

Supplementary material for paper DZ5093

Improving the scattering factor formalism in protein refinement. Application of the University at Buffalo Aspherical-Atom Databank to polypeptide structures.

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Figure S1. Residual Fourier difference maps in the plane N2-C1-O1 of YGG.
 Contour interval $0.05 \text{ e}\text{\AA}^{-3}$; positive – red, negative – blue.

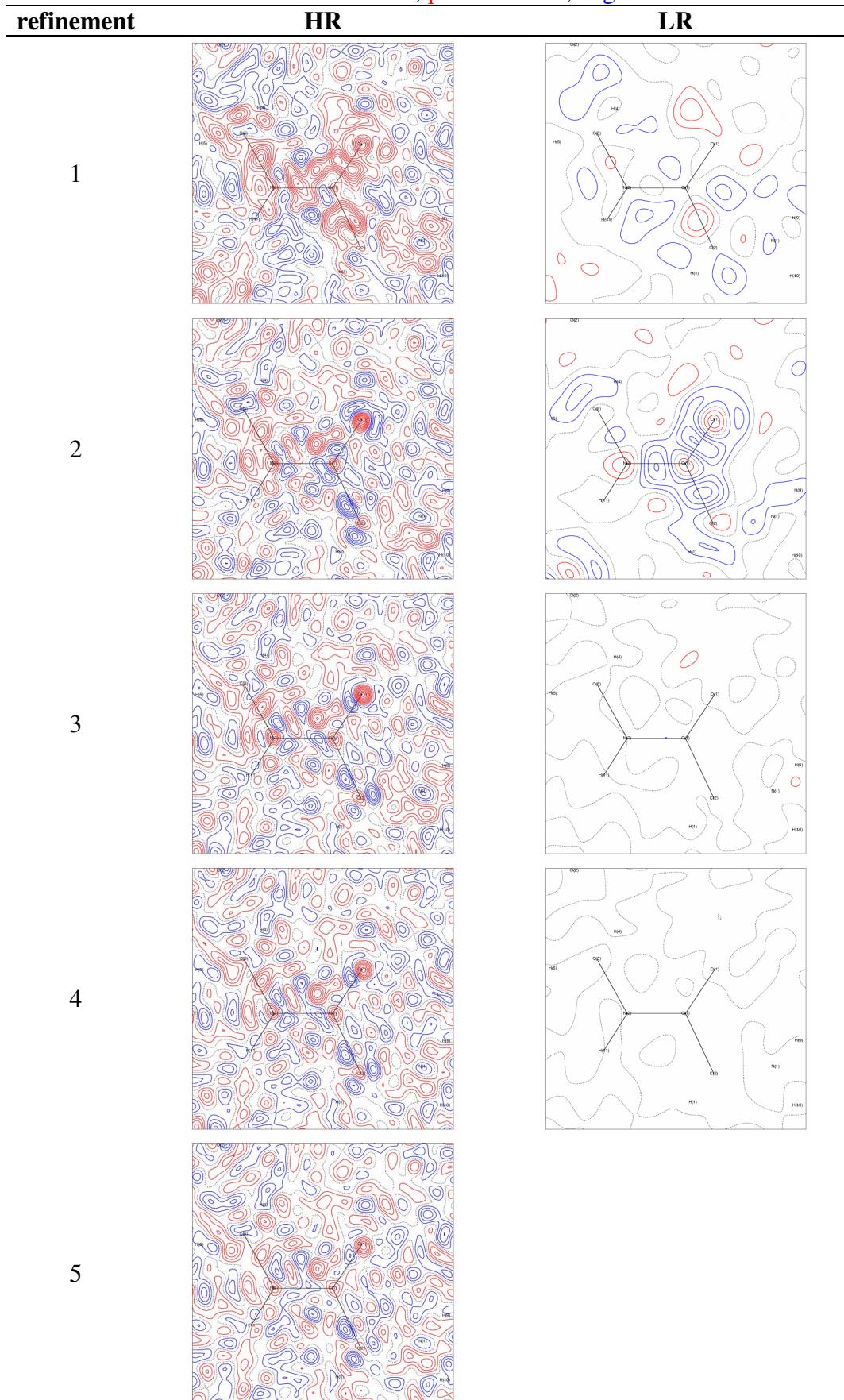


Figure S2. Residual Fourier difference maps in plane N3-C4-O2 in YGG.
 Contour interval $0.05 \text{ e}\text{\AA}^{-3}$; positive – red, negative – blue.

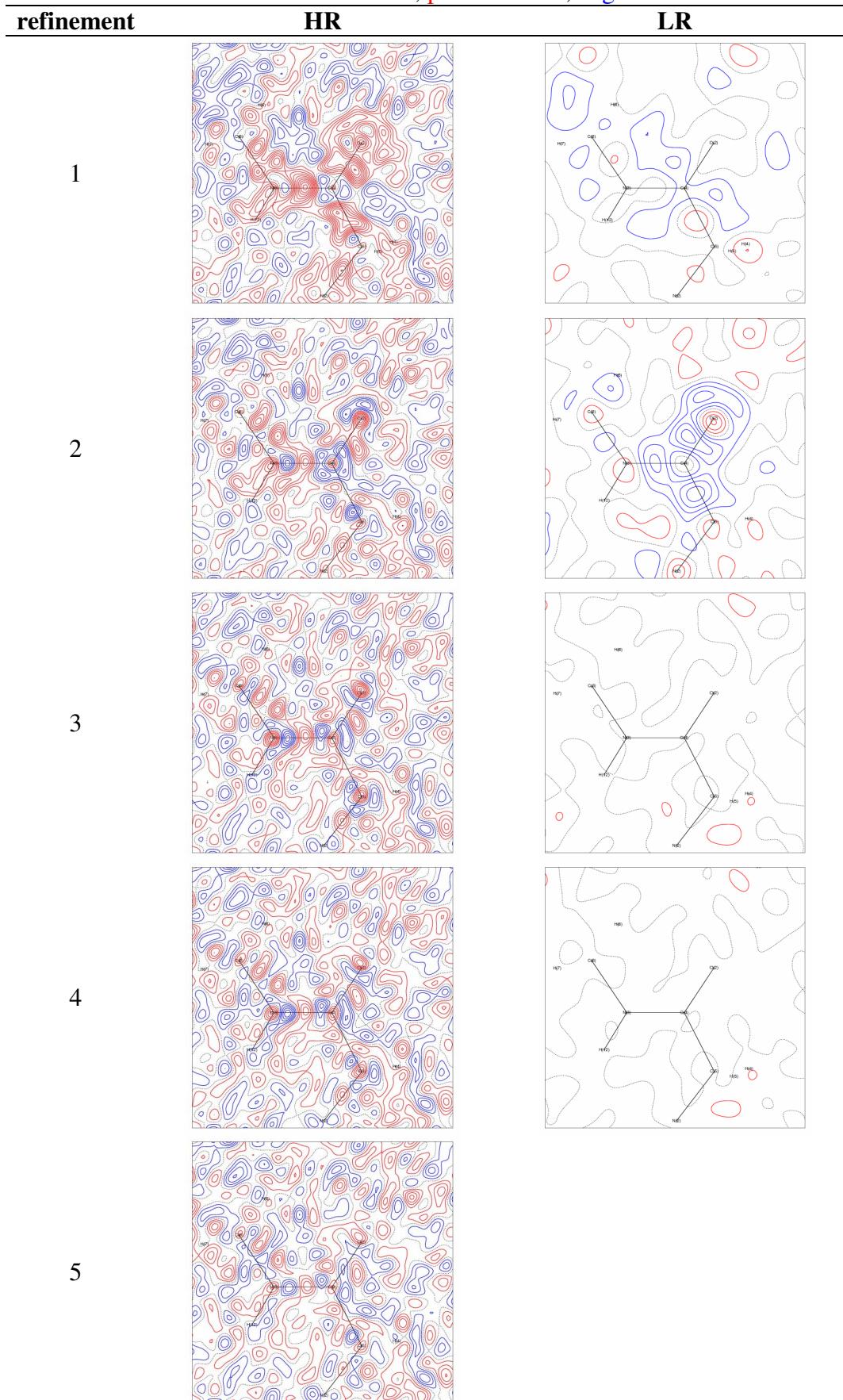


Figure S3. Residual Fourier difference maps in plane O4-C7-O3 in YGG.
 Contour interval $0.05 \text{ e}\text{\AA}^{-3}$; positive – red, negative – blue.

