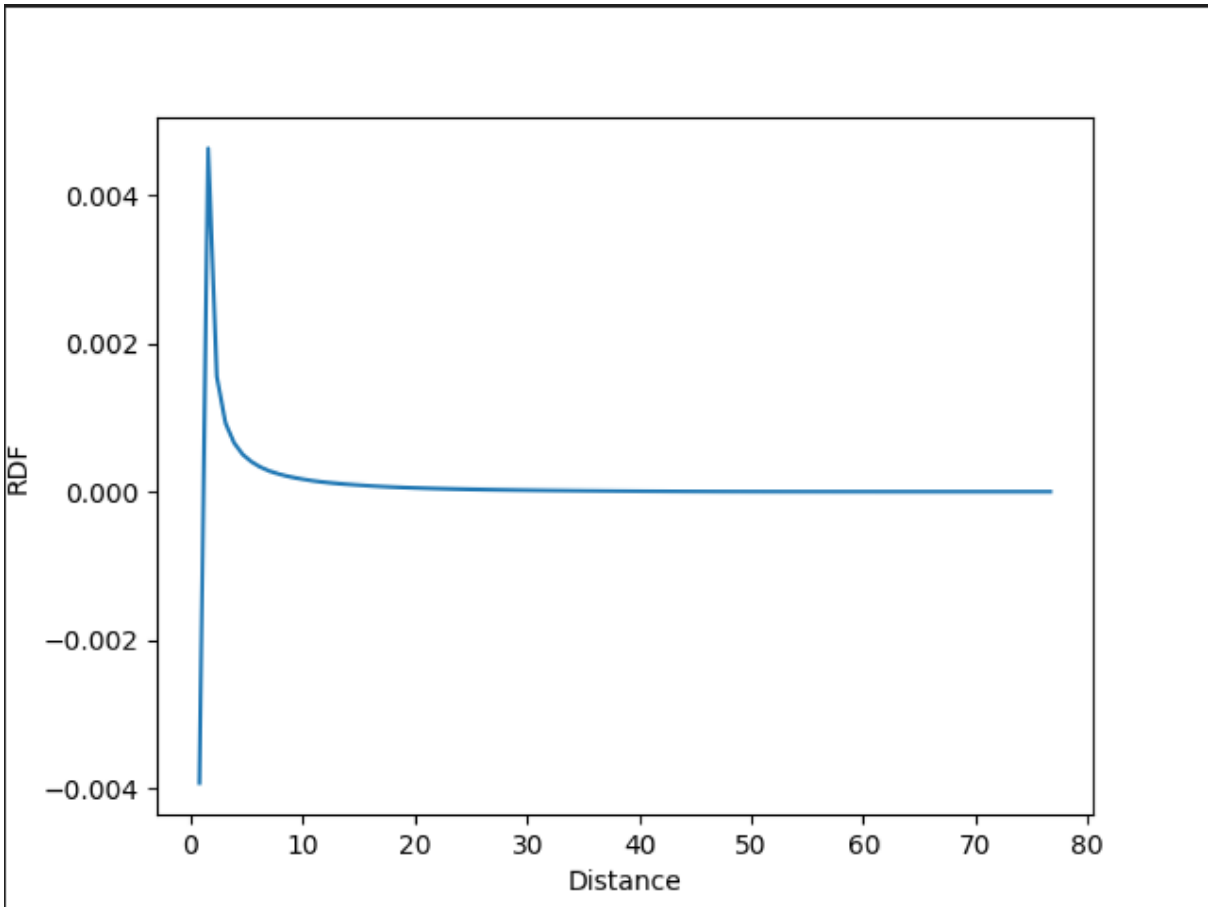
Sma86

M6 MD Supo 1: Q2

Q2.1

Ideal gas:



RDF constant with distance as expected; ideal gas has no potential energy/interactions so particles equally likely to be anywhere in system. Discrepancy at small distances where RDF is large?

