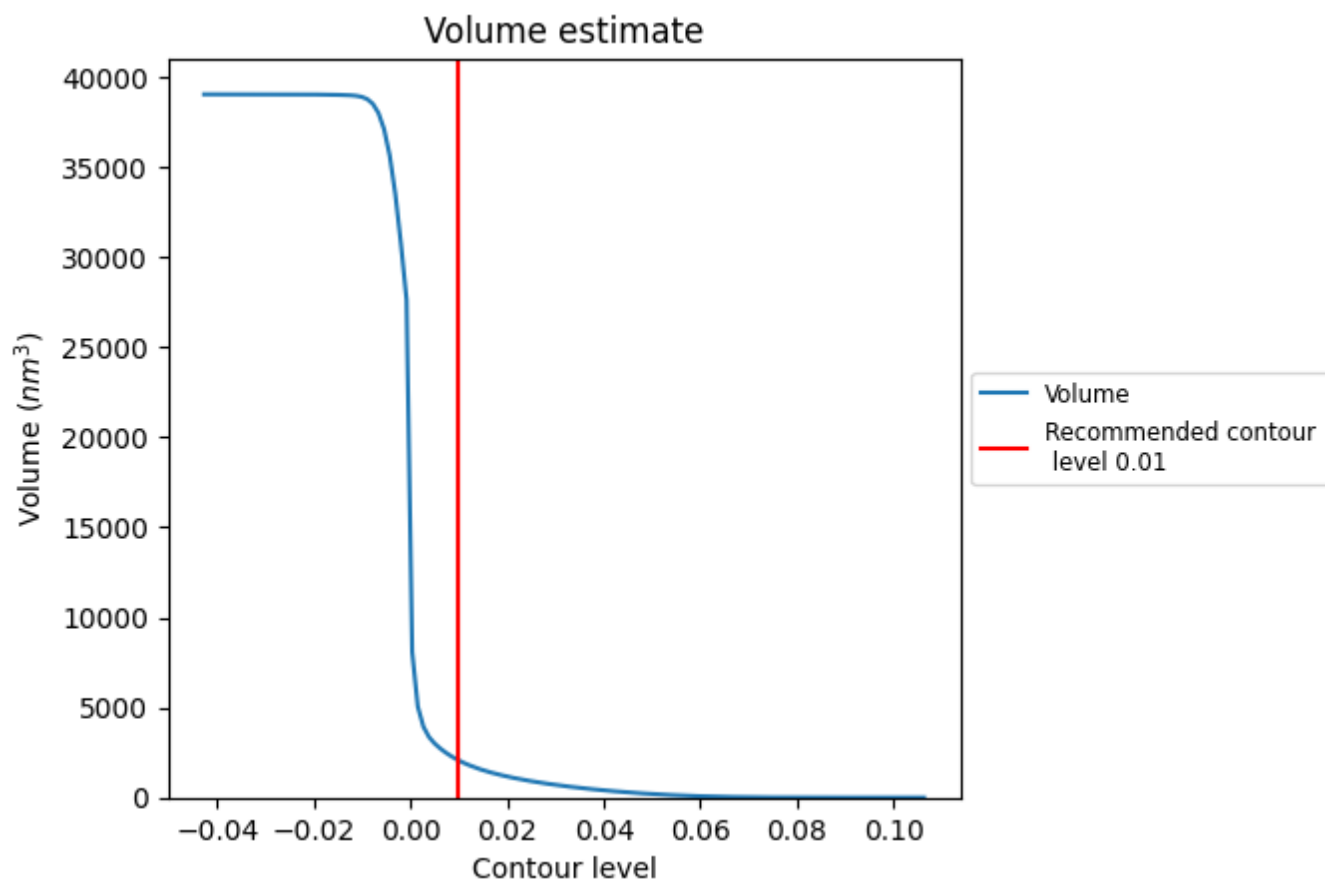
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