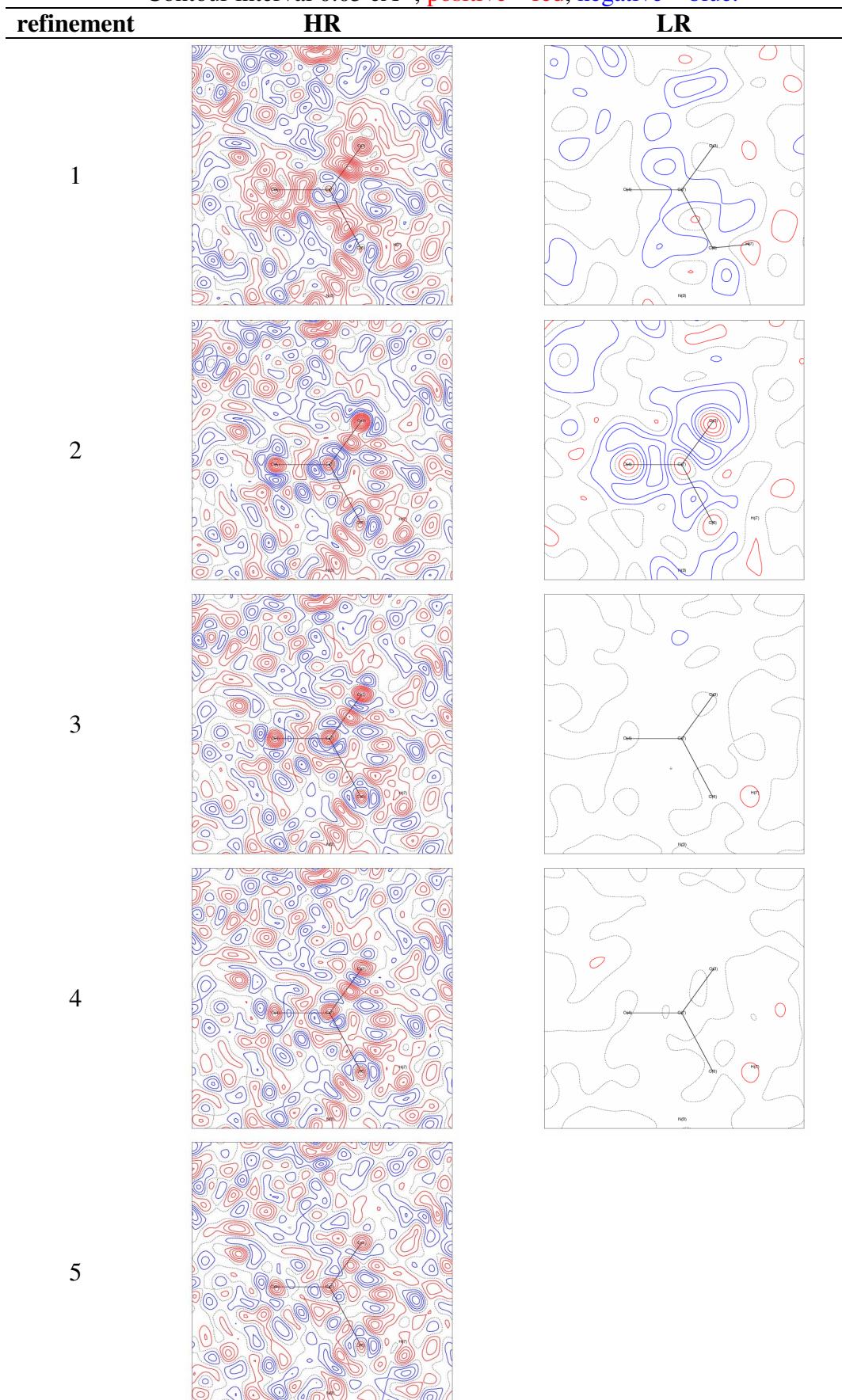


Figure S4. Residual Fourier difference maps in the plane N11-C21-O21 in P2A4.
 Contour interval $0.05 \text{ e}\text{\AA}^{-3}$; positive – red, negative – blue.

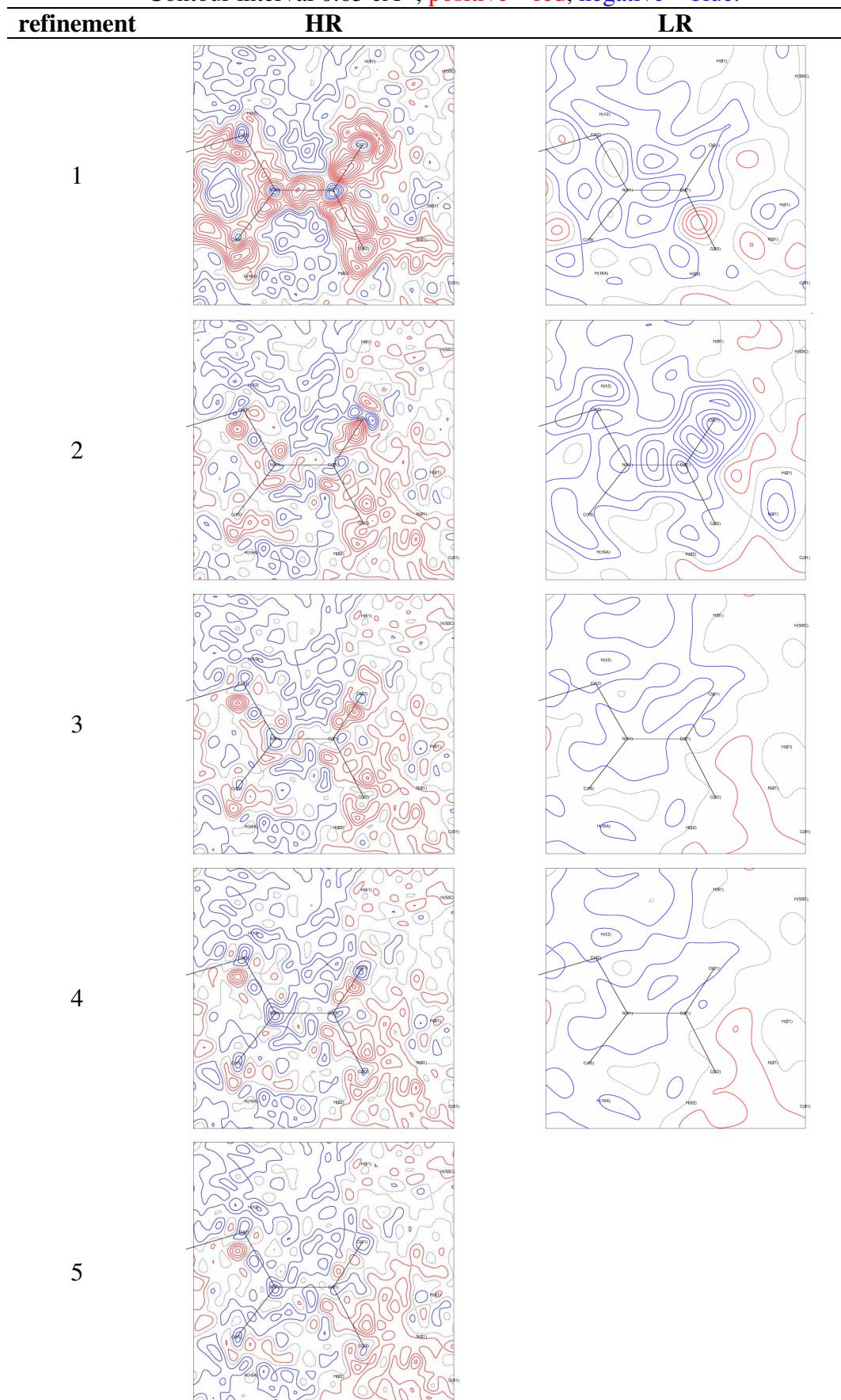


Figure S5. Residual Fourier difference maps map in the plane N21-C31-O31 in P2A4.
 Contour interval $0.05 \text{ e}\text{\AA}^{-3}$; positive – red, negative – blue.

