STRUCTURAL SCIENCE
CRYSTAL ENGINEERING
MATERIALS

Volume 73 (2017)

Supporting information for article:

A Theoretical Electron Density Databank using a Model of Real and Virtual Spherical Atoms

Ayoub Nassour, Slawomir Domagala, Benoit Guillot, Theo Leduc, Claude Lecomte and Christian Jelsch

Supplementary Materials.

A Theoretical Electron Density Databank using a Model of Real and Virtual Spherical Atoms.

Ayoub Nassour, Sławomir Domagała, Benoît Guillot , Theo Leduc, Claude Lecomte & Christian Jelsch Acta Crystallographica B. 2017.

Table Sup1. Valence populations and kappa1 (KP1) values of the urea atoms for the different models. *Q* are the fitted point charges.

	DB_VIR		THEO_VIR		FITQ
atom	P_{val}	KP1	P_{val}	KP1	*Q*
O	6.112	0.9536	6.453	0.9396	-0.646
C	2.947	1.0392	2.617	1.0569	0.750
N	5.101	1.0003	5.236	0.9894	-0.806
H1	0.634	1.1605	0.555	1.1600	0.365
H2	0.634	1.1605	0.652	1.1600	0.389
QCO	0.149	1.1352	0.149	1.1352	
QCN	0.427	0.9061	0.427	0.9061	
QNH1	0.207	1.1993	0.174	1.1612	
QNH2	0.207	1.1993	0.240	1.2374	
LPO	0.159	1.5735	0.106	1.9696	

atom	ELMAM2		UBDB	
atom	P_{val}	KP1	P_{val}	KP1
O	6.32969	0.98741	6.23783	0.986
C	4.16311	0.99407	4.19538	0.990
N	5.20125	0.99603	4.93228	1.003
H1	0.77617	1.17316	0.92556	1.155
H2	0.77617	1.17316	0.92556	1.155

Table Sup2. Discrepancies between streptavidin - biotin hydrogen bonds critical points found using ELMAM2 and DB_VIR models.
Hessian eigenvalues are given for both models and their relative discrepancy:

$$\Delta\lambda/\lambda = (\lambda_{ELMAM2} - \lambda_{DB\_VIR}) / | \lambda_{ELMAM2} + \lambda_{DB\_VIR} |$$

Strepdavidin	biotin	ELMAM2			DBVIR			(%)		
								$\Delta\lambda_1$	$\Delta\lambda_2$	$\Delta\lambda_3$
atom	**atom**	$\lambda 1$	$\lambda 2$	$\lambda 3$	$\lambda 1$	$\lambda 2$	$\lambda 3$	$/\lambda_1$	$/\lambda_2$	$/\lambda_3$
HD21_asn_10	O3	-0.69	-0.60	2.77	-0.67	-0.67	3.23	-1	5	-8
HG_ser_14	O3	-2.00	-1.95	5.37	-1.52	-1.49	6.23	-14	-13	-7
HH_tyr_30	O3	-1.88	-1.85	5.08	-1.36	-1.35	5.66	-16	-16	-5
OD2_asp_115	HN1	-1.92	-1.92	5.87	-1.64	-1.63	6.58	-8	-8	-6
OG_ser_32	HN2	-1.01	-0.98	3.45	-0.86	-0.86	3.91	-8	-6	-6
OG_ser_32	H71	-0.15	-0.12	0.94	-0.15	-0.12	0.98	3	2	-2
O_val_34	H72				-0.04	-0.01	0.31			
O_asn_36	H102	-0.14	-0.13	0.76	-0.13	-0.13	0.83	-3	0	-4
H_asn_36	O11	-1.39	-1.37	4.51	-1.24	-1.24	5.24	-6	-5	-8
HD11_leu_97	O12	-0.08	-0.07	0.43	-0.07	-0.07	0.46	-6	-4	-4
HD21_leu_97	O12	-0.03	-0.02	0.18	-0.02	-0.01	0.19	-11	-24	-2
HB1_ala_73	O12	-0.04	-0.03	0.33	-0.05	-0.04	0.36	7	17	-4
HG21_thr_77	S1	-0.14	-0.09	0.68	-0.12	-0.11	0.77	-6	9	-6
HZ2_trp_66	S1	-0.14	-0.08	0.81	-0.13	-0.13	0.82	-2	20	-1
HG1_thr_77	S1	-0.65	-0.61	1.95	-0.46	-0.46	2.17	-16	-14	-5

Table Sup3: List of crystal structures used for building the theoretical database.

