How long will my crystal last?

The quality of data you get from your crystal before it is hopelessly damaged will (all things being equal) not change no matter how intense the x-ray beam is. Cryo-cooled crystals are killed by photons/area, not time. Therefore, the amount of time your crystal can survive in the x-ray beam depends on flux density (photons/area/time) of the beamline you use.

The following table lists flux densities derived from beamline flux (photons/s) and beam size (used to compute area) parameters extracted from the `biosync.rcsb.org` website. **DISCLAIMER:** Flux depends on a lot of factors. You should check with your beamline scientist about what it is the day you collect data. It is intended here that these numbers reflect a "worst case scenario" at each beamline. This is because BioSync usually lists the maximum available flux and many ultra-bright sources are attenuated in practice. If you attenuate by 10x, then your crystal will last 10x longer. In as many cases as possible, beamline scientist have been contacted for up-to-date values. For example, Gerd Rosenbaum kindly provided the “typical” attenuated flux and beam size used at APS 22-ID, 23-ID-C and 23-ID-D for the “APS typical” entry below. In some cases below (indicated by a "?") one or more parameters were not provided in BioSync and had to be inferred or guessed at. For example, some entries report a "flux", but do not specify the x-ray wavelength. In these cases, 1 Å was assumed.

In addition to flux density (photons/area/time), the lifetime of a protein crystal will depend on a number of other parameters, such as photon energy (wavelength) and the concentration of heavy atoms. So, for this example a "typical" crystal is taken as a 100 μm thick lysozyme crystal, and the photon energy at which each beamline flux is reported is taken as the "typical" photon energy. All these "typical" values are taken together to compute a "typical" rate at which the sample absorbs energy: the “dose rate" (Gy/s). Dose is expressed in Gray (Gy) or Joules/kg.

The "`max xtal lifetime`" column is the time it will take a lysozyme crystal to absorb 30 MGy at the rate given in the "`dose rate`" column. 30 MGy has been described as a maximum recommended dose to a protein crystal (Owen et. al. *PNAS* 2006). This is what I would recommend as the maximum **total** exposure time of a native data set. The last column "`min site lifetime`" is the time it will take lysozyme to absorb 2 MGy, which represents the fastest SeMet damage rate I am aware of (Holton *JSR* 2007). The fastest damage half-life of any kind reported so far is 0.5 MGy for a Br-C bond in a nucleic acid (Oliéric et. al. *ACTA* D 2007). Therefore, the last column is the maximum **total** exposure time I would recommend for the first complete data set of a SeMet MAD, SAD or multi-SAD experiment (this includes the inverse-beam pass and all wavelengths). This is also an advisable maximum shutter-open time for a native experiment where the chemical integrity of a binding site is important. A second pass with longer exposures is always possible (you can merge it with the first), but you want to make sure you get complete data before the heavy atom sites change and/or before you get bonds breaking in your active site or ligand.

These are guidelines. Real life can be a lot more complicated than this. Some sites decay quickly, and others are quite "robust". Crystal lifetime also depends on your sample composition. For example, 2M KCl instead of 2M NaCl in your solvent channels will cut the lifetime of your crystal roughly in half. A table of commonly-used elements and the concentration that will cut the crystal lifetime in half is listed in the second table below. This table was calculated for the Se edge: 0.9793 Å. Changing the wavelength will change the dose-doubling concentration. As an extreme example, the dose-doubling concentration of Br is 1.5 M at 0.9793 Å ("below the edge") but this will drop to 270 mM at 0.9193 Å ("above the edge"). To calculate how long your particular crystal composition will behave at a particular wavelength, you can use the program RADDOSE (Murray et.al. *J. Apl. Cr.* 2004).

Radiation damage can get complicated, but, in general, the "lethal dose" for any two crystals of the same protein in the same buffer that are cooled under the same conditions at shot at the same wavelength … will be the same. This means that as you move from beamline to beamline or attenuate a given beamline, the lifetime of your crystals will be inversely proportional to photons/μm^2/s. You should bear these differences in mind when planning your experiments.