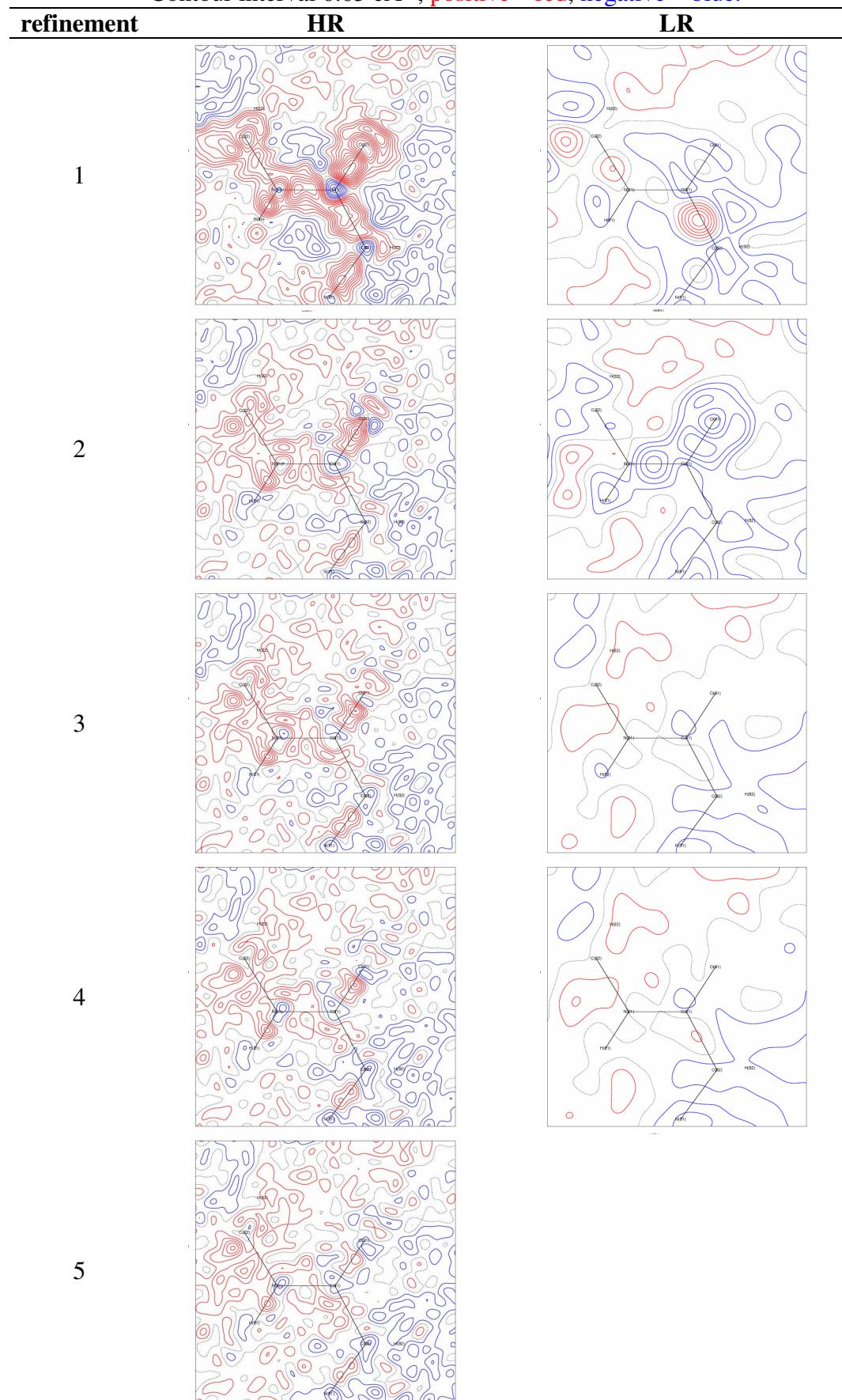


Figure S6. Residual Fourier difference maps in the plane N41-C51-O51 in P2A4.
 Contour interval $0.05 \text{ e}\text{\AA}^{-3}$; positive – red, negative – blue.

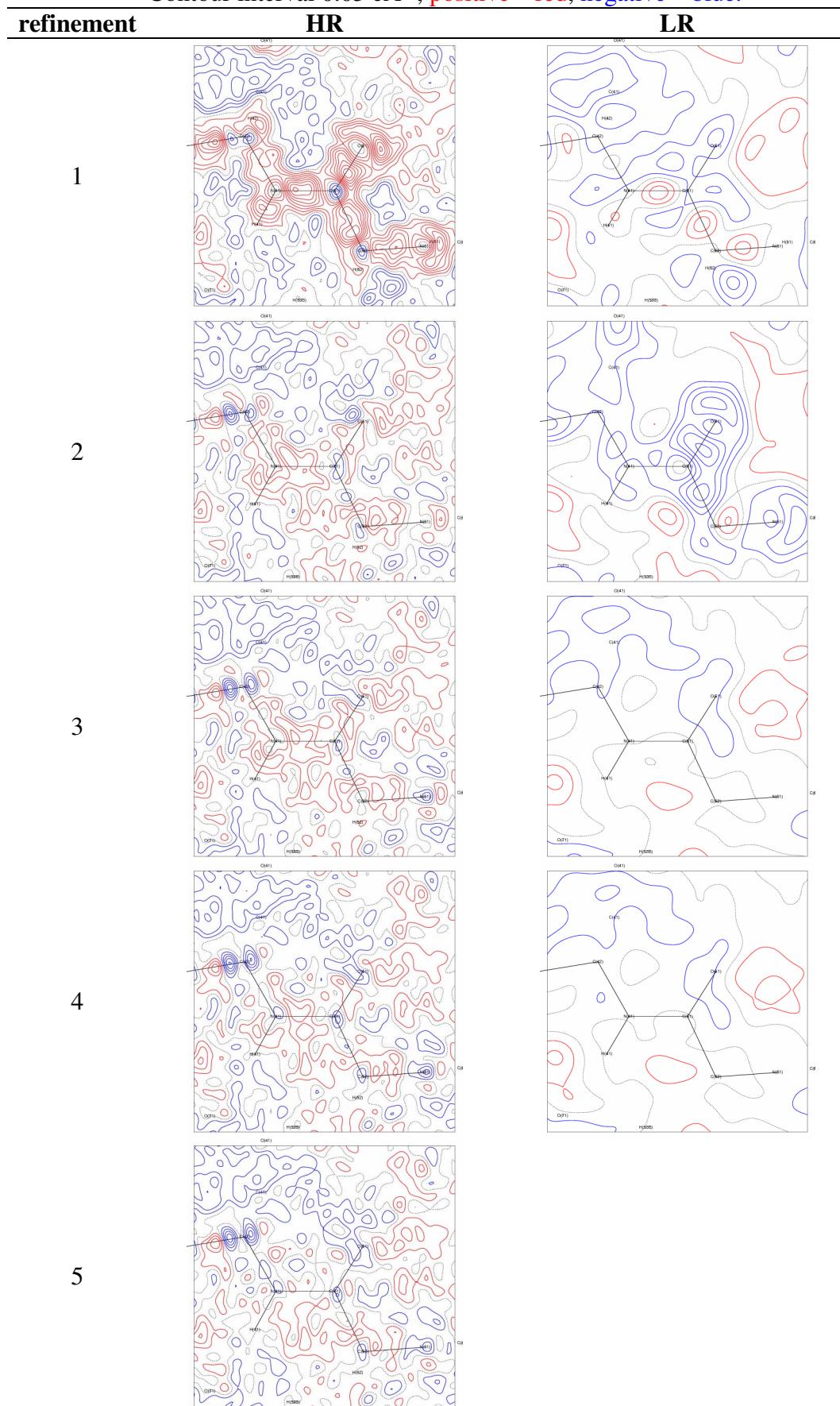


Figure S7. Residual Fourier difference maps in the plane N51-C61-O61 in P2A4.
 Contour interval $0.05 \text{ e}\text{\AA}^{-3}$; positive – red, negative – blue.