Q2.2

Water O-O:

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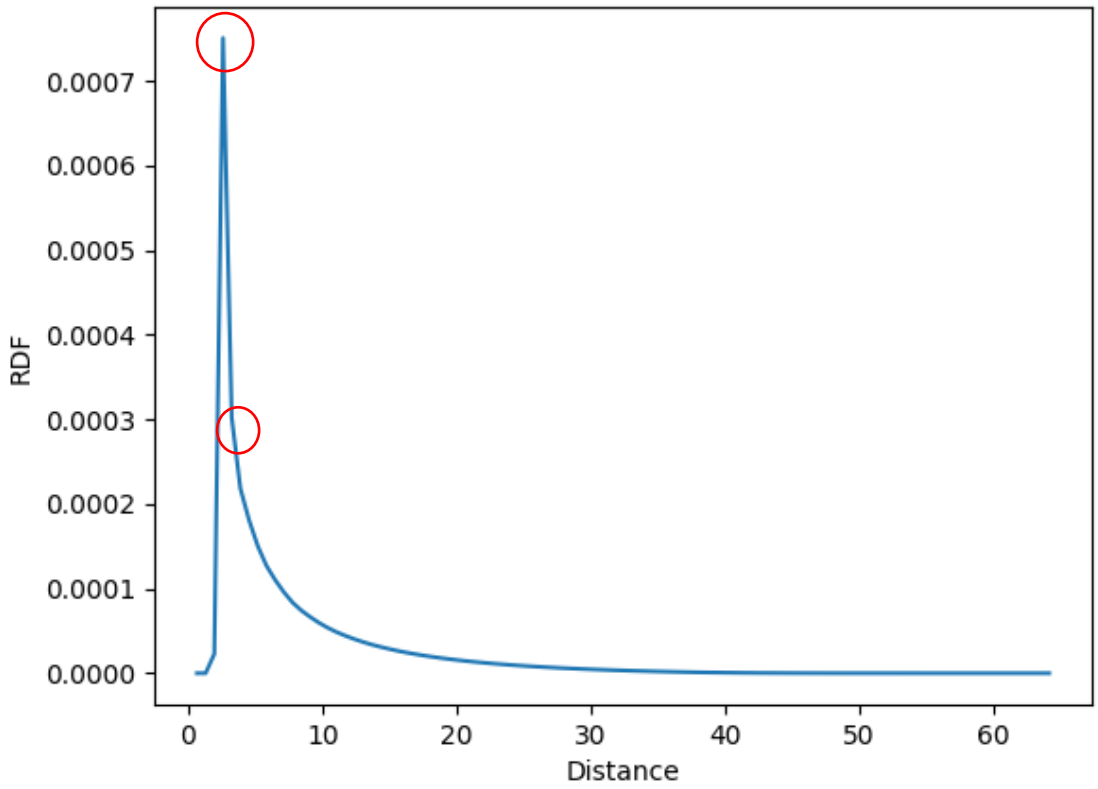
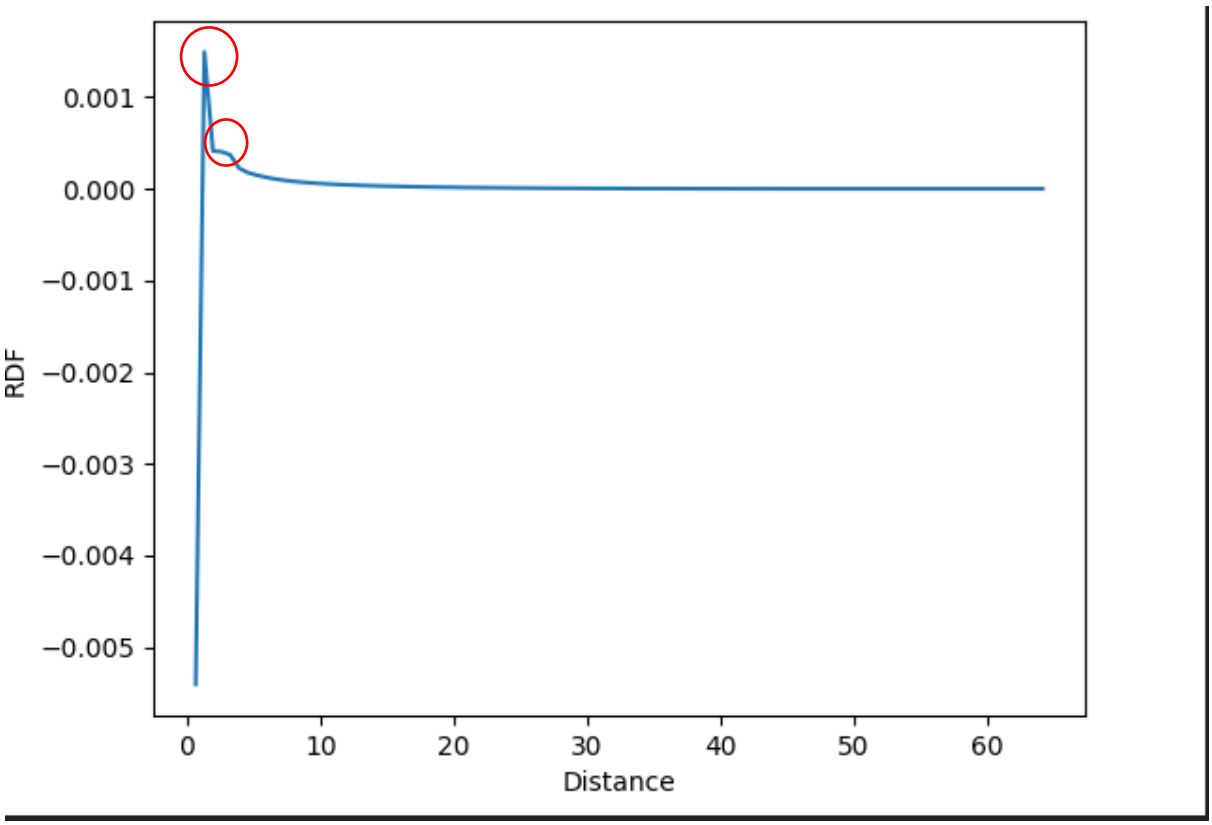


