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PDB ID	:	6QL6
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 (i) 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 (1)) were used in the production of this report:

EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7(2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 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.



Motrie	Whole archive	EM structures
Metric	$(\# { m Entries})$	$(\# { m Entries})$
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=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 <=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	А	1887	6% 80%	12% • 7%
1	В	1887	6% 80%	12% • 7%
1	С	1887	80%	11% • 7%
1	D	1887	80%	11% • 7%
1	Е	1887	80%	12% • 7%
1	F	1887	80%	12% • 7%
2	G	2040	86%	12% •
2	Н	2040	86%	13% •



Mol	Chain	Length	Quality of chain		
2	Ι	2040	86%	13%	
2	J	2040	86%	13%	•
2	K	2040	86%	13%	•
2	L	2040	86%	13%	



2 Entry composition (i)

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.

Mol	Chain	Residues		Α	toms			AltConf	Trace		
1	Δ	1757	Total	С	Ν	Ο	S	0	0		
1 I	Π	1101	13665	8650	2305	2658	52	0	0		
1	В	1757	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	0		
1	D	1101	13665	8650	2305	2658	52	0	0		
1	С	1757	Total	С	Ν	Ο	\mathbf{S}	0	0		
1	U	1101	13665	8650	2305	2658	52	0	0		
1	Л	1757	Total	С	Ν	Ο	\mathbf{S}	0	0		
1	D	1757	13665	8650	2305	2658	52	0	0		
1	F	1757	Total	С	Ν	Ο	\mathbf{S}	0	0		
L	Ľ	1101	13665	8650	2305	2658	52	0	0		
1	F	1757	Total	С	Ν	Ο	S	0	0		
		1757	1757	1757	13665	8650	2305	2658	52		0

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

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

Mol	Chain	Residues		At	toms			AltConf	Trace
9	С	2036	Total	С	Ν	Ο	\mathbf{S}	0	0
	G	2030	16018	10265	2663	3034	56	0	0
9	ц	2036	Total	С	Ν	Ο	\mathbf{S}	0	0
	11	2030	16018	10265	2663	3034	56	0	0
9	т	2036	Total	С	Ν	Ο	\mathbf{S}	0	0
	1	2030	16018	10265	2663	3034	56	0	0
9	т	2036	Total	С	Ν	Ο	\mathbf{S}	0	0
	J	2030	16018	10265	2663	3034	56	0	0
9	K	2036	Total	С	Ν	Ο	\mathbf{S}	0	0
	Γ	2030	16018	10265	2663	3034	56	0	0
2	Т	2036	Total	C	N	Ō	S	0	0
		2030	16018	10265	2663	3034	56	0	0

• Molecule 3 is [(3 {R})-4-azanyl-2,2-dimethyl-3-oxidanyl-4-oxidanylidene-butyl] dihydrogen phosphate (three-letter code: J8T) (formula: $C_6H_{14}NO_6P$).





Mol	Chain	Residues		AltConf				
3	Λ	1	Total	С	Ν	0	Р	0
0	Л	T	13	6	1	5	1	0
3	В	1	Total	С	Ν	0	Р	0
0	D	T	13	6	1	5	1	0
3	С	1	Total	С	Ν	0	Р	0
0	U	T	13	6	1	5	1	0
3	Л	1	Total	С	Ν	0	Р	0
0	D	T	13	6	1	5	1	0
3	F	1	Total	С	Ν	0	Р	0
0	Ľ	T	13	6	1	5	1	0
3	F	1	Total	С	Ν	0	Р	0
0	T,		13	6	1	5	1	

• Molecule 4 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).





Mol	Chain	Residues			AltConf			
4	С	1	Total	С	Ν	0	Р	0
4	G	1	31	17	4	9	1	0
4	н	1	Total	С	Ν	Ο	Р	0
4	11	T	31	17	4	9	1	0
4	T	1	Total	С	Ν	Ο	Р	0
4	L	T	31	17	4	9	1	0
4	T	1	Total	С	Ν	Ο	Р	0
-1	0	T	31	17	4	9	1	0
4	K	1	Total	С	Ν	Ο	Р	0
T	17	1	31	17	4	9	1	0
1	T.	1	Total	C	N	Ō	Р	0
		1	31	17	4	9	1	0



3 Residue-property plots (i)

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

• Molecule 1: Fatty acid synthase subunit alpha



N1780 M1580 N1780 01541 V1781 01545 N1783 01577 N1783 01577 N1784 01577 N1785 01576 N1785 01577 N1785 01576 R1785 01612 C1831 01612 C1832 01612 C1833 01612 C1834 01612 C1833 01643 L1334 01643 A1845 01643 A1843 01643 A1843 01643 A1844 01643 A1845 11641 A1844 017673 A1845 11643 A1846 01717 A1845 11643 A1845 11766 A1845 11764 A1845 1176 A1855 1176 A1856 1176 A1866 11764 A1866





• Molecule 1: Fatty acid synthase subunit alpha









• Molecule 2: Fatty acid synthase subunit beta





E1333 S1763 II 490 M.26 M.297 M.293 M.293 M.293 M.201 M.297 M.297 M.297 M.293 <th

• Molecule 2: Fatty acid synthase subunit beta

Chain H:	86%	13% •
55 R 7 P 8 L 9 L 9 C 2 Q 3 Q 3 Q 3 Q 3 Q 3 Q 3 Q 3 Q 3 Q 3 Q 3	E46 B52 KG3 E90 E90 C94 C94 C94 C94 C94 C94 C94 C94 C94 C94	L122 K140 F146 T166 T166 L173 L173 L173 L173 F190 F190
T194 1198 223 223 233 233 233 233 233 233 233 23	L267 A270 1277 1277 1285 1285 1285 1286 1285 1286 1285 1286 1286 13915 1286 1339 13315 13315 13315 1332 1332 1332 1332 1	L346 T345 T345 V355 V355 V355 V355 R419 R419 R419 R419 V433 V433 V433
A435 8436 8436 1448 1448 1448 1448 1490 1493 1493 1493	F4995 F4995 K497 S510 S510 S510 F515 F515 F546 E546 E546 E546 F545 F545 F545 F546 F546 F546 F546 F	1558 P599 P699 P602 1663 1663 1663 1663 1663 1663 1663 166
1717 1730 1730 1730 1730 1730 1772 1772 1777 1777	P7779 M794 M794 W805 V805 V805 V805 V805 V805 V846 V805 V846 V805 V846 V805 V846 V805 V846 V805 V805 V805 V805 V805 V805 V805 V805	E810 1874 887 8834 8834 1894 1946 1946 1947 1947
E965 K962 L972 K975 K975 A997 A997 D1000 D1000 D1001 K1031 K1031 S1033	L1040 V1044 V1048 L1054 L1054 L1056 H1061 L1065 F1103 F1103 F1103 CML G110 G111 G1121 CML	51131 11142 11142 11149 11150 11150 11155 51157 51157 51158 51157 11158 11158 11158
L1213 L1236 L1236 C1247 P1250 M1265 S1313 S1313 R1317 R1318 R1317	11.320 11.320 11.320 11.320 11.332 11.347 11.347 11.348 11.348 11.348 11.348 11.348 11.348 11.348 11.374 11.374	11389 N1398 S1408 N1415 T1422 T1422 T1422 T1428 N1441 V1443 V1443 V1445 V1445 V1445
F1466 E1466 E1468 E1468 E1468 E1468 F1470 F1476 F1476 F1476 F1476 F1486 F1486 F1486 F1486 F1486 F1551	F1652 R1567 F1569 M1583 M1583 R1590 R1590 R1590 A1597 V1615 V1615 L1638 L1638	KL639 TL663 VL665 L1680 D1689 D1689 R1683 R1693 R1736 R1735 F1738 F1738 T1741



VIB78 V1742 V1878 V1742 Q1896 K1745 Q1907 K1745 L1907 K1745 L19127 S1769 L1927 S1769 L1927 S1769 L1927 L1770 L1927 L1776 L1927 L1776 L1927 L1776 L1927 L1776 L1927 L1776 L1927 L1770 L1927 L1776 L1927 L1776 L1926 Q1775 P1968 Q1776 L1981 L1783 K1986 Q1776 P1987 L1778 K1986 L1778 K1986 L1778 K1986 L1778 K1986 L1783 K1986 L1803 K1986 L1803 K1986 L1804 K1986 L1805 K1986 L1805 K1986 L1806 K1986 L1807 K1986 L1806 K1986 L1806 K1986 L1806 K1986 L1806 K1986 L1806 K1986

• Molecule 2: Fatty acid synthase subunit beta







S223	L231	L232	S233 1234	P235	1236	L240		9 <u>4</u> 2	L267		A270 T271	1 1 7 1	L277	TORS		T286		R297	T301		P315	D326		L339	834 7	N343	L344 T345		D351	Y352 V353		N372	N376		K419	S425		H430	L431 L432	V433	P434 A435	S436	V448	
	007 A	1479	T 484		T492	1493 T494	0495	F496 K497		G505	8610		L515	T516	R526		F543	K544 0545	E546		V550	199.I	L593		M597 T598	P599	VEOD		T616	1922		1663 D664	L665		L669 R670		L679		F LOO	1717	L730		H741	•
Y754	H760		S769	G772	1	D//10	Y778	6/14	M794		L800	V805		V827	T845	V846	R847	S848	I854	H855		L864 W865		F868	D869 F870		N874	K887		K894	D898	1001		0010	1,914		N936	T077	1947	E955	K962	-	L972	•
K975	A997		11000		K1031	S1033	1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	L1040	V1044		V1048	L1054		11070	H1081		L1085	F1103		D1110	VAL	GLN	ASP	S1121	81131		L1142	W1149	R1150	41151 A1152		C1156	F1158	10	SI16/	T1189		V1195	L1205		L1213	L1236	G1247	
D10E0	06217	S1313	R1314	R1317	T1318	M1319 L1320		G1330 W1331	R1332		F1339 P1340		V1343	11247	L1348		S1354	N1355	01367		T1374	9/211	11389		S1408	N1415	T1400		T1426	T1441	A1442	V1443	S1446	i i	41451	F1466	E1467	T1468	T1470		F1474 K1475	N1476	F1486	
11/00	11403	E1551	P1552	R1567			M1583	S1586		V1589	R1590	A1597		V1605 P1606		V1616		T1624	R1635	K1636	L1637	L1638 K1639	F1640		T1663 F1664	V1665			D1689	V 1690	R1693	01710	27 JT N	M1736	L1/3/ F1738	E1739	T1740	11741	V1/42 D1743	G1744	K1745	L1746 K1747	T1748	E1749
K1750	S1759	T1760	S1761	L1770		T1774	Q1775	01778		L1781	T1782		D1791	T1 803	F1804	A1805		S1808	E1811		11824	9781H	V1828		V1831	M1836	T1837 M1838		R1844	D1845	L1840 L1847		M1854 T1855		V1862	F1866	S1867		A1870	V1878	04 806	OFOTH	L1907	
L1914	L1927		E1934 F1035		V1953	N1954 P1955	R1956	P195/	P1968		S1973	F1976	H1977	S1978	L1981	M1982	N1983	G1984 V1985	K1986	P1987	-	12010	T2015	A2016	K2017	T2022	F 2040		E2046	02050														

 \bullet Molecule 2: Fatty acid synthase subunit beta

Chain K:		86%	13% •
S5 T6 R7 P8 L9 L9	(32 (33 (34 (34 (33 (33 (34 (33 (35 (34 (33 (35 (34) (35 (35) (35) (35) (35) (35) (35) (35)	N99 1101 1101 1114 1114 1121 1122 1123 1124 1128 1129 1129	1166 L173 V184 1188 K189 F190 F190
L198 2223 L231 L232 S233	1234 1235 1236 1240 1246 1246 1246 1277 1271 1283 1283 1283	R297 1301 1339 13326 1339 1332 1334 1345 1345 1345 1345 1345 1345 1345	N376 N376 R419 8425 H430 L431 L431 L433 V435 P434 P434
S436 448 1448 1459 1479	1484 14490 14490 14493 1493 1494 1493 1494 1494 1495 1495 1495 1515 1515 1515	No.44 No.44 06.44 06.54 15.47 15.47 15.47 15.51 15.93 15.93 15.93 15.93 15.93 15.93 15.93 15.93 15.93 15.93 15.93 15.93 15.93 15.93 15.93 15.93 15.93 15.93 15.93 15.93 15.93 15.93 16.93 15.93 16.93 15.93 16.93 16.93 16.93 16.93 16.93 16.93 16.93 16.93 16.93 16.93 16.93 16.93 16.94 16.94 16.95 16.94 16.95 16.94 16.95 16.94 16.95 16.94 16.95 16.95 16.95 16.95 16.95 16.95 16.95 <td>L669 R670 L679 L700 L700 L717</td>	L669 R670 L679 L700 L700 L717
H741 7754 H760 S769	6772 1776 1776 1779 1779 1779 1779 1779 1779 1779 1800 1800 1800 1845 1845 1847 1845 1847 1845	2540 1854 1855 1864 1864 1864 1864 1864 1864 1864 1864	910 1914 1914 1947 1947 1947 1947 1965
L972 K975 A997 11000	D1 001 K1 031 D1 032 S1 033 L1 040 L1 044 L1 048 L1 048 L1 051 H1 081 L1 085	F1103 D1110 VAL VAL GLN GLN GLN SER ASP SER ASP CI142 H1151 H1151 H1151 H1152 C1156 C1156 C1156 C1156	11189 11189 11189 11189 11189 11286 11213
G1247 P1250 M1265	81313 R1314 R1317 T1319 R1319 R1319 R1330 R1330 R1332 F1339 F1340 V1343 L1347 L1347 L1348	81354 N1355 Q1367 T1374 T1375 T1375 T1375 T1375 T1375 T1375 T1375 T1375 T1375 T1375 T1425 T1422 T1422 T1443 T1443	81446 81446 01451 F1466 E1466 E1466 E1468 E1468 E1474 F1474