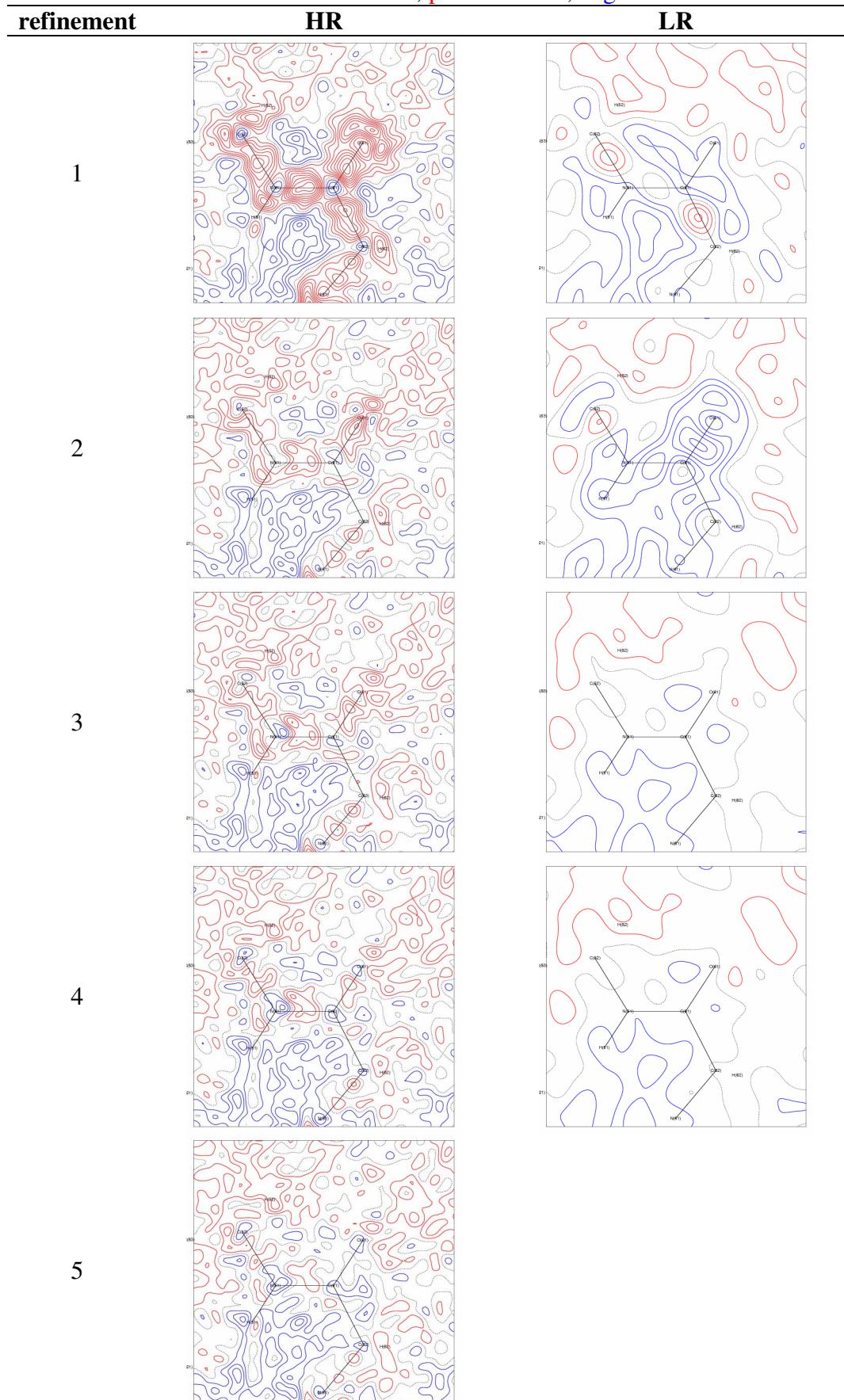


Figure S8. Residual Fourier difference maps in the plane N61-C11-O11 in P2A4.
 Contour interval $0.05 \text{ e}\text{\AA}^{-3}$; positive – red, negative – blue.

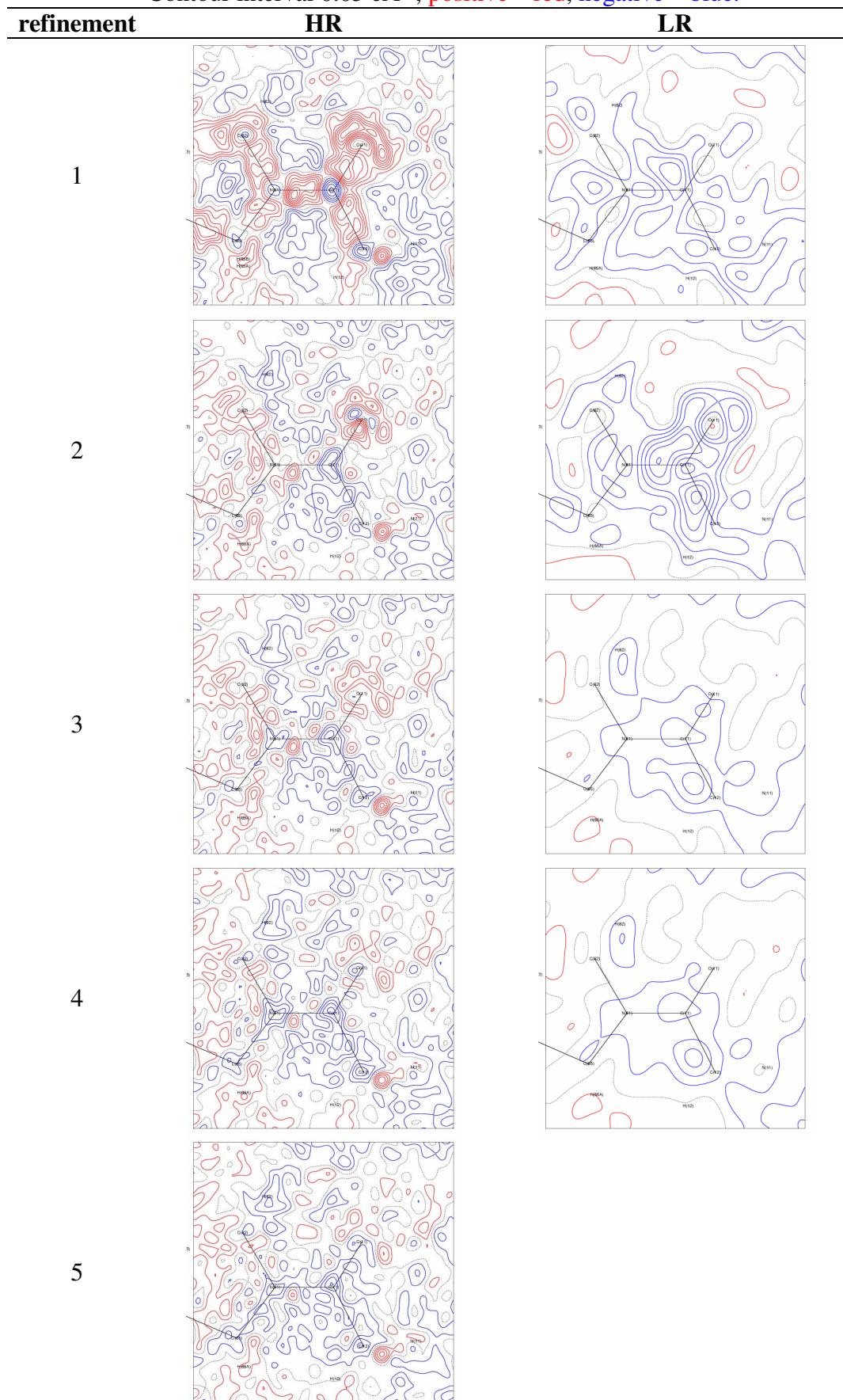


Figure S9. Residual Fourier difference maps in the plane of the water molecule in P2A4.
 Contour interval $0.05 \text{ e}\AA^{-3}$; positive – red, negative – blue.

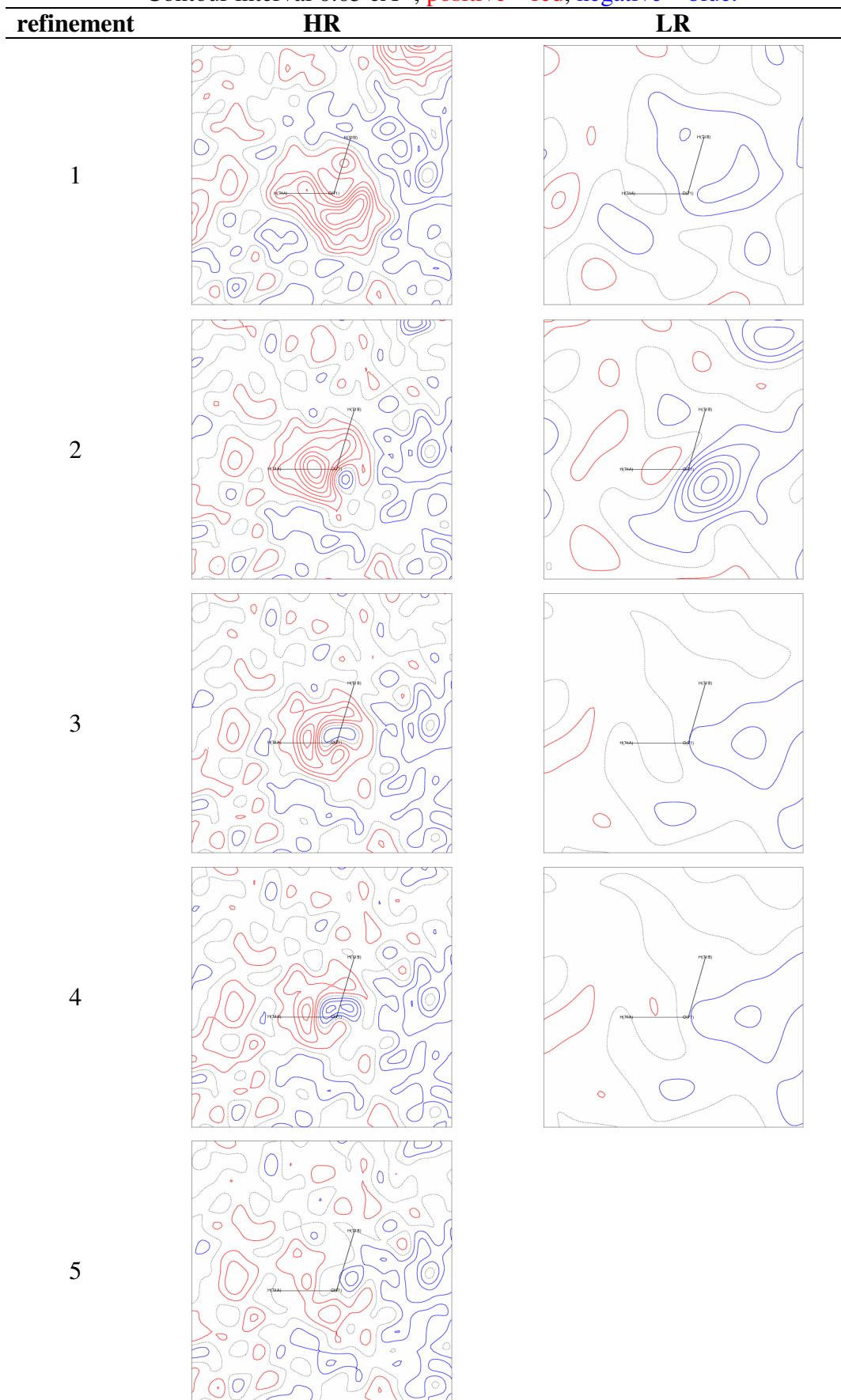


Figure S10. Differences of Mean-Squared Displacement Amplitudes (DMSDA) along interatomic vectors ($\times 10^4 \text{ \AA}^2$) from refinements of HR datasets in YGG.

