On the quality of protein crystals grown under diffusion mass-transport controlled regime, part I

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Supplementary material

Figure S1. The plot shows the first and third dimensions of the PC analysis. The projected direction of each indicator "axis" is indicated by arrows. The indicators for all the crystals in the dataset are plotted as blue/yellow circles for ground/space grown crystals. The same colors are used to indicate the ellipses encompassing the representative points within the two groups.

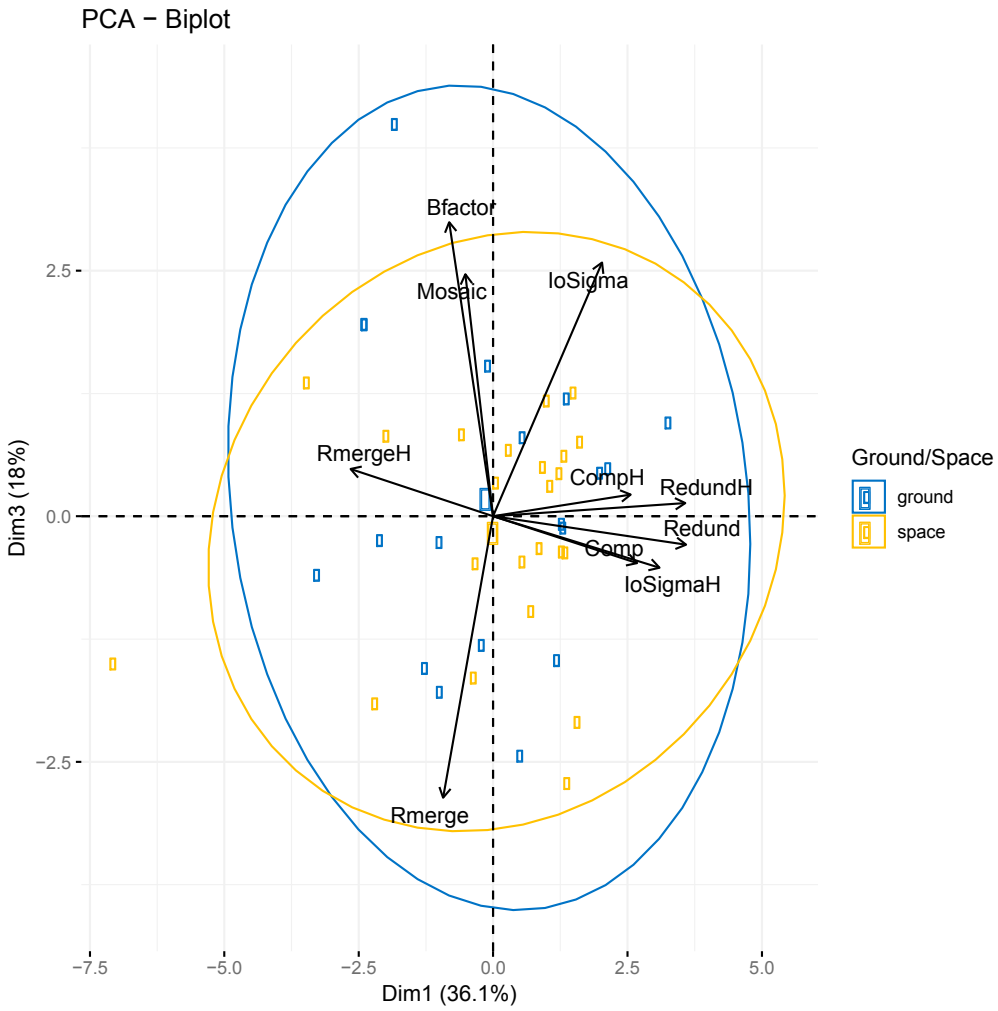

Table S1. Resume of data collection and refinement statistics for oxy-hemoglobin II crystals grown in space and on ground.