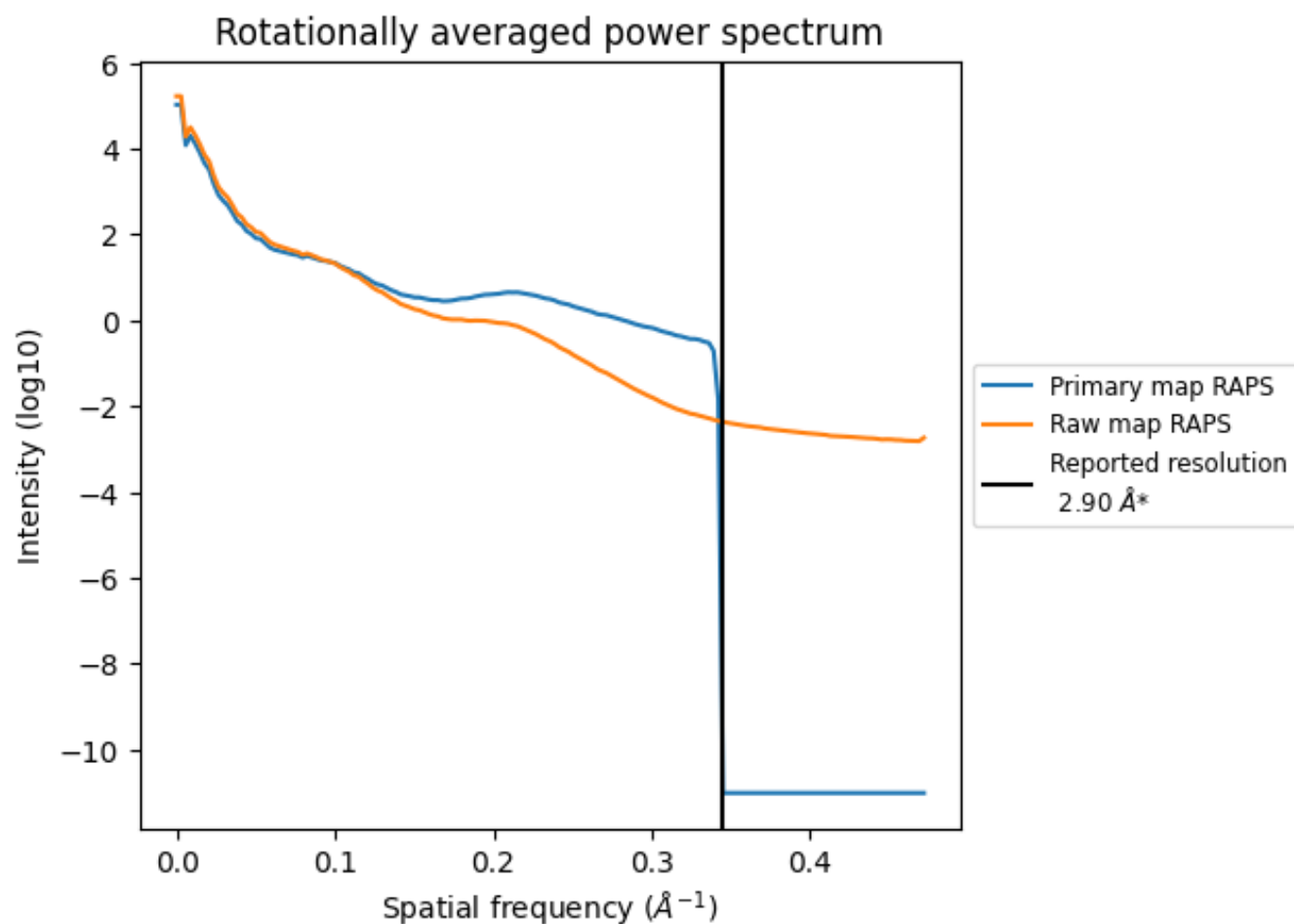
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2062 nm³; this corresponds to an approximate mass of 1862 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 ⓘ