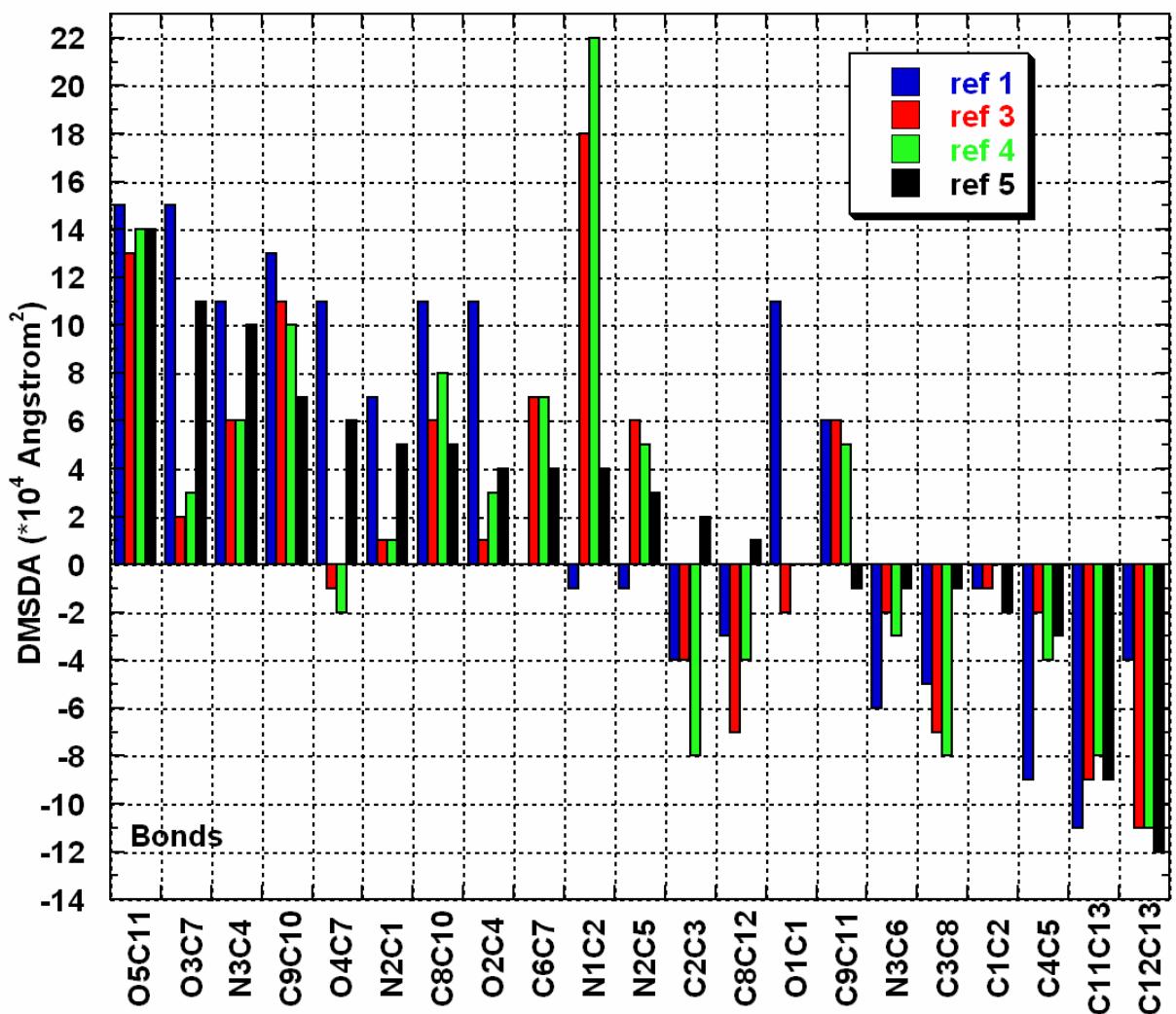


Figure S11. DMSDA ($\times 10^4 \text{ \AA}^2$) from LR refinements and from refinement 5 (KRMM) of HR data in YGG.

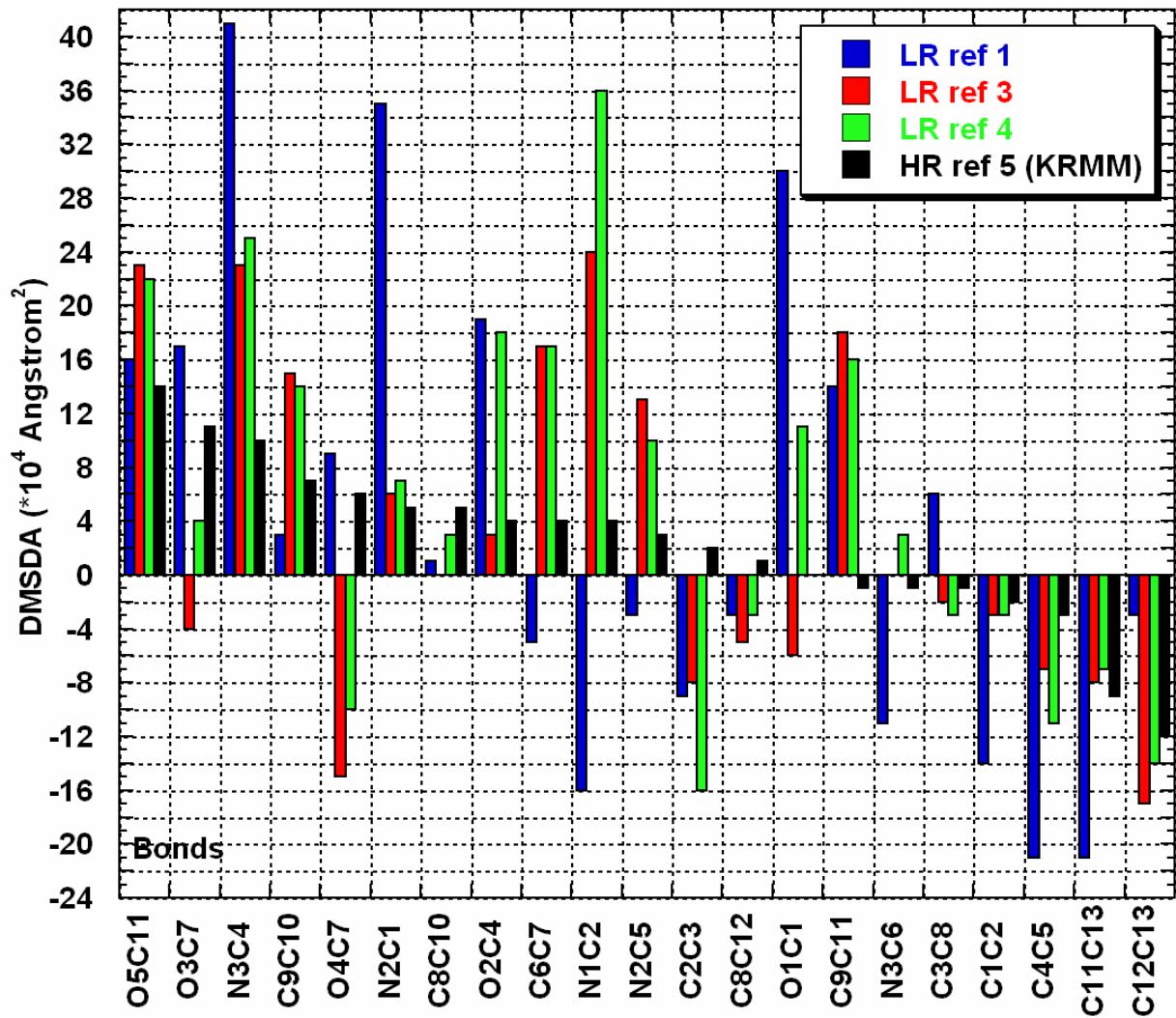


Figure S12. Differences of Mean-Squared Displacement Amplitudes (DMSDA) along interatomic vectors ($\times 10^4 \text{ \AA}^2$) from refinements of HR datasets in P2A4.