GI744 K1476 K1747 F1466 K1747 F1466 K1747 F1466 K1747 F1466 K1749 F1466 K1749 F1552 S1761 F1563 S1761 F1563 S1761 F1563 L1770 F1569 L1770 F1569 L1770 F1569 L1781 F1569 L1783 L1578 L1783 L1667 L1783 L1683 L1783 L1669 L1783 L1666 L1783 L1669 L1783 L1669 L1783 L1666 L1834 L1666 L1835 L1689 L1836 L1689 L1834 L1669 L1834 L1689 L1836 L1689 L1844 L1689 L1844 L1689 L1844 L1689 L1846</

L1907 L1907 L1914 L1914 L1926 L1926 L1955 L1955 R1956 P1955 P1955 P1958 R1976 P1968 R1976 P1981 R1982 R1982 R1982 R1982 R1986 P1987 C1982 R1986 P1987 R1986 P1987 C1986 P1987 R1986 P1987 C1986 P1987 C1986 P1987 R1986 P1987 C1986 P1987 C1986 P1987 C1986 P1987 C1986 P1987 C1986 P1987 C1986 C19866 C1986 C1986 C1986 C1986 C1986 C1986 C1986 C1986 C1986 C1986

• Molecule 2: Fatty acid synthase subunit beta





4 Experimental information (i)

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	Depositor
	CORRECTION	
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 $(^{\circ})$	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor



5 Model quality (i)

5.1 Standard geometry (i)

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

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			
1VIOI	Unain	RMSZ	# Z > 5	RMSZ	# Z > 5		
1	А	0.75	0/13918	0.93	5/18809~(0.0%)		
1	В	0.75	0/13918	0.93	5/18809~(0.0%)		
1	С	0.75	0/13918	0.93	5/18809~(0.0%)		
1	D	0.75	0/13918	0.93	5/18809~(0.0%)		
1	Е	0.75	0/13918	0.93	5/18809~(0.0%)		
1	F	0.75	0/13918	0.93	5/18809~(0.0%)		
2	G	0.68	0/16383	0.86	0/22229		
2	Н	0.68	0/16383	0.86	0/22229		
2	Ι	0.68	0/16383	0.86	0/22229		
2	J	0.68	0/16383	0.86	0/22229		
2	K	0.68	0/16383	0.86	0/22229		
2	L	0.68	0/16383	0.86	0/22229		
All	All	0.71	0/181806	0.89	30/246228~(0.0%)		

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	А	0	1
1	В	0	1
1	С	0	1
1	D	0	1
1	Ε	0	1
1	F	0	1
2	G	0	3
2	Н	0	3
2	Ι	0	3
2	J	0	3
2	Κ	0	3



Continued from previous page...

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

There are no bond length outliers.

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	1017	ARG	CB-CA-C	6.41	123.22	110.40
1	С	1017	ARG	CB-CA-C	6.40	123.21	110.40
1	F	1017	ARG	CB-CA-C	6.39	123.18	110.40
1	В	1017	ARG	CB-CA-C	6.39	123.17	110.40
1	D	1017	ARG	CB-CA-C	6.38	123.16	110.40
1	Е	1017	ARG	CB-CA-C	6.34	123.08	110.40
1	А	1585	LYS	CB-CA-C	6.32	123.04	110.40
1	С	1585	LYS	CB-CA-C	6.30	123.00	110.40
1	Е	1585	LYS	CB-CA-C	6.24	122.88	110.40
1	В	1585	LYS	CB-CA-C	6.22	122.85	110.40
1	F	1585	LYS	CB-CA-C	6.22	122.83	110.40
1	D	1585	LYS	CB-CA-C	6.14	122.69	110.40
1	F	1680	ARG	CG-CD-NE	-6.09	99.01	111.80
1	Е	1680	ARG	CG-CD-NE	-6.07	99.05	111.80
1	А	1680	ARG	CG-CD-NE	-6.07	99.06	111.80
1	D	1680	ARG	CG-CD-NE	-6.07	99.06	111.80
1	С	1680	ARG	CG-CD-NE	-6.06	99.07	111.80
1	В	1680	ARG	CG-CD-NE	-6.04	99.12	111.80
1	А	1566	ARG	NE-CZ-NH1	5.63	123.12	120.30
1	В	1566	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	F	1566	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	D	1566	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	Е	1566	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	С	1566	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	Е	1264	ARG	CG-CD-NE	-5.14	101.00	111.80
1	А	1264	ARG	CG-CD-NE	-5.14	101.01	111.80
1	D	1264	ARG	CG-CD-NE	-5.12	101.06	111.80
1	С	1264	ARG	CG-CD-NE	-5.12	101.06	111.80
1	F	1264	ARG	CG-CD-NE	-5.08	101.14	111.80
1	В	1264	ARG	CG-CD-NE	-5.05	101.20	111.80

There are no chirality outliers.

All (24) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	А	1565	GLY	Peptide
1	В	1565	GLY	Peptide
1	С	1565	GLY	Peptide
1	D	1565	GLY	Peptide
1	Е	1565	GLY	Peptide
1	F	1565	GLY	Peptide
2	G	1605	VAL	Peptide
2	G	2046	GLU	Peptide
2	G	975	LYS	Peptide
2	Н	1605	VAL	Peptide
2	Н	2046	GLU	Peptide
2	Н	975	LYS	Peptide
2	Ι	1605	VAL	Peptide
2	Ι	2046	GLU	Peptide
2	Ι	975	LYS	Peptide
2	J	1605	VAL	Peptide
2	J	2046	GLU	Peptide
2	J	975	LYS	Peptide
2	Κ	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	А	13665	0	13647	107	0
1	В	13665	0	13647	103	0
1	С	13665	0	13647	99	0
1	D	13665	0	13647	100	0
1	Е	13665	0	13647	107	0
1	F	13665	0	13647	103	0
2	G	16018	0	15993	110	0
2	Н	16018	0	15993	114	0
2	I	16018	0	15993	111	0
2	J	16018	0	15993	111	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	K	16018	0	15993	112	0
2	L	16018	0	15993	115	0
3	А	13	0	0	1	0
3	В	13	0	0	1	0
3	С	13	0	0	1	0
3	D	13	0	0	1	0
3	Е	13	0	0	1	0
3	F	13	0	0	1	0
4	G	31	0	19	2	0
4	Н	31	0	19	2	0
4	Ι	31	0	19	2	0
4	J	31	0	19	2	0
4	Κ	31	0	19	2	0
4	L	31	0	19	2	0
All	All	178362	0	177954	1206	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 3.

All (1206)	close	$\operatorname{contacts}$	within	the sa	me	$\operatorname{asymmetric}$	unit	are	listed	below,	sorted	by	their	clash
magnitude).													

Atom 1	Atom 2	Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	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	
1:C:1417:SER:OG	3:D:1901:J8T:O4	2.01	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	



	1.5	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
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	0.75
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
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
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
2:L:870:GLU:O	2:L:874:ASN:ND2	2.31	0.63
2:H:870:GLU:O	2:H:874:ASN:ND2	2.31	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
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:H:245:GLN:HE21	2:H:505:GLY:HA2	1.66	0.61
2:J:1314:ARG:NH2	2:L:315:PRO:O	2.34	0.60
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: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



At and 1		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
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: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: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
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: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: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
1:B:717:TYR:CZ	1:B:721:ILE:HD11	2.37	0.58
2:I:1054:LEU:HB2	4:I:2101:FMN:HM72	1.84	0.58
2:J:1054:LEU:HB2	4:J:2101:FMN:HM72	1.84	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:K:1054:LEU:HB2	4:K:2101:FMN:HM72	1.86	0.58
2:G:1745:LYS:CE	2:G:1745:LYS:HA	2.34	0.58



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:K:1745:LYS:HA	2:K:1745:LYS:CE	2.34	0.58
2:G:1054:LEU:HB2	4:G:2101:FMN:HM72	1.86	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:L:1054:LEU:HB2	4:L:2101:FMN:HM72	1.85	0.57
2:H:1054:LEU:HB2	4:H:2101:FMN:HM72	1.85	0.57
2:K:1156:CYS:SG	2:K:1250:PRO:HD2	2.45	0.57
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



A + a 1	At arra 0	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
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
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



A 4 1	A t and D	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
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
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
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
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



A 4 1	A + 0	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
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: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
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
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



A 4 1	A + 0	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
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
1:F:1030:TRP:O	1:F:1035:THR:OG1	2.27	0.51
2:I:90:GLU:O	2:I:94:CYS:SG	2.65	0.51
2:J:1343:VAL:O	2:J:1343:VAL:HG22	2.11	0.51
2:G:1804:PHE:CZ	2:G:2010:TYR:HB2	2.46	0.51
2:H:1330:GLY:HA2	2:H:1374:THR:HG21	1.91	0.51
2:I:1343:VAL:HG22	2:I:1343:VAL:O	2.11	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
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
1:B:1248:GLY:O	1:B:1331:GLY:HA2	2.11	0.51
2:J:90:GLU:O	2:J:94:CYS:SG	2.65	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: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



	1.0	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
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: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
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



	A + 0	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
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: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
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
1:E:89:TYR:OH	2:K:1791:ASP:OD2	2.17	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
1:F:901:MET:HE1	1:F:926:LEU:HB3	1.95	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: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:J:372:ASN:HB3	2:J:515:LEU:HD21	1.95	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
1:A:89:TYR:OH	2:G:1791:ASP:OD2	2.18	0.48
2:H:1331:TRP:O	2:H:1332:ARG:C	2.52	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:L:1331:TRP:O	2:L:1332:ARG:C	2.52	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
2:J:297:ARG:O	2:J:301:THR:HG22	2.13	0.48



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
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
1:A:198:PRO:HG3	1:A:212:THR:HG21	1.95	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
2:H:90:GLU:O	2:H:94:CYS:SG	2.65	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:B:901:MET:HE1	1:B:926:LEU:HB3	1.96	0.48
1:D:1036:ARG:NH1	1:D:1040:GLU:OE1	2.41	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: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
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
1:B:400:ARG:NH1	1:B:715:THR:HG21	2.29	0.47
1:D:44:VAL:CG1	1:D:78:ILE:HG13	2.45	0.47
2:H:848:SER:HB3	2:H:854:ILE:HD11	1.96	0.47
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



	1 J	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
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: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: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:J:1331:TRP:O	2:J:1332:ARG:C	2.52	0.47
2:K:1331:TRP:O	2:K:1332:ARG:C	2.52	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
2:G:1331:TRP:O	2:G:1332:ARG:C	2.52	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:I:1331:TRP:O	2:I:1332:ARG:C	2.52	0.47
2:J:597:MET:HA	4:J:2101:FMN:N5	2.30	0.47
2:L:372:ASN:HB3	2:L:515:LEU:HD21	1.95	0.47



A 4 1	A + 0	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
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:1486:LEU:HG	1:A:1756:ILE:HD11	1.96	0.47
1:B:901:MET:CE	1:B:926:LEU:HB3	2.45	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:F:901:MET:CE	1:F:926:LEU:HB3	2.45	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:529:MET:HE2	1:E:896:PHE:HE1	1.80	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



A 4 1	1 J	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	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:1745:LYS:HA	2:H:1745:LYS:HE2	1.97	0.46
2:L:234:ILE:HG21	2:L:425:SER:HB3	1.96	0.46
1:A:529:MET:HE2	1:A:896:PHE:HE1	1.80	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: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
1:A:901:MET:CE	1:A:926:LEU:HB3	2.45	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:I:1313:SER:HB2	2:I:1319:MET:HE3	1.98	0.46
2:J:1313:SER:HB2	2:J:1319:MET:HE3	1.98	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: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: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
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



