Supplementary Materials

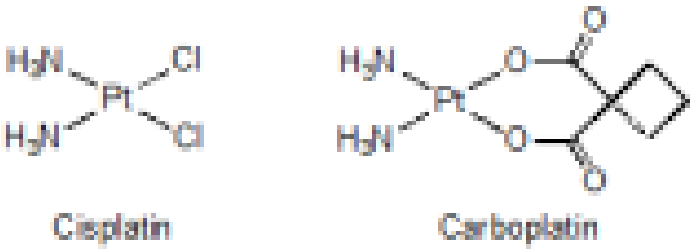

Figure S1 Chemical structures of cisplatin and carboplatin.

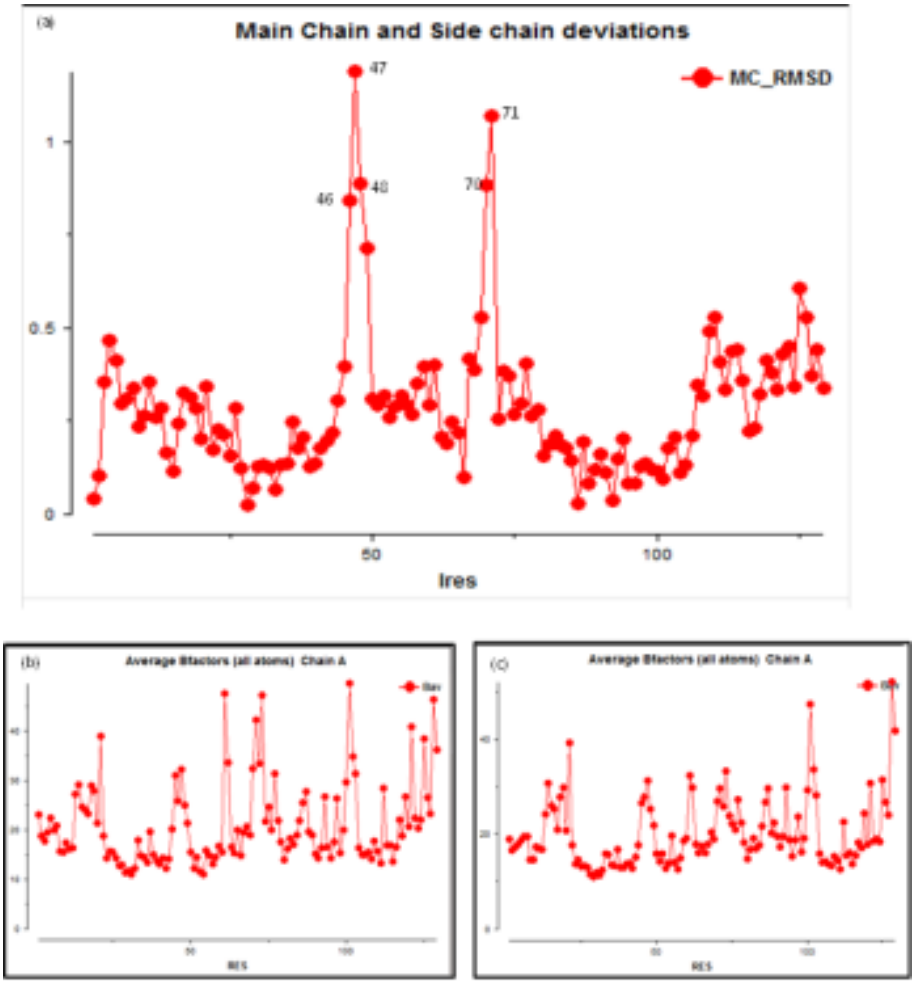

Figure S2 (a) RMS difference plot between the RT and 100K structures for the carboplatin_DMSO case after 13 months of prolonged chemical storage. Asn-46, Try-47, Asp-48, Pro-70 and Gly-71 show the biggest RMS differences (but see Table S2 for the significant statistical evaluations) and these residues all lie in loop regions of the protein and are, to our knowledge, not chemically

significant. However, the shift between Pro-70 is not significant to a 3σlevel. (b) Average B factors for the 100K crystal structure of carboplatin_DMSO case after 13months of prolonged chemical storage and (c) the average B factors for the RT crystal structure of carboplatin_DMSO after 13 months prolonged chemical storage. The trend in the B factors for both structures is the same, with the RT crystal structure having overall higher B factors as expected.