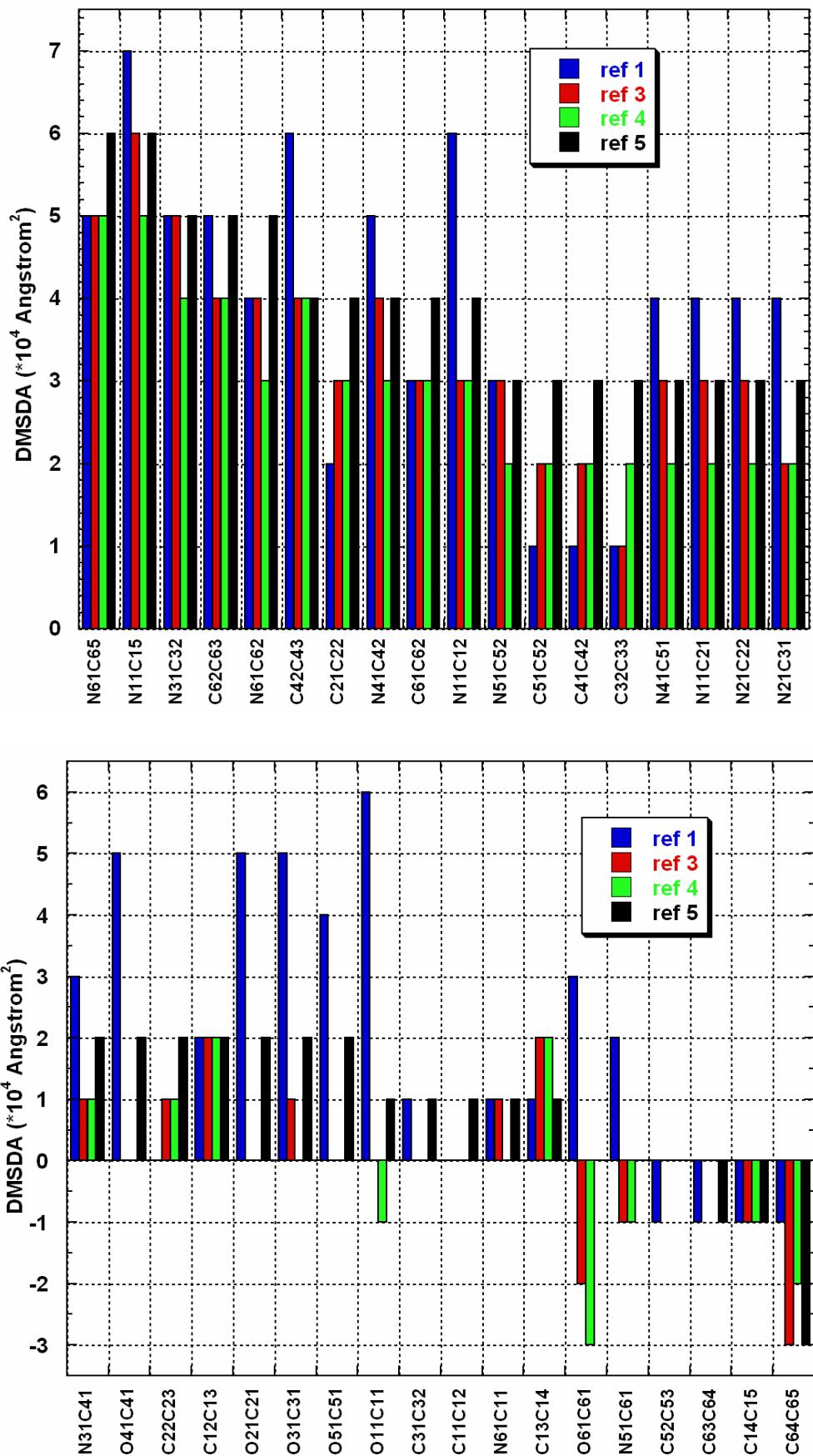


Figure S13. Differences of Mean-Squared Displacement Amplitudes (DMSDA) along interatomic vectors ($\times 10^4 \text{ \AA}^2$) from refinements of LR datasets in P2A4.

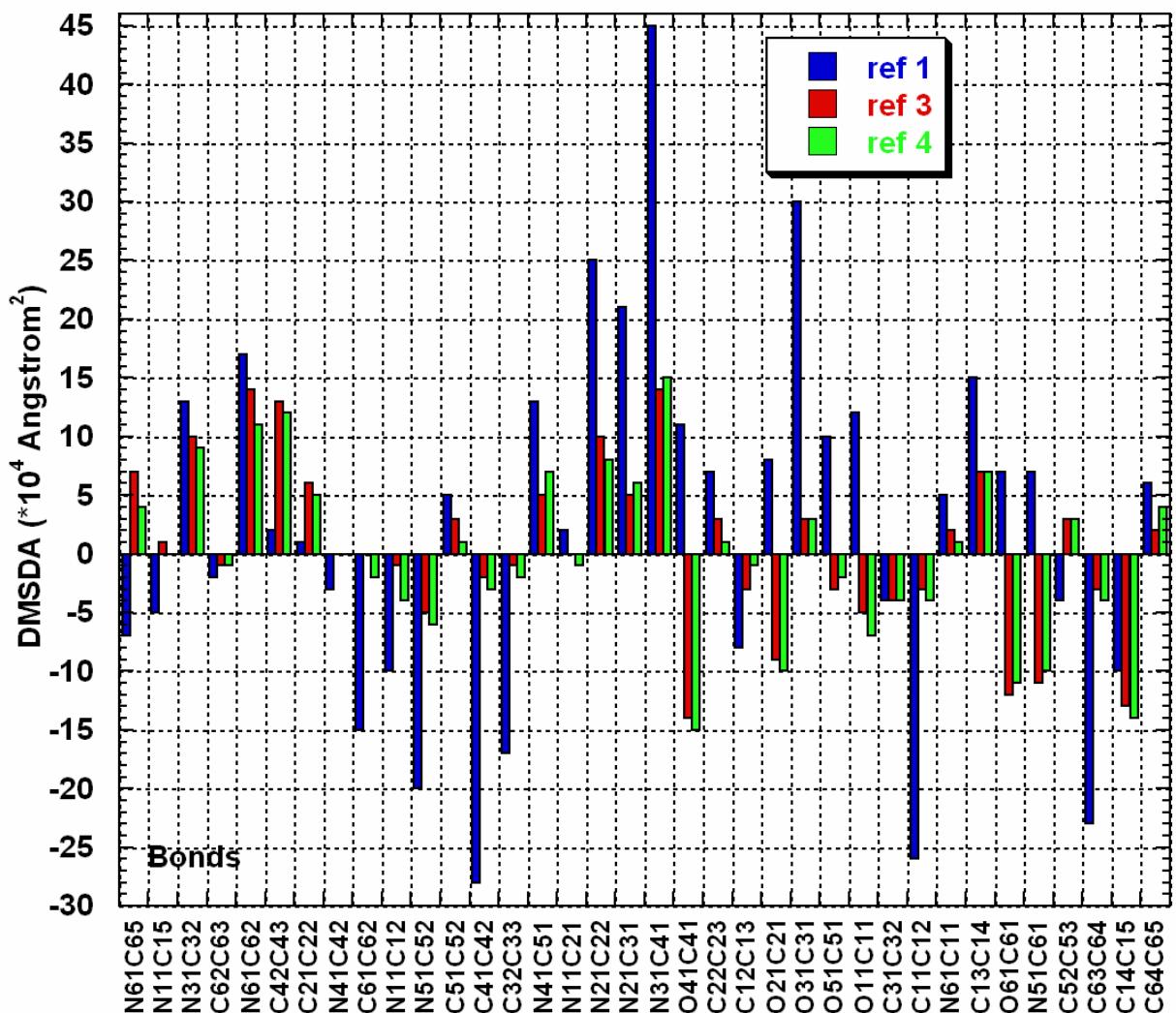


Figure S14. Differences in phase angles ($^{\circ}$) between HR KRMM refinement and HR refinements 1 and 3 as a function of $\sin\theta/\lambda$ in YGG (a) and P2A4 (b).