	SPACE			GROUND		
	hb2_naf5_1	hb2_naf5_2	hb2_naf5_3	hb2_naf5_1	hb2_naf5_2	hb2_naf5_3
Wavelength (Å)	0.886	0.886	0.886	0.886	0.886	0.886
Space group	P42212	P42212	P42212	P42212	P42212	P42212
Cell parameters (Å)	a=b=74.30, c=153.63	a=b=73.97, c=153.19	a=b=73.99, c=153.15	a=b=74.30, c=154.23	a=b=74.14, c=153.85	a=b=73.98, c=153.51
Resolution range (Å)	20.0-2.00 (2.07-2.00)	20.0-2.00 (2.07-2.00)	20.0-2.00 (2.07-2.00)	20.0-2.00 (2.07-2.00)	20.0-2.00 (2.07-2.00)	20.0-2.00 (2.07-2.00)
Observed reflections	285305	309606	268187	259362	316319	340167
Independent reflections	29991	29560	28943	29003	29639	29767
Data completeness (%)	99.2 (99.9)	99.9 (100.0)	99.0 (98.1)	97.8 (100.0)	99.2 (98.2)	99.2 (100.0)
Rmerge (%)†	11.8 (44.0)	13.8 (33.4)	14.8 (45.3)	11.4 (58.3)	9.2 (57.9)	8.9 (30.3)
Average I/σ (I)	17.4 (5.7)	16.2 (8.2)	13.0 (3.6)	15.2 (3.6)	24.4 (4.3)	24.8 (9.0)
Redundancy	9.6 (8.5)	10.5 (9.5)	9.4 (7.7)	8.9 (9.2)	10.7 (10.2)	11.5 (11.8)
Mosaicity	0.58	0.43	0.51	0.96	0.60	0.717
B factor	30.9	28.6	29.8	38.5	34.9	30.8

Table S2. Resume of data collection and refinement statistics for cyano-hemoglobin II-III crystals grown in space and on ground.

	SPACE				GROUND		
	hb23cnM_naf5_1	hb23cnM_naf5_2	hb23cnM_naf5_3	hb23cnM_naf5_4	hb23cnM_naf5_1	hb23cnM_naf5_2	hb23cnM_naf5_3
Wavelength (Å)	0.886	0.886	0.886	0.886	0.886	0.886	0.886
Space group	P42212	P42212	P42212	P42212	P42212	P42212	P42212
Cell parameters (Å)	a=b=73.94, c=152.70	a=b=73.64, c=152.60	a=b=73.79, c=152.68	a=b=73.82, c=152.56	a=b=73.93, c=152.74	a=b=74.02, c=152.72	a=b=73.83, c=152.49
Resolution range (Å)	20.0-2.45 (2.54-2.45)	20.0-2.75 (2.85-2.75)	20.0-2.50 (2.59-2.50)	20.0-2.75 (2.85-2.75)	20.0-2.40 (2.49-2.40)	20.0-2.25 (2.33-2.25)	20.0-2.20 (2.28-2.20)
Observed reflections	169888	117999	146886	117227	163687	202448	165962
Independent reflections	16481	11585	15209	11672	17275	20762	20530
Data completeness (%)	99.7 (100.0)	99.3 (100.0)	99.7 (99.9)	99.9 (100.0)	99.6 (100.0)	99.4 (100.0)	92.2 (89.2)
Rmerge (%)†	9.5 (45.9)	9.6 (49.4)	8.6 (49.0)	9.3 (47.2)	10.6 (48.4)	10.6 (53.5)	7.7 (32.9)
Average I/σ (I)	19.5 (4.6)	17.2 (4.4)	19.3 (4.8)	20.2 (5.1)	18.12 (5.1)	17.4 (4.11)	20.9 (5.6)
Redundancy	10.4 (10.7)	10.3 (10.7)	9.7 (9.7)	10.1 (10.6)	9.4 (9.5)	9.8 (9.9)	8.1 (7.4)
Mosaicity	1.15	1.36	1.13	1.27	0.94	0.87	0.69
B factor	48.4	59.2		55.9	45.9	43.4	35.4

Table S3. Resume of data collection and refinement statistics of insulin crystals grown in space and on ground.