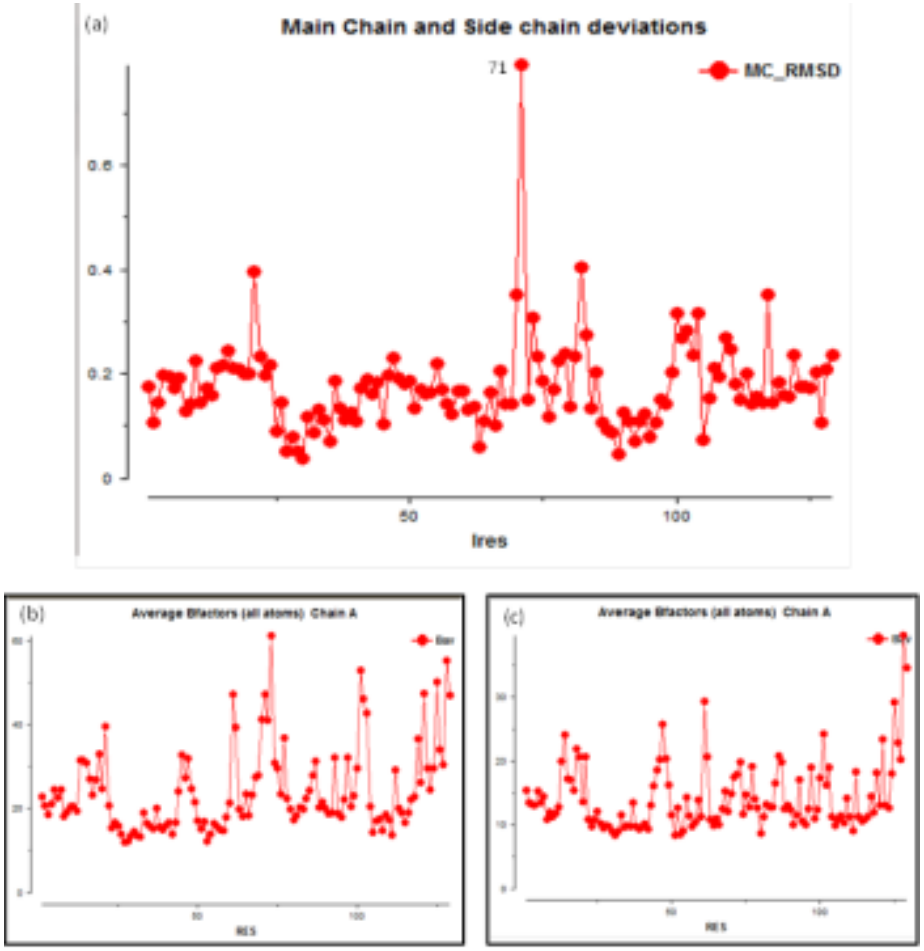

Figure S3 (a) RMS difference plot between the RT carboplatin_DMSO case after 13 months of prolonged chemical storage and the 100K Carboplatin_DMSO_Glycerol case after 8 days of crystallisation. Gly 71 again shows the biggest RMS differences between the structures (labelled). (b) Average B factors for the RT crystal structure of carboplatin_DMSO case after 13months of prolonged chemical storage and (c) the average B factors for the 100K crystal structure of carboplatin_DMSO_Glycerol after 8 days of co-crystallisation. The trend in the B factors for both structures is the same, with the RT crystal structure having overall higher B factors as expected.