Nr	Abbreviation	Name, formula	Reference
1	Ala	L-Alanine, $C_3H_7NO_2$	Destro *et al.*, 1988
2	Argphos	L-Arginine Phosphate Monohydrate, $C_6H_{15}N_4O_2^+$ $H_2PO_4^-$ H_2O	Espinosa *et al.*, 1996
3	His	DL-Histidine, $C_6H_9N_3O_2$	Coppens *et al.*, 1999
4	Actyr	N-acetyl-L-tyrosine ethyl ester monohydrate, $C_{13}H_{19}NO_5$	Dahaoui *et al.*, 1999
5	Gythr	Glycyl-L-threonine dihydrate, $C_6H_{12}N_2O_4$ $2H_2O$	Benabicha *et al.*, 2000
6	Urea	Urea, CH_4N_2O	Birkedal *et al.*, 2004
7	Trp	L-tryptophan formic acid, $C_{11}H_{12}N_2O_2$ CH_2O_2	Scheins *et al.*, 2004
9	Cytosine_hyd	Cytosine monohydrate, $C_4H_5N_3O$ H_2O	Munshi *et al.*, 2006b
10	Alaproala	L-alanyl-L-prolyl-L-alanine hydrate, $C_{11}H_{19}N_3O_4$ H_2O	Kalinowski *et al.*, 2007
11	Thymidine	Thymidine, $C_{10}H_{14}N_2O_5$	Hübschle *et al.*, 2008
12	Glycine	Glycine, $C_2H_5NO_2$	Destro *et al.*, 2008
13	Benzene	Benzene, C_6H_6	Bacon *et al.*, 1964
14	Catechol	Catechol, $C_6H_6O_2$	Fronczek *et al* , 2002
15	Resorcinol	Resorcinol, $C_6H_6O_2$	Bacon *et al.*, 1973
16	*P*-nitrophenol α -form	*P*-nitrophenol α -form, $C_6H_5NO_5$	Kulkarni *et al*, 1998
17	*P*-nitrophenol β-form	*P*-nitrophenol β-form, $C_6H_5NO_5$	Kulkarni *et al*, 1998
18	2,5-dihydroxybenzoic acid	2,5-dihydroxybenzoic acid, $C_7H_6O_7$	Cohen *et al*, 2007
19	*p*-dinitrobenzene	*p*-dinitrobenzene, $C_6H_4N_2O_4$	Tonogaki *et al*, 1993

20	Quercetin monohydrate	Quercetin monohydrate, $C_{15}H_{10}O_7H_2O$	Domagała *et al*, 2011
21	Fidarestat	Fidarestat, $C_{12}H_{10}N_3O_4F$	Fournier *et al.*, 2009
22	AMB	2-Carboxy-4-methylanilinium chloride monohydrate, $HOOC\text{-}C_7H_6\text{-}NH_3^+ Cl^- H_2O$	Dadda *et al*, 2012
23	Acgln	*N*-acetyl-L-glutamine, $C_7H_{12}N_2O_4$	Narasimhamurthy *et al*, 1976
24	Adenosine	2-(6-aminopurin-9-yl)-5-(hydroxyméthyl)oxolane-3,4-diol, $C_{10}H_{13}N_5O_4$	Lai *et al*, 1972
25	Alamet	DL-alanyl-methionine, C8H16N2O3S	Guillot *et al*, 2011
26	His_glutaric	L-Arginine-Glutaricacid-complex, $C_{17}H_{40}N_8O_{10}$	Saraswathi *et al*, 2001
27	Nitramine	Nitramine, $C_8H_8N_2O_2$	Zarychta *et al*, 2011
28	Coumarin	Coumarin, $C_9H_6O_2$	Munshi *et al*, 2010
29	TRP_VER	L-Tryptophan Formic acid, $C_{12}H_{14}N_2O_4$	Scheins *et al*, 2004
30	M11	1,4-bis (5-hexyl-2-thienyl) butane-1,4 dione, $C_{24}H_{34}O_2S_2$	Ahmed *et al*. (in preparation)
31	M12	4,4'-diphosphonate-2,2'-bipyridine, $H_{30}N_2O_6P_2$	Ahmed *et al*. (in preparation)
32	Cystine	L-Cystine, $C_6H_{12}N_2O_4S_2$	Dahaoui *et al*, 1999

33	Cysteine	L-cysteine, $C_3H_7NO_2S$	Harding *et al*, 1968
34	Hisphos	l-Histidinephosphate tert-Bu-l-Pro-His-NHMe,	Mata *et al*. (2006)
35	Nitril	2-methyl-4-nitro-1-phenyl-1Himidazole-5-carbonitrile	Poulain-Paul *et al*. (2012)
36	Adenine	adenine, $C_5H_5N_5$	Tret'yak *et al*, 1987
37	Guanine	guanine, $C_5H_5N_5O$	Guille et al, 2006
38	Guanosine	guanosine, $C_{10}H_{13}N_5O_5$	Sugawara et al, 1994

References.