Water O-H



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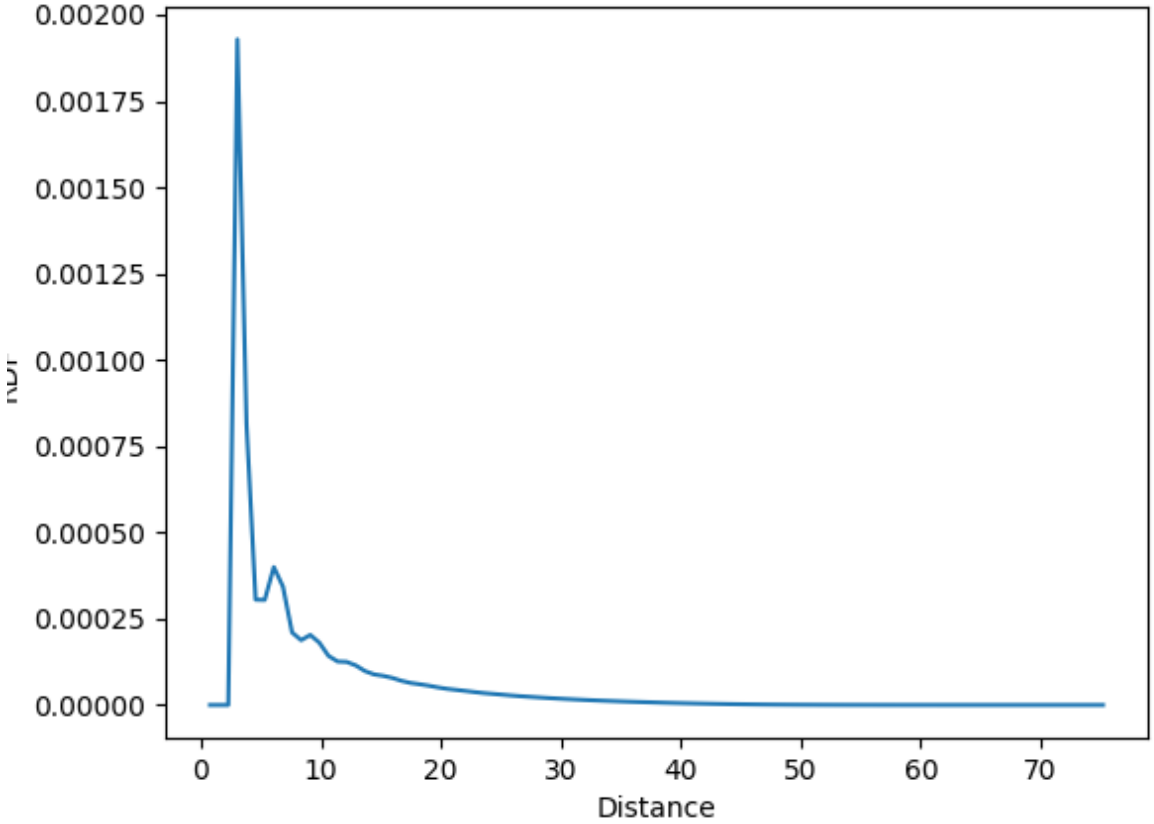
Both RDF show liquid behaviour. Primary RDF peak at small distance corresponding to first coordination shell in water hydrogen bonded network. Very weak secondary RDF peak (especially subtle in O-O RDF) present corresponding to second coordination shell. No more peaks present because of fluxional liquid behaviour destroying position correlations for third nearest neighbours and greater.