SPACE						
	Ins3ls41_2	Ins3ls41_3	Ins3ls41_4	Ins3ls41_4b	Ins3ls41_5	Ins3ls42_4
Wavelength (Å)	0.886	0.886	0.886	0.886	0.886	0.886
Space group	I213	I213	I213	I213	I213	I213
Cell parameters (Å)	a=b=c=78.42	a=b=c=77.52	a=b=c=77.78	a=b=c=77.80	a=b=c=77.84	a=b=c=77.4
Resolution range (Å)	20.0-1.55 (1.61-1.55)	20.0-1.80 (1.86-1.80)	20.0-1.50 (1.55-1.50)	20.0-1.40 (1.45-1.40)	20.0-1.45 (1.50-1.45)	20.0-1.81 (1.87-1.81)
Observed reflections	98160	63466	107411	80041	121185	38110
Independent reflections	11485	7347	12612	15192	13894	7098
Data completeness (%)	97.2 (100.0)	99.7 (100.0)	99.3 (100.0)	97.5 (100.0)	99.0 (100.0)	98.8 (99.9)
Rmerge (%)†	10.2 (37.1)	11.0 (39.1)	8.3 (35.3)	5.6 (46.4)	15.6 (36.0)	9.0 (43.8.)
Average I/σ (I)	16.4 (5.9)	15.6 (6.2)	19.44 (3.5)	22.3 (3.5)	10.1 (6.3)	14.7 (3.7)
Redundancy	8.6 (8.9)	8.6 (8.5)	8.5 (8.6)	5.3 (5.5)	8.7 (8.8)	5.4 (5.4)
Mosaicity	0.64	0.63	0.295	0.27	0.32	0.508
B factor	22.9	27.0	21.4	20.0	19.5	31.7

GROUND						
	Ins3lg39_1	Ins3lg39_3	Ins3lg39_4	Ins3lg39_5	Ins3lg41_3	Ins3lg41_4
Wavelength (Å)	0.886	0.886	0.886	0.886	0.886	0.886
Space group	I213	I213	I213	I213	I213	I213
Cell parameters (Å)	a=b=c=77.85	a=b=c=77.61	a=b=c=77.63	a=b=c=77.3	a=b=c=77.81	a=b=c=77.95
Resolution range (Å)	20.0-1.48 (1.53-1.48)	20.0-1.60 (1.66-1.60)	20.0-1.55 (1.61-1.55)	20.0-1.75 (1.81-1.75)	20.0-1.60 (1.66-1.60)	20.0-1.65 (1.71-1.65)
Observed reflections	112775	84060	62931	38319	88833	76345
Independent reflections	13058	10338	11267	7606	10436	9641
Data completeness (%)	98.5 (100.0)	99.2 (100.0)	98.4 (100.0)	95.9 (100.0)	99.2 (100.0)	99.7 (100.0)
Rmerge (%)†	8.0 (35.8)	9.5 (37.0)	11.1 (40.6)	8.5 (34.6)	14.3 (35.3)	18.4 (39.4)
Average I/σ (I)	21.2 (6.1)	17.1 (5.7)	10.6 (3.8)	14.2 (4.3)	11.4 (5.8)	11.4 (5.8)
Redundancy	8.6 (8.7)	8.1 (8.2)	5.6 (5.6)	5.0 (5.1)	8.5 (8.6)	7.9 (8.0)
Mosaicity	0.46	0.36	0.54	0.70	0.49	0.31
B factor	21.1	24.8	24.2	30.7	22.2	23.2

Table S4. Resume of data collection and refinement statistics of thaumatin crystals grown in space and on ground.

	SPACE									
	th_s1	th_s5	th_s7	th_s10	th_s11	th_s13	th_s15	th_s17	th_s19	th_s22
Wavelength (Å)	0.9779	0.9779	0.9779	0.9779	0.9779	0.9779	0.9779	0.9779	0.9779	0.9779
Space group	P41212	P41212	P41212	P41212	P41212	P41212	P41212	P41212	P41212	P41212
Cell parameters (Å)	a=b=58.59	a=b=58.61	a=b=58.61	a=b=58.61	a=b=58.60	a=b=58.60	a=b=58.54	a=b=58.60	a=b= 58.59	a=b=58.53
	c=151.54	c=151.54	c=151.54	c=151.53	c=151.53	c=151.52	c=151.55	c=151.53	c=151.53	c=151.46
Resolution range (Å) 20.0-1.5 (1.55-1.50)										
Observed reflections	306591	304279	304984	306374	306702	307475	307562	304279	306603	186981
Independent reflections	43190	43085	43114	43158	40767	43154	43161	40772	43152	30932
Data completeness (%)	99.7 (100)	99.5 (100)	99.5 (100)	99.7 (100)	94.2 (97.3)	99.6 (100)	99.8 (100)	94.0 (97.0)	99.8 (100)	71.5 (71.0)
Rmerge (%)†	4.7 (26.99	5.1 (32.7)	4.3 (25.8)	4.9 (30.9)	4.9 (31.8)	5.2 (29.3)	6.1 (43.8)	4.4 (30.8)	5.0 (41.2)	5.2 (46.2)
Average I/σ (I)	35.2 (7.4)	30.5 (6.8)	38.6 (8.2)	33.4 (6.9)	34.9 (6.9)	31.4 (6.5)	28.5 (5.0)	36.6 (7.0)	36.0 (4.9)	24.8 (3.4)
Redundancy	7.1 (7.2)	7.1 (7.2)	7.1 (7.2)	7.1 (7.2)	7.5 (7.4)	7.1 (7.2)	7.1 (7.2)	7.5 (7.2)	7.1 (7.1)	6.0 (5.7)
Mosaicity	0.08	0.14	0.11	0.10	0.08	0.06	0.07	0.11	0.11	0.06
B factor	15.2	15.4	15.7	15.4	15.3	15.4	15.3	15.5	15.7	14.8