source	model	optic	flux ph/s	beamsize μm	flux density ph/μm^2/s	dose rate	max xtal lifetime	min site lifetime
home	RU-200	Yale	1.5e8	300	2.1e+03	4.3 Gy/s	81 d	5.4 d
home	RU-200	blue	3.2e7	100	4.1e+03	8.26 Gy/s	42 d	67 h
home	FR-E	Cu	9.8e8	100	1.2e+05	253 Gy/s	33 h	2.2 h
home	FR-E+	Cu	1.2e9	100	1.5e+05	310 Gy/s	27 h	1.8 h
source	model	optic	flux ph/s	beamsize μm	flux density ph/μm^2/s	dose rate	max xtal lifetime	min site lifetime

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synch	line	type	flux ph/s	beamsize μm	flux density ph/μm^2/s	dose rate	max xtal lifetime	min site lifetime
ALS	4.2.2	MAD	2.4e11	100?	2.4e+07	13.5 kGy/s	37 m	2.5 m
ALS	5.0.1	mono	1.2e11	100	1.5e+07	7.77 kGy/s	64 m	4.3 m
ALS	5.0.2	MAD	5.5e11	100	7.0e+07	35.6 kGy/s	14 m	56 s
ALS	5.0.3	mono	1.6e11	100	2.0e+07	10.4 kGy/s	48 m	3.2 m
ALS	8.2.1	MAD	1.6e11	100	2.0e+07	10.4 kGy/s	48 m	3.2 m
ALS	8.2.2	MAD	2.1e11	100	2.7e+07	13.6 kGy/s	37 m	2.5 m
ALS	8.3.1	MAD	1.8e11	100	2.3e+07	11.7 kGy/s	43 m	2.9 m
ALS	12.3.1	MAD	1.8e11	100	2.3e+07	11.7 kGy/s	43 m	2.9 m
ALS	12.3.1	ML	4.0e12	100	5.1e+08	513 kGy/s	58 s	3.9 s
APS	"typical"	MAD	1.5e12	80	2.3e+08	119 kGy/s	4.2 m	17 s
APS	19-ID-attn	MAD	5.5e11	100x100	5.5e+07	28 kGy/s	18 m	71 s
APS	8-BM	MAD	1e11	200	2.5e+06	1.27 kGy/s	6.6 h	26 m
APS	14-BM-C	mono	5.8e10	200	1.4e+06	738 Gy/s	11 h	45 m
APS	14-BM-D	MAD	3.3e9	200	8.2e+04	42 Gy/s	8.3 d	13 h
APS	14-ID-B	MAD	6.0e10	200	1.5e+06	763 Gy/s	11 h	44 m
APS	17-BM	MAD	1.1e11	200	2.8e+06	1.4 kGy/s	6 h	24 m
APS	17-ID	MAD	2.3e11	200	5.8e+06	2.93 kGy/s	2.8 h	11 m
APS	19-BM	MAD	2.0e11	70x60	4.8e+07	24.2 kGy/s	21 m	83 s
APS	22-BM	MAD	7e12	80x40	2.2e+09	1.23 MGy/s	24 s	1.6 s
APS	23-ID-B	MAD	1e13	75x25	5.3e+09	3.01 MGy/s	10 s	0.66 s
APS	24-ID-C	MAD	1.3e13	20x60	1.1e+10	5.23 MGy/s	5.7 s	0.38 s
APS	24-ID-E	MAD	0.5e13	20x100	2.5e+09	1.19 MGy/s	25 s	1.7 s
APS	31-ID	MAD	2e12	70	4.1e+08	194 kGy/s	2.6 m	10 s
synch	line	type	flux ph/s	beamsize μm	flux density ph/μm^2/s	dose rate	max xtal lifetime	min site lifetime