2.3

Set 1



Set 2

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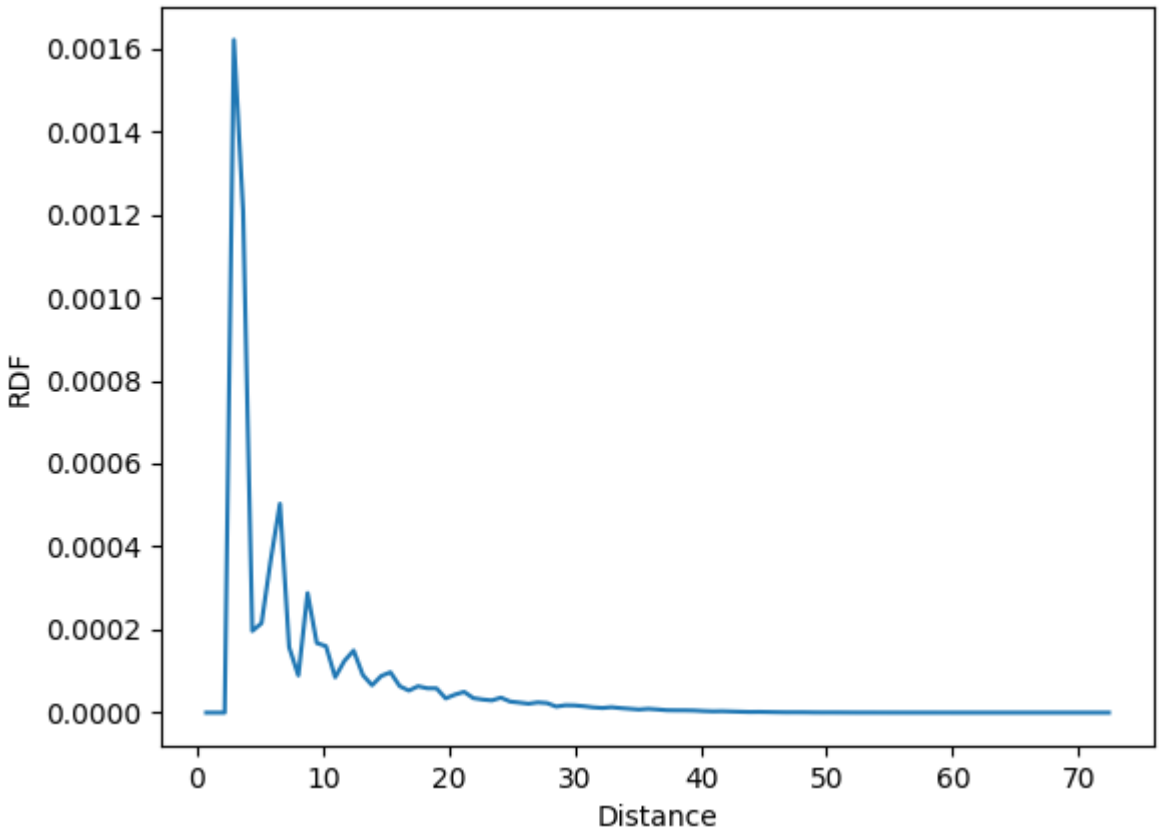
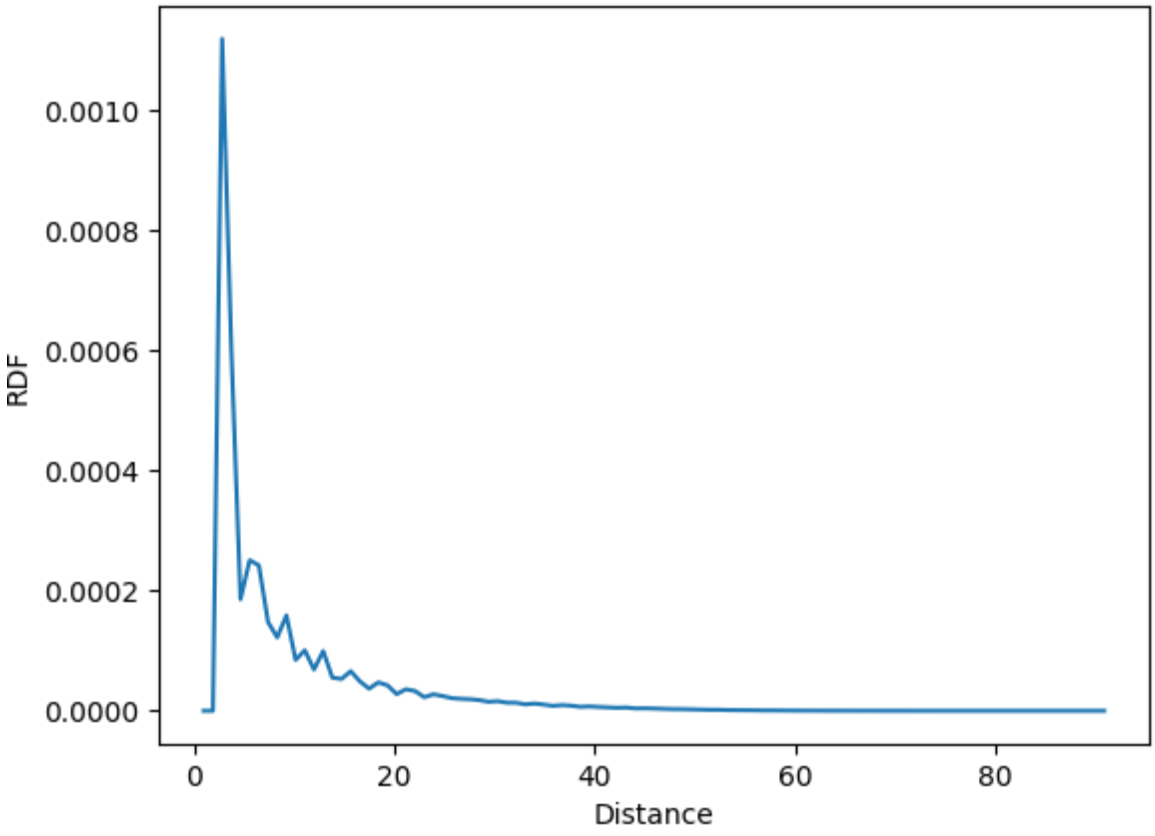

0.0016
0.0014
0.0012
0.0010
0.0008
0.0006
0.0004
0.0002
0.0000
RDF
0
10
20
30
40
50
60
70
Distance

Set 3


0.0010
0.0008
0.0006
0.0004
0.0002
0.0000
RDF
0
20
40
60
80
Distance

Set 1 is liquid phase (only two strong peaks before RDF decays). Sets 2 and 3 are crystalline (many peaks in RDF, showing that there is long-range order).