Bacon, G. E.; Curry, N. A.; Wilson, S. A. (1964). *Proc. R. Soc. London Ser. A,* 279, 98-110. [BENZENE]

Bacon, G. E. & Jude, R. J. (1973). Z. Kristallogr. 138, 19–40. [RESORCINOL]

Birkedal, H., Madsen, D., Mathiesen, R. H., Knudsen, K., Weber, H.-P., Pattisond, P. & Schwarzenbach, D. (2004). Acta Cryst. A60, 371-381. [UREA]

Benabicha, F., Pichon-Pesme, V., Jelsch, C., Lecomte, C. & Khmou, A. (2000). Acta Cryst. B56, 155-165. [GYTHR]

Cohen, D. E., Benedict, J. B., Morlan, B., Chiu, D. T. & Kahr, B. (2007). Crystal Growth Des. 7, 492–495. [DIHYDROXYBENZOIC]

Coppens, P., Abramov, Y., Carducci, M., Korjov, B., Novozhilova, I., Alhambra, C. & Pressprich, M. R. (1999). J. Am. Chem. Soc. 121, 2585-2593. [HIS]

Dadda, N., Nassour, A ., Guillot, B., Benalicherif, N. & Jelsch, C. *Acta Cryst.* (2012). *A68*, 452-463. [AMB]

Dahaoui, S., Jelsch, C., Howard, J. A. K. & Lecomte, C. (1999). Acta Cryst. B55, 226-230. [ACTYR]

Dahaoui, S., Pichon-Pesme, V., Howard, J. A. K. & Lecomte, C.(1999). J. Phys. Chem. A103, 6240–6250.[CYSTINE]

Domagała, S., Munshi, P., Ahmed, M., Guillot, B. & Jelsch, C. (2011).Acta Cryst. B67, 63–78. [QUERCETIN]

Destro, R., Marsh, R. E. & Bianchi, R. (1988). J. Phys. Chem. 92, 966-973. [ALA]

Destro, R.; Roversi, P.; Barzaghi, M.; Marsh, R. E. (2000). *J. Phys. Chem. A. 104*, 1047-1054. [GLYCINE]

Espinosa, E., Lecomte, C., Molins, E., Veintemillas, S., Cousson, A. & Paulus, W. (1996). Acta Cryst. B52, 519-534. [ARGPHOS]

Fournier, B., Bendeif, el-E., Guillot, B., Podjarny, A., Lecomte, C. & Jelsch, C. (2009). J. Am. Chem. Soc. 131, 10929–10941. [FIDARESTAT]

Fronczek, F. R., Kim, K. K. & Strongin, R. M. (2002). Private communication (refcode: CATCOL13). [CATECHOL]

Guillot.R, Nicolas Muzet. N, Dahaoui. S, Lecomte. C & Jelsch. C. (2001).Acta Cryst. B57, 567-578.[ALAMET]

Guille. K and Clegg. W. (2006). Acta Cryst. C62, o515-o517.[GUANINE]

Hübschle, C. B., Dittrich, B., Grabowsky, S., Messerschmidt, M. & Luger, P. (2008). Acta Cryst. B64, 363-374. [THYMIDINE]

Harding. M. M & Long. H. A.(1968). *Acta Cryst*. B24, 1096-1102.[CYSTEINE]

Kalinowski, R., Dittrich, B., Hübschle, C. B., Paulmann, C. & Luger, P. (2007). Acta Cryst. B63, 753-767. [ALAPROALA]

Kulkarni, G. U., Kumaradhas, P. & Rao, C. N. R. (1998). Chem. Mater. 10, 3498–3505. [NITROPHENOL_Alpha/BETA]

Lai. T.F & Marsh. R. E.(1972). *Acta Cryst.* B28, 1982. [ADENOSINE]

Munshi, P. & Guru Row, T. N. (2006b). Acta Cryst. B62, 612-626. [CYTOSINE_HYD]

Munshi. P, Jelsch. C, Hathwar. VR, Guru Row. TN . (2010). Crystal growth & Design. 10, 1516-1526.[COUMARIN]

Narasimhamurthy. M. R, Venkatesan. K & Winkler. F. (1976). *J. Chem. Soc., Perkin Trans. 2*, 768-771. [ACGLN]

Tret'yak. S. M, V.V.Mitkevich. V.V & L.F.Sukhodub. L. F. (1987). Kristallografiya(Russ.)(Crystallogr.Rep.). 32, 1268. [ADENINE]

Scheins, S., Dittrich, B., Messerschmidt, M., Paulmann, C. & Luger, P. (2004). Acta Cryst. B60, 184-190. [TRP]