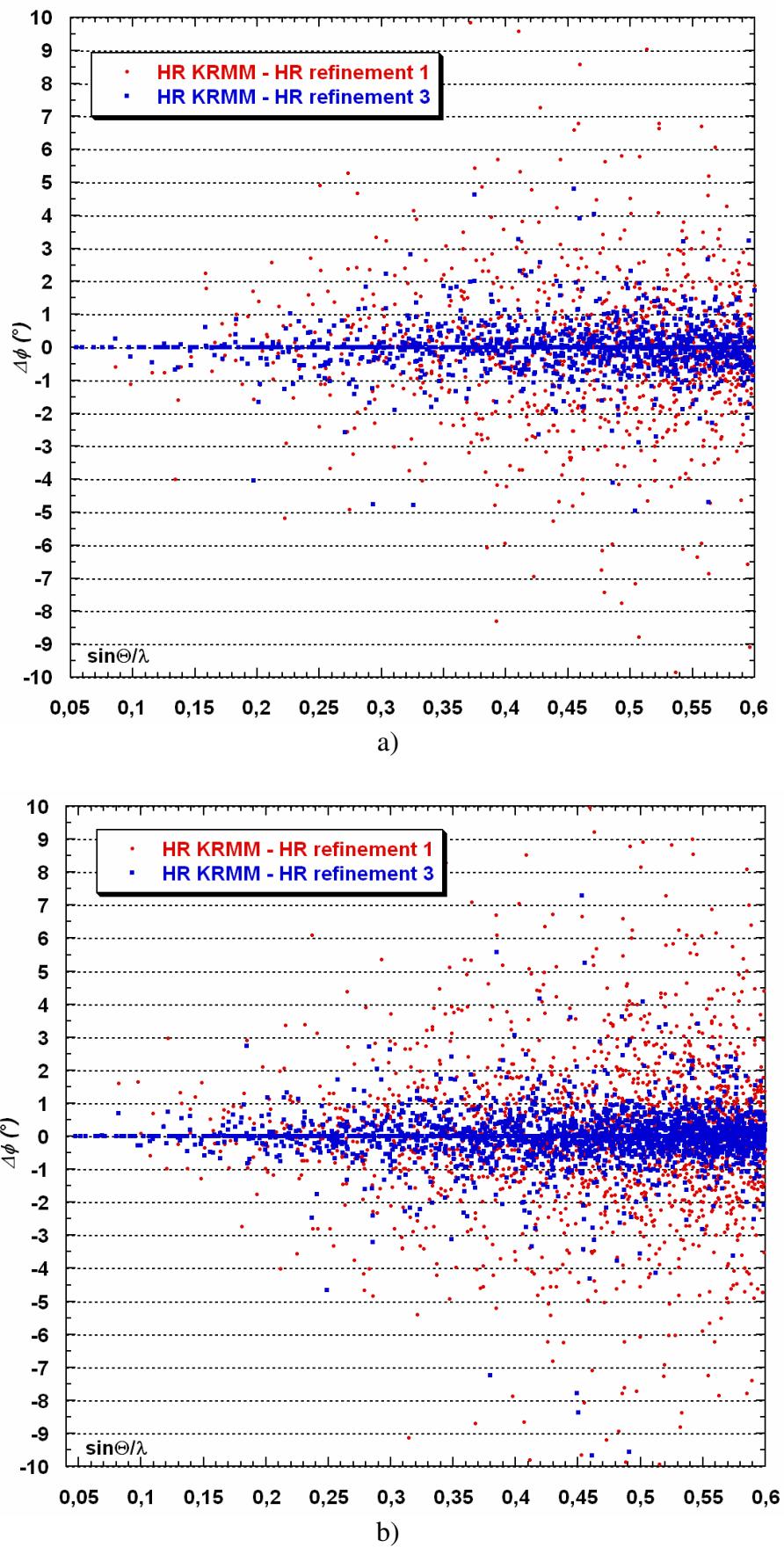


Table S1. U_{ii} (U_{11} , U_{22} and U_{33}) parameters (\AA^2) of YGG from all refinements sorted in the descending order of KRMM values

Atom/ U_{ii}	HR				LR		
	ref. 1	ref. 3	ref. 4	ref. 5	ref. 1	ref. 3	ref. 4
O5/U33	0.024	0.023	0.022	0.024	0.027	0.023	0.023
O1/U22	0.022	0.022	0.022	0.023	0.025	0.023	0.022
O4/U33	0.021	0.022	0.021	0.022	0.024	0.023	0.022
O3/U33	0.018	0.019	0.019	0.019	0.021	0.020	0.019
O2/U11	0.018	0.018	0.018	0.019	0.020	0.019	0.018
C6/U33	0.019	0.018	0.018	0.019	0.020	0.018	0.019
O5/U11	0.019	0.020	0.019	0.018	0.023	0.021	0.020
O6/U11	0.018	0.017	0.016	0.017	0.021	0.017	0.016
N3/U11	0.017	0.016	0.016	0.017	0.020	0.016	0.016
O6/U33	0.016	0.016	0.015	0.016	0.020	0.017	0.016
C5/U11	0.015	0.015	0.015	0.015	0.017	0.015	0.016
O5/U22	0.015	0.015	0.015	0.015	0.018	0.016	0.016
C10/U11	0.013	0.014	0.014	0.015	0.015	0.015	0.015
C13/U33	0.014	0.014	0.014	0.014	0.016	0.015	0.015
C10/U22	0.015	0.014	0.014	0.014	0.019	0.016	0.016
O3/U11	0.015	0.014	0.014	0.014	0.018	0.014	0.014
C11/U33	0.014	0.014	0.014	0.014	0.020	0.015	0.016
C3/U22	0.014	0.014	0.014	0.014	0.020	0.015	0.015
O6/U22	0.013	0.016	0.015	0.014	0.016	0.017	0.016
C13/U11	0.013	0.013	0.013	0.014	0.015	0.015	0.015
C9/U11	0.013	0.014	0.014	0.014	0.015	0.014	0.014
C9/U22	0.014	0.013	0.014	0.013	0.018	0.015	0.015
C12/U33	0.013	0.013	0.013	0.013	0.017	0.014	0.015
N1/U11	0.014	0.013	0.013	0.013	0.017	0.014	0.013
C13/U22	0.014	0.013	0.013	0.013	0.018	0.014	0.014
C12/U22	0.013	0.013	0.013	0.013	0.016	0.014	0.014
O2/U22	0.014	0.013	0.013	0.013	0.018	0.014	0.014
C4/U11	0.011	0.012	0.013	0.013	0.010	0.012	0.013
N1/U22	0.013	0.013	0.013	0.013	0.016	0.015	0.013
O4/U22	0.013	0.012	0.012	0.013	0.016	0.013	0.012
N2/U22	0.012	0.011	0.011	0.013	0.016	0.012	0.012
O4/U11	0.013	0.014	0.013	0.013	0.018	0.015	0.015
C2/U11	0.012	0.013	0.013	0.012	0.015	0.015	0.015
C11/U11	0.012	0.012	0.012	0.012	0.014	0.012	0.013
C6/U11	0.013	0.013	0.013	0.012	0.017	0.015	0.015
C11/U22	0.012	0.013	0.013	0.012	0.015	0.014	0.014
C1/U22	0.010	0.011	0.012	0.012	0.009	0.012	0.013
N3/U33	0.012	0.013	0.013	0.012	0.014	0.013	0.013
C12/U11	0.011	0.012	0.012	0.012	0.013	0.013	0.013
C9/U33	0.012	0.012	0.012	0.012	0.016	0.012	0.013
C8/U22	0.012	0.012	0.012	0.012	0.018	0.014	0.014
C2/U22	0.011	0.011	0.012	0.012	0.014	0.012	0.012
C3/U11	0.011	0.012	0.012	0.012	0.014	0.013	0.013
O1/U11	0.012	0.012	0.012	0.012	0.015	0.014	0.013
N2/U11	0.012	0.012	0.012	0.012	0.014	0.013	0.013
C7/U11	0.012	0.012	0.012	0.012	0.016	0.012	0.012
C7/U33	0.009	0.011	0.011	0.011	0.010	0.012	0.013
C8/U11	0.011	0.011	0.011	0.011	0.013	0.011	0.012

C5/U22	0.011	0.011	0.011	0.011	0.014	0.011	0.012
C3/U33	0.011	0.011	0.011	0.011	0.013	0.012	0.012
O1/U33	0.012	0.011	0.011	0.011	0.016	0.013	0.012
C1/U11	0.012	0.012	0.012	0.011	0.017	0.013	0.014
C6/U22	0.010	0.011	0.011	0.011	0.014	0.012	0.012
N1/U33	0.010	0.011	0.011	0.011	0.013	0.012	0.011
C8/U33	0.010	0.010	0.011	0.010	0.013	0.011	0.012
C5/U33	0.010	0.011	0.011	0.010	0.014	0.013	0.013
C4/U22	0.010	0.010	0.010	0.010	0.016	0.013	0.013
C10/U33	0.010	0.010	0.010	0.010	0.012	0.011	0.011
N2/U33	0.010	0.010	0.010	0.010	0.014	0.012	0.012
C7/U22	0.010	0.010	0.010	0.010	0.015	0.012	0.012
C4/U33	0.011	0.010	0.010	0.010	0.016	0.011	0.012
O2/U33	0.010	0.010	0.010	0.010	0.014	0.011	0.010
O3/U22	0.010	0.011	0.010	0.010	0.015	0.012	0.012
N3/U22	0.009	0.010	0.010	0.009	0.013	0.011	0.011
C1/U33	0.009	0.008	0.009	0.009	0.015	0.009	0.010
C2/U33	0.009	0.009	0.009	0.009	0.014	0.009	0.010

Table S2. U_{ii} (U_{11} , U_{22} and U_{33}) parameters (\AA^2) of P2A4 from all refinements sorted in the descending order of KRMM values