	GROUND						
	th_g6	th_g7	th_g10	th_g14	th_g16	th_g18	th_g19
Wavelength (Å)	0.9779	0.9779	0.9779	0.9779	0.9779	0.9779	0.9779
Space group	P41212	P41212	P41212	P41212	P41212	P41212	P41212
Cell parameters (Å)	a=b=58.54	a=b=58.58	a=b=58.49	a=b=58.58	a=b=58.43	a=b=58.61	a=b= 58.48
	c=151.54	c=151.51	c=151.57	c=151.48	c=151.58	c=151.54	c=151.55
Resolution range (Å)	20.0-1.5 (1.55-1.50)	20.0-1.5 (1.55-1.50)	20.0-1.5 (1.55-1.50)	20.0-1.5 (1.55-1.50)	20.0-1.5 (1.55-1.50)	20.0-1.5 (1.55-1.50)	
Observed reflections	285390	307733	294403	305675	298887	306241	289531
Independent reflections	42968	43229	41570	43161	42815	43174	42951
Data completeness (%)	99.4 (100)	99.9 (100)	96.3 (98.8)	99.6 (100)	99.3 (100)	99.6 (100)	99.5 (100)
Rmerge (%)†	7.1 (56.5)	6.7 (46.2)	4.6 (29.4)	4.6 (24.5)	4.1 (19.3)	4.1 (26.9)	4.7 (53.9)
Average I/σ (I)	24.1 (3.4)	26 (4.4)	34.7 (7.5)	35.4 (7.8)	37.7 (10.8)	39.4 (7.0)	38.6 (4.1)
Redundancy	6.6 (6.6)	7.1 (7.1)	7.0 (7.1)	7.1 (7.1)	7.1 (7.0)	7.1 (7.2)	6.7 (6.8)
Mosaicity	0.28	0.08	0.26	0.10	0.14	0.10	0.27
B factor	16.0	15.8	15.1	15.3	15.3	16.0	18.3

Table S5. Quality indicators from dataset processing including the completeness of the full data set and the highest resolution shell (Comp, CompH), redundancy (Redund, RedundH), R_merge (Rmerge, RmergeH), intensity over noise (IoSigma, IoSigmaH), B factor (Bfactor) and mosaic spread (Mosaic). The codes identifies the protein (hb2= oxy-hemoglobin II, hb23= cyano-hemoglobin II-III, ins= insulin, th= thaumatin) and enviromen (s=space and g=ground).