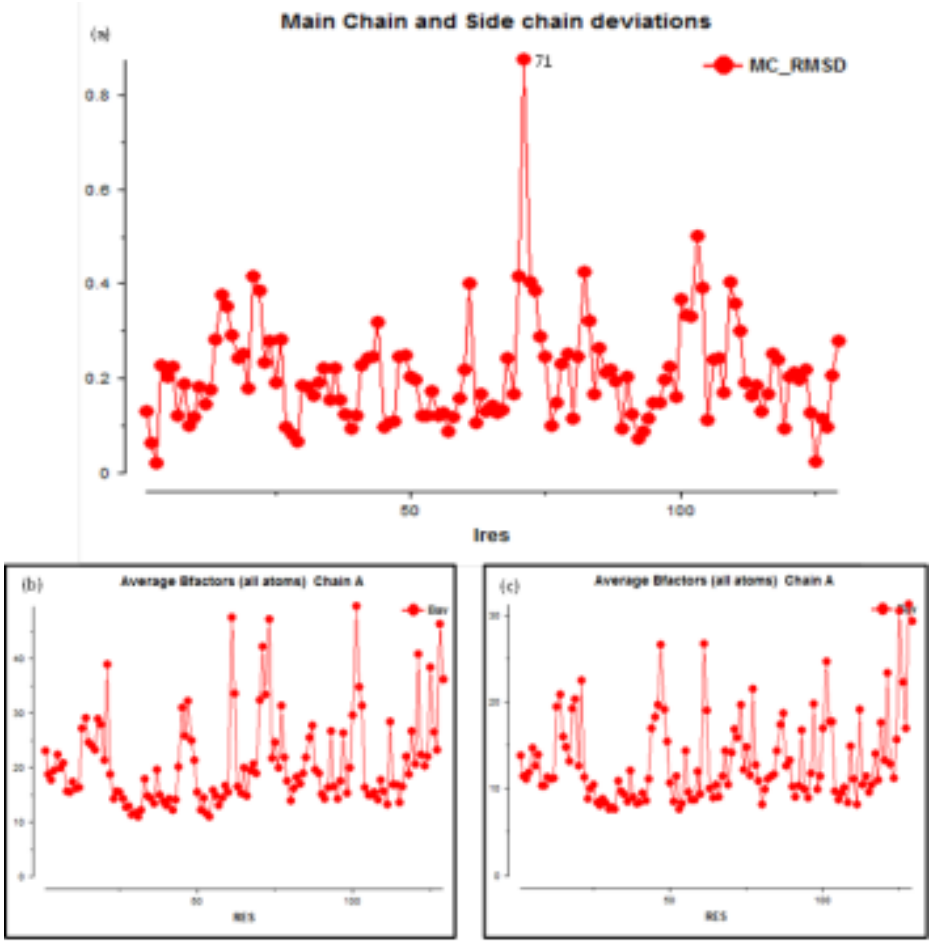

Figure S4 (a) RMS difference plot between the RT cisplatin_DMSO case after 13 months of prolonged chemical storage and the 100K cisplatin_DMSO_Glycerol case after 8 days of crystallisation. Gly 71 again shows the biggest RMS differences between the structures (labelled), but this shift is not significant at the 3σlevel. (b) Average B factors for the RT crystal structure of cisplatin_DMSO case after 13months of prolonged chemical storage and (c) the average B factors for the 100K crystal structure of cisplatin_DMSO_Glycerol after 8 days of co-crystallisation. The trend in the B factors for both structures is the same, with the RT crystal structure having overall higher B factors as expected.