Atom/ U_{ii}	HR				LR		
	ref. 1	ref. 3	ref. 4	ref. 5	ref. 1	ref. 3	ref. 4
O41/U22	0.031	0.032	0.032	0.032	0.033	0.033	0.033
C43/U11	0.031	0.032	0.031	0.031	0.033	0.032	0.032
O51/U33	0.029	0.029	0.029	0.029	0.031	0.030	0.030
C53/U33	0.029	0.029	0.028	0.028	0.035	0.031	0.030
O31/U11	0.025	0.025	0.025	0.025	0.025	0.026	0.026
O61/U11	0.025	0.025	0.025	0.025	0.025	0.025	0.025
C63/U11	0.024	0.024	0.024	0.024	0.029	0.025	0.024
O11/U22	0.023	0.024	0.024	0.024	0.025	0.024	0.024
C64/U22	0.023	0.023	0.023	0.023	0.026	0.025	0.024
C65/U22	0.022	0.022	0.022	0.022	0.026	0.023	0.023
C64/U11	0.021	0.021	0.021	0.021	0.024	0.021	0.021
C23/U11	0.020	0.020	0.019	0.019	0.022	0.021	0.020
C14/U11	0.019	0.019	0.019	0.019	0.021	0.019	0.019
C43/U33	0.018	0.019	0.018	0.018	0.021	0.020	0.019
O21/U11	0.018	0.018	0.018	0.018	0.019	0.018	0.018
C33/U33	0.018	0.018	0.018	0.018	0.020	0.019	0.018
O61/U33	0.017	0.018	0.018	0.017	0.022	0.020	0.020
O51/U22	0.018	0.017	0.017	0.017	0.022	0.019	0.019
O11/U33	0.018	0.017	0.017	0.017	0.023	0.018	0.018
O41/U33	0.017	0.017	0.017	0.017	0.021	0.018	0.018
O71/U22	0.017	0.017	0.017	0.017	0.020	0.018	0.018
C15/U11	0.017	0.017	0.017	0.017	0.019	0.018	0.017
N21/U11	0.017	0.017	0.017	0.017	0.020	0.017	0.017
C23/U33	0.017	0.017	0.016	0.017	0.020	0.018	0.017
C42/U22	0.017	0.017	0.017	0.016	0.022	0.018	0.018
C33/U11	0.016	0.017	0.016	0.016	0.018	0.018	0.017
N51/U11	0.016	0.016	0.016	0.016	0.020	0.016	0.016
O71/U33	0.016	0.016	0.016	0.016	0.020	0.017	0.017
C41/U22	0.015	0.016	0.015	0.016	0.013	0.016	0.016
C13/U11	0.016	0.016	0.015	0.015	0.017	0.016	0.016
O61/U22	0.016	0.015	0.015	0.015	0.020	0.016	0.016
N11/U11	0.015	0.015	0.014	0.015	0.017	0.014	0.014
O51/U11	0.014	0.014	0.014	0.014	0.018	0.016	0.015
O31/U22	0.015	0.014	0.014	0.014	0.019	0.015	0.015
O71/U11	0.014	0.014	0.014	0.014	0.017	0.015	0.015
C33/U22	0.014	0.014	0.014	0.014	0.018	0.015	0.014
C63/U22	0.014	0.014	0.014	0.014	0.016	0.016	0.015
C43/U22	0.014	0.014	0.014	0.014	0.019	0.016	0.016
C65/U11	0.014	0.014	0.014	0.014	0.017	0.015	0.015
C22/U11	0.014	0.014	0.014	0.014	0.015	0.015	0.014
C63/U33	0.014	0.014	0.014	0.014	0.018	0.016	0.015
C51/U33	0.013	0.013	0.013	0.013	0.015	0.015	0.014
C13/U33	0.013	0.013	0.013	0.013	0.017	0.014	0.013
C31/U11	0.013	0.013	0.013	0.013	0.013	0.014	0.014
O31/U33	0.013	0.013	0.013	0.013	0.018	0.015	0.015
C64/U33	0.013	0.013	0.013	0.013	0.019	0.014	0.014
C14/U33	0.013	0.013	0.013	0.013	0.017	0.014	0.013
C23/U22	0.013	0.013	0.013	0.013	0.018	0.015	0.014

N31/U22	0.013	0.013	0.013	0.013	0.017	0.013	0.012
C65/U33	0.013	0.013	0.013	0.013	0.019	0.015	0.014
C53/U22	0.013	0.013	0.013	0.013	0.015	0.014	0.013
C61/U11	0.013	0.013	0.013	0.013	0.013	0.013	0.013
C62/U11	0.013	0.013	0.013	0.013	0.016	0.014	0.014
C21/U11	0.012	0.013	0.013	0.013	0.013	0.014	0.014
N41/U33	0.013	0.012	0.012	0.013	0.015	0.013	0.012
C62/U33	0.013	0.013	0.013	0.013	0.017	0.015	0.014
C42/U11	0.013	0.013	0.012	0.012	0.014	0.013	0.013
C52/U11	0.013	0.012	0.012	0.012	0.017	0.013	0.013
C41/U33	0.012	0.012	0.012	0.012	0.021	0.015	0.014
C52/U33	0.012	0.012	0.012	0.012	0.017	0.014	0.014
C51/U22	0.012	0.012	0.012	0.012	0.017	0.014	0.014
C61/U33	0.012	0.012	0.012	0.012	0.017	0.013	0.013
N61/U22	0.012	0.012	0.011	0.012	0.015	0.012	0.011
C42/U33	0.012	0.012	0.011	0.012	0.017	0.013	0.013
C11/U33	0.012	0.012	0.012	0.012	0.019	0.014	0.014
C15/U33	0.011	0.011	0.011	0.011	0.015	0.013	0.013
C11/U22	0.011	0.011	0.011	0.011	0.011	0.012	0.012
C32/U33	0.011	0.011	0.011	0.011	0.017	0.014	0.013
C53/U11	0.011	0.011	0.011	0.011	0.013	0.012	0.012
N41/U22	0.011	0.011	0.011	0.011	0.015	0.013	0.013
N41/U11	0.011	0.011	0.011	0.011	0.015	0.012	0.012
O21/U33	0.011	0.011	0.011	0.011	0.016	0.013	0.013
C62/U22	0.011	0.011	0.011	0.011	0.015	0.012	0.011
C12/U33	0.011	0.011	0.011	0.011	0.016	0.013	0.013
N31/U33	0.011	0.011	0.011	0.011	0.015	0.013	0.013
N51/U33	0.011	0.011	0.011	0.011	0.014	0.013	0.013
N61/U33	0.011	0.011	0.011	0.011	0.016	0.012	0.012
C61/U22	0.011	0.011	0.011	0.011	0.016	0.012	0.012
C31/U33	0.011	0.011	0.010	0.011	0.017	0.012	0.012
N61/U11	0.011	0.011	0.011	0.010	0.014	0.012	0.012
C15/U22	0.011	0.011	0.010	0.010	0.015	0.012	0.011
N21/U33	0.010	0.011	0.011	0.010	0.014	0.013	0.012
C22/U33	0.010	0.010	0.010	0.010	0.015	0.012	0.011
N11/U33	0.010	0.011	0.010	0.010	0.012	0.012	0.011
C32/U11	0.010	0.010	0.010	0.010	0.012	0.011	0.011
O21/U22	0.011	0.010	0.010	0.010	0.014	0.010	0.010
C52/U22	0.010	0.010	0.010	0.010	0.013	0.011	0.011
C51/U11	0.010	0.010	0.010	0.010	0.014	0.011	0.011
C21/U33	0.010	0.010	0.010	0.010	0.015	0.011	0.011
C14/U22	0.010	0.010	0.010	0.010	0.014	0.012	0.011
N51/U22	0.010	0.010	0.010	0.010	0.014	0.012	0.011
C12/U11	0.010	0.010	0.010	0.010	0.014	0.011	0.010
O11/U11	0.010	0.010	0.010	0.010	0.014	0.011	0.011
N21/U22	0.010	0.010	0.010	0.010	0.013	0.011	0.011
C31/U22	0.010	0.010	0.010	0.010	0.013	0.011	0.010
C12/U22	0.010	0.009	0.009	0.009	0.012	0.010	0.009
C32/U22	0.009	0.009	0.009	0.009	0.013	0.010	0.009
C13/U22	0.009	0.009	0.009	0.009	0.013	0.010	0.010
C22/U22	0.009	0.009	0.009	0.009	0.014	0.011	0.010
C11/U11	0.009	0.009	0.009	0.009	0.014	0.010	0.009
C41/U11	0.009	0.009	0.008	0.008	0.014	0.009	0.009

C21/U22	0.009	0.009	0.008	0.008	0.013	0.010	0.010
O41/U11	0.008	0.009	0.008	0.008	0.013	0.010	0.010
N31/U11	0.008	0.008	0.008	0.008	0.010	0.010	0.010
N11/U22	0.008	0.008	0.008	0.008	0.014	0.011	0.011