Table 11.3.6.1. *Rating of lattice types implied by a given reduced cell*

Lattice type	Quality index	Conventional cell constants (Å, °)						Reindexing transformation
		a	*b*	*c*	α	β	γ	
1 *cF*	999.0	119.3	137.3	119.1	121.1	77.5	122.6	$11\bar{1}0/1\bar{1}10/\bar{1}\bar{1}\bar{1}0$
2 *hR*	770.1	74.6	111.7	137.4	103.6	89.1	108.8	$1100/\bar{1}0\bar{1}0/\bar{1}110$
3 *cP*	769.7	62.1	63.5	92.9	90.0	90.1	107.2	1000/0100/0010
5 *cI*	936.0	111.7	74.6	112.6	70.1	53.6	71.2	1010/1100/0110
4 *hR*	769.5	101.1	111.9	119.1	116.5	89.1	116.4	$1\bar{1}00/\bar{1}010/\bar{1}\bar{1}\bar{1}0$
6 *tI*	999.0	112.6	111.7	74.6	71.2	70.1	53.6	0110/1010/1100
7 *tI*	999.0	111.7	74.6	112.6	70.1	53.6	71.2	1010/1100/0110
8 *oI*	999.0	74.6	111.7	112.6	53.6	70.1	71.2	$\bar{1}\bar{1}00/\bar{1}0\bar{1}0/0\bar{1}\bar{1}0$
9 *hR*	772.7	62.1	74.6	296.6	90.5	105.8	125.5	$1000/\bar{1}\bar{1}00/\bar{1}\bar{1}\bar{3}0$
10 *mC*	24.0	101.1	74.6	92.9	90.1	90.0	91.3	$1\bar{1}00/1100/0010$
11 *tP*	174.8	62.1	63.5	92.9	90.0	90.1	107.2	1000/0100/0010
12 *hP*	122.8	62.1	63.5	92.9	90.0	90.1	107.2	1000/0100/0010
13 *oC*	**23.8**	74.6	101.1	92.9	90.0	90.1	88.7	$1100/\bar{1}100/0010$
15 *tI*	672.7	62.1	63.5	200.2	77.0	77.6	107.2	1000/0100/1120
16 *oF*	999.0	74.6	101.1	200.2	90.5	111.8	88.7	$\bar{1}\bar{1}00/1\bar{1}00/1120$
14 *mC*	23.4	74.6	101.1	92.9	90.0	90.1	88.7	$1100/\bar{1}100/0010$
17 *mC*	999.0	101.1	74.6	111.7	71.2	116.4	88.7	$1\bar{1}00/\bar{1}\bar{1}00/\bar{1}0\bar{1}0$
18 *tI*	999.0	112.6	119.1	62.1	68.7	99.5	115.4	$01\bar{1}0/1110/1000$
19 *oI*	999.0	62.1	112.6	119.1	64.6	68.7	80.5	$\bar{1}000/01\bar{1}0/\bar{1}\bar{1}\bar{1}0$
20 *mC*	746.3	112.6	112.6	62.1	99.5	99.6	111.3	$0\bar{1}\bar{1}0/0\bar{1}10/\bar{1}000$
21 *tP*	748.0	63.5	92.9	62.1	90.1	107.2	90.0	0100/0010/1000
22 *hP*	999.0	63.5	92.9	62.1	90.1	107.2	90.0	0100/0010/1000
23 *oC*	747.8	112.6	112.6	62.1	80.5	99.6	68.7	$0110/0\bar{1}10/1000$
24 *hR*	999.0	154.8	112.6	62.1	80.5	80.9	84.3	$1210/0\bar{1}10/1000$
25 *mC*	746.1	112.6	112.6	62.1	80.5	99.6	68.7	$0110/0\bar{1}10/1000$
26 *oF*	624.9	62.1	123.9	195.9	86.4	108.4	101.5	$1000/\bar{1}\bar{2}00/\bar{1}0\bar{2}0$
27 *mC*	499.7	123.9	62.1	112.6	80.5	119.7	78.5	$\bar{1}\bar{2}00/\bar{1}000/01\bar{1}0$
28 *mC*	325.0	62.1	195.9	63.5	95.4	107.2	71.6	$\bar{1}000/\bar{1}0\bar{2}0/0\bar{1}00$
29 *mC*	99.8	62.1	123.9	92.9	90.0	90.1	78.5	1000/1200/0010
30 *mC*	336.4	63.5	196.5	62.1	95.4	107.2	71.1	$0\bar{1}00/0\bar{1}20/\bar{1}000$
31 *aP*	0.2	62.1	63.5	92.9	90.0	89.9	72.8	$1000/0\bar{1}00/00\bar{1}0$
32 *oP*	152.0	62.1	63.5	92.9	90.0	90.1	107.2	1000/0100/0010
40 *oC*	413.0	63.5	196.4	62.1	84.5	107.2	108.9	$0\bar{1}00/0120/\bar{1}000$
35 *mP*	151.8	63.5	62.1	92.9	90.1	90.0	107.2	$0\bar{1}00/\bar{1}000/00\bar{1}0$
36 *oC*	400.3	62.1	195.9	63.5	84.6	107.2	108.4	$1000/\bar{1}0\bar{2}0/0100$
33 *mP*	151.2	62.1	63.5	92.9	90.0	90.1	107.2	1000/0100/0010
38 *oC*	100.1	62.1	123.9	92.9	90.0	90.1	101.5	$\bar{1}000/1200/00\bar{1}0$
34 *mP*	1.0	62.1	92.9	63.5	90.0	107.2	90.1	$\bar{1}000/00\bar{1}0/0\bar{1}00$
42 *oI*	661.3	62.1	63.5	200.2	103.0	102.4	107.2	$\bar{1}000/0\bar{1}00/1120$
41 *mC*	412.2	196.4	63.5	62.1	107.2	95.5	71.1	$0\bar{1}\bar{2}0/0\bar{1}00/\bar{1}000$
37 *mC*	400.1	195.9	62.1	63.5	107.2	95.4	71.6	1020/1000/0100
39 *mC*	99.9	123.9	62.1	92.9	90.1	90.0	78.5	$\bar{1}\bar{2}00/\bar{1}000/00\bar{1}0$
43 *mI*	999.0	74.6	200.2	63.5	103.0	127.3	68.2	$1100/1120/0\bar{1}00$
44 *aP*	0.0	62.1	63.5	92.9	90.0	90.1	107.2	1000/0100/0010

compatible with the observed diffraction pattern. The highest lattice symmetry is orthorhombic (character 13, Bravais type *oC*), which limits the possible space groups for protein crystals to either $C222_1$ or $C222$. Processing of all films in the data set was completed in space group $P1$ using the cell constants shown for lattice character 44. To test whether the crystal has space-group symmetry $C222$ and conventional cell constants $a = 74.6, b = 101.1, c = 92.9$ Å, the final steps of data processing were repeated after reindexing the reflections by the transformation $h' = 1 \cdot h + 1 \cdot k + 0 \cdot l + 0$, $k' = -1 \cdot h + 1 \cdot k + 0 \cdot l + 0$, $l' = 0 \cdot h + 0 \cdot k + 1 \cdot l + 0$ as specified for lattice character 13. Note that the transformation also provides a simple tool for correcting the indices if all reflections are misindexed by a constant. The results clearly show that the crystal has space-group symmetry $C222_1$. The presence of the 2_1 axis was deduced from the rather weak intensities observed for reflections of type $00l' = \text{odd}$.

references