Saraswathi. N. T & M. Vijayan. M. *Acta Cryst.* (2001). B**57**, 842-849. [HIS_GLUTARIC]

Scheins. S, Dittrich. B, Messerschmidt. M, Paulmann. C and Luger. P.(2004). Acta Cryst. B60, 184-190.[TRP_VER]

Sugawara. Y, Iimura. Y, Iwasaki.Y, Urabe. H, Saito. H.(1994). J.Biomol.Struct.Dyn. 11. 721.[GUANOSINE]

Tonogaki, M., Kawata, T., Ohba, S., Iwata, Y. & Shibuya, I. (1993). Acta Cryst. B49, 1031–1039. [DINITROBENZENE]

Zarychta. B, Zaleski. J, Kyzioł. J, Daszkiewicza. Z & Jelsch.C. (2011). Acta Cryst. B67, 250–262. [NITRAMINES]

Poulain-Paul.A , Nassour. A, Jelsch. C, Guillot. B, Kubicki. M and Lecomte. C. Acta Cryst. (2012). A68, 715-728.[NITRIL]

Table Sup4. Exemple of atoms types in the Databank_VIR_2017.

```
Urea atoms:
============================================================
ATOM  C13  C    XY O N  -    ONN     Con[hh]n[hh]           1
NBOND     3   CYCLE   0       CHIV    0.000  CHIR    0
SYMPLM    1   CONVAL  -   CONPLM  -    CONKAP  -
DIST      C-O  1.258   C-N  1.348   C-N  1.348
ANGL      O-C-N  118.9   O-C-N  118.9   N-C-N  122.1
KMD       1.06478 1.00000  2.594  0.000
KMD_ESD   0.01267 0.00000  0.109  0.000
TEXT      C_onn urea  sp2
============================================================
ATOM   O34   O    XY  C   N   -   C  Oc[n(hh)n(hh)]         1
NBOND     1   CYCLE   0       CHIV    -    CHIR    0
SYMPLM    1   CONVAL  -   CONPLM  -    CONKAP  -
DIST      O-C  1.258
KMD       0.93463 1.00000  6.480  0.000
KMD_ESD   0.00401 0.00000  0.065  0.000
TEXT      O=c_n(hh)n(hh) urea
============================================================
ATOM      N7    N     bZX   H   H   -   CHH    Nc[on(xx)]hh 1
NBOND     3   CYCLE   0       CHIV    0.000  CHIR    0
SYMPLM    1   CONVAL  -   CONPLM  -    CONKAP  -
DIST      N-H  1.015   N-H  1.014   N-C  1.348
ANGL      H-N-H  119.5   C-N-H  120.6   C-N-H  119.9
KMD       0.98776 1.00000  5.299  0.000
KMD_ESD   0.00322 0.00000  0.054  0.000
WILDCARD  x=c|h;
TEXT      N_c(on)hh urea
============================================================
ATOM      H10   H    ZX    N   C   -   N        Hn[ch]      12
NBOND     1   CYCLE   0       CHIV    -    CHIR    0
SYMPLM    1   CONVAL  -   CONPLM  -    CONKAP  -
DIST      H-N  1.004
DIST_ESD      0.042
KMD       1.16044 1.00000  0.660  0.000
KMD_ESD   0.00039 0.00000  0.028  0.000
TEXT      Hn NH2-C
============================================================
ATOM      Q43   Q    XY    O   C   -   OC       Qoc[nn]      4
NBOND     2   CYCLE   0       CHIV    -    CHIR    0
SYMPLM    1   CONVAL  -   CONPLM  -    CONKAP  -
DIST      Q-O  0.706   Q-C  0.539
DIST_ESD      0.055        0.061
ANGL      O-Q-C  180.0
ANGL_ESD           0.0
KMD       0.99879 1.00000  0.251  0.000
KMD_ESD   0.13145 0.00000  0.138  0.000
TEXT      Qo=c_nn urea
============================================================
ATOM      Q78   Q    XY    C   N   -   NC       Qn[hh]c[on]  1
NBOND     2   CYCLE   0       CHIV    -    CHIR    0
SYMPLM    1   CONVAL  -   CONPLM  -    CONKAP  -
DIST      Q-N  0.737   Q-C  0.612
ANGL      N-Q-C  180.0
KMD       0.85762 1.00000  0.418  0.000
KMD_ESD   0.03490 0.00000  0.048  0.000
TEXT      Qnc HH_N-C=O urea
============================================================
```

```
ATOM      Q50   Q    XY    N   H   -   NH       Qn[ch]h      6
NBOND     2   CYCLE   0       CHIV    -    CHIR    0
SYMPLM    1   CONVAL  -   CONPLM  -    CONKAP  -
DIST      Q-N  0.674   Q-H  0.340
DIST_ESD       0.006        0.001
ANGL      N-Q-H  180.0
ANGL_ESD           0.0
KMD       1.12412 1.00000  0.189  0.000
KMD_ESD   0.03128 0.00000  0.027  0.000
TEXT      Qnh_ch  general
============================================================
ATOM     LP13   Q    XY    O   C   -   O        Qo[c(nn)]    4
NBOND     1   CYCLE   0       CHIV    -    CHIR    0
SYMPLM    1   CONVAL  -   CONPLM  -    CONKAP  -
DIST      Q-O  0.279
DIST_ESD       0.000
ANGL      Q-O-Q  119.7
ANGL_ESD           0.1
KMD       1.57000 1.00000  0.104  0.000
KMD_ESD   0.06000 0.00000  0.030  0.000
TEXT      LP O=c_nn
```

```
Polypeptide mainchain atoms.
====================================================================
ATOM      N11   N       bXY   C   C   -   CCH      Nc[oc]c[xxx]h
10
NBOND     3   CYCLE   0       CHIV    0.058  CHIR    0
SYMPLM    1   CONVAL  -   CONPLM  -    CONKAP  -