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synch	line	type	flux ph/s	beamsize μm	flux density ph/μm^2/s	dose rate	max xtal lifetime	min site lifetime
CAMD	GCPCC	MAD	5.0e9	200	1.2e+05	179 Gy/s	47 h	3.1 h
CHESS	A1	mono	1.23e11	100	1.6e+07	7.44 kGy/s	67 m	4.5 m
CHESS	F1	mono	1.21e11	100	1.5e+07	5.98 kGy/s	84 m	5.6 m
CHESS	F1	micro	2.8e10	18	1.1e+08	42.7 kGy/s	12 m	47 s
CHESS	F2	MAD	1.91e10	150	1.1e+06	514 Gy/s	16 h	65 m
NSLS	X3A	MAD	2.4e10	200	6.0e+05	305 Gy/s	27 h	1.8 h
NSLS	X4A	MAD	2.0e10	200	5.0e+05	254 Gy/s	33 h	2.2 h
NSLS	X8C	MAD	1.1e10	200	2.8e+05	140 Gy/s	60 h	4 h
NSLS	X9A	MAD	2.4e10?	200	6.0e+05	285 Gy/s	29 h	1.9 h
NSLS	X9B	MAD	2.4e10?	200	6.0e+05	285 Gy/s	29 h	1.9 h
NSLS	X12B	MAD	2.0e10	200	5.0e+05	254 Gy/s	33 h	2.2 h
NSLS	X12C	MAD	2.0e10	200	5.0e+05	254 Gy/s	33 h	2.2 h
NSLS	X25	MAD	2.4e11	100	2.4e+07	16.5 kGy/s	30 m	2 m
NSLS	X26C	MAD	2.0e10	200	5.0e+05	344 Gy/s	24 h	97 m
NSLS	X29A	MAD	2.9e11	100	2.9e+07	14.8 kGy/s	34 m	2.3 m
SSRL	1-5	MAD	1.7e10	200	4.2e+05	202 Gy/s	41 h	2.8 h
SSRL	7-1	mono	2.6e11	200	6.5e+06	3.09 kGy/s	2.7 h	11 m
SSRL	9-1	mono	3.9e10	200	9.8e+05	463 Gy/s	18 h	72 m
SSRL	9-2	MAD	4.8e11	200	1.2e+07	5.7 kGy/s	88 m	5.8 m
SSRL	11-1	MAD	3.9e11	200	9.8e+06	4.63 kGy/s	1.8 h	7.2 m
SSRL	11-3	mono	2.6e10	200	6.5e+05	302 Gy/s	28 h	1.8 h
SSRL	12-2	MAD	4e12	90x5	8.9e+09	5.01 MGy/s	6 s	0.4 s
BESSY	14.1	MAD	1.6e11	340x800	5.9e+05	298 Gy/s	28 h	1.9 h
BESSY	14.2	MAD	1.9e11	190x90	1.1e+07	5.63 kGy/s	89 m	5.9 m
BESSY	14.3	mono	0.9e11	255x40	8.8e+06	3.18 kGy/s	2.6 h	10 m
BSRF	3W1A	MAD	5e10?	800x600	1.0e+05	53 Gy/s	6.6 d	10 h
synch	line	type	flux ph/s	beamsize μm	flux density ph/μm^2/s	dose rate	max xtal lifetime	min site lifetime

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synch	line	type	flux ph/s	beamsize μm	flux density ph/μm^2/s	dose rate	max xtal lifetime	min site lifetime
CLSI	08ID-1	MAD	6.5e12	167x500	7.8e+07	43.9 kGy/s	11 m	46 s
DIAMOND	I02	MAD	1e12	100	1.0e+08	50.9 kGy/s	9.8 m	39 s
DIAMOND	I03	MAD	1e12	100	1.0e+08	50.9 kGy/s	9.8 m	39 s
DIAMOND	I04	MAD	1e12	100	1.0e+08	50.9 kGy/s	9.8 m	39 s
DIAMOND	I04.1	MAD	1e12	100	1.0e+08	50.9 kGy/s	9.8 m	39 s
ESRF	ID14-1	MAD	?					
ESRF	ID14-2	MAD	?					
ESRF	ID14-3	MAD	?					
ESRF	ID14-4	MAD	?					
ESRF	BM30A	MAD	0.5e11	300	5.6e+05	275 Gy/s	30 h	2 h
LNLS	W01B-MX2	MAD	6.3e10	250x500	5.0e+05	1.03 kGy/s	8.1 h	32 m
MAXLAB	I711	MAD	6e12	300	6.7e+07	18.4 kGy/s	27 m	1.8 m
MAXLAB	I911-1	MAD	5e11	400x200	6.2e+06	6.46 kGy/s	77 m	5.2 m
MAXLAB	I911-2	MAD	5e11	400x200	6.2e+06	6.46 kGy/s	77 m	5.2 m
MAXLAB	I911-3	MAD	1e12	300	1.1e+07	5.65 kGy/s	88 m	5.9 m
MAXLAB	I911-4	mono	5e11	400x200	6.2e+06	3.18 kGy/s	2.6 h	10 m
MAXLAB	I911-5	mono	2e11	400x200	2.5e+06	1.27 kGy/s	6.6 h	26 m
NSRRC	BL13B1	MAD	4e11	200	1.3e+07	6.05 kGy/s	83 m	5.5 m
NSRRC	BL13C1	MAD	4e10	200	1.3e+06	598 Gy/s	14 h	56 m
NSRRC	BL17B1	MAD	4e9	200	1.3e+05	71.8 Gy/s	4.8 d	7.7 h
PAL/PLS	4A	MAD	1e12	300x3000	1.1e+06	565 Gy/s	15 h	59 m
PAL/PLS	6B	MAD	1e11	300	1.1e+06	565 Gy/s	15 h	59 m
PAL/PLS	6C1	MAD	1e11	300	1.1e+06	565 Gy/s	15 h	59 m
synch	line	type	flux	beamsize	flux density	dose	max xtal	min site
			ph/s	μm	ph/μm^2/s	rate	lifetime	lifetime