	1.5	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
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
1:C:901:MET:CE	1:C:926:LEU:HB3	2.45	0.46
1:E:901:MET:CE	1:E:926:LEU:HB3	2.45	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:K:90:GLU:O	2:K:94:CYS:SG	2.65	0.46
2:L:1081:HIS:O	2:L:1085:LEU:HB2	2.16	0.46
2:G:90:GLU:O	2:G:94:CYS:SG	2.65	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:1313:SER:HB2	2:K:1319:MET:HE3	1.98	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: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
1:B:1302:VAL:CG2	1:D:1302:VAL:CG2	2.94	0.45



A 4 a 1	1 0 Atom 9	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:C:1625:LEU:HD23	1:C:1626:TYR:N	2.31	0.45
1:D:901:MET:CE	1:D:926:LEU:HB3	2.45	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: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: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
2:G:1313:SER:HB2	2:G:1319:MET:HE3	1.98	0.45
1:B:966:LYS:HE3	1:B:971:ASN:HD21	1.81	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: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: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
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: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


A 4 a 1	A 4 ama 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:E:1625:LEU:HD23	1:E:1626:TYR:N	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: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
2:H:1313:SER:HB2	2:H:1319:MET:HE3	1.98	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
2:L:194:THR:O	2:L:198:LEU:HD23	2.17	0.45
2:L:1313:SER:HB2	2:L:1319:MET:HE3	1.98	0.45
2:G:96:LEU:HD11	2:G:101:ILE:HA	1.99	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: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:1370:THR:HG22	1:B:1372:THR:H	1.82	0.45
1:C:966:LYS:HE2	1:C:971:ASN:HD21	1.82	0.45
2:H:430:HIS:CE1	2:H:431:LEU:HD13	2.52	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
1:A:176:VAL:HG11	1:A:179:LYS:O	2.17	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:F:1673:TYR:CZ	1:F:1677:VAL:HG21	2.52	0.44
2:H:190:PHE:O	2:H:194:THR:OG1	2.28	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



A 4 a 1	1 0 Atom 9	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:B:529:MET:HE2	1:B:896:PHE:HE1	1.82	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:E:176:VAL:HG11	1:E:179:LYS:O	2.18	0.44
1:F:529:MET:HE2	1:F:896:PHE:HE1	1.82	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:J:1081:HIS:O	2:J:1085:LEU:HB2	2.16	0.44
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
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
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: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



A 4 a 1	1 0 Atom 9	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
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: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: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: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
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
1:A:337:VAL:HG12	1:A:341:GLN:HE21	1.83	0.44
1:A:472:LEU:HD13	1:A:472:LEU:C	2.39	0.44
2:G:1422:THR:HG22	2:G:1474:PHE:CD1	2.53	0.44
1:C:472:LEU:HD13	1:C:472:LEU:C	2.39	0.44
1:C:768:ILE:HD11	1:C:806:VAL:HG11	2.00	0.44
1:D:472:LEU:C	1:D:472:LEU:HD13	2.39	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:E:472:LEU:C	1:E:472:LEU:HD13	2.39	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:679:LEU:HB3	2:I:700:LEU:HD13	2.00	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: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



A 4 a 1	1 0 Atom 9	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
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
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
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
1:B:700:GLY:HA2	1:B:730:SER:HB3	2.01	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
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: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: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
1:C:529:MET:HE2	1:C:896:PHE:HE1	1.83	0.43



	1 0 At arra 0	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:D:529:MET:HE2	1:D:896:PHE:HE1	1.83	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
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
1:A:901:MET:HE1	1:A:926:LEU:HB3	1.99	0.43
1:E:850:PHE:HZ	1:E:866:GLY:HA3	1.84	0.43
1:F:472:LEU:HD13	1:F:472:LEU:C	2.39	0.43
2:H:101:ILE:HD11	2:H:122:LEU:CD2	2.48	0.43
2:H:1265:MET:HE1	2:H:1569:PHE:CZ	2.54	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:B:472:LEU:C	1:B:472:LEU:HD13	2.39	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: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
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
1:E:901:MET:HE1	1:E:926:LEU:HB3	2.00	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



A 4 1	A + 0	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:L:1265:MET:HE1	2:L:1569:PHE:CZ	2.54	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
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:1838:MET:HE3	2:J:1976:PHE:CD1	2.54	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
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
1:F:901:MET:HE3	1:F:904:ASN:HB2	2.01	0.42
2:H:717:ILE:HG23	2:H:760:HIS:CE1	2.54	0.42



	1.5	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:H:1738:PHE:CE1	2:H:1837:THR:HG23	2.54	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
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
2:I:1838:MET:HE3	2:I:1976:PHE:CD1	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: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
1:A:529:MET:HE2	1:A:896:PHE:CE1	2.54	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: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:B:901:MET:HE3	1:B:904:ASN:HB2	2.01	0.42
1:C:666:ALA:O	1:C:670:GLY:HA2	2.20	0.42
1:C:901:MET:HE1	1:C:926:LEU:HB3	2.01	0.42
1:C:1716:LEU:HD21	1:F:1426:LEU:HD22	2.01	0.42



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
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:E:529:MET:HE2	1:E:896:PHE:CE1	2.54	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: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
1:A:359:ARG:NH1	1:C:1153:ASP:OD2	2.51	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



A 4 a ma 1	A4.000 0	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:I:1149:TRP:CE2	2:I:1213:LEU:HD23	2.55	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: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:D:901:MET:HE1	1:D:926:LEU:HB3	2.01	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:D:1694:TYR:OH	2:J:1001:ASP:OD2	2.31	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



	1 J	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:G:741:HIS:CD2	2:G:855:HIS:ND1	2.88	0.41
1:C:652:ASP:OD2	1:C:655:LEU:HG	2.19	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
1:F:1308:SER:O	1:F:1311:SER:HB3	2.20	0.41
2:I:233:SER:C	2:I:235:PRO:HD2	2.41	0.41
2:J:233:SER:C	2:J:235:PRO:HD2	2.41	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: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: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: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:G:1862:VAL:HG11	2:G:1866:PHE:CD2	2.55	0.41



A + 1	A4	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:C:1694:TYR:OH	2:I:1001:ASP:OD2	2.32	0.41
1:E:839:TYR:O	1:E:842:SER:HB2	2.20	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: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:A:901:MET:HE3	1:A:904:ASN:HB2	2.02	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:F:1413:LYS:O	1:F:1648:GLN:NE2	2.43	0.41
2:H:233:SER:C	2:H:235:PRO:HD2	2.41	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:1838:MET:HE3	2:H:1976:PHE:CD1	2.55	0.41
2:H:1976:PHE:HA	2:H:1981:LEU:HD21	2.03	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:L:233:SER:C	2:L:235:PRO:HD2	2.41	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
2:L:1149:TRP:CE2	2:L:1213:LEU:HD23	2.55	0.41



A 4 1	A + 0	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:L:1838:MET:HE3	2:L:1976:PHE:CD1	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
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:E:901:MET:HE3	1:E:904:ASN:HB2	2.02	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
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:B:529:MET:HE2	1:B:896:PHE:CE1	2.56	0.41
1:C:442:ARG:HD3	1:C:726:GLY:O	2.21	0.41
1:C:901:MET:HE3	1:C:904:ASN:HB2	2.02	0.41
1:D:20:TYR:CE1	2:J:1985:VAL:HG11	2.56	0.41
1:D:901:MET:HE3	1:D:904:ASN:HB2	2.02	0.41
1:E:1076:VAL:HG13	1:E:1081:LYS:HA	2.01	0.41
1:F:529:MET:HE2	1:F:896:PHE:CE1	2.56	0.41
2:H:1693:ARG:HD3	2:H:1825:GLU:OE2	2.21	0.41



A 4 1	A + 0	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:J:663:ILE:HB	2:J:664:PRO:HD3	2.03	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: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: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:K:1702:TYR:O	2:K:1733:TYR:OH	2.31	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:G:233:SER:C	2:G:235:PRO:HD2	2.41	0.40
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: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:K:143:SER:OG	2:K:547:ILE:O	2.35	0.40
2:L:599:PRO:O	2:L:602:VAL:HG12	2.21	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
2:G:1265:MET:HE1	2:G:1569:PHE:CZ	2.57	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: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
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:233:SER:C	2:K:235:PRO:HD2	2.41	0.40
1:A:377:TYR:O	1:A:380:ALA:HB3	2.21	0.40



A 4 1	A + 0	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
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: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:846:VAL:HG13	2:J:865:TRP:CD1	2.56	0.40
2:K:1265:MET:HE1	2:K:1569:PHE:CZ	2.57	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
1:B:490:TYR:CD1	1:B:695:GLY:HA2	2.57	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
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)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	F	Perce	entiles
1	А	1749/1887~(93%)	1614 (92%)	118 (7%)	17 (1%)		15	45
1	В	1749/1887~(93%)	1613 (92%)	119 (7%)	17 (1%)		15	45
1	С	1749/1887~(93%)	1614 (92%)	118 (7%)	17 (1%)		15	45
1	D	1749/1887~(93%)	1613 (92%)	119 (7%)	17 (1%)		15	45
1	Ε	1749/1887~(93%)	1614 (92%)	118 (7%)	17 (1%)		15	45
1	F	1749/1887~(93%)	1615 (92%)	117 (7%)	17 (1%)		15	45
2	G	2032/2040~(100%)	1834 (90%)	174 (9%)	24 (1%)		13	40
2	Н	2032/2040~(100%)	1832 (90%)	176 (9%)	24 (1%)		13	40
2	Ι	2032/2040~(100%)	1834 (90%)	174 (9%)	24 (1%)		13	40
2	J	2032/2040~(100%)	1835 (90%)	173 (8%)	24 (1%)		13	40
2	Κ	2032/2040~(100%)	1833 (90%)	175~(9%)	24 (1%)		13	40
2	L	2032/2040~(100%)	1834 (90%)	174 (9%)	24 (1%)		13	40
All	All	22686/23562~(96%)	20685 (91%)	1755 (8%)	246 (1%)		18	42

All (246) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	22	PHE
1	А	812	ALA
1	А	1127	VAL
1	А	1240	VAL
1	А	1585	LYS
2	G	1739	GLU
1	В	22	PHE
1	В	812	ALA
1	В	1127	VAL
1	В	1240	VAL
1	В	1585	LYS
1	С	22	PHE



Mol	Chain	Res	Type
1	С	812	ALA
1	С	1127	VAL
1	С	1240	VAL
1	С	1585	LYS
1	D	22	PHE
1	D	812	ALA
1	D	1127	VAL
1	D	1240	VAL
1	D	1585	LYS
1	Е	22	PHE
1	Е	812	ALA
1	Е	1127	VAL
1	Е	1240	VAL
1	Е	1585	LYS
1	F	22	PHE
1	F	812	ALA
1	F	1127	VAL
1	F	1240	VAL
1	F	1585	LYS
2	Н	1739	GLU
2	Ι	1739	GLU
2	J	1739	GLU
2	K	1739	GLU
2	L	1739	GLU
1	А	730	SER
1	А	874	GLY
1	А	1207	GLN
1	А	1608	ASN
2	G	97	GLU
2	G	772	GLY
2	G	1953	VAL
2	G	1956	ARG
1	В	730	SER
1	В	874	GLY
1	В	$1\overline{207}$	GLN
1	В	1608	ASN
1	C	874	GLY
1	C	1207	GLN
1	C	1608	ASN
1	D	874	GLY
1	D	1207	GLN
1	D	1608	ASN



Mol	Chain	Res	Type
1	Е	874	GLY
1	Е	1207	GLN
1	Е	1608	ASN
1	F	874	GLY
1	F	1207	GLN
1	F	1608	ASN
2	Н	97	GLU
2	Н	772	GLY
2	Н	1953	VAL
2	Н	1956	ARG
2	Ι	97	GLU
2	Ι	772	GLY
2	Ι	1953	VAL
2	Ι	1956	ARG
2	J	97	GLU
2	J	772	GLY
2	J	1953	VAL
2	J	1956	ARG
2	Κ	97	GLU
2	K	772	GLY
2	Κ	1953	VAL
2	K	1956	ARG
2	L	97	GLU
2	L	772	GLY
2	L	1953	VAL
2	L	1956	ARG
1	А	1321	SER
1	А	1844	LYS
2	G	46	GLU
2	G	551	THR
1	В	1321	SER
1	В	1844	LYS
1	С	730	SER
1	С	1321	SER
1	С	1844	LYS
1	D	730	SER
1	D	1321	SER
1	D	1844	LYS
1	E	730	SER
1	Е	1321	SER
1	E	1844	LYS
1	F	730	SER