DIST      N-H  0.987   N-C  1.453   N-C  1.337
DIST_ESD       0.051        0.008        0.008
ANGL      C-N-H  120.8   C-N-H  117.1   C-N-C  121.8
ANGL_ESD           1.6           1.5           1.4
KMD       0.99422 1.00000  5.179  0.000
KMD_ESD   0.00541 0.00000  0.085  0.000
WILDCARD  x=c|h;
TEXT      N_peptide
====================================================================
ATOM      C15   C       bXY   O   N   -   ONC      Con[xx]c[xxx]
13
NBOND     3   CYCLE   0       CHIV    0.026  CHIR    0
SYMPLM    1   CONVAL  -   CONPLM  -    CONKAP  -
DIST      C-O  1.238   C-N  1.341   C-C  1.523
DIST_ESD       0.010        0.011        0.013
ANGL      O-C-N  123.5   O-C-C  121.6   N-C-C  114.8
ANGL_ESD           1.5           1.6           2.7
KMD       1.03634 1.00000  2.695  0.000
KMD_ESD   0.01379 0.00000  0.118  0.000
WILDCARD  x=h|c|n;
TEXT      C_onc_peptide sp2
====================================================================
ATOM      O28   O       XY    C   N   -   C        Oc[n(xx)c(xxx)]
11
NBOND     1   CYCLE   0       CHIV    -    CHIR    0
SYMPLM    1   CONVAL  -   CONPLM  -    CONKAP  -
DIST      O-C  1.237
DIST_ESD       0.011
KMD       0.94802 1.00000  6.312  0.000
KMD_ESD   0.00278 0.00000  0.079  0.000
WILDCARD  x=c|h|n;
TEXT      O=c_nc peptide
```

```
=====================================================================
ATOM      C34   C       bZX   C   C   -   NCCH     Cncch
22
NBOND     4   CYCLE   0       CHIV    0.878  CHIR    +
SYMPLM    1   CONVAL  -   CONPLM  -    CONKAP  -
DIST      C-N  1.475   C-H  1.075   C-C  1.538   C-C  1.529
DIST_ESD       0.018        0.037        0.008        0.008
ANGL      N-C-H  107.7   N-C-C  111.1   N-C-C  109.1   C-C-H  109.7   C-C-H
107.9   C-C-C  111.2
ANGL_ESD           1.4            1.1            1.8            1.5
1.1            2.0
KMD       1.09148 1.00000  2.569  0.000
KMD_ESD   0.01045 0.00000  0.112  0.000
TEXT      C_ncch sp3  Ca_peptide
=====================================================================
ATOM      Q63   Q       XY    N   C   -   NC       Qn[ch]c[xxx]
13
NBOND     2   CYCLE   0       CHIV    -    CHIR    0
SYMPLM    1   CONVAL  -   CONPLM  -    CONKAP  -
DIST      Q-N  0.765   Q-C  0.689
DIST_ESD       0.019        0.020
ANGL      N-Q-C  180.0
ANGL_ESD           0.0
KMD       1.00724 1.00000  0.208  0.000
KMD_ESD   0.05256 0.00000  0.034  0.000
WILDCARD  x=c|h;
TEXT      Qnc peptide N-Ca
=====================================================================
ATOM      Q104  Q       XY    C   C   -   CC       Qc[on]c[nch]
7
NBOND     2   CYCLE   0       CHIV    -    CHIR    0
SYMPLM    1   CONVAL  -   CONPLM  -    CONKAP  -
DIST      Q-C  0.756   Q-C  0.775
DIST_ESD       0.025        0.020
ANGL      C-Q-C  180.0
ANGL_ESD           0.0
KMD       0.79439 1.00000  0.666  0.000
KMD_ESD   0.01134 0.00000  0.021  0.000
TEXT      Qcc C-Ca peptide
=====================================================================
ATOM      Q49   Q       XY    N   H   -   NH       Qn[cc]h
17
NBOND     2   CYCLE   0       CHIV    -    CHIR    0
SYMPLM    1   CONVAL  -   CONPLM  -    CONKAP  -
DIST      Q-N  0.665   Q-H  0.331
DIST_ESD       0.060        0.033
ANGL      N-Q-H  180.0
ANGL_ESD           0.0
KMD       1.09647 1.00000  0.219  0.000
KMD_ESD   0.03586 0.00000  0.047  0.000
TEXT      Qnh_cc Q_NH_peptide
=====================================================================
ATOM      Q31   Q       XY    C   O   -   OC       Qoc[nc]
14
NBOND     2   CYCLE   0       CHIV    -    CHIR    0
SYMPLM    1   CONVAL  -   CONPLM  -    CONKAP  -
DIST      Q-O  0.714   Q-C  0.525
DIST_ESD       0.026        0.020
ANGL      O-Q-C  180.0
ANGL_ESD           0.0
KMD       0.96948 1.00000  0.299  0.000
```

```
KMD_ESD   0.07707 0.00000  0.080  0.000
TEXT      Qo=c amide
=====================================================================
ATOM     LP4    Q       XY    O   C   -   O        Qo[c(nc)]
18
NBOND     1   CYCLE   0       CHIV    -    CHIR    0
SYMPLM    1   CONVAL  -   CONPLM  -    CONKAP  -
DIST      Q-O  0.282
DIST_ESD       0.009
ANGL      Q-O-Q  122.0
ANGL_ESD           5.8
KMD       1.53773 1.00000  0.110  0.000
KMD_ESD   0.06187 0.00000  0.019  0.000
TEXT      LP_O peptide
=====================================================================
```