The coordination number corresponding to a crystalline peak in the RDF is given by:

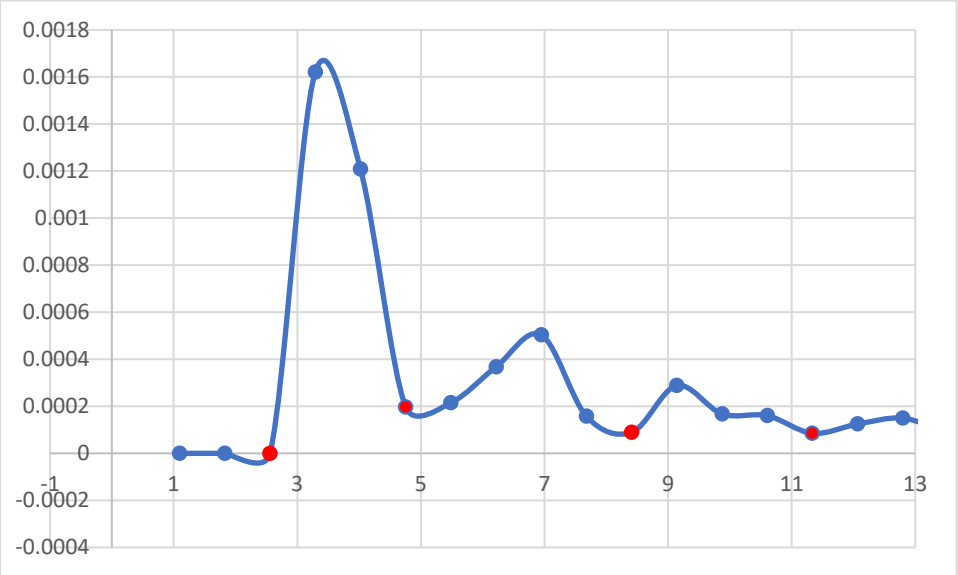
$$n_c = 4\pi \frac{N}{V} \int_{r_{min}}^{r_{\max}} r^2 g(r)\, dr$$

This numerically approximates to

$$n_c = 4\pi \frac{N}{V} \sum_i (\Delta r) r_i^2 g_i$$

Where the sum is over all bins, i, corresponding to the crystalline peak and Δr is the bin width.

For set 2: Looking at first three peaks in more detail. Judge minima by eye (marked as red circles).



bin_width	0.731395					Peak	Sum	Coord no.	Ratio
						1	0.041552	1.43E-02	1
Lmin	4.84E+01		N	2000		2	0.060606	2.08E-02	1.46E+00
Lmax	6.60E+00		V	7.31E+04		3	0.069381	2.39E-02	1.67E+00

bin	r_min	r_mid	RDF	r^2 * g(r)	
0	0.731395	1.097093	0	0	
1	1.46279	1.828488	0	0	
2	2.194185	2.559883	0	0	Peak 1 start
3	2.92558	3.291278	0.001621	0.017554	
4	3.656975	4.022673	0.001208	0.019551	
5	4.38837	4.754068	0.000197	0.004447	Peak 1 end
6	5.119765	5.485463	0.000215	0.006482	Peak 2 start
7	5.85116	6.216858	0.000368	0.014213	
8	6.582555	6.948253	0.000503	0.024291	
9	7.31395	7.679648	0.000157	0.009284	
10	8.045345	8.411043	8.96E-05	0.006337	Peak 2 end
11	8.77674	9.142438	0.000288	0.02407	Peak 3 start
12	9.508136	9.873833	0.000168	0.016351	
13	10.23953	10.60523	0.00016	0.018005	
14	10.97093	11.33662	8.52E-05	0.010956	Peak 3 end