Mol	Chain	Res	Type
1	F	1321	SER
1	F	1844	LYS
2	Н	46	GLU
2	Н	551	THR
2	Ι	46	GLU
2	Ι	551	THR
2	J	46	GLU
2	J	551	THR
2	K	46	GLU
2	K	551	THR
2	L	46	GLU
2	L	551	THR
1	А	515	PRO
1	А	1545	SER
2	G	343	ASN
2	G	622	GLY
2	G	769	SER
2	G	1578	THR
2	G	1808	SER
2	G	1847	LEU
2	G	1878	VAL
2	G	2016	ALA
1	В	515	PRO
1	В	1545	SER
1	С	515	PRO
1	С	977	TYR
1	С	1545	SER
1	D	515	PRO
1	D	977	TYR
1	D	1545	SER
1	Ε	515	PRO
1	E	1545	SER
1	F	515	PRO
1	F	977	TYR
1	F	1545	SER
2	Н	343	ASN
2	Н	622	GLY
2	Н	769	SER
2	H	1578	THR
2	Н	1808	SER
2	H	1847	LEU
$\overline{2}$	Н	1878	VAL



Mol	Chain	Res	Type
2	Н	2016	ALA
2	Ι	343	ASN
2	Ι	622	GLY
2	Ι	769	SER
2	Ι	1189	THR
2	Ι	1578	THR
2	Ι	1808	SER
2	Ι	1847	LEU
2	Ι	1878	VAL
2	Ι	2016	ALA
2	J	343	ASN
2	J	622	GLY
2	J	769	SER
2	J	1578	THR
2	J	1808	SER
2	J	1847	LEU
2	J	1878	VAL
2	J	2016	ALA
2	K	343	ASN
2	K	622	GLY
2	K	769	SER
2	K	1578	THR
2	K	1808	SER
2	K	1847	LEU
2	Κ	1878	VAL
2	Κ	2016	ALA
2	L	343	ASN
2	L	622	GLY
2	L	769	SER
2	L	1578	THR
2	L	1808	SER
2	L	1847	LEU
2	L	1878	VAL
2	L	2016	ALA
1	A	618	ASN
1	A	977	TYR
1	А	1566	ARG
2	G	1031	LYS
2	G	1189	THR
2	G	1896	GLN
1	В	618	ASN
1	В	977	TYR



Mol	Chain	Res	Type
1	В	1566	ARG
1	С	618	ASN
1	С	1566	ARG
1	D	618	ASN
1	D	1566	ARG
1	Е	618	ASN
1	Е	977	TYR
1	Е	1566	ARG
1	F	618	ASN
1	F	1566	ARG
2	Н	1031	LYS
2	Н	1189	THR
2	Н	1896	GLN
2	Ι	1031	LYS
2	Ι	1896	GLN
2	J	1031	LYS
2	J	1189	THR
2	J	1896	GLN
2	Κ	1031	LYS
2	Κ	1189	THR
2	Κ	1896	GLN
2	L	1031	LYS
2	L	1189	THR
2	L	1896	GLN
1	А	949	GLU
2	G	496	PHE
2	G	1044	VAL
2	G	1048	VAL
2	G	1167	SER
1	В	949	GLU
1	С	949	GLU
1	D	949	GLU
1	Е	949	GLU
1	F	949	GLU
2	Н	496	PHE
2	Н	1044	VAL
2	Н	1048	VAL
2	Н	1167	SER
2	Ι	496	PHE
2	Ι	1044	VAL
2	I	1048	VAL
2	Ι	1167	SER



Mol	Chain	Res	Type
2	J	496	PHE
2	J	1044	VAL
2	J	1048	VAL
2	J	1167	SER
2	K	496	PHE
2	К	1044	VAL
2	K	1048	VAL
2	K	1167	SER
2	L	496	PHE
2	L	1044	VAL
2	L	1048	VAL
2	L	1167	SER
2	G	1955	PRO
2	Н	1955	PRO
2	Ι	1955	PRO
2	J	1955	PRO
2	K	1955	PRO
2	L	1955	PRO
2	G	484	ILE
2	Н	484	ILE
2	Ι	484	ILE
2	J	484	ILE
2	Κ	484	ILE
2	L	484	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	А	1481/1566~(95%)	1383~(93%)	98~(7%)	16 44
1	В	1481/1566~(95%)	1384 (94%)	97~(6%)	17 45
1	С	1481/1566~(95%)	1384~(94%)	97~(6%)	17 45
1	D	1481/1566~(95%)	1384 (94%)	97~(6%)	17 45
1	Е	1481/1566~(95%)	1384 (94%)	97~(6%)	17 45



Mol	Chain	Analysed	Rotameric	Outliers	Perce	entiles
1	F	1481/1566~(95%)	1383 (93%)	98~(7%)	16	44
2	G	1775/1779~(100%)	1657~(93%)	118 (7%)	16	44
2	Н	1775/1779~(100%)	1656~(93%)	119~(7%)	16	43
2	Ι	1775/1779~(100%)	1657~(93%)	118 (7%)	16	44
2	J	1775/1779~(100%)	1658~(93%)	117 (7%)	16	44
2	Κ	1775/1779~(100%)	1657~(93%)	118 (7%)	16	44
2	L	1775/1779~(100%)	1657~(93%)	118 (7%)	16	44
All	All	19536/20070~(97%)	18244 (93%)	1292 (7%)	20	44

All (1292) residues with a non-rotameric sidechain are listed below:

Mol	Chain	\mathbf{Res}	Type
1	А	2	LYS
1	А	15	THR
1	А	21	GLN
1	А	27	ARG
1	А	42	GLU
1	А	140	ILE
1	А	168	MET
1	А	179	LYS
1	А	225	SER
1	А	301	ASP
1	А	363	LYS
1	А	390	VAL
1	А	392	THR
1	А	401	THR
1	А	432	VAL
1	А	443	SER
1	А	458	THR
1	А	489	VAL
1	А	493	VAL
1	А	515	PRO
1	А	527	GLN
1	А	537	LYS
1	А	538	GLU
1	А	599	MET
1	А	708	SER
1	А	719	GLN
1	А	731	THR
1	А	748	LEU



Mol	Chain	Res	Type
1	А	750	GLU
1	А	761	LEU
1	А	776	GLU
1	А	777	GLN
1	А	788	SER
1	А	789	GLU
1	А	797	THR
1	А	806	VAL
1	А	824	LEU
1	А	827	SER
1	А	862	LEU
1	А	864	VAL
1	А	875	THR
1	A	878	MET
1	А	894	ARG
1	А	913	VAL
1	А	916	LEU
1	А	923	MET
1	А	937	LYS
1	А	945	LYS
1	А	987	ASN
1	А	1001	VAL
1	А	1020	VAL
1	А	1022	THR
1	А	1047	LEU
1	А	1050	CYS
1	А	1061	SER
1	А	1073	THR
1	А	1079	LYS
1	A	1096	SER
1	A	1130	ASP
1	A	1164	SER
1	A	1166	LYS
1	А	1184	LEU
1	A	1197	THR
1	A	1203	ASP
1	А	1208	VAL
1	A	1238	VAL
1	A	1240	VAL
1	А	1254	VAL
1	A	1260	MET
1	А	1262	LYS



Mol	Chain	Res	Type
1	А	1283	MET
1	А	1327	CYS
1	А	1329	VAL
1	А	1333	ASP
1	А	1338	GLU
1	А	1392	LEU
1	А	1426	LEU
1	А	1430	ARG
1	А	1442	ASN
1	А	1471	LYS
1	А	1507	GLN
1	А	1528	THR
1	А	1544	THR
1	А	1556	THR
1	А	1566	ARG
1	А	1577	GLN
1	А	1580	LEU
1	А	1585	LYS
1	А	1640	SER
1	А	1642	THR
1	А	1643	SER
1	А	1649	LYS
1	А	1680	ARG
1	А	1681	GLU
1	А	1706	TYR
1	А	1722	VAL
1	А	1780	ASN
1	А	1828	LEU
2	G	7	ARG
2	G	34	GLN
2	G	38	ASN
2	G	99	ASN
2	G	109	LEU
2	G	114	THR
2	G	121	GLU
2	G	166	THR
2	G	173	LEU
2	G	194	THR
2	G	223	SER
2	G	236	ILE
2	G	240	LEU
2	G	267	LEU



Mol	Chain	Res	Type
2	G	277	LEU
2	G	326	ASP
2	G	339	LEU
2	G	342	SER
2	G	345	THR
2	G	351	ASP
2	G	353	VAL
2	G	376	ASN
2	G	419	ARG
2	G	425	SER
2	G	431	LEU
2	G	436	SER
2	G	492	THR
2	G	494	THR
2	G	497	LYS
2	G	510	SER
2	G	516	THR
2	G	545	GLN
2	G	598	THR
2	G	616	THR
2	G	665	LEU
2	G	669	LEU
2	G	670	ARG
2	G	730	LEU
2	G	776	ASP
2	G	805	VAL
2	G	827	VAL
2	G	845	THR
2	G	846	VAL
2	G	887	LYS
2	G	907	VAL
2	G	910	GLN
2	G	914	LEU
2	G	936	ASN
2	G	947	THR
2	G	972	LEU
2	G	1033	SER
2	G	1040	LEU
2	G	1110	ASP
2	G	1131	SER
2	G	1157	SER
2	G	1158	PHE



Mol	Chain	Res	Type
2	G	1167	SER
2	G	1189	THR
2	G	1195	VAL
2	G	1205	LEU
2	G	1213	LEU
2	G	1236	LEU
2	G	1317	ARG
2	G	1320	LEU
2	G	1343	VAL
2	G	1347	LEU
2	G	1348	LEU
2	G	1354	SER
2	G	1367	GLN
2	G	1375	THR
2	G	1389	ILE
2	G	1415	ASN
2	G	1422	THR
2	G	1441	ILE
2	G	1446	SER
2	G	1451	GLN
2	G	1468	THR
2	G	1470	THR
2	G	1476	ASN
2	G	1486	PHE
2	G	1567	ARG
2	G	1583	MET
2	G	1586	SER
2	G	1590	ARG
2	G	1616	VAL
2	G	1624	THR
2	G	1637	LEU
2	G	1639	LYS
2	G	1680	LEU
2	G	1693	ARG
2	G	1712	ASN
2	G	1736	MET
2	G	1740	THR
2	G	1741	ILE
2	G	1745	LYS
2	G	1747	LYS
2	G	1748	THR
2	G	1750	LYS



Mol	Chain	Res	Type
2	G	1759	SER
2	G	1761	SER
2	G	1770	LEU
2	G	1775	GLN
2	G	1781	LEU
2	G	1811	GLU
2	G	1844	ARG
2	G	1845	ASP
2	G	1846	GLU
2	G	1847	LEU
2	G	1862	VAL
2	G	1914	LEU
2	G	1927	LEU
2	G	1934	GLU
2	G	1935	GLU
2	G	1973	SER
2	G	1976	PHE
2	G	1978	SER
2	G	2022	THR
2	G	2040	GLU
1	В	2	LYS
1	В	15	THR
1	В	21	GLN
1	В	27	ARG
1	В	42	GLU
1	В	140	ILE
1	В	168	MET
1	В	179	LYS
1	В	225	SER
1	В	301	ASP
1	В	363	LYS
1	В	390	VAL
1	В	392	THR
1	В	401	THR
1	В	432	VAL
1	B	443	SER
1	В	458	THR
1	B	489	VAL
1	В	493	VAL
1	B	515	PRO
1	В	527	GLN
1	В	537	LYS



Mol	Chain	Res	Type
1	В	538	GLU
1	В	599	MET
1	В	708	SER
1	В	719	GLN
1	В	731	THR
1	В	748	LEU
1	В	750	GLU
1	В	761	LEU
1	В	776	GLU
1	В	777	GLN
1	В	788	SER
1	В	789	GLU
1	В	797	THR
1	В	806	VAL
1	В	824	LEU
1	В	827	SER
1	В	862	LEU
1	В	864	VAL
1	В	875	THR
1	В	878	MET
1	В	894	ARG
1	В	913	VAL
1	В	916	LEU
1	В	923	MET
1	В	937	LYS
1	В	945	LYS
1	В	987	ASN
1	В	1001	VAL
1	В	1020	VAL
1	В	1022	THR
1	В	1047	LEU
1	В	1050	CYS
1	В	1061	SER
1	В	1073	THR
1	В	1079	LYS
1	В	1096	SER
1	В	1130	ASP
1	В	1164	SER
1	B	1166	LYS
1	В	1184	LEU
1	В	1197	THR
1	В	1203	ASP