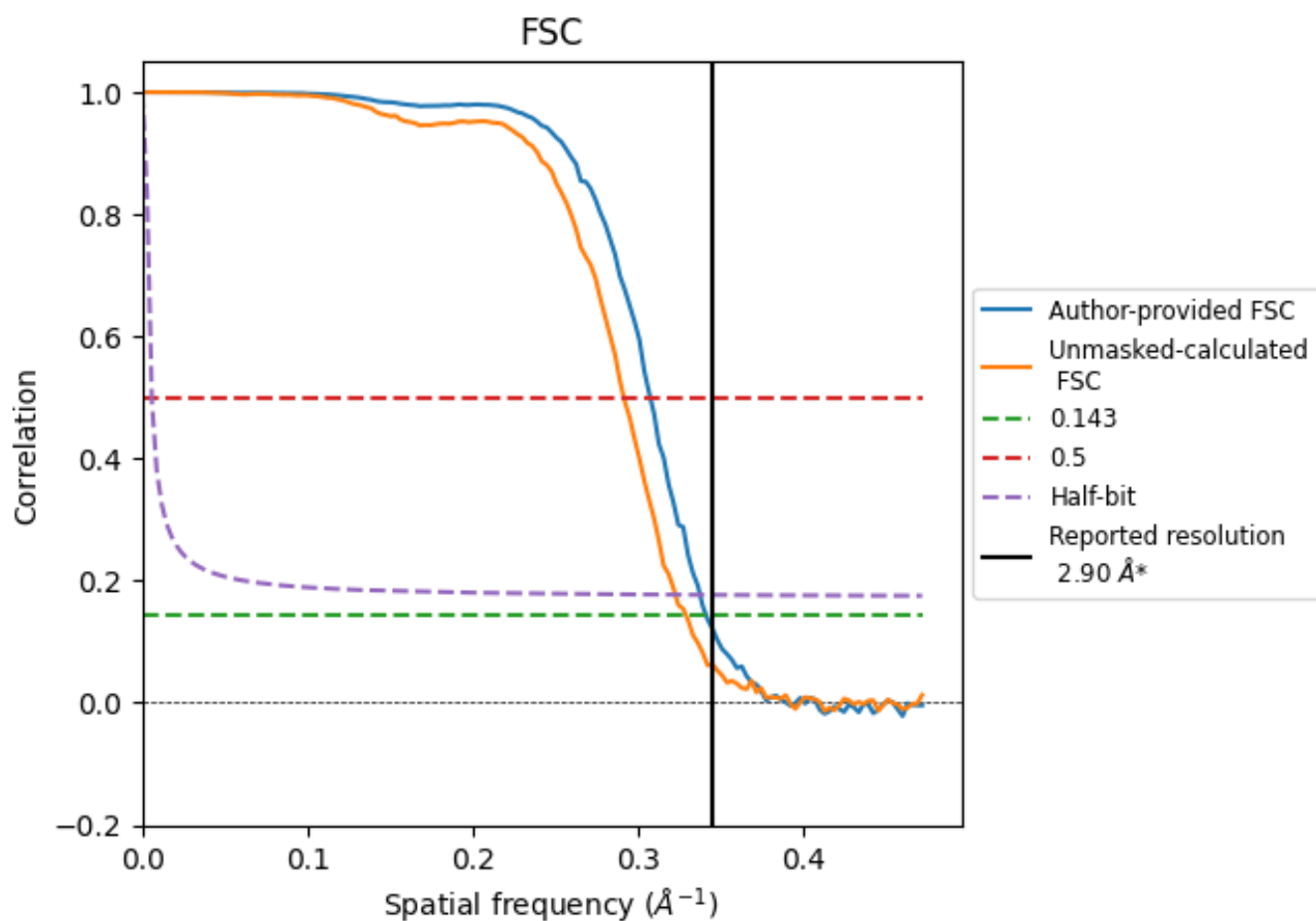


*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.345 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.93	3.25	2.96
Unmasked-calculated*	3.04	3.43	3.10

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

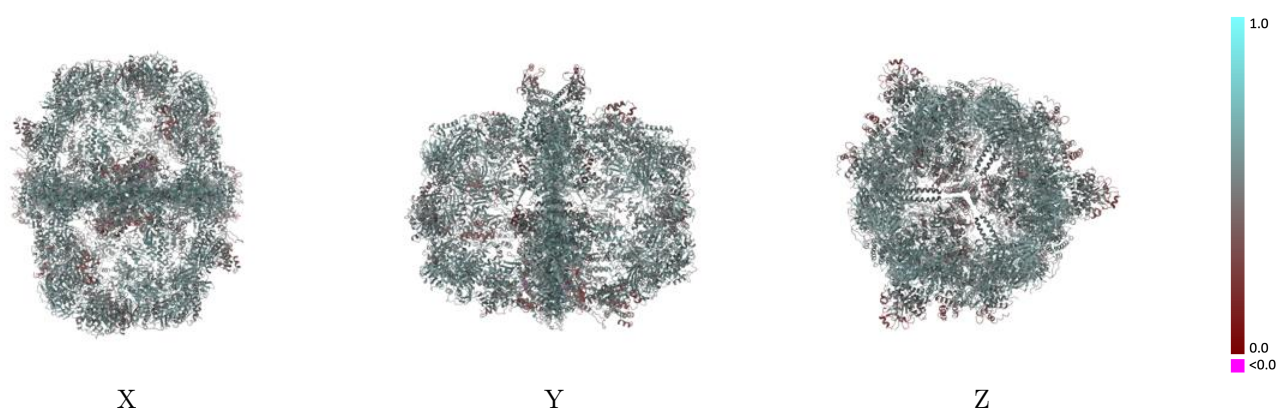
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-4578 and PDB model 6QL6. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)

This section was not generated.