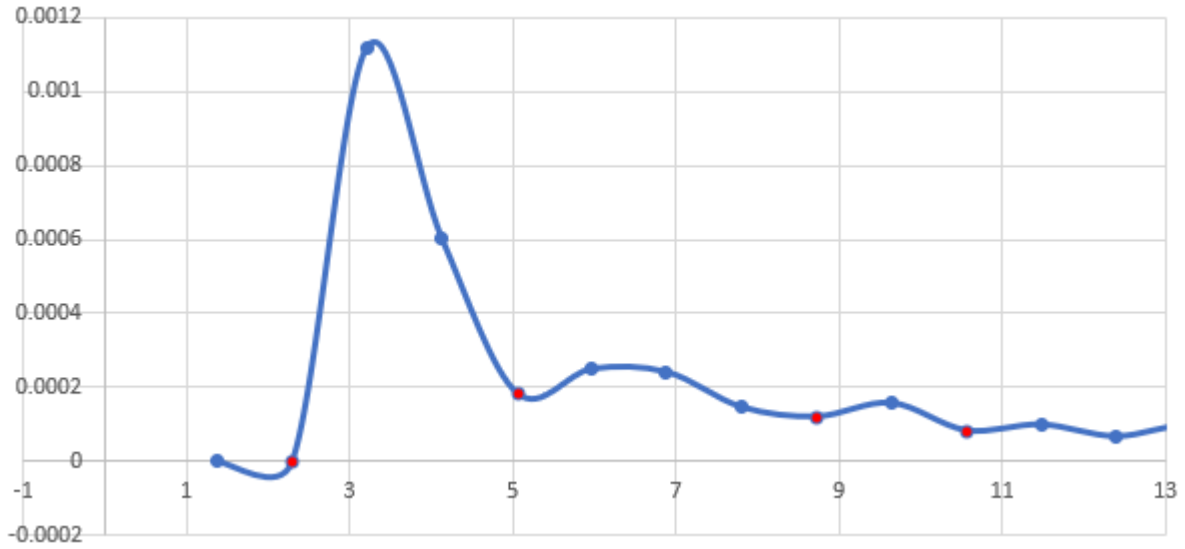
Coordination no. for first three peaks are 0.0143, 0.0208 and 0.0239 respectively. These numbers are too small so likely a normalisation error during RDF calculation (perhaps I wasn't meant to divide by no of atom pairs?). However, can still work out ratios of coordination numbers relative to first peak as approximately 1, 1.5 and 1.7 for the respective peak.

Use this table of data to identify crystalline phase based off coordination number ratio of peaks.

Crystal structure	1st nearest neighbours	2nd nearest neighbours	3rd nearest neighbours	Expected ratio pattern
Fcc	12	6	24	1, 0.5, 3
Bcc	8	6	12	1, 0.75, 2
Hcp	12	6		1, 0.5,

Set 1 does not correspond to any of these crystal structures. No. of bins should be increased to give more accurate values (I used N_bins = 100).

For set 3:



bin_width	0.918044					Peak	Sum	Coord no.	Ratio
						1	0.020523	6.55E-03	1
Lmin	5.17E+01		N	4000		2	0.025572	8.17E-03	1.25E+00
Lmax	-8.06E-01		V	1.44E+05		3	0.030378	9.70E-03	1.48E+00

bin	r_min	r_mid	RDF	r^2 * g(r)	
0	0.918044	1.377066	0	0	
1	1.836087	2.295109	0	0	Peak 1 starts
2	2.754131	3.213153	0.001119	0.008487	
3	3.672175	4.131197	0.000602	0.008123	
4	4.590219	5.049241	0.000186	0.003914	Peak 1 ends
5	5.508262	5.967284	0.000251	0.007608	Peak 2 starts
6	6.426306	6.885328	0.000242	0.009999	
7	7.34435	7.803372	0.000148	0.007966	Peak 2 ends
8	8.262394	8.721415	0.000122	0.008344	Peak 3 starts
9	9.180437	9.639459	0.000159	0.013385	
10	10.09848	10.5575	8.48E-05	0.008649	Peak 3 ends
11	11.01652	11.47555	0.000101	0.01221	
12	11.93457	12.39359	6.87E-05	0.009792	
13	12.85261	13.31163	9.94E-05	0.016425	
14	13.77066	14.22968	5.52E-05	0.010477	
15	14.6887	15.14772	5.30E-05	0.011434	
16	15.60674	16.06577	6.59E-05	0.016049	

Again, ratio pattern 1, 1.25, 1.48 doesn't match any of the crystal structures in the table. Conclusion: no. of bins too small to get an accurate value of coordination number.