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synch	line	optic	flux ph/s	beamsize µm	flux density ph/µm²/s	dose rate	max xtal lifetime	min site lifetime
PF	BL5A	MAD	2e11	200?	5.0e+06	2.54 kGy/s	3.3 h	13 m
PF	BL6A	MAD	1e10	200?	2.5e+05	127 Gy/s	66 h	4.4 h
PF	BL17A	MAD	6.6e9	200?	1.6e+05	83.9 Gy/s	99 h	6.6 h
PF	BBL18B	MAD	4.0e10	400x500	2.0e+05	102 Gy/s	82 h	5.5 h
PF	NW12A	MAD	2e10	200?	5.0e+05	254 Gy/s	33 h	2.2 h
SLS/PSI	X06SA	MAD	4e12	85x10	4.7e+09	2.39 MGy/s	13 s	0.84 s
SLS/PSI	X06SA	micro	1e12	25x5	8.0e+09	3.8 MGy/s	7.9 s	0.53 s
SLS/PSI	X10SA	MAD	2.5e12	50x10	5.0e+09	2.54 MGy/s	12 s	0.79 s
SOLEIL	ID-10C	MAD	5e12	250	8.0e+07	40.7 kGy/s	12 m	49 s
SPRING8	BL12B2	MAD	6e10	250	1.2e+06	619 Gy/s	13 h	54 m
SPRING8	BL24XU	MAD	1e12	1000?	1.0e+06	509 Gy/s	16 h	66 m
SPRING8	BL26B1	MAD	1e11	200?	2.5e+06	1.41 kGy/s	5.9 h	24 m
SPRING8	BL26B2	MAD	1e11	200?	2.5e+06	1.41 kGy/s	5.9 h	24 m
SPRING8	BL32B2	MAD	1e10	200	2.5e+05	127 Gy/s	66 h	4.4 h
SPRING8	BL38B1	mono	1e11	200?	2.5e+06	1.27 kGy/s	6.6 h	26 m
SPRING8	BL40B2	SAXS	1e11	250x200	2.0e+06	1.13 kGy/s	7.4 h	30 m
SPRING8	BL41XU	mono	1e13	25x25	1.6e+10	8.14 MGy/s	3.7 s	0.25 s
SPRING8	BL44B2	MAD	1.1e11	200?	2.8e+06	1.39 kGy/s	6 h	24 m
SPRING8	BL44XU	MAD	1e12	25x25	1.6e+09	814 kGy/s	37 s	2.5 s
SPRING8	BL45XU	SAXS	3e11	400x200	3.7e+06	1.91 kGy/s	4.4 h	17 m
SRS-UK	PX10.1	MAD	1e13	1000x300	3.3e+07	17 kGy/s	29 m	2 m
SRS-UK	14.2	MAD	1.4e13	300x400	1.2e+08	55.4 kGy/s	9 m	36 s
synch	line	optic	flux ph/s	beamsize µm	flux density ph/µm²/s	dose rate	max xtal lifetime	min site lifetime

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Dose-doubling concentration

(the concentration of something that will cut your crystal lifetime in half)

at the Se edge **based on μ_{en} from Seltzer (1993)**

Na	12 M	As	283 mM
Mg	8.8 M	Se	268 mM
P	4.0 M	Br	1.47 M
S	3.1 M	I	252 mM
Cl	2.5 M	Gd	122 mM
K	1.7 M	Ta	84 mM
Ca	1.4 M	Pt	113 mM
Fe	540 mM	Au	108 mM
Cu	380 mM	Hg	102 mM
Zn	340 mM	U	120 mM

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