Mol	Chain	Res	Type
1	В	1208	VAL
1	В	1238	VAL
1	В	1240	VAL
1	В	1254	VAL
1	В	1260	MET
1	В	1262	LYS
1	В	1283	MET
1	В	1327	CYS
1	В	1329	VAL
1	В	1333	ASP
1	В	1338	GLU
1	В	1392	LEU
1	В	1426	LEU
1	В	1430	ARG
1	В	1442	ASN
1	В	1471	LYS
1	В	1507	GLN
1	В	1528	THR
1	В	1556	THR
1	В	1566	ARG
1	В	1577	GLN
1	В	1580	LEU
1	В	1585	LYS
1	В	1640	SER
1	В	1642	THR
1	В	1643	SER
1	В	1649	LYS
1	В	1680	ARG
1	В	1681	GLU
1	В	1706	TYR
1	В	1722	VAL
1	В	1780	ASN
1	В	1828	LEU
1	C	2	LYS
1	C	15	THR
1	C	21	GLN
1	С	27	ARG
1	С	42	GLU
1	C	140	ILE
1	С	168	MET
1	С	179	LYS
1	С	225	SER



Mol	Chain	Res	Type
1	С	301	ASP
1	С	363	LYS
1	С	390	VAL
1	С	392	THR
1	С	401	THR
1	С	432	VAL
1	С	443	SER
1	С	458	THR
1	С	489	VAL
1	С	493	VAL
1	С	515	PRO
1	С	527	GLN
1	С	537	LYS
1	С	538	GLU
1	С	599	MET
1	С	708	SER
1	С	719	GLN
1	С	731	THR
1	С	748	LEU
1	С	750	GLU
1	С	761	LEU
1	С	776	GLU
1	С	777	GLN
1	С	788	SER
1	С	789	GLU
1	С	797	THR
1	С	806	VAL
1	С	824	LEU
1	С	827	SER
1	С	862	LEU
1	С	864	VAL
1	С	875	THR
1	С	878	MET
1	С	894	ARG
1	С	913	VAL
1	С	916	LEU
1	С	923	MET
1	С	937	LYS
1	C	945	LYS
1	С	987	ASN
1	С	1001	VAL
1	С	1020	VAL



Mol	Chain	Res	Type
1	С	1022	THR
1	С	1047	LEU
1	С	1050	CYS
1	С	1061	SER
1	С	1073	THR
1	С	1079	LYS
1	С	1096	SER
1	С	1130	ASP
1	С	1164	SER
1	С	1166	LYS
1	С	1184	LEU
1	С	1197	THR
1	С	1203	ASP
1	С	1208	VAL
1	С	1238	VAL
1	С	1240	VAL
1	С	1254	VAL
1	С	1260	MET
1	С	1262	LYS
1	С	1283	MET
1	С	1327	CYS
1	С	1329	VAL
1	С	1333	ASP
1	С	1338	GLU
1	С	1392	LEU
1	С	1426	LEU
1	С	1430	ARG
1	С	1442	ASN
1	С	1471	LYS
1	С	1507	GLN
1	С	1528	THR
1	C	1556	THR
1	С	1566	ARG
1	C	1577	GLN
1	С	1580	LEU
1	С	1585	LYS
1	С	1640	SER
1	С	1642	THR
1	С	1643	SER
1	С	1649	LYS
1	С	1680	ARG
1	С	1681	GLU



Mol	Chain	Res	Type
1	С	1706	TYR
1	С	1722	VAL
1	С	1780	ASN
1	С	1828	LEU
1	D	2	LYS
1	D	15	THR
1	D	21	GLN
1	D	27	ARG
1	D	42	GLU
1	D	140	ILE
1	D	168	MET
1	D	179	LYS
1	D	225	SER
1	D	301	ASP
1	D	363	LYS
1	D	390	VAL
1	D	392	THR
1	D	401	THR
1	D	432	VAL
1	D	443	SER
1	D	458	THR
1	D	489	VAL
1	D	493	VAL
1	D	515	PRO
1	D	527	GLN
1	D	537	LYS
1	D	538	GLU
1	D	599	MET
1	D	708	SER
1	D	719	GLN
1	D	731	THR
1	D	748	LEU
1	D	750	GLU
1	D	761	LEU
1	D	776	GLU
1	D	777	GLN
1	D	788	SER
1	D	789	GLU
1	D	797	THR
1	D	806	VAL
1	D	824	LEU
1	D	827	SER



Mol	Chain	Res	Type
1	D	862	LEU
1	D	864	VAL
1	D	875	THR
1	D	878	MET
1	D	894	ARG
1	D	913	VAL
1	D	916	LEU
1	D	923	MET
1	D	937	LYS
1	D	945	LYS
1	D	987	ASN
1	D	1001	VAL
1	D	1020	VAL
1	D	1022	THR
1	D	1047	LEU
1	D	1050	CYS
1	D	1061	SER
1	D	1073	THR
1	D	1079	LYS
1	D	1096	SER
1	D	1130	ASP
1	D	1164	SER
1	D	1166	LYS
1	D	1184	LEU
1	D	1197	THR
1	D	1203	ASP
1	D	1208	VAL
1	D	1238	VAL
1	D	1240	VAL
1	D	1254	VAL
1	D	1260	MET
1	D	1262	LYS
1	D	1283	MET
1	D	1327	CYS
1	D	1329	VAL
1	D	1333	ASP
1	D	1338	GLU
1	D	1392	LEU
1	D	1426	LEU
1	D	1430	ARG
1	D	1442	ASN
1	D	1471	LYS



Mol	Chain	Res	Type
1	D	1507	GLN
1	D	1528	THR
1	D	1556	THR
1	D	1566	ARG
1	D	1577	GLN
1	D	1580	LEU
1	D	1585	LYS
1	D	1640	SER
1	D	1642	THR
1	D	1643	SER
1	D	1649	LYS
1	D	1680	ARG
1	D	1681	GLU
1	D	1706	TYR
1	D	1722	VAL
1	D	1780	ASN
1	D	1828	LEU
1	Е	2	LYS
1	Е	15	THR
1	Е	21	GLN
1	Е	27	ARG
1	Е	42	GLU
1	Е	140	ILE
1	Е	168	MET
1	Е	179	LYS
1	Е	225	SER
1	Е	301	ASP
1	Е	363	LYS
1	Е	390	VAL
1	Е	392	THR
1	Е	401	THR
1	Е	432	VAL
1	Е	443	SER
1	Е	458	THR
1	Е	489	VAL
1	Е	493	VAL
1	E	515	PRO
1	Е	527	GLN
1	Е	537	LYS
1	Е	538	GLU
1	Е	599	MET
1	Е	708	SER



Mol	Chain	Res	Type
1	Е	719	GLN
1	Е	731	THR
1	Е	748	LEU
1	Е	750	GLU
1	Е	761	LEU
1	Е	776	GLU
1	Е	777	GLN
1	Е	788	SER
1	Е	789	GLU
1	Е	797	THR
1	Е	806	VAL
1	Е	824	LEU
1	Е	827	SER
1	Е	862	LEU
1	Е	864	VAL
1	Е	875	THR
1	Е	878	MET
1	Е	894	ARG
1	Е	913	VAL
1	Е	916	LEU
1	Е	923	MET
1	Е	937	LYS
1	Е	945	LYS
1	Е	987	ASN
1	Е	1001	VAL
1	Е	1020	VAL
1	Е	1022	THR
1	Ε	1047	LEU
1	Ε	1050	CYS
1	Ε	1061	SER
1	Е	1073	THR
1	E	1079	LYS
1	Е	1096	SER
1	E	1130	ASP
1	Е	1164	SER
1	E	1166	LYS
1	Е	1184	LEU
1	Е	1197	THR
1	E	1203	ASP
1	Е	1208	VAL
1	E	1238	VAL
1	Е	1240	VAL



Mol	Chain	Res	Type
1	Е	1254	VAL
1	Е	1260	MET
1	Е	1262	LYS
1	Е	1283	MET
1	Е	1327	CYS
1	Е	1329	VAL
1	Е	1333	ASP
1	Е	1338	GLU
1	Е	1392	LEU
1	Е	1426	LEU
1	Е	1430	ARG
1	Е	1442	ASN
1	Е	1471	LYS
1	Е	1507	GLN
1	E	1528	THR
1	Е	1556	THR
1	Е	1566	ARG
1	Е	1577	GLN
1	Е	1580	LEU
1	Е	1585	LYS
1	Ε	1640	SER
1	Е	1642	THR
1	Ε	1643	SER
1	Е	1649	LYS
1	Е	1680	ARG
1	Е	1681	GLU
1	Е	1706	TYR
1	Ε	1722	VAL
1	Е	1780	ASN
1	Е	1828	LEU
1	F	2	LYS
1	F	15	THR
1	F	21	GLN
1	F	27	ARG
1	F	42	GLU
1	F	140	ILE
1	F	168	MET
1	F	179	LYS
1	F	225	SER
1	F	301	ASP
1	F	363	LYS
1	F	390	VAL


Mol	Chain	Res	Type
1	F	392	THR
1	F	401	THR
1	F	432	VAL
1	F	443	SER
1	F	458	THR
1	F	489	VAL
1	F	493	VAL
1	F	515	PRO
1	F	527	GLN
1	F	537	LYS
1	F	538	GLU
1	F	599	MET
1	F	708	SER
1	F	709	ARG
1	F	719	GLN
1	F	731	THR
1	F	748	LEU
1	F	750	GLU
1	F	761	LEU
1	F	776	GLU
1	F	777	GLN
1	F	788	SER
1	F	789	GLU
1	F	797	THR
1	F	806	VAL
1	F	824	LEU
1	F	827	SER
1	F	862	LEU
1	F	864	VAL
1	F	875	THR
1	F	878	MET
1	F	894	ARG
1	F	913	VAL
1	F	916	LEU
1	F	923	MET
1	F	937	LYS
1	F	945	LYS
1	F	987	ASN
1	F	1001	VAL
1	F	1020	VAL
1	F	1022	THR
1	F	1047	LEU



Mol	Chain	Res	Type
1	F	1050	CYS
1	F	1061	SER
1	F	1073	THR
1	F	1079	LYS
1	F	1096	SER
1	F	1130	ASP
1	F	1164	SER
1	F	1166	LYS
1	F	1184	LEU
1	F	1197	THR
1	F	1203	ASP
1	F	1208	VAL
1	F	1238	VAL
1	F	1240	VAL
1	F	1254	VAL
1	F	1260	MET
1	F	1262	LYS
1	F	1283	MET
1	F	1327	CYS
1	F	1329	VAL
1	F	1333	ASP
1	F	1338	GLU
1	F	1392	LEU
1	F	1426	LEU
1	F	1430	ARG
1	F	1442	ASN
1	F	1471	LYS
1	F	1507	GLN
1	F	1528	THR
1	F	1556	THR
1	F	1566	ARG
1	F	1577	GLN
1	F	1580	LEU
1	F	1585	LYS
1	F	1640	SER
1	F	1642	THR
1	F	1643	SER
1	F	1649	LYS
1	F	1680	ARG
1	F	1681	GLU
1	F	1706	TYR
1	F	1722	VAL



Mol	Chain	Res	Type
1	F	1780	ASN
1	F	1828	LEU
2	Н	7	ARG
2	Н	24	THR
2	Н	34	GLN
2	Н	38	ASN
2	Н	99	ASN
2	Н	109	LEU
2	Н	114	THR
2	Н	121	GLU
2	Н	140	LYS
2	Н	166	THR
2	Н	173	LEU
2	Н	194	THR
2	Н	223	SER
2	Н	236	ILE
2	Н	240	LEU
2	Н	267	LEU
2	Н	277	LEU
2	Н	326	ASP
2	Н	339	LEU
2	Н	342	SER
2	Н	345	THR
2	Н	351	ASP
2	Н	353	VAL
2	Н	376	ASN
2	Н	419	ARG
2	Н	425	SER
2	Н	431	LEU
2	Н	436	SER
2	Н	492	THR
2	Н	494	THR
2	Н	497	LYS
2	Н	510	SER
2	Н	516	THR
2	Н	545	GLN
2	Н	598	THR
2	Н	616	THR
2	Η	665	LEU
2	Н	669	LEU
2	Н	670	ARG
2	Н	730	LEU



Mol	Chain	Res	Type
2	Н	776	ASP
2	Н	805	VAL
2	Н	827	VAL
2	Н	845	THR
2	Н	846	VAL
2	Н	887	LYS
2	Н	907	VAL
2	Н	910	GLN
2	Н	914	LEU
2	Н	936	ASN
2	Н	947	THR
2	Н	972	LEU
2	Н	1033	SER
2	Н	1040	LEU
2	Н	1110	ASP
2	Н	1131	SER
2	Н	1157	SER
2	Н	1158	PHE
2	Н	1167	SER
2	Н	1189	THR
2	Н	1195	VAL
2	Н	1205	LEU
2	Н	1213	LEU
2	Н	1236	LEU
2	Н	1317	ARG
2	Н	1320	LEU
2	Н	1343	VAL
2	Н	1347	LEU
2	Н	1348	LEU
2	Н	1354	SER
2	Н	1367	GLN
2	Н	1375	THR
2	Н	1389	ILE
2	Н	1415	ASN
2	Н	1441	ILE
2	Н	1446	SER
2	Н	1451	GLN
2	Н	1468	THR
2	Н	1470	THR
2	Н	1476	ASN
2	Н	1486	PHE
2	Н	1567	ARG