	code		Comp	CompH	Rmerge	RmergeH	IoSigma	IoSigmaH	Redund	RedundH	Mosaic	Bfactor
1	hb2	s1	99.2	99.9	11.80	44.00	17.40	5.70	9.60	8.50	0.58	30.90
2	hb2	s2	99.9	100.0	13.80	33.40	16.20	8.20	10.50	9.50	0.43	28.60
3	hb2	s3	99.0	98.1	14.80	45.30	13.00	3.60	9.40	7.70	0.51	29.80
4	hb2	g1	97.8	100.0	11.40	58.30	15.20	3.60	8.90	9.20	0.96	38.50
5	hb2	g2	99.2	98.2	9.20	57.90	24.40	4.30	10.70	10.20	0.60	34.90
6	hb2	g3	99.2	100.0	8.90	30.30	24.80	9.00	11.50	11.80	0.72	30.80
7	hb23	s1	99.7	100.0	9.50	45.90	19.50	4.60	10.40	10.70	1.15	48.40
8	hb23	s2	99.3	100.0	9.60	49.40	17.20	4.40	10.30	10.70	1.36	59.20
9	hb23	s3	99.7	99.9	8.60	49.00	19.30	4.80	9.70	9.70	1.13	-
10	hb23	s4	99.9	100.0	9.30	47.20	20.20	5.10	10.10	10.60	1.27	55.90
11	hb23	g1	99.6	100.0	10.60	48.40	18.12	5.10	9.40	9.50	0.94	45.90
12	hb23	g2	99.4	100.0	10.60	53.50	17.40	4.11	9.80	9.90	0.87	43.40
13	hb23	g3	99.2	89.2	7.70	32.90	20.90	5.60	8.10	7.40	0.69	35.40
14	ins	g1	98.5	100.0	8.00	35.80	21.20	6.10	8.60	8.70	0.46	21.10
15	ins	g3	99.2	100.0	9.50	37.00	17.10	5.70	8.10	8.20	0.36	24.80
16	ins	g4	98.4	100.0	11.10	40.60	10.60	3.80	5.60	5.60	0.54	24.20
17	ins	g5	95.9	100.0	8.50	34.60	14.20	4.30	5.00	5.10	0.70	30.70
18	ins	g3	99.2	100.0	14.30	35.30	11.40	5.80	8.50	8.60	0.49	22.20
19	ins	g4	99.7	100.0	18.40	39.40	11.40	5.80	7.90	8.00	0.31	23.20
20	ins	s2	97.2	100.0	10.20	37.10	16.40	5.90	8.60	8.90	0.64	22.90
21	ins	s3	99.7	100.0	11.00	39.10	15.60	6.20	8.60	8.50	0.63	27.00
22	ins	s4	99.3	100.0	8.30	35.30	19.44	3.50	8.50	8.60	0.29	31.40
23	ins	s4b	97.5	100.0	5.60	46.40	22.30	3.50	5.30	5.50	0.27	20.00
24	ins	s5	99.0	100.0	15.60	36.00	10.10	6.30	8.70	8.80	0.32	19.50
25	ins	s4	98.8	99.9	9.00	43.80	14.70	3.70	5.40	5.40	0.51	31.70
26	th	g6	99.4	100.0	7.10	56.50	24.10	3.40	6.60	6.60	0.28	16.00
27	th	g7	99.9	100.0	6.70	46.20	26.00	4.40	7.10	7.10	0.08	15.80
28	th	g10	96.3	98.8	4.60	29.40	34.70	7.50	7.00	7.10	0.26	15.10
29	th	g14	99.6	100.0	4.60	24.50	35.40	7.80	7.10	7.10	0.10	15.30
30	th	g16	99.3	100.0	4.10	19.30	37.70	10.80	7.10	7.00	0.14	15.30
31	th	g18	99.6	100.0	4.10	26.90	39.40	7.00	7.10	7.20	0.10	16.00
32	th	g19	99.5	100.0	4.70	53.90	38.60	4.10	6.70	6.80	0.27	18.30
33	th	s1	99.7	100.0	4.70	26.90	35.20	7.40	7.10	7.20	0.08	15.20
34	th	s5	99.5	100.0	5.10	32.70	30.50	6.80	7.10	7.20	0.14	15.40
35	th	s7	99.5	100.0	4.30	25.80	38.60	8.20	7.10	7.20	0.11	15.70
36	th	s10	99.7	100.0	4.90	30.90	33.40	6.90	7.10	7.20	0.10	15.40
37	th	s11	94.2	97.3	4.90	31.80	34.90	6.90	7.50	7.40	0.08	15.30
38	th	s13	99.6	100.0	5.20	29.30	31.40	6.50	7.10	7.20	0.06	15.40
39	th	s15	99.8	100.0	6.10	43.80	28.50	5.00	7.10	7.20	0.07	15.30
40	th	s17	94.0	97.0	4.40	30.80	36.60	7.00	7.50	7.20	0.11	15.50
41	th	s19	99.8	100.0	5.00	41.20	36.00	4.90	7.10	7.10	0.11	15.70
42	th	s22	71.5	71.0	5.20	46.20	24.80	3.40	6.00	5.70	0.06	14.80