Figure Sup1. Residual Fourier electron density map in the plane of urea molecule for the six compared models at 0.6 Å resolution after refinement vs. theoretical F_{hkl} data.
Contour level: ± 0.05 e/Å^3. Blue solid, and red dashed lines denote positive and negative contours, respectively. The additional VIR atoms are visible on each covalent bond and close to the oxygen atom on figures (b) and (c).

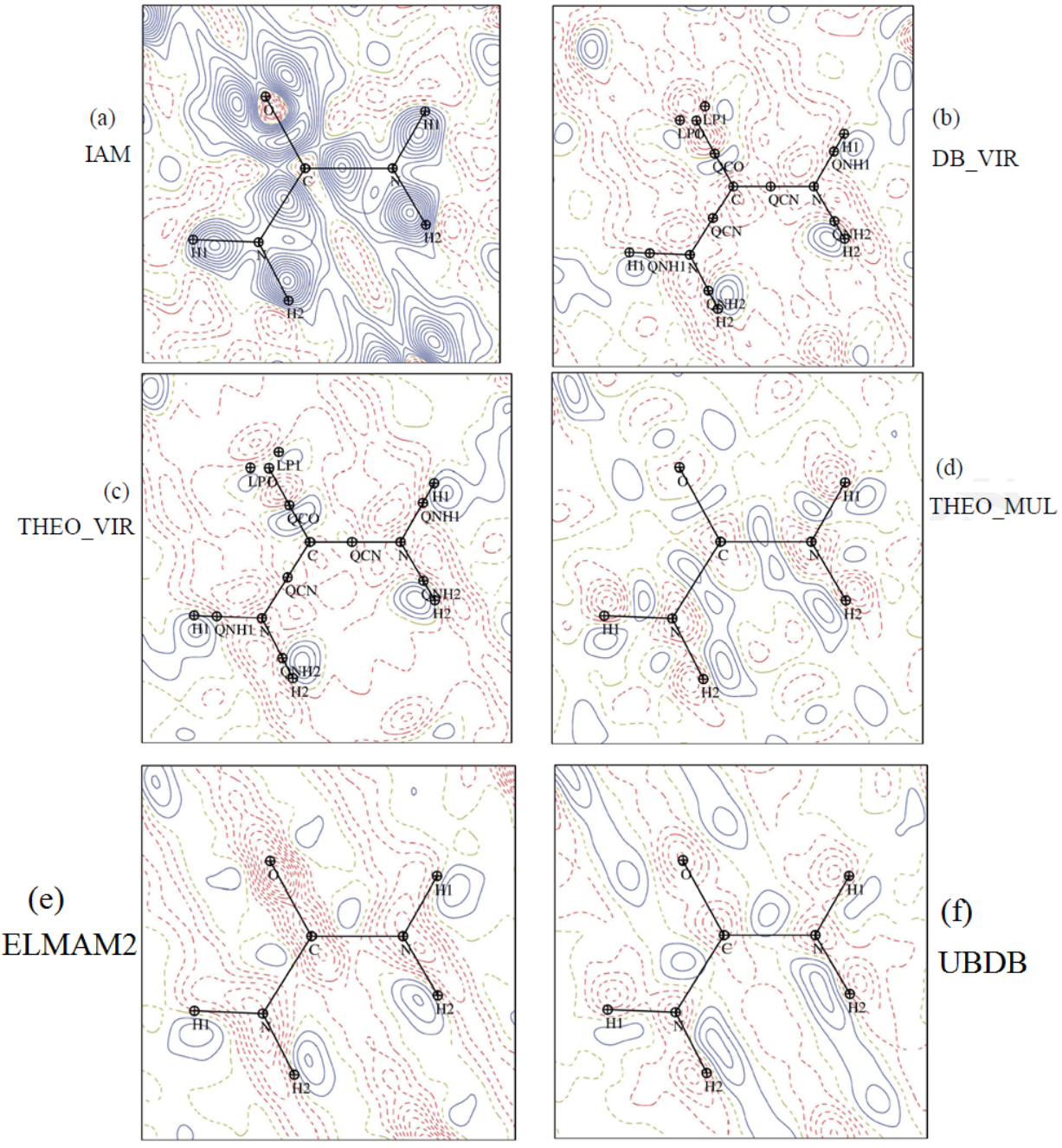


Figure Sup2. Residual Fourier electron density maps as in Fig. Sup1, but computed at 0.4 Å resolution.