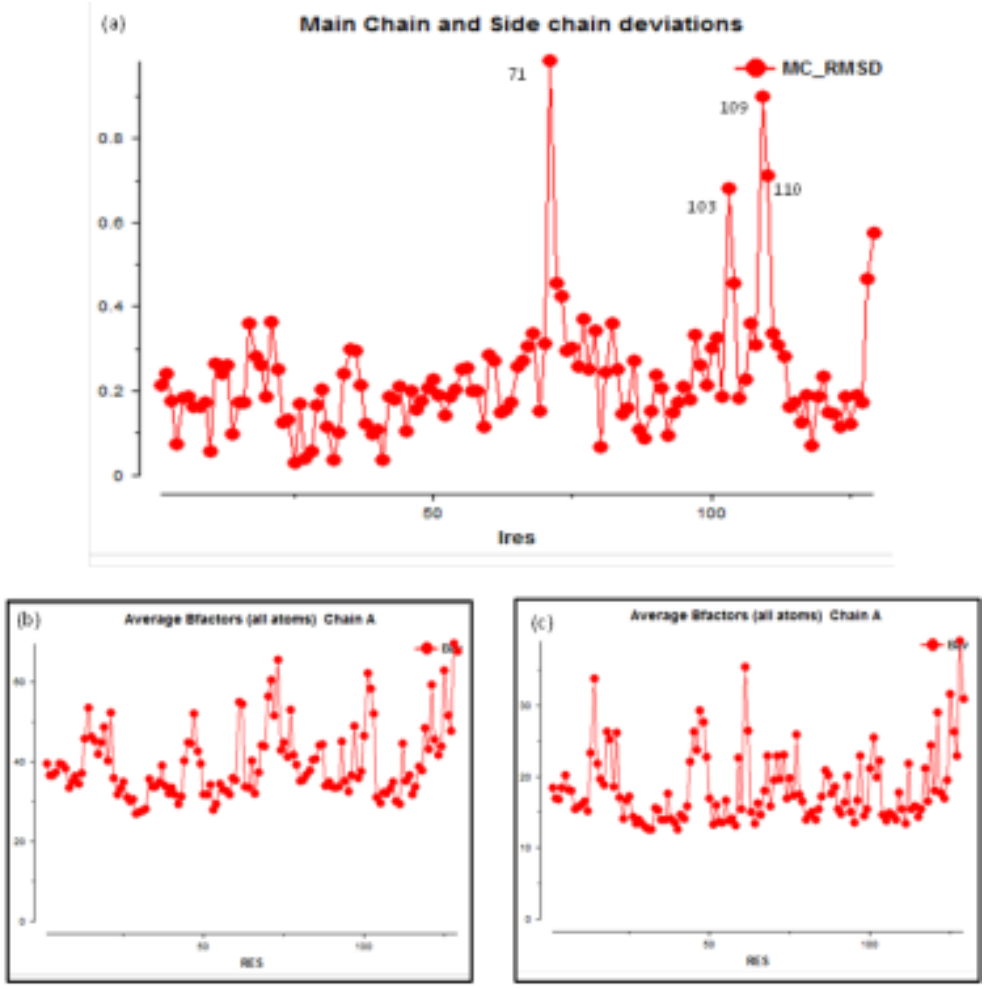

Figure S5 (a) RMS difference plot between the RT cisplatin_aqueous case after 13 months of prolonged chemical storage and the 100K cisplatin_aqueous_Glycerol case after 8 days of crystallisation. Gly 71, Asn 103, Val 109 and Ala 110 shows the biggest RMS differences between the structures (labelled) and these residues lie in loop regions of the protein and to our knowledge, are not chemically significant. However, these changes are not significant at a 3σlevel. (b) Average B factors for the RT crystal structure of cisplatin_aqueous case after 13months of prolonged chemical storage and (c) the average B factors for the 100K crystal structure of cisplatin_aqueous_Glycerol after 4 days of co-crystallisation. The trend in the B factors for both structures is the same, with the RT crystal structure having overall higher B factors as expected.