Table S6. Normalized quality indicators for each dataset

	code		Comp	CompH	Rmerge	RmergeH	IoSigma	IoSigmaH	Redund	RedundH	Mosaic	Bfactor
1	hb2	s1	0.22	0.57	0.06	-0.07	-0.22	-0.01	-0.52	-0.69	-0.28	-0.36
2	hb2	s2	1.24	0.67	0.91	-0.97	-0.47	1.04	0.41	0.01	-1.09	-0.98
3	hb2	s3	-0.07	-1.34	1.33	0.04	-1.11	-0.90	-0.73	-1.25	-0.66	-0.66
4	hb2	g1	-1.82	0.67	-0.11	1.14	-0.67	-0.90	-1.24	-0.20	1.75	1.68
5	hb2	g2	0.22	-1.24	-1.03	1.11	1.19	-0.61	0.62	0.50	-0.18	0.71
6	hb2	g3	0.22	0.67	-1.16	-1.24	1.27	1.38	1.45	1.63	0.45	-0.39
7	hb23	s1	0.63	0.38	0.08	-0.11	0.39	-0.43	0.91	0.79	0.39	0.04
8	hb23	s2	-0.97	0.38	0.18	0.43	-1.24	-0.83	0.79	0.79	1.28	1.29
9	hb23	s3	0.63	0.36	-0.78	0.37	0.25	-0.03	0.02	-0.07	0.30	
10	hb23	s4	1.42	0.38	-0.11	0.09	0.89	0.57	0.53	0.70	0.90	0.91
11	hb23	g1	0.23	0.38	1.14	0.28	-0.59	0.57	-0.37	-0.25	-0.50	-0.25
12	hb23	g2	-0.57	0.38	1.14	1.06	-1.10	-1.41	0.15	0.10	-0.80	-0.54
13	hb23	g3	-1.37	-2.27	-1.65	-2.11	1.39	1.57	-2.03	-2.05	-1.56	-1.46
14	ins	g1	-0.03	0.29	-0.77	-0.70	1.42	0.90	0.77	0.77	-0.00	-0.87
15	ins	g3	0.58	0.29	-0.36	-0.37	0.42	0.56	0.45	0.45	-0.67	-0.02
16	ins	g4	-0.12	0.29	0.08	0.61	-1.16	-1.07	-1.16	-1.21	0.54	-0.16
17	ins	g5	-2.31	0.29	-0.63	-1.02	-0.28	-0.64	-1.54	-1.53	1.61	1.33
18	ins	g3	0.58	0.29	0.97	-0.83	-0.96	0.64	0.71	0.71	0.20	-0.62
19	ins	g4	1.02	0.29	2.10	0.28	-0.96	0.64	0.32	0.32	-1.01	-0.39
20	ins	s2	-1.17	0.29	-0.16	-0.34	0.25	0.73	0.77	0.90	1.21	-0.46
21	ins	s3	1.02	0.29	0.06	0.20	0.06	0.98	0.77	0.64	1.14	0.48
22	ins	s4	0.67	0.29	-0.69	-0.83	0.99	-1.33	0.71	0.71	-1.11	1.49
23	ins	s4b	-0.91	0.29	-1.43	2.18	1.68	-1.33	-1.35	-1.27	-1.28	-1.12
24	ins	s5	0.41	0.29	1.32	-0.64	-1.28	1.07	0.84	0.83	-0.94	-1.24
25	ins	s4	0.23	-3.18	-0.49	1.47	-0.16	-1.16	-1.29	-1.33	0.32	1.56
26	th	g6	0.33	0.30	2.42	1.98	-1.86	-1.53	-1.25	-1.11	2.12	0.50
27	th	g7	0.41	0.30	1.95	1.03	-1.48	-1.01	0.22	0.18	-0.64	0.24
28	th	g10	-0.12	0.13	-0.52	-0.52	0.29	0.59	-0.07	0.18	1.85	-0.68
29	th	g14	0.36	0.30	-0.52	-0.98	0.43	0.75	0.22	0.18	-0.37	-0.42
30	th	g16	0.32	0.30	-1.11	-1.46	0.90	2.30	0.22	-0.08	0.19	-0.42
31	th	g18	0.36	0.30	-1.11	-0.75	1.24	0.34	0.22	0.44	-0.37	0.50
32	th	g19	0.35	0.30	-0.40	1.74	1.08	-1.17	-0.95	-0.59	1.98	3.54
33	th	s1	0.38	0.30	-0.40	-0.75	0.39	0.54	0.22	0.44	-0.64	-0.55
34	th	s5	0.35	0.30	0.07	-0.22	-0.56	0.23	0.22	0.44	0.19	-0.29
35	th	s7	0.35	0.30	-0.87	-0.86	1.08	0.96	0.22	0.44	-0.23	0.11
36	th	s10	0.38	0.30	-0.17	-0.38	0.02	0.28	0.22	0.44	-0.37	-0.29
37	th	s11	-0.42	-0.08	-0.17	-0.30	0.33	0.28	1.40	0.96	-0.64	-0.42
38	th	s13	0.36	0.30	0.19	-0.53	-0.38	0.08	0.22	0.44	-0.92	-0.29
39	th	s15	0.39	0.30	1.25	0.81	-0.97	-0.70	0.22	0.44	-0.78	-0.42
40	th	s17	-0.45	-0.13	-0.75	-0.39	0.67	0.34	1.40	0.44	-0.23	-0.16
41	th	s19	0.39	0.30	-0.05	0.57	0.55	-0.75	0.22	0.18	-0.23	0.11
42	th	s22	-3.73	-3.84	0.19	1.03	-1.72	-1.53	-3.01	-3.44	-0.92	-1.08