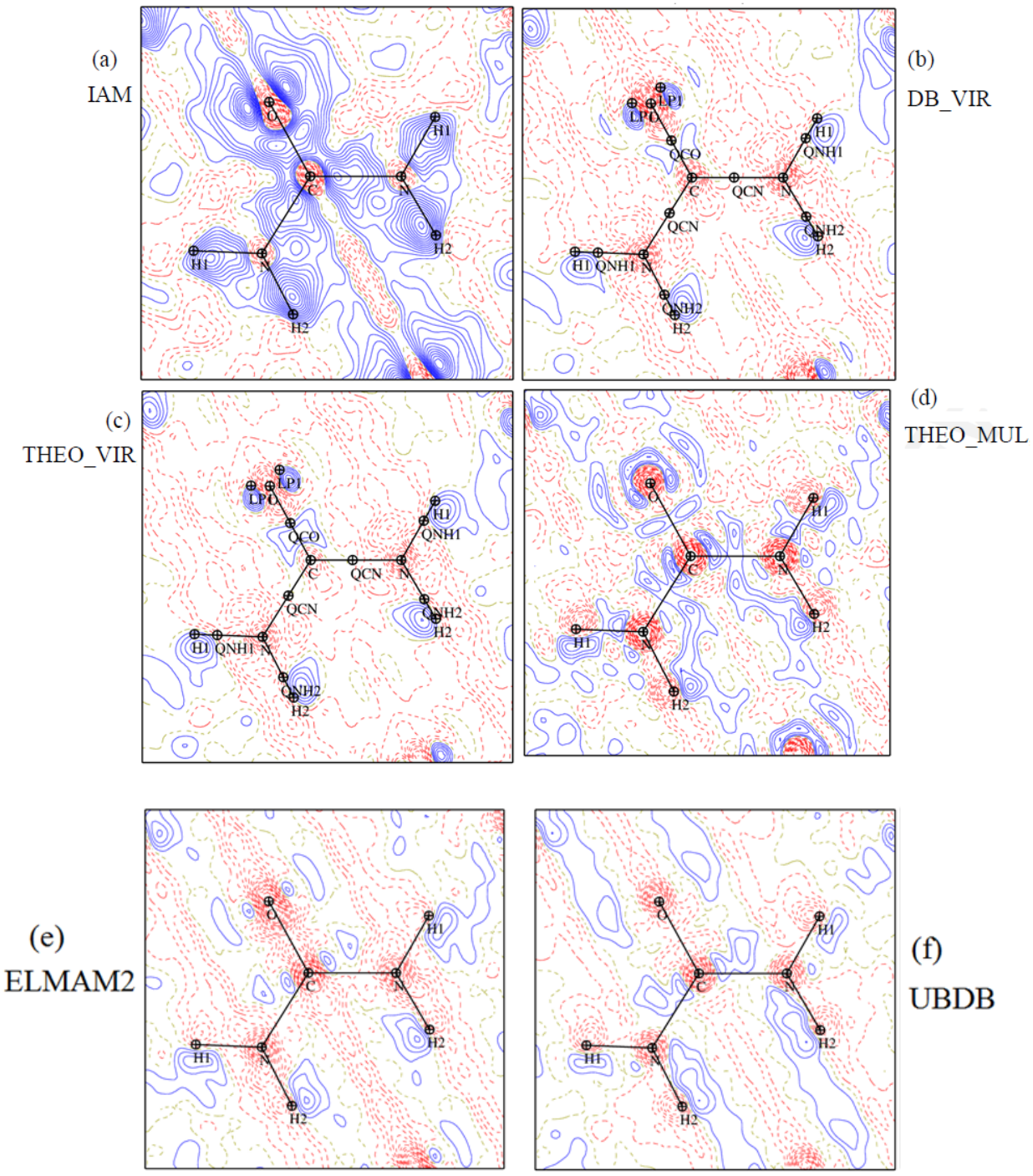
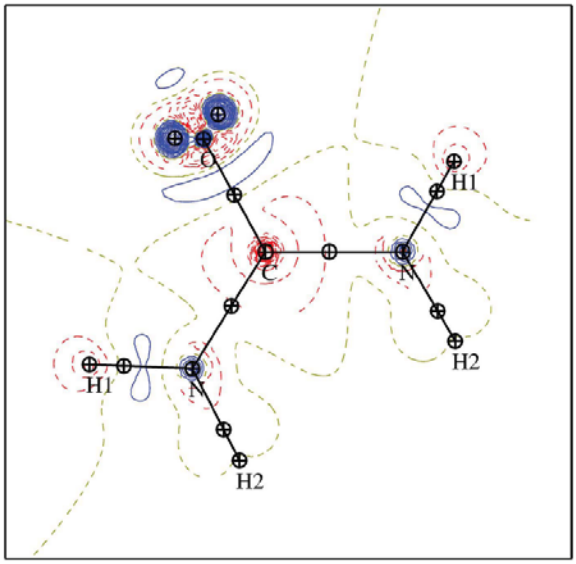
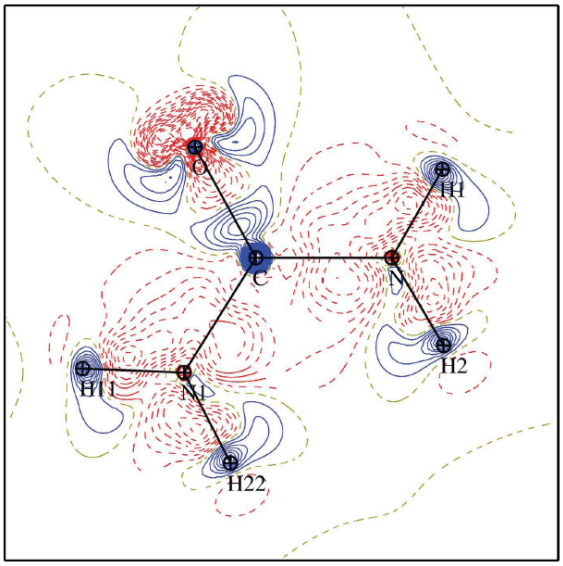


Figure Sup3
Difference between models of static deformation electron densities shown for urea.
Contour level: 0.05 e/Å^3. Blue solid lines and red dashed lines denote positive and negative