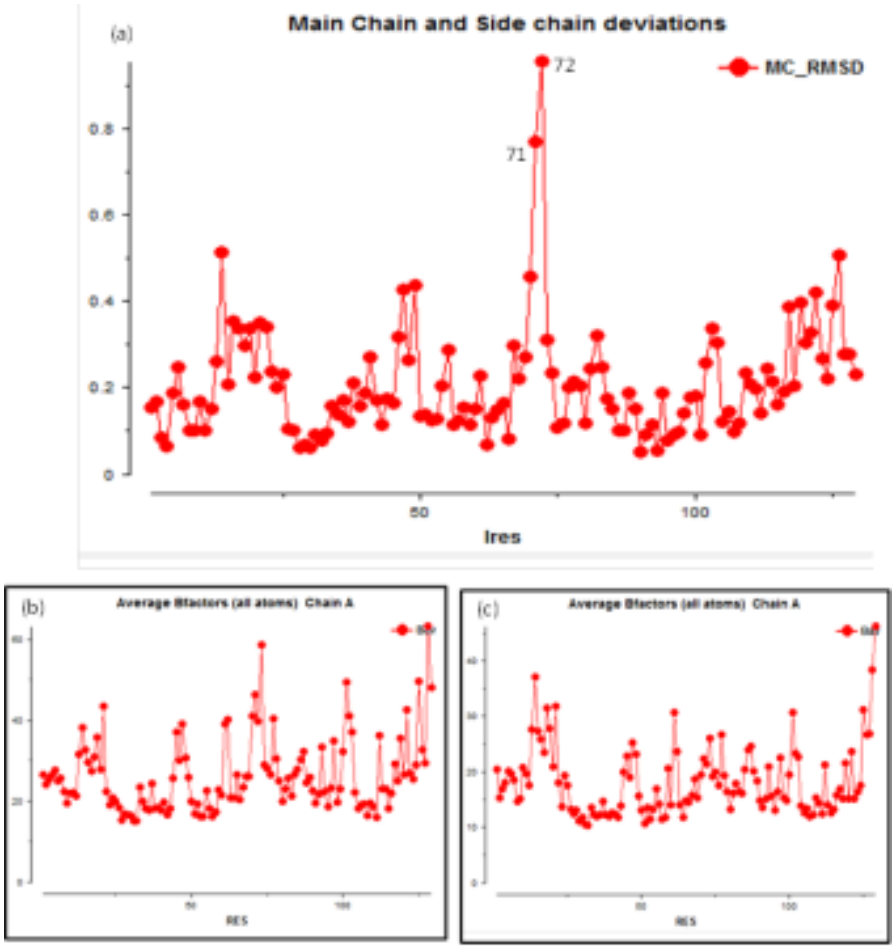

Figure S6 (a) RMS difference plot between the RT cisplatin_NAG_DMSO case after 13 months of prolonged chemical storage and the 100K ciaplatin_NAG_DMSO_Glycerol case after 8 days of crystallisation. Gly 71 and Ser-72 show the biggest RMS differences between the structures (labelled) and these residues lie in loop regions of the protein and to our knowledge, are not chemically significant. (b) Average B factors for the RT crystal structure of cisplatin_NAG_DMSO case after 13months of prolonged chemical storage and (c) the average B factors for the 100K crystal structure of cisplatin_NAG_DMSO_Glycerol after 8 days of co-crystallisation. The trend in the B factors for both structures is the same, with the RT crystal structure having overall higher B factors as expected.

Table S1 Data-collection strategy for each crystal.

	Swing around Phi (degrees)	**Sweep (degrees)**
Cisplatin_aq	25.0	189.0ω
	20.0	101.0Φ
	25.0	101.0Φ
	5.0	156.5ω
	-15.0	174.0Φ
Cisplatin_DMSO	-15.0	173.5ω
	5.0	100.0ω
	-15.0	117.5Φ
	5.0	152.0Φ
	-5.0	157.0Φ
	25.0	174.5Φ
	0.0	189.0ω
	25.0	292.0Φ
	20.0	329.0Φ
Cisplatin_DMSO_NAG	-25.0	360.0Φ
	-25.0	188.5ω
	25.0	188.5ω
	30.0	103.5ω
	25.0	73.0Φ
	10.0	90.0Φ
	30.0	27.5Φ
Carboplatin_DMSO_RT	25.0	176.0ω
	5.0	89.5Φ
	-5.0	115.0ω
	-10.0	138.0ω
	20.0	141.0ω
	-25.0	348.0Φ

Carboplatin_DMSO_100K	-25.0	331.5 Φ
	-5.0	124.0 Φ
	-5.0	152.5 Φ
	5.0	359.5 Φ
	10.0	73.0 Φ
	15.0	360.0 Φ
	25.0	275.0 Φ
	25.0	359.5 Φ

Table S2 Significant RMS differences (at 3σ level) between RT and 100K structures for each pair wise comparison with a standard deviation value for each calculated using equations 1 and 2

Pair-wise Comparisons	Significant changes to amino acids	RMS difference (Å) between structures with standard deviations calculated from equations 1 and 2.
RT prolonged chemical exposure carboplatin DMSO with 100K prolonged chemical exposure carboplatin DMSO	Asn 46	0.8 +/- 0.3
	Thr 47	1.2 +/- 0.3
	Asp 48	0.9 +/- 0.3
	Gly 71	1.1 +/- 0.3
RT prolonged chemical exposure carboplatin DMSO with 100K 8 day crystallisation carboplatin DMSO Glycerol	Gly 71	0.8 +/- 0.2
RT prolonged chemical exposure cisplatin NAG DMSO with 100K 8 day crystallisation cisplatin NAG DMSO Glycerol	Gly 71	0.9 +/- 0.3
	Ser 72	0.8 +/- 0.3