Table S7. Statistics comparing the crystals grown in space and ground conditions.

	indicator	min	low hinge	media	high hinge	max
1	Comp (space)	-3.73	-0.25	0.36	0.52	1.42
2	Comp (ground)	-2.31	-0.12	0.23	0.36	1.02
3	CompH (space)	-3.84	0.29	0.30	0.33	0.67
4	CompH (ground)	-2.27	0.29	0.30	0.30	0.67
5	Rmerge (space)	-1.43	-0.45	-0.05	0.18	1.33
6	Rmerge (ground)	-1.65	-0.90	-0.40	1.05	2.42
7	RmergeH (space)	-0.97	-0.46	-0.11	0.40	2.18
8	RmergeH (ground)	-2.11	-0.90	-0.37	1.04	1.98
9	IoSigma (space)	-1.72	-0.52	0.06	0.47	1.68
10	IoSigma (ground)	-1.86	-0.96	0.29	1.14	1.42
11	IoSigmaH (space)	-1.53	-0.79	0.08	0.56	1.07
12	IoSigmaH (ground)	-1.53	-0.96	0.56	0.70	2.30
13	Redund (space)	-3.01	0.12	0.22	0.77	1.40
14	Redund (ground)	-2.03	-1.05	0.22	0.39	1.45
15	RedundH (space)	-3.44	-0.03	0.44	0.70	0.96
16	RedundH (ground)	-2.05	-0.42	0.18	0.45	1.63
17	Mosaic (space)	-1.28	-0.85	-0.28	0.31	1.28
18	Mosaic (ground)	-1.56	-0.57	-0.00	1.07	2.12
19	Bfactor (space)	-1.24	-0.55	-0.29	0.11	1.56
20	Bfactor (ground)	-1.46	-0.48	-0.25	0.50	3.54

Table S8. Percentage of variance explained by each of the ten dimension obtained by PCA analysis of the quality indicators.

	Eigenvalue	Variance (%)	Cumulative variance (%)
Dim.1	3.61	36.14	36.14
Dim.2	2.22	22.19	58.33
Dim.3	1.80	17.99	76.33
Dim.4	0.86	8.61	84.94
Dim.5	0.52	5.21	90.15
Dim.6	0.44	4.38	94.52
Dim.7	0.32	3.21	97.73
Dim.8	0.13	1.26	98.99
Dim.9	0.07	0.68	99.68
Dim.10	0.03	0.32	100.00

Table S9. Contribution (percent) of each indicator to the five first dimensions.

	Dim.1	Dim.2	Dim.3	Dim.4	Dim.5
Comp	11.61	7.71	0.74	13.90	45.91
CompH	10.59	12.34	0.16	3.28	11.85
Rmerge	1.39	18.32	26.63	1.15	2.98
RmergeH	11.35	12.74	0.75	16.22	2.03
IoSigma	6.62	9.67	21.67	11.39	0.00
IoSigmaH	15.48	7.46	0.89	13.90	12.98
Redund	20.80	3.86	0.27	1.38	7.28
RedundH	20.65	6.48	0.06	0.36	7.87
Mosaic	0.43	10.00	19.72	38.00	1.39
Bfactor	1.08	11.43	29.10	0.42	7.71