contours, respectively. The zero contour is shown as a yellow dashed line.

(a) THEO_VIR – DB_VIR



(b) THEO_MUL – DB_VIR



(c) ELMAM2 – DB_VIR.

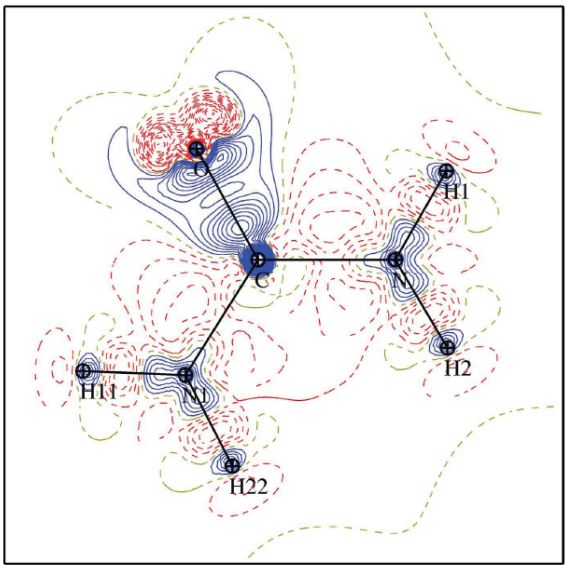


Figure Sup4. Electron density and Laplacian values on the H-bond Critical Points of the biotin/streptavidin complex, for the ELMAM2 and DB_VIR models.