Mol	Chain	Res	Type
2	Н	1583	MET
2	Н	1586	SER
2	Н	1590	ARG
2	Н	1616	VAL
2	Н	1624	THR
2	Н	1637	LEU
2	Н	1639	LYS
2	Н	1680	LEU
2	Н	1693	ARG
2	Н	1712	ASN
2	Н	1736	MET
2	Н	1740	THR
2	Н	1741	ILE
2	Н	1745	LYS
2	Н	1747	LYS
2	Н	1748	THR
2	Н	1750	LYS
2	Н	1759	SER
2	Н	1761	SER
2	Н	1770	LEU
2	Н	1775	GLN
2	Н	1781	LEU
2	Н	1811	GLU
2	Н	1844	ARG
2	Н	1845	ASP
2	Н	1846	GLU
2	Н	1847	LEU
2	Н	1862	VAL
2	Н	1914	LEU
2	Н	1927	LEU
2	Н	1934	GLU
2	Н	1935	GLU
2	Н	1973	SER
2	Н	1976	PHE
2	Н	1978	SER
2	Н	2022	THR
2	Н	2040	GLU
2	Ι	7	ARG
2	Ι	34	GLN
2	Ι	38	ASN
2	Ι	99	ASN
2	Ι	109	LEU



Mol	Chain	Res	Type
2	Ι	114	THR
2	Ι	121	GLU
2	Ι	140	LYS
2	Ι	166	THR
2	Ι	173	LEU
2	Ι	194	THR
2	Ι	223	SER
2	Ι	236	ILE
2	Ι	240	LEU
2	Ι	267	LEU
2	Ι	277	LEU
2	Ι	326	ASP
2	Ι	339	LEU
2	Ι	342	SER
2	Ι	345	THR
2	Ι	351	ASP
2	Ι	353	VAL
2	Ι	376	ASN
2	Ι	419	ARG
2	Ι	425	SER
2	Ι	431	LEU
2	Ι	436	SER
2	Ι	492	THR
2	Ι	494	THR
2	Ι	497	LYS
2	Ι	510	SER
2	Ι	516	THR
2	Ι	545	GLN
2	Ι	598	THR
2	Ι	616	THR
2	Ι	665	LEU
2	Ι	669	LEU
2	Ι	670	ARG
2	Ι	730	LEU
2	Ι	776	ASP
2	Ι	805	VAL
2	Ι	827	VAL
2	Ι	845	THR
2	Ι	846	VAL
2	Ι	887	LYS
2	Ι	907	VAL
2	Ι	910	GLN



Mol	Chain	Res	Type
2	Ι	914	LEU
2	Ι	936	ASN
2	Ι	947	THR
2	Ι	972	LEU
2	Ι	1033	SER
2	Ι	1040	LEU
2	Ι	1110	ASP
2	Ι	1131	SER
2	Ι	1157	SER
2	Ι	1158	PHE
2	Ι	1167	SER
2	Ι	1189	THR
2	Ι	1195	VAL
2	Ι	1205	LEU
2	Ι	1213	LEU
2	Ι	1236	LEU
2	Ι	1317	ARG
2	Ι	1320	LEU
2	Ι	1343	VAL
2	Ι	1347	LEU
2	Ι	1348	LEU
2	Ι	1354	SER
2	Ι	1367	GLN
2	Ι	1375	THR
2	Ι	1389	ILE
2	Ι	1415	ASN
2	Ι	1441	ILE
2	Ι	1446	SER
2	Ι	1451	GLN
2	Ι	1468	THR
2	Ι	1470	THR
2	Ι	1476	ASN
2	Ι	1486	PHE
2	Ι	1567	ARG
2	Ι	1583	MET
2	Ι	1586	SER
2	Ι	1590	ARG
2	Ι	1616	VAL
2	Ι	1624	THR
2	Ι	1637	LEU
2	Ι	1639	LYS
2	Ι	1680	LEU



Mol	Chain	Res	Type
2	Ι	1693	ARG
2	Ι	1712	ASN
2	Ι	1736	MET
2	Ι	1740	THR
2	Ι	1741	ILE
2	Ι	1745	LYS
2	Ι	1747	LYS
2	Ι	1748	THR
2	Ι	1750	LYS
2	Ι	1759	SER
2	Ι	1761	SER
2	Ι	1770	LEU
2	Ι	1775	GLN
2	Ι	1781	LEU
2	Ι	1811	GLU
2	Ι	1844	ARG
2	Ι	1845	ASP
2	Ι	1846	GLU
2	Ι	1847	LEU
2	Ι	1862	VAL
2	Ι	1914	LEU
2	Ι	1927	LEU
2	Ι	1934	GLU
2	Ι	1935	GLU
2	Ι	1973	SER
2	Ι	1976	PHE
2	Ι	1978	SER
2	Ι	2022	THR
2	Ι	2040	GLU
2	J	7	ARG
2	J	34	GLN
2	J	38	ASN
2	J	99	ASN
2	J	109	LEU
2	J	114	THR
2	J	121	GLU
2	J	166	THR
2	J	173	LEU
2	J	194	THR
2	J	223	SER
2	J	236	ILE
2	J	240	LEU



Mol	Chain	Res	Type
2	J	267	LEU
2	J	277	LEU
2	J	326	ASP
2	J	339	LEU
2	J	342	SER
2	J	345	THR
2	J	351	ASP
2	J	353	VAL
2	J	376	ASN
2	J	419	ARG
2	J	425	SER
2	J	431	LEU
2	J	436	SER
2	J	492	THR
2	J	494	THR
2	J	497	LYS
2	J	510	SER
2	J	516	THR
2	J	545	GLN
2	J	598	THR
2	J	616	THR
2	J	665	LEU
2	J	669	LEU
2	J	670	ARG
2	J	730	LEU
2	J	776	ASP
2	J	805	VAL
2	J	827	VAL
2	J	845	THR
2	J	846	VAL
2	J	887	LYS
2	J	907	VAL
2	J	910	GLN
2	J	914	LEU
2	J	936	ASN
2	J	947	THR
2	J	972	LEU
2	J	1033	SER
2	J	1040	LEU
2	J	1110	ASP
2	J	1131	SER
2	J	1157	SER



Mol	Chain	Res	Type
2	J	1158	PHE
2	J	1167	SER
2	J	1189	THR
2	J	1195	VAL
2	J	1205	LEU
2	J	1213	LEU
2	J	1236	LEU
2	J	1317	ARG
2	J	1320	LEU
2	J	1343	VAL
2	J	1347	LEU
2	J	1348	LEU
2	J	1354	SER
2	J	1367	GLN
2	J	1375	THR
2	J	1389	ILE
2	J	1415	ASN
2	J	1441	ILE
2	J	1446	SER
2	J	1451	GLN
2	J	1468	THR
2	J	1470	THR
2	J	1476	ASN
2	J	1486	PHE
2	J	1567	ARG
2	J	1583	MET
2	J	1586	SER
2	J	1590	ARG
2	J	1616	VAL
2	J	1624	THR
2	J	1637	LEU
2	J	1639	LYS
2	J	1680	LEU
2	J	1693	ARG
2	J	1712	ASN
2	J	1736	MET
2	J	1740	THR
2	J	1741	ILE
2	J	1745	LYS
2	J	1747	LYS
2	J	1748	THR
2	J	1750	LYS



Mol	Chain	Res	Type
2	J	1759	SER
2	J	1761	SER
2	J	1770	LEU
2	J	1775	GLN
2	J	1781	LEU
2	J	1811	GLU
2	J	1844	ARG
2	J	1845	ASP
2	J	1846	GLU
2	J	1847	LEU
2	J	1862	VAL
2	J	1914	LEU
2	J	1927	LEU
2	J	1934	GLU
2	J	1935	GLU
2	J	1973	SER
2	J	1976	PHE
2	J	1978	SER
2	J	2022	THR
2	J	2040	GLU
2	K	7	ARG
2	K	34	GLN
2	K	38	ASN
2	K	99	ASN
2	K	109	LEU
2	K	114	THR
2	K	121	GLU
2	K	166	THR
2	K	173	LEU
2	K	194	THR
2	K	223	SER
2	K	236	ILE
2	K	240	LEU
2	K	267	LEU
2	Κ	277	LEU
2	K	326	ASP
2	К	339	LEU
2	К	342	SER
2	K	345	THR
2	Κ	351	ASP
2	Κ	353	VAL
2	K	376	ASN



Mol	Chain	Res	Type
2	K	419	ARG
2	K	425	SER
2	K	431	LEU
2	K	436	SER
2	К	492	THR
2	К	494	THR
2	K	497	LYS
2	K	510	SER
2	K	516	THR
2	K	545	GLN
2	K	598	THR
2	K	616	THR
2	K	665	LEU
2	K	669	LEU
2	K	670	ARG
2	K	730	LEU
2	K	776	ASP
2	Κ	805	VAL
2	Κ	827	VAL
2	K	845	THR
2	Κ	846	VAL
2	K	887	LYS
2	Κ	907	VAL
2	K	910	GLN
2	K	914	LEU
2	Κ	936	ASN
2	K	947	THR
2	K	972	LEU
2	K	1033	SER
2	K	1040	LEU
2	K	1110	ASP
2	K	1131	SER
2	K	1157	SER
2	K	1158	PHE
2	K	1167	SER
2	K	1189	THR
2	K	1195	VAL
2	K	1205	LEU
2	K	1213	LEU
2	K	1236	LEU
2	K	1317	ARG
2	K	1320	LEU



Mol	Chain	Res	Type
2	K	1343	VAL
2	K	1347	LEU
2	K	1348	LEU
2	К	1354	SER
2	K	1367	GLN
2	K	1375	THR
2	K	1389	ILE
2	K	1415	ASN
2	K	1422	THR
2	K	1441	ILE
2	Κ	1446	SER
2	K	1451	GLN
2	K	1468	THR
2	K	1470	THR
2	K	1476	ASN
2	K	1486	PHE
2	K	1567	ARG
2	K	1583	MET
2	K	1586	SER
2	K	1590	ARG
2	K	1616	VAL
2	K	1624	THR
2	K	1637	LEU
2	K	1639	LYS
2	K	1680	LEU
2	K	1693	ARG
2	K	1712	ASN
2	K	1736	MET
2	K	1740	THR
2	K	1741	ILE
2	K	1745	LYS
2	K	1747	LYS
2	K	1748	THR
2	K	1750	LYS
2	Κ	1759	SER
2	K	1761	SER
2	К	1770	LEU
2	K	1775	GLN
2	K	1781	LEU
2	К	1811	GLU
2	К	1844	ARG
2	K	1845	ASP



Mol	Chain	Res	Type
2	K	1846	GLU
2	K	1847	LEU
2	K	1862	VAL
2	K	1914	LEU
2	K	1927	LEU
2	K	1934	GLU
2	K	1935	GLU
2	K	1973	SER
2	K	1976	PHE
2	K	1978	SER
2	K	2022	THR
2	K	2040	GLU
2	L	7	ARG
2	L	24	THR
2	L	34	GLN
2	L	38	ASN
2	L	99	ASN
2	L	109	LEU
2	L	114	THR
2	L	121	GLU
2	L	166	THR
2	L	173	LEU
2	L	194	THR
2	L	223	SER
2	L	236	ILE
2	L	240	LEU
2	L	267	LEU
2	L	277	LEU
2	L	326	ASP
2	L	339	LEU
2	L	342	SER
2	L	345	THR
2	L	351	ASP
2	L	353	VAL
2	L	376	ASN
2	L	419	ARG
2	L	425	SER
2	L	431	LEU
2	L	436	SER
2	L	492	THR
2	L	494	THR
2	L	497	LYS



Mol	Chain	Res	Type
2	L	510	SER
2	L	516	THR
2	L	545	GLN
2	L	598	THR
2	L	616	THR
2	L	665	LEU
2	L	669	LEU
2	L	670	ARG
2	L	730	LEU
2	L	776	ASP
2	L	805	VAL
2	L	827	VAL
2	L	845	THR
2	L	846	VAL
2	L	887	LYS
2	L	907	VAL
2	L	910	GLN
2	L	914	LEU
2	L	936	ASN
2	L	947	THR
2	L	972	LEU
2	L	1033	SER
2	L	1040	LEU
2	L	1110	ASP
2	L	1131	SER
2	L	1157	SER
2	L	1158	PHE
2	L	1167	SER
2	L	1189	THR
2	L	1195	VAL
2	L	1205	LEU
2	L	1213	LEU
2	L	1236	LEU
2	L	1317	ARG
2	L	1320	LEU
2	L	1343	VAL
2	L	1347	LEU
2	L	1348	LEU
2	L	1354	SER
2	L	1367	GLN
2	L	1375	THR
2	L	1389	ILE



Mol	Chain	Res	Type
2	L	1415	ASN
2	L	1441	ILE
2	L	1446	SER
2	L	1451	GLN
2	L	1468	THR
2	L	1470	THR
2	L	1476	ASN
2	L	1486	PHE
2	L	1567	ARG
2	L	1583	MET
2	L	1586	SER
2	L	1590	ARG
2	L	1616	VAL
2	L	1624	THR
2	L	1637	LEU
2	L	1639	LYS
2	L	1680	LEU
2	L	1693	ARG
2	L	1712	ASN
2	L	1736	MET
2	L	1740	THR
2	L	1741	ILE
2	L	1745	LYS
2	L	1747	LYS
2	L	1748	THR
2	L	1750	LYS
2	L	1759	SER
2	L	1761	SER
2	L	1770	LEU
2	L	1775	GLN
2	L	1781	LEU
2	L	1811	GLU
2	L	1844	ARG
2	L	1845	ASP
2	L	1846	GLU
2	L	1847	LEU
2	L	1862	VAL
2	L	1914	LEU
2	L	1927	LEU
2	L	1934	GLU
2	L	1935	GLU
2	L	1973	SER



Continued from previous page...