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

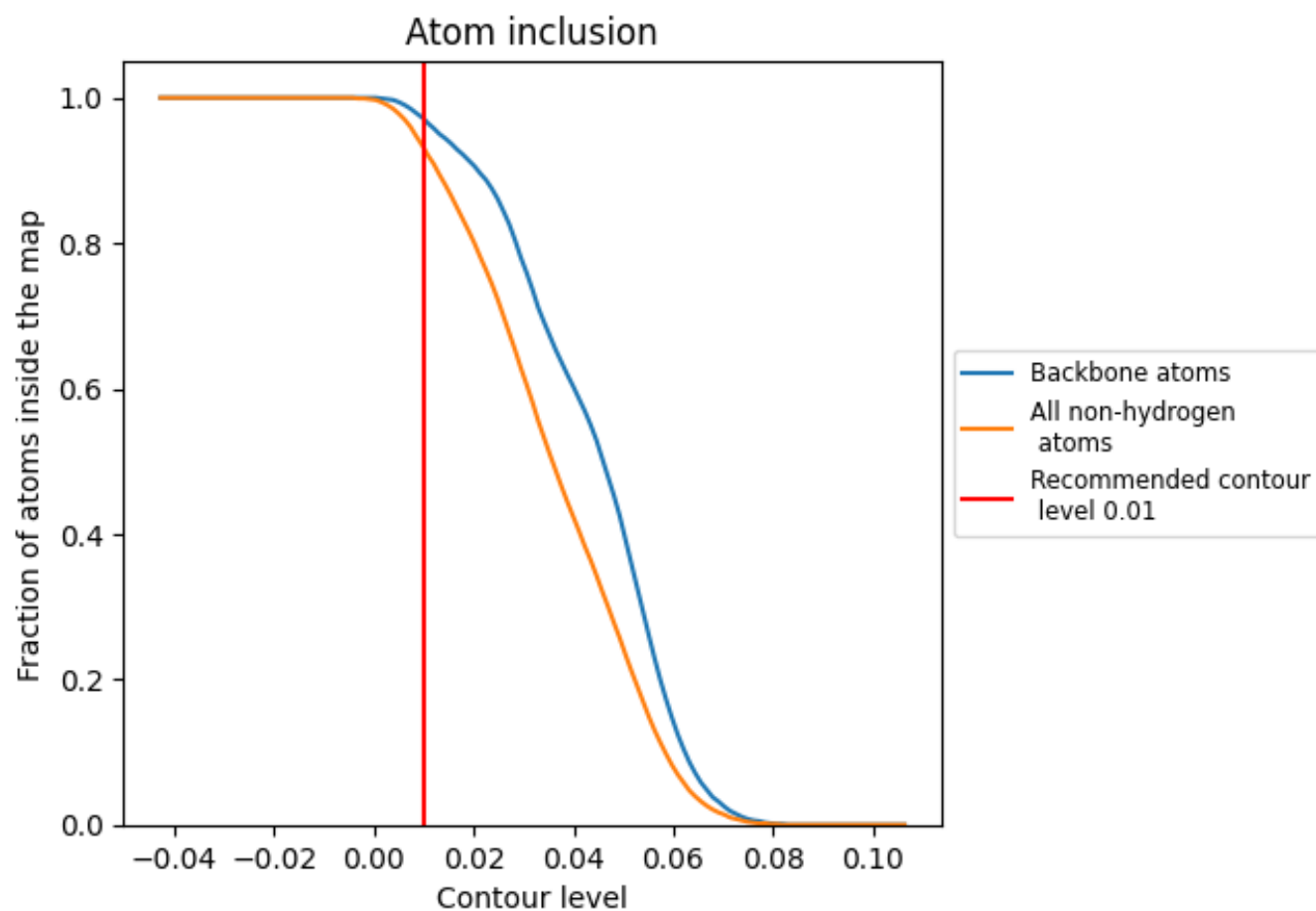


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion ⓘ



At the recommended contour level, 97% of all backbone atoms, 93% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9310	0.5370
A	0.8830	0.5440
B	0.8840	0.5440
C	0.8830	0.5440
D	0.8840	0.5440
E	0.8830	0.5450
F	0.8830	0.5450
G	0.9720	0.5320
H	0.9720	0.5310
I	0.9720	0.5300
J	0.9720	0.5310
K	0.9720	0.5310
L	0.9710	0.5310

1.0

0.0

<0.0