Mol	Chain	Res	Type
2	L	1976	PHE
2	L	1978	SER
2	L	2022	THR
2	Ĺ	2040	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (361) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	21	GLN
1	А	342	GLN
1	А	344	GLN
1	А	438	ASN
1	А	506	ASN
1	А	618	ASN
1	А	719	GLN
1	А	738	ASN
1	А	904	ASN
1	А	971	ASN
1	А	983	GLN
1	А	987	ASN
1	А	1064	ASN
1	А	1066	ASN
1	А	1146	HIS
1	А	1239	HIS
1	А	1288	ASN
1	А	1432	HIS
1	А	1442	ASN
1	А	1507	GLN
1	А	1510	ASN
1	А	1577	GLN
1	А	1610	ASN
1	А	1657	HIS
2	G	99	ASN
2	G	155	GLN
2	G	354	ASN
2	G	376	ASN
2	G	390	ASN
2	G	428	HIS
2	G	440	ASN
2	G	447	ASN
2	G	500	HIS
2	G	545	GLN



Mol	Chain	Res	Type
2	G	558	ASN
2	G	572	ASN
2	G	612	ASN
2	G	718	ASN
2	G	747	HIS
2	G	760	HIS
2	G	908	ASN
2	G	910	GLN
2	G	936	ASN
2	G	1046	GLN
2	G	1049	GLN
2	G	1061	GLN
2	G	1217	ASN
2	G	1307	ASN
2	G	1355	ASN
2	G	1383	ASN
2	G	1384	GLN
2	G	1415	ASN
2	G	1451	GLN
2	G	1619	ASN
2	G	1712	ASN
2	G	1775	GLN
2	G	1890	ASN
2	G	1983	ASN
2	G	2020	GLN
1	В	21	GLN
1	В	342	GLN
1	В	344	GLN
1	В	438	ASN
1	В	506	ASN
1	В	618	ASN
1	В	719	GLN
1	В	738	ASN
1	В	904	ASN
1	B	971	ASN
1	В	983	GLN
1	В	987	ASN
1	B	1064	ASN
1	В	1066	ASN
1	B	1146	HIS
1	В	1239	HIS
1	В	1288	ASN



Mol	Chain	Res	Type
1	В	1432	HIS
1	В	1442	ASN
1	В	1507	GLN
1	В	1510	ASN
1	В	1577	GLN
1	В	1610	ASN
1	В	1657	HIS
1	С	21	GLN
1	С	342	GLN
1	С	344	GLN
1	С	438	ASN
1	С	506	ASN
1	С	618	ASN
1	С	719	GLN
1	С	738	ASN
1	С	904	ASN
1	С	971	ASN
1	С	983	GLN
1	С	987	ASN
1	С	1064	ASN
1	С	1066	ASN
1	С	1146	HIS
1	С	1239	HIS
1	С	1288	ASN
1	С	1432	HIS
1	С	1442	ASN
1	С	1483	ASN
1	С	1507	GLN
1	С	1510	ASN
1	С	1577	GLN
1	С	1610	ASN
1	С	1657	HIS
1	С	1845	ASN
1	D	21	GLN
1	D	342	GLN
1	D	344	GLN
1	D	438	ASN
1	D	506	ASN
1	D	618	ASN
1	D	719	GLN
1	D	738	ASN
1	D	904	ASN



Mol	Chain	Res	Type
1	D	971	ASN
1	D	983	GLN
1	D	987	ASN
1	D	1064	ASN
1	D	1066	ASN
1	D	1146	HIS
1	D	1239	HIS
1	D	1288	ASN
1	D	1432	HIS
1	D	1442	ASN
1	D	1483	ASN
1	D	1507	GLN
1	D	1510	ASN
1	D	1577	GLN
1	D	1610	ASN
1	D	1657	HIS
1	D	1845	ASN
1	Е	21	GLN
1	Е	342	GLN
1	Е	344	GLN
1	Е	438	ASN
1	Е	506	ASN
1	Е	618	ASN
1	Е	719	GLN
1	Е	738	ASN
1	Е	904	ASN
1	Е	971	ASN
1	Е	983	GLN
1	Е	987	ASN
1	Е	1064	ASN
1	Е	1066	ASN
1	Е	1146	HIS
1	E	1239	HIS
1	Е	1288	ASN
1	Е	1432	HIS
1	Е	1442	ASN
1	Е	1507	GLN
1	E	1510	ASN
1	Е	1577	GLN
1	Е	1610	ASN
1	Е	1657	HIS
1	F	21	GLN



Mol	Chain	Res	Type
1	F	342	GLN
1	F	344	GLN
1	F	438	ASN
1	F	506	ASN
1	F	618	ASN
1	F	719	GLN
1	F	738	ASN
1	F	904	ASN
1	F	971	ASN
1	F	983	GLN
1	F	987	ASN
1	F	1064	ASN
1	F	1066	ASN
1	F	1146	HIS
1	F	1239	HIS
1	F	1288	ASN
1	F	1432	HIS
1	F	1442	ASN
1	F	1507	GLN
1	F	1510	ASN
1	F	1577	GLN
1	F	1610	ASN
1	F	1657	HIS
1	F	1845	ASN
2	Н	99	ASN
2	Н	155	GLN
2	Н	330	ASN
2	Н	354	ASN
2	Н	376	ASN
2	Н	390	ASN
2	Н	428	HIS
2	Н	440	ASN
2	Н	447	ASN
2	Н	500	HIS
2	Н	545	GLN
2	H	558	ASN
2	H	572	ASN
2	H	612	ASN
2	H	715	GLN
2	Н	718	ASN
2	H	747	HIS
2	Н	760	HIS



Mol	Chain	Res	Type
2	Н	908	ASN
2	Н	910	GLN
2	Н	936	ASN
2	Н	1046	GLN
2	Н	1049	GLN
2	Н	1061	GLN
2	Н	1217	ASN
2	Н	1307	ASN
2	Н	1355	ASN
2	Н	1383	ASN
2	Н	1384	GLN
2	Н	1415	ASN
2	Н	1451	GLN
2	Н	1581	HIS
2	Н	1619	ASN
2	Н	1712	ASN
2	Н	1775	GLN
2	Н	1890	ASN
2	Н	1983	ASN
2	Н	2020	GLN
2	Ι	99	ASN
2	Ι	155	GLN
2	Ι	354	ASN
2	Ι	376	ASN
2	Ι	390	ASN
2	Ι	428	HIS
2	Ι	447	ASN
2	Ι	500	HIS
2	Ι	545	GLN
2	Ι	572	ASN
2	Ι	612	ASN
2	Ι	715	GLN
2	Ι	718	ASN
2	Ι	747	HIS
2	Ι	760	HIS
2	Ι	908	ASN
2	Ι	910	GLN
2	Ι	936	ASN
2	Ι	1046	GLN
2	Ι	1217	ASN
2	Ι	1307	ASN
2	Ι	1355	ASN



Mol	Chain	Res	Type
2	Ι	1383	ASN
2	Ι	1384	GLN
2	Ι	1415	ASN
2	Ι	1451	GLN
2	Ι	1581	HIS
2	Ι	1619	ASN
2	Ι	1712	ASN
2	Ι	1775	GLN
2	Ι	1890	ASN
2	Ι	1983	ASN
2	Ι	2020	GLN
2	J	99	ASN
2	J	155	GLN
2	J	354	ASN
2	J	359	HIS
2	J	376	ASN
2	J	390	ASN
2	J	428	HIS
2	J	447	ASN
2	J	500	HIS
2	J	545	GLN
2	J	572	ASN
2	J	612	ASN
2	J	715	GLN
2	J	718	ASN
2	J	747	HIS
2	J	760	HIS
2	J	908	ASN
2	J	910	GLN
2	J	936	ASN
2	J	1046	GLN
2	J	1049	GLN
2	J	1217	ASN
2	J	1307	ASN
2	J	1355	ASN
2	J	1383	ASN
2	J	1415	ASN
2	J	1451	GLN
2	J	1581	HIS
2	J	1619	ASN
2	J	1712	ASN
2	J	1775	GLN



Mol	Chain	Res	Type
2	J	1890	ASN
2	J	1983	ASN
2	J	2020	GLN
2	K	99	ASN
2	K	155	GLN
2	K	354	ASN
2	K	359	HIS
2	K	376	ASN
2	K	390	ASN
2	K	428	HIS
2	K	447	ASN
2	K	500	HIS
2	K	545	GLN
2	K	558	ASN
2	K	572	ASN
2	K	612	ASN
2	K	715	GLN
2	K	718	ASN
2	K	747	HIS
2	К	760	HIS
2	K	908	ASN
2	К	910	GLN
2	K	936	ASN
2	K	1046	GLN
2	K	1049	GLN
2	K	1061	GLN
2	K	1217	ASN
2	K	1307	ASN
2	K	1355	ASN
2	Κ	1383	ASN
2	Κ	1384	GLN
2	Κ	1415	ASN
2	Κ	$1\overline{451}$	GLN
2	K	1619	ASN
2	K	1712	ASN
2	K	1775	GLN
2	K	1890	ASN
2	K	1983	ASN
2	K	2020	GLN
2	L	99	ASN
2	L	155	GLN
2	L	354	ASN



Mol	Chain	Res	Type
2	L	376	ASN
2	L	390	ASN
2	L	428	HIS
2	L	440	ASN
2	L	447	ASN
2	L	500	HIS
2	L	545	GLN
2	L	558	ASN
2	L	572	ASN
2	L	612	ASN
2	L	715	GLN
2	L	718	ASN
2	L	747	HIS
2	L	760	HIS
2	L	908	ASN
2	L	910	GLN
2	L	936	ASN
2	L	1046	GLN
2	L	1049	GLN
2	L	1217	ASN
2	L	1307	ASN
2	L	1355	ASN
2	L	1383	ASN
2	L	1384	GLN
2	L	1415	ASN
2	L	1451	GLN
2	L	1581	HIS
2	L	1619	ASN
2	L	1712	ASN
2	L	1775	GLN
2	L	1890	ASN
2	L	1983	ASN
2	L	2020	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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



5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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).

Mal	Type	Chain	Bos	Link	Bond lengths			E	ond ang	gles
WIOI	туре	Ullalli	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
3	J8T	А	1901	1	7,12,13	0.82	0	$11,\!17,\!20$	1.21	1 (9%)
3	J8T	Е	1901	1	$7,\!12,\!13$	0.82	0	$11,\!17,\!20$	1.20	1 (9%)
4	FMN	G	2101	-	33,33,33	1.51	6 (18%)	$48,\!50,\!50$	1.47	10 (20%)
3	J8T	В	1901	1	$7,\!12,\!13$	0.83	0	$11,\!17,\!20$	1.19	1 (9%)
4	FMN	L	2101	-	33,33,33	1.53	7 (21%)	48,50,50	1.47	9 (18%)
4	FMN	J	2101	-	33,33,33	1.52	7 (21%)	48,50,50	1.46	9 (18%)
4	FMN	К	2101	-	33,33,33	1.51	6 (18%)	48,50,50	1.47	10 (20%)
3	J8T	D	1901	1	7,12,13	0.84	0	11,17,20	1.21	1 (9%)
4	FMN	Ι	2101	-	33,33,33	1.53	7 (21%)	$48,\!50,\!50$	1.45	9 (18%)
3	J8T	С	1901	1	$7,\!12,\!13$	0.81	0	$11,\!17,\!20$	1.20	1 (9%)
4	FMN	Н	2101	-	33,33,33	1.53	6 (18%)	48,50,50	1.46	10 (20%)
3	J8T	F	1901	1	7,12,13	0.83	0	11,17,20	1.20	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	А	1901	1	-	4/13/16/17	-
3	J8T	Е	1901	1	-	4/13/16/17	-
4	FMN	G	2101	-	-	2/18/18/18	0/3/3/3
3	J8T	В	1901	1	-	4/13/16/17	-



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FMN	L	2101	-	-	2/18/18/18	0/3/3/3
4	FMN	J	2101	-	-	1/18/18/18	0/3/3/3
4	FMN	К	2101	-	-	2/18/18/18	0/3/3/3
3	J8T	D	1901	1	-	4/13/16/17	-
4	FMN	Ι	2101	-	-	1/18/18/18	0/3/3/3
3	J8T	С	1901	1	-	4/13/16/17	-
4	FMN	Н	2101	-	-	1/18/18/18	0/3/3/3
3	J8T	F	1901	1	-	4/13/16/17	-

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
4	Κ	2101	FMN	C9A-C5A	3.47	1.47	1.41
4	Н	2101	FMN	C9A-C5A	3.44	1.46	1.41
4	G	2101	FMN	C9A-C5A	3.44	1.46	1.41
4	L	2101	FMN	C9A-C5A	3.43	1.46	1.41
4	Ι	2101	FMN	C9A-C5A	3.37	1.46	1.41
4	J	2101	FMN	C9A-C5A	3.34	1.46	1.41
4	Н	2101	FMN	C5A-N5	-3.30	1.33	1.39
4	L	2101	FMN	C5A-N5	-3.28	1.33	1.39
4	J	2101	FMN	C5A-N5	-3.27	1.33	1.39
4	Ι	2101	FMN	C5A-N5	-3.22	1.33	1.39
4	Κ	2101	FMN	C5A-N5	-3.22	1.33	1.39
4	G	2101	FMN	C5A-N5	-3.17	1.33	1.39
4	G	2101	FMN	C8-C7	2.71	1.47	1.40
4	Κ	2101	FMN	C8-C7	2.71	1.47	1.40
4	Н	2101	FMN	C8-C7	2.68	1.47	1.40
4	L	2101	FMN	C8-C7	2.63	1.47	1.40
4	Н	2101	FMN	C4-N3	-2.62	1.34	1.38
4	Ι	2101	FMN	C6-C5A	-2.62	1.35	1.40
4	Ι	2101	FMN	C8-C7	2.61	1.47	1.40
4	J	2101	FMN	C8-C7	2.60	1.47	1.40
4	L	2101	FMN	C6-C5A	-2.56	1.35	1.40
4	Ι	2101	FMN	C4-N3	-2.55	1.34	1.38
4	J	2101	FMN	C6-C5A	-2.55	1.36	1.40
4	G	2101	FMN	C6-C5A	-2.55	1.36	1.40
4	J	2101	FMN	C4-N3	-2.55	1.34	1.38
4	Н	2101	FMN	C6-C5A	-2.53	1.36	1.40
4	Κ	2101	FMN	C6-C5A	-2.52	1.36	1.40
4	L	2101	FMN	C4-N3	-2.51	1.34	1.38
4	Κ	2101	FMN	C4-N3	-2.51	1.34	1.38



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	2101	FMN	C4-N3	-2.50	1.34	1.38
4	J	2101	FMN	C9-C8	-2.17	1.36	1.39
4	G	2101	FMN	C9-C8	-2.16	1.36	1.39
4	Ι	2101	FMN	C6-C7	-2.12	1.36	1.39
4	Ι	2101	FMN	C9-C8	-2.10	1.36	1.39
4	L	2101	FMN	C9-C8	-2.10	1.36	1.39
4	K	2101	FMN	C9-C8	-2.08	1.36	1.39
4	J	2101	FMN	C6-C7	-2.05	1.36	1.39
4	Н	2101	FMN	C9-C8	-2.04	1.36	1.39
4	L	2101	FMN	C6-C7	-2.04	1.36	1.39

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
4	G	2101	FMN	O4'-C4'-C5'	-3.35	102.39	109.92
4	Κ	2101	FMN	O4'-C4'-C5'	-3.35	102.39	109.92
4	L	2101	FMN	O4'-C4'-C5'	-3.30	102.50	109.92
4	Н	2101	FMN	O4'-C4'-C5'	-3.29	102.53	109.92
4	J	2101	FMN	O4'-C4'-C5'	-3.27	102.56	109.92
4	Ι	2101	FMN	O4'-C4'-C5'	-3.24	102.64	109.92
3	F	1901	J8T	C5-C8-C9	2.97	119.49	113.70
3	А	1901	J8T	C5-C8-C9	2.97	119.49	113.70
3	D	1901	J8T	C5-C8-C9	2.96	119.47	113.70
3	Е	1901	J8T	C5-C8-C9	2.96	119.47	113.70
3	С	1901	J8T	C5-C8-C9	2.95	119.45	113.70
3	В	1901	J8T	C5-C8-C9	2.94	119.44	113.70
4	Н	2101	FMN	C4A-C10-N1	-2.91	117.98	124.73
4	Ι	2101	FMN	C4A-C10-N1	-2.89	118.03	124.73
4	J	2101	FMN	C4A-C10-N1	-2.87	118.08	124.73
4	L	2101	FMN	C4A-C10-N1	-2.86	118.10	124.73
4	Κ	2101	FMN	C4A-C10-N1	-2.85	118.13	124.73
4	J	2101	FMN	C4-C4A-N5	2.80	122.22	118.23
4	G	2101	FMN	C4A-C10-N1	-2.79	118.26	124.73
4	Ι	2101	FMN	C4-C4A-N5	2.77	122.18	118.23
4	L	2101	FMN	O2-C2-N1	-2.76	117.26	121.83
4	L	2101	FMN	C4-C4A-N5	2.75	122.14	118.23
4	Κ	2101	FMN	O3P-P-O5'	-2.74	99.44	106.73
4	Κ	2101	FMN	C4-C4A-N5	2.74	122.13	118.23
4	G	2101	FMN	O2-C2-N1	-2.74	117.29	121.83
4	G	2101	FMN	O3P-P-O5'	-2.73	99.47	106.73
4	G	2101	FMN	C4-C4A-N5	2.73	122.12	118.23
4	Н	2101	FMN	C4-C4A-N5	2.72	122.10	118.23



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
4	Н	2101	FMN	O2-C2-N1	-2.71	117.34	121.83
4	J	2101	FMN	O2-C2-N1	-2.71	117.34	121.83
4	Κ	2101	FMN	O2-C2-N1	-2.70	117.35	121.83
4	L	2101	FMN	O3P-P-O5'	-2.67	99.64	106.73
4	Ι	2101	FMN	O3P-P-O5'	-2.66	99.65	106.73
4	J	2101	FMN	O3P-P-O5'	-2.66	99.66	106.73
4	Ι	2101	FMN	O2-C2-N1	-2.65	117.44	121.83
4	Н	2101	FMN	O3P-P-O5'	-2.65	99.69	106.73
4	J	2101	FMN	C10-N1-C2	2.64	122.18	116.90
4	Ι	2101	FMN	C10-N1-C2	2.61	122.12	116.90
4	Κ	2101	FMN	O4-C4-C4A	-2.59	119.74	126.60
4	G	2101	FMN	O4-C4-C4A	-2.58	119.75	126.60
4	Н	2101	FMN	C10-N1-C2	2.56	122.02	116.90
4	L	2101	FMN	C10-N1-C2	2.56	122.02	116.90
4	Κ	2101	FMN	C10-N1-C2	2.54	121.98	116.90
4	J	2101	FMN	O4-C4-C4A	-2.53	119.88	126.60
4	G	2101	FMN	C10-N1-C2	2.51	121.91	116.90
4	Ι	2101	FMN	O4-C4-C4A	-2.47	120.04	126.60
4	L	2101	FMN	O4-C4-C4A	-2.47	120.06	126.60
4	Н	2101	FMN	O4-C4-C4A	-2.46	120.07	126.60
4	Ι	2101	FMN	C10-C4A-N5	-2.20	120.18	124.86
4	L	2101	FMN	C10-C4A-N5	-2.18	120.22	124.86
4	Н	2101	FMN	C10-C4A-N5	-2.18	120.24	124.86
4	Κ	2101	FMN	C10-C4A-N5	-2.18	120.24	124.86
4	J	2101	FMN	C10-C4A-N5	-2.18	120.24	124.86
4	G	2101	FMN	C10-C4A-N5	-2.13	120.33	124.86
4	Ι	2101	FMN	C5A-N5-C4A	2.10	121.57	118.07
4	Κ	2101	FMN	C5A-N5-C4A	2.07	121.52	118.07
4	Н	2101	FMN	C4-N3-C2	-2.05	121.85	125.64
4	G	2101	FMN	C5A-N5-C4A	2.05	121.48	118.07
4	Κ	2101	FMN	C4-N3-C2	-2.03	121.89	125.64
4	L	2101	FMN	C4-N3-C2	-2.02	121.90	125.64
4	Н	2101	FMN	C5A-N5-C4A	2.02	121.44	118.07
4	J	2101	FMN	C5A-N5-C4A	2.02	121.43	118.07
4	G	2101	FMN	C4-N3-C2	-2.02	121.92	125.64

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There are no chirality outliers.

All (33) torsion outliers are listed below:

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



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	J	1	1 5	
Mol	Chain	Res	Type	Atoms
3	В	1901	J8T	O6-C8-C9-O7
3	В	1901	J8T	O6-C8-C9-N2
3	С	1901	J8T	O6-C8-C9-O7
3	С	1901	J8T	O6-C8-C9-N2
3	D	1901	J8T	O6-C8-C9-O7
3	D	1901	J8T	O6-C8-C9-N2
3	Е	1901	J8T	O6-C8-C9-O7
3	Е	1901	J8T	O6-C8-C9-N2
3	F	1901	J8T	O6-C8-C9-O7
3	F	1901	J8T	O6-C8-C9-N2
3	А	1901	J8T	O5-C4-C5-C6
3	В	1901	J8T	O5-C4-C5-C6
3	С	1901	J8T	O5-C4-C5-C6
3	D	1901	J8T	O5-C4-C5-C6
3	F	1901	J8T	O5-C4-C5-C6
4	G	2101	FMN	C4'-C5'-O5'-P
4	Н	2101	FMN	C4'-C5'-O5'-P
4	Ι	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
3	А	1901	J8T	O5-C4-C5-C7
3	В	1901	J8T	O5-C4-C5-C7
3	С	1901	J8T	O5-C4-C5-C7
3	D	1901	J8T	O5-C4-C5-C7
3	Е	1901	J8T	O5-C4-C5-C6
3	Е	1901	J8T	O5-C4-C5-C7
3	F	1901	J8T	O5-C4-C5-C7
4	G	2101	FMN	C2'-C3'-C4'-C5'
4	L	2101	FMN	C2'-C3'-C4'-C5'
4	K	2101	FMN	C2'-C3'-C4'-C5'

There are no ring outliers.

12 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	А	1901	J8T	1	0
3	Е	1901	J8T	1	0
4	G	2101	FMN	2	0
3	В	1901	J8T	1	0
4	L	2101	FMN	2	0
4	J	2101	FMN	2	0



Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	K	2101	FMN	2	0
3	D	1901	J8T	1	0
4	Ι	2101	FMN	2	0
3	С	1901	J8T	1	0
4	Н	2101	FMN	2	0
3	F	1901	J8T	1	0

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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 then 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 sufficient 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.

Orthogonal projections (i) 6.1

6.1.1**Primary** map









6.1.2Raw map



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



Z Index: 157

6.3.2 Raw map



X Index: 216

Y Index: 99



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



6.4 Orthogonal surface views (i)

6.4.1 Primary map



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.

6.4.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

6.5 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 nm^3 ; 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 (i)



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



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 $\mathrm{\AA^{-1}}$



8.2 Resolution estimates (i)

$\mathbf{Bosolution ostimato}(\mathbf{\hat{A}})$	Estimation criterion (FSC cut-off)		
Resolution estimate (A)	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)



The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.



9.2 Q-score mapped to coordinate model (i)



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

9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.01).



9.4 Atom inclusion (i)



At the recommended contour level, 97% of all backbone atoms, 93% of all non-hydrogen atoms, are inside the map.



Map-model fit summary (i) 9.5

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	0.9311	0.5370	_ 10
А	0.8833	0.5440	1.0
В	0.8841	0.5440	
С	0.8832	0.5440	
D	0.8841	0.5440	
Е	0.8831	0.5450	
F	0.8834	0.5450	
G	0.9716	0.5320	
Н	0.9716	0.5310	
Ι	0.9719	0.5300	0.0
J	0.9719	0.5310	<0.0
K	0.9716	0.5310	
L	0.9713	0.5310	

